



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:44 PM UTC

PDB ID : 9WG7 / pdb_00009wg7
EMDB ID : EMD-65950
Title : The structure of phycobilisome with a bicylindrical core from the cyanobacterium *Synechococcus elongatus* PCC 7942
Authors : Zheng, Z.G.; Ma, C.Y.; Wang, H.R.; Wang, G.P.; Dong, C.X.; Gao, N.; Zhao, J.D.
Deposited on : 2025-08-23
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

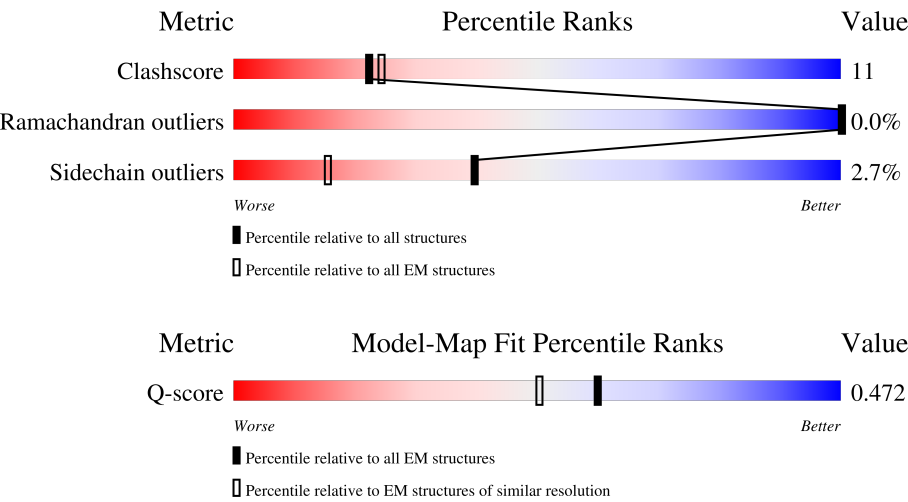
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









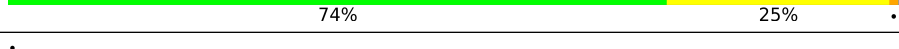
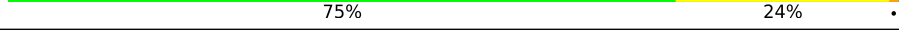
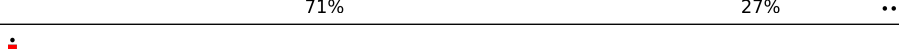
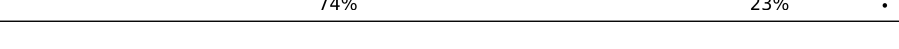
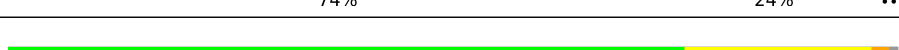

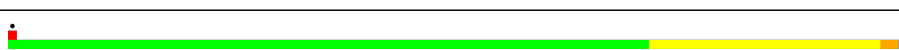

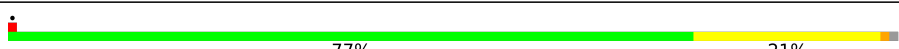





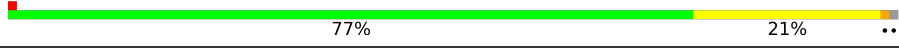
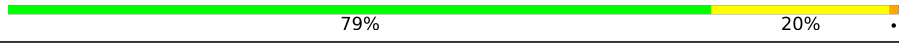



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	22	250	
1	32	250	
1	42	250	
1	52	250	



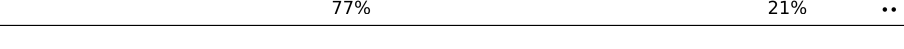
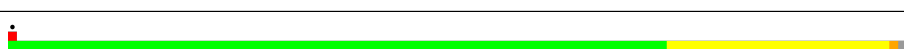



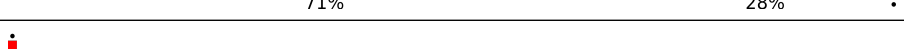



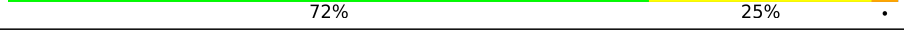

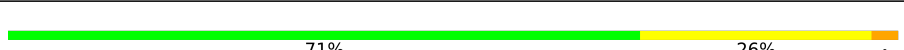


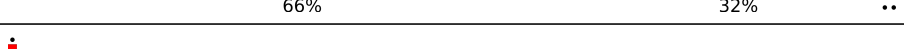







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Mol	Chain	Length	Quality of chain
1	A1	250	
1	A6	250	
2	B1	163	
2	B3	163	
2	B4	163	
2	B5	163	
2	B6	163	
2	B7	163	
2	F1	163	
2	F3	163	
2	F4	163	
2	F5	163	
2	F6	163	
2	F7	163	
2	G1	163	
2	G3	163	
2	G4	163	
2	G5	163	
2	G6	163	
2	G7	163	
2	H1	163	
2	H3	163	
2	H4	163	
2	H5	163	
2	H6	163	







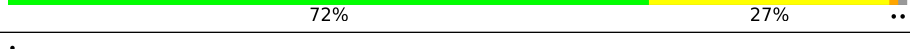
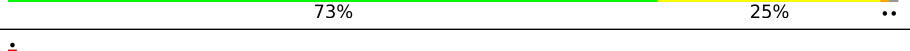
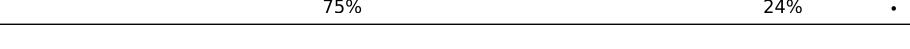
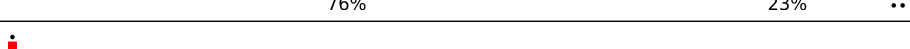
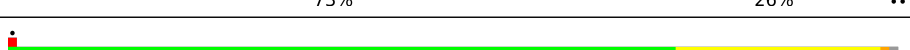

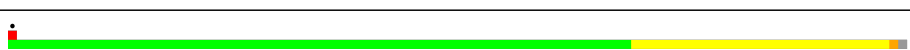

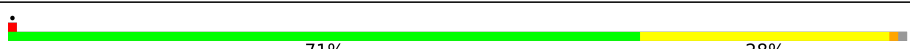





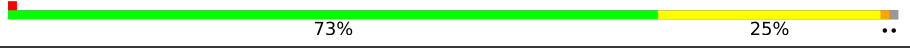
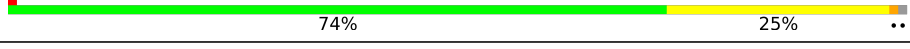



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Mol	Chain	Length	Quality of chain
2	H7	163	
2	I1	163	
2	I3	163	
2	I4	163	
2	I5	163	
2	I6	163	
2	I7	163	
2	K1	163	
2	K3	163	
2	K4	163	
2	K5	163	
2	K6	163	
2	K7	163	
2	N1	163	
2	N3	163	
2	N4	163	
2	N5	163	
2	N6	163	
2	N7	163	
2	R1	163	
2	R3	163	
2	R4	163	
2	R5	163	
2	R6	163	
2	R7	163	




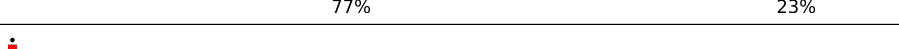

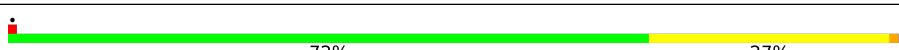



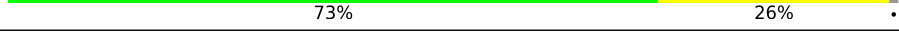

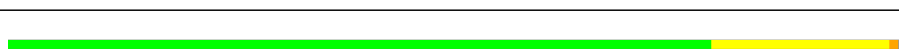




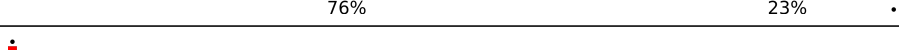




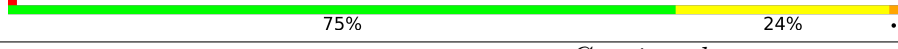



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Mol	Chain	Length	Quality of chain
2	S1	163	 75% 24% ..
2	S3	163	 74% 24% ..
2	S4	163	 74% 25% ..
2	S5	163	 75% 23% ..
2	S6	163	 75% 23% ..
2	S7	163	 74% 25% ..
2	T1	163	 72% 27% ..
2	T3	163	 73% 25% ..
2	T4	163	 75% 24% .
2	T5	163	 76% 23% ..
2	T6	163	 73% 26% ..
2	T7	163	 75% 23% ..
2	U1	163	 75% 24% ..
2	U3	163	 70% 29% ..
2	U4	163	 74% 25% ..
2	U5	163	 71% 28% ..
2	U6	163	 74% 24% ..
2	U7	163	 72% 27% ..
2	W1	163	 72% 27% .
2	W3	163	 72% 26% ..
2	W4	163	 74% 25% ..
2	W5	163	 73% 25% ..
2	W6	163	 74% 25% ..
2	W7	163	 71% 28% .
3	C1	173	 79% 21%


























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Mol	Chain	Length	Quality of chain
3	C3	173	
3	C4	173	
3	C5	173	
3	C6	173	
3	C7	173	
3	D1	173	
3	D3	173	
3	D4	173	
3	D5	173	
3	D6	173	
3	D7	173	
3	E1	173	
3	E3	173	
3	E4	173	
3	E5	173	
3	E6	173	
3	E7	173	
3	J1	173	
3	J3	173	
3	J4	173	
3	J5	173	
3	J6	173	
3	J7	173	
3	L1	173	
3	L3	173	







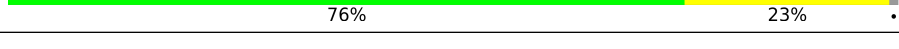
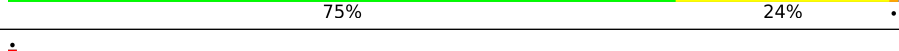
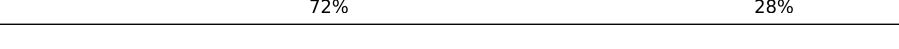
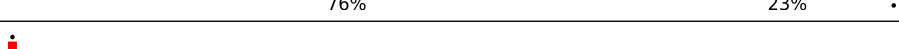
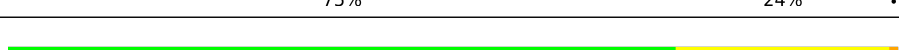

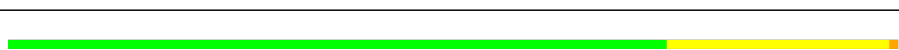

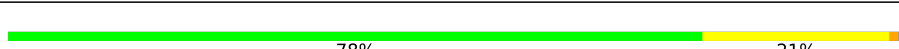










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Mol	Chain	Length	Quality of chain
3	L4	173	 77% 23% .
3	L5	173	 79% 18% .
3	L6	173	 74% 25% .
3	L7	173	 72% 27% .
3	M1	173	 72% 28%
3	M3	173	 79% 21%
3	M4	173	 77% 23%
3	M5	173	 75% 25%
3	M6	173	 74% 26%
3	M7	173	 79% 21%
3	O1	173	 75% 24% .
3	O3	173	 76% 23% .
3	O4	173	 72% 26% .
3	O5	173	 73% 27% .
3	O6	173	 73% 26% .
3	O7	173	 76% 24%
3	P1	173	 80% 19% .
3	P3	173	 75% 24% .
3	P4	173	 76% 24% .
3	P5	173	 77% 23% .
3	P6	173	 71% 29% .
3	P7	173	 78% 21% .
3	Q1	173	 76% 23% ..
3	Q3	173	 76% 22% ..
3	Q4	173	 79% 20% ..






















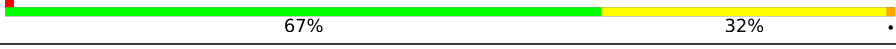
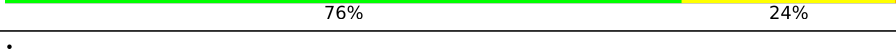
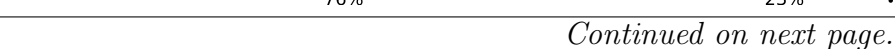

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Mol	Chain	Length	Quality of chain
3	Q5	173	
3	Q6	173	
3	Q7	173	
3	V1	173	
3	V3	173	
3	V4	173	
3	V5	173	
3	V6	173	
3	V7	173	
3	X1	173	
3	X3	173	
3	X4	173	
3	X5	173	
3	X6	173	
3	X7	173	
3	a1	173	
3	a3	173	
3	a4	173	
3	a5	173	
3	a6	173	
3	a7	173	
4	Y1	273	
4	Y3	273	
4	Y4	273	
4	Y5	273	

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Mol	Chain	Length	Quality of chain
4	Y6	273	
4	Y7	273	
5	Z1	289	
5	Z3	289	
5	Z4	289	
5	Z5	289	
5	Z6	289	
5	Z7	289	
6	O2	67	
6	Y2	67	
6	Z2	67	
6	z2	67	
7	12	110	
7	b2	110	
8	A2	161	
8	B2	161	
8	C2	161	
8	F2	161	
8	K2	161	
8	L2	161	
8	M2	161	
8	O2	161	
8	T2	161	
8	V2	161	
8	X2	161	

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Mol	Chain	Length	Quality of chain
8	a2	161	
8	c2	161	
8	d2	161	
8	g2	161	
8	l2	161	
8	m2	161	
8	n2	161	
8	p2	161	
8	u2	161	
8	w2	161	
8	y2	161	
9	D2	161	
9	E2	161	
9	G2	161	
9	H2	161	
9	I2	161	
9	J2	161	
9	Q2	161	
9	R2	161	
9	U2	161	
9	W2	161	
9	e2	161	
9	f2	161	
9	h2	161	
9	i2	161	

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Mol	Chain	Length	Quality of chain
9	j2	161	
9	k2	161	
9	r2	161	
9	s2	161	
9	v2	161	
9	x2	161	
10	N2	705	
10	o2	705	
11	P2	169	
11	q2	169	
12	S2	163	
12	t2	163	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 287122 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	196	Total	C	N	O	S	0	0
			1609	1029	280	299	1		
1	22	248	Total	C	N	O	S	0	0
			1989	1270	350	368	1		
1	32	248	Total	C	N	O	S	0	0
			1989	1270	350	368	1		
1	42	247	Total	C	N	O	S	0	0
			1980	1264	348	367	1		
1	52	247	Total	C	N	O	S	0	0
			1980	1264	348	367	1		
1	A6	196	Total	C	N	O	S	0	0
			1609	1029	280	299	1		

- Molecule 2 is a protein called C-phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	F1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	G1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	H1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	I1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	K1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	N1	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S1	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	T1	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	U1	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	W1	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	B3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	F3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	G3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	H3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	I3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	K3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	N3	163	Total 1221	C 771	N 205	O 243	S 2	0	0
2	R3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	S3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	T3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	U3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	W3	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	B4	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	F4	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	G4	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	H4	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	I4	162	Total 1213	C 766	N 204	O 242	S 1	0	0
2	K4	162	Total 1213	C 766	N 204	O 242	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N4	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R4	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S4	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	T4	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	U4	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	W4	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	B5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	F5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	G5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	H5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	I5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	K5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	N5	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	T5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	U5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	W5	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	B6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	F6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	G6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	I6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	K6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	N6	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	T6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	U6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	W6	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	B7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	F7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	G7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	H7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	I7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	K7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	N7	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	T7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	U7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	W7	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		

- Molecule 3 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D1	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E1	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q1	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V1	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X1	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a1	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	C3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D3	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E3	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q3	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	V3	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X3	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a3	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	C4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D4	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E4	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q4	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V4	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X4	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a4	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	C5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D5	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E5	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	O5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q5	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V5	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X5	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a5	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	C6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D6	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E6	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q6	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V6	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X6	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a6	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	C7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D7	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E7	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q7	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V7	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X7	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a7	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		

- Molecule 4 is a protein called Phycobilisome rod linker polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Y1	57	Total	C	N	O	0	0
			457	279	94	84		
4	Y3	57	Total	C	N	O	0	0
			457	279	94	84		
4	Y4	57	Total	C	N	O	0	0
			457	279	94	84		
4	Y5	57	Total	C	N	O	0	0
			457	279	94	84		
4	Y6	57	Total	C	N	O	0	0
			457	279	94	84		
4	Y7	57	Total	C	N	O	0	0
			457	279	94	84		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	51	GLY	SER	conflict	UNP Q31PE0
Y1	207	ASP	GLY	conflict	UNP Q31PE0
Y3	51	GLY	SER	conflict	UNP Q31PE0
Y3	207	ASP	GLY	conflict	UNP Q31PE0
Y4	51	GLY	SER	conflict	UNP Q31PE0

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Chain	Residue	Modelled	Actual	Comment	Reference
Y4	207	ASP	GLY	conflict	UNP Q31PE0
Y5	51	GLY	SER	conflict	UNP Q31PE0
Y5	207	ASP	GLY	conflict	UNP Q31PE0
Y6	51	GLY	SER	conflict	UNP Q31PE0
Y6	207	ASP	GLY	conflict	UNP Q31PE0
Y7	51	GLY	SER	conflict	UNP Q31PE0
Y7	207	ASP	GLY	conflict	UNP Q31PE0

- Molecule 5 is a protein called Phycobilisome rod linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z1	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		
5	Z3	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		
5	Z4	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		
5	Z5	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		
5	Z6	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		
5	Z7	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		

- Molecule 6 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	02	67	Total	C	N	O	S	0	0
			549	350	102	94	3		
6	Y2	67	Total	C	N	O	S	0	0
			549	350	102	94	3		
6	Z2	67	Total	C	N	O	S	0	0
			549	350	102	94	3		
6	z2	67	Total	C	N	O	S	0	0
			549	350	102	94	3		

- Molecule 7 is a protein called ApcG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	12	37	Total	C	N	O	0	0
			274	176	46	52		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	b2	37	Total	C	N	O	0	0
			274	176	46	52		

- Molecule 8 is a protein called Allophycocyanin, beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	B2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	C2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	F2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	K2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	L2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	M2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	O2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	T2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	V2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	X2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	a2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	c2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	d2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	g2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	l2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	m2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	n2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	p2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	u2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	w2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		
8	y2	161	Total	C	N	O	S	0	0
			1221	766	207	243	5		

- Molecule 9 is a protein called Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	E2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	G2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	H2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	I2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	J2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	Q2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	R2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	U2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	W2	160	Total	C	N	O	S	0	0
			1216	761	209	243	3		
9	e2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	f2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	h2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	i2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	j2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	k2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	r2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	s2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	v2	161	Total	C	N	O	S	0	0
			1224	766	210	244	4		
9	x2	160	Total	C	N	O	S	0	0
			1216	761	209	243	3		

- Molecule 10 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N2	658	Total	C	N	O	S	0	0
			5242	3317	948	971	6		
10	o2	658	Total	C	N	O	S	0	0
			5242	3317	948	971	6		

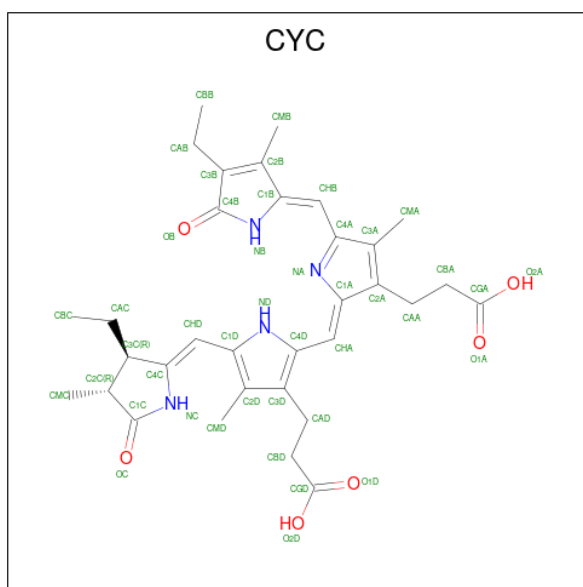
- Molecule 11 is a protein called Allophycocyanin, beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P2	169	Total	C	N	O	S	0	0
			1310	817	237	254	2		
11	q2	169	Total	C	N	O	S	0	0
			1310	817	237	254	2		

- Molecule 12 is a protein called Allophycocyanin alpha-B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S2	162	Total	C	N	O	S	0	0
			1268	805	220	239	4		
12	t2	162	Total	C	N	O	S	0	0
			1268	805	220	239	4		

- Molecule 13 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				AltConf
13	A1	1	Total 43	C 33	N 4	O 6	0
13	A1	1	Total 43	C 33	N 4	O 6	0
13	B1	1	Total 43	C 33	N 4	O 6	0
13	C1	1	Total 43	C 33	N 4	O 6	0
13	C1	1	Total 43	C 33	N 4	O 6	0
13	D1	1	Total 43	C 33	N 4	O 6	0
13	E1	1	Total 43	C 33	N 4	O 6	0
13	F1	1	Total 43	C 33	N 4	O 6	0
13	F1	1	Total 43	C 33	N 4	O 6	0
13	G1	1	Total 43	C 33	N 4	O 6	0
13	H1	1	Total 43	C 33	N 4	O 6	0
13	I1	1	Total 43	C 33	N 4	O 6	0
13	J1	1	Total 43	C 33	N 4	O 6	0
13	J1	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	K1	1	Total 43	C 33	N 4	O 6	0
13	L1	1	Total 43	C 33	N 4	O 6	0
13	M1	1	Total 43	C 33	N 4	O 6	0
13	N1	1	Total 43	C 33	N 4	O 6	0
13	P1	1	Total 43	C 33	N 4	O 6	0
13	P1	1	Total 43	C 33	N 4	O 6	0
13	Q1	1	Total 43	C 33	N 4	O 6	0
13	Q1	1	Total 43	C 33	N 4	O 6	0
13	R1	1	Total 43	C 33	N 4	O 6	0
13	S1	1	Total 43	C 33	N 4	O 6	0
13	T1	1	Total 43	C 33	N 4	O 6	0
13	T1	1	Total 43	C 33	N 4	O 6	0
13	U1	1	Total 43	C 33	N 4	O 6	0
13	V1	1	Total 43	C 33	N 4	O 6	0
13	V1	1	Total 43	C 33	N 4	O 6	0
13	W1	1	Total 43	C 33	N 4	O 6	0
13	X1	1	Total 43	C 33	N 4	O 6	0
13	Z1	1	Total 43	C 33	N 4	O 6	0
13	a1	1	Total 43	C 33	N 4	O 6	0
13	a1	1	Total 43	C 33	N 4	O 6	0
13	22	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
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13	32	1	Total 43	C 33	N 4	O 6	0
13	42	1	Total 43	C 33	N 4	O 6	0
13	42	1	Total 43	C 33	N 4	O 6	0
13	52	1	Total 43	C 33	N 4	O 6	0
13	52	1	Total 43	C 33	N 4	O 6	0
13	A2	1	Total 43	C 33	N 4	O 6	0
13	A2	1	Total 43	C 33	N 4	O 6	0
13	B2	1	Total 43	C 33	N 4	O 6	0
13	B2	1	Total 43	C 33	N 4	O 6	0
13	C2	1	Total 43	C 33	N 4	O 6	0
13	D2	1	Total 43	C 33	N 4	O 6	0
13	E2	1	Total 43	C 33	N 4	O 6	0
13	F2	1	Total 43	C 33	N 4	O 6	0
13	G2	1	Total 43	C 33	N 4	O 6	0
13	H2	1	Total 43	C 33	N 4	O 6	0
13	L2	1	Total 43	C 33	N 4	O 6	0
13	M2	1	Total 43	C 33	N 4	O 6	0
13	N2	1	Total 43	C 33	N 4	O 6	0
13	N2	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
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13	Q2	1	Total 43	C 33	N 4	O 6	0
13	R2	1	Total 43	C 33	N 4	O 6	0
13	S2	1	Total 43	C 33	N 4	O 6	0
13	T2	1	Total 43	C 33	N 4	O 6	0
13	U2	1	Total 43	C 33	N 4	O 6	0
13	V2	1	Total 43	C 33	N 4	O 6	0
13	W2	1	Total 43	C 33	N 4	O 6	0
13	X2	1	Total 43	C 33	N 4	O 6	0
13	a2	1	Total 43	C 33	N 4	O 6	0
13	c2	1	Total 43	C 33	N 4	O 6	0
13	d2	1	Total 43	C 33	N 4	O 6	0
13	e2	1	Total 43	C 33	N 4	O 6	0
13	f2	1	Total 43	C 33	N 4	O 6	0
13	g2	1	Total 43	C 33	N 4	O 6	0
13	h2	1	Total 43	C 33	N 4	O 6	0
13	i2	1	Total 43	C 33	N 4	O 6	0
13	j2	1	Total 43	C 33	N 4	O 6	0
13	k2	1	Total 43	C 33	N 4	O 6	0
13	l2	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
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13	n2	1	Total 43	C 33	N 4	O 6	0
13	o2	1	Total 43	C 33	N 4	O 6	0
13	p2	1	Total 43	C 33	N 4	O 6	0
13	q2	1	Total 43	C 33	N 4	O 6	0
13	r2	1	Total 43	C 33	N 4	O 6	0
13	s2	1	Total 43	C 33	N 4	O 6	0
13	t2	1	Total 43	C 33	N 4	O 6	0
13	v2	1	Total 43	C 33	N 4	O 6	0
13	w2	1	Total 43	C 33	N 4	O 6	0
13	x2	1	Total 43	C 33	N 4	O 6	0
13	y2	1	Total 43	C 33	N 4	O 6	0
13	z2	1	Total 43	C 33	N 4	O 6	0
13	B3	1	Total 43	C 33	N 4	O 6	0
13	C3	1	Total 43	C 33	N 4	O 6	0
13	C3	1	Total 43	C 33	N 4	O 6	0
13	D3	1	Total 43	C 33	N 4	O 6	0
13	E3	1	Total 43	C 33	N 4	O 6	0
13	F3	1	Total 43	C 33	N 4	O 6	0
13	F3	1	Total 43	C 33	N 4	O 6	0
13	G3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	H3	1	Total 43	C 33	N 4	O 6	0
13	I3	1	Total 43	C 33	N 4	O 6	0
13	J3	1	Total 43	C 33	N 4	O 6	0
13	J3	1	Total 43	C 33	N 4	O 6	0
13	K3	1	Total 43	C 33	N 4	O 6	0
13	L3	1	Total 43	C 33	N 4	O 6	0
13	M3	1	Total 43	C 33	N 4	O 6	0
13	N3	1	Total 43	C 33	N 4	O 6	0
13	P3	1	Total 43	C 33	N 4	O 6	0
13	P3	1	Total 43	C 33	N 4	O 6	0
13	Q3	1	Total 43	C 33	N 4	O 6	0
13	Q3	1	Total 43	C 33	N 4	O 6	0
13	R3	1	Total 43	C 33	N 4	O 6	0
13	S3	1	Total 43	C 33	N 4	O 6	0
13	T3	1	Total 43	C 33	N 4	O 6	0
13	T3	1	Total 43	C 33	N 4	O 6	0
13	U3	1	Total 43	C 33	N 4	O 6	0
13	V3	1	Total 43	C 33	N 4	O 6	0
13	V3	1	Total 43	C 33	N 4	O 6	0
13	W3	1	Total 43	C 33	N 4	O 6	0
13	X3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	Z3	1	Total 43	C 33	N 4	O 6	0
13	a3	1	Total 43	C 33	N 4	O 6	0
13	a3	1	Total 43	C 33	N 4	O 6	0
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13	C4	1	Total 43	C 33	N 4	O 6	0
13	C4	1	Total 43	C 33	N 4	O 6	0
13	D4	1	Total 43	C 33	N 4	O 6	0
13	E4	1	Total 43	C 33	N 4	O 6	0
13	F4	1	Total 43	C 33	N 4	O 6	0
13	F4	1	Total 43	C 33	N 4	O 6	0
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13	H4	1	Total 43	C 33	N 4	O 6	0
13	I4	1	Total 43	C 33	N 4	O 6	0
13	J4	1	Total 43	C 33	N 4	O 6	0
13	J4	1	Total 43	C 33	N 4	O 6	0
13	K4	1	Total 43	C 33	N 4	O 6	0
13	L4	1	Total 43	C 33	N 4	O 6	0
13	M4	1	Total 43	C 33	N 4	O 6	0
13	N4	1	Total 43	C 33	N 4	O 6	0
13	P4	1	Total 43	C 33	N 4	O 6	0
13	P4	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	Q4	1	Total 43	C 33	N 4	O 6	0
13	Q4	1	Total 43	C 33	N 4	O 6	0
13	R4	1	Total 43	C 33	N 4	O 6	0
13	S4	1	Total 43	C 33	N 4	O 6	0
13	T4	1	Total 43	C 33	N 4	O 6	0
13	T4	1	Total 43	C 33	N 4	O 6	0
13	U4	1	Total 43	C 33	N 4	O 6	0
13	V4	1	Total 43	C 33	N 4	O 6	0
13	V4	1	Total 43	C 33	N 4	O 6	0
13	W4	1	Total 43	C 33	N 4	O 6	0
13	X4	1	Total 43	C 33	N 4	O 6	0
13	Z4	1	Total 43	C 33	N 4	O 6	0
13	a4	1	Total 43	C 33	N 4	O 6	0
13	a4	1	Total 43	C 33	N 4	O 6	0
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13	C5	1	Total 43	C 33	N 4	O 6	0
13	D5	1	Total 43	C 33	N 4	O 6	0
13	E5	1	Total 43	C 33	N 4	O 6	0
13	F5	1	Total 43	C 33	N 4	O 6	0
13	F5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	G5	1	Total 43	C 33	N 4	O 6	0
13	H5	1	Total 43	C 33	N 4	O 6	0
13	I5	1	Total 43	C 33	N 4	O 6	0
13	J5	1	Total 43	C 33	N 4	O 6	0
13	J5	1	Total 43	C 33	N 4	O 6	0
13	K5	1	Total 43	C 33	N 4	O 6	0
13	L5	1	Total 43	C 33	N 4	O 6	0
13	M5	1	Total 43	C 33	N 4	O 6	0
13	N5	1	Total 43	C 33	N 4	O 6	0
13	P5	1	Total 43	C 33	N 4	O 6	0
13	P5	1	Total 43	C 33	N 4	O 6	0
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13	Q5	1	Total 43	C 33	N 4	O 6	0
13	R5	1	Total 43	C 33	N 4	O 6	0
13	S5	1	Total 43	C 33	N 4	O 6	0
13	T5	1	Total 43	C 33	N 4	O 6	0
13	T5	1	Total 43	C 33	N 4	O 6	0
13	U5	1	Total 43	C 33	N 4	O 6	0
13	V5	1	Total 43	C 33	N 4	O 6	0
13	V5	1	Total 43	C 33	N 4	O 6	0
13	W5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	X5	1	Total 43	C 33	N 4	O 6	0
13	Z5	1	Total 43	C 33	N 4	O 6	0
13	a5	1	Total 43	C 33	N 4	O 6	0
13	a5	1	Total 43	C 33	N 4	O 6	0
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13	A6	1	Total 43	C 33	N 4	O 6	0
13	B6	1	Total 43	C 33	N 4	O 6	0
13	C6	1	Total 43	C 33	N 4	O 6	0
13	C6	1	Total 43	C 33	N 4	O 6	0
13	D6	1	Total 43	C 33	N 4	O 6	0
13	E6	1	Total 43	C 33	N 4	O 6	0
13	F6	1	Total 43	C 33	N 4	O 6	0
13	F6	1	Total 43	C 33	N 4	O 6	0
13	G6	1	Total 43	C 33	N 4	O 6	0
13	H6	1	Total 43	C 33	N 4	O 6	0
13	I6	1	Total 43	C 33	N 4	O 6	0
13	J6	1	Total 43	C 33	N 4	O 6	0
13	J6	1	Total 43	C 33	N 4	O 6	0
13	K6	1	Total 43	C 33	N 4	O 6	0
13	L6	1	Total 43	C 33	N 4	O 6	0
13	M6	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	N6	1	Total 43	C 33	N 4	O 6	0
13	P6	1	Total 43	C 33	N 4	O 6	0
13	P6	1	Total 43	C 33	N 4	O 6	0
13	Q6	1	Total 43	C 33	N 4	O 6	0
13	Q6	1	Total 43	C 33	N 4	O 6	0
13	R6	1	Total 43	C 33	N 4	O 6	0
13	S6	1	Total 43	C 33	N 4	O 6	0
13	T6	1	Total 43	C 33	N 4	O 6	0
13	T6	1	Total 43	C 33	N 4	O 6	0
13	U6	1	Total 43	C 33	N 4	O 6	0
13	V6	1	Total 43	C 33	N 4	O 6	0
13	V6	1	Total 43	C 33	N 4	O 6	0
13	W6	1	Total 43	C 33	N 4	O 6	0
13	X6	1	Total 43	C 33	N 4	O 6	0
13	Z6	1	Total 43	C 33	N 4	O 6	0
13	a6	1	Total 43	C 33	N 4	O 6	0
13	a6	1	Total 43	C 33	N 4	O 6	0
13	B7	1	Total 43	C 33	N 4	O 6	0
13	C7	1	Total 43	C 33	N 4	O 6	0
13	C7	1	Total 43	C 33	N 4	O 6	0
13	D7	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
13	E7	1	Total 43	C 33	N 4	O 6	0
13	F7	1	Total 43	C 33	N 4	O 6	0
13	F7	1	Total 43	C 33	N 4	O 6	0
13	G7	1	Total 43	C 33	N 4	O 6	0
13	H7	1	Total 43	C 33	N 4	O 6	0
13	I7	1	Total 43	C 33	N 4	O 6	0
13	J7	1	Total 43	C 33	N 4	O 6	0
13	J7	1	Total 43	C 33	N 4	O 6	0
13	K7	1	Total 43	C 33	N 4	O 6	0
13	L7	1	Total 43	C 33	N 4	O 6	0
13	M7	1	Total 43	C 33	N 4	O 6	0
13	N7	1	Total 43	C 33	N 4	O 6	0
13	P7	1	Total 43	C 33	N 4	O 6	0
13	P7	1	Total 43	C 33	N 4	O 6	0
13	Q7	1	Total 43	C 33	N 4	O 6	0
13	Q7	1	Total 43	C 33	N 4	O 6	0
13	R7	1	Total 43	C 33	N 4	O 6	0
13	S7	1	Total 43	C 33	N 4	O 6	0
13	T7	1	Total 43	C 33	N 4	O 6	0
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13	U7	1	Total 43	C 33	N 4	O 6	0

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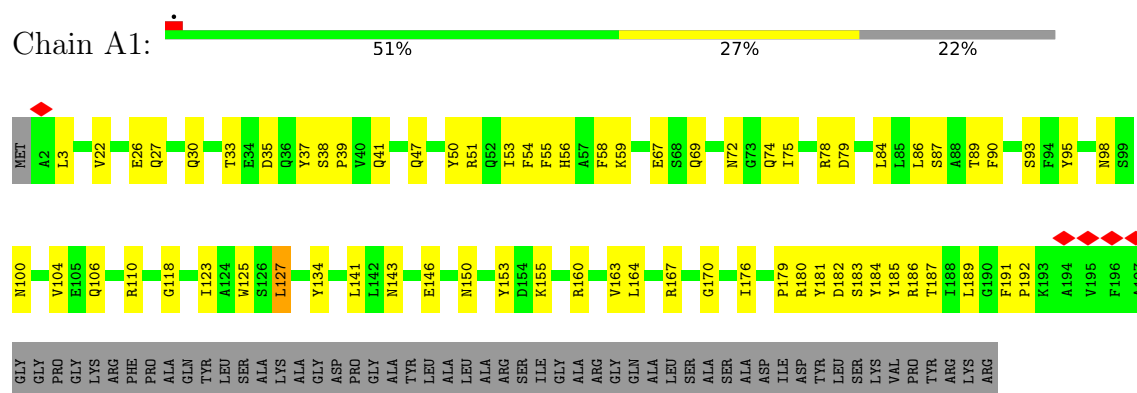
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Mol	Chain	Residues	Atoms				AltConf
13	V7	1	Total	C	N	O	0
			43	33	4	6	
13	V7	1	Total	C	N	O	0
			43	33	4	6	
13	W7	1	Total	C	N	O	0
			43	33	4	6	
13	X7	1	Total	C	N	O	0
			43	33	4	6	
13	Z7	1	Total	C	N	O	0
			43	33	4	6	
13	a7	1	Total	C	N	O	0
			43	33	4	6	
13	a7	1	Total	C	N	O	0
			43	33	4	6	

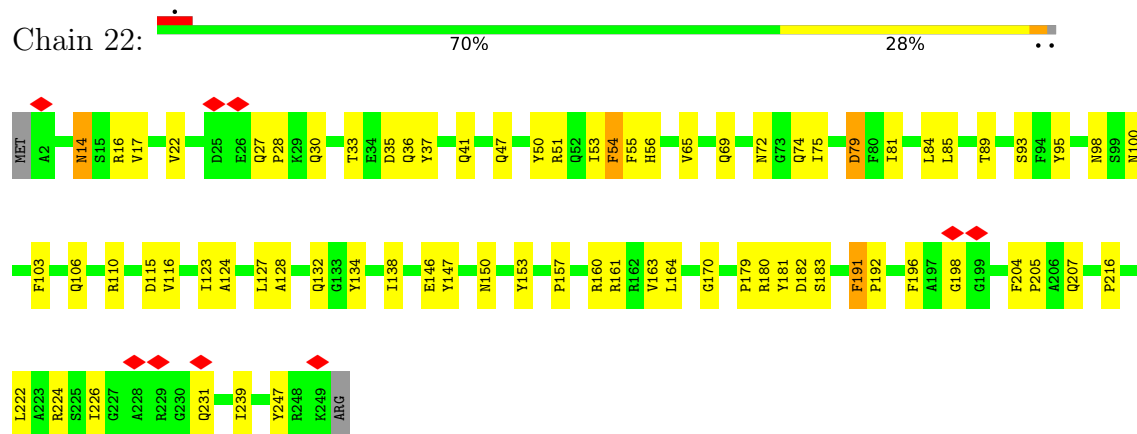
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

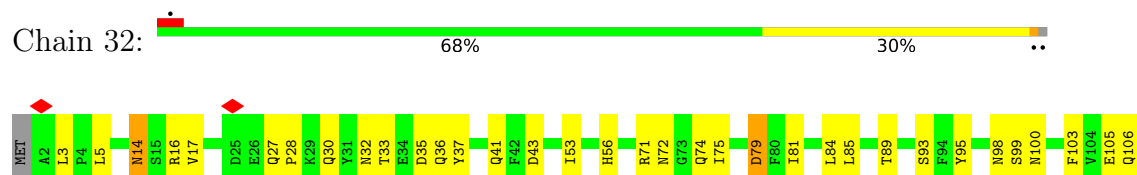
- Molecule 1: Phycobilisome rod-core linker polypeptide

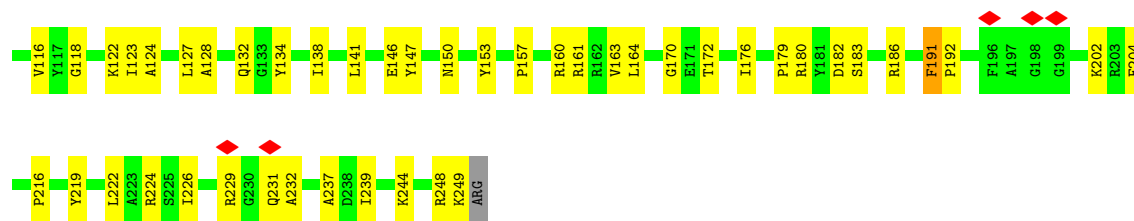


- Molecule 1: Phycobilisome rod-core linker polypeptide

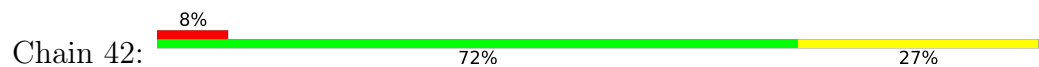


- Molecule 1: Phycobilisome rod-core linker polypeptide

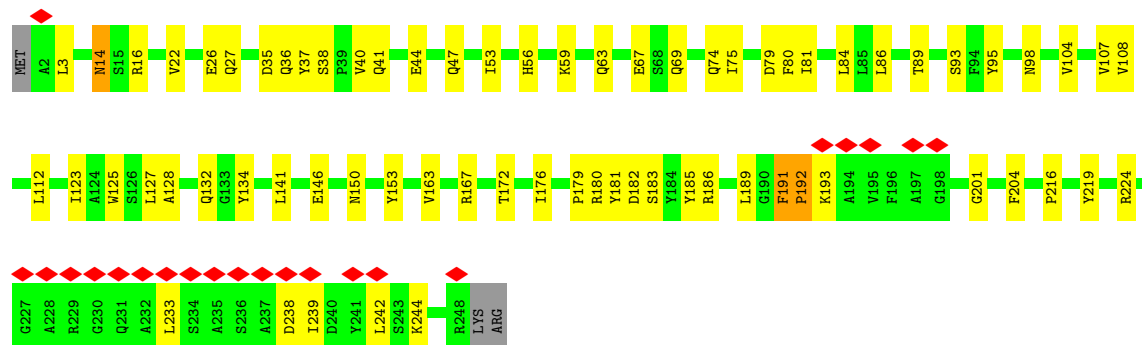




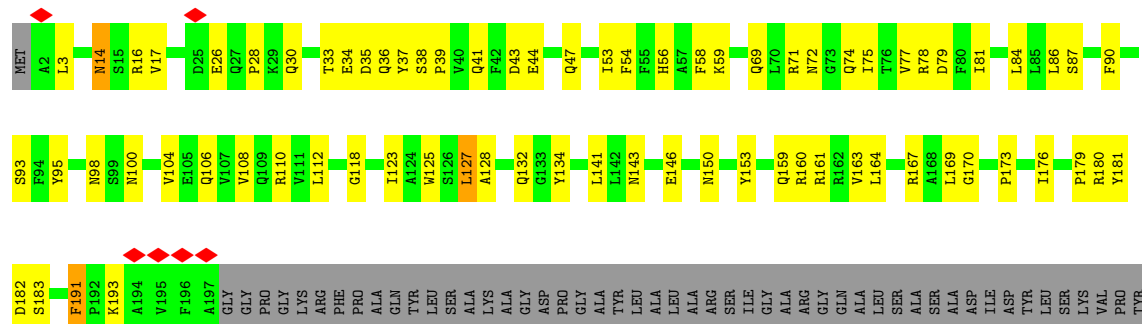
• Molecule 1: Phycobilisome rod-core linker polypeptide



• Molecule 1: Phycobilisome rod-core linker polypeptide




• Molecule 1: Phycobilisome rod-core linker polypeptide



ARG
LYS
ARG

• Molecule 2: C-phycoerythrin alpha subunit

Chain B1:  79% 18% ..


MET S2 A9 L20 S21 S22 T23 E24 L25 Q26 V27 A28 R31 F32 R33 A41 D50 N74 C85 R94 I95 V101 G106 P107 I108 D109 L113 I119 T122 A126 W129 L134 K138 H141 D146 S147 I155 S163

• Molecule 2: C-phycoerythrin alpha subunit

Chain F1:  71% 27% ..

MET S2 K3 E8 A9 V10 D14 S15 L20 S21 S22 T23 E24 L25 Q26 V27 A28 F29 R31 F32 R33 Q34 A41 L45 S62 N74 T78 F79 E80 G81 C85 I89 G90 Y91 R94 I95 Y98 A99 L100 V101 I108 D109 E110 T122 F123
D124 L125 P127 A128 W129 L134 K138 H141 S147 E150 Y154 I155 L162 S163

• Molecule 2: C-phycoerythrin alpha subunit

Chain G1:  78% 21% ..

MET S2 K3 T4 P5 E8 R18 T23 E24 L25 Q26 V27 R31 F32 R33 Q34 A41 D50 P71 N74 E80 C85 Y91 I95 A99 L100 V101 G103 G104 T105 I108 L113 E118 I119 T122 L134 L143 D146 S147
E150 Y154 I155 A161 L162 S163

• Molecule 2: C-phycoerythrin alpha subunit

Chain H1:  74% 26% .

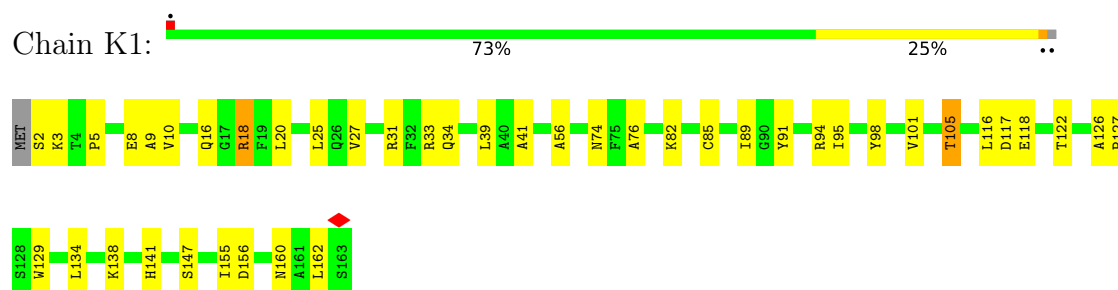
MET S2 K3 E8 A9 Q16 G17 F19 L20 T23 E24 L25 Q26 V27 R31 F32 R33 A41 K63 T78 P79 E80 G81 C85 A86 R87 Y91 R94 I95 Y98 A99 L100 V101 I108 D109 L112 L113 E118 T122 A126 W129
E132 A133 L134 H141 D146 S147 E150 Y154 I155 S163

• Molecule 2: C-phycoerythrin alpha subunit

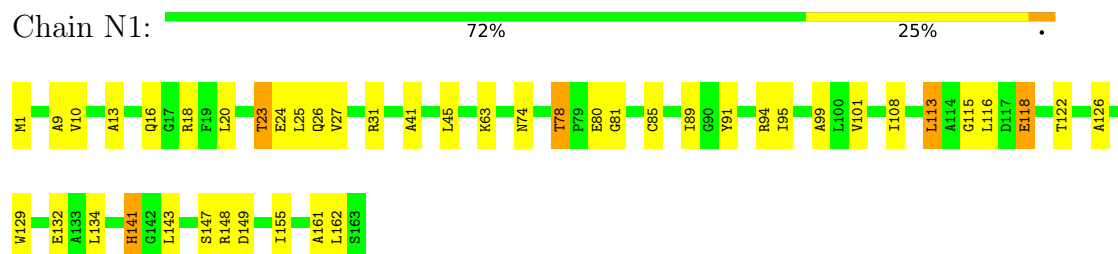
Chain I1:  75% 24% ..

MET S2 Q16 R18 F19 E24 Q26 V27 A28 R31 Q34 A35 A41 N48 A49 D50 S51 F64 P65 Y66 T67 T68 N74 T78 F79 E80 G81 C85 I89 G90 Y91 R94 I95 V101 I108 E118 K121 T122 A126 W129
L134 K138 L143 S147 R148 I155 D156 S163

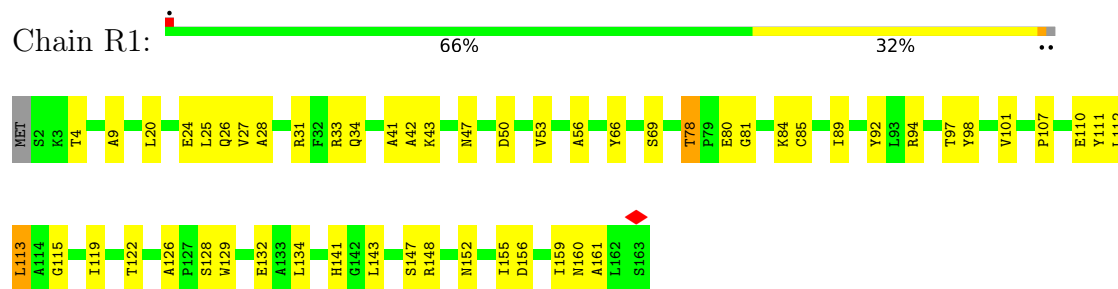
● Molecule 2: C-phycoerythrin alpha subunit



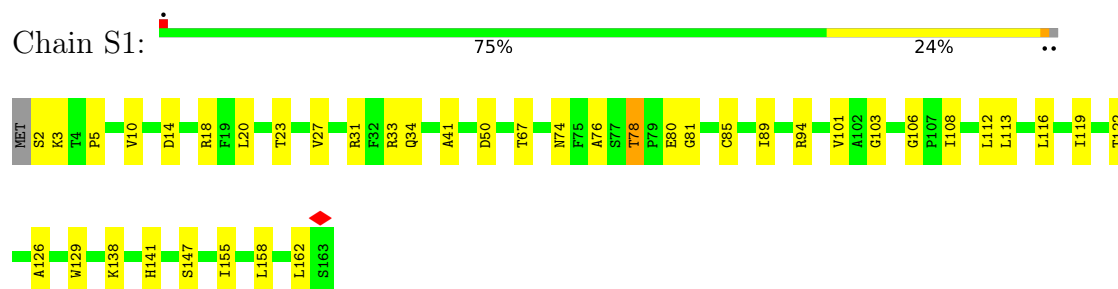
● Molecule 2: C-phycoerythrin alpha subunit



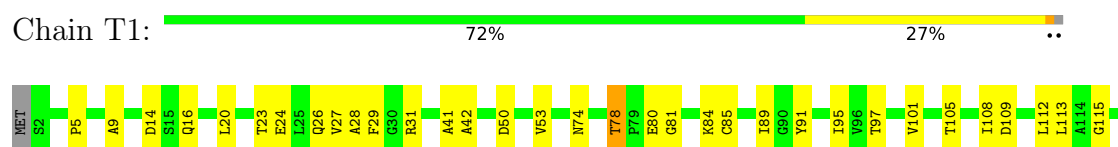
● Molecule 2: C-phycoerythrin alpha subunit



● Molecule 2: C-phycoerythrin alpha subunit



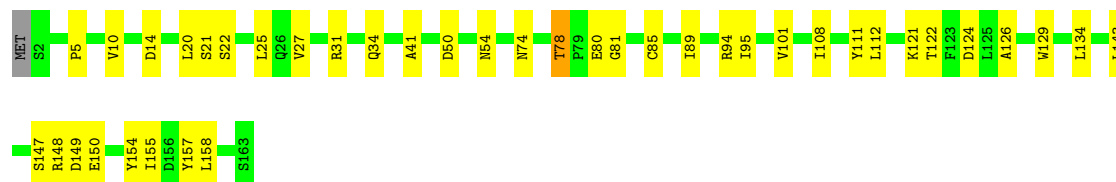
● Molecule 2: C-phycoerythrin alpha subunit





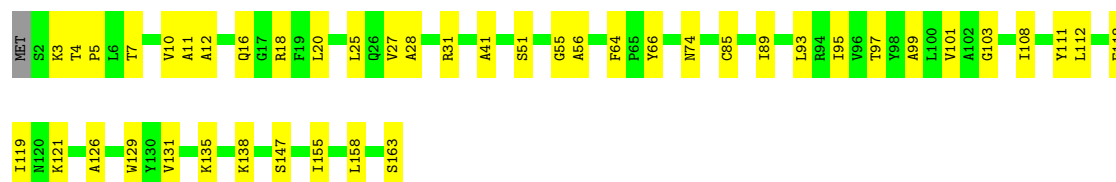
- Molecule 2: C-phycoerythrin alpha subunit

Chain U1: 75% 24% ..



- Molecule 2: C-phycoerythrin alpha subunit

Chain W1: 72% 27% .



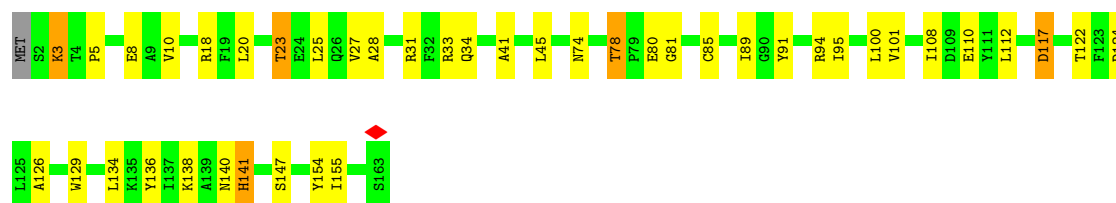
- Molecule 2: C-phycoerythrin alpha subunit

Chain B3: 76% 23% ..



- Molecule 2: C-phycoerythrin alpha subunit

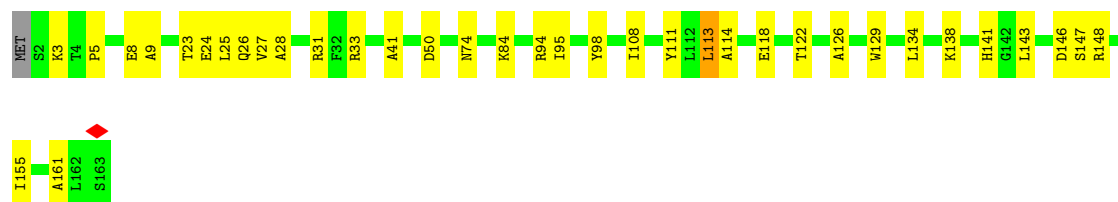
Chain F3: 74% 23% ..



- Molecule 2: C-phycoerythrin alpha subunit

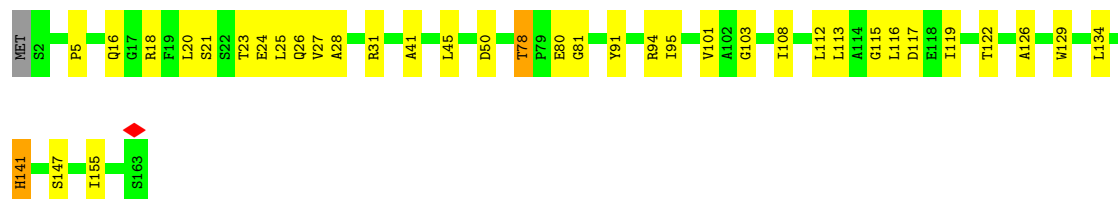
Chain G3: 77% 21% ..





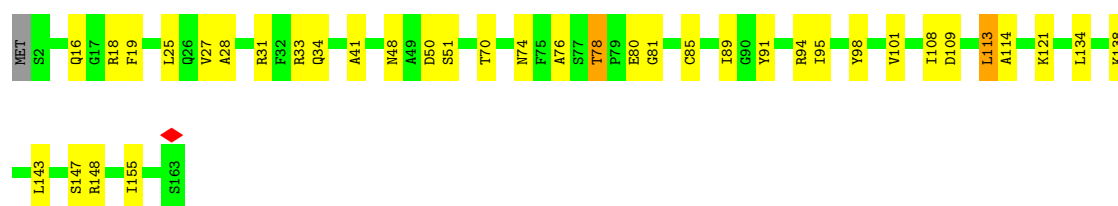
- Molecule 2: C-phycoerythrin alpha subunit

Chain H3: 77% 21% ..



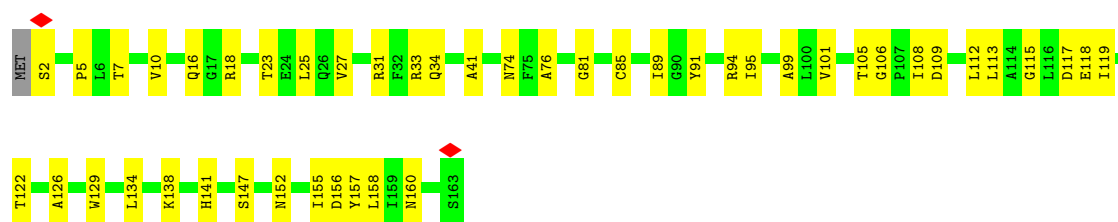
- Molecule 2: C-phycoerythrin alpha subunit

Chain I3: 77% 21% ..



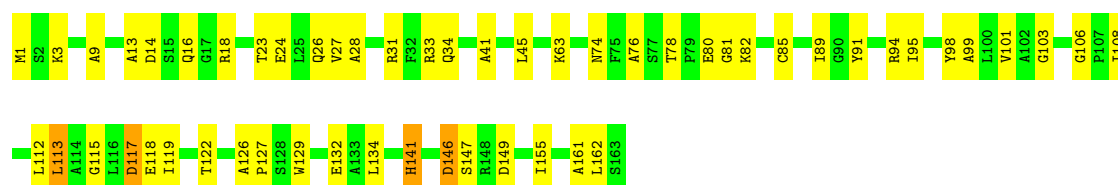
- Molecule 2: C-phycoerythrin alpha subunit

Chain K3: 71% 28% .



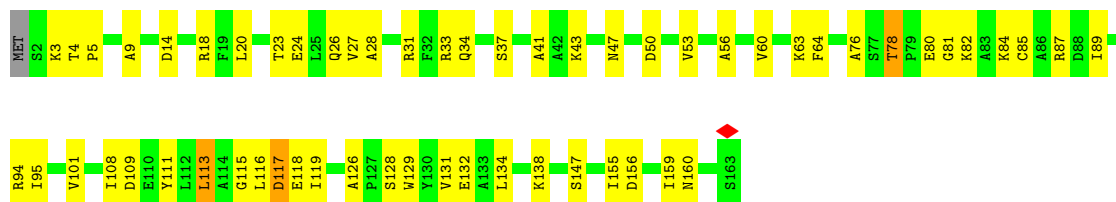
- Molecule 2: C-phycoerythrin alpha subunit

Chain N3: 67% 31% .




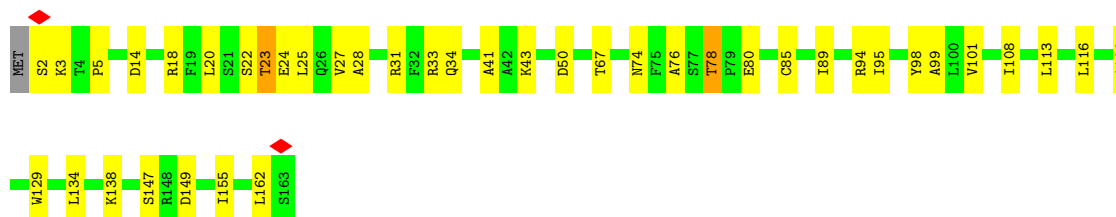
- Molecule 2: C-phycoerythrin alpha subunit

Chain R3:  64% 34% ..




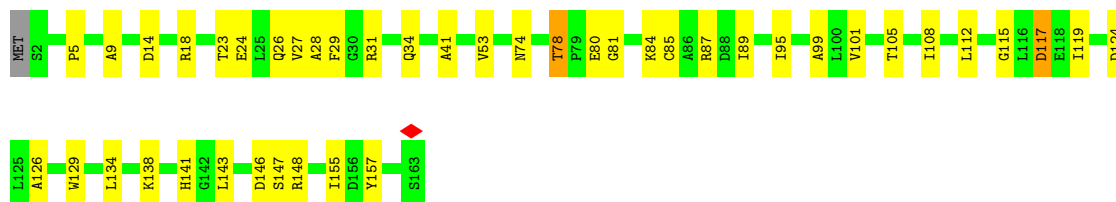
- Molecule 2: C-phycoerythrin alpha subunit

Chain S3:  74% 24% ..



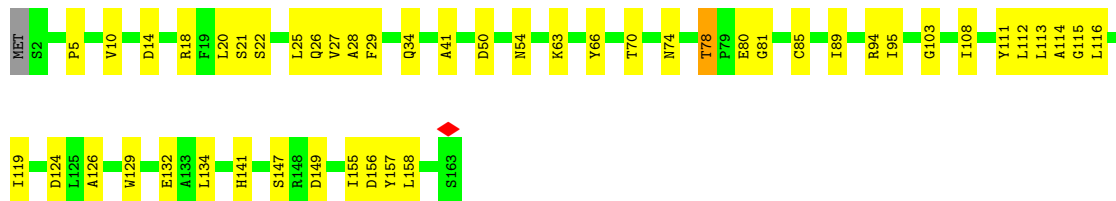
- Molecule 2: C-phycoerythrin alpha subunit

Chain T3:  73% 25% ..




- Molecule 2: C-phycoerythrin alpha subunit

Chain U3:  70% 29% ..



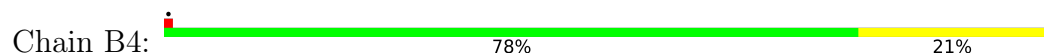
- Molecule 2: C-phycoerythrin alpha subunit

Chain W3:  72% 26% ..

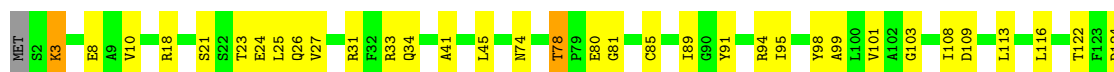
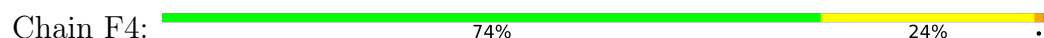




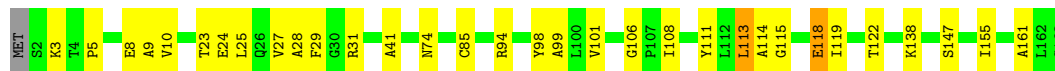
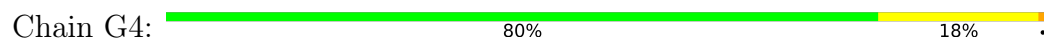
- Molecule 2: C-phycoerythrin alpha subunit



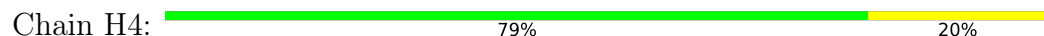
- Molecule 2: C-phycoerythrin alpha subunit



- Molecule 2: C-phycoerythrin alpha subunit



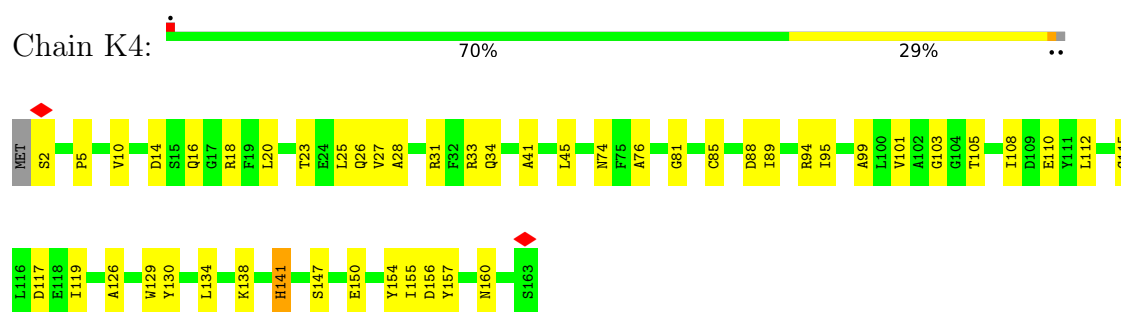
- Molecule 2: C-phycoerythrin alpha subunit



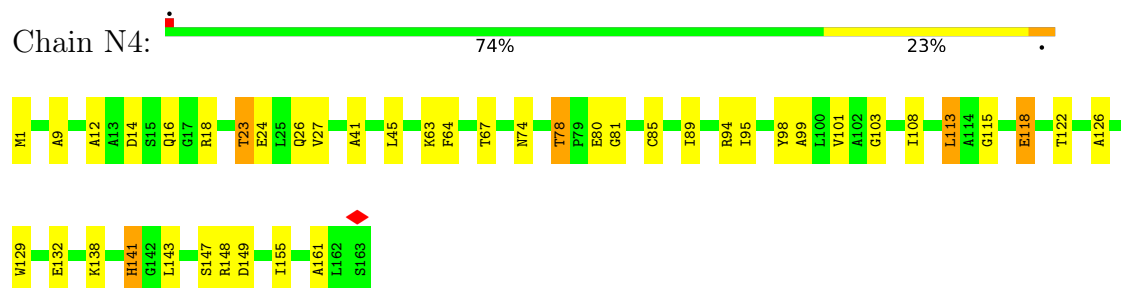
- Molecule 2: C-phycoerythrin alpha subunit



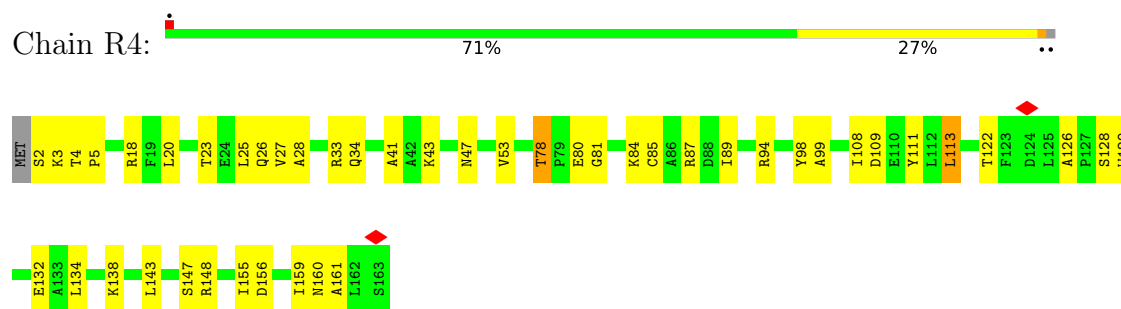
- Molecule 2: C-phycoerythrin alpha subunit



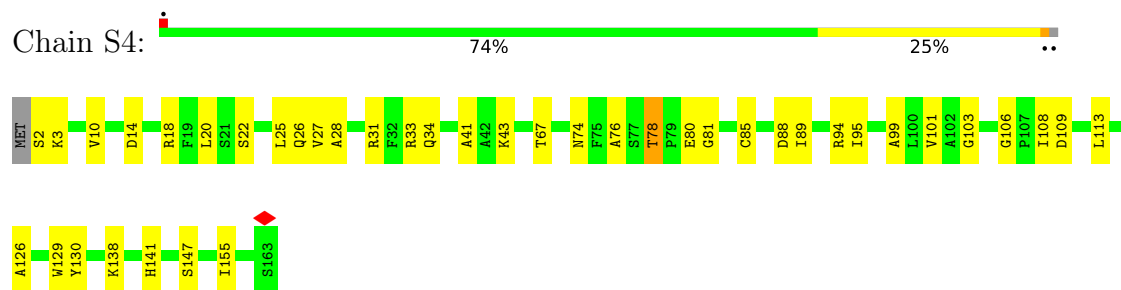
- Molecule 2: C-phycoerythrin alpha subunit



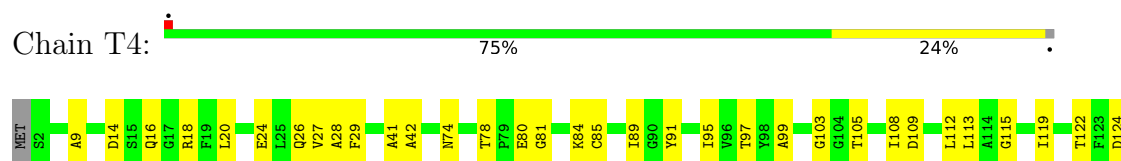
- Molecule 2: C-phycoerythrin alpha subunit

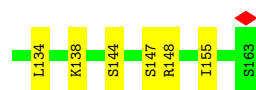


- Molecule 2: C-phycoerythrin alpha subunit



- Molecule 2: C-phycoerythrin alpha subunit





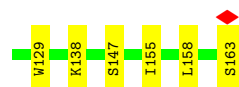
- Molecule 2: C-phycocyanin alpha subunit

Chain U4: 74% 25% ..



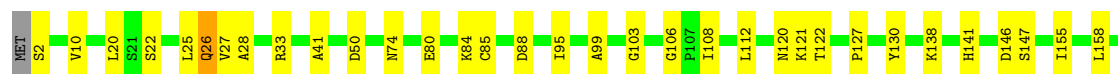
- Molecule 2: C-phycocyanin alpha subunit

Chain W4: 74% 25% ..



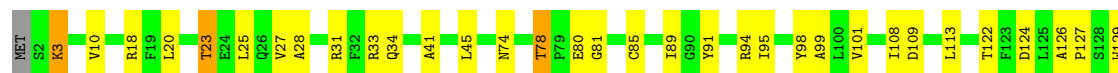
- Molecule 2: C-phycocyanin alpha subunit

Chain B5: 79% 20% ..



- Molecule 2: C-phycocyanin alpha subunit

Chain F5: 76% 21% ..

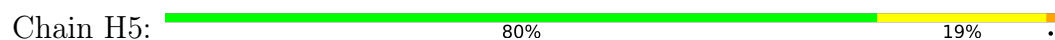


- Molecule 2: C-phycocyanin alpha subunit

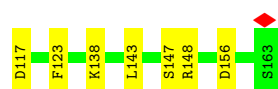
Chain G5: 81% 17% ..



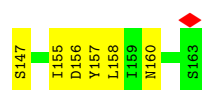
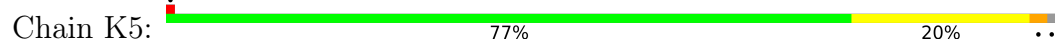
- Molecule 2: C-phycoerythrin alpha subunit



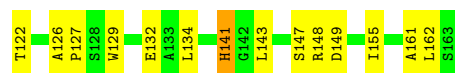
- Molecule 2: C-phycoerythrin alpha subunit



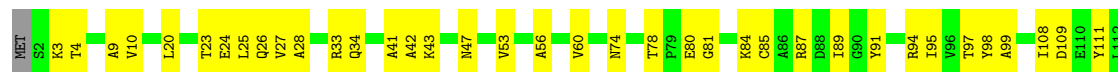
- Molecule 2: C-phycoerythrin alpha subunit

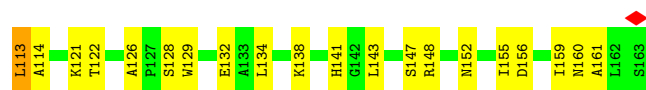


- Molecule 2: C-phycoerythrin alpha subunit



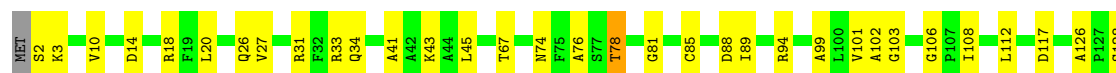
- Molecule 2: C-phycoerythrin alpha subunit





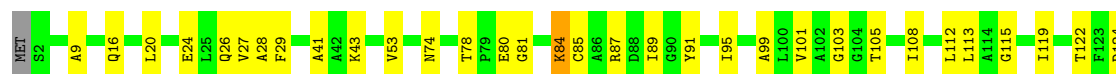
- Molecule 2: C-phycoerythrin alpha subunit

Chain S5: 75% 23% ..



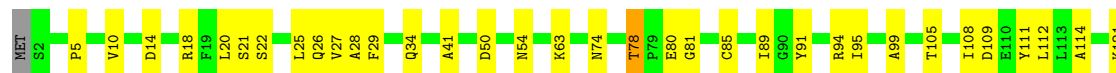
- Molecule 2: C-phycoerythrin alpha subunit

Chain T5: 76% 23% ..



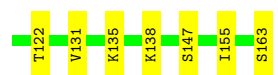
- Molecule 2: C-phycoerythrin alpha subunit

Chain U5: 71% 28% ..



- Molecule 2: C-phycoerythrin alpha subunit

Chain W5: 73% 25% ..



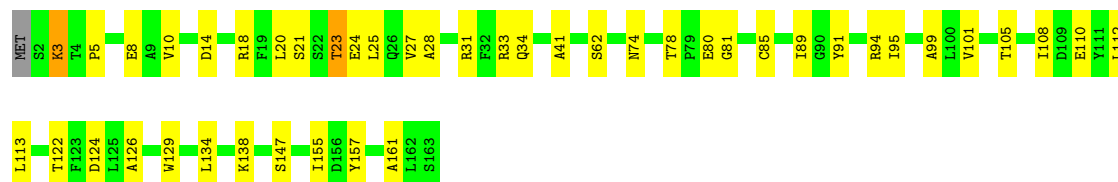
- Molecule 2: C-phycoerythrin alpha subunit

Chain B6: 74% 25% ..



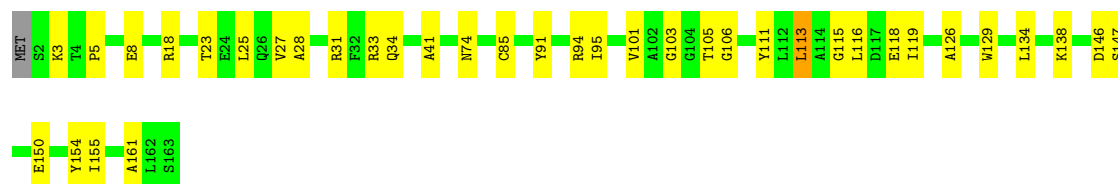
- Molecule 2: C-phycocyanin alpha subunit

Chain F6: 72% 26% ..



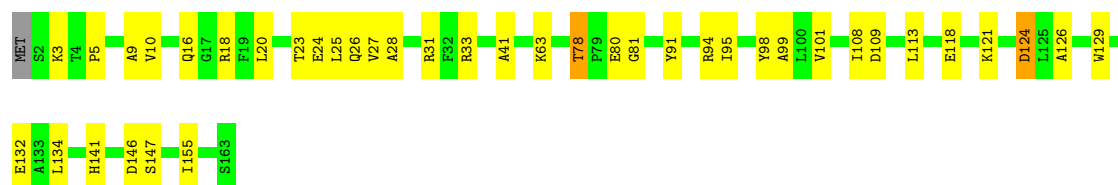
- Molecule 2: C-phycocyanin alpha subunit

Chain G6: 77% 22% ..



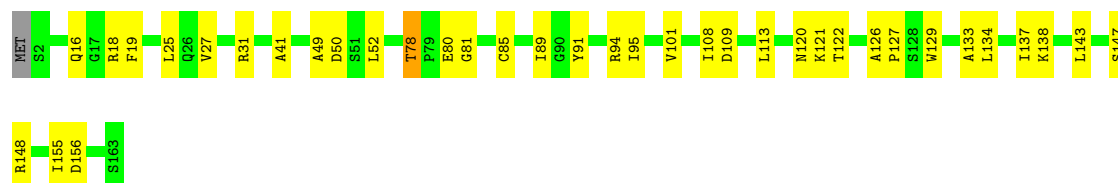
- Molecule 2: C-phycocyanin alpha subunit

Chain H6: 75% 23% ..




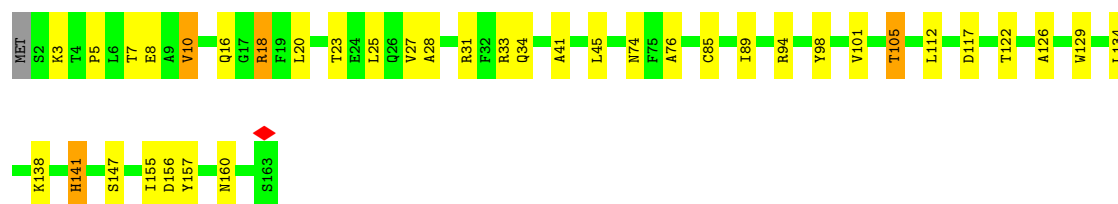
- Molecule 2: C-phycocyanin alpha subunit

Chain I6: 77% 22% ..




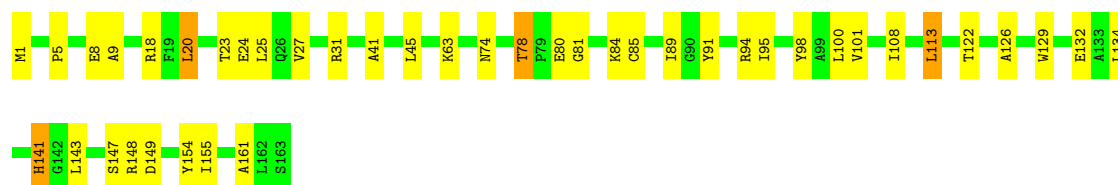
- Molecule 2: C-phycocyanin alpha subunit

Chain K6:  76% 21% ..



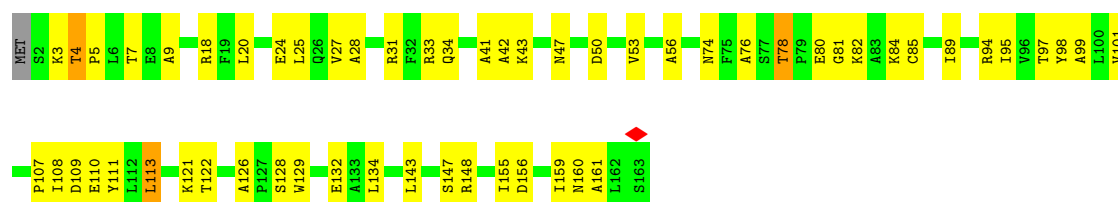
• Molecule 2: C-phycocyanin alpha subunit

Chain N6:  74% 23% .



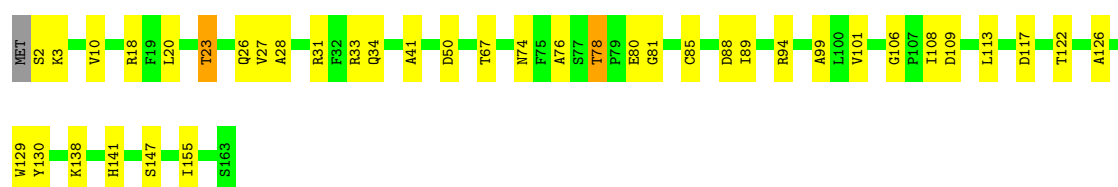
• Molecule 2: C-phycocyanin alpha subunit

Chain R6:  64% 33% ..



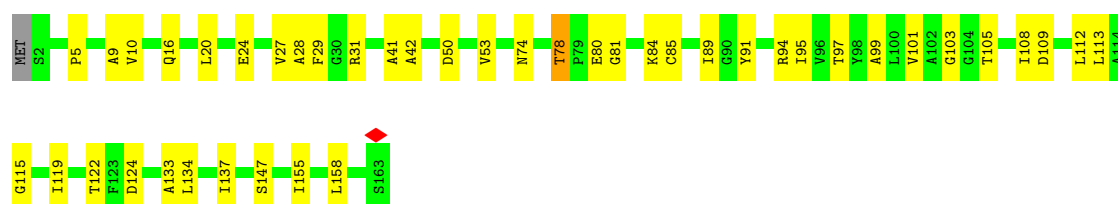
• Molecule 2: C-phycocyanin alpha subunit

Chain S6:  75% 23% ..

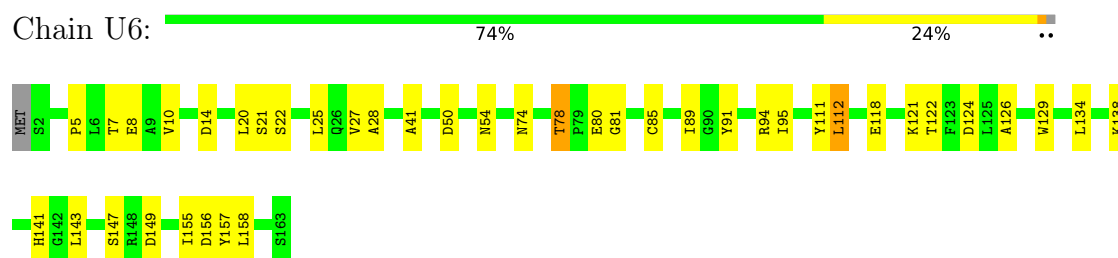


• Molecule 2: C-phycocyanin alpha subunit

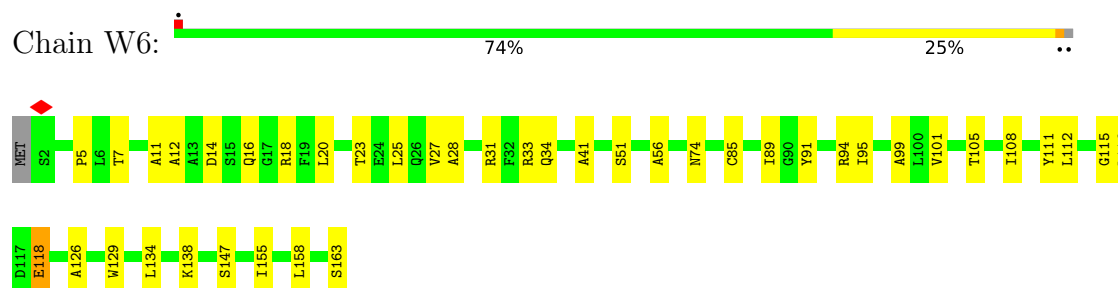
Chain T6:  73% 26% ..



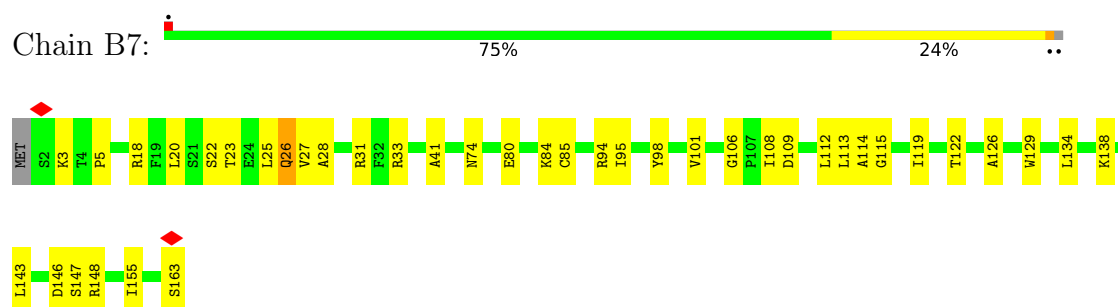
- Molecule 2: C-phycoerythrin alpha subunit



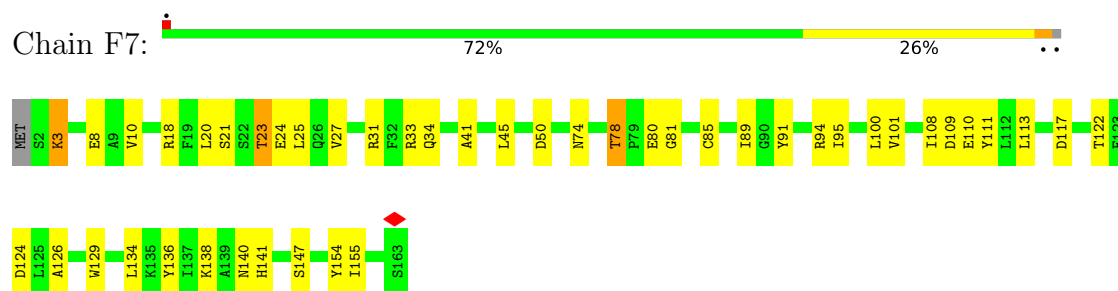
- Molecule 2: C-phycoerythrin alpha subunit



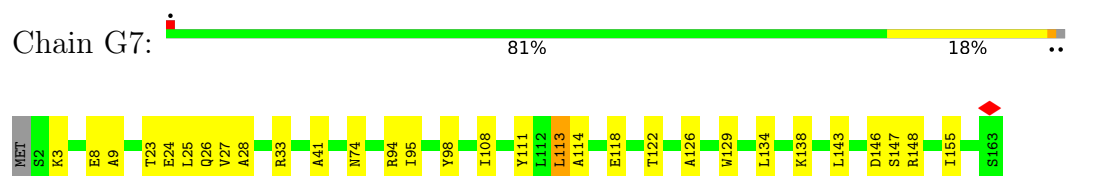
- Molecule 2: C-phycoerythrin alpha subunit



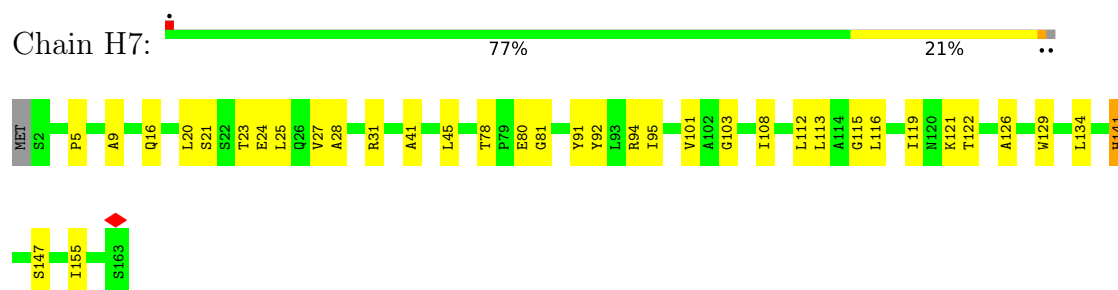
- Molecule 2: C-phycoerythrin alpha subunit



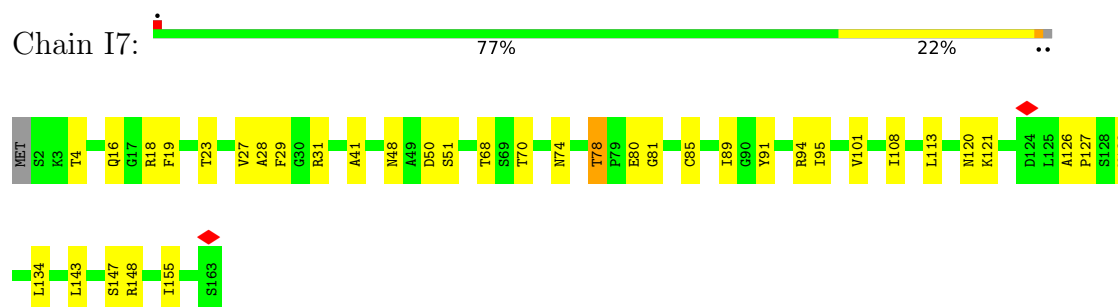
- Molecule 2: C-phycoerythrin alpha subunit



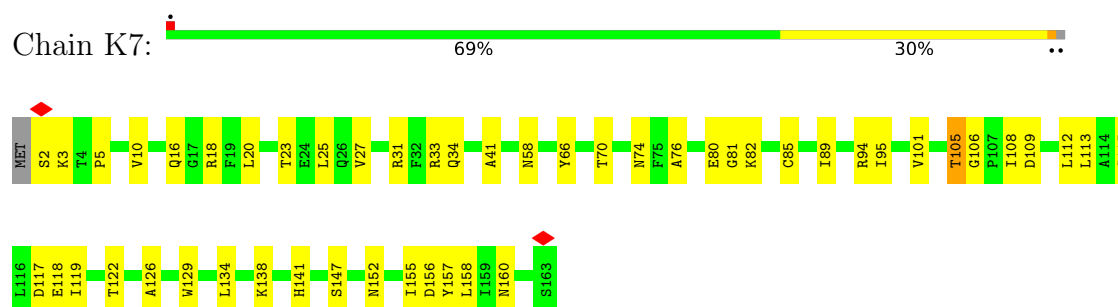
- Molecule 2: C-phycoerythrin alpha subunit



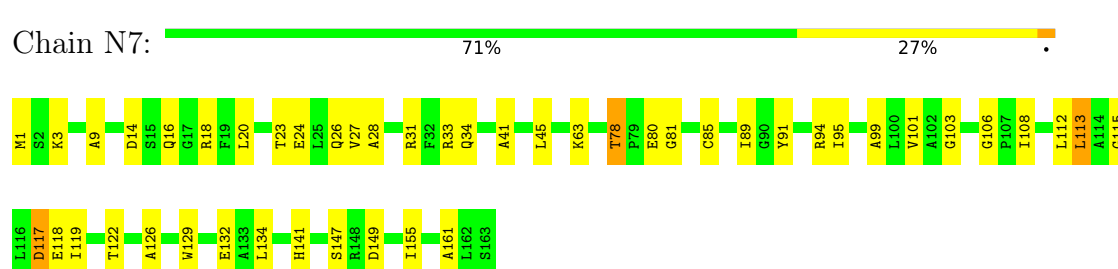
- Molecule 2: C-phycoerythrin alpha subunit



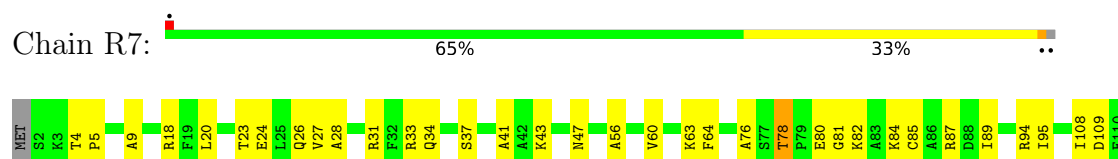
- Molecule 2: C-phycoerythrin alpha subunit



- Molecule 2: C-phycoerythrin alpha subunit



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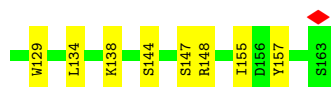
- Molecule 2: C-phycocyanin alpha subunit

Chain S7: 74% 25% ..



- Molecule 2: C-phycocyanin alpha subunit

Chain T7: 75% 23% ..



- Molecule 2: C-phycocyanin alpha subunit

Chain U7: 72% 27% ..

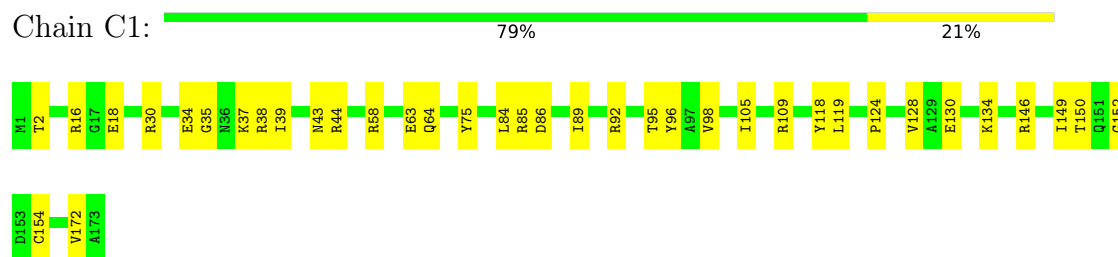


- Molecule 2: C-phycocyanin alpha subunit

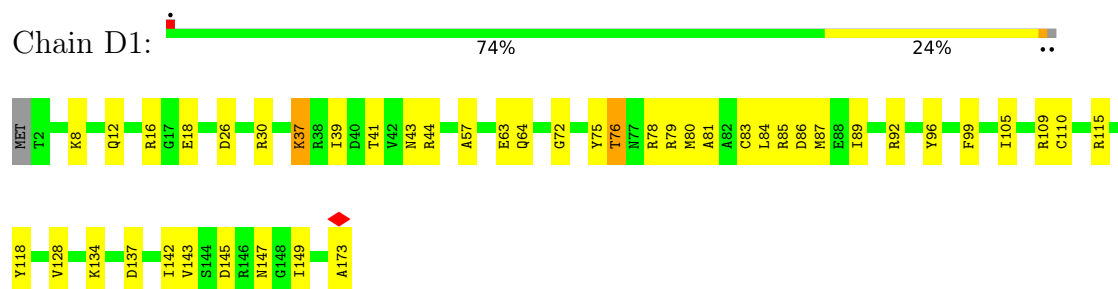
Chain W7: 71% 28% .



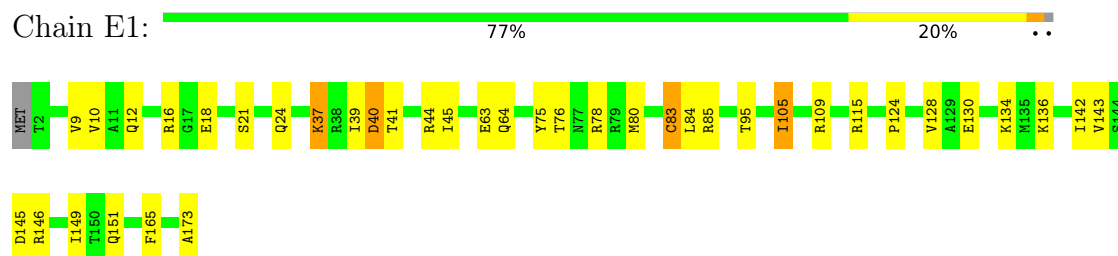
- Molecule 3: C-phycocyanin beta subunit



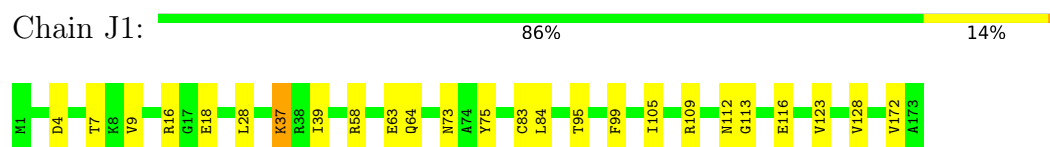
- Molecule 3: C-phycoerythrin beta subunit



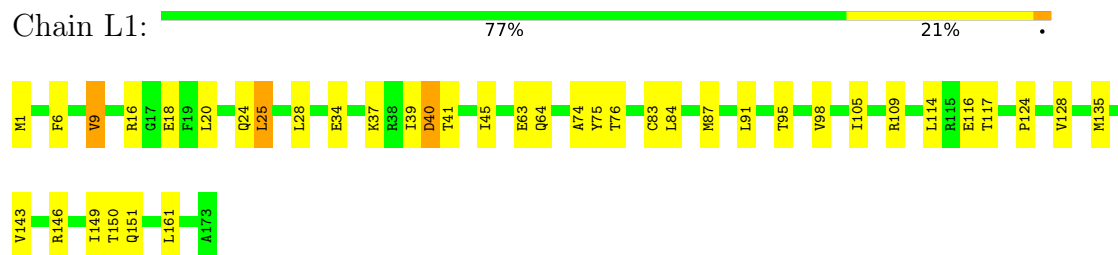
- Molecule 3: C-phycoerythrin beta subunit



- Molecule 3: C-phycoerythrin beta subunit

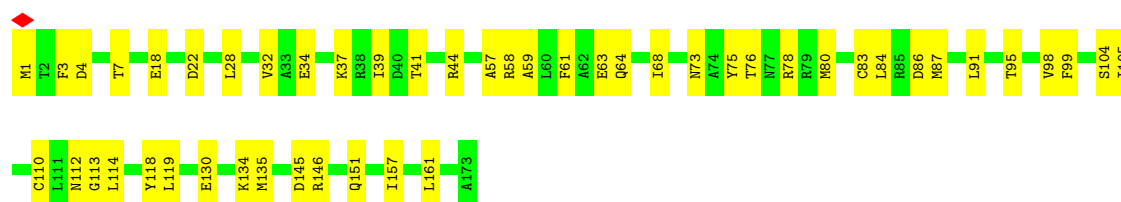


- Molecule 3: C-phycoerythrin beta subunit



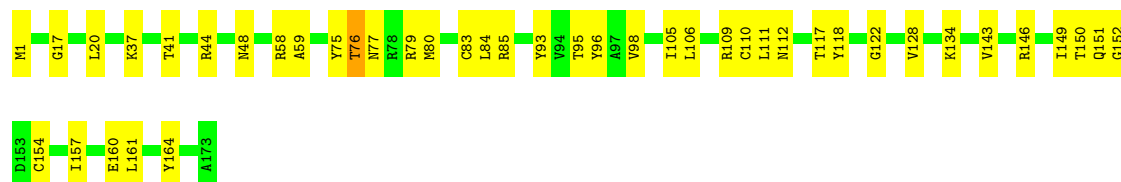
- Molecule 3: C-phycoerythrin beta subunit





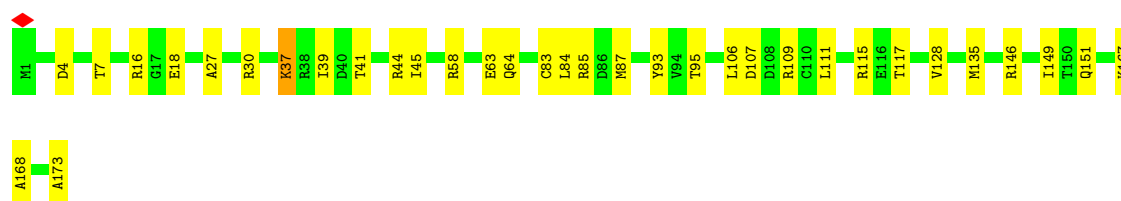
• Molecule 3: C-phycocyanin beta subunit

Chain O1: 75% 24%



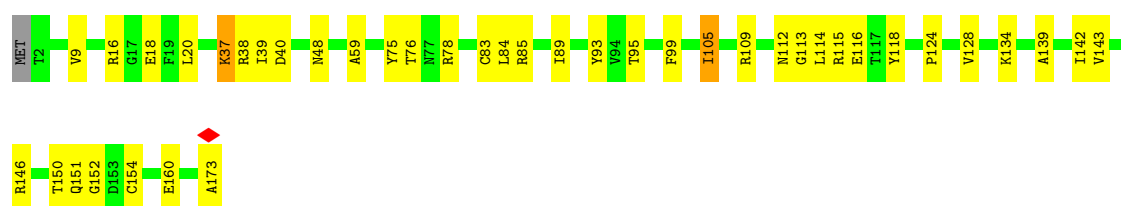
• Molecule 3: C-phycocyanin beta subunit

Chain P1: 80% 19%



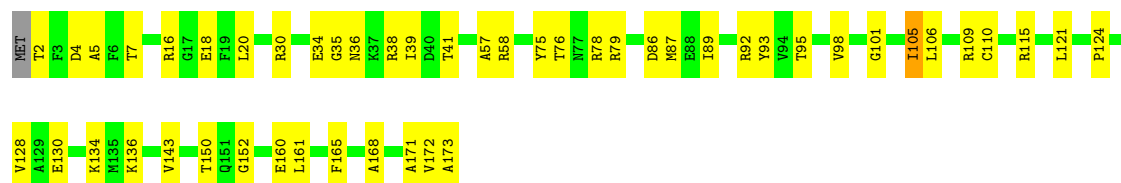
• Molecule 3: C-phycocyanin beta subunit

Chain Q1: 76% 23%

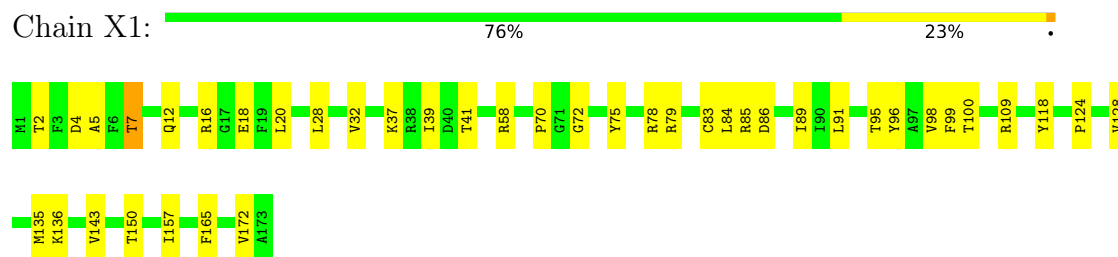


• Molecule 3: C-phycocyanin beta subunit

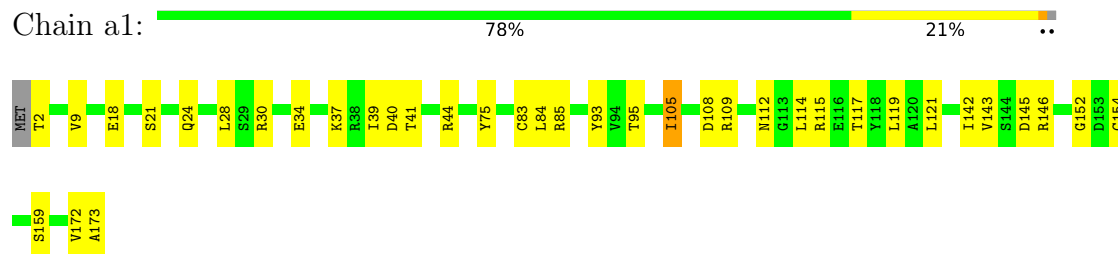
Chain V1: 71% 28%



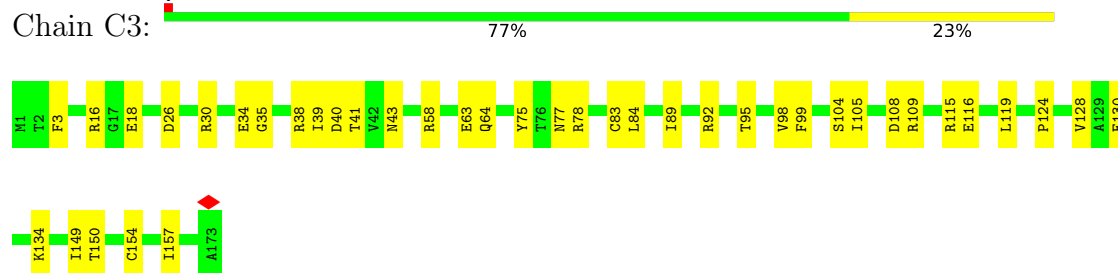
• Molecule 3: C-phycocyanin beta subunit



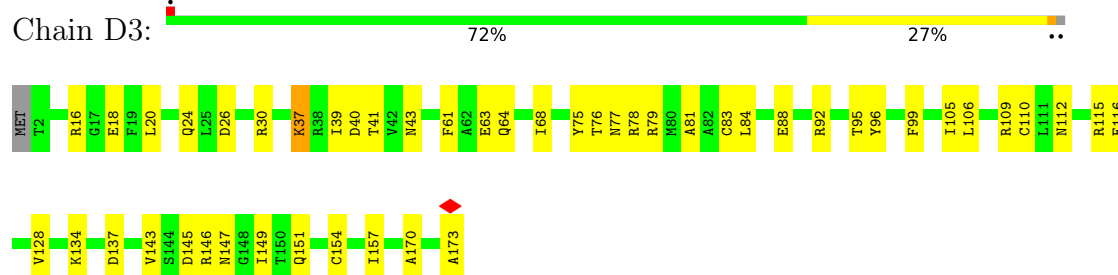
• Molecule 3: C-phycoerythrin beta subunit



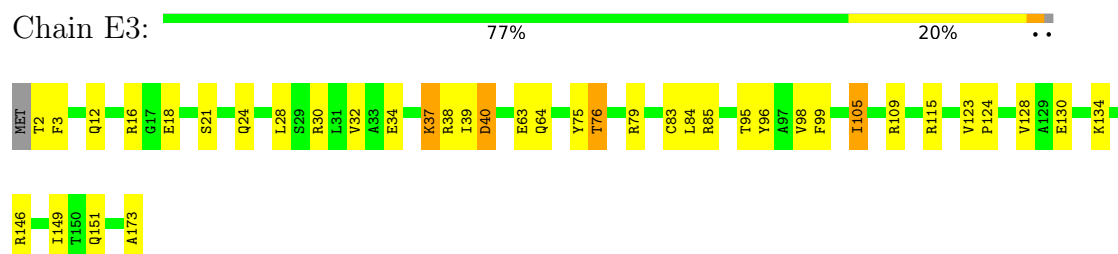
• Molecule 3: C-phycoerythrin beta subunit



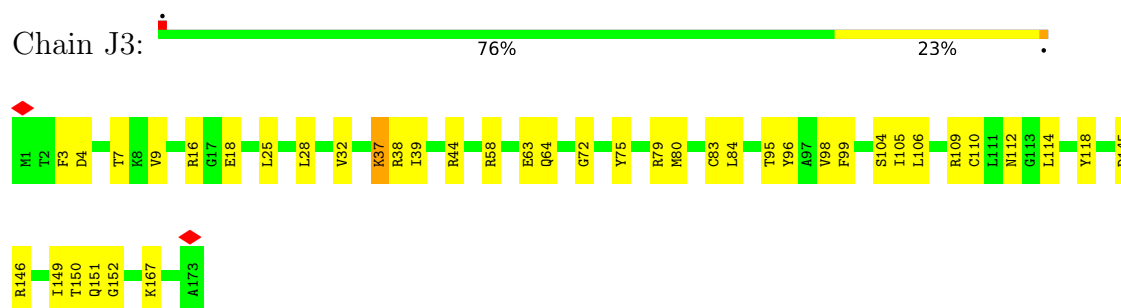
• Molecule 3: C-phycoerythrin beta subunit



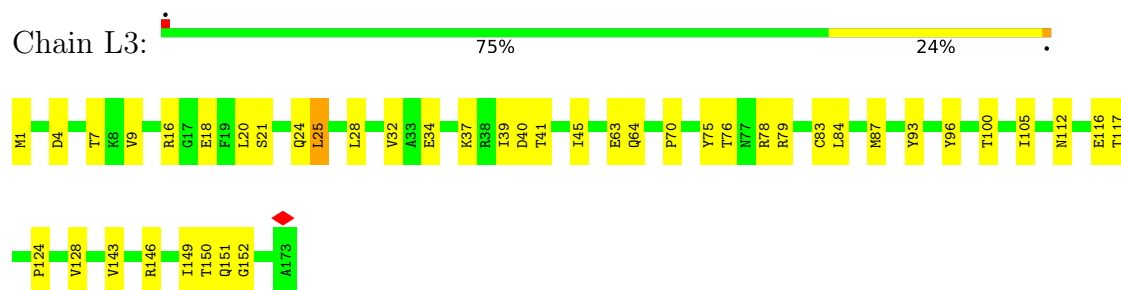
• Molecule 3: C-phycoerythrin beta subunit



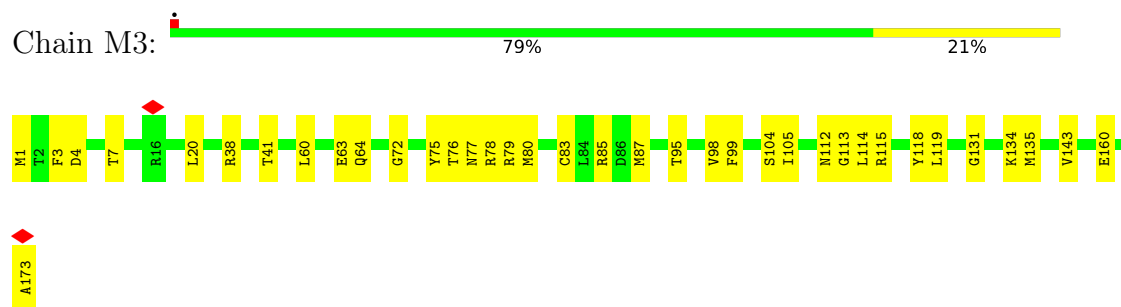
- Molecule 3: C-phycoerythrin beta subunit



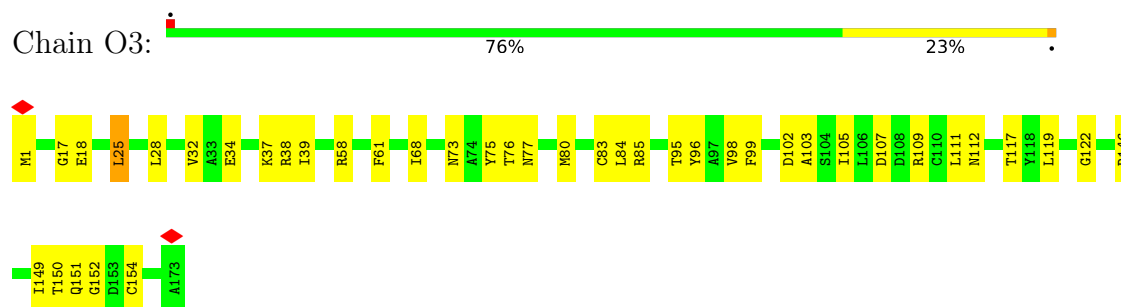
- Molecule 3: C-phycoerythrin beta subunit



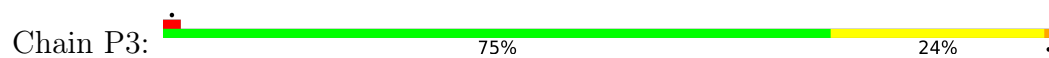
- Molecule 3: C-phycoerythrin beta subunit

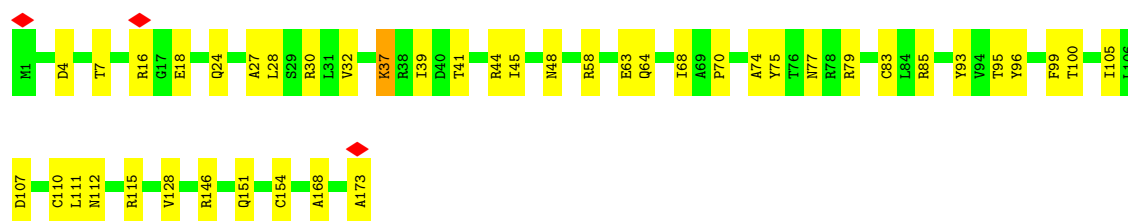


- Molecule 3: C-phycoerythrin beta subunit

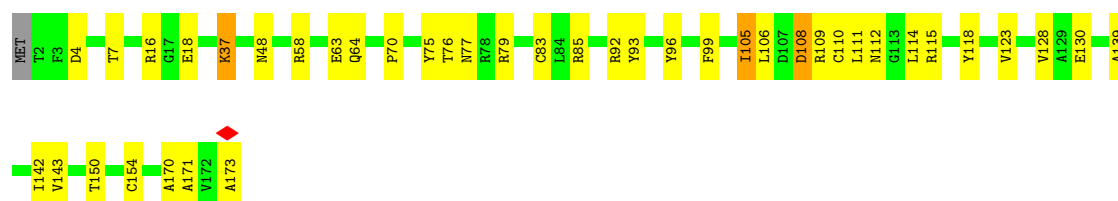
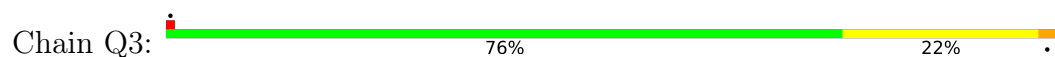


- Molecule 3: C-phycoerythrin beta subunit

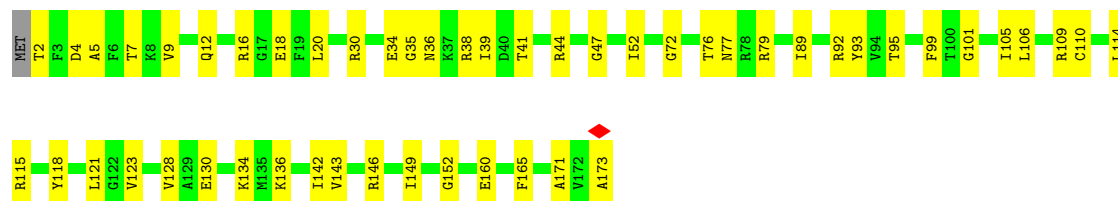




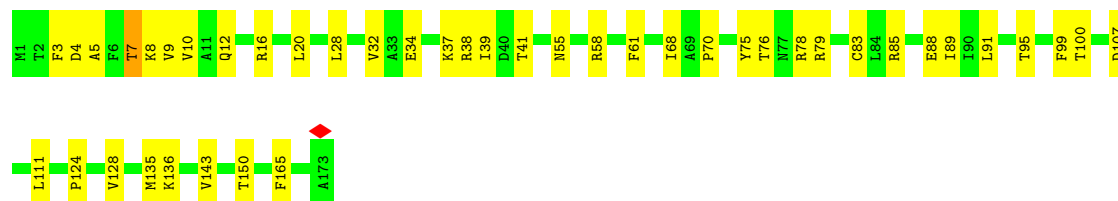
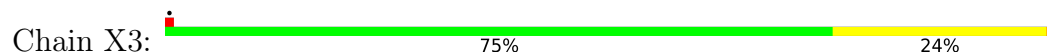
- Molecule 3: C-phycocyanin beta subunit



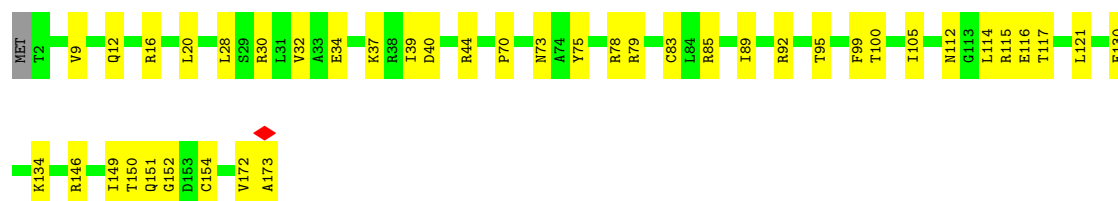
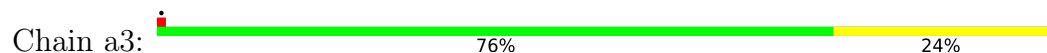
- Molecule 3: C-phycocyanin beta subunit



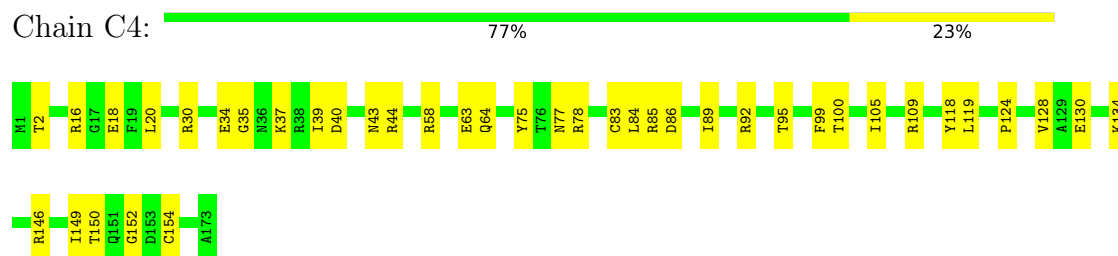
- Molecule 3: C-phycocyanin beta subunit



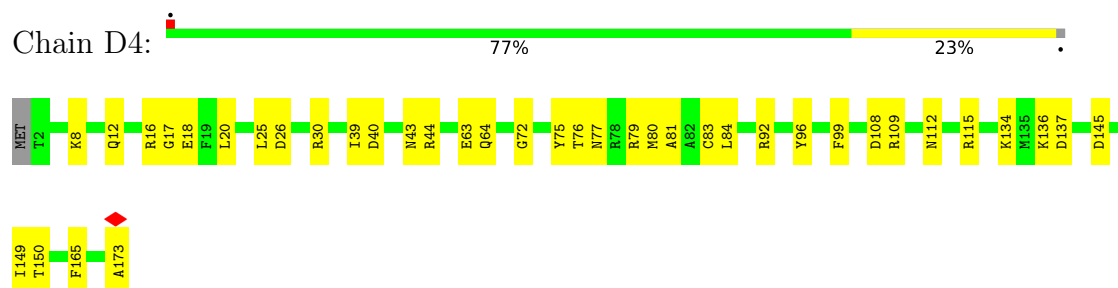
- Molecule 3: C-phycocyanin beta subunit



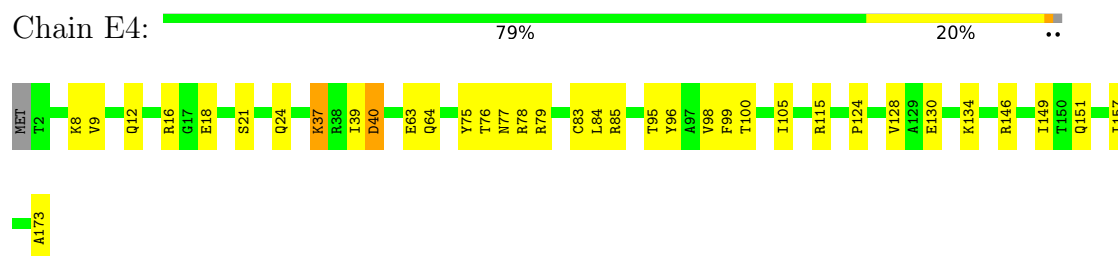
• Molecule 3: C-phycoerythrin beta subunit



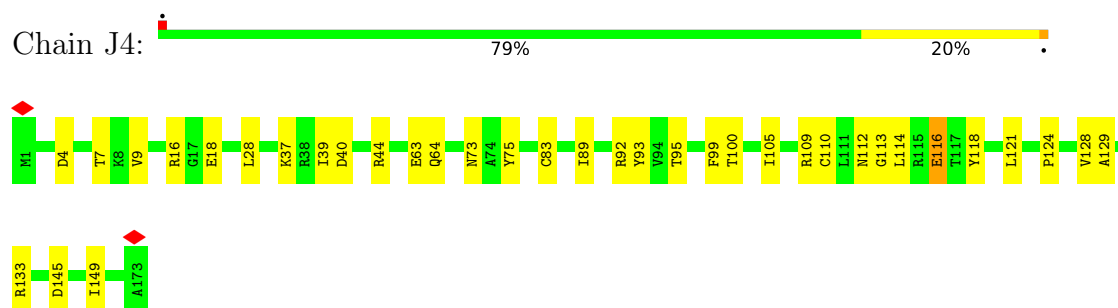
• Molecule 3: C-phycoerythrin beta subunit



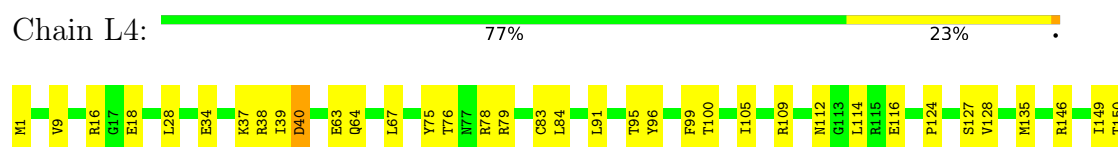
• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit

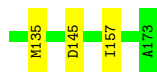
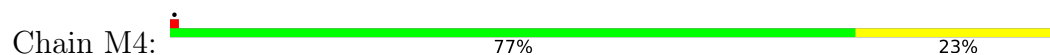


• Molecule 3: C-phycoerythrin beta subunit





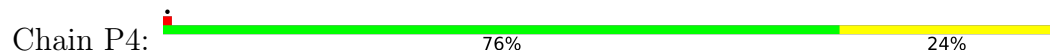
- Molecule 3: C-phycoerythrin beta subunit



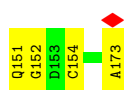
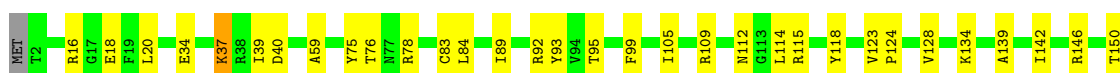
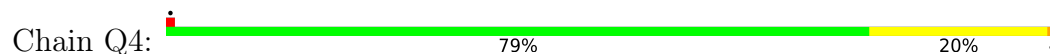
- Molecule 3: C-phycoerythrin beta subunit



- Molecule 3: C-phycoerythrin beta subunit

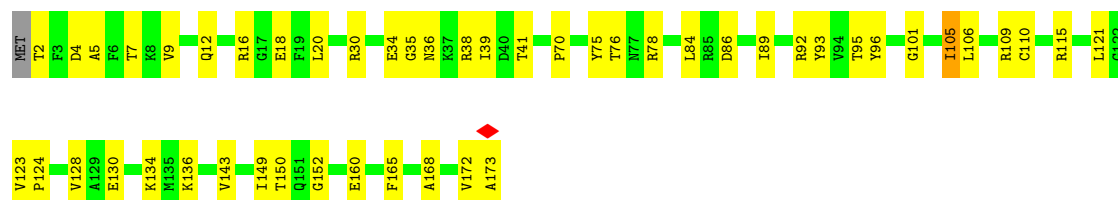


- Molecule 3: C-phycoerythrin beta subunit



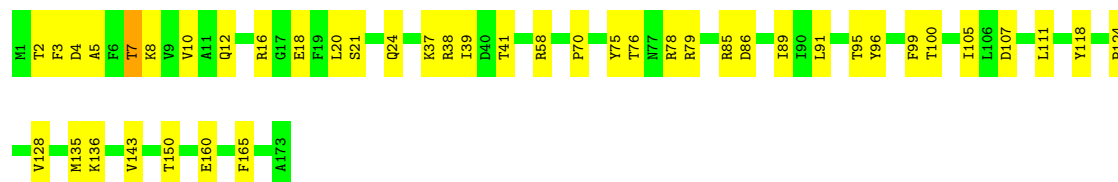
- Molecule 3: C-phycoerythrin beta subunit





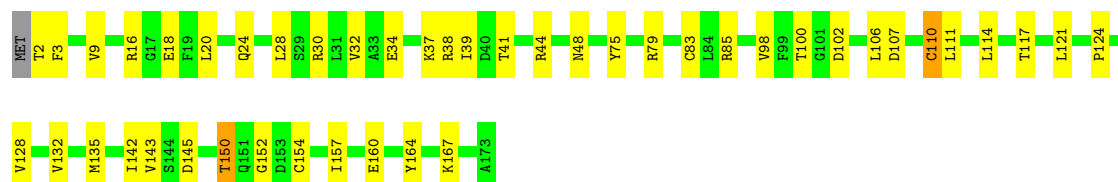
• Molecule 3: C-phycocyanin beta subunit

Chain X4: 75% 24%



• Molecule 3: C-phycocyanin beta subunit

Chain a4: 73% 25%



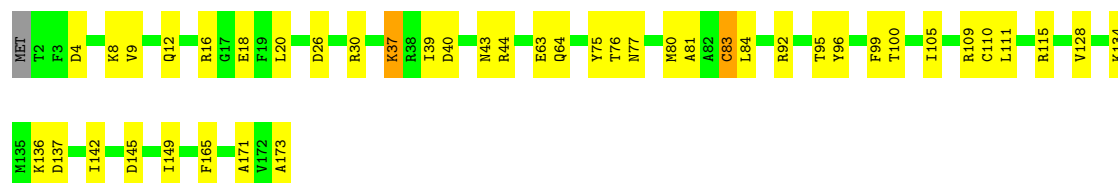
• Molecule 3: C-phycocyanin beta subunit

Chain C5: 76% 24%




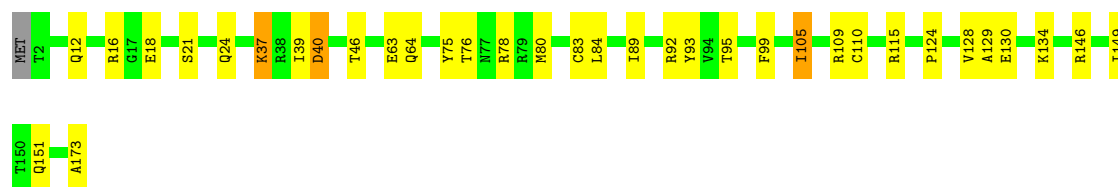
• Molecule 3: C-phycocyanin beta subunit

Chain D5: 75% 24%




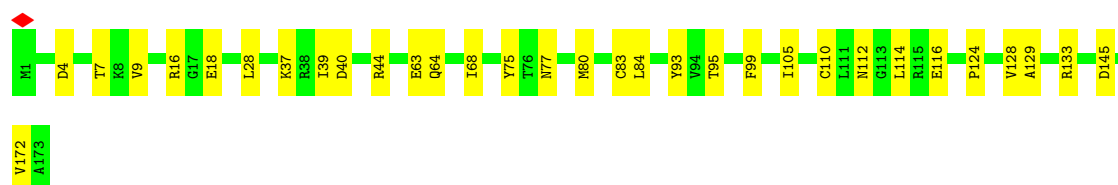
• Molecule 3: C-phycocyanin beta subunit

Chain E5:  79% 18% ..




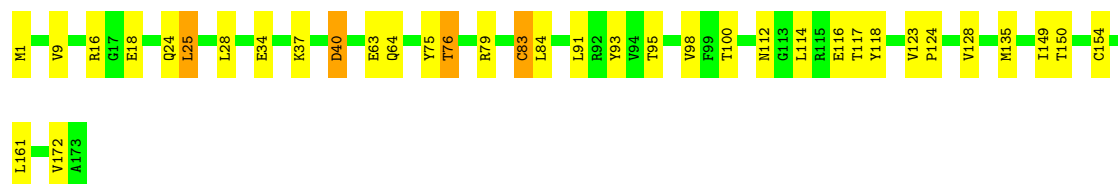
• Molecule 3: C-phycoerythrin beta subunit

Chain J5:  82% 18%




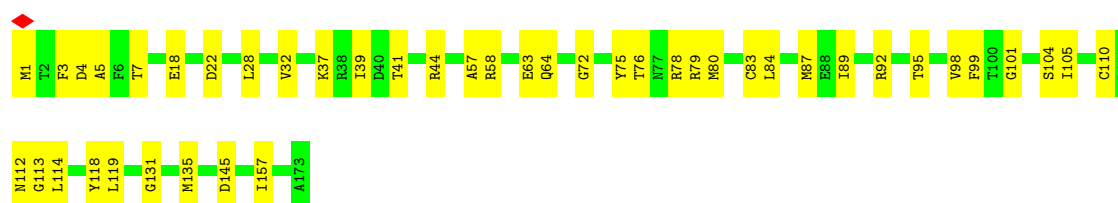
• Molecule 3: C-phycoerythrin beta subunit

Chain L5:  79% 18%




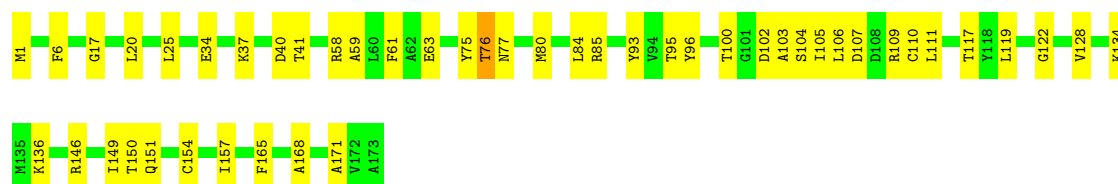
• Molecule 3: C-phycoerythrin beta subunit

Chain M5:  75% 25%

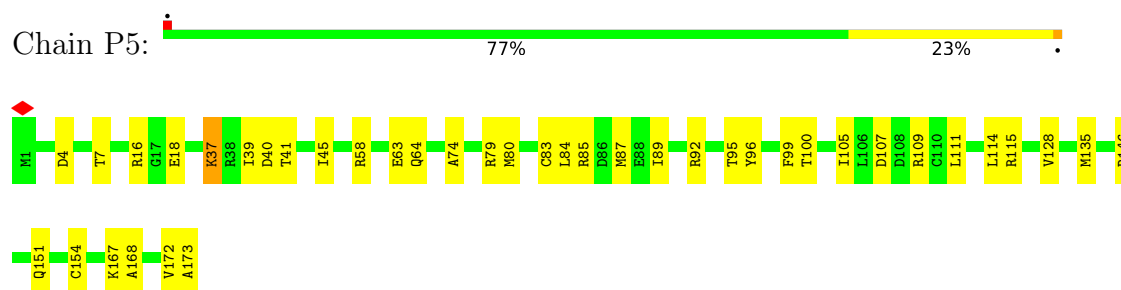


• Molecule 3: C-phycoerythrin beta subunit

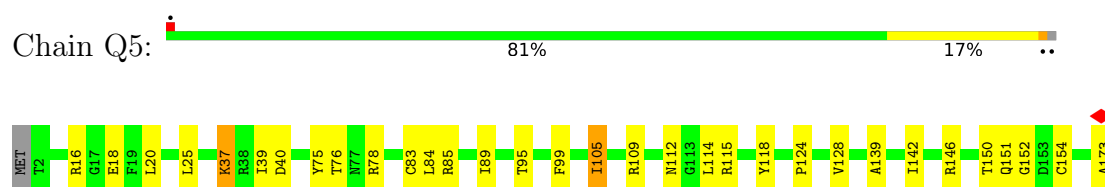
Chain O5:  73% 27%



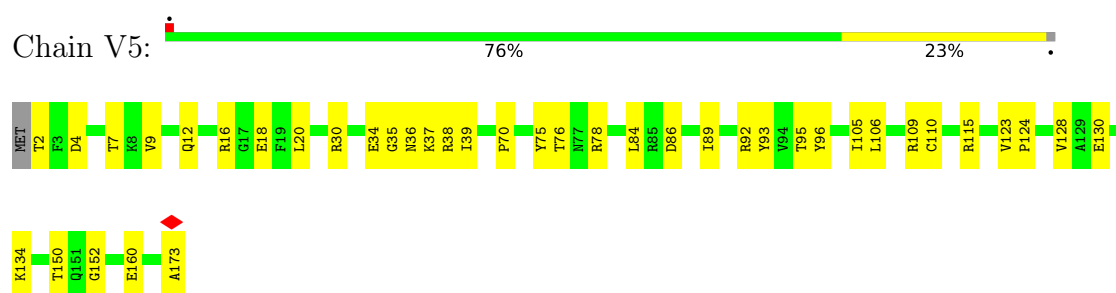
- Molecule 3: C-phycoerythrin beta subunit



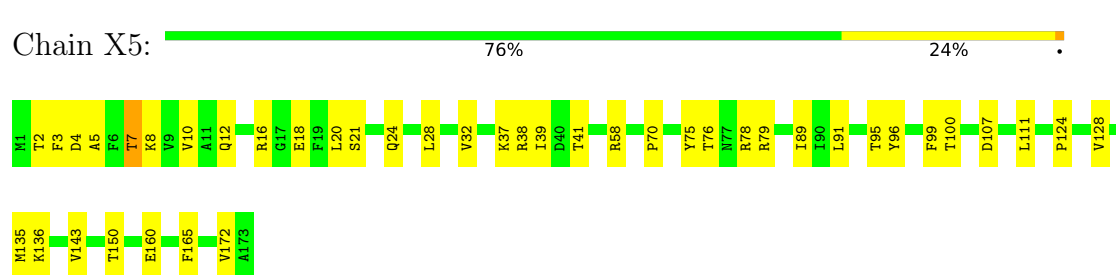
- Molecule 3: C-phycoerythrin beta subunit



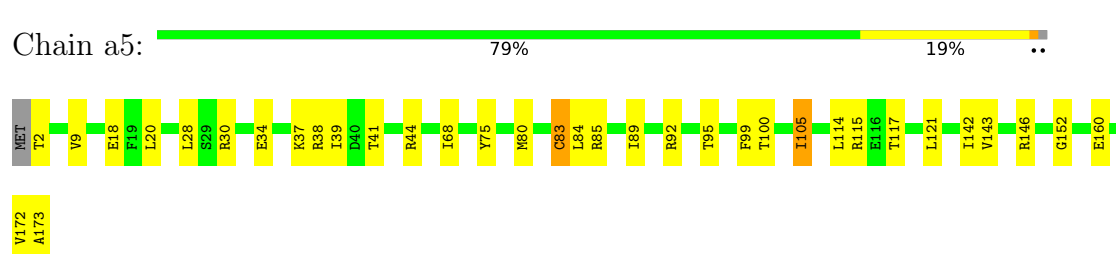
- Molecule 3: C-phycoerythrin beta subunit



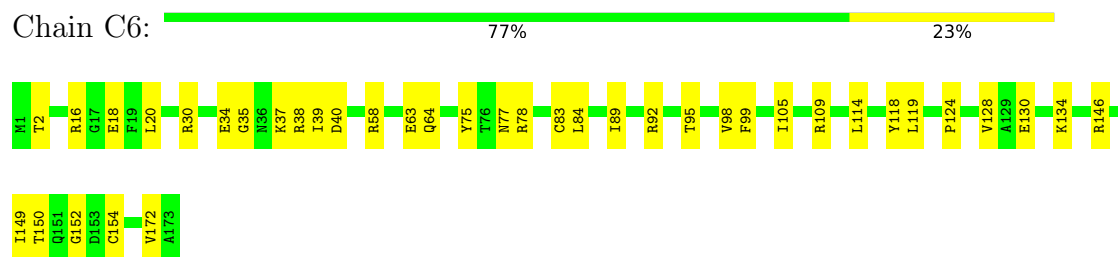
- Molecule 3: C-phycoerythrin beta subunit



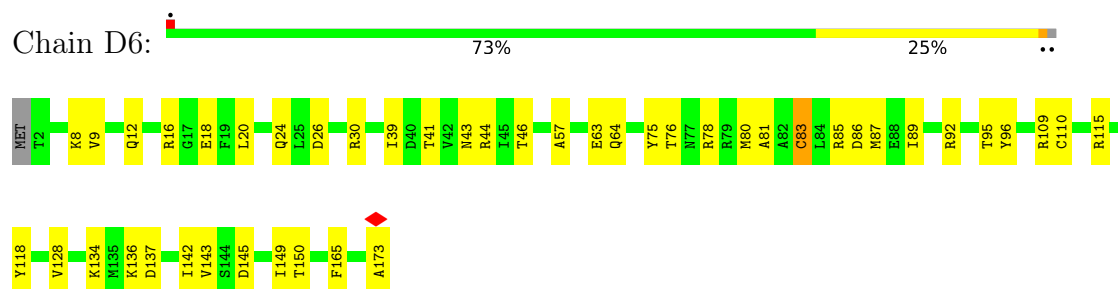
- Molecule 3: C-phycoerythrin beta subunit



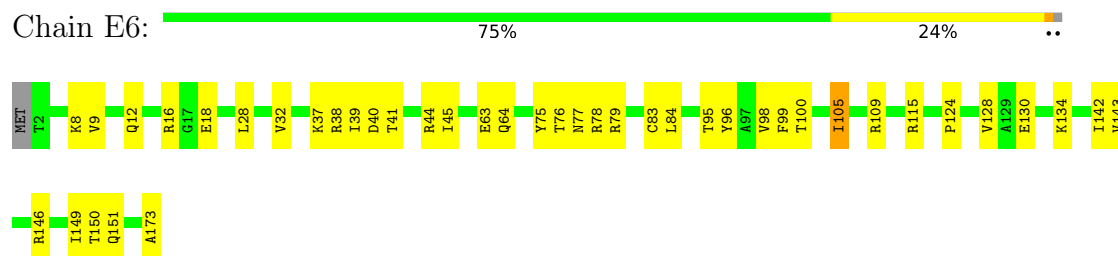
- Molecule 3: C-phycoerythrin beta subunit



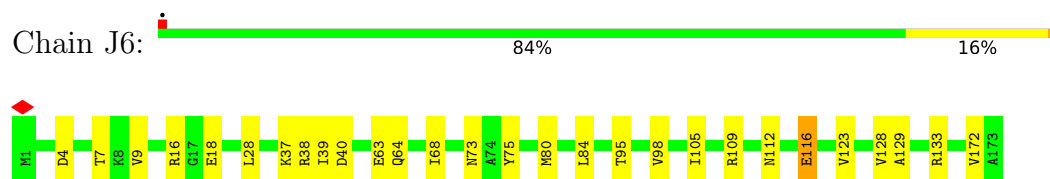
- Molecule 3: C-phycoerythrin beta subunit



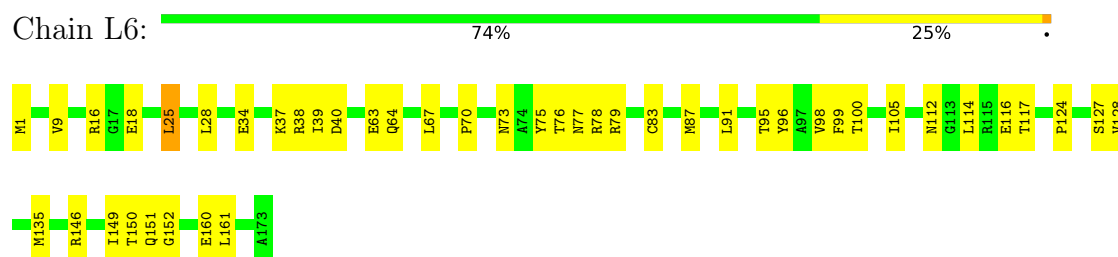
- Molecule 3: C-phycoerythrin beta subunit



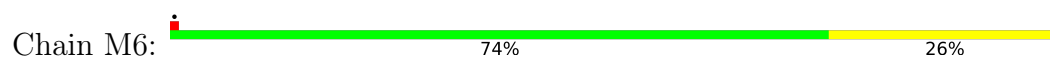
- Molecule 3: C-phycoerythrin beta subunit

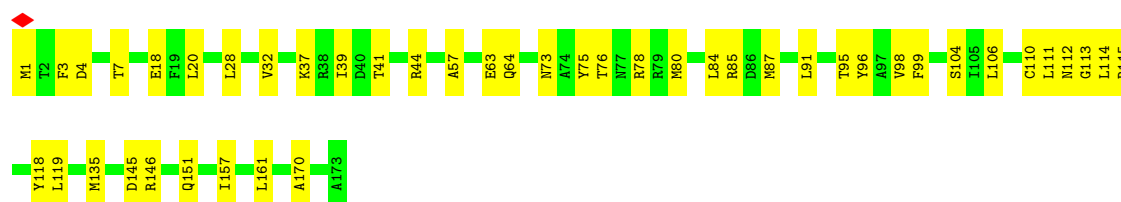


- Molecule 3: C-phycoerythrin beta subunit



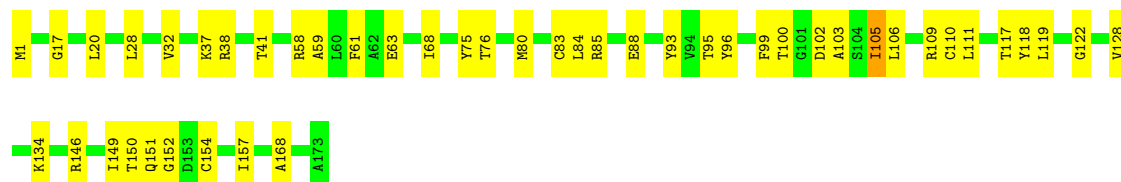
- Molecule 3: C-phycoerythrin beta subunit





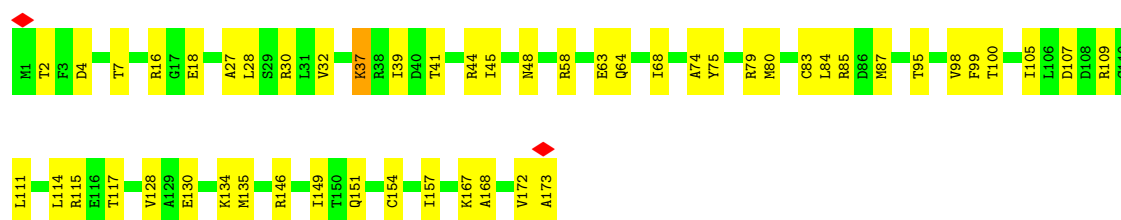
- Molecule 3: C-phycoerythrin beta subunit

Chain O6: 73% 26%



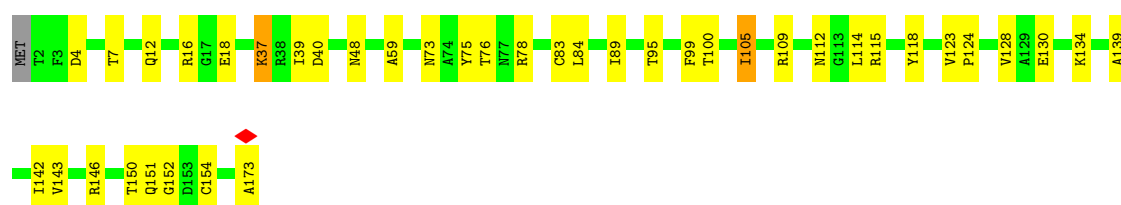
- Molecule 3: C-phycoerythrin beta subunit

Chain P6: 71% 29%



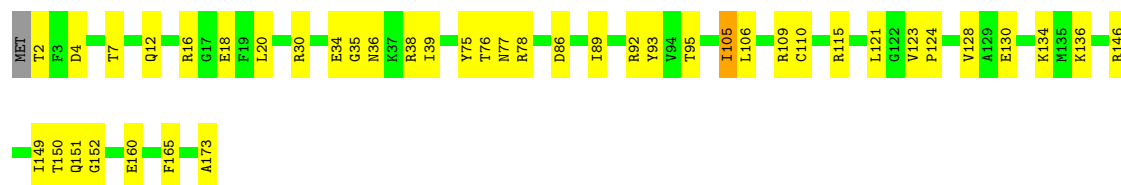
- Molecule 3: C-phycoerythrin beta subunit

Chain Q6: 76% 22%

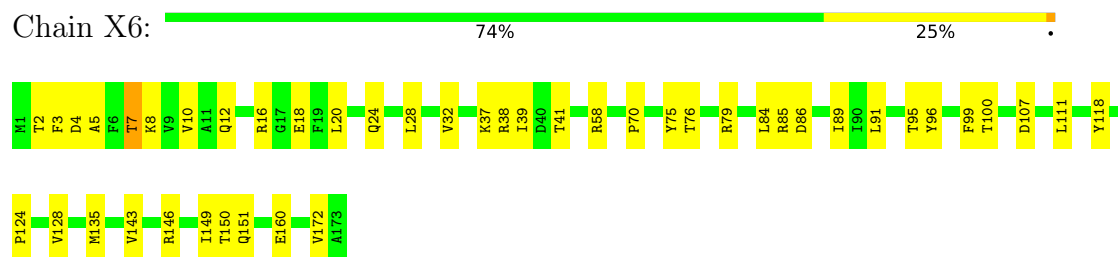


- Molecule 3: C-phycoerythrin beta subunit

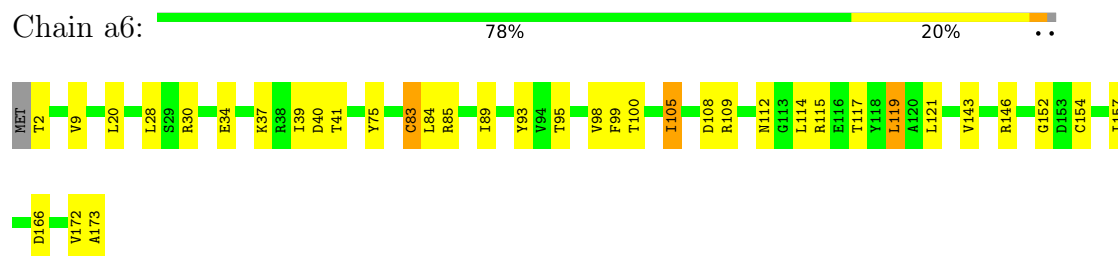
Chain V6: 75% 24%



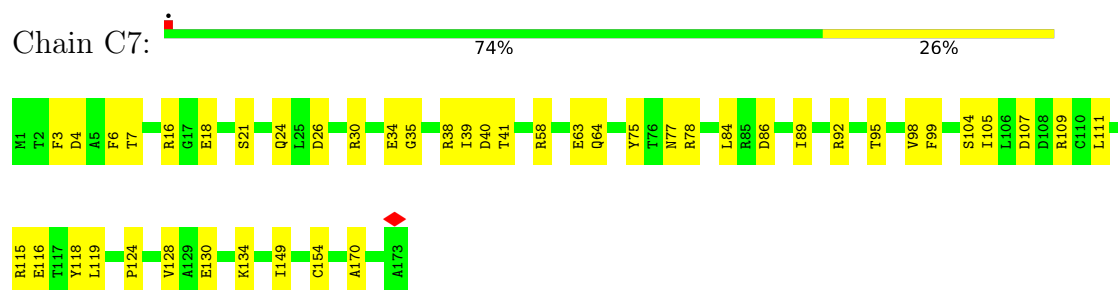
- Molecule 3: C-phycoerythrin beta subunit



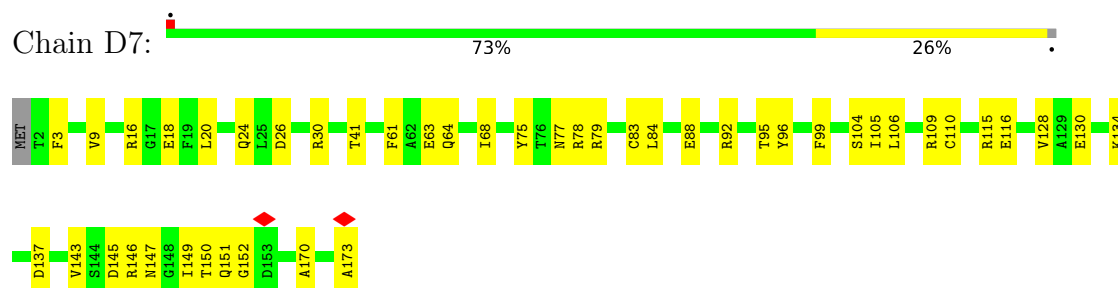
- Molecule 3: C-phycoerythrin beta subunit



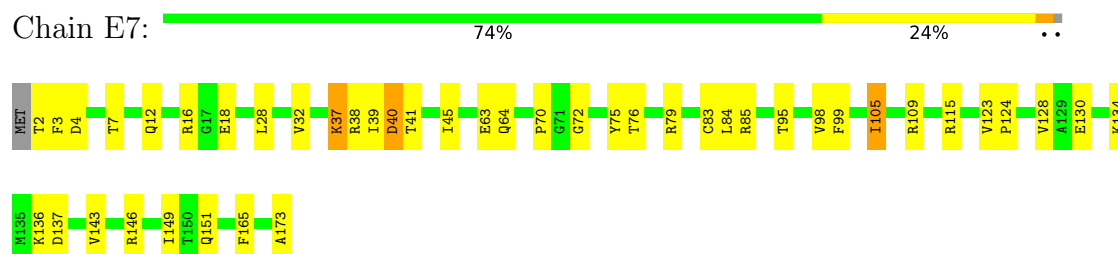
- Molecule 3: C-phycoerythrin beta subunit



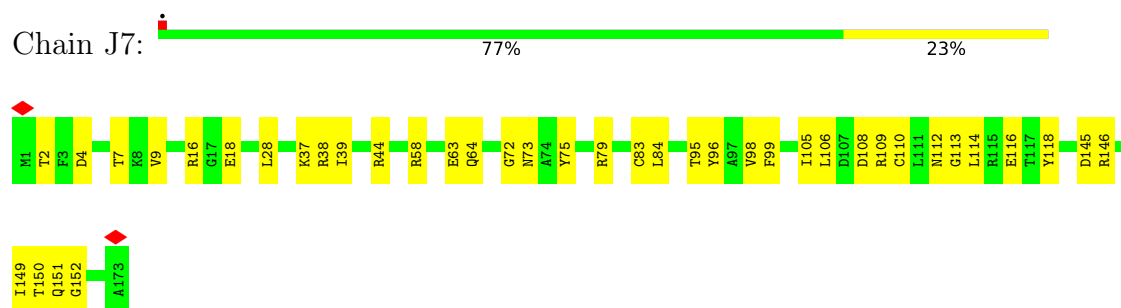
- Molecule 3: C-phycoerythrin beta subunit



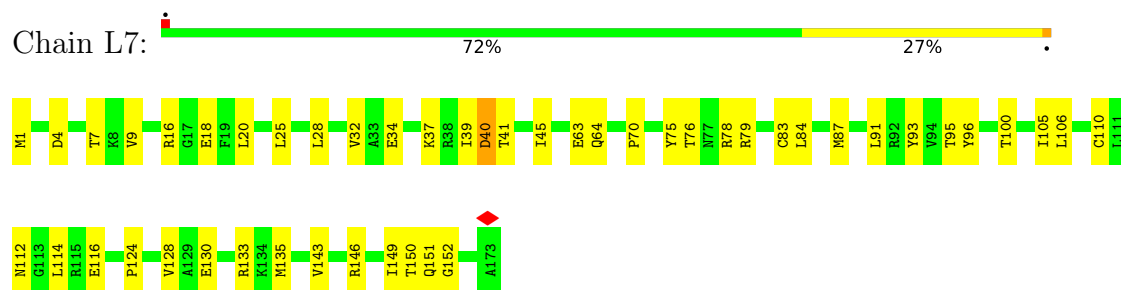
- Molecule 3: C-phycoerythrin beta subunit



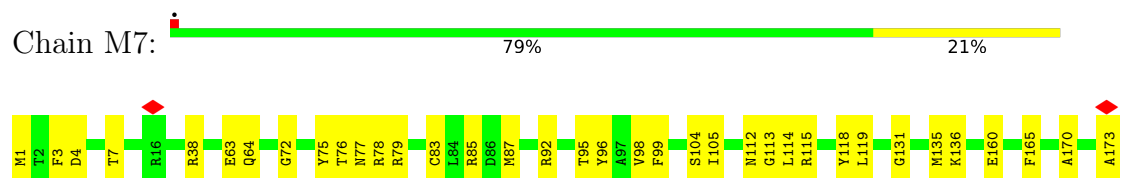
- Molecule 3: C-phycoerythrin beta subunit



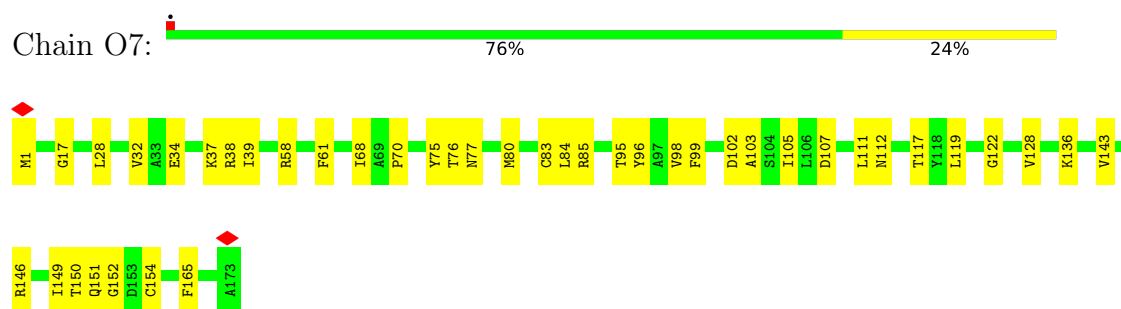
- Molecule 3: C-phycoerythrin beta subunit



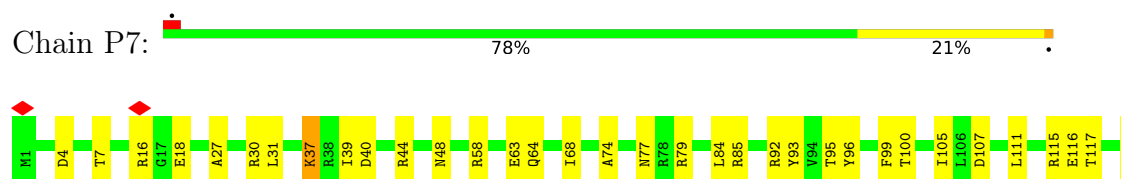
- Molecule 3: C-phycoerythrin beta subunit



- Molecule 3: C-phycoerythrin beta subunit



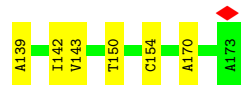
- Molecule 3: C-phycoerythrin beta subunit





- Molecule 3: C-phycocyanin beta subunit

Chain Q7: 76% 23% ..



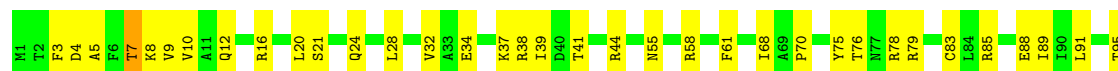
- Molecule 3: C-phycocyanin beta subunit

Chain V7: 72% 28% .



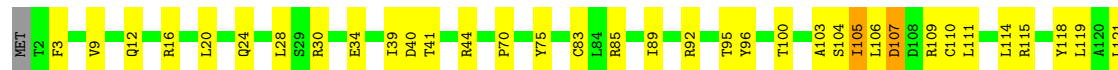
- Molecule 3: C-phycocyanin beta subunit

Chain X7: 71% 28% .



- Molecule 3: C-phycocyanin beta subunit

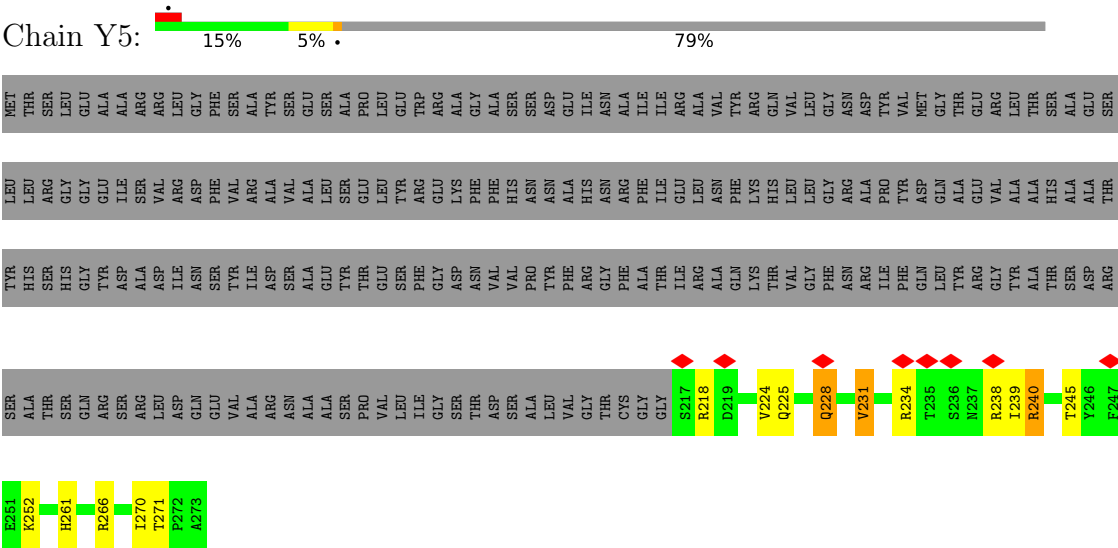
Chain a7: 72% 26% ..



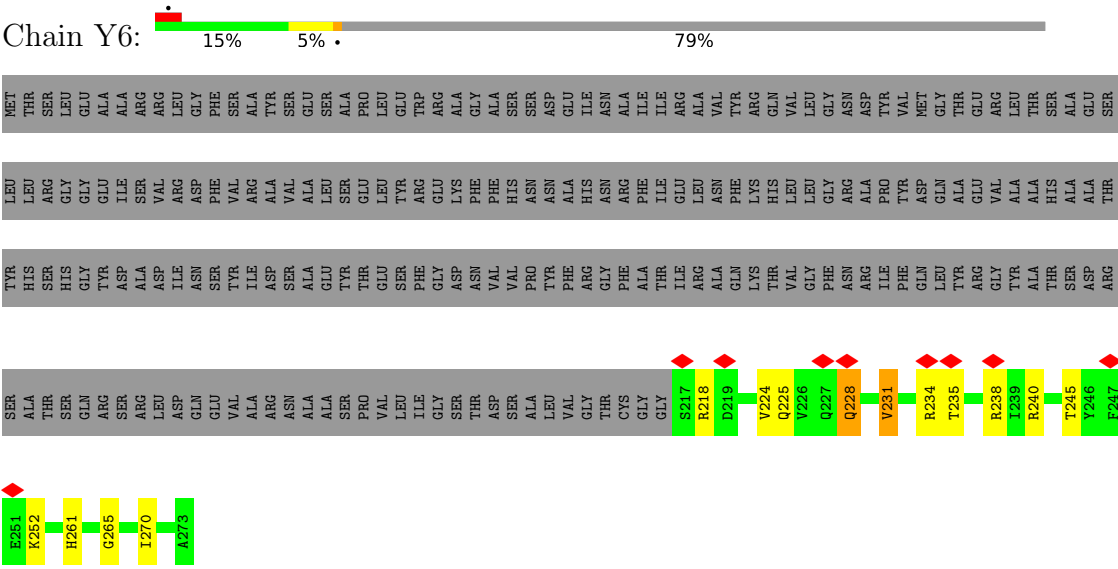
- Molecule 4: Phycobilisome rod linker polypeptide

Chain Y1: 15% 5% 79%

• Molecule 4: Phycobilisome rod linker polypeptide

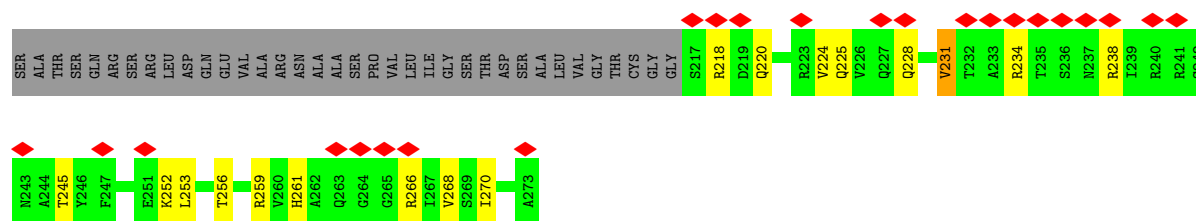


• Molecule 4: Phycobilisome rod linker polypeptide



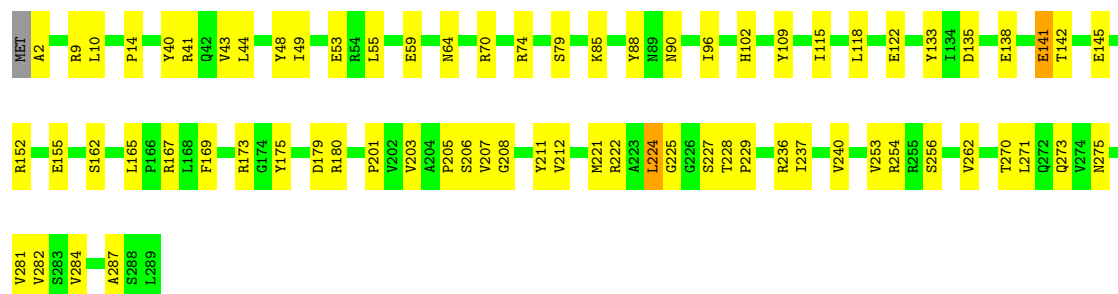
• Molecule 4: Phycobilisome rod linker polypeptide





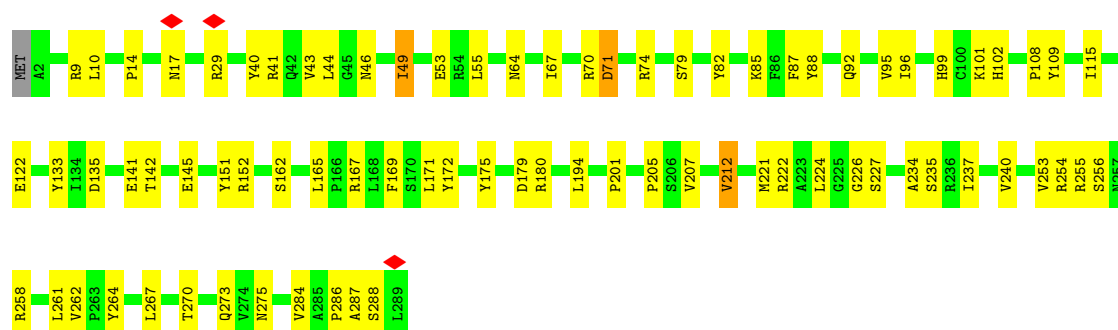
• Molecule 5: Phycobilisome rod linker polypeptide

Chain Z1: .



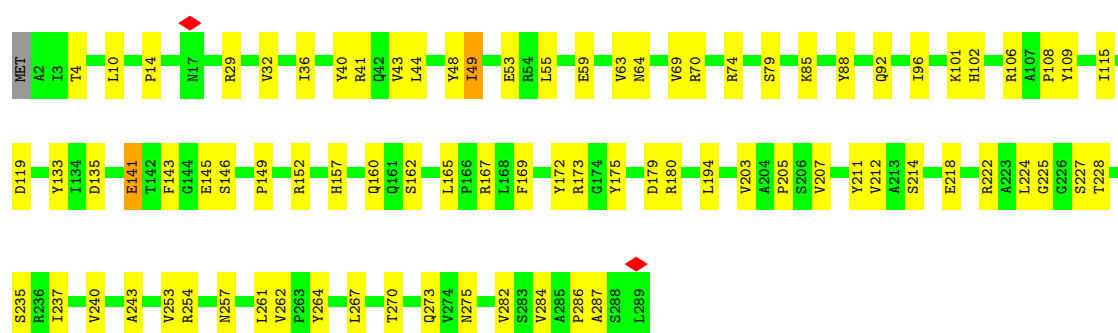
• Molecule 5: Phycobilisome rod linker polypeptide

Chain Z3: .




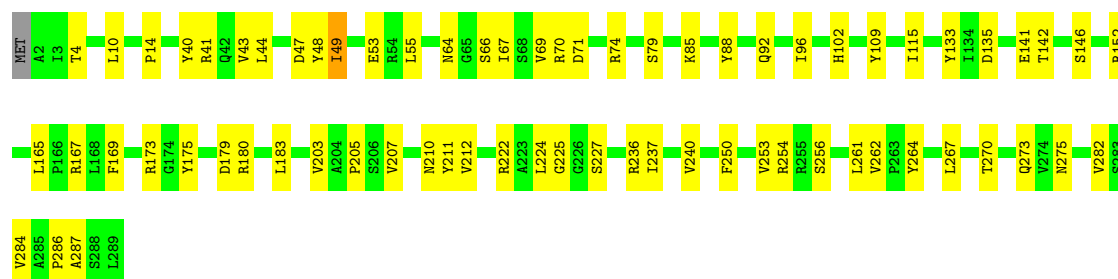
• Molecule 5: Phycobilisome rod linker polypeptide

Chain Z4: .




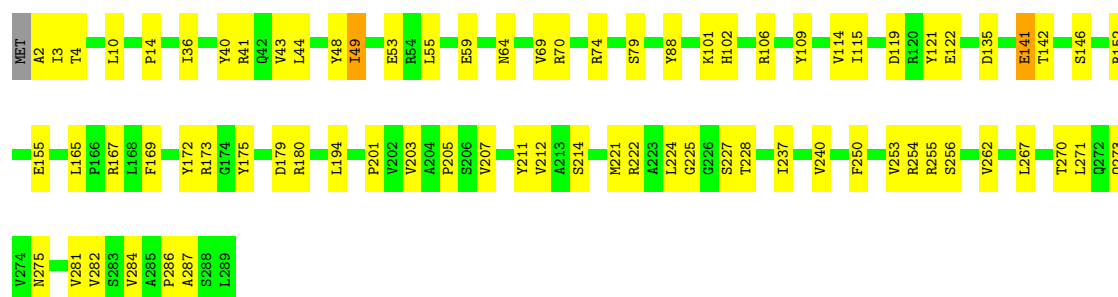
• Molecule 5: Phycobilisome rod linker polypeptide

Chain Z5:  76% 24%



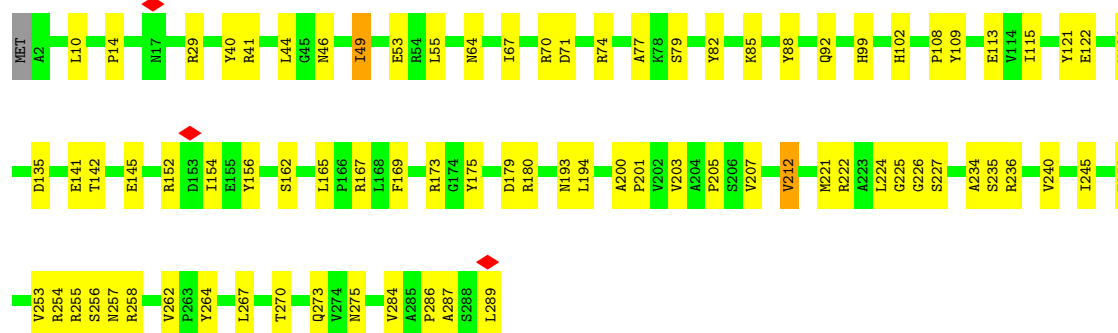
- Molecule 5: Phycobilisome rod linker polypeptide

Chain Z6:  73% 26%



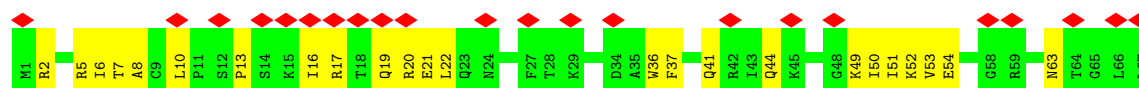
- Molecule 5: Phycobilisome rod linker polypeptide

Chain Z7:  72% 27%



- Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 02:  33% 64% 36%

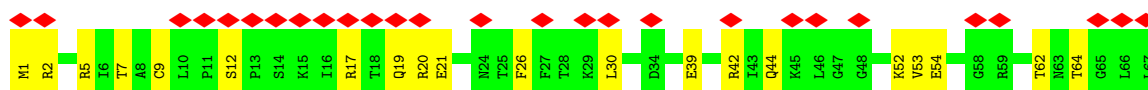
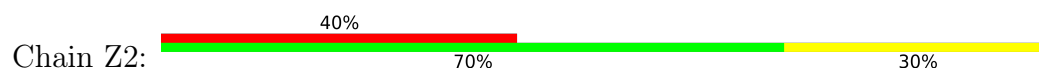


- Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

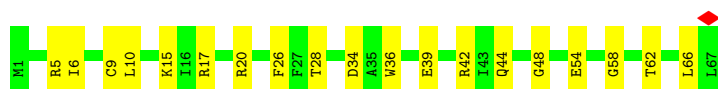
Chain Y2:  69% 30%



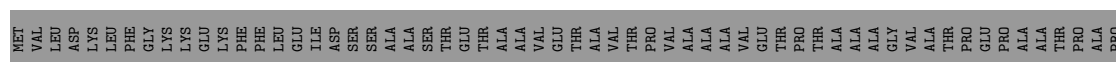
- Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



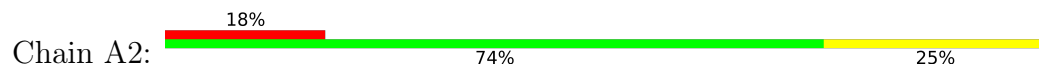
- Molecule 7: ApcG



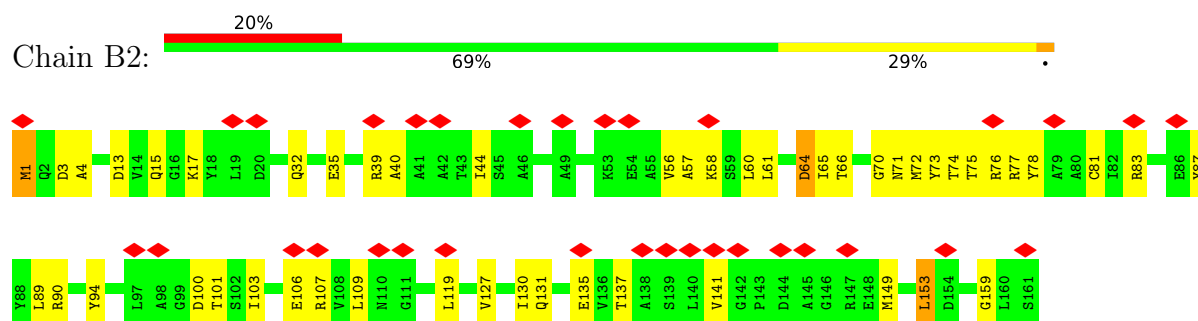
- Molecule 7: ApcG



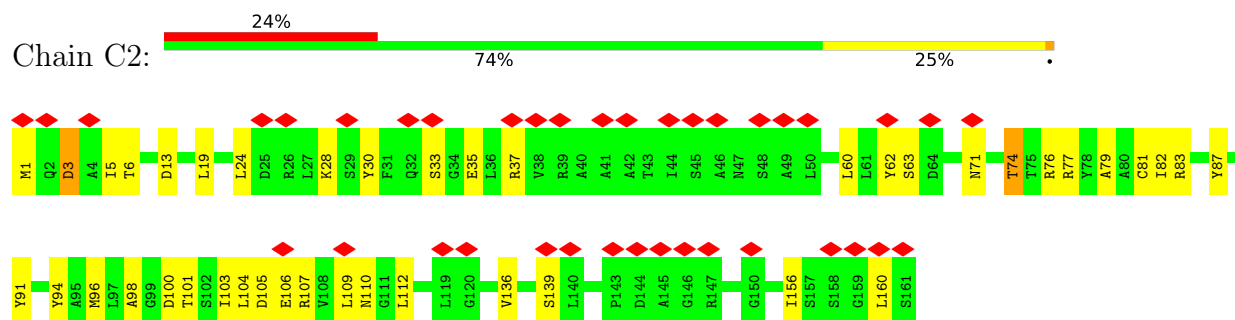
- Molecule 8: Allophycocyanin, beta subunit



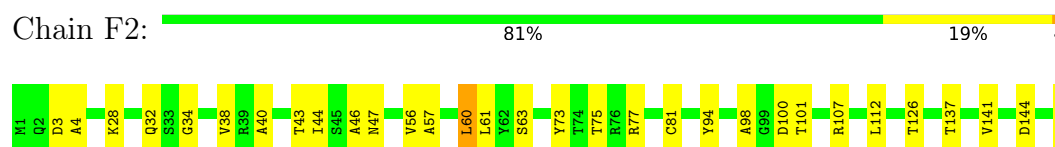
- Molecule 8: Allophycocyanin, beta subunit



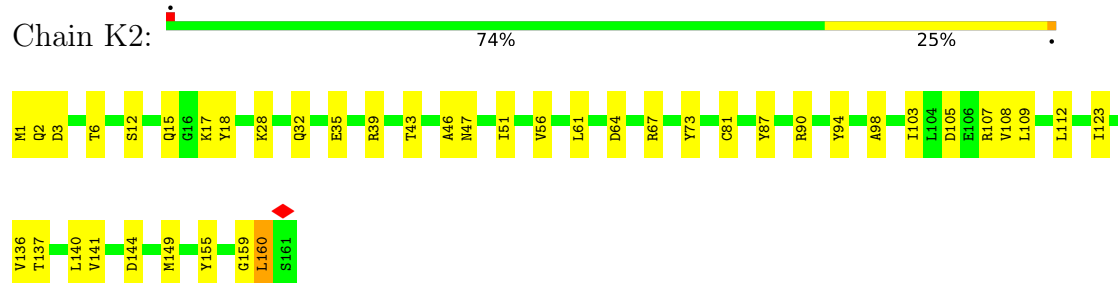
- Molecule 8: Allophycocyanin, beta subunit



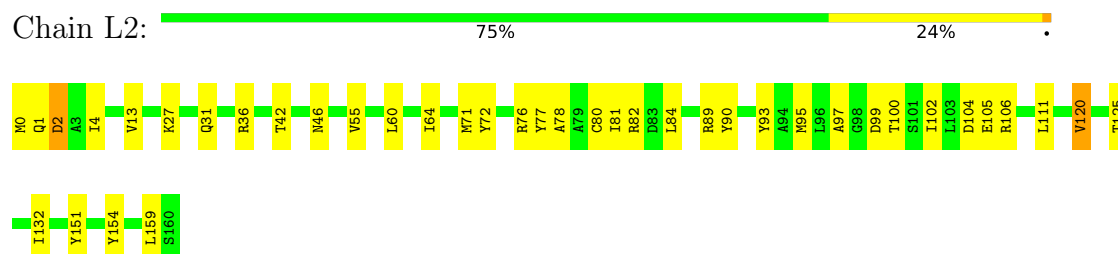
- Molecule 8: Allophycocyanin, beta subunit



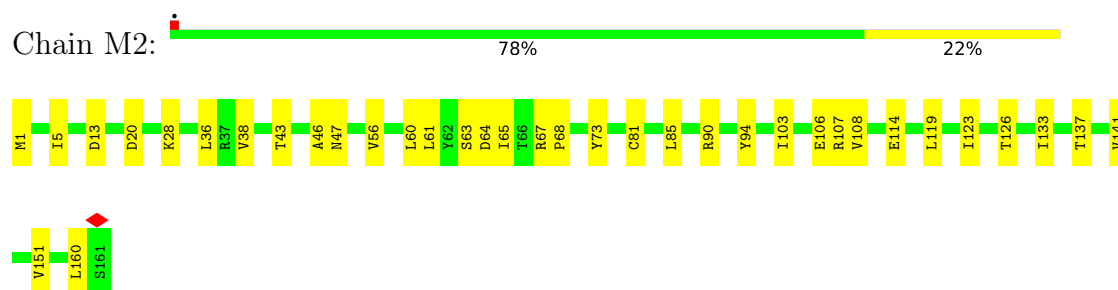
- Molecule 8: Allophycocyanin, beta subunit



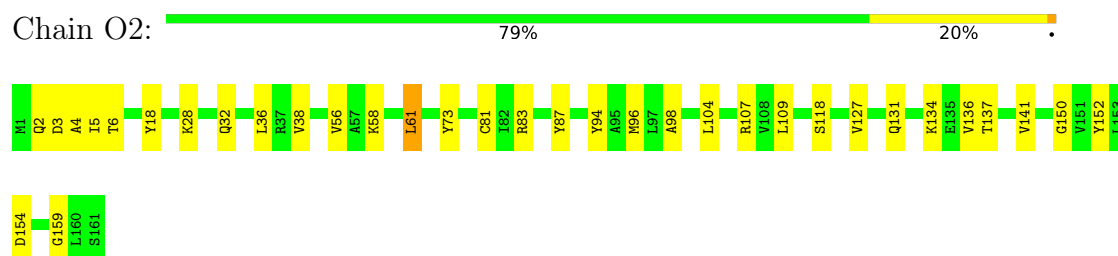
- Molecule 8: Allophycocyanin, beta subunit



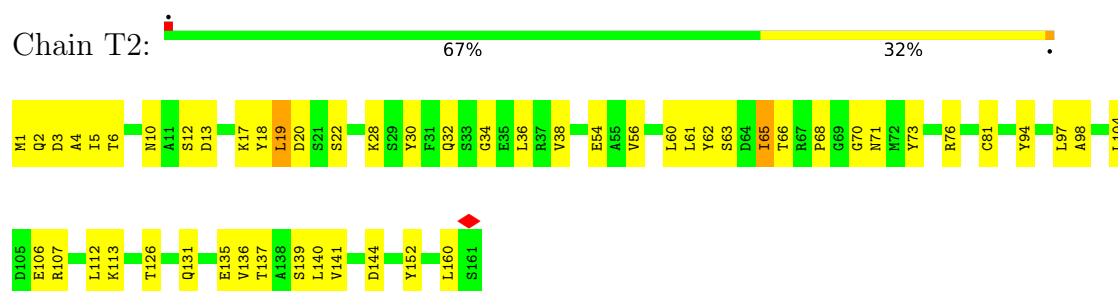
- Molecule 8: Allophycocyanin, beta subunit



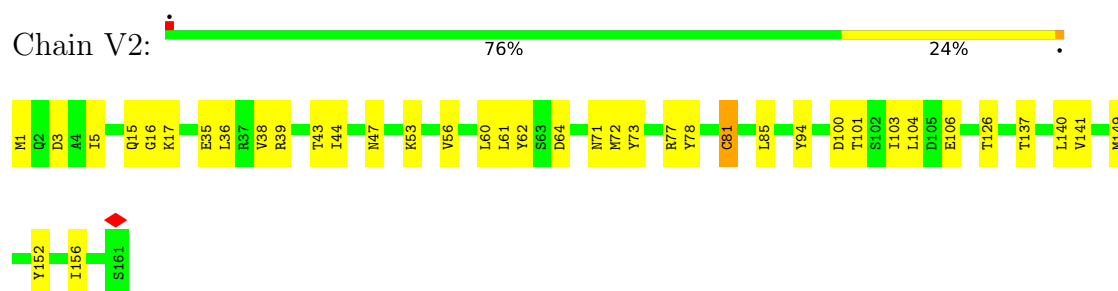
- Molecule 8: Allophycocyanin, beta subunit



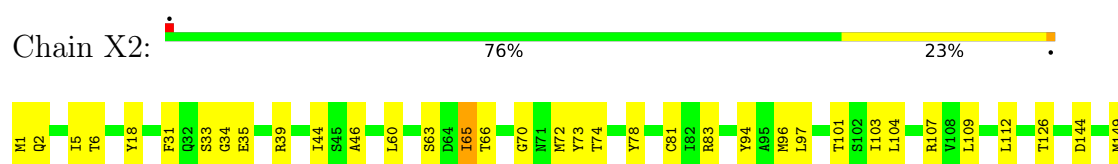
- Molecule 8: Allophycocyanin, beta subunit

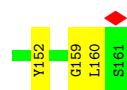


- Molecule 8: Allophycocyanin, beta subunit

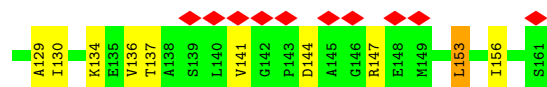
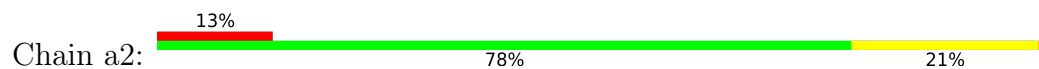


- Molecule 8: Allophycocyanin, beta subunit

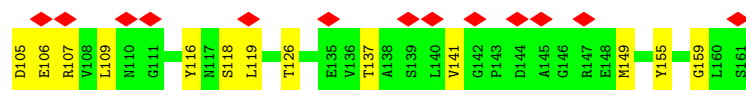
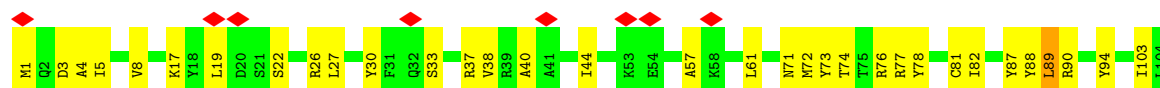
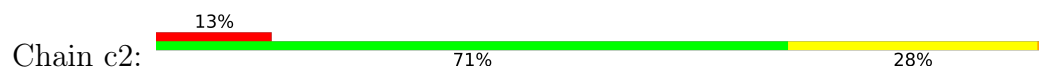




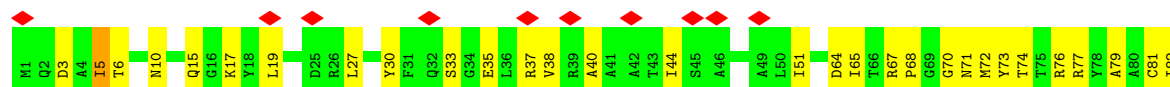
- Molecule 8: Allophycocyanin, beta subunit



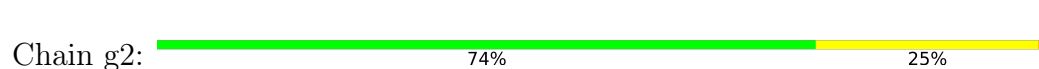
- Molecule 8: Allophycocyanin, beta subunit



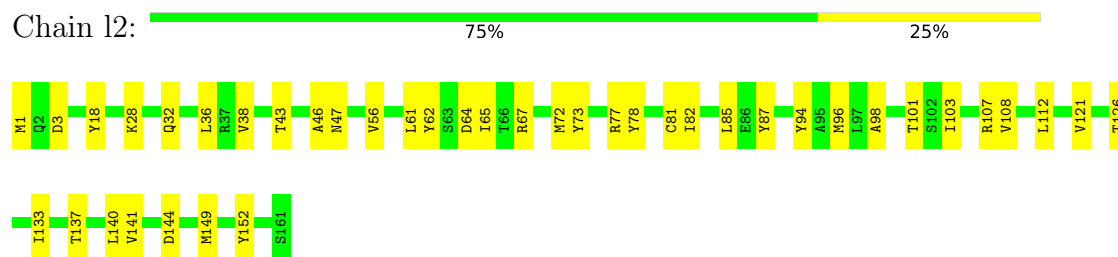
- Molecule 8: Allophycocyanin, beta subunit



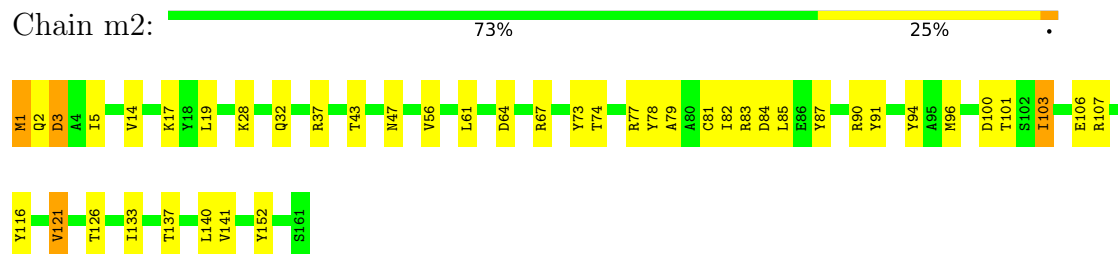
- Molecule 8: Allophycocyanin, beta subunit



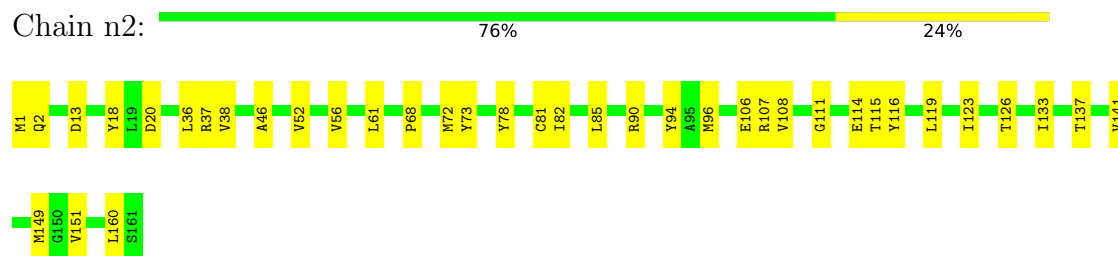
- Molecule 8: Allophycocyanin, beta subunit



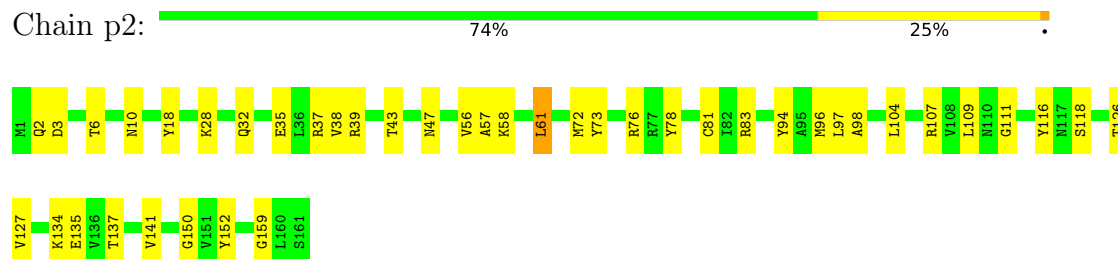
• Molecule 8: Allophycocyanin, beta subunit



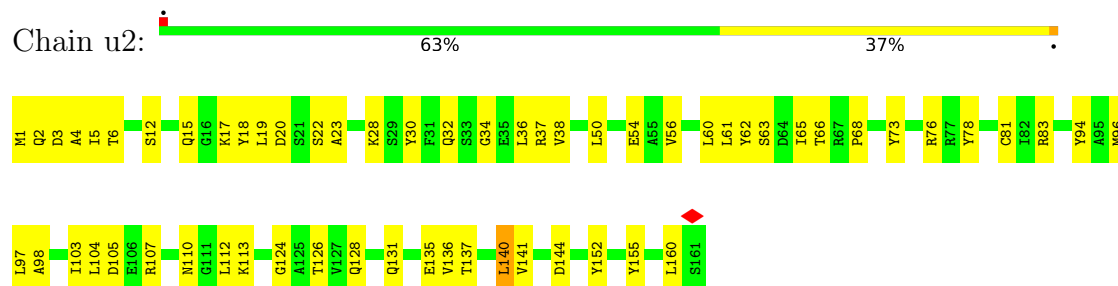
• Molecule 8: Allophycocyanin, beta subunit




• Molecule 8: Allophycocyanin, beta subunit



• Molecule 8: Allophycocyanin, beta subunit




- Molecule 8: Allophycocyanin, beta subunit

Chain w2:  82% 18%



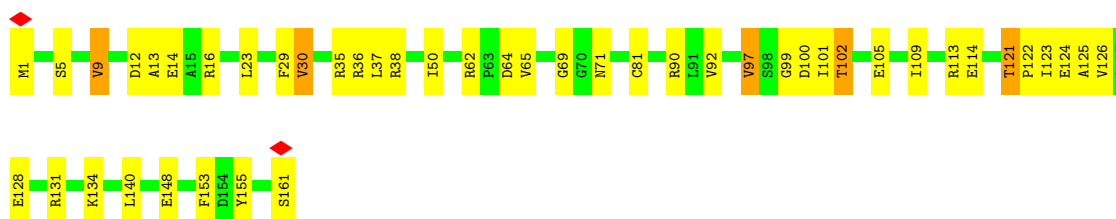
- Molecule 8: Allophycocyanin, beta subunit

Chain y2:  75% 25%



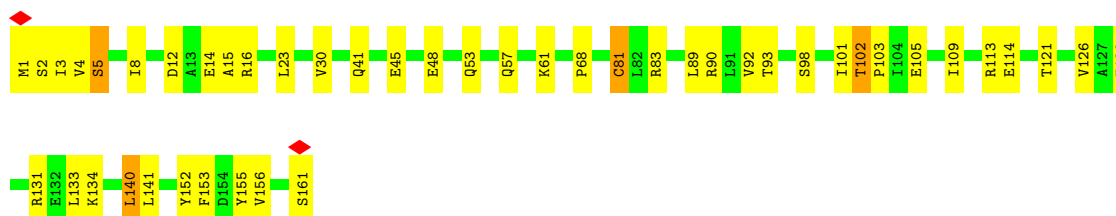
- Molecule 9: Allophycocyanin alpha chain

Chain D2:  71% 25%



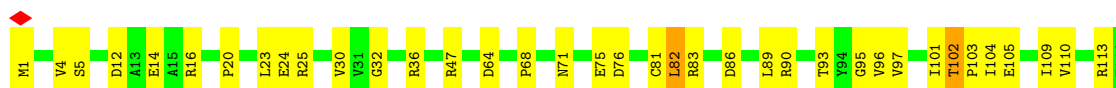
- Molecule 9: Allophycocyanin alpha chain

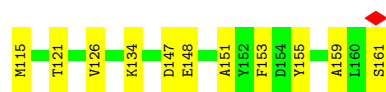
Chain E2:  71% 26%



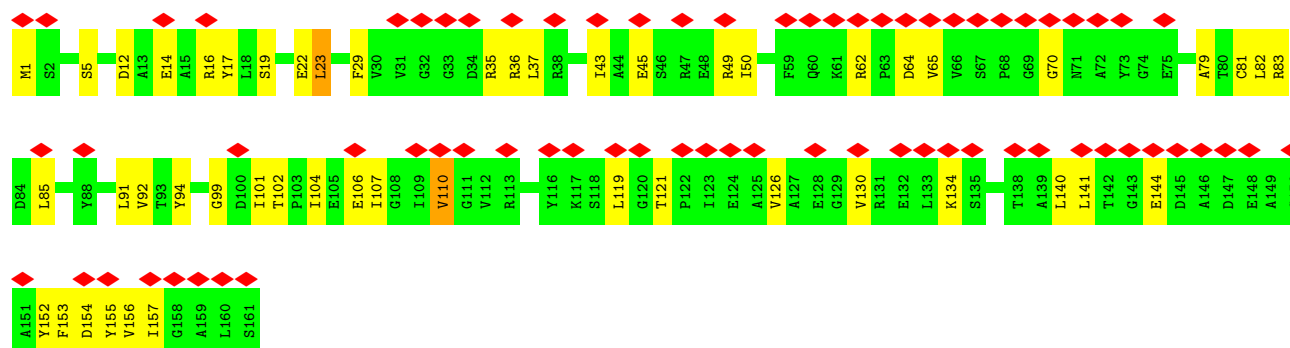
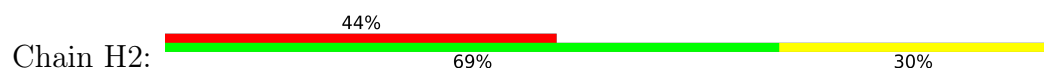
- Molecule 9: Allophycocyanin alpha chain

Chain G2:  70% 29%

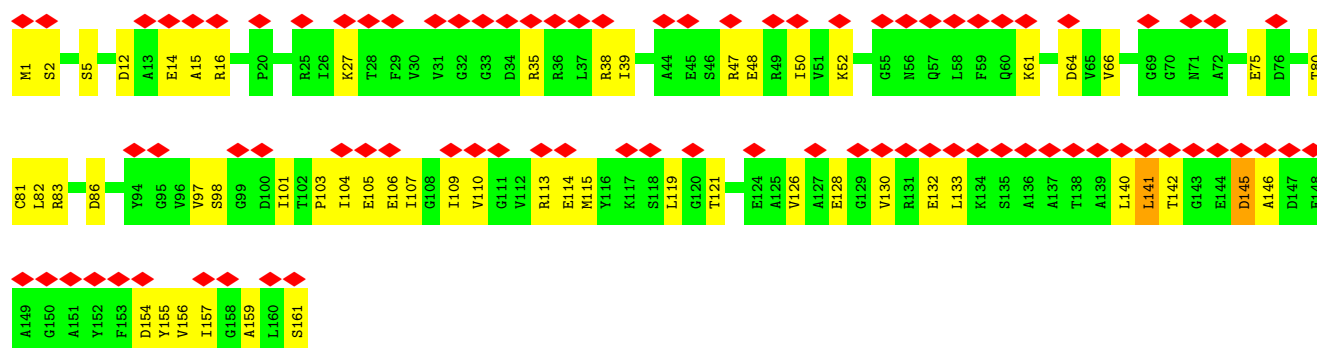




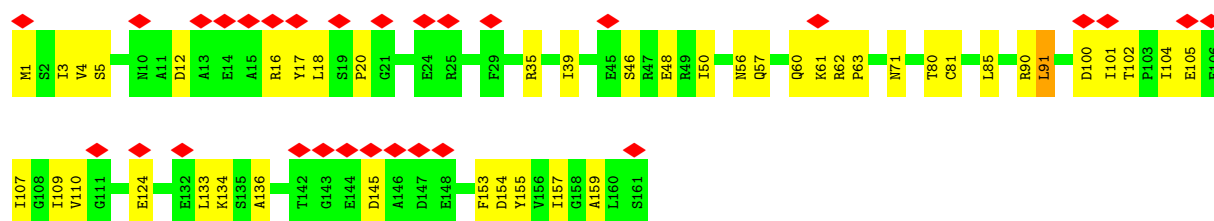
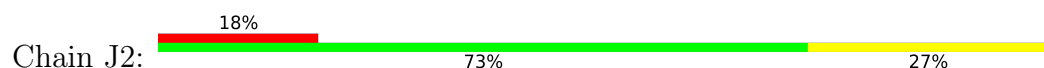
• Molecule 9: Allophycocyanin alpha chain



• Molecule 9: Allophycocyanin alpha chain

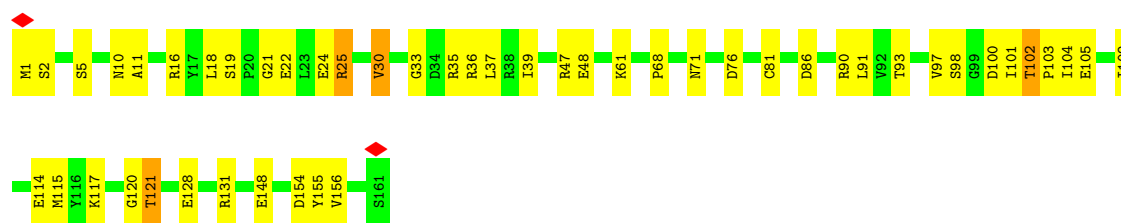


• Molecule 9: Allophycocyanin alpha chain

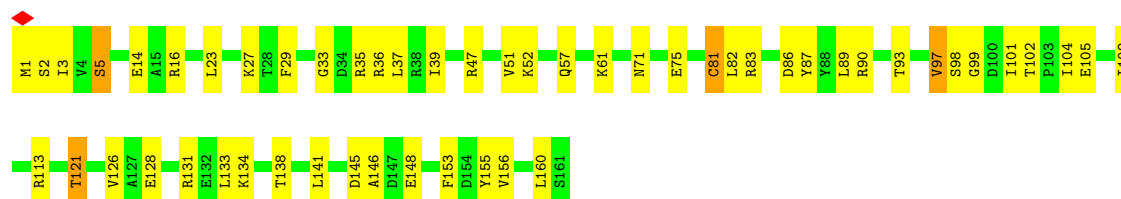


• Molecule 9: Allophycocyanin alpha chain

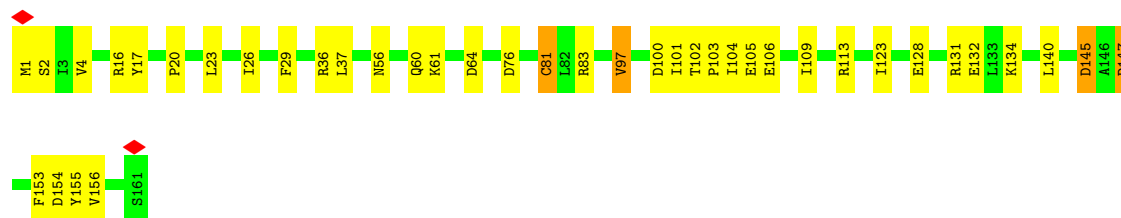
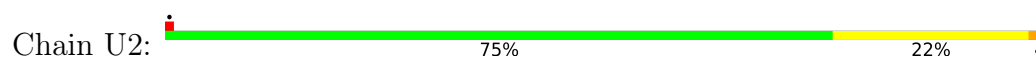




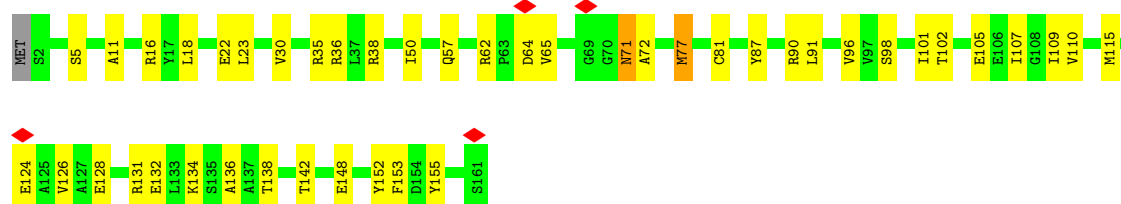
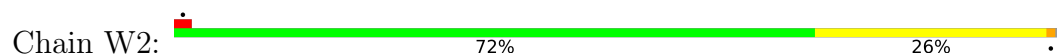
• Molecule 9: Allophycocyanin alpha chain



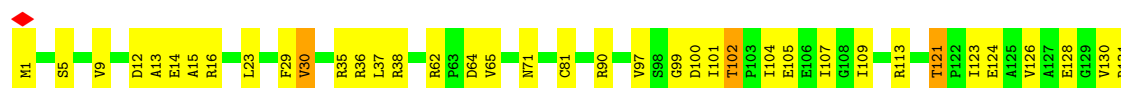
• Molecule 9: Allophycocyanin alpha chain

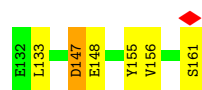


• Molecule 9: Allophycocyanin alpha chain



• Molecule 9: Allophycocyanin alpha chain

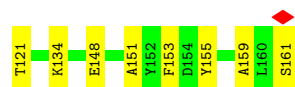
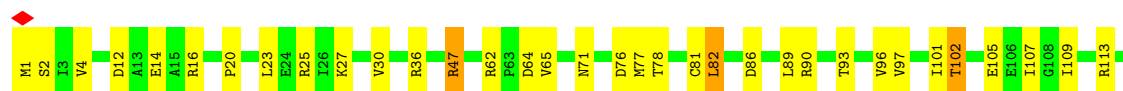
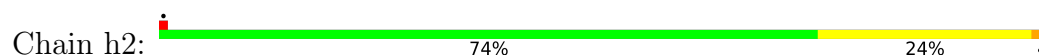




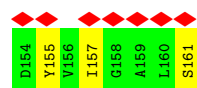
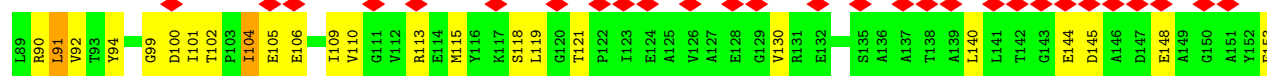
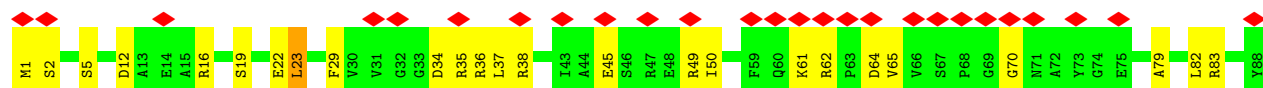
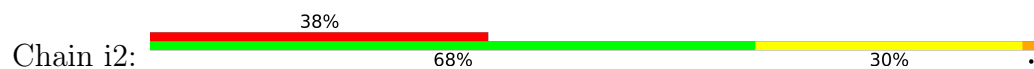
• Molecule 9: Allophycocyanin alpha chain



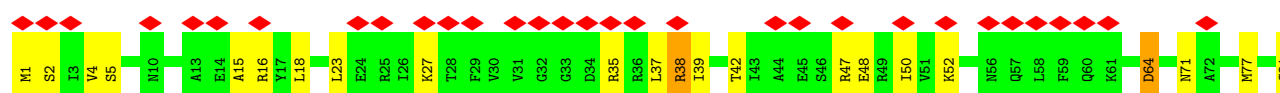
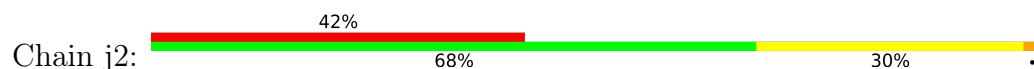
• Molecule 9: Allophycocyanin alpha chain

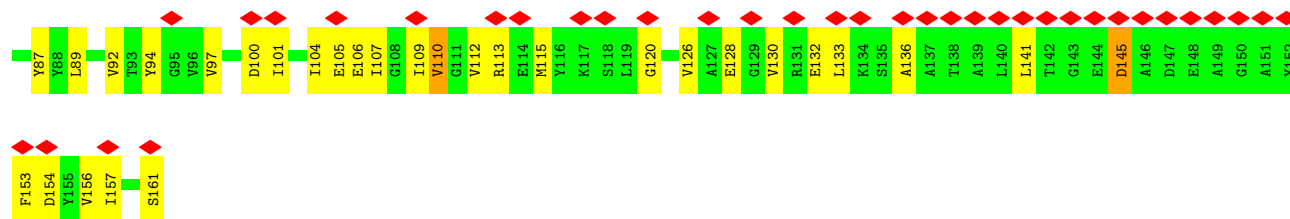


• Molecule 9: Allophycocyanin alpha chain

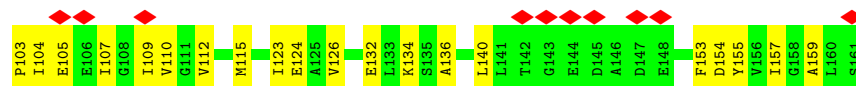
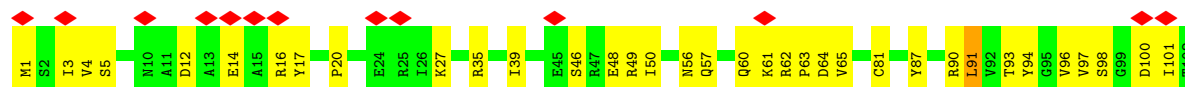


• Molecule 9: Allophycocyanin alpha chain

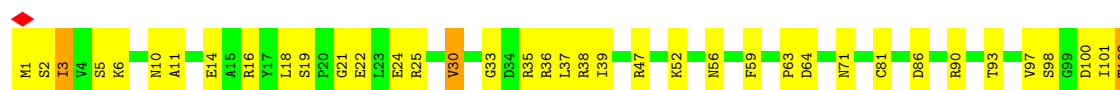




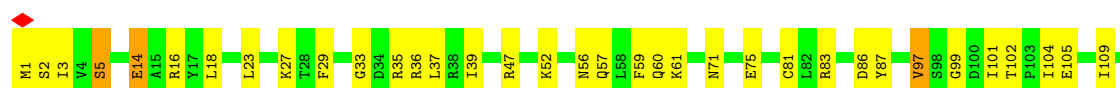
• Molecule 9: Allophycocyanin alpha chain



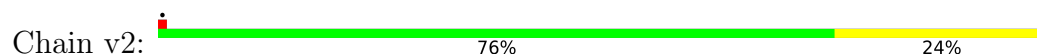
• Molecule 9: Allophycocyanin alpha chain



• Molecule 9: Allophycocyanin alpha chain



• Molecule 9: Allophycocyanin alpha chain

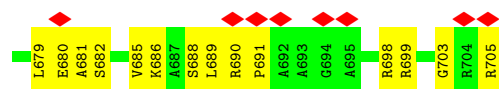
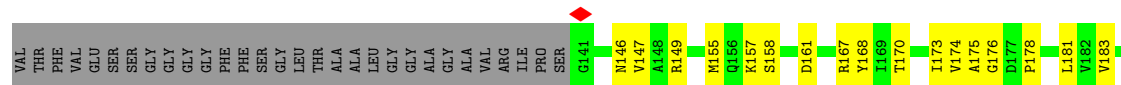
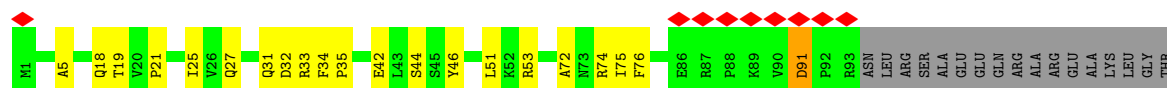




• Molecule 9: Allophycocyanin alpha chain

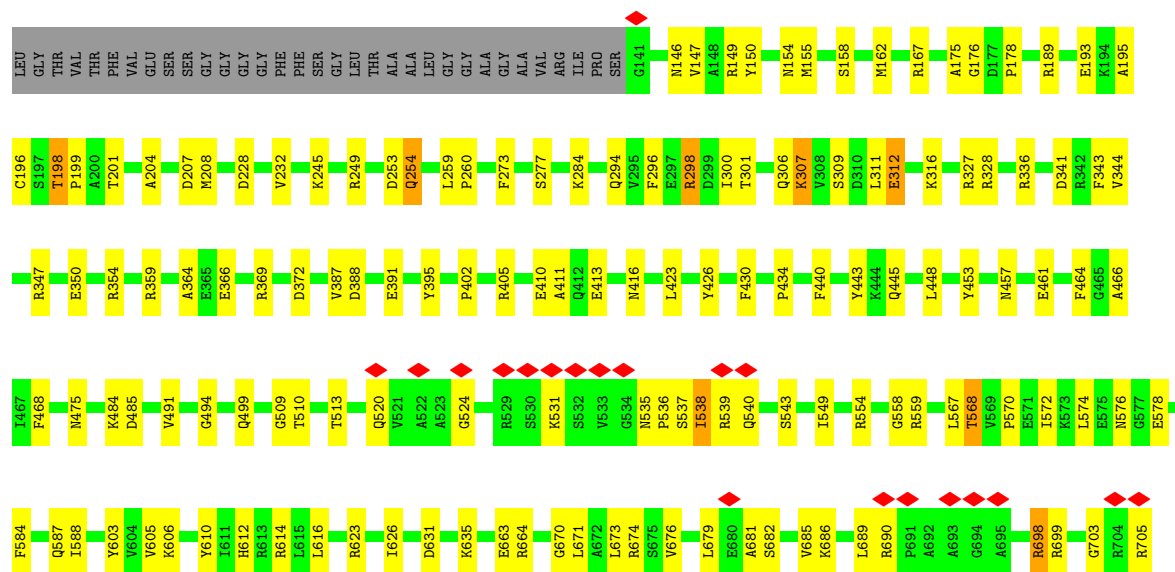


• Molecule 10: Phycobiliprotein ApcE



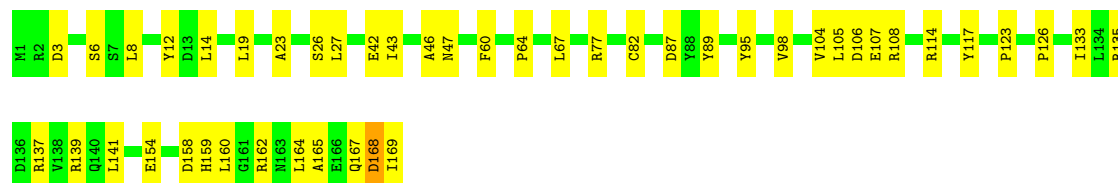
• Molecule 10: Phycobiliprotein ApcE





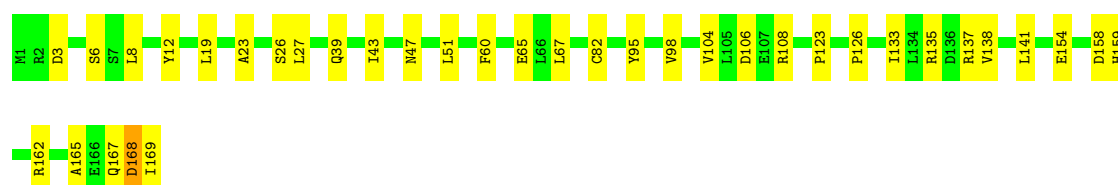
• Molecule 11: Allophycocyanin, beta subunit

Chain P2: 73% 27%



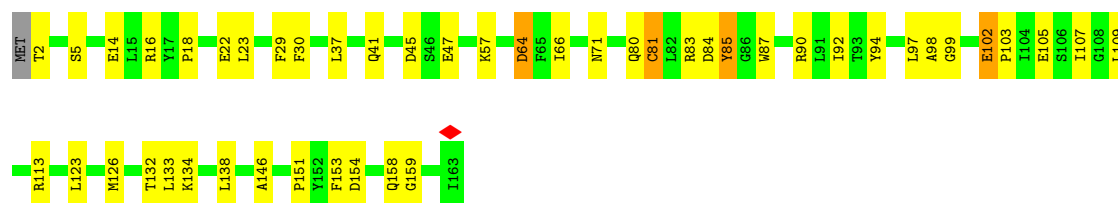
• Molecule 11: Allophycocyanin, beta subunit

Chain q2: 79% 21%

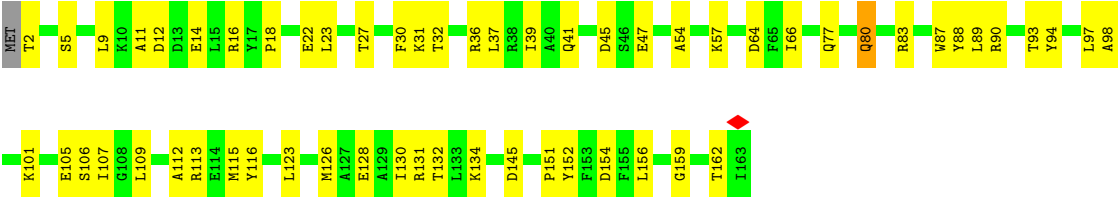


• Molecule 12: Allophycocyanin alpha-B chain

Chain S2: 71% 26%



• Molecule 12: Allophycocyanin alpha-B chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258722	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	599.2, 599.2, 599.2	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	22	0.26	0/2038	0.40	0/2760
1	32	0.31	0/2038	0.45	0/2760
1	42	0.35	0/2029	0.50	0/2749
1	52	0.52	0/2029	0.76	1/2749 (0.0%)
1	A1	0.33	0/1649	0.46	1/2235 (0.0%)
1	A6	0.28	0/1649	0.45	0/2235
2	B1	0.17	0/1237	0.27	0/1681
2	B3	0.12	0/1237	0.26	0/1681
2	B4	0.14	0/1237	0.26	0/1681
2	B5	0.16	0/1237	0.27	0/1681
2	B6	0.16	0/1237	0.28	0/1681
2	B7	0.11	0/1237	0.26	0/1681
2	F1	0.16	0/1237	0.23	0/1681
2	F3	0.11	0/1237	0.23	0/1681
2	F4	0.14	0/1237	0.22	0/1681
2	F5	0.15	0/1237	0.23	0/1681
2	F6	0.15	0/1237	0.23	0/1681
2	F7	0.11	0/1237	0.23	0/1681
2	G1	0.17	0/1237	0.27	0/1681
2	G3	0.12	0/1237	0.25	0/1681
2	G4	0.14	0/1237	0.25	0/1681
2	G5	0.16	0/1237	0.27	0/1681
2	G6	0.15	0/1237	0.25	0/1681
2	G7	0.11	0/1237	0.25	0/1681
2	H1	0.16	0/1237	0.24	0/1681
2	H3	0.11	0/1237	0.23	0/1681
2	H4	0.13	0/1237	0.23	0/1681
2	H5	0.15	0/1237	0.24	0/1681
2	H6	0.14	0/1237	0.23	0/1681
2	H7	0.10	0/1237	0.23	0/1681
2	I1	0.17	0/1237	0.25	0/1681
2	I3	0.24	0/1237	0.36	0/1681

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	I4	0.25	0/1237	0.38	0/1681
2	I5	0.23	0/1237	0.38	0/1681
2	I6	0.27	0/1237	0.40	0/1681
2	I7	0.11	0/1237	0.25	0/1681
2	K1	0.16	0/1237	0.24	0/1681
2	K3	0.12	0/1237	0.23	0/1681
2	K4	0.13	0/1237	0.23	0/1681
2	K5	0.15	0/1237	0.24	0/1681
2	K6	0.14	0/1237	0.22	0/1681
2	K7	0.11	0/1237	0.23	0/1681
2	N1	0.16	0/1245	0.26	0/1691
2	N3	0.12	0/1245	0.24	0/1691
2	N4	0.14	0/1245	0.25	0/1691
2	N5	0.15	0/1245	0.26	0/1691
2	N6	0.15	0/1245	0.26	0/1691
2	N7	0.11	0/1245	0.24	0/1691
2	R1	0.15	0/1237	0.25	0/1681
2	R3	0.11	0/1237	0.26	0/1681
2	R4	0.13	0/1237	0.24	0/1681
2	R5	0.14	0/1237	0.25	0/1681
2	R6	0.14	0/1237	0.25	0/1681
2	R7	0.11	0/1237	0.25	0/1681
2	S1	0.14	0/1237	0.24	0/1681
2	S3	0.11	0/1237	0.23	0/1681
2	S4	0.13	0/1237	0.23	0/1681
2	S5	0.14	0/1237	0.24	0/1681
2	S6	0.13	0/1237	0.24	0/1681
2	S7	0.10	0/1237	0.23	0/1681
2	T1	0.15	0/1237	0.25	0/1681
2	T3	0.11	0/1237	0.22	0/1681
2	T4	0.13	0/1237	0.24	0/1681
2	T5	0.15	0/1237	0.24	0/1681
2	T6	0.14	0/1237	0.24	0/1681
2	T7	0.10	0/1237	0.22	0/1681
2	U1	0.14	0/1237	0.25	0/1681
2	U3	0.10	0/1237	0.23	0/1681
2	U4	0.12	0/1237	0.24	0/1681
2	U5	0.13	0/1237	0.25	0/1681
2	U6	0.13	0/1237	0.25	0/1681
2	U7	0.09	0/1237	0.23	0/1681
2	W1	0.16	0/1237	0.26	0/1681
2	W3	0.11	0/1237	0.24	0/1681
2	W4	0.14	0/1237	0.25	0/1681

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	W5	0.15	0/1237	0.25	0/1681
2	W6	0.15	0/1237	0.27	0/1681
2	W7	0.11	0/1237	0.23	0/1681
3	C1	0.18	0/1293	0.25	0/1748
3	C3	0.12	0/1293	0.24	0/1748
3	C4	0.14	0/1293	0.24	0/1748
3	C5	0.16	0/1293	0.25	0/1748
3	C6	0.16	0/1293	0.24	0/1748
3	C7	0.11	0/1293	0.23	0/1748
3	D1	0.18	0/1285	0.28	0/1738
3	D3	0.12	0/1285	0.27	0/1738
3	D4	0.14	0/1285	0.26	0/1738
3	D5	0.16	0/1285	0.27	0/1738
3	D6	0.16	0/1285	0.26	0/1738
3	D7	0.11	0/1285	0.26	0/1738
3	E1	0.17	0/1285	0.26	0/1738
3	E3	0.11	0/1285	0.24	0/1738
3	E4	0.13	0/1285	0.24	0/1738
3	E5	0.15	0/1285	0.25	0/1738
3	E6	0.15	0/1285	0.26	0/1738
3	E7	0.10	0/1285	0.23	0/1738
3	J1	0.17	0/1293	0.25	0/1748
3	J3	0.12	0/1293	0.23	0/1748
3	J4	0.14	0/1293	0.24	0/1748
3	J5	0.15	0/1293	0.25	0/1748
3	J6	0.15	0/1293	0.25	0/1748
3	J7	0.12	0/1293	0.23	0/1748
3	L1	0.17	0/1293	0.26	0/1748
3	L3	0.12	0/1293	0.24	0/1748
3	L4	0.14	0/1293	0.23	0/1748
3	L5	0.15	0/1293	0.24	0/1748
3	L6	0.16	0/1293	0.24	0/1748
3	L7	0.11	0/1293	0.23	0/1748
3	M1	0.14	0/1293	0.25	0/1748
3	M3	0.10	0/1293	0.24	0/1748
3	M4	0.13	0/1293	0.24	0/1748
3	M5	0.14	0/1293	0.24	0/1748
3	M6	0.13	0/1293	0.25	0/1748
3	M7	0.10	0/1293	0.24	0/1748
3	O1	0.17	0/1293	0.25	0/1748
3	O3	0.12	0/1293	0.24	0/1748
3	O4	0.14	0/1293	0.24	0/1748
3	O5	0.15	0/1293	0.25	0/1748

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	O6	0.15	0/1293	0.25	0/1748
3	O7	0.11	0/1293	0.24	0/1748
3	P1	0.14	0/1293	0.23	0/1748
3	P3	0.10	0/1293	0.22	0/1748
3	P4	0.13	0/1293	0.22	0/1748
3	P5	0.14	0/1293	0.23	0/1748
3	P6	0.13	0/1293	0.23	0/1748
3	P7	0.10	0/1293	0.21	0/1748
3	Q1	0.14	0/1285	0.25	0/1738
3	Q3	0.10	0/1285	0.24	0/1738
3	Q4	0.12	0/1285	0.24	0/1738
3	Q5	0.14	0/1285	0.24	0/1738
3	Q6	0.13	0/1285	0.25	0/1738
3	Q7	0.10	0/1285	0.24	0/1738
3	V1	0.17	0/1285	0.26	0/1738
3	V3	0.12	0/1285	0.24	0/1738
3	V4	0.14	0/1285	0.25	0/1738
3	V5	0.16	0/1285	0.26	0/1738
3	V6	0.15	0/1285	0.25	0/1738
3	V7	0.11	0/1285	0.24	0/1738
3	X1	0.23	0/1293	0.38	0/1748
3	X3	0.11	0/1293	0.26	0/1748
3	X4	0.13	0/1293	0.26	0/1748
3	X5	0.14	0/1293	0.26	0/1748
3	X6	0.14	0/1293	0.27	0/1748
3	X7	0.11	0/1293	0.25	0/1748
3	a1	0.17	0/1285	0.26	0/1738
3	a3	0.13	0/1285	0.25	0/1738
3	a4	0.61	0/1285	0.89	0/1738
3	a5	0.23	0/1285	0.34	0/1738
3	a6	0.16	0/1285	0.28	0/1738
3	a7	0.35	0/1285	0.55	1/1738 (0.1%)
4	Y1	0.12	0/462	0.28	0/621
4	Y3	0.11	0/462	0.28	0/621
4	Y4	0.45	0/462	0.58	0/621
4	Y5	0.10	0/462	0.25	0/621
4	Y6	0.10	0/462	0.26	0/621
4	Y7	0.09	0/462	0.27	0/621
5	Z1	0.17	0/2272	0.29	0/3083
5	Z3	0.13	0/2272	0.28	0/3083
5	Z4	0.14	0/2272	0.28	0/3083
5	Z5	0.16	0/2272	0.29	0/3083
5	Z6	0.16	0/2272	0.29	0/3083

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Z7	0.12	0/2272	0.28	0/3083
6	O2	0.12	0/559	0.30	0/750
6	Y2	0.17	0/559	0.33	0/750
6	Z2	0.09	0/559	0.27	0/750
6	z2	0.20	0/559	0.34	0/750
7	l2	0.16	0/280	0.37	0/386
7	b2	0.14	0/280	0.30	0/386
8	A2	0.09	0/1236	0.27	0/1673
8	B2	0.10	0/1236	0.24	0/1673
8	C2	0.09	0/1236	0.25	0/1673
8	F2	0.17	0/1236	0.25	0/1673
8	K2	0.18	0/1236	0.30	0/1673
8	L2	0.19	0/1236	0.26	0/1673
8	M2	0.19	0/1236	0.28	0/1673
8	O2	0.18	0/1236	0.27	0/1673
8	T2	0.15	0/1236	0.24	0/1673
8	V2	0.15	0/1236	0.27	0/1673
8	X2	0.16	0/1236	0.29	0/1673
8	a2	0.09	0/1236	0.25	0/1673
8	c2	0.10	0/1236	0.25	0/1673
8	d2	0.10	0/1236	0.26	0/1673
8	g2	0.20	0/1236	0.30	0/1673
8	l2	0.20	0/1236	0.29	0/1673
8	m2	0.22	0/1236	0.27	0/1673
8	n2	0.22	0/1236	0.29	0/1673
8	p2	0.21	0/1236	0.29	0/1673
8	u2	0.16	0/1236	0.27	0/1673
8	w2	0.17	0/1236	0.27	0/1673
8	y2	0.19	0/1236	0.30	0/1673
9	D2	0.15	0/1239	0.27	0/1674
9	E2	0.27	0/1239	0.43	0/1674
9	G2	0.27	0/1239	0.41	0/1674
9	H2	0.10	0/1239	0.25	0/1674
9	I2	0.09	0/1239	0.23	0/1674
9	J2	0.11	0/1239	0.29	0/1674
9	Q2	0.15	0/1239	0.28	0/1674
9	R2	0.17	0/1239	0.30	0/1674
9	U2	0.17	0/1239	0.29	0/1674
9	W2	0.13	0/1231	0.28	0/1664
9	e2	0.17	0/1239	0.27	0/1674
9	f2	0.18	0/1239	0.30	0/1674
9	h2	0.18	0/1239	0.29	0/1674
9	i2	0.10	0/1239	0.25	0/1674

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	j2	0.10	0/1239	0.26	0/1674
9	k2	0.12	0/1239	0.29	0/1674
9	r2	0.25	0/1239	0.43	0/1674
9	s2	0.20	0/1239	0.31	0/1674
9	v2	0.20	0/1239	0.31	0/1674
9	x2	0.15	0/1231	0.28	0/1664
10	N2	0.26	0/5348	0.38	1/7227 (0.0%)
10	o2	0.25	0/5348	0.33	0/7227
11	P2	0.19	0/1329	0.28	0/1803
11	q2	0.23	0/1329	0.30	0/1803
12	S2	0.17	0/1290	0.30	0/1741
12	t2	0.19	0/1290	0.31	0/1741
All	All	0.17	0/280490	0.29	4/379940 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a7	107	ASP	CA-CB-CG	5.87	118.47	112.60
10	N2	317	ASN	N-CA-C	-5.34	107.41	114.04
1	52	201	GLY	CA-C-O	-5.16	118.15	122.33
1	A1	55	PHE	N-CA-C	-5.09	105.38	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	22	1989	0	1948	61	0
1	32	1989	0	1948	60	0
1	42	1980	0	1935	50	0
1	52	1980	0	1935	53	0
1	A1	1609	0	1561	56	0
1	A6	1609	0	1561	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B1	1213	0	1180	25	0
2	B3	1213	0	1180	30	0
2	B4	1213	0	1180	24	0
2	B5	1213	0	1180	24	0
2	B6	1213	0	1180	29	0
2	B7	1213	0	1180	33	0
2	F1	1213	0	1181	37	0
2	F3	1213	0	1181	35	0
2	F4	1213	0	1181	35	0
2	F5	1213	0	1181	32	0
2	F6	1213	0	1181	41	0
2	F7	1213	0	1181	36	0
2	G1	1213	0	1180	27	0
2	G3	1213	0	1180	32	0
2	G4	1213	0	1180	29	0
2	G5	1213	0	1180	28	0
2	G6	1213	0	1180	29	0
2	G7	1213	0	1180	25	0
2	H1	1213	0	1180	32	0
2	H3	1213	0	1180	32	0
2	H4	1213	0	1180	29	0
2	H5	1213	0	1180	29	0
2	H6	1213	0	1180	34	0
2	H7	1213	0	1180	31	0
2	I1	1213	0	1180	32	0
2	I3	1213	0	1180	33	0
2	I4	1213	0	1180	37	0
2	I5	1213	0	1180	36	0
2	I6	1213	0	1180	30	0
2	I7	1213	0	1180	27	0
2	K1	1213	0	1180	33	0
2	K3	1213	0	1180	37	0
2	K4	1213	0	1180	37	0
2	K5	1213	0	1180	28	0
2	K6	1213	0	1180	36	0
2	K7	1213	0	1180	41	0
2	N1	1221	0	1192	33	0
2	N3	1221	0	1192	42	0
2	N4	1221	0	1192	36	0
2	N5	1221	0	1192	37	0
2	N6	1221	0	1192	33	0
2	N7	1221	0	1192	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R1	1213	0	1181	39	0
2	R3	1213	0	1181	49	0
2	R4	1213	0	1181	35	0
2	R5	1213	0	1181	44	0
2	R6	1213	0	1181	46	0
2	R7	1213	0	1181	43	0
2	S1	1213	0	1180	34	0
2	S3	1213	0	1180	36	0
2	S4	1213	0	1180	35	0
2	S5	1213	0	1180	33	0
2	S6	1213	0	1180	33	0
2	S7	1213	0	1180	36	0
2	T1	1213	0	1177	33	0
2	T3	1213	0	1177	31	0
2	T4	1213	0	1177	30	0
2	T5	1213	0	1177	32	0
2	T6	1213	0	1177	33	0
2	T7	1213	0	1177	30	0
2	U1	1213	0	1180	29	0
2	U3	1213	0	1180	40	0
2	U4	1213	0	1180	35	0
2	U5	1213	0	1180	40	0
2	U6	1213	0	1180	34	0
2	U7	1213	0	1180	37	0
2	W1	1213	0	1180	35	0
2	W3	1213	0	1180	35	0
2	W4	1213	0	1180	36	0
2	W5	1213	0	1180	36	0
2	W6	1213	0	1180	36	0
2	W7	1213	0	1180	35	0
3	C1	1280	0	1282	28	0
3	C3	1280	0	1282	34	0
3	C4	1280	0	1282	32	0
3	C5	1280	0	1282	33	0
3	C6	1280	0	1282	28	0
3	C7	1280	0	1282	33	0
3	D1	1272	0	1270	35	0
3	D3	1272	0	1270	42	0
3	D4	1272	0	1270	35	0
3	D5	1272	0	1270	37	0
3	D6	1272	0	1270	38	0
3	D7	1272	0	1270	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E1	1272	0	1270	32	0
3	E3	1272	0	1271	33	0
3	E4	1272	0	1270	32	0
3	E5	1272	0	1270	32	0
3	E6	1272	0	1271	34	0
3	E7	1272	0	1271	36	0
3	J1	1280	0	1280	20	0
3	J3	1280	0	1280	31	0
3	J4	1280	0	1280	27	0
3	J5	1280	0	1280	21	0
3	J6	1280	0	1280	21	0
3	J7	1280	0	1280	29	0
3	L1	1280	0	1285	31	0
3	L3	1280	0	1285	39	0
3	L4	1280	0	1285	32	0
3	L5	1280	0	1285	32	0
3	L6	1280	0	1285	39	0
3	L7	1280	0	1285	41	0
3	M1	1280	0	1283	35	0
3	M3	1280	0	1283	29	0
3	M4	1280	0	1283	28	0
3	M5	1280	0	1283	34	0
3	M6	1280	0	1283	35	0
3	M7	1280	0	1283	28	0
3	O1	1280	0	1285	37	0
3	O3	1280	0	1285	37	0
3	O4	1280	0	1285	41	0
3	O5	1280	0	1285	41	0
3	O6	1280	0	1285	35	0
3	O7	1280	0	1285	37	0
3	P1	1280	0	1282	23	0
3	P3	1280	0	1282	30	0
3	P4	1280	0	1282	25	0
3	P5	1280	0	1282	26	0
3	P6	1280	0	1282	34	0
3	P7	1280	0	1282	26	0
3	Q1	1272	0	1270	38	0
3	Q3	1272	0	1270	40	0
3	Q4	1272	0	1270	29	0
3	Q5	1272	0	1270	30	0
3	Q6	1272	0	1270	36	0
3	Q7	1272	0	1270	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V1	1272	0	1271	39	0
3	V3	1272	0	1271	38	0
3	V4	1272	0	1271	41	0
3	V5	1272	0	1271	34	0
3	V6	1272	0	1271	37	0
3	V7	1272	0	1271	33	0
3	X1	1280	0	1284	31	0
3	X3	1280	0	1284	32	0
3	X4	1280	0	1284	33	0
3	X5	1280	0	1284	30	0
3	X6	1280	0	1284	36	0
3	X7	1280	0	1284	36	0
3	a1	1272	0	1272	30	0
3	a3	1272	0	1271	33	0
3	a4	1272	0	1273	38	0
3	a5	1272	0	1271	30	0
3	a6	1272	0	1272	32	0
3	a7	1272	0	1271	41	0
4	Y1	457	0	462	17	0
4	Y3	457	0	462	19	0
4	Y4	457	0	464	21	0
4	Y5	457	0	462	15	0
4	Y6	457	0	462	16	0
4	Y7	457	0	462	16	0
5	Z1	2229	0	2209	61	0
5	Z3	2229	0	2209	62	0
5	Z4	2229	0	2209	59	0
5	Z5	2229	0	2209	54	0
5	Z6	2229	0	2209	59	0
5	Z7	2229	0	2209	62	0
6	02	549	0	580	19	0
6	Y2	549	0	580	16	0
6	Z2	549	0	580	20	0
6	z2	549	0	580	16	0
7	12	274	0	280	11	0
7	b2	274	0	280	8	0
8	A2	1221	0	1234	34	0
8	B2	1221	0	1234	38	0
8	C2	1221	0	1234	38	0
8	F2	1221	0	1234	28	0
8	K2	1221	0	1234	25	0
8	L2	1221	0	1234	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M2	1221	0	1234	30	0
8	O2	1221	0	1234	28	0
8	T2	1221	0	1234	41	0
8	V2	1221	0	1234	30	0
8	X2	1221	0	1234	31	0
8	a2	1221	0	1234	30	0
8	c2	1221	0	1234	36	0
8	d2	1221	0	1234	45	0
8	g2	1221	0	1234	39	0
8	l2	1221	0	1234	33	0
8	m2	1221	0	1234	38	0
8	n2	1221	0	1234	28	0
8	p2	1221	0	1234	34	0
8	u2	1221	0	1234	44	0
8	w2	1221	0	1234	26	0
8	y2	1221	0	1234	34	0
9	D2	1224	0	1232	35	0
9	E2	1224	0	1232	31	0
9	G2	1224	0	1232	39	0
9	H2	1224	0	1232	39	0
9	I2	1224	0	1232	49	0
9	J2	1224	0	1232	36	0
9	Q2	1224	0	1232	46	0
9	R2	1224	0	1232	41	0
9	U2	1224	0	1232	29	0
9	W2	1216	0	1220	32	0
9	e2	1224	0	1232	33	0
9	f2	1224	0	1231	33	0
9	h2	1224	0	1232	36	0
9	i2	1224	0	1232	36	0
9	j2	1224	0	1232	49	0
9	k2	1224	0	1232	51	0
9	r2	1224	0	1232	45	0
9	s2	1224	0	1232	41	0
9	v2	1224	0	1232	28	0
9	x2	1216	0	1219	34	0
10	N2	5242	0	5263	137	0
10	o2	5242	0	5262	133	0
11	P2	1310	0	1297	34	0
11	q2	1310	0	1297	28	0
12	S2	1268	0	1283	44	0
12	t2	1268	0	1279	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	22	86	0	74	12	0
13	32	86	0	74	12	0
13	42	86	0	74	14	0
13	52	86	0	74	13	0
13	A1	86	0	74	13	0
13	A2	86	0	76	10	0
13	A6	86	0	74	14	0
13	B1	43	0	35	7	0
13	B2	86	0	76	8	0
13	B3	43	0	35	5	0
13	B4	43	0	35	5	0
13	B5	43	0	35	7	0
13	B6	43	0	35	9	0
13	B7	43	0	35	5	0
13	C1	86	0	74	13	0
13	C2	43	0	38	5	0
13	C3	86	0	73	8	0
13	C4	86	0	74	13	0
13	C5	86	0	73	14	0
13	C6	86	0	74	11	0
13	C7	86	0	74	8	0
13	D1	43	0	38	2	0
13	D2	43	0	38	8	0
13	D3	43	0	38	3	0
13	D4	43	0	38	4	0
13	D5	43	0	38	2	0
13	D6	43	0	38	3	0
13	D7	43	0	38	5	0
13	E1	43	0	37	5	0
13	E2	43	0	38	7	0
13	E3	43	0	36	3	0
13	E4	43	0	37	4	0
13	E5	43	0	37	4	0
13	E6	43	0	36	5	0
13	E7	43	0	37	5	0
13	F1	86	0	74	6	0
13	F2	43	0	38	8	0
13	F3	86	0	74	7	0
13	F4	86	0	74	8	0
13	F5	86	0	74	7	0
13	F6	86	0	74	8	0
13	F7	86	0	74	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	G1	43	0	36	4	0
13	G2	43	0	38	8	0
13	G3	43	0	35	2	0
13	G4	43	0	35	3	0
13	G5	43	0	35	3	0
13	G6	43	0	35	2	0
13	G7	43	0	35	1	0
13	H1	43	0	36	3	0
13	H2	43	0	38	8	0
13	H3	43	0	35	1	0
13	H4	43	0	35	3	0
13	H5	43	0	35	3	0
13	H6	43	0	35	1	0
13	H7	43	0	35	1	0
13	I1	43	0	35	5	0
13	I3	43	0	35	4	0
13	I4	43	0	35	3	0
13	I5	43	0	35	3	0
13	I6	43	0	35	3	0
13	I7	43	0	35	2	0
13	J1	86	0	73	7	0
13	J3	86	0	73	4	0
13	J4	86	0	73	10	0
13	J5	86	0	73	4	0
13	J6	86	0	73	6	0
13	J7	86	0	73	6	0
13	K1	43	0	35	4	0
13	K3	43	0	35	3	0
13	K4	43	0	35	4	0
13	K5	43	0	36	4	0
13	K6	43	0	35	5	0
13	K7	43	0	35	2	0
13	L1	43	0	38	5	0
13	L2	43	0	38	7	0
13	L3	43	0	38	3	0
13	L4	43	0	38	1	0
13	L5	43	0	38	5	0
13	L6	43	0	38	5	0
13	L7	43	0	38	4	0
13	M1	43	0	37	6	0
13	M2	43	0	38	8	0
13	M3	43	0	37	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M4	43	0	37	4	0
13	M5	43	0	37	7	0
13	M6	43	0	37	7	0
13	M7	43	0	37	6	0
13	N1	43	0	36	5	0
13	N2	86	0	76	10	0
13	N3	43	0	36	4	0
13	N4	43	0	35	5	0
13	N5	43	0	36	5	0
13	N6	43	0	36	4	0
13	N7	43	0	36	3	0
13	O2	43	0	38	5	0
13	P1	86	0	75	4	0
13	P2	43	0	38	3	0
13	P3	86	0	75	4	0
13	P4	86	0	75	5	0
13	P5	86	0	75	4	0
13	P6	86	0	75	4	0
13	P7	86	0	75	2	0
13	Q1	86	0	76	11	0
13	Q2	43	0	38	7	0
13	Q3	86	0	76	11	0
13	Q4	86	0	76	11	0
13	Q5	86	0	76	12	0
13	Q6	86	0	76	12	0
13	Q7	86	0	76	11	0
13	R1	43	0	38	4	0
13	R2	43	0	38	9	0
13	R3	43	0	38	6	0
13	R4	43	0	38	3	0
13	R5	43	0	38	5	0
13	R6	43	0	38	5	0
13	R7	43	0	38	3	0
13	S1	43	0	36	7	0
13	S2	43	0	38	9	0
13	S3	43	0	36	6	0
13	S4	43	0	37	6	0
13	S5	43	0	35	7	0
13	S6	43	0	36	5	0
13	S7	43	0	36	6	0
13	T1	86	0	73	9	0
13	T2	43	0	38	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	T3	86	0	72	7	0
13	T4	86	0	73	7	0
13	T5	86	0	73	8	0
13	T6	86	0	73	7	0
13	T7	86	0	73	8	0
13	U1	43	0	36	2	0
13	U2	43	0	38	7	0
13	U3	43	0	35	1	0
13	U4	43	0	35	3	0
13	U5	43	0	36	4	0
13	U6	43	0	36	3	0
13	U7	43	0	35	1	0
13	V1	86	0	72	11	0
13	V2	43	0	38	2	0
13	V3	86	0	72	9	0
13	V4	86	0	72	10	0
13	V5	86	0	72	8	0
13	V6	86	0	72	11	0
13	V7	86	0	73	10	0
13	W1	43	0	36	6	0
13	W2	43	0	38	7	0
13	W3	43	0	35	3	0
13	W4	43	0	36	6	0
13	W5	43	0	36	5	0
13	W6	43	0	36	3	0
13	W7	43	0	35	2	0
13	X1	43	0	36	9	0
13	X2	43	0	38	8	0
13	X3	43	0	36	7	0
13	X4	43	0	37	8	0
13	X5	43	0	37	9	0
13	X6	43	0	37	5	0
13	X7	43	0	36	9	0
13	Z1	43	0	38	6	0
13	Z3	43	0	38	7	0
13	Z4	43	0	38	5	0
13	Z5	43	0	38	5	0
13	Z6	43	0	38	4	0
13	Z7	43	0	38	7	0
13	a1	86	0	75	9	0
13	a2	43	0	38	7	0
13	a3	86	0	75	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a4	86	0	76	12	0
13	a5	86	0	75	10	0
13	a6	86	0	75	13	0
13	a7	86	0	75	10	0
13	c2	43	0	36	7	0
13	d2	43	0	38	6	0
13	e2	43	0	38	8	0
13	f2	43	0	36	5	0
13	g2	43	0	38	10	0
13	h2	43	0	38	9	0
13	i2	43	0	38	3	0
13	j2	43	0	38	5	0
13	k2	43	0	38	6	0
13	l2	43	0	38	8	0
13	m2	43	0	38	6	0
13	n2	43	0	38	7	0
13	o2	43	0	38	8	0
13	p2	43	0	38	7	0
13	q2	43	0	38	2	0
13	r2	43	0	38	6	0
13	s2	43	0	38	9	0
13	t2	43	0	34	2	0
13	v2	43	0	38	6	0
13	w2	43	0	38	3	0
13	x2	43	0	37	3	0
13	y2	43	0	38	6	0
13	z2	43	0	38	6	0
All	All	287122	0	283564	6523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (6523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O2:201:CYC:HMA1	13:O2:201:CYC:HB	1.33	0.93
3:a7:104:SER:HA	3:a7:107:ASP:CG	2.01	0.86
3:Q1:83:CYS:HA	13:Q1:201:CYC:HHD	1.60	0.84
3:Q4:83:CYS:HA	13:Q4:201:CYC:HHD	1.61	0.83
13:X7:201:CYC:HB	13:X7:201:CYC:HMA1	1.42	0.83
13:A2:201:CYC:HB	13:A2:201:CYC:HMA1	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e2:201:CYC:HB	13:e2:201:CYC:HMA1	1.42	0.82
8:g2:81:CYS:HA	13:g2:201:CYC:HHD	1.61	0.82
3:Q5:83:CYS:HA	13:Q5:201:CYC:HHD	1.62	0.82
9:D2:81:CYS:HA	13:D2:201:CYC:HHD	1.61	0.82
3:a4:44:ARG:HH12	3:a4:145:ASP:HB3	1.44	0.82
9:R2:81:CYS:HA	13:R2:201:CYC:HHD	1.62	0.81
9:s2:81:CYS:HA	13:s2:201:CYC:HHD	1.63	0.81
9:U2:105:GLU:HA	9:U2:109:ILE:HB	1.63	0.81
13:U2:201:CYC:HB	13:U2:201:CYC:HMA1	1.44	0.81
13:R2:201:CYC:HMA3	13:R2:201:CYC:HB	1.46	0.81
8:d2:103:ILE:HG13	8:d2:107:ARG:HD3	1.64	0.80
3:a4:154:CYS:SG	13:a4:202:CYC:HBC2	2.21	0.80
9:R2:105:GLU:HA	9:R2:109:ILE:HB	1.63	0.80
3:Q3:83:CYS:HA	13:Q3:201:CYC:HHD	1.64	0.80
1:52:93:SER:HB3	1:52:180:ARG:HD2	1.65	0.79
3:Q7:83:CYS:HA	13:Q7:201:CYC:HHD	1.64	0.79
10:N2:703:GLY:H	9:W2:142:THR:HG22	1.45	0.78
10:o2:703:GLY:H	9:x2:142:THR:HG22	1.45	0.78
9:v2:105:GLU:HA	9:v2:109:ILE:HB	1.66	0.78
2:S7:41:ALA:HB2	2:S7:147:SER:HB3	1.66	0.78
3:Q6:83:CYS:HA	13:Q6:201:CYC:HHD	1.64	0.78
2:S3:41:ALA:HB2	2:S3:147:SER:HB3	1.66	0.78
3:a7:105:ILE:HD12	3:a7:109:ARG:HG3	1.66	0.78
8:M2:81:CYS:HA	13:M2:201:CYC:HHD	1.67	0.77
9:r2:81:CYS:HA	13:r2:201:CYC:HHD	1.64	0.77
3:a7:3:PHE:H	3:a7:104:SER:CB	1.97	0.77
8:n2:126:THR:HG23	13:n2:201:CYC:HBC3	1.66	0.77
2:N7:41:ALA:HB2	2:N7:147:SER:HB3	1.67	0.77
8:n2:73:TYR:O	13:s2:201:CYC:OB	2.03	0.77
9:s2:105:GLU:HA	9:s2:109:ILE:HB	1.65	0.77
9:G2:105:GLU:HA	9:G2:109:ILE:HB	1.67	0.77
3:C4:149:ILE:HG21	13:C4:202:CYC:HMC3	1.66	0.76
8:m2:106:GLU:HG3	8:m2:107:ARG:HG2	1.67	0.76
13:32:302:CYC:HHD	3:E3:83:CYS:HA	1.67	0.76
8:m2:14:VAL:HG21	11:q2:165:ALA:HB1	1.68	0.76
9:E2:105:GLU:HA	9:E2:109:ILE:HB	1.67	0.76
10:o2:623:ARG:HA	10:o2:626:ILE:HG22	1.67	0.76
8:u2:76:ARG:HB3	9:x2:110:VAL:HG23	1.68	0.75
13:Z1:301:CYC:HMA3	13:Z1:301:CYC:HB	1.52	0.75
8:a2:90:ARG:HH12	9:i2:12:ASP:HA	1.50	0.75
8:A2:90:ARG:HH12	9:H2:12:ASP:HA	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e2:81:CYS:HA	13:e2:201:CYC:HHD	1.67	0.75
8:M2:73:TYR:O	13:R2:201:CYC:OB	2.04	0.75
9:h2:105:GLU:HA	9:h2:109:ILE:HB	1.69	0.75
9:E2:81:CYS:HA	13:E2:201:CYC:HHD	1.68	0.75
2:N3:41:ALA:HB2	2:N3:147:SER:HB3	1.68	0.74
13:L1:201:CYC:HB	13:L1:201:CYC:HMA1	1.53	0.74
3:a3:146:ARG:HD3	13:a3:202:CYC:HMC2	1.67	0.74
3:a1:108:ASP:O	10:N2:699:ARG:NH2	2.21	0.74
13:X1:201:CYC:HMA3	13:X1:201:CYC:HB	1.51	0.74
2:W4:5:PRO:HG2	2:W4:31:ARG:HD3	1.70	0.74
3:C1:149:ILE:HG21	13:C1:202:CYC:HMC3	1.69	0.74
3:M1:63:GLU:HG3	3:M1:64:GLN:HG3	1.70	0.74
13:22:302:CYC:HHD	3:E7:83:CYS:HA	1.69	0.74
13:e2:201:CYC:OB	8:m2:73:TYR:O	2.06	0.74
2:B3:41:ALA:HB2	2:B3:147:SER:HB3	1.70	0.74
13:M2:201:CYC:HAA1	10:N2:430:PHE:HZ	1.51	0.74
8:O2:73:TYR:O	13:U2:201:CYC:OB	2.05	0.73
13:T2:201:CYC:HB	13:T2:201:CYC:HMA3	1.53	0.73
8:g2:126:THR:HG23	13:g2:201:CYC:HBC3	1.70	0.73
9:v2:81:CYS:HA	13:v2:201:CYC:HHD	1.70	0.73
2:S4:41:ALA:HB2	2:S4:147:SER:HB3	1.70	0.73
8:n2:81:CYS:HA	13:n2:201:CYC:HHD	1.70	0.73
2:G6:41:ALA:HB2	2:G6:147:SER:HB3	1.71	0.73
2:W7:41:ALA:HB2	2:W7:147:SER:HB3	1.71	0.73
2:W3:41:ALA:HB2	2:W3:147:SER:HB3	1.70	0.73
1:A6:56:HIS:HB3	3:a6:85:ARG:HH11	1.54	0.73
13:N2:802:CYC:HB	13:N2:802:CYC:HMA1	1.53	0.73
13:Z4:301:CYC:HB	13:Z4:301:CYC:HMA3	1.52	0.73
1:A6:98:ASN:O	3:D6:109:ARG:NH1	2.21	0.73
2:F7:41:ALA:HB2	2:F7:147:SER:HB3	1.69	0.73
8:B2:83:ARG:HE	10:N2:572:ILE:HD11	1.52	0.73
3:a7:146:ARG:HD3	13:a7:202:CYC:HMC2	1.70	0.73
3:V1:109:ARG:HG2	5:Z1:14:PRO:HG3	1.70	0.73
13:B4:201:CYC:O2D	3:C4:58:ARG:NH1	2.22	0.73
2:R5:78:THR:HG23	2:R5:81:GLY:H	1.53	0.73
1:42:98:ASN:O	3:D4:109:ARG:NH1	2.22	0.72
13:n2:201:CYC:HAA1	10:o2:430:PHE:HZ	1.53	0.72
2:W3:3:LYS:H	2:W3:106:GLY:HA3	1.53	0.72
2:S5:41:ALA:HB2	2:S5:147:SER:HB3	1.71	0.72
2:B7:41:ALA:HB2	2:B7:147:SER:HB3	1.72	0.72
2:W7:3:LYS:H	2:W7:106:GLY:HA3	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:32:56:HIS:HB3	3:a3:85:ARG:HH11	1.55	0.72
8:g2:73:TYR:OH	9:h2:90:ARG:NH2	2.20	0.72
2:W6:31:ARG:NH2	2:W6:101:VAL:O	2.22	0.72
9:e2:35:ARG:NH1	9:e2:148:GLU:OE1	2.23	0.72
3:M6:63:GLU:HG3	3:M6:64:GLN:HG3	1.72	0.72
2:R6:156:ASP:O	2:R6:160:ASN:ND2	2.22	0.72
3:V6:109:ARG:HG2	5:Z6:14:PRO:HG3	1.71	0.72
2:H7:41:ALA:HB2	2:H7:147:SER:HB3	1.70	0.72
9:G2:1:MET:HG3	9:G2:5:SER:HB3	1.70	0.72
10:o2:284:LYS:HD3	10:o2:316:LYS:HB2	1.71	0.72
2:H3:41:ALA:HB2	2:H3:147:SER:HB3	1.69	0.72
3:C5:149:ILE:HG21	13:C5:202:CYC:HMC3	1.69	0.72
13:f2:201:CYC:OB	8:l2:73:TYR:O	2.07	0.72
10:o2:685:VAL:HG22	8:p2:58:LYS:HB3	1.69	0.72
2:R1:156:ASP:O	2:R1:160:ASN:ND2	2.23	0.71
13:t2:201:CYC:OB	8:y2:73:TYR:O	2.06	0.71
13:X6:201:CYC:HMA3	13:X6:201:CYC:HB	1.54	0.71
13:V1:201:CYC:O1A	5:Z1:180:ARG:NH2	2.23	0.71
13:h2:201:CYC:HMA3	13:h2:201:CYC:HB	1.55	0.71
10:o2:699:ARG:NH2	3:a6:108:ASP:O	2.23	0.71
8:y2:81:CYS:HA	13:y2:201:CYC:HHD	1.72	0.71
13:Z5:301:CYC:HMA3	13:Z5:301:CYC:HB	1.53	0.71
2:K1:101:VAL:HG21	3:L1:20:LEU:HD12	1.72	0.71
1:22:75:ILE:HB	1:22:79:ASP:HB2	1.70	0.71
8:l2:81:CYS:HA	13:l2:201:CYC:HHD	1.72	0.71
13:X5:201:CYC:HB	13:X5:201:CYC:HMA1	1.54	0.71
2:S6:41:ALA:HB2	2:S6:147:SER:HB3	1.70	0.71
8:L2:13:VAL:HG21	11:P2:165:ALA:HB1	1.72	0.71
3:M4:1:MET:HG3	4:Y4:218:ARG:HH21	1.55	0.71
2:H5:95:ILE:HG22	2:H5:108:ILE:HD13	1.72	0.71
8:T2:76:ARG:HB3	9:W2:110:VAL:HG23	1.73	0.71
8:d2:30:TYR:O	8:d2:37:ARG:NH2	2.24	0.71
2:N1:101:VAL:HG21	3:V1:20:LEU:HD12	1.73	0.71
10:N2:491:VAL:HG11	10:N2:671:LEU:HD22	1.73	0.71
9:h2:81:CYS:HA	13:h2:201:CYC:HHD	1.71	0.71
5:Z5:10:LEU:HA	5:Z5:205:PRO:HD2	1.72	0.71
13:c2:801:CYC:HB	10:o2:572:ILE:HG21	1.56	0.71
8:d2:3:ASP:HB3	8:d2:98:ALA:HB1	1.72	0.71
8:l2:126:THR:HG23	13:l2:201:CYC:HBC3	1.72	0.71
2:N3:1:MET:SD	3:V3:2:THR:N	2.64	0.71
2:G5:41:ALA:HB2	2:G5:147:SER:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P5:58:ARG:NH1	13:T5:202:CYC:O2D	2.23	0.71
2:K6:41:ALA:HB2	2:K6:147:SER:HB3	1.72	0.71
1:32:75:ILE:HB	1:32:79:ASP:HB2	1.71	0.70
3:O4:117:THR:HG23	5:Z4:165:LEU:HD22	1.71	0.70
3:P6:58:ARG:NH1	13:T6:202:CYC:O2D	2.24	0.70
8:F2:81:CYS:HA	13:F2:201:CYC:HHD	1.71	0.70
2:N4:18:ARG:NH1	2:U4:157:TYR:OH	2.24	0.70
2:R4:78:THR:HG23	2:R4:81:GLY:H	1.55	0.70
2:N5:113:LEU:HD21	2:N5:161:ALA:HB1	1.73	0.70
13:V5:201:CYC:O1A	5:Z5:180:ARG:NH2	2.24	0.70
2:F3:41:ALA:HB2	2:F3:147:SER:HB3	1.72	0.70
8:L2:80:CYS:HA	13:L2:201:CYC:HHD	1.73	0.70
13:p2:201:CYC:HMA3	13:p2:201:CYC:HB	1.56	0.70
3:P4:58:ARG:NH1	13:T4:202:CYC:O2D	2.23	0.70
3:E7:63:GLU:HG3	3:E7:64:GLN:HG3	1.74	0.70
3:M1:1:MET:HG3	4:Y1:218:ARG:HH21	1.56	0.70
2:U1:41:ALA:HB2	2:U1:147:SER:HB3	1.73	0.70
9:k2:91:LEU:HD12	9:k2:104:ILE:HA	1.73	0.70
3:D3:115:ARG:NH1	3:D3:173:ALA:O	2.25	0.70
2:K5:41:ALA:HB2	2:K5:147:SER:HB3	1.72	0.70
3:X5:89:ILE:HG21	13:X5:201:CYC:HAB1	1.74	0.70
2:U7:41:ALA:HB2	2:U7:147:SER:HB3	1.74	0.70
8:p2:73:TYR:O	13:v2:201:CYC:OB	2.10	0.70
9:I2:12:ASP:OD2	6:Z2:20:ARG:NH2	2.25	0.70
13:B3:201:CYC:O2D	3:C3:58:ARG:NH1	2.24	0.70
2:H1:95:ILE:HG22	2:H1:108:ILE:HD13	1.74	0.70
8:m2:81:CYS:HA	13:m2:201:CYC:HHD	1.74	0.70
10:o2:491:VAL:HG11	10:o2:671:LEU:HD22	1.73	0.70
3:C6:149:ILE:HG21	13:C6:202:CYC:HMC3	1.72	0.70
8:g2:77:ARG:HD3	13:g2:201:CYC:HAD2	1.74	0.69
2:G1:41:ALA:HB2	2:G1:147:SER:HB3	1.74	0.69
9:I2:15:ALA:HB2	6:Z2:19:GLN:HG2	1.74	0.69
8:c2:119:LEU:HD13	13:c2:801:CYC:HBD1	1.72	0.69
8:g2:73:TYR:O	13:h2:201:CYC:OB	2.10	0.69
2:G4:41:ALA:HB2	2:G4:147:SER:HB3	1.74	0.69
2:N5:101:VAL:HG21	3:V5:20:LEU:HD12	1.74	0.69
13:B1:201:CYC:O2D	3:C1:58:ARG:NH1	2.23	0.69
3:O1:85:ARG:NH1	13:Z1:301:CYC:O1A	2.23	0.69
8:u2:81:CYS:HA	13:z2:201:CYC:HHD	1.74	0.69
2:W3:5:PRO:HG2	2:W3:31:ARG:HD3	1.73	0.69
13:B5:201:CYC:O2D	3:C5:58:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W5:5:PRO:HG2	2:W5:31:ARG:HD3	1.74	0.69
1:A6:153:TYR:OH	5:Z6:273:GLN:OE1	2.11	0.69
3:Q6:75:TYR:OH	2:R6:94:ARG:NH2	2.25	0.69
2:W7:101:VAL:HG21	3:X7:20:LEU:HD12	1.75	0.69
1:52:186:ARG:HG2	1:52:192:PRO:HD3	1.74	0.69
8:C2:30:TYR:O	8:C2:37:ARG:NH2	2.25	0.69
13:G2:201:CYC:HMA3	13:G2:201:CYC:HB	1.57	0.69
3:P3:63:GLU:HG3	3:P3:64:GLN:HG3	1.75	0.69
2:I6:95:ILE:HG22	2:I6:108:ILE:HD13	1.73	0.69
9:D2:105:GLU:HA	9:D2:109:ILE:HB	1.75	0.69
9:R2:138:THR:HG23	9:R2:146:ALA:HB1	1.75	0.69
3:C3:16:ARG:NH1	3:C3:18:GLU:OE2	2.26	0.69
2:K3:156:ASP:O	2:K3:160:ASN:ND2	2.25	0.69
2:H4:9:ALA:HB1	2:H4:24:GLU:HG3	1.75	0.69
13:B7:201:CYC:O2D	3:C7:58:ARG:NH1	2.24	0.69
13:y2:201:CYC:HMA3	13:y2:201:CYC:HB	1.56	0.69
3:M4:63:GLU:HG3	3:M4:64:GLN:HG3	1.74	0.69
2:R5:156:ASP:O	2:R5:160:ASN:ND2	2.26	0.69
8:B2:74:THR:HB	8:B2:77:ARG:HG2	1.75	0.69
8:F2:73:TYR:OH	9:G2:90:ARG:NH2	2.26	0.69
13:o2:801:CYC:HB	13:o2:801:CYC:HMA1	1.57	0.69
8:u2:73:TYR:OH	9:x2:90:ARG:NH2	2.26	0.69
4:Y3:231:VAL:HG23	4:Y3:234:ARG:HB2	1.74	0.69
2:R4:156:ASP:O	2:R4:160:ASN:ND2	2.26	0.69
3:M5:1:MET:HG3	4:Y5:218:ARG:HH21	1.57	0.69
3:Q1:75:TYR:OH	2:R1:94:ARG:NH2	2.25	0.69
3:Q3:150:THR:O	13:Q3:202:CYC:NC	2.24	0.69
2:R3:41:ALA:HB2	2:R3:147:SER:HB3	1.75	0.69
13:V4:201:CYC:O1A	5:Z4:180:ARG:NH2	2.25	0.69
3:D7:115:ARG:NH1	3:D7:173:ALA:O	2.26	0.69
3:J7:16:ARG:HG3	3:J7:18:GLU:HG2	1.74	0.69
2:K1:41:ALA:HB2	2:K1:147:SER:HB3	1.75	0.69
1:A6:100:ASN:ND2	3:D6:109:ARG:O	2.25	0.69
3:V1:105:ILE:HD12	3:V1:109:ARG:HD3	1.75	0.68
2:I3:31:ARG:NH2	2:I3:101:VAL:O	2.26	0.68
13:N3:201:CYC:O2D	3:O3:58:ARG:NH1	2.26	0.68
2:H3:95:ILE:HG22	2:H3:108:ILE:HD13	1.74	0.68
13:N4:201:CYC:O2D	3:O4:58:ARG:NH1	2.25	0.68
2:R6:78:THR:HG23	2:R6:81:GLY:H	1.56	0.68
13:Z6:301:CYC:HMA3	13:Z6:301:CYC:HB	1.58	0.68
3:P7:63:GLU:HG3	3:P7:64:GLN:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J3:16:ARG:HG3	3:J3:18:GLU:HG2	1.74	0.68
2:N3:78:THR:HG23	2:N3:81:GLY:H	1.55	0.68
3:D4:115:ARG:NH1	3:D4:173:ALA:O	2.26	0.68
2:K4:41:ALA:HB2	2:K4:147:SER:HB3	1.73	0.68
1:32:232:ALA:HB1	9:r2:63:PRO:HB2	1.75	0.68
2:N6:41:ALA:HB2	2:N6:147:SER:HB3	1.75	0.68
9:s2:39:ILE:HG23	9:s2:141:LEU:HD21	1.75	0.68
3:P5:16:ARG:NH1	3:P5:18:GLU:OE2	2.27	0.68
2:K7:156:ASP:O	2:K7:160:ASN:ND2	2.27	0.68
4:Y7:231:VAL:HG23	4:Y7:234:ARG:HB2	1.76	0.68
1:A1:100:ASN:ND2	3:D1:109:ARG:O	2.26	0.68
9:e2:9:VAL:HG13	10:o2:513:THR:HA	1.75	0.68
3:Q4:150:THR:O	13:Q4:202:CYC:NC	2.27	0.68
2:S4:138:LYS:HB2	2:S4:155:ILE:HG21	1.75	0.68
13:N7:201:CYC:O2D	3:O7:58:ARG:NH1	2.26	0.68
2:R7:41:ALA:HB2	2:R7:147:SER:HB3	1.76	0.68
13:E2:201:CYC:OB	8:K2:73:TYR:O	2.11	0.68
2:N3:18:ARG:NH1	2:U3:157:TYR:OH	2.27	0.68
3:J5:9:VAL:HG11	3:J5:28:LEU:HD11	1.73	0.68
3:Q6:150:THR:O	13:Q6:202:CYC:NC	2.22	0.68
13:V6:201:CYC:O1A	5:Z6:180:ARG:NH2	2.26	0.68
2:G7:41:ALA:HB2	2:G7:147:SER:HB3	1.76	0.68
13:N1:201:CYC:O2D	3:O1:58:ARG:NH1	2.27	0.68
8:F2:126:THR:HG23	13:F2:201:CYC:HBC3	1.76	0.68
13:F5:202:CYC:NC	3:L5:150:THR:O	2.27	0.68
3:D7:63:GLU:HG3	3:D7:64:GLN:HG3	1.75	0.68
3:M7:63:GLU:HG3	3:M7:64:GLN:HG3	1.74	0.68
2:W7:31:ARG:NH2	2:W7:101:VAL:O	2.26	0.68
3:P1:115:ARG:NH1	3:P1:173:ALA:O	2.27	0.68
8:F2:73:TYR:O	13:G2:201:CYC:OB	2.11	0.68
8:V2:1:MET:HG3	8:V2:103:ILE:HB	1.76	0.68
3:M3:75:TYR:OH	2:U3:94:ARG:NH2	2.27	0.68
2:F1:78:THR:HG23	2:F1:81:GLY:H	1.58	0.68
13:F1:202:CYC:NC	3:L1:150:THR:O	2.27	0.68
8:B2:60:LEU:HB3	8:B2:72:MET:HE1	1.76	0.68
10:N2:689:LEU:HD21	8:O2:136:VAL:HG22	1.76	0.68
13:F4:202:CYC:NC	3:L4:150:THR:O	2.26	0.68
2:N4:113:LEU:HD21	2:N4:161:ALA:HB1	1.74	0.68
3:D6:115:ARG:NH1	3:D6:173:ALA:O	2.26	0.68
2:S1:41:ALA:HB2	2:S1:147:SER:HB3	1.76	0.67
1:22:56:HIS:HB3	3:a7:85:ARG:HH11	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W2:72:ALA:HA	9:W2:77:MET:HB2	1.75	0.67
2:G3:41:ALA:HB2	2:G3:147:SER:HB3	1.76	0.67
5:Z6:10:LEU:HA	5:Z6:205:PRO:HD2	1.75	0.67
3:C7:16:ARG:NH1	3:C7:18:GLU:OE2	2.27	0.67
2:K7:41:ALA:HB2	2:K7:147:SER:HB3	1.76	0.67
2:W1:5:PRO:HG2	2:W1:31:ARG:HD3	1.76	0.67
1:22:106:GLN:NE2	1:22:179:PRO:O	2.27	0.67
9:k2:105:GLU:HA	9:k2:109:ILE:HB	1.76	0.67
2:U4:78:THR:HG23	2:U4:81:GLY:H	1.59	0.67
2:F7:18:ARG:NH2	2:K7:157:TYR:OH	2.27	0.67
2:N7:78:THR:HG23	2:N7:81:GLY:H	1.59	0.67
3:D1:115:ARG:NH1	3:D1:173:ALA:O	2.27	0.67
8:c2:22:SER:HB2	8:c2:26:ARG:HH21	1.59	0.67
2:G1:103:GLY:O	2:H1:26:GLN:NE2	2.26	0.67
1:22:95:TYR:O	3:D7:109:ARG:NH1	2.28	0.67
11:P2:123:PRO:HB2	11:P2:126:PRO:HD2	1.75	0.67
13:S2:201:CYC:OB	8:X2:73:TYR:O	2.13	0.67
2:F6:78:THR:HG23	2:F6:81:GLY:H	1.57	0.67
9:f2:105:GLU:HA	9:f2:109:ILE:HB	1.76	0.67
2:H4:41:ALA:HB2	2:H4:147:SER:HB3	1.76	0.67
3:L4:76:THR:HB	3:L4:79:ARG:HG3	1.77	0.67
2:N7:1:MET:SD	3:V7:2:THR:N	2.67	0.67
3:P1:58:ARG:NH1	13:T1:202:CYC:O2D	2.27	0.67
3:M5:63:GLU:HG3	3:M5:64:GLN:HG3	1.76	0.67
2:U6:41:ALA:HB2	2:U6:147:SER:HB3	1.77	0.67
2:W1:138:LYS:HB2	2:W1:155:ILE:HG21	1.77	0.67
2:F3:95:ILE:HG22	2:F3:108:ILE:HD13	1.74	0.67
2:W3:31:ARG:NH2	2:W3:101:VAL:O	2.27	0.67
2:N4:101:VAL:HG21	3:V4:20:LEU:HD12	1.76	0.67
2:K6:156:ASP:O	2:K6:160:ASN:ND2	2.27	0.67
2:R1:78:THR:HG23	2:R1:81:GLY:H	1.59	0.67
3:V1:16:ARG:NH1	3:V1:18:GLU:OE2	2.28	0.67
2:N6:78:THR:HG23	2:N6:81:GLY:H	1.60	0.67
9:D2:9:VAL:HG13	10:N2:513:THR:HA	1.77	0.67
13:E2:201:CYC:HMA3	13:E2:201:CYC:HB	1.58	0.67
8:M2:106:GLU:HG3	8:M2:107:ARG:HG2	1.77	0.67
9:Q2:105:GLU:HA	9:Q2:109:ILE:HB	1.76	0.67
3:L5:16:ARG:NH1	3:L5:18:GLU:OE2	2.28	0.67
13:N6:201:CYC:O2D	3:O6:58:ARG:NH1	2.27	0.67
3:M7:75:TYR:OH	2:U7:94:ARG:NH2	2.27	0.67
8:A2:73:TYR:OH	9:J2:90:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L2:105:GLU:HG3	8:L2:106:ARG:HG2	1.76	0.67
11:P2:106:ASP:OD1	11:P2:159:HIS:NE2	2.25	0.67
9:s2:138:THR:HG23	9:s2:146:ALA:HB1	1.77	0.67
2:F4:78:THR:HG23	2:F4:81:GLY:H	1.60	0.67
3:D5:115:ARG:NH1	3:D5:173:ALA:O	2.28	0.67
2:N1:78:THR:HG23	2:N1:81:GLY:H	1.58	0.66
10:o2:312:GLU:HG2	10:o2:316:LYS:HE3	1.77	0.66
3:a5:68:ILE:HG22	3:a5:80:MET:HE1	1.77	0.66
3:Q6:115:ARG:NH1	3:Q6:173:ALA:O	2.28	0.66
2:H7:78:THR:HG23	2:H7:81:GLY:H	1.59	0.66
3:O7:146:ARG:HD2	13:T7:201:CYC:HMC2	1.77	0.66
1:32:3:LEU:HD21	3:D3:81:ALA:HB3	1.76	0.66
13:D2:201:CYC:OB	8:L2:72:TYR:O	2.13	0.66
9:H2:35:ARG:NH2	9:H2:144:GLU:OE1	2.28	0.66
2:G3:3:LYS:HD2	2:H3:16:GLN:HE22	1.58	0.66
2:W5:41:ALA:HB2	2:W5:147:SER:HB3	1.76	0.66
1:A6:95:TYR:O	3:D6:109:ARG:NH1	2.28	0.66
3:E6:146:ARG:HD2	3:E6:151:GLN:HG3	1.77	0.66
2:I7:31:ARG:NH2	2:I7:101:VAL:O	2.28	0.66
5:Z1:10:LEU:HA	5:Z1:205:PRO:HD2	1.77	0.66
1:32:95:TYR:O	3:D3:109:ARG:NH1	2.28	0.66
3:E3:76:THR:HG22	3:E3:79:ARG:H	1.60	0.66
3:V3:16:ARG:NH1	3:V3:18:GLU:OE2	2.29	0.66
3:E5:95:THR:HG22	2:H5:20:LEU:HD12	1.77	0.66
3:D6:57:ALA:HB2	3:D6:87:MET:HE1	1.78	0.66
9:J2:105:GLU:HA	9:J2:109:ILE:HB	1.76	0.66
11:q2:123:PRO:HB2	11:q2:126:PRO:HD2	1.76	0.66
2:F3:18:ARG:NH2	2:K3:157:TYR:OH	2.29	0.66
2:S3:67:THR:HG22	2:S3:76:ALA:H	1.60	0.66
5:Z4:10:LEU:HA	5:Z4:205:PRO:HD2	1.78	0.66
3:D5:26:ASP:OD2	3:D5:30:ARG:NH1	2.28	0.66
2:T5:78:THR:HG23	2:T5:81:GLY:H	1.60	0.66
3:E6:115:ARG:NH1	3:E6:173:ALA:O	2.29	0.66
2:F6:3:LYS:HZ2	2:K6:18:ARG:HE	1.43	0.66
2:R7:156:ASP:O	2:R7:160:ASN:ND2	2.24	0.66
2:K1:156:ASP:O	2:K1:160:ASN:ND2	2.29	0.66
9:r2:1:MET:HE2	8:y2:6:THR:HG23	1.78	0.66
3:V5:16:ARG:NH1	3:V5:18:GLU:OE2	2.28	0.66
10:N2:698:ARG:NH1	9:W2:138:THR:O	2.29	0.66
2:K3:41:ALA:HB2	2:K3:147:SER:HB3	1.78	0.66
3:O3:146:ARG:HD2	13:T3:201:CYC:HMC2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V7:16:ARG:NH1	3:V7:18:GLU:OE2	2.29	0.66
3:C1:16:ARG:NH1	3:C1:18:GLU:OE2	2.29	0.66
5:Z1:109:TYR:O	5:Z1:167:ARG:NH1	2.29	0.66
1:32:98:ASN:O	3:D3:109:ARG:NH1	2.28	0.66
13:O2:201:CYC:HMA1	13:O2:201:CYC:NB	2.10	0.66
10:o2:75:ILE:HD13	10:o2:204:ALA:HB2	1.78	0.66
2:N5:78:THR:HG23	2:N5:81:GLY:H	1.61	0.66
3:O5:117:THR:HG23	5:Z5:165:LEU:HD22	1.78	0.66
2:U5:78:THR:HG23	2:U5:81:GLY:H	1.60	0.66
3:a7:104:SER:HA	3:a7:107:ASP:OD2	1.95	0.66
2:B1:20:LEU:HD12	3:J1:95:THR:HG22	1.78	0.66
3:E1:115:ARG:NH1	3:E1:173:ALA:O	2.29	0.66
3:J1:9:VAL:HG11	3:J1:28:LEU:HD11	1.78	0.66
1:32:98:ASN:ND2	1:32:180:ARG:O	2.28	0.66
9:j2:1:MET:HE3	10:o2:540:GLN:HG3	1.78	0.66
2:B4:138:LYS:HB2	2:B4:155:ILE:HG21	1.77	0.66
2:S5:138:LYS:HB2	2:S5:155:ILE:HG21	1.78	0.66
1:A6:35:ASP:OD1	5:Z6:254:ARG:NH1	2.29	0.66
2:I6:41:ALA:HB2	2:I6:147:SER:HB3	1.78	0.66
2:U6:78:THR:HG23	2:U6:81:GLY:H	1.61	0.66
13:D2:201:CYC:HMA3	13:D2:201:CYC:HB	1.59	0.65
9:v2:29:PHE:O	9:v2:36:ARG:NH2	2.28	0.65
3:E3:63:GLU:HG3	3:E3:64:GLN:HG3	1.77	0.65
2:W4:31:ARG:NH2	2:W4:101:VAL:O	2.29	0.65
2:W5:138:LYS:HB2	2:W5:155:ILE:HG21	1.78	0.65
1:A1:153:TYR:OH	5:Z1:273:GLN:OE1	2.12	0.65
1:22:205:PRO:HB2	1:22:207:GLN:HG2	1.77	0.65
1:52:146:GLU:O	1:52:150:ASN:ND2	2.29	0.65
9:e2:12:ASP:OD2	8:g2:107:ARG:NH1	2.30	0.65
9:i2:19:SER:OG	9:i2:22:GLU:OE1	2.14	0.65
2:H5:9:ALA:HB1	2:H5:24:GLU:HG3	1.77	0.65
9:D2:12:ASP:OD2	8:F2:107:ARG:NH1	2.30	0.65
12:S2:105:GLU:HA	12:S2:109:LEU:HB3	1.77	0.65
8:n2:106:GLU:HG3	8:n2:107:ARG:HG2	1.78	0.65
8:w2:1:MET:HG3	8:w2:103:ILE:HB	1.77	0.65
3:D3:75:TYR:OH	2:H3:94:ARG:NH2	2.27	0.65
2:N3:94:ARG:NH2	3:O3:75:TYR:OH	2.26	0.65
2:U3:41:ALA:HB2	2:U3:147:SER:HB3	1.77	0.65
3:O4:85:ARG:NH1	13:Z4:301:CYC:O1A	2.29	0.65
2:G7:3:LYS:HD2	2:H7:16:GLN:HE22	1.61	0.65
2:G7:111:TYR:HA	3:L7:76:THR:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E2:2:SER:N	9:E2:5:SER:OG	2.29	0.65
10:N2:685:VAL:HG22	8:O2:58:LYS:HB3	1.78	0.65
2:F3:3:LYS:O	2:K3:23:THR:OG1	2.14	0.65
3:P6:63:GLU:HG3	3:P6:64:GLN:HG3	1.76	0.65
3:M7:114:LEU:HD13	13:M7:201:CYC:HMB1	1.79	0.65
1:42:95:TYR:O	3:D4:109:ARG:NH1	2.29	0.65
10:N2:405:ARG:NH1	10:N2:410:GLU:OE2	2.30	0.65
8:I2:64:ASP:OD1	8:I2:67:ARG:NH2	2.27	0.65
12:t2:113:ARG:HH12	12:t2:162:THR:HG22	1.61	0.65
2:W3:101:VAL:HG21	3:X3:20:LEU:HD12	1.78	0.65
2:W4:138:LYS:HB2	2:W4:155:ILE:HG21	1.78	0.65
2:U5:41:ALA:HB2	2:U5:147:SER:HB3	1.78	0.65
2:N6:101:VAL:HG21	3:V6:20:LEU:HD12	1.77	0.65
3:O1:117:THR:HG23	5:Z1:165:LEU:HD22	1.79	0.65
1:32:106:GLN:NE2	1:32:179:PRO:O	2.30	0.65
2:I4:41:ALA:HB2	2:I4:147:SER:HB3	1.79	0.65
2:N4:78:THR:HG23	2:N4:81:GLY:H	1.61	0.65
5:Z5:109:TYR:O	5:Z5:167:ARG:NH1	2.29	0.65
2:N1:41:ALA:HB2	2:N1:147:SER:HB3	1.79	0.65
1:52:153:TYR:OH	5:Z5:273:GLN:OE1	2.13	0.65
8:M2:126:THR:HG23	13:M2:201:CYC:HBC3	1.79	0.65
2:H3:78:THR:HG23	2:H3:81:GLY:H	1.61	0.65
2:B4:22:SER:O	2:B4:26:GLN:HG2	1.96	0.65
13:N5:201:CYC:O2D	3:O5:58:ARG:NH1	2.25	0.65
1:A6:26:GLU:OE2	3:a6:2:THR:N	2.29	0.65
1:42:37:TYR:HB3	1:42:41:GLN:HB2	1.77	0.65
10:N2:75:ILE:HD13	10:N2:204:ALA:HB2	1.79	0.65
3:J3:9:VAL:HG11	3:J3:28:LEU:HD11	1.79	0.65
3:E7:12:GLN:OE1	3:E7:16:ARG:NH1	2.28	0.65
2:W7:5:PRO:HG2	2:W7:31:ARG:HD3	1.79	0.65
1:A1:186:ARG:HG3	1:A1:191:PHE:HB2	1.79	0.65
1:32:146:GLU:O	1:32:150:ASN:ND2	2.29	0.65
9:H2:19:SER:OG	9:H2:22:GLU:OE1	2.15	0.65
9:s2:56:ASN:O	9:s2:60:GLN:NE2	2.29	0.65
2:B4:41:ALA:HB2	2:B4:147:SER:HB3	1.78	0.65
2:H6:78:THR:HG23	2:H6:81:GLY:H	1.60	0.65
3:E3:146:ARG:HD2	3:E3:151:GLN:HG3	1.79	0.65
2:R4:43:LYS:O	2:R4:47:ASN:ND2	2.30	0.65
3:V4:16:ARG:NH1	3:V4:18:GLU:OE2	2.30	0.65
2:B5:41:ALA:HB2	2:B5:147:SER:HB3	1.79	0.65
2:N5:18:ARG:NH1	2:U5:157:TYR:OH	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q1:150:THR:O	13:Q1:202:CYC:NC	2.26	0.64
9:D2:126:VAL:HG22	13:D2:201:CYC:H3C	1.80	0.64
10:N2:296:PHE:O	10:N2:298:ARG:NH1	2.28	0.64
8:a2:76:ARG:HB2	9:k2:110:VAL:HG23	1.78	0.64
5:Z3:142:THR:HG21	5:Z3:152:ARG:HD2	1.79	0.64
3:a3:115:ARG:NH1	3:a3:173:ALA:O	2.29	0.64
3:E4:12:GLN:OE1	3:E4:16:ARG:NH1	2.28	0.64
2:F5:95:ILE:HG22	2:F5:108:ILE:HD13	1.79	0.64
2:G6:111:TYR:HA	3:L6:76:THR:HG23	1.79	0.64
3:L1:109:ARG:O	5:Z1:254:ARG:NH2	2.31	0.64
1:22:98:ASN:O	3:D7:109:ARG:NH1	2.30	0.64
1:42:146:GLU:O	1:42:150:ASN:ND2	2.30	0.64
9:f2:1:MET:HB3	9:f2:5:SER:HB2	1.79	0.64
9:r2:105:GLU:HA	9:r2:109:ILE:HB	1.78	0.64
8:u2:126:THR:HG23	13:z2:201:CYC:HBC3	1.79	0.64
3:C4:16:ARG:NH1	3:C4:18:GLU:OE2	2.30	0.64
3:L4:63:GLU:HG3	3:L4:64:GLN:HG3	1.77	0.64
2:H5:78:THR:HG23	2:H5:81:GLY:H	1.60	0.64
2:B6:41:ALA:HB2	2:B6:147:SER:HB3	1.80	0.64
2:I7:78:THR:HG23	2:I7:81:GLY:H	1.61	0.64
2:F1:95:ILE:HG22	2:F1:108:ILE:HD13	1.80	0.64
2:S1:78:THR:HG23	2:S1:81:GLY:H	1.62	0.64
8:n2:13:ASP:OD1	10:o2:167:ARG:NH2	2.30	0.64
10:o2:689:LEU:HD11	8:p2:135:GLU:HB3	1.79	0.64
3:E3:12:GLN:OE1	3:E3:16:ARG:NH1	2.30	0.64
2:I1:31:ARG:NH2	2:I1:101:VAL:O	2.30	0.64
8:d2:51:ILE:HG12	8:d2:140:LEU:HD21	1.79	0.64
13:C3:201:CYC:HAA1	5:Z3:267:LEU:HD23	1.79	0.64
2:B5:22:SER:O	2:B5:26:GLN:HG2	1.97	0.64
3:J5:63:GLU:HG3	3:J5:64:GLN:HG3	1.79	0.64
1:52:37:TYR:HB3	1:52:41:GLN:HB2	1.78	0.64
9:j2:71:ASN:HB3	13:j2:201:CYC:HMD1	1.79	0.64
12:t2:90:ARG:NH1	8:y2:73:TYR:OH	2.31	0.64
3:V4:130:GLU:OE2	3:V4:134:LYS:NZ	2.31	0.64
2:B5:138:LYS:HB2	2:B5:155:ILE:HG21	1.78	0.64
3:E5:130:GLU:OE2	3:E5:134:LYS:NZ	2.31	0.64
4:Y5:231:VAL:HG23	4:Y5:234:ARG:HB2	1.80	0.64
13:B6:201:CYC:O2D	3:C6:58:ARG:NH1	2.22	0.64
3:C6:16:ARG:NH1	3:C6:18:GLU:OE2	2.31	0.64
2:H6:41:ALA:HB2	2:H6:147:SER:HB3	1.79	0.64
2:B7:108:ILE:HG22	2:B7:113:LEU:HG	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E7:146:ARG:HD2	3:E7:151:GLN:HG3	1.79	0.64
9:Q2:35:ARG:HH12	9:Q2:148:GLU:HG3	1.63	0.64
9:e2:105:GLU:HA	9:e2:109:ILE:HB	1.78	0.64
13:f2:201:CYC:HMA3	13:f2:201:CYC:HB	1.63	0.64
3:a4:152:GLY:HA3	13:a4:202:CYC:HMD2	1.80	0.64
2:W5:31:ARG:NH2	2:W5:101:VAL:O	2.31	0.64
1:A6:93:SER:HB3	1:A6:180:ARG:HD2	1.79	0.64
1:A6:146:GLU:O	1:A6:150:ASN:ND2	2.31	0.64
2:S6:67:THR:HG22	2:S6:76:ALA:H	1.63	0.64
3:V6:105:ILE:HD12	3:V6:109:ARG:HD3	1.79	0.64
3:X6:89:ILE:HG21	13:X6:201:CYC:HAB1	1.80	0.64
8:A2:94:TYR:OH	9:H2:16:ARG:O	2.16	0.64
2:H4:95:ILE:HG22	2:H4:108:ILE:HD13	1.80	0.64
3:P4:16:ARG:NH1	3:P4:18:GLU:OE2	2.31	0.64
3:C5:16:ARG:NH1	3:C5:18:GLU:OE2	2.30	0.64
2:W7:33:ARG:NH2	2:W7:34:GLN:OE1	2.31	0.64
1:A1:98:ASN:O	3:D1:109:ARG:NH1	2.31	0.64
13:F2:201:CYC:HMA3	13:F2:201:CYC:HB	1.62	0.64
2:I6:78:THR:HG23	2:I6:81:GLY:H	1.63	0.64
3:E7:75:TYR:OH	2:F7:94:ARG:NH2	2.29	0.64
2:N7:94:ARG:NH2	3:O7:75:TYR:OH	2.29	0.64
3:a7:103:ALA:O	3:a7:107:ASP:N	2.30	0.64
9:Q2:102:THR:HG23	9:Q2:103:PRO:HD3	1.79	0.64
3:L4:16:ARG:NH1	3:L4:18:GLU:OE2	2.30	0.64
2:U5:149:ASP:HB3	13:V5:202:CYC:HAB2	1.79	0.64
2:G6:3:LYS:HD2	2:H6:16:GLN:HE22	1.63	0.64
2:S7:67:THR:HG22	2:S7:76:ALA:H	1.63	0.64
3:Q1:115:ARG:NH1	3:Q1:173:ALA:O	2.30	0.63
1:22:37:TYR:HB3	1:22:41:GLN:HB2	1.80	0.63
13:32:302:CYC:H3C	3:E3:128:VAL:HG22	1.80	0.63
10:N2:195:ALA:HB3	13:N2:802:CYC:HBD2	1.80	0.63
13:r2:201:CYC:OB	8:w2:73:TYR:O	2.15	0.63
2:G3:111:TYR:HA	3:L3:76:THR:HG23	1.80	0.63
3:J4:9:VAL:HG11	3:J4:28:LEU:HD11	1.79	0.63
3:J4:63:GLU:HG3	3:J4:64:GLN:HG3	1.80	0.63
3:a6:152:GLY:O	13:a6:202:CYC:OC	2.17	0.63
2:B1:41:ALA:HB2	2:B1:147:SER:HB3	1.80	0.63
2:U1:78:THR:HG23	2:U1:81:GLY:H	1.63	0.63
8:A2:76:ARG:HB2	9:J2:110:VAL:HG23	1.78	0.63
6:Y2:10:LEU:HD13	6:Y2:48:GLY:HA3	1.80	0.63
6:Y2:34:ASP:OD1	6:Y2:34:ASP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:y2:83:ARG:NH1	13:y2:201:CYC:O1A	2.30	0.63
2:K4:156:ASP:O	2:K4:160:ASN:ND2	2.31	0.63
2:U4:149:ASP:HB3	13:V4:202:CYC:HAB2	1.81	0.63
2:N5:63:LYS:HD2	2:N5:132:GLU:HG3	1.79	0.63
2:N7:18:ARG:NH1	2:U7:157:TYR:OH	2.30	0.63
1:A1:35:ASP:OD1	5:Z1:254:ARG:NH1	2.28	0.63
9:i2:35:ARG:NH2	9:i2:144:GLU:OE1	2.32	0.63
8:n2:56:VAL:HG12	8:n2:61:LEU:HG	1.79	0.63
11:q2:135:ARG:NH1	11:q2:158:ASP:OD1	2.30	0.63
2:H4:78:THR:HG23	2:H4:81:GLY:H	1.62	0.63
3:O5:146:ARG:HH21	3:O5:151:GLN:HB3	1.62	0.63
3:D7:75:TYR:OH	2:H7:94:ARG:NH2	2.25	0.63
3:E7:84:LEU:HD13	2:F7:122:THR:HG21	1.79	0.63
9:r2:102:THR:HG23	9:r2:103:PRO:HD3	1.79	0.63
12:t2:105:GLU:OE2	6:z2:17:ARG:NH2	2.31	0.63
6:z2:5:ARG:NH1	6:z2:54:GLU:OE2	2.32	0.63
3:V3:130:GLU:OE2	3:V3:134:LYS:NZ	2.32	0.63
2:T4:78:THR:HG23	2:T4:81:GLY:H	1.64	0.63
13:X5:201:CYC:HMA1	13:X5:201:CYC:NB	2.13	0.63
3:P6:115:ARG:NH1	3:P6:173:ALA:O	2.32	0.63
2:S6:138:LYS:HB2	2:S6:155:ILE:HG21	1.80	0.63
2:W6:41:ALA:HB2	2:W6:147:SER:HB3	1.80	0.63
3:D7:115:ARG:NH2	3:D7:170:ALA:O	2.31	0.63
2:K7:33:ARG:NH2	2:K7:34:GLN:OE1	2.30	0.63
2:N7:103:GLY:O	2:U7:26:GLN:NE2	2.31	0.63
13:V7:201:CYC:O1A	5:Z7:180:ARG:NH2	2.29	0.63
1:A1:93:SER:HB3	1:A1:180:ARG:HD2	1.80	0.63
3:E1:130:GLU:OE2	3:E1:134:LYS:NZ	2.32	0.63
2:N1:1:MET:SD	3:V1:2:THR:N	2.71	0.63
9:G2:64:ASP:HB2	9:I2:64:ASP:HB2	1.81	0.63
3:D4:63:GLU:HG3	3:D4:64:GLN:HG3	1.81	0.63
2:U4:41:ALA:HB2	2:U4:147:SER:HB3	1.79	0.63
1:A6:37:TYR:HB3	1:A6:41:GLN:HB2	1.80	0.63
3:J6:9:VAL:HG11	3:J6:28:LEU:HD11	1.79	0.63
5:Z7:10:LEU:HA	5:Z7:205:PRO:HD2	1.80	0.63
8:T2:73:TYR:OH	9:W2:90:ARG:NH2	2.32	0.63
9:W2:81:CYS:HA	13:W2:201:CYC:HHD	1.79	0.63
2:R3:156:ASP:O	2:R3:160:ASN:ND2	2.25	0.63
2:S5:33:ARG:NH2	2:S5:34:GLN:OE1	2.32	0.63
5:Z5:49:ILE:HD12	5:Z5:53:GLU:HG3	1.80	0.63
1:A1:146:GLU:O	1:A1:150:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D1:26:ASP:OD2	3:D1:30:ARG:NH1	2.32	0.63
8:B2:65:ILE:HG13	8:B2:71:ASN:H	1.63	0.63
12:S2:102:GLU:HG3	12:S2:103:PRO:HD3	1.80	0.63
8:X2:83:ARG:NH1	13:X2:201:CYC:O1A	2.30	0.63
8:w2:81:CYS:HA	13:w2:201:CYC:HHD	1.81	0.63
2:B3:31:ARG:NH2	2:B3:101:VAL:O	2.31	0.63
2:N3:103:GLY:O	2:U3:26:GLN:NE2	2.30	0.63
3:Q4:115:ARG:NH1	3:Q4:173:ALA:O	2.32	0.63
2:W4:41:ALA:HB2	2:W4:147:SER:HB3	1.79	0.63
3:V6:16:ARG:NH1	3:V6:18:GLU:OE2	2.31	0.63
4:Y6:231:VAL:HG23	4:Y6:234:ARG:HB2	1.81	0.63
5:Z6:2:ALA:N	5:Z6:155:GLU:OE1	2.32	0.63
2:N1:31:ARG:NH2	2:N1:101:VAL:O	2.32	0.63
2:F3:74:ASN:ND2	2:F3:124:ASP:OD2	2.32	0.63
3:C4:63:GLU:HG3	3:C4:64:GLN:HG3	1.79	0.63
1:22:146:GLU:O	1:22:150:ASN:ND2	2.30	0.63
1:32:100:ASN:ND2	3:D3:109:ARG:O	2.32	0.63
1:42:53:ILE:HD11	1:42:81:ILE:HG23	1.80	0.63
9:D2:35:ARG:NH1	9:D2:148:GLU:OE1	2.31	0.63
8:d2:33:SER:OG	8:d2:37:ARG:NH1	2.31	0.63
3:E3:84:LEU:HD13	2:F3:122:THR:HG21	1.80	0.63
3:E5:12:GLN:OE1	3:E5:16:ARG:NH1	2.31	0.63
2:R6:41:ALA:HB2	2:R6:147:SER:HB3	1.79	0.63
2:F7:74:ASN:ND2	2:F7:124:ASP:OD2	2.32	0.63
3:X1:89:ILE:HG21	13:X1:201:CYC:HAB1	1.81	0.62
9:R2:39:ILE:HG23	9:R2:141:LEU:HD21	1.80	0.62
13:n2:201:CYC:HAA1	10:o2:430:PHE:CZ	2.33	0.62
9:r2:126:VAL:HG22	13:r2:201:CYC:H3C	1.80	0.62
13:s2:201:CYC:HB	13:s2:201:CYC:HMA1	1.64	0.62
2:R3:18:ARG:NH2	2:W3:105:THR:OG1	2.30	0.62
5:Z3:10:LEU:HA	5:Z3:205:PRO:HD2	1.80	0.62
3:a4:154:CYS:HB3	3:a4:157:ILE:HG22	1.81	0.62
2:N5:41:ALA:HB2	2:N5:147:SER:HB3	1.81	0.62
3:P5:115:ARG:NH1	3:P5:173:ALA:O	2.32	0.62
3:E7:76:THR:HG23	2:F7:111:TYR:HA	1.79	0.62
2:R1:33:ARG:NH2	2:R1:34:GLN:OE1	2.31	0.62
3:P3:4:ASP:N	3:P3:7:THR:OG1	2.31	0.62
2:S5:78:THR:HG23	2:S5:81:GLY:H	1.64	0.62
2:H6:95:ILE:HG22	2:H6:108:ILE:HD13	1.80	0.62
3:L6:16:ARG:NH1	3:L6:18:GLU:OE2	2.33	0.62
3:M6:1:MET:HG3	4:Y6:218:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E7:38:ARG:NH1	3:E7:98:VAL:O	2.30	0.62
3:P7:4:ASP:N	3:P7:7:THR:OG1	2.31	0.62
5:Z1:201:PRO:HD3	5:Z1:221:MET:HE1	1.81	0.62
3:a1:152:GLY:O	13:a1:202:CYC:OC	2.16	0.62
1:22:100:ASN:ND2	3:D7:109:ARG:O	2.33	0.62
13:c2:801:CYC:HBA1	10:o2:572:ILE:HG23	1.80	0.62
13:l2:201:CYC:HMA3	13:l2:201:CYC:HB	1.65	0.62
2:B4:85:CYS:HA	13:B4:201:CYC:HHD	1.80	0.62
3:V4:109:ARG:HG2	5:Z4:14:PRO:HG3	1.80	0.62
3:Q5:150:THR:O	13:Q5:202:CYC:NC	2.29	0.62
4:Y1:231:VAL:HG23	4:Y1:234:ARG:HB2	1.82	0.62
5:Z1:43:VAL:HA	5:Z1:102:HIS:HB3	1.81	0.62
1:42:72:ASN:OD1	1:42:74:GLN:NE2	2.33	0.62
1:42:153:TYR:OH	5:Z4:273:GLN:OE1	2.14	0.62
13:A2:201:CYC:HMA1	13:A2:201:CYC:NB	2.13	0.62
8:K2:137:THR:HG21	8:K2:149:MET:HG2	1.80	0.62
8:a2:94:TYR:OH	9:i2:16:ARG:O	2.16	0.62
11:q2:82:CYS:HA	13:q2:201:CYC:HHD	1.81	0.62
9:r2:19:SER:OG	9:r2:22:GLU:OE1	2.17	0.62
2:W3:25:LEU:HD22	3:X3:39:ILE:HG23	1.81	0.62
2:W3:33:ARG:NH2	2:W3:34:GLN:OE1	2.32	0.62
2:B6:31:ARG:NH2	2:B6:101:VAL:O	2.32	0.62
13:52:301:CYC:HC	13:52:301:CYC:HMD1	1.62	0.62
8:C2:33:SER:OG	8:C2:37:ARG:NH1	2.32	0.62
9:I2:104:ILE:HG21	9:I2:156:VAL:HG22	1.82	0.62
9:e2:13:ALA:HB2	10:o2:513:THR:HB	1.82	0.62
2:R3:117:ASP:OD1	2:R3:117:ASP:N	2.31	0.62
1:A1:106:GLN:NE2	1:A1:179:PRO:O	2.33	0.62
10:N2:520:GLN:OE1	6:Z2:20:ARG:NH1	2.33	0.62
8:p2:109:LEU:HD13	8:p2:159:GLY:HA3	1.81	0.62
2:R3:78:THR:HG23	2:R3:81:GLY:H	1.63	0.62
3:X3:85:ARG:HG3	5:Z3:122:GLU:HG2	1.81	0.62
3:O5:85:ARG:NH1	13:Z5:301:CYC:O1A	2.30	0.62
2:F6:95:ILE:HG22	2:F6:108:ILE:HD13	1.81	0.62
2:G1:3:LYS:HD2	2:H1:16:GLN:HE22	1.65	0.62
8:B2:1:MET:HG2	8:B2:103:ILE:HB	1.81	0.62
8:l2:137:THR:HG21	8:l2:149:MET:HG2	1.81	0.62
10:o2:195:ALA:HB3	13:o2:801:CYC:HBD2	1.81	0.62
8:u2:3:ASP:HA	8:u2:98:ALA:HB1	1.82	0.62
2:F4:18:ARG:NH2	2:K4:157:TYR:OH	2.33	0.62
2:F5:78:THR:HG23	2:F5:81:GLY:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K5:33:ARG:NH2	2:K5:34:GLN:OE1	2.32	0.62
3:V5:76:THR:HG23	2:W5:111:TYR:HA	1.81	0.62
3:V5:130:GLU:OE2	3:V5:134:LYS:NZ	2.32	0.62
2:B6:33:ARG:NH1	2:B6:146:ASP:OD2	2.31	0.62
2:I6:138:LYS:NZ	2:I6:156:ASP:OD1	2.28	0.62
3:X6:3:PHE:HA	3:X6:7:THR:HG23	1.81	0.62
13:G1:201:CYC:OB	3:L1:75:TYR:O	2.18	0.62
3:J1:63:GLU:HG3	3:J1:64:GLN:HG3	1.82	0.62
2:K1:33:ARG:NH2	2:K1:34:GLN:OE1	2.32	0.62
3:P1:93:TYR:OH	2:U1:14:ASP:OD1	2.18	0.62
1:22:98:ASN:ND2	1:22:180:ARG:O	2.32	0.62
9:D2:90:ARG:HH22	8:L2:72:TYR:HH	1.45	0.62
8:M2:56:VAL:HG12	8:M2:61:LEU:HG	1.81	0.62
8:d2:15:GLN:OE1	8:d2:17:LYS:NZ	2.31	0.62
3:D4:26:ASP:OD2	3:D4:30:ARG:NH1	2.33	0.62
9:Q2:16:ARG:O	8:X2:94:TYR:OH	2.18	0.62
12:S2:80:GLN:NE2	12:S2:84:ASP:OD1	2.32	0.62
13:X2:201:CYC:HMA3	13:X2:201:CYC:HB	1.64	0.62
9:i2:1:MET:HB3	9:i2:102:THR:HG21	1.82	0.62
3:E3:95:THR:HG22	2:H3:20:LEU:HD12	1.82	0.62
3:P3:115:ARG:NH1	3:P3:173:ALA:O	2.32	0.62
3:J6:16:ARG:HG3	3:J6:18:GLU:HG2	1.82	0.62
1:32:27:GLN:OE1	1:32:30:GLN:NE2	2.33	0.61
9:I2:1:MET:H2	9:I2:103:PRO:HG3	1.65	0.61
13:M2:201:CYC:HAA1	10:N2:430:PHE:CZ	2.33	0.61
8:p2:94:TYR:OH	9:s2:16:ARG:O	2.16	0.61
3:D3:146:ARG:HH21	3:D3:151:GLN:HB3	1.65	0.61
3:L3:93:TYR:OH	5:Z3:254:ARG:NH2	2.33	0.61
2:U3:50:ASP:O	2:U3:54:ASN:ND2	2.31	0.61
2:T5:95:ILE:HG13	2:T5:112:LEU:HD13	1.82	0.61
2:B6:109:ASP:HA	2:B6:113:LEU:HB2	1.81	0.61
3:P7:107:ASP:HA	3:P7:111:LEU:HB2	1.80	0.61
3:P7:115:ARG:NH1	3:P7:173:ALA:O	2.33	0.61
2:R7:18:ARG:NH2	2:W7:105:THR:OG1	2.33	0.61
2:H1:78:THR:HG23	2:H1:81:GLY:H	1.64	0.61
3:L1:16:ARG:NH1	3:L1:18:GLU:OE2	2.33	0.61
3:P1:107:ASP:HA	3:P1:111:LEU:HB2	1.82	0.61
2:W1:31:ARG:NH2	2:W1:101:VAL:O	2.33	0.61
1:32:172:THR:HA	3:a3:112:ASN:HD21	1.65	0.61
9:E2:2:SER:HA	9:E2:98:SER:HB3	1.82	0.61
3:M3:63:GLU:HG3	3:M3:64:GLN:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X3:201:CYC:HB	13:X3:201:CYC:CMA	2.13	0.61
2:S4:18:ARG:NH2	2:T4:105:THR:OG1	2.32	0.61
3:C5:89:ILE:HG12	3:C5:92:ARG:HH21	1.64	0.61
2:B6:2:SER:HB3	2:B6:106:GLY:HA3	1.80	0.61
2:S6:78:THR:HG23	2:S6:81:GLY:H	1.64	0.61
2:F7:3:LYS:O	2:K7:23:THR:OG1	2.15	0.61
2:H7:95:ILE:HG22	2:H7:108:ILE:HD13	1.82	0.61
3:Q7:150:THR:O	13:Q7:202:CYC:NC	2.19	0.61
1:32:226:ILE:HG21	9:s2:59:PHE:HD2	1.65	0.61
8:c2:8:VAL:HG21	8:c2:27:LEU:HD21	1.81	0.61
3:C7:78:ARG:NH1	13:C7:201:CYC:O1D	2.32	0.61
13:X7:201:CYC:HMA1	13:X7:201:CYC:NB	2.14	0.61
3:P1:109:ARG:NH1	2:U1:14:ASP:OD2	2.33	0.61
1:22:72:ASN:OD1	1:22:74:GLN:NE2	2.32	0.61
1:42:35:ASP:OD1	5:Z4:254:ARG:NH1	2.32	0.61
10:N2:340:HIS:O	8:O2:107:ARG:NH1	2.33	0.61
3:O4:17:GLY:HA3	3:X4:70:PRO:HB3	1.81	0.61
2:B5:85:CYS:HA	13:B5:201:CYC:HH2	1.82	0.61
3:Q5:75:TYR:OH	2:R5:94:ARG:NH2	2.29	0.61
2:W5:95:ILE:HG13	2:W5:112:LEU:HD13	1.81	0.61
13:M6:201:CYC:HAA1	5:Z6:64:ASN:HB2	1.82	0.61
10:N2:623:ARG:HA	10:N2:626:ILE:HG22	1.81	0.61
9:k2:81:CYS:HA	13:k2:201:CYC:HAC2	1.82	0.61
8:n2:90:ARG:NH2	10:o2:32:ASP:OD1	2.33	0.61
10:o2:699:ARG:NH2	3:a6:112:ASN:OD1	2.33	0.61
2:S4:78:THR:HG23	2:S4:81:GLY:H	1.66	0.61
3:J5:75:TYR:OH	2:K5:94:ARG:NH2	2.27	0.61
2:N5:103:GLY:O	2:U5:26:GLN:NE2	2.34	0.61
2:R5:43:LYS:O	2:R5:47:ASN:ND2	2.29	0.61
2:S6:3:LYS:HD3	2:T6:16:GLN:HE22	1.64	0.61
3:V6:76:THR:HG23	2:W6:111:TYR:HA	1.82	0.61
8:C2:3:ASP:H	8:C2:6:THR:HB	1.63	0.61
8:M2:85:LEU:HB3	8:M2:133:ILE:HD11	1.82	0.61
9:R2:29:PHE:HE1	9:R2:99:GLY:HA3	1.64	0.61
8:c2:30:TYR:O	8:c2:37:ARG:NH2	2.34	0.61
12:t2:16:ARG:O	8:u2:94:TYR:OH	2.19	0.61
12:t2:107:ILE:HA	8:y2:74:THR:HG23	1.83	0.61
3:J3:63:GLU:HG3	3:J3:64:GLN:HG3	1.81	0.61
2:K3:33:ARG:NH2	2:K3:34:GLN:OE1	2.34	0.61
5:Z6:43:VAL:HA	5:Z6:102:HIS:HB3	1.82	0.61
3:L7:93:TYR:OH	5:Z7:254:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O7:117:THR:HG23	5:Z7:165:LEU:HD22	1.81	0.61
1:42:193:LYS:NZ	1:42:194:ALA:O	2.33	0.61
12:S2:14:GLU:HG3	12:S2:16:ARG:HG2	1.82	0.61
8:g2:76:ARG:NH1	13:g2:201:CYC:O1D	2.33	0.61
3:M3:114:LEU:HD13	13:M3:201:CYC:HMB1	1.83	0.61
2:T5:74:ASN:ND2	2:T5:124:ASP:OD2	2.34	0.61
1:A6:106:GLN:NE2	1:A6:179:PRO:O	2.33	0.61
3:D6:149:ILE:HG21	13:D6:201:CYC:HMC3	1.82	0.61
2:F6:41:ALA:HB2	2:F6:147:SER:HB3	1.82	0.61
3:M6:75:TYR:OH	2:U6:94:ARG:NH2	2.26	0.61
2:U6:74:ASN:HA	13:U6:201:CYC:HBD2	1.82	0.61
3:J7:63:GLU:HG3	3:J7:64:GLN:HG3	1.82	0.61
3:Q7:75:TYR:OH	2:R7:94:ARG:NH2	2.33	0.61
2:S7:108:ILE:HG22	2:S7:113:LEU:HG	1.83	0.61
1:42:93:SER:HB3	1:42:180:ARG:HD2	1.81	0.61
9:Q2:71:ASN:ND2	9:Q2:120:GLY:O	2.31	0.61
3:P4:115:ARG:NH1	3:P4:173:ALA:O	2.32	0.61
2:N5:1:MET:SD	3:V5:2:THR:N	2.74	0.61
2:R5:113:LEU:HD11	2:R5:161:ALA:HB1	1.83	0.61
13:F6:202:CYC:NC	3:L6:150:THR:O	2.34	0.61
3:D7:77:ASN:ND2	2:H7:112:LEU:O	2.31	0.61
3:X7:78:ARG:NH2	13:X7:201:CYC:O1D	2.34	0.61
3:E1:44:ARG:NH1	3:E1:142:ILE:O	2.34	0.61
8:T2:3:ASP:HA	8:T2:98:ALA:HB1	1.81	0.61
10:o2:347:ARG:NH1	10:o2:350:GLU:OE1	2.32	0.61
9:s2:29:PHE:HE1	9:s2:99:GLY:HA3	1.66	0.61
9:s2:83:ARG:HH22	13:s2:201:CYC:HBA2	1.66	0.61
3:D3:115:ARG:NH2	3:D3:170:ALA:O	2.33	0.61
2:T3:78:THR:HG23	2:T3:81:GLY:H	1.66	0.61
2:N4:63:LYS:HD2	2:N4:132:GLU:HG3	1.82	0.61
2:S4:33:ARG:NH2	2:S4:34:GLN:OE1	2.34	0.61
13:C5:201:CYC:NC	13:C5:201:CYC:HMD1	2.16	0.61
2:B7:109:ASP:HA	2:B7:113:LEU:HB2	1.81	0.61
2:T7:78:THR:HG23	2:T7:81:GLY:H	1.66	0.61
1:A1:176:ILE:O	3:a1:117:THR:OG1	2.17	0.61
13:42:301:CYC:HMD1	13:42:301:CYC:HC	1.64	0.61
1:52:176:ILE:O	3:a5:117:THR:OG1	2.18	0.61
8:c2:87:TYR:OH	10:o2:568:THR:OG1	2.18	0.61
9:j2:77:MET:N	9:j2:77:MET:SD	2.74	0.61
2:R3:138:LYS:HB2	2:R3:155:ILE:HG21	1.83	0.61
4:Y3:256:THR:OG1	4:Y3:259:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R4:33:ARG:NH2	2:R4:34:GLN:OE1	2.34	0.61
2:F5:18:ARG:NH2	2:K5:157:TYR:OH	2.33	0.61
2:B6:138:LYS:HB2	2:B6:155:ILE:HG21	1.82	0.61
3:P6:16:ARG:NH1	3:P6:18:GLU:OE2	2.33	0.61
2:B7:31:ARG:NH2	2:B7:101:VAL:O	2.33	0.61
8:B2:90:ARG:HH12	9:J2:12:ASP:HA	1.66	0.60
8:d2:19:LEU:HD11	9:j2:97:VAL:HG11	1.83	0.60
9:h2:1:MET:O	9:h2:102:THR:OG1	2.14	0.60
2:I3:41:ALA:HB2	2:I3:147:SER:HB3	1.81	0.60
3:E4:63:GLU:HG3	3:E4:64:GLN:HG3	1.83	0.60
3:E5:115:ARG:NH1	3:E5:173:ALA:O	2.34	0.60
3:J5:44:ARG:NH1	3:J5:145:ASP:O	2.28	0.60
2:I6:31:ARG:NH2	2:I6:101:VAL:O	2.34	0.60
3:M7:76:THR:HG23	2:U7:111:TYR:HA	1.83	0.60
2:R7:78:THR:HG23	2:R7:81:GLY:H	1.65	0.60
3:X7:55:ASN:OD1	3:X7:58:ARG:NH2	2.34	0.60
8:L2:0:MET:N	10:N2:485:ASP:OD2	2.34	0.60
9:f2:8:ILE:HG21	8:m2:1:MET:HE3	1.83	0.60
9:j2:104:ILE:HG21	9:j2:156:VAL:HG22	1.83	0.60
3:X4:78:ARG:NH2	13:X4:201:CYC:O1D	2.35	0.60
3:E5:75:TYR:OH	2:F5:94:ARG:NH2	2.28	0.60
2:I5:94:ARG:NH2	3:a5:75:TYR:OH	2.27	0.60
3:P5:109:ARG:NH1	2:U5:14:ASP:OD2	2.34	0.60
3:V6:130:GLU:OE2	3:V6:134:LYS:NZ	2.33	0.60
5:Z1:55:LEU:HD21	5:Z1:79:SER:HB3	1.83	0.60
5:Z1:85:LYS:HG3	5:Z1:180:ARG:HD3	1.84	0.60
13:Z1:301:CYC:HB	13:Z1:301:CYC:CMA	2.14	0.60
3:a1:159:SER:HB3	10:N2:691:PRO:HG3	1.82	0.60
8:A2:57:ALA:HA	8:A2:61:LEU:HB2	1.83	0.60
8:T2:76:ARG:NH2	6:Y2:62:THR:O	2.34	0.60
9:s2:52:LYS:O	9:s2:56:ASN:ND2	2.33	0.60
3:X3:37:LYS:NZ	3:X3:150:THR:OG1	2.35	0.60
13:X3:201:CYC:HB	13:X3:201:CYC:HMA3	1.64	0.60
2:I4:94:ARG:NH2	3:a4:75:TYR:OH	2.29	0.60
3:E6:130:GLU:OE2	3:E6:134:LYS:NZ	2.35	0.60
13:C7:201:CYC:HAA1	5:Z7:267:LEU:HD23	1.83	0.60
13:M1:201:CYC:HAA1	5:Z1:64:ASN:HB2	1.84	0.60
3:P1:16:ARG:NH1	3:P1:18:GLU:OE2	2.34	0.60
3:V1:130:GLU:OE2	3:V1:134:LYS:NZ	2.33	0.60
9:H2:1:MET:HB3	9:H2:102:THR:HG21	1.83	0.60
3:D3:77:ASN:ND2	2:H3:112:LEU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I4:78:THR:HG23	2:I4:81:GLY:H	1.67	0.60
3:X4:4:ASP:OD1	3:X4:5:ALA:N	2.31	0.60
3:O6:85:ARG:NH1	13:Z6:301:CYC:O1A	2.33	0.60
3:D1:39:ILE:HG23	2:I1:25:LEU:HG	1.84	0.60
3:M1:4:ASP:H	3:M1:7:THR:HG1	1.47	0.60
2:S1:138:LYS:HB2	2:S1:155:ILE:HG21	1.83	0.60
8:O2:81:CYS:HA	13:O2:201:CYC:HHD	1.84	0.60
8:c2:3:ASP:OD1	8:c2:4:ALA:N	2.35	0.60
8:c2:73:TYR:O	13:j2:201:CYC:OB	2.18	0.60
10:o2:690:ARG:NH1	3:a6:166:ASP:OD2	2.35	0.60
10:o2:698:ARG:NH1	9:x2:138:THR:O	2.25	0.60
9:s2:126:VAL:HG22	13:s2:201:CYC:H3C	1.83	0.60
8:w2:94:TYR:OH	9:x2:16:ARG:O	2.18	0.60
3:E3:130:GLU:OE2	3:E3:134:LYS:NZ	2.34	0.60
3:E4:130:GLU:OE2	3:E4:134:LYS:NZ	2.35	0.60
3:E5:89:ILE:HG12	3:E5:92:ARG:HH21	1.67	0.60
2:N5:18:ARG:NH2	2:U5:105:THR:OG1	2.34	0.60
3:X6:4:ASP:HA	3:X6:100:THR:HB	1.84	0.60
3:J7:9:VAL:HG11	3:J7:28:LEU:HD11	1.83	0.60
2:R7:33:ARG:NH2	2:R7:34:GLN:OE1	2.35	0.60
3:X7:37:LYS:NZ	3:X7:150:THR:OG1	2.34	0.60
2:F1:33:ARG:NH2	2:F1:34:GLN:OE1	2.35	0.60
13:22:301:CYC:O2A	3:D7:78:ARG:NH2	2.35	0.60
10:N2:196:CYS:SG	10:N2:201:THR:OG1	2.58	0.60
9:Q2:1:MET:HE2	8:X2:6:THR:HG23	1.83	0.60
9:e2:16:ARG:O	8:g2:94:TYR:OH	2.17	0.60
8:m2:37:ARG:NH1	8:m2:96:MET:O	2.32	0.60
3:D3:149:ILE:HG21	13:D3:201:CYC:HMC3	1.83	0.60
13:M3:201:CYC:HAA1	5:Z3:64:ASN:HB2	1.84	0.60
2:U3:78:THR:OG1	2:U3:80:GLU:OE1	2.19	0.60
5:Z3:235:SER:HB3	5:Z3:264:TYR:HB3	1.83	0.60
4:Y4:225:GLN:HG2	4:Y4:245:THR:HG22	1.83	0.60
5:Z6:49:ILE:HD12	5:Z6:53:GLU:HG3	1.83	0.60
2:B1:138:LYS:HB2	2:B1:155:ILE:HG21	1.84	0.60
13:C1:201:CYC:NC	13:C1:201:CYC:HMD1	2.16	0.60
13:22:302:CYC:H3C	3:E7:128:VAL:HG22	1.83	0.60
8:A2:107:ARG:NH1	9:H2:12:ASP:OD2	2.35	0.60
10:N2:249:ARG:HB3	10:N2:254:GLN:HG3	1.82	0.60
8:a2:17:LYS:NZ	8:a2:18:TYR:O	2.35	0.60
8:c2:74:THR:HB	8:c2:77:ARG:HG3	1.83	0.60
10:o2:253:ASP:OD2	10:o2:369:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p2:2:GLN:OE1	8:p2:10:ASN:ND2	2.35	0.60
13:V3:201:CYC:O1A	5:Z3:180:ARG:NH2	2.31	0.60
3:Q4:75:TYR:OH	2:R4:94:ARG:NH2	2.33	0.60
2:B5:2:SER:HB3	2:B5:106:GLY:HA3	1.84	0.60
3:D6:26:ASP:OD2	3:D6:30:ARG:NH1	2.34	0.60
3:J6:75:TYR:OH	2:K6:94:ARG:NH2	2.28	0.60
2:G7:94:ARG:NH2	3:L7:75:TYR:OH	2.33	0.60
3:J1:75:TYR:O	13:K1:201:CYC:OB	2.20	0.60
1:32:72:ASN:OD1	1:32:74:GLN:NE2	2.34	0.60
9:G2:126:VAL:HG22	13:G2:201:CYC:H3C	1.84	0.60
9:I2:12:ASP:O	6:Z2:19:GLN:NE2	2.33	0.60
10:N2:294:GLN:HG2	10:N2:402:PRO:HB2	1.83	0.60
8:n2:85:LEU:HB3	8:n2:133:ILE:HD11	1.83	0.60
10:o2:461:GLU:HG3	10:o2:670:GLY:HA3	1.84	0.60
2:N4:94:ARG:NH2	3:O4:75:TYR:OH	2.28	0.60
2:B6:85:CYS:HA	13:B6:201:CYC:HHD	1.84	0.60
2:B7:33:ARG:NH1	2:B7:146:ASP:OD2	2.35	0.60
2:B7:138:LYS:HB2	2:B7:155:ILE:HG21	1.84	0.60
2:W7:25:LEU:HD22	3:X7:39:ILE:HG23	1.82	0.60
3:P1:63:GLU:HG3	3:P1:64:GLN:HG3	1.84	0.60
2:S1:33:ARG:NH2	2:S1:34:GLN:OE1	2.35	0.60
9:W2:35:ARG:HG2	9:W2:38:ARG:HH22	1.67	0.60
9:i2:29:PHE:O	9:i2:36:ARG:NH2	2.31	0.60
13:P3:202:CYC:HMD3	13:P3:202:CYC:HC	1.67	0.60
3:V7:130:GLU:OE2	3:V7:134:LYS:NZ	2.34	0.60
8:A2:90:ARG:NH1	8:A2:94:TYR:OH	2.35	0.60
8:L2:1:GLN:NE2	11:P2:167:GLN:OE1	2.35	0.60
8:c2:44:ILE:HG13	8:c2:149:MET:HE3	1.83	0.60
2:I4:85:CYS:HA	13:I4:201:CYC:HHD	1.82	0.60
3:O5:95:THR:HG22	2:S5:20:LEU:HD12	1.82	0.60
3:M6:76:THR:HG23	2:U6:111:TYR:HA	1.84	0.60
3:O6:100:THR:HG23	2:S6:10:VAL:HG21	1.84	0.60
2:W6:74:ASN:HA	13:W6:201:CYC:HBD2	1.84	0.60
2:B1:22:SER:O	2:B1:26:GLN:HG2	2.00	0.59
3:J1:16:ARG:HG3	3:J1:18:GLU:HG2	1.83	0.59
2:T1:78:THR:HG23	2:T1:81:GLY:H	1.67	0.59
2:W1:41:ALA:HB2	2:W1:147:SER:HB3	1.83	0.59
5:Z1:49:ILE:HD12	5:Z1:53:GLU:HG3	1.82	0.59
9:I2:50:ILE:HD11	9:I2:140:LEU:HD13	1.84	0.59
13:h2:201:CYC:HB	13:h2:201:CYC:CMA	2.14	0.59
2:N3:1:MET:N	3:V3:2:THR:OG1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W3:74:ASN:HA	13:W3:201:CYC:HBD2	1.84	0.59
3:V5:109:ARG:HG2	5:Z5:14:PRO:HG3	1.83	0.59
3:C6:63:GLU:HG3	3:C6:64:GLN:HG3	1.83	0.59
2:B7:94:ARG:NH2	3:C7:75:TYR:OH	2.32	0.59
3:X7:107:ASP:HA	3:X7:111:LEU:HB2	1.84	0.59
5:Z7:142:THR:HG21	5:Z7:152:ARG:HD2	1.84	0.59
2:N1:113:LEU:HD21	2:N1:161:ALA:HB1	1.84	0.59
3:X1:37:LYS:NZ	3:X1:150:THR:OG1	2.34	0.59
8:A2:75:THR:HG23	13:A2:202:CYC:HBB2	1.84	0.59
9:G2:113:ARG:NH2	9:G2:161:SER:OXT	2.35	0.59
8:M2:108:VAL:O	10:N2:426:TYR:OH	2.18	0.59
3:P3:107:ASP:HA	3:P3:111:LEU:HB2	1.83	0.59
2:B4:33:ARG:NH1	2:B4:146:ASP:OD2	2.35	0.59
5:Z4:49:ILE:HD12	5:Z4:53:GLU:HG3	1.84	0.59
2:F6:8:GLU:OE2	2:K6:16:GLN:NE2	2.35	0.59
2:F1:20:LEU:HD12	3:a1:95:THR:HG22	1.83	0.59
2:S1:31:ARG:NH2	2:S1:101:VAL:O	2.35	0.59
10:o2:453:TYR:CD2	10:o2:605:VAL:HG11	2.36	0.59
2:B3:109:ASP:HA	2:B3:113:LEU:HB2	1.84	0.59
2:F5:41:ALA:HB2	2:F5:147:SER:HB3	1.83	0.59
2:S5:94:ARG:NH2	3:X5:75:TYR:OH	2.32	0.59
13:Z5:301:CYC:HB	13:Z5:301:CYC:CMA	2.14	0.59
13:G6:201:CYC:OB	3:L6:75:TYR:O	2.20	0.59
2:W6:5:PRO:HG2	2:W6:31:ARG:HD3	1.84	0.59
3:O7:95:THR:HG22	2:S7:20:LEU:HD12	1.84	0.59
2:K1:25:LEU:HD22	3:L1:39:ILE:HG23	1.84	0.59
8:B2:74:THR:HG22	8:B2:76:ARG:H	1.68	0.59
9:I2:80:THR:HG23	9:I2:83:ARG:HH21	1.68	0.59
9:j2:39:ILE:HG13	9:j2:145:ASP:HB3	1.84	0.59
8:p2:81:CYS:HA	13:p2:201:CYC:HH2	1.85	0.59
3:C4:130:GLU:OE2	3:C4:134:LYS:NZ	2.36	0.59
13:Z4:301:CYC:HB	13:Z4:301:CYC:CMA	2.15	0.59
13:J6:201:CYC:HMA3	5:Z6:224:LEU:HD23	1.84	0.59
3:Q6:112:ASN:O	4:Y6:261:HIS:NE2	2.33	0.59
2:R6:43:LYS:O	2:R6:47:ASN:ND2	2.31	0.59
3:D7:96:TYR:OH	2:I7:18:ARG:O	2.20	0.59
3:E7:95:THR:HG22	2:H7:20:LEU:HD12	1.83	0.59
3:O7:1:MET:SD	2:S7:2:SER:N	2.76	0.59
3:P7:58:ARG:NH1	13:T7:202:CYC:O2D	2.31	0.59
2:S1:3:LYS:HD3	2:T1:16:GLN:HE22	1.67	0.59
1:42:238:ASP:HA	9:j2:52:LYS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E3:75:TYR:OH	2:F3:94:ARG:NH2	2.29	0.59
2:N3:9:ALA:HB1	2:N3:24:GLU:HG3	1.85	0.59
5:Z3:109:TYR:O	5:Z3:167:ARG:NH1	2.36	0.59
3:a3:130:GLU:OE2	3:a3:134:LYS:NZ	2.35	0.59
13:Z6:301:CYC:HB	13:Z6:301:CYC:CMA	2.15	0.59
2:F7:78:THR:HG23	2:F7:81:GLY:H	1.68	0.59
3:D1:44:ARG:NH1	3:D1:142:ILE:O	2.35	0.59
8:a2:107:ARG:NH1	9:i2:12:ASP:OD2	2.35	0.59
2:F4:74:ASN:ND2	2:F4:124:ASP:OD2	2.35	0.59
3:P4:109:ARG:NH1	2:U4:14:ASP:OD2	2.35	0.59
2:H5:41:ALA:HB2	2:H5:147:SER:HB3	1.85	0.59
3:L6:63:GLU:HG3	3:L6:64:GLN:HG3	1.85	0.59
3:C1:130:GLU:OE2	3:C1:134:LYS:NZ	2.36	0.59
3:O3:117:THR:HG23	5:Z3:165:LEU:HD22	1.84	0.59
3:X3:78:ARG:NH2	13:X3:201:CYC:O1D	2.35	0.59
2:N4:41:ALA:HB2	2:N4:147:SER:HB3	1.83	0.59
3:J5:16:ARG:HG3	3:J5:18:GLU:HG2	1.83	0.59
3:X5:3:PHE:HA	3:X5:7:THR:HG23	1.84	0.59
3:O6:117:THR:HG23	5:Z6:165:LEU:HD22	1.85	0.59
2:S6:33:ARG:NH2	2:S6:34:GLN:OE1	2.36	0.59
3:L7:34:GLU:HG3	3:L7:37:LYS:HD2	1.84	0.59
4:Y7:225:GLN:HG2	4:Y7:245:THR:HG22	1.85	0.59
5:Z7:41:ARG:NH2	5:Z7:175:TYR:O	2.36	0.59
5:Z1:138:GLU:OE2	5:Z1:152:ARG:NH2	2.35	0.59
9:H2:81:CYS:HA	13:H2:201:CYC:HAC2	1.82	0.59
12:S2:64:ASP:OD1	12:S2:64:ASP:N	2.32	0.59
3:L4:34:GLU:HG3	3:L4:37:LYS:HD2	1.83	0.59
3:Q5:128:VAL:HG22	13:Q5:201:CYC:H3C	1.82	0.59
2:W5:33:ARG:NH2	2:W5:34:GLN:OE1	2.35	0.59
4:Y5:252:LYS:HZ1	5:Z5:70:ARG:HH22	1.50	0.59
13:C6:201:CYC:NC	13:C6:201:CYC:HMD1	2.18	0.59
2:I6:85:CYS:HA	13:I6:201:CYC:HH2	1.84	0.59
3:P6:109:ARG:NH1	2:U6:14:ASP:OD2	2.36	0.59
2:R6:33:ARG:NH2	2:R6:34:GLN:OE1	2.36	0.59
5:Z7:49:ILE:HD12	5:Z7:53:GLU:HG3	1.84	0.59
2:H1:63:LYS:HG2	2:H1:132:GLU:HG3	1.85	0.59
3:Q1:112:ASN:O	4:Y1:261:HIS:NE2	2.33	0.59
10:N2:681:ALA:HB3	10:N2:686:LYS:HE3	1.85	0.59
9:R2:121:THR:OG1	13:R2:201:CYC:NC	2.36	0.59
9:U2:29:PHE:O	9:U2:36:ARG:NH2	2.36	0.59
3:P3:58:ARG:NH1	13:T3:202:CYC:O2D	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P4:107:ASP:HA	3:P4:111:LEU:HB2	1.85	0.59
2:F5:20:LEU:HD12	3:a5:95:THR:HG22	1.85	0.59
2:N6:31:ARG:NH2	2:N6:101:VAL:O	2.36	0.59
3:O6:95:THR:HG22	2:S6:20:LEU:HD12	1.84	0.59
2:R6:5:PRO:HG3	2:W6:23:THR:HA	1.84	0.59
2:S6:31:ARG:NH2	2:S6:101:VAL:O	2.36	0.59
2:S6:78:THR:OG1	2:S6:80:GLU:OE1	2.21	0.59
1:32:37:TYR:HB3	1:32:41:GLN:HB2	1.85	0.59
8:F2:56:VAL:HG12	8:F2:61:LEU:HG	1.83	0.59
8:g2:58:LYS:NZ	8:g2:135:GLU:OE1	2.34	0.59
8:n2:108:VAL:O	10:o2:426:TYR:OH	2.19	0.59
10:o2:311:LEU:HD11	10:o2:328:ARG:HD2	1.85	0.59
10:o2:509:GLY:HA3	10:o2:664:ARG:HB3	1.84	0.59
9:r2:16:ARG:O	8:y2:94:TYR:OH	2.19	0.59
5:Z3:74:ARG:NH2	5:Z3:135:ASP:OD1	2.36	0.59
3:J4:75:TYR:OH	2:K4:94:ARG:NH2	2.32	0.59
3:P4:128:VAL:HG22	13:P4:201:CYC:H3C	1.84	0.59
2:B5:33:ARG:NH1	2:B5:146:ASP:OD2	2.36	0.59
3:C7:63:GLU:HG3	3:C7:64:GLN:HG3	1.85	0.59
3:a7:130:GLU:OE2	3:a7:134:LYS:NZ	2.36	0.59
1:A1:167:ARG:NH1	13:A1:302:CYC:O2D	2.35	0.58
4:Y1:228:GLN:HG2	4:Y1:266:ARG:HG2	1.86	0.58
13:D2:201:CYC:HB	13:D2:201:CYC:CMA	2.15	0.58
9:h2:16:ARG:O	8:l2:94:TYR:OH	2.21	0.58
9:r2:18:LEU:HD12	8:y2:97:LEU:HD13	1.85	0.58
8:w2:107:ARG:NH1	9:x2:12:ASP:OD2	2.36	0.58
2:F3:20:LEU:HD12	3:a3:95:THR:HG22	1.83	0.58
3:L3:34:GLU:HG3	3:L3:37:LYS:HD2	1.85	0.58
3:X3:55:ASN:OD1	3:X3:58:ARG:NH2	2.36	0.58
3:E4:75:TYR:OH	2:F4:94:ARG:NH2	2.29	0.58
3:E4:95:THR:HG22	2:H4:20:LEU:HD12	1.84	0.58
2:K4:33:ARG:NH2	2:K4:34:GLN:OE1	2.36	0.58
3:E5:84:LEU:HD13	2:F5:122:THR:HG21	1.85	0.58
2:R5:33:ARG:NH2	2:R5:34:GLN:OE1	2.36	0.58
5:Z6:55:LEU:HD21	5:Z6:79:SER:HB3	1.85	0.58
2:F7:10:VAL:HG21	3:a7:100:THR:HG23	1.85	0.58
2:F7:95:ILE:HG22	2:F7:108:ILE:HD13	1.84	0.58
3:L7:16:ARG:NH1	3:L7:18:GLU:OE2	2.36	0.58
2:S7:78:THR:OG1	2:S7:80:GLU:OE1	2.21	0.58
5:Z7:85:LYS:HG3	5:Z7:180:ARG:HD3	1.85	0.58
2:F1:41:ALA:HB2	2:F1:147:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V1:201:CYC:NC	13:V1:201:CYC:HMD1	2.17	0.58
13:B2:202:CYC:HBC2	9:I2:126:VAL:HG22	1.85	0.58
8:M2:46:ALA:HB1	9:Q2:154:ASP:HB3	1.85	0.58
13:N2:801:CYC:NC	13:N2:801:CYC:HMD1	2.18	0.58
9:Q2:22:GLU:HG3	9:Q2:25:ARG:HH21	1.68	0.58
9:r2:35:ARG:HG3	9:r2:38:ARG:HH22	1.68	0.58
2:I5:31:ARG:NH2	2:I5:101:VAL:O	2.36	0.58
3:E6:75:TYR:OH	2:F6:94:ARG:NH2	2.27	0.58
2:G6:31:ARG:NH2	2:G6:101:VAL:O	2.36	0.58
3:V7:152:GLY:HA3	13:V7:202:CYC:HMD2	1.85	0.58
2:H1:41:ALA:HB2	2:H1:147:SER:HB3	1.86	0.58
1:32:229:ARG:NH2	3:D4:17:GLY:O	2.36	0.58
8:O2:94:TYR:OH	9:R2:16:ARG:O	2.19	0.58
3:L3:63:GLU:HG3	3:L3:64:GLN:HG3	1.85	0.58
3:M3:76:THR:HG23	2:U3:111:TYR:HA	1.85	0.58
2:N3:33:ARG:NH2	2:N3:34:GLN:OE1	2.35	0.58
2:R3:26:GLN:NE2	2:W3:103:GLY:O	2.36	0.58
3:O5:1:MET:SD	3:O5:1:MET:N	2.74	0.58
2:W5:74:ASN:HA	13:W5:201:CYC:HBD2	1.86	0.58
1:A6:78:ARG:NH1	1:A6:143:ASN:OD1	2.36	0.58
2:S1:94:ARG:NH2	3:X1:75:TYR:OH	2.26	0.58
2:T1:74:ASN:ND2	2:T1:124:ASP:OD2	2.37	0.58
3:V1:76:THR:HG22	3:V1:78:ARG:H	1.67	0.58
1:22:41:GLN:HG2	3:L7:1:MET:HA	1.86	0.58
9:D2:14:GLU:OE1	9:D2:16:ARG:NE	2.30	0.58
9:W2:105:GLU:HA	9:W2:109:ILE:HB	1.85	0.58
9:h2:47:ARG:NH2	9:h2:86:ASP:OD2	2.37	0.58
9:h2:113:ARG:NH2	9:h2:161:SER:OXT	2.36	0.58
8:u2:62:TYR:OH	13:x2:201:CYC:O1D	2.20	0.58
2:B3:138:LYS:HB2	2:B3:155:ILE:HG21	1.86	0.58
3:O4:146:ARG:HD2	13:T4:201:CYC:HMC2	1.84	0.58
2:F5:33:ARG:NH2	2:F5:34:GLN:OE1	2.36	0.58
1:A6:72:ASN:OD1	1:A6:74:GLN:NE2	2.37	0.58
3:E7:130:GLU:OE2	3:E7:134:LYS:NZ	2.36	0.58
3:X7:4:ASP:OD1	3:X7:5:ALA:N	2.34	0.58
2:B1:2:SER:HB3	2:B1:106:GLY:HA3	1.84	0.58
3:E1:84:LEU:HD13	2:F1:122:THR:HG21	1.84	0.58
13:J1:201:CYC:HMA3	5:Z1:224:LEU:HD23	1.85	0.58
8:B2:58:LYS:NZ	8:B2:135:GLU:OE1	2.31	0.58
9:E2:1:MET:O	9:E2:102:THR:OG1	2.15	0.58
3:D3:63:GLU:HG3	3:D3:64:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D3:96:TYR:OH	2:I3:18:ARG:O	2.20	0.58
2:W4:33:ARG:NH2	2:W4:34:GLN:OE1	2.36	0.58
3:E6:63:GLU:HG3	3:E6:64:GLN:HG3	1.84	0.58
3:X6:37:LYS:NZ	3:X6:150:THR:OG1	2.35	0.58
3:V7:121:LEU:HD13	13:V7:201:CYC:HBD1	1.84	0.58
13:A2:201:CYC:O2D	6:Z2:2:ARG:NH1	2.36	0.58
9:I2:47:ARG:NH2	9:I2:86:ASP:OD2	2.33	0.58
11:P2:135:ARG:NH1	11:P2:158:ASP:OD1	2.32	0.58
8:g2:110:ASN:ND2	10:o2:461:GLU:O	2.36	0.58
11:q2:106:ASP:OD1	11:q2:159:HIS:NE2	2.31	0.58
9:r2:35:ARG:HH12	9:r2:148:GLU:HG3	1.68	0.58
3:O3:83:CYS:HA	13:Z3:301:CYC:HAC2	1.86	0.58
3:X3:4:ASP:OD1	3:X3:5:ALA:N	2.35	0.58
3:V4:76:THR:HG23	2:W4:111:TYR:HA	1.85	0.58
2:U6:74:ASN:ND2	2:U6:124:ASP:OD2	2.36	0.58
2:G7:8:GLU:HG3	2:H7:23:THR:HG21	1.86	0.58
3:C1:154:CYS:SG	13:C1:202:CYC:OC	2.61	0.58
9:D2:113:ARG:NH2	9:D2:161:SER:OXT	2.36	0.58
8:O2:3:ASP:HA	8:O2:98:ALA:HB1	1.86	0.58
9:h2:36:ARG:NE	9:h2:148:GLU:OE2	2.37	0.58
10:o2:294:GLN:HG2	10:o2:402:PRO:HB2	1.84	0.58
8:u2:60:LEU:O	8:u2:63:SER:OG	2.21	0.58
2:K4:95:ILE:HG13	2:K4:112:LEU:HD13	1.86	0.58
2:N5:94:ARG:NH2	3:O5:75:TYR:OH	2.29	0.58
5:Z5:74:ARG:NH2	5:Z5:135:ASP:OD1	2.37	0.58
3:D7:26:ASP:OD2	3:D7:30:ARG:NH1	2.36	0.58
1:A1:75:ILE:HB	1:A1:79:ASP:HB2	1.85	0.58
13:A1:301:CYC:NC	13:A1:301:CYC:HMD1	2.19	0.58
3:X1:16:ARG:NE	3:X1:18:GLU:OE2	2.37	0.58
1:52:35:ASP:OD1	5:Z5:254:ARG:NH1	2.36	0.58
2:G3:9:ALA:HB1	2:G3:24:GLU:HG3	1.86	0.58
2:F4:41:ALA:HB2	2:F4:147:SER:HB3	1.85	0.58
3:C5:68:ILE:HG22	3:C5:80:MET:HE1	1.85	0.58
2:F5:3:LYS:HZ2	2:K5:18:ARG:HE	1.52	0.58
3:D6:39:ILE:HG23	2:I6:25:LEU:HG	1.84	0.58
13:F7:202:CYC:NC	3:L7:150:THR:O	2.36	0.58
2:N7:1:MET:N	3:V7:2:THR:OG1	2.36	0.58
2:W7:74:ASN:HA	13:W7:201:CYC:HBD2	1.86	0.58
2:G1:8:GLU:HG3	2:H1:23:THR:HG21	1.84	0.58
13:32:301:CYC:O2A	3:D3:78:ARG:NH2	2.37	0.58
10:N2:42:GLU:OE1	9:Q2:25:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k2:56:ASN:ND2	9:k2:60:GLN:OE1	2.36	0.58
2:G3:8:GLU:HG3	2:H3:23:THR:HG21	1.86	0.58
3:M3:78:ARG:NH1	13:M3:201:CYC:O1D	2.36	0.58
4:Y3:218:ARG:NH1	4:Y3:220:GLN:OE1	2.37	0.58
4:Y4:231:VAL:HA	4:Y4:234:ARG:NH2	2.19	0.58
3:D5:63:GLU:HG3	3:D5:64:GLN:HG3	1.85	0.58
2:S6:18:ARG:NH2	2:T6:105:THR:OG1	2.36	0.58
2:S6:94:ARG:NH2	3:X6:75:TYR:OH	2.25	0.58
3:X6:4:ASP:OD1	3:X6:5:ALA:N	2.34	0.58
3:E1:95:THR:HG22	2:H1:20:LEU:HD12	1.84	0.58
2:I1:85:CYS:HA	13:I1:201:CYC:HHD	1.85	0.58
2:K1:31:ARG:NH2	2:K1:101:VAL:O	2.37	0.58
8:B2:3:ASP:OD1	8:B2:4:ALA:N	2.37	0.58
8:n2:46:ALA:HB1	9:r2:154:ASP:HB3	1.86	0.58
2:K4:20:LEU:HD12	3:L4:95:THR:HG22	1.85	0.58
3:X4:4:ASP:HA	3:X4:100:THR:HB	1.86	0.58
5:Z4:109:TYR:O	5:Z4:167:ARG:NH1	2.36	0.58
3:X5:4:ASP:OD1	3:X5:5:ALA:N	2.33	0.58
2:F6:31:ARG:NH2	2:F6:101:VAL:O	2.36	0.58
3:J6:63:GLU:HG3	3:J6:64:GLN:HG3	1.86	0.58
2:U6:121:LYS:NZ	2:W6:163:SER:OXT	2.33	0.58
2:I7:16:GLN:OE1	2:I7:18:ARG:NE	2.37	0.58
2:U7:78:THR:OG1	2:U7:80:GLU:OE1	2.21	0.58
3:X7:3:PHE:HA	3:X7:7:THR:HG23	1.85	0.58
3:P1:128:VAL:HG22	13:P1:202:CYC:H3C	1.84	0.57
2:T1:78:THR:OG1	2:T1:80:GLU:OE1	2.22	0.57
1:22:53:ILE:HD11	1:22:81:ILE:HG23	1.86	0.57
1:32:17:VAL:O	1:32:161:ARG:NH1	2.36	0.57
9:Q2:47:ARG:NH1	9:Q2:86:ASP:OD2	2.37	0.57
8:m2:1:MET:N	10:o2:485:ASP:OD2	2.35	0.57
3:V3:121:LEU:HD13	13:V3:201:CYC:HBD1	1.86	0.57
2:F4:33:ARG:NH2	2:F4:34:GLN:OE1	2.37	0.57
2:I4:121:LYS:NZ	2:K4:117:ASP:OD1	2.36	0.57
2:W4:74:ASN:HA	13:W4:201:CYC:HBD2	1.86	0.57
3:E5:12:GLN:NE2	3:E5:24:GLN:OE1	2.32	0.57
5:Z5:262:VAL:HG11	5:Z5:270:THR:HG21	1.85	0.57
3:E7:40:ASP:HB3	13:E7:201:CYC:HBC3	1.84	0.57
2:G1:31:ARG:NH2	2:G1:101:VAL:O	2.37	0.57
6:02:2:ARG:NH1	13:a2:201:CYC:O2D	2.37	0.57
1:22:216:PRO:HB2	1:52:204:PHE:CZ	2.39	0.57
8:V2:106:GLU:OE1	6:Y2:58:GLY:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W2:126:VAL:HG22	13:W2:201:CYC:H3C	1.86	0.57
8:w2:126:THR:HG23	13:w2:201:CYC:HBC3	1.86	0.57
3:V3:89:ILE:HD13	13:V3:201:CYC:HBB3	1.85	0.57
3:J4:4:ASP:N	3:J4:7:THR:OG1	2.37	0.57
2:R4:41:ALA:HB2	2:R4:147:SER:HB3	1.85	0.57
2:I5:85:CYS:HA	13:I5:201:CYC:HHD	1.86	0.57
1:A6:146:GLU:OE2	1:A6:160:ARG:NH2	2.37	0.57
2:G6:8:GLU:HG3	2:H6:23:THR:HG21	1.86	0.57
2:T6:42:ALA:HB1	2:T6:97:THR:HG23	1.86	0.57
2:W1:74:ASN:HA	13:W1:201:CYC:HBD2	1.86	0.57
5:Z1:102:HIS:NE2	5:Z1:179:ASP:OD2	2.32	0.57
8:c2:118:SER:HA	10:o2:531:LYS:HD3	1.85	0.57
9:k2:1:MET:HE2	9:k2:5:SER:HB2	1.86	0.57
11:q2:168:ASP:N	11:q2:168:ASP:OD1	2.36	0.57
8:u2:76:ARG:NH2	6:z2:62:THR:O	2.36	0.57
2:I5:41:ALA:HB2	2:I5:147:SER:HB3	1.86	0.57
4:Y5:225:GLN:HG2	4:Y5:245:THR:HG22	1.84	0.57
1:A6:54:PHE:HE1	1:A6:90:PHE:HB2	1.70	0.57
2:B6:22:SER:O	2:B6:26:GLN:HG2	2.05	0.57
3:J6:68:ILE:HG22	3:J6:80:MET:HE1	1.86	0.57
2:T6:74:ASN:ND2	2:T6:124:ASP:OD2	2.37	0.57
2:R7:138:LYS:HB2	2:R7:155:ILE:HG21	1.87	0.57
2:U7:50:ASP:O	2:U7:54:ASN:ND2	2.31	0.57
3:X7:41:THR:HG23	3:X7:143:VAL:HG11	1.86	0.57
5:Z7:235:SER:HB3	5:Z7:264:TYR:HB3	1.85	0.57
1:A1:72:ASN:OD1	1:A1:74:GLN:NE2	2.37	0.57
3:O1:20:LEU:HD22	2:S1:101:VAL:HG21	1.86	0.57
5:Z1:142:THR:OG1	5:Z1:152:ARG:NH1	2.37	0.57
13:a1:201:CYC:HB	13:a1:201:CYC:CMA	2.18	0.57
1:32:219:TYR:OH	9:s2:86:ASP:OD2	2.21	0.57
13:G2:201:CYC:HB	13:G2:201:CYC:CMA	2.17	0.57
8:m2:2:GLN:NE2	11:q2:167:GLN:OE1	2.37	0.57
2:I4:31:ARG:NH2	2:I4:101:VAL:O	2.38	0.57
3:O4:95:THR:HG22	2:S4:20:LEU:HD12	1.86	0.57
3:O4:100:THR:HG23	2:S4:10:VAL:HG21	1.87	0.57
3:D5:149:ILE:HD13	13:D5:201:CYC:H3C	1.87	0.57
2:K5:85:CYS:HA	13:K5:201:CYC:HHD	1.86	0.57
3:Q5:115:ARG:NH1	3:Q5:173:ALA:O	2.36	0.57
2:F6:20:LEU:HD12	3:a6:95:THR:HG22	1.85	0.57
3:J6:4:ASP:N	3:J6:7:THR:OG1	2.36	0.57
4:Y6:225:GLN:HG2	4:Y6:245:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a6:201:CYC:NC	13:a6:201:CYC:HMD1	2.18	0.57
3:Q7:109:ARG:O	4:Y7:261:HIS:ND1	2.38	0.57
3:L1:9:VAL:HG21	3:L1:28:LEU:HD11	1.86	0.57
2:R1:41:ALA:HB2	2:R1:147:SER:HB3	1.85	0.57
9:I2:39:ILE:HG13	9:I2:145:ASP:HB3	1.86	0.57
8:X2:1:MET:HG3	8:X2:103:ILE:HB	1.87	0.57
6:Z2:12:SER:OG	6:Z2:17:ARG:NH1	2.37	0.57
8:d2:94:TYR:OH	9:j2:16:ARG:O	2.21	0.57
9:e2:1:MET:O	9:e2:102:THR:OG1	2.19	0.57
2:G3:94:ARG:NH2	3:L3:75:TYR:OH	2.33	0.57
3:X3:3:PHE:HA	3:X3:7:THR:HG23	1.86	0.57
2:K6:33:ARG:NH2	2:K6:34:GLN:OE1	2.37	0.57
2:U6:78:THR:OG1	2:U6:80:GLU:OE1	2.21	0.57
2:W6:25:LEU:HD22	3:X6:39:ILE:HG23	1.86	0.57
2:H7:78:THR:OG1	2:H7:80:GLU:OE1	2.21	0.57
2:I7:41:ALA:HB2	2:I7:147:SER:HB3	1.86	0.57
2:I7:94:ARG:NH2	3:a7:75:TYR:OH	2.33	0.57
3:M7:78:ARG:NH1	13:M7:201:CYC:O1D	2.35	0.57
9:H2:29:PHE:O	9:H2:36:ARG:NH2	2.33	0.57
8:T2:107:ARG:HA	6:Y2:44:GLN:HB3	1.86	0.57
8:d2:35:GLU:HG3	9:j2:27:LYS:HE3	1.87	0.57
8:u2:12:SER:OG	8:u2:17:LYS:O	2.21	0.57
6:z2:15:LYS:HG2	6:z2:20:ARG:HB3	1.87	0.57
2:B3:22:SER:O	2:B3:26:GLN:HG2	2.04	0.57
3:J3:58:ARG:NH1	13:K3:201:CYC:O2D	2.38	0.57
2:K3:101:VAL:HG21	3:L3:20:LEU:HD12	1.86	0.57
5:Z3:49:ILE:HD12	5:Z3:53:GLU:HG3	1.86	0.57
2:S4:3:LYS:HD3	2:T4:16:GLN:HE22	1.68	0.57
13:G5:201:CYC:OB	3:L5:75:TYR:O	2.22	0.57
3:X6:16:ARG:NE	3:X6:18:GLU:OE2	2.38	0.57
5:Z6:109:TYR:O	5:Z6:167:ARG:NH1	2.36	0.57
3:D7:146:ARG:HH21	3:D7:151:GLN:HB3	1.69	0.57
13:M7:201:CYC:HAA1	5:Z7:64:ASN:HB2	1.86	0.57
3:V1:76:THR:HG23	2:W1:111:TYR:HA	1.86	0.57
13:42:301:CYC:HAC1	3:D4:83:CYS:HA	1.86	0.57
8:d2:112:LEU:HD23	8:d2:160:LEU:HD21	1.86	0.57
3:D3:145:ASP:OD1	3:D3:147:ASN:ND2	2.33	0.57
2:F3:117:ASP:N	2:F3:117:ASP:OD1	2.37	0.57
3:O3:95:THR:HG22	2:S3:20:LEU:HD12	1.87	0.57
2:W3:117:ASP:N	2:W3:117:ASP:OD1	2.37	0.57
2:G4:111:TYR:HA	3:L4:76:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a5:152:GLY:O	13:a5:202:CYC:OC	2.23	0.57
2:N6:1:MET:N	3:V6:2:THR:OG1	2.36	0.57
2:N7:78:THR:OG1	2:N7:80:GLU:OE1	2.23	0.57
2:R1:134:LEU:HB2	2:R1:159:ILE:HD11	1.86	0.57
11:P2:77:ARG:NH2	13:P2:201:CYC:O1D	2.38	0.57
11:P2:89:TYR:HH	11:P2:117:TYR:HH	1.51	0.57
8:V2:126:THR:HG23	13:V2:201:CYC:HBC2	1.85	0.57
10:o2:189:ARG:O	10:o2:193:GLU:HB3	2.05	0.57
5:Z3:142:THR:OG1	5:Z3:152:ARG:NH1	2.38	0.57
2:S4:67:THR:HG22	2:S4:76:ALA:H	1.70	0.57
1:A6:176:ILE:O	3:a6:117:THR:OG1	2.19	0.57
2:K6:25:LEU:HD22	3:L6:39:ILE:HG23	1.87	0.57
4:Y7:256:THR:OG1	4:Y7:259:ARG:NH2	2.36	0.57
1:A1:95:TYR:O	3:D1:109:ARG:NH1	2.37	0.57
3:D1:8:LYS:NZ	3:D1:12:GLN:OE1	2.38	0.57
3:O1:95:THR:HG22	2:S1:20:LEU:HD12	1.87	0.57
6:O2:19:GLN:HG3	9:j2:15:ALA:HB2	1.87	0.57
8:A2:70:GLY:O	8:A2:77:ARG:NH1	2.38	0.57
9:E2:16:ARG:O	8:L2:93:TYR:OH	2.22	0.57
8:c2:57:ALA:HA	8:c2:61:LEU:HB2	1.86	0.57
8:c2:90:ARG:HH12	9:k2:12:ASP:HA	1.70	0.57
9:f2:12:ASP:OD1	8:m2:91:TYR:OH	2.15	0.57
9:i2:1:MET:HG3	9:i2:5:SER:HB2	1.87	0.57
10:o2:453:TYR:HD2	10:o2:605:VAL:HG11	1.68	0.57
3:E4:146:ARG:HD2	3:E4:151:GLN:HG3	1.87	0.57
3:Q4:128:VAL:HG22	13:Q4:201:CYC:H3C	1.86	0.57
5:Z4:173:ARG:NH1	5:Z4:203:VAL:O	2.33	0.57
3:Q6:84:LEU:HD13	2:R6:122:THR:HG21	1.86	0.57
2:U6:149:ASP:HB3	13:V6:202:CYC:HAB2	1.87	0.57
5:Z7:109:TYR:O	5:Z7:167:ARG:NH1	2.38	0.57
1:A1:51:ARG:NH2	2:F1:15:SER:O	2.38	0.57
2:I1:78:THR:HG23	2:I1:81:GLY:H	1.70	0.57
8:C2:94:TYR:OH	9:I2:16:ARG:O	2.23	0.57
8:T2:71:ASN:ND2	6:Y2:61:ASN:OD1	2.35	0.57
2:S3:20:LEU:HA	2:S3:24:GLU:HG3	1.87	0.57
3:X3:41:THR:HG23	3:X3:143:VAL:HG11	1.87	0.57
3:X3:61:PHE:HB3	3:X3:68:ILE:HD13	1.87	0.57
3:X3:107:ASP:HA	3:X3:111:LEU:HB2	1.87	0.57
3:E5:63:GLU:HG3	3:E5:64:GLN:HG3	1.87	0.57
3:L5:63:GLU:HG3	3:L5:64:GLN:HG3	1.85	0.57
3:M5:57:ALA:HB2	3:M5:87:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A6:301:CYC:HC	13:A6:301:CYC:HMD1	1.68	0.57
2:W6:138:LYS:HB2	2:W6:155:ILE:HG21	1.87	0.57
5:Z7:102:HIS:NE2	5:Z7:179:ASP:OD2	2.37	0.57
3:Q1:16:ARG:HG3	3:Q1:18:GLU:HG2	1.86	0.56
8:A2:17:LYS:NZ	8:A2:18:TYR:O	2.37	0.56
9:J2:91:LEU:HD12	9:J2:104:ILE:HA	1.87	0.56
3:J3:72:GLY:O	3:J3:79:ARG:NH2	2.37	0.56
5:Z3:67:ILE:HB	5:Z3:71:ASP:HB2	1.87	0.56
5:Z3:85:LYS:HG3	5:Z3:180:ARG:HD3	1.85	0.56
2:F4:95:ILE:HG22	2:F4:108:ILE:HD13	1.87	0.56
3:J4:16:ARG:HG3	3:J4:18:GLU:HG2	1.87	0.56
3:O5:146:ARG:HD2	13:T5:201:CYC:HMC2	1.86	0.56
13:A6:301:CYC:HMD1	13:A6:301:CYC:NC	2.20	0.56
5:Z6:211:TYR:HB2	5:Z6:282:VAL:HG21	1.86	0.56
2:I7:121:LYS:NZ	2:K7:117:ASP:OD1	2.35	0.56
3:J7:38:ARG:NH1	3:J7:98:VAL:O	2.33	0.56
2:R7:43:LYS:O	2:R7:47:ASN:ND2	2.31	0.56
1:A1:78:ARG:NH1	1:A1:143:ASN:OD1	2.38	0.56
3:D1:149:ILE:HG21	13:D1:201:CYC:HMC3	1.87	0.56
3:M1:39:ILE:HG23	2:R1:25:LEU:HD22	1.86	0.56
3:a1:114:LEU:HD23	3:a1:172:VAL:HG12	1.86	0.56
8:C2:104:LEU:HD22	8:C2:156:ILE:HD11	1.86	0.56
11:q2:19:LEU:HD12	9:v2:97:VAL:HG21	1.86	0.56
2:B3:108:ILE:HG22	2:B3:113:LEU:HG	1.87	0.56
2:F3:78:THR:HG23	2:F3:81:GLY:H	1.70	0.56
3:Q3:109:ARG:O	4:Y3:261:HIS:ND1	2.37	0.56
2:R3:5:PRO:HG3	2:W3:23:THR:HA	1.87	0.56
13:C4:201:CYC:HAA1	5:Z4:267:LEU:HD23	1.86	0.56
2:N4:85:CYS:HA	13:N4:201:CYC:HHD	1.87	0.56
3:E6:95:THR:HG22	2:H6:20:LEU:HD12	1.87	0.56
13:Q7:202:CYC:HBB3	2:S7:149:ASP:HB3	1.87	0.56
13:S7:201:CYC:O2D	3:X7:58:ARG:NH1	2.38	0.56
3:X7:85:ARG:HG3	5:Z7:122:GLU:HG2	1.86	0.56
2:F1:74:ASN:ND2	2:F1:124:ASP:OD2	2.38	0.56
2:I1:41:ALA:HB2	2:I1:147:SER:HB3	1.86	0.56
3:Q1:76:THR:HG22	3:Q1:78:ARG:H	1.71	0.56
2:U1:121:LYS:NZ	2:W1:163:SER:OXT	2.39	0.56
6:O2:63:ASN:OD1	8:a2:77:ARG:NH2	2.38	0.56
13:42:302:CYC:HHD	3:E4:83:CYS:HA	1.87	0.56
8:A2:74:THR:HG22	8:A2:76:ARG:H	1.71	0.56
9:D2:1:MET:O	9:D2:102:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E2:126:VAL:HG22	13:E2:201:CYC:H3C	1.87	0.56
9:I2:14:GLU:HB3	9:I2:16:ARG:HG2	1.85	0.56
13:N2:801:CYC:HB	13:N2:801:CYC:HMA3	1.69	0.56
9:R2:35:ARG:NH1	9:R2:148:GLU:OE1	2.38	0.56
8:w2:106:GLU:OE1	6:z2:58:GLY:N	2.36	0.56
9:x2:105:GLU:HA	9:x2:109:ILE:HB	1.86	0.56
3:E3:12:GLN:NE2	3:E3:24:GLN:OE1	2.36	0.56
2:H3:78:THR:OG1	2:H3:80:GLU:OE1	2.22	0.56
2:N3:78:THR:OG1	2:N3:80:GLU:OE1	2.24	0.56
3:P3:85:ARG:HD2	4:Y3:238:ARG:HE	1.71	0.56
2:R3:33:ARG:NH2	2:R3:34:GLN:OE1	2.38	0.56
3:D4:75:TYR:OH	2:H4:94:ARG:NH2	2.32	0.56
2:G4:9:ALA:HB1	2:G4:24:GLU:HG3	1.87	0.56
2:I4:95:ILE:HG22	2:I4:108:ILE:HD13	1.87	0.56
4:Y4:228:GLN:HG2	4:Y4:266:ARG:HG2	1.88	0.56
3:C5:130:GLU:OE2	3:C5:134:LYS:NZ	2.38	0.56
2:K5:2:SER:O	3:L5:1:MET:N	2.38	0.56
2:R5:78:THR:OG1	2:R5:80:GLU:OE1	2.23	0.56
13:a5:201:CYC:NC	13:a5:201:CYC:HMD1	2.20	0.56
2:H6:31:ARG:NH2	2:H6:101:VAL:O	2.39	0.56
3:M6:4:ASP:H	3:M6:7:THR:HG1	1.51	0.56
2:N6:94:ARG:NH2	3:O6:75:TYR:OH	2.29	0.56
2:I7:120:ASN:HD22	2:I7:127:PRO:HG3	1.70	0.56
3:L7:63:GLU:HG3	3:L7:64:GLN:HG3	1.86	0.56
3:M7:4:ASP:H	3:M7:7:THR:HG1	1.53	0.56
2:N7:101:VAL:HG21	3:V7:20:LEU:HD12	1.86	0.56
2:S7:20:LEU:HA	2:S7:24:GLU:HG3	1.87	0.56
2:T7:41:ALA:HB2	2:T7:147:SER:HB3	1.87	0.56
2:T7:78:THR:OG1	2:T7:80:GLU:OE1	2.24	0.56
2:T7:95:ILE:HG13	2:T7:112:LEU:HD13	1.87	0.56
2:B1:122:THR:HG21	3:C1:84:LEU:HD13	1.87	0.56
2:S1:78:THR:OG1	2:S1:80:GLU:OE1	2.24	0.56
5:Z1:74:ARG:NH2	5:Z1:135:ASP:OD1	2.38	0.56
8:C2:3:ASP:HB3	8:C2:98:ALA:HB1	1.87	0.56
13:E2:201:CYC:HB	13:E2:201:CYC:CMA	2.18	0.56
9:G2:12:ASP:OD2	8:K2:107:ARG:NH1	2.38	0.56
8:K2:43:THR:O	8:K2:47:ASN:ND2	2.38	0.56
13:S2:201:CYC:HBA1	8:X2:66:THR:HG21	1.87	0.56
13:o2:801:CYC:HB	13:o2:801:CYC:CMA	2.18	0.56
8:y2:126:THR:HG23	13:y2:201:CYC:HBC3	1.88	0.56
3:D4:16:ARG:NE	3:D4:18:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V4:89:ILE:HG12	3:V4:92:ARG:HH21	1.70	0.56
3:P5:128:VAL:HG22	13:P5:202:CYC:H3C	1.87	0.56
2:U5:63:LYS:HD3	2:U5:132:GLU:HG3	1.87	0.56
3:E6:84:LEU:HD13	2:F6:122:THR:HG21	1.87	0.56
2:R6:85:CYS:HB2	13:R6:201:CYC:H2C	1.86	0.56
1:A1:186:ARG:HA	1:A1:191:PHE:HD2	1.70	0.56
13:A1:302:CYC:NC	13:A1:302:CYC:HMD1	2.19	0.56
3:E1:75:TYR:OH	2:F1:94:ARG:NH2	2.24	0.56
2:F1:78:THR:OG1	2:F1:80:GLU:OE1	2.23	0.56
1:22:93:SER:HB3	1:22:180:ARG:HD2	1.88	0.56
8:V2:94:TYR:OH	9:W2:16:ARG:O	2.23	0.56
6:Y2:5:ARG:NH1	6:Y2:54:GLU:OE2	2.39	0.56
9:f2:128:GLU:OE1	9:f2:131:ARG:NH1	2.38	0.56
8:p2:56:VAL:HG12	8:p2:61:LEU:HD13	1.87	0.56
2:B3:20:LEU:HD12	3:J3:95:THR:HG22	1.87	0.56
13:S3:201:CYC:O2D	3:X3:58:ARG:NH1	2.39	0.56
2:N4:103:GLY:O	2:U4:26:GLN:NE2	2.38	0.56
2:R4:78:THR:OG1	2:R4:80:GLU:OE1	2.24	0.56
2:S4:103:GLY:O	2:T4:26:GLN:NE2	2.38	0.56
2:S5:67:THR:HG22	2:S5:76:ALA:H	1.71	0.56
3:O6:146:ARG:HH21	3:O6:151:GLN:HB3	1.70	0.56
3:V6:121:LEU:HD13	13:V6:201:CYC:HBD1	1.87	0.56
2:G7:9:ALA:HB1	2:G7:24:GLU:HG3	1.88	0.56
2:S7:31:ARG:NH2	2:S7:101:VAL:O	2.39	0.56
5:Z7:142:THR:OG1	5:Z7:152:ARG:NH1	2.39	0.56
3:a1:115:ARG:NH1	3:a1:173:ALA:O	2.39	0.56
1:52:123:ILE:HG23	13:52:301:CYC:HMA1	1.87	0.56
9:H2:126:VAL:HG12	13:H2:201:CYC:HBC3	1.88	0.56
8:L2:89:ARG:NH2	10:N2:499:GLN:OE1	2.36	0.56
13:z2:201:CYC:HMA1	13:z2:201:CYC:HB	1.70	0.56
2:B4:74:ASN:HA	13:B4:201:CYC:HBD2	1.88	0.56
3:E4:149:ILE:HG21	13:E4:201:CYC:HMC3	1.88	0.56
2:R4:85:CYS:HA	13:R4:201:CYC:HH2	1.87	0.56
2:B7:122:THR:HG21	3:C7:84:LEU:HD13	1.88	0.56
3:C7:3:PHE:O	3:C7:104:SER:OG	2.23	0.56
3:X7:44:ARG:NH1	3:X7:145:ASP:O	2.28	0.56
3:D1:149:ILE:HD13	13:D1:201:CYC:H3C	1.87	0.56
2:I1:94:ARG:NH2	3:a1:75:TYR:OH	2.30	0.56
2:S1:18:ARG:NH2	2:T1:105:THR:OG1	2.39	0.56
10:N2:682:SER:HB2	10:N2:685:VAL:HG23	1.87	0.56
8:d2:10:ASN:OD1	10:o2:537:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o2:631:ASP:OD1	10:o2:635:LYS:NZ	2.33	0.56
13:y2:201:CYC:HMA3	13:y2:201:CYC:NB	2.20	0.56
3:C3:38:ARG:NH1	3:C3:98:VAL:O	2.34	0.56
3:X3:12:GLN:O	3:X3:16:ARG:HG2	2.05	0.56
2:G5:85:CYS:HA	13:G5:201:CYC:HHD	1.88	0.56
2:N6:18:ARG:NH1	2:U6:157:TYR:OH	2.39	0.56
1:22:123:ILE:HG23	13:22:301:CYC:HMA1	1.88	0.56
13:52:301:CYC:HAC1	3:D5:83:CYS:HA	1.88	0.56
9:R2:126:VAL:HG22	13:R2:201:CYC:H3C	1.88	0.56
13:e2:201:CYC:HMA1	13:e2:201:CYC:NB	2.17	0.56
9:s2:104:ILE:HG21	9:s2:156:VAL:HG22	1.88	0.56
8:w2:15:GLN:HG2	8:w2:17:LYS:HG2	1.88	0.56
9:x2:35:ARG:HG2	9:x2:38:ARG:HH22	1.70	0.56
2:N3:101:VAL:HG21	3:V3:20:LEU:HD12	1.86	0.56
3:Q3:77:ASN:HD21	2:R3:116:LEU:HD13	1.71	0.56
3:P4:95:THR:HG22	2:U4:20:LEU:HD12	1.87	0.56
13:X4:201:CYC:CMA	13:X4:201:CYC:HB	2.19	0.56
3:C5:146:ARG:NH2	3:C5:152:GLY:O	2.39	0.56
2:K5:20:LEU:HD12	3:L5:95:THR:HG22	1.87	0.56
3:V6:93:TYR:CG	3:V6:110:CYS:HB2	2.41	0.56
3:O7:149:ILE:HD13	13:T7:201:CYC:H3C	1.88	0.56
3:P7:16:ARG:NH1	3:P7:18:GLU:OE2	2.38	0.56
2:R7:5:PRO:HG3	2:W7:23:THR:HA	1.88	0.56
3:V7:72:GLY:O	3:V7:79:ARG:NH2	2.39	0.56
3:C1:146:ARG:NH2	3:C1:152:GLY:O	2.39	0.56
2:R1:85:CYS:HB2	13:R1:201:CYC:H2C	1.88	0.56
13:a1:201:CYC:HB	13:a1:201:CYC:HMA3	1.70	0.56
9:J2:39:ILE:HG21	9:J2:145:ASP:HB3	1.88	0.56
8:M2:123:ILE:HG23	8:M2:160:LEU:HG	1.87	0.56
9:Q2:18:LEU:HD12	8:X2:97:LEU:HD13	1.86	0.56
8:c2:126:THR:HG23	13:c2:801:CYC:HBC3	1.88	0.56
9:h2:25:ARG:HH22	9:k2:3:ILE:HD11	1.70	0.56
9:h2:71:ASN:OD1	9:h2:121:THR:OG1	2.21	0.56
8:m2:56:VAL:HG12	8:m2:61:LEU:HG	1.87	0.56
3:L3:16:ARG:NH1	3:L3:18:GLU:OE2	2.39	0.56
2:K4:10:VAL:HG21	3:L4:100:THR:HG23	1.88	0.56
13:M4:201:CYC:HAA1	5:Z4:64:ASN:HB2	1.88	0.56
3:D5:16:ARG:NE	3:D5:18:GLU:OE2	2.38	0.56
2:S5:3:LYS:HD3	2:T5:16:GLN:HE22	1.69	0.56
2:F6:85:CYS:HA	13:F6:201:CYC:HHD	1.88	0.56
3:P6:4:ASP:N	3:P6:7:THR:OG1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q6:76:THR:HG22	3:Q6:78:ARG:H	1.70	0.56
2:W6:18:ARG:O	3:X6:96:TYR:OH	2.24	0.56
2:B7:20:LEU:HD12	3:J7:95:THR:HG22	1.87	0.56
3:M1:146:ARG:O	3:M1:151:GLN:NE2	2.36	0.56
1:42:3:LEU:HD21	3:D4:81:ALA:HB3	1.87	0.56
8:A2:64:ASP:OD1	8:A2:67:ARG:NH1	2.39	0.56
13:X2:201:CYC:HBA2	6:Y2:12:SER:HB3	1.87	0.56
9:h2:2:SER:OG	8:l2:3:ASP:OD2	2.18	0.56
10:o2:464:PHE:HB3	10:o2:558:GLY:HA3	1.88	0.56
2:R3:43:LYS:O	2:R3:47:ASN:ND2	2.32	0.56
3:V3:152:GLY:HA3	13:V3:202:CYC:HMD2	1.87	0.56
3:C4:154:CYS:SG	13:C4:202:CYC:OC	2.64	0.56
3:O4:149:ILE:HD13	13:T4:201:CYC:H3C	1.88	0.56
3:J5:4:ASP:N	3:J5:7:THR:OG1	2.39	0.56
3:O5:100:THR:HG23	2:S5:10:VAL:HG21	1.87	0.56
2:G6:33:ARG:NH1	2:G6:146:ASP:OD2	2.38	0.56
3:D7:149:ILE:HG21	13:D7:201:CYC:HMC3	1.87	0.56
2:K1:105:THR:O	2:K1:105:THR:OG1	2.23	0.55
3:M1:91:LEU:HB2	3:M1:135:MET:HE3	1.86	0.55
6:02:20:ARG:HH21	8:d2:107:ARG:HA	1.71	0.55
9:H2:91:LEU:HD12	9:H2:104:ILE:HA	1.88	0.55
8:c2:103:ILE:HG13	8:c2:107:ARG:HD2	1.87	0.55
10:o2:445:GLN:NE2	8:p2:118:SER:O	2.39	0.55
9:s2:29:PHE:O	9:s2:36:ARG:NH2	2.39	0.55
5:Z5:102:HIS:NE2	5:Z5:179:ASP:OD2	2.38	0.55
3:a5:114:LEU:HD23	3:a5:172:VAL:HG12	1.87	0.55
3:C6:130:GLU:OE2	3:C6:134:LYS:NZ	2.39	0.55
2:U6:95:ILE:HG13	2:U6:112:LEU:HD13	1.88	0.55
3:D7:145:ASP:OD1	3:D7:147:ASN:ND2	2.32	0.55
2:I7:78:THR:OG1	2:I7:80:GLU:OE1	2.24	0.55
4:Y7:218:ARG:NH1	4:Y7:220:GLN:OE1	2.40	0.55
3:P1:4:ASP:N	3:P1:7:THR:OG1	2.38	0.55
1:32:41:GLN:HG2	3:L3:1:MET:HA	1.87	0.55
1:42:69:GLN:HE21	5:Z4:225:GLY:HA3	1.70	0.55
8:C2:19:LEU:HD11	9:I2:97:VAL:HG11	1.88	0.55
9:i2:65:VAL:HA	9:i2:70:GLY:HA3	1.87	0.55
3:L3:1:MET:SD	3:L3:1:MET:N	2.79	0.55
3:E4:115:ARG:NH1	3:E4:173:ALA:O	2.39	0.55
3:X4:37:LYS:NZ	3:X4:150:THR:OG1	2.37	0.55
4:Y4:234:ARG:H	4:Y4:234:ARG:NE	2.04	0.55
3:O5:96:TYR:OH	2:S5:18:ARG:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L6:34:GLU:HG3	3:L6:37:LYS:HD2	1.87	0.55
2:T6:95:ILE:HG13	2:T6:112:LEU:HD13	1.88	0.55
8:F2:60:LEU:O	8:F2:63:SER:OG	2.23	0.55
9:H2:91:LEU:HD13	9:H2:94:TYR:HD2	1.71	0.55
10:N2:178:PRO:HB2	10:N2:232:VAL:HG11	1.89	0.55
10:N2:445:GLN:NE2	8:O2:118:SER:O	2.39	0.55
13:N2:801:CYC:HB	13:N2:801:CYC:CMA	2.19	0.55
9:e2:1:MET:HB2	9:e2:5:SER:HB3	1.89	0.55
8:y2:60:LEU:O	8:y2:63:SER:OG	2.24	0.55
3:D3:26:ASP:OD2	3:D3:30:ARG:NH1	2.39	0.55
2:T3:78:THR:OG1	2:T3:80:GLU:OE1	2.24	0.55
2:U4:74:ASN:ND2	2:U4:124:ASP:OD2	2.40	0.55
2:F5:85:CYS:HB2	13:F5:201:CYC:H2C	1.88	0.55
2:R5:41:ALA:HB2	2:R5:147:SER:HB3	1.87	0.55
3:X5:4:ASP:HA	3:X5:100:THR:HB	1.89	0.55
2:F6:78:THR:OG1	2:F6:80:GLU:OE1	2.24	0.55
3:Q6:16:ARG:HG3	3:Q6:18:GLU:HG2	1.88	0.55
1:A1:37:TYR:HB3	1:A1:41:GLN:HB2	1.86	0.55
3:E1:63:GLU:HG3	3:E1:64:GLN:HG3	1.87	0.55
2:F1:25:LEU:HD22	3:a1:39:ILE:HG23	1.88	0.55
13:L1:201:CYC:HMA1	13:L1:201:CYC:NB	2.19	0.55
8:B2:103:ILE:HG13	8:B2:107:ARG:HD2	1.87	0.55
10:N2:509:GLY:HA3	10:N2:664:ARG:HB3	1.88	0.55
12:S2:90:ARG:NH1	8:T2:13:ASP:OD1	2.38	0.55
6:Z2:62:THR:OG1	6:Z2:64:THR:O	2.22	0.55
9:e2:81:CYS:SG	13:e2:201:CYC:HAC2	2.47	0.55
9:i2:100:ASP:OD1	9:i2:101:ILE:N	2.40	0.55
8:n2:123:ILE:HG23	8:n2:160:LEU:HG	1.87	0.55
10:o2:457:ASN:HD21	10:o2:605:VAL:HG12	1.71	0.55
2:I3:78:THR:HG23	2:I3:81:GLY:H	1.70	0.55
3:J3:150:THR:O	13:J3:202:CYC:NC	2.28	0.55
3:M3:87:MET:HG3	13:M3:201:CYC:HBC1	1.88	0.55
3:O3:1:MET:SD	2:S3:2:SER:N	2.79	0.55
3:D4:8:LYS:NZ	3:D4:12:GLN:OE1	2.38	0.55
2:R5:85:CYS:HA	13:R5:201:CYC:HHH	1.87	0.55
2:T5:41:ALA:HB2	2:T5:147:SER:HB3	1.89	0.55
3:E6:77:ASN:HD21	13:F6:201:CYC:HMB1	1.71	0.55
2:T6:78:THR:OG1	2:T6:80:GLU:OE1	2.25	0.55
2:F7:20:LEU:HD12	3:a7:95:THR:HG22	1.88	0.55
2:K7:76:ALA:O	2:K7:82:LYS:NZ	2.32	0.55
2:F1:62:SER:HB3	2:I7:70:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:146:ARG:HD2	13:T1:201:CYC:HMC2	1.88	0.55
3:X1:128:VAL:HG22	13:X1:201:CYC:H3C	1.88	0.55
3:a1:44:ARG:NH1	3:a1:142:ILE:O	2.40	0.55
1:22:17:VAL:O	1:22:161:ARG:NH1	2.40	0.55
12:S2:151:PRO:HB2	9:U2:20:PRO:HB3	1.88	0.55
8:c2:1:MET:N	8:c2:106:GLU:OE1	2.40	0.55
9:h2:81:CYS:SG	13:h2:201:CYC:HAC2	2.46	0.55
9:r2:52:LYS:O	9:r2:56:ASN:ND2	2.34	0.55
2:K4:85:CYS:HA	13:K4:201:CYC:HHH	1.88	0.55
3:Q4:109:ARG:O	4:Y4:261:HIS:ND1	2.39	0.55
3:V4:89:ILE:HD13	13:V4:201:CYC:HBB3	1.89	0.55
2:I7:48:ASN:OD1	2:I7:51:SER:OG	2.22	0.55
2:R1:78:THR:OG1	2:R1:80:GLU:OE1	2.25	0.55
2:R1:128:SER:O	2:R1:132:GLU:HG3	2.05	0.55
3:V1:4:ASP:N	3:V1:7:THR:OG1	2.37	0.55
9:G2:36:ARG:NE	9:G2:148:GLU:OE2	2.39	0.55
9:H2:1:MET:HG3	9:H2:5:SER:HB2	1.88	0.55
8:K2:64:ASP:OD1	8:K2:67:ARG:NH2	2.34	0.55
9:R2:1:MET:HG3	9:R2:5:SER:HB2	1.87	0.55
9:h2:64:ASP:HB2	9:j2:64:ASP:HB3	1.87	0.55
9:v2:81:CYS:SG	13:v2:201:CYC:HAC2	2.46	0.55
2:I3:48:ASN:OD1	2:I3:51:SER:OG	2.22	0.55
3:M3:38:ARG:NH1	3:M3:98:VAL:O	2.34	0.55
2:N5:122:THR:HG21	3:O5:84:LEU:HD13	1.89	0.55
5:Z5:142:THR:OG1	5:Z5:152:ARG:NH1	2.40	0.55
13:A6:302:CYC:NC	13:A6:302:CYC:HMD1	2.21	0.55
2:G1:33:ARG:NH1	2:G1:146:ASP:OD2	2.40	0.55
2:N1:63:LYS:HD2	2:N1:132:GLU:HG3	1.88	0.55
3:V1:121:LEU:HD13	13:V1:201:CYC:HBD1	1.88	0.55
1:32:176:ILE:O	3:a3:117:THR:OG1	2.20	0.55
8:C2:112:LEU:HD23	8:C2:160:LEU:HD21	1.89	0.55
9:R2:1:MET:HB3	9:R2:102:THR:HG21	1.89	0.55
8:d2:70:GLY:O	8:d2:77:ARG:NH2	2.39	0.55
2:B3:27:VAL:HG22	2:I3:27:VAL:HG22	1.88	0.55
3:L3:76:THR:HB	3:L3:79:ARG:HG3	1.89	0.55
2:T4:78:THR:OG1	2:T4:80:GLU:OE1	2.25	0.55
4:Y4:218:ARG:HG2	4:Y4:250:TYR:HB3	1.87	0.55
4:Y4:234:ARG:HG2	4:Y4:235:THR:HG23	1.89	0.55
3:V5:76:THR:HG22	3:V5:78:ARG:H	1.70	0.55
13:V5:201:CYC:NC	13:V5:201:CYC:HMD1	2.22	0.55
2:F6:157:TYR:OH	2:K6:18:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M6:39:ILE:HG23	2:R6:25:LEU:HD22	1.87	0.55
3:X7:3:PHE:HB3	3:X7:8:LYS:HB2	1.89	0.55
2:T1:95:ILE:HG13	2:T1:112:LEU:HD13	1.87	0.55
1:22:153:TYR:OH	5:Z7:273:GLN:OE1	2.20	0.55
8:V2:15:GLN:HG2	8:V2:17:LYS:HG2	1.87	0.55
9:h2:36:ARG:HG3	9:h2:96:VAL:O	2.07	0.55
9:j2:113:ARG:NH2	9:j2:161:SER:OXT	2.38	0.55
9:k2:153:PHE:O	9:k2:157:ILE:HG12	2.07	0.55
9:r2:128:GLU:OE1	9:r2:131:ARG:NH1	2.39	0.55
12:t2:41:GLN:NE2	12:t2:45:ASP:OD2	2.39	0.55
2:N3:63:LYS:HD2	2:N3:132:GLU:HG3	1.88	0.55
2:B4:20:LEU:HD12	3:J4:95:THR:HG22	1.88	0.55
2:I4:108:ILE:HG22	2:I4:113:LEU:HG	1.89	0.55
2:N5:149:ASP:HB3	13:P5:201:CYC:H2C	1.87	0.55
3:Q5:84:LEU:HD13	2:R5:122:THR:HG21	1.89	0.55
3:V5:93:TYR:CG	3:V5:110:CYS:HB2	2.41	0.55
3:M6:91:LEU:HB2	3:M6:135:MET:HE3	1.89	0.55
3:X6:3:PHE:HB3	3:X6:8:LYS:HB2	1.88	0.55
2:B7:27:VAL:HG22	2:I7:27:VAL:HG22	1.89	0.55
3:D7:16:ARG:NE	3:D7:18:GLU:OE2	2.39	0.55
3:C1:128:VAL:HG22	13:C1:201:CYC:H3C	1.89	0.55
3:Q1:20:LEU:H	3:Q1:20:LEU:HD12	1.72	0.55
9:E2:41:GLN:NE2	9:E2:45:GLU:OE2	2.40	0.55
9:G2:81:CYS:HA	13:G2:201:CYC:HHD	1.87	0.55
8:T2:1:MET:N	8:T2:106:GLU:OE1	2.40	0.55
8:T2:2:GLN:OE1	8:T2:10:ASN:ND2	2.40	0.55
6:Y2:9:CYS:HB2	6:Y2:26:PHE:HD1	1.71	0.55
11:q2:108:ARG:NH1	9:v2:12:ASP:OD2	2.35	0.55
2:I3:94:ARG:NH2	3:a3:75:TYR:OH	2.30	0.55
3:P3:16:ARG:NH1	3:P3:18:GLU:OE2	2.36	0.55
2:T3:74:ASN:ND2	2:T3:124:ASP:OD2	2.40	0.55
5:Z3:262:VAL:HG11	5:Z3:270:THR:HG21	1.89	0.55
13:a3:201:CYC:CMA	13:a3:201:CYC:HB	2.20	0.55
2:I6:121:LYS:NZ	2:K6:117:ASP:OD1	2.40	0.55
3:M6:76:THR:HG22	3:M6:78:ARG:H	1.71	0.55
3:P6:39:ILE:HG23	2:U6:25:LEU:HD22	1.88	0.55
3:X7:12:GLN:O	3:X7:16:ARG:HG2	2.06	0.55
3:a7:30:ARG:O	3:a7:34:GLU:HG2	2.07	0.55
3:E1:12:GLN:OE1	3:E1:16:ARG:NH1	2.30	0.55
3:Q1:128:VAL:HG22	13:Q1:201:CYC:H3C	1.89	0.55
1:32:53:ILE:HD11	1:32:81:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a2:90:ARG:NH1	8:a2:94:TYR:OH	2.38	0.55
3:a3:114:LEU:HD23	3:a3:172:VAL:HG12	1.89	0.55
2:S5:103:GLY:O	2:T5:26:GLN:NE2	2.39	0.55
2:W5:85:CYS:HA	13:W5:201:CYC:HAC2	1.89	0.55
3:a5:34:GLU:OE1	3:a5:37:LYS:NZ	2.34	0.55
2:U6:138:LYS:NZ	2:U6:156:ASP:OD1	2.28	0.55
13:a6:201:CYC:HB	13:a6:201:CYC:CMA	2.20	0.55
2:N7:113:LEU:HD21	2:N7:161:ALA:HB1	1.88	0.55
3:C1:119:LEU:HD22	3:O1:122:GLY:HA2	1.89	0.54
3:D1:96:TYR:OH	2:I1:18:ARG:O	2.21	0.54
9:G2:83:ARG:HH12	13:G2:201:CYC:CGA	2.20	0.54
8:M2:13:ASP:OD1	10:N2:167:ARG:NH2	2.40	0.54
10:N2:46:TYR:OH	10:N2:174:VAL:O	2.21	0.54
11:P2:168:ASP:OD1	11:P2:168:ASP:N	2.40	0.54
8:d2:3:ASP:OD1	8:d2:6:THR:OG1	2.16	0.54
13:f2:201:CYC:HB	13:f2:201:CYC:CMA	2.20	0.54
8:g2:37:ARG:NH1	8:g2:96:MET:O	2.33	0.54
8:g2:60:LEU:O	8:g2:63:SER:OG	2.25	0.54
8:w2:38:VAL:HG23	9:x2:23:LEU:HD22	1.89	0.54
9:x2:72:ALA:HA	9:x2:77:MET:HB3	1.87	0.54
6:z2:9:CYS:HB2	6:z2:26:PHE:HD1	1.72	0.54
3:O3:146:ARG:HH21	3:O3:151:GLN:HB3	1.72	0.54
2:N4:149:ASP:HB3	13:P4:202:CYC:H2C	1.89	0.54
3:Q4:16:ARG:HG3	3:Q4:18:GLU:HG2	1.89	0.54
3:X4:89:ILE:HG21	13:X4:201:CYC:HAB1	1.87	0.54
2:G5:122:THR:HG21	3:L5:84:LEU:HD13	1.89	0.54
2:H5:108:ILE:HG22	2:H5:113:LEU:HG	1.89	0.54
13:J5:201:CYC:NB	13:J5:201:CYC:HMA1	2.21	0.54
1:A6:41:GLN:HG2	3:L6:1:MET:HA	1.89	0.54
3:X6:128:VAL:HG22	13:X6:201:CYC:H3C	1.89	0.54
3:Q7:77:ASN:HD21	2:R7:116:LEU:HD13	1.72	0.54
3:M1:57:ALA:HB2	3:M1:87:MET:HE1	1.88	0.54
2:W1:20:LEU:HD12	3:X1:95:THR:HG22	1.89	0.54
1:42:100:ASN:ND2	3:D4:109:ARG:O	2.32	0.54
1:52:86:LEU:HA	1:52:134:TYR:HE1	1.72	0.54
9:D2:50:ILE:HD11	9:D2:140:LEU:HD21	1.88	0.54
9:J2:56:ASN:ND2	9:J2:60:GLN:OE1	2.41	0.54
9:W2:16:ARG:NH1	9:W2:22:GLU:OE2	2.32	0.54
8:g2:56:VAL:HG12	8:g2:61:LEU:HG	1.88	0.54
2:B3:94:ARG:NH2	3:C3:75:TYR:OH	2.33	0.54
13:V3:201:CYC:NC	13:V3:201:CYC:HMD1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z3:41:ARG:NH2	5:Z3:175:TYR:O	2.40	0.54
13:G4:201:CYC:OB	3:L4:75:TYR:O	2.25	0.54
3:P4:37:LYS:HE2	3:P4:154:CYS:HB3	1.89	0.54
2:R4:134:LEU:HB2	2:R4:159:ILE:HD11	1.89	0.54
3:a4:128:VAL:HG22	13:a4:201:CYC:H3C	1.89	0.54
2:B5:25:LEU:HD22	3:J5:39:ILE:HG23	1.90	0.54
2:G5:23:THR:HA	2:H5:5:PRO:HG3	1.88	0.54
13:M5:201:CYC:HAA1	5:Z5:64:ASN:HB2	1.90	0.54
2:I6:52:LEU:HB3	2:I6:137:ILE:HD12	1.88	0.54
2:N6:149:ASP:HB3	13:P6:201:CYC:H2C	1.90	0.54
3:O6:149:ILE:HD13	13:T6:201:CYC:H3C	1.89	0.54
2:B7:85:CYS:HA	13:B7:201:CYC:HHH	1.88	0.54
3:C7:38:ARG:NH1	3:C7:98:VAL:O	2.34	0.54
3:D1:75:TYR:OH	2:H1:94:ARG:NH2	2.32	0.54
2:I1:91:TYR:O	2:I1:95:ILE:HG12	2.07	0.54
3:J1:4:ASP:N	3:J1:7:THR:OG1	2.39	0.54
1:32:164:LEU:HD21	13:32:302:CYC:HBA2	1.89	0.54
1:42:55:PHE:HD2	13:a4:201:CYC:HBA1	1.72	0.54
8:B2:3:ASP:HB2	9:J2:5:SER:HB3	1.90	0.54
8:L2:1:GLN:OE1	11:P2:162:ARG:NH1	2.36	0.54
8:O2:109:LEU:HD13	8:O2:159:GLY:HA3	1.89	0.54
9:Q2:19:SER:OG	9:Q2:22:GLU:OE1	2.25	0.54
9:e2:113:ARG:NH2	9:e2:161:SER:OXT	2.39	0.54
9:r2:30:VAL:HG21	8:y2:34:GLY:HA3	1.87	0.54
3:a3:30:ARG:O	3:a3:34:GLU:HG2	2.08	0.54
2:N4:1:MET:N	3:V4:2:THR:OG1	2.40	0.54
2:R5:134:LEU:HB2	2:R5:159:ILE:HD11	1.89	0.54
1:A6:179:PRO:HB2	3:a6:121:LEU:HD21	1.89	0.54
2:W6:20:LEU:HD12	3:X6:95:THR:HG22	1.89	0.54
5:Z6:173:ARG:NH1	5:Z6:203:VAL:O	2.32	0.54
3:C1:109:ARG:HD3	5:Z1:275:ASN:HB3	1.89	0.54
3:E1:146:ARG:HD2	3:E1:151:GLN:HG3	1.88	0.54
2:N1:1:MET:N	3:V1:2:THR:OG1	2.40	0.54
3:a1:112:ASN:HB3	10:N2:699:ARG:NH1	2.22	0.54
13:a1:202:CYC:NB	13:a1:202:CYC:HMA3	2.23	0.54
1:32:93:SER:HB3	1:32:180:ARG:HD2	1.90	0.54
1:32:153:TYR:OH	5:Z3:273:GLN:OE1	2.19	0.54
1:52:69:GLN:HE21	5:Z5:225:GLY:HA3	1.72	0.54
10:N2:631:ASP:OD1	10:N2:635:LYS:NZ	2.32	0.54
13:R2:201:CYC:HB	13:R2:201:CYC:CMA	2.18	0.54
8:T2:60:LEU:O	8:T2:63:SER:OG	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p2:37:ARG:NH1	8:p2:96:MET:O	2.35	0.54
2:B3:25:LEU:HD22	3:J3:39:ILE:HG23	1.90	0.54
2:F3:8:GLU:HG3	2:K3:23:THR:HG21	1.89	0.54
2:I3:16:GLN:OE1	2:I3:18:ARG:NE	2.39	0.54
3:D4:44:ARG:HH12	3:D4:145:ASP:HB3	1.73	0.54
3:a4:83:CYS:SG	13:a4:201:CYC:HAC2	2.47	0.54
3:M5:76:THR:HG23	2:U5:111:TYR:HA	1.89	0.54
2:W5:85:CYS:HA	13:W5:201:CYC:HHD	1.89	0.54
3:X5:16:ARG:NE	3:X5:18:GLU:OE2	2.41	0.54
5:Z6:4:THR:OG1	13:Z6:301:CYC:O1D	2.26	0.54
3:a6:114:LEU:HD23	3:a6:172:VAL:HG12	1.88	0.54
3:P7:74:ALA:HA	3:P7:79:ARG:HB3	1.89	0.54
3:Q7:16:ARG:HG3	3:Q7:18:GLU:HG2	1.89	0.54
13:L1:201:CYC:HB	13:L1:201:CYC:CMA	2.20	0.54
9:I2:113:ARG:NH2	9:I2:161:SER:OXT	2.40	0.54
13:P2:201:CYC:NC	13:P2:201:CYC:HMD1	2.22	0.54
3:M4:44:ARG:NH2	3:M4:145:ASP:O	2.40	0.54
2:I5:91:TYR:O	2:I5:95:ILE:HG12	2.07	0.54
2:U5:74:ASN:HA	13:U5:201:CYC:HBD2	1.88	0.54
13:a5:201:CYC:HB	13:a5:201:CYC:CMA	2.19	0.54
3:C7:130:GLU:OE2	3:C7:134:LYS:NZ	2.41	0.54
1:A1:30:GLN:OE1	1:A1:155:LYS:NZ	2.35	0.54
8:C2:74:THR:HA	13:H2:201:CYC:HBB2	1.90	0.54
13:N2:802:CYC:HB	13:N2:802:CYC:CMA	2.20	0.54
8:V2:3:ASP:OD2	9:W2:5:SER:OG	2.23	0.54
8:a2:75:THR:HG23	13:k2:201:CYC:HBB2	1.89	0.54
8:c2:81:CYS:HA	13:c2:801:CYC:HHD	1.89	0.54
9:f2:16:ARG:O	8:m2:94:TYR:OH	2.26	0.54
13:p2:201:CYC:HB	13:p2:201:CYC:CMA	2.20	0.54
2:B4:2:SER:HB3	2:B4:106:GLY:HA3	1.89	0.54
2:B4:109:ASP:HA	2:B4:113:LEU:HB2	1.90	0.54
3:E4:12:GLN:NE2	3:E4:24:GLN:OE1	2.33	0.54
3:P4:4:ASP:N	3:P4:7:THR:OG1	2.38	0.54
3:V4:4:ASP:N	3:V4:7:THR:OG1	2.38	0.54
3:V4:105:ILE:HD12	3:V4:109:ARG:HD3	1.90	0.54
3:M5:75:TYR:OH	2:U5:94:ARG:NH2	2.34	0.54
13:S6:201:CYC:O2D	3:X6:58:ARG:NH1	2.41	0.54
2:T6:78:THR:HG23	2:T6:81:GLY:H	1.73	0.54
3:L7:1:MET:SD	3:L7:1:MET:N	2.81	0.54
3:O7:17:GLY:HA3	3:X7:70:PRO:HB3	1.89	0.54
3:V7:4:ASP:N	3:V7:7:THR:OG1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:14:ASP:OD1	3:a1:93:TYR:OH	2.20	0.54
2:H1:31:ARG:NH2	2:H1:101:VAL:O	2.40	0.54
3:O1:76:THR:HG23	3:O1:79:ARG:HG3	1.90	0.54
3:Q1:84:LEU:HD13	2:R1:122:THR:HG21	1.88	0.54
2:R1:31:ARG:NH2	2:R1:101:VAL:O	2.40	0.54
3:V1:93:TYR:CG	3:V1:110:CYS:HB2	2.43	0.54
3:X1:78:ARG:NH2	13:X1:201:CYC:O1D	2.41	0.54
8:A2:85:LEU:HD21	8:A2:129:ALA:HB1	1.89	0.54
8:B2:70:GLY:O	10:N2:535:ASN:ND2	2.41	0.54
9:E2:113:ARG:NH2	9:E2:161:SER:OXT	2.40	0.54
13:F2:201:CYC:HB	13:F2:201:CYC:CMA	2.20	0.54
9:H2:65:VAL:HA	9:H2:70:GLY:HA3	1.89	0.54
8:d2:68:PRO:HA	8:d2:73:TYR:CG	2.42	0.54
9:f2:76:ASP:OD1	9:f2:76:ASP:N	2.40	0.54
13:g2:201:CYC:CMA	13:g2:201:CYC:HB	2.20	0.54
13:m2:201:CYC:NC	13:m2:201:CYC:HMD1	2.23	0.54
9:r2:104:ILE:HG21	9:r2:156:VAL:HG22	1.90	0.54
9:s2:37:LEU:HD23	9:s2:97:VAL:HG22	1.90	0.54
8:y2:144:ASP:N	8:y2:144:ASP:OD1	2.40	0.54
13:D3:201:CYC:HMA3	13:D3:201:CYC:HB	1.71	0.54
2:T3:95:ILE:HG13	2:T3:112:LEU:HD13	1.90	0.54
2:U3:149:ASP:HB3	13:V3:202:CYC:HAB2	1.90	0.54
3:M4:72:GLY:O	3:M4:79:ARG:NH2	2.38	0.54
3:D5:75:TYR:O	13:H5:201:CYC:OB	2.26	0.54
2:I5:9:ALA:HB1	2:I5:24:GLU:HG3	1.88	0.54
3:P5:95:THR:HG22	2:U5:20:LEU:HD12	1.89	0.54
3:Q5:112:ASN:O	4:Y5:261:HIS:NE2	2.34	0.54
3:a6:146:ARG:NH1	3:a6:152:GLY:O	2.40	0.54
3:L7:9:VAL:HG21	3:L7:28:LEU:HD11	1.90	0.54
2:S7:27:VAL:HG22	2:T7:27:VAL:HG23	1.90	0.54
2:U1:149:ASP:HB3	13:V1:202:CYC:HAB2	1.90	0.54
3:V1:38:ARG:NH2	3:V1:160:GLU:OE1	2.41	0.54
8:C2:71:ASN:ND2	13:C2:201:CYC:OC	2.41	0.54
9:D2:13:ALA:HB2	10:N2:513:THR:HB	1.90	0.54
9:J2:91:LEU:HD11	9:J2:107:ILE:HB	1.90	0.54
10:N2:461:GLU:OE2	10:N2:613:ARG:NH1	2.40	0.54
8:c2:74:THR:HG23	9:j2:107:ILE:HA	1.90	0.54
9:e2:30:VAL:HG21	8:g2:34:GLY:HA3	1.90	0.54
10:o2:520:GLN:HB3	10:o2:524:GLY:HA2	1.90	0.54
8:p2:38:VAL:HG11	9:s2:27:LYS:HG3	1.89	0.54
2:B4:94:ARG:NH2	3:C4:75:TYR:OH	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E4:18:GLU:O	2:H4:98:TYR:OH	2.25	0.54
2:F4:10:VAL:HG21	3:a4:100:THR:HG23	1.89	0.54
2:N4:78:THR:OG1	2:N4:80:GLU:OE1	2.25	0.54
3:Q4:84:LEU:HD13	2:R4:122:THR:HG21	1.89	0.54
5:Z4:106:ARG:HD3	5:Z4:152:ARG:HH21	1.73	0.54
5:Z4:235:SER:HB3	5:Z4:264:TYR:HB3	1.90	0.54
2:B7:22:SER:O	2:B7:26:GLN:HG2	2.08	0.54
3:E7:115:ARG:NH1	3:E7:173:ALA:O	2.41	0.54
2:S7:33:ARG:NH2	2:S7:34:GLN:OE1	2.40	0.54
2:W7:134:LEU:HB3	2:W7:155:ILE:HG23	1.90	0.54
3:C1:63:GLU:HG3	3:C1:64:GLN:HG3	1.89	0.54
3:D1:63:GLU:HG3	3:D1:64:GLN:HG3	1.88	0.54
2:F1:31:ARG:NH2	2:F1:101:VAL:O	2.38	0.54
2:U1:50:ASP:O	2:U1:54:ASN:ND2	2.34	0.54
1:32:191:PHE:CE1	3:a3:73:ASN:HA	2.43	0.54
1:52:191:PHE:O	1:52:193:LYS:N	2.40	0.54
13:A2:202:CYC:HAC2	9:J2:81:CYS:HA	1.89	0.54
8:K2:12:SER:HA	8:K2:15:GLN:HE21	1.73	0.54
8:L2:99:ASP:OD1	8:L2:100:THR:N	2.41	0.54
13:U2:201:CYC:HB	13:U2:201:CYC:CMA	2.19	0.54
8:a2:64:ASP:OD1	8:a2:67:ARG:NH1	2.41	0.54
8:a2:85:LEU:HD21	8:a2:129:ALA:HB1	1.90	0.54
9:e2:35:ARG:HG3	9:e2:38:ARG:HH21	1.73	0.54
10:o2:699:ARG:HD3	1:A6:169:LEU:HD23	1.90	0.54
3:C3:130:GLU:OE2	3:C3:134:LYS:NZ	2.41	0.54
2:R3:78:THR:OG1	2:R3:80:GLU:OE1	2.25	0.54
2:S3:27:VAL:HG22	2:T3:27:VAL:HG23	1.90	0.54
2:U4:78:THR:OG1	2:U4:80:GLU:OE1	2.26	0.54
2:F5:85:CYS:HA	13:F5:201:CYC:HH2	1.90	0.54
2:I6:94:ARG:NH2	3:a6:75:TYR:OH	2.27	0.54
3:L6:116:GLU:HG3	5:Z6:212:VAL:HG22	1.90	0.54
3:P1:117:THR:HG21	13:P1:202:CYC:HMA1	1.90	0.54
3:V1:78:ARG:NH1	13:V1:201:CYC:O1D	2.40	0.54
8:A2:137:THR:O	8:A2:141:VAL:HG22	2.08	0.54
9:G2:1:MET:HG3	9:G2:5:SER:CB	2.38	0.54
12:S2:2:THR:N	12:S2:5:SER:HG	2.06	0.54
8:d2:64:ASP:HA	8:d2:67:ARG:HB2	1.89	0.54
9:r2:121:THR:OG1	13:r2:201:CYC:NC	2.40	0.54
13:Q3:202:CYC:HBB3	2:S3:149:ASP:HB3	1.89	0.54
3:C4:109:ARG:HD3	5:Z4:275:ASN:HB3	1.90	0.54
13:P4:201:CYC:O2A	4:Y4:238:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V4:152:GLY:HA3	13:V4:202:CYC:HMD2	1.88	0.54
2:G5:8:GLU:HG3	2:H5:23:THR:HG21	1.88	0.54
3:Q5:95:THR:HG22	2:T5:20:LEU:HD12	1.90	0.54
5:Z5:43:VAL:HA	5:Z5:102:HIS:HB3	1.90	0.54
3:L6:76:THR:HB	3:L6:79:ARG:HG3	1.89	0.54
3:P6:128:VAL:HG22	13:P6:202:CYC:H3C	1.88	0.54
2:W6:16:GLN:HG3	2:W6:18:ARG:HG2	1.90	0.54
2:B1:25:LEU:HD22	3:J1:39:ILE:HG23	1.90	0.53
13:C1:202:CYC:HMA3	13:C1:202:CYC:HB	1.73	0.53
3:E1:44:ARG:HH12	3:E1:145:ASP:HB3	1.74	0.53
2:W1:95:ILE:HG13	2:W1:112:LEU:HD13	1.91	0.53
5:Z1:211:TYR:HB2	5:Z1:282:VAL:HG21	1.89	0.53
5:Z1:262:VAL:HG11	5:Z1:270:THR:HG21	1.91	0.53
8:M2:1:MET:N	10:N2:268:GLU:OE2	2.41	0.53
8:X2:60:LEU:O	8:X2:63:SER:OG	2.25	0.53
9:i2:113:ARG:NH2	9:i2:161:SER:OXT	2.41	0.53
12:t2:2:THR:HG22	12:t2:98:ALA:HB1	1.90	0.53
13:F3:202:CYC:NC	3:L3:150:THR:O	2.41	0.53
3:P5:4:ASP:N	3:P5:7:THR:OG1	2.40	0.53
2:R6:128:SER:O	2:R6:132:GLU:HG3	2.08	0.53
3:P7:27:ALA:HA	3:P7:30:ARG:HE	1.73	0.53
1:A1:47:GLN:OE1	1:A1:51:ARG:NH1	2.40	0.53
3:C1:30:ARG:O	3:C1:34:GLU:HG2	2.09	0.53
3:L1:116:GLU:HG3	5:Z1:212:VAL:HG22	1.90	0.53
2:N1:94:ARG:NH2	3:O1:75:TYR:OH	2.26	0.53
2:R1:85:CYS:HA	13:R1:201:CYC:HAC2	1.91	0.53
8:A2:130:ILE:HG22	8:A2:134:LYS:HE3	1.89	0.53
9:U2:36:ARG:NH1	9:U2:97:VAL:O	2.41	0.53
10:o2:311:LEU:HD21	10:o2:328:ARG:HB3	1.89	0.53
8:w2:5:ILE:HG21	9:x2:98:SER:HA	1.90	0.53
3:O3:61:PHE:HB3	3:O3:68:ILE:HD13	1.89	0.53
2:S3:18:ARG:NH2	2:T3:105:THR:OG1	2.40	0.53
3:L4:9:VAL:HG21	3:L4:28:LEU:HD11	1.89	0.53
3:V5:38:ARG:NH2	3:V5:160:GLU:OE1	2.41	0.53
3:C6:37:LYS:HE2	13:C6:202:CYC:HMD2	1.89	0.53
3:V6:4:ASP:N	3:V6:7:THR:OG1	2.33	0.53
3:a6:115:ARG:NH1	3:a6:173:ALA:O	2.41	0.53
2:N7:23:THR:HA	2:U7:5:PRO:HG3	1.90	0.53
2:I1:78:THR:OG1	2:I1:80:GLU:OE1	2.26	0.53
4:Y1:225:GLN:HG2	4:Y1:245:THR:HG22	1.91	0.53
1:42:43:ASP:OD1	1:42:71:ARG:NH2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:52:26:GLU:OE2	3:a5:2:THR:N	2.42	0.53
13:52:302:CYC:NC	13:52:302:CYC:HMD1	2.24	0.53
8:A2:81:CYS:HA	13:A2:201:CYC:HHH	1.90	0.53
10:N2:364:ALA:HB2	10:N2:440:PHE:HB3	1.90	0.53
8:T2:12:SER:OG	8:T2:17:LYS:O	2.25	0.53
9:f2:89:LEU:HB2	9:f2:133:LEU:HD21	1.90	0.53
2:F3:23:THR:HA	2:K3:5:PRO:HG3	1.89	0.53
2:I3:78:THR:OG1	2:I3:80:GLU:OE1	2.25	0.53
2:N4:18:ARG:NH2	2:U4:105:THR:OG1	2.40	0.53
13:X4:201:CYC:HB	13:X4:201:CYC:HMA3	1.74	0.53
13:X4:201:CYC:NC	13:X4:201:CYC:HMD1	2.22	0.53
5:Z4:262:VAL:HG11	5:Z4:270:THR:HG21	1.89	0.53
2:K5:74:ASN:HA	13:K5:201:CYC:HBD2	1.90	0.53
3:V5:152:GLY:HA3	13:V5:202:CYC:HMD2	1.89	0.53
3:V6:150:THR:O	13:V6:202:CYC:NC	2.40	0.53
2:W6:33:ARG:NH2	2:W6:34:GLN:OE1	2.41	0.53
2:K7:118:GLU:OE1	2:K7:118:GLU:N	2.36	0.53
13:N7:201:CYC:HMB2	3:O7:77:ASN:HD21	1.74	0.53
2:R7:78:THR:OG1	2:R7:80:GLU:OE1	2.25	0.53
3:V7:52:ILE:HD11	3:V7:142:ILE:HD12	1.90	0.53
13:B1:201:CYC:OB	3:C1:75:TYR:O	2.26	0.53
3:P1:84:LEU:HD13	2:T1:122:THR:HG21	1.90	0.53
2:S1:67:THR:HG22	2:S1:76:ALA:H	1.74	0.53
2:W1:25:LEU:HD22	3:X1:39:ILE:HG23	1.90	0.53
9:G2:25:ARG:HH22	9:J2:3:ILE:HD11	1.73	0.53
8:T2:81:CYS:HA	13:T2:201:CYC:HAC1	1.89	0.53
8:a2:57:ALA:HA	8:a2:61:LEU:HB2	1.91	0.53
8:d2:74:THR:HG22	8:d2:76:ARG:H	1.73	0.53
8:l2:43:THR:O	8:l2:47:ASN:ND2	2.42	0.53
12:t2:105:GLU:HA	12:t2:109:LEU:HB3	1.90	0.53
3:O3:17:GLY:HA3	3:X3:70:PRO:HB3	1.89	0.53
2:U3:78:THR:HG23	2:U3:81:GLY:H	1.73	0.53
2:N4:1:MET:SD	3:V4:2:THR:N	2.81	0.53
2:N5:1:MET:N	3:V5:2:THR:OG1	2.42	0.53
3:P5:85:ARG:NE	4:Y5:238:ARG:HH21	2.07	0.53
2:R6:134:LEU:HB3	2:R6:155:ILE:HG23	1.91	0.53
5:Z6:106:ARG:HD3	5:Z6:152:ARG:HH21	1.72	0.53
13:a6:202:CYC:NB	13:a6:202:CYC:HMA3	2.24	0.53
3:E7:16:ARG:NE	3:E7:18:GLU:OE2	2.37	0.53
2:G7:26:GLN:NE2	2:H7:103:GLY:O	2.41	0.53
3:M7:87:MET:HG3	13:M7:201:CYC:HBC1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V7:109:ARG:HG2	5:Z7:14:PRO:HG3	1.90	0.53
1:A1:53:ILE:O	1:A1:110:ARG:HD3	2.08	0.53
3:O1:96:TYR:OH	2:S1:18:ARG:O	2.24	0.53
1:22:85:LEU:HD13	1:22:138:ILE:HD12	1.91	0.53
13:B2:202:CYC:HBB1	9:I2:107:ILE:HG22	1.91	0.53
12:S2:107:ILE:HA	8:X2:74:THR:HG23	1.90	0.53
13:g2:201:CYC:HB	13:g2:201:CYC:HMA3	1.73	0.53
9:k2:91:LEU:HD11	9:k2:107:ILE:HB	1.89	0.53
9:s2:1:MET:HB3	9:s2:102:THR:HG21	1.90	0.53
8:y2:1:MET:HG3	8:y2:103:ILE:HB	1.91	0.53
3:C3:63:GLU:HG3	3:C3:64:GLN:HG3	1.89	0.53
3:O3:119:LEU:HD11	5:Z3:286:PRO:HD2	1.91	0.53
2:S3:33:ARG:NH2	2:S3:34:GLN:OE1	2.41	0.53
2:T3:41:ALA:HB2	2:T3:147:SER:HB3	1.90	0.53
2:S4:78:THR:OG1	2:S4:80:GLU:OE1	2.27	0.53
3:V4:93:TYR:CG	3:V4:110:CYS:HB2	2.43	0.53
3:C5:154:CYS:SG	13:C5:202:CYC:OC	2.67	0.53
2:R5:128:SER:O	2:R5:132:GLU:HG3	2.09	0.53
2:B6:122:THR:HG21	3:C6:84:LEU:HD13	1.90	0.53
3:C6:154:CYS:SG	13:C6:202:CYC:OC	2.64	0.53
3:L7:91:LEU:HB2	3:L7:135:MET:HE3	1.90	0.53
2:S7:18:ARG:NH2	2:T7:105:THR:OG1	2.42	0.53
2:S7:18:ARG:NH1	2:T7:157:TYR:OH	2.39	0.53
3:V7:89:ILE:HD13	13:V7:201:CYC:HBB3	1.91	0.53
3:E1:149:ILE:HG21	13:E1:201:CYC:HMC3	1.90	0.53
13:N1:201:CYC:OB	3:O1:75:TYR:O	2.26	0.53
7:12:93:PRO:HG2	9:f2:76:ASP:HB2	1.91	0.53
1:32:85:LEU:HD13	1:32:138:ILE:HD12	1.91	0.53
9:D2:16:ARG:O	8:F2:94:TYR:OH	2.20	0.53
11:P2:95:TYR:OH	9:U2:16:ARG:O	2.26	0.53
9:s2:81:CYS:SG	13:s2:201:CYC:HAC2	2.48	0.53
3:D4:96:TYR:OH	2:I4:18:ARG:O	2.24	0.53
2:R4:113:LEU:HD11	2:R4:161:ALA:HB1	1.91	0.53
13:S4:201:CYC:O2D	3:X4:58:ARG:NH1	2.41	0.53
3:D5:77:ASN:ND2	2:H5:112:LEU:O	2.35	0.53
3:O5:17:GLY:HA3	3:X5:70:PRO:HB3	1.91	0.53
1:A6:43:ASP:OD1	1:A6:71:ARG:NH2	2.32	0.53
3:J7:84:LEU:HD13	2:K7:122:THR:HG21	1.91	0.53
3:Q7:109:ARG:HD3	4:Y7:261:HIS:HB3	1.90	0.53
5:Z1:41:ARG:NH2	5:Z1:175:TYR:O	2.40	0.53
1:22:28:PRO:O	1:22:30:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:32:301:CYC:H3C	3:D3:128:VAL:HG22	1.90	0.53
9:E2:81:CYS:SG	13:E2:201:CYC:HAC2	2.49	0.53
8:g2:44:ILE:HD11	8:g2:137:THR:HG23	1.91	0.53
12:t2:90:ARG:HD3	12:t2:94:TYR:CZ	2.44	0.53
3:V3:72:GLY:O	3:V3:79:ARG:NH2	2.36	0.53
3:M4:89:ILE:HG12	3:M4:92:ARG:HH21	1.72	0.53
13:a5:202:CYC:HMA3	13:a5:202:CYC:NB	2.24	0.53
2:G6:103:GLY:O	2:H6:26:GLN:NE2	2.42	0.53
2:H6:78:THR:OG1	2:H6:80:GLU:OE1	2.27	0.53
3:V6:78:ARG:NH1	13:V6:201:CYC:O1D	2.42	0.53
2:U7:78:THR:HG23	2:U7:81:GLY:H	1.74	0.53
2:T1:42:ALA:HB1	2:T1:97:THR:HG23	1.91	0.53
5:Z1:142:THR:HG21	5:Z1:152:ARG:HD2	1.90	0.53
1:42:191:PHE:O	1:42:193:LYS:N	2.41	0.53
10:N2:158:SER:HA	13:N2:802:CYC:HH2	1.91	0.53
9:Q2:22:GLU:HG3	9:Q2:25:ARG:NH2	2.24	0.53
9:R2:14:GLU:HG3	9:R2:16:ARG:HG2	1.90	0.53
13:X2:201:CYC:HC	13:X2:201:CYC:HMD1	1.74	0.53
8:d2:74:THR:HB	8:d2:77:ARG:HD3	1.90	0.53
12:t2:16:ARG:NH2	12:t2:22:GLU:OE2	2.35	0.53
12:t2:113:ARG:HA	12:t2:123:LEU:HD21	1.91	0.53
2:G4:122:THR:HG21	3:L4:84:LEU:HD13	1.91	0.53
3:L4:91:LEU:HB2	3:L4:135:MET:HE3	1.91	0.53
2:N4:9:ALA:HB1	2:N4:24:GLU:HG3	1.91	0.53
3:Q4:95:THR:HG22	2:T4:20:LEU:HD12	1.90	0.53
3:M5:78:ARG:NH1	13:M5:201:CYC:O1D	2.38	0.53
3:O5:106:LEU:HG	3:O5:111:LEU:HD22	1.89	0.53
3:C6:119:LEU:HD22	3:O6:122:GLY:HA2	1.90	0.53
3:X6:85:ARG:HG3	5:Z6:122:GLU:HG2	1.91	0.53
1:A1:179:PRO:HB2	3:a1:121:LEU:HD21	1.91	0.53
2:U1:112:LEU:HD23	2:U1:158:LEU:HD21	1.91	0.53
3:a1:154:CYS:SG	13:a1:202:CYC:HBC2	2.49	0.53
1:52:53:ILE:HD11	1:52:81:ILE:HG23	1.91	0.53
9:D2:128:GLU:OE1	9:D2:131:ARG:NH1	2.41	0.53
10:o2:300:ILE:HG22	10:o2:306:GLN:HB2	1.91	0.53
12:t2:18:PRO:HD3	8:u2:94:TYR:HE1	1.73	0.53
8:u2:113:LYS:NZ	8:u2:160:LEU:O	2.36	0.53
9:x2:134:LYS:HB2	9:x2:153:PHE:HB3	1.91	0.53
3:E3:21:SER:H	3:E3:24:GLN:HE21	1.56	0.53
2:G3:33:ARG:NH1	2:G3:146:ASP:OD2	2.42	0.53
2:G3:122:THR:HG21	3:L3:84:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M3:95:THR:HG22	2:R3:20:LEU:HD12	1.91	0.53
2:S3:108:ILE:HG22	2:S3:113:LEU:HG	1.91	0.53
5:Z3:222:ARG:HA	5:Z3:287:ALA:HB1	1.90	0.53
13:Z3:301:CYC:HB	13:Z3:301:CYC:CMA	2.22	0.53
3:O4:37:LYS:NZ	13:T4:201:CYC:O1D	2.40	0.53
3:X4:128:VAL:HG22	13:X4:201:CYC:H3C	1.90	0.53
5:Z4:240:VAL:HG12	5:Z4:284:VAL:HG22	1.90	0.53
3:C5:30:ARG:O	3:C5:34:GLU:HG2	2.08	0.53
3:J5:75:TYR:O	13:K5:201:CYC:OB	2.27	0.53
13:J5:202:CYC:NB	13:J5:202:CYC:HMA3	2.23	0.53
2:N5:9:ALA:HB1	2:N5:24:GLU:HG3	1.91	0.53
3:Q5:16:ARG:HG3	3:Q5:18:GLU:HG2	1.90	0.53
2:T5:78:THR:OG1	2:T5:80:GLU:OE1	2.27	0.53
3:E6:75:TYR:O	13:F6:201:CYC:OB	2.27	0.53
3:O6:119:LEU:HD11	5:Z6:286:PRO:HD2	1.91	0.53
2:I1:95:ILE:HG22	2:I1:108:ILE:HD13	1.91	0.53
3:V1:115:ARG:NH2	3:V1:173:ALA:O	2.36	0.53
5:Z1:271:LEU:HD12	5:Z1:281:VAL:HG21	1.91	0.53
8:B2:74:THR:HG23	9:I2:107:ILE:HA	1.90	0.53
10:N2:650:GLU:OE2	10:N2:664:ARG:NH2	2.34	0.53
9:R2:104:ILE:HG21	9:R2:156:VAL:HG22	1.89	0.53
6:Z2:5:ARG:NH2	6:Z2:54:GLU:OE1	2.40	0.53
10:o2:178:PRO:HB2	10:o2:232:VAL:HG11	1.90	0.53
10:o2:395:TYR:OH	10:o2:410:GLU:OE1	2.23	0.53
9:s2:2:SER:N	9:s2:5:SER:OG	2.38	0.53
9:v2:126:VAL:HG22	13:v2:201:CYC:H3C	1.90	0.53
3:X3:75:TYR:HB3	3:X3:79:ARG:HH21	1.73	0.53
2:G4:85:CYS:HA	13:G4:201:CYC:HH2	1.91	0.53
3:a4:160:GLU:HG2	3:a4:164:TYR:CE2	2.44	0.53
13:a4:202:CYC:NB	13:a4:202:CYC:HMA3	2.24	0.53
3:D5:96:TYR:OH	2:I5:18:ARG:O	2.21	0.53
3:M6:95:THR:HG22	2:R6:20:LEU:HD12	1.91	0.53
2:N6:78:THR:OG1	2:N6:80:GLU:OE1	2.27	0.53
3:Q6:48:ASN:HB2	3:Q6:142:ILE:HD13	1.90	0.53
3:Q6:75:TYR:O	13:R6:201:CYC:OB	2.27	0.53
13:V6:201:CYC:NC	13:V6:201:CYC:HMD1	2.24	0.53
5:Z7:262:VAL:HG11	5:Z7:270:THR:HG21	1.91	0.53
2:F1:85:CYS:HB2	13:F1:201:CYC:H2C	1.91	0.52
3:a1:9:VAL:HG11	3:a1:28:LEU:HD11	1.89	0.52
1:22:198:GLY:H	9:G2:68:PRO:HB3	1.74	0.52
9:E2:8:ILE:HD12	8:L2:0:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T2:104:LEU:HD11	8:T2:152:TYR:HB3	1.91	0.52
13:T2:201:CYC:NC	13:T2:201:CYC:HMD1	2.24	0.52
3:P3:27:ALA:HA	3:P3:30:ARG:HE	1.74	0.52
3:Q5:152:GLY:O	13:Q5:202:CYC:OC	2.27	0.52
3:X5:78:ARG:NH2	13:X5:201:CYC:O1D	2.42	0.52
13:X6:201:CYC:HB	13:X6:201:CYC:CMA	2.22	0.52
2:H7:134:LEU:HB3	2:H7:155:ILE:HG23	1.92	0.52
2:N7:63:LYS:HD2	2:N7:132:GLU:HG3	1.91	0.52
3:O7:119:LEU:HD11	5:Z7:286:PRO:HD2	1.92	0.52
3:P7:146:ARG:NE	3:P7:151:GLN:OE1	2.34	0.52
13:a7:201:CYC:HB	13:a7:201:CYC:CMA	2.22	0.52
2:B1:85:CYS:HA	13:B1:201:CYC:HHH	1.91	0.52
3:X1:109:ARG:NH1	5:Z1:90:ASN:O	2.39	0.52
3:a1:34:GLU:OE1	3:a1:37:LYS:NZ	2.41	0.52
1:32:179:PRO:HB2	3:a3:121:LEU:HD21	1.91	0.52
1:42:56:HIS:HB3	3:a4:85:ARG:HH11	1.74	0.52
1:42:78:ARG:NH1	1:42:143:ASN:OD1	2.42	0.52
8:C2:3:ASP:OD2	9:I2:5:SER:OG	2.25	0.52
10:N2:157:LYS:NZ	13:N2:802:CYC:O1A	2.40	0.52
3:Q3:115:ARG:NH2	3:Q3:173:ALA:O	2.41	0.52
3:M5:76:THR:HG22	3:M5:78:ARG:H	1.74	0.52
1:A6:69:GLN:HE21	5:Z6:225:GLY:HA3	1.74	0.52
2:K6:20:LEU:HD12	3:L6:95:THR:HG22	1.91	0.52
2:F7:78:THR:OG1	2:F7:80:GLU:OE1	2.26	0.52
13:V7:201:CYC:NC	13:V7:201:CYC:HMD1	2.24	0.52
2:W7:11:ALA:HB1	5:Z7:88:TYR:CZ	2.44	0.52
3:C1:85:ARG:NH2	13:C1:201:CYC:O2A	2.42	0.52
2:I1:134:LEU:HB3	2:I1:155:ILE:HG23	1.92	0.52
2:K1:20:LEU:HD12	3:L1:95:THR:HG22	1.91	0.52
1:52:238:ASP:HA	9:I2:52:LYS:HD3	1.90	0.52
9:D2:1:MET:HB2	9:D2:5:SER:HB3	1.91	0.52
9:f2:113:ARG:NH2	9:f2:161:SER:OXT	2.40	0.52
8:m2:126:THR:HG23	13:m2:201:CYC:HBC3	1.91	0.52
2:H3:31:ARG:NH2	2:H3:101:VAL:O	2.42	0.52
3:J3:84:LEU:HD13	2:K3:122:THR:HG21	1.92	0.52
3:M3:1:MET:HG3	4:Y3:218:ARG:HH21	1.73	0.52
13:N3:201:CYC:HMB2	3:O3:77:ASN:HD21	1.75	0.52
3:P4:84:LEU:HD13	2:T4:122:THR:HG21	1.90	0.52
3:X4:3:PHE:HA	3:X4:7:THR:HG23	1.92	0.52
5:Z5:240:VAL:HG12	5:Z5:284:VAL:HG22	1.92	0.52
1:A6:53:ILE:HD11	1:A6:81:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:123:ILE:HG23	13:A6:301:CYC:HMA1	1.91	0.52
2:B6:27:VAL:HG22	2:I6:27:VAL:HG22	1.92	0.52
3:Q6:128:VAL:HG22	13:Q6:201:CYC:HBC3	1.92	0.52
5:Z6:102:HIS:NE2	5:Z6:179:ASP:OD2	2.38	0.52
5:Z6:240:VAL:HG12	5:Z6:284:VAL:HG22	1.92	0.52
3:D7:84:LEU:HD13	2:H7:122:THR:HG21	1.91	0.52
3:J7:72:GLY:O	3:J7:79:ARG:NH2	2.38	0.52
5:Z7:67:ILE:HB	5:Z7:71:ASP:HB2	1.91	0.52
1:42:26:GLU:OE2	3:a4:2:THR:N	2.42	0.52
8:B2:15:GLN:HG3	8:B2:17:LYS:H	1.73	0.52
8:B2:56:VAL:HG22	8:B2:60:LEU:HD12	1.90	0.52
8:T2:30:TYR:OH	8:T2:97:LEU:O	2.26	0.52
9:U2:102:THR:HA	9:U2:105:GLU:HG2	1.90	0.52
8:c2:5:ILE:HD13	8:c2:27:LEU:HD22	1.90	0.52
10:o2:359:ARG:NE	10:o2:391:GLU:OE2	2.36	0.52
3:C3:3:PHE:O	3:C3:104:SER:OG	2.28	0.52
3:L3:9:VAL:HG21	3:L3:28:LEU:HD11	1.91	0.52
5:Z3:55:LEU:HD21	5:Z3:79:SER:HB3	1.91	0.52
3:D4:149:ILE:HD13	13:D4:201:CYC:H3C	1.92	0.52
2:U5:78:THR:OG1	2:U5:80:GLU:OE1	2.28	0.52
2:F6:3:LYS:HG3	2:K6:18:ARG:HH21	1.74	0.52
2:R7:85:CYS:HA	13:R7:201:CYC:HAC2	1.91	0.52
2:W7:112:LEU:HD23	2:W7:158:LEU:HD21	1.90	0.52
3:D1:57:ALA:HB2	3:D1:87:MET:HE1	1.92	0.52
2:I1:48:ASN:OD1	2:I1:51:SER:OG	2.27	0.52
2:R1:85:CYS:HA	13:R1:201:CYC:HHD	1.91	0.52
3:X1:79:ARG:HD2	13:X1:201:CYC:HBD2	1.91	0.52
1:32:186:ARG:HH11	1:32:192:PRO:HG3	1.74	0.52
13:52:301:CYC:HMD1	13:52:301:CYC:NC	2.24	0.52
8:F2:44:ILE:HD11	8:F2:137:THR:HG23	1.92	0.52
6:Z2:5:ARG:HH12	6:Z2:52:LYS:HE2	1.74	0.52
8:p2:18:TYR:OH	9:s2:86:ASP:OD1	2.23	0.52
2:I3:95:ILE:HG22	2:I3:108:ILE:HD13	1.91	0.52
3:O4:1:MET:SD	3:O4:1:MET:N	2.72	0.52
2:W4:85:CYS:HA	13:W4:201:CYC:HHD	1.90	0.52
5:Z4:41:ARG:NH2	5:Z4:175:TYR:O	2.42	0.52
13:a4:201:CYC:HB	13:a4:201:CYC:HMA1	1.74	0.52
2:F5:74:ASN:ND2	2:F5:124:ASP:OD2	2.42	0.52
2:N5:78:THR:OG1	2:N5:80:GLU:OE1	2.28	0.52
2:S5:18:ARG:NH2	2:T5:105:THR:OG1	2.43	0.52
5:Z5:55:LEU:HD21	5:Z5:79:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J6:202:CYC:HMA3	13:J6:202:CYC:NB	2.25	0.52
2:N6:23:THR:HA	2:U6:5:PRO:HG3	1.92	0.52
2:S7:94:ARG:NH2	3:X7:75:TYR:OH	2.31	0.52
2:B1:26:GLN:HE22	2:I1:34:GLN:HG2	1.75	0.52
8:L2:2:ASP:OD1	8:L2:4:ILE:N	2.41	0.52
8:O2:38:VAL:HG11	9:R2:27:LYS:HG3	1.92	0.52
9:k2:109:ILE:HG23	9:k2:159:ALA:HB1	1.92	0.52
13:l2:201:CYC:HB	13:l2:201:CYC:CMA	2.22	0.52
10:o2:249:ARG:HB3	10:o2:254:GLN:HG3	1.92	0.52
10:o2:336:ARG:NH1	10:o2:341:ASP:OD2	2.43	0.52
12:t2:106:SER:O	8:y2:76:ARG:NH1	2.42	0.52
3:D3:20:LEU:HD22	2:I3:101:VAL:HG21	1.92	0.52
2:G4:138:LYS:HB2	2:G4:155:ILE:HG21	1.91	0.52
3:V5:75:TYR:OH	2:W5:94:ARG:NH2	2.32	0.52
13:B6:201:CYC:HMB2	3:C6:77:ASN:HD21	1.73	0.52
2:F6:33:ARG:NH2	2:F6:34:GLN:OE1	2.43	0.52
3:Q6:95:THR:HG22	2:T6:20:LEU:HD12	1.91	0.52
2:R6:134:LEU:HB2	2:R6:159:ILE:HD11	1.92	0.52
9:D2:29:PHE:HE1	9:D2:99:GLY:HA3	1.74	0.52
9:H2:64:ASP:OD1	9:H2:65:VAL:N	2.43	0.52
10:N2:522:ALA:O	10:N2:539:ARG:NH1	2.42	0.52
11:P2:12:TYR:CZ	11:P2:23:ALA:HB2	2.45	0.52
9:R2:37:LEU:HD23	9:R2:97:VAL:HG22	1.92	0.52
9:W2:11:ALA:HB2	9:W2:18:LEU:HD23	1.90	0.52
8:m2:2:GLN:OE1	11:q2:162:ARG:NH1	2.43	0.52
10:o2:158:SER:HA	13:o2:801:CYC:HHD	1.92	0.52
12:t2:128:GLU:OE1	12:t2:131:ARG:NH1	2.43	0.52
8:w2:104:LEU:HD11	8:w2:152:TYR:HB3	1.90	0.52
2:F3:85:CYS:HB2	13:F3:201:CYC:H2C	1.92	0.52
2:H3:134:LEU:HB3	2:H3:155:ILE:HG23	1.92	0.52
3:O3:149:ILE:HD13	13:T3:201:CYC:H3C	1.91	0.52
13:J4:202:CYC:NB	13:J4:202:CYC:HMA3	2.25	0.52
3:M4:39:ILE:HG23	2:R4:25:LEU:HD22	1.90	0.52
2:U4:74:ASN:HA	13:U4:201:CYC:HBD2	1.90	0.52
2:W4:20:LEU:HD12	3:X4:95:THR:HG22	1.91	0.52
3:a4:34:GLU:OE1	3:a4:37:LYS:NZ	2.43	0.52
13:B5:201:CYC:OB	3:C5:75:TYR:O	2.28	0.52
2:U5:74:ASN:ND2	2:U5:124:ASP:OD2	2.42	0.52
1:A6:127:LEU:HD13	3:D6:89:ILE:HD12	1.91	0.52
2:I6:91:TYR:O	2:I6:95:ILE:HG12	2.10	0.52
2:T6:31:ARG:NH2	2:T6:101:VAL:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B7:25:LEU:HD22	3:J7:39:ILE:HG23	1.92	0.52
3:L7:78:ARG:NH1	13:L7:201:CYC:O1D	2.40	0.52
3:O7:83:CYS:HA	13:Z7:301:CYC:HAC2	1.92	0.52
13:C1:202:CYC:HMA3	13:C1:202:CYC:NB	2.25	0.52
2:H1:33:ARG:NH1	2:H1:146:ASP:OD2	2.42	0.52
2:S1:18:ARG:NH1	2:T1:109:ASP:OD2	2.43	0.52
13:X1:201:CYC:HB	13:X1:201:CYC:CMA	2.19	0.52
8:F2:75:THR:HG22	9:G2:115:MET:HE2	1.92	0.52
13:M2:201:CYC:NC	13:M2:201:CYC:HMD1	2.24	0.52
8:O2:56:VAL:HG12	8:O2:61:LEU:HD13	1.92	0.52
9:k2:46:SER:O	9:k2:50:ILE:HG22	2.10	0.52
10:o2:434:PRO:HD2	8:p2:111:GLY:HA3	1.91	0.52
12:t2:64:ASP:N	12:t2:64:ASP:OD1	2.43	0.52
3:L5:116:GLU:HG3	5:Z5:212:VAL:HG22	1.92	0.52
3:D6:75:TYR:OH	2:H6:94:ARG:NH2	2.33	0.52
3:P6:84:LEU:HD13	2:T6:122:THR:HG21	1.89	0.52
3:P6:85:ARG:NE	4:Y6:238:ARG:HH21	2.08	0.52
2:R6:78:THR:OG1	2:R6:80:GLU:OE1	2.28	0.52
5:Z6:262:VAL:HG11	5:Z6:270:THR:HG21	1.91	0.52
3:a6:9:VAL:HG11	3:a6:28:LEU:HD11	1.90	0.52
2:F7:33:ARG:NH2	2:F7:34:GLN:OE1	2.41	0.52
3:L7:76:THR:HB	3:L7:79:ARG:HG3	1.91	0.52
2:W7:108:ILE:HG22	2:W7:113:LEU:HG	1.92	0.52
13:X7:201:CYC:HB	13:X7:201:CYC:CMA	2.18	0.52
1:A1:41:GLN:HG2	3:L1:1:MET:HA	1.91	0.52
8:C2:76:ARG:NH1	9:H2:106:GLU:OE2	2.42	0.52
9:D2:81:CYS:SG	13:D2:201:CYC:HAC2	2.50	0.52
8:F2:100:ASP:OD1	8:F2:101:THR:N	2.42	0.52
3:M3:72:GLY:O	3:M3:79:ARG:NH2	2.42	0.52
3:Q3:76:THR:HG23	2:R3:111:TYR:HA	1.92	0.52
2:W3:134:LEU:HB3	2:W3:155:ILE:HG23	1.92	0.52
3:M4:4:ASP:H	3:M4:7:THR:HG1	1.58	0.52
3:P4:130:GLU:OE2	3:P4:134:LYS:NZ	2.43	0.52
5:Z4:222:ARG:HA	5:Z4:287:ALA:HB1	1.92	0.52
3:C6:30:ARG:O	3:C6:34:GLU:HG2	2.10	0.52
3:C6:89:ILE:HD13	13:C6:201:CYC:HBB3	1.91	0.52
3:D6:44:ARG:HH12	3:D6:145:ASP:HB3	1.75	0.52
1:A1:186:ARG:HG2	1:A1:192:PRO:HD3	1.93	0.52
2:B1:33:ARG:NH1	2:B1:146:ASP:OD2	2.42	0.52
3:M1:3:PHE:O	3:M1:104:SER:OG	2.27	0.52
3:O1:149:ILE:HD13	13:T1:201:CYC:H3C	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R1:113:LEU:HD11	2:R1:161:ALA:HB1	1.91	0.52
8:B2:35:GLU:OE1	8:B2:39:ARG:NH2	2.43	0.52
9:I2:145:ASP:N	9:I2:145:ASP:OD1	2.43	0.52
8:g2:40:ALA:O	8:g2:44:ILE:HG12	2.10	0.52
13:P3:202:CYC:HMD3	13:P3:202:CYC:NC	2.24	0.52
3:a3:12:GLN:HB3	3:a3:16:ARG:HH12	1.75	0.52
3:O4:1:MET:SD	2:S4:2:SER:N	2.82	0.52
5:Z5:211:TYR:HB2	5:Z5:282:VAL:HG21	1.92	0.52
3:D6:8:LYS:NZ	3:D6:12:GLN:OE1	2.43	0.52
3:E7:2:THR:HG23	3:E7:3:PHE:HD2	1.75	0.52
3:X7:61:PHE:HB3	3:X7:68:ILE:HD13	1.92	0.52
3:a7:111:LEU:HD22	3:a7:171:ALA:HB3	1.91	0.52
3:J1:58:ARG:NH1	13:K1:201:CYC:O2D	2.43	0.51
3:X1:72:GLY:O	3:X1:79:ARG:NH2	2.41	0.51
8:C2:103:ILE:HG23	8:C2:107:ARG:HD2	1.92	0.51
9:H2:16:ARG:NH1	9:H2:17:TYR:O	2.41	0.51
10:N2:520:GLN:NE2	10:N2:524:GLY:O	2.43	0.51
9:Q2:22:GLU:OE1	9:Q2:22:GLU:N	2.43	0.51
9:R2:2:SER:N	9:R2:5:SER:OG	2.39	0.51
12:S2:2:THR:HG22	12:S2:98:ALA:HB1	1.92	0.51
8:g2:3:ASP:HA	8:g2:98:ALA:HB1	1.91	0.51
9:i2:105:GLU:HA	9:i2:109:ILE:HB	1.92	0.51
10:o2:27:GLN:OE1	9:r2:10:ASN:ND2	2.44	0.51
3:D3:146:ARG:NE	3:D3:151:GLN:OE1	2.40	0.51
3:Q3:16:ARG:HG3	3:Q3:18:GLU:HG2	1.92	0.51
3:L4:116:GLU:HG3	5:Z4:212:VAL:HG22	1.92	0.51
13:N5:201:CYC:OB	3:O5:75:TYR:O	2.28	0.51
3:M6:44:ARG:NH2	3:M6:145:ASP:O	2.43	0.51
5:Z6:74:ARG:NH2	5:Z6:135:ASP:OD1	2.43	0.51
2:F7:85:CYS:HB2	13:F7:201:CYC:H2C	1.92	0.51
3:P7:95:THR:HG22	2:U7:20:LEU:HD12	1.92	0.51
3:X7:75:TYR:HB3	3:X7:79:ARG:HH21	1.75	0.51
3:Q1:76:THR:HG23	2:R1:111:TYR:HA	1.92	0.51
2:T1:31:ARG:NH2	2:T1:101:VAL:O	2.43	0.51
2:W1:4:THR:HG21	3:X1:7:THR:HG22	1.93	0.51
2:W1:16:GLN:HG3	2:W1:18:ARG:HG2	1.93	0.51
10:N2:345:ASN:OD1	8:O2:107:ARG:NH2	2.43	0.51
3:M3:85:ARG:HH12	13:M3:201:CYC:HB	1.58	0.51
13:X3:201:CYC:OB	5:Z3:92:GLN:HB3	2.09	0.51
3:E5:146:ARG:HB3	3:E5:151:GLN:HE21	1.74	0.51
2:I5:48:ASN:OD1	2:I5:51:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O5:109:ARG:NH1	2:S5:14:ASP:OD2	2.42	0.51
2:U5:50:ASP:O	2:U5:54:ASN:ND2	2.35	0.51
3:E6:39:ILE:HG23	2:H6:25:LEU:HD22	1.91	0.51
2:K6:31:ARG:NH2	2:K6:101:VAL:O	2.43	0.51
3:M6:20:LEU:HD13	2:R6:101:VAL:HG21	1.92	0.51
3:O7:37:LYS:NZ	13:T7:201:CYC:O1D	2.38	0.51
2:H1:108:ILE:HG22	2:H1:113:LEU:HG	1.91	0.51
2:T1:9:ALA:HB2	2:T1:27:VAL:HG11	1.92	0.51
8:d2:17:LYS:O	9:j2:94:TYR:OH	2.22	0.51
8:u2:1:MET:N	8:u2:1:MET:SD	2.83	0.51
8:u2:104:LEU:HD11	8:u2:152:TYR:HB3	1.91	0.51
3:M3:131:GLY:O	3:M3:135:MET:HG3	2.10	0.51
3:E4:84:LEU:HD13	2:F4:122:THR:HG21	1.91	0.51
2:F4:85:CYS:HB2	13:F4:201:CYC:H2C	1.92	0.51
2:G4:23:THR:HA	2:H4:5:PRO:HG3	1.92	0.51
3:O4:146:ARG:HH21	3:O4:151:GLN:HB3	1.74	0.51
2:R4:128:SER:O	2:R4:132:GLU:HG3	2.09	0.51
2:U4:121:LYS:NZ	2:W4:163:SER:OXT	2.40	0.51
3:X4:16:ARG:NE	3:X4:18:GLU:OE2	2.44	0.51
2:G5:113:LEU:HD11	2:G5:161:ALA:HB1	1.93	0.51
2:I5:16:GLN:OE1	2:I5:18:ARG:NE	2.34	0.51
2:I5:78:THR:HG23	2:I5:81:GLY:H	1.75	0.51
5:Z5:173:ARG:NH1	5:Z5:203:VAL:O	2.35	0.51
1:A6:167:ARG:NH1	13:A6:302:CYC:O2D	2.41	0.51
4:Y6:218:ARG:HG2	4:Y6:250:TYR:HB3	1.92	0.51
3:C7:92:ARG:O	3:C7:95:THR:OG1	2.25	0.51
13:F7:202:CYC:OC	3:L7:152:GLY:O	2.28	0.51
3:M7:85:ARG:HH12	13:M7:201:CYC:HB	1.56	0.51
3:Q7:76:THR:HG23	2:R7:111:TYR:HA	1.92	0.51
3:E1:39:ILE:HG23	2:H1:25:LEU:HD22	1.91	0.51
3:M1:18:GLU:O	2:R1:98:TYR:OH	2.28	0.51
7:12:93:PRO:HB3	7:12:97:LEU:HD21	1.93	0.51
1:32:35:ASP:OD1	5:Z3:254:ARG:NH1	2.43	0.51
1:32:123:ILE:HG23	13:32:301:CYC:HMA1	1.92	0.51
9:G2:14:GLU:OE1	9:G2:16:ARG:NE	2.33	0.51
10:N2:372:ASP:OD1	8:O2:83:ARG:NH1	2.38	0.51
11:P2:3:ASP:N	11:P2:6:SER:OG	2.43	0.51
13:T2:201:CYC:HMD1	13:T2:201:CYC:HC	1.75	0.51
8:V2:60:LEU:HD13	8:V2:72:MET:HE1	1.93	0.51
8:p2:38:VAL:HG13	9:s2:23:LEU:HB3	1.91	0.51
8:w2:35:GLU:HG2	8:w2:36:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G3:84:LYS:NZ	13:G3:201:CYC:O1A	2.41	0.51
2:W3:108:ILE:HG22	2:W3:113:LEU:HG	1.91	0.51
4:Y3:225:GLN:HG2	4:Y3:245:THR:HG22	1.92	0.51
3:M4:57:ALA:HB2	3:M4:87:MET:HE1	1.93	0.51
4:Y4:229:GLN:HB2	4:Y4:242:SER:HA	1.92	0.51
2:G5:74:ASN:HA	13:G5:201:CYC:HBD2	1.92	0.51
2:S5:74:ASN:HA	13:S5:201:CYC:HBD2	1.93	0.51
2:W5:20:LEU:HD12	3:X5:95:THR:HG22	1.92	0.51
2:H6:63:LYS:HG2	2:H6:132:GLU:HG3	1.92	0.51
3:E7:72:GLY:O	3:E7:79:ARG:NH2	2.43	0.51
3:V7:149:ILE:HG21	13:V7:202:CYC:HMC3	1.92	0.51
3:E1:75:TYR:O	13:F1:201:CYC:OB	2.28	0.51
1:42:17:VAL:O	1:42:161:ARG:NH1	2.44	0.51
6:Y2:5:ARG:HB2	6:Y2:56:ALA:HB2	1.92	0.51
8:l2:65:ILE:HG22	8:l2:72:MET:HB2	1.92	0.51
10:o2:682:SER:HB2	10:o2:685:VAL:HG23	1.91	0.51
11:q2:12:TYR:CZ	11:q2:23:ALA:HB2	2.45	0.51
13:v2:201:CYC:HB	13:v2:201:CYC:CMA	2.23	0.51
6:z2:10:LEU:HD13	6:z2:48:GLY:HA3	1.90	0.51
2:I3:109:ASP:HA	2:I3:113:LEU:HB2	1.93	0.51
3:O4:25:LEU:HD22	2:S4:43:LYS:HB2	1.93	0.51
3:C5:96:TYR:OH	2:G5:18:ARG:O	2.29	0.51
3:D5:92:ARG:HG2	2:I5:19:PHE:CZ	2.46	0.51
3:M5:131:GLY:O	3:M5:135:MET:HG3	2.10	0.51
2:R5:141:HIS:NE2	2:R5:152:ASN:OD1	2.39	0.51
1:A6:16:ARG:NH2	3:E6:109:ARG:O	2.31	0.51
3:M6:78:ARG:NH1	13:M6:201:CYC:O1D	2.42	0.51
2:F7:109:ASP:HA	2:F7:113:LEU:HB3	1.92	0.51
2:H7:31:ARG:NH2	2:H7:101:VAL:O	2.43	0.51
3:J7:58:ARG:NH1	13:K7:201:CYC:O2D	2.43	0.51
2:G1:85:CYS:HA	13:G1:201:CYC:HHD	1.91	0.51
2:U1:78:THR:OG1	2:U1:80:GLU:OE1	2.28	0.51
3:V1:150:THR:O	13:V1:202:CYC:NC	2.39	0.51
9:R2:89:LEU:HB2	9:R2:133:LEU:HD21	1.92	0.51
9:j2:35:ARG:O	9:j2:39:ILE:HG12	2.11	0.51
9:j2:38:ARG:NH1	9:j2:42:THR:OG1	2.44	0.51
12:t2:14:GLU:HG3	12:t2:16:ARG:HG2	1.91	0.51
9:x2:87:TYR:O	9:x2:91:LEU:HG	2.11	0.51
3:D3:84:LEU:HD13	2:H3:122:THR:HG21	1.91	0.51
2:F4:78:THR:OG1	2:F4:80:GLU:OE1	2.28	0.51
13:V4:201:CYC:NC	13:V4:201:CYC:HMD1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C5:109:ARG:HD3	5:Z5:275:ASN:HB3	1.92	0.51
2:B6:160:ASN:ND2	3:D6:46:THR:O	2.44	0.51
5:Z6:271:LEU:HD12	5:Z6:281:VAL:HG21	1.93	0.51
3:P7:100:THR:HG23	2:U7:10:VAL:HG21	1.93	0.51
3:J1:84:LEU:HD13	2:K1:122:THR:HG21	1.92	0.51
13:42:302:CYC:H3C	3:E4:128:VAL:HG22	1.92	0.51
8:C2:60:LEU:O	8:C2:63:SER:OG	2.27	0.51
9:D2:124:GLU:OE1	9:D2:124:GLU:N	2.43	0.51
8:M2:119:LEU:HD13	13:M2:201:CYC:HBD1	1.92	0.51
9:e2:29:PHE:O	9:e2:36:ARG:NH2	2.32	0.51
12:t2:57:LYS:HB3	12:t2:132:THR:HG21	1.93	0.51
2:G3:74:ASN:O	13:G3:201:CYC:NC	2.41	0.51
3:M3:38:ARG:NH2	3:M3:160:GLU:OE1	2.44	0.51
2:N3:27:VAL:HG22	2:U3:27:VAL:HG22	1.92	0.51
3:D4:43:ASN:HB2	2:I4:25:LEU:HD21	1.92	0.51
2:G4:94:ARG:NH2	3:L4:75:TYR:OH	2.29	0.51
3:L4:67:LEU:HD21	3:L4:127:SER:HB3	1.93	0.51
3:M4:95:THR:HG22	2:R4:20:LEU:HD12	1.93	0.51
2:W4:18:ARG:O	3:X4:96:TYR:OH	2.25	0.51
5:Z4:102:HIS:NE2	5:Z4:179:ASP:OD2	2.41	0.51
3:P5:111:LEU:HD21	3:P5:168:ALA:HA	1.93	0.51
2:W5:99:ALA:HB2	2:W5:108:ILE:HG13	1.93	0.51
3:D6:96:TYR:OH	2:I6:18:ARG:O	2.24	0.51
3:D6:149:ILE:HD13	13:D6:201:CYC:H3C	1.93	0.51
3:Q6:109:ARG:O	4:Y6:261:HIS:ND1	2.44	0.51
5:Z6:201:PRO:HD3	5:Z6:221:MET:HE1	1.91	0.51
3:C7:109:ARG:HD3	5:Z7:275:ASN:HB3	1.92	0.51
3:D7:92:ARG:NH1	3:D7:96:TYR:OH	2.44	0.51
2:G7:23:THR:HA	2:H7:5:PRO:HG3	1.91	0.51
1:A1:84:LEU:O	1:A1:87:SER:OG	2.26	0.51
3:L1:63:GLU:HG3	3:L1:64:GLN:HG3	1.93	0.51
3:M1:76:THR:HG22	3:M1:78:ARG:H	1.76	0.51
2:U1:74:ASN:ND2	2:U1:124:ASP:OD2	2.44	0.51
8:B2:75:THR:HG23	13:B2:202:CYC:HAB2	1.92	0.51
9:J2:153:PHE:O	9:J2:157:ILE:HG12	2.10	0.51
10:N2:327:ARG:HB2	10:N2:387:VAL:HG11	1.92	0.51
11:P2:42:GLU:HG2	9:U2:23:LEU:HD13	1.93	0.51
8:T2:4:ALA:N	8:T2:98:ALA:O	2.44	0.51
8:T2:112:LEU:HG	8:T2:160:LEU:HD21	1.91	0.51
9:W2:36:ARG:NH1	9:W2:148:GLU:OE2	2.42	0.51
9:h2:113:ARG:NH2	9:h2:159:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:s2:128:GLU:OE1	9:s2:131:ARG:NH1	2.44	0.51
9:x2:11:ALA:HB2	9:x2:18:LEU:HD23	1.92	0.51
3:M3:4:ASP:H	3:M3:7:THR:HG1	1.54	0.51
3:O3:107:ASP:HA	3:O3:111:LEU:HB2	1.93	0.51
3:P3:100:THR:HG23	2:U3:10:VAL:HG21	1.91	0.51
2:R3:63:LYS:HD3	2:R3:132:GLU:HG2	1.93	0.51
5:Z3:101:LYS:HD2	5:Z3:171:LEU:HB3	1.93	0.51
2:I4:91:TYR:O	2:I4:95:ILE:HG12	2.11	0.51
3:O4:112:ASN:O	5:Z4:162:SER:OG	2.26	0.51
1:A6:28:PRO:O	1:A6:30:GLN:NE2	2.39	0.51
1:A6:44:GLU:O	1:A6:47:GLN:HG3	2.10	0.51
13:A6:302:CYC:O1A	3:E6:78:ARG:NH2	2.41	0.51
13:C6:201:CYC:HAA1	5:Z6:267:LEU:HD23	1.92	0.51
2:F6:105:THR:OG1	2:K6:18:ARG:NH2	2.43	0.51
3:J6:38:ARG:NH1	3:J6:98:VAL:O	2.33	0.51
2:N6:1:MET:SD	3:V6:2:THR:N	2.84	0.51
3:O6:105:ILE:HD12	3:O6:109:ARG:HG3	1.92	0.51
3:Q6:146:ARG:HB3	3:Q6:151:GLN:HE22	1.76	0.51
3:J7:75:TYR:OH	2:K7:94:ARG:NH2	2.33	0.51
3:L7:116:GLU:OE1	3:L7:116:GLU:N	2.34	0.51
1:42:102:ARG:HH22	1:42:179:PRO:HD2	1.76	0.51
8:B2:44:ILE:HG13	8:B2:149:MET:HE3	1.92	0.51
9:H2:29:PHE:HE1	9:H2:99:GLY:HA3	1.76	0.51
8:X2:144:ASP:N	8:X2:144:ASP:OD1	2.40	0.51
10:o2:354:ARG:HB2	10:o2:423:LEU:HD21	1.93	0.51
6:z2:34:ASP:OD1	6:z2:34:ASP:N	2.43	0.51
2:H3:45:LEU:HD21	2:H3:141:HIS:HB2	1.92	0.51
2:H3:108:ILE:HG22	2:H3:113:LEU:HG	1.93	0.51
3:C4:30:ARG:O	3:C4:34:GLU:HG2	2.11	0.51
3:L4:83:CYS:SG	13:L4:201:CYC:HAC2	2.50	0.51
3:V4:30:ARG:O	3:V4:34:GLU:HG2	2.11	0.51
2:B5:122:THR:HG21	3:C5:84:LEU:HD13	1.93	0.51
3:E5:149:ILE:HG21	13:E5:201:CYC:HMC3	1.93	0.51
2:S5:112:LEU:HD23	2:S5:158:LEU:HD21	1.92	0.51
3:D6:16:ARG:NE	3:D6:18:GLU:OE2	2.44	0.51
2:U6:50:ASP:O	2:U6:54:ASN:ND2	2.33	0.51
3:M7:38:ARG:NH1	3:M7:98:VAL:O	2.36	0.51
3:P7:85:ARG:HD2	4:Y7:238:ARG:HE	1.75	0.51
13:a7:201:CYC:HC	13:a7:201:CYC:HMD1	1.75	0.51
2:K1:39:LEU:HD22	3:L1:25:LEU:HD12	1.92	0.51
3:L1:146:ARG:HH21	3:L1:151:GLN:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A2:1:MET:HE1	8:A2:103:ILE:HD12	1.92	0.51
8:B2:106:GLU:OE1	6:Z2:1:MET:N	2.41	0.51
9:D2:35:ARG:HG3	9:D2:38:ARG:HH21	1.76	0.51
9:Q2:104:ILE:HG21	9:Q2:156:VAL:HG22	1.92	0.51
8:T2:144:ASP:OD1	8:T2:144:ASP:N	2.40	0.51
8:a2:1:MET:HE1	8:a2:103:ILE:HD12	1.93	0.51
9:j2:106:GLU:HB2	10:o2:538:ILE:HG22	1.93	0.51
13:s2:201:CYC:HMA1	13:s2:201:CYC:NB	2.26	0.51
2:S3:31:ARG:NH2	2:S3:101:VAL:O	2.44	0.51
3:D4:77:ASN:HD21	13:H4:201:CYC:HMB2	1.76	0.51
3:M4:76:THR:HG23	2:U4:111:TYR:HA	1.93	0.51
2:N4:23:THR:HA	2:U4:5:PRO:HG3	1.91	0.51
13:N4:201:CYC:OB	3:O4:75:TYR:O	2.28	0.51
2:W4:3:LYS:H	2:W4:106:GLY:HA3	1.76	0.51
3:V5:4:ASP:OD1	3:V5:7:THR:OG1	2.22	0.51
3:V5:92:ARG:O	3:V5:95:THR:OG1	2.25	0.51
1:A6:75:ILE:HB	1:A6:79:ASP:HB2	1.93	0.51
2:T6:41:ALA:HB2	2:T6:147:SER:HB3	1.93	0.51
2:K7:134:LEU:HB3	2:K7:155:ILE:HG23	1.92	0.51
3:P7:77:ASN:ND2	2:T7:112:LEU:O	2.37	0.51
2:U7:149:ASP:HB3	13:V7:202:CYC:HAB2	1.92	0.51
2:W7:16:GLN:HG3	2:W7:18:ARG:HG2	1.93	0.51
13:a7:201:CYC:HMD1	13:a7:201:CYC:NC	2.26	0.51
2:B1:27:VAL:HG22	2:I1:27:VAL:HG22	1.92	0.50
3:L1:34:GLU:HG3	3:L1:37:LYS:HD2	1.92	0.50
3:O1:146:ARG:HH21	3:O1:151:GLN:HB3	1.76	0.50
2:R1:42:ALA:HB1	2:R1:97:THR:HG23	1.93	0.50
1:22:16:ARG:NH2	3:E7:109:ARG:O	2.29	0.50
1:22:224:ARG:NE	9:R2:75:GLU:OE2	2.44	0.50
1:22:231:GLN:NE2	3:D5:16:ARG:O	2.29	0.50
8:F2:40:ALA:O	8:F2:44:ILE:HG12	2.11	0.50
10:N2:391:GLU:OE2	10:N2:405:ARG:NH2	2.45	0.50
8:O2:18:TYR:OH	9:R2:86:ASP:OD1	2.26	0.50
10:o2:466:ALA:HB1	10:o2:468:PHE:HE1	1.76	0.50
9:s2:35:ARG:NH1	9:s2:148:GLU:OE1	2.44	0.50
8:u2:2:GLN:HB2	8:u2:6:THR:HB	1.93	0.50
8:w2:3:ASP:OD2	9:x2:2:SER:OG	2.25	0.50
8:y2:137:THR:HG21	8:y2:149:MET:HG2	1.92	0.50
2:B3:122:THR:HG21	3:C3:84:LEU:HD13	1.91	0.50
2:F3:78:THR:OG1	2:F3:80:GLU:OE1	2.28	0.50
3:J3:75:TYR:OH	2:K3:94:ARG:NH2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K3:10:VAL:HG21	3:L3:100:THR:HG23	1.93	0.50
2:R3:128:SER:O	2:R3:132:GLU:HG3	2.10	0.50
3:a3:44:ARG:HH21	3:a3:149:ILE:HG12	1.76	0.50
3:C5:128:VAL:HG22	13:C5:201:CYC:H3C	1.93	0.50
2:K5:156:ASP:O	2:K5:160:ASN:ND2	2.26	0.50
3:M5:95:THR:HG22	2:R5:20:LEU:HD12	1.92	0.50
13:X5:201:CYC:CGA	5:Z5:115:ILE:HG12	2.41	0.50
3:D6:63:GLU:HG3	3:D6:64:GLN:HG3	1.91	0.50
2:N6:63:LYS:HD2	2:N6:132:GLU:HG3	1.93	0.50
2:R6:85:CYS:HA	13:R6:201:CYC:HHD	1.92	0.50
2:K7:112:LEU:HD23	2:K7:158:LEU:HD21	1.93	0.50
2:T7:117:ASP:OD1	2:T7:117:ASP:N	2.42	0.50
3:D1:76:THR:HG23	3:D1:79:ARG:HG3	1.93	0.50
3:Q1:48:ASN:HB2	3:Q1:142:ILE:HD13	1.92	0.50
1:22:36:GLN:OE1	3:L7:112:ASN:ND2	2.45	0.50
1:22:182:ASP:OD1	1:22:183:SER:N	2.38	0.50
1:52:95:TYR:O	3:D5:109:ARG:NH1	2.44	0.50
8:m2:28:LYS:O	8:m2:32:GLN:HG2	2.10	0.50
9:r2:117:LYS:O	8:w2:53:LYS:NZ	2.44	0.50
9:s2:1:MET:HG3	9:s2:5:SER:HB2	1.93	0.50
3:J4:44:ARG:NH1	3:J4:145:ASP:O	2.30	0.50
5:Z4:43:VAL:HA	5:Z4:102:HIS:HB3	1.94	0.50
2:F5:3:LYS:NZ	2:K5:16:GLN:OE1	2.29	0.50
2:F5:78:THR:OG1	2:F5:80:GLU:OE1	2.29	0.50
3:O5:102:ASP:OD1	3:O5:103:ALA:N	2.43	0.50
2:S5:99:ALA:HB2	2:S5:108:ILE:HG13	1.94	0.50
3:L6:9:VAL:HG21	3:L6:28:LEU:HD11	1.92	0.50
3:Q6:76:THR:HG23	2:R6:111:TYR:HA	1.93	0.50
3:E7:37:LYS:HA	13:E7:201:CYC:HHD	1.94	0.50
2:N7:122:THR:HG21	3:O7:84:LEU:HD13	1.93	0.50
2:R7:128:SER:O	2:R7:132:GLU:HG3	2.11	0.50
2:H1:78:THR:OG1	2:H1:80:GLU:OE1	2.29	0.50
3:V1:152:GLY:HA3	13:V1:202:CYC:HMD2	1.94	0.50
1:22:51:ARG:HA	1:22:55:PHE:O	2.11	0.50
1:42:167:ARG:NH1	13:42:302:CYC:O2D	2.44	0.50
8:B2:78:TYR:CD2	9:I2:115:MET:HG3	2.46	0.50
9:U2:147:ASP:OD1	9:U2:147:ASP:N	2.42	0.50
8:a2:40:ALA:O	8:a2:44:ILE:HG12	2.11	0.50
8:d2:40:ALA:O	8:d2:44:ILE:HG12	2.11	0.50
8:g2:144:ASP:OD1	8:g2:144:ASP:N	2.43	0.50
9:i2:91:LEU:HD12	9:i2:104:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t2:32:THR:O	12:t2:36:ARG:HG3	2.11	0.50
3:D3:16:ARG:HH22	3:D3:24:GLN:HE22	1.59	0.50
2:N3:14:ASP:OD2	3:V3:109:ARG:NE	2.44	0.50
2:N3:134:LEU:HB3	2:N3:155:ILE:HG23	1.93	0.50
2:W3:14:ASP:OD1	5:Z3:121:TYR:OH	2.29	0.50
13:X3:201:CYC:CGA	5:Z3:115:ILE:HG12	2.42	0.50
3:D4:80:MET:HE3	3:D4:80:MET:O	2.10	0.50
3:Q4:152:GLY:O	13:Q4:202:CYC:OC	2.29	0.50
3:a4:9:VAL:HG11	3:a4:28:LEU:HD11	1.93	0.50
2:N5:26:GLN:HG2	2:U5:34:GLN:HG3	1.93	0.50
2:R5:99:ALA:HB2	2:R5:108:ILE:HG13	1.93	0.50
2:G6:113:LEU:HD11	2:G6:161:ALA:HB1	1.94	0.50
2:I6:78:THR:OG1	2:I6:80:GLU:OE1	2.29	0.50
3:L6:83:CYS:SG	13:L6:201:CYC:HAC2	2.52	0.50
3:M6:3:PHE:O	3:M6:104:SER:OG	2.29	0.50
2:R6:113:LEU:HD11	2:R6:161:ALA:HB1	1.93	0.50
5:Z6:222:ARG:HA	5:Z6:287:ALA:HB1	1.92	0.50
13:a6:201:CYC:HB	13:a6:201:CYC:HMA3	1.75	0.50
2:N7:27:VAL:HG22	2:U7:27:VAL:HG22	1.94	0.50
2:N7:33:ARG:NH2	2:N7:34:GLN:OE1	2.40	0.50
5:Z7:240:VAL:HG12	5:Z7:284:VAL:HG22	1.92	0.50
2:I1:138:LYS:NZ	2:I1:156:ASP:OD1	2.28	0.50
2:W1:112:LEU:HD12	13:W1:201:CYC:HAB1	1.94	0.50
8:T2:2:GLN:HB2	8:T2:6:THR:HB	1.93	0.50
9:W2:134:LYS:HB2	9:W2:153:PHE:HB3	1.94	0.50
13:X2:201:CYC:HMD1	13:X2:201:CYC:NC	2.27	0.50
8:g2:71:ASN:O	8:g2:77:ARG:HD2	2.11	0.50
8:g2:100:ASP:OD1	8:g2:101:THR:N	2.45	0.50
11:q2:3:ASP:N	11:q2:6:SER:OG	2.44	0.50
3:D3:154:CYS:HB3	3:D3:157:ILE:HG22	1.93	0.50
3:E3:38:ARG:NH1	3:E3:98:VAL:O	2.33	0.50
2:K3:134:LEU:HB3	2:K3:155:ILE:HG23	1.94	0.50
2:N3:113:LEU:HD21	2:N3:161:ALA:HB1	1.93	0.50
2:T4:95:ILE:HG13	2:T4:112:LEU:HD13	1.93	0.50
2:W4:101:VAL:HG21	3:X4:20:LEU:HD12	1.94	0.50
3:C5:154:CYS:HG	13:C5:202:CYC:HAC2	1.77	0.50
2:G5:138:LYS:HB2	2:G5:155:ILE:HG21	1.92	0.50
2:U5:95:ILE:HG13	2:U5:112:LEU:HD13	1.94	0.50
2:U5:138:LYS:NZ	2:U5:156:ASP:OD1	2.30	0.50
3:V5:4:ASP:N	3:V5:7:THR:OG1	2.37	0.50
3:D7:92:ARG:HG2	2:I7:19:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R1:43:LYS:O	2:R1:47:ASN:ND2	2.34	0.50
2:U1:21:SER:OG	2:U1:22:SER:N	2.45	0.50
1:52:167:ARG:NH1	13:52:302:CYC:O2D	2.44	0.50
13:A2:202:CYC:HMD2	9:J2:71:ASN:HB3	1.94	0.50
10:N2:91:ASP:N	10:N2:91:ASP:OD1	2.44	0.50
10:N2:181:LEU:HD22	10:N2:233:LEU:HD13	1.93	0.50
8:V2:43:THR:O	8:V2:47:ASN:ND2	2.45	0.50
9:r2:71:ASN:ND2	9:r2:120:GLY:O	2.34	0.50
2:R3:95:ILE:HG22	2:R3:108:ILE:HG12	1.93	0.50
2:S3:74:ASN:O	13:S3:201:CYC:NC	2.44	0.50
2:T3:117:ASP:N	2:T3:117:ASP:OD1	2.41	0.50
2:I5:138:LYS:NZ	2:I5:156:ASP:OD1	2.37	0.50
3:V5:30:ARG:O	3:V5:34:GLU:HG2	2.12	0.50
3:a5:9:VAL:HG11	3:a5:28:LEU:HD11	1.93	0.50
3:O6:146:ARG:NE	3:O6:151:GLN:OE1	2.43	0.50
5:Z7:201:PRO:HD3	5:Z7:221:MET:HE1	1.94	0.50
1:32:182:ASP:OD1	1:32:183:SER:N	2.38	0.50
8:C2:74:THR:OG1	9:H2:107:ILE:O	2.20	0.50
9:G2:16:ARG:O	8:K2:94:TYR:OH	2.29	0.50
9:I2:35:ARG:O	9:I2:39:ILE:HG12	2.12	0.50
9:J2:16:ARG:NH1	9:J2:17:TYR:O	2.44	0.50
8:X2:103:ILE:HG13	8:X2:107:ARG:HD2	1.93	0.50
9:e2:124:GLU:N	9:e2:124:GLU:OE1	2.45	0.50
10:o2:5:ALA:HB3	10:o2:443:TYR:CD1	2.47	0.50
8:u2:37:ARG:NH1	8:u2:96:MET:O	2.40	0.50
3:P3:146:ARG:NE	3:P3:151:GLN:OE1	2.35	0.50
2:R3:85:CYS:HA	13:R3:201:CYC:HAC2	1.93	0.50
2:B4:25:LEU:HD22	3:J4:39:ILE:HG23	1.93	0.50
2:F5:99:ALA:HB2	2:F5:108:ILE:HG12	1.92	0.50
3:L5:9:VAL:HG21	3:L5:28:LEU:HD11	1.92	0.50
2:R5:134:LEU:HB3	2:R5:155:ILE:HG23	1.92	0.50
4:Y5:218:ARG:HG2	4:Y5:250:TYR:HB3	1.93	0.50
5:Z5:41:ARG:NH2	5:Z5:175:TYR:O	2.42	0.50
3:D6:43:ASN:HB2	2:I6:25:LEU:HD21	1.93	0.50
2:K6:85:CYS:HA	13:K6:201:CYC:HHD	1.94	0.50
3:M6:80:MET:HE3	3:M6:80:MET:O	2.11	0.50
3:M1:44:ARG:NH2	3:M1:145:ASP:O	2.44	0.50
3:P1:85:ARG:NE	4:Y1:238:ARG:HH21	2.09	0.50
1:42:84:LEU:O	1:42:87:SER:OG	2.26	0.50
8:B2:1:MET:N	8:B2:106:GLU:OE1	2.44	0.50
13:B2:201:CYC:HB	10:N2:572:ILE:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N2:189:ARG:O	10:N2:193:GLU:HB3	2.12	0.50
10:N2:603:TYR:HD2	10:N2:606:LYS:HG3	1.74	0.50
12:S2:80:GLN:NE2	12:S2:80:GLN:O	2.45	0.50
8:m2:81:CYS:SG	13:m2:201:CYC:HAC2	2.51	0.50
13:z2:201:CYC:HMA1	13:z2:201:CYC:NB	2.25	0.50
2:B3:85:CYS:HA	13:B3:201:CYC:HHD	1.92	0.50
3:E3:149:ILE:HG21	13:E3:201:CYC:HMC3	1.94	0.50
2:S3:138:LYS:HB2	2:S3:155:ILE:HG21	1.93	0.50
13:D4:201:CYC:HAB1	2:I4:25:LEU:HD23	1.94	0.50
3:Q4:112:ASN:O	4:Y4:261:HIS:NE2	2.36	0.50
2:T4:41:ALA:HB2	2:T4:147:SER:HB3	1.94	0.50
3:L5:34:GLU:HG3	3:L5:37:LYS:HD2	1.94	0.50
2:U5:121:LYS:NZ	2:W5:163:SER:OXT	2.44	0.50
3:X5:128:VAL:HG22	13:X5:201:CYC:H3C	1.93	0.50
2:N7:134:LEU:HB3	2:N7:155:ILE:HG23	1.94	0.50
3:P7:96:TYR:OH	2:U7:18:ARG:O	2.26	0.50
1:A1:191:PHE:N	1:A1:192:PRO:HD2	2.26	0.50
3:M1:78:ARG:NH1	13:M1:201:CYC:O1D	2.43	0.50
1:52:44:GLU:O	1:52:47:GLN:HG3	2.12	0.50
8:B2:57:ALA:HA	8:B2:61:LEU:HG	1.94	0.50
9:E2:128:GLU:OE1	9:E2:131:ARG:NH1	2.44	0.50
9:H2:101:ILE:HG12	9:H2:155:TYR:CD1	2.47	0.50
8:X2:126:THR:HG23	13:X2:201:CYC:HBC2	1.92	0.50
6:Z2:19:GLN:OE1	6:Z2:20:ARG:N	2.44	0.50
9:i2:50:ILE:HD11	9:i2:140:LEU:HD12	1.93	0.50
9:i2:130:VAL:HG13	9:i2:157:ILE:HG12	1.94	0.50
9:j2:81:CYS:HB2	13:j2:201:CYC:NC	2.27	0.50
9:k2:14:GLU:OE1	9:k2:16:ARG:NE	2.39	0.50
12:t2:14:GLU:OE2	12:t2:16:ARG:NE	2.34	0.50
8:u2:30:TYR:OH	8:u2:97:LEU:O	2.26	0.50
8:u2:107:ARG:HA	6:z2:44:GLN:HB3	1.93	0.50
13:L3:201:CYC:OB	5:Z3:254:ARG:O	2.30	0.50
3:P3:77:ASN:ND2	2:T3:112:LEU:O	2.36	0.50
3:V3:4:ASP:N	3:V3:7:THR:OG1	2.36	0.50
3:P4:146:ARG:NE	3:P4:151:GLN:OE1	2.44	0.50
2:S4:99:ALA:HB2	2:S4:108:ILE:HG13	1.93	0.50
3:E5:40:ASP:HB3	13:E5:201:CYC:HBC3	1.94	0.50
2:N5:99:ALA:HB2	2:N5:108:ILE:HG13	1.94	0.50
3:O5:37:LYS:NZ	13:T5:201:CYC:O1D	2.40	0.50
2:W5:28:ALA:HB2	3:X5:99:PHE:CZ	2.47	0.50
1:A6:182:ASP:OD1	1:A6:183:SER:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C6:128:VAL:HG22	13:C6:201:CYC:H3C	1.94	0.50
3:P6:146:ARG:O	3:P6:151:GLN:NE2	2.41	0.50
2:U6:21:SER:OG	2:U6:22:SER:N	2.45	0.50
3:V6:30:ARG:O	3:V6:34:GLU:HG2	2.11	0.50
2:W6:7:THR:HG23	3:X6:2:THR:HB	1.93	0.50
3:D7:77:ASN:HD21	2:H7:116:LEU:HD13	1.75	0.50
2:R7:80:GLU:O	2:R7:84:LYS:HG2	2.12	0.50
2:N1:78:THR:OG1	2:N1:80:GLU:OE1	2.28	0.50
3:a1:30:ARG:O	3:a1:34:GLU:HG2	2.11	0.50
8:K2:109:LEU:HD13	8:K2:159:GLY:HA3	1.93	0.50
10:N2:284:LYS:HD3	10:N2:316:LYS:HB2	1.93	0.50
9:R2:128:GLU:OE1	9:R2:131:ARG:NH1	2.45	0.50
9:h2:151:ALA:HB1	9:k2:20:PRO:HB3	1.94	0.50
9:j2:47:ARG:HG2	9:j2:48:GLU:HG3	1.93	0.50
11:q2:8:LEU:HD23	11:q2:27:LEU:HG	1.93	0.50
8:u2:83:ARG:HH22	13:z2:201:CYC:HBA2	1.77	0.50
3:L3:76:THR:HG22	3:L3:78:ARG:H	1.77	0.50
2:T3:24:GLU:O	2:T3:27:VAL:HG12	2.12	0.50
2:I4:45:LEU:HD21	2:I4:141:HIS:HB2	1.93	0.50
3:M4:131:GLY:O	3:M4:135:MET:HG3	2.12	0.50
3:P4:74:ALA:HA	3:P4:79:ARG:HB3	1.93	0.50
2:H5:63:LYS:HG2	2:H5:132:GLU:HG3	1.94	0.50
2:H5:78:THR:OG1	2:H5:80:GLU:OE1	2.30	0.50
3:X5:3:PHE:HB3	3:X5:8:LYS:HB2	1.93	0.50
3:C6:92:ARG:O	3:C6:95:THR:OG1	2.27	0.50
3:D6:80:MET:O	3:D6:80:MET:HE3	2.11	0.50
3:a6:30:ARG:O	3:a6:34:GLU:HG2	2.11	0.50
13:Z7:301:CYC:CMA	13:Z7:301:CYC:HB	2.25	0.50
1:A1:186:ARG:CG	1:A1:192:PRO:HD3	2.42	0.49
13:A1:301:CYC:HMD1	13:A1:301:CYC:HC	1.77	0.49
3:C1:89:ILE:HD13	13:C1:201:CYC:HBB3	1.93	0.49
2:I1:16:GLN:OE1	2:I1:18:ARG:NE	2.34	0.49
3:M1:114:LEU:HD11	3:M1:118:TYR:CZ	2.46	0.49
3:Q1:95:THR:HG22	2:T1:20:LEU:HD12	1.94	0.49
3:Q1:109:ARG:HA	4:Y1:261:HIS:HB3	1.94	0.49
1:52:16:ARG:NH2	3:E5:109:ARG:O	2.31	0.49
9:Q2:100:ASP:OD1	9:Q2:101:ILE:N	2.44	0.49
12:S2:83:ARG:NH2	13:S2:201:CYC:O2A	2.42	0.49
9:j2:145:ASP:OD1	9:j2:145:ASP:N	2.45	0.49
13:F3:202:CYC:HMD2	3:L3:152:GLY:HA3	1.93	0.49
5:Z3:102:HIS:NE2	5:Z3:179:ASP:OD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C5:119:LEU:HD22	3:O5:122:GLY:HA2	1.94	0.49
3:M5:44:ARG:NH2	3:M5:145:ASP:O	2.45	0.49
3:O5:149:ILE:HD13	13:T5:201:CYC:H3C	1.94	0.49
3:P5:37:LYS:HE2	3:P5:154:CYS:HB3	1.93	0.49
3:a5:115:ARG:NH1	3:a5:173:ALA:O	2.45	0.49
2:I6:134:LEU:HB3	2:I6:155:ILE:HG23	1.93	0.49
3:O6:20:LEU:HD22	2:S6:101:VAL:HG21	1.93	0.49
3:X6:41:THR:HG23	3:X6:143:VAL:HG11	1.93	0.49
3:X6:91:LEU:HB2	3:X6:135:MET:HE3	1.94	0.49
3:M7:1:MET:HG3	4:Y7:218:ARG:HH21	1.77	0.49
2:U7:95:ILE:HG22	2:U7:108:ILE:HG12	1.94	0.49
2:W7:138:LYS:HB2	2:W7:155:ILE:HG21	1.93	0.49
5:Z7:55:LEU:HD21	5:Z7:79:SER:HB3	1.94	0.49
2:R1:134:LEU:HB3	2:R1:155:ILE:HG23	1.94	0.49
2:T1:24:GLU:HA	2:T1:27:VAL:HG12	1.93	0.49
13:42:301:CYC:HMD1	13:42:301:CYC:NC	2.27	0.49
8:A2:104:LEU:HB3	8:A2:156:ILE:HD11	1.94	0.49
12:S2:16:ARG:NH2	12:S2:22:GLU:OE2	2.33	0.49
13:e2:201:CYC:HB	13:e2:201:CYC:CMA	2.20	0.49
8:g2:73:TYR:HH	9:h2:90:ARG:HH22	1.55	0.49
8:n2:114:GLU:OE1	8:n2:114:GLU:N	2.41	0.49
13:o2:801:CYC:HMA1	13:o2:801:CYC:NB	2.24	0.49
8:w2:137:THR:HG21	8:w2:149:MET:HG2	1.94	0.49
2:W3:4:THR:HG22	2:W3:102:ALA:HB1	1.94	0.49
3:a3:154:CYS:SG	13:a3:202:CYC:HBC2	2.51	0.49
3:a4:30:ARG:O	3:a4:34:GLU:HG2	2.11	0.49
3:a4:107:ASP:HA	3:a4:111:LEU:HB2	1.93	0.49
2:B5:74:ASN:HA	13:B5:201:CYC:HBD2	1.95	0.49
2:K5:138:LYS:HB2	2:K5:155:ILE:HG21	1.93	0.49
1:A6:53:ILE:O	1:A6:110:ARG:HD3	2.11	0.49
3:L7:146:ARG:HH21	3:L7:151:GLN:HB3	1.77	0.49
2:R7:63:LYS:HD3	2:R7:132:GLU:HG2	1.93	0.49
2:S7:138:LYS:HB2	2:S7:155:ILE:HG21	1.94	0.49
2:T7:74:ASN:ND2	2:T7:124:ASP:OD2	2.45	0.49
5:Z7:82:TYR:HE1	5:Z7:99:HIS:HE1	1.59	0.49
5:Z7:222:ARG:HA	5:Z7:287:ALA:HB1	1.92	0.49
2:F1:45:LEU:HD21	2:F1:141:HIS:HB2	1.93	0.49
2:T1:91:TYR:O	2:T1:95:ILE:HG12	2.13	0.49
3:V1:75:TYR:O	13:W1:201:CYC:OB	2.30	0.49
1:I2:239:ILE:HD12	9:I2:82:LEU:HD11	1.95	0.49
9:G2:1:MET:HB3	9:G2:102:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I2:1:MET:HE3	10:N2:540:GLN:HG2	1.94	0.49
9:Q2:101:ILE:HD12	9:Q2:155:TYR:CE1	2.48	0.49
8:g2:4:ALA:N	8:g2:98:ALA:O	2.44	0.49
8:p2:126:THR:HG23	13:p2:201:CYC:HBC3	1.94	0.49
3:C3:26:ASP:OD1	3:C3:30:ARG:NH1	2.44	0.49
2:F3:25:LEU:HD22	3:a3:39:ILE:HG23	1.95	0.49
2:I3:70:THR:HA	2:F6:62:SER:HB3	1.94	0.49
2:K3:141:HIS:NE2	2:K3:152:ASN:OD1	2.43	0.49
2:N3:122:THR:HG21	3:O3:84:LEU:HD13	1.94	0.49
3:P3:95:THR:HG22	2:U3:20:LEU:HD12	1.94	0.49
3:X3:4:ASP:HA	3:X3:100:THR:HB	1.95	0.49
2:R4:99:ALA:HB2	2:R4:108:ILE:HG13	1.93	0.49
3:V4:121:LEU:HD13	13:V4:201:CYC:HBD1	1.93	0.49
3:E5:39:ILE:HG23	2:H5:25:LEU:HD22	1.94	0.49
2:U5:21:SER:OG	2:U5:22:SER:N	2.45	0.49
3:V6:38:ARG:NH2	3:V6:160:GLU:OE1	2.45	0.49
3:X6:107:ASP:HA	3:X6:111:LEU:HB2	1.93	0.49
2:N7:9:ALA:HB1	2:N7:24:GLU:HG3	1.94	0.49
3:O7:107:ASP:HA	3:O7:111:LEU:HB2	1.92	0.49
3:Q7:58:ARG:NE	13:R7:201:CYC:O2D	2.45	0.49
3:V7:136:LYS:HB2	3:V7:165:PHE:CG	2.47	0.49
2:K1:85:CYS:HA	13:K1:201:CYC:HHB	1.94	0.49
3:M1:80:MET:O	3:M1:80:MET:HE3	2.12	0.49
1:32:222:LEU:O	1:32:226:ILE:HG12	2.12	0.49
9:I2:140:LEU:HD23	9:I2:141:LEU:HB2	1.94	0.49
9:i2:34:ASP:O	9:i2:38:ARG:HG2	2.10	0.49
10:o2:307:LYS:HE2	10:o2:309:SER:HB2	1.94	0.49
9:v2:71:ASN:ND2	9:v2:120:GLY:O	2.46	0.49
3:D3:16:ARG:NE	3:D3:18:GLU:OE2	2.45	0.49
2:N3:117:ASP:N	2:N3:117:ASP:OD1	2.43	0.49
2:R3:80:GLU:O	2:R3:84:LYS:HG2	2.12	0.49
2:S3:5:PRO:HG3	2:T3:23:THR:HA	1.95	0.49
2:W3:16:GLN:HG3	2:W3:18:ARG:HG2	1.95	0.49
2:B4:27:VAL:HG22	2:I4:27:VAL:HG22	1.92	0.49
3:C4:146:ARG:NH2	3:C4:152:GLY:O	2.46	0.49
4:Y4:252:LYS:HZ1	5:Z4:70:ARG:HH22	1.58	0.49
3:M5:4:ASP:H	3:M5:7:THR:HG1	1.60	0.49
2:R5:85:CYS:HB2	13:R5:201:CYC:H2C	1.92	0.49
2:B6:94:ARG:NH2	3:C6:75:TYR:OH	2.32	0.49
2:F6:85:CYS:HB2	13:F6:201:CYC:H2C	1.93	0.49
2:R6:50:ASP:N	2:R6:50:ASP:OD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U6:112:LEU:HD23	2:U6:158:LEU:HD21	1.95	0.49
3:J7:109:ARG:HG2	5:Z7:226:GLY:HA3	1.94	0.49
3:Q7:106:LEU:HD12	3:Q7:110:CYS:HB3	1.93	0.49
8:B2:137:THR:O	8:B2:141:VAL:HG12	2.12	0.49
11:P2:114:ARG:NH2	11:P2:164:LEU:O	2.45	0.49
12:S2:87:TRP:CD1	12:S2:90:ARG:HH21	2.30	0.49
8:T2:113:LYS:NZ	8:T2:160:LEU:O	2.40	0.49
3:D3:99:PHE:CZ	2:I3:28:ALA:HB2	2.47	0.49
2:H3:5:PRO:HD2	2:H3:31:ARG:HD3	1.93	0.49
2:N3:74:ASN:O	13:N3:201:CYC:NC	2.39	0.49
2:U3:95:ILE:HG22	2:U3:108:ILE:HG12	1.93	0.49
3:C4:89:ILE:HD13	13:C4:201:CYC:HBB3	1.94	0.49
3:M4:84:LEU:HD13	2:U4:122:THR:HG21	1.94	0.49
3:P4:114:LEU:HD23	3:P4:172:VAL:HG12	1.94	0.49
2:S4:26:GLN:NE2	2:T4:103:GLY:O	2.41	0.49
3:V4:38:ARG:NH2	3:V4:160:GLU:OE1	2.46	0.49
3:a4:38:ARG:HA	3:a4:157:ILE:HG12	1.95	0.49
2:K5:105:THR:O	2:K5:105:THR:OG1	2.29	0.49
3:Q5:109:ARG:O	4:Y5:261:HIS:ND1	2.46	0.49
2:R5:23:THR:HG21	2:W5:8:GLU:HG3	1.93	0.49
2:F7:8:GLU:HG3	2:K7:23:THR:HG21	1.95	0.49
2:K7:31:ARG:NH2	2:K7:101:VAL:O	2.45	0.49
3:L7:70:PRO:HA	3:L7:75:TYR:CG	2.48	0.49
1:A1:3:LEU:HD22	3:D1:78:ARG:HG2	1.95	0.49
2:B1:95:ILE:HG22	2:B1:108:ILE:HG12	1.94	0.49
13:J1:202:CYC:HMA3	13:J1:202:CYC:NB	2.27	0.49
1:22:179:PRO:HB2	3:a7:121:LEU:HD21	1.95	0.49
1:32:105:GLU:HB2	1:32:122:LYS:HD3	1.94	0.49
1:52:219:TYR:OH	9:G2:86:ASP:OD2	2.22	0.49
10:N2:461:GLU:HG3	10:N2:670:GLY:HA3	1.95	0.49
8:m2:3:ASP:OD1	8:m2:5:ILE:N	2.42	0.49
3:O3:149:ILE:HG21	13:T3:201:CYC:HMC3	1.95	0.49
2:N4:18:ARG:O	3:V4:96:TYR:OH	2.28	0.49
3:O4:80:MET:HE3	3:O4:80:MET:O	2.13	0.49
3:V4:84:LEU:HD13	2:W4:122:THR:HG21	1.95	0.49
3:a4:154:CYS:HB3	3:a4:157:ILE:CG2	2.42	0.49
3:D5:44:ARG:HH12	3:D5:145:ASP:HB3	1.78	0.49
3:E5:46:THR:HG23	2:H5:19:PHE:HB3	1.95	0.49
3:M5:80:MET:O	3:M5:80:MET:HE3	2.11	0.49
3:a5:44:ARG:NH1	3:a5:142:ILE:O	2.46	0.49
3:V6:89:ILE:HG12	3:V6:92:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q7:109:ARG:HA	4:Y7:261:HIS:HB3	1.94	0.49
3:P1:39:ILE:HG23	2:U1:25:LEU:HD22	1.95	0.49
2:R1:107:PRO:HA	2:R1:110:GLU:HG2	1.95	0.49
2:W1:51:SER:OG	2:S7:80:GLU:OE2	2.28	0.49
13:32:302:CYC:O2A	3:E3:85:ARG:NH1	2.45	0.49
9:D2:30:VAL:HG21	8:F2:34:GLY:HA3	1.94	0.49
10:N2:609:GLU:OE1	10:N2:620:THR:OG1	2.27	0.49
8:p2:104:LEU:HD11	8:p2:152:TYR:HB3	1.95	0.49
9:s2:35:ARG:NH2	9:s2:145:ASP:OD1	2.43	0.49
9:x2:96:VAL:HA	9:x2:152:TYR:HE2	1.78	0.49
3:C3:78:ARG:NH1	13:C3:201:CYC:O1D	2.43	0.49
2:F3:45:LEU:HD21	2:F3:141:HIS:HB2	1.95	0.49
3:J3:38:ARG:NH1	3:J3:98:VAL:O	2.35	0.49
13:J3:201:CYC:HMA1	13:J3:201:CYC:NB	2.28	0.49
3:P3:16:ARG:NH2	3:P3:24:GLN:OE1	2.46	0.49
2:W3:11:ALA:HB1	5:Z3:88:TYR:CZ	2.48	0.49
3:O4:102:ASP:OD1	3:O4:103:ALA:N	2.46	0.49
3:a4:41:THR:HG23	3:a4:143:VAL:HG21	1.95	0.49
3:D5:80:MET:O	3:D5:80:MET:HE3	2.12	0.49
2:G5:5:PRO:HG3	2:H5:23:THR:HA	1.95	0.49
2:G5:94:ARG:NH2	3:L5:75:TYR:OH	2.27	0.49
2:I5:78:THR:OG1	2:I5:80:GLU:OE1	2.30	0.49
3:O5:20:LEU:HD22	2:S5:101:VAL:HG21	1.94	0.49
1:A6:3:LEU:HD21	3:D6:81:ALA:HB3	1.95	0.49
3:C6:109:ARG:HD3	5:Z6:275:ASN:HB3	1.94	0.49
3:E6:105:ILE:HD12	3:E6:109:ARG:HG3	1.93	0.49
3:V7:75:TYR:OH	2:W7:94:ARG:NH2	2.37	0.49
3:a7:154:CYS:SG	13:a7:202:CYC:HBC2	2.52	0.49
1:A1:58:PHE:O	1:A1:59:LYS:C	2.56	0.49
3:D1:43:ASN:HB2	2:I1:25:LEU:HD21	1.95	0.49
3:D1:80:MET:HE3	3:D1:80:MET:O	2.13	0.49
3:D1:145:ASP:OD1	3:D1:147:ASN:ND2	2.41	0.49
3:Q1:139:ALA:HA	3:Q1:142:ILE:HG12	1.95	0.49
13:42:302:CYC:O2A	3:E4:85:ARG:NH2	2.45	0.49
9:J2:46:SER:O	9:J2:50:ILE:HG22	2.12	0.49
10:N2:349:ILE:HG22	10:N2:361:ILE:HD11	1.95	0.49
9:Q2:128:GLU:OE1	9:Q2:131:ARG:NH1	2.46	0.49
9:f2:12:ASP:OD1	10:o2:499:GLN:NE2	2.45	0.49
3:D3:43:ASN:HB2	2:I3:25:LEU:HD21	1.94	0.49
2:F3:136:TYR:O	2:F3:140:ASN:ND2	2.38	0.49
2:K3:118:GLU:OE1	2:K3:118:GLU:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X3:91:LEU:HB2	3:X3:135:MET:HE3	1.94	0.49
2:S4:94:ARG:NH2	3:X4:75:TYR:OH	2.27	0.49
3:V4:92:ARG:O	3:V4:95:THR:OG1	2.26	0.49
2:W4:11:ALA:HB1	5:Z4:88:TYR:CZ	2.47	0.49
2:F5:109:ASP:HA	2:F5:113:LEU:HB3	1.95	0.49
2:F6:18:ARG:NH2	2:K6:157:TYR:OH	2.46	0.49
2:R6:107:PRO:HA	2:R6:110:GLU:HG2	1.95	0.49
3:X6:146:ARG:O	3:X6:151:GLN:NE2	2.45	0.49
3:E7:136:LYS:NZ	3:E7:137:ASP:OD1	2.38	0.49
3:V7:41:THR:HG23	3:V7:143:VAL:HG21	1.93	0.49
3:a7:3:PHE:H	3:a7:104:SER:HB3	1.73	0.49
2:G1:74:ASN:HA	13:G1:201:CYC:HBD2	1.94	0.49
3:V1:30:ARG:O	3:V1:34:GLU:HG2	2.12	0.49
6:O2:44:GLN:HE22	13:a2:201:CYC:HBB2	1.78	0.49
8:F2:46:ALA:HB2	9:I2:154:ASP:HB3	1.95	0.49
8:L2:125:THR:HG23	13:L2:201:CYC:HBC3	1.95	0.49
9:Q2:98:SER:HA	8:X2:5:ILE:HG21	1.95	0.49
12:S2:41:GLN:NE2	12:S2:45:ASP:OD2	2.45	0.49
8:V2:16:GLY:O	9:W2:90:ARG:NH1	2.46	0.49
8:a2:130:ILE:HG23	8:a2:153:LEU:HD12	1.94	0.49
13:l2:201:CYC:O1A	10:o2:453:TYR:OH	2.28	0.49
12:t2:115:MET:SD	8:y2:75:THR:HG22	2.52	0.49
3:D3:116:GLU:OE1	3:D3:116:GLU:N	2.37	0.49
2:G3:113:LEU:HD11	2:G3:161:ALA:HB1	1.95	0.49
2:R3:37:SER:OG	2:R3:147:SER:N	2.46	0.49
5:Z3:201:PRO:HD3	5:Z3:221:MET:HE1	1.95	0.49
3:O4:146:ARG:NE	3:O4:151:GLN:OE1	2.46	0.49
3:D5:18:GLU:O	2:I5:98:TYR:OH	2.28	0.49
3:V5:150:THR:O	13:V5:202:CYC:NC	2.44	0.49
2:G6:105:THR:OG1	2:H6:18:ARG:NH2	2.46	0.49
2:H6:108:ILE:HG22	2:H6:113:LEU:HG	1.95	0.49
2:K6:138:LYS:HB2	2:K6:155:ILE:HG21	1.95	0.49
2:T6:9:ALA:HB2	2:T6:27:VAL:HG11	1.94	0.49
3:V6:76:THR:HG22	3:V6:78:ARG:H	1.77	0.49
3:D7:150:THR:O	13:D7:201:CYC:NC	2.41	0.49
3:L7:76:THR:HG22	3:L7:78:ARG:H	1.78	0.49
3:M7:131:GLY:O	3:M7:135:MET:HG3	2.12	0.49
3:O7:149:ILE:HG21	13:T7:201:CYC:HMC3	1.94	0.49
5:Z7:74:ARG:NH2	5:Z7:135:ASP:OD1	2.45	0.49
3:a7:12:GLN:HB3	3:a7:16:ARG:HH12	1.77	0.49
3:a7:96:TYR:HB3	3:a7:105:ILE:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:302:CYC:H3C	3:E1:128:VAL:HG22	1.95	0.49
2:W1:99:ALA:HB2	2:W1:108:ILE:HG13	1.95	0.49
1:32:43:ASP:OD1	1:32:71:ARG:NH2	2.40	0.49
1:52:242:LEU:HD23	1:52:242:LEU:H	1.78	0.49
13:L2:201:CYC:NC	13:L2:201:CYC:HMD1	2.27	0.49
10:N2:18:GLN:OE1	10:N2:269:ARG:NH1	2.46	0.49
10:N2:354:ARG:HB2	10:N2:423:LEU:HD21	1.93	0.49
11:P2:98:VAL:HG11	9:U2:26:ILE:HD13	1.95	0.49
9:R2:29:PHE:O	9:R2:36:ARG:NH2	2.46	0.49
12:S2:113:ARG:HA	12:S2:123:LEU:HD21	1.95	0.49
9:U2:61:LYS:HE3	9:i2:61:LYS:HE2	1.94	0.49
8:g2:121:VAL:HG22	13:g2:201:CYC:HC	1.77	0.49
10:o2:147:VAL:HG13	10:o2:155:MET:HG3	1.95	0.49
2:I4:16:GLN:OE1	2:I4:18:ARG:NE	2.39	0.49
2:N4:98:TYR:OH	3:V4:18:GLU:O	2.31	0.49
2:T4:108:ILE:HG22	2:T4:113:LEU:HG	1.95	0.49
3:J5:112:ASN:O	5:Z5:224:LEU:HA	2.12	0.49
2:T5:138:LYS:HB2	2:T5:155:ILE:HG21	1.95	0.49
4:Y5:228:GLN:OE1	4:Y5:266:ARG:NE	2.40	0.49
2:N6:122:THR:HG21	3:O6:84:LEU:HD13	1.93	0.49
3:X6:76:THR:HG23	3:X6:79:ARG:H	1.78	0.49
3:C7:26:ASP:OD1	3:C7:30:ARG:NH1	2.45	0.49
3:D7:20:LEU:HD12	3:D7:20:LEU:H	1.78	0.49
13:F7:202:CYC:H3C	3:L7:149:ILE:HD13	1.95	0.49
2:G7:122:THR:HG21	3:L7:84:LEU:HD13	1.93	0.49
2:N7:14:ASP:OD2	3:V7:109:ARG:NE	2.46	0.49
3:P7:44:ARG:O	3:P7:48:ASN:ND2	2.42	0.49
2:N1:134:LEU:HB3	2:N1:155:ILE:HG23	1.95	0.48
3:Q1:37:LYS:N	3:Q1:37:LYS:HE2	2.28	0.48
3:Q1:109:ARG:O	4:Y1:261:HIS:ND1	2.46	0.48
9:D2:113:ARG:HH22	9:D2:161:SER:C	2.21	0.48
9:I2:2:SER:HA	9:I2:98:SER:HB2	1.95	0.48
8:d2:81:CYS:HA	13:d2:201:CYC:HH2	1.94	0.48
8:n2:94:TYR:HE1	10:o2:35:PRO:HD3	1.77	0.48
11:q2:135:ARG:HD2	11:q2:154:GLU:HB3	1.94	0.48
9:r2:3:ILE:HG22	9:r2:100:ASP:HB2	1.95	0.48
8:u2:105:ASP:OD1	8:u2:155:TYR:OH	2.29	0.48
9:x2:21:GLY:O	9:x2:24:GLU:HG2	2.13	0.48
3:D3:39:ILE:HG23	2:I3:25:LEU:HG	1.94	0.48
2:N3:23:THR:HA	2:U3:5:PRO:HG3	1.94	0.48
4:Y3:252:LYS:HZ1	5:Z3:70:ARG:HH22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G4:8:GLU:HG3	2:H4:23:THR:HG21	1.95	0.48
2:B5:26:GLN:HE22	2:I5:34:GLN:HG2	1.78	0.48
3:M5:18:GLU:O	2:R5:98:TYR:OH	2.29	0.48
2:S5:2:SER:HB2	2:S5:106:GLY:HA3	1.94	0.48
2:S5:26:GLN:NE2	2:T5:103:GLY:O	2.41	0.48
2:G6:94:ARG:NH2	3:L6:75:TYR:OH	2.31	0.48
2:N6:25:LEU:HD22	3:V6:39:ILE:HG23	1.94	0.48
2:T6:134:LEU:HB3	2:T6:155:ILE:HG23	1.93	0.48
13:X6:201:CYC:CGA	5:Z6:115:ILE:HG12	2.43	0.48
4:Y6:252:LYS:NZ	5:Z6:70:ARG:HH22	2.11	0.48
13:a6:201:CYC:HMD1	13:a6:201:CYC:HC	1.75	0.48
3:C7:119:LEU:HD22	3:O7:122:GLY:HA2	1.94	0.48
3:Q7:115:ARG:NH2	3:Q7:170:ALA:O	2.46	0.48
2:R7:26:GLN:NE2	2:W7:103:GLY:O	2.45	0.48
3:E1:12:GLN:O	3:E1:16:ARG:NH1	2.47	0.48
13:E1:201:CYC:NB	13:E1:201:CYC:HMA3	2.28	0.48
2:I1:118:GLU:OE1	2:I1:118:GLU:N	2.42	0.48
2:K1:76:ALA:HB1	2:K1:82:LYS:HD3	1.95	0.48
3:O1:44:ARG:O	3:O1:48:ASN:ND2	2.38	0.48
3:O1:154:CYS:HB3	3:O1:157:ILE:HG22	1.95	0.48
1:22:191:PHE:N	1:22:192:PRO:HD2	2.28	0.48
13:22:301:CYC:H3C	3:D7:128:VAL:HG22	1.95	0.48
9:E2:83:ARG:HH22	13:E2:201:CYC:HBA2	1.77	0.48
9:H2:121:THR:OG1	13:H2:201:CYC:NC	2.46	0.48
12:S2:16:ARG:O	8:T2:94:TYR:OH	2.28	0.48
8:c2:5:ILE:HG21	9:k2:98:SER:HA	1.95	0.48
9:i2:29:PHE:HE1	9:i2:99:GLY:HA3	1.78	0.48
8:l2:36:LEU:H	8:l2:36:LEU:HD12	1.78	0.48
8:m2:1:MET:HE2	8:m2:103:ILE:HB	1.95	0.48
10:o2:445:GLN:NE2	10:o2:448:LEU:HD21	2.28	0.48
3:J3:109:ARG:HG2	5:Z3:226:GLY:HA3	1.94	0.48
3:Q3:109:ARG:HA	4:Y3:261:HIS:HB3	1.94	0.48
2:N4:26:GLN:HG2	2:U4:34:GLN:HG3	1.95	0.48
3:X4:86:ASP:OD2	3:X4:118:TYR:OH	2.30	0.48
3:M6:57:ALA:HB2	3:M6:87:MET:HE1	1.95	0.48
13:S1:201:CYC:O2D	3:X1:58:ARG:NH1	2.45	0.48
1:22:164:LEU:HD21	13:22:302:CYC:HBA2	1.94	0.48
8:A2:40:ALA:O	8:A2:44:ILE:HG12	2.14	0.48
8:F2:144:ASP:N	8:F2:144:ASP:OD1	2.46	0.48
12:S2:23:LEU:HB3	8:T2:38:VAL:HG13	1.94	0.48
2:S3:85:CYS:O	2:S3:89:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U4:99:ALA:HB2	2:U4:108:ILE:HG13	1.95	0.48
5:Z4:101:LYS:HE2	5:Z4:172:TYR:HB2	1.94	0.48
3:J5:84:LEU:HD13	2:K5:122:THR:HG21	1.95	0.48
2:U5:99:ALA:HB2	2:U5:108:ILE:HG13	1.94	0.48
5:Z5:222:ARG:HA	5:Z5:287:ALA:HB1	1.96	0.48
3:P6:107:ASP:HA	3:P6:111:LEU:HB2	1.94	0.48
2:S6:27:VAL:HG22	2:T6:27:VAL:HG23	1.96	0.48
2:W6:118:GLU:OE1	2:W6:118:GLU:N	2.43	0.48
3:X6:38:ARG:NH2	3:X6:160:GLU:OE1	2.43	0.48
3:a7:9:VAL:HG11	3:a7:28:LEU:HD11	1.95	0.48
13:A1:301:CYC:H3C	3:D1:128:VAL:HG22	1.95	0.48
2:F1:23:THR:HA	2:K1:5:PRO:HG3	1.96	0.48
2:F1:99:ALA:HB2	2:F1:108:ILE:HG12	1.95	0.48
2:H1:134:LEU:HB3	2:H1:155:ILE:HG23	1.95	0.48
13:V1:201:CYC:HMD1	13:V1:201:CYC:HC	1.77	0.48
1:32:180:ARG:NH2	13:a3:201:CYC:O1D	2.46	0.48
8:C2:74:THR:HG23	8:C2:77:ARG:HG2	1.94	0.48
9:J2:62:ARG:HH12	9:J2:124:GLU:HG2	1.78	0.48
8:L2:106:ARG:HH11	10:N2:487:ARG:HB2	1.78	0.48
9:Q2:81:CYS:HA	13:Q2:201:CYC:HAC2	1.94	0.48
9:R2:113:ARG:NH1	9:R2:160:LEU:O	2.45	0.48
9:U2:145:ASP:OD1	9:U2:145:ASP:N	2.44	0.48
8:a2:130:ILE:HG22	8:a2:134:LYS:HE3	1.94	0.48
9:i2:101:ILE:HG12	9:i2:155:TYR:CD1	2.49	0.48
13:v2:201:CYC:HB	13:v2:201:CYC:HMA3	1.79	0.48
2:I3:74:ASN:HA	13:I3:201:CYC:HBD2	1.96	0.48
2:K3:31:ARG:NH2	2:K3:101:VAL:O	2.45	0.48
3:L3:146:ARG:HH21	3:L3:151:GLN:HB3	1.79	0.48
3:Q3:75:TYR:OH	2:R3:94:ARG:NH2	2.40	0.48
2:S3:94:ARG:NH2	3:X3:75:TYR:OH	2.33	0.48
2:W3:95:ILE:HG22	2:W3:108:ILE:HG12	1.95	0.48
2:R4:85:CYS:HB2	13:R4:201:CYC:H2C	1.94	0.48
3:V4:78:ARG:NH1	13:V4:201:CYC:O1D	2.47	0.48
2:N5:85:CYS:HA	13:N5:201:CYC:HHD	1.95	0.48
3:P5:39:ILE:HG23	2:U5:25:LEU:HD22	1.95	0.48
2:K7:74:ASN:HA	13:K7:201:CYC:HBD2	1.95	0.48
3:Q7:128:VAL:HG22	13:Q7:201:CYC:H3C	1.94	0.48
3:C1:154:CYS:SG	13:C1:202:CYC:HAC2	2.53	0.48
3:V1:89:ILE:HD13	13:V1:201:CYC:HBB3	1.96	0.48
2:W1:7:THR:HG23	3:X1:2:THR:HB	1.96	0.48
13:X1:201:CYC:CGA	5:Z1:115:ILE:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:42:102:ARG:NH2	1:42:179:PRO:HD2	2.29	0.48
13:52:302:CYC:O1A	3:E5:78:ARG:NH2	2.45	0.48
9:Q2:30:VAL:HG21	8:X2:34:GLY:HA3	1.95	0.48
8:X2:112:LEU:HG	8:X2:160:LEU:HD21	1.95	0.48
9:i2:64:ASP:OD1	9:i2:65:VAL:N	2.46	0.48
9:j2:1:MET:HB3	9:j2:5:SER:HB2	1.95	0.48
10:o2:327:ARG:HH12	10:o2:388:ASP:CG	2.21	0.48
10:o2:520:GLN:NE2	10:o2:524:GLY:O	2.46	0.48
3:C3:109:ARG:HD3	5:Z3:275:ASN:HB3	1.96	0.48
3:E3:16:ARG:NE	3:E3:18:GLU:OE2	2.40	0.48
3:M3:78:ARG:HD2	5:Z3:29:ARG:HH21	1.77	0.48
2:R3:64:PHE:HE2	2:R3:132:GLU:HG2	1.78	0.48
2:F4:101:VAL:HG21	3:a4:20:LEU:HD13	1.95	0.48
2:I4:9:ALA:HB1	2:I4:24:GLU:HG3	1.94	0.48
2:K4:112:LEU:HD12	13:K4:201:CYC:HAB1	1.93	0.48
2:N4:99:ALA:HB2	2:N4:108:ILE:HG13	1.96	0.48
3:C5:86:ASP:OD2	3:C5:118:TYR:OH	2.21	0.48
5:Z5:47:ASP:OD2	5:Z5:180:ARG:NE	2.34	0.48
3:D6:150:THR:O	13:D6:201:CYC:NC	2.41	0.48
3:E6:12:GLN:OE1	3:E6:16:ARG:NH1	2.29	0.48
2:H6:134:LEU:HB3	2:H6:155:ILE:HG23	1.95	0.48
3:L6:67:LEU:HD21	3:L6:127:SER:HB3	1.96	0.48
3:V6:92:ARG:O	3:V6:95:THR:OG1	2.24	0.48
5:Z6:227:SER:HA	5:Z6:237:ILE:HD11	1.94	0.48
2:B7:5:PRO:HG3	2:I7:23:THR:HA	1.96	0.48
2:F7:3:LYS:NZ	2:K7:18:ARG:HE	2.11	0.48
3:V7:5:ALA:HB2	3:V7:101:GLY:HA3	1.95	0.48
3:a7:104:SER:HA	3:a7:107:ASP:OD1	2.13	0.48
1:A1:69:GLN:NE2	5:Z1:225:GLY:HA3	2.28	0.48
2:K1:2:SER:O	3:L1:1:MET:N	2.47	0.48
2:N1:18:ARG:NH1	2:U1:157:TYR:OH	2.47	0.48
4:Y1:218:ARG:HG2	4:Y1:250:TYR:HB3	1.95	0.48
13:42:302:CYC:HMD3	13:42:302:CYC:HC	1.79	0.48
8:A2:72:MET:SD	13:A2:201:CYC:OC	2.72	0.48
10:N2:518:LEU:HB2	10:N2:548:VAL:HG11	1.96	0.48
9:Q2:71:ASN:HB3	13:Q2:201:CYC:HMD2	1.96	0.48
9:R2:81:CYS:SG	13:R2:201:CYC:HAC2	2.54	0.48
12:S2:105:GLU:OE2	6:Y2:17:ARG:NH2	2.42	0.48
8:V2:104:LEU:HD11	8:V2:152:TYR:HB3	1.95	0.48
8:g2:112:LEU:HG	8:g2:160:LEU:HD21	1.94	0.48
9:j2:71:ASN:ND2	9:j2:120:GLY:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p2:3:ASP:HA	8:p2:98:ALA:HB1	1.95	0.48
8:w2:3:ASP:OD2	9:x2:5:SER:OG	2.25	0.48
3:C3:89:ILE:HD13	13:C3:201:CYC:HBB3	1.94	0.48
3:C3:92:ARG:O	3:C3:95:THR:OG1	2.25	0.48
5:Z3:82:TYR:HE1	5:Z3:99:HIS:HE1	1.61	0.48
3:C4:37:LYS:HE2	13:C4:202:CYC:HMD2	1.95	0.48
2:G4:113:LEU:HD11	2:G4:161:ALA:HB1	1.95	0.48
2:W4:99:ALA:HB2	2:W4:108:ILE:HG13	1.95	0.48
4:Y4:234:ARG:O	5:Z4:141:GLU:HG3	2.14	0.48
3:D5:75:TYR:OH	2:H5:94:ARG:NH2	2.30	0.48
13:A6:302:CYC:H3C	3:E6:128:VAL:HG22	1.96	0.48
2:H6:33:ARG:NH1	2:H6:146:ASP:OD2	2.45	0.48
3:M6:114:LEU:HD11	3:M6:118:TYR:CZ	2.48	0.48
3:O6:17:GLY:HA3	3:X6:70:PRO:HB3	1.95	0.48
3:O6:80:MET:O	3:O6:80:MET:HE3	2.14	0.48
2:R6:155:ILE:O	2:R6:159:ILE:HG12	2.14	0.48
2:W6:11:ALA:HB1	5:Z6:88:TYR:CZ	2.48	0.48
3:O7:152:GLY:HA3	13:T7:201:CYC:HMD2	1.95	0.48
3:Q1:105:ILE:HD12	3:Q1:109:ARG:HG3	1.96	0.48
2:T1:53:VAL:HG13	2:T1:89:ILE:HB	1.95	0.48
5:Z1:227:SER:HA	5:Z1:237:ILE:HD11	1.95	0.48
1:42:186:ARG:HH11	1:42:192:PRO:HG2	1.79	0.48
1:52:26:GLU:HB3	1:52:163:VAL:HG21	1.94	0.48
8:C2:37:ARG:HD2	8:C2:96:MET:O	2.13	0.48
10:N2:567:LEU:HB3	10:N2:570:PRO:HD2	1.94	0.48
13:P2:201:CYC:HB	13:P2:201:CYC:CMA	2.27	0.48
8:T2:54:GLU:HG3	8:T2:136:VAL:HG21	1.94	0.48
8:X2:104:LEU:HD11	8:X2:152:TYR:HB3	1.94	0.48
8:l2:137:THR:O	8:l2:141:VAL:HG22	2.14	0.48
13:n2:201:CYC:NC	13:n2:201:CYC:HMD1	2.28	0.48
3:M3:114:LEU:HD11	3:M3:118:TYR:CZ	2.48	0.48
2:W3:112:LEU:HD23	2:W3:158:LEU:HD21	1.95	0.48
2:W3:138:LYS:HB2	2:W3:155:ILE:HG21	1.95	0.48
2:H4:78:THR:OG1	2:H4:80:GLU:OE1	2.31	0.48
3:P4:111:LEU:HD21	3:P4:168:ALA:HA	1.96	0.48
3:Q4:83:CYS:SG	13:Q4:201:CYC:HAC2	2.54	0.48
3:C5:37:LYS:HE2	13:C5:202:CYC:HMD2	1.95	0.48
3:D5:20:LEU:HD13	2:I5:101:VAL:HG21	1.95	0.48
3:a5:30:ARG:O	3:a5:34:GLU:HG2	2.13	0.48
2:F6:23:THR:HA	2:K6:5:PRO:HG3	1.95	0.48
2:K6:105:THR:O	2:K6:105:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L6:117:THR:HG23	5:Z6:256:SER:HB2	1.96	0.48
2:N6:27:VAL:HG22	2:U6:27:VAL:HG22	1.95	0.48
3:Q6:109:ARG:HA	4:Y6:261:HIS:HB3	1.95	0.48
2:S6:26:GLN:NE2	2:T6:103:GLY:O	2.46	0.48
3:M7:95:THR:HG22	2:R7:20:LEU:HD12	1.94	0.48
2:T7:99:ALA:HB2	2:T7:108:ILE:HG13	1.95	0.48
3:E1:105:ILE:HD12	3:E1:109:ARG:HG3	1.95	0.48
3:J1:37:LYS:HE2	3:J1:37:LYS:N	2.29	0.48
13:P1:201:CYC:HAC1	13:P1:201:CYC:HHD	1.44	0.48
3:V1:86:ASP:OD1	5:Z1:48:TYR:OH	2.30	0.48
3:V1:92:ARG:O	3:V1:95:THR:OG1	2.24	0.48
3:V1:115:ARG:HD2	5:Z1:208:GLY:HA3	1.95	0.48
2:W1:11:ALA:HB1	5:Z1:88:TYR:CZ	2.48	0.48
3:X1:91:LEU:HB2	3:X1:135:MET:HE3	1.95	0.48
9:H2:152:TYR:O	9:H2:156:VAL:HG23	2.14	0.48
10:N2:259:LEU:HB2	10:N2:411:ALA:HB2	1.95	0.48
8:O2:38:VAL:HG13	9:R2:23:LEU:HB3	1.96	0.48
8:O2:127:VAL:O	8:O2:131:GLN:HG2	2.13	0.48
8:X2:109:LEU:HD13	8:X2:159:GLY:HA3	1.96	0.48
8:d2:5:ILE:HG12	9:j2:2:SER:HB3	1.94	0.48
10:o2:72:ALA:O	10:o2:76:PHE:HB2	2.14	0.48
8:u2:137:THR:O	8:u2:141:VAL:HG22	2.14	0.48
9:v2:102:THR:HA	9:v2:105:GLU:HG2	1.96	0.48
2:B3:18:ARG:O	3:J3:96:TYR:OH	2.29	0.48
3:O3:152:GLY:HA3	13:T3:201:CYC:HMD2	1.95	0.48
2:K4:138:LYS:HB2	2:K4:155:ILE:HG21	1.95	0.48
2:R4:5:PRO:HG3	2:W4:23:THR:HA	1.94	0.48
3:V4:76:THR:HG22	3:V4:78:ARG:H	1.79	0.48
2:K5:120:ASN:HD22	2:K5:127:PRO:HG3	1.79	0.48
3:O5:61:PHE:CZ	3:O5:80:MET:HE1	2.48	0.48
3:P5:107:ASP:HA	3:P5:111:LEU:HB2	1.95	0.48
2:U5:112:LEU:HD23	2:U5:158:LEU:HD21	1.95	0.48
2:F6:74:ASN:ND2	2:F6:124:ASP:OD2	2.47	0.48
2:W6:85:CYS:HA	13:W6:201:CYC:HAC2	1.96	0.48
4:Y6:252:LYS:HZ1	5:Z6:70:ARG:HH22	1.59	0.48
3:D7:61:PHE:HB3	3:D7:68:ILE:HD13	1.96	0.48
2:U7:134:LEU:HB3	2:U7:155:ILE:HG23	1.95	0.48
2:W7:20:LEU:HD12	3:X7:95:THR:HG22	1.96	0.48
3:a7:89:ILE:HG12	3:a7:92:ARG:HH21	1.77	0.48
2:F1:91:TYR:O	2:F1:95:ILE:HG12	2.14	0.48
2:K1:138:LYS:HB2	2:K1:155:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L1:98:VAL:HG21	3:L1:161:LEU:HD13	1.95	0.48
3:M1:76:THR:HG23	2:U1:111:TYR:HA	1.95	0.48
2:N1:23:THR:HA	2:U1:5:PRO:HG3	1.94	0.48
7:12:97:LEU:HB2	7:12:100:PHE:HB2	1.96	0.48
1:22:14:ASN:N	1:22:14:ASN:OD1	2.47	0.48
1:42:41:GLN:HG2	3:L4:1:MET:HA	1.94	0.48
13:42:302:CYC:HAD2	3:E4:78:ARG:HH21	1.78	0.48
8:L2:64:ILE:HG22	8:L2:71:MET:HB2	1.94	0.48
10:N2:167:ARG:O	10:N2:170:THR:OG1	2.28	0.48
8:O2:4:ALA:N	8:O2:98:ALA:O	2.47	0.48
9:Q2:11:ALA:HB2	9:Q2:18:LEU:HD23	1.96	0.48
6:Z2:7:THR:HB	6:Z2:52:LYS:HB3	1.95	0.48
8:d2:37:ARG:HD2	8:d2:96:MET:O	2.14	0.48
9:h2:12:ASP:OD2	8:l2:107:ARG:NH1	2.38	0.48
2:N3:99:ALA:HB2	2:N3:108:ILE:HG13	1.96	0.48
3:Q3:106:LEU:HD12	3:Q3:110:CYS:HB3	1.95	0.48
2:F4:3:LYS:O	2:K4:23:THR:OG1	2.24	0.48
3:J4:75:TYR:O	13:K4:201:CYC:OB	2.32	0.48
2:K4:28:ALA:HB2	3:L4:99:PHE:CZ	2.49	0.48
2:K4:85:CYS:O	2:K4:89:ILE:HG12	2.14	0.48
3:O4:61:PHE:HB3	3:O4:68:ILE:HD13	1.95	0.48
2:F5:101:VAL:HG21	3:a5:20:LEU:HD13	1.96	0.48
3:L5:93:TYR:OH	5:Z5:254:ARG:NH2	2.46	0.48
3:M5:114:LEU:HD11	3:M5:118:TYR:CZ	2.49	0.48
2:S5:85:CYS:HA	13:S5:201:CYC:HHD	1.96	0.48
3:M6:98:VAL:HG13	3:M6:157:ILE:HD11	1.94	0.48
2:N6:85:CYS:HA	13:N6:201:CYC:HHD	1.95	0.48
3:D7:146:ARG:NE	3:D7:151:GLN:OE1	2.44	0.48
3:J7:150:THR:O	13:J7:202:CYC:NC	2.28	0.48
2:K7:18:ARG:O	3:L7:96:TYR:OH	2.27	0.48
3:O7:61:PHE:HB3	3:O7:68:ILE:HD13	1.94	0.48
2:S7:74:ASN:O	13:S7:201:CYC:NC	2.47	0.48
2:B1:94:ARG:NH2	3:C1:75:TYR:OH	2.28	0.48
6:02:7:THR:HB	6:02:52:LYS:HB3	1.94	0.48
1:52:3:LEU:HD21	3:D5:81:ALA:HB3	1.95	0.48
9:E2:89:LEU:HB2	9:E2:133:LEU:HD21	1.95	0.48
9:G2:151:ALA:HB1	9:J2:20:PRO:HB3	1.96	0.48
8:c2:119:LEU:HD11	13:c2:801:CYC:HAA2	1.95	0.48
9:e2:113:ARG:HH22	9:e2:161:SER:C	2.22	0.48
9:j2:105:GLU:HA	9:j2:109:ILE:HB	1.96	0.48
8:l2:56:VAL:HG12	8:l2:61:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D3:37:LYS:H	3:D3:37:LYS:HG2	1.44	0.48
3:P3:39:ILE:HG23	2:U3:25:LEU:HD22	1.96	0.48
3:V3:136:LYS:HB2	3:V3:165:PHE:CG	2.49	0.48
2:B5:28:ALA:HB2	3:J5:99:PHE:CZ	2.49	0.48
13:F5:201:CYC:HHA	13:F5:201:CYC:HBD2	1.95	0.48
3:O5:154:CYS:HB3	3:O5:157:ILE:HG22	1.96	0.48
3:Q5:99:PHE:CZ	2:T5:28:ALA:HB2	2.49	0.48
3:Q5:109:ARG:HA	4:Y5:261:HIS:HB3	1.96	0.48
2:B6:80:GLU:O	2:B6:84:LYS:HG2	2.13	0.48
13:B6:201:CYC:OB	3:C6:75:TYR:O	2.31	0.48
2:K6:98:TYR:OH	3:L6:18:GLU:O	2.31	0.48
3:L6:128:VAL:HG13	13:L6:201:CYC:HBC3	1.96	0.48
3:O6:102:ASP:OD1	3:O6:103:ALA:N	2.47	0.48
2:S6:74:ASN:HA	13:S6:201:CYC:HBD2	1.95	0.48
2:K7:105:THR:O	2:K7:105:THR:OG1	2.30	0.48
3:O7:80:MET:O	3:O7:80:MET:HE3	2.14	0.48
3:O7:85:ARG:NH1	13:Z7:301:CYC:O1A	2.47	0.48
2:B1:134:LEU:HB3	2:B1:155:ILE:HG23	1.96	0.47
2:F1:85:CYS:HA	13:F1:201:CYC:HHD	1.96	0.47
3:J1:112:ASN:O	5:Z1:224:LEU:HA	2.14	0.47
3:Q1:83:CYS:SG	13:Q1:201:CYC:HAC2	2.54	0.47
2:R1:155:ILE:O	2:R1:159:ILE:HG12	2.14	0.47
2:S1:85:CYS:HA	13:S1:201:CYC:HAC1	1.70	0.47
1:52:74:GLN:HA	5:Z5:261:LEU:HD12	1.96	0.47
13:52:301:CYC:H3C	3:D5:128:VAL:HG22	1.96	0.47
10:N2:31:GLN:HG2	10:N2:273:PHE:HZ	1.79	0.47
10:N2:300:ILE:CG2	10:N2:306:GLN:HB2	2.43	0.47
10:N2:308:VAL:HG11	10:N2:311:LEU:HD22	1.96	0.47
12:S2:2:THR:HG21	8:T2:5:ILE:HB	1.96	0.47
8:V2:5:ILE:HG21	9:W2:98:SER:HA	1.96	0.47
8:X2:81:CYS:HA	13:X2:201:CYC:HAC1	1.95	0.47
9:j2:50:ILE:HG22	9:j2:133:LEU:HD12	1.95	0.47
9:k2:50:ILE:HG13	9:k2:136:ALA:HB3	1.95	0.47
8:m2:78:TYR:O	8:m2:82:ILE:HG12	2.13	0.47
8:p2:2:GLN:HB2	8:p2:6:THR:HB	1.95	0.47
9:r2:37:LEU:HD23	9:r2:97:VAL:HG22	1.96	0.47
12:t2:83:ARG:HD3	12:t2:87:TRP:CE2	2.49	0.47
3:D3:92:ARG:O	3:D3:95:THR:OG1	2.30	0.47
2:F3:95:ILE:HG21	2:F3:112:LEU:HB2	1.95	0.47
2:H3:80:GLU:OE1	2:H3:80:GLU:N	2.39	0.47
3:O3:37:LYS:NZ	13:T3:201:CYC:O1D	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R3:134:LEU:HB2	2:R3:159:ILE:HD11	1.95	0.47
3:a3:79:ARG:HB3	13:a3:201:CYC:HMD1	1.95	0.47
3:Q4:20:LEU:H	3:Q4:20:LEU:HD12	1.79	0.47
2:H5:85:CYS:HA	13:H5:201:CYC:HHD	1.95	0.47
3:M5:58:ARG:NE	13:U5:201:CYC:O2D	2.35	0.47
3:M5:89:ILE:HG12	3:M5:92:ARG:HH21	1.79	0.47
2:N5:31:ARG:NH2	2:N5:101:VAL:O	2.47	0.47
3:E6:12:GLN:O	3:E6:16:ARG:NH1	2.47	0.47
2:K6:112:LEU:HD12	13:K6:201:CYC:HAB1	1.95	0.47
2:R6:18:ARG:NH2	2:W6:105:THR:OG1	2.47	0.47
3:D7:106:LEU:HD12	3:D7:110:CYS:HB3	1.95	0.47
3:M7:38:ARG:NH2	3:M7:160:GLU:OE1	2.44	0.47
2:N7:117:ASP:OD1	2:N7:117:ASP:N	2.46	0.47
2:R7:95:ILE:HG22	2:R7:108:ILE:HG12	1.95	0.47
5:Z7:70:ARG:NE	5:Z7:145:GLU:OE1	2.37	0.47
2:K1:85:CYS:O	2:K1:89:ILE:HG12	2.14	0.47
1:32:116:VAL:HG23	1:32:118:GLY:H	1.79	0.47
1:32:248:ARG:HH12	1:32:249:LYS:HE2	1.79	0.47
1:42:123:ILE:HG23	13:42:301:CYC:HMA1	1.95	0.47
9:Q2:117:LYS:O	8:V2:53:LYS:NZ	2.47	0.47
9:R2:39:ILE:HG12	9:R2:145:ASP:HB3	1.95	0.47
9:U2:83:ARG:NH2	13:U2:201:CYC:O2A	2.44	0.47
9:W2:71:ASN:HD21	13:W2:201:CYC:HBD2	1.78	0.47
8:d2:71:ASN:O	8:d2:77:ARG:NE	2.37	0.47
8:p2:43:THR:O	8:p2:47:ASN:ND2	2.40	0.47
13:s2:201:CYC:HB	13:s2:201:CYC:CMA	2.25	0.47
9:x2:16:ARG:NH1	9:x2:22:GLU:OE2	2.40	0.47
2:I3:121:LYS:NZ	2:K3:117:ASP:OD1	2.41	0.47
3:X3:3:PHE:HB3	3:X3:8:LYS:HB2	1.95	0.47
13:B4:201:CYC:OB	3:C4:75:TYR:O	2.33	0.47
2:H4:63:LYS:HG2	2:H4:132:GLU:HG3	1.96	0.47
3:M4:75:TYR:OH	2:U4:94:ARG:NH2	2.33	0.47
2:R4:3:LYS:HB3	2:W4:18:ARG:HH12	1.79	0.47
3:C5:43:ASN:HB2	2:G5:25:LEU:HD21	1.96	0.47
2:H5:138:LYS:HB2	2:H5:155:ILE:HG21	1.96	0.47
3:L5:98:VAL:HG21	3:L5:161:LEU:HD13	1.96	0.47
3:Q5:37:LYS:HE2	3:Q5:37:LYS:N	2.29	0.47
2:B6:25:LEU:HD22	3:J6:39:ILE:HG23	1.95	0.47
2:G6:116:LEU:HD13	3:L6:77:ASN:HD21	1.80	0.47
13:N6:201:CYC:OB	3:O6:75:TYR:O	2.32	0.47
2:F7:25:LEU:HD22	3:a7:39:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O7:96:TYR:OH	2:S7:18:ARG:O	2.31	0.47
2:R7:37:SER:OG	2:R7:147:SER:N	2.47	0.47
13:X7:201:CYC:CGA	5:Z7:115:ILE:HG12	2.43	0.47
2:W1:112:LEU:HD23	2:W1:158:LEU:HD21	1.95	0.47
6:O2:16:ILE:HG22	8:d2:83:ARG:HD3	1.96	0.47
13:A2:201:CYC:HBB2	6:Z2:44:GLN:HE22	1.80	0.47
8:C2:76:ARG:HB2	9:H2:110:VAL:HG23	1.96	0.47
8:C2:110:ASN:OD1	8:C2:110:ASN:N	2.46	0.47
8:K2:15:GLN:HG3	8:K2:17:LYS:HG2	1.96	0.47
9:h2:20:PRO:HD2	9:k2:101:ILE:HG21	1.96	0.47
8:m2:64:ASP:HA	8:m2:67:ARG:HB2	1.96	0.47
8:m2:79:ALA:O	8:m2:83:ARG:HG3	2.15	0.47
9:v2:36:ARG:NH1	9:v2:97:VAL:O	2.47	0.47
3:C3:115:ARG:HD3	5:Z3:9:ARG:HD3	1.97	0.47
3:E3:115:ARG:NH1	3:E3:173:ALA:O	2.46	0.47
2:G3:95:ILE:HG22	2:G3:108:ILE:HG12	1.96	0.47
3:L3:83:CYS:SG	13:L3:201:CYC:HAC2	2.54	0.47
3:X3:34:GLU:OE2	3:X3:38:ARG:NH2	2.38	0.47
3:M4:1:MET:HA	2:R4:2:SER:HB2	1.95	0.47
3:X4:3:PHE:HB3	3:X4:8:LYS:HB2	1.96	0.47
13:X4:201:CYC:CGA	5:Z4:115:ILE:HG12	2.44	0.47
3:C5:92:ARG:O	3:C5:95:THR:OG1	2.27	0.47
13:C5:201:CYC:HAA1	5:Z5:267:LEU:HD23	1.96	0.47
3:D5:99:PHE:CZ	2:I5:28:ALA:HB2	2.49	0.47
3:M5:39:ILE:HG23	2:R5:25:LEU:HD22	1.95	0.47
3:Q5:83:CYS:SG	13:Q5:201:CYC:HAC2	2.55	0.47
2:T5:95:ILE:HG22	2:T5:108:ILE:HG12	1.95	0.47
2:W5:25:LEU:HD22	3:X5:39:ILE:HG23	1.95	0.47
2:K6:10:VAL:HG21	3:L6:100:THR:HG23	1.96	0.47
3:M6:85:ARG:HH12	13:M6:201:CYC:HB	1.62	0.47
3:M7:83:CYS:HA	13:M7:201:CYC:HAC1	1.42	0.47
2:R7:131:VAL:HG13	2:R7:159:ILE:HD12	1.97	0.47
3:a7:83:CYS:HA	13:a7:201:CYC:HAC2	1.95	0.47
2:W1:85:CYS:HA	13:W1:201:CYC:HAC2	1.96	0.47
4:Y1:238:ARG:NH1	4:Y1:240:ARG:HH21	2.13	0.47
1:22:196:PHE:HB3	9:I2:61:LYS:HA	1.96	0.47
1:32:28:PRO:O	1:32:30:GLN:NE2	2.48	0.47
8:T2:65:ILE:HA	8:T2:70:GLY:HA3	1.96	0.47
9:W2:87:TYR:O	9:W2:91:LEU:HG	2.14	0.47
8:a2:134:LYS:HE2	8:a2:153:LEU:HB3	1.96	0.47
8:l2:144:ASP:N	8:l2:144:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m2:100:ASP:OD1	8:m2:101:THR:N	2.47	0.47
8:y2:65:ILE:H	8:y2:65:ILE:HG12	1.38	0.47
6:z2:6:ILE:O	6:z2:6:ILE:HG13	2.14	0.47
3:J3:146:ARG:NH2	3:J3:152:GLY:H	2.12	0.47
3:L3:4:ASP:OD1	3:L3:7:THR:OG1	2.26	0.47
3:O3:80:MET:O	3:O3:80:MET:HE3	2.14	0.47
2:R3:85:CYS:HB2	13:R3:201:CYC:H2C	1.95	0.47
2:W3:20:LEU:HD12	3:X3:95:THR:HG22	1.97	0.47
3:V4:9:VAL:HG12	3:V4:20:LEU:HD21	1.96	0.47
3:E5:18:GLU:O	2:H5:98:TYR:OH	2.25	0.47
1:A6:108:VAL:HG13	1:A6:112:LEU:HD12	1.96	0.47
2:N6:9:ALA:HB1	2:N6:24:GLU:HG3	1.96	0.47
3:P6:117:THR:HG21	13:P6:202:CYC:HMA1	1.96	0.47
3:X6:7:THR:HA	3:X6:10:VAL:HB	1.97	0.47
3:X6:85:ARG:NH1	5:Z6:119:ASP:OD1	2.47	0.47
3:E7:149:ILE:HG21	13:E7:201:CYC:HMC3	1.96	0.47
3:V7:92:ARG:O	3:V7:95:THR:OG1	2.29	0.47
3:L1:91:LEU:HB2	3:L1:135:MET:HE3	1.97	0.47
2:U1:134:LEU:HB3	2:U1:155:ILE:HG23	1.97	0.47
3:a1:2:THR:HG23	3:a1:105:ILE:HB	1.96	0.47
6:O2:5:ARG:NH2	6:O2:54:GLU:OE1	2.47	0.47
8:A2:130:ILE:O	8:A2:134:LYS:HG3	2.14	0.47
9:H2:50:ILE:HD11	9:H2:140:LEU:HD12	1.96	0.47
8:L2:27:LYS:O	8:L2:31:GLN:HG2	2.13	0.47
8:L2:120:VAL:HB	13:L2:201:CYC:HC	1.79	0.47
8:M2:64:ASP:OD1	8:M2:67:ARG:NH2	2.34	0.47
8:g2:30:TYR:OH	8:g2:97:LEU:O	2.32	0.47
9:v2:128:GLU:O	9:v2:132:GLU:HG2	2.15	0.47
9:x2:105:GLU:O	9:x2:110:VAL:HG22	2.15	0.47
2:B3:33:ARG:NH1	2:B3:146:ASP:OD2	2.46	0.47
3:E3:2:THR:HG23	3:E3:3:PHE:HD2	1.79	0.47
2:B4:28:ALA:HB2	3:J4:99:PHE:CZ	2.50	0.47
3:C4:154:CYS:SG	13:C4:202:CYC:HAC2	2.55	0.47
2:F4:85:CYS:HA	13:F4:201:CYC:HHD	1.95	0.47
2:N4:74:ASN:HA	13:N4:201:CYC:HBD2	1.96	0.47
2:F5:45:LEU:HD21	2:F5:141:HIS:HB2	1.96	0.47
3:O5:146:ARG:NE	3:O5:151:GLN:OE1	2.42	0.47
3:V5:2:THR:HG21	3:V5:109:ARG:HH11	1.80	0.47
5:Z5:183:LEU:HD23	5:Z5:210:ASN:HB3	1.96	0.47
3:E6:150:THR:O	13:E6:201:CYC:NC	2.43	0.47
3:J6:37:LYS:N	3:J6:37:LYS:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L6:91:LEU:HB2	3:L6:135:MET:HE3	1.96	0.47
2:R6:80:GLU:O	2:R6:84:LYS:HG2	2.14	0.47
13:a6:202:CYC:HMA3	13:a6:202:CYC:HB	1.80	0.47
2:I7:91:TYR:O	2:I7:95:ILE:HG12	2.14	0.47
2:I7:134:LEU:HB3	2:I7:155:ILE:HG23	1.96	0.47
1:A1:26:GLU:OE2	3:a1:2:THR:N	2.48	0.47
2:B1:109:ASP:HA	2:B1:113:LEU:HB2	1.96	0.47
3:J1:75:TYR:OH	2:K1:94:ARG:NH2	2.27	0.47
3:X1:41:THR:HG23	3:X1:143:VAL:HG11	1.96	0.47
5:Z1:173:ARG:NH1	5:Z1:203:VAL:O	2.33	0.47
8:F2:81:CYS:SG	13:F2:201:CYC:HAC2	2.55	0.47
9:G2:36:ARG:HG3	9:G2:96:VAL:O	2.15	0.47
12:t2:23:LEU:HB3	8:u2:38:VAL:HG13	1.96	0.47
12:t2:112:ALA:HA	12:t2:115:MET:HG2	1.95	0.47
2:B3:114:ALA:HB3	3:C3:78:ARG:HB2	1.97	0.47
2:I4:138:LYS:NZ	2:I4:156:ASP:OD1	2.37	0.47
3:M4:80:MET:O	3:M4:80:MET:HE3	2.14	0.47
3:P4:20:LEU:HD13	2:U4:101:VAL:HG21	1.96	0.47
3:Q4:37:LYS:N	3:Q4:37:LYS:HE2	2.30	0.47
2:B5:99:ALA:HB2	2:B5:108:ILE:HG13	1.97	0.47
2:B5:103:GLY:O	2:I5:26:GLN:NE2	2.47	0.47
3:C5:99:PHE:CZ	2:G5:28:ALA:HB2	2.49	0.47
3:O5:80:MET:O	3:O5:80:MET:HE3	2.14	0.47
13:S5:201:CYC:O2D	3:X5:58:ARG:NH1	2.47	0.47
3:a5:146:ARG:NH1	3:a5:152:GLY:O	2.48	0.47
2:F6:138:LYS:HB2	2:F6:155:ILE:HG21	1.95	0.47
2:H6:91:TYR:O	2:H6:95:ILE:HG12	2.15	0.47
3:P6:95:THR:HG22	2:U6:20:LEU:HD12	1.96	0.47
2:W6:112:LEU:HD23	2:W6:158:LEU:HD21	1.96	0.47
2:B7:84:LYS:NZ	13:B7:201:CYC:O1A	2.46	0.47
2:F7:23:THR:HA	2:K7:5:PRO:HG3	1.96	0.47
1:A1:123:ILE:HG23	13:A1:301:CYC:HMA1	1.95	0.47
2:K1:134:LEU:HB3	2:K1:155:ILE:HG23	1.97	0.47
2:N1:45:LEU:HD21	2:N1:141:HIS:HB2	1.96	0.47
2:N1:122:THR:HG21	3:O1:84:LEU:HD13	1.96	0.47
3:O1:80:MET:HE3	3:O1:80:MET:O	2.14	0.47
3:Q1:75:TYR:O	13:R1:201:CYC:OB	2.33	0.47
2:W1:28:ALA:HB2	3:X1:99:PHE:CZ	2.49	0.47
2:W1:95:ILE:HG22	2:W1:108:ILE:HG12	1.96	0.47
3:X1:85:ARG:HG3	5:Z1:122:GLU:HG2	1.97	0.47
1:32:5:LEU:HG	1:32:124:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:52:41:GLN:HG2	3:L5:1:MET:HA	1.96	0.47
8:A2:107:ARG:HA	6:Z2:44:GLN:HB2	1.96	0.47
13:B2:202:CYC:HMC3	9:I2:121:THR:HG23	1.97	0.47
8:C2:28:LYS:HZ1	9:I2:38:ARG:HH22	1.63	0.47
8:C2:136:VAL:O	8:C2:139:SER:OG	2.28	0.47
9:D2:69:GLY:HA2	9:v2:56:ASN:HA	1.96	0.47
8:K2:28:LYS:O	8:K2:32:GLN:HG2	2.15	0.47
10:N2:445:GLN:NE2	10:N2:448:LEU:HD21	2.29	0.47
10:N2:557:PHE:HD1	10:N2:597:LEU:HD12	1.80	0.47
9:Q2:115:MET:HE1	13:Q2:201:CYC:HMB3	1.97	0.47
8:T2:137:THR:O	8:T2:141:VAL:HG22	2.14	0.47
9:i2:91:LEU:HD13	9:i2:94:TYR:HD2	1.79	0.47
9:k2:90:ARG:O	9:k2:93:THR:OG1	2.29	0.47
9:r2:37:LEU:HD22	8:y2:24:LEU:HD22	1.97	0.47
9:r2:101:ILE:HD12	9:r2:155:TYR:CE1	2.49	0.47
9:s2:71:ASN:OD1	9:s2:121:THR:OG1	2.25	0.47
3:C3:83:CYS:HA	13:C3:201:CYC:HAC2	1.96	0.47
2:K3:74:ASN:HA	13:K3:201:CYC:HBD2	1.97	0.47
3:O3:85:ARG:NH1	13:Z3:301:CYC:O1A	2.39	0.47
3:P3:96:TYR:OH	2:U3:18:ARG:O	2.26	0.47
3:Q3:79:ARG:HG2	13:Q3:201:CYC:HAD1	1.95	0.47
13:a3:202:CYC:NB	13:a3:202:CYC:HMA3	2.30	0.47
3:D4:149:ILE:HG21	13:D4:201:CYC:HMC3	1.97	0.47
2:F4:141:HIS:HE1	2:F4:148:ARG:HG3	1.79	0.47
3:J4:93:TYR:CG	3:J4:110:CYS:HB2	2.50	0.47
3:M4:3:PHE:O	3:M4:104:SER:OG	2.33	0.47
2:W4:7:THR:HG23	3:X4:2:THR:HB	1.96	0.47
3:X4:38:ARG:NH2	3:X4:160:GLU:OE1	2.44	0.47
2:B5:88:ASP:HB3	2:B5:130:TYR:HE1	1.78	0.47
2:B5:95:ILE:HG22	2:B5:108:ILE:HG12	1.96	0.47
3:D5:149:ILE:HG21	13:D5:201:CYC:HMC3	1.97	0.47
2:I5:74:ASN:HA	13:I5:201:CYC:HBD2	1.96	0.47
13:a5:201:CYC:HB	13:a5:201:CYC:HMA3	1.78	0.47
1:A6:163:VAL:HG12	1:A6:170:GLY:HA3	1.97	0.47
13:F6:202:CYC:H3C	3:L6:149:ILE:HD13	1.96	0.47
2:K6:85:CYS:O	2:K6:89:ILE:HG12	2.14	0.47
3:M6:18:GLU:O	2:R6:98:TYR:OH	2.31	0.47
2:N6:113:LEU:HA	2:N6:113:LEU:HD23	1.68	0.47
5:Z6:40:TYR:O	5:Z6:44:LEU:HB2	2.14	0.47
5:Z6:101:LYS:HE2	5:Z6:172:TYR:HB2	1.97	0.47
3:D7:99:PHE:CZ	2:I7:28:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F7:45:LEU:HD21	2:F7:141:HIS:HB2	1.96	0.47
2:R7:5:PRO:HD2	2:R7:31:ARG:HD3	1.96	0.47
13:V7:201:CYC:HAC2	13:V7:201:CYC:HHD	1.37	0.47
3:C1:89:ILE:HG12	3:C1:92:ARG:HH21	1.80	0.47
3:D1:86:ASP:OD2	3:D1:118:TYR:OH	2.30	0.47
13:E1:201:CYC:HMA3	13:E1:201:CYC:HB	1.79	0.47
2:I1:74:ASN:O	13:I1:201:CYC:NC	2.48	0.47
3:J1:73:ASN:OD1	13:J1:201:CYC:NC	2.48	0.47
3:V1:124:PRO:O	3:V1:128:VAL:HG23	2.15	0.47
13:52:302:CYC:HC	3:E5:83:CYS:HB2	1.80	0.47
13:B2:202:CYC:HHA	9:I2:119:LEU:HD22	1.97	0.47
9:D2:29:PHE:O	9:D2:36:ARG:NH2	2.33	0.47
8:V2:36:LEU:HD22	8:V2:36:LEU:H	1.80	0.47
8:d2:76:ARG:HB2	9:i2:110:VAL:HG23	1.96	0.47
9:j2:154:ASP:HA	9:j2:157:ILE:HG12	1.96	0.47
9:x2:64:ASP:OD1	9:x2:64:ASP:N	2.45	0.47
9:x2:81:CYS:HA	13:x2:201:CYC:HAC1	1.45	0.47
2:G3:126:ALA:HB3	2:G3:129:TRP:CE2	2.50	0.47
2:N3:126:ALA:HB3	2:N3:129:TRP:CE2	2.50	0.47
3:Q4:76:THR:HG22	3:Q4:78:ARG:H	1.79	0.47
2:S4:18:ARG:NH1	2:T4:109:ASP:OD2	2.48	0.47
2:T4:138:LYS:HB2	2:T4:155:ILE:HG21	1.96	0.47
13:X4:201:CYC:OB	5:Z4:92:GLN:HB3	2.15	0.47
5:Z4:74:ARG:NH2	5:Z4:135:ASP:OD1	2.48	0.47
3:D5:20:LEU:H	3:D5:20:LEU:HD12	1.80	0.47
3:E5:146:ARG:O	3:E5:151:GLN:NE2	2.48	0.47
13:F5:202:CYC:H3C	3:L5:149:ILE:HD13	1.96	0.47
3:M5:84:LEU:HD13	2:U5:122:THR:HG21	1.97	0.47
2:R5:9:ALA:HB1	2:R5:24:GLU:HG3	1.97	0.47
2:U5:85:CYS:O	2:U5:89:ILE:HG12	2.15	0.47
1:A6:191:PHE:O	1:A6:193:LYS:N	2.43	0.47
2:B6:120:ASN:HD22	2:B6:127:PRO:HG3	1.78	0.47
2:F6:85:CYS:O	2:F6:89:ILE:HG12	2.15	0.47
3:L6:73:ASN:OD1	13:L6:201:CYC:NC	2.47	0.47
3:Q6:37:LYS:HE2	3:Q6:37:LYS:N	2.29	0.47
3:J7:109:ARG:NH2	5:Z7:227:SER:OG	2.48	0.47
2:U7:108:ILE:HG22	2:U7:113:LEU:HG	1.97	0.47
2:W7:14:ASP:OD1	5:Z7:121:TYR:OH	2.33	0.47
5:Z7:41:ARG:O	5:Z7:46:ASN:N	2.42	0.47
3:a7:16:ARG:NH2	3:a7:24:GLN:OE1	2.48	0.47
2:G1:113:LEU:HD11	2:G1:161:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:109:ARG:NH1	2:S1:14:ASP:OD2	2.48	0.47
2:R1:27:VAL:HG22	2:W1:27:VAL:HG22	1.96	0.47
13:a1:202:CYC:HMA3	13:a1:202:CYC:HB	1.80	0.47
10:N2:235:ARG:CZ	8:X2:46:ALA:HB1	2.43	0.47
13:c2:801:CYC:NB	10:o2:572:ILE:HG21	2.28	0.47
9:e2:128:GLU:OE1	9:e2:131:ARG:NH1	2.48	0.47
9:h2:27:LYS:HG3	8:l2:38:VAL:HG11	1.96	0.47
9:v2:76:ASP:OD1	9:v2:76:ASP:N	2.46	0.47
3:E3:40:ASP:HB3	13:E3:201:CYC:HBC3	1.96	0.47
2:N3:85:CYS:O	2:N3:89:ILE:HG12	2.15	0.47
3:O3:38:ARG:NH1	3:O3:98:VAL:O	2.36	0.47
3:P3:74:ALA:HA	3:P3:79:ARG:HB3	1.97	0.47
3:X3:76:THR:HG23	3:X3:79:ARG:H	1.80	0.47
2:K4:99:ALA:HB2	2:K4:108:ILE:HG13	1.95	0.47
3:O4:96:TYR:OH	2:S4:18:ARG:O	2.30	0.47
3:O5:93:TYR:CG	3:O5:110:CYS:HB2	2.50	0.47
3:P5:100:THR:HG23	2:U5:10:VAL:HG21	1.96	0.47
5:Z5:142:THR:HG21	5:Z5:152:ARG:HD2	1.97	0.47
1:A6:36:GLN:OE1	3:L6:112:ASN:ND2	2.48	0.47
3:D6:9:VAL:HG12	3:D6:20:LEU:HD23	1.97	0.47
3:J6:112:ASN:O	5:Z6:224:LEU:HA	2.15	0.47
3:Q6:152:GLY:O	13:Q6:202:CYC:OC	2.33	0.47
2:B7:18:ARG:O	3:J7:96:TYR:OH	2.30	0.47
2:G7:114:ALA:HB3	3:L7:78:ARG:HB2	1.97	0.47
2:K7:101:VAL:HG21	3:L7:20:LEU:HD12	1.97	0.47
2:R7:64:PHE:HE2	2:R7:132:GLU:HG2	1.79	0.47
2:U7:74:ASN:ND2	2:U7:124:ASP:OD2	2.48	0.47
13:A1:301:CYC:HAB2	3:D1:110:CYS:HA	1.96	0.47
3:D1:75:TYR:O	13:H1:201:CYC:OB	2.32	0.47
2:N1:27:VAL:HG22	2:U1:27:VAL:HG22	1.97	0.47
2:R1:80:GLU:O	2:R1:84:LYS:HG2	2.15	0.47
13:32:302:CYC:HMD1	3:E3:79:ARG:HB3	1.97	0.47
9:D2:100:ASP:OD1	9:D2:101:ILE:N	2.48	0.47
9:G2:95:GLY:HA3	9:G2:104:ILE:HD11	1.96	0.47
9:I2:106:GLU:OE1	10:N2:539:ARG:N	2.43	0.47
8:K2:35:GLU:OE1	8:K2:39:ARG:NH1	2.48	0.47
9:Q2:33:GLY:O	9:Q2:36:ARG:HG2	2.14	0.47
9:Q2:81:CYS:HA	13:Q2:201:CYC:HHD	1.97	0.47
8:T2:126:THR:HG23	13:T2:201:CYC:HBC2	1.97	0.47
8:a2:137:THR:O	8:a2:141:VAL:HG22	2.14	0.47
10:o2:31:GLN:HG2	10:o2:273:PHE:HZ	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o2:53:ARG:HH21	10:o2:176:GLY:HA2	1.80	0.47
10:o2:603:TYR:HD2	10:o2:606:LYS:HG3	1.79	0.47
9:r2:100:ASP:OD1	9:r2:101:ILE:N	2.43	0.47
12:t2:151:PRO:HB2	9:v2:20:PRO:HB3	1.97	0.47
9:v2:128:GLU:OE1	9:v2:131:ARG:NH1	2.47	0.47
9:v2:134:LYS:HB2	9:v2:153:PHE:HB3	1.97	0.47
3:C3:99:PHE:CZ	2:G3:28:ALA:HB2	2.50	0.47
2:F3:31:ARG:NH2	2:F3:101:VAL:O	2.38	0.47
2:G3:138:LYS:HB2	2:G3:155:ILE:HG21	1.97	0.47
3:P3:111:LEU:HD21	3:P3:168:ALA:HA	1.96	0.47
2:I4:52:LEU:HB3	2:I4:137:ILE:HD12	1.97	0.47
2:I4:109:ASP:HA	2:I4:113:LEU:HB2	1.96	0.47
3:J4:37:LYS:HE2	3:J4:37:LYS:N	2.30	0.47
3:O4:119:LEU:HD11	5:Z4:286:PRO:HD2	1.97	0.47
2:T4:9:ALA:HB2	2:T4:27:VAL:HG11	1.96	0.47
3:V4:136:LYS:HB2	3:V4:165:PHE:CG	2.50	0.47
3:O5:119:LEU:HD11	5:Z5:286:PRO:HD2	1.97	0.47
3:C6:89:ILE:HG12	3:C6:92:ARG:HH21	1.80	0.47
2:K6:45:LEU:HD21	2:K6:141:HIS:HB2	1.97	0.47
3:M6:146:ARG:O	3:M6:151:GLN:NE2	2.39	0.47
2:G7:95:ILE:HG22	2:G7:108:ILE:HG12	1.97	0.47
2:H7:5:PRO:HD2	2:H7:31:ARG:HD3	1.95	0.47
2:S7:85:CYS:O	2:S7:89:ILE:HG12	2.14	0.47
3:V7:30:ARG:O	3:V7:34:GLU:HG2	2.15	0.47
3:X7:4:ASP:HA	3:X7:100:THR:HB	1.97	0.47
3:Q1:152:GLY:O	13:Q1:202:CYC:OC	2.33	0.46
2:W1:56:ALA:HB3	2:W1:89:ILE:HG21	1.97	0.46
1:22:69:GLN:HE21	5:Z7:225:GLY:HA3	1.80	0.46
1:32:163:VAL:HG12	1:32:170:GLY:HA3	1.97	0.46
9:G2:90:ARG:HB3	8:K2:18:TYR:CZ	2.50	0.46
8:M2:90:ARG:NH2	10:N2:32:ASP:OD1	2.48	0.46
8:O2:104:LEU:HD11	8:O2:152:TYR:HB3	1.98	0.46
9:Q2:2:SER:H	9:Q2:5:SER:HG	1.62	0.46
13:S2:201:CYC:HB	13:S2:201:CYC:CMA	2.28	0.46
9:h2:90:ARG:HB3	8:l2:18:TYR:CZ	2.49	0.46
2:F3:85:CYS:HA	13:F3:201:CYC:HAC2	1.97	0.46
13:F3:202:CYC:OC	3:L3:152:GLY:O	2.32	0.46
3:Q3:128:VAL:HG22	13:Q3:201:CYC:H3C	1.96	0.46
2:S3:80:GLU:OE2	2:W6:51:SER:OG	2.26	0.46
2:B4:108:ILE:HG22	2:B4:113:LEU:HG	1.96	0.46
3:C4:99:PHE:CZ	2:G4:28:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K4:2:SER:O	3:L4:1:MET:N	2.47	0.46
3:O4:20:LEU:HD22	2:S4:101:VAL:HG21	1.97	0.46
2:U4:50:ASP:O	2:U4:54:ASN:ND2	2.35	0.46
4:Y4:252:LYS:NZ	5:Z4:70:ARG:HH22	2.13	0.46
3:E5:124:PRO:O	3:E5:128:VAL:HG23	2.15	0.46
2:G5:23:THR:HG23	2:H5:5:PRO:HA	1.98	0.46
2:N5:45:LEU:HD21	2:N5:141:HIS:HB2	1.97	0.46
13:F6:202:CYC:OC	3:L6:152:GLY:O	2.32	0.46
3:P6:27:ALA:HA	3:P6:30:ARG:HE	1.80	0.46
3:Q6:128:VAL:HG22	13:Q6:201:CYC:H3C	1.96	0.46
3:a6:2:THR:HG23	3:a6:105:ILE:HB	1.97	0.46
3:C7:99:PHE:CZ	2:G7:28:ALA:HB2	2.50	0.46
2:H7:91:TYR:O	2:H7:95:ILE:HG12	2.15	0.46
2:H7:108:ILE:HG22	2:H7:113:LEU:HG	1.97	0.46
3:L7:83:CYS:SG	13:L7:201:CYC:HAC2	2.55	0.46
3:V7:118:TYR:HE2	3:V7:128:VAL:HG11	1.81	0.46
3:X7:91:LEU:HB2	3:X7:135:MET:HE3	1.97	0.46
2:B1:9:ALA:HB1	2:B1:24:GLU:HB3	1.97	0.46
2:W1:10:VAL:HG21	3:X1:100:THR:HG23	1.97	0.46
9:J2:109:ILE:HG23	9:J2:159:ALA:HB1	1.98	0.46
9:Q2:91:LEU:HB3	9:Q2:104:ILE:HG23	1.98	0.46
8:a2:130:ILE:O	8:a2:134:LYS:HG3	2.15	0.46
8:c2:40:ALA:O	8:c2:44:ILE:HG12	2.15	0.46
9:e2:147:ASP:OD1	9:e2:147:ASP:N	2.48	0.46
9:j2:50:ILE:HG23	9:j2:136:ALA:HB3	1.97	0.46
9:k2:16:ARG:NH1	9:k2:17:TYR:O	2.46	0.46
10:o2:364:ALA:HB2	10:o2:440:PHE:HB3	1.96	0.46
6:z2:6:ILE:HD13	6:z2:36:TRP:HZ3	1.80	0.46
2:U3:112:LEU:HD23	2:U3:158:LEU:HD21	1.97	0.46
2:U3:134:LEU:HB3	2:U3:155:ILE:HG23	1.96	0.46
3:M4:58:ARG:HE	13:U4:201:CYC:CGD	2.29	0.46
3:O4:99:PHE:CZ	2:S4:28:ALA:HB2	2.51	0.46
2:R4:155:ILE:O	2:R4:159:ILE:HG12	2.15	0.46
3:D5:8:LYS:NZ	3:D5:12:GLN:OE1	2.49	0.46
2:N5:74:ASN:HA	13:N5:201:CYC:HBD2	1.97	0.46
3:V5:115:ARG:NH2	3:V5:173:ALA:O	2.37	0.46
4:Y5:252:LYS:NZ	5:Z5:70:ARG:HH22	2.12	0.46
1:A6:17:VAL:O	1:A6:161:ARG:NH1	2.48	0.46
13:J6:202:CYC:HMA3	13:J6:202:CYC:HB	1.79	0.46
3:C7:30:ARG:O	3:C7:34:GLU:HG2	2.14	0.46
3:D7:16:ARG:HH22	3:D7:24:GLN:HE22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:116:GLU:OE1	3:D7:116:GLU:N	2.40	0.46
3:M7:76:THR:HG22	3:M7:78:ARG:H	1.81	0.46
3:P7:37:LYS:HE2	3:P7:154:CYS:HB3	1.96	0.46
2:R7:85:CYS:HB2	13:R7:201:CYC:H2C	1.96	0.46
2:U7:112:LEU:HD23	2:U7:158:LEU:HD21	1.96	0.46
1:52:56:HIS:HB3	3:a5:85:ARG:HH11	1.79	0.46
8:C2:79:ALA:HA	8:C2:82:ILE:HG12	1.98	0.46
10:N2:464:PHE:HB3	10:N2:558:GLY:HA3	1.97	0.46
9:h2:47:ARG:H	9:h2:47:ARG:HG3	1.51	0.46
8:m2:100:ASP:OD2	11:q2:162:ARG:NH2	2.49	0.46
10:o2:196:CYS:SG	10:o2:201:THR:OG1	2.74	0.46
10:o2:494:GLY:O	10:o2:510:THR:HG21	2.15	0.46
9:s2:57:GLN:HB3	9:s2:61:LYS:HZ3	1.80	0.46
12:t2:47:GLU:OE1	8:u2:18:TYR:OH	2.32	0.46
2:B3:74:ASN:OD1	2:B3:74:ASN:N	2.48	0.46
2:K3:112:LEU:HD23	2:K3:158:LEU:HD21	1.97	0.46
3:Q3:96:TYR:OH	2:T3:18:ARG:O	2.33	0.46
2:T3:134:LEU:HB3	2:T3:155:ILE:HG23	1.96	0.46
3:E4:75:TYR:O	13:F4:201:CYC:OB	2.33	0.46
2:I4:78:THR:OG1	2:I4:80:GLU:OE1	2.32	0.46
3:Q4:99:PHE:CZ	2:T4:28:ALA:HB2	2.51	0.46
2:T4:74:ASN:ND2	2:T4:124:ASP:OD2	2.47	0.46
3:a4:3:PHE:O	3:a4:102:ASP:HB3	2.15	0.46
3:M5:3:PHE:O	3:M5:104:SER:OG	2.32	0.46
3:P5:114:LEU:HD23	3:P5:172:VAL:HG12	1.96	0.46
13:A6:302:CYC:HBC2	13:A6:302:CYC:H2C	1.77	0.46
2:B6:74:ASN:HA	13:B6:201:CYC:HBD2	1.97	0.46
3:O6:37:LYS:O	3:O6:41:THR:HG23	2.15	0.46
3:J7:44:ARG:NH1	3:J7:145:ASP:O	2.31	0.46
2:K7:20:LEU:HD12	3:L7:95:THR:HG22	1.97	0.46
3:M7:114:LEU:HD11	3:M7:118:TYR:CZ	2.49	0.46
3:O7:38:ARG:NH1	3:O7:98:VAL:O	2.34	0.46
3:Q7:154:CYS:SG	13:Q7:202:CYC:H2C	2.56	0.46
13:C1:201:CYC:O2D	5:Z1:236:ARG:NH2	2.49	0.46
1:22:204:PHE:CZ	1:52:216:PRO:HB2	2.51	0.46
1:52:98:ASN:OD1	1:52:181:TYR:HA	2.16	0.46
1:52:179:PRO:HB2	3:a5:121:LEU:HD21	1.98	0.46
13:52:302:CYC:HBC2	13:52:302:CYC:H2C	1.76	0.46
9:E2:12:ASP:OD1	8:L2:90:TYR:CZ	2.68	0.46
8:M2:94:TYR:OH	10:N2:33:ARG:O	2.34	0.46
8:O2:28:LYS:O	8:O2:32:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d2:104:LEU:HD22	8:d2:156:ILE:HD11	1.96	0.46
8:m2:43:THR:O	8:m2:47:ASN:ND2	2.45	0.46
9:s2:101:ILE:HD12	9:s2:155:TYR:CE1	2.49	0.46
12:t2:77:GLN:OE1	12:t2:77:GLN:N	2.43	0.46
3:Q3:154:CYS:SG	13:Q3:202:CYC:H2C	2.56	0.46
3:V3:106:LEU:HD12	3:V3:110:CYS:HB3	1.97	0.46
5:Z3:240:VAL:HG12	5:Z3:284:VAL:HG22	1.97	0.46
3:E4:100:THR:HG23	2:H4:10:VAL:HG21	1.96	0.46
3:O4:34:GLU:HG3	3:O4:37:LYS:HD2	1.98	0.46
5:Z4:55:LEU:HD21	5:Z4:79:SER:HB3	1.97	0.46
2:N5:23:THR:HA	2:U5:5:PRO:HG3	1.97	0.46
2:F6:91:TYR:O	2:F6:95:ILE:HG12	2.16	0.46
2:K6:134:LEU:HB3	2:K6:155:ILE:HG23	1.98	0.46
3:P6:44:ARG:HH21	3:P6:149:ILE:HB	1.79	0.46
3:P6:74:ALA:HA	3:P6:79:ARG:HB3	1.97	0.46
2:K7:25:LEU:HD22	3:L7:39:ILE:HG23	1.96	0.46
2:T7:138:LYS:HB2	2:T7:155:ILE:HG21	1.96	0.46
3:a7:146:ARG:NH1	3:a7:152:GLY:H	2.13	0.46
3:D1:99:PHE:CZ	2:I1:28:ALA:HB2	2.51	0.46
2:F1:3:LYS:HZ2	2:K1:18:ARG:HE	1.63	0.46
2:N1:24:GLU:OE1	2:N1:24:GLU:N	2.43	0.46
2:S1:27:VAL:HG22	2:T1:27:VAL:HG23	1.97	0.46
2:W1:18:ARG:O	3:X1:96:TYR:OH	2.28	0.46
3:X1:86:ASP:OD2	3:X1:118:TYR:OH	2.33	0.46
5:Z1:222:ARG:HA	5:Z1:287:ALA:HB1	1.96	0.46
1:32:16:ARG:NH2	3:E3:109:ARG:O	2.28	0.46
9:E2:12:ASP:OD1	8:L2:90:TYR:OH	2.30	0.46
9:I2:1:MET:HB3	9:I2:2:SER:H	1.57	0.46
9:I2:154:ASP:HA	9:I2:157:ILE:HG12	1.98	0.46
8:K2:56:VAL:HG12	8:K2:61:LEU:HG	1.97	0.46
10:N2:72:ALA:O	10:N2:76:PHE:HB2	2.16	0.46
10:N2:680:GLU:HG3	10:N2:681:ALA:H	1.80	0.46
8:O2:2:GLN:HB2	8:O2:6:THR:HB	1.97	0.46
8:T2:56:VAL:HG12	8:T2:61:LEU:HG	1.98	0.46
8:V2:81:CYS:HA	13:V2:201:CYC:HAC1	1.96	0.46
8:m2:137:THR:O	8:m2:141:VAL:HG22	2.16	0.46
11:q2:60:PHE:HB3	11:q2:67:LEU:HD11	1.97	0.46
9:r2:39:ILE:HG12	9:r2:145:ASP:HB3	1.97	0.46
8:u2:4:ALA:N	8:u2:98:ALA:O	2.46	0.46
6:z2:6:ILE:HD13	6:z2:36:TRP:CZ3	2.50	0.46
3:C3:119:LEU:HD22	3:O3:122:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W3:28:ALA:HB2	3:X3:99:PHE:CZ	2.50	0.46
3:C4:43:ASN:HB2	2:G4:25:LEU:HD21	1.98	0.46
13:J4:201:CYC:HMA1	13:J4:201:CYC:NB	2.31	0.46
2:R4:23:THR:HG21	2:W4:8:GLU:HG3	1.97	0.46
2:W4:16:GLN:HG3	2:W4:18:ARG:HG2	1.97	0.46
3:a4:128:VAL:HG13	13:a4:201:CYC:HBC3	1.98	0.46
3:O5:63:GLU:OE2	3:O5:134:LYS:NZ	2.43	0.46
3:C6:154:CYS:SG	13:C6:202:CYC:HAC2	2.56	0.46
3:E6:38:ARG:NH1	3:E6:98:VAL:O	2.40	0.46
2:N6:126:ALA:HB3	2:N6:129:TRP:CE2	2.50	0.46
3:J7:112:ASN:O	5:Z7:224:LEU:HA	2.15	0.46
3:M7:78:ARG:HD2	5:Z7:29:ARG:HH21	1.80	0.46
2:F1:98:TYR:OH	3:a1:18:GLU:O	2.32	0.46
13:22:301:CYC:HMD1	3:D7:79:ARG:HB3	1.96	0.46
13:52:302:CYC:H3C	3:E5:128:VAL:HG22	1.96	0.46
8:B2:94:TYR:OH	9:J2:16:ARG:O	2.32	0.46
9:J2:154:ASP:O	8:K2:46:ALA:HB2	2.15	0.46
12:S2:109:LEU:HD11	12:S2:159:GLY:HA3	1.97	0.46
8:c2:19:LEU:HD12	9:k2:97:VAL:HG21	1.95	0.46
10:o2:536:PRO:HB2	10:o2:539:ARG:HH11	1.81	0.46
8:p2:137:THR:O	8:p2:141:VAL:HG22	2.16	0.46
9:r2:47:ARG:NH1	9:r2:86:ASP:OD2	2.48	0.46
13:r2:201:CYC:CMA	13:r2:201:CYC:HB	2.28	0.46
12:t2:2:THR:HG21	8:u2:5:ILE:HB	1.98	0.46
8:w2:56:VAL:HG12	8:w2:61:LEU:HG	1.96	0.46
2:K3:95:ILE:HG22	2:K3:108:ILE:HG12	1.98	0.46
2:T3:99:ALA:HB2	2:T3:108:ILE:HG13	1.98	0.46
3:V3:76:THR:HG23	2:W3:111:TYR:HA	1.96	0.46
3:V3:115:ARG:NH2	3:V3:173:ALA:O	2.36	0.46
3:a3:83:CYS:HA	13:a3:201:CYC:HAC2	1.96	0.46
2:F4:85:CYS:O	2:F4:89:ILE:HG12	2.16	0.46
2:F4:138:LYS:HB2	2:F4:155:ILE:HG21	1.96	0.46
3:L4:76:THR:HG22	3:L4:78:ARG:H	1.81	0.46
3:Q4:114:LEU:HD11	3:Q4:118:TYR:CZ	2.50	0.46
3:C5:154:CYS:SG	13:C5:202:CYC:HAC2	2.55	0.46
13:L5:201:CYC:HBB3	5:Z5:250:PHE:HE1	1.81	0.46
2:R5:155:ILE:O	2:R5:159:ILE:HG12	2.15	0.46
2:F6:10:VAL:HG21	3:a6:100:THR:HG23	1.97	0.46
3:Q6:59:ALA:HB3	3:Q6:134:LYS:HD3	1.97	0.46
2:T6:24:GLU:HA	2:T6:27:VAL:HG12	1.97	0.46
3:J7:4:ASP:N	3:J7:7:THR:OG1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K7:141:HIS:NE2	2:K7:152:ASN:OD1	2.44	0.46
3:L7:76:THR:OG1	3:L7:79:ARG:NH1	2.49	0.46
3:M7:115:ARG:NH2	3:M7:170:ALA:O	2.48	0.46
2:T7:9:ALA:HB2	2:T7:27:VAL:HG11	1.98	0.46
3:V7:115:ARG:NH2	3:V7:173:ALA:O	2.37	0.46
1:A1:56:HIS:HB3	3:a1:85:ARG:HH11	1.80	0.46
13:B1:201:CYC:HHD	13:B1:201:CYC:HAC1	1.64	0.46
3:M1:84:LEU:HD13	2:U1:122:THR:HG21	1.98	0.46
3:M1:130:GLU:HG3	3:M1:134:LYS:HE2	1.98	0.46
2:N1:85:CYS:O	2:N1:89:ILE:HG12	2.16	0.46
2:T1:150:GLU:HG2	2:T1:154:TYR:CE2	2.51	0.46
2:W1:85:CYS:HA	13:W1:201:CYC:HHD	1.98	0.46
1:42:36:GLN:OE1	3:L4:112:ASN:ND2	2.48	0.46
9:D2:64:ASP:N	9:D2:64:ASP:OD1	2.46	0.46
8:F2:3:ASP:HA	8:F2:98:ALA:HB1	1.98	0.46
9:G2:81:CYS:SG	13:G2:201:CYC:HAC2	2.56	0.46
9:J2:50:ILE:HG13	9:J2:136:ALA:HB3	1.98	0.46
8:L2:120:VAL:HB	13:L2:201:CYC:NC	2.31	0.46
10:N2:27:GLN:OE1	9:Q2:10:ASN:HB3	2.16	0.46
10:N2:521:VAL:HG22	10:N2:526:SER:HB2	1.97	0.46
9:e2:14:GLU:OE1	9:e2:16:ARG:NE	2.30	0.46
9:e2:15:ALA:HB2	10:o2:554:ARG:HD3	1.97	0.46
9:k2:48:GLU:H	9:k2:48:GLU:CD	2.23	0.46
8:l2:1:MET:SD	8:l2:103:ILE:HB	2.55	0.46
10:o2:372:ASP:OD1	8:p2:83:ARG:NH1	2.45	0.46
8:p2:134:LYS:HG3	8:p2:150:GLY:HA2	1.97	0.46
3:C3:30:ARG:O	3:C3:34:GLU:HG2	2.15	0.46
3:L3:149:ILE:O	3:L3:151:GLN:NE2	2.48	0.46
3:M3:3:PHE:O	3:M3:104:SER:OG	2.34	0.46
3:M3:75:TYR:HH	2:U3:94:ARG:HH22	1.60	0.46
2:N3:45:LEU:HD21	2:N3:141:HIS:HB2	1.98	0.46
3:a3:9:VAL:HG11	3:a3:28:LEU:HD11	1.98	0.46
3:C4:92:ARG:O	3:C4:95:THR:OG1	2.26	0.46
3:C4:124:PRO:O	3:C4:128:VAL:HG23	2.15	0.46
2:S4:85:CYS:O	2:S4:89:ILE:HG12	2.16	0.46
3:X5:91:LEU:HB2	3:X5:135:MET:HE3	1.98	0.46
3:D6:20:LEU:HD13	2:I6:101:VAL:HG21	1.97	0.46
3:D6:41:THR:HG23	3:D6:143:VAL:HG21	1.98	0.46
3:O6:106:LEU:HG	3:O6:111:LEU:HD22	1.98	0.46
3:V6:124:PRO:O	3:V6:128:VAL:HG23	2.15	0.46
2:G7:94:ARG:HG2	2:G7:98:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P7:116:GLU:OE1	3:P7:116:GLU:N	2.43	0.46
3:Q7:79:ARG:O	13:Q7:201:CYC:HMD2	2.16	0.46
2:F1:8:GLU:OE2	2:K1:16:GLN:NE2	2.32	0.46
3:P1:106:LEU:HG	3:P1:111:LEU:HD22	1.98	0.46
2:R1:53:VAL:HG23	2:R1:89:ILE:HB	1.97	0.46
2:S1:74:ASN:HA	13:S1:201:CYC:HBD2	1.97	0.46
2:T1:134:LEU:HB3	2:T1:155:ILE:HG23	1.97	0.46
2:U1:95:ILE:HG22	2:U1:108:ILE:HG12	1.98	0.46
9:G2:1:MET:SD	9:G2:102:THR:HG21	2.55	0.46
9:Q2:1:MET:SD	9:Q2:103:PRO:HA	2.56	0.46
9:U2:56:ASN:O	9:U2:60:GLN:HG2	2.16	0.46
8:V2:56:VAL:HG12	8:V2:61:LEU:HG	1.98	0.46
8:a2:38:VAL:HG13	9:i2:23:LEU:HD12	1.97	0.46
9:f2:134:LYS:HB2	9:f2:153:PHE:HB3	1.98	0.46
10:o2:663:GLU:OE2	10:o2:674:ARG:NH2	2.44	0.46
9:r2:1:MET:SD	9:r2:103:PRO:HA	2.56	0.46
13:C3:202:CYC:HBC2	13:C3:202:CYC:H2C	1.72	0.46
2:G3:26:GLN:NE2	2:H3:103:GLY:O	2.46	0.46
3:J3:149:ILE:HG21	13:J3:202:CYC:HMC3	1.97	0.46
2:T3:9:ALA:HB2	2:T3:27:VAL:HG11	1.98	0.46
5:Z3:41:ARG:O	5:Z3:46:ASN:N	2.41	0.46
13:Z3:301:CYC:HC	13:Z3:301:CYC:HMD1	1.81	0.46
3:D4:44:ARG:HE	3:D4:149:ILE:HD12	1.80	0.46
3:E4:96:TYR:OH	2:H4:18:ARG:O	2.28	0.46
13:F4:202:CYC:H3C	3:L4:149:ILE:HD13	1.96	0.46
2:H4:85:CYS:HA	13:H4:201:CYC:HHD	1.98	0.46
2:K4:18:ARG:O	3:L4:96:TYR:OH	2.31	0.46
2:R4:80:GLU:O	2:R4:84:LYS:HG2	2.15	0.46
2:U4:21:SER:OG	2:U4:22:SER:N	2.48	0.46
2:U4:126:ALA:HB3	2:U4:129:TRP:CE2	2.51	0.46
2:F5:10:VAL:HG21	3:a5:100:THR:HG23	1.98	0.46
3:M5:83:CYS:HA	13:M5:201:CYC:HAC1	1.48	0.46
3:P5:89:ILE:HG12	3:P5:92:ARG:HH21	1.80	0.46
3:D6:20:LEU:H	3:D6:20:LEU:HD12	1.80	0.46
2:N6:98:TYR:OH	3:V6:18:GLU:O	2.32	0.46
3:Q6:4:ASP:OD1	3:Q6:7:THR:N	2.40	0.46
2:R6:31:ARG:NH2	2:R6:101:VAL:O	2.48	0.46
3:V6:86:ASP:OD1	5:Z6:48:TYR:OH	2.28	0.46
2:F7:21:SER:N	2:F7:24:GLU:OE1	2.48	0.46
2:K7:10:VAL:HG21	3:L7:100:THR:HG23	1.97	0.46
3:L7:4:ASP:OD1	3:L7:7:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N7:85:CYS:O	2:N7:89:ILE:HG12	2.15	0.46
3:O7:146:ARG:HH21	3:O7:151:GLN:HB3	1.80	0.46
3:Q7:112:ASN:O	4:Y7:261:HIS:NE2	2.41	0.46
2:W7:115:GLY:O	2:W7:119:ILE:HG12	2.16	0.46
3:a7:44:ARG:HH21	3:a7:149:ILE:HG12	1.80	0.46
2:S1:2:SER:HB2	2:S1:106:GLY:HA3	1.96	0.46
4:Y1:248:VAL:HG11	4:Y1:256:THR:HG21	1.97	0.46
7:12:78:ALA:HB1	8:n2:151:VAL:HG11	1.98	0.46
1:52:185:TYR:CE2	1:52:189:LEU:HD11	2.51	0.46
8:B2:65:ILE:HG23	8:B2:72:MET:HE2	1.98	0.46
9:H2:14:GLU:HB2	9:H2:16:ARG:HG2	1.98	0.46
9:R2:101:ILE:HD12	9:R2:155:TYR:CE1	2.51	0.46
8:T2:1:MET:N	8:T2:1:MET:SD	2.89	0.46
8:V2:36:LEU:HD12	8:V2:39:ARG:HH21	1.80	0.46
8:V2:137:THR:HG21	8:V2:149:MET:HG2	1.98	0.46
9:W2:87:TYR:HB3	13:W2:201:CYC:HBB3	1.98	0.46
8:l2:3:ASP:HA	8:l2:98:ALA:HB1	1.97	0.46
13:z2:201:CYC:NC	13:z2:201:CYC:HMD1	2.31	0.46
3:J3:44:ARG:NH1	3:J3:145:ASP:O	2.32	0.46
3:C4:128:VAL:HG22	13:C4:201:CYC:H3C	1.97	0.46
2:F4:31:ARG:NH2	2:F4:101:VAL:O	2.49	0.46
3:M4:114:LEU:HD11	3:M4:118:TYR:CZ	2.50	0.46
2:W4:85:CYS:HA	13:W4:201:CYC:HAC2	1.98	0.46
3:J5:83:CYS:HA	13:J5:201:CYC:HAC1	1.48	0.46
3:P5:99:PHE:CZ	2:U5:28:ALA:HB2	2.51	0.46
2:W5:16:GLN:HG3	2:W5:18:ARG:HG2	1.98	0.46
13:C6:202:CYC:NB	13:C6:202:CYC:HMA3	2.31	0.46
3:P6:41:THR:O	3:P6:45:ILE:HG12	2.16	0.46
3:X6:149:ILE:O	3:X6:151:GLN:NE2	2.49	0.46
2:F7:85:CYS:HA	13:F7:201:CYC:HAC2	1.98	0.46
4:Y7:224:VAL:HG13	4:Y7:270:ILE:HG12	1.97	0.46
2:N1:85:CYS:HA	13:N1:201:CYC:HHH	1.98	0.46
3:Q1:99:PHE:CZ	2:T1:28:ALA:HB2	2.50	0.46
3:Q1:154:CYS:SG	13:Q1:202:CYC:H2C	2.56	0.46
1:22:128:ALA:O	1:22:132:GLN:HG2	2.16	0.46
1:22:180:ARG:NH2	13:a7:201:CYC:O1D	2.49	0.46
9:E2:48:GLU:H	9:E2:48:GLU:CD	2.24	0.46
8:F2:137:THR:O	8:F2:141:VAL:HG22	2.16	0.46
9:J2:1:MET:HE2	9:J2:5:SER:HB2	1.98	0.46
8:M2:38:VAL:HG11	10:N2:44:SER:OG	2.16	0.46
8:M2:43:THR:O	8:M2:47:ASN:ND2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q2:201:CYC:OB	8:V2:73:TYR:O	2.34	0.46
7:b2:93:PRO:HB2	7:b2:97:LEU:HD11	1.97	0.46
8:c2:137:THR:O	8:c2:141:VAL:HG12	2.16	0.46
9:e2:29:PHE:HE1	9:e2:99:GLY:HA3	1.80	0.46
9:e2:100:ASP:OD1	9:e2:101:ILE:N	2.49	0.46
8:m2:90:ARG:NH2	10:o2:499:GLN:OE1	2.45	0.46
8:n2:116:TYR:HE2	8:n2:126:THR:HG21	1.79	0.46
8:n2:119:LEU:HD13	13:n2:201:CYC:HBD1	1.97	0.46
10:o2:74:ARG:HE	10:o2:207:ASP:HB2	1.80	0.46
10:o2:296:PHE:O	10:o2:298:ARG:NH1	2.40	0.46
2:K3:85:CYS:O	2:K3:89:ILE:HG12	2.15	0.46
3:M3:83:CYS:HA	13:M3:201:CYC:HAC1	1.42	0.46
2:N3:146:ASP:N	2:N3:146:ASP:OD1	2.49	0.46
3:O3:39:ILE:HG22	13:T3:201:CYC:HMB1	1.97	0.46
2:S3:50:ASP:N	2:S3:50:ASP:OD1	2.49	0.46
2:W3:115:GLY:O	2:W3:118:GLU:HG2	2.16	0.46
5:Z3:101:LYS:NZ	5:Z3:151:TYR:OH	2.42	0.46
2:I4:95:ILE:HG21	2:I4:112:LEU:HG	1.98	0.46
3:J4:89:ILE:HD13	13:J4:201:CYC:HBB3	1.96	0.46
2:R4:143:LEU:C	2:R4:148:ARG:HB2	2.41	0.46
2:S4:74:ASN:HA	13:S4:201:CYC:HBD2	1.98	0.46
2:T4:24:GLU:HA	2:T4:27:VAL:HG12	1.97	0.46
5:Z4:108:PRO:HG2	5:Z4:194:LEU:HD11	1.98	0.46
3:D5:77:ASN:HD21	13:H5:201:CYC:HMB1	1.81	0.46
2:S5:67:THR:HG21	13:S5:201:CYC:HMC2	1.98	0.46
3:a5:83:CYS:HA	13:a5:201:CYC:HAC2	1.98	0.46
3:M6:84:LEU:HD13	2:U6:122:THR:HG21	1.98	0.46
2:B7:3:LYS:H	2:B7:106:GLY:HA3	1.81	0.46
3:C7:4:ASP:OD2	3:C7:7:THR:OG1	2.25	0.46
3:E7:105:ILE:HD12	3:E7:109:ARG:HG3	1.97	0.46
2:H7:45:LEU:HD21	2:H7:141:HIS:HB2	1.98	0.46
2:T7:53:VAL:HG13	2:T7:89:ILE:HB	1.97	0.46
1:A1:3:LEU:HD21	3:D1:81:ALA:HB3	1.98	0.45
1:A1:75:ILE:HG21	5:Z1:229:PRO:HB2	1.98	0.45
3:O1:17:GLY:HA3	3:X1:70:PRO:HB3	1.98	0.45
2:R1:141:HIS:NE2	2:R1:152:ASN:OD1	2.41	0.45
7:12:96:SER:N	11:q2:65:GLU:OE2	2.48	0.45
1:22:50:TYR:CD1	1:22:54:PHE:HE2	2.34	0.45
1:32:14:ASN:OD1	1:32:14:ASN:N	2.49	0.45
1:52:14:ASN:N	1:52:14:ASN:OD1	2.48	0.45
8:C2:35:GLU:HG3	9:I2:27:LYS:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F2:112:LEU:HG	8:F2:160:LEU:HD21	1.98	0.45
9:H2:130:VAL:HG13	9:H2:157:ILE:HG12	1.97	0.45
12:S2:92:ILE:HG21	12:S2:153:PHE:CZ	2.51	0.45
9:U2:100:ASP:OD1	9:U2:101:ILE:N	2.48	0.45
13:U2:201:CYC:HMA1	13:U2:201:CYC:NB	2.22	0.45
8:c2:94:TYR:OH	9:k2:16:ARG:O	2.33	0.45
8:n2:38:VAL:HG11	10:o2:44:SER:OG	2.16	0.45
10:o2:33:ARG:HG2	10:o2:34:PHE:O	2.17	0.45
10:o2:68:VAL:HG13	10:o2:162:MET:HE2	1.98	0.45
3:E3:99:PHE:CZ	2:H3:28:ALA:HB2	2.50	0.45
3:J3:109:ARG:NH2	5:Z3:227:SER:OG	2.49	0.45
3:M3:80:MET:HE3	3:M3:80:MET:O	2.16	0.45
5:Z3:70:ARG:NE	5:Z3:145:GLU:OE1	2.38	0.45
2:G4:27:VAL:HG13	2:H4:27:VAL:HG22	1.98	0.45
3:J4:112:ASN:O	5:Z4:224:LEU:HA	2.16	0.45
3:Q4:109:ARG:HA	4:Y4:261:HIS:HB3	1.98	0.45
3:V4:75:TYR:OH	2:W4:94:ARG:NH2	2.33	0.45
3:X4:85:ARG:NH1	5:Z4:119:ASP:OD1	2.48	0.45
13:a4:202:CYC:HMA3	13:a4:202:CYC:HB	1.80	0.45
13:F5:202:CYC:H2C	3:L5:154:CYS:SG	2.56	0.45
2:N5:14:ASP:OD2	3:V5:109:ARG:NE	2.49	0.45
3:P5:84:LEU:HD13	2:T5:122:THR:HG21	1.96	0.45
3:V5:84:LEU:HD13	2:W5:122:THR:HG21	1.98	0.45
2:F6:113:LEU:HD11	2:F6:161:ALA:HB1	1.98	0.45
3:V6:115:ARG:NH2	3:V6:173:ALA:O	2.40	0.45
5:Z6:41:ARG:NH2	5:Z6:175:TYR:O	2.44	0.45
2:B7:85:CYS:CA	13:B7:201:CYC:HHD	2.46	0.45
3:E7:99:PHE:CZ	2:H7:28:ALA:HB2	2.51	0.45
13:J7:201:CYC:HMA3	5:Z7:224:LEU:HD23	1.97	0.45
2:N7:126:ALA:HB3	2:N7:129:TRP:CE2	2.51	0.45
2:S7:85:CYS:HA	13:S7:201:CYC:HAC1	1.75	0.45
13:S7:201:CYC:HAC1	13:S7:201:CYC:HHD	1.55	0.45
3:V7:77:ASN:HD21	13:W7:201:CYC:HMB2	1.81	0.45
2:S1:103:GLY:O	2:T1:26:GLN:NE2	2.45	0.45
5:Z1:40:TYR:OH	5:Z1:59:GLU:OE2	2.27	0.45
1:22:65:VAL:HG13	13:J7:201:CYC:HBB2	1.97	0.45
1:42:28:PRO:O	1:42:30:GLN:NE2	2.47	0.45
1:42:40:VAL:HB	2:K4:110:GLU:HG3	1.98	0.45
1:42:163:VAL:HG12	1:42:170:GLY:HA3	1.98	0.45
8:C2:81:CYS:HB2	13:C2:201:CYC:NC	2.30	0.45
8:L2:76:ARG:O	13:L2:201:CYC:HMD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e2:90:ARG:NH2	8:m2:73:TYR:OH	2.27	0.45
9:f2:1:MET:O	9:f2:102:THR:OG1	2.19	0.45
9:f2:53:GLN:OE1	9:f2:57:GLN:NE2	2.47	0.45
9:h2:14:GLU:OE1	9:h2:16:ARG:NE	2.35	0.45
8:l2:108:VAL:O	8:l2:112:LEU:HB2	2.16	0.45
11:q2:95:TYR:OH	9:v2:16:ARG:O	2.31	0.45
9:s2:71:ASN:OD1	13:s2:201:CYC:NC	2.44	0.45
9:x2:76:ASP:O	9:x2:80:THR:OG1	2.33	0.45
3:C3:18:GLU:O	2:G3:98:TYR:OH	2.30	0.45
2:G3:114:ALA:HB3	3:L3:78:ARG:HB2	1.97	0.45
3:O3:112:ASN:O	5:Z3:162:SER:OG	2.28	0.45
2:S3:85:CYS:HA	13:S3:201:CYC:HAC1	1.73	0.45
2:U3:108:ILE:HG22	2:U3:113:LEU:HG	1.98	0.45
5:Z3:43:VAL:HA	5:Z3:102:HIS:HB3	1.98	0.45
5:Z3:87:PHE:HD1	5:Z3:95:VAL:HG11	1.80	0.45
3:D4:20:LEU:HD13	2:I4:101:VAL:HG21	1.98	0.45
2:K5:39:LEU:HD22	3:L5:25:LEU:HD12	1.98	0.45
2:W5:7:THR:HG23	3:X5:2:THR:HB	1.97	0.45
3:X5:37:LYS:NZ	3:X5:150:THR:OG1	2.45	0.45
5:Z5:10:LEU:HD13	5:Z5:169:PHE:CE2	2.52	0.45
3:D6:75:TYR:O	13:H6:201:CYC:OB	2.33	0.45
3:D6:92:ARG:O	3:D6:95:THR:OG1	2.29	0.45
2:G6:5:PRO:HG3	2:H6:23:THR:HA	1.97	0.45
3:M6:75:TYR:HH	2:U6:94:ARG:HH22	1.57	0.45
3:P6:68:ILE:HG22	3:P6:80:MET:HE1	1.99	0.45
3:Q6:114:LEU:HD11	3:Q6:118:TYR:CZ	2.51	0.45
2:N7:20:LEU:HD12	2:N7:24:GLU:HG2	1.98	0.45
2:R7:134:LEU:HB2	2:R7:159:ILE:HD11	1.97	0.45
2:T7:115:GLY:O	2:T7:119:ILE:HG12	2.16	0.45
3:V7:39:ILE:HG22	13:V7:202:CYC:HMB2	1.98	0.45
2:W7:4:THR:HG22	2:W7:102:ALA:HB1	1.98	0.45
13:C1:202:CYC:HBC2	13:C1:202:CYC:H2C	1.75	0.45
3:D1:37:LYS:N	3:D1:37:LYS:HE2	2.31	0.45
2:G1:122:THR:HG21	3:L1:84:LEU:HD13	1.98	0.45
2:H1:91:TYR:O	2:H1:95:ILE:HG12	2.15	0.45
8:A2:134:LYS:HE2	8:A2:153:LEU:HB3	1.97	0.45
8:K2:144:ASP:N	8:K2:144:ASP:OD1	2.47	0.45
8:M2:114:GLU:OE1	8:M2:114:GLU:N	2.43	0.45
9:W2:105:GLU:O	9:W2:110:VAL:HG22	2.15	0.45
8:a2:74:THR:HG23	9:k2:107:ILE:HA	1.98	0.45
9:e2:64:ASP:OD1	9:e2:64:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g2:160:LEU:HD23	8:g2:160:LEU:HA	1.83	0.45
9:v2:126:VAL:HG12	9:v2:160:LEU:HD13	1.98	0.45
3:C3:35:GLY:O	3:C3:39:ILE:HG12	2.16	0.45
2:I3:91:TYR:O	2:I3:95:ILE:HG12	2.16	0.45
3:L3:70:PRO:HA	3:L3:75:TYR:CG	2.52	0.45
2:W3:131:VAL:HG12	2:W3:135:LYS:HE2	1.97	0.45
3:X3:7:THR:HA	3:X3:10:VAL:HB	1.98	0.45
3:D4:39:ILE:HG23	2:I4:25:LEU:HG	1.97	0.45
2:K4:74:ASN:HA	13:K4:201:CYC:HBD2	1.98	0.45
2:U4:85:CYS:O	2:U4:89:ILE:HG12	2.16	0.45
3:Q5:76:THR:HG23	2:R5:111:TYR:HA	1.99	0.45
3:Q5:128:VAL:HG13	13:Q5:201:CYC:HBC3	1.97	0.45
2:R5:143:LEU:C	2:R5:148:ARG:HB2	2.42	0.45
3:E6:18:GLU:O	2:H6:98:TYR:OH	2.29	0.45
3:E6:96:TYR:OH	2:H6:18:ARG:O	2.34	0.45
5:Z6:40:TYR:OH	5:Z6:59:GLU:OE2	2.31	0.45
3:C7:18:GLU:O	2:G7:98:TYR:OH	2.28	0.45
2:F7:27:VAL:HG22	2:K7:27:VAL:HG22	1.97	0.45
2:I7:74:ASN:HA	13:I7:201:CYC:HBD2	1.99	0.45
2:K7:115:GLY:O	2:K7:119:ILE:HG12	2.17	0.45
2:N7:31:ARG:NH2	2:N7:101:VAL:O	2.49	0.45
3:Q7:114:LEU:HD11	3:Q7:118:TYR:CZ	2.51	0.45
2:T7:24:GLU:O	2:T7:27:VAL:HG12	2.16	0.45
1:A1:189:LEU:HB2	1:A1:191:PHE:CE2	2.51	0.45
2:R1:26:GLN:NE2	2:W1:103:GLY:O	2.49	0.45
2:T1:108:ILE:HG22	2:T1:113:LEU:HG	1.97	0.45
1:32:224:ARG:HB3	9:s2:75:GLU:OE2	2.17	0.45
1:52:244:LYS:NZ	9:I2:75:GLU:OE2	2.37	0.45
9:I2:39:ILE:HG23	9:I2:141:LEU:HD13	1.97	0.45
9:J2:48:GLU:CD	9:J2:48:GLU:H	2.24	0.45
8:a2:75:THR:HG22	9:k2:115:MET:HE2	1.98	0.45
9:k2:154:ASP:O	8:l2:46:ALA:HB2	2.16	0.45
8:u2:54:GLU:HG3	8:u2:136:VAL:HG21	1.98	0.45
9:x2:90:ARG:O	9:x2:93:THR:OG1	2.26	0.45
9:x2:128:GLU:O	9:x2:131:ARG:HG2	2.16	0.45
13:D3:201:CYC:HMA3	13:D3:201:CYC:NB	2.31	0.45
3:E3:21:SER:H	3:E3:24:GLN:NE2	2.14	0.45
2:F3:91:TYR:O	2:F3:95:ILE:HG12	2.16	0.45
2:I3:50:ASP:OD1	2:I3:50:ASP:N	2.48	0.45
3:J3:106:LEU:HD12	3:J3:110:CYS:HB3	1.98	0.45
2:K3:18:ARG:O	3:L3:96:TYR:OH	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:73:ASN:OD1	13:a3:201:CYC:NC	2.41	0.45
13:I4:201:CYC:HHD	13:I4:201:CYC:HAC1	1.56	0.45
3:P4:89:ILE:HD13	13:P4:201:CYC:HBB3	1.98	0.45
2:I5:50:ASP:N	2:I5:50:ASP:OD1	2.50	0.45
3:O5:37:LYS:O	3:O5:41:THR:HG23	2.17	0.45
3:L6:124:PRO:O	3:L6:128:VAL:HG23	2.16	0.45
3:Q6:99:PHE:CZ	2:T6:28:ALA:HB2	2.51	0.45
2:R6:85:CYS:HA	13:R6:201:CYC:HAC2	1.99	0.45
3:V6:136:LYS:HB2	3:V6:165:PHE:CG	2.51	0.45
2:G7:138:LYS:HB2	2:G7:155:ILE:HG21	1.98	0.45
2:I7:85:CYS:O	2:I7:89:ILE:HG12	2.16	0.45
3:J7:146:ARG:NH2	3:J7:152:GLY:H	2.14	0.45
5:Z7:109:TYR:N	5:Z7:113:GLU:OE1	2.50	0.45
2:K1:8:GLU:HG3	2:K1:9:ALA:N	2.31	0.45
3:O1:106:LEU:HG	3:O1:111:LEU:HD22	1.98	0.45
1:22:27:GLN:HE21	2:K7:16:GLN:HG2	1.81	0.45
1:32:128:ALA:O	1:32:132:GLN:HG2	2.16	0.45
1:32:216:PRO:HB2	1:42:204:PHE:CZ	2.50	0.45
9:E2:134:LYS:HB2	9:E2:153:PHE:HB3	1.99	0.45
9:H2:43:ILE:HD11	9:H2:141:LEU:HD11	1.98	0.45
9:I2:105:GLU:HA	9:I2:109:ILE:HB	1.98	0.45
8:L2:42:THR:O	8:L2:46:ASN:ND2	2.46	0.45
10:N2:53:ARG:HH21	10:N2:176:GLY:HA2	1.82	0.45
11:P2:89:TYR:OH	11:P2:117:TYR:OH	2.26	0.45
8:a2:104:LEU:HD22	8:a2:156:ILE:HD11	1.99	0.45
8:n2:72:MET:HE2	8:n2:78:TYR:CD2	2.51	0.45
10:o2:681:ALA:HB3	10:o2:686:LYS:NZ	2.31	0.45
9:s2:39:ILE:HG12	9:s2:145:ASP:HB3	1.97	0.45
2:F3:33:ARG:NH2	2:F3:34:GLN:OE1	2.50	0.45
3:P3:37:LYS:HE2	3:P3:154:CYS:HB3	1.97	0.45
3:V3:109:ARG:HG2	5:Z3:14:PRO:HG3	1.98	0.45
2:W3:115:GLY:O	2:W3:119:ILE:HG12	2.17	0.45
2:B4:98:TYR:OH	3:J4:18:GLU:O	2.30	0.45
3:M4:83:CYS:HA	13:M4:201:CYC:HAC1	1.46	0.45
5:Z4:243:ALA:HA	5:Z4:257:ASN:HD22	1.82	0.45
2:F5:98:TYR:OH	3:a5:18:GLU:O	2.31	0.45
3:J5:37:LYS:HE2	3:J5:37:LYS:N	2.32	0.45
3:C6:35:GLY:O	3:C6:39:ILE:HG12	2.16	0.45
2:F6:95:ILE:HG21	2:F6:112:LEU:HB2	1.97	0.45
3:O6:61:PHE:HB3	3:O6:68:ILE:HD13	1.98	0.45
2:T6:53:VAL:HG13	2:T6:89:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T6:115:GLY:O	2:T6:119:ILE:HG12	2.17	0.45
2:F7:134:LEU:HB3	2:F7:155:ILE:HG23	1.99	0.45
2:K7:85:CYS:O	2:K7:89:ILE:HG12	2.16	0.45
5:Z7:108:PRO:HG2	5:Z7:194:LEU:HD11	1.98	0.45
1:A1:127:LEU:HD12	3:D1:85:ARG:NE	2.32	0.45
2:G1:27:VAL:HG22	2:H1:27:VAL:HG22	1.97	0.45
2:G1:150:GLU:HG2	2:G1:154:TYR:CE2	2.51	0.45
3:M1:44:ARG:HH21	3:M1:145:ASP:HB3	1.82	0.45
3:M1:83:CYS:HA	13:M1:201:CYC:HAC1	1.43	0.45
2:N1:126:ALA:HB3	2:N1:129:TRP:CE2	2.52	0.45
2:U1:85:CYS:O	2:U1:89:ILE:HG12	2.16	0.45
1:22:207:GLN:NE2	8:F2:57:ALA:O	2.50	0.45
8:C2:87:TYR:OH	6:Z2:17:ARG:O	2.34	0.45
9:D2:37:LEU:HD23	9:D2:97:VAL:HG22	1.97	0.45
12:S2:18:PRO:HD3	8:T2:94:TYR:HE1	1.81	0.45
6:Y2:10:LEU:HB2	6:Y2:25:THR:HB	1.98	0.45
8:c2:17:LYS:O	9:k2:94:TYR:OH	2.34	0.45
9:h2:78:THR:O	9:h2:82:LEU:HD22	2.16	0.45
9:k2:87:TYR:CE1	13:k2:201:CYC:HAB2	2.51	0.45
10:o2:75:ILE:HG21	10:o2:204:ALA:HB2	1.98	0.45
10:o2:567:LEU:HB3	10:o2:570:PRO:HD2	1.98	0.45
13:B3:201:CYC:HMB1	3:C3:77:ASN:HD21	1.82	0.45
3:E3:37:LYS:H	3:E3:37:LYS:HG2	1.38	0.45
2:I3:85:CYS:O	2:I3:89:ILE:HG12	2.16	0.45
3:V3:52:ILE:HD11	3:V3:142:ILE:HD12	1.98	0.45
3:M4:99:PHE:CZ	2:R4:28:ALA:HB2	2.52	0.45
3:C5:63:GLU:HG3	3:C5:64:GLN:HG3	1.97	0.45
2:F5:23:THR:HA	2:K5:5:PRO:HG3	1.99	0.45
2:F5:31:ARG:NH2	2:F5:101:VAL:O	2.49	0.45
3:a5:146:ARG:HD3	13:a5:202:CYC:HMC2	1.99	0.45
1:A6:84:LEU:O	1:A6:87:SER:OG	2.28	0.45
13:F6:202:CYC:HHD	13:F6:202:CYC:HAC1	1.54	0.45
13:I6:201:CYC:HHD	13:I6:201:CYC:HAC1	1.57	0.45
3:M6:73:ASN:OD1	13:M6:201:CYC:NC	2.47	0.45
3:O6:93:TYR:CG	3:O6:110:CYS:HB2	2.51	0.45
2:S6:85:CYS:HA	13:S6:201:CYC:HAC1	1.69	0.45
2:S6:109:ASP:HA	2:S6:113:LEU:HB2	1.99	0.45
2:W6:14:ASP:OD1	5:Z6:121:TYR:OH	2.34	0.45
3:C1:37:LYS:HE2	13:C1:202:CYC:HMD2	1.97	0.45
3:D1:134:LYS:HA	3:D1:137:ASP:OD2	2.16	0.45
13:I1:201:CYC:OB	3:a1:75:TYR:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M1:98:VAL:HG13	3:M1:157:ILE:HD11	1.98	0.45
3:O1:76:THR:OG1	3:O1:77:ASN:N	2.50	0.45
3:P1:27:ALA:HA	3:P1:30:ARG:HE	1.80	0.45
1:22:53:ILE:O	1:22:110:ARG:HD3	2.16	0.45
13:22:302:CYC:O2A	3:E7:85:ARG:NH1	2.49	0.45
1:42:226:ILE:HD11	9:h2:78:THR:HG21	1.98	0.45
1:52:128:ALA:O	1:52:132:GLN:HG2	2.16	0.45
1:52:141:LEU:HD12	1:52:141:LEU:HA	1.82	0.45
10:N2:592:GLU:OE1	10:N2:595:ARG:NH2	2.46	0.45
9:Q2:37:LEU:HD23	9:Q2:97:VAL:HG22	1.98	0.45
13:R2:201:CYC:HMA3	13:R2:201:CYC:NB	2.24	0.45
13:S2:201:CYC:HB	13:S2:201:CYC:HMA1	1.82	0.45
9:U2:76:ASP:N	9:U2:76:ASP:OD1	2.50	0.45
8:X2:35:GLU:HG2	8:X2:39:ARG:HH11	1.81	0.45
8:d2:81:CYS:HA	13:d2:201:CYC:HAC2	1.99	0.45
9:i2:35:ARG:NH2	9:i2:148:GLU:OE1	2.42	0.45
8:l2:28:LYS:O	8:l2:32:GLN:HG2	2.17	0.45
8:m2:121:VAL:HB	13:m2:201:CYC:NC	2.32	0.45
10:o2:198:THR:HG23	10:o2:199:PRO:HD3	1.97	0.45
8:p2:116:TYR:HE2	8:p2:126:THR:HG21	1.82	0.45
2:B3:28:ALA:HB2	3:J3:99:PHE:CE1	2.51	0.45
3:C3:109:ARG:O	5:Z3:275:ASN:ND2	2.50	0.45
3:J3:112:ASN:O	5:Z3:224:LEU:HA	2.17	0.45
2:K3:115:GLY:O	2:K3:119:ILE:HG12	2.17	0.45
3:M3:112:ASN:OD1	3:M3:113:GLY:N	2.49	0.45
3:O3:18:GLU:O	2:S3:98:TYR:OH	2.28	0.45
3:V3:92:ARG:O	3:V3:95:THR:OG1	2.29	0.45
3:J4:4:ASP:OD1	3:J4:7:THR:OG1	2.35	0.45
2:G5:99:ALA:HB2	2:G5:108:ILE:HG13	1.99	0.45
3:L5:118:TYR:HE2	3:L5:128:VAL:HG11	1.82	0.45
3:O5:76:THR:OG1	3:O5:77:ASN:N	2.49	0.45
3:Q5:154:CYS:SG	13:Q5:202:CYC:HAC2	2.57	0.45
2:U5:85:CYS:HA	13:U5:201:CYC:HHH	1.98	0.45
3:C6:99:PHE:CZ	2:G6:28:ALA:HB2	2.51	0.45
2:I6:122:THR:HG21	3:a6:84:LEU:HD13	1.98	0.45
3:L7:116:GLU:HG3	5:Z7:212:VAL:HG22	1.99	0.45
1:A1:50:TYR:OH	1:A1:67:GLU:OE2	2.33	0.45
2:H1:109:ASP:HA	2:H1:113:LEU:HB2	1.98	0.45
2:K1:74:ASN:HA	13:K1:201:CYC:HBD2	1.98	0.45
3:M1:75:TYR:OH	2:U1:94:ARG:NH2	2.28	0.45
2:T1:85:CYS:O	2:T1:89:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:42:302:CYC:O1A	3:E4:78:ARG:NH2	2.50	0.45
13:52:302:CYC:NC	3:E5:83:CYS:HB2	2.32	0.45
8:A2:74:THR:HG23	9:J2:107:ILE:HA	1.98	0.45
9:G2:113:ARG:NH2	9:G2:159:ALA:O	2.50	0.45
9:i2:79:ALA:O	9:i2:82:LEU:HG	2.16	0.45
9:k2:81:CYS:HA	13:k2:201:CYC:HHD	1.99	0.45
8:m2:103:ILE:HD12	8:m2:107:ARG:HG3	1.98	0.45
2:N3:31:ARG:NH2	2:N3:101:VAL:O	2.50	0.45
2:T3:53:VAL:HG13	2:T3:89:ILE:HB	1.98	0.45
3:X3:124:PRO:O	3:X3:128:VAL:HG23	2.17	0.45
4:Y3:248:VAL:HG11	4:Y3:256:THR:HG21	1.99	0.45
3:E4:39:ILE:HG23	2:H4:25:LEU:HD22	1.99	0.45
2:N4:85:CYS:O	2:N4:89:ILE:HG12	2.16	0.45
3:Q4:89:ILE:HG12	3:Q4:92:ARG:HH21	1.81	0.45
3:V4:5:ALA:HB2	3:V4:101:GLY:HA3	1.99	0.45
3:X4:91:LEU:HB2	3:X4:135:MET:HE3	1.98	0.45
2:T5:24:GLU:HA	2:T5:27:VAL:HG12	1.98	0.45
1:A6:98:ASN:OD1	1:A6:181:TYR:HA	2.17	0.45
2:N6:74:ASN:HA	13:N6:201:CYC:HBD2	1.98	0.45
3:X6:75:TYR:HB3	3:X6:79:ARG:HH21	1.81	0.45
5:Z6:69:VAL:HB	5:Z6:146:SER:HA	1.99	0.45
13:C7:202:CYC:HBC2	13:C7:202:CYC:H2C	1.71	0.45
2:G7:126:ALA:HB3	2:G7:129:TRP:CE2	2.52	0.45
2:N7:23:THR:HG22	2:U7:5:PRO:HD3	1.98	0.45
2:T7:24:GLU:HA	2:T7:27:VAL:HG12	1.99	0.45
3:X7:124:PRO:O	3:X7:128:VAL:HG23	2.17	0.45
2:F1:29:PHE:HE2	13:a1:202:CYC:HBB3	1.82	0.45
2:R1:143:LEU:C	2:R1:148:ARG:HB2	2.42	0.45
2:S1:122:THR:HG21	3:X1:84:LEU:HD23	1.99	0.45
1:32:36:GLN:OE1	3:L3:112:ASN:ND2	2.50	0.45
10:N2:569:VAL:HB	10:N2:570:PRO:HD3	1.98	0.45
10:N2:582:ARG:NH1	10:N2:647:ASP:OD1	2.46	0.45
9:U2:134:LYS:HB2	9:U2:153:PHE:HB3	1.98	0.45
8:X2:72:MET:HE2	8:X2:78:TYR:CE2	2.51	0.45
8:c2:109:LEU:HD13	8:c2:159:GLY:HA3	1.99	0.45
9:f2:68:PRO:O	9:k2:63:PRO:HG2	2.17	0.45
9:j2:81:CYS:HA	13:j2:201:CYC:HAC1	1.99	0.45
8:u2:28:LYS:O	8:u2:32:GLN:HG2	2.17	0.45
8:u2:76:ARG:NE	6:z2:66:LEU:HD11	2.31	0.45
3:C3:154:CYS:SG	13:C3:202:CYC:HAC2	2.57	0.45
3:D3:92:ARG:HG2	2:I3:19:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G3:23:THR:HA	2:H3:5:PRO:HG3	1.99	0.45
2:I3:85:CYS:HA	13:I3:201:CYC:HHD	1.99	0.45
5:Z3:10:LEU:HB3	5:Z3:169:PHE:CE1	2.52	0.45
2:F4:8:GLU:OE2	2:K4:16:GLN:NE2	2.33	0.45
2:F4:99:ALA:HB2	2:F4:108:ILE:HG12	1.98	0.45
2:H4:91:TYR:O	2:H4:95:ILE:HG12	2.17	0.45
3:V4:123:VAL:HG13	13:V4:201:CYC:HMC3	1.99	0.45
5:Z4:40:TYR:OH	5:Z4:59:GLU:OE2	2.31	0.45
2:B5:20:LEU:HD12	3:J5:95:THR:HG22	1.98	0.45
3:D5:92:ARG:O	3:D5:95:THR:OG1	2.30	0.45
13:E5:201:CYC:NB	13:E5:201:CYC:HMA3	2.31	0.45
2:I6:16:GLN:OE1	2:I6:18:ARG:NE	2.38	0.45
3:O6:96:TYR:OH	2:S6:18:ARG:O	2.26	0.45
3:Q6:139:ALA:HA	3:Q6:142:ILE:HG12	1.99	0.45
2:S6:18:ARG:NH1	2:T6:109:ASP:OD2	2.49	0.45
2:S6:67:THR:HG21	13:S6:201:CYC:HMC2	1.99	0.45
2:S6:94:ARG:HH22	3:X6:75:TYR:HH	1.58	0.45
2:U6:85:CYS:O	2:U6:89:ILE:HG12	2.17	0.45
3:V6:89:ILE:HD13	13:V6:201:CYC:HBB3	1.99	0.45
2:B7:114:ALA:HB3	3:C7:78:ARG:HB2	1.99	0.45
3:D7:9:VAL:HG12	3:D7:20:LEU:HD23	1.98	0.45
3:E7:4:ASP:OD1	3:E7:7:THR:N	2.37	0.45
2:F7:18:ARG:HH22	2:K7:109:ASP:CG	2.25	0.45
2:K7:95:ILE:HG22	2:K7:108:ILE:HG12	1.99	0.45
3:P7:39:ILE:HG23	2:U7:25:LEU:HD22	1.99	0.45
3:Q7:4:ASP:H	3:Q7:7:THR:HB	1.80	0.45
3:X7:146:ARG:O	3:X7:151:GLN:NE2	2.46	0.45
5:Z7:10:LEU:HB3	5:Z7:169:PHE:CE1	2.52	0.45
1:A1:164:LEU:HD21	13:A1:302:CYC:HBA2	1.99	0.45
2:B1:31:ARG:NH2	2:B1:101:VAL:O	2.51	0.45
2:I1:122:THR:HG21	3:a1:84:LEU:HD13	1.98	0.45
2:N1:149:ASP:HB3	13:P1:201:CYC:H2C	1.98	0.45
8:B2:65:ILE:HA	8:B2:70:GLY:HA3	1.99	0.45
9:E2:90:ARG:O	9:E2:93:THR:OG1	2.32	0.45
9:G2:105:GLU:HG2	9:G2:110:VAL:HG23	1.98	0.45
8:K2:3:ASP:HA	8:K2:98:ALA:HB1	1.98	0.45
8:K2:64:ASP:HB3	11:P2:123:PRO:HB3	1.99	0.45
9:R2:52:LYS:HZ3	9:R2:82:LEU:HD13	1.82	0.45
12:S2:84:ASP:HB2	13:S2:201:CYC:HBC3	1.98	0.45
12:S2:90:ARG:HD2	12:S2:94:TYR:CZ	2.52	0.45
9:f2:90:ARG:NH2	8:l2:73:TYR:OH	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j2:126:VAL:HG22	13:j2:201:CYC:HBC2	1.98	0.45
10:o2:72:ALA:HB2	10:o2:162:MET:HE1	1.99	0.45
8:p2:81:CYS:SG	13:p2:201:CYC:HAC2	2.57	0.45
2:B3:113:LEU:HD23	2:B3:113:LEU:HA	1.82	0.45
3:E3:39:ILE:HG23	2:H3:25:LEU:HD22	1.98	0.45
2:K3:2:SER:HA	2:K3:106:GLY:HA3	1.99	0.45
3:E4:98:VAL:HG13	3:E4:157:ILE:HD11	1.99	0.45
2:F4:26:GLN:NE2	2:K4:103:GLY:O	2.50	0.45
2:G4:3:LYS:HB2	2:G4:106:GLY:HA2	1.99	0.45
13:J4:201:CYC:NC	13:J4:201:CYC:HMD1	2.32	0.45
3:P4:39:ILE:HG23	2:U4:25:LEU:HD22	1.99	0.45
3:D5:100:THR:HG23	2:I5:10:VAL:HG21	1.99	0.45
13:J5:202:CYC:HMA3	13:J5:202:CYC:HB	1.81	0.45
3:V5:20:LEU:HD23	3:V5:20:LEU:HA	1.79	0.45
3:C6:124:PRO:O	3:C6:128:VAL:HG23	2.17	0.45
3:C6:146:ARG:NH2	3:C6:152:GLY:O	2.50	0.45
13:C6:202:CYC:H2C	13:C6:202:CYC:HBC2	1.72	0.45
3:E6:9:VAL:HG13	3:E6:12:GLN:HE21	1.81	0.45
13:E6:201:CYC:HMA3	13:E6:201:CYC:HB	1.80	0.45
3:P6:87:MET:HG2	3:P6:135:MET:SD	2.57	0.45
3:P6:130:GLU:HG3	3:P6:134:LYS:HZ3	1.81	0.45
2:T6:95:ILE:HG22	2:T6:108:ILE:HG12	1.98	0.45
2:T6:99:ALA:HB2	2:T6:108:ILE:HG13	1.99	0.45
2:S7:33:ARG:NH1	2:S7:146:ASP:OD2	2.45	0.45
3:V7:106:LEU:HD12	3:V7:110:CYS:HB3	1.99	0.45
3:C1:92:ARG:O	3:C1:95:THR:OG1	2.30	0.44
2:I1:18:ARG:NH2	2:I1:24:GLU:OE2	2.45	0.44
3:O1:37:LYS:O	3:O1:41:THR:HG23	2.17	0.44
3:X1:4:ASP:O	3:X1:5:ALA:C	2.61	0.44
1:22:146:GLU:OE2	1:22:160:ARG:NH2	2.50	0.44
1:42:65:VAL:HG13	13:J4:201:CYC:HBB2	2.00	0.44
1:42:184:TYR:OH	3:D4:108:ASP:OD1	2.29	0.44
9:I2:113:ARG:NH2	9:I2:159:ALA:O	2.51	0.44
10:N2:147:VAL:HG13	10:N2:155:MET:HG3	1.99	0.44
10:N2:288:ILE:HD11	10:N2:315:VAL:HG11	1.99	0.44
10:N2:616:LEU:HD23	10:N2:616:LEU:HA	1.84	0.44
8:O2:61:LEU:HG	13:U2:201:CYC:HBA1	1.99	0.44
8:O2:137:THR:O	8:O2:141:VAL:HG22	2.17	0.44
13:a2:201:CYC:HMA3	13:a2:201:CYC:HB	1.82	0.44
8:c2:3:ASP:HB2	9:k2:5:SER:HB3	1.98	0.44
10:o2:391:GLU:OE2	10:o2:405:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r2:47:ARG:HD2	8:y2:18:TYR:CE1	2.52	0.44
12:t2:134:LYS:NZ	12:t2:154:ASP:OD1	2.32	0.44
8:w2:36:LEU:HD22	8:w2:36:LEU:H	1.82	0.44
2:F3:85:CYS:O	2:F3:89:ILE:HG12	2.17	0.44
3:J3:4:ASP:N	3:J3:7:THR:OG1	2.48	0.44
3:L3:116:GLU:OE1	3:L3:116:GLU:N	2.36	0.44
3:M3:99:PHE:CZ	2:R3:28:ALA:HB2	2.51	0.44
2:R3:85:CYS:HA	13:R3:201:CYC:HHD	1.99	0.44
2:B4:122:THR:HG21	3:C4:84:LEU:HD13	1.99	0.44
3:E4:124:PRO:O	3:E4:128:VAL:HG23	2.16	0.44
2:H4:108:ILE:HG22	2:H4:113:LEU:HG	1.98	0.44
2:K4:88:ASP:HB3	2:K4:130:TYR:HE1	1.82	0.44
2:U5:126:ALA:HB3	2:U5:129:TRP:CE2	2.52	0.44
3:X5:38:ARG:NH2	3:X5:160:GLU:OE1	2.44	0.44
3:D6:16:ARG:HH22	3:D6:24:GLN:HE22	1.65	0.44
2:F6:14:ASP:OD1	3:a6:93:TYR:OH	2.25	0.44
2:F6:25:LEU:HD22	3:a6:39:ILE:HG23	1.98	0.44
2:N6:1:MET:H1	3:V6:2:THR:N	2.15	0.44
2:F7:85:CYS:O	2:F7:89:ILE:HG12	2.17	0.44
3:X7:76:THR:HG23	3:X7:79:ARG:H	1.82	0.44
3:D1:16:ARG:NE	3:D1:18:GLU:OE2	2.50	0.44
3:E1:124:PRO:O	3:E1:128:VAL:HG23	2.17	0.44
2:N1:74:ASN:HA	13:N1:201:CYC:HBD2	1.99	0.44
2:W1:55:GLY:HA2	2:S7:79:PRO:HD3	1.98	0.44
8:F2:4:ALA:N	8:F2:98:ALA:O	2.47	0.44
9:G2:101:ILE:HD12	9:G2:155:TYR:CE1	2.53	0.44
9:G2:134:LYS:HB2	9:G2:153:PHE:HB3	1.98	0.44
10:N2:196:CYS:SG	13:N2:802:CYC:OC	2.62	0.44
11:P2:133:ILE:O	11:P2:137:ARG:HG2	2.17	0.44
9:R2:57:GLN:O	9:R2:61:LYS:HG2	2.17	0.44
12:S2:37:LEU:HD23	12:S2:97:LEU:HD22	1.99	0.44
9:h2:1:MET:HB3	9:h2:102:THR:HB	1.98	0.44
11:q2:133:ILE:O	11:q2:137:ARG:HG2	2.17	0.44
3:C3:39:ILE:HG23	2:G3:25:LEU:HG	2.00	0.44
2:F3:10:VAL:HG21	3:a3:100:THR:HG23	1.98	0.44
3:M3:76:THR:HG22	3:M3:78:ARG:H	1.82	0.44
3:P3:128:VAL:HG22	13:P3:202:CYC:H3C	1.99	0.44
3:V3:4:ASP:H	3:V3:7:THR:HG1	1.62	0.44
3:E4:149:ILE:HD13	13:E4:201:CYC:H3C	1.99	0.44
3:O4:93:TYR:CG	3:O4:110:CYS:HB2	2.52	0.44
3:Q4:93:TYR:OH	2:T4:14:ASP:OD1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T4:99:ALA:HB2	2:T4:108:ILE:HG13	1.99	0.44
2:W4:95:ILE:HG22	2:W4:108:ILE:HG12	1.98	0.44
2:H5:91:TYR:O	2:H5:95:ILE:HG12	2.17	0.44
3:L5:40:ASP:CG	3:L5:149:ILE:HD11	2.42	0.44
2:N5:12:ALA:O	2:N5:16:GLN:HG2	2.17	0.44
2:N5:85:CYS:O	2:N5:89:ILE:HG12	2.17	0.44
2:R5:85:CYS:HA	13:R5:201:CYC:HAC2	1.99	0.44
2:W5:131:VAL:HG12	2:W5:135:LYS:HE2	1.99	0.44
3:C6:38:ARG:NH1	3:C6:98:VAL:O	2.39	0.44
3:J6:109:ARG:HD3	5:Z6:228:THR:OG1	2.17	0.44
3:P6:111:LEU:HD21	3:P6:168:ALA:HA	1.99	0.44
2:S6:88:ASP:HB3	2:S6:130:TYR:HE1	1.83	0.44
2:T6:85:CYS:O	2:T6:89:ILE:HG12	2.18	0.44
13:T6:201:CYC:NB	13:T6:201:CYC:HMA3	2.32	0.44
3:X6:37:LYS:HD3	3:X6:37:LYS:HA	1.79	0.44
2:B7:134:LEU:HB3	2:B7:155:ILE:HG23	1.99	0.44
3:J7:108:ASP:HA	5:Z7:289:LEU:HB3	1.98	0.44
3:Q7:139:ALA:HA	3:Q7:142:ILE:HG12	1.99	0.44
2:T7:134:LEU:HB3	2:T7:155:ILE:HG23	1.99	0.44
3:a7:41:THR:HG23	3:a7:143:VAL:HG21	1.98	0.44
1:A1:184:TYR:O	1:A1:187:THR:HG22	2.18	0.44
2:N1:25:LEU:HD22	3:V1:39:ILE:HG23	1.98	0.44
3:Q1:128:VAL:HG22	13:Q1:201:CYC:HBC3	1.98	0.44
2:U1:126:ALA:HB3	2:U1:129:TRP:CE2	2.52	0.44
3:V1:35:GLY:O	3:V1:39:ILE:HG13	2.18	0.44
3:X1:37:LYS:HD3	3:X1:37:LYS:HA	1.78	0.44
1:22:53:ILE:HG21	1:22:84:LEU:HB3	2.00	0.44
1:22:205:PRO:HG2	1:22:207:GLN:HE21	1.82	0.44
1:32:103:PHE:HZ	1:32:134:TYR:HE2	1.65	0.44
1:42:74:GLN:HA	5:Z4:261:LEU:HD12	1.99	0.44
8:B2:119:LEU:HD13	13:B2:201:CYC:HBD2	2.00	0.44
8:C2:87:TYR:CG	13:C2:201:CYC:HBB3	2.52	0.44
8:K2:137:THR:O	8:K2:141:VAL:HG22	2.17	0.44
8:M2:28:LYS:HG3	10:N2:51:LEU:HD11	1.99	0.44
10:N2:74:ARG:HH21	10:N2:207:ASP:HB2	1.81	0.44
10:N2:584:PHE:O	10:N2:588:ILE:HG12	2.18	0.44
9:Q2:48:GLU:H	9:Q2:48:GLU:CD	2.26	0.44
12:S2:71:ASN:OD1	13:S2:201:CYC:NC	2.48	0.44
13:a2:201:CYC:HB	13:a2:201:CYC:CMA	2.31	0.44
9:e2:37:LEU:HD23	9:e2:97:VAL:HG22	1.98	0.44
9:j2:39:ILE:HD12	9:j2:141:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o2:201:THR:HG23	13:o2:801:CYC:HBC2	1.98	0.44
12:t2:2:THR:N	12:t2:5:SER:HG	2.15	0.44
8:y2:109:LEU:HD13	8:y2:159:GLY:HA3	1.99	0.44
3:D3:77:ASN:HD21	2:H3:116:LEU:HD13	1.82	0.44
3:J3:83:CYS:HA	13:J3:201:CYC:HAC1	1.47	0.44
2:K3:91:TYR:HB3	13:K3:201:CYC:HBB3	1.99	0.44
2:N3:149:ASP:HB3	13:P3:201:CYC:HAC2	1.98	0.44
3:O3:96:TYR:OH	2:S3:18:ARG:O	2.33	0.44
2:B4:10:VAL:HG21	3:J4:100:THR:HG23	1.98	0.44
3:J4:89:ILE:HG12	3:J4:92:ARG:HH21	1.81	0.44
2:S4:31:ARG:NH2	2:S4:101:VAL:O	2.50	0.44
3:X4:21:SER:H	3:X4:24:GLN:HE21	1.64	0.44
3:C5:44:ARG:NE	13:C5:202:CYC:HMC1	2.32	0.44
3:D5:84:LEU:HD13	2:H5:122:THR:HG21	1.98	0.44
2:F5:85:CYS:O	2:F5:89:ILE:HG12	2.17	0.44
2:H5:9:ALA:HB2	2:H5:27:VAL:HG11	1.99	0.44
3:J5:124:PRO:O	3:J5:128:VAL:HG23	2.18	0.44
2:T5:115:GLY:O	2:T5:119:ILE:HG12	2.17	0.44
3:X5:7:THR:HA	3:X5:10:VAL:HB	1.98	0.44
2:B6:98:TYR:OH	3:J6:18:GLU:O	2.33	0.44
3:M6:96:TYR:OH	2:R6:18:ARG:O	2.33	0.44
2:S6:2:SER:HB2	2:S6:106:GLY:HA3	1.99	0.44
2:I7:95:ILE:HG22	2:I7:108:ILE:HD13	1.99	0.44
2:K7:76:ALA:HA	2:K7:81:GLY:HA3	2.00	0.44
2:R7:115:GLY:O	2:R7:119:ILE:HG12	2.18	0.44
3:V7:86:ASP:OD2	3:V7:118:TYR:OH	2.29	0.44
2:W7:95:ILE:HG22	2:W7:108:ILE:HG12	1.99	0.44
5:Z7:77:ALA:O	5:Z7:126:TYR:OH	2.30	0.44
3:E1:37:LYS:H	3:E1:37:LYS:HG2	1.54	0.44
3:P1:41:THR:O	3:P1:45:ILE:HG12	2.17	0.44
2:S1:112:LEU:HD23	2:S1:158:LEU:HD21	2.00	0.44
3:V1:20:LEU:HD23	3:V1:20:LEU:HA	1.81	0.44
3:X1:28:LEU:O	3:X1:32:VAL:HG23	2.17	0.44
8:C2:24:LEU:HD13	9:I2:38:ARG:HH21	1.81	0.44
8:O2:5:ILE:HG21	9:R2:98:SER:HA	1.99	0.44
8:V2:35:GLU:HG2	8:V2:36:LEU:HD22	1.98	0.44
8:d2:15:GLN:HB2	8:d2:17:LYS:HZ2	1.82	0.44
9:e2:130:VAL:HA	9:e2:133:LEU:HD12	1.99	0.44
8:l2:72:MET:HE2	8:l2:78:TYR:CE2	2.52	0.44
9:r2:6:LYS:HE2	9:r2:102:THR:HB	2.00	0.44
9:s2:2:SER:OG	9:s2:3:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:u2:56:VAL:HG12	8:u2:61:LEU:HG	1.99	0.44
2:B3:85:CYS:CA	13:B3:201:CYC:HHD	2.47	0.44
3:Q3:63:GLU:HG2	3:Q3:64:GLN:HG3	1.98	0.44
3:Q3:92:ARG:HH12	2:T3:14:ASP:HA	1.82	0.44
2:T3:143:LEU:C	2:T3:148:ARG:HB3	2.43	0.44
3:V3:44:ARG:NH1	3:V3:142:ILE:O	2.51	0.44
3:V3:44:ARG:HE	3:V3:149:ILE:HD12	1.82	0.44
3:V3:89:ILE:HG12	3:V3:92:ARG:HH21	1.83	0.44
13:V3:201:CYC:HMD1	13:V3:201:CYC:HC	1.81	0.44
3:X3:128:VAL:HG22	13:X3:201:CYC:H3C	1.98	0.44
3:C4:85:ARG:NH2	13:C4:201:CYC:O2A	2.48	0.44
3:D4:134:LYS:HA	3:D4:137:ASP:OD2	2.17	0.44
2:K4:14:ASP:OD2	3:L4:109:ARG:NH1	2.46	0.44
2:K4:134:LEU:HB3	2:K4:155:ILE:HG23	1.98	0.44
3:Q4:76:THR:HG23	2:R4:111:TYR:HA	1.99	0.44
2:R4:134:LEU:HB3	2:R4:155:ILE:HG23	1.98	0.44
2:T4:42:ALA:HB1	2:T4:97:THR:HG23	2.00	0.44
3:V4:20:LEU:HD23	3:V4:20:LEU:HA	1.76	0.44
3:V4:150:THR:O	13:V4:202:CYC:NC	2.49	0.44
2:B5:27:VAL:HG22	2:I5:27:VAL:HG22	1.99	0.44
3:J5:114:LEU:HD23	3:J5:172:VAL:HG22	1.99	0.44
2:N5:98:TYR:OH	3:V5:18:GLU:O	2.33	0.44
3:Q5:20:LEU:HD22	2:T5:101:VAL:HG21	1.99	0.44
2:R5:138:LYS:HB2	2:R5:155:ILE:HG21	1.99	0.44
3:V5:123:VAL:HG13	13:V5:201:CYC:HMC3	2.00	0.44
5:Z5:69:VAL:HB	5:Z5:146:SER:HA	1.99	0.44
2:B6:134:LEU:HB3	2:B6:155:ILE:HG23	1.99	0.44
2:F6:101:VAL:HG21	3:a6:20:LEU:HD13	1.99	0.44
3:L6:40:ASP:CG	3:L6:149:ILE:HD11	2.42	0.44
13:L6:201:CYC:HBB3	5:Z6:250:PHE:HE1	1.82	0.44
3:O6:149:ILE:HG21	13:T6:201:CYC:HMC3	2.00	0.44
3:Q6:83:CYS:SG	13:Q6:201:CYC:HAC2	2.57	0.44
2:R6:27:VAL:HG22	2:W6:27:VAL:HG22	1.99	0.44
2:W6:12:ALA:O	2:W6:16:GLN:HG2	2.18	0.44
3:X6:124:PRO:O	3:X6:128:VAL:HG23	2.16	0.44
3:D7:134:LYS:HA	3:D7:137:ASP:OD2	2.18	0.44
3:M7:3:PHE:O	3:M7:104:SER:OG	2.36	0.44
3:O7:39:ILE:HG22	13:T7:201:CYC:HMB1	1.99	0.44
2:B1:50:ASP:N	2:B1:50:ASP:OD1	2.49	0.44
3:C1:39:ILE:HG23	2:G1:25:LEU:HG	1.99	0.44
2:F1:85:CYS:O	2:F1:89:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J1:201:CYC:NC	13:J1:201:CYC:HMD1	2.32	0.44
3:M1:37:LYS:O	3:M1:41:THR:HG23	2.18	0.44
2:R1:9:ALA:HB1	2:R1:24:GLU:HG3	1.98	0.44
3:a1:21:SER:H	3:a1:24:GLN:HE21	1.64	0.44
3:a1:37:LYS:HE3	13:a1:202:CYC:HMD1	1.99	0.44
1:42:179:PRO:HB2	3:a4:121:LEU:HD21	2.00	0.44
13:42:302:CYC:HMD1	3:E4:79:ARG:HB3	1.98	0.44
8:C2:28:LYS:NZ	9:I2:38:ARG:HH22	2.15	0.44
8:C2:106:GLU:O	8:C2:110:ASN:ND2	2.48	0.44
8:L2:77:TYR:O	8:L2:81:ILE:HG12	2.17	0.44
8:M2:5:ILE:HD12	10:N2:21:PRO:HG2	1.99	0.44
10:N2:33:ARG:HG2	10:N2:34:PHE:O	2.17	0.44
10:N2:75:ILE:HG21	10:N2:204:ALA:HB2	1.98	0.44
9:Q2:30:VAL:HG11	8:X2:34:GLY:HA3	1.99	0.44
9:R2:101:ILE:HB	9:R2:155:TYR:CE2	2.53	0.44
6:Z2:20:ARG:HE	6:Z2:20:ARG:HB3	1.62	0.44
9:f2:48:GLU:H	9:f2:48:GLU:CD	2.26	0.44
9:f2:104:ILE:HG21	9:f2:156:VAL:HG22	1.99	0.44
9:j2:105:GLU:OE1	10:o2:543:SER:OG	2.28	0.44
11:q2:39:GLN:O	11:q2:43:ILE:HG12	2.18	0.44
9:r2:90:ARG:O	9:r2:93:THR:OG1	2.29	0.44
12:t2:115:MET:HG3	12:t2:116:TYR:N	2.31	0.44
9:x2:85:LEU:HG	13:x2:201:CYC:HBC1	2.00	0.44
3:D3:106:LEU:HD12	3:D3:110:CYS:HB3	1.99	0.44
2:F3:5:PRO:HA	2:K3:23:THR:HG23	2.00	0.44
3:L3:116:GLU:HG3	5:Z3:212:VAL:HG22	1.99	0.44
3:Q3:4:ASP:H	3:Q3:7:THR:HB	1.81	0.44
3:Q3:109:ARG:HD3	4:Y3:261:HIS:HB3	1.99	0.44
3:V3:5:ALA:HB2	3:V3:101:GLY:HA3	2.00	0.44
4:Y3:224:VAL:HG13	4:Y3:270:ILE:HG12	1.98	0.44
2:I4:5:PRO:HG2	2:I4:31:ARG:HD3	1.99	0.44
5:Z4:211:TYR:HB2	5:Z4:282:VAL:HG21	1.98	0.44
13:B5:201:CYC:HHH	13:B5:201:CYC:HAC1	1.61	0.44
3:E5:37:LYS:H	3:E5:37:LYS:HG2	1.51	0.44
2:G5:27:VAL:HG22	2:H5:27:VAL:HG13	2.00	0.44
2:H5:112:LEU:HD23	2:H5:158:LEU:HD21	1.99	0.44
3:M5:87:MET:HE2	13:M5:201:CYC:HBC1	2.00	0.44
3:P5:96:TYR:OH	2:U5:18:ARG:O	2.31	0.44
3:V5:86:ASP:OD1	5:Z5:48:TYR:OH	2.30	0.44
13:A6:301:CYC:HAC1	3:D6:83:CYS:HA	1.98	0.44
3:P6:75:TYR:OH	2:T6:94:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y6:228:GLN:O	4:Y6:265:GLY:HA2	2.18	0.44
3:C7:149:ILE:HG21	13:C7:202:CYC:HMC3	2.00	0.44
3:Q7:85:ARG:NH2	13:Q7:201:CYC:O2A	2.40	0.44
2:W7:115:GLY:O	2:W7:118:GLU:HG2	2.17	0.44
2:F1:14:ASP:OD2	3:a1:109:ARG:NH1	2.48	0.44
3:M1:22:ASP:OD1	2:R1:43:LYS:NZ	2.51	0.44
3:Q1:142:ILE:HG13	3:Q1:143:VAL:N	2.32	0.44
3:a1:41:THR:HG23	3:a1:143:VAL:HG21	2.00	0.44
6:02:37:PHE:HB2	13:a2:201:CYC:HBA1	2.00	0.44
1:22:192:PRO:O	1:52:233:LEU:HB3	2.17	0.44
13:52:301:CYC:HAB2	3:D5:110:CYS:HA	1.99	0.44
9:D2:81:CYS:CA	13:D2:201:CYC:HHB	2.41	0.44
9:E2:68:PRO:O	9:J2:63:PRO:HG2	2.17	0.44
8:F2:43:THR:O	8:F2:47:ASN:ND2	2.45	0.44
8:K2:1:MET:SD	8:K2:103:ILE:HB	2.58	0.44
13:Q2:201:CYC:HBD2	8:V2:62:TYR:OH	2.18	0.44
9:R2:52:LYS:HA	9:R2:52:LYS:HD3	1.76	0.44
12:S2:80:GLN:HE22	12:S2:83:ARG:CZ	2.31	0.44
8:T2:68:PRO:HG3	8:T2:73:TYR:CE1	2.52	0.44
9:W2:96:VAL:HA	9:W2:152:TYR:CE2	2.52	0.44
8:g2:46:ALA:HB2	9:j2:154:ASP:HB3	1.98	0.44
9:i2:92:VAL:HG11	9:i2:153:PHE:CE2	2.53	0.44
9:j2:87:TYR:OH	9:j2:107:ILE:HG22	2.17	0.44
10:o2:19:THR:HG22	10:o2:175:ALA:HB1	2.00	0.44
10:o2:245:LYS:HE2	10:o2:245:LYS:HB3	1.81	0.44
10:o2:584:PHE:O	10:o2:588:ILE:HG12	2.18	0.44
9:s2:14:GLU:HG3	9:s2:16:ARG:HG2	1.98	0.44
12:t2:27:THR:O	12:t2:31:LYS:HG3	2.18	0.44
9:v2:100:ASP:OD1	9:v2:101:ILE:N	2.49	0.44
3:D3:92:ARG:HG2	2:I3:19:PHE:CE2	2.53	0.44
3:D3:134:LYS:HA	3:D3:137:ASP:OD2	2.17	0.44
3:E3:28:LEU:O	3:E3:32:VAL:HG23	2.18	0.44
3:P3:93:TYR:OH	2:U3:14:ASP:OD1	2.22	0.44
3:V3:41:THR:HG23	3:V3:143:VAL:HG21	1.98	0.44
5:Z3:40:TYR:O	5:Z3:44:LEU:HB2	2.17	0.44
3:a3:89:ILE:HG12	3:a3:92:ARG:HH21	1.82	0.44
3:D4:18:GLU:O	2:I4:98:TYR:OH	2.30	0.44
3:D4:75:TYR:O	13:H4:201:CYC:OB	2.34	0.44
2:F4:27:VAL:HG22	2:K4:27:VAL:HG13	2.00	0.44
2:F4:98:TYR:OH	3:a4:18:GLU:O	2.33	0.44
3:O4:107:ASP:HA	3:O4:111:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S4:67:THR:HG21	13:S4:201:CYC:HMC2	2.00	0.44
2:U4:85:CYS:HA	13:U4:201:CYC:HHD	1.98	0.44
3:V4:35:GLY:O	3:V4:39:ILE:HG13	2.17	0.44
5:Z4:85:LYS:HG3	5:Z4:180:ARG:HD3	1.99	0.44
5:Z4:227:SER:HA	5:Z4:237:ILE:HD11	2.00	0.44
3:C5:89:ILE:HD13	13:C5:201:CYC:HBB3	1.98	0.44
3:D5:39:ILE:HG23	2:I5:25:LEU:HG	1.99	0.44
3:D5:43:ASN:HB2	2:I5:25:LEU:HD21	1.99	0.44
2:I5:109:ASP:HA	2:I5:113:LEU:HB2	1.99	0.44
2:S5:85:CYS:O	2:S5:89:ILE:HG12	2.17	0.44
13:X5:201:CYC:HB	13:X5:201:CYC:CMA	2.26	0.44
5:Z5:203:VAL:HG13	5:Z5:282:VAL:HB	2.00	0.44
3:D6:44:ARG:NH1	3:D6:142:ILE:O	2.49	0.44
3:D6:86:ASP:OD2	3:D6:118:TYR:OH	2.33	0.44
3:E6:44:ARG:NH1	3:E6:142:ILE:O	2.51	0.44
3:E6:100:THR:HG23	2:H6:10:VAL:HG21	2.00	0.44
2:G6:85:CYS:HA	13:G6:201:CYC:HHD	1.99	0.44
3:P6:100:THR:HG23	2:U6:10:VAL:HG21	2.00	0.44
3:Q6:109:ARG:HD3	4:Y6:261:HIS:HB3	1.99	0.44
3:Q6:124:PRO:O	3:Q6:128:VAL:HG23	2.18	0.44
2:N7:3:LYS:H	2:N7:106:GLY:HA3	1.83	0.44
2:U7:26:GLN:HA	2:U7:29:PHE:HB2	1.99	0.44
3:a7:96:TYR:CB	3:a7:105:ILE:HG12	2.47	0.44
3:V1:136:LYS:HB2	3:V1:165:PHE:CG	2.53	0.44
5:Z1:40:TYR:HA	5:Z1:44:LEU:HD23	2.00	0.44
1:22:22:VAL:HG21	2:F7:113:LEU:HG	2.00	0.44
8:M2:94:TYR:HE1	10:N2:35:PRO:HD3	1.83	0.44
10:N2:5:ALA:HB3	10:N2:443:TYR:CD1	2.53	0.44
10:N2:53:ARG:NH2	10:N2:176:GLY:HA2	2.33	0.44
9:e2:62:ARG:O	9:e2:65:VAL:HG22	2.18	0.44
9:h2:101:ILE:HD12	9:h2:155:TYR:CE1	2.52	0.44
10:o2:67:ILE:HG22	10:o2:208:MET:HG2	1.99	0.44
10:o2:475:ASN:O	10:o2:475:ASN:ND2	2.51	0.44
11:q2:51:LEU:HD13	11:q2:138:VAL:HG22	2.00	0.44
8:y2:72:MET:HE2	8:y2:78:TYR:CE2	2.52	0.44
3:D3:61:PHE:HB3	3:D3:68:ILE:HD13	1.99	0.44
13:F3:202:CYC:H3C	3:L3:149:ILE:HD13	1.99	0.44
2:N3:26:GLN:HG2	2:U3:34:GLN:HG3	2.00	0.44
3:P3:85:ARG:NE	4:Y3:238:ARG:HH21	2.15	0.44
3:Q3:70:PRO:HA	3:Q3:75:TYR:CG	2.53	0.44
3:Q3:115:ARG:NH2	3:Q3:170:ALA:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R3:9:ALA:HB1	2:R3:24:GLU:HG3	1.99	0.44
3:C4:119:LEU:HD22	3:O4:122:GLY:HA2	1.98	0.44
2:F4:45:LEU:HD21	2:F4:141:HIS:HB2	2.00	0.44
13:F4:202:CYC:OC	3:L4:152:GLY:O	2.35	0.44
2:G4:114:ALA:HB3	3:L4:78:ARG:HB2	2.00	0.44
2:N4:95:ILE:HG22	2:N4:108:ILE:HG12	1.99	0.44
2:T4:91:TYR:O	2:T4:95:ILE:HG12	2.18	0.44
2:I5:108:ILE:HG22	2:I5:113:LEU:HG	2.00	0.44
3:Q5:76:THR:HG22	3:Q5:78:ARG:H	1.83	0.44
3:V5:9:VAL:HG12	3:V5:20:LEU:HD21	2.00	0.44
3:X5:107:ASP:HA	3:X5:111:LEU:HB2	2.00	0.44
5:Z5:40:TYR:O	5:Z5:44:LEU:HB2	2.18	0.44
1:A6:164:LEU:HD21	13:A6:302:CYC:HBA2	2.00	0.44
3:J6:75:TYR:O	13:K6:201:CYC:OB	2.35	0.44
2:N6:134:LEU:HB3	2:N6:155:ILE:HG23	2.00	0.44
2:R6:99:ALA:HB2	2:R6:108:ILE:HG13	1.99	0.44
3:D7:41:THR:HG23	3:D7:143:VAL:HG21	2.00	0.44
3:Q7:93:TYR:CG	3:Q7:110:CYS:HB2	2.53	0.44
13:Z7:301:CYC:H2C	13:Z7:301:CYC:HBC2	1.77	0.44
3:a7:114:LEU:HD23	3:a7:172:VAL:HG12	2.00	0.44
2:H1:87:ARG:NH1	13:H1:201:CYC:O2A	2.45	0.44
3:M1:86:ASP:OD2	3:M1:118:TYR:OH	2.32	0.44
2:S1:85:CYS:HA	13:S1:201:CYC:HHH	2.00	0.44
2:W1:3:LYS:HD3	2:W1:3:LYS:HA	1.74	0.44
8:B2:72:MET:HG2	8:B2:81:CYS:SG	2.58	0.44
8:O2:134:LYS:HZ3	8:O2:154:ASP:CG	2.25	0.44
9:Q2:76:ASP:N	9:Q2:76:ASP:OD1	2.50	0.44
8:d2:65:ILE:HG13	8:d2:71:ASN:HB3	2.00	0.44
8:d2:76:ARG:NE	13:d2:201:CYC:O1D	2.47	0.44
13:h2:201:CYC:HMA3	13:h2:201:CYC:NB	2.28	0.44
9:j2:128:GLU:O	9:j2:132:GLU:HG2	2.18	0.44
9:k2:105:GLU:O	9:k2:110:VAL:HG22	2.17	0.44
8:n2:20:ASP:OD1	8:n2:20:ASP:N	2.47	0.44
11:q2:98:VAL:HG11	9:v2:26:ILE:HD13	2.00	0.44
8:w2:60:LEU:HD13	8:w2:72:MET:HE1	1.99	0.44
3:P3:68:ILE:HD12	2:T3:87:ARG:HH12	1.82	0.44
5:Z3:108:PRO:HG2	5:Z3:194:LEU:HD11	1.99	0.44
3:Q4:146:ARG:NH1	3:Q4:151:GLN:OE1	2.43	0.44
2:R4:109:ASP:HA	2:R4:113:LEU:HB2	1.98	0.44
2:S4:27:VAL:HG22	2:T4:27:VAL:HG23	1.99	0.44
2:U4:112:LEU:HD23	2:U4:158:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J5:68:ILE:HG22	3:J5:80:MET:HE1	2.00	0.44
2:K5:85:CYS:O	2:K5:89:ILE:HG12	2.18	0.44
2:N5:18:ARG:NH1	2:U5:109:ASP:OD2	2.51	0.44
3:L6:98:VAL:HG21	3:L6:161:LEU:HD13	2.00	0.44
3:M6:106:LEU:HG	3:M6:111:LEU:HD12	1.98	0.44
3:Q6:142:ILE:HG13	3:Q6:143:VAL:N	2.33	0.44
2:R6:143:LEU:C	2:R6:148:ARG:HB2	2.43	0.44
2:S6:85:CYS:O	2:S6:89:ILE:HG12	2.17	0.44
2:T6:50:ASP:OD1	2:T6:50:ASP:N	2.51	0.44
2:U6:134:LEU:HB3	2:U6:155:ILE:HG23	2.00	0.44
3:C7:35:GLY:O	3:C7:39:ILE:HG12	2.17	0.44
2:F7:31:ARG:NH2	2:F7:101:VAL:O	2.40	0.44
13:F7:202:CYC:HMD2	3:L7:152:GLY:HA3	2.00	0.44
2:H7:80:GLU:OE1	2:H7:80:GLU:N	2.41	0.44
3:V7:93:TYR:CG	3:V7:110:CYS:HB2	2.53	0.44
2:W7:28:ALA:HB2	3:X7:99:PHE:CZ	2.53	0.44
3:X7:7:THR:HA	3:X7:10:VAL:HB	2.00	0.44
2:I1:121:LYS:NZ	2:K1:117:ASP:OD1	2.50	0.44
3:M1:34:GLU:HG3	3:M1:37:LYS:HE2	2.00	0.44
3:M1:95:THR:HG22	2:R1:20:LEU:HD12	2.00	0.44
3:V1:57:ALA:HB2	3:V1:87:MET:HE1	1.99	0.44
8:A2:2:GLN:HB2	8:A2:6:THR:HB	2.00	0.44
8:B2:64:ASP:OD1	8:B2:64:ASP:N	2.49	0.44
9:E2:53:GLN:OE1	9:E2:57:GLN:NE2	2.47	0.44
9:I2:128:GLU:O	9:I2:132:GLU:HG2	2.18	0.44
12:S2:126:MET:HE1	13:S2:201:CYC:HBC2	1.99	0.44
9:W2:128:GLU:O	9:W2:131:ARG:HG2	2.18	0.44
7:b2:99:PRO:O	7:b2:103:ILE:HG13	2.18	0.44
9:k2:49:ARG:HH12	9:k2:140:LEU:HD21	1.83	0.44
8:p2:96:MET:HE2	8:p2:96:MET:HB3	1.87	0.44
12:t2:80:GLN:HE22	12:t2:83:ARG:HH21	1.66	0.44
3:E3:105:ILE:HD12	3:E3:109:ARG:HG3	1.98	0.44
2:I3:114:ALA:HB3	3:a3:78:ARG:HB2	2.00	0.44
2:R3:131:VAL:HG13	2:R3:159:ILE:HD12	2.00	0.44
4:Y3:225:GLN:HB2	4:Y3:268:VAL:HB	1.99	0.44
13:Z3:301:CYC:HBC2	13:Z3:301:CYC:H2C	1.83	0.44
3:E4:9:VAL:HG13	3:E4:12:GLN:HE21	1.83	0.44
2:N4:27:VAL:HG22	2:U4:27:VAL:HG22	2.00	0.44
3:X4:21:SER:H	3:X4:24:GLN:NE2	2.16	0.44
5:Z4:157:HIS:CE1	5:Z4:160:GLN:HB2	2.53	0.44
2:I5:85:CYS:O	2:I5:89:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N5:126:ALA:HB3	2:N5:129:TRP:CE2	2.53	0.44
13:N5:201:CYC:HHD	13:N5:201:CYC:HAC2	1.67	0.44
2:T5:9:ALA:HB2	2:T5:27:VAL:HG11	1.99	0.44
3:L6:1:MET:SD	3:L6:1:MET:N	2.84	0.44
3:O6:154:CYS:HB3	3:O6:157:ILE:HG22	2.00	0.44
3:Q6:100:THR:HG23	2:T6:10:VAL:HG21	2.00	0.44
3:Q6:105:ILE:HD12	3:Q6:109:ARG:HG3	2.00	0.44
3:Q6:154:CYS:SG	13:Q6:202:CYC:H2C	2.57	0.44
2:R6:74:ASN:OD1	2:R6:74:ASN:N	2.51	0.44
2:S6:99:ALA:HB2	2:S6:108:ILE:HG13	2.00	0.44
2:B7:115:GLY:O	2:B7:119:ILE:HG12	2.17	0.44
3:E7:149:ILE:HD13	13:E7:201:CYC:HMC3	1.99	0.44
2:K7:108:ILE:HG22	2:K7:113:LEU:HG	2.00	0.44
2:N7:85:CYS:HA	13:N7:201:CYC:HHD	1.99	0.44
2:N7:149:ASP:HB3	13:P7:201:CYC:HAC2	1.99	0.44
2:T7:126:ALA:HB3	2:T7:129:TRP:CE2	2.53	0.44
3:C1:96:TYR:OH	2:G1:18:ARG:O	2.31	0.43
2:G1:134:LEU:HB3	2:G1:155:ILE:HG23	2.00	0.43
3:M1:112:ASN:OD1	3:M1:113:GLY:N	2.51	0.43
2:S1:33:ARG:HE	2:S1:33:ARG:HB3	1.70	0.43
1:52:69:GLN:NE2	5:Z5:225:GLY:HA3	2.33	0.43
8:A2:144:ASP:O	8:A2:147:ARG:HG2	2.17	0.43
13:B2:201:CYC:HBA1	10:N2:572:ILE:HG23	2.00	0.43
8:L2:95:MET:HE2	8:L2:95:MET:HB3	1.91	0.43
10:N2:555:GLN:HG2	10:N2:661:PRO:HB2	2.00	0.43
8:T2:28:LYS:O	8:T2:32:GLN:HG2	2.18	0.43
9:U2:101:ILE:HD12	9:U2:155:TYR:CE1	2.53	0.43
9:U2:128:GLU:O	9:U2:132:GLU:HG2	2.17	0.43
8:X2:44:ILE:HD13	8:X2:149:MET:HE2	1.99	0.43
9:f2:71:ASN:OD1	13:f2:201:CYC:NC	2.41	0.43
9:f2:97:VAL:HG21	8:m2:19:LEU:HD12	2.00	0.43
2:B3:80:GLU:O	2:B3:84:LYS:HG2	2.18	0.43
2:B3:84:LYS:NZ	13:B3:201:CYC:O1A	2.47	0.43
2:F3:3:LYS:NZ	2:K3:18:ARG:HE	2.16	0.43
2:K3:76:ALA:HA	2:K3:81:GLY:HA3	2.00	0.43
3:Q3:114:LEU:HD11	3:Q3:118:TYR:CZ	2.53	0.43
2:S3:85:CYS:HA	13:S3:201:CYC:HHD	2.00	0.43
2:T3:31:ARG:NH2	2:T3:101:VAL:O	2.51	0.43
2:W3:100:LEU:HA	2:W3:154:TYR:HE2	1.83	0.43
3:C4:100:THR:HG23	2:G4:10:VAL:HG21	1.99	0.43
13:F4:201:CYC:HBD2	13:F4:201:CYC:HHA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H4:95:ILE:HG21	2:H4:112:LEU:HB2	1.99	0.43
3:M4:89:ILE:HG21	13:M4:201:CYC:HAB2	2.00	0.43
2:N4:14:ASP:OD2	3:V4:109:ARG:NE	2.50	0.43
3:O4:111:LEU:HD21	3:O4:168:ALA:HA	1.99	0.43
2:W4:115:GLY:O	2:W4:118:GLU:HG2	2.17	0.43
3:O5:6:PHE:HB3	2:S5:102:ALA:HA	2.00	0.43
3:P5:107:ASP:OD1	3:P5:167:LYS:HD3	2.18	0.43
2:W5:3:LYS:HD3	2:W5:3:LYS:HA	1.75	0.43
13:a5:201:CYC:HMD1	13:a5:201:CYC:HC	1.83	0.43
1:A6:141:LEU:HD12	1:A6:141:LEU:HA	1.80	0.43
2:G6:138:LYS:HB2	2:G6:155:ILE:HG21	2.00	0.43
2:N7:99:ALA:HB2	2:N7:108:ILE:HG13	1.99	0.43
3:P7:111:LEU:HD21	3:P7:168:ALA:HA	1.99	0.43
2:R7:109:ASP:HA	2:R7:113:LEU:HB2	2.00	0.43
3:X7:128:VAL:HG22	13:X7:201:CYC:H3C	1.99	0.43
1:A1:180:ARG:HG3	13:a1:201:CYC:HBA2	2.00	0.43
2:K1:98:TYR:OH	3:L1:18:GLU:O	2.35	0.43
3:O1:44:ARG:HD3	3:O1:143:VAL:HA	1.99	0.43
3:Q1:59:ALA:HB3	3:Q1:134:LYS:HD3	2.00	0.43
2:R1:50:ASP:N	2:R1:50:ASP:OD1	2.50	0.43
2:T1:50:ASP:OD1	2:T1:50:ASP:N	2.50	0.43
1:22:27:GLN:OE1	1:22:30:GLN:NE2	2.51	0.43
1:42:99:SER:HB3	3:D4:112:ASN:ND2	2.33	0.43
1:42:238:ASP:OD1	9:j2:52:LYS:NZ	2.47	0.43
1:52:63:GLN:O	1:52:67:GLU:HG3	2.18	0.43
1:52:224:ARG:NH1	9:G2:75:GLU:OE1	2.51	0.43
9:D2:114:GLU:OE1	9:D2:114:GLU:N	2.41	0.43
8:L2:111:LEU:HG	8:L2:159:LEU:HD21	1.99	0.43
9:e2:71:ASN:OD1	9:e2:121:THR:OG1	2.35	0.43
9:f2:41:GLN:NE2	9:f2:45:GLU:OE2	2.50	0.43
10:o2:69:SER:HA	10:o2:82:LEU:HD21	1.99	0.43
3:C3:109:ARG:HA	5:Z3:275:ASN:HB3	1.99	0.43
2:F3:27:VAL:HG22	2:K3:27:VAL:HG22	1.99	0.43
2:K3:25:LEU:HD22	3:L3:39:ILE:HG23	2.01	0.43
3:P3:37:LYS:HB3	3:P3:37:LYS:HE3	1.81	0.43
3:Q3:48:ASN:HB2	3:Q3:142:ILE:HD13	1.99	0.43
2:U3:74:ASN:HA	13:U3:201:CYC:HBD2	1.99	0.43
3:a3:146:ARG:NH1	3:a3:152:GLY:H	2.16	0.43
3:M4:98:VAL:HG13	3:M4:157:ILE:HD11	2.01	0.43
13:C5:202:CYC:HMA3	13:C5:202:CYC:NB	2.32	0.43
2:K5:76:ALA:HA	2:K5:81:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P5:146:ARG:NE	3:P5:151:GLN:OE1	2.49	0.43
2:T5:108:ILE:HG22	2:T5:113:LEU:HG	2.00	0.43
2:W5:95:ILE:HG22	2:W5:108:ILE:HG12	2.00	0.43
2:B6:114:ALA:HB3	3:C6:78:ARG:HB2	2.00	0.43
2:F6:23:THR:HG21	2:K6:3:LYS:HE2	2.00	0.43
2:G6:126:ALA:HB3	2:G6:129:TRP:CE2	2.53	0.43
2:I6:52:LEU:HB3	2:I6:137:ILE:CD1	2.47	0.43
3:L6:25:LEU:HD13	3:L6:25:LEU:HA	1.89	0.43
3:M6:87:MET:HE2	13:M6:201:CYC:HBC1	1.99	0.43
2:S6:126:ALA:HB3	2:S6:129:TRP:CE2	2.53	0.43
2:K7:2:SER:HA	2:K7:106:GLY:HA3	2.01	0.43
2:S7:5:PRO:HG3	2:T7:23:THR:HA	1.99	0.43
2:U7:63:LYS:HD3	2:U7:132:GLU:HG3	2.00	0.43
4:Y7:252:LYS:NZ	5:Z7:70:ARG:HH22	2.15	0.43
3:a7:96:TYR:HB3	3:a7:105:ILE:HG12	2.00	0.43
3:Q1:146:ARG:HB3	3:Q1:151:GLN:HE22	1.83	0.43
3:Q1:154:CYS:SG	13:Q1:202:CYC:HAC2	2.58	0.43
2:U1:85:CYS:HA	13:U1:201:CYC:HHH	1.99	0.43
2:U1:143:LEU:C	2:U1:148:ARG:HB2	2.43	0.43
13:X1:201:CYC:HMA2	5:Z1:118:LEU:HD22	2.01	0.43
5:Z1:40:TYR:O	5:Z1:44:LEU:HB2	2.19	0.43
6:02:13:PRO:HA	8:d2:76:ARG:HD2	1.99	0.43
9:G2:89:LEU:O	9:G2:93:THR:HG23	2.17	0.43
10:N2:300:ILE:HG22	10:N2:306:GLN:O	2.18	0.43
11:P2:46:ALA:O	12:S2:158:GLN:NE2	2.52	0.43
9:Q2:21:GLY:O	9:Q2:24:GLU:HG3	2.18	0.43
12:S2:2:THR:OG1	8:T2:3:ASP:OD2	2.33	0.43
9:W2:64:ASP:OD1	9:W2:64:ASP:N	2.50	0.43
9:r2:14:GLU:OE1	9:r2:16:ARG:NE	2.38	0.43
8:u2:20:ASP:OD1	8:u2:22:SER:OG	2.23	0.43
9:v2:7:SER:HB3	9:v2:22:GLU:HB3	1.99	0.43
3:C3:43:ASN:HB2	2:G3:25:LEU:HD21	2.00	0.43
3:J3:37:LYS:N	3:J3:37:LYS:HE2	2.32	0.43
3:Q3:128:VAL:HG22	13:Q3:201:CYC:HBC3	2.00	0.43
2:T3:115:GLY:O	2:T3:119:ILE:HG12	2.17	0.43
5:Z3:237:ILE:H	5:Z3:288:SER:HB3	1.82	0.43
2:G4:31:ARG:NH2	2:G4:101:VAL:O	2.51	0.43
2:H4:74:ASN:ND2	2:H4:124:ASP:O	2.41	0.43
2:I4:85:CYS:HA	13:I4:201:CYC:HAC1	1.77	0.43
3:J4:129:ALA:O	3:J4:133:ARG:HG3	2.18	0.43
2:K4:76:ALA:HA	2:K4:81:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K5:14:ASP:OD1	3:L5:93:TYR:OH	2.25	0.43
2:R5:42:ALA:HB1	2:R5:97:THR:HG23	2.00	0.43
2:R5:80:GLU:O	2:R5:84:LYS:HG2	2.18	0.43
2:U5:95:ILE:HG22	2:U5:108:ILE:HG12	2.00	0.43
2:W5:11:ALA:HB1	5:Z5:88:TYR:CZ	2.54	0.43
3:E6:149:ILE:HG21	13:E6:201:CYC:HMC3	2.00	0.43
3:M6:146:ARG:NE	3:M6:151:GLN:OE1	2.51	0.43
2:N6:143:LEU:C	2:N6:148:ARG:HB2	2.44	0.43
2:F7:85:CYS:HA	13:F7:201:CYC:HHD	2.00	0.43
2:I7:85:CYS:HA	13:I7:201:CYC:HAC1	1.95	0.43
1:A1:69:GLN:HE21	5:Z1:225:GLY:HA3	1.83	0.43
3:E1:9:VAL:HG13	3:E1:12:GLN:HE21	1.83	0.43
3:L1:146:ARG:HB3	3:L1:151:GLN:OE1	2.19	0.43
2:T1:95:ILE:HG22	2:T1:108:ILE:HG12	1.99	0.43
3:X1:136:LYS:HB2	3:X1:165:PHE:CG	2.54	0.43
1:22:54:PHE:O	1:22:55:PHE:C	2.62	0.43
1:32:164:LEU:HD11	13:32:302:CYC:HAA2	2.00	0.43
1:32:248:ARG:HA	1:32:248:ARG:HD2	1.82	0.43
8:B2:13:ASP:OD1	9:J2:90:ARG:NH1	2.51	0.43
8:C2:100:ASP:OD1	8:C2:101:THR:N	2.50	0.43
9:D2:23:LEU:HB3	8:F2:38:VAL:HG13	1.99	0.43
9:J2:101:ILE:HD12	9:J2:155:TYR:CZ	2.53	0.43
9:Q2:86:ASP:OD1	8:X2:18:TYR:OH	2.26	0.43
9:W2:101:ILE:HD12	9:W2:155:TYR:CE1	2.54	0.43
8:g2:60:LEU:HD21	8:g2:129:ALA:HB2	1.99	0.43
8:g2:126:THR:O	8:g2:130:ILE:HG13	2.18	0.43
9:k2:87:TYR:OH	9:k2:107:ILE:HG22	2.19	0.43
8:m2:140:LEU:HD23	8:m2:140:LEU:HA	1.85	0.43
8:p2:57:ALA:HA	8:p2:61:LEU:HB2	2.00	0.43
8:p2:72:MET:HE2	8:p2:78:TYR:CE2	2.53	0.43
12:t2:9:LEU:HD21	8:u2:1:MET:HG3	2.00	0.43
9:v2:61:LYS:HB2	9:v2:61:LYS:HE3	1.78	0.43
3:L3:28:LEU:O	3:L3:32:VAL:HG23	2.18	0.43
3:O3:34:GLU:HG3	3:O3:37:LYS:HD2	2.00	0.43
2:N4:115:GLY:O	2:N4:118:GLU:HG2	2.18	0.43
3:Q4:154:CYS:SG	13:Q4:202:CYC:HAC2	2.58	0.43
2:R4:138:LYS:HB2	2:R4:155:ILE:HG21	2.00	0.43
3:V4:75:TYR:O	13:W4:201:CYC:OB	2.36	0.43
3:X4:12:GLN:O	3:X4:16:ARG:HG2	2.19	0.43
3:a4:48:ASN:CB	3:a4:142:ILE:HD13	2.48	0.43
2:B5:112:LEU:HD23	2:B5:158:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C5:35:GLY:O	3:C5:39:ILE:HG12	2.19	0.43
3:C5:83:CYS:HA	13:C5:201:CYC:HAC2	1.98	0.43
3:O5:25:LEU:HD13	2:S5:43:LYS:HB2	2.00	0.43
13:P5:201:CYC:HAC1	13:P5:201:CYC:HHD	1.45	0.43
2:T5:112:LEU:HD23	2:T5:158:LEU:HD21	2.00	0.43
2:W5:12:ALA:O	2:W5:16:GLN:HG2	2.18	0.43
4:Y5:234:ARG:HD2	4:Y5:239:ILE:HG13	2.01	0.43
4:Y5:238:ARG:NH1	4:Y5:240:ARG:HH21	2.17	0.43
2:F6:27:VAL:HG22	2:K6:27:VAL:HG22	2.00	0.43
2:G6:33:ARG:NH2	2:G6:34:GLN:OE1	2.51	0.43
3:O6:111:LEU:HD21	3:O6:168:ALA:HA	1.99	0.43
13:P6:201:CYC:HHD	13:P6:201:CYC:HAC1	1.44	0.43
2:G7:134:LEU:HB3	2:G7:155:ILE:HG23	1.99	0.43
3:L7:41:THR:HG23	3:L7:143:VAL:HG21	2.00	0.43
2:S7:3:LYS:HG3	2:T7:18:ARG:NH1	2.34	0.43
2:S7:50:ASP:OD1	2:S7:50:ASP:N	2.50	0.43
2:U7:21:SER:O	2:U7:25:LEU:HG	2.19	0.43
3:X7:21:SER:H	3:X7:24:GLN:NE2	2.16	0.43
1:A1:22:VAL:HB	2:F1:109:ASP:HB3	2.00	0.43
3:C1:86:ASP:OD2	3:C1:118:TYR:OH	2.23	0.43
3:E1:44:ARG:HD3	3:E1:143:VAL:HA	2.00	0.43
2:F1:27:VAL:HG13	2:K1:27:VAL:HG22	2.00	0.43
2:K1:118:GLU:OE1	2:K1:118:GLU:N	2.45	0.43
3:M1:87:MET:HE2	13:M1:201:CYC:HBC1	2.00	0.43
3:V1:4:ASP:OD1	3:V1:7:THR:OG1	2.28	0.43
13:32:301:CYC:HMD1	3:D3:79:ARG:HB3	1.99	0.43
8:B2:87:TYR:OH	10:N2:568:THR:OG1	2.15	0.43
9:D2:122:PRO:HG2	9:D2:125:ALA:HB3	2.00	0.43
13:M2:201:CYC:HHD	13:M2:201:CYC:HAC2	1.62	0.43
9:R2:33:GLY:HA2	9:R2:36:ARG:CZ	2.49	0.43
12:S2:134:LYS:HB2	12:S2:153:PHE:HB3	2.01	0.43
8:T2:62:TYR:OH	13:W2:201:CYC:O1D	2.32	0.43
8:c2:76:ARG:HB3	9:j2:110:VAL:HG13	2.01	0.43
8:g2:28:LYS:HE3	8:g2:28:LYS:HB2	1.81	0.43
9:h2:89:LEU:O	9:h2:93:THR:HG23	2.18	0.43
9:k2:105:GLU:OE2	9:k2:155:TYR:OH	2.30	0.43
8:m2:17:LYS:HE2	8:m2:17:LYS:HB2	1.79	0.43
9:r2:21:GLY:O	9:r2:24:GLU:HG3	2.19	0.43
8:u2:19:LEU:HD12	8:u2:23:ALA:HB1	1.99	0.43
8:u2:112:LEU:HG	8:u2:160:LEU:HD21	2.00	0.43
8:y2:2:GLN:HB2	8:y2:6:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:112:LEU:HD12	3:C3:77:ASN:ND2	2.33	0.43
3:Q3:58:ARG:NE	13:R3:201:CYC:O2D	2.51	0.43
4:Y3:252:LYS:NZ	5:Z3:70:ARG:HH22	2.15	0.43
5:Z3:255:ARG:HH21	5:Z3:258:ARG:HH11	1.67	0.43
3:P4:44:ARG:HH21	3:P4:149:ILE:HB	1.82	0.43
3:P4:99:PHE:CZ	2:U4:28:ALA:HB2	2.54	0.43
3:X4:124:PRO:O	3:X4:128:VAL:HG23	2.18	0.43
2:B5:121:LYS:HE2	2:B5:121:LYS:HB2	1.90	0.43
13:C5:201:CYC:O2D	5:Z5:236:ARG:NH2	2.51	0.43
3:E5:21:SER:H	3:E5:24:GLN:NE2	2.17	0.43
3:L5:124:PRO:O	3:L5:128:VAL:HG23	2.18	0.43
3:X5:124:PRO:O	3:X5:128:VAL:HG23	2.18	0.43
3:a5:2:THR:HG23	3:a5:105:ILE:HB	2.01	0.43
1:A6:58:PHE:O	1:A6:59:LYS:C	2.60	0.43
2:F6:27:VAL:HG22	2:K6:27:VAL:HG13	2.01	0.43
3:V6:149:ILE:HD13	13:V6:202:CYC:HMC3	2.00	0.43
2:W6:5:PRO:CG	2:W6:31:ARG:HD3	2.48	0.43
2:W6:115:GLY:O	2:W6:118:GLU:HG2	2.19	0.43
3:E7:70:PRO:HA	3:E7:75:TYR:CG	2.54	0.43
2:G7:74:ASN:O	13:G7:201:CYC:NC	2.43	0.43
2:H7:126:ALA:HB3	2:H7:129:TRP:CE2	2.54	0.43
3:O7:112:ASN:O	5:Z7:162:SER:OG	2.28	0.43
2:R7:76:ALA:HB1	2:R7:82:LYS:HD3	2.01	0.43
3:V7:84:LEU:HD13	2:W7:122:THR:HG21	1.99	0.43
3:X7:70:PRO:HA	3:X7:75:TYR:CD1	2.54	0.43
3:X7:89:ILE:HG21	13:X7:201:CYC:HAB1	2.01	0.43
1:A1:104:VAL:HG11	1:A1:125:TRP:HB2	2.00	0.43
1:A1:163:VAL:HG12	1:A1:170:GLY:HA3	2.00	0.43
3:D1:41:THR:HG23	3:D1:143:VAL:HG21	2.00	0.43
3:D1:72:GLY:O	3:D1:79:ARG:NH2	2.44	0.43
3:E1:149:ILE:HD13	13:E1:201:CYC:H3C	2.01	0.43
2:F1:23:THR:HG21	2:K1:3:LYS:HE2	2.00	0.43
2:F1:138:LYS:HB2	2:F1:155:ILE:HG21	1.98	0.43
2:G1:113:LEU:HD22	2:G1:113:LEU:HA	1.82	0.43
3:J1:109:ARG:HD3	5:Z1:228:THR:OG1	2.19	0.43
3:J1:116:GLU:OE1	3:J1:116:GLU:N	2.50	0.43
3:L1:83:CYS:HA	13:L1:201:CYC:HAC2	2.01	0.43
3:M1:28:LEU:O	3:M1:32:VAL:HG23	2.19	0.43
2:T1:126:ALA:HB3	2:T1:129:TRP:CE2	2.54	0.43
2:W1:126:ALA:HB3	2:W1:129:TRP:CE2	2.53	0.43
1:22:163:VAL:HG12	1:22:170:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:22:222:LEU:O	1:22:226:ILE:HG22	2.19	0.43
8:K2:123:ILE:HG23	8:K2:160:LEU:HD22	2.01	0.43
8:L2:36:ARG:NH1	8:L2:95:MET:O	2.46	0.43
8:V2:137:THR:O	8:V2:141:VAL:HG22	2.19	0.43
7:b2:97:LEU:H	7:b2:97:LEU:HG	1.68	0.43
8:d2:6:THR:OG1	9:j2:1:MET:HA	2.18	0.43
8:n2:126:THR:HB	8:n2:160:LEU:HD21	2.00	0.43
10:o2:259:LEU:HB2	10:o2:411:ALA:HB2	2.00	0.43
9:r2:90:ARG:HB2	8:y2:18:TYR:CZ	2.54	0.43
8:u2:144:ASP:OD1	8:u2:144:ASP:N	2.45	0.43
2:H3:91:TYR:O	2:H3:95:ILE:HG12	2.18	0.43
3:O3:28:LEU:O	3:O3:32:VAL:HG23	2.18	0.43
3:Q3:93:TYR:CG	3:Q3:110:CYS:HB2	2.54	0.43
2:T3:34:GLN:HE22	2:T3:146:ASP:HB3	1.84	0.43
3:a3:9:VAL:HG11	3:a3:28:LEU:HD21	2.01	0.43
2:B4:99:ALA:HA	2:B4:107:PRO:HG2	2.01	0.43
3:D4:150:THR:O	13:D4:201:CYC:NC	2.44	0.43
3:E4:99:PHE:CZ	2:H4:28:ALA:HB2	2.53	0.43
3:J4:83:CYS:HA	13:J4:201:CYC:HAC1	1.48	0.43
3:X4:70:PRO:HA	3:X4:75:TYR:CD1	2.54	0.43
5:Z4:36:ILE:HD13	5:Z4:59:GLU:HG2	2.01	0.43
2:F5:28:ALA:HB2	3:a5:99:PHE:CZ	2.53	0.43
2:G5:5:PRO:HA	2:H5:23:THR:HG23	1.99	0.43
2:K5:134:LEU:HB3	2:K5:155:ILE:HG23	1.99	0.43
3:P5:87:MET:HG2	3:P5:135:MET:SD	2.58	0.43
3:Q5:124:PRO:O	3:Q5:128:VAL:HG23	2.19	0.43
13:S5:201:CYC:HHD	13:S5:201:CYC:HAC1	1.59	0.43
2:T5:99:ALA:HB2	2:T5:108:ILE:HG13	2.01	0.43
1:A6:191:PHE:HD1	1:A6:191:PHE:HA	1.73	0.43
3:D6:134:LYS:HA	3:D6:137:ASP:OD2	2.18	0.43
13:E6:201:CYC:HMA3	13:E6:201:CYC:NB	2.33	0.43
2:G6:18:ARG:NH1	2:H6:3:LYS:HE2	2.33	0.43
3:J6:123:VAL:HG13	13:J6:201:CYC:NC	2.34	0.43
3:M6:37:LYS:O	3:M6:41:THR:HG23	2.18	0.43
3:P6:99:PHE:CZ	2:U6:28:ALA:HB2	2.54	0.43
2:W6:28:ALA:HB2	3:X6:99:PHE:CZ	2.53	0.43
2:W6:95:ILE:HG22	2:W6:108:ILE:HG12	2.00	0.43
3:a6:83:CYS:HA	13:a6:201:CYC:HAC2	2.00	0.43
2:B7:28:ALA:HB2	3:J7:99:PHE:CE1	2.52	0.43
2:H7:9:ALA:HB1	2:H7:24:GLU:HG3	2.01	0.43
3:O7:28:LEU:O	3:O7:32:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X7:136:LYS:HB2	3:X7:165:PHE:CG	2.53	0.43
2:H1:150:GLU:HG2	2:H1:154:TYR:CE2	2.54	0.43
3:J1:123:VAL:HG13	13:J1:201:CYC:NC	2.34	0.43
3:M1:59:ALA:HB3	3:M1:134:LYS:HD3	2.01	0.43
3:P1:87:MET:HG2	3:P1:135:MET:SD	2.59	0.43
1:22:79:ASP:OD1	1:22:79:ASP:N	2.49	0.43
13:22:302:CYC:HC	3:E7:123:VAL:HG22	1.83	0.43
1:52:75:ILE:HB	1:52:79:ASP:HB2	2.00	0.43
8:A2:130:ILE:HG23	8:A2:153:LEU:HD12	2.00	0.43
13:F2:201:CYC:NC	13:F2:201:CYC:HMD1	2.34	0.43
8:M2:94:TYR:HB3	8:M2:103:ILE:HD13	2.01	0.43
10:N2:298:ARG:NH2	10:N2:300:ILE:HD11	2.34	0.43
8:g2:110:ASN:OD1	10:o2:673:LEU:HB3	2.19	0.43
9:s2:101:ILE:HB	9:s2:155:TYR:CE2	2.54	0.43
8:y2:101:THR:HG22	8:y2:152:TYR:HD1	1.84	0.43
2:B3:134:LEU:HB3	2:B3:155:ILE:HG23	2.01	0.43
3:C3:149:ILE:HG21	13:C3:202:CYC:HMC3	2.01	0.43
2:G3:74:ASN:OD1	2:G3:74:ASN:N	2.47	0.43
2:I3:33:ARG:NH2	2:I3:34:GLN:OE1	2.52	0.43
2:K3:126:ALA:HB3	2:K3:129:TRP:CE2	2.53	0.43
2:K3:138:LYS:HB2	2:K3:155:ILE:HG21	2.00	0.43
3:P3:44:ARG:O	3:P3:48:ASN:ND2	2.38	0.43
2:U3:115:GLY:O	2:U3:119:ILE:HG12	2.18	0.43
3:O4:109:ARG:NH1	2:S4:14:ASP:OD2	2.51	0.43
2:W4:115:GLY:O	2:W4:119:ILE:HG12	2.18	0.43
3:D5:37:LYS:HE2	3:D5:37:LYS:N	2.34	0.43
2:G5:113:LEU:HD22	2:G5:113:LEU:HA	1.75	0.43
3:M5:28:LEU:O	3:M5:32:VAL:HG23	2.19	0.43
2:T5:85:CYS:O	2:T5:89:ILE:HG12	2.19	0.43
2:U5:26:GLN:HA	2:U5:29:PHE:HB2	2.00	0.43
13:A6:301:CYC:H3C	3:D6:128:VAL:HG22	2.00	0.43
2:F6:28:ALA:HB2	3:a6:99:PHE:CZ	2.54	0.43
2:F6:126:ALA:HB3	2:F6:129:TRP:CE2	2.54	0.43
2:N6:85:CYS:O	2:N6:89:ILE:HG12	2.19	0.43
3:O6:99:PHE:CZ	2:S6:28:ALA:HB2	2.54	0.43
3:V6:146:ARG:HH21	3:V6:151:GLN:HB3	1.84	0.43
2:I7:108:ILE:HG22	2:I7:113:LEU:HG	2.01	0.43
3:O7:99:PHE:CZ	2:S7:28:ALA:HB2	2.54	0.43
3:P7:84:LEU:HD13	2:T7:122:THR:HG21	1.99	0.43
3:Q7:92:ARG:NH1	3:Q7:96:TYR:OH	2.46	0.43
2:U7:74:ASN:O	13:U7:201:CYC:NC	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z7:40:TYR:O	5:Z7:44:LEU:HB2	2.18	0.43
3:a7:89:ILE:HG21	13:a7:201:CYC:HAB1	1.99	0.43
13:A1:302:CYC:HBC2	13:A1:302:CYC:H2C	1.68	0.43
3:E1:136:LYS:HB2	3:E1:165:PHE:CG	2.53	0.43
2:F1:27:VAL:HG22	2:K1:27:VAL:HG22	2.00	0.43
13:G1:201:CYC:NC	13:G1:201:CYC:HMD1	2.33	0.43
2:N1:9:ALA:HB1	2:N1:24:GLU:HG3	2.01	0.43
13:V1:201:CYC:HAC2	13:V1:201:CYC:HHH	1.57	0.43
4:Y1:228:GLN:OE1	4:Y1:266:ARG:NE	2.49	0.43
1:22:204:PHE:CE1	9:G2:76:ASP:HB3	2.54	0.43
13:32:302:CYC:HBC3	3:E3:128:VAL:HG13	2.00	0.43
1:52:22:VAL:HB	2:F5:109:ASP:HB3	2.00	0.43
10:N2:578:GLU:O	6:Z2:30:LEU:N	2.48	0.43
10:N2:610:TYR:O	10:N2:614:ARG:HG2	2.19	0.43
12:S2:57:LYS:HB3	12:S2:132:THR:HG21	2.01	0.43
8:a2:76:ARG:NH1	13:a2:201:CYC:O2D	2.52	0.43
8:d2:147:ARG:HD3	8:d2:147:ARG:HA	1.85	0.43
9:e2:104:ILE:HG21	9:e2:156:VAL:HG22	2.00	0.43
8:g2:137:THR:O	8:g2:141:VAL:HG22	2.19	0.43
10:o2:33:ARG:NH2	10:o2:39:GLU:OE2	2.43	0.43
9:x2:50:ILE:HG23	9:x2:136:ALA:HB3	2.00	0.43
2:G3:134:LEU:HB3	2:G3:155:ILE:HG23	2.01	0.43
3:L3:41:THR:O	3:L3:45:ILE:HG12	2.19	0.43
3:L3:117:THR:HG23	5:Z3:256:SER:HB2	1.99	0.43
3:M3:41:THR:HG22	3:M3:143:VAL:HG13	2.00	0.43
2:R3:115:GLY:O	2:R3:119:ILE:HG12	2.18	0.43
3:D4:92:ARG:HG2	2:I4:19:PHE:CE2	2.54	0.43
2:F4:25:LEU:HD22	3:a4:39:ILE:HG23	2.01	0.43
2:I4:143:LEU:C	2:I4:148:ARG:HB2	2.43	0.43
3:O4:37:LYS:O	3:O4:41:THR:HG23	2.18	0.43
3:O4:152:GLY:N	13:T4:201:CYC:OC	2.50	0.43
3:Q4:124:PRO:O	3:Q4:128:VAL:HG23	2.19	0.43
2:T4:74:ASN:HA	13:T4:202:CYC:HBD2	1.99	0.43
3:V4:106:LEU:HD12	3:V4:110:CYS:HB3	2.00	0.43
3:V4:149:ILE:HD13	13:V4:202:CYC:HMC3	1.99	0.43
2:W4:12:ALA:O	2:W4:16:GLN:HG2	2.19	0.43
3:X4:41:THR:HG23	3:X4:143:VAL:HG11	1.99	0.43
3:D5:4:ASP:HA	3:D5:100:THR:HB	2.01	0.43
2:G5:3:LYS:HB2	2:G5:106:GLY:HA2	2.01	0.43
2:I5:95:ILE:HG22	2:I5:108:ILE:HD13	2.01	0.43
2:I5:143:LEU:C	2:I5:148:ARG:HB2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J5:129:ALA:O	3:J5:133:ARG:HG3	2.18	0.43
2:K5:112:LEU:HD23	2:K5:158:LEU:HD21	2.01	0.43
3:L5:16:ARG:HH21	3:L5:24:GLN:HE22	1.65	0.43
3:M5:89:ILE:HG21	13:M5:201:CYC:HAB2	2.01	0.43
2:N5:127:PRO:HB3	2:N5:162:LEU:HD22	2.01	0.43
2:R5:109:ASP:HA	2:R5:113:LEU:HB2	1.99	0.43
3:X5:12:GLN:O	3:X5:16:ARG:HG2	2.19	0.43
2:H6:124:ASP:N	2:H6:124:ASP:OD1	2.51	0.43
3:J6:116:GLU:N	3:J6:116:GLU:OE1	2.52	0.43
2:T6:91:TYR:O	2:T6:95:ILE:HG12	2.18	0.43
2:W6:91:TYR:O	2:W6:95:ILE:HG12	2.19	0.43
3:a6:37:LYS:HE3	13:a6:202:CYC:HMD1	1.99	0.43
2:B7:74:ASN:OD1	2:B7:74:ASN:N	2.51	0.43
3:C7:4:ASP:OD1	3:C7:6:PHE:N	2.51	0.43
3:C7:86:ASP:OD2	3:C7:118:TYR:OH	2.24	0.43
2:H7:21:SER:N	2:H7:24:GLU:OE1	2.51	0.43
2:R7:84:LYS:HE2	2:R7:87:ARG:HH21	1.84	0.43
2:R7:134:LEU:HB3	2:R7:155:ILE:HG23	2.01	0.43
5:Z7:193:ASN:HD21	5:Z7:200:ALA:HB2	1.84	0.43
2:G1:105:THR:OG1	2:H1:18:ARG:NH2	2.51	0.43
13:M1:201:CYC:NC	13:M1:201:CYC:HMD1	2.33	0.43
2:N1:13:ALA:HA	2:N1:16:GLN:HE21	1.83	0.43
3:O1:93:TYR:CG	3:O1:110:CYS:HB2	2.53	0.43
3:O1:160:GLU:HG2	3:O1:164:TYR:CE2	2.54	0.43
13:Q1:202:CYC:HMA1	2:T1:29:PHE:CZ	2.54	0.43
13:T1:201:CYC:HMA3	13:T1:201:CYC:NB	2.34	0.43
2:W1:121:LYS:HE2	2:W1:121:LYS:HB3	1.89	0.43
4:Y1:252:LYS:HZ1	5:Z1:70:ARG:HH22	1.66	0.43
5:Z1:203:VAL:HG13	5:Z1:282:VAL:HB	2.00	0.43
1:52:86:LEU:HD23	1:52:134:TYR:CE1	2.53	0.43
9:E2:101:ILE:HD13	9:E2:155:TYR:CZ	2.54	0.43
9:H2:134:LYS:HB2	9:H2:153:PHE:HB3	1.99	0.43
9:Q2:121:THR:OG1	13:Q2:201:CYC:NC	2.52	0.43
9:R2:52:LYS:NZ	9:R2:82:LEU:HD13	2.34	0.43
9:W2:71:ASN:HD22	13:W2:201:CYC:HMD2	1.84	0.43
8:a2:144:ASP:O	8:a2:147:ARG:HG2	2.19	0.43
8:c2:105:ASP:OD1	8:c2:155:TYR:OH	2.23	0.43
9:i2:101:ILE:HG12	9:i2:155:TYR:CG	2.54	0.43
10:o2:612:HIS:NE2	10:o2:616:LEU:HD12	2.33	0.43
11:q2:82:CYS:HA	13:q2:201:CYC:CHD	2.46	0.43
12:t2:39:ILE:HG12	12:t2:145:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D3:37:LYS:N	3:D3:37:LYS:HE2	2.34	0.43
2:H3:126:ALA:HB3	2:H3:129:TRP:CE2	2.54	0.43
3:Q3:92:ARG:NH1	3:Q3:96:TYR:OH	2.45	0.43
2:R3:76:ALA:HB1	2:R3:82:LYS:HD3	2.01	0.43
3:V3:38:ARG:NH2	3:V3:160:GLU:OE1	2.52	0.43
3:E4:21:SER:H	3:E4:24:GLN:NE2	2.17	0.43
2:F4:21:SER:N	2:F4:24:GLU:OE1	2.50	0.43
2:G4:113:LEU:HA	2:G4:113:LEU:HD22	1.74	0.43
3:M4:96:TYR:OH	2:R4:18:ARG:O	2.34	0.43
2:N4:45:LEU:HD21	2:N4:141:HIS:HB2	2.01	0.43
3:O4:102:ASP:OD1	3:O4:104:SER:N	2.51	0.43
13:P4:202:CYC:HHH	13:P4:202:CYC:HAC1	1.45	0.43
3:Q4:123:VAL:HG22	13:Q4:201:CYC:HC	1.83	0.43
2:T4:144:SER:HA	2:T4:148:ARG:HD3	2.01	0.43
3:X4:107:ASP:HA	3:X4:111:LEU:HB2	2.01	0.43
3:D5:134:LYS:HA	3:D5:137:ASP:OD2	2.19	0.43
2:F5:25:LEU:HD22	3:a5:39:ILE:HG23	2.00	0.43
3:J5:93:TYR:CG	3:J5:110:CYS:HB2	2.54	0.43
2:K5:45:LEU:HD21	2:K5:141:HIS:HB2	2.01	0.43
3:Q5:146:ARG:HB3	3:Q5:151:GLN:HE22	1.83	0.43
3:V5:34:GLU:OE1	3:V5:37:LYS:NZ	2.47	0.43
1:A6:69:GLN:NE2	5:Z6:225:GLY:HA3	2.33	0.43
2:F6:14:ASP:OD2	3:a6:109:ARG:NH1	2.44	0.43
2:G6:23:THR:HG23	2:H6:5:PRO:HA	2.01	0.43
2:I6:108:ILE:HG22	2:I6:113:LEU:HG	2.01	0.43
2:I6:143:LEU:C	2:I6:148:ARG:HB2	2.42	0.43
3:V6:123:VAL:HG13	13:V6:201:CYC:HMC3	2.00	0.43
3:X6:28:LEU:O	3:X6:32:VAL:HG23	2.18	0.43
2:B7:112:LEU:HD12	3:C7:77:ASN:ND2	2.33	0.43
3:C7:154:CYS:SG	13:C7:202:CYC:HAC2	2.59	0.43
3:D7:149:ILE:HD13	13:D7:201:CYC:H3C	2.01	0.43
3:E7:28:LEU:O	3:E7:32:VAL:HG23	2.19	0.43
2:F7:101:VAL:HG21	3:a7:20:LEU:HD13	2.00	0.43
2:G7:33:ARG:NH1	2:G7:146:ASP:OD2	2.51	0.43
3:J7:146:ARG:NE	3:J7:151:GLN:OE1	2.52	0.43
3:O7:102:ASP:OD1	3:O7:103:ALA:N	2.51	0.43
3:a7:106:LEU:HD12	3:a7:110:CYS:SG	2.59	0.43
1:A1:98:ASN:OD1	1:A1:181:TYR:HA	2.19	0.43
3:C1:38:ARG:NH1	3:C1:98:VAL:O	2.40	0.43
3:D1:92:ARG:HG2	2:I1:19:PHE:CZ	2.54	0.43
3:E1:41:THR:O	3:E1:45:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G1:33:ARG:NH2	2:G1:34:GLN:OE1	2.51	0.43
2:S1:85:CYS:O	2:S1:89:ILE:HG12	2.18	0.43
3:a1:146:ARG:NH1	3:a1:152:GLY:H	2.16	0.43
1:32:53:ILE:HG21	1:32:84:LEU:HB3	2.01	0.43
8:C2:83:ARG:NH2	13:C2:201:CYC:O2A	2.38	0.43
9:E2:140:LEU:HD12	9:E2:140:LEU:HA	1.75	0.43
9:H2:91:LEU:HD13	9:H2:91:LEU:HA	1.92	0.43
10:N2:490:LEU:HD12	10:N2:505:PHE:HZ	1.83	0.43
10:N2:511:THR:HB	10:N2:662:TYR:CD1	2.54	0.43
12:S2:81:CYS:CB	13:S2:201:CYC:HAC1	2.49	0.43
8:T2:139:SER:O	9:i2:49:ARG:NH2	2.51	0.43
8:V2:38:VAL:HG23	9:W2:23:LEU:HD22	2.01	0.43
8:c2:78:TYR:O	8:c2:82:ILE:HG12	2.19	0.43
8:d2:38:VAL:HG23	9:j2:23:LEU:HD22	2.01	0.43
9:e2:126:VAL:HG22	13:e2:201:CYC:H3C	2.01	0.43
9:f2:1:MET:O	9:f2:103:PRO:HD3	2.19	0.43
8:l2:64:ASP:HB3	11:q2:123:PRO:HB3	2.00	0.43
8:m2:85:LEU:HB3	8:m2:133:ILE:HD11	2.01	0.43
10:o2:484:LYS:HE2	11:q2:169:ILE:HD12	2.01	0.43
10:o2:676:VAL:CG1	8:p2:127:VAL:HG21	2.49	0.43
8:w2:60:LEU:O	8:w2:63:SER:OG	2.36	0.43
3:C3:41:THR:OG1	13:C3:202:CYC:HBC1	2.18	0.43
3:D3:16:ARG:NH2	3:D3:24:GLN:HE22	2.17	0.43
2:F3:100:LEU:HA	2:F3:154:TYR:HE2	1.82	0.43
2:I3:134:LEU:HB3	2:I3:155:ILE:HG23	2.01	0.43
2:N3:28:ALA:HB2	3:V3:99:PHE:CE1	2.53	0.43
3:V3:93:TYR:HE2	3:V3:109:ARG:HD3	1.83	0.43
3:X3:70:PRO:HA	3:X3:75:TYR:CD1	2.54	0.43
4:Y3:238:ARG:HD3	4:Y3:240:ARG:HH21	1.84	0.43
13:B4:201:CYC:HMB1	3:C4:77:ASN:HD21	1.83	0.43
2:G4:23:THR:HG23	2:H4:5:PRO:HA	2.01	0.43
2:I4:112:LEU:O	2:I4:116:LEU:HB2	2.18	0.43
3:Q4:128:VAL:HG13	13:Q4:201:CYC:HBC3	1.99	0.43
2:R4:27:VAL:HG22	2:W4:27:VAL:HG22	2.01	0.43
3:V4:70:PRO:HA	3:V4:75:TYR:CD1	2.54	0.43
3:X4:4:ASP:H	3:X4:7:THR:HG23	1.84	0.43
5:Z4:4:THR:OG1	13:Z4:301:CYC:O1D	2.33	0.43
3:a4:44:ARG:NH1	3:a4:142:ILE:O	2.52	0.43
3:C5:18:GLU:O	2:G5:98:TYR:OH	2.33	0.43
2:F5:138:LYS:HB2	2:F5:155:ILE:HG21	1.99	0.43
2:R5:3:LYS:HB3	2:W5:18:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S5:45:LEU:HD21	2:S5:141:HIS:HB2	2.01	0.43
3:X5:21:SER:H	3:X5:24:GLN:HE21	1.67	0.43
13:a5:202:CYC:HMA3	13:a5:202:CYC:HB	1.83	0.43
1:A6:34:GLU:OE1	5:Z6:255:ARG:NE	2.50	0.43
3:E6:41:THR:HG23	3:E6:143:VAL:HG21	2.01	0.43
3:E6:124:PRO:O	3:E6:128:VAL:HG23	2.19	0.43
2:F6:134:LEU:HB3	2:F6:155:ILE:HG23	2.00	0.43
3:J6:129:ALA:O	3:J6:133:ARG:HG3	2.18	0.43
2:K6:74:ASN:HA	13:K6:201:CYC:HBD2	2.00	0.43
2:U6:126:ALA:HB3	2:U6:129:TRP:CE2	2.54	0.43
3:V6:20:LEU:HD23	3:V6:20:LEU:HA	1.83	0.43
3:X6:16:ARG:NH2	3:X6:24:GLN:OE1	2.52	0.43
5:Z6:214:SER:OG	5:Z6:255:ARG:NH1	2.52	0.43
13:D7:201:CYC:HMA1	2:I7:29:PHE:CE1	2.54	0.43
2:K7:138:LYS:HB2	2:K7:155:ILE:HG21	2.01	0.43
13:L7:201:CYC:OB	5:Z7:254:ARG:O	2.36	0.43
3:O7:1:MET:SD	3:O7:1:MET:N	2.74	0.43
3:P7:117:THR:HG21	13:P7:202:CYC:HMA1	2.01	0.43
5:Z7:70:ARG:HE	5:Z7:145:GLU:CD	2.25	0.43
13:A1:302:CYC:O1A	3:E1:78:ARG:NH2	2.47	0.42
2:F1:126:ALA:HB3	2:F1:129:TRP:CE2	2.54	0.42
13:F1:202:CYC:H3C	3:L1:149:ILE:HD13	2.00	0.42
3:J1:83:CYS:HA	13:J1:201:CYC:HAC1	1.46	0.42
3:O1:37:LYS:NZ	13:T1:201:CYC:O1D	2.43	0.42
3:O1:59:ALA:HB3	3:O1:134:LYS:HD3	2.01	0.42
3:O1:112:ASN:O	5:Z1:162:SER:OG	2.27	0.42
4:Y1:252:LYS:NZ	5:Z1:70:ARG:HH22	2.17	0.42
1:22:231:GLN:HG3	9:Q2:68:PRO:HG2	2.01	0.42
13:32:302:CYC:HC	3:E3:123:VAL:HG22	1.83	0.42
1:52:59:LYS:HD2	2:I5:117:ASP:HB2	2.01	0.42
1:52:107:VAL:HG12	1:52:141:LEU:HD23	2.00	0.42
9:D2:62:ARG:O	9:D2:65:VAL:HG22	2.19	0.42
9:G2:64:ASP:N	9:G2:64:ASP:OD1	2.50	0.42
8:L2:104:ASP:OD1	8:L2:154:TYR:OH	2.37	0.42
10:N2:466:ALA:HB1	10:N2:468:PHE:HE1	1.84	0.42
11:P2:64:PRO:HG2	7:b2:95:PRO:HG2	2.01	0.42
9:R2:90:ARG:O	9:R2:93:THR:OG1	2.30	0.42
9:f2:113:ARG:HH22	9:f2:161:SER:C	2.27	0.42
9:i2:62:ARG:HG3	9:i2:64:ASP:OD1	2.19	0.42
9:j2:89:LEU:HB2	9:j2:133:LEU:HD21	2.00	0.42
9:k2:1:MET:H2	9:k2:103:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o2:53:ARG:NH2	10:o2:176:GLY:HA2	2.34	0.42
12:t2:115:MET:HB2	12:t2:115:MET:HE3	1.70	0.42
13:y2:201:CYC:HHD	13:y2:201:CYC:HAC2	1.71	0.42
2:I3:138:LYS:HB2	2:I3:155:ILE:HG21	2.00	0.42
2:R3:85:CYS:O	2:R3:89:ILE:HG12	2.18	0.42
2:S3:3:LYS:HG3	2:T3:18:ARG:NH1	2.34	0.42
2:T3:126:ALA:HB3	2:T3:129:TRP:CE2	2.54	0.42
2:U3:21:SER:O	2:U3:25:LEU:HG	2.19	0.42
3:V3:77:ASN:HD21	13:W3:201:CYC:HMB2	1.84	0.42
3:D4:25:LEU:HD13	2:I4:43:LYS:HB2	2.01	0.42
3:E4:16:ARG:NE	3:E4:18:GLU:OE2	2.51	0.42
2:T4:85:CYS:O	2:T4:89:ILE:HG12	2.19	0.42
4:Y4:248:VAL:HG11	4:Y4:256:THR:HG21	2.00	0.42
2:B5:80:GLU:O	2:B5:84:LYS:HG2	2.19	0.42
3:E5:105:ILE:HD12	3:E5:109:ARG:HG3	2.01	0.42
3:E5:149:ILE:HD13	13:E5:201:CYC:H3C	2.01	0.42
2:I5:5:PRO:HG2	2:I5:31:ARG:HD3	2.00	0.42
13:K5:201:CYC:HHD	13:K5:201:CYC:HAC2	1.69	0.42
3:M5:99:PHE:CE1	2:R5:28:ALA:HB2	2.54	0.42
3:Q5:78:ARG:HB2	2:R5:114:ALA:HB3	2.00	0.42
3:Q5:89:ILE:HD13	13:Q5:201:CYC:HBB3	2.01	0.42
3:Q5:139:ALA:O	3:Q5:142:ILE:HG13	2.19	0.42
2:R5:27:VAL:HG22	2:W5:27:VAL:HG22	2.01	0.42
3:a5:37:LYS:HE3	13:a5:202:CYC:HMD1	2.00	0.42
13:A6:302:CYC:HMD2	3:E6:79:ARG:O	2.19	0.42
2:B6:163:SER:OXT	2:H6:121:LYS:NZ	2.48	0.42
2:H6:126:ALA:HB3	2:H6:129:TRP:CE2	2.54	0.42
2:I6:120:ASN:HD22	2:I6:127:PRO:HG3	1.84	0.42
3:Q6:154:CYS:SG	13:Q6:202:CYC:HAC2	2.59	0.42
2:R6:95:ILE:HG22	2:R6:108:ILE:HG12	2.01	0.42
3:V6:35:GLY:O	3:V6:39:ILE:HG13	2.19	0.42
3:V6:75:TYR:OH	2:W6:94:ARG:NH2	2.29	0.42
13:V6:201:CYC:HHD	13:V6:201:CYC:HAC2	1.72	0.42
2:B7:126:ALA:HB3	2:B7:129:TRP:CE2	2.54	0.42
2:B7:163:SER:OXT	2:H7:121:LYS:NZ	2.43	0.42
3:D7:130:GLU:HG3	3:D7:134:LYS:HE2	2.01	0.42
3:J7:37:LYS:HE2	3:J7:37:LYS:N	2.33	0.42
2:N7:45:LEU:HD21	2:N7:141:HIS:HB2	2.00	0.42
2:N7:112:LEU:HD12	3:O7:77:ASN:ND2	2.34	0.42
3:O7:143:VAL:HG13	13:T7:201:CYC:HBC1	2.01	0.42
3:a7:9:VAL:HG11	3:a7:28:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M1:61:PHE:HB3	3:M1:68:ILE:HD13	2.00	0.42
3:Q1:37:LYS:HB3	3:Q1:154:CYS:SG	2.60	0.42
6:02:6:ILE:HG21	6:02:36:TRP:CZ3	2.54	0.42
1:22:124:ALA:HA	13:22:301:CYC:HBA2	2.00	0.42
8:C2:71:ASN:O	8:C2:77:ARG:HD3	2.19	0.42
9:R2:71:ASN:OD1	9:R2:121:THR:OG1	2.35	0.42
12:S2:138:LEU:HD22	12:S2:146:ALA:HA	2.00	0.42
9:U2:64:ASP:OD1	9:U2:64:ASP:N	2.52	0.42
9:U2:113:ARG:HD2	9:U2:123:ILE:HD13	2.01	0.42
9:e2:23:LEU:HB3	8:g2:38:VAL:HG13	2.00	0.42
9:f2:101:ILE:HD13	9:f2:155:TYR:CZ	2.54	0.42
9:j2:92:VAL:HA	9:j2:104:ILE:HD11	2.00	0.42
9:j2:100:ASP:OD1	9:j2:101:ILE:N	2.53	0.42
10:o2:91:ASP:OD1	10:o2:91:ASP:N	2.50	0.42
10:o2:201:THR:OG1	13:o2:801:CYC:HMC3	2.19	0.42
9:r2:11:ALA:HB2	9:r2:18:LEU:HD23	2.01	0.42
9:s2:134:LYS:HB2	9:s2:153:PHE:HB3	2.00	0.42
9:v2:90:ARG:O	9:v2:93:THR:OG1	2.31	0.42
8:y2:85:LEU:HB3	8:y2:133:ILE:HD11	2.01	0.42
2:B3:115:GLY:O	2:B3:119:ILE:HG12	2.18	0.42
2:B3:126:ALA:HB3	2:B3:129:TRP:CE2	2.54	0.42
3:E3:37:LYS:HA	13:E3:201:CYC:HHH	2.00	0.42
2:F3:18:ARG:HH22	2:K3:109:ASP:CG	2.27	0.42
2:K3:99:ALA:HB2	2:K3:108:ILE:HG13	2.01	0.42
3:Q3:79:ARG:O	13:Q3:201:CYC:HMD2	2.20	0.42
3:Q3:111:LEU:HD13	3:Q3:171:ALA:HB2	2.01	0.42
2:S3:95:ILE:HG22	2:S3:108:ILE:HG12	2.02	0.42
2:U3:66:TYR:O	2:U3:70:THR:OG1	2.33	0.42
3:V3:123:VAL:HG13	13:V3:201:CYC:HMC3	2.00	0.42
3:V3:146:ARG:HD2	13:V3:202:CYC:HMC2	2.00	0.42
5:Z3:227:SER:HB2	5:Z3:234:ALA:HB3	2.00	0.42
3:a3:151:GLN:CD	3:L6:151:GLN:HG3	2.44	0.42
2:B4:50:ASP:N	2:B4:50:ASP:OD1	2.52	0.42
3:O4:76:THR:OG1	3:O4:77:ASN:N	2.52	0.42
3:V4:86:ASP:OD1	5:Z4:48:TYR:OH	2.30	0.42
5:Z4:203:VAL:HG13	5:Z4:282:VAL:HB	2.01	0.42
3:a4:132:VAL:HA	3:a4:135:MET:HE2	2.00	0.42
3:E5:93:TYR:CG	3:E5:110:CYS:HB2	2.53	0.42
2:R5:87:ARG:NH2	13:R5:201:CYC:O2A	2.52	0.42
2:T5:53:VAL:HG13	2:T5:89:ILE:HB	2.00	0.42
13:V5:201:CYC:HMD1	13:V5:201:CYC:HC	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:127:LEU:HD12	3:D6:85:ARG:NE	2.34	0.42
2:B6:85:CYS:CA	13:B6:201:CYC:HHD	2.48	0.42
3:C6:83:CYS:HA	13:C6:201:CYC:HAC2	2.01	0.42
2:K6:18:ARG:O	3:L6:96:TYR:OH	2.32	0.42
2:K6:76:ALA:HB2	13:K6:201:CYC:OC	2.19	0.42
2:N6:84:LYS:HE3	2:N6:84:LYS:HB2	1.95	0.42
2:N6:113:LEU:HD21	2:N6:161:ALA:HB1	2.01	0.42
2:R6:3:LYS:O	2:W6:23:THR:OG1	2.23	0.42
3:D7:92:ARG:O	3:D7:95:THR:OG1	2.30	0.42
2:F1:21:SER:N	2:F1:24:GLU:OE1	2.49	0.42
2:F1:150:GLU:HG2	2:F1:154:TYR:CE2	2.54	0.42
2:G1:80:GLU:H	2:G1:80:GLU:CD	2.27	0.42
2:G1:91:TYR:O	2:G1:95:ILE:HG12	2.20	0.42
2:H1:9:ALA:HB1	2:H1:24:GLU:HG3	2.01	0.42
2:K1:126:ALA:HB3	2:K1:129:TRP:CE2	2.54	0.42
3:L1:16:ARG:HH21	3:L1:24:GLN:HE22	1.67	0.42
3:Q1:9:VAL:HG12	3:Q1:20:LEU:HD23	2.00	0.42
6:02:49:LYS:NZ	6:02:50:ILE:O	2.52	0.42
1:32:146:GLU:OE2	1:32:160:ARG:NH2	2.52	0.42
1:42:240:ASP:OD1	1:42:240:ASP:N	2.53	0.42
8:F2:77:ARG:HG2	13:F2:201:CYC:HAD1	2.02	0.42
9:J2:1:MET:H3	9:J2:102:THR:HB	1.84	0.42
12:S2:80:GLN:HE22	12:S2:83:ARG:NE	2.17	0.42
9:U2:128:GLU:OE1	9:U2:131:ARG:NH1	2.52	0.42
8:d2:100:ASP:OD1	8:d2:101:THR:N	2.52	0.42
8:d2:112:LEU:HD11	8:d2:116:TYR:CZ	2.54	0.42
9:h2:134:LYS:HB2	9:h2:153:PHE:HB3	2.00	0.42
10:o2:301:THR:OG1	10:o2:307:LYS:HB3	2.19	0.42
8:p2:61:LEU:HA	8:p2:61:LEU:HD12	1.76	0.42
9:s2:2:SER:H	9:s2:5:SER:HG	1.61	0.42
2:G3:113:LEU:HD22	2:G3:113:LEU:HA	1.83	0.42
2:H3:115:GLY:O	2:H3:119:ILE:HG12	2.19	0.42
3:M3:60:LEU:HA	3:M3:134:LYS:HE3	2.01	0.42
3:Q3:76:THR:OG1	3:Q3:79:ARG:NH2	2.48	0.42
2:R3:118:GLU:OE1	2:R3:118:GLU:N	2.41	0.42
2:W3:19:PHE:HZ	3:X3:88:GLU:HG2	1.85	0.42
2:B4:31:ARG:NH2	2:B4:101:VAL:O	2.52	0.42
3:C4:35:GLY:O	3:C4:39:ILE:HG12	2.19	0.42
3:C4:89:ILE:HG12	3:C4:92:ARG:HH21	1.84	0.42
13:E4:201:CYC:NB	13:E4:201:CYC:HMA3	2.34	0.42
2:F4:23:THR:HA	2:K4:5:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H4:99:ALA:HB2	2:H4:108:ILE:HG12	2.01	0.42
2:I4:45:LEU:HD23	2:I4:45:LEU:HA	1.91	0.42
3:X4:7:THR:HA	3:X4:10:VAL:HB	2.01	0.42
4:Y4:234:ARG:HE	4:Y4:235:THR:H	1.68	0.42
2:B5:120:ASN:HD22	2:B5:127:PRO:HG3	1.84	0.42
3:X5:79:ARG:HD2	13:X5:201:CYC:HBD2	2.01	0.42
4:Y5:224:VAL:HG13	4:Y5:270:ILE:HG12	2.01	0.42
5:Z5:85:LYS:HG3	5:Z5:180:ARG:HD3	2.01	0.42
3:E6:41:THR:O	3:E6:45:ILE:HG12	2.20	0.42
2:R6:53:VAL:HG23	2:R6:89:ILE:HB	2.00	0.42
2:T6:133:ALA:O	2:T6:137:ILE:HG12	2.19	0.42
2:U6:118:GLU:OE1	2:U6:118:GLU:N	2.42	0.42
3:J7:73:ASN:OD1	13:J7:201:CYC:NC	2.51	0.42
3:L7:41:THR:O	3:L7:45:ILE:HG12	2.19	0.42
3:Q7:123:VAL:HG22	13:Q7:201:CYC:HC	1.84	0.42
2:R7:9:ALA:HB1	2:R7:24:GLU:HG3	2.00	0.42
2:B1:85:CYS:HA	13:B1:201:CYC:HAC1	1.75	0.42
3:C1:43:ASN:HB2	2:G1:25:LEU:HD21	2.01	0.42
3:D1:92:ARG:NH1	3:D1:96:TYR:OH	2.52	0.42
2:G1:5:PRO:HG3	2:H1:23:THR:HA	2.01	0.42
2:I1:50:ASP:OD1	2:I1:50:ASP:N	2.50	0.42
2:S1:67:THR:HG21	13:S1:201:CYC:HMC2	2.00	0.42
2:S1:126:ALA:HB3	2:S1:129:TRP:CE2	2.54	0.42
6:02:41:GLN:HE21	13:a2:201:CYC:HBB3	1.84	0.42
7:12:93:PRO:HB2	7:12:97:LEU:HD11	2.01	0.42
1:22:47:GLN:OE1	1:22:51:ARG:NH1	2.53	0.42
1:22:147:TYR:HE2	1:22:157:PRO:HG3	1.85	0.42
1:32:204:PHE:CE1	9:h2:76:ASP:HB2	2.53	0.42
8:A2:66:THR:HA	8:A2:72:MET:HB2	2.02	0.42
9:E2:1:MET:O	9:E2:103:PRO:HD3	2.18	0.42
9:G2:81:CYS:CA	13:G2:201:CYC:HHD	2.50	0.42
9:W2:62:ARG:O	9:W2:65:VAL:HG22	2.19	0.42
7:b2:102:GLN:O	7:b2:105:SER:OG	2.33	0.42
8:c2:88:TYR:HH	8:c2:116:TYR:HH	1.67	0.42
8:l2:77:ARG:HB3	13:l2:201:CYC:HMD1	2.01	0.42
8:n2:96:MET:SD	8:n2:149:MET:HG2	2.60	0.42
12:t2:11:ALA:HB1	12:t2:16:ARG:O	2.20	0.42
2:G3:94:ARG:HG2	2:G3:98:TYR:CZ	2.55	0.42
2:H3:95:ILE:HG13	2:H3:112:LEU:HD13	2.01	0.42
2:I3:108:ILE:HG22	2:I3:113:LEU:HG	2.00	0.42
2:N3:115:GLY:O	2:N3:119:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q3:99:PHE:CZ	2:T3:28:ALA:HB2	2.55	0.42
3:Q3:139:ALA:HA	3:Q3:142:ILE:HG12	2.01	0.42
2:S3:67:THR:HG21	13:S3:201:CYC:HMC2	2.00	0.42
2:T3:138:LYS:HB2	2:T3:155:ILE:HG21	2.00	0.42
2:U3:112:LEU:O	2:U3:116:LEU:HB2	2.19	0.42
5:Z3:71:ASP:OD1	5:Z3:71:ASP:N	2.52	0.42
3:C4:44:ARG:NE	13:C4:202:CYC:HMC1	2.34	0.42
3:D4:72:GLY:O	3:D4:79:ARG:NH2	2.44	0.42
2:F4:109:ASP:HA	2:F4:113:LEU:HB3	2.01	0.42
2:I4:134:LEU:HB3	2:I4:155:ILE:HG23	2.01	0.42
2:N4:122:THR:HG21	3:O4:84:LEU:HD13	2.00	0.42
3:O4:154:CYS:HB3	3:O4:157:ILE:HG22	2.00	0.42
5:Z4:40:TYR:O	5:Z4:44:LEU:HB2	2.19	0.42
3:E5:99:PHE:CZ	2:H5:28:ALA:HB2	2.54	0.42
13:Q5:202:CYC:HMA1	2:T5:29:PHE:CZ	2.54	0.42
2:S5:27:VAL:HG22	2:T5:27:VAL:HG23	2.00	0.42
2:T5:85:CYS:HA	13:T5:202:CYC:HHD	2.02	0.42
2:W5:5:PRO:CG	2:W5:31:ARG:HD3	2.45	0.42
2:W5:18:ARG:O	3:X5:96:TYR:OH	2.27	0.42
4:Y5:238:ARG:HD3	4:Y5:240:ARG:NH2	2.35	0.42
2:B6:50:ASP:N	2:B6:50:ASP:OD1	2.51	0.42
2:G6:23:THR:HA	2:H6:5:PRO:HG3	2.02	0.42
2:I6:85:CYS:O	2:I6:89:ILE:HG12	2.20	0.42
3:O6:152:GLY:N	13:T6:201:CYC:OC	2.52	0.42
2:R6:76:ALA:HB1	2:R6:82:LYS:HD3	2.00	0.42
3:X6:146:ARG:HH21	3:X6:151:GLN:HB3	1.84	0.42
3:C7:39:ILE:HG23	2:G7:25:LEU:HG	2.01	0.42
2:K7:74:ASN:OD1	2:K7:74:ASN:N	2.50	0.42
3:L7:116:GLU:HB3	5:Z7:257:ASN:HD22	1.84	0.42
3:L7:130:GLU:HG2	3:L7:133:ARG:HH21	1.83	0.42
3:P7:68:ILE:HD12	2:T7:87:ARG:HH12	1.83	0.42
3:Q7:20:LEU:HD22	2:T7:101:VAL:HG21	2.01	0.42
3:Q7:99:PHE:CZ	2:T7:28:ALA:HB2	2.55	0.42
3:Q7:142:ILE:HG13	3:Q7:143:VAL:N	2.34	0.42
2:R7:113:LEU:HD11	2:R7:161:ALA:HB1	2.01	0.42
2:T7:31:ARG:NH2	2:T7:101:VAL:O	2.53	0.42
2:U7:85:CYS:O	2:U7:89:ILE:HG12	2.19	0.42
2:U7:112:LEU:O	2:U7:116:LEU:HB2	2.19	0.42
3:a7:150:THR:O	13:a7:202:CYC:NC	2.53	0.42
2:B1:126:ALA:HB3	2:B1:129:TRP:CE2	2.55	0.42
13:J1:202:CYC:HMA3	13:J1:202:CYC:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L1:40:ASP:CG	3:L1:149:ILE:HD11	2.44	0.42
3:Q1:85:ARG:NH2	13:Q1:201:CYC:O2A	2.51	0.42
3:V1:115:ARG:NH2	3:V1:171:ALA:O	2.53	0.42
5:Z1:10:LEU:HD13	5:Z1:169:PHE:CE2	2.55	0.42
13:22:302:CYC:HMD1	3:E7:79:ARG:HB3	2.01	0.42
1:32:99:SER:HB3	3:D3:112:ASN:ND2	2.34	0.42
8:C2:1:MET:N	8:C2:106:GLU:OE2	2.46	0.42
9:D2:121:THR:OG1	13:D2:201:CYC:NC	2.34	0.42
10:N2:19:THR:HG22	10:N2:175:ALA:HB1	2.00	0.42
11:P2:43:ILE:O	11:P2:47:ASN:ND2	2.46	0.42
11:P2:47:ASN:HB2	11:P2:141:LEU:HD21	2.00	0.42
11:P2:60:PHE:HB3	11:P2:67:LEU:HD11	2.01	0.42
12:S2:47:GLU:OE1	8:T2:18:TYR:OH	2.32	0.42
8:T2:76:ARG:NE	6:Y2:66:LEU:HD11	2.34	0.42
8:a2:104:LEU:HB3	8:a2:156:ILE:HD11	2.01	0.42
8:d2:76:ARG:NH1	9:i2:106:GLU:OE2	2.52	0.42
9:e2:101:ILE:HD12	9:e2:155:TYR:CE1	2.55	0.42
9:f2:1:MET:HE2	8:m2:1:MET:HB3	2.00	0.42
13:g2:201:CYC:NC	13:g2:201:CYC:HMD1	2.34	0.42
10:o2:616:LEU:HD23	10:o2:616:LEU:HA	1.79	0.42
10:o2:705:ARG:NE	1:A6:118:GLY:HA2	2.35	0.42
9:s2:57:GLN:O	9:s2:61:LYS:HG2	2.19	0.42
9:x2:48:GLU:H	9:x2:48:GLU:CD	2.28	0.42
9:x2:115:MET:HE3	9:x2:115:MET:HB3	1.94	0.42
8:y2:71:ASN:O	8:y2:77:ARG:HD3	2.20	0.42
3:L3:41:THR:HG23	3:L3:143:VAL:HG21	2.01	0.42
3:O3:99:PHE:CZ	2:S3:28:ALA:HB2	2.55	0.42
3:P3:99:PHE:CZ	2:U3:28:ALA:HB2	2.54	0.42
3:V3:118:TYR:HE2	3:V3:128:VAL:HG11	1.84	0.42
2:W3:34:GLN:HE21	2:W3:150:GLU:HB2	1.85	0.42
3:a3:37:LYS:HE3	13:a3:202:CYC:HMD1	2.01	0.42
3:D4:77:ASN:ND2	2:H4:112:LEU:O	2.37	0.42
2:F4:3:LYS:HZ2	2:K4:18:ARG:HE	1.66	0.42
2:I4:85:CYS:O	2:I4:89:ILE:HG12	2.19	0.42
2:K4:25:LEU:HD22	3:L4:39:ILE:HG23	2.00	0.42
3:L4:124:PRO:O	3:L4:128:VAL:HG23	2.20	0.42
3:Q4:139:ALA:O	3:Q4:142:ILE:HG13	2.20	0.42
2:R4:126:ALA:HB3	2:R4:129:TRP:CE2	2.54	0.42
3:a4:98:VAL:HG13	3:a4:157:ILE:HD11	2.01	0.42
3:E5:21:SER:H	3:E5:24:GLN:HE21	1.68	0.42
3:O5:102:ASP:OD1	3:O5:104:SER:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O5:154:CYS:SG	13:T5:201:CYC:HAC1	2.60	0.42
2:S5:85:CYS:HA	13:S5:201:CYC:HAC1	1.68	0.42
2:U5:112:LEU:HD12	13:U5:201:CYC:HAB1	2.00	0.42
3:C6:20:LEU:HD22	2:G6:101:VAL:HG21	2.01	0.42
3:E6:44:ARG:HD3	3:E6:143:VAL:HA	2.01	0.42
2:G6:150:GLU:HG2	2:G6:154:TYR:CE2	2.54	0.42
2:I6:126:ALA:HB3	2:I6:129:TRP:CE2	2.54	0.42
2:K6:7:THR:HG22	3:L6:1:MET:HB2	2.00	0.42
3:L6:70:PRO:HA	3:L6:75:TYR:CG	2.54	0.42
3:O6:38:ARG:O	3:O6:41:THR:OG1	2.32	0.42
3:O6:146:ARG:HD2	13:T6:201:CYC:HMC2	2.02	0.42
2:R6:126:ALA:HB3	2:R6:129:TRP:CE2	2.54	0.42
3:D7:88:GLU:O	3:D7:92:ARG:HG3	2.19	0.42
3:M7:1:MET:HG3	4:Y7:218:ARG:HE	1.85	0.42
2:R7:85:CYS:O	2:R7:89:ILE:HG12	2.19	0.42
2:W7:34:GLN:HE21	2:W7:150:GLU:HB2	1.84	0.42
1:A1:54:PHE:HE1	1:A1:90:PHE:HB2	1.84	0.42
1:A1:146:GLU:OE2	1:A1:160:ARG:NH2	2.51	0.42
2:B1:108:ILE:HG22	2:B1:113:LEU:HG	2.01	0.42
2:I1:85:CYS:CA	13:I1:201:CYC:HHD	2.49	0.42
3:P1:107:ASP:OD1	3:P1:167:LYS:HD3	2.19	0.42
2:T1:85:CYS:HA	13:T1:202:CYC:HHD	2.01	0.42
13:42:302:CYC:HAC2	3:E4:83:CYS:HA	2.02	0.42
8:A2:38:VAL:HG13	9:H2:23:LEU:HD12	2.00	0.42
8:L2:55:VAL:HG12	8:L2:60:LEU:HG	2.02	0.42
8:M2:65:ILE:HD11	13:M2:201:CYC:HMC2	2.01	0.42
10:N2:192:ILE:O	10:N2:196:CYS:HB3	2.20	0.42
10:N2:298:ARG:CZ	10:N2:300:ILE:HD11	2.49	0.42
10:N2:520:GLN:HE21	10:N2:524:GLY:C	2.28	0.42
10:N2:579:ILE:HB	10:N2:583:GLU:HB3	2.01	0.42
11:P2:3:ASP:H	11:P2:6:SER:HG	1.68	0.42
9:W2:50:ILE:HG23	9:W2:136:ALA:HB3	2.00	0.42
6:Y2:3:MET:N	6:Y2:57:THR:OG1	2.48	0.42
8:g2:100:ASP:OD1	8:g2:102:SER:N	2.49	0.42
9:k2:134:LYS:HB2	9:k2:153:PHE:HB3	2.01	0.42
13:k2:201:CYC:HBB2	13:k2:201:CYC:HMB1	2.01	0.42
8:l2:101:THR:HG22	8:l2:152:TYR:HD1	1.85	0.42
8:n2:68:PRO:HD3	9:s2:87:TYR:OH	2.20	0.42
10:o2:549:ILE:HG12	10:o2:574:LEU:HD23	2.01	0.42
9:r2:33:GLY:O	9:r2:36:ARG:HG2	2.20	0.42
3:E3:30:ARG:O	3:E3:34:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F3:134:LEU:HB3	2:F3:155:ILE:HG23	2.02	0.42
2:H3:21:SER:N	2:H3:24:GLU:OE1	2.51	0.42
3:J3:114:LEU:HD11	3:J3:118:TYR:CZ	2.55	0.42
2:N3:115:GLY:O	2:N3:118:GLU:HG2	2.20	0.42
13:N3:201:CYC:OB	3:O3:75:TYR:O	2.38	0.42
3:O3:61:PHE:CZ	3:O3:80:MET:HE1	2.55	0.42
3:Q3:123:VAL:HG22	13:Q3:201:CYC:HC	1.85	0.42
2:R3:23:THR:HG23	2:W3:5:PRO:HA	2.00	0.42
2:R3:27:VAL:HG22	2:W3:27:VAL:HG22	2.00	0.42
2:R3:155:ILE:O	2:R3:159:ILE:HG12	2.20	0.42
3:V3:35:GLY:O	3:V3:39:ILE:HG13	2.20	0.42
3:X3:28:LEU:O	3:X3:32:VAL:HG23	2.20	0.42
13:a3:201:CYC:NC	13:a3:201:CYC:HMD3	2.35	0.42
2:S4:88:ASP:HB3	2:S4:130:TYR:HE1	1.85	0.42
3:V4:115:ARG:NH2	3:V4:173:ALA:O	2.41	0.42
3:a4:16:ARG:NH2	3:a4:24:GLN:OE1	2.52	0.42
3:C5:100:THR:HG23	2:G5:10:VAL:HG21	2.02	0.42
3:D5:9:VAL:HG12	3:D5:20:LEU:HD23	2.00	0.42
3:P5:63:GLU:HG3	3:P5:64:GLN:HG3	2.01	0.42
3:Q5:154:CYS:SG	13:Q5:202:CYC:H2C	2.59	0.42
2:R5:126:ALA:HB3	2:R5:129:TRP:CE2	2.54	0.42
2:T5:91:TYR:O	2:T5:95:ILE:HG12	2.19	0.42
2:U5:138:LYS:HB2	2:U5:155:ILE:HG21	2.01	0.42
3:V5:35:GLY:O	3:V5:39:ILE:HG13	2.20	0.42
2:W5:50:ASP:OD1	2:W5:51:SER:N	2.53	0.42
3:X5:136:LYS:HB2	3:X5:165:PHE:CG	2.54	0.42
13:A6:301:CYC:HAB2	3:D6:110:CYS:HA	2.02	0.42
13:A6:302:CYC:NC	3:E6:83:CYS:HB2	2.34	0.42
3:E6:8:LYS:HE2	3:E6:8:LYS:HB2	1.91	0.42
2:G6:3:LYS:HB2	2:G6:106:GLY:HA2	2.02	0.42
3:J6:128:VAL:HB	3:J6:172:VAL:HG11	2.01	0.42
2:N6:45:LEU:HD21	2:N6:141:HIS:HB2	2.02	0.42
2:S6:85:CYS:HA	13:S6:201:CYC:HHH	2.01	0.42
3:V6:12:GLN:O	3:V6:16:ARG:HG3	2.19	0.42
3:V6:77:ASN:HD21	2:W6:116:LEU:HD13	1.85	0.42
3:V6:106:LEU:HD12	3:V6:110:CYS:HB3	2.02	0.42
4:Y6:238:ARG:NH1	4:Y6:240:ARG:HH21	2.16	0.42
5:Z6:10:LEU:HD13	5:Z6:169:PHE:CE2	2.54	0.42
3:a6:41:THR:HG23	3:a6:143:VAL:HG21	2.00	0.42
3:a6:154:CYS:SG	13:a6:202:CYC:HBC2	2.60	0.42
2:B7:95:ILE:HG22	2:B7:108:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C7:89:ILE:HD13	13:C7:201:CYC:HBB3	2.01	0.42
13:C7:201:CYC:O2D	5:Z7:236:ARG:NH2	2.53	0.42
3:D7:3:PHE:O	3:D7:104:SER:OG	2.38	0.42
3:E7:146:ARG:HB3	3:E7:151:GLN:HE21	1.85	0.42
3:P7:99:PHE:CZ	2:U7:28:ALA:HB2	2.54	0.42
2:R7:155:ILE:O	2:R7:159:ILE:HG12	2.18	0.42
2:B1:85:CYS:CA	13:B1:201:CYC:HHD	2.49	0.42
3:C1:35:GLY:O	3:C1:39:ILE:HG12	2.20	0.42
2:H1:85:CYS:HA	13:H1:201:CYC:HHD	2.01	0.42
2:I1:85:CYS:O	2:I1:89:ILE:HG12	2.19	0.42
2:N1:74:ASN:O	13:N1:201:CYC:NC	2.48	0.42
2:N1:91:TYR:O	2:N1:95:ILE:HG12	2.20	0.42
2:S1:108:ILE:HG22	2:S1:113:LEU:HG	2.01	0.42
4:Y1:228:GLN:O	4:Y1:265:GLY:HA2	2.20	0.42
6:O2:21:GLU:OE1	13:d2:201:CYC:HBA1	2.18	0.42
8:F2:77:ARG:O	13:F2:201:CYC:HMD2	2.20	0.42
10:N2:198:THR:HG23	10:N2:199:PRO:HD3	2.01	0.42
10:N2:395:TYR:HA	6:Y2:20:ARG:HE	1.85	0.42
9:Q2:61:LYS:HE2	9:Q2:61:LYS:HB2	1.89	0.42
8:V2:71:ASN:O	8:V2:77:ARG:HD3	2.19	0.42
13:o2:801:CYC:CGA	11:q2:67:LEU:HD13	2.50	0.42
12:t2:101:LYS:HE2	9:v2:16:ARG:NE	2.34	0.42
8:u2:50:LEU:O	8:u2:54:GLU:HG2	2.19	0.42
8:w2:68:PRO:HG3	8:w2:73:TYR:CE1	2.54	0.42
3:E3:124:PRO:O	3:E3:128:VAL:HG23	2.19	0.42
2:N3:91:TYR:O	2:N3:95:ILE:HG12	2.20	0.42
2:N3:112:LEU:HD12	3:O3:77:ASN:ND2	2.35	0.42
3:Q3:142:ILE:HG13	3:Q3:143:VAL:N	2.34	0.42
2:T3:26:GLN:HA	2:T3:29:PHE:HD2	1.84	0.42
2:U3:63:LYS:HD3	2:U3:132:GLU:HG3	2.01	0.42
2:U3:126:ALA:HB3	2:U3:129:TRP:CE2	2.55	0.42
2:W3:85:CYS:HA	13:W3:201:CYC:HHD	2.02	0.42
13:C4:202:CYC:HMA3	13:C4:202:CYC:NB	2.35	0.42
3:E4:77:ASN:ND2	2:F4:116:LEU:HD13	2.34	0.42
3:P4:63:GLU:HG3	3:P4:64:GLN:HG3	2.01	0.42
3:Q4:154:CYS:SG	13:Q4:202:CYC:H2C	2.59	0.42
13:Q4:201:CYC:HAD2	4:Y4:250:TYR:HH	1.84	0.42
2:W4:28:ALA:HB2	3:X4:99:PHE:CZ	2.55	0.42
5:Z4:10:LEU:HD13	5:Z4:169:PHE:CE2	2.55	0.42
3:a4:9:VAL:HG11	3:a4:28:LEU:HD21	2.01	0.42
3:a4:28:LEU:O	3:a4:32:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F5:126:ALA:HB3	2:F5:129:TRP:CE2	2.55	0.42
3:L5:91:LEU:HB2	3:L5:135:MET:HE3	2.01	0.42
2:R5:121:LYS:NZ	2:S5:117:ASP:OD1	2.47	0.42
2:H6:99:ALA:HB2	2:H6:108:ILE:HG12	2.01	0.42
2:I6:85:CYS:HA	13:I6:201:CYC:HAC1	1.81	0.42
3:J6:73:ASN:OD1	13:J6:201:CYC:NC	2.52	0.42
2:K6:28:ALA:HB2	3:L6:99:PHE:CZ	2.55	0.42
3:O6:28:LEU:O	3:O6:32:VAL:HG23	2.20	0.42
3:P6:98:VAL:HG13	3:P6:157:ILE:HD11	2.00	0.42
2:R6:109:ASP:HA	2:R6:113:LEU:HB2	2.02	0.42
3:V6:89:ILE:HG12	3:V6:92:ARG:NH2	2.34	0.42
2:W6:99:ALA:HB2	2:W6:108:ILE:HG13	2.00	0.42
3:X6:86:ASP:OD2	3:X6:118:TYR:OH	2.32	0.42
3:C7:21:SER:N	3:C7:24:GLN:OE1	2.48	0.42
3:D7:92:ARG:HG2	2:I7:19:PHE:CE2	2.54	0.42
2:K7:126:ALA:HB3	2:K7:129:TRP:CE2	2.53	0.42
3:L7:146:ARG:NE	3:L7:151:GLN:OE1	2.50	0.42
2:G1:71:PRO:HG2	2:K7:58:ASN:O	2.20	0.42
3:J1:128:VAL:HB	3:J1:172:VAL:HG11	2.02	0.42
3:P1:37:LYS:HE3	3:P1:37:LYS:HB3	1.72	0.42
1:32:32:ASN:N	1:32:37:TYR:OH	2.53	0.42
8:B2:130:ILE:HG23	8:B2:153:LEU:HG	2.02	0.42
9:E2:8:ILE:CD1	8:L2:0:MET:HE1	2.50	0.42
9:I2:1:MET:N	10:N2:538:ILE:HD12	2.35	0.42
8:K2:105:ASP:OD1	8:K2:155:TYR:OH	2.27	0.42
10:N2:284:LYS:O	10:N2:288:ILE:HG12	2.18	0.42
9:U2:1:MET:HB2	9:U2:102:THR:HG21	2.01	0.42
8:V2:44:ILE:HD13	8:V2:149:MET:HE2	2.02	0.42
9:k2:39:ILE:HD11	9:k2:96:VAL:HG11	2.00	0.42
9:k2:126:VAL:HG22	13:k2:201:CYC:HBC3	2.01	0.42
8:m2:77:ARG:O	13:m2:201:CYC:HMD2	2.20	0.42
10:o2:300:ILE:CG2	10:o2:306:GLN:HB2	2.50	0.42
9:r2:33:GLY:O	9:r2:37:LEU:HG	2.20	0.42
8:y2:44:ILE:HD13	8:y2:149:MET:HE2	2.00	0.42
2:F3:138:LYS:HB2	2:F3:155:ILE:HG21	2.01	0.42
3:L3:76:THR:OG1	3:L3:79:ARG:NH1	2.53	0.42
3:M3:115:ARG:CZ	3:M3:173:ALA:HB2	2.49	0.42
2:S3:126:ALA:HB3	2:S3:129:TRP:CE2	2.54	0.42
2:T3:138:LYS:HA	2:T3:141:HIS:CD2	2.55	0.42
2:U3:26:GLN:HA	2:U3:29:PHE:HB2	2.00	0.42
3:X3:12:GLN:HB3	3:X3:16:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G4:5:PRO:HG3	2:H4:23:THR:HA	2.00	0.42
2:G4:115:GLY:O	2:G4:118:GLU:HG2	2.20	0.42
3:J4:113:GLY:O	3:J4:116:GLU:HG2	2.20	0.42
13:J4:202:CYC:HMA3	13:J4:202:CYC:HB	1.83	0.42
3:L4:40:ASP:CG	3:L4:149:ILE:HD11	2.44	0.42
13:M4:201:CYC:NC	13:M4:201:CYC:HMD1	2.34	0.42
2:N4:64:PHE:O	2:N4:67:THR:OG1	2.35	0.42
3:V4:41:THR:HG23	3:V4:143:VAL:HG21	2.02	0.42
2:B5:28:ALA:HB2	3:J5:99:PHE:CE1	2.55	0.42
3:M5:22:ASP:OD1	2:R5:43:LYS:NZ	2.51	0.42
3:M5:99:PHE:CZ	2:R5:28:ALA:HB2	2.55	0.42
2:N5:115:GLY:O	2:N5:118:GLU:HG2	2.19	0.42
3:Q5:85:ARG:NH2	13:Q5:201:CYC:O2A	2.45	0.42
2:R5:53:VAL:HG23	2:R5:89:ILE:HB	2.00	0.42
3:V5:89:ILE:HD13	13:V5:201:CYC:HBB3	2.00	0.42
3:V5:124:PRO:O	3:V5:128:VAL:HG23	2.19	0.42
2:W5:112:LEU:O	2:W5:116:LEU:HB2	2.20	0.42
5:Z5:227:SER:HA	5:Z5:237:ILE:HD11	2.01	0.42
3:E6:149:ILE:HD13	13:E6:201:CYC:H3C	2.01	0.42
2:H6:109:ASP:HA	2:H6:113:LEU:HB2	2.01	0.42
3:M6:99:PHE:CZ	2:R6:28:ALA:HB2	2.54	0.42
3:P6:146:ARG:NE	3:P6:151:GLN:OE1	2.53	0.42
2:T6:108:ILE:HG22	2:T6:113:LEU:HG	2.01	0.42
2:B7:94:ARG:HG2	2:B7:98:TYR:CZ	2.54	0.42
3:C7:115:ARG:NH2	3:C7:170:ALA:O	2.53	0.42
3:Q7:70:PRO:HA	3:Q7:75:TYR:CG	2.55	0.42
2:S7:23:THR:HA	2:T7:5:PRO:HG3	2.02	0.42
2:S7:95:ILE:HG22	2:S7:108:ILE:HG12	2.02	0.42
2:U7:50:ASP:OD1	2:U7:50:ASP:N	2.52	0.42
1:A1:38:SER:OG	1:A1:41:GLN:HG3	2.19	0.42
1:A1:127:LEU:HD13	3:D1:89:ILE:HD12	2.00	0.42
3:C1:44:ARG:NE	13:C1:202:CYC:HMC1	2.34	0.42
3:E1:18:GLU:O	2:H1:98:TYR:OH	2.28	0.42
3:E1:21:SER:H	3:E1:24:GLN:NE2	2.17	0.42
2:F1:134:LEU:HB3	2:F1:155:ILE:HG23	2.01	0.42
2:H1:126:ALA:HB3	2:H1:129:TRP:CE2	2.55	0.42
2:K1:91:TYR:O	2:K1:95:ILE:HG12	2.20	0.42
3:L1:117:THR:HG23	5:Z1:256:SER:HB2	2.01	0.42
3:M1:99:PHE:CE1	2:R1:28:ALA:HB2	2.55	0.42
3:P1:111:LEU:HD21	3:P1:168:ALA:HA	2.01	0.42
2:R1:132:GLU:HG3	2:R1:132:GLU:H	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W1:131:VAL:HG12	2:W1:135:LYS:HE2	2.01	0.42
7:12:93:PRO:HA	8:12:62:TYR:CD1	2.54	0.42
1:42:55:PHE:CD2	13:a4:201:CYC:HBA1	2.52	0.42
1:52:108:VAL:HG13	1:52:112:LEU:HD12	2.02	0.42
1:52:191:PHE:HD2	1:52:191:PHE:HA	1.67	0.42
8:C2:105:ASP:HA	8:C2:109:LEU:HB2	2.02	0.42
8:F2:28:LYS:O	8:F2:32:GLN:HG2	2.20	0.42
9:I2:48:GLU:H	9:I2:48:GLU:CD	2.27	0.42
8:L2:99:ASP:OD2	11:P2:162:ARG:NH2	2.53	0.42
10:N2:306:GLN:HB3	10:N2:334:LEU:HD21	2.00	0.42
13:O2:201:CYC:HC	13:O2:201:CYC:CMD	2.32	0.42
11:P2:107:GLU:HG2	11:P2:108:ARG:HG3	2.02	0.42
9:Q2:101:ILE:HB	9:Q2:155:TYR:CE2	2.55	0.42
8:g2:81:CYS:HA	13:g2:201:CYC:HAC2	2.02	0.42
8:m2:84:ASP:OD2	8:m2:116:TYR:OH	2.29	0.42
10:o2:45:SER:OG	9:r2:24:GLU:OE2	2.31	0.42
9:s2:33:GLY:HA2	9:s2:36:ARG:CZ	2.50	0.42
12:t2:30:PHE:CD2	8:u2:34:GLY:HA3	2.55	0.42
8:u2:131:GLN:O	8:u2:135:GLU:HG2	2.20	0.42
9:x2:101:ILE:HD12	9:x2:155:TYR:CE1	2.55	0.42
2:B3:95:ILE:HG22	2:B3:108:ILE:HG12	2.02	0.42
3:O3:37:LYS:HB3	3:O3:154:CYS:SG	2.60	0.42
3:C4:83:CYS:HA	13:C4:201:CYC:HAC2	2.02	0.42
3:P4:28:LEU:O	3:P4:32:VAL:HG23	2.20	0.42
2:S4:85:CYS:HA	13:S4:201:CYC:HAC1	1.69	0.42
4:Y4:224:VAL:HG13	4:Y4:270:ILE:HG12	2.02	0.42
3:a4:107:ASP:HB3	3:a4:167:LYS:HE3	2.01	0.42
3:E5:75:TYR:O	13:F5:201:CYC:OB	2.37	0.42
2:G5:18:ARG:NH1	2:H5:3:LYS:HE2	2.35	0.42
2:N5:24:GLU:OE1	2:N5:24:GLU:N	2.50	0.42
3:V5:70:PRO:HA	3:V5:75:TYR:CG	2.55	0.42
1:A6:86:LEU:HA	1:A6:134:TYR:HE1	1.84	0.42
3:C6:114:LEU:HD11	3:C6:118:TYR:CZ	2.55	0.42
2:I6:49:ALA:O	2:I6:50:ASP:C	2.63	0.42
2:R6:9:ALA:HB1	2:R6:24:GLU:HG3	2.00	0.42
2:S6:23:THR:HA	2:T6:5:PRO:HG3	2.02	0.42
3:E7:41:THR:HG23	3:E7:143:VAL:HG21	2.01	0.42
2:F7:50:ASP:N	2:F7:50:ASP:OD1	2.53	0.42
2:F7:100:LEU:HA	2:F7:154:TYR:HE2	1.84	0.42
2:H7:92:TYR:HE1	13:H7:201:CYC:HMB2	1.84	0.42
3:L7:40:ASP:CG	3:L7:149:ILE:HD11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N7:16:GLN:HG3	2:N7:18:ARG:HB2	2.01	0.42
2:N7:26:GLN:HG2	2:U7:34:GLN:HG3	2.00	0.42
2:R7:118:GLU:OE1	2:R7:118:GLU:N	2.40	0.42
2:S7:112:LEU:HD23	2:S7:158:LEU:HD21	2.01	0.42
3:V7:35:GLY:O	3:V7:39:ILE:HG13	2.19	0.42
2:W7:100:LEU:HA	2:W7:154:TYR:HE2	1.85	0.42
13:A1:302:CYC:O2A	3:E1:85:ARG:NH1	2.53	0.42
2:K1:127:PRO:HB3	2:K1:162:LEU:HD22	2.01	0.42
3:L1:151:GLN:HG3	3:a7:151:GLN:CD	2.45	0.42
3:O1:146:ARG:NE	3:O1:151:GLN:OE1	2.50	0.42
3:Q1:124:PRO:O	3:Q1:128:VAL:HG23	2.20	0.42
2:S1:85:CYS:CA	13:S1:201:CYC:HH2	2.50	0.42
3:V1:89:ILE:HG12	3:V1:92:ARG:HH21	1.85	0.42
5:Z1:142:THR:HG21	5:Z1:152:ARG:CD	2.49	0.42
1:52:233:LEU:HD12	9:I2:66:VAL:HG21	2.01	0.42
8:B2:40:ALA:O	8:B2:44:ILE:HG12	2.20	0.42
10:N2:257:LEU:HD11	10:N2:413:GLU:HB3	2.02	0.42
10:N2:690:ARG:O	10:N2:691:PRO:C	2.63	0.42
12:S2:29:PHE:CE1	12:S2:99:GLY:HA3	2.55	0.42
9:U2:81:CYS:SG	13:U2:201:CYC:HAC2	2.59	0.42
8:d2:79:ALA:HA	8:d2:82:ILE:HG12	2.01	0.42
9:k2:35:ARG:O	9:k2:39:ILE:HG23	2.20	0.42
10:o2:296:PHE:HB3	10:o2:300:ILE:HD11	2.02	0.42
2:G3:5:PRO:HD2	2:G3:31:ARG:HD3	2.02	0.42
3:Q3:4:ASP:OD1	3:Q3:7:THR:N	2.41	0.42
3:J4:114:LEU:HD11	3:J4:118:TYR:CZ	2.55	0.42
3:O4:128:VAL:HG22	13:Z4:301:CYC:H3C	2.02	0.42
2:T4:115:GLY:O	2:T4:119:ILE:HG12	2.20	0.42
3:V4:124:PRO:O	3:V4:128:VAL:HG23	2.19	0.42
2:W4:4:THR:HG22	2:W4:102:ALA:HB1	2.02	0.42
5:Z4:69:VAL:HB	5:Z4:146:SER:HA	2.02	0.42
3:a4:124:PRO:O	3:a4:128:VAL:HG23	2.19	0.42
2:B5:85:CYS:HA	13:B5:201:CYC:HAC1	1.75	0.42
13:B5:201:CYC:HMB1	3:C5:77:ASN:HD21	1.85	0.42
3:E5:80:MET:O	3:E5:84:LEU:HG	2.20	0.42
2:N5:27:VAL:HG13	2:U5:27:VAL:HG22	2.01	0.42
2:W5:115:GLY:O	2:W5:118:GLU:HG2	2.20	0.42
5:Z5:40:TYR:HA	5:Z5:44:LEU:HD23	2.01	0.42
1:A6:38:SER:HB2	1:A6:39:PRO:HD2	2.02	0.42
1:A6:180:ARG:NH2	13:a6:201:CYC:O1D	2.53	0.42
2:G6:27:VAL:HG22	2:H6:27:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J6:201:CYC:NC	13:J6:201:CYC:HMD1	2.35	0.42
3:L6:76:THR:HG22	3:L6:78:ARG:H	1.85	0.42
2:R6:74:ASN:O	13:R6:201:CYC:NC	2.50	0.42
3:D7:16:ARG:NH2	3:D7:24:GLN:HE22	2.17	0.42
2:F7:91:TYR:O	2:F7:95:ILE:HG12	2.19	0.42
3:M7:99:PHE:CZ	2:R7:28:ALA:HB2	2.54	0.42
3:P7:93:TYR:OH	2:U7:14:ASP:OD1	2.26	0.42
3:Q7:128:VAL:HG22	13:Q7:201:CYC:HBC3	2.02	0.42
13:Q7:201:CYC:HBA2	4:Y7:253:LEU:HB2	2.00	0.42
2:R7:56:ALA:O	2:R7:60:VAL:HG23	2.20	0.42
2:R7:126:ALA:HB3	2:R7:129:TRP:CE2	2.55	0.42
2:S7:116:LEU:HD21	2:S7:162:LEU:HD21	2.02	0.42
2:T7:85:CYS:O	2:T7:89:ILE:HG12	2.19	0.42
3:V7:38:ARG:NH2	3:V7:160:GLU:OE1	2.53	0.42
5:Z7:245:ILE:N	5:Z7:256:SER:OG	2.52	0.42
1:A1:181:TYR:HB2	1:A1:185:TYR:HB3	2.01	0.41
3:E1:80:MET:O	3:E1:84:LEU:HG	2.19	0.41
2:K1:56:ALA:HB3	2:K1:89:ILE:HG21	2.02	0.41
2:K1:116:LEU:HD21	2:K1:162:LEU:HD21	2.02	0.41
3:O1:96:TYR:HD1	2:S1:20:LEU:HD11	1.85	0.41
5:Z1:85:LYS:HE2	5:Z1:85:LYS:HB2	1.89	0.41
1:32:202:LYS:HD3	9:h2:77:MET:HE2	2.02	0.41
1:42:69:GLN:NE2	5:Z4:225:GLY:HA3	2.35	0.41
13:42:302:CYC:HC	13:42:302:CYC:CMD	2.33	0.41
9:J2:134:LYS:HB2	9:J2:153:PHE:HB3	2.01	0.41
8:K2:108:VAL:O	8:K2:112:LEU:HB2	2.20	0.41
8:L2:84:LEU:HB3	8:L2:132:ILE:HD11	2.02	0.41
8:M2:151:VAL:HG11	7:b2:78:ALA:HB1	2.02	0.41
10:N2:327:ARG:HH12	10:N2:388:ASP:CG	2.28	0.41
8:O2:81:CYS:SG	13:O2:201:CYC:HAC2	2.60	0.41
11:P2:19:LEU:HD12	9:U2:97:VAL:HG21	2.02	0.41
9:Q2:115:MET:HG3	8:V2:78:TYR:CD1	2.55	0.41
8:V2:140:LEU:HD23	8:V2:140:LEU:HA	1.90	0.41
8:d2:3:ASP:HB2	8:d2:98:ALA:O	2.20	0.41
8:d2:97:LEU:HD13	9:j2:18:LEU:HD12	2.02	0.41
8:n2:52:VAL:HG11	8:n2:82:ILE:HG23	2.02	0.41
10:o2:42:GLU:OE1	9:r2:25:ARG:NH2	2.43	0.41
10:o2:576:ASN:HB2	10:o2:578:GLU:HG3	2.01	0.41
9:r2:98:SER:HA	8:y2:5:ILE:HG21	2.02	0.41
9:v2:46:SER:O	9:v2:49:ARG:HG2	2.20	0.41
8:w2:96:MET:HA	8:w2:152:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:y2:2:GLN:HB2	8:y2:6:THR:CG2	2.50	0.41
3:C3:98:VAL:HG13	3:C3:157:ILE:HD11	2.01	0.41
3:D3:18:GLU:O	2:I3:98:TYR:OH	2.37	0.41
2:F3:28:ALA:HB2	3:a3:99:PHE:CZ	2.55	0.41
3:L3:21:SER:N	3:L3:24:GLN:OE1	2.44	0.41
3:O3:25:LEU:HD22	2:S3:43:LYS:HB2	2.02	0.41
2:T3:85:CYS:O	2:T3:89:ILE:HG12	2.20	0.41
13:a3:201:CYC:HB	13:a3:201:CYC:HMA3	1.84	0.41
2:B4:99:ALA:HB2	2:B4:108:ILE:HG13	2.02	0.41
2:B4:114:ALA:HB3	3:C4:78:ARG:HB2	2.01	0.41
2:G4:99:ALA:HB2	2:G4:108:ILE:HG13	2.01	0.41
3:O4:59:ALA:HB3	3:O4:134:LYS:HD3	2.01	0.41
2:G5:27:VAL:HG13	2:H5:27:VAL:HG22	2.02	0.41
2:S5:126:ALA:HB3	2:S5:129:TRP:CE2	2.55	0.41
2:W5:112:LEU:HD12	13:W5:201:CYC:HAB1	2.02	0.41
1:A6:14:ASN:OD1	1:A6:14:ASN:N	2.53	0.41
2:N6:95:ILE:HG22	2:N6:108:ILE:HG12	2.01	0.41
3:P6:114:LEU:HD23	3:P6:172:VAL:HG12	2.02	0.41
2:U6:91:TYR:O	2:U6:95:ILE:HG12	2.19	0.41
13:U6:201:CYC:HHH	13:U6:201:CYC:HAC2	1.78	0.41
3:C7:124:PRO:O	3:C7:128:VAL:HG23	2.20	0.41
3:E7:124:PRO:O	3:E7:128:VAL:HG23	2.19	0.41
3:J7:106:LEU:HD12	3:J7:110:CYS:HB3	2.02	0.41
3:P7:92:ARG:HH12	2:U7:14:ASP:HA	1.85	0.41
2:U7:126:ALA:HB3	2:U7:129:TRP:CE2	2.55	0.41
4:Y7:225:GLN:HB2	4:Y7:268:VAL:HB	2.01	0.41
2:G1:99:ALA:HB2	2:G1:108:ILE:HG13	2.02	0.41
2:I1:143:LEU:C	2:I1:148:ARG:HB2	2.44	0.41
3:L1:41:THR:O	3:L1:45:ILE:HG12	2.20	0.41
3:L1:124:PRO:O	3:L1:128:VAL:HG23	2.20	0.41
3:Q1:38:ARG:HH12	3:Q1:160:GLU:CD	2.28	0.41
2:S1:5:PRO:HG3	2:T1:23:THR:HA	2.02	0.41
3:X1:85:ARG:NH1	13:X1:201:CYC:O1A	2.37	0.41
7:12:98:ASP:HA	7:12:101:VAL:HG22	2.02	0.41
1:42:38:SER:OG	1:42:41:GLN:HG3	2.20	0.41
8:M2:13:ASP:OD2	10:N2:168:TYR:OH	2.27	0.41
10:N2:161:ASP:CG	13:N2:802:CYC:HHB	2.45	0.41
9:R2:134:LYS:HB2	9:R2:153:PHE:HB3	2.01	0.41
12:S2:30:PHE:CD2	8:T2:34:GLY:HA3	2.55	0.41
12:S2:154:ASP:O	12:S2:158:GLN:HG2	2.19	0.41
8:X2:65:ILE:H	8:X2:65:ILE:HG12	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c2:38:VAL:HG11	9:k2:27:LYS:HG2	2.02	0.41
9:f2:12:ASP:O	10:o2:499:GLN:NE2	2.51	0.41
9:i2:83:ARG:HH21	13:i2:201:CYC:HB	1.68	0.41
8:l2:96:MET:HE3	8:l2:96:MET:HB3	1.86	0.41
8:u2:68:PRO:HG3	8:u2:73:TYR:CE1	2.55	0.41
9:v2:14:GLU:OE1	9:v2:16:ARG:NE	2.38	0.41
9:x2:62:ARG:O	9:x2:65:VAL:HG22	2.20	0.41
13:I3:201:CYC:OB	3:a3:75:TYR:O	2.38	0.41
3:L3:25:LEU:HD13	3:L3:25:LEU:HA	1.87	0.41
3:Q3:112:ASN:O	4:Y3:261:HIS:NE2	2.43	0.41
2:R3:53:VAL:HG23	2:R3:89:ILE:HB	2.01	0.41
3:a3:70:PRO:HA	3:a3:75:TYR:CD1	2.55	0.41
3:M4:28:LEU:O	3:M4:32:VAL:HG23	2.20	0.41
2:R4:53:VAL:HG23	2:R4:89:ILE:HB	2.02	0.41
3:V4:12:GLN:O	3:V4:16:ARG:HG3	2.19	0.41
13:W4:201:CYC:HHD	13:W4:201:CYC:HAC2	1.65	0.41
4:Y4:234:ARG:HD2	4:Y4:263:GLN:NE2	2.35	0.41
2:B5:50:ASP:OD1	2:B5:50:ASP:N	2.53	0.41
3:C5:149:ILE:HD12	3:C5:149:ILE:HA	1.93	0.41
2:G5:33:ARG:HE	2:G5:33:ARG:HB3	1.74	0.41
2:I5:85:CYS:CA	13:I5:201:CYC:HHD	2.50	0.41
3:P5:80:MET:HG3	2:T5:119:ILE:HD12	2.02	0.41
3:Q5:25:LEU:HD13	2:T5:43:LYS:HB2	2.02	0.41
13:T5:202:CYC:HHD	13:T5:202:CYC:HAC2	1.78	0.41
5:Z5:4:THR:OG1	13:Z5:301:CYC:O1D	2.26	0.41
3:D6:92:ARG:HG2	2:I6:19:PHE:CZ	2.55	0.41
3:D6:136:LYS:HB2	3:D6:165:PHE:HB3	2.03	0.41
2:F6:28:ALA:HB2	3:a6:99:PHE:CE1	2.56	0.41
3:M6:112:ASN:OD1	3:M6:113:GLY:N	2.52	0.41
2:R6:121:LYS:NZ	2:S6:117:ASP:OD1	2.53	0.41
2:S6:50:ASP:OD1	2:S6:50:ASP:N	2.52	0.41
2:U6:85:CYS:HA	13:U6:201:CYC:HHD	2.02	0.41
4:Y6:224:VAL:HG22	4:Y6:270:ILE:HG12	2.01	0.41
3:a6:98:VAL:HG13	3:a6:157:ILE:HD11	2.02	0.41
3:C7:41:THR:OG1	13:C7:202:CYC:HBC1	2.20	0.41
3:M7:77:ASN:ND2	2:U7:116:LEU:HD13	2.36	0.41
3:O7:85:ARG:HD2	5:Z7:156:TYR:CD2	2.55	0.41
2:R7:27:VAL:HG22	2:W7:27:VAL:HG22	2.02	0.41
3:a7:118:TYR:HB3	3:a7:123:VAL:HB	2.02	0.41
1:A1:26:GLU:OE2	3:a1:2:THR:OG1	2.31	0.41
2:N1:115:GLY:O	2:N1:118:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:98:VAL:HG21	3:O1:161:LEU:HD13	2.02	0.41
3:O1:152:GLY:HA3	13:T1:201:CYC:HMD2	2.02	0.41
3:X1:124:PRO:O	3:X1:128:VAL:HG23	2.20	0.41
4:Y1:235:THR:HB	5:Z1:141:GLU:HA	2.01	0.41
5:Z1:9:ARG:HA	5:Z1:206:SER:HB3	2.02	0.41
7:12:106:GLU:H	7:12:106:GLU:HG2	1.70	0.41
8:B2:71:ASN:C	8:B2:77:ARG:HD3	2.45	0.41
8:C2:3:ASP:OD1	8:C2:6:THR:OG1	2.28	0.41
9:E2:114:GLU:OE1	9:E2:114:GLU:N	2.42	0.41
9:G2:12:ASP:HA	8:K2:90:ARG:HH12	1.85	0.41
9:J2:105:GLU:O	9:J2:110:VAL:HG22	2.20	0.41
10:N2:602:LEU:HD23	10:N2:602:LEU:HA	1.94	0.41
9:R2:14:GLU:H	9:R2:14:GLU:HG2	1.74	0.41
8:X2:96:MET:HA	8:X2:152:TYR:CE2	2.55	0.41
9:h2:77:MET:HE1	13:h2:201:CYC:CGD	2.51	0.41
9:j2:92:VAL:HG11	9:j2:153:PHE:CZ	2.54	0.41
9:k2:109:ILE:O	9:k2:112:VAL:HG12	2.20	0.41
8:n2:18:TYR:CZ	10:o2:167:ARG:HG3	2.55	0.41
8:n2:37:ARG:HD2	8:n2:96:MET:O	2.20	0.41
9:r2:101:ILE:HB	9:r2:155:TYR:CE2	2.55	0.41
8:u2:124:GLY:O	8:u2:128:GLN:HG2	2.20	0.41
3:C3:124:PRO:O	3:C3:128:VAL:HG23	2.19	0.41
2:N3:95:ILE:HG22	2:N3:108:ILE:HG12	2.01	0.41
3:P3:70:PRO:HA	3:P3:75:TYR:CD1	2.55	0.41
2:R3:50:ASP:N	2:R3:50:ASP:OD1	2.53	0.41
2:S3:99:ALA:HB2	2:S3:108:ILE:HG13	2.02	0.41
3:C4:18:GLU:O	2:G4:98:TYR:OH	2.33	0.41
2:F4:27:VAL:HG13	2:K4:27:VAL:HG22	2.01	0.41
2:K4:31:ARG:NH2	2:K4:101:VAL:O	2.53	0.41
2:R4:26:GLN:NE2	2:W4:103:GLY:O	2.54	0.41
2:W4:112:LEU:HD12	13:W4:201:CYC:HAB1	2.02	0.41
3:L5:114:LEU:HD23	3:L5:114:LEU:HA	1.90	0.41
13:L5:201:CYC:OB	5:Z5:254:ARG:O	2.37	0.41
13:M5:201:CYC:NC	13:M5:201:CYC:HMD1	2.35	0.41
3:Q5:105:ILE:HD12	3:Q5:109:ARG:HG3	2.02	0.41
3:a5:41:THR:HG23	3:a5:143:VAL:HG21	2.01	0.41
2:B6:95:ILE:HG22	2:B6:108:ILE:HG12	2.02	0.41
2:I6:133:ALA:O	2:I6:137:ILE:HG12	2.21	0.41
2:N6:100:LEU:HA	2:N6:154:TYR:HE2	1.85	0.41
3:P6:146:ARG:HB3	3:P6:151:GLN:OE1	2.20	0.41
3:V6:152:GLY:HA3	13:V6:202:CYC:HMD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W6:85:CYS:HA	13:W6:201:CYC:HHD	2.03	0.41
5:Z6:142:THR:HG21	5:Z6:152:ARG:HD2	2.03	0.41
2:B7:85:CYS:HA	13:B7:201:CYC:HAC1	1.94	0.41
3:J7:83:CYS:HA	13:J7:201:CYC:HAC1	1.47	0.41
3:L7:28:LEU:O	3:L7:32:VAL:HG23	2.20	0.41
2:N7:28:ALA:HB2	3:V7:99:PHE:CE1	2.55	0.41
3:O7:37:LYS:HB3	3:O7:154:CYS:SG	2.60	0.41
2:U7:115:GLY:O	2:U7:119:ILE:HG12	2.20	0.41
2:N1:99:ALA:HB2	2:N1:108:ILE:HG13	2.02	0.41
3:O1:110:CYS:HA	13:Z1:301:CYC:HAB2	2.02	0.41
3:O1:149:ILE:HG21	13:T1:201:CYC:HMC3	2.03	0.41
3:O1:154:CYS:SG	13:T1:201:CYC:HAC1	2.60	0.41
2:T1:133:ALA:O	2:T1:137:ILE:HG12	2.20	0.41
2:W1:12:ALA:O	2:W1:16:GLN:HG2	2.21	0.41
1:32:192:PRO:HB2	1:42:233:LEU:O	2.20	0.41
8:A2:104:LEU:HD22	8:A2:156:ILE:HD11	2.02	0.41
8:F2:28:LYS:HE3	8:F2:28:LYS:HB2	1.84	0.41
9:G2:20:PRO:O	9:G2:24:GLU:HG2	2.20	0.41
9:G2:82:LEU:HD13	9:G2:82:LEU:HA	1.86	0.41
8:L2:100:THR:HG22	8:L2:151:TYR:HD1	1.85	0.41
10:N2:146:ASN:OD1	10:N2:149:ARG:HG2	2.20	0.41
10:N2:522:ALA:N	10:N2:541:THR:OG1	2.53	0.41
9:Q2:47:ARG:HD2	8:X2:18:TYR:CE1	2.54	0.41
9:R2:83:ARG:NH2	13:R2:201:CYC:O1A	2.53	0.41
9:W2:124:GLU:H	9:W2:124:GLU:CD	2.28	0.41
8:a2:51:ILE:HG23	8:a2:136:VAL:HG13	2.03	0.41
8:c2:33:SER:OG	8:c2:37:ARG:NH2	2.54	0.41
9:f2:64:ASP:OD1	9:f2:64:ASP:N	2.53	0.41
9:i2:37:LEU:HD13	9:i2:37:LEU:HA	1.95	0.41
8:l2:121:VAL:HG22	13:l2:201:CYC:HC	1.85	0.41
8:m2:87:TYR:OH	10:o2:499:GLN:N	2.53	0.41
8:y2:56:VAL:HG12	8:y2:61:LEU:HG	2.02	0.41
2:B3:3:LYS:H	2:B3:106:GLY:HA3	1.85	0.41
3:D3:88:GLU:O	3:D3:92:ARG:HG3	2.20	0.41
2:F3:85:CYS:HA	13:F3:201:CYC:HHD	2.02	0.41
2:K3:7:THR:HG22	3:L3:1:MET:HB2	2.02	0.41
3:M3:20:LEU:HD22	2:R3:101:VAL:HG21	2.02	0.41
3:Q3:108:ASP:N	3:Q3:108:ASP:OD1	2.51	0.41
2:R3:126:ALA:HB3	2:R3:129:TRP:CE2	2.56	0.41
13:a3:202:CYC:HMA3	13:a3:202:CYC:HB	1.85	0.41
3:D4:84:LEU:HD13	2:H4:122:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G4:115:GLY:O	2:G4:119:ILE:HG12	2.20	0.41
2:H4:138:LYS:HB2	2:H4:155:ILE:HG21	2.02	0.41
3:O4:2:THR:HG21	3:O4:105:ILE:HA	2.02	0.41
2:S4:126:ALA:HB3	2:S4:129:TRP:CE2	2.56	0.41
5:Z4:70:ARG:HE	5:Z4:145:GLU:CD	2.28	0.41
5:Z4:214:SER:N	5:Z4:218:GLU:OE2	2.50	0.41
3:M5:98:VAL:HG13	3:M5:157:ILE:HD11	2.02	0.41
13:X5:201:CYC:HBB2	5:Z5:92:GLN:HB2	2.02	0.41
5:Z5:96:ILE:HG23	5:Z5:133:TYR:OH	2.20	0.41
3:a5:9:VAL:HG11	3:a5:28:LEU:HD21	2.02	0.41
1:A6:69:GLN:HB3	1:A6:74:GLN:HB2	2.02	0.41
1:A6:128:ALA:O	1:A6:132:GLN:HG2	2.20	0.41
2:B6:113:LEU:HD23	2:B6:113:LEU:HA	1.70	0.41
2:F6:3:LYS:HE3	2:K6:16:GLN:HE22	1.85	0.41
2:K6:126:ALA:HB3	2:K6:129:TRP:CE2	2.55	0.41
3:P6:44:ARG:O	3:P6:48:ASN:ND2	2.46	0.41
3:Q6:37:LYS:HB3	3:Q6:154:CYS:SG	2.61	0.41
3:a6:119:LEU:HD13	3:a6:119:LEU:HA	1.83	0.41
2:H7:115:GLY:O	2:H7:119:ILE:HG12	2.20	0.41
2:K7:3:LYS:HE2	2:K7:3:LYS:HB3	1.88	0.41
2:K7:16:GLN:OE1	2:K7:18:ARG:HD3	2.20	0.41
3:M7:112:ASN:OD1	3:M7:113:GLY:N	2.52	0.41
3:Q7:37:LYS:N	3:Q7:37:LYS:HE2	2.35	0.41
3:V7:79:ARG:O	13:V7:201:CYC:HMD2	2.21	0.41
13:Z7:301:CYC:HB	13:Z7:301:CYC:HMA2	1.85	0.41
5:Z1:2:ALA:N	5:Z1:155:GLU:OE1	2.54	0.41
1:32:237:ALA:HB2	9:r2:59:PHE:CD2	2.54	0.41
8:A2:126:THR:O	8:A2:130:ILE:HG12	2.20	0.41
8:B2:100:ASP:OD1	8:B2:101:THR:N	2.54	0.41
8:C2:91:TYR:HE2	13:C2:201:CYC:HBB1	1.85	0.41
9:J2:35:ARG:HH11	9:J2:35:ARG:HA	1.85	0.41
8:T2:73:TYR:HE2	9:W2:107:ILE:HD11	1.84	0.41
6:Z2:9:CYS:HB2	6:Z2:26:PHE:HD1	1.85	0.41
8:d2:109:LEU:HD11	8:d2:159:GLY:HA3	2.02	0.41
8:g2:65:ILE:HD11	13:g2:201:CYC:OC	2.21	0.41
9:k2:57:GLN:NE2	9:k2:132:GLU:OE1	2.53	0.41
10:o2:344:VAL:HG12	8:p2:107:ARG:C	2.45	0.41
13:p2:201:CYC:HC	13:p2:201:CYC:CMD	2.34	0.41
12:t2:57:LYS:HB3	12:t2:132:THR:CG2	2.50	0.41
8:y2:137:THR:O	8:y2:141:VAL:HG22	2.21	0.41
2:G3:27:VAL:HG22	2:H3:27:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J3:3:PHE:O	3:J3:104:SER:OG	2.39	0.41
3:J3:80:MET:HG3	2:K3:119:ILE:HD12	2.02	0.41
3:M3:77:ASN:ND2	2:U3:116:LEU:HD13	2.35	0.41
3:Q3:37:LYS:HE2	3:Q3:37:LYS:N	2.35	0.41
2:R3:56:ALA:HB3	2:R3:89:ILE:HG21	2.03	0.41
2:R3:56:ALA:O	2:R3:60:VAL:HG23	2.21	0.41
2:S3:116:LEU:HD21	2:S3:162:LEU:HD21	2.01	0.41
3:a3:28:LEU:O	3:a3:32:VAL:HG23	2.20	0.41
3:E4:37:LYS:H	3:E4:37:LYS:HG2	1.56	0.41
2:G4:74:ASN:HA	13:G4:201:CYC:HBD2	2.03	0.41
3:J4:149:ILE:HD13	13:J4:202:CYC:H3C	2.03	0.41
3:L4:146:ARG:HH21	3:L4:151:GLN:HB3	1.86	0.41
2:S4:109:ASP:HA	2:S4:113:LEU:HB2	2.02	0.41
2:U4:26:GLN:HA	2:U4:29:PHE:HB2	2.02	0.41
3:V4:168:ALA:O	3:V4:172:VAL:HG12	2.20	0.41
4:Y4:234:ARG:H	4:Y4:234:ARG:HE	1.67	0.41
5:Z4:32:VAL:HG11	5:Z4:63:VAL:HA	2.01	0.41
3:a4:79:ARG:HB3	13:a4:201:CYC:HMD1	2.03	0.41
3:a4:150:THR:HG21	13:a4:202:CYC:O2A	2.20	0.41
3:C5:20:LEU:HD22	2:G5:101:VAL:HG21	2.02	0.41
2:I5:123:PHE:HE2	3:a5:84:LEU:HD11	1.85	0.41
2:N5:27:VAL:HG22	2:U5:27:VAL:HG22	2.03	0.41
3:O5:1:MET:H2	2:S5:2:SER:N	2.18	0.41
2:S5:88:ASP:HB3	2:S5:130:TYR:HE1	1.85	0.41
2:W5:4:THR:HG22	2:W5:102:ALA:HB1	2.02	0.41
1:A6:104:VAL:HG11	1:A6:125:TRP:HB2	2.02	0.41
13:B6:201:CYC:HHH	13:B6:201:CYC:HAC1	1.65	0.41
3:J6:84:LEU:HD13	2:K6:122:THR:HG21	2.03	0.41
2:N6:91:TYR:O	2:N6:95:ILE:HG12	2.20	0.41
2:R6:42:ALA:HB1	2:R6:97:THR:HG23	2.01	0.41
2:B7:80:GLU:O	2:B7:84:LYS:HG2	2.21	0.41
3:E7:39:ILE:HG23	2:H7:25:LEU:HD22	2.01	0.41
2:F7:126:ALA:HB3	2:F7:129:TRP:CE2	2.56	0.41
2:I7:126:ALA:HB3	2:I7:129:TRP:CE2	2.55	0.41
3:Q7:95:THR:HG22	2:T7:20:LEU:HD12	2.03	0.41
3:Q7:124:PRO:O	3:Q7:128:VAL:HG23	2.20	0.41
2:S7:84:LYS:HE2	2:S7:84:LYS:HB2	1.90	0.41
2:W7:19:PHE:HZ	3:X7:88:GLU:HG2	1.86	0.41
3:a7:70:PRO:HA	3:a7:75:TYR:CD1	2.56	0.41
13:A1:302:CYC:HAC2	3:E1:83:CYS:HA	2.02	0.41
3:E1:41:THR:HG23	3:E1:143:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G1:50:ASP:OD1	2:G1:50:ASP:N	2.54	0.41
13:I1:201:CYC:HHD	13:I1:201:CYC:HAC1	1.58	0.41
3:Q1:114:LEU:HD11	3:Q1:118:TYR:CZ	2.55	0.41
2:S1:23:THR:HA	2:T1:5:PRO:HG3	2.03	0.41
2:U1:31:ARG:NH2	2:U1:101:VAL:O	2.53	0.41
5:Z1:179:ASP:OD1	5:Z1:179:ASP:N	2.53	0.41
6:O2:17:ARG:HG3	6:O2:21:GLU:HB3	2.02	0.41
8:A2:112:LEU:HD23	8:A2:160:LEU:HD21	2.02	0.41
9:I2:126:VAL:O	9:I2:130:VAL:HG23	2.21	0.41
9:J2:91:LEU:HD13	9:J2:91:LEU:HA	1.87	0.41
10:N2:676:VAL:CG1	8:O2:127:VAL:HG21	2.50	0.41
9:R2:51:VAL:HG12	9:R2:52:LYS:HE2	2.02	0.41
12:S2:102:GLU:HG3	12:S2:103:PRO:CD	2.48	0.41
7:b2:98:ASP:HA	7:b2:101:VAL:HG22	2.03	0.41
8:g2:61:LEU:HD22	13:h2:201:CYC:HAA1	2.02	0.41
9:h2:81:CYS:CA	13:h2:201:CYC:HHD	2.45	0.41
10:o2:343:PHE:HB3	10:o2:347:ARG:HB3	2.03	0.41
10:o2:359:ARG:NH2	10:o2:366:GLU:OE2	2.45	0.41
9:r2:2:SER:H	9:r2:5:SER:HG	1.68	0.41
12:t2:54:ALA:HA	12:t2:132:THR:HG22	2.03	0.41
8:y2:31:PHE:C	8:y2:33:SER:H	2.28	0.41
2:G3:143:LEU:C	2:G3:148:ARG:HB2	2.46	0.41
2:N3:3:LYS:H	2:N3:106:GLY:HA3	1.85	0.41
2:N3:23:THR:HG22	2:U3:5:PRO:HD3	2.03	0.41
3:O3:109:ARG:NH1	2:S3:14:ASP:OD2	2.53	0.41
3:Q3:85:ARG:NH2	13:Q3:201:CYC:O2A	2.43	0.41
3:Q3:118:TYR:HE2	3:Q3:128:VAL:HG11	1.86	0.41
2:R3:109:ASP:HA	2:R3:113:LEU:HB2	2.03	0.41
2:S3:23:THR:HA	2:T3:5:PRO:HG3	2.03	0.41
2:S3:78:THR:OG1	2:S3:80:GLU:OE1	2.26	0.41
13:C4:202:CYC:HBC2	13:C4:202:CYC:H2C	1.72	0.41
13:C4:202:CYC:HBB3	2:G4:29:PHE:HE2	1.86	0.41
13:F4:202:CYC:H2C	3:L4:154:CYS:SG	2.60	0.41
2:N4:12:ALA:O	2:N4:16:GLN:HG2	2.20	0.41
2:N4:126:ALA:HB3	2:N4:129:TRP:CE2	2.56	0.41
2:T4:134:LEU:HB3	2:T4:155:ILE:HG23	2.02	0.41
2:U4:63:LYS:HD3	2:U4:132:GLU:HG3	2.01	0.41
2:U4:95:ILE:HG13	2:U4:112:LEU:HD13	2.02	0.41
2:F5:27:VAL:HG13	2:K5:27:VAL:HG22	2.01	0.41
2:F5:91:TYR:O	2:F5:95:ILE:HG12	2.20	0.41
3:L5:83:CYS:SG	13:L5:201:CYC:HAC2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M5:37:LYS:O	3:M5:41:THR:HG23	2.20	0.41
3:O5:111:LEU:HG	3:O5:171:ALA:HB3	2.01	0.41
3:O5:136:LYS:HB2	3:O5:165:PHE:HB3	2.03	0.41
3:P5:41:THR:O	3:P5:45:ILE:HG12	2.19	0.41
2:G6:115:GLY:O	2:G6:118:GLU:HG2	2.21	0.41
13:Q6:202:CYC:HMA1	2:T6:29:PHE:CZ	2.55	0.41
13:T6:201:CYC:HMA3	13:T6:201:CYC:HB	1.85	0.41
2:W6:56:ALA:HB3	2:W6:89:ILE:HG21	2.03	0.41
2:F7:136:TYR:O	2:F7:140:ASN:ND2	2.38	0.41
2:F7:138:LYS:HB2	2:F7:155:ILE:HG21	2.01	0.41
3:J7:114:LEU:HD11	3:J7:118:TYR:CZ	2.55	0.41
3:M7:78:ARG:HB2	2:U7:114:ALA:HB3	2.03	0.41
3:O7:128:VAL:HG22	13:Z7:301:CYC:HBC3	2.02	0.41
2:S7:134:LEU:HB3	2:S7:155:ILE:HG23	2.03	0.41
4:Y7:228:GLN:OE1	4:Y7:266:ARG:NE	2.41	0.41
1:A1:38:SER:HB2	1:A1:39:PRO:HD2	2.02	0.41
3:M1:58:ARG:HE	13:U1:201:CYC:CGD	2.34	0.41
2:R1:115:GLY:O	2:R1:119:ILE:HG12	2.21	0.41
2:S1:116:LEU:HD21	2:S1:162:LEU:HD21	2.02	0.41
2:U1:95:ILE:HG13	2:U1:112:LEU:HD13	2.03	0.41
3:V1:106:LEU:HD12	3:V1:110:CYS:HB3	2.03	0.41
3:V1:168:ALA:O	3:V1:172:VAL:HG12	2.21	0.41
5:Z1:240:VAL:HG12	5:Z1:284:VAL:HG13	2.03	0.41
1:22:247:TYR:OH	8:V2:64:ASP:OD1	2.36	0.41
1:42:22:VAL:HG21	2:F4:113:LEU:HG	2.02	0.41
1:42:128:ALA:O	1:42:132:GLN:HG2	2.20	0.41
1:52:36:GLN:OE1	3:L5:112:ASN:ND2	2.54	0.41
8:A2:27:LEU:HD12	9:H2:37:LEU:HD21	2.01	0.41
9:D2:134:LYS:HB2	9:D2:153:PHE:HB3	2.02	0.41
9:H2:81:CYS:SG	13:H2:201:CYC:H2C	2.60	0.41
8:M2:137:THR:O	8:M2:141:VAL:HG22	2.21	0.41
11:P2:8:LEU:HD23	11:P2:27:LEU:HG	2.01	0.41
11:P2:87:ASP:OD1	9:U2:17:TYR:OH	2.32	0.41
9:Q2:114:GLU:OE1	9:Q2:114:GLU:N	2.48	0.41
8:c2:78:TYR:CD2	9:j2:115:MET:HG3	2.55	0.41
8:d2:27:LEU:HB2	9:j2:37:LEU:HD21	2.02	0.41
13:i2:201:CYC:H2C	13:i2:201:CYC:HBC2	1.85	0.41
9:k2:61:LYS:HE3	9:k2:61:LYS:HB3	1.89	0.41
9:k2:104:ILE:O	9:k2:109:ILE:HG12	2.21	0.41
8:n2:1:MET:HG2	10:o2:26:VAL:HG23	2.02	0.41
13:n2:201:CYC:HHD	13:n2:201:CYC:HAC2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:o2:146:ASN:OD1	10:o2:149:ARG:HG2	2.20	0.41
9:x2:80:THR:HG22	9:x2:83:ARG:HH21	1.85	0.41
8:y2:96:MET:HA	8:y2:152:TYR:CE2	2.56	0.41
2:G3:31:ARG:HD2	2:H3:26:GLN:OE1	2.21	0.41
3:J3:28:LEU:O	3:J3:32:VAL:HG23	2.20	0.41
2:R3:3:LYS:HG3	2:W3:18:ARG:HH12	1.86	0.41
13:Z3:301:CYC:HB	13:Z3:301:CYC:HMA3	1.84	0.41
2:B4:143:LEU:C	2:B4:148:ARG:HB2	2.46	0.41
2:G4:5:PRO:HA	2:H4:23:THR:HG23	2.02	0.41
2:I4:117:ASP:OD1	2:I4:117:ASP:N	2.51	0.41
2:T4:109:ASP:HA	2:T4:113:LEU:HB2	2.03	0.41
3:D5:44:ARG:NH1	3:D5:142:ILE:O	2.53	0.41
2:F5:127:PRO:HB3	2:F5:162:LEU:HD22	2.02	0.41
2:G5:23:THR:OG1	2:H5:3:LYS:O	2.26	0.41
2:N5:91:TYR:O	2:N5:95:ILE:HG12	2.21	0.41
3:O5:107:ASP:HA	3:O5:111:LEU:HB2	2.02	0.41
2:S5:31:ARG:NH2	2:S5:101:VAL:O	2.54	0.41
2:B6:20:LEU:HD12	3:J6:95:THR:HG22	2.03	0.41
2:B6:66:TYR:O	2:B6:70:THR:OG1	2.32	0.41
2:F6:21:SER:N	2:F6:24:GLU:OE1	2.53	0.41
3:P6:107:ASP:OD1	3:P6:167:LYS:HD3	2.20	0.41
13:E7:201:CYC:HAA1	13:E7:201:CYC:HBD1	2.03	0.41
2:G7:113:LEU:HD22	2:G7:113:LEU:HA	1.90	0.41
3:J7:149:ILE:HD13	13:J7:202:CYC:H3C	2.01	0.41
3:O7:136:LYS:HB2	3:O7:165:PHE:CG	2.55	0.41
3:Q7:78:ARG:HB2	2:R7:114:ALA:HB3	2.03	0.41
2:T7:144:SER:HA	2:T7:148:ARG:HD3	2.02	0.41
5:Z7:154:ILE:O	13:Z7:301:CYC:HBA2	2.21	0.41
3:L1:6:PHE:HD1	3:L1:28:LEU:HD13	1.85	0.41
2:N1:26:GLN:HG2	2:U1:34:GLN:HG3	2.03	0.41
3:P1:95:THR:HG22	2:U1:20:LEU:HD12	2.03	0.41
3:Q1:93:TYR:OH	2:T1:14:ASP:OD1	2.26	0.41
2:R1:126:ALA:HB3	2:R1:129:TRP:CE2	2.55	0.41
3:V1:79:ARG:O	13:V1:201:CYC:HMD2	2.21	0.41
5:Z1:96:ILE:HG23	5:Z1:133:TYR:OH	2.20	0.41
6:02:44:GLN:HB2	8:a2:106:GLU:O	2.20	0.41
7:12:99:PRO:O	7:12:103:ILE:HG13	2.21	0.41
13:22:302:CYC:HBC3	3:E7:128:VAL:HG13	2.02	0.41
1:42:129:VAL:HG22	1:42:137:PHE:CG	2.56	0.41
9:E2:113:ARG:HH22	9:E2:161:SER:C	2.28	0.41
9:E2:152:TYR:O	9:E2:156:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I2:50:ILE:HG22	9:I2:133:LEU:HD12	2.02	0.41
9:J2:85:LEU:HB3	9:J2:133:LEU:HD11	2.03	0.41
8:L2:71:MET:HE2	8:L2:77:TYR:CE2	2.56	0.41
8:L2:95:MET:HA	8:L2:151:TYR:CE2	2.56	0.41
12:S2:85:TYR:HE1	12:S2:133:LEU:HB2	1.86	0.41
9:U2:104:ILE:HG21	9:U2:156:VAL:HG22	2.02	0.41
6:Z2:17:ARG:HH11	6:Z2:21:GLU:HG3	1.85	0.41
8:a2:126:THR:O	8:a2:130:ILE:HG12	2.21	0.41
13:f2:201:CYC:HMA3	13:f2:201:CYC:NB	2.33	0.41
8:g2:15:GLN:H	8:g2:15:GLN:HG2	1.70	0.41
8:m2:101:THR:HG22	8:m2:152:TYR:HD1	1.86	0.41
8:p2:28:LYS:O	8:p2:32:GLN:HG2	2.20	0.41
11:q2:47:ASN:HB2	11:q2:141:LEU:HD21	2.03	0.41
13:r2:201:CYC:HAD2	8:w2:62:TYR:OH	2.21	0.41
12:t2:37:LEU:HD23	12:t2:97:LEU:HD22	2.03	0.41
8:u2:78:TYR:CD1	9:x2:115:MET:HG2	2.55	0.41
6:z2:39:GLU:OE2	6:z2:42:ARG:NH2	2.33	0.41
2:B3:94:ARG:HG2	2:B3:98:TYR:CZ	2.55	0.41
2:R3:5:PRO:HD2	2:R3:31:ARG:HD3	2.02	0.41
3:V3:12:GLN:O	3:V3:16:ARG:HG3	2.21	0.41
3:J4:73:ASN:OD1	13:J4:201:CYC:NC	2.52	0.41
2:N4:26:GLN:NE2	2:U4:103:GLY:O	2.39	0.41
2:N4:143:LEU:C	2:N4:148:ARG:HB2	2.46	0.41
3:O4:149:ILE:HG21	13:T4:201:CYC:HMC3	2.03	0.41
2:F5:28:ALA:HB2	3:a5:99:PHE:CE1	2.55	0.41
2:K5:10:VAL:HG21	3:L5:100:THR:HG23	2.03	0.41
2:K5:56:ALA:HB3	2:K5:89:ILE:HG21	2.02	0.41
3:L5:128:VAL:HG22	13:L5:201:CYC:H3C	2.02	0.41
3:M5:5:ALA:HB2	3:M5:101:GLY:HA3	2.03	0.41
3:M5:72:GLY:O	3:M5:79:ARG:NH2	2.46	0.41
3:P5:89:ILE:HD13	13:P5:202:CYC:HBB3	2.02	0.41
13:W5:201:CYC:HAC2	13:W5:201:CYC:HHD	1.61	0.41
5:Z5:64:ASN:OD1	5:Z5:66:SER:OG	2.35	0.41
3:a5:89:ILE:HG12	3:a5:92:ARG:HH21	1.85	0.41
2:F6:5:PRO:HA	2:K6:23:THR:HG23	2.02	0.41
3:P6:37:LYS:HE2	3:P6:154:CYS:HB3	2.02	0.41
2:R6:4:THR:HG23	2:R6:7:THR:HB	2.01	0.41
4:Y6:235:THR:HB	5:Z6:141:GLU:HA	2.02	0.41
2:G7:3:LYS:NZ	2:H7:16:GLN:OE1	2.33	0.41
2:K7:80:GLU:OE1	2:K7:80:GLU:N	2.39	0.41
3:M7:115:ARG:CZ	3:M7:173:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N7:115:GLY:O	2:N7:119:ILE:HG12	2.21	0.41
2:R7:163:SER:OXT	2:S7:121:LYS:NZ	2.49	0.41
2:S7:85:CYS:HA	13:S7:201:CYC:HHD	2.02	0.41
1:A1:26:GLU:HB3	1:A1:163:VAL:HG21	2.02	0.41
2:B1:28:ALA:HB2	3:J1:99:PHE:CE1	2.55	0.41
3:E1:40:ASP:HB3	13:E1:201:CYC:HBC3	2.03	0.41
13:F1:202:CYC:HHD	13:F1:202:CYC:HAC1	1.60	0.41
2:G1:23:THR:OG1	2:H1:3:LYS:O	2.32	0.41
2:I1:31:ARG:CZ	2:I1:35:ALA:HB2	2.50	0.41
3:L1:41:THR:HG23	3:L1:143:VAL:HG21	2.03	0.41
3:L1:74:ALA:HB2	13:L1:201:CYC:OC	2.19	0.41
2:N1:116:LEU:HD21	2:N1:162:LEU:HD21	2.02	0.41
3:P1:44:ARG:HH21	3:P1:149:ILE:HB	1.86	0.41
3:Q1:89:ILE:HD13	13:Q1:201:CYC:HBB3	2.03	0.41
2:S1:50:ASP:OD1	2:S1:50:ASP:N	2.53	0.41
3:V1:58:ARG:NE	13:W1:201:CYC:O2D	2.38	0.41
3:V1:98:VAL:HG21	3:V1:161:LEU:HD13	2.03	0.41
2:W1:64:PHE:HB3	2:W1:66:TYR:CE1	2.55	0.41
3:X1:98:VAL:HG13	3:X1:157:ILE:HD11	2.03	0.41
4:Y1:235:THR:HB	5:Z1:141:GLU:O	2.21	0.41
5:Z1:70:ARG:HE	5:Z1:145:GLU:CD	2.29	0.41
1:22:103:PHE:HZ	1:22:134:TYR:HE2	1.68	0.41
1:42:75:ILE:HB	1:42:79:ASP:HB2	2.03	0.41
1:52:40:VAL:HB	2:K5:110:GLU:HG3	2.03	0.41
8:C2:62:TYR:H	13:H2:201:CYC:HBA2	1.86	0.41
9:H2:62:ARG:HG3	9:H2:64:ASP:OD1	2.21	0.41
8:L2:78:ALA:O	8:L2:82:ARG:HG3	2.21	0.41
10:N2:183:VAL:HG11	10:N2:266:ALA:HB2	2.03	0.41
10:N2:310:ASP:OD2	10:N2:310:ASP:N	2.51	0.41
10:N2:321:SER:OG	10:N2:398:GLU:OE2	2.31	0.41
8:O2:96:MET:HE2	8:O2:96:MET:HB3	1.98	0.41
6:Y2:6:ILE:O	6:Y2:28:THR:HA	2.21	0.41
7:b2:97:LEU:O	7:b2:101:VAL:HG13	2.21	0.41
8:d2:73:TYR:OH	9:i2:90:ARG:NH1	2.53	0.41
9:f2:115:MET:HG3	8:l2:78:TYR:CD1	2.56	0.41
9:j2:126:VAL:O	9:j2:130:VAL:HG23	2.21	0.41
9:k2:62:ARG:O	9:k2:65:VAL:HG22	2.21	0.41
9:k2:64:ASP:OD1	9:k2:64:ASP:N	2.52	0.41
8:p2:76:ARG:NH1	13:p2:201:CYC:O2D	2.42	0.41
9:r2:36:ARG:HA	9:r2:39:ILE:HD12	2.02	0.41
9:r2:64:ASP:OD1	9:r2:64:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t2:12:ASP:OD2	8:u2:107:ARG:NH1	2.48	0.41
9:v2:64:ASP:OD1	9:v2:64:ASP:N	2.54	0.41
2:F3:101:VAL:HG21	3:a3:20:LEU:HD13	2.03	0.41
2:K3:16:GLN:OE1	2:K3:18:ARG:HD3	2.21	0.41
3:L3:124:PRO:O	3:L3:128:VAL:HG23	2.21	0.41
3:M3:78:ARG:HB2	2:U3:114:ALA:HB3	2.03	0.41
2:N3:1:MET:O	5:Z3:17:ASN:ND2	2.54	0.41
2:N3:13:ALA:HA	2:N3:16:GLN:HE21	1.86	0.41
2:N3:127:PRO:HB3	2:N3:162:LEU:HD22	2.03	0.41
3:P3:41:THR:O	3:P3:45:ILE:HG12	2.21	0.41
2:R3:87:ARG:NH2	13:R3:201:CYC:O2A	2.53	0.41
2:S3:22:SER:HA	2:S3:25:LEU:HG	2.03	0.41
13:S3:201:CYC:HAC1	13:S3:201:CYC:HHD	1.55	0.41
2:U3:85:CYS:O	2:U3:89:ILE:HG12	2.21	0.41
2:U3:156:ASP:HB3	3:V3:47:GLY:HA2	2.03	0.41
3:V3:30:ARG:O	3:V3:34:GLU:HG2	2.20	0.41
3:X3:136:LYS:HB2	3:X3:165:PHE:CG	2.55	0.41
4:Y3:228:GLN:OE1	4:Y3:266:ARG:NE	2.42	0.41
5:Z3:101:LYS:HE2	5:Z3:172:TYR:HB2	2.03	0.41
3:a3:116:GLU:OE1	3:a3:116:GLU:N	2.46	0.41
2:B4:80:GLU:O	2:B4:84:LYS:HG2	2.21	0.41
3:D4:99:PHE:CZ	2:I4:28:ALA:HB2	2.56	0.41
2:F4:91:TYR:O	2:F4:95:ILE:HG12	2.20	0.41
2:F4:103:GLY:O	2:K4:26:GLN:NE2	2.54	0.41
2:F4:126:ALA:HB3	2:F4:129:TRP:CE2	2.56	0.41
2:G4:27:VAL:HG22	2:H4:27:VAL:HG22	2.03	0.41
3:J4:109:ARG:HD3	5:Z4:228:THR:OG1	2.20	0.41
2:K4:45:LEU:HD21	2:K4:141:HIS:HB2	2.03	0.41
2:K4:150:GLU:HG2	2:K4:154:TYR:CE2	2.56	0.41
3:M4:18:GLU:O	2:R4:98:TYR:OH	2.37	0.41
3:M4:78:ARG:HD2	5:Z4:29:ARG:HH21	1.86	0.41
3:O4:136:LYS:HB2	3:O4:165:PHE:HB3	2.03	0.41
3:P4:27:ALA:HA	3:P4:30:ARG:HE	1.85	0.41
3:P4:100:THR:HG23	2:U4:10:VAL:HG21	2.02	0.41
3:Q4:59:ALA:HB3	3:Q4:134:LYS:HD3	2.02	0.41
13:Q4:202:CYC:HMA1	2:T4:29:PHE:CZ	2.56	0.41
2:R4:87:ARG:NH2	13:R4:201:CYC:O2A	2.54	0.41
2:S4:22:SER:HA	2:S4:25:LEU:HG	2.01	0.41
2:U4:91:TYR:O	2:U4:95:ILE:HG12	2.21	0.41
2:W4:3:LYS:HD3	2:W4:3:LYS:HA	1.78	0.41
5:Z4:143:PHE:CE1	5:Z4:149:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a4:114:LEU:HD12	3:a4:114:LEU:HA	1.88	0.41
3:C5:124:PRO:O	3:C5:128:VAL:HG23	2.20	0.41
3:D5:111:LEU:HD22	3:D5:171:ALA:HB3	2.03	0.41
3:L5:25:LEU:HD13	3:L5:25:LEU:HA	1.88	0.41
3:M5:78:ARG:HB2	2:U5:114:ALA:HB3	2.02	0.41
3:M5:114:LEU:HD13	13:M5:201:CYC:HMB1	2.03	0.41
3:O5:34:GLU:HG3	3:O5:37:LYS:HD2	2.02	0.41
13:Q5:201:CYC:HHD	13:Q5:201:CYC:HAC1	1.74	0.41
2:R5:26:GLN:NE2	2:W5:103:GLY:O	2.53	0.41
2:R5:74:ASN:OD1	2:R5:74:ASN:N	2.53	0.41
5:Z5:67:ILE:HB	5:Z5:71:ASP:HB2	2.03	0.41
1:A6:159:GLN:OE1	1:A6:173:PRO:HA	2.21	0.41
3:J6:16:ARG:NH1	3:O6:63:GLU:OE2	2.49	0.41
3:M6:115:ARG:NH2	3:M6:170:ALA:O	2.54	0.41
3:O6:1:MET:SD	3:O6:1:MET:N	2.81	0.41
3:O6:118:TYR:HE2	3:O6:128:VAL:HG11	1.85	0.41
3:P6:28:LEU:O	3:P6:32:VAL:HG23	2.21	0.41
3:Q6:73:ASN:OD1	13:Q6:201:CYC:NC	2.53	0.41
3:Q6:89:ILE:HD13	13:Q6:201:CYC:HBB3	2.02	0.41
2:R6:56:ALA:HB3	2:R6:89:ILE:HG21	2.03	0.41
2:U6:5:PRO:O	2:U6:8:GLU:HG3	2.21	0.41
2:W6:134:LEU:HB3	2:W6:155:ILE:HG23	2.02	0.41
5:Z6:36:ILE:HD13	5:Z6:59:GLU:HG2	2.02	0.41
5:Z6:267:LEU:HD12	5:Z6:267:LEU:HA	1.84	0.41
2:B7:3:LYS:HA	2:B7:3:LYS:HD3	1.90	0.41
3:C7:107:ASP:HA	3:C7:111:LEU:HB2	2.01	0.41
3:D7:152:GLY:O	13:D7:201:CYC:OC	2.39	0.41
2:G7:27:VAL:HG22	2:H7:27:VAL:HG22	2.03	0.41
3:J7:75:TYR:HB3	3:J7:79:ARG:NH2	2.35	0.41
3:L7:106:LEU:HD12	3:L7:110:CYS:HB3	2.03	0.41
2:S7:67:THR:HG21	13:S7:201:CYC:HMC2	2.01	0.41
2:W7:131:VAL:HG12	2:W7:135:LYS:HE2	2.02	0.41
3:a7:39:ILE:HG22	13:a7:202:CYC:HMB1	2.03	0.41
3:a7:115:ARG:NH1	3:a7:173:ALA:O	2.54	0.41
2:B1:23:THR:O	2:B1:27:VAL:HG23	2.21	0.41
2:B1:74:ASN:HA	13:B1:201:CYC:HBD2	2.03	0.41
2:I1:64:PHE:HB3	2:I1:66:TYR:CE2	2.55	0.41
3:M1:98:VAL:HG21	3:M1:161:LEU:HD13	2.03	0.41
2:R1:66:TYR:HA	2:R1:69:SER:HG	1.86	0.41
2:T1:41:ALA:HB2	2:T1:147:SER:HB3	2.02	0.41
2:T1:115:GLY:O	2:T1:119:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V1:5:ALA:HB2	3:V1:101:GLY:HA3	2.02	0.41
6:O2:22:LEU:N	13:d2:201:CYC:OB	2.54	0.41
1:52:38:SER:OG	1:52:41:GLN:HG3	2.21	0.41
13:A2:202:CYC:HHD	9:J2:81:CYS:HA	2.03	0.41
9:E2:92:VAL:HG11	9:E2:153:PHE:CE2	2.56	0.41
9:G2:1:MET:N	9:G2:103:PRO:HG3	2.36	0.41
9:G2:109:ILE:HD13	9:G2:109:ILE:HA	1.90	0.41
9:H2:83:ARG:HH22	13:H2:201:CYC:C3A	2.33	0.41
10:N2:300:ILE:HD13	10:N2:300:ILE:HA	1.93	0.41
10:N2:312:GLU:O	10:N2:315:VAL:HG12	2.21	0.41
10:N2:546:GLN:NE2	10:N2:575:GLU:OE2	2.54	0.41
11:P2:8:LEU:HD21	11:P2:23:ALA:HA	2.03	0.41
8:T2:131:GLN:O	8:T2:135:GLU:HG2	2.21	0.41
9:f2:92:VAL:HG11	9:f2:153:PHE:CE2	2.56	0.41
9:j2:106:GLU:OE2	10:o2:540:GLN:HA	2.21	0.41
9:k2:57:GLN:O	9:k2:61:LYS:HG2	2.21	0.41
2:B3:43:LYS:HB2	3:J3:25:LEU:HD13	2.03	0.41
2:H3:112:LEU:HD12	13:H3:201:CYC:HAB1	2.03	0.41
3:J3:146:ARG:NE	3:J3:151:GLN:OE1	2.51	0.41
2:N3:26:GLN:NE2	2:U3:103:GLY:O	2.54	0.41
3:O3:102:ASP:OD1	3:O3:103:ALA:N	2.53	0.41
3:P3:107:ASP:O	3:P3:112:ASN:N	2.54	0.41
3:Q3:105:ILE:O	3:Q3:109:ARG:HB2	2.20	0.41
2:R3:84:LYS:NZ	13:R3:201:CYC:O1A	2.43	0.41
2:R3:134:LEU:HB3	2:R3:155:ILE:HG23	2.03	0.41
3:X3:89:ILE:HG21	13:X3:201:CYC:HAB1	2.03	0.41
3:C4:86:ASP:OD2	3:C4:118:TYR:OH	2.21	0.41
2:I4:74:ASN:OD1	2:I4:74:ASN:N	2.54	0.41
2:S4:85:CYS:HA	13:S4:201:CYC:HHD	2.03	0.41
13:S4:201:CYC:HAC1	13:S4:201:CYC:HHD	1.59	0.41
5:Z4:40:TYR:HA	5:Z4:44:LEU:HD23	2.02	0.41
3:J5:77:ASN:HD21	2:K5:116:LEU:HD13	1.85	0.41
3:Q5:114:LEU:HD11	3:Q5:118:TYR:CZ	2.56	0.41
2:T5:84:LYS:HE3	2:T5:87:ARG:NH2	2.36	0.41
3:X5:28:LEU:O	3:X5:32:VAL:HG23	2.21	0.41
1:A6:3:LEU:HD22	3:D6:78:ARG:HG2	2.03	0.41
2:G6:91:TYR:O	2:G6:95:ILE:HG12	2.20	0.41
2:G6:134:LEU:HB3	2:G6:155:ILE:HG23	2.01	0.41
2:H6:9:ALA:HB1	2:H6:24:GLU:HG3	2.03	0.41
2:I6:109:ASP:HA	2:I6:113:LEU:HB2	2.02	0.41
3:L6:38:ARG:HH12	3:L6:160:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U6:141:HIS:CE1	2:U6:143:LEU:HB2	2.56	0.41
2:G7:143:LEU:C	2:G7:148:ARG:HB2	2.46	0.41
2:I7:143:LEU:C	2:I7:148:ARG:HB2	2.46	0.41
2:K7:66:TYR:O	2:K7:70:THR:OG1	2.31	0.41
2:S7:141:HIS:NE2	2:S7:152:ASN:OD1	2.53	0.41
5:Z7:255:ARG:HH21	5:Z7:258:ARG:HH11	1.69	0.41
1:A1:118:GLY:HA2	10:N2:705:ARG:NE	2.36	0.40
3:D1:84:LEU:HD13	2:H1:122:THR:HG21	2.03	0.40
2:H1:3:LYS:HD2	2:H1:8:GLU:OE2	2.20	0.40
2:H1:95:ILE:HG21	2:H1:112:LEU:HB2	2.03	0.40
3:M1:73:ASN:OD1	13:M1:201:CYC:NC	2.52	0.40
3:Q1:113:GLY:HA2	3:Q1:116:GLU:HG2	2.01	0.40
1:32:74:GLN:HA	5:Z3:261:LEU:HD12	2.03	0.40
9:D2:92:VAL:HG11	9:D2:153:PHE:CZ	2.56	0.40
9:D2:101:ILE:HD12	9:D2:155:TYR:CE1	2.56	0.40
8:F2:107:ARG:HB3	10:N2:463:GLN:HE21	1.86	0.40
9:H2:49:ARG:HH22	8:u2:140:LEU:HA	1.86	0.40
9:H2:91:LEU:HB3	9:H2:104:ILE:HD12	2.02	0.40
9:I2:101:ILE:HD12	9:I2:155:TYR:CE1	2.57	0.40
8:L2:159:LEU:HD23	8:L2:159:LEU:HA	1.93	0.40
13:L2:201:CYC:HHD	13:L2:201:CYC:HAC2	1.72	0.40
10:N2:484:LYS:HE2	11:P2:169:ILE:HD12	2.02	0.40
9:Q2:36:ARG:HA	9:Q2:39:ILE:HD12	2.02	0.40
9:Q2:90:ARG:O	9:Q2:93:THR:OG1	2.28	0.40
12:S2:57:LYS:HB3	12:S2:132:THR:CG2	2.51	0.40
9:U2:103:PRO:HA	9:U2:106:GLU:HG2	2.03	0.40
8:c2:71:ASN:HB3	8:c2:72:MET:HE2	2.03	0.40
9:k2:35:ARG:HH11	9:k2:35:ARG:HA	1.86	0.40
9:k2:100:ASP:OD1	9:k2:101:ILE:N	2.54	0.40
10:o2:327:ARG:HB2	10:o2:387:VAL:HG11	2.02	0.40
8:p2:97:LEU:HD13	9:s2:18:LEU:HD22	2.03	0.40
12:t2:109:LEU:HD11	12:t2:159:GLY:HA3	2.03	0.40
8:u2:15:GLN:H	8:u2:15:GLN:HG2	1.59	0.40
9:x2:14:GLU:HG3	9:x2:16:ARG:HE	1.86	0.40
6:z2:6:ILE:O	6:z2:28:THR:HA	2.22	0.40
3:O3:73:ASN:OD1	13:Z3:301:CYC:NC	2.54	0.40
3:P3:28:LEU:O	3:P3:32:VAL:HG23	2.21	0.40
2:R3:23:THR:HG21	2:W3:8:GLU:HG3	2.04	0.40
3:V3:114:LEU:HD11	3:V3:118:TYR:CZ	2.56	0.40
3:C4:20:LEU:HD22	2:G4:101:VAL:HG21	2.03	0.40
3:D4:136:LYS:HB2	3:D4:165:PHE:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N4:27:VAL:HG22	2:U4:27:VAL:HG13	2.03	0.40
3:P4:98:VAL:HG13	3:P4:157:ILE:HD11	2.02	0.40
3:X4:136:LYS:HB2	3:X4:165:PHE:CG	2.55	0.40
3:E5:129:ALA:HB2	3:E5:173:ALA:HB2	2.03	0.40
2:N5:134:LEU:HB3	2:N5:155:ILE:HG23	2.03	0.40
2:R5:84:LYS:NZ	13:R5:201:CYC:O1A	2.47	0.40
2:U5:91:TYR:O	2:U5:95:ILE:HG12	2.21	0.40
2:F6:99:ALA:HB2	2:F6:108:ILE:HG12	2.02	0.40
2:H6:5:PRO:HD2	2:H6:31:ARG:HD3	2.03	0.40
3:L6:128:VAL:HG22	13:L6:201:CYC:H3C	2.03	0.40
3:M6:78:ARG:HH12	13:M6:201:CYC:CGD	2.31	0.40
3:M6:99:PHE:CE1	2:R6:28:ALA:HB2	2.56	0.40
13:M6:201:CYC:NC	13:M6:201:CYC:HMD1	2.35	0.40
2:S6:122:THR:HG21	3:X6:84:LEU:HD23	2.03	0.40
2:W6:126:ALA:HB3	2:W6:129:TRP:CE2	2.56	0.40
3:a6:114:LEU:HD12	3:a6:114:LEU:HA	1.87	0.40
3:E7:136:LYS:HB2	3:E7:165:PHE:CG	2.57	0.40
2:G7:23:THR:HG23	2:H7:5:PRO:HA	2.03	0.40
3:M7:72:GLY:O	3:M7:79:ARG:NH2	2.52	0.40
2:R7:23:THR:HG21	2:W7:8:GLU:HG3	2.02	0.40
2:H1:99:ALA:HB2	2:H1:108:ILE:HG12	2.03	0.40
2:I1:74:ASN:OD1	2:I1:74:ASN:N	2.50	0.40
2:I1:126:ALA:HB3	2:I1:129:TRP:CE2	2.56	0.40
2:N1:113:LEU:HD23	2:N1:113:LEU:HA	1.72	0.40
2:R1:56:ALA:HB3	2:R1:89:ILE:HG21	2.03	0.40
2:U1:150:GLU:HG2	2:U1:154:TYR:CE2	2.56	0.40
3:X1:12:GLN:O	3:X1:16:ARG:HG2	2.20	0.40
1:22:115:ASP:OD1	1:22:116:VAL:N	2.55	0.40
1:42:182:ASP:OD1	1:42:183:SER:N	2.49	0.40
8:B2:73:TYR:OH	8:C2:13:ASP:OD1	2.31	0.40
8:B2:109:LEU:HD22	8:B2:159:GLY:HA3	2.02	0.40
9:H2:92:VAL:HG11	9:H2:153:PHE:CE2	2.57	0.40
9:I2:142:THR:HA	9:I2:146:ALA:HB2	2.02	0.40
8:M2:60:LEU:O	8:M2:63:SER:OG	2.27	0.40
8:O2:134:LYS:HG3	8:O2:150:GLY:HA2	2.03	0.40
9:U2:37:LEU:HD23	9:U2:97:VAL:HG22	2.03	0.40
9:U2:134:LYS:NZ	9:U2:154:ASP:OD1	2.48	0.40
13:W2:201:CYC:HHD	13:W2:201:CYC:HAC2	1.74	0.40
8:X2:31:PHE:C	8:X2:33:SER:H	2.29	0.40
8:X2:101:THR:HG22	8:X2:152:TYR:HD1	1.86	0.40
8:c2:89:LEU:HD13	8:c2:89:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:f2:126:VAL:HG12	9:f2:160:LEU:HD13	2.03	0.40
9:h2:62:ARG:O	9:h2:65:VAL:HG22	2.21	0.40
13:t2:201:CYC:O2D	8:y2:62:TYR:OH	2.19	0.40
3:C3:116:GLU:OE1	3:C3:116:GLU:N	2.43	0.40
2:F3:126:ALA:HB3	2:F3:129:TRP:CE2	2.56	0.40
2:G3:50:ASP:N	2:G3:50:ASP:OD1	2.55	0.40
3:P3:93:TYR:CD2	3:P3:110:CYS:HB2	2.57	0.40
2:R3:9:ALA:HB2	2:R3:27:VAL:HG11	2.04	0.40
2:S3:18:ARG:NH1	2:T3:157:TYR:OH	2.51	0.40
2:U3:21:SER:OG	2:U3:22:SER:N	2.54	0.40
2:U3:63:LYS:CD	2:U3:132:GLU:HG3	2.51	0.40
2:U3:74:ASN:ND2	2:U3:124:ASP:OD2	2.54	0.40
2:W4:25:LEU:HD22	3:X4:39:ILE:HG23	2.03	0.40
3:a4:106:LEU:O	3:a4:110:CYS:HB3	2.21	0.40
2:I5:95:ILE:HD12	2:I5:111:TYR:CD2	2.56	0.40
3:P5:74:ALA:HA	3:P5:79:ARG:HB3	2.02	0.40
2:R5:91:TYR:O	2:R5:95:ILE:HG12	2.22	0.40
3:V5:106:LEU:HD12	3:V5:110:CYS:HB3	2.04	0.40
3:a5:38:ARG:HH12	3:a5:160:GLU:CD	2.29	0.40
3:E6:99:PHE:CZ	2:H6:28:ALA:HB2	2.56	0.40
3:L6:146:ARG:NH2	3:L6:151:GLN:HB3	2.36	0.40
3:O6:59:ALA:HB3	3:O6:134:LYS:HD3	2.04	0.40
2:T6:112:LEU:HD23	2:T6:158:LEU:HD21	2.02	0.40
4:Y6:235:THR:HB	5:Z6:141:GLU:O	2.21	0.40
5:Z6:114:VAL:HG21	5:Z6:194:LEU:HD13	2.03	0.40
2:B7:113:LEU:HD23	2:B7:113:LEU:HA	1.88	0.40
3:E7:41:THR:O	3:E7:45:ILE:HG12	2.20	0.40
2:I7:50:ASP:N	2:I7:50:ASP:OD1	2.51	0.40
3:L7:124:PRO:O	3:L7:128:VAL:HG23	2.22	0.40
3:M7:92:ARG:HG2	3:M7:96:TYR:CZ	2.55	0.40
3:M7:136:LYS:HB2	3:M7:165:PHE:CG	2.56	0.40
3:O7:34:GLU:HG3	3:O7:37:LYS:HD2	2.03	0.40
2:U7:3:LYS:H	2:U7:106:GLY:HA3	1.85	0.40
5:Z7:173:ARG:NH1	5:Z7:203:VAL:O	2.37	0.40
1:A1:182:ASP:OD1	1:A1:183:SER:N	2.49	0.40
3:E1:146:ARG:O	3:E1:151:GLN:NE2	2.55	0.40
2:N1:143:LEU:C	2:N1:148:ARG:HB2	2.46	0.40
6:O2:8:ALA:HA	6:O2:51:ILE:HD12	2.03	0.40
1:22:35:ASP:OD1	5:Z7:254:ARG:NH1	2.54	0.40
9:E2:14:GLU:O	9:E2:15:ALA:C	2.64	0.40
9:H2:79:ALA:O	9:H2:82:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H2:134:LYS:NZ	9:H2:154:ASP:OD1	2.44	0.40
9:J2:57:GLN:O	9:J2:61:LYS:HG2	2.22	0.40
9:J2:100:ASP:OD1	9:J2:101:ILE:N	2.55	0.40
8:M2:1:MET:HE1	10:N2:25:ILE:HG21	2.02	0.40
8:M2:68:PRO:HD3	9:R2:87:TYR:OH	2.21	0.40
11:P2:60:PHE:CD2	11:P2:67:LEU:HD21	2.56	0.40
11:P2:105:LEU:HD22	11:P2:160:LEU:HD21	2.03	0.40
12:S2:14:GLU:H	12:S2:14:GLU:HG2	1.74	0.40
8:T2:19:LEU:HD13	8:T2:19:LEU:HA	1.92	0.40
8:X2:2:GLN:HB2	8:X2:6:THR:CG2	2.51	0.40
13:X2:201:CYC:HB	13:X2:201:CYC:CMA	2.34	0.40
6:Z2:39:GLU:OE2	6:Z2:42:ARG:NH2	2.34	0.40
8:a2:3:ASP:OD2	9:i2:2:SER:OG	2.35	0.40
8:d2:65:ILE:HD11	8:d2:72:MET:HG3	2.04	0.40
13:d2:201:CYC:HMA1	13:d2:201:CYC:NB	2.36	0.40
8:g2:74:THR:HG22	9:h2:107:ILE:HG23	2.03	0.40
9:i2:121:THR:HG21	13:i2:201:CYC:H3C	2.03	0.40
9:j2:2:SER:OG	9:j2:4:VAL:HG22	2.21	0.40
9:k2:62:ARG:HH12	9:k2:124:GLU:HG2	1.85	0.40
10:o2:259:LEU:HD12	10:o2:260:PRO:HD2	2.04	0.40
10:o2:453:TYR:HB2	10:o2:457:ASN:HD22	1.87	0.40
10:o2:535:ASN:ND2	10:o2:535:ASN:O	2.55	0.40
10:o2:610:TYR:O	10:o2:614:ARG:HG2	2.21	0.40
11:q2:12:TYR:CE1	11:q2:23:ALA:HB2	2.57	0.40
12:t2:36:ARG:NH2	12:t2:152:TYR:OH	2.55	0.40
8:w2:140:LEU:HD23	8:w2:140:LEU:HA	1.92	0.40
2:G3:138:LYS:HA	2:G3:141:HIS:CD2	2.56	0.40
2:H3:50:ASP:OD1	2:H3:50:ASP:N	2.54	0.40
2:I3:85:CYS:CA	13:I3:201:CYC:HHD	2.51	0.40
13:M3:201:CYC:HMD1	13:M3:201:CYC:NC	2.36	0.40
2:N3:98:TYR:OH	3:V3:18:GLU:O	2.37	0.40
13:Q3:201:CYC:HBA2	4:Y3:253:LEU:HB2	2.02	0.40
2:S3:134:LEU:HB3	2:S3:155:ILE:HG23	2.03	0.40
3:E4:40:ASP:HB3	13:E4:201:CYC:HBC3	2.02	0.40
2:I4:31:ARG:CZ	2:I4:35:ALA:HB2	2.51	0.40
3:L4:38:ARG:HH12	3:L4:160:GLU:CD	2.29	0.40
3:M4:44:ARG:HH21	3:M4:145:ASP:HB3	1.85	0.40
2:S4:3:LYS:HG3	2:T4:18:ARG:NH1	2.36	0.40
2:S4:95:ILE:HG22	2:S4:108:ILE:HG12	2.03	0.40
2:W4:126:ALA:HB3	2:W4:129:TRP:CE2	2.56	0.40
2:W4:158:LEU:HD23	2:W4:158:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X4:76:THR:HG23	3:X4:79:ARG:H	1.86	0.40
5:Z4:96:ILE:HG23	5:Z4:133:TYR:OH	2.21	0.40
13:C5:201:CYC:HAD2	5:Z5:264:TYR:HH	1.87	0.40
3:L5:76:THR:HG22	3:L5:79:ARG:H	1.86	0.40
3:L5:117:THR:HG23	5:Z5:256:SER:HB2	2.03	0.40
3:L5:123:VAL:HG13	13:L5:201:CYC:NC	2.36	0.40
3:O5:128:VAL:HG22	13:Z5:301:CYC:H3C	2.04	0.40
2:R5:56:ALA:O	2:R5:60:VAL:HG23	2.21	0.40
2:T5:126:ALA:HB3	2:T5:129:TRP:CE2	2.56	0.40
2:W5:88:ASP:O	2:W5:92:TYR:HD1	2.04	0.40
3:X5:76:THR:HG23	3:X5:79:ARG:H	1.85	0.40
1:A6:180:ARG:HG3	13:a6:201:CYC:HBA2	2.04	0.40
2:B6:126:ALA:HB3	2:B6:129:TRP:CE2	2.56	0.40
3:E6:28:LEU:O	3:E6:32:VAL:HG23	2.21	0.40
3:M6:28:LEU:O	3:M6:32:VAL:HG23	2.22	0.40
2:N6:5:PRO:O	2:N6:8:GLU:HG3	2.21	0.40
2:N6:20:LEU:HD12	2:N6:24:GLU:HG2	2.02	0.40
3:a6:89:ILE:HG21	13:a6:201:CYC:HAB1	2.03	0.40
3:C7:116:GLU:OE1	3:C7:116:GLU:N	2.44	0.40
13:L7:201:CYC:HMA1	5:Z7:250:PHE:HD1	1.86	0.40
3:P7:37:LYS:HB3	3:P7:37:LYS:HE3	1.81	0.40
3:Q7:48:ASN:HB2	3:Q7:142:ILE:HD13	2.02	0.40
2:W7:16:GLN:OE1	2:W7:18:ARG:NE	2.55	0.40
2:W7:126:ALA:HB3	2:W7:129:TRP:CE2	2.57	0.40
3:X7:24:GLN:HE21	3:X7:24:GLN:HB2	1.68	0.40
3:X7:34:GLU:OE2	3:X7:38:ARG:NH2	2.42	0.40
5:Z7:227:SER:HB2	5:Z7:234:ALA:HB3	2.03	0.40
3:a7:103:ALA:O	3:a7:104:SER:C	2.64	0.40
3:C1:124:PRO:O	3:C1:128:VAL:HG23	2.22	0.40
2:G1:18:ARG:NH1	2:H1:3:LYS:HE2	2.36	0.40
3:O1:128:VAL:HG22	13:Z1:301:CYC:H3C	2.03	0.40
2:R1:92:TYR:CD2	2:R1:112:LEU:HD21	2.57	0.40
3:V1:41:THR:HG23	3:V1:143:VAL:HG21	2.03	0.40
3:a1:44:ARG:HH12	3:a1:145:ASP:HB3	1.87	0.40
6:O2:44:GLN:HB2	8:a2:107:ARG:HA	2.03	0.40
7:12:97:LEU:O	7:12:101:VAL:HG13	2.21	0.40
1:22:98:ASN:OD1	1:22:181:TYR:HA	2.21	0.40
1:52:182:ASP:OD1	1:52:183:SER:N	2.54	0.40
8:B2:127:VAL:O	8:B2:131:GLN:HG2	2.22	0.40
9:G2:32:GLY:O	9:G2:36:ARG:HD3	2.21	0.40
9:H2:81:CYS:HA	13:H2:201:CYC:HHD	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K2:2:GLN:HB2	8:K2:6:THR:HB	2.04	0.40
10:N2:374:LEU:HD22	10:N2:382:LEU:HD22	2.04	0.40
11:P2:139:ARG:HD2	11:P2:154:GLU:CD	2.46	0.40
8:T2:20:ASP:OD1	8:T2:22:SER:OG	2.24	0.40
8:V2:100:ASP:OD1	8:V2:101:THR:N	2.55	0.40
8:V2:104:LEU:HD22	8:V2:156:ILE:HD11	2.03	0.40
9:f2:131:ARG:HA	9:f2:157:ILE:HD11	2.02	0.40
9:h2:64:ASP:N	9:h2:64:ASP:OD1	2.53	0.40
9:k2:50:ILE:HG13	9:k2:136:ALA:CB	2.52	0.40
8:l2:78:TYR:O	8:l2:82:ILE:HG12	2.22	0.40
8:n2:137:THR:O	8:n2:141:VAL:HG22	2.20	0.40
10:o2:413:GLU:HG3	10:o2:416:ASN:OD1	2.20	0.40
10:o2:699:ARG:HD2	1:A6:170:GLY:O	2.22	0.40
9:s2:61:LYS:HE3	9:s2:61:LYS:HB3	1.89	0.40
8:w2:60:LEU:HB3	8:w2:72:MET:HE1	2.03	0.40
8:w2:81:CYS:HA	13:w2:201:CYC:HAC2	2.03	0.40
3:C3:108:ASP:N	3:C3:108:ASP:OD1	2.55	0.40
3:D3:41:THR:HG23	3:D3:143:VAL:HG21	2.03	0.40
2:G3:23:THR:HG23	2:H3:5:PRO:HA	2.04	0.40
2:I3:143:LEU:C	2:I3:148:ARG:HB2	2.46	0.40
3:J3:4:ASP:OD1	3:J3:7:THR:OG1	2.40	0.40
3:J3:167:LYS:HB2	3:J3:167:LYS:HE3	1.87	0.40
2:K3:108:ILE:HG22	2:K3:113:LEU:HG	2.03	0.40
3:L3:78:ARG:NH1	13:L3:201:CYC:O1D	2.52	0.40
2:N3:76:ALA:HB1	2:N3:82:LYS:HD3	2.04	0.40
2:K4:126:ALA:HB3	2:K4:129:TRP:CE2	2.56	0.40
2:N4:74:ASN:O	13:N4:201:CYC:NC	2.52	0.40
2:S4:2:SER:HB2	2:S4:106:GLY:HA3	2.03	0.40
3:a4:157:ILE:HD12	3:a4:157:ILE:HA	1.96	0.40
2:G5:115:GLY:O	2:G5:118:GLU:HG2	2.21	0.40
3:M5:44:ARG:HH21	3:M5:145:ASP:HB3	1.86	0.40
2:N5:20:LEU:HD21	3:V5:96:TYR:HD1	1.87	0.40
2:N5:143:LEU:C	2:N5:148:ARG:HB2	2.46	0.40
3:O5:59:ALA:HB3	3:O5:134:LYS:HD3	2.04	0.40
2:S5:85:CYS:CA	13:S5:201:CYC:HHD	2.52	0.40
1:A6:77:VAL:O	1:A6:81:ILE:HG12	2.22	0.40
2:B6:76:ALA:N	13:B6:201:CYC:OC	2.55	0.40
2:G6:5:PRO:HA	2:H6:23:THR:HG23	2.03	0.40
2:T6:24:GLU:OE1	2:T6:24:GLU:N	2.49	0.40
2:U6:50:ASP:OD1	2:U6:50:ASP:N	2.55	0.40
5:Z6:203:VAL:HG13	5:Z6:282:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C7:109:ARG:HA	5:Z7:275:ASN:HB3	2.03	0.40
2:N7:91:TYR:O	2:N7:95:ILE:HG12	2.22	0.40
2:N7:115:GLY:O	2:N7:118:GLU:HG2	2.22	0.40
3:O7:70:PRO:HA	3:O7:75:TYR:CD1	2.57	0.40
3:Q7:154:CYS:SG	13:Q7:202:CYC:HAC2	2.62	0.40
13:X7:201:CYC:OB	5:Z7:92:GLN:HB3	2.21	0.40
1:A1:86:LEU:HD23	1:A1:134:TYR:CE1	2.56	0.40
2:F1:23:THR:O	2:F1:27:VAL:HG23	2.21	0.40
2:F1:127:PRO:HB3	2:F1:162:LEU:HD22	2.04	0.40
3:J1:113:GLY:O	3:J1:116:GLU:HG2	2.22	0.40
3:O1:118:TYR:HE2	3:O1:128:VAL:HG11	1.86	0.40
3:P1:146:ARG:HB3	3:P1:151:GLN:OE1	2.21	0.40
3:Q1:37:LYS:H	3:Q1:37:LYS:HG2	1.60	0.40
13:S1:201:CYC:HAC1	13:S1:201:CYC:HHD	1.57	0.40
2:W1:93:LEU:O	2:W1:97:THR:HG23	2.21	0.40
13:Z1:301:CYC:HBC2	13:Z1:301:CYC:H2C	1.94	0.40
1:32:147:TYR:HE2	1:32:157:PRO:HG3	1.87	0.40
1:32:239:ILE:HD12	1:32:244:LYS:HD2	2.03	0.40
1:52:80:PHE:CE2	1:52:84:LEU:HD11	2.57	0.40
1:52:104:VAL:HG11	1:52:125:TRP:HB2	2.03	0.40
8:A2:68:PRO:HG3	8:A2:73:TYR:CE1	2.56	0.40
9:E2:61:LYS:HB3	9:E2:61:LYS:HE2	1.83	0.40
8:K2:51:ILE:HA	8:K2:136:VAL:HG11	2.03	0.40
8:L2:2:ASP:HA	8:L2:97:ALA:HB1	2.03	0.40
8:M2:20:ASP:OD1	8:M2:20:ASP:N	2.52	0.40
9:R2:2:SER:OG	9:R2:3:ILE:N	2.54	0.40
8:V2:85:LEU:HD23	8:V2:85:LEU:HA	1.91	0.40
9:W2:115:MET:HE3	9:W2:115:MET:HB3	1.92	0.40
8:X2:65:ILE:HA	8:X2:70:GLY:HA3	2.04	0.40
9:e2:107:ILE:HG23	8:m2:74:THR:HG22	2.02	0.40
13:e2:201:CYC:HHD	13:e2:201:CYC:HAC1	1.72	0.40
9:f2:23:LEU:HD12	9:f2:23:LEU:HA	1.93	0.40
9:f2:152:TYR:O	9:f2:156:VAL:HG23	2.22	0.40
9:i2:115:MET:O	9:i2:118:SER:OG	2.40	0.40
9:j2:109:ILE:O	9:j2:112:VAL:HG12	2.22	0.40
8:l2:81:CYS:SG	13:l2:201:CYC:HAC2	2.62	0.40
8:l2:85:LEU:HD22	8:l2:133:ILE:HD11	2.02	0.40
8:n2:111:GLY:O	8:n2:115:THR:HG23	2.22	0.40
10:o2:150:TYR:CZ	10:o2:154:ASN:HB3	2.56	0.40
8:p2:35:GLU:O	8:p2:39:ARG:HG2	2.21	0.40
12:t2:88:TYR:CD1	12:t2:156:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t2:89:LEU:O	12:t2:93:THR:HG23	2.20	0.40
12:t2:126:MET:O	12:t2:130:ILE:HG12	2.22	0.40
8:u2:110:ASN:HB3	6:z2:44:GLN:HG2	2.03	0.40
9:v2:145:ASP:N	9:v2:145:ASP:OD1	2.55	0.40
2:B3:99:ALA:HB2	2:B3:108:ILE:HG13	2.04	0.40
3:D3:37:LYS:HB3	3:D3:154:CYS:SG	2.62	0.40
3:E3:96:TYR:OH	2:H3:18:ARG:O	2.32	0.40
2:I3:76:ALA:HA	2:I3:81:GLY:HA3	2.04	0.40
3:V3:115:ARG:NH2	3:V3:171:ALA:O	2.54	0.40
5:Z3:96:ILE:HG23	5:Z3:133:TYR:OH	2.22	0.40
3:J4:121:LEU:HD13	13:J4:201:CYC:HBD1	2.03	0.40
3:J4:124:PRO:O	3:J4:128:VAL:HG23	2.22	0.40
2:K4:115:GLY:O	2:K4:119:ILE:HG12	2.22	0.40
3:M4:53:VAL:HG22	3:M4:135:MET:HE3	2.04	0.40
2:N4:138:LYS:HB2	2:N4:155:ILE:HG21	2.04	0.40
3:D5:136:LYS:HB2	3:D5:165:PHE:HB3	2.04	0.40
2:G5:126:ALA:HB3	2:G5:129:TRP:CE2	2.57	0.40
2:I5:95:ILE:HD12	2:I5:111:TYR:HD2	1.86	0.40
2:I5:99:ALA:HB2	2:I5:108:ILE:HG12	2.04	0.40
3:M5:112:ASN:OD1	3:M5:113:GLY:N	2.55	0.40
3:O5:111:LEU:HD21	3:O5:168:ALA:HA	2.04	0.40
2:T5:112:LEU:HD12	2:T5:112:LEU:HA	1.95	0.40
13:T5:201:CYC:HMA3	13:T5:201:CYC:NB	2.37	0.40
3:V5:12:GLN:O	3:V5:16:ARG:HG3	2.21	0.40
3:X5:37:LYS:HA	3:X5:37:LYS:HD3	1.79	0.40
3:X5:41:THR:HG23	3:X5:143:VAL:HG11	2.03	0.40
2:B6:85:CYS:HA	13:B6:201:CYC:HAC1	1.76	0.40
2:G6:74:ASN:OD1	2:G6:74:ASN:N	2.54	0.40
3:M6:98:VAL:HG21	3:M6:161:LEU:HD13	2.04	0.40
3:P6:2:THR:HG22	2:U6:7:THR:HG22	2.03	0.40
3:Q6:123:VAL:HG22	13:Q6:201:CYC:HC	1.86	0.40
3:X6:12:GLN:O	3:X6:16:ARG:HG2	2.21	0.40
5:Z6:3:ILE:HD11	5:Z6:165:LEU:HD11	2.03	0.40
2:B7:143:LEU:C	2:B7:148:ARG:HB2	2.47	0.40
3:J7:113:GLY:HA2	3:J7:116:GLU:CD	2.47	0.40
2:R7:23:THR:HG23	2:W7:5:PRO:HA	2.03	0.40
3:V7:132:VAL:HA	3:V7:135:MET:HE2	2.03	0.40
3:X7:28:LEU:O	3:X7:32:VAL:HG23	2.21	0.40
3:X7:128:VAL:HG22	13:X7:201:CYC:HMC3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	22	246/250 (98%)	233 (95%)	13 (5%)	0	100	100
1	32	246/250 (98%)	236 (96%)	10 (4%)	0	100	100
1	42	245/250 (98%)	236 (96%)	9 (4%)	0	100	100
1	52	245/250 (98%)	231 (94%)	13 (5%)	1 (0%)	30	62
1	A1	194/250 (78%)	186 (96%)	8 (4%)	0	100	100
1	A6	194/250 (78%)	186 (96%)	8 (4%)	0	100	100
2	B1	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B3	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B4	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B5	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	B6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	B7	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F1	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	F3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	F4	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	F5	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	F6	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	F7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	G1	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	G3	160/163 (98%)	160 (100%)	0	0	100	100
2	G4	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	G5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	G6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	G7	160/163 (98%)	160 (100%)	0	0	100	100
2	H1	160/163 (98%)	157 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H4	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	H5	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H6	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	H7	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	I1	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	I3	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	I4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	I5	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	I6	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	I7	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K1	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K3	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	K4	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K5	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K6	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	N1	161/163 (99%)	161 (100%)	0	0	100	100
2	N3	161/163 (99%)	160 (99%)	1 (1%)	0	100	100
2	N4	161/163 (99%)	160 (99%)	1 (1%)	0	100	100
2	N5	161/163 (99%)	160 (99%)	1 (1%)	0	100	100
2	N6	161/163 (99%)	161 (100%)	0	0	100	100
2	N7	161/163 (99%)	161 (100%)	0	0	100	100
2	R1	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	R3	160/163 (98%)	160 (100%)	0	0	100	100
2	R4	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	R5	160/163 (98%)	160 (100%)	0	0	100	100
2	R6	160/163 (98%)	160 (100%)	0	0	100	100
2	R7	160/163 (98%)	160 (100%)	0	0	100	100
2	S1	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	S3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S4	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	S5	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	S6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	S7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	T1	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	T3	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	T4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	T5	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	T6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	T7	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	U1	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	U4	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U5	160/163 (98%)	160 (100%)	0	0	100	100
2	U6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	W1	160/163 (98%)	160 (100%)	0	0	100	100
2	W3	160/163 (98%)	160 (100%)	0	0	100	100
2	W4	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	W5	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	W6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	W7	160/163 (98%)	160 (100%)	0	0	100	100
3	C1	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	C3	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	C4	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	C5	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	C6	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	C7	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	D1	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	D3	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	D4	170/173 (98%)	168 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	D6	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	D7	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	E1	170/173 (98%)	170 (100%)	0	0	100	100
3	E3	170/173 (98%)	170 (100%)	0	0	100	100
3	E4	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	E5	170/173 (98%)	170 (100%)	0	0	100	100
3	E6	170/173 (98%)	170 (100%)	0	0	100	100
3	E7	170/173 (98%)	170 (100%)	0	0	100	100
3	J1	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	J3	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	J4	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	J5	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	J6	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	J7	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	L1	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	L3	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	L4	171/173 (99%)	171 (100%)	0	0	100	100
3	L5	171/173 (99%)	171 (100%)	0	0	100	100
3	L6	171/173 (99%)	171 (100%)	0	0	100	100
3	L7	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	M1	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	M3	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	M4	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	M5	171/173 (99%)	171 (100%)	0	0	100	100
3	M6	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	M7	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	O1	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	O3	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	O4	171/173 (99%)	171 (100%)	0	0	100	100
3	O5	171/173 (99%)	169 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O6	171/173 (99%)	171 (100%)	0	0	100	100
3	O7	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	P1	171/173 (99%)	171 (100%)	0	0	100	100
3	P3	171/173 (99%)	171 (100%)	0	0	100	100
3	P4	171/173 (99%)	171 (100%)	0	0	100	100
3	P5	171/173 (99%)	171 (100%)	0	0	100	100
3	P6	171/173 (99%)	171 (100%)	0	0	100	100
3	P7	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	Q1	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	Q3	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	Q4	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	Q5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	Q6	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	Q7	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	V1	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	V3	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	V4	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	V5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	V6	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	V7	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	X1	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	X3	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	X4	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	X5	171/173 (99%)	167 (98%)	4 (2%)	0	100	100
3	X6	171/173 (99%)	166 (97%)	5 (3%)	0	100	100
3	X7	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	a1	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	a3	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	a4	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	21	56
3	a5	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
3	a6	170/173 (98%)	167 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a7	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
4	Y1	55/273 (20%)	51 (93%)	4 (7%)	0	100	100
4	Y3	55/273 (20%)	52 (94%)	3 (6%)	0	100	100
4	Y4	55/273 (20%)	52 (94%)	3 (6%)	0	100	100
4	Y5	55/273 (20%)	53 (96%)	2 (4%)	0	100	100
4	Y6	55/273 (20%)	51 (93%)	4 (7%)	0	100	100
4	Y7	55/273 (20%)	52 (94%)	3 (6%)	0	100	100
5	Z1	286/289 (99%)	272 (95%)	14 (5%)	0	100	100
5	Z3	286/289 (99%)	276 (96%)	10 (4%)	0	100	100
5	Z4	286/289 (99%)	275 (96%)	11 (4%)	0	100	100
5	Z5	286/289 (99%)	276 (96%)	10 (4%)	0	100	100
5	Z6	286/289 (99%)	274 (96%)	12 (4%)	0	100	100
5	Z7	286/289 (99%)	272 (95%)	14 (5%)	0	100	100
6	02	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
6	Y2	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
6	Z2	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
6	z2	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
7	12	35/110 (32%)	33 (94%)	2 (6%)	0	100	100
7	b2	35/110 (32%)	33 (94%)	2 (6%)	0	100	100
8	A2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
8	B2	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
8	C2	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	F2	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
8	K2	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
8	L2	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
8	M2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
8	O2	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	T2	159/161 (99%)	159 (100%)	0	0	100	100
8	V2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
8	X2	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
8	a2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
8	d2	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	g2	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
8	l2	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
8	m2	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	n2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
8	p2	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	u2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
8	w2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
8	y2	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
9	D2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	E2	159/161 (99%)	159 (100%)	0	0	100	100
9	G2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	H2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	I2	159/161 (99%)	159 (100%)	0	0	100	100
9	J2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	Q2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	R2	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
9	U2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	W2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
9	e2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	f2	159/161 (99%)	159 (100%)	0	0	100	100
9	h2	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
9	i2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	j2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	k2	159/161 (99%)	159 (100%)	0	0	100	100
9	r2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	s2	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
9	v2	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
9	x2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
10	N2	654/705 (93%)	632 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	o2	654/705 (93%)	628 (96%)	26 (4%)	0	100	100
11	P2	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
11	q2	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
12	S2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
12	t2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
All	All	36192/38388 (94%)	35631 (98%)	559 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	a4	110	CYS
1	52	192	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	22	206/208 (99%)	198 (96%)	8 (4%)	28	62
1	32	206/208 (99%)	198 (96%)	8 (4%)	28	62
1	42	205/208 (99%)	197 (96%)	8 (4%)	28	62
1	52	205/208 (99%)	199 (97%)	6 (3%)	37	67
1	A1	171/208 (82%)	166 (97%)	5 (3%)	37	67
1	A6	171/208 (82%)	167 (98%)	4 (2%)	44	70
2	B1	122/123 (99%)	117 (96%)	5 (4%)	27	60
2	B3	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	B4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	B5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	B6	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	B7	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	F1	122/123 (99%)	118 (97%)	4 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F3	122/123 (99%)	116 (95%)	6 (5%)	22	55
2	F4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	F5	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	F6	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	F7	122/123 (99%)	117 (96%)	5 (4%)	27	60
2	G1	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	G3	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	G4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	G5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	G6	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	G7	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	H1	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	H3	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	H4	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	H5	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	H6	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	H7	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	I1	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	I3	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	I4	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	I5	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	I6	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	I7	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	K1	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	K3	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	K4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	K5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	K6	122/123 (99%)	117 (96%)	5 (4%)	27	60
2	K7	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	N1	123/123 (100%)	116 (94%)	7 (6%)	18	51
2	N3	123/123 (100%)	119 (97%)	4 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N4	123/123 (100%)	118 (96%)	5 (4%)	27	60
2	N5	123/123 (100%)	117 (95%)	6 (5%)	22	55
2	N6	123/123 (100%)	119 (97%)	4 (3%)	33	65
2	N7	123/123 (100%)	120 (98%)	3 (2%)	43	70
2	R1	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	R3	122/123 (99%)	117 (96%)	5 (4%)	27	60
2	R4	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	R5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	R6	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	R7	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	S1	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	S3	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	S4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	S5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	S6	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	S7	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	T1	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	T3	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	T4	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	T5	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	T6	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	T7	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	U1	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	U3	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	U4	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	U5	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	U6	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	U7	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	W1	122/123 (99%)	120 (98%)	2 (2%)	55	75
2	W3	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	W4	122/123 (99%)	121 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W5	122/123 (99%)	119 (98%)	3 (2%)	42	69
2	W6	122/123 (99%)	121 (99%)	1 (1%)	73	82
2	W7	122/123 (99%)	121 (99%)	1 (1%)	73	82
3	C1	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	C3	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	C4	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	C5	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	C6	129/129 (100%)	124 (96%)	5 (4%)	28	62
3	C7	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	D1	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	D3	128/129 (99%)	123 (96%)	5 (4%)	28	62
3	D4	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	D5	128/129 (99%)	123 (96%)	5 (4%)	28	62
3	D6	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	D7	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	E1	128/129 (99%)	122 (95%)	6 (5%)	23	57
3	E3	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	E4	128/129 (99%)	123 (96%)	5 (4%)	28	62
3	E5	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	E6	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	E7	128/129 (99%)	125 (98%)	3 (2%)	44	70
3	J1	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	J3	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	J4	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	J5	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	J6	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	J7	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	L1	129/129 (100%)	122 (95%)	7 (5%)	20	53
3	L3	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	L4	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	L5	129/129 (100%)	124 (96%)	5 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L6	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	L7	129/129 (100%)	124 (96%)	5 (4%)	28	62
3	M1	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	M3	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	M4	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	M5	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	M6	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	M7	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	O1	129/129 (100%)	124 (96%)	5 (4%)	28	62
3	O3	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	O4	129/129 (100%)	124 (96%)	5 (4%)	28	62
3	O5	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	O6	129/129 (100%)	124 (96%)	5 (4%)	28	62
3	O7	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	P1	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	P3	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	P4	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	P5	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	P6	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	P7	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	Q1	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	Q3	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	Q4	128/129 (99%)	123 (96%)	5 (4%)	28	62
3	Q5	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	Q6	128/129 (99%)	122 (95%)	6 (5%)	23	57
3	Q7	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	V1	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	V3	128/129 (99%)	125 (98%)	3 (2%)	44	70
3	V4	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	V5	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	V6	128/129 (99%)	126 (98%)	2 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	V7	128/129 (99%)	125 (98%)	3 (2%)	44	70
3	X1	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	X3	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	X4	129/129 (100%)	127 (98%)	2 (2%)	55	75
3	X5	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	X6	129/129 (100%)	126 (98%)	3 (2%)	44	70
3	X7	129/129 (100%)	125 (97%)	4 (3%)	35	66
3	a1	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	a3	128/129 (99%)	125 (98%)	3 (2%)	44	70
3	a4	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	a5	128/129 (99%)	126 (98%)	2 (2%)	55	75
3	a6	128/129 (99%)	124 (97%)	4 (3%)	35	66
3	a7	128/129 (99%)	124 (97%)	4 (3%)	35	66
4	Y1	49/221 (22%)	47 (96%)	2 (4%)	27	60
4	Y3	49/221 (22%)	48 (98%)	1 (2%)	48	72
4	Y4	49/221 (22%)	46 (94%)	3 (6%)	17	49
4	Y5	49/221 (22%)	45 (92%)	4 (8%)	10	39
4	Y6	49/221 (22%)	47 (96%)	2 (4%)	27	60
4	Y7	49/221 (22%)	48 (98%)	1 (2%)	48	72
5	Z1	239/240 (100%)	235 (98%)	4 (2%)	53	75
5	Z3	239/240 (100%)	233 (98%)	6 (2%)	42	69
5	Z4	239/240 (100%)	235 (98%)	4 (2%)	53	75
5	Z5	239/240 (100%)	235 (98%)	4 (2%)	53	75
5	Z6	239/240 (100%)	235 (98%)	4 (2%)	53	75
5	Z7	239/240 (100%)	234 (98%)	5 (2%)	47	71
6	02	60/60 (100%)	58 (97%)	2 (3%)	33	65
6	Y2	60/60 (100%)	59 (98%)	1 (2%)	53	75
6	Z2	60/60 (100%)	59 (98%)	1 (2%)	53	75
6	z2	60/60 (100%)	60 (100%)	0	100	100
7	12	32/86 (37%)	30 (94%)	2 (6%)	16	48
7	b2	32/86 (37%)	30 (94%)	2 (6%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A2	128/128 (100%)	125 (98%)	3 (2%)	44	70
8	B2	128/128 (100%)	122 (95%)	6 (5%)	23	57
8	C2	128/128 (100%)	125 (98%)	3 (2%)	44	70
8	F2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	K2	128/128 (100%)	124 (97%)	4 (3%)	35	66
8	L2	128/128 (100%)	125 (98%)	3 (2%)	44	70
8	M2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	O2	128/128 (100%)	125 (98%)	3 (2%)	44	70
8	T2	128/128 (100%)	123 (96%)	5 (4%)	28	62
8	V2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	X2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	a2	128/128 (100%)	124 (97%)	4 (3%)	35	66
8	c2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	d2	128/128 (100%)	125 (98%)	3 (2%)	44	70
8	g2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	l2	128/128 (100%)	126 (98%)	2 (2%)	55	75
8	m2	128/128 (100%)	124 (97%)	4 (3%)	35	66
8	n2	128/128 (100%)	126 (98%)	2 (2%)	55	75
8	p2	128/128 (100%)	127 (99%)	1 (1%)	73	82
8	u2	128/128 (100%)	123 (96%)	5 (4%)	28	62
8	w2	128/128 (100%)	128 (100%)	0	100	100
8	y2	128/128 (100%)	127 (99%)	1 (1%)	73	82
9	D2	128/128 (100%)	121 (94%)	7 (6%)	19	52
9	E2	128/128 (100%)	118 (92%)	10 (8%)	11	41
9	G2	128/128 (100%)	118 (92%)	10 (8%)	11	41
9	H2	128/128 (100%)	123 (96%)	5 (4%)	28	62
9	I2	128/128 (100%)	123 (96%)	5 (4%)	28	62
9	J2	128/128 (100%)	124 (97%)	4 (3%)	35	66
9	Q2	128/128 (100%)	124 (97%)	4 (3%)	35	66
9	R2	128/128 (100%)	123 (96%)	5 (4%)	28	62
9	U2	128/128 (100%)	121 (94%)	7 (6%)	19	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W2	127/128 (99%)	121 (95%)	6 (5%)	23	57
9	e2	128/128 (100%)	123 (96%)	5 (4%)	28	62
9	f2	128/128 (100%)	118 (92%)	10 (8%)	11	41
9	h2	128/128 (100%)	121 (94%)	7 (6%)	19	52
9	i2	128/128 (100%)	122 (95%)	6 (5%)	23	57
9	j2	128/128 (100%)	124 (97%)	4 (3%)	35	66
9	k2	128/128 (100%)	125 (98%)	3 (2%)	44	70
9	r2	128/128 (100%)	124 (97%)	4 (3%)	35	66
9	s2	128/128 (100%)	122 (95%)	6 (5%)	23	57
9	v2	128/128 (100%)	123 (96%)	5 (4%)	28	62
9	x2	127/128 (99%)	119 (94%)	8 (6%)	16	48
10	N2	553/584 (95%)	541 (98%)	12 (2%)	45	71
10	o2	553/584 (95%)	537 (97%)	16 (3%)	37	67
11	P2	133/133 (100%)	128 (96%)	5 (4%)	29	62
11	q2	133/133 (100%)	130 (98%)	3 (2%)	44	70
12	S2	132/133 (99%)	127 (96%)	5 (4%)	29	62
12	t2	132/133 (99%)	130 (98%)	2 (2%)	57	76
All	All	28254/29646 (95%)	27493 (97%)	761 (3%)	40	68

All (761) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	27	GLN
1	A1	33	THR
1	A1	89	THR
1	A1	127	LEU
1	A1	141	LEU
2	B1	23	THR
2	B1	24	GLU
2	B1	26	GLN
2	B1	119	ILE
2	B1	141	HIS
3	C1	2	THR
3	C1	105	ILE
3	C1	150	THR
3	C1	172	VAL

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Mol	Chain	Res	Type
3	D1	37	LYS
3	D1	76	THR
3	D1	83	CYS
3	D1	105	ILE
3	E1	10	VAL
3	E1	37	LYS
3	E1	40	ASP
3	E1	76	THR
3	E1	83	CYS
3	E1	105	ILE
2	F1	3	LYS
2	F1	10	VAL
2	F1	23	THR
2	F1	110	GLU
2	G1	113	LEU
2	G1	118	GLU
2	G1	119	ILE
2	G1	143	LEU
2	H1	118	GLU
2	H1	141	HIS
2	I1	68	THR
2	I1	78	THR
3	J1	37	LYS
3	J1	105	ILE
2	K1	10	VAL
2	K1	18	ARG
2	K1	105	THR
2	K1	141	HIS
3	L1	9	VAL
3	L1	25	LEU
3	L1	40	ASP
3	L1	76	THR
3	L1	87	MET
3	L1	105	ILE
3	L1	114	LEU
3	M1	105	ILE
3	M1	110	CYS
3	M1	119	LEU
2	N1	10	VAL
2	N1	20	LEU
2	N1	23	THR
2	N1	78	THR

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Mol	Chain	Res	Type
2	N1	113	LEU
2	N1	118	GLU
2	N1	141	HIS
3	O1	1	MET
3	O1	76	THR
3	O1	83	CYS
3	O1	105	ILE
3	O1	150	THR
3	P1	37	LYS
3	P1	83	CYS
3	Q1	37	LYS
3	Q1	39	ILE
3	Q1	40	ASP
3	Q1	105	ILE
2	R1	4	THR
2	R1	78	THR
2	R1	113	LEU
2	S1	10	VAL
2	S1	78	THR
2	S1	119	ILE
2	S1	141	HIS
2	T1	78	THR
2	T1	84	LYS
2	U1	10	VAL
2	U1	78	THR
3	V1	36	ASN
3	V1	105	ILE
2	W1	118	GLU
2	W1	119	ILE
3	X1	7	THR
3	X1	20	LEU
3	X1	83	CYS
3	X1	172	VAL
4	Y1	231	VAL
4	Y1	240	ARG
5	Z1	141	GLU
5	Z1	207	VAL
5	Z1	224	LEU
5	Z1	253	VAL
3	a1	40	ASP
3	a1	83	CYS
3	a1	105	ILE

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Mol	Chain	Res	Type
3	a1	119	LEU
6	02	10	LEU
6	02	53	VAL
7	12	88	THR
7	12	97	LEU
1	22	14	ASN
1	22	33	THR
1	22	54	PHE
1	22	79	ASP
1	22	89	THR
1	22	127	LEU
1	22	191	PHE
1	22	239	ILE
1	32	14	ASN
1	32	33	THR
1	32	79	ASP
1	32	89	THR
1	32	127	LEU
1	32	141	LEU
1	32	191	PHE
1	32	231	GLN
1	42	27	GLN
1	42	33	THR
1	42	89	THR
1	42	127	LEU
1	42	172	THR
1	42	191	PHE
1	42	207	GLN
1	42	209	LEU
1	52	14	ASN
1	52	27	GLN
1	52	89	THR
1	52	127	LEU
1	52	172	THR
1	52	191	PHE
8	A2	61	LEU
8	A2	113	LYS
8	A2	153	LEU
8	B2	1	MET
8	B2	32	GLN
8	B2	64	ASP
8	B2	66	THR

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Mol	Chain	Res	Type
8	B2	89	LEU
8	B2	153	LEU
8	C2	3	ASP
8	C2	5	ILE
8	C2	74	THR
9	D2	9	VAL
9	D2	30	VAL
9	D2	71	ASN
9	D2	97	VAL
9	D2	102	THR
9	D2	121	THR
9	D2	123	ILE
9	E2	3	ILE
9	E2	4	VAL
9	E2	5	SER
9	E2	23	LEU
9	E2	30	VAL
9	E2	81	CYS
9	E2	102	THR
9	E2	121	THR
9	E2	140	LEU
9	E2	141	LEU
8	F2	60	LEU
9	G2	4	VAL
9	G2	23	LEU
9	G2	30	VAL
9	G2	47	ARG
9	G2	71	ASN
9	G2	82	LEU
9	G2	97	VAL
9	G2	102	THR
9	G2	121	THR
9	G2	147	ASP
9	H2	23	LEU
9	H2	45	GLU
9	H2	85	LEU
9	H2	110	VAL
9	H2	119	LEU
9	I2	81	CYS
9	I2	110	VAL
9	I2	114	GLU
9	I2	141	LEU

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Mol	Chain	Res	Type
9	I2	145	ASP
9	J2	4	VAL
9	J2	18	LEU
9	J2	80	THR
9	J2	91	LEU
8	K2	81	CYS
8	K2	87	TYR
8	K2	140	LEU
8	K2	160	LEU
8	L2	2	ASP
8	L2	102	ILE
8	L2	120	VAL
8	M2	36	LEU
10	N2	91	ASP
10	N2	173	ILE
10	N2	198	THR
10	N2	316	LYS
10	N2	533	VAL
10	N2	538	ILE
10	N2	539	ARG
10	N2	559	ARG
10	N2	587	GLN
10	N2	605	VAL
10	N2	679	LEU
10	N2	688	SER
8	O2	36	LEU
8	O2	61	LEU
8	O2	87	TYR
11	P2	14	LEU
11	P2	26	SER
11	P2	82	CYS
11	P2	104	VAL
11	P2	168	ASP
9	Q2	25	ARG
9	Q2	30	VAL
9	Q2	102	THR
9	Q2	121	THR
9	R2	5	SER
9	R2	47	ARG
9	R2	81	CYS
9	R2	97	VAL
9	R2	121	THR

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Mol	Chain	Res	Type
12	S2	64	ASP
12	S2	66	ILE
12	S2	81	CYS
12	S2	85	TYR
12	S2	102	GLU
8	T2	19	LEU
8	T2	36	LEU
8	T2	65	ILE
8	T2	66	THR
8	T2	140	LEU
9	U2	2	SER
9	U2	4	VAL
9	U2	81	CYS
9	U2	97	VAL
9	U2	140	LEU
9	U2	145	ASP
9	U2	147	ASP
8	V2	81	CYS
9	W2	30	VAL
9	W2	57	GLN
9	W2	71	ASN
9	W2	77	MET
9	W2	102	THR
9	W2	132	GLU
8	X2	65	ILE
6	Y2	34	ASP
6	Z2	53	VAL
8	a2	61	LEU
8	a2	71	ASN
8	a2	113	LYS
8	a2	153	LEU
7	b2	88	THR
7	b2	97	LEU
8	c2	89	LEU
8	d2	5	ILE
8	d2	109	LEU
8	d2	141	VAL
9	e2	30	VAL
9	e2	102	THR
9	e2	121	THR
9	e2	123	ILE
9	e2	147	ASP

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Mol	Chain	Res	Type
9	f2	3	ILE
9	f2	4	VAL
9	f2	5	SER
9	f2	23	LEU
9	f2	30	VAL
9	f2	81	CYS
9	f2	98	SER
9	f2	102	THR
9	f2	140	LEU
9	f2	141	LEU
8	g2	60	LEU
9	h2	4	VAL
9	h2	23	LEU
9	h2	30	VAL
9	h2	47	ARG
9	h2	82	LEU
9	h2	97	VAL
9	h2	102	THR
9	i2	23	LEU
9	i2	45	GLU
9	i2	91	LEU
9	i2	104	ILE
9	i2	119	LEU
9	i2	145	ASP
9	j2	38	ARG
9	j2	64	ASP
9	j2	110	VAL
9	j2	145	ASP
9	k2	4	VAL
9	k2	91	LEU
9	k2	123	ILE
8	l2	87	TYR
8	l2	140	LEU
8	m2	1	MET
8	m2	3	ASP
8	m2	103	ILE
8	m2	121	VAL
8	n2	2	GLN
8	n2	36	LEU
10	o2	26	VAL
10	o2	37	GLN
10	o2	91	ASP

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Mol	Chain	Res	Type
10	o2	198	THR
10	o2	228	ASP
10	o2	254	GLN
10	o2	277	SER
10	o2	298	ARG
10	o2	307	LYS
10	o2	312	GLU
10	o2	538	ILE
10	o2	559	ARG
10	o2	568	THR
10	o2	587	GLN
10	o2	679	LEU
10	o2	698	ARG
8	p2	61	LEU
11	q2	26	SER
11	q2	104	VAL
11	q2	168	ASP
9	r2	3	ILE
9	r2	30	VAL
9	r2	102	THR
9	r2	121	THR
9	s2	5	SER
9	s2	14	GLU
9	s2	47	ARG
9	s2	97	VAL
9	s2	121	THR
9	s2	133	LEU
12	t2	66	ILE
12	t2	80	GLN
8	u2	36	LEU
8	u2	65	ILE
8	u2	66	THR
8	u2	103	ILE
8	u2	140	LEU
9	v2	2	SER
9	v2	4	VAL
9	v2	30	VAL
9	v2	121	THR
9	v2	140	LEU
9	x2	14	GLU
9	x2	30	VAL
9	x2	57	GLN

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Mol	Chain	Res	Type
9	x2	97	VAL
9	x2	102	THR
9	x2	114	GLU
9	x2	132	GLU
9	x2	140	LEU
8	y2	65	ILE
2	B3	23	THR
2	B3	26	GLN
3	C3	40	ASP
3	C3	105	ILE
3	C3	150	THR
3	D3	37	LYS
3	D3	40	ASP
3	D3	76	THR
3	D3	83	CYS
3	D3	105	ILE
3	E3	37	LYS
3	E3	40	ASP
3	E3	76	THR
3	E3	105	ILE
2	F3	3	LYS
2	F3	23	THR
2	F3	78	THR
2	F3	110	GLU
2	F3	117	ASP
2	F3	141	HIS
2	G3	113	LEU
2	G3	118	GLU
2	H3	78	THR
2	H3	117	ASP
2	H3	141	HIS
2	I3	78	THR
2	I3	113	LEU
3	J3	37	LYS
3	J3	105	ILE
2	K3	105	THR
3	L3	25	LEU
3	L3	40	ASP
3	L3	87	MET
3	L3	105	ILE
3	M3	105	ILE
3	M3	119	LEU

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Mol	Chain	Res	Type
2	N3	113	LEU
2	N3	117	ASP
2	N3	141	HIS
2	N3	146	ASP
3	O3	25	LEU
3	O3	76	THR
3	O3	105	ILE
3	O3	150	THR
3	P3	37	LYS
3	P3	83	CYS
3	P3	105	ILE
3	Q3	37	LYS
3	Q3	105	ILE
3	Q3	108	ASP
3	Q3	130	GLU
2	R3	4	THR
2	R3	14	ASP
2	R3	78	THR
2	R3	113	LEU
2	R3	117	ASP
2	S3	23	THR
2	S3	78	THR
2	T3	78	THR
2	T3	84	LYS
2	T3	117	ASP
2	U3	78	THR
2	U3	141	HIS
3	V3	9	VAL
3	V3	36	ASN
3	V3	105	ILE
2	W3	117	ASP
2	W3	118	GLU
2	W3	141	HIS
3	X3	7	THR
3	X3	9	VAL
3	X3	83	CYS
4	Y3	231	VAL
5	Z3	49	ILE
5	Z3	71	ASP
5	Z3	141	GLU
5	Z3	207	VAL
5	Z3	212	VAL

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Mol	Chain	Res	Type
5	Z3	253	VAL
3	a3	40	ASP
3	a3	105	ILE
3	a3	150	THR
2	B4	23	THR
2	B4	141	HIS
3	C4	2	THR
3	C4	40	ASP
3	C4	105	ILE
3	C4	150	THR
3	D4	40	ASP
3	D4	76	THR
3	E4	8	LYS
3	E4	37	LYS
3	E4	40	ASP
3	E4	76	THR
3	E4	105	ILE
2	F4	3	LYS
2	F4	78	THR
2	G4	113	LEU
2	G4	118	GLU
2	H4	4	THR
2	H4	78	THR
2	H4	141	HIS
2	I4	10	VAL
2	I4	68	THR
2	I4	78	THR
2	I4	117	ASP
3	J4	40	ASP
3	J4	105	ILE
3	J4	116	GLU
2	K4	105	THR
2	K4	141	HIS
3	L4	40	ASP
3	L4	105	ILE
3	L4	114	LEU
3	M4	105	ILE
3	M4	110	CYS
3	M4	119	LEU
2	N4	23	THR
2	N4	78	THR
2	N4	113	LEU

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Mol	Chain	Res	Type
2	N4	118	GLU
2	N4	141	HIS
3	O4	25	LEU
3	O4	76	THR
3	O4	83	CYS
3	O4	105	ILE
3	O4	150	THR
3	P4	37	LYS
3	P4	40	ASP
3	P4	83	CYS
3	P4	105	ILE
3	Q4	34	GLU
3	Q4	37	LYS
3	Q4	39	ILE
3	Q4	40	ASP
3	Q4	105	ILE
2	R4	4	THR
2	R4	78	THR
2	R4	113	LEU
2	S4	78	THR
2	S4	141	HIS
2	T4	84	LYS
2	U4	10	VAL
2	U4	78	THR
3	V4	36	ASN
3	V4	105	ILE
2	W4	118	GLU
3	X4	7	THR
3	X4	105	ILE
4	Y4	234	ARG
4	Y4	237	ASN
4	Y4	240	ARG
5	Z4	49	ILE
5	Z4	141	GLU
5	Z4	207	VAL
5	Z4	253	VAL
3	a4	117	THR
3	a4	150	THR
2	B5	10	VAL
2	B5	26	GLN
2	B5	141	HIS
3	C5	2	THR

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Mol	Chain	Res	Type
3	C5	40	ASP
3	C5	105	ILE
3	C5	150	THR
3	D5	37	LYS
3	D5	40	ASP
3	D5	76	THR
3	D5	83	CYS
3	D5	105	ILE
3	E5	37	LYS
3	E5	40	ASP
3	E5	76	THR
3	E5	105	ILE
2	F5	3	LYS
2	F5	23	THR
2	F5	78	THR
2	F5	141	HIS
2	G5	10	VAL
2	G5	113	LEU
2	G5	119	ILE
2	H5	4	THR
2	H5	10	VAL
2	H5	78	THR
2	H5	141	HIS
2	I5	68	THR
2	I5	78	THR
3	J5	40	ASP
3	J5	105	ILE
3	J5	116	GLU
2	K5	10	VAL
2	K5	105	THR
2	K5	141	HIS
3	L5	25	LEU
3	L5	40	ASP
3	L5	76	THR
3	L5	83	CYS
3	L5	172	VAL
3	M5	105	ILE
3	M5	110	CYS
3	M5	119	LEU
2	N5	10	VAL
2	N5	23	THR
2	N5	78	THR

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Mol	Chain	Res	Type
2	N5	113	LEU
2	N5	118	GLU
2	N5	141	HIS
3	O5	40	ASP
3	O5	76	THR
3	O5	105	ILE
3	O5	150	THR
3	P5	37	LYS
3	P5	40	ASP
3	P5	83	CYS
3	P5	105	ILE
3	Q5	37	LYS
3	Q5	39	ILE
3	Q5	40	ASP
3	Q5	105	ILE
2	R5	4	THR
2	R5	10	VAL
2	R5	113	LEU
2	S5	78	THR
2	S5	128	SER
2	S5	141	HIS
2	T5	84	LYS
2	U5	78	THR
3	V5	36	ASN
3	V5	105	ILE
2	W5	112	LEU
2	W5	118	GLU
2	W5	119	ILE
3	X5	7	THR
3	X5	20	LEU
3	X5	172	VAL
4	Y5	228	GLN
4	Y5	231	VAL
4	Y5	240	ARG
4	Y5	271	THR
5	Z5	49	ILE
5	Z5	141	GLU
5	Z5	207	VAL
5	Z5	253	VAL
3	a5	83	CYS
3	a5	105	ILE
1	A6	14	ASN

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Mol	Chain	Res	Type
1	A6	33	THR
1	A6	127	LEU
1	A6	191	PHE
2	B6	23	THR
2	B6	24	GLU
2	B6	26	GLN
2	B6	141	HIS
3	C6	2	THR
3	C6	40	ASP
3	C6	105	ILE
3	C6	150	THR
3	C6	172	VAL
3	D6	76	THR
3	D6	83	CYS
3	E6	37	LYS
3	E6	40	ASP
3	E6	76	THR
3	E6	105	ILE
2	F6	3	LYS
2	F6	23	THR
2	F6	110	GLU
2	G6	25	LEU
2	G6	113	LEU
2	G6	119	ILE
2	H6	78	THR
2	H6	118	GLU
2	H6	124	ASP
2	H6	141	HIS
2	I6	78	THR
3	J6	40	ASP
3	J6	105	ILE
3	J6	116	GLU
2	K6	8	GLU
2	K6	10	VAL
2	K6	18	ARG
2	K6	105	THR
2	K6	141	HIS
3	L6	25	LEU
3	L6	87	MET
3	L6	105	ILE
3	L6	114	LEU
3	M6	110	CYS

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Mol	Chain	Res	Type
3	M6	119	LEU
2	N6	20	LEU
2	N6	78	THR
2	N6	113	LEU
2	N6	141	HIS
3	O6	76	THR
3	O6	83	CYS
3	O6	88	GLU
3	O6	105	ILE
3	O6	150	THR
3	P6	37	LYS
3	P6	83	CYS
3	P6	105	ILE
3	Q6	12	GLN
3	Q6	37	LYS
3	Q6	39	ILE
3	Q6	40	ASP
3	Q6	105	ILE
3	Q6	130	GLU
2	R6	4	THR
2	R6	78	THR
2	R6	113	LEU
2	S6	23	THR
2	S6	78	THR
2	S6	141	HIS
2	T6	78	THR
2	T6	84	LYS
2	U6	78	THR
2	U6	112	LEU
3	V6	36	ASN
3	V6	105	ILE
2	W6	118	GLU
3	X6	7	THR
3	X6	20	LEU
3	X6	172	VAL
4	Y6	228	GLN
4	Y6	231	VAL
5	Z6	49	ILE
5	Z6	141	GLU
5	Z6	207	VAL
5	Z6	253	VAL
3	a6	40	ASP

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Mol	Chain	Res	Type
3	a6	83	CYS
3	a6	105	ILE
3	a6	119	LEU
2	B7	23	THR
2	B7	26	GLN
3	C7	40	ASP
3	C7	105	ILE
3	D7	83	CYS
3	D7	105	ILE
3	E7	37	LYS
3	E7	40	ASP
3	E7	105	ILE
2	F7	3	LYS
2	F7	23	THR
2	F7	78	THR
2	F7	110	GLU
2	F7	117	ASP
2	G7	113	LEU
2	G7	118	GLU
2	H7	141	HIS
2	I7	4	THR
2	I7	68	THR
2	I7	78	THR
3	J7	2	THR
3	J7	105	ILE
2	K7	105	THR
3	L7	25	LEU
3	L7	40	ASP
3	L7	87	MET
3	L7	105	ILE
3	L7	114	LEU
3	M7	105	ILE
3	M7	119	LEU
2	N7	78	THR
2	N7	113	LEU
2	N7	117	ASP
3	O7	76	THR
3	O7	105	ILE
3	O7	150	THR
3	P7	31	LEU
3	P7	37	LYS
3	P7	40	ASP

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Mol	Chain	Res	Type
3	P7	105	ILE
3	Q7	37	LYS
3	Q7	105	ILE
3	Q7	108	ASP
3	Q7	130	GLU
2	R7	4	THR
2	R7	78	THR
2	R7	113	LEU
2	R7	117	ASP
2	S7	78	THR
2	T7	78	THR
2	T7	84	LYS
2	T7	117	ASP
2	U7	78	THR
2	U7	141	HIS
3	V7	9	VAL
3	V7	36	ASN
3	V7	105	ILE
2	W7	117	ASP
3	X7	7	THR
3	X7	9	VAL
3	X7	83	CYS
3	X7	105	ILE
4	Y7	231	VAL
5	Z7	49	ILE
5	Z7	141	GLU
5	Z7	207	VAL
5	Z7	212	VAL
5	Z7	253	VAL
3	a7	40	ASP
3	a7	105	ILE
3	a7	119	LEU
3	a7	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (155) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	56	HIS
3	C1	36	ASN
3	D1	43	ASN
3	D1	77	ASN
3	E1	77	ASN

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Mol	Chain	Res	Type
2	H1	73	ASN
2	I1	34	GLN
2	K1	140	ASN
3	L1	112	ASN
3	P1	43	ASN
3	Q1	147	ASN
2	S1	54	ASN
2	S1	73	ASN
2	T1	160	ASN
3	X1	147	ASN
3	a1	112	ASN
3	a1	147	ASN
6	02	44	GLN
1	22	56	HIS
1	22	106	GLN
1	32	106	GLN
1	42	56	HIS
1	52	106	GLN
8	A2	10	ASN
8	A2	47	ASN
9	H2	53	GLN
9	H2	57	GLN
8	K2	15	GLN
8	L2	130	GLN
10	N2	254	GLN
10	N2	420	GLN
10	N2	445	GLN
10	N2	600	ASN
10	N2	627	ASN
12	S2	80	GLN
8	T2	47	ASN
9	U2	41	GLN
9	W2	71	ASN
6	Y2	19	GLN
6	Z2	44	GLN
9	i2	53	GLN
9	i2	57	GLN
10	o2	30	GLN
10	o2	37	GLN
10	o2	63	ASN
10	o2	254	GLN
10	o2	255	GLN

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Mol	Chain	Res	Type
10	o2	294	GLN
10	o2	306	GLN
10	o2	445	GLN
10	o2	457	ASN
10	o2	520	GLN
10	o2	546	GLN
10	o2	600	ASN
10	o2	627	ASN
9	r2	10	ASN
8	u2	47	ASN
6	z2	44	GLN
2	B3	120	ASN
3	D3	48	ASN
3	E3	147	ASN
2	F3	160	ASN
2	H3	34	GLN
2	I3	120	ASN
3	J3	48	ASN
2	K3	140	ASN
2	N3	16	GLN
3	O3	77	ASN
2	S3	54	ASN
2	T3	34	GLN
2	T3	160	ASN
2	U3	140	ASN
2	U3	160	ASN
3	V3	77	ASN
2	W3	120	ASN
3	X3	77	ASN
4	Y3	225	GLN
3	a3	43	ASN
3	a3	112	ASN
2	B4	160	ASN
3	C4	77	ASN
3	D4	48	ASN
3	D4	77	ASN
2	G4	160	ASN
2	I4	120	ASN
3	L4	77	ASN
3	L4	147	ASN
3	O4	77	ASN
3	P4	24	GLN

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Mol	Chain	Res	Type
3	Q4	112	ASN
3	Q4	147	ASN
3	V4	77	ASN
2	W4	54	ASN
3	X4	77	ASN
3	X4	147	ASN
4	Y4	228	GLN
4	Y4	258	GLN
4	Y4	263	GLN
5	Z4	17	ASN
5	Z4	257	ASN
3	a4	64	GLN
3	a4	147	ASN
2	B5	120	ASN
3	C5	77	ASN
3	D5	43	ASN
3	D5	48	ASN
2	F5	47	ASN
2	H5	73	ASN
3	J5	48	ASN
2	K5	120	ASN
2	K5	140	ASN
3	L5	112	ASN
3	L5	147	ASN
3	O5	77	ASN
3	P5	24	GLN
3	Q5	112	ASN
2	U5	140	ASN
3	X5	24	GLN
4	Y5	263	GLN
5	Z5	17	ASN
3	a5	147	ASN
2	B6	120	ASN
3	C6	77	ASN
3	D6	43	ASN
3	D6	48	ASN
3	D6	77	ASN
3	E6	77	ASN
2	F6	160	ASN
2	I6	34	GLN
2	I6	120	ASN
3	J6	64	GLN

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Mol	Chain	Res	Type
3	M6	64	GLN
3	O6	77	ASN
3	O6	147	ASN
3	Q6	112	ASN
3	Q6	147	ASN
2	S6	73	ASN
4	Y6	254	ASN
5	Z6	269	ASN
3	D7	48	ASN
2	H7	73	ASN
2	I7	73	ASN
2	I7	120	ASN
3	J7	48	ASN
3	L7	147	ASN
3	O7	77	ASN
3	P7	24	GLN
2	U7	140	ASN
3	V7	77	ASN
2	W7	120	ASN
3	X7	12	GLN
3	X7	77	ASN
3	X7	147	ASN
5	Z7	17	ASN
3	a7	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

252 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	U2	201	-	46,46,46	6.27	23 (50%)	63,67,67	3.92	20 (31%)
13	CYC	w2	201	-	46,46,46	6.34	23 (50%)	63,67,67	3.92	16 (25%)
13	CYC	P7	201	-	46,46,46	6.30	22 (47%)	63,67,67	4.16	16 (25%)
13	CYC	o2	801	-	46,46,46	6.39	24 (52%)	63,67,67	4.42	14 (22%)
13	CYC	S2	201	-	46,46,46	6.34	23 (50%)	63,67,67	4.14	19 (30%)
13	CYC	a2	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.07	13 (20%)
13	CYC	I6	201	2	46,46,46	6.37	22 (47%)	63,67,67	3.99	14 (22%)
13	CYC	L1	201	-	46,46,46	6.33	23 (50%)	63,67,67	4.17	18 (28%)
13	CYC	F7	201	-	46,46,46	6.33	22 (47%)	63,67,67	4.08	14 (22%)
13	CYC	a5	201	-	46,46,46	6.29	23 (50%)	63,67,67	3.91	18 (28%)
13	CYC	A2	202	-	46,46,46	6.33	22 (47%)	63,67,67	4.13	14 (22%)
13	CYC	32	301	-	46,46,46	6.36	23 (50%)	63,67,67	3.93	17 (26%)
13	CYC	F6	202	-	46,46,46	6.36	22 (47%)	63,67,67	4.12	14 (22%)
13	CYC	v2	201	-	46,46,46	6.38	23 (50%)	63,67,67	3.98	18 (28%)
13	CYC	A2	201	-	46,46,46	6.34	22 (47%)	63,67,67	4.06	15 (23%)
13	CYC	M5	201	3	46,46,46	6.32	23 (50%)	63,67,67	4.03	18 (28%)
13	CYC	X4	201	3	46,46,46	6.28	23 (50%)	63,67,67	3.85	18 (28%)
13	CYC	Q5	202	-	46,46,46	6.37	22 (47%)	63,67,67	4.08	17 (26%)
13	CYC	S7	201	2	46,46,46	6.38	22 (47%)	63,67,67	3.84	15 (23%)
13	CYC	y2	201	-	46,46,46	6.32	23 (50%)	63,67,67	3.92	16 (25%)
13	CYC	W5	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.03	16 (25%)
13	CYC	E4	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.07	16 (25%)
13	CYC	C1	201	3	46,46,46	6.28	23 (50%)	63,67,67	3.92	16 (25%)
13	CYC	C5	202	-	46,46,46	6.38	22 (47%)	63,67,67	4.13	15 (23%)
13	CYC	Q6	201	-	46,46,46	6.36	22 (47%)	63,67,67	3.89	16 (25%)
13	CYC	T1	202	2	46,46,46	6.35	22 (47%)	63,67,67	4.06	14 (22%)
13	CYC	P3	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.14	14 (22%)
13	CYC	B1	201	2	46,46,46	6.37	23 (50%)	63,67,67	4.03	16 (25%)
13	CYC	J3	201	3	46,46,46	6.31	23 (50%)	63,67,67	4.03	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	C5	201	3	46,46,46	6.30	23 (50%)	63,67,67	3.90	17 (26%)
13	CYC	I7	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.11	14 (22%)
13	CYC	V7	201	3	46,46,46	6.31	23 (50%)	63,67,67	4.04	16 (25%)
13	CYC	C3	202	-	46,46,46	6.34	22 (47%)	63,67,67	4.16	15 (23%)
13	CYC	Q3	202	-	46,46,46	6.34	22 (47%)	63,67,67	4.12	15 (23%)
13	CYC	V3	201	3	46,46,46	6.33	23 (50%)	63,67,67	4.01	17 (26%)
13	CYC	T5	201	-	46,46,46	6.30	23 (50%)	63,67,67	4.13	15 (23%)
13	CYC	T6	202	2	46,46,46	6.35	22 (47%)	63,67,67	4.07	14 (22%)
13	CYC	T1	201	-	46,46,46	6.33	22 (47%)	63,67,67	4.00	15 (23%)
13	CYC	N2	801	-	46,46,46	6.33	23 (50%)	63,67,67	4.15	20 (31%)
13	CYC	a7	202	-	46,46,46	6.31	22 (47%)	63,67,67	3.98	15 (23%)
13	CYC	U3	201	2	46,46,46	6.30	23 (50%)	63,67,67	4.07	14 (22%)
13	CYC	J4	201	3	46,46,46	6.35	23 (50%)	63,67,67	3.99	18 (28%)
13	CYC	H5	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.11	16 (25%)
13	CYC	Q3	201	-	46,46,46	6.34	22 (47%)	63,67,67	3.96	14 (22%)
13	CYC	P4	201	-	46,46,46	6.34	23 (50%)	63,67,67	3.97	13 (20%)
13	CYC	W6	201	2	46,46,46	6.35	22 (47%)	63,67,67	4.11	15 (23%)
13	CYC	A1	302	-	46,46,46	6.39	23 (50%)	63,67,67	4.07	22 (34%)
13	CYC	J6	202	3	46,46,46	6.30	22 (47%)	63,67,67	4.03	15 (23%)
13	CYC	V1	202	3	46,46,46	6.32	23 (50%)	63,67,67	4.08	15 (23%)
13	CYC	W1	201	2	46,46,46	6.33	23 (50%)	63,67,67	4.18	17 (26%)
13	CYC	A6	301	-	46,46,46	6.37	23 (50%)	63,67,67	4.00	17 (26%)
13	CYC	R1	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.08	16 (25%)
13	CYC	H1	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.11	15 (23%)
13	CYC	C3	201	3	46,46,46	6.28	23 (50%)	63,67,67	3.96	16 (25%)
13	CYC	J5	202	3	46,46,46	6.31	22 (47%)	63,67,67	4.04	15 (23%)
13	CYC	42	301	-	46,46,46	6.39	23 (50%)	63,67,67	3.93	15 (23%)
13	CYC	U5	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.14	15 (23%)
13	CYC	C7	202	-	46,46,46	6.34	22 (47%)	63,67,67	4.18	12 (19%)
13	CYC	G6	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.05	15 (23%)
13	CYC	R6	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.07	15 (23%)
13	CYC	G7	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.17	15 (23%)
13	CYC	T4	201	-	46,46,46	6.30	22 (47%)	63,67,67	4.12	14 (22%)
13	CYC	B4	201	2	46,46,46	6.33	22 (47%)	63,67,67	4.03	14 (22%)
13	CYC	x2	201	9	46,46,46	6.37	23 (50%)	63,67,67	3.95	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	P7	202	-	46,46,46	6.36	22 (47%)	63,67,67	4.01	12 (19%)
13	CYC	N5	201	2	46,46,46	6.35	22 (47%)	63,67,67	4.03	15 (23%)
13	CYC	H6	201	2	46,46,46	6.32	23 (50%)	63,67,67	4.10	16 (25%)
13	CYC	F1	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.06	17 (26%)
13	CYC	22	302	-	46,46,46	6.38	22 (47%)	63,67,67	3.92	17 (26%)
13	CYC	S5	201	2	46,46,46	6.38	22 (47%)	63,67,67	3.84	17 (26%)
13	CYC	X6	201	3	46,46,46	6.32	23 (50%)	63,67,67	3.88	19 (30%)
13	CYC	a6	201	-	46,46,46	6.30	23 (50%)	63,67,67	3.93	18 (28%)
13	CYC	W7	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.12	13 (20%)
13	CYC	M7	201	3	46,46,46	6.33	23 (50%)	63,67,67	3.98	18 (28%)
13	CYC	U4	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.09	16 (25%)
13	CYC	H4	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.05	15 (23%)
13	CYC	X2	201	-	46,46,46	6.36	23 (50%)	63,67,67	3.97	17 (26%)
13	CYC	W3	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.10	13 (20%)
13	CYC	H2	201	-	46,46,46	6.28	22 (47%)	63,67,67	4.19	14 (22%)
13	CYC	K7	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.21	14 (22%)
13	CYC	K4	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.03	16 (25%)
13	CYC	M2	201	-	46,46,46	6.27	23 (50%)	63,67,67	3.95	17 (26%)
13	CYC	R5	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.05	16 (25%)
13	CYC	V5	201	3	46,46,46	6.34	23 (50%)	63,67,67	4.04	19 (30%)
13	CYC	W4	201	2	46,46,46	6.35	22 (47%)	63,67,67	4.04	15 (23%)
13	CYC	T3	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.06	13 (20%)
13	CYC	f2	201	9	46,46,46	6.36	23 (50%)	63,67,67	3.99	18 (28%)
13	CYC	V4	202	3	46,46,46	6.31	22 (47%)	63,67,67	4.08	16 (25%)
13	CYC	L6	201	-	46,46,46	6.32	23 (50%)	63,67,67	4.02	18 (28%)
13	CYC	P3	202	-	46,46,46	6.34	22 (47%)	63,67,67	3.99	13 (20%)
13	CYC	Z4	301	-	46,46,46	6.31	23 (50%)	63,67,67	3.93	18 (28%)
13	CYC	J3	202	3	46,46,46	6.30	22 (47%)	63,67,67	4.04	15 (23%)
13	CYC	t2	201	12	46,46,46	6.29	24 (52%)	63,67,67	3.89	19 (30%)
13	CYC	D6	201	-	46,46,46	6.32	23 (50%)	63,67,67	3.99	18 (28%)
13	CYC	a3	202	-	46,46,46	6.33	22 (47%)	63,67,67	3.94	15 (23%)
13	CYC	B7	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.02	13 (20%)
13	CYC	U6	201	2	46,46,46	6.37	22 (47%)	63,67,67	4.05	16 (25%)
13	CYC	T7	202	2	46,46,46	6.34	22 (47%)	63,67,67	4.08	14 (22%)
13	CYC	F3	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.07	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	Q4	201	-	46,46,46	6.36	22 (47%)	63,67,67	3.93	15 (23%)
13	CYC	g2	201	-	46,46,46	6.25	23 (50%)	63,67,67	3.90	17 (26%)
13	CYC	N3	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.15	15 (23%)
13	CYC	I1	201	2	46,46,46	6.38	22 (47%)	63,67,67	4.01	14 (22%)
13	CYC	l2	201	-	46,46,46	6.33	23 (50%)	63,67,67	3.96	20 (31%)
13	CYC	K3	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.14	15 (23%)
13	CYC	J1	201	3	46,46,46	6.35	23 (50%)	63,67,67	4.00	17 (26%)
13	CYC	p2	201	-	46,46,46	6.37	23 (50%)	63,67,67	4.02	19 (30%)
13	CYC	E2	201	-	46,46,46	6.38	23 (50%)	63,67,67	3.96	15 (23%)
13	CYC	K5	201	2	46,46,46	6.35	23 (50%)	63,67,67	4.01	16 (25%)
13	CYC	T2	201	-	46,46,46	6.37	24 (52%)	63,67,67	3.96	18 (28%)
13	CYC	N2	802	-	46,46,46	6.38	23 (50%)	63,67,67	4.23	16 (25%)
13	CYC	X7	201	3	46,46,46	6.37	23 (50%)	63,67,67	3.96	16 (25%)
13	CYC	B5	201	2	46,46,46	6.37	23 (50%)	63,67,67	4.04	14 (22%)
13	CYC	V1	201	3	46,46,46	6.37	23 (50%)	63,67,67	4.03	19 (30%)
13	CYC	S4	201	2	46,46,46	6.37	22 (47%)	63,67,67	3.86	15 (23%)
13	CYC	F3	202	-	46,46,46	6.34	22 (47%)	63,67,67	4.16	15 (23%)
13	CYC	Z7	301	-	46,46,46	6.31	22 (47%)	63,67,67	3.88	16 (25%)
13	CYC	I5	201	2	46,46,46	6.35	22 (47%)	63,67,67	4.04	13 (20%)
13	CYC	C4	202	-	46,46,46	6.37	22 (47%)	63,67,67	4.13	15 (23%)
13	CYC	N4	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.07	14 (22%)
13	CYC	Z1	301	-	46,46,46	6.31	23 (50%)	63,67,67	3.96	20 (31%)
13	CYC	L2	201	-	46,46,46	6.32	23 (50%)	63,67,67	3.95	15 (23%)
13	CYC	B6	201	2	46,46,46	6.37	22 (47%)	63,67,67	4.02	14 (22%)
13	CYC	22	301	-	46,46,46	6.35	23 (50%)	63,67,67	3.93	15 (23%)
13	CYC	B3	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.00	13 (20%)
13	CYC	P5	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.10	14 (22%)
13	CYC	H7	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.14	15 (23%)
13	CYC	Q7	202	-	46,46,46	6.33	22 (47%)	63,67,67	4.11	15 (23%)
13	CYC	S3	201	2	46,46,46	6.39	22 (47%)	63,67,67	3.82	15 (23%)
13	CYC	D3	201	-	46,46,46	6.29	22 (47%)	63,67,67	4.05	16 (25%)
13	CYC	a5	202	-	46,46,46	6.34	22 (47%)	63,67,67	3.98	17 (26%)
13	CYC	V2	201	-	46,46,46	6.33	23 (50%)	63,67,67	4.11	17 (26%)
13	CYC	G5	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.04	15 (23%)
13	CYC	T3	202	2	46,46,46	6.36	22 (47%)	63,67,67	4.08	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	F2	201	-	46,46,46	6.34	23 (50%)	63,67,67	3.93	17 (26%)
13	CYC	I3	201	2	46,46,46	6.32	22 (47%)	63,67,67	4.10	14 (22%)
13	CYC	D7	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.03	18 (28%)
13	CYC	P1	201	-	46,46,46	6.33	22 (47%)	63,67,67	4.06	16 (25%)
13	CYC	M3	201	3	46,46,46	6.34	23 (50%)	63,67,67	3.98	19 (30%)
13	CYC	D2	201	-	46,46,46	6.36	22 (47%)	63,67,67	3.98	16 (25%)
13	CYC	P6	202	-	46,46,46	6.34	23 (50%)	63,67,67	3.98	14 (22%)
13	CYC	Q5	201	-	46,46,46	6.39	22 (47%)	63,67,67	3.89	16 (25%)
13	CYC	P2	201	-	46,46,46	6.34	23 (50%)	63,67,67	4.00	20 (31%)
13	CYC	B2	202	-	46,46,46	6.26	22 (47%)	63,67,67	3.81	14 (22%)
13	CYC	Q2	201	-	46,46,46	6.37	22 (47%)	63,67,67	4.08	16 (25%)
13	CYC	a4	201	-	46,46,46	0.82	0	63,67,67	1.01	2 (3%)
13	CYC	E1	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.06	16 (25%)
13	CYC	G1	201	2	46,46,46	6.32	23 (50%)	63,67,67	4.14	16 (25%)
13	CYC	a6	202	-	46,46,46	6.33	22 (47%)	63,67,67	4.04	17 (26%)
13	CYC	d2	201	-	46,46,46	6.30	22 (47%)	63,67,67	4.08	13 (20%)
13	CYC	R3	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.01	15 (23%)
13	CYC	M6	201	3	46,46,46	6.32	23 (50%)	63,67,67	4.01	20 (31%)
13	CYC	A1	301	-	46,46,46	6.38	23 (50%)	63,67,67	4.00	19 (30%)
13	CYC	B2	201	-	46,46,46	6.36	22 (47%)	63,67,67	3.91	13 (20%)
13	CYC	D1	201	-	46,46,46	6.31	22 (47%)	63,67,67	3.92	18 (28%)
13	CYC	L7	201	-	46,46,46	6.33	23 (50%)	63,67,67	4.02	18 (28%)
13	CYC	L4	201	-	46,46,46	6.36	23 (50%)	63,67,67	3.94	16 (25%)
13	CYC	h2	201	-	46,46,46	6.36	23 (50%)	63,67,67	3.95	18 (28%)
13	CYC	F4	202	-	46,46,46	6.35	22 (47%)	63,67,67	4.11	16 (25%)
13	CYC	L5	201	-	46,46,46	6.36	23 (50%)	63,67,67	3.98	17 (26%)
13	CYC	J6	201	3	46,46,46	6.33	23 (50%)	63,67,67	3.99	17 (26%)
13	CYC	a1	202	-	46,46,46	6.34	22 (47%)	63,67,67	4.01	17 (26%)
13	CYC	S1	201	2	46,46,46	6.38	22 (47%)	63,67,67	3.85	17 (26%)
13	CYC	P6	201	-	46,46,46	6.34	22 (47%)	63,67,67	4.08	14 (22%)
13	CYC	C4	201	3	46,46,46	6.29	23 (50%)	63,67,67	3.89	17 (26%)
13	CYC	C7	201	3	46,46,46	6.27	23 (50%)	63,67,67	3.91	15 (23%)
13	CYC	L3	201	-	46,46,46	6.33	24 (52%)	63,67,67	4.03	19 (30%)
13	CYC	n2	201	-	46,46,46	6.32	23 (50%)	63,67,67	3.93	17 (26%)
13	CYC	E7	201	-	46,46,46	6.30	23 (50%)	63,67,67	4.12	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	H3	201	2	46,46,46	6.29	22 (47%)	63,67,67	4.11	15 (23%)
13	CYC	J7	202	3	46,46,46	6.32	22 (47%)	63,67,67	4.03	15 (23%)
13	CYC	Q1	202	-	46,46,46	6.37	22 (47%)	63,67,67	4.08	18 (28%)
13	CYC	T4	202	2	46,46,46	6.33	22 (47%)	63,67,67	4.08	14 (22%)
13	CYC	V7	202	3	46,46,46	6.29	22 (47%)	63,67,67	4.09	15 (23%)
13	CYC	Q1	201	-	46,46,46	6.37	22 (47%)	63,67,67	3.88	16 (25%)
13	CYC	K6	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.16	16 (25%)
13	CYC	V3	202	3	46,46,46	6.31	22 (47%)	63,67,67	4.05	16 (25%)
13	CYC	U1	201	2	46,46,46	6.32	23 (50%)	63,67,67	4.13	16 (25%)
13	CYC	N6	201	2	46,46,46	6.32	23 (50%)	63,67,67	4.15	15 (23%)
13	CYC	C6	201	3	46,46,46	6.27	23 (50%)	63,67,67	3.94	17 (26%)
13	CYC	C2	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.05	14 (22%)
13	CYC	a1	201	-	46,46,46	6.30	23 (50%)	63,67,67	3.96	21 (33%)
13	CYC	q2	201	-	46,46,46	0.82	1 (2%)	63,67,67	1.04	3 (4%)
13	CYC	K1	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.17	16 (25%)
13	CYC	k2	201	-	46,46,46	6.28	22 (47%)	63,67,67	4.21	15 (23%)
13	CYC	R2	201	-	46,46,46	6.38	23 (50%)	63,67,67	4.01	19 (30%)
13	CYC	G4	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.05	15 (23%)
13	CYC	F7	202	-	46,46,46	6.35	22 (47%)	63,67,67	4.15	15 (23%)
13	CYC	D4	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.00	19 (30%)
13	CYC	z2	201	-	46,46,46	6.29	23 (50%)	63,67,67	3.98	16 (25%)
13	CYC	Q4	202	-	46,46,46	6.35	22 (47%)	63,67,67	4.10	16 (25%)
13	CYC	R4	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.05	15 (23%)
13	CYC	52	302	-	46,46,46	6.36	23 (50%)	63,67,67	4.06	22 (34%)
13	CYC	s2	201	-	46,46,46	6.39	23 (50%)	63,67,67	4.02	17 (26%)
13	CYC	52	301	-	46,46,46	6.39	23 (50%)	63,67,67	3.96	17 (26%)
13	CYC	F4	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.09	17 (26%)
13	CYC	M4	201	3	46,46,46	6.33	23 (50%)	63,67,67	4.02	20 (31%)
13	CYC	T6	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.02	15 (23%)
13	CYC	J1	202	3	46,46,46	6.32	22 (47%)	63,67,67	3.99	15 (23%)
13	CYC	E5	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.05	16 (25%)
13	CYC	V6	202	3	46,46,46	6.30	22 (47%)	63,67,67	4.08	17 (26%)
13	CYC	a7	201	-	46,46,46	6.29	23 (50%)	63,67,67	3.91	16 (25%)
13	CYC	a3	201	-	46,46,46	6.29	23 (50%)	63,67,67	3.91	16 (25%)
13	CYC	e2	201	-	46,46,46	6.37	23 (50%)	63,67,67	3.99	19 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	V6	201	3	46,46,46	6.32	23 (50%)	63,67,67	4.05	18 (28%)
13	CYC	G3	201	2	46,46,46	6.31	22 (47%)	63,67,67	4.17	15 (23%)
13	CYC	F1	202	-	46,46,46	6.35	22 (47%)	63,67,67	4.10	14 (22%)
13	CYC	A6	302	-	46,46,46	6.38	23 (50%)	63,67,67	4.05	22 (34%)
13	CYC	S6	201	2	46,46,46	6.38	22 (47%)	63,67,67	3.84	17 (26%)
13	CYC	N1	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.13	16 (25%)
13	CYC	F5	202	-	46,46,46	6.36	22 (47%)	63,67,67	4.13	15 (23%)
13	CYC	I4	201	2	46,46,46	6.36	22 (47%)	63,67,67	3.99	14 (22%)
13	CYC	Z5	301	-	46,46,46	6.29	23 (50%)	63,67,67	3.92	19 (30%)
13	CYC	M1	201	3	46,46,46	6.33	23 (50%)	63,67,67	4.02	20 (31%)
13	CYC	Q6	202	-	46,46,46	6.36	22 (47%)	63,67,67	4.07	15 (23%)
13	CYC	G2	201	-	46,46,46	6.38	23 (50%)	63,67,67	4.03	17 (26%)
13	CYC	X3	201	3	46,46,46	6.36	23 (50%)	63,67,67	3.97	17 (26%)
13	CYC	J5	201	3	46,46,46	6.34	23 (50%)	63,67,67	4.00	18 (28%)
13	CYC	Z6	301	-	46,46,46	6.32	23 (50%)	63,67,67	3.97	19 (30%)
13	CYC	J7	201	3	46,46,46	6.31	23 (50%)	63,67,67	4.04	17 (26%)
13	CYC	V4	201	3	46,46,46	6.32	23 (50%)	63,67,67	4.03	17 (26%)
13	CYC	U7	201	2	46,46,46	6.29	22 (47%)	63,67,67	4.18	14 (22%)
13	CYC	F5	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.12	17 (26%)
13	CYC	a4	202	-	46,46,46	6.34	22 (47%)	63,67,67	3.95	17 (26%)
13	CYC	T5	202	2	46,46,46	6.34	22 (47%)	63,67,67	4.06	14 (22%)
13	CYC	32	302	-	46,46,46	6.37	22 (47%)	63,67,67	3.94	18 (28%)
13	CYC	c2	801	-	46,46,46	6.31	22 (47%)	63,67,67	3.99	13 (20%)
13	CYC	T7	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.06	13 (20%)
13	CYC	P1	202	-	46,46,46	6.35	23 (50%)	63,67,67	3.98	16 (25%)
13	CYC	r2	201	-	46,46,46	6.32	22 (47%)	63,67,67	4.03	17 (26%)
13	CYC	F6	201	-	46,46,46	6.37	22 (47%)	63,67,67	4.08	17 (26%)
13	CYC	R7	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.05	15 (23%)
13	CYC	j2	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.08	14 (22%)
13	CYC	J4	202	3	46,46,46	6.32	22 (47%)	63,67,67	4.03	16 (25%)
13	CYC	X5	201	3	46,46,46	6.27	23 (50%)	63,67,67	3.87	19 (30%)
13	CYC	V5	202	3	46,46,46	6.31	23 (50%)	63,67,67	4.10	15 (23%)
13	CYC	P4	202	-	46,46,46	6.35	22 (47%)	63,67,67	4.10	13 (20%)
13	CYC	O2	201	-	46,46,46	6.35	23 (50%)	63,67,67	3.96	18 (28%)
13	CYC	E3	201	-	46,46,46	6.30	23 (50%)	63,67,67	4.08	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	C1	202	-	46,46,46	6.40	22 (47%)	63,67,67	4.17	14 (22%)
13	CYC	N7	201	2	46,46,46	6.30	22 (47%)	63,67,67	4.17	15 (23%)
13	CYC	Q7	201	-	46,46,46	6.34	22 (47%)	63,67,67	3.97	14 (22%)
13	CYC	E6	201	-	46,46,46	6.32	23 (50%)	63,67,67	4.07	16 (25%)
13	CYC	i2	201	-	46,46,46	6.30	22 (47%)	63,67,67	4.00	16 (25%)
13	CYC	W2	201	-	46,46,46	6.31	22 (47%)	63,67,67	4.11	18 (28%)
13	CYC	D5	201	-	46,46,46	6.30	22 (47%)	63,67,67	3.94	18 (28%)
13	CYC	X1	201	3	46,46,46	6.31	23 (50%)	63,67,67	3.88	19 (30%)
13	CYC	P5	202	-	46,46,46	6.34	23 (50%)	63,67,67	3.97	15 (23%)
13	CYC	C6	202	-	46,46,46	6.36	22 (47%)	63,67,67	4.16	14 (22%)
13	CYC	m2	201	-	46,46,46	6.36	23 (50%)	63,67,67	3.95	16 (25%)
13	CYC	Z3	301	-	46,46,46	6.33	22 (47%)	63,67,67	3.88	16 (25%)
13	CYC	42	302	-	46,46,46	6.38	23 (50%)	63,67,67	3.93	21 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	U2	201	-	-	13/26/74/74	0/4/4/4
13	CYC	w2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	P7	201	-	-	18/26/74/74	0/4/4/4
13	CYC	o2	801	-	-	10/26/74/74	0/4/4/4
13	CYC	S2	201	-	-	15/26/74/74	0/4/4/4
13	CYC	a2	201	-	-	18/26/74/74	0/4/4/4
13	CYC	I6	201	2	-	12/26/74/74	0/4/4/4
13	CYC	L1	201	-	-	11/26/74/74	0/4/4/4
13	CYC	F7	201	-	-	14/26/74/74	0/4/4/4
13	CYC	a5	201	-	-	14/26/74/74	0/4/4/4
13	CYC	A2	202	-	-	12/26/74/74	0/4/4/4
13	CYC	32	301	-	-	14/26/74/74	0/4/4/4
13	CYC	F6	202	-	-	15/26/74/74	0/4/4/4
13	CYC	v2	201	-	-	13/26/74/74	0/4/4/4
13	CYC	A2	201	-	-	15/26/74/74	0/4/4/4
13	CYC	M5	201	3	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	X4	201	3	-	15/26/74/74	0/4/4/4
13	CYC	Q5	202	-	-	10/26/74/74	0/4/4/4
13	CYC	S7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	y2	201	-	-	11/26/74/74	0/4/4/4
13	CYC	W5	201	2	-	10/26/74/74	0/4/4/4
13	CYC	E4	201	-	-	18/26/74/74	0/4/4/4
13	CYC	C1	201	3	-	13/26/74/74	0/4/4/4
13	CYC	C5	202	-	-	15/26/74/74	0/4/4/4
13	CYC	Q6	201	-	-	13/26/74/74	0/4/4/4
13	CYC	T1	202	2	-	10/26/74/74	0/4/4/4
13	CYC	P3	201	-	-	19/26/74/74	0/4/4/4
13	CYC	B1	201	2	-	11/26/74/74	0/4/4/4
13	CYC	J3	201	3	-	10/26/74/74	0/4/4/4
13	CYC	C5	201	3	-	13/26/74/74	0/4/4/4
13	CYC	I7	201	2	-	11/26/74/74	0/4/4/4
13	CYC	V7	201	3	-	12/26/74/74	0/4/4/4
13	CYC	C3	202	-	-	18/26/74/74	0/4/4/4
13	CYC	Q3	202	-	-	15/26/74/74	0/4/4/4
13	CYC	V3	201	3	-	12/26/74/74	0/4/4/4
13	CYC	T5	201	-	-	18/26/74/74	0/4/4/4
13	CYC	T6	202	2	-	10/26/74/74	0/4/4/4
13	CYC	T1	201	-	-	18/26/74/74	0/4/4/4
13	CYC	N2	801	-	-	12/26/74/74	0/4/4/4
13	CYC	a7	202	-	-	16/26/74/74	0/4/4/4
13	CYC	U3	201	2	-	14/26/74/74	0/4/4/4
13	CYC	J4	201	3	-	13/26/74/74	0/4/4/4
13	CYC	H5	201	2	-	11/26/74/74	0/4/4/4
13	CYC	Q3	201	-	-	13/26/74/74	0/4/4/4
13	CYC	P4	201	-	-	14/26/74/74	0/4/4/4
13	CYC	W6	201	2	-	11/26/74/74	0/4/4/4
13	CYC	A1	302	-	-	11/26/74/74	0/4/4/4
13	CYC	J6	202	3	-	19/26/74/74	0/4/4/4
13	CYC	V1	202	3	-	21/26/74/74	0/4/4/4
13	CYC	W1	201	2	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	A6	301	-	-	14/26/74/74	0/4/4/4
13	CYC	R1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	H1	201	2	-	15/26/74/74	0/4/4/4
13	CYC	C3	201	3	-	13/26/74/74	0/4/4/4
13	CYC	J5	202	3	-	17/26/74/74	0/4/4/4
13	CYC	42	301	-	-	14/26/74/74	0/4/4/4
13	CYC	U5	201	2	-	13/26/74/74	0/4/4/4
13	CYC	C7	202	-	-	18/26/74/74	0/4/4/4
13	CYC	G6	201	2	-	12/26/74/74	0/4/4/4
13	CYC	R6	201	-	-	13/26/74/74	0/4/4/4
13	CYC	G7	201	2	-	13/26/74/74	0/4/4/4
13	CYC	T4	201	-	-	18/26/74/74	0/4/4/4
13	CYC	B4	201	2	-	11/26/74/74	0/4/4/4
13	CYC	x2	201	9	-	11/26/74/74	0/4/4/4
13	CYC	P7	202	-	-	16/26/74/74	0/4/4/4
13	CYC	N5	201	2	-	11/26/74/74	0/4/4/4
13	CYC	H6	201	2	-	13/26/74/74	0/4/4/4
13	CYC	F1	201	-	-	14/26/74/74	0/4/4/4
13	CYC	22	302	-	-	12/26/74/74	0/4/4/4
13	CYC	S5	201	2	-	12/26/74/74	0/4/4/4
13	CYC	X6	201	3	-	14/26/74/74	0/4/4/4
13	CYC	a6	201	-	-	13/26/74/74	0/4/4/4
13	CYC	W7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	M7	201	3	-	9/26/74/74	0/4/4/4
13	CYC	U4	201	2	-	13/26/74/74	0/4/4/4
13	CYC	H4	201	2	-	12/26/74/74	0/4/4/4
13	CYC	X2	201	-	-	14/26/74/74	0/4/4/4
13	CYC	W3	201	2	-	14/26/74/74	0/4/4/4
13	CYC	H2	201	-	-	15/26/74/74	0/4/4/4
13	CYC	K7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	K4	201	2	-	12/26/74/74	0/4/4/4
13	CYC	M2	201	-	-	11/26/74/74	0/4/4/4
13	CYC	R5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	V5	201	3	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	W4	201	2	-	12/26/74/74	0/4/4/4
13	CYC	T3	201	-	-	18/26/74/74	0/4/4/4
13	CYC	f2	201	9	-	9/26/74/74	0/4/4/4
13	CYC	V4	202	3	-	22/26/74/74	0/4/4/4
13	CYC	L6	201	-	-	11/26/74/74	0/4/4/4
13	CYC	P3	202	-	-	14/26/74/74	0/4/4/4
13	CYC	Z4	301	-	-	14/26/74/74	0/4/4/4
13	CYC	J3	202	3	-	19/26/74/74	0/4/4/4
13	CYC	t2	201	12	-	14/26/74/74	0/4/4/4
13	CYC	D6	201	-	-	14/26/74/74	0/4/4/4
13	CYC	a3	202	-	-	17/26/74/74	0/4/4/4
13	CYC	B7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	U6	201	2	-	11/26/74/74	0/4/4/4
13	CYC	T7	202	2	-	10/26/74/74	0/4/4/4
13	CYC	F3	201	-	-	14/26/74/74	0/4/4/4
13	CYC	Q4	201	-	-	13/26/74/74	0/4/4/4
13	CYC	g2	201	-	-	11/26/74/74	0/4/4/4
13	CYC	N3	201	2	-	15/26/74/74	0/4/4/4
13	CYC	I1	201	2	-	14/26/74/74	0/4/4/4
13	CYC	l2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	K3	201	2	-	14/26/74/74	0/4/4/4
13	CYC	J1	201	3	-	13/26/74/74	0/4/4/4
13	CYC	p2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	E2	201	-	-	14/26/74/74	0/4/4/4
13	CYC	K5	201	2	-	10/26/74/74	0/4/4/4
13	CYC	T2	201	-	-	11/26/74/74	0/4/4/4
13	CYC	N2	802	-	-	14/26/74/74	0/4/4/4
13	CYC	X7	201	3	-	13/26/74/74	0/4/4/4
13	CYC	B5	201	2	-	11/26/74/74	0/4/4/4
13	CYC	V1	201	3	-	12/26/74/74	0/4/4/4
13	CYC	S4	201	2	-	12/26/74/74	0/4/4/4
13	CYC	F3	202	-	-	14/26/74/74	0/4/4/4
13	CYC	Z7	301	-	-	16/26/74/74	0/4/4/4
13	CYC	I5	201	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	C4	202	-	-	17/26/74/74	0/4/4/4
13	CYC	N4	201	2	-	13/26/74/74	0/4/4/4
13	CYC	Z1	301	-	-	13/26/74/74	0/4/4/4
13	CYC	L2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	B6	201	2	-	12/26/74/74	0/4/4/4
13	CYC	22	301	-	-	15/26/74/74	0/4/4/4
13	CYC	B3	201	2	-	12/26/74/74	0/4/4/4
13	CYC	P5	201	-	-	20/26/74/74	0/4/4/4
13	CYC	H7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	Q7	202	-	-	15/26/74/74	0/4/4/4
13	CYC	S3	201	2	-	14/26/74/74	0/4/4/4
13	CYC	D3	201	-	-	20/26/74/74	0/4/4/4
13	CYC	a5	202	-	-	17/26/74/74	0/4/4/4
13	CYC	V2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	G5	201	2	-	12/26/74/74	0/4/4/4
13	CYC	T3	202	2	-	11/26/74/74	0/4/4/4
13	CYC	F2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	I3	201	2	-	10/26/74/74	0/4/4/4
13	CYC	D7	201	-	-	14/26/74/74	0/4/4/4
13	CYC	P1	201	-	-	19/26/74/74	0/4/4/4
13	CYC	M3	201	3	-	9/26/74/74	0/4/4/4
13	CYC	D2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	P6	202	-	-	13/26/74/74	0/4/4/4
13	CYC	Q5	201	-	-	13/26/74/74	0/4/4/4
13	CYC	P2	201	-	-	13/26/74/74	0/4/4/4
13	CYC	B2	202	-	-	16/26/74/74	0/4/4/4
13	CYC	Q2	201	-	-	17/26/74/74	0/4/4/4
13	CYC	a4	201	-	-	13/26/74/74	0/4/4/4
13	CYC	E1	201	-	-	18/26/74/74	0/4/4/4
13	CYC	G1	201	2	-	12/26/74/74	0/4/4/4
13	CYC	a6	202	-	-	18/26/74/74	0/4/4/4
13	CYC	d2	201	-	-	18/26/74/74	0/4/4/4
13	CYC	R3	201	-	-	12/26/74/74	0/4/4/4
13	CYC	M6	201	3	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	A1	301	-	-	14/26/74/74	0/4/4/4
13	CYC	B2	201	-	-	18/26/74/74	0/4/4/4
13	CYC	D1	201	-	-	11/26/74/74	0/4/4/4
13	CYC	L7	201	-	-	15/26/74/74	0/4/4/4
13	CYC	L4	201	-	-	14/26/74/74	0/4/4/4
13	CYC	h2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	F4	202	-	-	14/26/74/74	0/4/4/4
13	CYC	L5	201	-	-	14/26/74/74	0/4/4/4
13	CYC	J6	201	3	-	12/26/74/74	0/4/4/4
13	CYC	a1	202	-	-	19/26/74/74	0/4/4/4
13	CYC	S1	201	2	-	12/26/74/74	0/4/4/4
13	CYC	P6	201	-	-	20/26/74/74	0/4/4/4
13	CYC	C4	201	3	-	13/26/74/74	0/4/4/4
13	CYC	C7	201	3	-	13/26/74/74	0/4/4/4
13	CYC	L3	201	-	-	14/26/74/74	0/4/4/4
13	CYC	n2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	E7	201	-	-	19/26/74/74	0/4/4/4
13	CYC	H3	201	2	-	14/26/74/74	0/4/4/4
13	CYC	J7	202	3	-	19/26/74/74	0/4/4/4
13	CYC	Q1	202	-	-	10/26/74/74	0/4/4/4
13	CYC	T4	202	2	-	12/26/74/74	0/4/4/4
13	CYC	V7	202	3	-	22/26/74/74	0/4/4/4
13	CYC	Q1	201	-	-	11/26/74/74	0/4/4/4
13	CYC	K6	201	2	-	14/26/74/74	0/4/4/4
13	CYC	V3	202	3	-	22/26/74/74	0/4/4/4
13	CYC	U1	201	2	-	13/26/74/74	0/4/4/4
13	CYC	N6	201	2	-	12/26/74/74	0/4/4/4
13	CYC	C6	201	3	-	11/26/74/74	0/4/4/4
13	CYC	C2	201	-	-	14/26/74/74	0/4/4/4
13	CYC	a1	201	-	-	11/26/74/74	0/4/4/4
13	CYC	q2	201	-	-	16/26/74/74	0/4/4/4
13	CYC	K1	201	2	-	12/26/74/74	0/4/4/4
13	CYC	k2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	R2	201	-	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	G4	201	2	-	12/26/74/74	0/4/4/4
13	CYC	F7	202	-	-	15/26/74/74	0/4/4/4
13	CYC	D4	201	-	-	16/26/74/74	0/4/4/4
13	CYC	z2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	Q4	202	-	-	10/26/74/74	0/4/4/4
13	CYC	R4	201	-	-	13/26/74/74	0/4/4/4
13	CYC	52	302	-	-	10/26/74/74	0/4/4/4
13	CYC	s2	201	-	-	13/26/74/74	0/4/4/4
13	CYC	52	301	-	-	15/26/74/74	0/4/4/4
13	CYC	F4	201	-	-	13/26/74/74	0/4/4/4
13	CYC	M4	201	3	-	10/26/74/74	0/4/4/4
13	CYC	T6	201	-	-	19/26/74/74	0/4/4/4
13	CYC	J1	202	3	-	18/26/74/74	0/4/4/4
13	CYC	E5	201	-	-	18/26/74/74	0/4/4/4
13	CYC	V6	202	3	-	21/26/74/74	0/4/4/4
13	CYC	a7	201	-	-	13/26/74/74	0/4/4/4
13	CYC	a3	201	-	-	13/26/74/74	0/4/4/4
13	CYC	e2	201	-	-	15/26/74/74	0/4/4/4
13	CYC	V6	201	3	-	13/26/74/74	0/4/4/4
13	CYC	G3	201	2	-	13/26/74/74	0/4/4/4
13	CYC	F1	202	-	-	14/26/74/74	0/4/4/4
13	CYC	A6	302	-	-	10/26/74/74	0/4/4/4
13	CYC	S6	201	2	-	13/26/74/74	0/4/4/4
13	CYC	N1	201	2	-	12/26/74/74	0/4/4/4
13	CYC	F5	202	-	-	16/26/74/74	0/4/4/4
13	CYC	I4	201	2	-	13/26/74/74	0/4/4/4
13	CYC	Z5	301	-	-	13/26/74/74	0/4/4/4
13	CYC	M1	201	3	-	9/26/74/74	0/4/4/4
13	CYC	Q6	202	-	-	10/26/74/74	0/4/4/4
13	CYC	G2	201	-	-	15/26/74/74	0/4/4/4
13	CYC	X3	201	3	-	10/26/74/74	0/4/4/4
13	CYC	J5	201	3	-	9/26/74/74	0/4/4/4
13	CYC	Z6	301	-	-	13/26/74/74	0/4/4/4
13	CYC	J7	201	3	-	13/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	V4	201	3	-	13/26/74/74	0/4/4/4
13	CYC	U7	201	2	-	13/26/74/74	0/4/4/4
13	CYC	F5	201	-	-	13/26/74/74	0/4/4/4
13	CYC	a4	202	-	-	18/26/74/74	0/4/4/4
13	CYC	T5	202	2	-	10/26/74/74	0/4/4/4
13	CYC	32	302	-	-	11/26/74/74	0/4/4/4
13	CYC	c2	801	-	-	14/26/74/74	0/4/4/4
13	CYC	T7	201	-	-	19/26/74/74	0/4/4/4
13	CYC	P1	202	-	-	13/26/74/74	0/4/4/4
13	CYC	r2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	F6	201	-	-	16/26/74/74	0/4/4/4
13	CYC	R7	201	-	-	12/26/74/74	0/4/4/4
13	CYC	j2	201	-	-	16/26/74/74	0/4/4/4
13	CYC	J4	202	3	-	18/26/74/74	0/4/4/4
13	CYC	X5	201	3	-	13/26/74/74	0/4/4/4
13	CYC	V5	202	3	-	22/26/74/74	0/4/4/4
13	CYC	P4	202	-	-	19/26/74/74	0/4/4/4
13	CYC	O2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	E3	201	-	-	19/26/74/74	0/4/4/4
13	CYC	C1	202	-	-	15/26/74/74	0/4/4/4
13	CYC	N7	201	2	-	14/26/74/74	0/4/4/4
13	CYC	Q7	201	-	-	13/26/74/74	0/4/4/4
13	CYC	E6	201	-	-	18/26/74/74	0/4/4/4
13	CYC	i2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	W2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	D5	201	-	-	13/26/74/74	0/4/4/4
13	CYC	X1	201	3	-	13/26/74/74	0/4/4/4
13	CYC	P5	202	-	-	14/26/74/74	0/4/4/4
13	CYC	C6	202	-	-	17/26/74/74	0/4/4/4
13	CYC	m2	201	-	-	10/26/74/74	0/4/4/4
13	CYC	Z3	301	-	-	14/26/74/74	0/4/4/4
13	CYC	42	302	-	-	9/26/74/74	0/4/4/4

All (5615) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	p2	201	CYC	C2C-C1C	-26.26	1.28	1.52
13	o2	801	CYC	C2C-C1C	-26.19	1.28	1.52
13	B5	201	CYC	C2C-C1C	-26.17	1.28	1.52
13	B1	201	CYC	C2C-C1C	-26.16	1.28	1.52
13	42	302	CYC	C2C-C1C	-26.11	1.28	1.52
13	m2	201	CYC	C2C-C1C	-26.08	1.28	1.52
13	B6	201	CYC	C2C-C1C	-26.03	1.28	1.52
13	A1	302	CYC	C2C-C1C	-26.01	1.28	1.52
13	I1	201	CYC	C2C-C1C	-25.99	1.28	1.52
13	V1	201	CYC	C2C-C1C	-25.98	1.28	1.52
13	s2	201	CYC	C2C-C1C	-25.98	1.28	1.52
13	O2	201	CYC	C2C-C1C	-25.96	1.29	1.52
13	A6	302	CYC	C2C-C1C	-25.94	1.29	1.52
13	e2	201	CYC	C2C-C1C	-25.94	1.29	1.52
13	R2	201	CYC	C2C-C1C	-25.93	1.29	1.52
13	v2	201	CYC	C2C-C1C	-25.87	1.29	1.52
13	Q5	201	CYC	C2C-C1C	-25.87	1.29	1.52
13	S1	201	CYC	C2C-C1C	-25.87	1.29	1.52
13	C1	202	CYC	C2C-C1C	-25.85	1.29	1.52
13	E2	201	CYC	C2C-C1C	-25.84	1.29	1.52
13	G2	201	CYC	C2C-C1C	-25.83	1.29	1.52
13	I6	201	CYC	C2C-C1C	-25.83	1.29	1.52
13	S5	201	CYC	C2C-C1C	-25.82	1.29	1.52
13	I4	201	CYC	C2C-C1C	-25.81	1.29	1.52
13	w2	201	CYC	C2C-C1C	-25.78	1.29	1.52
13	h2	201	CYC	C2C-C1C	-25.76	1.29	1.52
13	a2	201	CYC	C2C-C1C	-25.75	1.29	1.52
13	F5	202	CYC	C2C-C1C	-25.75	1.29	1.52
13	52	302	CYC	C2C-C1C	-25.74	1.29	1.52
13	N2	802	CYC	C2C-C1C	-25.71	1.29	1.52
13	S4	201	CYC	C2C-C1C	-25.71	1.29	1.52
13	F6	202	CYC	C2C-C1C	-25.71	1.29	1.52
13	S6	201	CYC	C2C-C1C	-25.69	1.29	1.52
13	F1	202	CYC	C2C-C1C	-25.68	1.29	1.52
13	S3	201	CYC	C2C-C1C	-25.68	1.29	1.52
13	C5	202	CYC	C2C-C1C	-25.67	1.29	1.52
13	P5	201	CYC	C2C-C1C	-25.67	1.29	1.52
13	Q4	201	CYC	C2C-C1C	-25.67	1.29	1.52
13	F5	201	CYC	C2C-C1C	-25.66	1.29	1.52
13	F2	201	CYC	C2C-C1C	-25.65	1.29	1.52
13	52	301	CYC	C2C-C1C	-25.65	1.29	1.52
13	Q2	201	CYC	C2C-C1C	-25.63	1.29	1.52
13	F1	201	CYC	C2C-C1C	-25.63	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F4	202	CYC	C2C-C1C	-25.63	1.29	1.52
13	U6	201	CYC	C2C-C1C	-25.62	1.29	1.52
13	C4	202	CYC	C2C-C1C	-25.62	1.29	1.52
13	S7	201	CYC	C2C-C1C	-25.62	1.29	1.52
13	I5	201	CYC	C2C-C1C	-25.61	1.29	1.52
13	P7	202	CYC	C2C-C1C	-25.58	1.29	1.52
13	K5	201	CYC	C2C-C1C	-25.56	1.29	1.52
13	Q1	202	CYC	C2C-C1C	-25.55	1.29	1.52
13	F6	201	CYC	C2C-C1C	-25.54	1.29	1.52
13	P4	202	CYC	C2C-C1C	-25.54	1.29	1.52
13	l2	201	CYC	C2C-C1C	-25.53	1.29	1.52
13	C6	202	CYC	C2C-C1C	-25.53	1.29	1.52
13	Q1	201	CYC	C2C-C1C	-25.53	1.29	1.52
13	W4	201	CYC	C2C-C1C	-25.52	1.29	1.52
13	n2	201	CYC	C2C-C1C	-25.52	1.29	1.52
13	D2	201	CYC	C2C-C1C	-25.52	1.29	1.52
13	N5	201	CYC	C2C-C1C	-25.52	1.29	1.52
13	22	302	CYC	C2C-C1C	-25.51	1.29	1.52
13	L2	201	CYC	C2C-C1C	-25.51	1.29	1.52
13	A1	301	CYC	C2C-C1C	-25.50	1.29	1.52
13	F3	202	CYC	C2C-C1C	-25.50	1.29	1.52
13	W6	201	CYC	C2C-C1C	-25.49	1.29	1.52
13	A6	301	CYC	C2C-C1C	-25.49	1.29	1.52
13	42	301	CYC	C2C-C1C	-25.49	1.29	1.52
13	32	302	CYC	C2C-C1C	-25.49	1.29	1.52
13	Q5	202	CYC	C2C-C1C	-25.48	1.29	1.52
13	F7	202	CYC	C2C-C1C	-25.48	1.29	1.52
13	Q6	202	CYC	C2C-C1C	-25.47	1.29	1.52
13	P6	201	CYC	C2C-C1C	-25.47	1.29	1.52
13	Q6	201	CYC	C2C-C1C	-25.45	1.29	1.52
13	F4	201	CYC	C2C-C1C	-25.42	1.29	1.52
13	P1	201	CYC	C2C-C1C	-25.42	1.29	1.52
13	B4	201	CYC	C2C-C1C	-25.41	1.29	1.52
13	x2	201	CYC	C2C-C1C	-25.40	1.29	1.52
13	Q3	202	CYC	C2C-C1C	-25.38	1.29	1.52
13	V5	201	CYC	C2C-C1C	-25.37	1.29	1.52
13	T3	202	CYC	C2C-C1C	-25.36	1.29	1.52
13	R5	201	CYC	C2C-C1C	-25.36	1.29	1.52
13	T1	202	CYC	C2C-C1C	-25.36	1.29	1.52
13	R1	201	CYC	C2C-C1C	-25.36	1.29	1.52
13	T6	202	CYC	C2C-C1C	-25.34	1.29	1.52
13	S2	201	CYC	C2C-C1C	-25.33	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R3	201	CYC	C2C-C1C	-25.33	1.29	1.52
13	Q4	202	CYC	C2C-C1C	-25.33	1.29	1.52
13	K1	201	CYC	C2C-C1C	-25.32	1.29	1.52
13	C3	202	CYC	C2C-C1C	-25.31	1.29	1.52
13	R6	201	CYC	C2C-C1C	-25.31	1.29	1.52
13	G1	201	CYC	C2C-C1C	-25.31	1.29	1.52
13	T5	202	CYC	C2C-C1C	-25.31	1.29	1.52
13	y2	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	J1	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	X2	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	r2	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	R4	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	Q7	201	CYC	C2C-C1C	-25.30	1.29	1.52
13	M2	201	CYC	C2C-C1C	-25.29	1.29	1.52
13	T2	201	CYC	C2C-C1C	-25.27	1.29	1.52
13	F3	201	CYC	C2C-C1C	-25.27	1.29	1.52
13	J4	201	CYC	C2C-C1C	-25.27	1.29	1.52
13	P3	202	CYC	C2C-C1C	-25.27	1.29	1.52
13	I3	201	CYC	C2C-C1C	-25.26	1.29	1.52
13	P6	202	CYC	C2C-C1C	-25.26	1.29	1.52
13	j2	201	CYC	C2C-C1C	-25.26	1.29	1.52
13	C7	202	CYC	C2C-C1C	-25.25	1.29	1.52
13	W1	201	CYC	C2C-C1C	-25.25	1.29	1.52
13	K6	201	CYC	C2C-C1C	-25.25	1.29	1.52
13	Q3	201	CYC	C2C-C1C	-25.24	1.29	1.52
13	R7	201	CYC	C2C-C1C	-25.23	1.29	1.52
13	Z3	301	CYC	C2C-C1C	-25.22	1.29	1.52
13	W5	201	CYC	C2C-C1C	-25.22	1.29	1.52
13	N6	201	CYC	C2C-C1C	-25.22	1.29	1.52
13	A2	202	CYC	C2C-C1C	-25.22	1.29	1.52
13	V6	201	CYC	C2C-C1C	-25.22	1.29	1.52
13	V7	201	CYC	C2C-C1C	-25.21	1.29	1.52
13	P1	202	CYC	C2C-C1C	-25.21	1.29	1.52
13	f2	201	CYC	C2C-C1C	-25.21	1.29	1.52
13	G5	201	CYC	C2C-C1C	-25.20	1.29	1.52
13	K4	201	CYC	C2C-C1C	-25.20	1.29	1.52
13	T7	202	CYC	C2C-C1C	-25.18	1.29	1.52
13	V4	201	CYC	C2C-C1C	-25.18	1.29	1.52
13	z2	201	CYC	C2C-C1C	-25.18	1.29	1.52
13	P4	201	CYC	C2C-C1C	-25.18	1.29	1.52
13	P5	202	CYC	C2C-C1C	-25.17	1.29	1.52
13	N1	201	CYC	C2C-C1C	-25.17	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L5	201	CYC	C2C-C1C	-25.16	1.29	1.52
13	H5	201	CYC	C2C-C1C	-25.15	1.29	1.52
13	U5	201	CYC	C2C-C1C	-25.15	1.29	1.52
13	B7	201	CYC	C2C-C1C	-25.15	1.29	1.52
13	N2	801	CYC	C2C-C1C	-25.15	1.29	1.52
13	H1	201	CYC	C2C-C1C	-25.14	1.29	1.52
13	T4	202	CYC	C2C-C1C	-25.14	1.29	1.52
13	I7	201	CYC	C2C-C1C	-25.14	1.29	1.52
13	G4	201	CYC	C2C-C1C	-25.13	1.29	1.52
13	C2	201	CYC	C2C-C1C	-25.13	1.29	1.52
13	B3	201	CYC	C2C-C1C	-25.13	1.29	1.52
13	U1	201	CYC	C2C-C1C	-25.13	1.29	1.52
13	Q7	202	CYC	C2C-C1C	-25.12	1.29	1.52
13	P2	201	CYC	C2C-C1C	-25.11	1.29	1.52
13	V3	201	CYC	C2C-C1C	-25.11	1.29	1.52
13	H6	201	CYC	C2C-C1C	-25.11	1.29	1.52
13	V2	201	CYC	C2C-C1C	-25.10	1.29	1.52
13	L4	201	CYC	C2C-C1C	-25.10	1.29	1.52
13	N4	201	CYC	C2C-C1C	-25.10	1.29	1.52
13	W2	201	CYC	C2C-C1C	-25.08	1.29	1.52
13	Z7	301	CYC	C2C-C1C	-25.08	1.29	1.52
13	F7	201	CYC	C2C-C1C	-25.08	1.29	1.52
13	J6	201	CYC	C2C-C1C	-25.07	1.29	1.52
13	L1	201	CYC	C2C-C1C	-25.07	1.29	1.52
13	J5	201	CYC	C2C-C1C	-25.07	1.29	1.52
13	P3	201	CYC	C2C-C1C	-25.07	1.29	1.52
13	G6	201	CYC	C2C-C1C	-25.07	1.29	1.52
13	A2	201	CYC	C2C-C1C	-25.06	1.29	1.52
13	22	301	CYC	C2C-C1C	-25.05	1.29	1.52
13	32	301	CYC	C2C-C1C	-25.04	1.29	1.52
13	M4	201	CYC	C2C-C1C	-25.02	1.29	1.52
13	M5	201	CYC	C2C-C1C	-25.02	1.29	1.52
13	N3	201	CYC	C2C-C1C	-25.02	1.29	1.52
13	D6	201	CYC	C2C-C1C	-25.01	1.29	1.52
13	X7	201	CYC	C2C-C1C	-25.00	1.29	1.52
13	K3	201	CYC	C2C-C1C	-25.00	1.29	1.52
13	M1	201	CYC	C2C-C1C	-24.99	1.29	1.52
13	H4	201	CYC	C2C-C1C	-24.99	1.29	1.52
13	G3	201	CYC	C2C-C1C	-24.98	1.29	1.52
13	U4	201	CYC	C2C-C1C	-24.97	1.29	1.52
13	K7	201	CYC	C2C-C1C	-24.96	1.29	1.52
13	D7	201	CYC	C2C-C1C	-24.95	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P7	201	CYC	C2C-C1C	-24.94	1.29	1.52
13	X3	201	CYC	C2C-C1C	-24.94	1.29	1.52
13	M6	201	CYC	C2C-C1C	-24.93	1.29	1.52
13	D4	201	CYC	C2C-C1C	-24.92	1.29	1.52
13	a1	201	CYC	C2C-C1C	-24.92	1.29	1.52
13	L6	201	CYC	C2C-C1C	-24.90	1.29	1.52
13	J1	202	CYC	C2C-C1C	-24.89	1.29	1.52
13	L3	201	CYC	C2C-C1C	-24.88	1.29	1.52
13	G7	201	CYC	C2C-C1C	-24.88	1.29	1.52
13	V1	202	CYC	C2C-C1C	-24.88	1.29	1.52
13	B2	201	CYC	C2C-C1C	-24.87	1.29	1.52
13	T1	201	CYC	C2C-C1C	-24.87	1.29	1.52
13	H7	201	CYC	C2C-C1C	-24.87	1.29	1.52
13	E6	201	CYC	C2C-C1C	-24.87	1.29	1.52
13	N7	201	CYC	C2C-C1C	-24.87	1.29	1.52
13	M3	201	CYC	C2C-C1C	-24.86	1.29	1.52
13	a1	202	CYC	C2C-C1C	-24.86	1.29	1.52
13	U3	201	CYC	C2C-C1C	-24.86	1.29	1.52
13	a6	201	CYC	C2C-C1C	-24.85	1.29	1.52
13	H3	201	CYC	C2C-C1C	-24.85	1.29	1.52
13	c2	801	CYC	C2C-C1C	-24.84	1.30	1.52
13	d2	201	CYC	C2C-C1C	-24.83	1.30	1.52
13	J5	202	CYC	C2C-C1C	-24.82	1.30	1.52
13	a5	202	CYC	C2C-C1C	-24.82	1.30	1.52
13	Z1	301	CYC	C2C-C1C	-24.82	1.30	1.52
13	L7	201	CYC	C2C-C1C	-24.80	1.30	1.52
13	V5	202	CYC	C2C-C1C	-24.80	1.30	1.52
13	U7	201	CYC	C2C-C1C	-24.80	1.30	1.52
13	g2	201	CYC	C2C-C1C	-24.80	1.30	1.52
13	E1	201	CYC	C2C-C1C	-24.79	1.30	1.52
13	V4	202	CYC	C2C-C1C	-24.78	1.30	1.52
13	M7	201	CYC	C2C-C1C	-24.78	1.30	1.52
13	J4	202	CYC	C2C-C1C	-24.78	1.30	1.52
13	J7	201	CYC	C2C-C1C	-24.77	1.30	1.52
13	W7	201	CYC	C2C-C1C	-24.77	1.30	1.52
13	J7	202	CYC	C2C-C1C	-24.77	1.30	1.52
13	Z6	301	CYC	C2C-C1C	-24.76	1.30	1.52
13	a3	201	CYC	C2C-C1C	-24.76	1.30	1.52
13	J3	201	CYC	C2C-C1C	-24.76	1.30	1.52
13	W3	201	CYC	C2C-C1C	-24.75	1.30	1.52
13	a7	201	CYC	C2C-C1C	-24.75	1.30	1.52
13	H2	201	CYC	C2C-C1C	-24.74	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E4	201	CYC	C2C-C1C	-24.74	1.30	1.52
13	a6	202	CYC	C2C-C1C	-24.74	1.30	1.52
13	a5	201	CYC	C2C-C1C	-24.73	1.30	1.52
13	T5	201	CYC	C2C-C1C	-24.72	1.30	1.52
13	J6	202	CYC	C2C-C1C	-24.72	1.30	1.52
13	k2	201	CYC	C2C-C1C	-24.72	1.30	1.52
13	E5	201	CYC	C2C-C1C	-24.72	1.30	1.52
13	T6	201	CYC	C2C-C1C	-24.71	1.30	1.52
13	V6	202	CYC	C2C-C1C	-24.70	1.30	1.52
13	J3	202	CYC	C2C-C1C	-24.70	1.30	1.52
13	t2	201	CYC	C2C-C1C	-24.68	1.30	1.52
13	Z4	301	CYC	C2C-C1C	-24.68	1.30	1.52
13	D1	201	CYC	C2C-C1C	-24.66	1.30	1.52
13	V3	202	CYC	C2C-C1C	-24.66	1.30	1.52
13	C5	201	CYC	C2C-C1C	-24.66	1.30	1.52
13	T7	201	CYC	C2C-C1C	-24.66	1.30	1.52
13	C3	201	CYC	C2C-C1C	-24.65	1.30	1.52
13	D5	201	CYC	C2C-C1C	-24.65	1.30	1.52
13	T4	201	CYC	C2C-C1C	-24.63	1.30	1.52
13	T3	201	CYC	C2C-C1C	-24.63	1.30	1.52
13	a4	202	CYC	C2C-C1C	-24.61	1.30	1.52
13	C1	201	CYC	C2C-C1C	-24.60	1.30	1.52
13	X1	201	CYC	C2C-C1C	-24.59	1.30	1.52
13	Z5	301	CYC	C2C-C1C	-24.58	1.30	1.52
13	E7	201	CYC	C2C-C1C	-24.58	1.30	1.52
13	C6	201	CYC	C2C-C1C	-24.57	1.30	1.52
13	E3	201	CYC	C2C-C1C	-24.54	1.30	1.52
13	V7	202	CYC	C2C-C1C	-24.53	1.30	1.52
13	X6	201	CYC	C2C-C1C	-24.52	1.30	1.52
13	a3	202	CYC	C2C-C1C	-24.50	1.30	1.52
13	C4	201	CYC	C2C-C1C	-24.50	1.30	1.52
13	i2	201	CYC	C2C-C1C	-24.49	1.30	1.52
13	D3	201	CYC	C2C-C1C	-24.49	1.30	1.52
13	a7	202	CYC	C2C-C1C	-24.45	1.30	1.52
13	C7	201	CYC	C2C-C1C	-24.37	1.30	1.52
13	U2	201	CYC	C2C-C1C	-24.32	1.30	1.52
13	X4	201	CYC	C2C-C1C	-24.31	1.30	1.52
13	X5	201	CYC	C2C-C1C	-24.12	1.30	1.52
13	B2	202	CYC	C2C-C1C	-24.00	1.30	1.52
13	a4	202	CYC	C1C-NC	16.58	1.59	1.37
13	a3	202	CYC	C1C-NC	16.57	1.59	1.37
13	R7	201	CYC	C1C-NC	16.54	1.59	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	202	CYC	C1C-NC	16.52	1.59	1.37
13	a7	202	CYC	C1C-NC	16.52	1.59	1.37
13	a6	202	CYC	C1C-NC	16.49	1.59	1.37
13	T7	201	CYC	C1C-NC	16.49	1.59	1.37
13	T3	201	CYC	C1C-NC	16.49	1.59	1.37
13	B2	202	CYC	C1C-NC	16.46	1.59	1.37
13	a5	202	CYC	C1C-NC	16.44	1.59	1.37
13	R1	201	CYC	C1C-NC	16.39	1.59	1.37
13	R3	201	CYC	C1C-NC	16.38	1.59	1.37
13	i2	201	CYC	C1C-NC	16.38	1.59	1.37
13	R5	201	CYC	C1C-NC	16.37	1.59	1.37
13	T6	201	CYC	C1C-NC	16.37	1.59	1.37
13	T4	201	CYC	C1C-NC	16.36	1.59	1.37
13	E7	201	CYC	C1C-NC	16.36	1.59	1.37
13	F7	201	CYC	C1C-NC	16.36	1.59	1.37
13	R6	201	CYC	C1C-NC	16.35	1.59	1.37
13	R4	201	CYC	C1C-NC	16.35	1.59	1.37
13	B2	201	CYC	C1C-NC	16.34	1.59	1.37
13	F3	201	CYC	C1C-NC	16.34	1.59	1.37
13	T1	201	CYC	C1C-NC	16.34	1.59	1.37
13	F4	201	CYC	C1C-NC	16.33	1.59	1.37
13	d2	201	CYC	C1C-NC	16.33	1.59	1.37
13	E3	201	CYC	C1C-NC	16.33	1.59	1.37
13	V3	202	CYC	C1C-NC	16.33	1.59	1.37
13	J3	202	CYC	C1C-NC	16.32	1.59	1.37
13	T5	201	CYC	C1C-NC	16.32	1.59	1.37
13	J7	202	CYC	C1C-NC	16.32	1.59	1.37
13	22	302	CYC	C1C-NC	16.29	1.59	1.37
13	V4	202	CYC	C1C-NC	16.28	1.59	1.37
13	V6	202	CYC	C1C-NC	16.28	1.59	1.37
13	A2	201	CYC	C1C-NC	16.28	1.59	1.37
13	X3	201	CYC	C1C-NC	16.28	1.59	1.37
13	Q7	201	CYC	C1C-NC	16.28	1.59	1.37
13	Q3	201	CYC	C1C-NC	16.28	1.59	1.37
13	F6	201	CYC	C1C-NC	16.28	1.59	1.37
13	W3	201	CYC	C1C-NC	16.27	1.59	1.37
13	X7	201	CYC	C1C-NC	16.26	1.59	1.37
13	U6	201	CYC	C1C-NC	16.26	1.59	1.37
13	Q7	202	CYC	C1C-NC	16.26	1.59	1.37
13	U3	201	CYC	C1C-NC	16.25	1.59	1.37
13	T3	202	CYC	C1C-NC	16.25	1.59	1.37
13	Q6	202	CYC	C1C-NC	16.25	1.59	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T7	202	CYC	C1C-NC	16.25	1.59	1.37
13	C3	202	CYC	C1C-NC	16.25	1.59	1.37
13	J4	202	CYC	C1C-NC	16.24	1.59	1.37
13	B3	201	CYC	C1C-NC	16.24	1.59	1.37
13	Q5	202	CYC	C1C-NC	16.24	1.59	1.37
13	W7	201	CYC	C1C-NC	16.24	1.59	1.37
13	E6	201	CYC	C1C-NC	16.24	1.59	1.37
13	G6	201	CYC	C1C-NC	16.24	1.59	1.37
13	J1	202	CYC	C1C-NC	16.23	1.59	1.37
13	H4	201	CYC	C1C-NC	16.23	1.59	1.37
13	F1	201	CYC	C1C-NC	16.23	1.59	1.37
13	E4	201	CYC	C1C-NC	16.23	1.59	1.37
13	Q4	202	CYC	C1C-NC	16.23	1.59	1.37
13	B7	201	CYC	C1C-NC	16.23	1.59	1.37
13	M7	201	CYC	C1C-NC	16.23	1.59	1.37
13	V1	202	CYC	C1C-NC	16.22	1.59	1.37
13	V7	202	CYC	C1C-NC	16.22	1.59	1.37
13	Q6	201	CYC	C1C-NC	16.22	1.59	1.37
13	A2	202	CYC	C1C-NC	16.21	1.59	1.37
13	M3	201	CYC	C1C-NC	16.21	1.59	1.37
13	C7	202	CYC	C1C-NC	16.21	1.59	1.37
13	K3	201	CYC	C1C-NC	16.21	1.59	1.37
13	E5	201	CYC	C1C-NC	16.21	1.59	1.37
13	T2	201	CYC	C1C-NC	16.20	1.59	1.37
13	32	302	CYC	C1C-NC	16.20	1.59	1.37
13	32	301	CYC	C1C-NC	16.20	1.59	1.37
13	J6	202	CYC	C1C-NC	16.20	1.59	1.37
13	G5	201	CYC	C1C-NC	16.19	1.59	1.37
13	P4	201	CYC	C1C-NC	16.19	1.59	1.37
13	U7	201	CYC	C1C-NC	16.18	1.59	1.37
13	U4	201	CYC	C1C-NC	16.18	1.59	1.37
13	J5	202	CYC	C1C-NC	16.17	1.59	1.37
13	Q1	201	CYC	C1C-NC	16.17	1.59	1.37
13	L7	201	CYC	C1C-NC	16.17	1.58	1.37
13	W5	201	CYC	C1C-NC	16.17	1.58	1.37
13	E1	201	CYC	C1C-NC	16.17	1.58	1.37
13	W4	201	CYC	C1C-NC	16.17	1.58	1.37
13	Q1	202	CYC	C1C-NC	16.16	1.58	1.37
13	F5	201	CYC	C1C-NC	16.16	1.58	1.37
13	I7	201	CYC	C1C-NC	16.16	1.58	1.37
13	C1	202	CYC	C1C-NC	16.16	1.58	1.37
13	f2	201	CYC	C1C-NC	16.15	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I3	201	CYC	C1C-NC	16.15	1.58	1.37
13	Q4	201	CYC	C1C-NC	16.15	1.58	1.37
13	T4	202	CYC	C1C-NC	16.15	1.58	1.37
13	H7	201	CYC	C1C-NC	16.15	1.58	1.37
13	T5	202	CYC	C1C-NC	16.15	1.58	1.37
13	G4	201	CYC	C1C-NC	16.15	1.58	1.37
13	T1	202	CYC	C1C-NC	16.15	1.58	1.37
13	W6	201	CYC	C1C-NC	16.15	1.58	1.37
13	V5	202	CYC	C1C-NC	16.15	1.58	1.37
13	G7	201	CYC	C1C-NC	16.14	1.58	1.37
13	G3	201	CYC	C1C-NC	16.14	1.58	1.37
13	C4	202	CYC	C1C-NC	16.14	1.58	1.37
13	T6	202	CYC	C1C-NC	16.14	1.58	1.37
13	W1	201	CYC	C1C-NC	16.14	1.58	1.37
13	x2	201	CYC	C1C-NC	16.14	1.58	1.37
13	K7	201	CYC	C1C-NC	16.13	1.58	1.37
13	P1	202	CYC	C1C-NC	16.13	1.58	1.37
13	Q5	201	CYC	C1C-NC	16.13	1.58	1.37
13	X6	201	CYC	C1C-NC	16.13	1.58	1.37
13	D2	201	CYC	C1C-NC	16.13	1.58	1.37
13	X1	201	CYC	C1C-NC	16.12	1.58	1.37
13	C6	202	CYC	C1C-NC	16.12	1.58	1.37
13	22	301	CYC	C1C-NC	16.12	1.58	1.37
13	U1	201	CYC	C1C-NC	16.12	1.58	1.37
13	c2	801	CYC	C1C-NC	16.12	1.58	1.37
13	K5	201	CYC	C1C-NC	16.12	1.58	1.37
13	D1	201	CYC	C1C-NC	16.11	1.58	1.37
13	L3	201	CYC	C1C-NC	16.11	1.58	1.37
13	H6	201	CYC	C1C-NC	16.11	1.58	1.37
13	H2	201	CYC	C1C-NC	16.11	1.58	1.37
13	42	301	CYC	C1C-NC	16.11	1.58	1.37
13	N4	201	CYC	C1C-NC	16.11	1.58	1.37
13	M4	201	CYC	C1C-NC	16.11	1.58	1.37
13	Q3	202	CYC	C1C-NC	16.10	1.58	1.37
13	B4	201	CYC	C1C-NC	16.10	1.58	1.37
13	X2	201	CYC	C1C-NC	16.10	1.58	1.37
13	N5	201	CYC	C1C-NC	16.10	1.58	1.37
13	C5	202	CYC	C1C-NC	16.10	1.58	1.37
13	r2	201	CYC	C1C-NC	16.09	1.58	1.37
13	H3	201	CYC	C1C-NC	16.09	1.58	1.37
13	K4	201	CYC	C1C-NC	16.09	1.58	1.37
13	D3	201	CYC	C1C-NC	16.09	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q2	201	CYC	C1C-NC	16.09	1.58	1.37
13	N2	802	CYC	C1C-NC	16.09	1.58	1.37
13	F7	202	CYC	C1C-NC	16.08	1.58	1.37
13	J7	201	CYC	C1C-NC	16.08	1.58	1.37
13	P3	202	CYC	C1C-NC	16.07	1.58	1.37
13	P7	202	CYC	C1C-NC	16.07	1.58	1.37
13	L4	201	CYC	C1C-NC	16.07	1.58	1.37
13	L5	201	CYC	C1C-NC	16.07	1.58	1.37
13	P5	202	CYC	C1C-NC	16.07	1.58	1.37
13	U2	201	CYC	C1C-NC	16.07	1.58	1.37
13	D5	201	CYC	C1C-NC	16.07	1.58	1.37
13	N7	201	CYC	C1C-NC	16.06	1.58	1.37
13	S3	201	CYC	C1C-NC	16.06	1.58	1.37
13	k2	201	CYC	C1C-NC	16.06	1.58	1.37
13	W2	201	CYC	C1C-NC	16.05	1.58	1.37
13	s2	201	CYC	C1C-NC	16.04	1.58	1.37
13	U5	201	CYC	C1C-NC	16.04	1.58	1.37
13	F3	202	CYC	C1C-NC	16.04	1.58	1.37
13	S6	201	CYC	C1C-NC	16.04	1.58	1.37
13	E2	201	CYC	C1C-NC	16.04	1.58	1.37
13	N3	201	CYC	C1C-NC	16.04	1.58	1.37
13	I5	201	CYC	C1C-NC	16.04	1.58	1.37
13	S7	201	CYC	C1C-NC	16.03	1.58	1.37
13	J3	201	CYC	C1C-NC	16.03	1.58	1.37
13	P6	202	CYC	C1C-NC	16.03	1.58	1.37
13	X4	201	CYC	C1C-NC	16.02	1.58	1.37
13	F4	202	CYC	C1C-NC	16.01	1.58	1.37
13	H1	201	CYC	C1C-NC	16.01	1.58	1.37
13	M5	201	CYC	C1C-NC	16.01	1.58	1.37
13	N1	201	CYC	C1C-NC	16.01	1.58	1.37
13	M6	201	CYC	C1C-NC	16.01	1.58	1.37
13	F5	202	CYC	C1C-NC	15.99	1.58	1.37
13	X5	201	CYC	C1C-NC	15.98	1.58	1.37
13	I6	201	CYC	C1C-NC	15.98	1.58	1.37
13	v2	201	CYC	C1C-NC	15.98	1.58	1.37
13	G1	201	CYC	C1C-NC	15.98	1.58	1.37
13	K1	201	CYC	C1C-NC	15.97	1.58	1.37
13	J1	201	CYC	C1C-NC	15.97	1.58	1.37
13	N6	201	CYC	C1C-NC	15.97	1.58	1.37
13	H5	201	CYC	C1C-NC	15.97	1.58	1.37
13	M1	201	CYC	C1C-NC	15.97	1.58	1.37
13	G2	201	CYC	C1C-NC	15.96	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e2	201	CYC	C1C-NC	15.96	1.58	1.37
13	K6	201	CYC	C1C-NC	15.95	1.58	1.37
13	D7	201	CYC	C1C-NC	15.95	1.58	1.37
13	A1	301	CYC	C1C-NC	15.95	1.58	1.37
13	F2	201	CYC	C1C-NC	15.94	1.58	1.37
13	S4	201	CYC	C1C-NC	15.94	1.58	1.37
13	52	301	CYC	C1C-NC	15.94	1.58	1.37
13	J5	201	CYC	C1C-NC	15.94	1.58	1.37
13	I1	201	CYC	C1C-NC	15.94	1.58	1.37
13	J6	201	CYC	C1C-NC	15.93	1.58	1.37
13	A6	301	CYC	C1C-NC	15.93	1.58	1.37
13	R2	201	CYC	C1C-NC	15.93	1.58	1.37
13	F1	202	CYC	C1C-NC	15.93	1.58	1.37
13	D4	201	CYC	C1C-NC	15.93	1.58	1.37
13	n2	201	CYC	C1C-NC	15.92	1.58	1.37
13	D6	201	CYC	C1C-NC	15.92	1.58	1.37
13	l2	201	CYC	C1C-NC	15.91	1.58	1.37
13	F6	202	CYC	C1C-NC	15.90	1.58	1.37
13	S1	201	CYC	C1C-NC	15.90	1.58	1.37
13	h2	201	CYC	C1C-NC	15.90	1.58	1.37
13	J4	201	CYC	C1C-NC	15.90	1.58	1.37
13	C7	201	CYC	C1C-NC	15.89	1.58	1.37
13	P2	201	CYC	C1C-NC	15.88	1.58	1.37
13	C2	201	CYC	C1C-NC	15.87	1.58	1.37
13	B6	201	CYC	C1C-NC	15.86	1.58	1.37
13	L6	201	CYC	C1C-NC	15.86	1.58	1.37
13	S5	201	CYC	C1C-NC	15.86	1.58	1.37
13	P7	201	CYC	C1C-NC	15.84	1.58	1.37
13	V2	201	CYC	C1C-NC	15.84	1.58	1.37
13	I4	201	CYC	C1C-NC	15.83	1.58	1.37
13	y2	201	CYC	C1C-NC	15.83	1.58	1.37
13	L2	201	CYC	C1C-NC	15.82	1.58	1.37
13	N2	801	CYC	C1C-NC	15.82	1.58	1.37
13	C4	201	CYC	C1C-NC	15.82	1.58	1.37
13	j2	201	CYC	C1C-NC	15.81	1.58	1.37
13	a2	201	CYC	C1C-NC	15.81	1.58	1.37
13	V3	201	CYC	C1C-NC	15.80	1.58	1.37
13	P3	201	CYC	C1C-NC	15.79	1.58	1.37
13	V5	201	CYC	C1C-NC	15.79	1.58	1.37
13	B1	201	CYC	C1C-NC	15.78	1.58	1.37
13	t2	201	CYC	C1C-NC	15.78	1.58	1.37
13	V6	201	CYC	C1C-NC	15.77	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z7	301	CYC	C1C-NC	15.77	1.58	1.37
13	V4	201	CYC	C1C-NC	15.75	1.58	1.37
13	L1	201	CYC	C1C-NC	15.73	1.58	1.37
13	g2	201	CYC	C1C-NC	15.71	1.58	1.37
13	B5	201	CYC	C1C-NC	15.70	1.58	1.37
13	z2	201	CYC	C1C-NC	15.70	1.58	1.37
13	m2	201	CYC	C1C-NC	15.70	1.58	1.37
13	Z4	301	CYC	C1C-NC	15.68	1.58	1.37
13	C5	201	CYC	C1C-NC	15.68	1.58	1.37
13	a3	201	CYC	C1C-NC	15.68	1.58	1.37
13	P6	201	CYC	C1C-NC	15.68	1.58	1.37
13	C1	201	CYC	C1C-NC	15.68	1.58	1.37
13	P4	202	CYC	C1C-NC	15.67	1.58	1.37
13	Z5	301	CYC	C1C-NC	15.67	1.58	1.37
13	Z6	301	CYC	C1C-NC	15.67	1.58	1.37
13	V7	201	CYC	C1C-NC	15.66	1.58	1.37
13	C3	201	CYC	C1C-NC	15.65	1.58	1.37
13	Z3	301	CYC	C1C-NC	15.65	1.58	1.37
13	P1	201	CYC	C1C-NC	15.64	1.58	1.37
13	a7	201	CYC	C1C-NC	15.64	1.58	1.37
13	P5	201	CYC	C1C-NC	15.64	1.58	1.37
13	Z1	301	CYC	C1C-NC	15.61	1.58	1.37
13	C6	201	CYC	C1C-NC	15.58	1.58	1.37
13	o2	801	CYC	C1C-NC	15.58	1.58	1.37
13	a6	201	CYC	C1C-NC	15.56	1.58	1.37
13	a5	201	CYC	C1C-NC	15.55	1.58	1.37
13	52	302	CYC	C1C-NC	15.54	1.58	1.37
13	S2	201	CYC	C1C-NC	15.54	1.58	1.37
13	A1	302	CYC	C1C-NC	15.53	1.58	1.37
13	a1	201	CYC	C1C-NC	15.53	1.58	1.37
13	A6	302	CYC	C1C-NC	15.52	1.58	1.37
13	w2	201	CYC	C1C-NC	15.47	1.58	1.37
13	V1	201	CYC	C1C-NC	15.46	1.58	1.37
13	M2	201	CYC	C1C-NC	15.45	1.58	1.37
13	O2	201	CYC	C1C-NC	15.39	1.57	1.37
13	42	302	CYC	C1C-NC	15.33	1.57	1.37
13	p2	201	CYC	C1C-NC	15.20	1.57	1.37
13	A1	302	CYC	CHD-C4C	13.31	1.58	1.36
13	42	302	CYC	CHD-C4C	13.30	1.58	1.36
13	S7	201	CYC	CHD-C4C	13.29	1.58	1.36
13	S3	201	CYC	CHD-C4C	13.27	1.58	1.36
13	V3	201	CYC	CHD-C4C	13.27	1.58	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A6	302	CYC	CHD-C4C	13.27	1.58	1.36
13	52	302	CYC	CHD-C4C	13.25	1.58	1.36
13	T1	202	CYC	CHD-C4C	13.21	1.58	1.36
13	S5	201	CYC	CHD-C4C	13.19	1.58	1.36
13	P6	201	CYC	CHD-C4C	13.19	1.58	1.36
13	p2	201	CYC	CHD-C4C	13.18	1.58	1.36
13	V7	201	CYC	CHD-C4C	13.18	1.58	1.36
13	Z6	301	CYC	CHD-C4C	13.18	1.58	1.36
13	T6	202	CYC	CHD-C4C	13.17	1.58	1.36
13	P5	201	CYC	CHD-C4C	13.16	1.58	1.36
13	a4	202	CYC	CHD-C4C	13.16	1.58	1.36
13	V4	201	CYC	CHD-C4C	13.16	1.58	1.36
13	S6	201	CYC	CHD-C4C	13.15	1.58	1.36
13	Z4	301	CYC	CHD-C4C	13.15	1.58	1.36
13	P1	201	CYC	CHD-C4C	13.15	1.58	1.36
13	F7	202	CYC	CHD-C4C	13.14	1.58	1.36
13	V2	201	CYC	CHD-C4C	13.13	1.58	1.36
13	N3	201	CYC	CHD-C4C	13.13	1.58	1.36
13	P4	202	CYC	CHD-C4C	13.13	1.58	1.36
13	T7	202	CYC	CHD-C4C	13.13	1.58	1.36
13	N2	801	CYC	CHD-C4C	13.13	1.58	1.36
13	Z5	301	CYC	CHD-C4C	13.13	1.58	1.36
13	i2	201	CYC	CHD-C4C	13.13	1.58	1.36
13	S4	201	CYC	CHD-C4C	13.13	1.58	1.36
13	I6	201	CYC	CHD-C4C	13.12	1.58	1.36
13	C5	201	CYC	CHD-C4C	13.12	1.58	1.36
13	I4	201	CYC	CHD-C4C	13.12	1.58	1.36
13	S1	201	CYC	CHD-C4C	13.12	1.58	1.36
13	D3	201	CYC	CHD-C4C	13.12	1.58	1.36
13	B5	201	CYC	CHD-C4C	13.11	1.58	1.36
13	T4	202	CYC	CHD-C4C	13.11	1.58	1.36
13	T5	202	CYC	CHD-C4C	13.11	1.58	1.36
13	V5	201	CYC	CHD-C4C	13.10	1.58	1.36
13	a7	202	CYC	CHD-C4C	13.10	1.58	1.36
13	32	301	CYC	CHD-C4C	13.10	1.58	1.36
13	C1	202	CYC	CHD-C4C	13.10	1.58	1.36
13	V6	201	CYC	CHD-C4C	13.09	1.58	1.36
13	C4	201	CYC	CHD-C4C	13.09	1.58	1.36
13	V1	201	CYC	CHD-C4C	13.09	1.58	1.36
13	C4	202	CYC	CHD-C4C	13.09	1.58	1.36
13	C5	202	CYC	CHD-C4C	13.09	1.58	1.36
13	U6	201	CYC	CHD-C4C	13.09	1.58	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	w2	201	CYC	CHD-C4C	13.09	1.58	1.36
13	T3	202	CYC	CHD-C4C	13.08	1.58	1.36
13	a3	202	CYC	CHD-C4C	13.08	1.58	1.36
13	J1	201	CYC	CHD-C4C	13.08	1.58	1.36
13	P7	201	CYC	CHD-C4C	13.08	1.58	1.36
13	H5	201	CYC	CHD-C4C	13.07	1.58	1.36
13	I5	201	CYC	CHD-C4C	13.07	1.58	1.36
13	O2	201	CYC	CHD-C4C	13.07	1.58	1.36
13	L5	201	CYC	CHD-C4C	13.07	1.58	1.36
13	C3	201	CYC	CHD-C4C	13.07	1.58	1.36
13	P3	201	CYC	CHD-C4C	13.07	1.58	1.36
13	C3	202	CYC	CHD-C4C	13.07	1.58	1.36
13	L4	201	CYC	CHD-C4C	13.06	1.58	1.36
13	N7	201	CYC	CHD-C4C	13.06	1.58	1.36
13	P2	201	CYC	CHD-C4C	13.06	1.58	1.36
13	N6	201	CYC	CHD-C4C	13.05	1.58	1.36
13	C6	202	CYC	CHD-C4C	13.05	1.58	1.36
13	K5	201	CYC	CHD-C4C	13.05	1.58	1.36
13	G7	201	CYC	CHD-C4C	13.05	1.58	1.36
13	H6	201	CYC	CHD-C4C	13.04	1.58	1.36
13	J7	201	CYC	CHD-C4C	13.04	1.58	1.36
13	J4	201	CYC	CHD-C4C	13.04	1.58	1.36
13	T7	201	CYC	CHD-C4C	13.04	1.58	1.36
13	a6	202	CYC	CHD-C4C	13.04	1.58	1.36
13	G1	201	CYC	CHD-C4C	13.04	1.58	1.36
13	F6	202	CYC	CHD-C4C	13.04	1.58	1.36
13	J5	201	CYC	CHD-C4C	13.04	1.58	1.36
13	B1	201	CYC	CHD-C4C	13.04	1.58	1.36
13	J3	201	CYC	CHD-C4C	13.04	1.58	1.36
13	C7	201	CYC	CHD-C4C	13.04	1.58	1.36
13	W4	201	CYC	CHD-C4C	13.04	1.58	1.36
13	T6	201	CYC	CHD-C4C	13.03	1.58	1.36
13	I1	201	CYC	CHD-C4C	13.03	1.58	1.36
13	F3	202	CYC	CHD-C4C	13.03	1.58	1.36
13	22	301	CYC	CHD-C4C	13.03	1.58	1.36
13	a1	202	CYC	CHD-C4C	13.02	1.58	1.36
13	X6	201	CYC	CHD-C4C	13.02	1.58	1.36
13	T3	201	CYC	CHD-C4C	13.02	1.58	1.36
13	C7	202	CYC	CHD-C4C	13.02	1.58	1.36
13	M7	201	CYC	CHD-C4C	13.02	1.58	1.36
13	N5	201	CYC	CHD-C4C	13.01	1.58	1.36
13	F4	202	CYC	CHD-C4C	13.01	1.58	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U1	201	CYC	CHD-C4C	13.01	1.58	1.36
13	Z1	301	CYC	CHD-C4C	13.01	1.57	1.36
13	L1	201	CYC	CHD-C4C	13.01	1.57	1.36
13	G3	201	CYC	CHD-C4C	13.01	1.57	1.36
13	F5	202	CYC	CHD-C4C	13.01	1.57	1.36
13	H3	201	CYC	CHD-C4C	13.01	1.57	1.36
13	A1	301	CYC	CHD-C4C	13.00	1.57	1.36
13	a5	202	CYC	CHD-C4C	13.00	1.57	1.36
13	R6	201	CYC	CHD-C4C	13.00	1.57	1.36
13	Q4	202	CYC	CHD-C4C	13.00	1.57	1.36
13	V5	202	CYC	CHD-C4C	13.00	1.57	1.36
13	F1	202	CYC	CHD-C4C	13.00	1.57	1.36
13	L6	201	CYC	CHD-C4C	13.00	1.57	1.36
13	T1	201	CYC	CHD-C4C	13.00	1.57	1.36
13	W7	201	CYC	CHD-C4C	12.99	1.57	1.36
13	N4	201	CYC	CHD-C4C	12.99	1.57	1.36
13	H2	201	CYC	CHD-C4C	12.99	1.57	1.36
13	H7	201	CYC	CHD-C4C	12.99	1.57	1.36
13	U7	201	CYC	CHD-C4C	12.99	1.57	1.36
13	E5	201	CYC	CHD-C4C	12.99	1.57	1.36
13	H4	201	CYC	CHD-C4C	12.98	1.57	1.36
13	V7	202	CYC	CHD-C4C	12.98	1.57	1.36
13	M3	201	CYC	CHD-C4C	12.98	1.57	1.36
13	B6	201	CYC	CHD-C4C	12.98	1.57	1.36
13	W3	201	CYC	CHD-C4C	12.98	1.57	1.36
13	c2	801	CYC	CHD-C4C	12.98	1.57	1.36
13	X1	201	CYC	CHD-C4C	12.98	1.57	1.36
13	S2	201	CYC	CHD-C4C	12.97	1.57	1.36
13	V1	202	CYC	CHD-C4C	12.97	1.57	1.36
13	m2	201	CYC	CHD-C4C	12.97	1.57	1.36
13	R7	201	CYC	CHD-C4C	12.97	1.57	1.36
13	K3	201	CYC	CHD-C4C	12.97	1.57	1.36
13	a6	201	CYC	CHD-C4C	12.97	1.57	1.36
13	R4	201	CYC	CHD-C4C	12.97	1.57	1.36
13	Q3	202	CYC	CHD-C4C	12.97	1.57	1.36
13	W6	201	CYC	CHD-C4C	12.97	1.57	1.36
13	T5	201	CYC	CHD-C4C	12.97	1.57	1.36
13	X3	201	CYC	CHD-C4C	12.97	1.57	1.36
13	M6	201	CYC	CHD-C4C	12.97	1.57	1.36
13	B2	202	CYC	CHD-C4C	12.97	1.57	1.36
13	X7	201	CYC	CHD-C4C	12.96	1.57	1.36
13	E4	201	CYC	CHD-C4C	12.96	1.57	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C1	201	CYC	CHD-C4C	12.96	1.57	1.36
13	Q2	201	CYC	CHD-C4C	12.96	1.57	1.36
13	M1	201	CYC	CHD-C4C	12.96	1.57	1.36
13	X4	201	CYC	CHD-C4C	12.96	1.57	1.36
13	A6	301	CYC	CHD-C4C	12.96	1.57	1.36
13	B3	201	CYC	CHD-C4C	12.96	1.57	1.36
13	H1	201	CYC	CHD-C4C	12.96	1.57	1.36
13	K4	201	CYC	CHD-C4C	12.96	1.57	1.36
13	E7	201	CYC	CHD-C4C	12.96	1.57	1.36
13	U5	201	CYC	CHD-C4C	12.96	1.57	1.36
13	U3	201	CYC	CHD-C4C	12.95	1.57	1.36
13	X5	201	CYC	CHD-C4C	12.95	1.57	1.36
13	E1	201	CYC	CHD-C4C	12.95	1.57	1.36
13	R1	201	CYC	CHD-C4C	12.95	1.57	1.36
13	V3	202	CYC	CHD-C4C	12.95	1.57	1.36
13	B4	201	CYC	CHD-C4C	12.95	1.57	1.36
13	W1	201	CYC	CHD-C4C	12.95	1.57	1.36
13	V4	202	CYC	CHD-C4C	12.95	1.57	1.36
13	a5	201	CYC	CHD-C4C	12.95	1.57	1.36
13	Q1	202	CYC	CHD-C4C	12.95	1.57	1.36
13	B2	201	CYC	CHD-C4C	12.95	1.57	1.36
13	W5	201	CYC	CHD-C4C	12.95	1.57	1.36
13	V6	202	CYC	CHD-C4C	12.94	1.57	1.36
13	K6	201	CYC	CHD-C4C	12.94	1.57	1.36
13	N1	201	CYC	CHD-C4C	12.94	1.57	1.36
13	C6	201	CYC	CHD-C4C	12.94	1.57	1.36
13	T4	201	CYC	CHD-C4C	12.94	1.57	1.36
13	K7	201	CYC	CHD-C4C	12.94	1.57	1.36
13	Q5	202	CYC	CHD-C4C	12.94	1.57	1.36
13	J3	202	CYC	CHD-C4C	12.94	1.57	1.36
13	U4	201	CYC	CHD-C4C	12.94	1.57	1.36
13	L3	201	CYC	CHD-C4C	12.94	1.57	1.36
13	R5	201	CYC	CHD-C4C	12.93	1.57	1.36
13	J6	201	CYC	CHD-C4C	12.93	1.57	1.36
13	P3	202	CYC	CHD-C4C	12.93	1.57	1.36
13	K1	201	CYC	CHD-C4C	12.93	1.57	1.36
13	52	301	CYC	CHD-C4C	12.93	1.57	1.36
13	R3	201	CYC	CHD-C4C	12.93	1.57	1.36
13	Q1	201	CYC	CHD-C4C	12.93	1.57	1.36
13	Q6	202	CYC	CHD-C4C	12.92	1.57	1.36
13	F6	201	CYC	CHD-C4C	12.92	1.57	1.36
13	Q7	202	CYC	CHD-C4C	12.91	1.57	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	201	CYC	CHD-C4C	12.91	1.57	1.36
13	42	301	CYC	CHD-C4C	12.91	1.57	1.36
13	E6	201	CYC	CHD-C4C	12.91	1.57	1.36
13	E3	201	CYC	CHD-C4C	12.90	1.57	1.36
13	I3	201	CYC	CHD-C4C	12.90	1.57	1.36
13	J1	202	CYC	CHD-C4C	12.90	1.57	1.36
13	L7	201	CYC	CHD-C4C	12.90	1.57	1.36
13	M4	201	CYC	CHD-C4C	12.90	1.57	1.36
13	G6	201	CYC	CHD-C4C	12.89	1.57	1.36
13	J4	202	CYC	CHD-C4C	12.89	1.57	1.36
13	F3	201	CYC	CHD-C4C	12.89	1.57	1.36
13	F7	201	CYC	CHD-C4C	12.89	1.57	1.36
13	P1	202	CYC	CHD-C4C	12.89	1.57	1.36
13	G5	201	CYC	CHD-C4C	12.89	1.57	1.36
13	P4	201	CYC	CHD-C4C	12.88	1.57	1.36
13	J7	202	CYC	CHD-C4C	12.88	1.57	1.36
13	D6	201	CYC	CHD-C4C	12.88	1.57	1.36
13	P7	202	CYC	CHD-C4C	12.88	1.57	1.36
13	x2	201	CYC	CHD-C4C	12.87	1.57	1.36
13	a7	201	CYC	CHD-C4C	12.87	1.57	1.36
13	Q5	201	CYC	CHD-C4C	12.87	1.57	1.36
13	I7	201	CYC	CHD-C4C	12.87	1.57	1.36
13	P6	202	CYC	CHD-C4C	12.87	1.57	1.36
13	T2	201	CYC	CHD-C4C	12.87	1.57	1.36
13	Q6	201	CYC	CHD-C4C	12.86	1.57	1.36
13	D1	201	CYC	CHD-C4C	12.86	1.57	1.36
13	B7	201	CYC	CHD-C4C	12.86	1.57	1.36
13	G4	201	CYC	CHD-C4C	12.86	1.57	1.36
13	P5	202	CYC	CHD-C4C	12.85	1.57	1.36
13	D7	201	CYC	CHD-C4C	12.85	1.57	1.36
13	a3	201	CYC	CHD-C4C	12.84	1.57	1.36
13	J5	202	CYC	CHD-C4C	12.84	1.57	1.36
13	M5	201	CYC	CHD-C4C	12.83	1.57	1.36
13	Z3	301	CYC	CHD-C4C	12.83	1.57	1.36
13	A2	202	CYC	CHD-C4C	12.82	1.57	1.36
13	22	302	CYC	CHD-C4C	12.81	1.57	1.36
13	D4	201	CYC	CHD-C4C	12.81	1.57	1.36
13	G2	201	CYC	CHD-C4C	12.81	1.57	1.36
13	D2	201	CYC	CHD-C4C	12.80	1.57	1.36
13	W2	201	CYC	CHD-C4C	12.80	1.57	1.36
13	32	302	CYC	CHD-C4C	12.79	1.57	1.36
13	Z7	301	CYC	CHD-C4C	12.79	1.57	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D5	201	CYC	CHD-C4C	12.79	1.57	1.36
13	L2	201	CYC	CHD-C4C	12.78	1.57	1.36
13	Q7	201	CYC	CHD-C4C	12.78	1.57	1.36
13	Q4	201	CYC	CHD-C4C	12.78	1.57	1.36
13	d2	201	CYC	CHD-C4C	12.77	1.57	1.36
13	F2	201	CYC	CHD-C4C	12.77	1.57	1.36
13	N2	802	CYC	CHD-C4C	12.77	1.57	1.36
13	v2	201	CYC	CHD-C4C	12.76	1.57	1.36
13	J6	202	CYC	CHD-C4C	12.76	1.57	1.36
13	Q3	201	CYC	CHD-C4C	12.76	1.57	1.36
13	t2	201	CYC	CHD-C4C	12.76	1.57	1.36
13	F1	201	CYC	CHD-C4C	12.75	1.57	1.36
13	X2	201	CYC	CHD-C4C	12.74	1.57	1.36
13	A2	201	CYC	CHD-C4C	12.73	1.57	1.36
13	F4	201	CYC	CHD-C4C	12.72	1.57	1.36
13	U2	201	CYC	CHD-C4C	12.72	1.57	1.36
13	g2	201	CYC	CHD-C4C	12.72	1.57	1.36
13	z2	201	CYC	CHD-C4C	12.71	1.57	1.36
13	F5	201	CYC	CHD-C4C	12.71	1.57	1.36
13	R2	201	CYC	CHD-C4C	12.70	1.57	1.36
13	C2	201	CYC	CHD-C4C	12.70	1.57	1.36
13	f2	201	CYC	CHD-C4C	12.70	1.57	1.36
13	E2	201	CYC	CHD-C4C	12.70	1.57	1.36
13	k2	201	CYC	CHD-C4C	12.69	1.57	1.36
13	y2	201	CYC	CHD-C4C	12.67	1.57	1.36
13	s2	201	CYC	CHD-C4C	12.65	1.57	1.36
13	l2	201	CYC	CHD-C4C	12.64	1.57	1.36
13	r2	201	CYC	CHD-C4C	12.64	1.57	1.36
13	j2	201	CYC	CHD-C4C	12.60	1.57	1.36
13	o2	801	CYC	CHD-C4C	12.59	1.57	1.36
13	e2	201	CYC	CHD-C4C	12.58	1.57	1.36
13	a2	201	CYC	CHD-C4C	12.57	1.57	1.36
13	h2	201	CYC	CHD-C4C	12.55	1.57	1.36
13	M2	201	CYC	CHD-C4C	12.48	1.57	1.36
13	n2	201	CYC	CHD-C4C	12.45	1.57	1.36
13	S7	201	CYC	C4C-NC	11.36	1.59	1.37
13	S3	201	CYC	C4C-NC	11.35	1.59	1.37
13	C5	202	CYC	C4C-NC	11.31	1.59	1.37
13	C1	202	CYC	C4C-NC	11.31	1.59	1.37
13	C4	202	CYC	C4C-NC	11.30	1.59	1.37
13	S4	201	CYC	C4C-NC	11.26	1.59	1.37
13	C6	202	CYC	C4C-NC	11.25	1.59	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S6	201	CYC	C4C-NC	11.23	1.59	1.37
13	B2	201	CYC	C4C-NC	11.20	1.59	1.37
13	Q5	201	CYC	C4C-NC	11.18	1.59	1.37
13	E2	201	CYC	C4C-NC	11.17	1.59	1.37
13	S5	201	CYC	C4C-NC	11.16	1.59	1.37
13	F7	202	CYC	C4C-NC	11.16	1.58	1.37
13	Q1	201	CYC	C4C-NC	11.16	1.58	1.37
13	S1	201	CYC	C4C-NC	11.15	1.58	1.37
13	N2	802	CYC	C4C-NC	11.14	1.58	1.37
13	F6	202	CYC	C4C-NC	11.14	1.58	1.37
13	P7	202	CYC	C4C-NC	11.14	1.58	1.37
13	S7	201	CYC	OC-C1C	11.14	1.44	1.23
13	F4	202	CYC	C4C-NC	11.13	1.58	1.37
13	C7	202	CYC	C4C-NC	11.13	1.58	1.37
13	F1	202	CYC	C4C-NC	11.13	1.58	1.37
13	S3	201	CYC	OC-C1C	11.13	1.44	1.23
13	h2	201	CYC	C4C-NC	11.13	1.58	1.37
13	o2	801	CYC	C4C-NC	11.12	1.58	1.37
13	F5	202	CYC	C4C-NC	11.12	1.58	1.37
13	Q1	202	CYC	C4C-NC	11.11	1.58	1.37
13	v2	201	CYC	C4C-NC	11.11	1.58	1.37
13	G2	201	CYC	C4C-NC	11.11	1.58	1.37
13	C3	202	CYC	C4C-NC	11.10	1.58	1.37
13	R2	201	CYC	C4C-NC	11.10	1.58	1.37
13	F3	202	CYC	C4C-NC	11.10	1.58	1.37
13	Q4	201	CYC	C4C-NC	11.08	1.58	1.37
13	22	302	CYC	C4C-NC	11.08	1.58	1.37
13	32	302	CYC	C4C-NC	11.08	1.58	1.37
13	Q6	201	CYC	C4C-NC	11.08	1.58	1.37
13	S5	201	CYC	OC-C1C	11.08	1.44	1.23
13	B2	201	CYC	OC-C1C	11.08	1.44	1.23
13	X3	201	CYC	C4C-NC	11.08	1.58	1.37
13	C2	201	CYC	C4C-NC	11.07	1.58	1.37
13	Q3	202	CYC	C4C-NC	11.07	1.58	1.37
13	Q6	202	CYC	C4C-NC	11.06	1.58	1.37
13	X7	201	CYC	C4C-NC	11.06	1.58	1.37
13	S6	201	CYC	OC-C1C	11.05	1.44	1.23
13	P3	202	CYC	C4C-NC	11.05	1.58	1.37
13	s2	201	CYC	C4C-NC	11.05	1.58	1.37
13	I1	201	CYC	C4C-NC	11.05	1.58	1.37
13	Q2	201	CYC	C4C-NC	11.04	1.58	1.37
13	P5	201	CYC	C4C-NC	11.04	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q5	202	CYC	C4C-NC	11.04	1.58	1.37
13	Q4	202	CYC	C4C-NC	11.04	1.58	1.37
13	Q7	201	CYC	C4C-NC	11.04	1.58	1.37
13	Q3	201	CYC	C4C-NC	11.03	1.58	1.37
13	S4	201	CYC	OC-C1C	11.03	1.44	1.23
13	e2	201	CYC	C4C-NC	11.03	1.58	1.37
13	P4	202	CYC	C4C-NC	11.03	1.58	1.37
13	T3	202	CYC	C4C-NC	11.02	1.58	1.37
13	A2	202	CYC	C4C-NC	11.01	1.58	1.37
13	c2	801	CYC	OC-C1C	11.01	1.44	1.23
13	I6	201	CYC	C4C-NC	11.01	1.58	1.37
13	52	301	CYC	C4C-NC	11.00	1.58	1.37
13	S1	201	CYC	OC-C1C	11.00	1.44	1.23
13	B6	201	CYC	C4C-NC	11.00	1.58	1.37
13	F6	201	CYC	C4C-NC	10.99	1.58	1.37
13	I4	201	CYC	C4C-NC	10.99	1.58	1.37
13	a2	201	CYC	C4C-NC	10.98	1.58	1.37
13	22	301	CYC	C4C-NC	10.97	1.58	1.37
13	A2	201	CYC	C4C-NC	10.97	1.58	1.37
13	P3	201	CYC	C4C-NC	10.97	1.58	1.37
13	R3	201	CYC	C4C-NC	10.97	1.58	1.37
13	a3	202	CYC	C4C-NC	10.97	1.58	1.37
13	B1	201	CYC	C4C-NC	10.97	1.58	1.37
13	T7	202	CYC	C4C-NC	10.96	1.58	1.37
13	P6	201	CYC	C4C-NC	10.96	1.58	1.37
13	x2	201	CYC	C4C-NC	10.96	1.58	1.37
13	42	301	CYC	C4C-NC	10.96	1.58	1.37
13	F2	201	CYC	C4C-NC	10.95	1.58	1.37
13	P7	201	CYC	C4C-NC	10.95	1.58	1.37
13	B7	201	CYC	C4C-NC	10.95	1.58	1.37
13	P4	201	CYC	C4C-NC	10.95	1.58	1.37
13	T1	202	CYC	C4C-NC	10.95	1.58	1.37
13	M3	201	CYC	C4C-NC	10.94	1.58	1.37
13	32	301	CYC	C4C-NC	10.94	1.58	1.37
13	F1	201	CYC	C4C-NC	10.94	1.58	1.37
13	j2	201	CYC	C4C-NC	10.94	1.58	1.37
13	R7	201	CYC	C4C-NC	10.94	1.58	1.37
13	Q7	202	CYC	C4C-NC	10.94	1.58	1.37
13	R4	201	CYC	C4C-NC	10.93	1.58	1.37
13	a4	202	CYC	C4C-NC	10.93	1.58	1.37
13	F3	201	CYC	C4C-NC	10.93	1.58	1.37
13	m2	201	CYC	C4C-NC	10.93	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I5	201	CYC	C4C-NC	10.92	1.58	1.37
13	F4	201	CYC	C4C-NC	10.92	1.58	1.37
13	M7	201	CYC	C4C-NC	10.92	1.58	1.37
13	T7	201	CYC	C4C-NC	10.92	1.58	1.37
13	F5	201	CYC	C4C-NC	10.92	1.58	1.37
13	T6	202	CYC	C4C-NC	10.91	1.58	1.37
13	P1	201	CYC	C4C-NC	10.91	1.58	1.37
13	F7	201	CYC	C4C-NC	10.91	1.58	1.37
13	B3	201	CYC	C4C-NC	10.91	1.58	1.37
13	a5	202	CYC	C4C-NC	10.91	1.58	1.37
13	a7	202	CYC	C4C-NC	10.91	1.58	1.37
13	U6	201	CYC	C4C-NC	10.91	1.58	1.37
13	V3	202	CYC	C4C-NC	10.91	1.58	1.37
13	P6	202	CYC	C4C-NC	10.91	1.58	1.37
13	t2	201	CYC	C4C-NC	10.91	1.58	1.37
13	R5	201	CYC	C4C-NC	10.91	1.58	1.37
13	J4	201	CYC	C4C-NC	10.90	1.58	1.37
13	R6	201	CYC	C4C-NC	10.90	1.58	1.37
13	T4	202	CYC	C4C-NC	10.90	1.58	1.37
13	M4	201	CYC	C4C-NC	10.90	1.58	1.37
13	a7	201	CYC	OC-C1C	10.89	1.44	1.23
13	R1	201	CYC	C4C-NC	10.89	1.58	1.37
13	T5	202	CYC	C4C-NC	10.89	1.58	1.37
13	E3	201	CYC	C4C-NC	10.89	1.58	1.37
13	T3	201	CYC	C4C-NC	10.89	1.58	1.37
13	a1	202	CYC	C4C-NC	10.89	1.58	1.37
13	W2	201	CYC	C4C-NC	10.89	1.58	1.37
13	Q6	201	CYC	OC-C1C	10.89	1.44	1.23
13	Z4	301	CYC	OC-C1C	10.88	1.44	1.23
13	l2	201	CYC	C4C-NC	10.88	1.58	1.37
13	H2	201	CYC	OC-C1C	10.88	1.44	1.23
13	M3	201	CYC	OC-C1C	10.88	1.44	1.23
13	B5	201	CYC	C4C-NC	10.88	1.58	1.37
13	a3	202	CYC	OC-C1C	10.88	1.44	1.23
13	J7	202	CYC	OC-C1C	10.88	1.44	1.23
13	P5	202	CYC	C4C-NC	10.87	1.58	1.37
13	42	302	CYC	C4C-NC	10.87	1.58	1.37
13	Z3	301	CYC	OC-C1C	10.87	1.44	1.23
13	C2	201	CYC	OC-C1C	10.87	1.44	1.23
13	V7	202	CYC	OC-C1C	10.87	1.44	1.23
13	T2	201	CYC	C4C-NC	10.87	1.58	1.37
13	B4	201	CYC	C4C-NC	10.87	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	i2	201	CYC	C4C-NC	10.87	1.58	1.37
13	Z7	301	CYC	OC-C1C	10.87	1.44	1.23
13	22	302	CYC	OC-C1C	10.87	1.44	1.23
13	c2	801	CYC	C4C-NC	10.87	1.58	1.37
13	C4	201	CYC	OC-C1C	10.87	1.44	1.23
13	I3	201	CYC	C4C-NC	10.87	1.58	1.37
13	A1	301	CYC	C4C-NC	10.86	1.58	1.37
13	K4	201	CYC	C4C-NC	10.86	1.58	1.37
13	D2	201	CYC	C4C-NC	10.86	1.58	1.37
13	A6	301	CYC	C4C-NC	10.86	1.58	1.37
13	E7	201	CYC	C4C-NC	10.86	1.58	1.37
13	B2	202	CYC	OC-C1C	10.86	1.44	1.23
13	d2	201	CYC	C4C-NC	10.86	1.58	1.37
13	V1	202	CYC	C4C-NC	10.86	1.58	1.37
13	T6	201	CYC	OC-C1C	10.85	1.44	1.23
13	P7	201	CYC	OC-C1C	10.85	1.44	1.23
13	P1	202	CYC	C4C-NC	10.85	1.58	1.37
13	V3	202	CYC	OC-C1C	10.85	1.44	1.23
13	D3	201	CYC	OC-C1C	10.85	1.44	1.23
13	X5	201	CYC	OC-C1C	10.85	1.44	1.23
13	T4	201	CYC	C4C-NC	10.85	1.58	1.37
13	J7	202	CYC	C4C-NC	10.85	1.58	1.37
13	Z7	301	CYC	C4C-NC	10.85	1.58	1.37
13	n2	201	CYC	C4C-NC	10.85	1.58	1.37
13	w2	201	CYC	C4C-NC	10.85	1.58	1.37
13	a3	201	CYC	OC-C1C	10.85	1.44	1.23
13	H2	201	CYC	C4C-NC	10.85	1.58	1.37
13	y2	201	CYC	C4C-NC	10.85	1.58	1.37
13	J4	202	CYC	OC-C1C	10.84	1.44	1.23
13	t2	201	CYC	OC-C1C	10.84	1.44	1.23
13	a1	201	CYC	OC-C1C	10.84	1.44	1.23
13	a6	201	CYC	OC-C1C	10.84	1.44	1.23
13	L5	201	CYC	C4C-NC	10.84	1.58	1.37
13	E3	201	CYC	OC-C1C	10.84	1.44	1.23
13	U4	201	CYC	C4C-NC	10.84	1.58	1.37
13	X1	201	CYC	C4C-NC	10.84	1.58	1.37
13	Q3	202	CYC	OC-C1C	10.84	1.44	1.23
13	T7	201	CYC	OC-C1C	10.84	1.44	1.23
13	N7	201	CYC	C4C-NC	10.84	1.58	1.37
13	T6	201	CYC	C4C-NC	10.84	1.58	1.37
13	k2	201	CYC	C4C-NC	10.83	1.58	1.37
13	V4	202	CYC	C4C-NC	10.83	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E7	201	CYC	OC-C1C	10.83	1.44	1.23
13	B2	202	CYC	C4C-NC	10.83	1.58	1.37
13	j2	201	CYC	OC-C1C	10.83	1.44	1.23
13	X4	201	CYC	OC-C1C	10.83	1.44	1.23
13	a7	202	CYC	OC-C1C	10.83	1.44	1.23
13	Q3	201	CYC	OC-C1C	10.83	1.44	1.23
13	X2	201	CYC	C4C-NC	10.83	1.58	1.37
13	V1	202	CYC	OC-C1C	10.83	1.44	1.23
13	f2	201	CYC	C4C-NC	10.83	1.58	1.37
13	T1	201	CYC	OC-C1C	10.83	1.44	1.23
13	E5	201	CYC	OC-C1C	10.83	1.44	1.23
13	r2	201	CYC	C4C-NC	10.83	1.58	1.37
13	z2	201	CYC	OC-C1C	10.83	1.44	1.23
13	Q7	202	CYC	OC-C1C	10.83	1.44	1.23
13	H7	201	CYC	OC-C1C	10.83	1.44	1.23
13	K5	201	CYC	C4C-NC	10.83	1.58	1.37
13	K6	201	CYC	C4C-NC	10.83	1.58	1.37
13	C5	201	CYC	OC-C1C	10.83	1.44	1.23
13	X6	201	CYC	OC-C1C	10.83	1.44	1.23
13	F1	202	CYC	OC-C1C	10.82	1.44	1.23
13	L7	201	CYC	C4C-NC	10.82	1.58	1.37
13	a5	201	CYC	OC-C1C	10.82	1.44	1.23
13	M7	201	CYC	OC-C1C	10.82	1.44	1.23
13	P3	201	CYC	OC-C1C	10.82	1.44	1.23
13	P5	201	CYC	OC-C1C	10.82	1.44	1.23
13	U1	201	CYC	C4C-NC	10.82	1.58	1.37
13	H6	201	CYC	C4C-NC	10.82	1.58	1.37
13	C7	201	CYC	OC-C1C	10.82	1.44	1.23
13	E5	201	CYC	C4C-NC	10.82	1.58	1.37
13	P5	202	CYC	OC-C1C	10.82	1.44	1.23
13	P3	202	CYC	OC-C1C	10.82	1.44	1.23
13	D7	201	CYC	OC-C1C	10.82	1.44	1.23
13	a6	202	CYC	C4C-NC	10.82	1.58	1.37
13	i2	201	CYC	OC-C1C	10.82	1.44	1.23
13	E4	201	CYC	C4C-NC	10.82	1.58	1.37
13	F6	202	CYC	OC-C1C	10.81	1.44	1.23
13	U5	201	CYC	C4C-NC	10.81	1.58	1.37
13	W7	201	CYC	C4C-NC	10.81	1.58	1.37
13	O2	201	CYC	C4C-NC	10.81	1.58	1.37
13	T3	201	CYC	OC-C1C	10.81	1.44	1.23
13	Q7	201	CYC	OC-C1C	10.81	1.44	1.23
13	W4	201	CYC	C4C-NC	10.81	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E1	201	CYC	OC-C1C	10.81	1.44	1.23
13	X6	201	CYC	C4C-NC	10.81	1.58	1.37
13	K7	201	CYC	C4C-NC	10.81	1.58	1.37
13	Q1	202	CYC	OC-C1C	10.81	1.44	1.23
13	L2	201	CYC	C4C-NC	10.81	1.58	1.37
13	V4	202	CYC	OC-C1C	10.81	1.44	1.23
13	N5	201	CYC	C4C-NC	10.81	1.58	1.37
13	I7	201	CYC	C4C-NC	10.81	1.58	1.37
13	P4	202	CYC	OC-C1C	10.81	1.44	1.23
13	E6	201	CYC	OC-C1C	10.81	1.44	1.23
13	A2	202	CYC	OC-C1C	10.81	1.44	1.23
13	V6	202	CYC	OC-C1C	10.81	1.44	1.23
13	a2	201	CYC	OC-C1C	10.81	1.44	1.23
13	P6	202	CYC	OC-C1C	10.81	1.44	1.23
13	G3	201	CYC	C4C-NC	10.81	1.58	1.37
13	N3	201	CYC	C4C-NC	10.81	1.58	1.37
13	H3	201	CYC	OC-C1C	10.81	1.44	1.23
13	E4	201	CYC	OC-C1C	10.81	1.44	1.23
13	X7	201	CYC	OC-C1C	10.81	1.44	1.23
13	J3	202	CYC	OC-C1C	10.81	1.44	1.23
13	X4	201	CYC	C4C-NC	10.81	1.58	1.37
13	V4	201	CYC	OC-C1C	10.80	1.44	1.23
13	y2	201	CYC	OC-C1C	10.80	1.44	1.23
13	Q6	202	CYC	OC-C1C	10.80	1.44	1.23
13	Z6	301	CYC	OC-C1C	10.80	1.44	1.23
13	J7	201	CYC	OC-C1C	10.80	1.44	1.23
13	H4	201	CYC	C4C-NC	10.80	1.58	1.37
13	X3	201	CYC	OC-C1C	10.80	1.44	1.23
13	E6	201	CYC	C4C-NC	10.80	1.58	1.37
13	H3	201	CYC	C4C-NC	10.80	1.58	1.37
13	M4	201	CYC	OC-C1C	10.80	1.44	1.23
13	T5	201	CYC	C4C-NC	10.80	1.58	1.37
13	Q1	201	CYC	OC-C1C	10.80	1.44	1.23
13	T1	201	CYC	C4C-NC	10.80	1.58	1.37
13	L4	201	CYC	C4C-NC	10.80	1.58	1.37
13	A6	302	CYC	C4C-NC	10.80	1.58	1.37
13	M6	201	CYC	C4C-NC	10.80	1.58	1.37
13	L3	201	CYC	C4C-NC	10.80	1.58	1.37
13	N4	201	CYC	C4C-NC	10.80	1.58	1.37
13	C3	201	CYC	OC-C1C	10.80	1.44	1.23
13	J4	201	CYC	OC-C1C	10.80	1.44	1.23
13	A2	201	CYC	OC-C1C	10.79	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H5	201	CYC	C4C-NC	10.79	1.58	1.37
13	P2	201	CYC	OC-C1C	10.79	1.44	1.23
13	D7	201	CYC	C4C-NC	10.79	1.58	1.37
13	V5	201	CYC	OC-C1C	10.79	1.44	1.23
13	P1	202	CYC	OC-C1C	10.79	1.44	1.23
13	T2	201	CYC	OC-C1C	10.79	1.44	1.23
13	J6	202	CYC	OC-C1C	10.79	1.44	1.23
13	32	302	CYC	OC-C1C	10.79	1.44	1.23
13	V3	201	CYC	OC-C1C	10.79	1.44	1.23
13	D5	201	CYC	OC-C1C	10.79	1.44	1.23
13	F7	201	CYC	OC-C1C	10.79	1.44	1.23
13	W2	201	CYC	OC-C1C	10.79	1.44	1.23
13	F3	202	CYC	OC-C1C	10.79	1.44	1.23
13	Q5	202	CYC	OC-C1C	10.79	1.44	1.23
13	U3	201	CYC	C4C-NC	10.79	1.58	1.37
13	H1	201	CYC	OC-C1C	10.79	1.44	1.23
13	J1	202	CYC	C4C-NC	10.78	1.58	1.37
13	Z5	301	CYC	OC-C1C	10.78	1.44	1.23
13	J3	201	CYC	C4C-NC	10.78	1.58	1.37
13	H7	201	CYC	C4C-NC	10.78	1.58	1.37
13	V7	202	CYC	C4C-NC	10.78	1.58	1.37
13	V2	201	CYC	OC-C1C	10.78	1.44	1.23
13	k2	201	CYC	OC-C1C	10.78	1.44	1.23
13	G5	201	CYC	C4C-NC	10.78	1.58	1.37
13	P6	201	CYC	OC-C1C	10.78	1.44	1.23
13	F7	202	CYC	OC-C1C	10.78	1.44	1.23
13	P1	201	CYC	OC-C1C	10.78	1.44	1.23
13	M5	201	CYC	C4C-NC	10.78	1.58	1.37
13	N1	201	CYC	C4C-NC	10.78	1.58	1.37
13	F4	202	CYC	OC-C1C	10.78	1.44	1.23
13	W6	201	CYC	C4C-NC	10.78	1.58	1.37
13	J1	202	CYC	OC-C1C	10.78	1.44	1.23
13	V5	202	CYC	OC-C1C	10.78	1.44	1.23
13	T4	201	CYC	OC-C1C	10.77	1.44	1.23
13	M5	201	CYC	OC-C1C	10.77	1.44	1.23
13	Z1	301	CYC	OC-C1C	10.77	1.44	1.23
13	J7	201	CYC	C4C-NC	10.77	1.58	1.37
13	B7	201	CYC	OC-C1C	10.77	1.44	1.23
13	U1	201	CYC	OC-C1C	10.77	1.44	1.23
13	a4	202	CYC	OC-C1C	10.77	1.44	1.23
13	H1	201	CYC	C4C-NC	10.77	1.58	1.37
13	z2	201	CYC	C4C-NC	10.77	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V7	201	CYC	C4C-NC	10.77	1.58	1.37
13	H5	201	CYC	OC-C1C	10.77	1.44	1.23
13	P7	202	CYC	OC-C1C	10.77	1.44	1.23
13	S2	201	CYC	C4C-NC	10.77	1.58	1.37
13	D4	201	CYC	C4C-NC	10.77	1.58	1.37
13	V6	202	CYC	C4C-NC	10.77	1.58	1.37
13	N3	201	CYC	OC-C1C	10.77	1.44	1.23
13	W1	201	CYC	C4C-NC	10.77	1.58	1.37
13	N7	201	CYC	OC-C1C	10.77	1.44	1.23
13	W3	201	CYC	C4C-NC	10.77	1.58	1.37
13	D3	201	CYC	C4C-NC	10.77	1.58	1.37
13	G7	201	CYC	C4C-NC	10.77	1.58	1.37
13	T7	202	CYC	OC-C1C	10.77	1.44	1.23
13	V3	201	CYC	C4C-NC	10.77	1.58	1.37
13	J5	201	CYC	C4C-NC	10.77	1.58	1.37
13	J6	201	CYC	C4C-NC	10.77	1.58	1.37
13	N6	201	CYC	C4C-NC	10.77	1.58	1.37
13	J5	201	CYC	OC-C1C	10.77	1.44	1.23
13	A1	302	CYC	C4C-NC	10.76	1.58	1.37
13	K6	201	CYC	OC-C1C	10.76	1.44	1.23
13	J1	201	CYC	C4C-NC	10.76	1.58	1.37
13	K1	201	CYC	C4C-NC	10.76	1.58	1.37
13	Z3	301	CYC	C4C-NC	10.76	1.58	1.37
13	R3	201	CYC	OC-C1C	10.76	1.44	1.23
13	Q4	201	CYC	OC-C1C	10.76	1.44	1.23
13	M1	201	CYC	OC-C1C	10.76	1.44	1.23
13	U7	201	CYC	C4C-NC	10.76	1.58	1.37
13	G4	201	CYC	C4C-NC	10.76	1.58	1.37
13	C1	201	CYC	OC-C1C	10.76	1.44	1.23
13	J5	202	CYC	OC-C1C	10.76	1.44	1.23
13	J4	202	CYC	C4C-NC	10.76	1.58	1.37
13	D4	201	CYC	OC-C1C	10.76	1.44	1.23
13	P4	201	CYC	OC-C1C	10.76	1.44	1.23
13	d2	201	CYC	OC-C1C	10.76	1.44	1.23
13	Q4	202	CYC	OC-C1C	10.76	1.44	1.23
13	E1	201	CYC	C4C-NC	10.76	1.58	1.37
13	T4	202	CYC	OC-C1C	10.76	1.44	1.23
13	C6	201	CYC	OC-C1C	10.76	1.44	1.23
13	V7	201	CYC	OC-C1C	10.76	1.44	1.23
13	K3	201	CYC	C4C-NC	10.76	1.58	1.37
13	C3	202	CYC	OC-C1C	10.76	1.44	1.23
13	D6	201	CYC	C4C-NC	10.76	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X1	201	CYC	OC-C1C	10.76	1.44	1.23
13	J6	201	CYC	OC-C1C	10.76	1.44	1.23
13	H4	201	CYC	OC-C1C	10.76	1.44	1.23
13	C7	202	CYC	OC-C1C	10.76	1.44	1.23
13	J5	202	CYC	C4C-NC	10.75	1.58	1.37
13	w2	201	CYC	OC-C1C	10.75	1.44	1.23
13	S2	201	CYC	OC-C1C	10.75	1.44	1.23
13	M1	201	CYC	C4C-NC	10.75	1.58	1.37
13	Q5	201	CYC	OC-C1C	10.75	1.44	1.23
13	U3	201	CYC	OC-C1C	10.75	1.44	1.23
13	52	302	CYC	C4C-NC	10.75	1.58	1.37
13	h2	201	CYC	OC-C1C	10.75	1.44	1.23
13	U7	201	CYC	OC-C1C	10.74	1.44	1.23
13	J3	201	CYC	OC-C1C	10.74	1.44	1.23
13	L7	201	CYC	OC-C1C	10.74	1.44	1.23
13	22	301	CYC	OC-C1C	10.74	1.44	1.23
13	D6	201	CYC	OC-C1C	10.74	1.44	1.23
13	G6	201	CYC	C4C-NC	10.74	1.58	1.37
13	M2	201	CYC	OC-C1C	10.74	1.44	1.23
13	T5	201	CYC	OC-C1C	10.74	1.44	1.23
13	D1	201	CYC	OC-C1C	10.74	1.44	1.23
13	G3	201	CYC	OC-C1C	10.74	1.44	1.23
13	N6	201	CYC	OC-C1C	10.74	1.44	1.23
13	F5	202	CYC	OC-C1C	10.74	1.44	1.23
13	H6	201	CYC	OC-C1C	10.74	1.44	1.23
13	M2	201	CYC	C4C-NC	10.73	1.58	1.37
13	f2	201	CYC	OC-C1C	10.73	1.44	1.23
13	C5	202	CYC	OC-C1C	10.73	1.44	1.23
13	G1	201	CYC	C4C-NC	10.73	1.58	1.37
13	M6	201	CYC	OC-C1C	10.73	1.44	1.23
13	42	301	CYC	OC-C1C	10.73	1.44	1.23
13	T5	202	CYC	OC-C1C	10.73	1.44	1.23
13	V5	202	CYC	C4C-NC	10.73	1.58	1.37
13	L2	201	CYC	OC-C1C	10.73	1.44	1.23
13	R7	201	CYC	OC-C1C	10.73	1.44	1.23
13	J3	202	CYC	C4C-NC	10.73	1.58	1.37
13	C7	201	CYC	C4C-NC	10.73	1.58	1.37
13	e2	201	CYC	OC-C1C	10.73	1.44	1.23
13	W5	201	CYC	C4C-NC	10.73	1.58	1.37
13	L3	201	CYC	OC-C1C	10.73	1.44	1.23
13	A1	301	CYC	OC-C1C	10.73	1.44	1.23
13	n2	201	CYC	OC-C1C	10.73	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F3	201	CYC	OC-C1C	10.73	1.44	1.23
13	I7	201	CYC	OC-C1C	10.72	1.44	1.23
13	N2	802	CYC	OC-C1C	10.72	1.44	1.23
13	T6	202	CYC	OC-C1C	10.72	1.44	1.23
13	U2	201	CYC	OC-C1C	10.72	1.44	1.23
13	C4	202	CYC	OC-C1C	10.72	1.44	1.23
13	L5	201	CYC	OC-C1C	10.72	1.44	1.23
13	p2	201	CYC	C4C-NC	10.72	1.58	1.37
13	G7	201	CYC	OC-C1C	10.72	1.44	1.23
13	42	302	CYC	OC-C1C	10.72	1.44	1.23
13	I4	201	CYC	OC-C1C	10.72	1.44	1.23
13	G1	201	CYC	OC-C1C	10.72	1.44	1.23
13	J1	201	CYC	OC-C1C	10.72	1.44	1.23
13	A6	301	CYC	OC-C1C	10.71	1.44	1.23
13	X2	201	CYC	OC-C1C	10.71	1.44	1.23
13	B3	201	CYC	OC-C1C	10.71	1.44	1.23
13	R4	201	CYC	OC-C1C	10.71	1.44	1.23
13	x2	201	CYC	OC-C1C	10.71	1.44	1.23
13	C3	201	CYC	C4C-NC	10.71	1.58	1.37
13	G4	201	CYC	OC-C1C	10.71	1.43	1.23
13	J6	202	CYC	C4C-NC	10.71	1.58	1.37
13	52	302	CYC	OC-C1C	10.71	1.43	1.23
13	T3	202	CYC	OC-C1C	10.71	1.43	1.23
13	V1	201	CYC	C4C-NC	10.71	1.58	1.37
13	V1	201	CYC	OC-C1C	10.71	1.43	1.23
13	U5	201	CYC	OC-C1C	10.71	1.43	1.23
13	A6	302	CYC	OC-C1C	10.70	1.43	1.23
13	T1	202	CYC	OC-C1C	10.70	1.43	1.23
13	U4	201	CYC	OC-C1C	10.70	1.43	1.23
13	52	301	CYC	OC-C1C	10.70	1.43	1.23
13	v2	201	CYC	OC-C1C	10.70	1.43	1.23
13	a5	202	CYC	OC-C1C	10.70	1.43	1.23
13	W7	201	CYC	OC-C1C	10.70	1.43	1.23
13	32	301	CYC	OC-C1C	10.70	1.43	1.23
13	N1	201	CYC	OC-C1C	10.70	1.43	1.23
13	B4	201	CYC	OC-C1C	10.70	1.43	1.23
13	W3	201	CYC	OC-C1C	10.70	1.43	1.23
13	R2	201	CYC	OC-C1C	10.69	1.43	1.23
13	X5	201	CYC	C4C-NC	10.69	1.58	1.37
13	D2	201	CYC	OC-C1C	10.69	1.43	1.23
13	o2	801	CYC	OC-C1C	10.69	1.43	1.23
13	D1	201	CYC	C4C-NC	10.69	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C1	202	CYC	OC-C1C	10.69	1.43	1.23
13	G2	201	CYC	OC-C1C	10.69	1.43	1.23
13	E2	201	CYC	OC-C1C	10.69	1.43	1.23
13	L4	201	CYC	OC-C1C	10.69	1.43	1.23
13	O2	201	CYC	OC-C1C	10.68	1.43	1.23
13	C6	202	CYC	OC-C1C	10.68	1.43	1.23
13	r2	201	CYC	OC-C1C	10.68	1.43	1.23
13	F6	201	CYC	OC-C1C	10.68	1.43	1.23
13	s2	201	CYC	OC-C1C	10.68	1.43	1.23
13	V6	201	CYC	OC-C1C	10.68	1.43	1.23
13	P2	201	CYC	C4C-NC	10.68	1.58	1.37
13	V4	201	CYC	C4C-NC	10.68	1.58	1.37
13	A1	302	CYC	OC-C1C	10.67	1.43	1.23
13	V6	201	CYC	C4C-NC	10.67	1.58	1.37
13	D5	201	CYC	C4C-NC	10.67	1.58	1.37
13	B1	201	CYC	OC-C1C	10.67	1.43	1.23
13	N2	801	CYC	OC-C1C	10.67	1.43	1.23
13	K4	201	CYC	OC-C1C	10.67	1.43	1.23
13	R5	201	CYC	OC-C1C	10.67	1.43	1.23
13	N4	201	CYC	OC-C1C	10.67	1.43	1.23
13	B5	201	CYC	OC-C1C	10.67	1.43	1.23
13	F4	201	CYC	OC-C1C	10.66	1.43	1.23
13	l2	201	CYC	OC-C1C	10.66	1.43	1.23
13	R1	201	CYC	OC-C1C	10.66	1.43	1.23
13	V5	201	CYC	C4C-NC	10.66	1.58	1.37
13	W1	201	CYC	OC-C1C	10.66	1.43	1.23
13	N5	201	CYC	OC-C1C	10.66	1.43	1.23
13	U6	201	CYC	OC-C1C	10.66	1.43	1.23
13	a6	202	CYC	OC-C1C	10.65	1.43	1.23
13	Q2	201	CYC	OC-C1C	10.65	1.43	1.23
13	I1	201	CYC	OC-C1C	10.65	1.43	1.23
13	G5	201	CYC	OC-C1C	10.65	1.43	1.23
13	K1	201	CYC	OC-C1C	10.65	1.43	1.23
13	a7	201	CYC	C4C-NC	10.65	1.58	1.37
13	F2	201	CYC	OC-C1C	10.65	1.43	1.23
13	L6	201	CYC	OC-C1C	10.65	1.43	1.23
13	K5	201	CYC	OC-C1C	10.64	1.43	1.23
13	R6	201	CYC	OC-C1C	10.64	1.43	1.23
13	g2	201	CYC	OC-C1C	10.64	1.43	1.23
13	I5	201	CYC	OC-C1C	10.64	1.43	1.23
13	C4	201	CYC	C4C-NC	10.64	1.57	1.37
13	K3	201	CYC	OC-C1C	10.64	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a3	201	CYC	C4C-NC	10.64	1.57	1.37
13	I3	201	CYC	OC-C1C	10.64	1.43	1.23
13	I6	201	CYC	OC-C1C	10.64	1.43	1.23
13	W4	201	CYC	OC-C1C	10.64	1.43	1.23
13	g2	201	CYC	C4C-NC	10.63	1.57	1.37
13	K7	201	CYC	OC-C1C	10.63	1.43	1.23
13	Z4	301	CYC	C4C-NC	10.62	1.57	1.37
13	a1	202	CYC	OC-C1C	10.62	1.43	1.23
13	U2	201	CYC	C4C-NC	10.62	1.57	1.37
13	W5	201	CYC	OC-C1C	10.61	1.43	1.23
13	W6	201	CYC	OC-C1C	10.61	1.43	1.23
13	G6	201	CYC	OC-C1C	10.61	1.43	1.23
13	B6	201	CYC	OC-C1C	10.60	1.43	1.23
13	C5	201	CYC	C4C-NC	10.60	1.57	1.37
13	F5	201	CYC	OC-C1C	10.59	1.43	1.23
13	L6	201	CYC	C4C-NC	10.58	1.57	1.37
13	N2	801	CYC	C4C-NC	10.58	1.57	1.37
13	V2	201	CYC	C4C-NC	10.58	1.57	1.37
13	Z6	301	CYC	C4C-NC	10.58	1.57	1.37
13	m2	201	CYC	OC-C1C	10.57	1.43	1.23
13	a5	201	CYC	C4C-NC	10.57	1.57	1.37
13	F1	201	CYC	OC-C1C	10.57	1.43	1.23
13	C1	201	CYC	C4C-NC	10.56	1.57	1.37
13	L1	201	CYC	OC-C1C	10.56	1.43	1.23
13	C6	201	CYC	C4C-NC	10.55	1.57	1.37
13	Z1	301	CYC	C4C-NC	10.54	1.57	1.37
13	a6	201	CYC	C4C-NC	10.54	1.57	1.37
13	p2	201	CYC	OC-C1C	10.54	1.43	1.23
13	Z5	301	CYC	C4C-NC	10.53	1.57	1.37
13	L1	201	CYC	C4C-NC	10.52	1.57	1.37
13	a1	201	CYC	C4C-NC	10.50	1.57	1.37
13	f2	201	CYC	C3C-C4C	-10.29	1.29	1.50
13	a1	202	CYC	C3C-C4C	-10.28	1.29	1.50
13	a5	202	CYC	C3C-C4C	-10.21	1.29	1.50
13	U2	201	CYC	C3C-C4C	-10.21	1.29	1.50
13	E1	201	CYC	C3C-C4C	-10.17	1.29	1.50
13	T5	201	CYC	C3C-C4C	-10.16	1.29	1.50
13	a4	202	CYC	C3C-C4C	-10.16	1.29	1.50
13	a6	202	CYC	C3C-C4C	-10.16	1.29	1.50
13	T4	201	CYC	C3C-C4C	-10.15	1.29	1.50
13	N2	801	CYC	C3C-C4C	-10.14	1.29	1.50
13	E6	201	CYC	C3C-C4C	-10.13	1.29	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a3	202	CYC	C3C-C4C	-10.12	1.29	1.50
13	T7	201	CYC	C3C-C4C	-10.12	1.29	1.50
13	X5	201	CYC	C3C-C4C	-10.12	1.29	1.50
13	E4	201	CYC	C3C-C4C	-10.12	1.29	1.50
13	X6	201	CYC	C3C-C4C	-10.12	1.29	1.50
13	V5	202	CYC	C3C-C4C	-10.11	1.29	1.50
13	X1	201	CYC	C3C-C4C	-10.11	1.29	1.50
13	J7	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	E7	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	M1	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	J5	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	T3	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	E5	201	CYC	C3C-C4C	-10.10	1.29	1.50
13	J6	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	M6	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	J1	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	J3	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	E3	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	V4	202	CYC	C3C-C4C	-10.09	1.29	1.50
13	M7	201	CYC	C3C-C4C	-10.09	1.29	1.50
13	T1	201	CYC	C3C-C4C	-10.08	1.29	1.50
13	a7	202	CYC	C3C-C4C	-10.08	1.29	1.50
13	T2	201	CYC	C3C-C4C	-10.08	1.29	1.50
13	V3	202	CYC	C3C-C4C	-10.08	1.29	1.50
13	J6	202	CYC	C3C-C4C	-10.07	1.29	1.50
13	V7	202	CYC	C3C-C4C	-10.07	1.29	1.50
13	M3	201	CYC	C3C-C4C	-10.07	1.29	1.50
13	D1	201	CYC	C3C-C4C	-10.06	1.29	1.50
13	J5	202	CYC	C3C-C4C	-10.06	1.29	1.50
13	L6	201	CYC	C3C-C4C	-10.06	1.29	1.50
13	V1	202	CYC	C3C-C4C	-10.06	1.29	1.50
13	V6	202	CYC	C3C-C4C	-10.06	1.29	1.50
13	M5	201	CYC	C3C-C4C	-10.06	1.29	1.50
13	T6	201	CYC	C3C-C4C	-10.06	1.29	1.50
13	P1	202	CYC	C3C-C4C	-10.05	1.29	1.50
13	M4	201	CYC	C3C-C4C	-10.05	1.29	1.50
13	P5	202	CYC	C3C-C4C	-10.05	1.29	1.50
13	X2	201	CYC	C3C-C4C	-10.04	1.29	1.50
13	X7	201	CYC	C3C-C4C	-10.04	1.29	1.50
13	B2	202	CYC	C3C-C4C	-10.04	1.29	1.50
13	X4	201	CYC	C3C-C4C	-10.04	1.29	1.50
13	D5	201	CYC	C3C-C4C	-10.04	1.29	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X3	201	CYC	C3C-C4C	-10.04	1.29	1.50
13	J4	201	CYC	C3C-C4C	-10.03	1.29	1.50
13	J4	202	CYC	C3C-C4C	-10.03	1.29	1.50
13	J1	202	CYC	C3C-C4C	-10.02	1.29	1.50
13	L7	201	CYC	C3C-C4C	-10.02	1.29	1.50
13	J7	202	CYC	C3C-C4C	-10.00	1.29	1.50
13	L1	201	CYC	C3C-C4C	-10.00	1.29	1.50
13	C1	201	CYC	C3C-C4C	-10.00	1.29	1.50
13	L3	201	CYC	C3C-C4C	-10.00	1.29	1.50
13	P2	201	CYC	C3C-C4C	-9.99	1.29	1.50
13	V2	201	CYC	C3C-C4C	-9.99	1.29	1.50
13	P4	201	CYC	C3C-C4C	-9.99	1.29	1.50
13	C6	201	CYC	C3C-C4C	-9.99	1.29	1.50
13	J3	202	CYC	C3C-C4C	-9.99	1.29	1.50
13	L5	201	CYC	C3C-C4C	-9.98	1.29	1.50
13	P6	202	CYC	C3C-C4C	-9.97	1.29	1.50
13	L4	201	CYC	C3C-C4C	-9.97	1.29	1.50
13	D3	201	CYC	C3C-C4C	-9.95	1.29	1.50
13	A1	301	CYC	C3C-C4C	-9.95	1.29	1.50
13	t2	201	CYC	C3C-C4C	-9.94	1.29	1.50
13	x2	201	CYC	C3C-C4C	-9.94	1.29	1.50
13	A6	301	CYC	C3C-C4C	-9.94	1.29	1.50
13	42	301	CYC	C3C-C4C	-9.93	1.29	1.50
13	B2	201	CYC	C3C-C4C	-9.93	1.29	1.50
13	Z1	301	CYC	C3C-C4C	-9.92	1.29	1.50
13	22	301	CYC	C3C-C4C	-9.91	1.29	1.50
13	C4	201	CYC	C3C-C4C	-9.91	1.29	1.50
13	32	301	CYC	C3C-C4C	-9.90	1.29	1.50
13	52	301	CYC	C3C-C4C	-9.90	1.29	1.50
13	Z6	301	CYC	C3C-C4C	-9.90	1.29	1.50
13	C5	201	CYC	C3C-C4C	-9.89	1.29	1.50
13	a1	201	CYC	C3C-C4C	-9.88	1.29	1.50
13	D4	201	CYC	C3C-C4C	-9.88	1.29	1.50
13	a7	201	CYC	C3C-C4C	-9.86	1.29	1.50
13	P3	202	CYC	C3C-C4C	-9.86	1.29	1.50
13	Z5	301	CYC	C3C-C4C	-9.86	1.29	1.50
13	C7	201	CYC	C3C-C4C	-9.85	1.29	1.50
13	a3	201	CYC	C3C-C4C	-9.85	1.29	1.50
13	D6	201	CYC	C3C-C4C	-9.84	1.29	1.50
13	Z4	301	CYC	C3C-C4C	-9.84	1.29	1.50
13	d2	201	CYC	C3C-C4C	-9.82	1.30	1.50
13	R7	201	CYC	C3C-C4C	-9.82	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C3	201	CYC	C3C-C4C	-9.81	1.30	1.50
13	D7	201	CYC	C3C-C4C	-9.80	1.30	1.50
13	i2	201	CYC	C3C-C4C	-9.79	1.30	1.50
13	a6	201	CYC	C3C-C4C	-9.79	1.30	1.50
13	R3	201	CYC	C3C-C4C	-9.78	1.30	1.50
13	A2	201	CYC	C3C-C4C	-9.77	1.30	1.50
13	D2	201	CYC	C3C-C4C	-9.77	1.30	1.50
13	a5	201	CYC	C3C-C4C	-9.74	1.30	1.50
13	P7	202	CYC	C3C-C4C	-9.74	1.30	1.50
13	S2	201	CYC	C3C-C4C	-9.71	1.30	1.50
13	V5	201	CYC	C3C-C4C	-9.70	1.30	1.50
13	j2	201	CYC	C3C-C4C	-9.69	1.30	1.50
13	F3	201	CYC	C3C-C4C	-9.68	1.30	1.50
13	F4	201	CYC	C3C-C4C	-9.68	1.30	1.50
13	A2	202	CYC	C3C-C4C	-9.68	1.30	1.50
13	F7	201	CYC	C3C-C4C	-9.68	1.30	1.50
13	k2	201	CYC	C3C-C4C	-9.68	1.30	1.50
13	R1	201	CYC	C3C-C4C	-9.65	1.30	1.50
13	R4	201	CYC	C3C-C4C	-9.65	1.30	1.50
13	V6	201	CYC	C3C-C4C	-9.64	1.30	1.50
13	F6	201	CYC	C3C-C4C	-9.63	1.30	1.50
13	R6	201	CYC	C3C-C4C	-9.63	1.30	1.50
13	a2	201	CYC	C3C-C4C	-9.63	1.30	1.50
13	Z3	301	CYC	C3C-C4C	-9.62	1.30	1.50
13	R5	201	CYC	C3C-C4C	-9.62	1.30	1.50
13	V4	201	CYC	C3C-C4C	-9.61	1.30	1.50
13	C2	201	CYC	C3C-C4C	-9.59	1.30	1.50
13	G2	201	CYC	C3C-C4C	-9.59	1.30	1.50
13	Q7	202	CYC	C3C-C4C	-9.59	1.30	1.50
13	F1	201	CYC	C3C-C4C	-9.58	1.30	1.50
13	Z7	301	CYC	C3C-C4C	-9.57	1.30	1.50
13	F5	201	CYC	C3C-C4C	-9.57	1.30	1.50
13	N2	802	CYC	C3C-C4C	-9.56	1.30	1.50
13	Q2	201	CYC	C3C-C4C	-9.55	1.30	1.50
13	Q3	201	CYC	C3C-C4C	-9.52	1.30	1.50
13	Q7	201	CYC	C3C-C4C	-9.52	1.30	1.50
13	C3	202	CYC	C3C-C4C	-9.52	1.30	1.50
13	W7	201	CYC	C3C-C4C	-9.52	1.30	1.50
13	C7	202	CYC	C3C-C4C	-9.52	1.30	1.50
13	V3	201	CYC	C3C-C4C	-9.51	1.30	1.50
13	Q4	202	CYC	C3C-C4C	-9.51	1.30	1.50
13	Q5	202	CYC	C3C-C4C	-9.51	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q6	202	CYC	C3C-C4C	-9.51	1.30	1.50
13	H7	201	CYC	C3C-C4C	-9.51	1.30	1.50
13	W3	201	CYC	C3C-C4C	-9.51	1.30	1.50
13	K3	201	CYC	C3C-C4C	-9.50	1.30	1.50
13	G7	201	CYC	C3C-C4C	-9.50	1.30	1.50
13	K7	201	CYC	C3C-C4C	-9.49	1.30	1.50
13	32	302	CYC	C3C-C4C	-9.49	1.30	1.50
13	52	302	CYC	C3C-C4C	-9.48	1.30	1.50
13	G6	201	CYC	C3C-C4C	-9.48	1.30	1.50
13	H3	201	CYC	C3C-C4C	-9.47	1.30	1.50
13	c2	801	CYC	C3C-C4C	-9.47	1.30	1.50
13	U7	201	CYC	C3C-C4C	-9.47	1.30	1.50
13	W6	201	CYC	C3C-C4C	-9.46	1.30	1.50
13	G3	201	CYC	C3C-C4C	-9.46	1.30	1.50
13	U3	201	CYC	C3C-C4C	-9.46	1.30	1.50
13	U4	201	CYC	C3C-C4C	-9.46	1.30	1.50
13	H6	201	CYC	C3C-C4C	-9.46	1.30	1.50
13	H2	201	CYC	C3C-C4C	-9.45	1.30	1.50
13	N7	201	CYC	C3C-C4C	-9.45	1.30	1.50
13	22	302	CYC	C3C-C4C	-9.45	1.30	1.50
13	g2	201	CYC	C3C-C4C	-9.45	1.30	1.50
13	Q6	201	CYC	C3C-C4C	-9.43	1.30	1.50
13	W1	201	CYC	C3C-C4C	-9.43	1.30	1.50
13	N1	201	CYC	C3C-C4C	-9.43	1.30	1.50
13	n2	201	CYC	C3C-C4C	-9.43	1.30	1.50
13	W5	201	CYC	C3C-C4C	-9.42	1.30	1.50
13	e2	201	CYC	C3C-C4C	-9.42	1.30	1.50
13	G5	201	CYC	C3C-C4C	-9.42	1.30	1.50
13	H1	201	CYC	C3C-C4C	-9.42	1.30	1.50
13	H4	201	CYC	C3C-C4C	-9.41	1.30	1.50
13	Q1	202	CYC	C3C-C4C	-9.41	1.30	1.50
13	C5	202	CYC	C3C-C4C	-9.41	1.30	1.50
13	A6	302	CYC	C3C-C4C	-9.41	1.30	1.50
13	V1	201	CYC	C3C-C4C	-9.40	1.30	1.50
13	h2	201	CYC	C3C-C4C	-9.40	1.30	1.50
13	N4	201	CYC	C3C-C4C	-9.40	1.30	1.50
13	Q4	201	CYC	C3C-C4C	-9.39	1.30	1.50
13	U5	201	CYC	C3C-C4C	-9.39	1.30	1.50
13	V7	201	CYC	C3C-C4C	-9.39	1.30	1.50
13	U6	201	CYC	C3C-C4C	-9.39	1.30	1.50
13	r2	201	CYC	C3C-C4C	-9.39	1.30	1.50
13	l2	201	CYC	C3C-C4C	-9.38	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G4	201	CYC	C3C-C4C	-9.38	1.30	1.50
13	U1	201	CYC	C3C-C4C	-9.38	1.30	1.50
13	N3	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	s2	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	R2	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	K1	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	H5	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	Q1	201	CYC	C3C-C4C	-9.37	1.30	1.50
13	A1	302	CYC	C3C-C4C	-9.36	1.30	1.50
13	W4	201	CYC	C3C-C4C	-9.36	1.30	1.50
13	G1	201	CYC	C3C-C4C	-9.36	1.30	1.50
13	M2	201	CYC	C3C-C4C	-9.36	1.30	1.50
13	K6	201	CYC	C3C-C4C	-9.36	1.30	1.50
13	E2	201	CYC	C3C-C4C	-9.36	1.31	1.50
13	Q3	202	CYC	C3C-C4C	-9.35	1.31	1.50
13	C4	202	CYC	C3C-C4C	-9.35	1.31	1.50
13	N5	201	CYC	C3C-C4C	-9.35	1.31	1.50
13	W2	201	CYC	C3C-C4C	-9.35	1.31	1.50
13	I7	201	CYC	C3C-C4C	-9.34	1.31	1.50
13	N6	201	CYC	C3C-C4C	-9.34	1.31	1.50
13	y2	201	CYC	C3C-C4C	-9.33	1.31	1.50
13	T7	202	CYC	C3C-C4C	-9.33	1.31	1.50
13	C1	202	CYC	C3C-C4C	-9.33	1.31	1.50
13	C6	202	CYC	C3C-C4C	-9.33	1.31	1.50
13	K4	201	CYC	C3C-C4C	-9.32	1.31	1.50
13	L2	201	CYC	C3C-C4C	-9.32	1.31	1.50
13	T3	202	CYC	C3C-C4C	-9.31	1.31	1.50
13	v2	201	CYC	C3C-C4C	-9.31	1.31	1.50
13	z2	201	CYC	C3C-C4C	-9.31	1.31	1.50
13	P7	201	CYC	C3C-C4C	-9.30	1.31	1.50
13	B7	201	CYC	C3C-C4C	-9.29	1.31	1.50
13	T4	202	CYC	C3C-C4C	-9.28	1.31	1.50
13	P3	201	CYC	C3C-C4C	-9.28	1.31	1.50
13	B3	201	CYC	C3C-C4C	-9.27	1.31	1.50
13	Q5	201	CYC	C3C-C4C	-9.26	1.31	1.50
13	T6	202	CYC	C3C-C4C	-9.26	1.31	1.50
13	I3	201	CYC	C3C-C4C	-9.25	1.31	1.50
13	T1	202	CYC	C3C-C4C	-9.24	1.31	1.50
13	T5	202	CYC	C3C-C4C	-9.24	1.31	1.50
13	F1	202	CYC	C3C-C4C	-9.24	1.31	1.50
13	o2	801	CYC	C3C-C4C	-9.23	1.31	1.50
13	P1	201	CYC	C3C-C4C	-9.23	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F2	201	CYC	C3C-C4C	-9.23	1.31	1.50
13	F4	202	CYC	C3C-C4C	-9.20	1.31	1.50
13	F5	202	CYC	C3C-C4C	-9.20	1.31	1.50
13	K5	201	CYC	C3C-C4C	-9.19	1.31	1.50
13	m2	201	CYC	C3C-C4C	-9.17	1.31	1.50
13	P6	201	CYC	C3C-C4C	-9.16	1.31	1.50
13	B4	201	CYC	C3C-C4C	-9.15	1.31	1.50
13	F7	202	CYC	C3C-C4C	-9.14	1.31	1.50
13	F3	202	CYC	C3C-C4C	-9.14	1.31	1.50
13	P5	201	CYC	C3C-C4C	-9.12	1.31	1.50
13	P4	202	CYC	C3C-C4C	-9.11	1.31	1.50
13	32	302	CYC	OB-C4B	9.09	1.40	1.23
13	22	302	CYC	OB-C4B	9.08	1.40	1.23
13	A1	301	CYC	OB-C4B	9.07	1.40	1.23
13	I5	201	CYC	C3C-C4C	-9.07	1.31	1.50
13	F6	202	CYC	C3C-C4C	-9.06	1.31	1.50
13	p2	201	CYC	C3C-C4C	-9.04	1.31	1.50
13	42	302	CYC	OB-C4B	9.04	1.40	1.23
13	B6	201	CYC	C3C-C4C	-9.03	1.31	1.50
13	A6	301	CYC	OB-C4B	9.03	1.40	1.23
13	T3	202	CYC	OB-C4B	9.03	1.40	1.23
13	I1	201	CYC	C3C-C4C	-9.02	1.31	1.50
13	B2	201	CYC	OB-C4B	9.01	1.40	1.23
13	P7	202	CYC	OB-C4B	9.01	1.40	1.23
13	32	301	CYC	OB-C4B	9.00	1.40	1.23
13	52	302	CYC	OB-C4B	9.00	1.40	1.23
13	52	301	CYC	OB-C4B	9.00	1.40	1.23
13	T7	202	CYC	OB-C4B	8.99	1.40	1.23
13	B1	201	CYC	C3C-C4C	-8.99	1.31	1.50
13	O2	201	CYC	C3C-C4C	-8.99	1.31	1.50
13	22	301	CYC	OB-C4B	8.99	1.40	1.23
13	42	301	CYC	OB-C4B	8.98	1.40	1.23
13	k2	201	CYC	OB-C4B	8.98	1.40	1.23
13	B2	202	CYC	OB-C4B	8.97	1.40	1.23
13	C5	201	CYC	OB-C4B	8.97	1.40	1.23
13	S6	201	CYC	C3C-C4C	-8.97	1.31	1.50
13	J5	201	CYC	OB-C4B	8.96	1.40	1.23
13	V3	201	CYC	OB-C4B	8.96	1.40	1.23
13	S1	201	CYC	C3C-C4C	-8.96	1.31	1.50
13	U6	201	CYC	OB-C4B	8.96	1.40	1.23
13	P3	202	CYC	OB-C4B	8.96	1.40	1.23
13	C7	201	CYC	OB-C4B	8.96	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c2	801	CYC	OB-C4B	8.96	1.40	1.23
13	R6	201	CYC	OB-C4B	8.96	1.40	1.23
13	T6	202	CYC	OB-C4B	8.96	1.40	1.23
13	J4	201	CYC	OB-C4B	8.96	1.40	1.23
13	Q5	201	CYC	OB-C4B	8.96	1.40	1.23
13	S5	201	CYC	C3C-C4C	-8.96	1.31	1.50
13	I6	201	CYC	C3C-C4C	-8.96	1.31	1.50
13	C2	201	CYC	OB-C4B	8.96	1.40	1.23
13	C6	201	CYC	OB-C4B	8.96	1.40	1.23
13	H7	201	CYC	OB-C4B	8.96	1.40	1.23
13	N7	201	CYC	OB-C4B	8.95	1.40	1.23
13	Z6	301	CYC	OB-C4B	8.95	1.40	1.23
13	P6	201	CYC	OB-C4B	8.95	1.40	1.23
13	I4	201	CYC	C3C-C4C	-8.95	1.31	1.50
13	I7	201	CYC	OB-C4B	8.95	1.40	1.23
13	w2	201	CYC	C3C-C4C	-8.95	1.31	1.50
13	X2	201	CYC	OB-C4B	8.95	1.40	1.23
13	R3	201	CYC	OB-C4B	8.95	1.40	1.23
13	C3	201	CYC	OB-C4B	8.95	1.40	1.23
13	K4	201	CYC	OB-C4B	8.95	1.40	1.23
13	I4	201	CYC	OB-C4B	8.95	1.40	1.23
13	S4	201	CYC	C3C-C4C	-8.95	1.31	1.50
13	P1	201	CYC	OB-C4B	8.95	1.40	1.23
13	W7	201	CYC	OB-C4B	8.95	1.40	1.23
13	Q3	201	CYC	OB-C4B	8.94	1.40	1.23
13	U7	201	CYC	OB-C4B	8.94	1.40	1.23
13	W3	201	CYC	OB-C4B	8.94	1.40	1.23
13	P4	201	CYC	OB-C4B	8.94	1.40	1.23
13	B7	201	CYC	OB-C4B	8.94	1.40	1.23
13	Q7	201	CYC	OB-C4B	8.94	1.40	1.23
13	I5	201	CYC	OB-C4B	8.94	1.40	1.23
13	P7	201	CYC	OB-C4B	8.94	1.40	1.23
13	F3	201	CYC	OB-C4B	8.94	1.40	1.23
13	B3	201	CYC	OB-C4B	8.94	1.40	1.23
13	F7	201	CYC	OB-C4B	8.94	1.40	1.23
13	P3	201	CYC	OB-C4B	8.94	1.40	1.23
13	F4	201	CYC	OB-C4B	8.94	1.40	1.23
13	I3	201	CYC	OB-C4B	8.94	1.40	1.23
13	42	302	CYC	C3C-C4C	-8.94	1.31	1.50
13	A6	302	CYC	OB-C4B	8.94	1.40	1.23
13	I1	201	CYC	OB-C4B	8.93	1.40	1.23
13	a1	201	CYC	OB-C4B	8.93	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R5	201	CYC	OB-C4B	8.93	1.40	1.23
13	G7	201	CYC	OB-C4B	8.93	1.40	1.23
13	C1	201	CYC	OB-C4B	8.93	1.40	1.23
13	Q4	201	CYC	OB-C4B	8.93	1.40	1.23
13	T1	202	CYC	OB-C4B	8.93	1.40	1.23
13	a5	201	CYC	OB-C4B	8.93	1.40	1.23
13	S3	201	CYC	C3C-C4C	-8.93	1.31	1.50
13	y2	201	CYC	OB-C4B	8.93	1.40	1.23
13	I6	201	CYC	OB-C4B	8.93	1.40	1.23
13	a7	201	CYC	OB-C4B	8.93	1.40	1.23
13	G3	201	CYC	OB-C4B	8.93	1.40	1.23
13	R4	201	CYC	OB-C4B	8.93	1.40	1.23
13	Z5	301	CYC	OB-C4B	8.93	1.40	1.23
13	H3	201	CYC	OB-C4B	8.93	1.40	1.23
13	Z1	301	CYC	OB-C4B	8.93	1.40	1.23
13	a2	201	CYC	OB-C4B	8.93	1.40	1.23
13	R1	201	CYC	OB-C4B	8.93	1.40	1.23
13	K3	201	CYC	OB-C4B	8.93	1.40	1.23
13	L3	201	CYC	OB-C4B	8.93	1.40	1.23
13	Z3	301	CYC	OB-C4B	8.92	1.40	1.23
13	a6	201	CYC	OB-C4B	8.92	1.40	1.23
13	U4	201	CYC	OB-C4B	8.92	1.40	1.23
13	N2	801	CYC	OB-C4B	8.92	1.40	1.23
13	H2	201	CYC	OB-C4B	8.92	1.40	1.23
13	p2	201	CYC	OB-C4B	8.92	1.40	1.23
13	S6	201	CYC	OB-C4B	8.92	1.40	1.23
13	A2	201	CYC	OB-C4B	8.92	1.40	1.23
13	M7	201	CYC	OB-C4B	8.92	1.40	1.23
13	C4	201	CYC	OB-C4B	8.92	1.40	1.23
13	V4	201	CYC	OB-C4B	8.92	1.40	1.23
13	S7	201	CYC	OB-C4B	8.91	1.40	1.23
13	O2	201	CYC	OB-C4B	8.91	1.40	1.23
13	F7	202	CYC	OB-C4B	8.91	1.40	1.23
13	A1	302	CYC	OB-C4B	8.91	1.40	1.23
13	U3	201	CYC	OB-C4B	8.91	1.40	1.23
13	L7	201	CYC	OB-C4B	8.91	1.40	1.23
13	K7	201	CYC	OB-C4B	8.91	1.40	1.23
13	M3	201	CYC	OB-C4B	8.91	1.40	1.23
13	S7	201	CYC	C3C-C4C	-8.91	1.31	1.50
13	U1	201	CYC	OB-C4B	8.91	1.40	1.23
13	U5	201	CYC	OB-C4B	8.91	1.40	1.23
13	S3	201	CYC	OB-C4B	8.91	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q1	201	CYC	OB-C4B	8.91	1.40	1.23
13	Z7	301	CYC	OB-C4B	8.91	1.40	1.23
13	P6	202	CYC	OB-C4B	8.91	1.40	1.23
13	N3	201	CYC	OB-C4B	8.91	1.40	1.23
13	K5	201	CYC	OB-C4B	8.91	1.40	1.23
13	T5	202	CYC	OB-C4B	8.91	1.40	1.23
13	B5	201	CYC	C3C-C4C	-8.90	1.31	1.50
13	L5	201	CYC	OB-C4B	8.90	1.40	1.23
13	J7	201	CYC	OB-C4B	8.90	1.40	1.23
13	F3	202	CYC	OB-C4B	8.90	1.40	1.23
13	F6	202	CYC	OB-C4B	8.90	1.40	1.23
13	J3	201	CYC	OB-C4B	8.90	1.40	1.23
13	S4	201	CYC	OB-C4B	8.90	1.40	1.23
13	G5	201	CYC	OB-C4B	8.90	1.40	1.23
13	J7	202	CYC	OB-C4B	8.90	1.40	1.23
13	R7	201	CYC	OB-C4B	8.90	1.40	1.23
13	F6	201	CYC	OB-C4B	8.90	1.40	1.23
13	H5	201	CYC	OB-C4B	8.90	1.40	1.23
13	B5	201	CYC	OB-C4B	8.89	1.40	1.23
13	W5	201	CYC	OB-C4B	8.89	1.40	1.23
13	P5	201	CYC	OB-C4B	8.89	1.40	1.23
13	Q6	201	CYC	OB-C4B	8.89	1.40	1.23
13	d2	201	CYC	OB-C4B	8.89	1.40	1.23
13	P4	202	CYC	OB-C4B	8.89	1.40	1.23
13	L6	201	CYC	OB-C4B	8.89	1.40	1.23
13	L1	201	CYC	OB-C4B	8.89	1.40	1.23
13	Z4	301	CYC	OB-C4B	8.89	1.40	1.23
13	W6	201	CYC	OB-C4B	8.88	1.40	1.23
13	S1	201	CYC	OB-C4B	8.88	1.40	1.23
13	i2	201	CYC	OB-C4B	8.88	1.40	1.23
13	x2	201	CYC	OB-C4B	8.88	1.40	1.23
13	z2	201	CYC	OB-C4B	8.88	1.40	1.23
13	V7	201	CYC	OB-C4B	8.88	1.40	1.23
13	J6	201	CYC	OB-C4B	8.88	1.40	1.23
13	T2	201	CYC	OB-C4B	8.88	1.40	1.23
13	H1	201	CYC	OB-C4B	8.88	1.40	1.23
13	j2	201	CYC	OB-C4B	8.88	1.40	1.23
13	a3	201	CYC	OB-C4B	8.88	1.40	1.23
13	B4	201	CYC	OB-C4B	8.88	1.40	1.23
13	P1	202	CYC	OB-C4B	8.88	1.40	1.23
13	V6	201	CYC	OB-C4B	8.88	1.40	1.23
13	D4	201	CYC	OB-C4B	8.88	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q2	201	CYC	OB-C4B	8.88	1.40	1.23
13	W4	201	CYC	OB-C4B	8.88	1.40	1.23
13	N6	201	CYC	OB-C4B	8.87	1.40	1.23
13	T3	201	CYC	OB-C4B	8.87	1.40	1.23
13	P5	202	CYC	OB-C4B	8.87	1.40	1.23
13	F4	202	CYC	OB-C4B	8.87	1.40	1.23
13	V1	201	CYC	OB-C4B	8.87	1.40	1.23
13	V5	201	CYC	OB-C4B	8.87	1.40	1.23
13	D6	201	CYC	OB-C4B	8.87	1.40	1.23
13	L4	201	CYC	OB-C4B	8.87	1.40	1.23
13	F5	201	CYC	OB-C4B	8.87	1.40	1.23
13	M1	201	CYC	OB-C4B	8.87	1.40	1.23
13	S5	201	CYC	OB-C4B	8.86	1.40	1.23
13	V7	202	CYC	OB-C4B	8.86	1.40	1.23
13	N4	201	CYC	OB-C4B	8.86	1.40	1.23
13	A2	202	CYC	OB-C4B	8.86	1.40	1.23
13	T4	202	CYC	OB-C4B	8.86	1.40	1.23
13	M6	201	CYC	OB-C4B	8.86	1.40	1.23
13	B6	201	CYC	OB-C4B	8.86	1.40	1.23
13	J1	201	CYC	OB-C4B	8.86	1.40	1.23
13	g2	201	CYC	OB-C4B	8.86	1.40	1.23
13	C3	202	CYC	OB-C4B	8.86	1.40	1.23
13	V2	201	CYC	OB-C4B	8.86	1.40	1.23
13	H4	201	CYC	OB-C4B	8.86	1.40	1.23
13	H6	201	CYC	OB-C4B	8.86	1.40	1.23
13	C7	202	CYC	OB-C4B	8.86	1.40	1.23
13	K6	201	CYC	OB-C4B	8.86	1.40	1.23
13	E3	201	CYC	OB-C4B	8.86	1.40	1.23
13	Q7	202	CYC	OB-C4B	8.86	1.40	1.23
13	L2	201	CYC	OB-C4B	8.85	1.40	1.23
13	F1	202	CYC	OB-C4B	8.85	1.40	1.23
13	w2	201	CYC	OB-C4B	8.85	1.40	1.23
13	r2	201	CYC	OB-C4B	8.85	1.40	1.23
13	Q1	202	CYC	OB-C4B	8.85	1.40	1.23
13	F2	201	CYC	OB-C4B	8.85	1.40	1.23
13	N5	201	CYC	OB-C4B	8.85	1.40	1.23
13	G4	201	CYC	OB-C4B	8.85	1.40	1.23
13	M4	201	CYC	OB-C4B	8.85	1.40	1.23
13	a3	202	CYC	OB-C4B	8.85	1.40	1.23
13	D7	201	CYC	OB-C4B	8.85	1.40	1.23
13	M2	201	CYC	OB-C4B	8.84	1.40	1.23
13	J4	202	CYC	OB-C4B	8.84	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F1	201	CYC	OB-C4B	8.84	1.40	1.23
13	J3	202	CYC	OB-C4B	8.84	1.40	1.23
13	E6	201	CYC	OB-C4B	8.84	1.40	1.23
13	W2	201	CYC	OB-C4B	8.84	1.40	1.23
13	B1	201	CYC	OB-C4B	8.84	1.40	1.23
13	n2	201	CYC	OB-C4B	8.84	1.40	1.23
13	l2	201	CYC	OB-C4B	8.84	1.40	1.23
13	T7	201	CYC	OB-C4B	8.83	1.40	1.23
13	D1	201	CYC	OB-C4B	8.83	1.40	1.23
13	D5	201	CYC	OB-C4B	8.83	1.40	1.23
13	F5	202	CYC	OB-C4B	8.83	1.40	1.23
13	V5	202	CYC	OB-C4B	8.83	1.40	1.23
13	C5	202	CYC	OB-C4B	8.83	1.40	1.23
13	N2	802	CYC	OB-C4B	8.83	1.40	1.23
13	a1	202	CYC	OB-C4B	8.83	1.40	1.23
13	a6	202	CYC	OB-C4B	8.83	1.40	1.23
13	N1	201	CYC	OB-C4B	8.83	1.40	1.23
13	P2	201	CYC	OB-C4B	8.83	1.40	1.23
13	D3	201	CYC	OB-C4B	8.83	1.40	1.23
13	W1	201	CYC	OB-C4B	8.82	1.40	1.23
13	C6	202	CYC	OB-C4B	8.82	1.40	1.23
13	K1	201	CYC	OB-C4B	8.82	1.40	1.23
13	a4	202	CYC	OB-C4B	8.82	1.40	1.23
13	a7	202	CYC	OB-C4B	8.82	1.40	1.23
13	E7	201	CYC	OB-C4B	8.82	1.40	1.23
13	E4	201	CYC	OB-C4B	8.82	1.40	1.23
13	C1	202	CYC	OB-C4B	8.81	1.40	1.23
13	M5	201	CYC	OB-C4B	8.81	1.40	1.23
13	Q6	202	CYC	OB-C4B	8.81	1.40	1.23
13	V1	202	CYC	OB-C4B	8.81	1.40	1.23
13	C4	202	CYC	OB-C4B	8.81	1.40	1.23
13	V4	202	CYC	OB-C4B	8.81	1.40	1.23
13	Q3	202	CYC	OB-C4B	8.80	1.40	1.23
13	a5	202	CYC	OB-C4B	8.80	1.40	1.23
13	X6	201	CYC	OB-C4B	8.80	1.40	1.23
13	o2	801	CYC	OB-C4B	8.80	1.40	1.23
13	G6	201	CYC	OB-C4B	8.80	1.40	1.23
13	E1	201	CYC	OB-C4B	8.80	1.40	1.23
13	T1	201	CYC	OB-C4B	8.80	1.40	1.23
13	G2	201	CYC	OB-C4B	8.79	1.40	1.23
13	Q5	202	CYC	OB-C4B	8.79	1.40	1.23
13	V6	202	CYC	OB-C4B	8.79	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V3	202	CYC	OB-C4B	8.78	1.40	1.23
13	Q4	202	CYC	OB-C4B	8.78	1.40	1.23
13	J5	202	CYC	OB-C4B	8.78	1.40	1.23
13	J1	202	CYC	OB-C4B	8.78	1.40	1.23
13	E5	201	CYC	OB-C4B	8.78	1.40	1.23
13	T4	201	CYC	OB-C4B	8.77	1.40	1.23
13	X7	201	CYC	OB-C4B	8.77	1.40	1.23
13	T5	201	CYC	OB-C4B	8.76	1.40	1.23
13	D2	201	CYC	OB-C4B	8.76	1.40	1.23
13	m2	201	CYC	OB-C4B	8.75	1.40	1.23
13	S2	201	CYC	OB-C4B	8.74	1.40	1.23
13	J6	202	CYC	OB-C4B	8.74	1.40	1.23
13	T6	201	CYC	OB-C4B	8.74	1.40	1.23
13	G1	201	CYC	OB-C4B	8.73	1.40	1.23
13	X5	201	CYC	OB-C4B	8.73	1.40	1.23
13	h2	201	CYC	OB-C4B	8.72	1.40	1.23
13	X1	201	CYC	OB-C4B	8.71	1.40	1.23
13	t2	201	CYC	OB-C4B	8.71	1.40	1.23
13	X3	201	CYC	OB-C4B	8.67	1.40	1.23
13	E2	201	CYC	OB-C4B	8.66	1.40	1.23
13	R2	201	CYC	OB-C4B	8.65	1.40	1.23
13	e2	201	CYC	OB-C4B	8.65	1.40	1.23
13	v2	201	CYC	OB-C4B	8.63	1.39	1.23
13	U2	201	CYC	OB-C4B	8.60	1.39	1.23
13	f2	201	CYC	OB-C4B	8.60	1.39	1.23
13	s2	201	CYC	OB-C4B	8.60	1.39	1.23
13	X4	201	CYC	OB-C4B	8.58	1.39	1.23
13	A2	201	CYC	CHA-C1A	8.00	1.53	1.38
13	Q3	201	CYC	CHA-C1A	8.00	1.53	1.38
13	Q7	201	CYC	CHA-C1A	7.96	1.53	1.38
13	22	302	CYC	CHA-C1A	7.95	1.53	1.38
13	Q4	201	CYC	CHA-C1A	7.91	1.53	1.38
13	Q1	201	CYC	CHA-C1A	7.88	1.53	1.38
13	B2	202	CYC	CHA-C1A	7.88	1.53	1.38
13	Q6	201	CYC	CHA-C1A	7.88	1.53	1.38
13	P3	201	CYC	CHA-C1A	7.88	1.53	1.38
13	x2	201	CYC	CHA-C1A	7.88	1.53	1.38
13	T2	201	CYC	CHA-C1A	7.88	1.53	1.38
13	T3	202	CYC	CHA-C1A	7.88	1.53	1.38
13	c2	801	CYC	CHA-C1A	7.87	1.53	1.38
13	T5	202	CYC	CHA-C1A	7.87	1.53	1.38
13	T7	202	CYC	CHA-C1A	7.87	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M7	201	CYC	CHA-C1A	7.87	1.53	1.38
13	S2	201	CYC	CHA-C1A	7.87	1.53	1.38
13	P5	201	CYC	CHA-C1A	7.87	1.53	1.38
13	T6	202	CYC	CHA-C1A	7.86	1.53	1.38
13	L4	201	CYC	CHA-C1A	7.86	1.53	1.38
13	32	302	CYC	CHA-C1A	7.86	1.53	1.38
13	V3	201	CYC	CHA-C1A	7.86	1.53	1.38
13	L3	201	CYC	CHA-C1A	7.85	1.53	1.38
13	Z3	301	CYC	CHA-C1A	7.85	1.53	1.38
13	Q5	201	CYC	CHA-C1A	7.85	1.53	1.38
13	T4	202	CYC	CHA-C1A	7.84	1.53	1.38
13	V6	201	CYC	CHA-C1A	7.84	1.53	1.38
13	P4	202	CYC	CHA-C1A	7.84	1.53	1.38
13	a2	201	CYC	CHA-C1A	7.84	1.53	1.38
13	Z7	301	CYC	CHA-C1A	7.84	1.53	1.38
13	P5	202	CYC	CHA-C1A	7.83	1.53	1.38
13	D7	201	CYC	CHA-C1A	7.83	1.53	1.38
13	C7	201	CYC	CHA-C1A	7.83	1.53	1.38
13	P7	201	CYC	CHA-C1A	7.83	1.53	1.38
13	M3	201	CYC	CHA-C1A	7.83	1.53	1.38
13	D1	201	CYC	CHA-C1A	7.82	1.53	1.38
13	P6	201	CYC	CHA-C1A	7.82	1.53	1.38
13	B7	201	CYC	CHA-C1A	7.82	1.53	1.38
13	T1	202	CYC	CHA-C1A	7.82	1.53	1.38
13	V7	201	CYC	CHA-C1A	7.82	1.53	1.38
13	a3	201	CYC	CHA-C1A	7.82	1.53	1.38
13	C4	201	CYC	CHA-C1A	7.82	1.53	1.38
13	W2	201	CYC	CHA-C1A	7.82	1.53	1.38
13	P1	202	CYC	CHA-C1A	7.82	1.53	1.38
13	H7	201	CYC	CHA-C1A	7.82	1.53	1.38
13	H3	201	CYC	CHA-C1A	7.81	1.53	1.38
13	W7	201	CYC	CHA-C1A	7.81	1.53	1.38
13	L7	201	CYC	CHA-C1A	7.81	1.53	1.38
13	j2	201	CYC	CHA-C1A	7.80	1.53	1.38
13	a7	201	CYC	CHA-C1A	7.80	1.53	1.38
13	P1	201	CYC	CHA-C1A	7.80	1.53	1.38
13	W3	201	CYC	CHA-C1A	7.80	1.53	1.38
13	H2	201	CYC	CHA-C1A	7.80	1.53	1.38
13	D5	201	CYC	CHA-C1A	7.80	1.53	1.38
13	D4	201	CYC	CHA-C1A	7.80	1.53	1.38
13	Z4	301	CYC	CHA-C1A	7.79	1.53	1.38
13	R6	201	CYC	CHA-C1A	7.79	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J1	202	CYC	CHA-C1A	7.79	1.53	1.38
13	F3	201	CYC	CHA-C1A	7.79	1.53	1.38
13	C2	201	CYC	CHA-C1A	7.78	1.53	1.38
13	S3	201	CYC	CHA-C1A	7.78	1.53	1.38
13	Z6	301	CYC	CHA-C1A	7.78	1.53	1.38
13	C5	201	CYC	CHA-C1A	7.78	1.53	1.38
13	I6	201	CYC	CHA-C1A	7.78	1.53	1.38
13	C3	201	CYC	CHA-C1A	7.77	1.53	1.38
13	V1	201	CYC	CHA-C1A	7.77	1.53	1.38
13	V4	201	CYC	CHA-C1A	7.77	1.53	1.38
13	C6	201	CYC	CHA-C1A	7.77	1.53	1.38
13	F6	201	CYC	CHA-C1A	7.77	1.53	1.38
13	P6	202	CYC	CHA-C1A	7.76	1.53	1.38
13	42	301	CYC	CHA-C1A	7.76	1.53	1.38
13	J5	201	CYC	CHA-C1A	7.76	1.53	1.38
13	E2	201	CYC	CHA-C1A	7.76	1.53	1.38
13	F5	201	CYC	CHA-C1A	7.76	1.53	1.38
13	U7	201	CYC	CHA-C1A	7.76	1.53	1.38
13	F2	201	CYC	CHA-C1A	7.76	1.53	1.38
13	D6	201	CYC	CHA-C1A	7.76	1.53	1.38
13	X7	201	CYC	CHA-C1A	7.76	1.53	1.38
13	C1	202	CYC	CHA-C1A	7.76	1.53	1.38
13	k2	201	CYC	CHA-C1A	7.76	1.53	1.38
13	F4	201	CYC	CHA-C1A	7.76	1.53	1.38
13	P4	201	CYC	CHA-C1A	7.75	1.53	1.38
13	F7	201	CYC	CHA-C1A	7.75	1.53	1.38
13	N7	201	CYC	CHA-C1A	7.75	1.53	1.38
13	J4	202	CYC	CHA-C1A	7.75	1.53	1.38
13	U3	201	CYC	CHA-C1A	7.75	1.53	1.38
13	Q1	202	CYC	CHA-C1A	7.75	1.53	1.38
13	S7	201	CYC	CHA-C1A	7.75	1.53	1.38
13	B3	201	CYC	CHA-C1A	7.75	1.53	1.38
13	J6	202	CYC	CHA-C1A	7.74	1.53	1.38
13	r2	201	CYC	CHA-C1A	7.73	1.53	1.38
13	U2	201	CYC	CHA-C1A	7.73	1.53	1.38
13	L5	201	CYC	CHA-C1A	7.73	1.53	1.38
13	a6	201	CYC	CHA-C1A	7.73	1.53	1.38
13	G7	201	CYC	CHA-C1A	7.73	1.53	1.38
13	22	301	CYC	CHA-C1A	7.72	1.53	1.38
13	B2	201	CYC	CHA-C1A	7.72	1.53	1.38
13	I3	201	CYC	CHA-C1A	7.72	1.53	1.38
13	W4	201	CYC	CHA-C1A	7.72	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V7	202	CYC	CHA-C1A	7.72	1.53	1.38
13	J5	202	CYC	CHA-C1A	7.72	1.53	1.38
13	Q4	202	CYC	CHA-C1A	7.72	1.53	1.38
13	V5	201	CYC	CHA-C1A	7.72	1.53	1.38
13	I4	201	CYC	CHA-C1A	7.72	1.53	1.38
13	D3	201	CYC	CHA-C1A	7.72	1.53	1.38
13	d2	201	CYC	CHA-C1A	7.72	1.53	1.38
13	I1	201	CYC	CHA-C1A	7.72	1.53	1.38
13	L1	201	CYC	CHA-C1A	7.72	1.53	1.38
13	s2	201	CYC	CHA-C1A	7.71	1.53	1.38
13	C1	201	CYC	CHA-C1A	7.71	1.53	1.38
13	F1	201	CYC	CHA-C1A	7.71	1.53	1.38
13	N3	201	CYC	CHA-C1A	7.71	1.53	1.38
13	C4	202	CYC	CHA-C1A	7.71	1.53	1.38
13	a5	201	CYC	CHA-C1A	7.71	1.53	1.38
13	U5	201	CYC	CHA-C1A	7.71	1.53	1.38
13	K3	201	CYC	CHA-C1A	7.71	1.53	1.38
13	Q6	202	CYC	CHA-C1A	7.71	1.53	1.38
13	P7	202	CYC	CHA-C1A	7.71	1.53	1.38
13	32	301	CYC	CHA-C1A	7.71	1.53	1.38
13	N2	802	CYC	CHA-C1A	7.70	1.53	1.38
13	Z5	301	CYC	CHA-C1A	7.70	1.53	1.38
13	V3	202	CYC	CHA-C1A	7.70	1.53	1.38
13	52	301	CYC	CHA-C1A	7.70	1.53	1.38
13	W1	201	CYC	CHA-C1A	7.70	1.53	1.38
13	e2	201	CYC	CHA-C1A	7.70	1.53	1.38
13	42	302	CYC	CHA-C1A	7.70	1.53	1.38
13	R2	201	CYC	CHA-C1A	7.70	1.53	1.38
13	Q7	202	CYC	CHA-C1A	7.70	1.53	1.38
13	I5	201	CYC	CHA-C1A	7.70	1.53	1.38
13	Q3	202	CYC	CHA-C1A	7.70	1.53	1.38
13	R5	201	CYC	CHA-C1A	7.70	1.53	1.38
13	U6	201	CYC	CHA-C1A	7.70	1.53	1.38
13	A6	302	CYC	CHA-C1A	7.70	1.53	1.38
13	t2	201	CYC	CHA-C1A	7.70	1.53	1.38
13	R3	201	CYC	CHA-C1A	7.69	1.53	1.38
13	F7	202	CYC	CHA-C1A	7.69	1.53	1.38
13	R1	201	CYC	CHA-C1A	7.69	1.53	1.38
13	L6	201	CYC	CHA-C1A	7.69	1.53	1.38
13	a1	201	CYC	CHA-C1A	7.69	1.53	1.38
13	Q5	202	CYC	CHA-C1A	7.69	1.53	1.38
13	C6	202	CYC	CHA-C1A	7.69	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z1	301	CYC	CHA-C1A	7.69	1.53	1.38
13	y2	201	CYC	CHA-C1A	7.69	1.53	1.38
13	X2	201	CYC	CHA-C1A	7.68	1.53	1.38
13	F4	202	CYC	CHA-C1A	7.68	1.53	1.38
13	S5	201	CYC	CHA-C1A	7.68	1.53	1.38
13	R7	201	CYC	CHA-C1A	7.68	1.53	1.38
13	P3	202	CYC	CHA-C1A	7.68	1.53	1.38
13	v2	201	CYC	CHA-C1A	7.68	1.53	1.38
13	z2	201	CYC	CHA-C1A	7.68	1.53	1.38
13	A2	202	CYC	CHA-C1A	7.68	1.53	1.38
13	K4	201	CYC	CHA-C1A	7.68	1.53	1.38
13	U4	201	CYC	CHA-C1A	7.68	1.53	1.38
13	I7	201	CYC	CHA-C1A	7.68	1.53	1.38
13	X3	201	CYC	CHA-C1A	7.68	1.53	1.38
13	G4	201	CYC	CHA-C1A	7.67	1.53	1.38
13	J4	201	CYC	CHA-C1A	7.67	1.53	1.38
13	G3	201	CYC	CHA-C1A	7.67	1.53	1.38
13	A1	302	CYC	CHA-C1A	7.67	1.53	1.38
13	F6	202	CYC	CHA-C1A	7.67	1.53	1.38
13	M1	201	CYC	CHA-C1A	7.67	1.53	1.38
13	E1	201	CYC	CHA-C1A	7.67	1.53	1.38
13	F3	202	CYC	CHA-C1A	7.67	1.53	1.38
13	W6	201	CYC	CHA-C1A	7.67	1.53	1.38
13	R4	201	CYC	CHA-C1A	7.67	1.53	1.38
13	H4	201	CYC	CHA-C1A	7.67	1.53	1.38
13	S6	201	CYC	CHA-C1A	7.66	1.53	1.38
13	V2	201	CYC	CHA-C1A	7.66	1.53	1.38
13	a3	202	CYC	CHA-C1A	7.66	1.53	1.38
13	M4	201	CYC	CHA-C1A	7.66	1.53	1.38
13	F1	202	CYC	CHA-C1A	7.65	1.53	1.38
13	H6	201	CYC	CHA-C1A	7.65	1.53	1.38
13	U1	201	CYC	CHA-C1A	7.65	1.53	1.38
13	i2	201	CYC	CHA-C1A	7.65	1.53	1.38
13	S4	201	CYC	CHA-C1A	7.65	1.53	1.38
13	V6	202	CYC	CHA-C1A	7.65	1.53	1.38
13	C7	202	CYC	CHA-C1A	7.65	1.53	1.38
13	E7	201	CYC	CHA-C1A	7.65	1.53	1.38
13	S1	201	CYC	CHA-C1A	7.65	1.53	1.38
13	L2	201	CYC	CHA-C1A	7.65	1.53	1.38
13	B6	201	CYC	CHA-C1A	7.65	1.53	1.38
13	V4	202	CYC	CHA-C1A	7.65	1.53	1.38
13	M6	201	CYC	CHA-C1A	7.65	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V5	202	CYC	CHA-C1A	7.64	1.53	1.38
13	a7	202	CYC	CHA-C1A	7.64	1.53	1.38
13	X5	201	CYC	CHA-C1A	7.64	1.53	1.38
13	G6	201	CYC	CHA-C1A	7.64	1.53	1.38
13	T1	201	CYC	CHA-C1A	7.64	1.53	1.38
13	B4	201	CYC	CHA-C1A	7.64	1.53	1.38
13	52	302	CYC	CHA-C1A	7.64	1.53	1.38
13	X6	201	CYC	CHA-C1A	7.64	1.53	1.38
13	J3	202	CYC	CHA-C1A	7.64	1.53	1.38
13	C3	202	CYC	CHA-C1A	7.64	1.53	1.38
13	E3	201	CYC	CHA-C1A	7.63	1.53	1.38
13	T3	201	CYC	CHA-C1A	7.63	1.53	1.38
13	T7	201	CYC	CHA-C1A	7.63	1.53	1.38
13	J3	201	CYC	CHA-C1A	7.63	1.53	1.38
13	a4	202	CYC	CHA-C1A	7.63	1.53	1.38
13	E6	201	CYC	CHA-C1A	7.62	1.53	1.38
13	f2	201	CYC	CHA-C1A	7.62	1.53	1.38
13	J1	201	CYC	CHA-C1A	7.62	1.53	1.38
13	K7	201	CYC	CHA-C1A	7.62	1.53	1.38
13	w2	201	CYC	CHA-C1A	7.62	1.53	1.38
13	a5	202	CYC	CHA-C1A	7.62	1.53	1.38
13	o2	801	CYC	CHA-C1A	7.62	1.53	1.38
13	G5	201	CYC	CHA-C1A	7.62	1.53	1.38
13	J6	201	CYC	CHA-C1A	7.62	1.53	1.38
13	D2	201	CYC	CHA-C1A	7.62	1.53	1.38
13	C5	202	CYC	CHA-C1A	7.61	1.53	1.38
13	V1	202	CYC	CHA-C1A	7.61	1.53	1.38
13	M5	201	CYC	CHA-C1A	7.61	1.53	1.38
13	J7	202	CYC	CHA-C1A	7.61	1.53	1.38
13	N4	201	CYC	CHA-C1A	7.61	1.53	1.38
13	a6	202	CYC	CHA-C1A	7.61	1.53	1.38
13	X1	201	CYC	CHA-C1A	7.61	1.53	1.38
13	J7	201	CYC	CHA-C1A	7.61	1.53	1.38
13	N2	801	CYC	CHA-C1A	7.61	1.53	1.38
13	F5	202	CYC	CHA-C1A	7.61	1.53	1.38
13	Q2	201	CYC	CHA-C1A	7.60	1.53	1.38
13	W5	201	CYC	CHA-C1A	7.60	1.53	1.38
13	K1	201	CYC	CHA-C1A	7.59	1.53	1.38
13	K6	201	CYC	CHA-C1A	7.59	1.53	1.38
13	E5	201	CYC	CHA-C1A	7.59	1.53	1.38
13	O2	201	CYC	CHA-C1A	7.59	1.53	1.38
13	K5	201	CYC	CHA-C1A	7.59	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G1	201	CYC	CHA-C1A	7.58	1.53	1.38
13	E4	201	CYC	CHA-C1A	7.58	1.53	1.38
13	H5	201	CYC	CHA-C1A	7.58	1.53	1.38
13	X4	201	CYC	CHA-C1A	7.57	1.53	1.38
13	A1	301	CYC	CHA-C1A	7.57	1.53	1.38
13	T6	201	CYC	CHA-C1A	7.57	1.53	1.38
13	a1	202	CYC	CHA-C1A	7.57	1.53	1.38
13	N1	201	CYC	CHA-C1A	7.56	1.53	1.38
13	P2	201	CYC	CHA-C1A	7.56	1.53	1.38
13	N5	201	CYC	CHA-C1A	7.56	1.53	1.38
13	N6	201	CYC	CHA-C1A	7.56	1.53	1.38
13	l2	201	CYC	CHA-C1A	7.56	1.53	1.38
13	h2	201	CYC	CHA-C1A	7.55	1.53	1.38
13	p2	201	CYC	CHA-C1A	7.55	1.52	1.38
13	B1	201	CYC	CHA-C1A	7.54	1.52	1.38
13	g2	201	CYC	CHA-C1A	7.53	1.52	1.38
13	A6	301	CYC	CHA-C1A	7.53	1.52	1.38
13	B5	201	CYC	CHA-C1A	7.53	1.52	1.38
13	H1	201	CYC	CHA-C1A	7.53	1.52	1.38
13	T4	201	CYC	CHA-C1A	7.53	1.52	1.38
13	G2	201	CYC	CHA-C1A	7.51	1.52	1.38
13	T5	201	CYC	CHA-C1A	7.49	1.52	1.38
13	m2	201	CYC	CHA-C1A	7.48	1.52	1.38
13	n2	201	CYC	CHA-C1A	7.47	1.52	1.38
13	M2	201	CYC	CHA-C1A	7.46	1.52	1.38
13	32	302	CYC	CHB-C1B	6.97	1.54	1.37
13	22	302	CYC	CHB-C1B	6.96	1.54	1.37
13	A1	301	CYC	CHB-C1B	6.95	1.54	1.37
13	42	302	CYC	CHB-C1B	6.94	1.54	1.37
13	52	302	CYC	CHB-C1B	6.91	1.54	1.37
13	A6	301	CYC	CHB-C1B	6.91	1.54	1.37
13	A6	302	CYC	CHB-C1B	6.90	1.54	1.37
13	42	301	CYC	CHB-C1B	6.89	1.54	1.37
13	A1	302	CYC	CHB-C1B	6.89	1.54	1.37
13	52	301	CYC	CHB-C1B	6.88	1.54	1.37
13	a6	201	CYC	CHB-C1B	6.88	1.54	1.37
13	a5	201	CYC	CHB-C1B	6.85	1.54	1.37
13	Z4	301	CYC	CHB-C1B	6.84	1.54	1.37
13	Z6	301	CYC	CHB-C1B	6.84	1.54	1.37
13	a1	201	CYC	CHB-C1B	6.84	1.54	1.37
13	a7	201	CYC	CHB-C1B	6.84	1.54	1.37
13	a3	201	CYC	CHB-C1B	6.83	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	32	301	CYC	CHB-C1B	6.83	1.54	1.37
13	A2	201	CYC	CHB-C1B	6.81	1.54	1.37
13	22	301	CYC	CHB-C1B	6.80	1.54	1.37
13	V5	202	CYC	CHB-C1B	6.78	1.54	1.37
13	Z3	301	CYC	CHB-C1B	6.78	1.54	1.37
13	D3	201	CYC	CHB-C1B	6.78	1.54	1.37
13	V6	202	CYC	CHB-C1B	6.78	1.54	1.37
13	D7	201	CYC	CHB-C1B	6.77	1.54	1.37
13	Z7	301	CYC	CHB-C1B	6.77	1.54	1.37
13	Z1	301	CYC	CHB-C1B	6.77	1.54	1.37
13	O2	201	CYC	CHB-C1B	6.76	1.54	1.37
13	J5	201	CYC	CHB-C1B	6.76	1.54	1.37
13	h2	201	CYC	CHB-C1B	6.76	1.54	1.37
13	e2	201	CYC	CHB-C1B	6.76	1.54	1.37
13	V4	202	CYC	CHB-C1B	6.75	1.54	1.37
13	E2	201	CYC	CHB-C1B	6.75	1.54	1.37
13	X7	201	CYC	CHB-C1B	6.75	1.54	1.37
13	W2	201	CYC	CHB-C1B	6.75	1.54	1.37
13	R2	201	CYC	CHB-C1B	6.73	1.54	1.37
13	G2	201	CYC	CHB-C1B	6.73	1.54	1.37
13	Z5	301	CYC	CHB-C1B	6.73	1.54	1.37
13	V3	202	CYC	CHB-C1B	6.73	1.54	1.37
13	D2	201	CYC	CHB-C1B	6.72	1.54	1.37
13	X1	201	CYC	CHB-C1B	6.72	1.54	1.37
13	V1	202	CYC	CHB-C1B	6.72	1.54	1.37
13	s2	201	CYC	CHB-C1B	6.72	1.54	1.37
13	a2	201	CYC	CHB-C1B	6.72	1.54	1.37
13	N2	801	CYC	CHB-C1B	6.71	1.54	1.37
13	Q2	201	CYC	CHB-C1B	6.71	1.53	1.37
13	D4	201	CYC	CHB-C1B	6.71	1.53	1.37
13	g2	201	CYC	CHB-C1B	6.70	1.53	1.37
13	X3	201	CYC	CHB-C1B	6.70	1.53	1.37
13	D6	201	CYC	CHB-C1B	6.70	1.53	1.37
13	Q5	201	CYC	CHB-C1B	6.70	1.53	1.37
13	X6	201	CYC	CHB-C1B	6.70	1.53	1.37
13	V7	202	CYC	CHB-C1B	6.70	1.53	1.37
13	T2	201	CYC	CHB-C1B	6.69	1.53	1.37
13	L1	201	CYC	CHB-C1B	6.69	1.53	1.37
13	Q4	201	CYC	CHB-C1B	6.69	1.53	1.37
13	V4	201	CYC	CHB-C1B	6.69	1.53	1.37
13	z2	201	CYC	CHB-C1B	6.69	1.53	1.37
13	x2	201	CYC	CHB-C1B	6.69	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d2	201	CYC	CHB-C1B	6.69	1.53	1.37
13	r2	201	CYC	CHB-C1B	6.68	1.53	1.37
13	C5	201	CYC	CHB-C1B	6.68	1.53	1.37
13	Q5	202	CYC	CHB-C1B	6.68	1.53	1.37
13	X5	201	CYC	CHB-C1B	6.68	1.53	1.37
13	p2	201	CYC	CHB-C1B	6.68	1.53	1.37
13	C4	201	CYC	CHB-C1B	6.68	1.53	1.37
13	Q4	202	CYC	CHB-C1B	6.67	1.53	1.37
13	X2	201	CYC	CHB-C1B	6.67	1.53	1.37
13	J6	202	CYC	CHB-C1B	6.67	1.53	1.37
13	P6	201	CYC	CHB-C1B	6.67	1.53	1.37
13	l2	201	CYC	CHB-C1B	6.67	1.53	1.37
13	Q6	201	CYC	CHB-C1B	6.67	1.53	1.37
13	Q7	202	CYC	CHB-C1B	6.67	1.53	1.37
13	Q6	202	CYC	CHB-C1B	6.66	1.53	1.37
13	V6	201	CYC	CHB-C1B	6.66	1.53	1.37
13	T7	202	CYC	CHB-C1B	6.66	1.53	1.37
13	Q7	201	CYC	CHB-C1B	6.66	1.53	1.37
13	v2	201	CYC	CHB-C1B	6.66	1.53	1.37
13	J4	202	CYC	CHB-C1B	6.66	1.53	1.37
13	D1	201	CYC	CHB-C1B	6.65	1.53	1.37
13	V1	201	CYC	CHB-C1B	6.65	1.53	1.37
13	y2	201	CYC	CHB-C1B	6.65	1.53	1.37
13	V3	201	CYC	CHB-C1B	6.65	1.53	1.37
13	P3	201	CYC	CHB-C1B	6.65	1.53	1.37
13	C6	202	CYC	CHB-C1B	6.65	1.53	1.37
13	M2	201	CYC	CHB-C1B	6.65	1.53	1.37
13	C2	201	CYC	CHB-C1B	6.65	1.53	1.37
13	Q1	201	CYC	CHB-C1B	6.64	1.53	1.37
13	J1	202	CYC	CHB-C1B	6.64	1.53	1.37
13	F2	201	CYC	CHB-C1B	6.64	1.53	1.37
13	P7	201	CYC	CHB-C1B	6.64	1.53	1.37
13	J4	201	CYC	CHB-C1B	6.64	1.53	1.37
13	V7	201	CYC	CHB-C1B	6.64	1.53	1.37
13	X4	201	CYC	CHB-C1B	6.64	1.53	1.37
13	Q1	202	CYC	CHB-C1B	6.64	1.53	1.37
13	C5	202	CYC	CHB-C1B	6.63	1.53	1.37
13	M3	201	CYC	CHB-C1B	6.63	1.53	1.37
13	P4	202	CYC	CHB-C1B	6.63	1.53	1.37
13	C1	202	CYC	CHB-C1B	6.63	1.53	1.37
13	L6	201	CYC	CHB-C1B	6.63	1.53	1.37
13	M1	201	CYC	CHB-C1B	6.63	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M7	201	CYC	CHB-C1B	6.63	1.53	1.37
13	J5	202	CYC	CHB-C1B	6.62	1.53	1.37
13	A2	202	CYC	CHB-C1B	6.62	1.53	1.37
13	B2	201	CYC	CHB-C1B	6.62	1.53	1.37
13	Q3	202	CYC	CHB-C1B	6.62	1.53	1.37
13	Q3	201	CYC	CHB-C1B	6.62	1.53	1.37
13	C1	201	CYC	CHB-C1B	6.62	1.53	1.37
13	I6	201	CYC	CHB-C1B	6.62	1.53	1.37
13	E1	201	CYC	CHB-C1B	6.62	1.53	1.37
13	a4	202	CYC	CHB-C1B	6.62	1.53	1.37
13	P5	201	CYC	CHB-C1B	6.62	1.53	1.37
13	J3	201	CYC	CHB-C1B	6.62	1.53	1.37
13	T3	202	CYC	CHB-C1B	6.62	1.53	1.37
13	M5	201	CYC	CHB-C1B	6.62	1.53	1.37
13	a6	202	CYC	CHB-C1B	6.61	1.53	1.37
13	P1	201	CYC	CHB-C1B	6.61	1.53	1.37
13	D5	201	CYC	CHB-C1B	6.61	1.53	1.37
13	C4	202	CYC	CHB-C1B	6.60	1.53	1.37
13	F3	201	CYC	CHB-C1B	6.60	1.53	1.37
13	S5	201	CYC	CHB-C1B	6.60	1.53	1.37
13	C7	201	CYC	CHB-C1B	6.60	1.53	1.37
13	N1	201	CYC	CHB-C1B	6.60	1.53	1.37
13	U1	201	CYC	CHB-C1B	6.60	1.53	1.37
13	G4	201	CYC	CHB-C1B	6.60	1.53	1.37
13	J6	201	CYC	CHB-C1B	6.60	1.53	1.37
13	a3	202	CYC	CHB-C1B	6.60	1.53	1.37
13	L4	201	CYC	CHB-C1B	6.60	1.53	1.37
13	V5	201	CYC	CHB-C1B	6.60	1.53	1.37
13	U2	201	CYC	CHB-C1B	6.60	1.53	1.37
13	P2	201	CYC	CHB-C1B	6.59	1.53	1.37
13	i2	201	CYC	CHB-C1B	6.59	1.53	1.37
13	M4	201	CYC	CHB-C1B	6.59	1.53	1.37
13	a5	202	CYC	CHB-C1B	6.59	1.53	1.37
13	f2	201	CYC	CHB-C1B	6.59	1.53	1.37
13	J1	201	CYC	CHB-C1B	6.59	1.53	1.37
13	S4	201	CYC	CHB-C1B	6.59	1.53	1.37
13	I3	201	CYC	CHB-C1B	6.59	1.53	1.37
13	M6	201	CYC	CHB-C1B	6.59	1.53	1.37
13	T5	202	CYC	CHB-C1B	6.59	1.53	1.37
13	a1	202	CYC	CHB-C1B	6.58	1.53	1.37
13	P4	201	CYC	CHB-C1B	6.58	1.53	1.37
13	C6	201	CYC	CHB-C1B	6.58	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N4	201	CYC	CHB-C1B	6.58	1.53	1.37
13	W5	201	CYC	CHB-C1B	6.58	1.53	1.37
13	W4	201	CYC	CHB-C1B	6.58	1.53	1.37
13	C7	202	CYC	CHB-C1B	6.58	1.53	1.37
13	I5	201	CYC	CHB-C1B	6.58	1.53	1.37
13	R6	201	CYC	CHB-C1B	6.58	1.53	1.37
13	C3	202	CYC	CHB-C1B	6.57	1.53	1.37
13	T1	202	CYC	CHB-C1B	6.57	1.53	1.37
13	J7	201	CYC	CHD-C1D	6.57	1.55	1.40
13	V2	201	CYC	CHD-C1D	6.57	1.55	1.40
13	E5	201	CYC	CHB-C1B	6.57	1.53	1.37
13	F6	201	CYC	CHB-C1B	6.57	1.53	1.37
13	L5	201	CYC	CHD-C1D	6.57	1.55	1.40
13	W6	201	CYC	CHB-C1B	6.57	1.53	1.37
13	U7	201	CYC	CHB-C1B	6.56	1.53	1.37
13	W3	201	CYC	CHB-C1B	6.56	1.53	1.37
13	L5	201	CYC	CHB-C1B	6.56	1.53	1.37
13	F4	201	CYC	CHB-C1B	6.56	1.53	1.37
13	c2	801	CYC	CHB-C1B	6.56	1.53	1.37
13	o2	801	CYC	CHB-C1B	6.56	1.53	1.37
13	S6	201	CYC	CHB-C1B	6.56	1.53	1.37
13	L7	201	CYC	CHB-C1B	6.56	1.53	1.37
13	K4	201	CYC	CHB-C1B	6.56	1.53	1.37
13	K6	201	CYC	CHB-C1B	6.56	1.53	1.37
13	G7	201	CYC	CHB-C1B	6.56	1.53	1.37
13	F5	201	CYC	CHB-C1B	6.56	1.53	1.37
13	F1	201	CYC	CHB-C1B	6.56	1.53	1.37
13	T1	201	CYC	CHB-C1B	6.55	1.53	1.37
13	W1	201	CYC	CHB-C1B	6.55	1.53	1.37
13	I4	201	CYC	CHB-C1B	6.55	1.53	1.37
13	U5	201	CYC	CHB-C1B	6.55	1.53	1.37
13	I1	201	CYC	CHB-C1B	6.55	1.53	1.37
13	S3	201	CYC	CHB-C1B	6.55	1.53	1.37
13	T6	201	CYC	CHB-C1B	6.55	1.53	1.37
13	Z6	301	CYC	CHD-C1D	6.55	1.55	1.40
13	K5	201	CYC	CHB-C1B	6.55	1.53	1.37
13	N7	201	CYC	CHB-C1B	6.55	1.53	1.37
13	P5	202	CYC	CHB-C1B	6.55	1.53	1.37
13	N5	201	CYC	CHB-C1B	6.54	1.53	1.37
13	F7	201	CYC	CHB-C1B	6.54	1.53	1.37
13	F5	202	CYC	CHB-C1B	6.54	1.53	1.37
13	H7	201	CYC	CHB-C1B	6.54	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J7	201	CYC	CHB-C1B	6.54	1.53	1.37
13	W7	201	CYC	CHB-C1B	6.54	1.53	1.37
13	32	301	CYC	CHD-C1D	6.54	1.55	1.40
13	C4	201	CYC	CHD-C1D	6.54	1.55	1.40
13	N6	201	CYC	CHB-C1B	6.54	1.53	1.37
13	G3	201	CYC	CHB-C1B	6.53	1.53	1.37
13	B6	201	CYC	CHB-C1B	6.53	1.53	1.37
13	U4	201	CYC	CHB-C1B	6.53	1.53	1.37
13	G6	201	CYC	CHB-C1B	6.53	1.53	1.37
13	V2	201	CYC	CHB-C1B	6.53	1.53	1.37
13	J3	201	CYC	CHD-C1D	6.53	1.55	1.40
13	Z5	301	CYC	CHD-C1D	6.53	1.55	1.40
13	U3	201	CYC	CHB-C1B	6.53	1.53	1.37
13	J7	202	CYC	CHB-C1B	6.53	1.53	1.37
13	C5	201	CYC	CHD-C1D	6.53	1.55	1.40
13	a7	202	CYC	CHB-C1B	6.53	1.53	1.37
13	G1	201	CYC	CHB-C1B	6.53	1.53	1.37
13	S1	201	CYC	CHB-C1B	6.53	1.53	1.37
13	E6	201	CYC	CHB-C1B	6.53	1.53	1.37
13	T6	202	CYC	CHB-C1B	6.53	1.53	1.37
13	Z4	301	CYC	CHD-C1D	6.53	1.55	1.40
13	B1	201	CYC	CHB-C1B	6.53	1.53	1.37
13	C3	201	CYC	CHB-C1B	6.53	1.53	1.37
13	B7	201	CYC	CHB-C1B	6.53	1.53	1.37
13	U6	201	CYC	CHB-C1B	6.53	1.53	1.37
13	I7	201	CYC	CHB-C1B	6.52	1.53	1.37
13	L2	201	CYC	CHB-C1B	6.52	1.53	1.37
13	E4	201	CYC	CHB-C1B	6.52	1.53	1.37
13	T4	201	CYC	CHB-C1B	6.52	1.53	1.37
13	P6	202	CYC	CHB-C1B	6.52	1.53	1.37
13	w2	201	CYC	CHB-C1B	6.52	1.53	1.37
13	J3	202	CYC	CHB-C1B	6.52	1.53	1.37
13	J5	201	CYC	CHD-C1D	6.52	1.55	1.40
13	P3	202	CYC	CHB-C1B	6.52	1.53	1.37
13	B4	201	CYC	CHB-C1B	6.52	1.53	1.37
13	G5	201	CYC	CHB-C1B	6.52	1.53	1.37
13	S2	201	CYC	CHB-C1B	6.52	1.53	1.37
13	J4	201	CYC	CHD-C1D	6.51	1.55	1.40
13	B3	201	CYC	CHB-C1B	6.51	1.53	1.37
13	j2	201	CYC	CHB-C1B	6.51	1.53	1.37
13	C3	201	CYC	CHD-C1D	6.51	1.55	1.40
13	P1	202	CYC	CHB-C1B	6.51	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R1	201	CYC	CHB-C1B	6.51	1.53	1.37
13	R3	201	CYC	CHB-C1B	6.51	1.53	1.37
13	N3	201	CYC	CHB-C1B	6.51	1.53	1.37
13	E3	201	CYC	CHB-C1B	6.51	1.53	1.37
13	F6	202	CYC	CHB-C1B	6.51	1.53	1.37
13	H1	201	CYC	CHB-C1B	6.51	1.53	1.37
13	T5	201	CYC	CHB-C1B	6.51	1.53	1.37
13	R5	201	CYC	CHB-C1B	6.51	1.53	1.37
13	L3	201	CYC	CHB-C1B	6.51	1.53	1.37
13	H6	201	CYC	CHB-C1B	6.50	1.53	1.37
13	E7	201	CYC	CHB-C1B	6.50	1.53	1.37
13	S2	201	CYC	CHD-C1D	6.50	1.55	1.40
13	H4	201	CYC	CHB-C1B	6.50	1.53	1.37
13	K7	201	CYC	CHB-C1B	6.50	1.53	1.37
13	H3	201	CYC	CHB-C1B	6.50	1.53	1.37
13	F7	202	CYC	CHB-C1B	6.50	1.53	1.37
13	T7	201	CYC	CHB-C1B	6.50	1.53	1.37
13	N2	801	CYC	CHD-C1D	6.50	1.55	1.40
13	P7	202	CYC	CHB-C1B	6.50	1.53	1.37
13	L4	201	CYC	CHD-C1D	6.49	1.55	1.40
13	H5	201	CYC	CHB-C1B	6.49	1.53	1.37
13	F1	202	CYC	CHB-C1B	6.49	1.53	1.37
13	M3	201	CYC	CHD-C1D	6.49	1.55	1.40
13	X4	201	CYC	CHD-C1D	6.49	1.55	1.40
13	T4	202	CYC	CHB-C1B	6.49	1.53	1.37
13	S7	201	CYC	CHB-C1B	6.49	1.53	1.37
13	T3	201	CYC	CHB-C1B	6.49	1.53	1.37
13	R4	201	CYC	CHB-C1B	6.49	1.53	1.37
13	t2	201	CYC	CHB-C1B	6.48	1.53	1.37
13	M7	201	CYC	CHD-C1D	6.48	1.55	1.40
13	K1	201	CYC	CHB-C1B	6.48	1.53	1.37
13	X6	201	CYC	CHD-C1D	6.48	1.55	1.40
13	X1	201	CYC	CHD-C1D	6.48	1.55	1.40
13	22	301	CYC	CHD-C1D	6.48	1.55	1.40
13	A1	301	CYC	CHD-C1D	6.48	1.55	1.40
13	C1	201	CYC	CHD-C1D	6.48	1.55	1.40
13	n2	201	CYC	CHB-C1B	6.48	1.53	1.37
13	Z1	301	CYC	CHD-C1D	6.48	1.55	1.40
13	R7	201	CYC	CHB-C1B	6.48	1.53	1.37
13	P2	201	CYC	CHD-C1D	6.48	1.55	1.40
13	N2	802	CYC	CHB-C1B	6.47	1.53	1.37
13	F3	202	CYC	CHB-C1B	6.47	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a5	201	CYC	CHD-C1D	6.47	1.55	1.40
13	i2	201	CYC	CHD-C1D	6.46	1.55	1.40
13	L1	201	CYC	CHD-C1D	6.46	1.55	1.40
13	J6	201	CYC	CHD-C1D	6.46	1.55	1.40
13	K3	201	CYC	CHB-C1B	6.46	1.53	1.37
13	B2	202	CYC	CHB-C1B	6.46	1.53	1.37
13	X5	201	CYC	CHD-C1D	6.46	1.55	1.40
13	L3	201	CYC	CHD-C1D	6.46	1.55	1.40
13	X3	201	CYC	CHD-C1D	6.46	1.55	1.40
13	F4	202	CYC	CHB-C1B	6.46	1.53	1.37
13	C6	201	CYC	CHD-C1D	6.45	1.55	1.40
13	H2	201	CYC	CHB-C1B	6.45	1.53	1.37
13	J1	201	CYC	CHD-C1D	6.45	1.55	1.40
13	L7	201	CYC	CHD-C1D	6.45	1.55	1.40
13	X7	201	CYC	CHD-C1D	6.44	1.54	1.40
13	C7	201	CYC	CHD-C1D	6.44	1.54	1.40
13	B5	201	CYC	CHB-C1B	6.44	1.53	1.37
13	M6	201	CYC	CHD-C1D	6.43	1.54	1.40
13	k2	201	CYC	CHB-C1B	6.42	1.53	1.37
13	A6	301	CYC	CHD-C1D	6.42	1.54	1.40
13	a1	201	CYC	CHD-C1D	6.40	1.54	1.40
13	D7	201	CYC	CHD-C1D	6.39	1.54	1.40
13	m2	201	CYC	CHB-C1B	6.37	1.53	1.37
13	L6	201	CYC	CHD-C1D	6.37	1.54	1.40
13	M1	201	CYC	CHD-C1D	6.37	1.54	1.40
13	P5	202	CYC	CHD-C1D	6.36	1.54	1.40
13	a6	201	CYC	CHD-C1D	6.36	1.54	1.40
13	M4	201	CYC	CHD-C1D	6.34	1.54	1.40
13	a3	201	CYC	CHD-C1D	6.33	1.54	1.40
13	M5	201	CYC	CHD-C1D	6.33	1.54	1.40
13	P1	202	CYC	CHD-C1D	6.32	1.54	1.40
13	a7	201	CYC	CHD-C1D	6.32	1.54	1.40
13	D4	201	CYC	CHD-C1D	6.32	1.54	1.40
13	x2	201	CYC	CHD-C1D	6.32	1.54	1.40
13	T2	201	CYC	CHD-C1D	6.32	1.54	1.40
13	D5	201	CYC	CHD-C1D	6.32	1.54	1.40
13	42	301	CYC	CHD-C1D	6.31	1.54	1.40
13	P6	202	CYC	CHD-C1D	6.31	1.54	1.40
13	52	301	CYC	CHD-C1D	6.30	1.54	1.40
13	J3	202	CYC	CHD-C1D	6.30	1.54	1.40
13	D6	201	CYC	CHD-C1D	6.30	1.54	1.40
13	B2	201	CYC	CHD-C1D	6.29	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P4	201	CYC	CHD-C1D	6.29	1.54	1.40
13	U2	201	CYC	CHD-C1D	6.29	1.54	1.40
13	J4	202	CYC	CHD-C1D	6.29	1.54	1.40
13	J7	202	CYC	CHD-C1D	6.29	1.54	1.40
13	J1	202	CYC	CHD-C1D	6.28	1.54	1.40
13	X2	201	CYC	CHD-C1D	6.28	1.54	1.40
13	D1	201	CYC	CHD-C1D	6.28	1.54	1.40
13	J5	202	CYC	CHD-C1D	6.26	1.54	1.40
13	V3	201	CYC	CHD-C1D	6.25	1.54	1.40
13	V5	201	CYC	CHD-C1D	6.24	1.54	1.40
13	A1	302	CYC	CHD-C1D	6.22	1.54	1.40
13	52	302	CYC	CHD-C1D	6.21	1.54	1.40
13	D3	201	CYC	CHD-C1D	6.20	1.54	1.40
13	J6	202	CYC	CHD-C1D	6.20	1.54	1.40
13	A6	302	CYC	CHD-C1D	6.20	1.54	1.40
13	V4	201	CYC	CHD-C1D	6.19	1.54	1.40
13	t2	201	CYC	CHD-C1D	6.18	1.54	1.40
13	V6	201	CYC	CHD-C1D	6.18	1.54	1.40
13	P3	202	CYC	CHD-C1D	6.16	1.54	1.40
13	a6	202	CYC	CHD-C1D	6.15	1.54	1.40
13	f2	201	CYC	CHD-C1D	6.14	1.54	1.40
13	V1	201	CYC	CHD-C1D	6.13	1.54	1.40
13	V7	201	CYC	CHD-C1D	6.13	1.54	1.40
13	a5	202	CYC	CHD-C1D	6.12	1.54	1.40
13	T6	201	CYC	CHD-C1D	6.12	1.54	1.40
13	P7	202	CYC	CHD-C1D	6.12	1.54	1.40
13	E5	201	CYC	CHD-C1D	6.11	1.54	1.40
13	E1	201	CYC	CHD-C1D	6.10	1.54	1.40
13	E4	201	CYC	CHD-C1D	6.10	1.54	1.40
13	Z3	301	CYC	CHD-C1D	6.10	1.54	1.40
13	a4	202	CYC	CHD-C1D	6.10	1.54	1.40
13	V1	202	CYC	CHD-C1D	6.10	1.54	1.40
13	V3	202	CYC	CHD-C1D	6.10	1.54	1.40
13	a3	202	CYC	CHD-C1D	6.09	1.54	1.40
13	a1	202	CYC	CHD-C1D	6.08	1.54	1.40
13	T1	201	CYC	CHD-C1D	6.08	1.54	1.40
13	V7	202	CYC	CHD-C1D	6.08	1.54	1.40
13	E6	201	CYC	CHD-C1D	6.08	1.54	1.40
13	E7	201	CYC	CHD-C1D	6.08	1.54	1.40
13	B2	202	CYC	CHD-C1D	6.08	1.54	1.40
13	Z6	301	CYC	CHB-C4A	6.07	1.54	1.40
13	V5	202	CYC	CHD-C1D	6.06	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	42	302	CYC	CHD-C1D	6.06	1.54	1.40
13	Z7	301	CYC	CHD-C1D	6.06	1.54	1.40
13	V6	202	CYC	CHD-C1D	6.06	1.54	1.40
13	E3	201	CYC	CHD-C1D	6.05	1.54	1.40
13	Z4	301	CYC	CHB-C4A	6.05	1.54	1.40
13	H6	201	CYC	CHD-C1D	6.04	1.54	1.40
13	T5	202	CYC	CHD-C1D	6.04	1.54	1.40
13	O2	201	CYC	CHD-C1D	6.04	1.54	1.40
13	a7	202	CYC	CHD-C1D	6.04	1.54	1.40
13	T1	202	CYC	CHD-C1D	6.03	1.54	1.40
13	T5	201	CYC	CHD-C1D	6.02	1.54	1.40
13	Z1	301	CYC	CHB-C4A	6.02	1.54	1.40
13	w2	201	CYC	CHD-C1D	6.02	1.54	1.40
13	X7	201	CYC	CHB-C4A	6.02	1.54	1.40
13	T7	201	CYC	CHD-C1D	6.02	1.54	1.40
13	Z5	301	CYC	CHB-C4A	6.02	1.54	1.40
13	22	302	CYC	CHB-C4A	6.01	1.54	1.40
13	N6	201	CYC	CHD-C1D	6.01	1.53	1.40
13	H5	201	CYC	CHD-C1D	6.00	1.53	1.40
13	a1	201	CYC	CHB-C4A	6.00	1.54	1.40
13	T4	201	CYC	CHD-C1D	6.00	1.53	1.40
13	H1	201	CYC	CHD-C1D	6.00	1.53	1.40
13	X3	201	CYC	CHB-C4A	6.00	1.54	1.40
13	T7	202	CYC	CHD-C1D	5.99	1.53	1.40
13	c2	801	CYC	CHD-C1D	5.99	1.53	1.40
13	S5	201	CYC	CHD-C1D	5.99	1.53	1.40
13	U6	201	CYC	CHD-C1D	5.99	1.53	1.40
13	G1	201	CYC	CHD-C1D	5.99	1.53	1.40
13	G7	201	CYC	CHD-C1D	5.99	1.53	1.40
13	32	302	CYC	CHB-C4A	5.99	1.54	1.40
13	T3	201	CYC	CHD-C1D	5.99	1.53	1.40
13	N1	201	CYC	CHD-C1D	5.99	1.53	1.40
13	E2	201	CYC	CHB-C4A	5.99	1.54	1.40
13	L1	201	CYC	CHB-C4A	5.98	1.54	1.40
13	F6	201	CYC	CHA-C4D	5.98	1.53	1.40
13	T4	202	CYC	CHD-C1D	5.97	1.53	1.40
13	T5	202	CYC	CHA-C4D	5.97	1.53	1.40
13	W1	201	CYC	CHD-C1D	5.97	1.53	1.40
13	V4	202	CYC	CHD-C1D	5.97	1.53	1.40
13	s2	201	CYC	CHB-C4A	5.97	1.54	1.40
13	H4	201	CYC	CHD-C1D	5.97	1.53	1.40
13	R6	201	CYC	CHD-C1D	5.97	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	p2	201	CYC	CHD-C1D	5.97	1.53	1.40
13	T6	202	CYC	CHD-C1D	5.96	1.53	1.40
13	S7	201	CYC	CHD-C1D	5.96	1.53	1.40
13	S4	201	CYC	CHD-C1D	5.96	1.53	1.40
13	Q2	201	CYC	CHD-C1D	5.96	1.53	1.40
13	N3	201	CYC	CHD-C1D	5.96	1.53	1.40
13	W6	201	CYC	CHD-C1D	5.96	1.53	1.40
13	o2	801	CYC	CHB-C4A	5.96	1.54	1.40
13	a6	201	CYC	CHB-C4A	5.96	1.54	1.40
13	y2	201	CYC	CHB-C4A	5.96	1.54	1.40
13	U5	201	CYC	CHD-C1D	5.95	1.53	1.40
13	N5	201	CYC	CHD-C1D	5.95	1.53	1.40
13	U1	201	CYC	CHD-C1D	5.95	1.53	1.40
13	T1	202	CYC	CHA-C4D	5.95	1.53	1.40
13	T3	202	CYC	CHD-C1D	5.95	1.53	1.40
13	G3	201	CYC	CHD-C1D	5.95	1.53	1.40
13	a5	201	CYC	CHB-C4A	5.95	1.54	1.40
13	S6	201	CYC	CHD-C1D	5.95	1.53	1.40
13	F7	201	CYC	CHD-C1D	5.95	1.53	1.40
13	K5	201	CYC	CHD-C1D	5.94	1.53	1.40
13	F6	202	CYC	CHD-C1D	5.94	1.53	1.40
13	X1	201	CYC	CHB-C4A	5.94	1.54	1.40
13	G2	201	CYC	CHB-C4A	5.94	1.54	1.40
13	F5	201	CYC	CHA-C4D	5.94	1.53	1.40
13	R7	201	CYC	CHD-C1D	5.94	1.53	1.40
13	42	302	CYC	CHB-C4A	5.94	1.54	1.40
13	c2	801	CYC	CHA-C4D	5.94	1.53	1.40
13	W5	201	CYC	CHD-C1D	5.94	1.53	1.40
13	I7	201	CYC	CHD-C1D	5.94	1.53	1.40
13	W4	201	CYC	CHD-C1D	5.94	1.53	1.40
13	Q5	202	CYC	CHD-C1D	5.93	1.53	1.40
13	F3	201	CYC	CHD-C1D	5.93	1.53	1.40
13	C1	202	CYC	CHA-C4D	5.93	1.53	1.40
13	W3	201	CYC	CHD-C1D	5.93	1.53	1.40
13	X5	201	CYC	CHB-C4A	5.93	1.54	1.40
13	O2	201	CYC	CHB-C4A	5.93	1.54	1.40
13	L6	201	CYC	CHB-C4A	5.93	1.54	1.40
13	R1	201	CYC	CHD-C1D	5.93	1.53	1.40
13	Q7	202	CYC	CHD-C1D	5.93	1.53	1.40
13	G5	201	CYC	CHD-C1D	5.93	1.53	1.40
13	B5	201	CYC	CHD-C1D	5.93	1.53	1.40
13	v2	201	CYC	CHB-C4A	5.93	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T6	202	CYC	CHA-C4D	5.92	1.53	1.40
13	T4	202	CYC	CHA-C4D	5.92	1.53	1.40
13	K1	201	CYC	CHD-C1D	5.92	1.53	1.40
13	Q3	202	CYC	CHD-C1D	5.92	1.53	1.40
13	R2	201	CYC	CHB-C4A	5.92	1.54	1.40
13	U7	201	CYC	CHD-C1D	5.92	1.53	1.40
13	R3	201	CYC	CHD-C1D	5.92	1.53	1.40
13	I6	201	CYC	CHD-C1D	5.92	1.53	1.40
13	T7	202	CYC	CHA-C4D	5.92	1.53	1.40
13	h2	201	CYC	CHB-C4A	5.92	1.54	1.40
13	L4	201	CYC	CHA-C4D	5.92	1.53	1.40
13	P4	202	CYC	CHB-C4A	5.92	1.54	1.40
13	a3	201	CYC	CHB-C4A	5.92	1.54	1.40
13	T3	202	CYC	CHA-C4D	5.91	1.53	1.40
13	K4	201	CYC	CHD-C1D	5.91	1.53	1.40
13	K7	201	CYC	CHD-C1D	5.91	1.53	1.40
13	l2	201	CYC	CHB-C4A	5.91	1.54	1.40
13	F4	201	CYC	CHD-C1D	5.91	1.53	1.40
13	Q6	202	CYC	CHD-C1D	5.91	1.53	1.40
13	S2	201	CYC	CHA-C4D	5.91	1.53	1.40
13	K6	201	CYC	CHD-C1D	5.91	1.53	1.40
13	S3	201	CYC	CHD-C1D	5.91	1.53	1.40
13	N2	802	CYC	CHA-C4D	5.91	1.53	1.40
13	Z3	301	CYC	CHB-C4A	5.91	1.54	1.40
13	m2	201	CYC	CHD-C1D	5.91	1.53	1.40
13	U2	201	CYC	CHB-C4A	5.91	1.54	1.40
13	I4	201	CYC	CHD-C1D	5.91	1.53	1.40
13	A2	201	CYC	CHA-C4D	5.91	1.53	1.40
13	S3	201	CYC	CHA-C4D	5.91	1.53	1.40
13	S7	201	CYC	CHA-C4D	5.91	1.53	1.40
13	U3	201	CYC	CHD-C1D	5.90	1.53	1.40
13	F1	201	CYC	CHA-C4D	5.90	1.53	1.40
13	A2	201	CYC	CHB-C4A	5.90	1.54	1.40
13	Q1	202	CYC	CHD-C1D	5.90	1.53	1.40
13	I3	201	CYC	CHD-C1D	5.90	1.53	1.40
13	F1	201	CYC	CHD-C1D	5.90	1.53	1.40
13	B6	201	CYC	CHD-C1D	5.90	1.53	1.40
13	F3	201	CYC	CHA-C4D	5.90	1.53	1.40
13	F6	201	CYC	CHD-C1D	5.90	1.53	1.40
13	52	302	CYC	CHB-C4A	5.90	1.54	1.40
13	k2	201	CYC	CHA-C4D	5.90	1.53	1.40
13	N4	201	CYC	CHD-C1D	5.90	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H3	201	CYC	CHD-C1D	5.90	1.53	1.40
13	F5	201	CYC	CHD-C1D	5.90	1.53	1.40
13	S1	201	CYC	CHD-C1D	5.90	1.53	1.40
13	D4	201	CYC	CHB-C4A	5.90	1.54	1.40
13	R5	201	CYC	CHD-C1D	5.90	1.53	1.40
13	X6	201	CYC	CHB-C4A	5.90	1.54	1.40
13	P6	201	CYC	CHB-C4A	5.89	1.54	1.40
13	F5	202	CYC	CHD-C1D	5.89	1.53	1.40
13	D2	201	CYC	CHB-C4A	5.89	1.54	1.40
13	C5	201	CYC	CHA-C4D	5.89	1.53	1.40
13	42	301	CYC	CHB-C4A	5.89	1.54	1.40
13	A1	302	CYC	CHB-C4A	5.89	1.54	1.40
13	D6	201	CYC	CHB-C4A	5.89	1.54	1.40
13	N7	201	CYC	CHD-C1D	5.89	1.53	1.40
13	W2	201	CYC	CHB-C4A	5.89	1.54	1.40
13	F4	202	CYC	CHD-C1D	5.89	1.53	1.40
13	K5	201	CYC	CHA-C4D	5.89	1.53	1.40
13	B3	201	CYC	CHA-C4D	5.89	1.53	1.40
13	P6	201	CYC	CHD-C1D	5.89	1.53	1.40
13	L5	201	CYC	CHA-C4D	5.89	1.53	1.40
13	W7	201	CYC	CHD-C1D	5.89	1.53	1.40
13	Q4	202	CYC	CHD-C1D	5.89	1.53	1.40
13	G6	201	CYC	CHD-C1D	5.88	1.53	1.40
13	F7	201	CYC	CHA-C4D	5.88	1.53	1.40
13	F1	202	CYC	CHD-C1D	5.88	1.53	1.40
13	P6	201	CYC	CHA-C4D	5.88	1.53	1.40
13	K3	201	CYC	CHD-C1D	5.88	1.53	1.40
13	R4	201	CYC	CHD-C1D	5.88	1.53	1.40
13	a7	201	CYC	CHB-C4A	5.88	1.54	1.40
13	S1	201	CYC	CHA-C4D	5.88	1.53	1.40
13	F3	202	CYC	CHD-C1D	5.88	1.53	1.40
13	S6	201	CYC	CHA-C4D	5.88	1.53	1.40
13	C4	201	CYC	CHA-C4D	5.88	1.53	1.40
13	C5	202	CYC	CHA-C4D	5.88	1.53	1.40
13	B7	201	CYC	CHA-C4D	5.88	1.53	1.40
13	P1	201	CYC	CHA-C4D	5.88	1.53	1.40
13	G4	201	CYC	CHD-C1D	5.88	1.53	1.40
13	U4	201	CYC	CHD-C1D	5.88	1.53	1.40
13	j2	201	CYC	CHB-C4A	5.88	1.54	1.40
13	e2	201	CYC	CHB-C4A	5.88	1.54	1.40
13	S4	201	CYC	CHA-C4D	5.88	1.53	1.40
13	P5	201	CYC	CHD-C1D	5.88	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H2	201	CYC	CHA-C4D	5.87	1.53	1.40
13	C4	202	CYC	CHA-C4D	5.87	1.53	1.40
13	f2	201	CYC	CHB-C4A	5.87	1.54	1.40
13	r2	201	CYC	CHB-C4A	5.87	1.54	1.40
13	R6	201	CYC	CHA-C4D	5.87	1.53	1.40
13	U6	201	CYC	CHA-C4D	5.87	1.53	1.40
13	N2	801	CYC	CHB-C4A	5.87	1.54	1.40
13	P4	202	CYC	CHA-C4D	5.87	1.53	1.40
13	T2	201	CYC	CHA-C4D	5.87	1.53	1.40
13	U7	201	CYC	CHA-C4D	5.87	1.53	1.40
13	W3	201	CYC	CHA-C4D	5.87	1.53	1.40
13	F7	202	CYC	CHD-C1D	5.87	1.53	1.40
13	P7	201	CYC	CHB-C4A	5.86	1.54	1.40
13	a2	201	CYC	CHD-C1D	5.86	1.53	1.40
13	A6	302	CYC	CHB-C4A	5.86	1.54	1.40
13	P5	201	CYC	CHB-C4A	5.86	1.54	1.40
13	d2	201	CYC	CHD-C1D	5.86	1.53	1.40
13	C7	201	CYC	CHA-C4D	5.86	1.53	1.40
13	B3	201	CYC	CHD-C1D	5.86	1.53	1.40
13	B6	201	CYC	CHA-C4D	5.86	1.53	1.40
13	B7	201	CYC	CHD-C1D	5.86	1.53	1.40
13	52	301	CYC	CHB-C4A	5.86	1.54	1.40
13	I5	201	CYC	CHD-C1D	5.86	1.53	1.40
13	P3	201	CYC	CHB-C4A	5.86	1.54	1.40
13	P1	201	CYC	CHD-C1D	5.86	1.53	1.40
13	K4	201	CYC	CHA-C4D	5.86	1.53	1.40
13	a2	201	CYC	CHA-C4D	5.86	1.53	1.40
13	R1	201	CYC	CHA-C4D	5.86	1.53	1.40
13	P4	202	CYC	CHD-C1D	5.86	1.53	1.40
13	32	301	CYC	CHB-C4A	5.85	1.54	1.40
13	I1	201	CYC	CHD-C1D	5.85	1.53	1.40
13	L4	201	CYC	CHB-C4A	5.85	1.54	1.40
13	P7	201	CYC	CHD-C1D	5.85	1.53	1.40
13	A1	301	CYC	CHB-C4A	5.85	1.54	1.40
13	B1	201	CYC	CHD-C1D	5.85	1.53	1.40
13	S5	201	CYC	CHA-C4D	5.85	1.53	1.40
13	J5	201	CYC	CHB-C4A	5.85	1.54	1.40
13	N2	802	CYC	CHD-C1D	5.85	1.53	1.40
13	P3	201	CYC	CHA-C4D	5.85	1.53	1.40
13	F6	202	CYC	CHA-C4D	5.85	1.53	1.40
13	B4	201	CYC	CHA-C4D	5.85	1.53	1.40
13	Z7	301	CYC	CHB-C4A	5.85	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L3	201	CYC	CHA-C4D	5.85	1.53	1.40
13	22	301	CYC	CHB-C4A	5.85	1.54	1.40
13	H2	201	CYC	CHD-C1D	5.85	1.53	1.40
13	C3	202	CYC	CHA-C4D	5.85	1.53	1.40
13	F4	201	CYC	CHA-C4D	5.85	1.53	1.40
13	H4	201	CYC	CHA-C4D	5.84	1.53	1.40
13	W4	201	CYC	CHA-C4D	5.84	1.53	1.40
13	Q1	202	CYC	CHB-C4A	5.84	1.54	1.40
13	B4	201	CYC	CHD-C1D	5.84	1.53	1.40
13	N4	201	CYC	CHA-C4D	5.84	1.53	1.40
13	Q2	201	CYC	CHB-C4A	5.84	1.54	1.40
13	H5	201	CYC	CHA-C4D	5.84	1.53	1.40
13	N5	201	CYC	CHA-C4D	5.84	1.53	1.40
13	C6	202	CYC	CHA-C4D	5.84	1.53	1.40
13	H6	201	CYC	CHA-C4D	5.84	1.53	1.40
13	C3	201	CYC	CHA-C4D	5.84	1.53	1.40
13	R4	201	CYC	CHA-C4D	5.84	1.53	1.40
13	G3	201	CYC	CHA-C4D	5.84	1.53	1.40
13	L7	201	CYC	CHA-C4D	5.84	1.53	1.40
13	W7	201	CYC	CHA-C4D	5.84	1.53	1.40
13	U3	201	CYC	CHA-C4D	5.84	1.53	1.40
13	P2	201	CYC	CHB-C4A	5.84	1.54	1.40
13	I5	201	CYC	CHA-C4D	5.83	1.53	1.40
13	B1	201	CYC	CHA-C4D	5.83	1.53	1.40
13	G4	201	CYC	CHA-C4D	5.83	1.53	1.40
13	j2	201	CYC	CHD-C1D	5.83	1.53	1.40
13	P3	201	CYC	CHD-C1D	5.83	1.53	1.40
13	F4	202	CYC	CHA-C4D	5.83	1.53	1.40
13	L5	201	CYC	CHB-C4A	5.83	1.54	1.40
13	G7	201	CYC	CHA-C4D	5.83	1.53	1.40
13	L2	201	CYC	CHD-C1D	5.83	1.53	1.40
13	Q5	201	CYC	CHB-C4A	5.83	1.54	1.40
13	P5	201	CYC	CHA-C4D	5.83	1.53	1.40
13	x2	201	CYC	CHB-C4A	5.83	1.54	1.40
13	F1	202	CYC	CHA-C4D	5.83	1.53	1.40
13	P1	201	CYC	CHB-C4A	5.83	1.54	1.40
13	W2	201	CYC	CHD-C1D	5.82	1.53	1.40
13	W5	201	CYC	CHA-C4D	5.82	1.53	1.40
13	Q5	201	CYC	CHD-C1D	5.82	1.53	1.40
13	R5	201	CYC	CHA-C4D	5.82	1.53	1.40
13	Q6	201	CYC	CHB-C4A	5.82	1.54	1.40
13	C1	201	CYC	CHA-C4D	5.82	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G6	201	CYC	CHA-C4D	5.82	1.53	1.40
13	Q6	202	CYC	CHA-C4D	5.82	1.53	1.40
13	H7	201	CYC	CHD-C1D	5.82	1.53	1.40
13	H7	201	CYC	CHA-C4D	5.82	1.53	1.40
13	Q1	201	CYC	CHD-C1D	5.82	1.53	1.40
13	L3	201	CYC	CHB-C4A	5.82	1.54	1.40
13	F2	201	CYC	CHA-C4D	5.82	1.53	1.40
13	C2	201	CYC	CHD-C1D	5.82	1.53	1.40
13	U4	201	CYC	CHA-C4D	5.82	1.53	1.40
13	N7	201	CYC	CHA-C4D	5.82	1.53	1.40
13	V2	201	CYC	CHA-C4D	5.82	1.53	1.40
13	Q1	202	CYC	CHA-C4D	5.81	1.53	1.40
13	K1	201	CYC	CHA-C4D	5.81	1.53	1.40
13	Q3	201	CYC	CHA-C4D	5.81	1.53	1.40
13	D7	201	CYC	CHB-C4A	5.81	1.54	1.40
13	A6	302	CYC	CHA-C4D	5.81	1.53	1.40
13	W6	201	CYC	CHA-C4D	5.81	1.53	1.40
13	Q5	202	CYC	CHB-C4A	5.81	1.54	1.40
13	F3	202	CYC	CHA-C4D	5.81	1.53	1.40
13	G2	201	CYC	CHD-C1D	5.81	1.53	1.40
13	p2	201	CYC	CHB-C4A	5.81	1.54	1.40
13	G5	201	CYC	CHA-C4D	5.81	1.53	1.40
13	R7	201	CYC	CHA-C4D	5.81	1.53	1.40
13	22	302	CYC	CHA-C4D	5.81	1.53	1.40
13	N6	201	CYC	CHA-C4D	5.81	1.53	1.40
13	H3	201	CYC	CHA-C4D	5.81	1.53	1.40
13	I1	201	CYC	CHA-C4D	5.81	1.53	1.40
13	A6	301	CYC	CHB-C4A	5.81	1.54	1.40
13	Q1	201	CYC	CHA-C4D	5.81	1.53	1.40
13	R3	201	CYC	CHA-C4D	5.80	1.53	1.40
13	F2	201	CYC	CHD-C1D	5.80	1.53	1.40
13	C6	201	CYC	CHA-C4D	5.80	1.53	1.40
13	Q4	202	CYC	CHB-C4A	5.80	1.54	1.40
13	Q7	201	CYC	CHA-C4D	5.80	1.53	1.40
13	Q1	201	CYC	CHB-C4A	5.80	1.54	1.40
13	B2	201	CYC	CHA-C4D	5.80	1.53	1.40
13	I6	201	CYC	CHA-C4D	5.80	1.53	1.40
13	K6	201	CYC	CHA-C4D	5.80	1.53	1.40
13	P7	201	CYC	CHA-C4D	5.80	1.53	1.40
13	z2	201	CYC	CHD-C1D	5.80	1.53	1.40
13	U5	201	CYC	CHA-C4D	5.80	1.53	1.40
13	S2	201	CYC	CHB-C4A	5.80	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	52	302	CYC	CHA-C4D	5.80	1.53	1.40
13	C7	202	CYC	CHA-C4D	5.80	1.53	1.40
13	Q6	202	CYC	CHB-C4A	5.80	1.54	1.40
13	W1	201	CYC	CHA-C4D	5.80	1.53	1.40
13	Q6	201	CYC	CHA-C4D	5.80	1.53	1.40
13	Q3	202	CYC	CHA-C4D	5.80	1.53	1.40
13	Q6	201	CYC	CHD-C1D	5.80	1.53	1.40
13	N3	201	CYC	CHA-C4D	5.80	1.53	1.40
13	V1	201	CYC	CHB-C4A	5.79	1.54	1.40
13	F2	201	CYC	CHB-C4A	5.79	1.54	1.40
13	F7	202	CYC	CHA-C4D	5.79	1.53	1.40
13	o2	801	CYC	CHD-C1D	5.79	1.53	1.40
13	V3	201	CYC	CHA-C4D	5.79	1.53	1.40
13	j2	201	CYC	CHA-C4D	5.79	1.53	1.40
13	Z4	301	CYC	CHA-C4D	5.79	1.53	1.40
13	32	301	CYC	CHA-C4D	5.78	1.53	1.40
13	I4	201	CYC	CHA-C4D	5.78	1.53	1.40
13	V6	201	CYC	CHB-C4A	5.78	1.54	1.40
13	X4	201	CYC	CHB-C4A	5.78	1.54	1.40
13	Q2	201	CYC	CHA-C4D	5.78	1.53	1.40
13	H1	201	CYC	CHA-C4D	5.78	1.53	1.40
13	Q5	202	CYC	CHA-C4D	5.78	1.53	1.40
13	Q4	201	CYC	CHB-C4A	5.78	1.54	1.40
13	22	302	CYC	CHD-C1D	5.78	1.53	1.40
13	I7	201	CYC	CHA-C4D	5.78	1.53	1.40
13	x2	201	CYC	CHA-C4D	5.78	1.53	1.40
13	W1	201	CYC	CHB-C4A	5.78	1.54	1.40
13	42	301	CYC	CHA-C4D	5.78	1.53	1.40
13	I3	201	CYC	CHA-C4D	5.78	1.53	1.40
13	A2	202	CYC	CHD-C1D	5.78	1.53	1.40
13	D3	201	CYC	CHA-C4D	5.78	1.53	1.40
13	22	301	CYC	CHA-C4D	5.78	1.53	1.40
13	C2	201	CYC	CHA-C4D	5.78	1.53	1.40
13	y2	201	CYC	CHD-C1D	5.78	1.53	1.40
13	Q4	202	CYC	CHA-C4D	5.78	1.53	1.40
13	32	302	CYC	CHA-C4D	5.77	1.53	1.40
13	W2	201	CYC	CHA-C4D	5.77	1.53	1.40
13	K3	201	CYC	CHA-C4D	5.77	1.53	1.40
13	T2	201	CYC	CHB-C4A	5.77	1.54	1.40
13	L6	201	CYC	CHA-C4D	5.77	1.53	1.40
13	B5	201	CYC	CHA-C4D	5.77	1.53	1.40
13	E6	201	CYC	CHA-C4D	5.77	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g2	201	CYC	CHB-C4A	5.77	1.54	1.40
13	L1	201	CYC	CHA-C4D	5.77	1.53	1.40
13	M2	201	CYC	CHD-C1D	5.77	1.53	1.40
13	U1	201	CYC	CHA-C4D	5.77	1.53	1.40
13	C4	202	CYC	CHD-C1D	5.77	1.53	1.40
13	Q5	201	CYC	CHA-C4D	5.77	1.53	1.40
13	N1	201	CYC	CHA-C4D	5.77	1.53	1.40
13	D1	201	CYC	CHB-C4A	5.77	1.54	1.40
13	J7	201	CYC	CHA-C4D	5.77	1.53	1.40
13	J1	202	CYC	CHA-C4D	5.77	1.53	1.40
13	E5	201	CYC	CHA-C4D	5.77	1.53	1.40
13	C1	202	CYC	CHD-C1D	5.77	1.53	1.40
13	C6	202	CYC	CHD-C1D	5.76	1.53	1.40
13	F5	202	CYC	CHA-C4D	5.76	1.53	1.40
13	Q3	201	CYC	CHD-C1D	5.76	1.53	1.40
13	A1	301	CYC	CHA-C4D	5.76	1.53	1.40
13	G1	201	CYC	CHA-C4D	5.76	1.53	1.40
13	Q7	202	CYC	CHA-C4D	5.76	1.53	1.40
13	K7	201	CYC	CHA-C4D	5.76	1.53	1.40
13	X2	201	CYC	CHB-C4A	5.76	1.53	1.40
13	v2	201	CYC	CHD-C1D	5.76	1.53	1.40
13	X7	201	CYC	CHA-C4D	5.76	1.53	1.40
13	Q3	201	CYC	CHB-C4A	5.76	1.53	1.40
13	Q4	201	CYC	CHA-C4D	5.76	1.53	1.40
13	J7	202	CYC	CHA-C4D	5.76	1.53	1.40
13	Q7	201	CYC	CHD-C1D	5.76	1.53	1.40
13	V5	201	CYC	CHB-C4A	5.76	1.53	1.40
13	C5	201	CYC	CHB-C4A	5.76	1.53	1.40
13	E1	201	CYC	CHA-C4D	5.76	1.53	1.40
13	k2	201	CYC	CHD-C1D	5.76	1.53	1.40
13	J6	201	CYC	CHB-C4A	5.76	1.53	1.40
13	A1	302	CYC	CHA-C4D	5.76	1.53	1.40
13	J4	201	CYC	CHA-C4D	5.75	1.53	1.40
13	a2	201	CYC	CHB-C4A	5.75	1.53	1.40
13	L7	201	CYC	CHB-C4A	5.75	1.53	1.40
13	g2	201	CYC	CHD-C1D	5.75	1.53	1.40
13	J5	202	CYC	CHA-C4D	5.75	1.53	1.40
13	X2	201	CYC	CHA-C4D	5.75	1.53	1.40
13	N2	802	CYC	CHB-C4A	5.75	1.53	1.40
13	d2	201	CYC	CHA-C4D	5.75	1.53	1.40
13	J4	201	CYC	CHB-C4A	5.75	1.53	1.40
13	J4	202	CYC	CHA-C4D	5.75	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A2	201	CYC	CHD-C1D	5.75	1.53	1.40
13	J3	202	CYC	CHA-C4D	5.74	1.53	1.40
13	C5	202	CYC	CHD-C1D	5.74	1.53	1.40
13	Z6	301	CYC	CHA-C4D	5.74	1.53	1.40
13	J1	201	CYC	CHA-C4D	5.74	1.53	1.40
13	52	301	CYC	CHA-C4D	5.74	1.53	1.40
13	t2	201	CYC	CHA-C4D	5.74	1.53	1.40
13	a7	201	CYC	CHA-C4D	5.74	1.53	1.40
13	T6	201	CYC	CHA-C4D	5.74	1.53	1.40
13	a6	202	CYC	CHA-C4D	5.74	1.53	1.40
13	32	302	CYC	CHD-C1D	5.74	1.53	1.40
13	Z3	301	CYC	CHA-C4D	5.74	1.53	1.40
13	V7	201	CYC	CHB-C4A	5.74	1.53	1.40
13	T1	201	CYC	CHA-C4D	5.74	1.53	1.40
13	C3	202	CYC	CHD-C1D	5.74	1.53	1.40
13	V4	201	CYC	CHB-C4A	5.74	1.53	1.40
13	E3	201	CYC	CHA-C4D	5.74	1.53	1.40
13	P7	202	CYC	CHA-C4D	5.74	1.53	1.40
13	C7	202	CYC	CHD-C1D	5.73	1.53	1.40
13	P1	202	CYC	CHA-C4D	5.73	1.53	1.40
13	J1	201	CYC	CHB-C4A	5.73	1.53	1.40
13	A2	202	CYC	CHA-C4D	5.73	1.53	1.40
13	v2	201	CYC	CHA-C4D	5.73	1.53	1.40
13	X3	201	CYC	CHA-C4D	5.73	1.53	1.40
13	V3	201	CYC	CHB-C4A	5.73	1.53	1.40
13	J6	201	CYC	CHA-C4D	5.73	1.53	1.40
13	E4	201	CYC	CHA-C4D	5.73	1.53	1.40
13	D7	201	CYC	CHA-C4D	5.73	1.53	1.40
13	J3	201	CYC	CHB-C4A	5.73	1.53	1.40
13	X1	201	CYC	CHA-C4D	5.73	1.53	1.40
13	J3	201	CYC	CHA-C4D	5.73	1.53	1.40
13	J5	201	CYC	CHA-C4D	5.73	1.53	1.40
13	V6	201	CYC	CHA-C4D	5.73	1.53	1.40
13	M3	201	CYC	CHA-C4D	5.73	1.53	1.40
13	C1	201	CYC	CHB-C4A	5.73	1.53	1.40
13	U1	201	CYC	CHB-C4A	5.73	1.53	1.40
13	D5	201	CYC	CHB-C4A	5.73	1.53	1.40
13	C6	201	CYC	CHB-C4A	5.73	1.53	1.40
13	M2	201	CYC	CHB-C4A	5.73	1.53	1.40
13	W6	201	CYC	CHB-C4A	5.73	1.53	1.40
13	a3	201	CYC	CHA-C4D	5.73	1.53	1.40
13	a7	202	CYC	CHA-C4D	5.72	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W4	201	CYC	CHB-C4A	5.72	1.53	1.40
13	Z5	301	CYC	CHA-C4D	5.72	1.53	1.40
13	D2	201	CYC	CHA-C4D	5.72	1.53	1.40
13	K4	201	CYC	CHB-C4A	5.72	1.53	1.40
13	g2	201	CYC	CHA-C4D	5.72	1.53	1.40
13	T5	201	CYC	CHA-C4D	5.72	1.53	1.40
13	M7	201	CYC	CHA-C4D	5.72	1.53	1.40
13	Q4	201	CYC	CHD-C1D	5.72	1.53	1.40
13	T6	202	CYC	CHB-C4A	5.71	1.53	1.40
13	C4	201	CYC	CHB-C4A	5.71	1.53	1.40
13	a4	202	CYC	CHA-C4D	5.71	1.53	1.40
13	J6	202	CYC	CHA-C4D	5.71	1.53	1.40
13	a3	202	CYC	CHA-C4D	5.71	1.53	1.40
13	l2	201	CYC	CHD-C1D	5.71	1.53	1.40
13	T7	201	CYC	CHA-C4D	5.71	1.53	1.40
13	Z1	301	CYC	CHA-C4D	5.71	1.53	1.40
13	J6	202	CYC	CHB-C4A	5.71	1.53	1.40
13	E7	201	CYC	CHA-C4D	5.71	1.53	1.40
13	A6	301	CYC	CHA-C4D	5.71	1.53	1.40
13	Z7	301	CYC	CHA-C4D	5.71	1.53	1.40
13	y2	201	CYC	CHA-C4D	5.71	1.53	1.40
13	n2	201	CYC	CHD-C1D	5.71	1.53	1.40
13	r2	201	CYC	CHA-C4D	5.70	1.53	1.40
13	t2	201	CYC	CHB-C4A	5.70	1.53	1.40
13	J4	202	CYC	CHB-C4A	5.70	1.53	1.40
13	a5	201	CYC	CHA-C4D	5.70	1.53	1.40
13	R2	201	CYC	CHA-C4D	5.70	1.53	1.40
13	J5	202	CYC	CHB-C4A	5.70	1.53	1.40
13	42	302	CYC	CHA-C4D	5.70	1.53	1.40
13	W5	201	CYC	CHB-C4A	5.70	1.53	1.40
13	a5	202	CYC	CHB-C4A	5.70	1.53	1.40
13	D1	201	CYC	CHA-C4D	5.70	1.53	1.40
13	V4	201	CYC	CHA-C4D	5.70	1.53	1.40
13	X6	201	CYC	CHA-C4D	5.70	1.53	1.40
13	T3	202	CYC	CHB-C4A	5.70	1.53	1.40
13	L2	201	CYC	CHA-C4D	5.69	1.53	1.40
13	M1	201	CYC	CHB-C4A	5.69	1.53	1.40
13	a4	202	CYC	CHB-C4A	5.69	1.53	1.40
13	D3	201	CYC	CHB-C4A	5.69	1.53	1.40
13	T1	202	CYC	CHB-C4A	5.69	1.53	1.40
13	Q7	201	CYC	CHB-C4A	5.69	1.53	1.40
13	z2	201	CYC	CHB-C4A	5.69	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a6	202	CYC	CHB-C4A	5.69	1.53	1.40
13	i2	201	CYC	CHA-C4D	5.69	1.53	1.40
13	V5	201	CYC	CHA-C4D	5.69	1.53	1.40
13	X4	201	CYC	CHA-C4D	5.69	1.53	1.40
13	E2	201	CYC	CHA-C4D	5.69	1.53	1.40
13	J1	202	CYC	CHB-C4A	5.69	1.53	1.40
13	S3	201	CYC	CHB-C4A	5.69	1.53	1.40
13	T7	202	CYC	CHB-C4A	5.69	1.53	1.40
13	U2	201	CYC	CHA-C4D	5.69	1.53	1.40
13	n2	201	CYC	CHB-C4A	5.69	1.53	1.40
13	V7	201	CYC	CHA-C4D	5.69	1.53	1.40
13	d2	201	CYC	CHB-C4A	5.69	1.53	1.40
13	p2	201	CYC	CHA-C4D	5.69	1.53	1.40
13	T4	201	CYC	CHA-C4D	5.69	1.53	1.40
13	U5	201	CYC	CHB-C4A	5.68	1.53	1.40
13	R2	201	CYC	CHD-C1D	5.68	1.53	1.40
13	m2	201	CYC	CHA-C4D	5.68	1.53	1.40
13	S7	201	CYC	CHB-C4A	5.68	1.53	1.40
13	z2	201	CYC	CHA-C4D	5.68	1.53	1.40
13	M5	201	CYC	CHA-C4D	5.68	1.53	1.40
13	r2	201	CYC	CHD-C1D	5.68	1.53	1.40
13	I6	201	CYC	CHB-C4A	5.68	1.53	1.40
13	T3	201	CYC	CHA-C4D	5.68	1.53	1.40
13	X5	201	CYC	CHA-C4D	5.68	1.53	1.40
13	I3	201	CYC	CHB-C4A	5.68	1.53	1.40
13	J7	201	CYC	CHB-C4A	5.68	1.53	1.40
13	C3	201	CYC	CHB-C4A	5.68	1.53	1.40
13	e2	201	CYC	CHA-C4D	5.68	1.53	1.40
13	w2	201	CYC	CHA-C4D	5.68	1.53	1.40
13	a1	202	CYC	CHB-C4A	5.68	1.53	1.40
13	P2	201	CYC	CHA-C4D	5.68	1.53	1.40
13	P3	202	CYC	CHA-C4D	5.68	1.53	1.40
13	H7	201	CYC	CHB-C4A	5.68	1.53	1.40
13	o2	801	CYC	CHA-C4D	5.67	1.53	1.40
13	P4	201	CYC	CHA-C4D	5.67	1.53	1.40
13	L2	201	CYC	CHB-C4A	5.67	1.53	1.40
13	P5	202	CYC	CHA-C4D	5.67	1.53	1.40
13	H3	201	CYC	CHB-C4A	5.67	1.53	1.40
13	M3	201	CYC	CHB-C4A	5.67	1.53	1.40
13	T4	202	CYC	CHB-C4A	5.67	1.53	1.40
13	F6	201	CYC	CHB-C4A	5.67	1.53	1.40
13	P5	202	CYC	CHB-C4A	5.66	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D2	201	CYC	CHD-C1D	5.66	1.53	1.40
13	D5	201	CYC	CHA-C4D	5.66	1.53	1.40
13	V1	202	CYC	CHA-C4D	5.66	1.53	1.40
13	a5	202	CYC	CHA-C4D	5.66	1.53	1.40
13	I7	201	CYC	CHB-C4A	5.66	1.53	1.40
13	a6	201	CYC	CHA-C4D	5.66	1.53	1.40
13	V3	202	CYC	CHA-C4D	5.66	1.53	1.40
13	s2	201	CYC	CHA-C4D	5.66	1.53	1.40
13	F1	201	CYC	CHB-C4A	5.66	1.53	1.40
13	B2	202	CYC	CHA-C4D	5.66	1.53	1.40
13	V6	202	CYC	CHA-C4D	5.66	1.53	1.40
13	T5	202	CYC	CHB-C4A	5.66	1.53	1.40
13	a1	202	CYC	CHA-C4D	5.65	1.53	1.40
13	S1	201	CYC	CHB-C4A	5.65	1.53	1.40
13	M5	201	CYC	CHB-C4A	5.65	1.53	1.40
13	D6	201	CYC	CHA-C4D	5.65	1.53	1.40
13	D4	201	CYC	CHA-C4D	5.65	1.53	1.40
13	s2	201	CYC	CHD-C1D	5.65	1.53	1.40
13	S4	201	CYC	CHB-C4A	5.65	1.53	1.40
13	G2	201	CYC	CHA-C4D	5.65	1.53	1.40
13	h2	201	CYC	CHA-C4D	5.65	1.53	1.40
13	F6	202	CYC	CHB-C4A	5.65	1.53	1.40
13	M7	201	CYC	CHB-C4A	5.65	1.53	1.40
13	S6	201	CYC	CHB-C4A	5.65	1.53	1.40
13	M6	201	CYC	CHB-C4A	5.64	1.53	1.40
13	K6	201	CYC	CHB-C4A	5.64	1.53	1.40
13	E2	201	CYC	CHD-C1D	5.64	1.53	1.40
13	V7	202	CYC	CHA-C4D	5.64	1.53	1.40
13	w2	201	CYC	CHB-C4A	5.64	1.53	1.40
13	P1	202	CYC	CHB-C4A	5.64	1.53	1.40
13	G7	201	CYC	CHB-C4A	5.64	1.53	1.40
13	V1	201	CYC	CHA-C4D	5.64	1.53	1.40
13	A2	202	CYC	CHB-C4A	5.64	1.53	1.40
13	F4	201	CYC	CHB-C4A	5.64	1.53	1.40
13	N5	201	CYC	CHB-C4A	5.64	1.53	1.40
13	S5	201	CYC	CHB-C4A	5.64	1.53	1.40
13	K5	201	CYC	CHB-C4A	5.64	1.53	1.40
13	a3	202	CYC	CHB-C4A	5.64	1.53	1.40
13	P6	202	CYC	CHA-C4D	5.64	1.53	1.40
13	M6	201	CYC	CHA-C4D	5.64	1.53	1.40
13	M1	201	CYC	CHA-C4D	5.63	1.53	1.40
13	C1	202	CYC	CHB-C4A	5.63	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c2	801	CYC	CHB-C4A	5.63	1.53	1.40
13	M4	201	CYC	CHB-C4A	5.63	1.53	1.40
13	W7	201	CYC	CHB-C4A	5.63	1.53	1.40
13	B4	201	CYC	CHB-C4A	5.63	1.53	1.40
13	V4	202	CYC	CHA-C4D	5.63	1.53	1.40
13	M4	201	CYC	CHA-C4D	5.63	1.53	1.40
13	H1	201	CYC	CHB-C4A	5.63	1.53	1.40
13	F1	202	CYC	CHB-C4A	5.63	1.53	1.40
13	N3	201	CYC	CHB-C4A	5.63	1.53	1.40
13	Q3	202	CYC	CHB-C4A	5.63	1.53	1.40
13	N4	201	CYC	CHB-C4A	5.63	1.53	1.40
13	h2	201	CYC	CHD-C1D	5.62	1.53	1.40
13	H6	201	CYC	CHB-C4A	5.62	1.53	1.40
13	C2	201	CYC	CHB-C4A	5.62	1.53	1.40
13	I4	201	CYC	CHB-C4A	5.62	1.53	1.40
13	F5	201	CYC	CHB-C4A	5.62	1.53	1.40
13	C7	201	CYC	CHB-C4A	5.62	1.53	1.40
13	B3	201	CYC	CHB-C4A	5.62	1.53	1.40
13	U4	201	CYC	CHB-C4A	5.62	1.53	1.40
13	a1	201	CYC	CHA-C4D	5.62	1.53	1.40
13	U3	201	CYC	CHB-C4A	5.61	1.53	1.40
13	B7	201	CYC	CHB-C4A	5.61	1.53	1.40
13	V5	202	CYC	CHA-C4D	5.61	1.53	1.40
13	I5	201	CYC	CHB-C4A	5.61	1.53	1.40
13	N7	201	CYC	CHB-C4A	5.61	1.53	1.40
13	V2	201	CYC	CHB-C4A	5.61	1.53	1.40
13	F5	202	CYC	CHB-C4A	5.61	1.53	1.40
13	N6	201	CYC	CHB-C4A	5.61	1.53	1.40
13	a7	202	CYC	CHB-C4A	5.61	1.53	1.40
13	B2	201	CYC	CHB-C4A	5.61	1.53	1.40
13	B5	201	CYC	CHB-C4A	5.61	1.53	1.40
13	F3	202	CYC	CHB-C4A	5.61	1.53	1.40
13	F7	202	CYC	CHB-C4A	5.61	1.53	1.40
13	E4	201	CYC	CHB-C4A	5.61	1.53	1.40
13	K7	201	CYC	CHB-C4A	5.61	1.53	1.40
13	Q7	202	CYC	CHB-C4A	5.61	1.53	1.40
13	N1	201	CYC	CHB-C4A	5.60	1.53	1.40
13	F4	202	CYC	CHB-C4A	5.60	1.53	1.40
13	C4	202	CYC	CHB-C4A	5.60	1.53	1.40
13	H5	201	CYC	CHB-C4A	5.60	1.53	1.40
13	K3	201	CYC	CHB-C4A	5.60	1.53	1.40
13	O2	201	CYC	CHA-C4D	5.59	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E1	201	CYC	CHB-C4A	5.59	1.53	1.40
13	N2	801	CYC	CHA-C4D	5.59	1.53	1.40
13	C6	202	CYC	CHB-C4A	5.59	1.53	1.40
13	E5	201	CYC	CHB-C4A	5.59	1.53	1.40
13	G1	201	CYC	CHB-C4A	5.59	1.53	1.40
13	U7	201	CYC	CHB-C4A	5.59	1.53	1.40
13	U6	201	CYC	CHB-C4A	5.59	1.53	1.40
13	G4	201	CYC	CHB-C4A	5.58	1.53	1.40
13	I1	201	CYC	CHB-C4A	5.58	1.53	1.40
13	B6	201	CYC	CHB-C4A	5.58	1.53	1.40
13	e2	201	CYC	CHD-C1D	5.58	1.53	1.40
13	P4	201	CYC	CHB-C4A	5.58	1.53	1.40
13	P6	202	CYC	CHB-C4A	5.58	1.53	1.40
13	T6	201	CYC	CHB-C4A	5.58	1.53	1.40
13	T1	201	CYC	CHB-C4A	5.57	1.53	1.40
13	C3	202	CYC	CHB-C4A	5.57	1.53	1.40
13	B1	201	CYC	CHB-C4A	5.57	1.53	1.40
13	n2	201	CYC	CHA-C4D	5.57	1.52	1.40
13	G3	201	CYC	CHB-C4A	5.57	1.53	1.40
13	C7	202	CYC	CHB-C4A	5.56	1.53	1.40
13	C5	202	CYC	CHB-C4A	5.56	1.53	1.40
13	f2	201	CYC	CHA-C4D	5.56	1.52	1.40
13	m2	201	CYC	CHB-C4A	5.56	1.53	1.40
13	K1	201	CYC	CHB-C4A	5.56	1.53	1.40
13	R6	201	CYC	CHB-C4A	5.56	1.53	1.40
13	F7	201	CYC	CHB-C4A	5.56	1.53	1.40
13	W3	201	CYC	CHB-C4A	5.56	1.53	1.40
13	M2	201	CYC	CHA-C4D	5.55	1.52	1.40
13	H4	201	CYC	CHB-C4A	5.55	1.53	1.40
13	E6	201	CYC	CHB-C4A	5.55	1.53	1.40
13	G5	201	CYC	CHB-C4A	5.55	1.53	1.40
13	i2	201	CYC	CHB-C4A	5.54	1.53	1.40
13	o2	801	CYC	C4B-C3B	-5.54	1.38	1.48
13	G6	201	CYC	CHB-C4A	5.54	1.53	1.40
13	V4	202	CYC	CHB-C4A	5.53	1.53	1.40
13	R4	201	CYC	CHB-C4A	5.52	1.53	1.40
13	R1	201	CYC	CHB-C4A	5.52	1.53	1.40
13	42	302	CYC	C2C-C3C	5.52	1.69	1.54
13	P3	202	CYC	CHB-C4A	5.51	1.53	1.40
13	F3	201	CYC	CHB-C4A	5.51	1.53	1.40
13	E3	201	CYC	CHB-C4A	5.51	1.53	1.40
13	Z6	301	CYC	C2C-C3C	5.50	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a7	201	CYC	C2C-C3C	5.50	1.69	1.54
13	J3	202	CYC	CHB-C4A	5.50	1.53	1.40
13	T7	201	CYC	CHB-C4A	5.50	1.53	1.40
13	T5	201	CYC	CHB-C4A	5.50	1.53	1.40
13	E7	201	CYC	CHB-C4A	5.49	1.53	1.40
13	V6	202	CYC	CHB-C4A	5.49	1.53	1.40
13	T4	201	CYC	CHB-C4A	5.49	1.53	1.40
13	Z4	301	CYC	C2C-C3C	5.49	1.69	1.54
13	P7	202	CYC	CHB-C4A	5.49	1.53	1.40
13	V7	201	CYC	C2C-C3C	5.48	1.69	1.54
13	B2	202	CYC	CHB-C4A	5.48	1.53	1.40
13	a3	201	CYC	C2C-C3C	5.48	1.69	1.54
13	Z5	301	CYC	C2C-C3C	5.48	1.69	1.54
13	N3	201	CYC	C2C-C3C	5.48	1.69	1.54
13	C5	201	CYC	C2C-C3C	5.48	1.69	1.54
13	v2	201	CYC	C4B-C3B	-5.47	1.38	1.48
13	l2	201	CYC	CHA-C4D	5.47	1.52	1.40
13	D4	201	CYC	C2C-C3C	5.47	1.69	1.54
13	J7	202	CYC	CHB-C4A	5.47	1.53	1.40
13	V5	202	CYC	CHB-C4A	5.47	1.53	1.40
13	G7	201	CYC	C2C-C3C	5.47	1.69	1.54
13	C3	201	CYC	C2C-C3C	5.47	1.69	1.54
13	H2	201	CYC	CHB-C4A	5.46	1.53	1.40
13	R3	201	CYC	CHB-C4A	5.46	1.53	1.40
13	V3	202	CYC	CHB-C4A	5.46	1.53	1.40
13	V1	202	CYC	CHB-C4A	5.46	1.53	1.40
13	D6	201	CYC	C2C-C3C	5.46	1.69	1.54
13	k2	201	CYC	CHB-C4A	5.45	1.53	1.40
13	R5	201	CYC	CHB-C4A	5.45	1.53	1.40
13	p2	201	CYC	C2C-C3C	5.45	1.69	1.54
13	D7	201	CYC	C2C-C3C	5.45	1.69	1.54
13	h2	201	CYC	C4B-C3B	-5.45	1.38	1.48
13	U5	201	CYC	C2C-C3C	5.45	1.69	1.54
13	W5	201	CYC	C2C-C3C	5.45	1.69	1.54
13	L1	201	CYC	C2C-C3C	5.45	1.69	1.54
13	H7	201	CYC	C2C-C3C	5.44	1.69	1.54
13	T3	201	CYC	CHB-C4A	5.44	1.53	1.40
13	N6	201	CYC	C2C-C3C	5.44	1.69	1.54
13	W1	201	CYC	C2C-C3C	5.44	1.69	1.54
13	k2	201	CYC	C2C-C3C	5.44	1.69	1.54
13	W3	201	CYC	C2C-C3C	5.44	1.69	1.54
13	N7	201	CYC	C2C-C3C	5.44	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R7	201	CYC	CHB-C4A	5.44	1.53	1.40
13	V7	202	CYC	CHB-C4A	5.43	1.53	1.40
13	G3	201	CYC	C2C-C3C	5.43	1.69	1.54
13	Z3	301	CYC	C2C-C3C	5.43	1.69	1.54
13	P6	201	CYC	C2C-C3C	5.43	1.69	1.54
13	K7	201	CYC	C2C-C3C	5.43	1.69	1.54
13	Z1	301	CYC	C2C-C3C	5.43	1.69	1.54
13	O2	201	CYC	C2C-C3C	5.43	1.69	1.54
13	P3	201	CYC	C2C-C3C	5.43	1.69	1.54
13	H1	201	CYC	C2C-C3C	5.43	1.69	1.54
13	c2	801	CYC	C2C-C3C	5.43	1.69	1.54
13	H6	201	CYC	C2C-C3C	5.43	1.69	1.54
13	H2	201	CYC	C2C-C3C	5.42	1.69	1.54
13	H5	201	CYC	C2C-C3C	5.42	1.69	1.54
13	P1	201	CYC	C2C-C3C	5.42	1.69	1.54
13	P4	202	CYC	C2C-C3C	5.42	1.69	1.54
13	C4	201	CYC	C2C-C3C	5.42	1.69	1.54
13	U7	201	CYC	C2C-C3C	5.42	1.69	1.54
13	P7	201	CYC	C2C-C3C	5.42	1.69	1.54
13	R2	201	CYC	C4B-C3B	-5.42	1.38	1.48
13	W2	201	CYC	C2C-C3C	5.42	1.69	1.54
13	H3	201	CYC	C2C-C3C	5.42	1.69	1.54
13	a6	201	CYC	C2C-C3C	5.41	1.69	1.54
13	V3	201	CYC	C2C-C3C	5.41	1.69	1.54
13	D5	201	CYC	C2C-C3C	5.41	1.69	1.54
13	G1	201	CYC	C2C-C3C	5.41	1.69	1.54
13	s2	201	CYC	C4B-C3B	-5.41	1.38	1.48
13	C7	201	CYC	C2C-C3C	5.41	1.69	1.54
13	e2	201	CYC	C4B-C3B	-5.41	1.38	1.48
13	V1	201	CYC	C2C-C3C	5.41	1.69	1.54
13	f2	201	CYC	C4B-C3B	-5.41	1.38	1.48
13	U4	201	CYC	C2C-C3C	5.41	1.69	1.54
13	U1	201	CYC	C2C-C3C	5.40	1.69	1.54
13	W7	201	CYC	C2C-C3C	5.40	1.69	1.54
13	A1	302	CYC	C2C-C3C	5.40	1.69	1.54
13	a5	201	CYC	C2C-C3C	5.40	1.69	1.54
13	C2	201	CYC	C2C-C3C	5.40	1.69	1.54
13	Z7	301	CYC	C2C-C3C	5.40	1.69	1.54
13	H4	201	CYC	C2C-C3C	5.39	1.69	1.54
13	N4	201	CYC	C2C-C3C	5.39	1.69	1.54
13	w2	201	CYC	C2C-C3C	5.39	1.69	1.54
13	T4	202	CYC	C2C-C3C	5.39	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W4	201	CYC	C2C-C3C	5.39	1.69	1.54
13	X5	201	CYC	C4B-C3B	-5.38	1.38	1.48
13	C6	201	CYC	C2C-C3C	5.38	1.69	1.54
13	P5	201	CYC	C2C-C3C	5.38	1.69	1.54
13	K1	201	CYC	C2C-C3C	5.38	1.69	1.54
13	K6	201	CYC	C2C-C3C	5.38	1.69	1.54
13	D1	201	CYC	C2C-C3C	5.38	1.69	1.54
13	A6	302	CYC	C2C-C3C	5.38	1.69	1.54
13	N1	201	CYC	C2C-C3C	5.37	1.69	1.54
13	U3	201	CYC	C2C-C3C	5.37	1.69	1.54
13	a1	201	CYC	C2C-C3C	5.37	1.69	1.54
13	X1	201	CYC	C4B-C3B	-5.37	1.38	1.48
13	T5	202	CYC	C2C-C3C	5.37	1.69	1.54
13	D3	201	CYC	C2C-C3C	5.36	1.69	1.54
13	K3	201	CYC	C2C-C3C	5.36	1.69	1.54
13	T6	202	CYC	C2C-C3C	5.36	1.69	1.54
13	W6	201	CYC	C2C-C3C	5.36	1.69	1.54
13	T1	202	CYC	C2C-C3C	5.36	1.69	1.54
13	T7	202	CYC	C2C-C3C	5.35	1.68	1.54
13	K5	201	CYC	C2C-C3C	5.35	1.68	1.54
13	X5	201	CYC	C2C-C3C	5.35	1.68	1.54
13	V6	201	CYC	C2C-C3C	5.34	1.68	1.54
13	N5	201	CYC	C2C-C3C	5.34	1.68	1.54
13	j2	201	CYC	C2C-C3C	5.34	1.68	1.54
13	U2	201	CYC	C4B-C3B	-5.34	1.38	1.48
13	C1	201	CYC	C2C-C3C	5.33	1.68	1.54
13	52	302	CYC	C2C-C3C	5.33	1.68	1.54
13	G2	201	CYC	C4B-C3B	-5.33	1.38	1.48
13	G4	201	CYC	C2C-C3C	5.33	1.68	1.54
13	S7	201	CYC	C2C-C3C	5.33	1.68	1.54
13	G6	201	CYC	C2C-C3C	5.33	1.68	1.54
13	L6	201	CYC	C2C-C3C	5.32	1.68	1.54
13	K4	201	CYC	C2C-C3C	5.32	1.68	1.54
13	D2	201	CYC	C4B-C3B	-5.32	1.38	1.48
13	T3	202	CYC	C2C-C3C	5.32	1.68	1.54
13	S5	201	CYC	C2C-C3C	5.32	1.68	1.54
13	V4	201	CYC	C2C-C3C	5.31	1.68	1.54
13	B3	201	CYC	C2C-C3C	5.31	1.68	1.54
13	I4	201	CYC	C2C-C3C	5.31	1.68	1.54
13	Q1	202	CYC	C4B-C3B	-5.31	1.38	1.48
13	Q5	202	CYC	C4B-C3B	-5.31	1.38	1.48
13	I7	201	CYC	C2C-C3C	5.30	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l2	201	CYC	C4B-C3B	-5.30	1.38	1.48
13	U6	201	CYC	C2C-C3C	5.30	1.68	1.54
13	G5	201	CYC	C2C-C3C	5.30	1.68	1.54
13	S3	201	CYC	C2C-C3C	5.30	1.68	1.54
13	g2	201	CYC	C2C-C3C	5.29	1.68	1.54
13	I3	201	CYC	C2C-C3C	5.29	1.68	1.54
13	E2	201	CYC	C4B-C3B	-5.29	1.38	1.48
13	M2	201	CYC	C2C-C3C	5.29	1.68	1.54
13	F3	202	CYC	C2C-C3C	5.29	1.68	1.54
13	I5	201	CYC	C2C-C3C	5.29	1.68	1.54
13	l2	201	CYC	C2C-C3C	5.29	1.68	1.54
13	F7	202	CYC	C2C-C3C	5.29	1.68	1.54
13	V5	201	CYC	C2C-C3C	5.28	1.68	1.54
13	y2	201	CYC	C2C-C3C	5.28	1.68	1.54
13	d2	201	CYC	C2C-C3C	5.28	1.68	1.54
13	n2	201	CYC	C2C-C3C	5.28	1.68	1.54
13	S6	201	CYC	C2C-C3C	5.27	1.68	1.54
13	S1	201	CYC	C2C-C3C	5.27	1.68	1.54
13	a2	201	CYC	C2C-C3C	5.27	1.68	1.54
13	S4	201	CYC	C2C-C3C	5.27	1.68	1.54
13	L2	201	CYC	C2C-C3C	5.27	1.68	1.54
13	B5	201	CYC	C2C-C3C	5.27	1.68	1.54
13	S2	201	CYC	C2C-C3C	5.27	1.68	1.54
13	L1	201	CYC	C4B-C3B	-5.27	1.38	1.48
13	B7	201	CYC	C2C-C3C	5.27	1.68	1.54
13	X4	201	CYC	C2C-C3C	5.26	1.68	1.54
13	J3	201	CYC	C2C-C3C	5.26	1.68	1.54
13	J5	201	CYC	C2C-C3C	5.26	1.68	1.54
13	t2	201	CYC	C2C-C3C	5.26	1.68	1.54
13	a6	201	CYC	C4B-C3B	-5.25	1.38	1.48
13	Q4	202	CYC	C4B-C3B	-5.25	1.38	1.48
13	C1	202	CYC	C2C-C3C	5.25	1.68	1.54
13	A2	202	CYC	C2C-C3C	5.25	1.68	1.54
13	Q6	202	CYC	C4B-C3B	-5.25	1.38	1.48
13	L3	201	CYC	C2C-C3C	5.24	1.68	1.54
13	N2	802	CYC	C4B-C3B	-5.24	1.38	1.48
13	I6	201	CYC	C2C-C3C	5.24	1.68	1.54
13	z2	201	CYC	C2C-C3C	5.24	1.68	1.54
13	F7	201	CYC	C2C-C3C	5.23	1.68	1.54
13	J7	201	CYC	C2C-C3C	5.23	1.68	1.54
13	R6	201	CYC	C2C-C3C	5.23	1.68	1.54
13	A1	302	CYC	C4B-C3B	-5.23	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F2	201	CYC	C4B-C3B	-5.23	1.38	1.48
13	F6	202	CYC	C2C-C3C	5.23	1.68	1.54
13	a1	201	CYC	C4B-C3B	-5.23	1.38	1.48
13	F3	201	CYC	C2C-C3C	5.23	1.68	1.54
13	r2	201	CYC	C2C-C3C	5.23	1.68	1.54
13	B2	202	CYC	C2C-C3C	5.23	1.68	1.54
13	Q3	202	CYC	C2C-C3C	5.23	1.68	1.54
13	Q7	202	CYC	C2C-C3C	5.22	1.68	1.54
13	R7	201	CYC	C2C-C3C	5.22	1.68	1.54
13	p2	201	CYC	C4B-C3B	-5.22	1.38	1.48
13	V7	202	CYC	C2C-C3C	5.22	1.68	1.54
13	m2	201	CYC	C2C-C3C	5.22	1.68	1.54
13	A6	302	CYC	C4B-C3B	-5.22	1.38	1.48
13	M5	201	CYC	C2C-C3C	5.21	1.68	1.54
13	R3	201	CYC	C2C-C3C	5.21	1.68	1.54
13	X6	201	CYC	C4B-C3B	-5.21	1.38	1.48
13	a7	202	CYC	C2C-C3C	5.21	1.68	1.54
13	B2	201	CYC	C2C-C3C	5.21	1.68	1.54
13	i2	201	CYC	C2C-C3C	5.21	1.68	1.54
13	I1	201	CYC	C2C-C3C	5.21	1.68	1.54
13	J3	202	CYC	C2C-C3C	5.21	1.68	1.54
13	L7	201	CYC	C2C-C3C	5.21	1.68	1.54
13	F4	202	CYC	C2C-C3C	5.21	1.68	1.54
13	R4	201	CYC	C2C-C3C	5.20	1.68	1.54
13	S2	201	CYC	C4B-C3B	-5.20	1.38	1.48
13	V5	202	CYC	C2C-C3C	5.20	1.68	1.54
13	M6	201	CYC	C2C-C3C	5.20	1.68	1.54
13	Z6	301	CYC	C4B-C3B	-5.20	1.38	1.48
13	a3	202	CYC	C2C-C3C	5.20	1.68	1.54
13	B4	201	CYC	C2C-C3C	5.20	1.68	1.54
13	Q3	201	CYC	C2C-C3C	5.20	1.68	1.54
13	C7	202	CYC	C2C-C3C	5.19	1.68	1.54
13	P3	202	CYC	C2C-C3C	5.19	1.68	1.54
13	Q7	202	CYC	C4B-C3B	-5.19	1.38	1.48
13	Q7	201	CYC	C2C-C3C	5.19	1.68	1.54
13	r2	201	CYC	C4B-C3B	-5.19	1.38	1.48
13	X4	201	CYC	C4B-C3B	-5.19	1.38	1.48
13	Z1	301	CYC	C4B-C3B	-5.19	1.38	1.48
13	E1	201	CYC	C4B-C3B	-5.19	1.38	1.48
13	E5	201	CYC	C4B-C3B	-5.19	1.38	1.48
13	Q2	201	CYC	C2C-C3C	5.19	1.68	1.54
13	B1	201	CYC	C2C-C3C	5.19	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C5	202	CYC	C2C-C3C	5.19	1.68	1.54
13	V6	202	CYC	C2C-C3C	5.19	1.68	1.54
13	M1	201	CYC	C2C-C3C	5.19	1.68	1.54
13	22	301	CYC	C2C-C3C	5.19	1.68	1.54
13	C6	202	CYC	C2C-C3C	5.18	1.68	1.54
13	J7	202	CYC	C2C-C3C	5.18	1.68	1.54
13	M2	201	CYC	C1A-C2A	-5.18	1.37	1.45
13	R5	201	CYC	C2C-C3C	5.18	1.68	1.54
13	M1	201	CYC	C4B-C3B	-5.18	1.38	1.48
13	B6	201	CYC	C2C-C3C	5.18	1.68	1.54
13	M4	201	CYC	C2C-C3C	5.18	1.68	1.54
13	E7	201	CYC	C2C-C3C	5.18	1.68	1.54
13	R1	201	CYC	C2C-C3C	5.18	1.68	1.54
13	Q3	202	CYC	C4B-C3B	-5.18	1.38	1.48
13	a5	201	CYC	C4B-C3B	-5.18	1.38	1.48
13	C1	202	CYC	C4B-C3B	-5.17	1.38	1.48
13	P2	201	CYC	C4B-C3B	-5.17	1.38	1.48
13	C3	202	CYC	C2C-C3C	5.17	1.68	1.54
13	O2	201	CYC	C4B-C3B	-5.17	1.38	1.48
13	C4	202	CYC	C2C-C3C	5.17	1.68	1.54
13	M7	201	CYC	C2C-C3C	5.17	1.68	1.54
13	X6	201	CYC	C2C-C3C	5.17	1.68	1.54
13	Z5	301	CYC	C4B-C3B	-5.17	1.38	1.48
13	E6	201	CYC	C4B-C3B	-5.17	1.38	1.48
13	f2	201	CYC	C1A-C2A	-5.17	1.37	1.45
13	Q6	202	CYC	C2C-C3C	5.16	1.68	1.54
13	F1	202	CYC	C2C-C3C	5.16	1.68	1.54
13	V4	202	CYC	C4B-C3B	-5.16	1.38	1.48
13	A2	201	CYC	C2C-C3C	5.16	1.68	1.54
13	Q5	202	CYC	C2C-C3C	5.16	1.68	1.54
13	L4	201	CYC	C2C-C3C	5.16	1.68	1.54
13	F2	201	CYC	C2C-C3C	5.16	1.68	1.54
13	E4	201	CYC	C2C-C3C	5.16	1.68	1.54
13	D1	201	CYC	C4B-C3B	-5.15	1.38	1.48
13	M3	201	CYC	C2C-C3C	5.15	1.68	1.54
13	22	302	CYC	C2C-C3C	5.15	1.68	1.54
13	32	302	CYC	C2C-C3C	5.15	1.68	1.54
13	N2	801	CYC	C2C-C3C	5.15	1.68	1.54
13	Q1	202	CYC	C2C-C3C	5.15	1.68	1.54
13	N2	801	CYC	C4B-C3B	-5.15	1.38	1.48
13	h2	201	CYC	C2C-C3C	5.15	1.68	1.54
13	Q1	201	CYC	C2C-C3C	5.14	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L5	201	CYC	C2C-C3C	5.14	1.68	1.54
13	P2	201	CYC	C2C-C3C	5.14	1.68	1.54
13	Q4	201	CYC	C2C-C3C	5.14	1.68	1.54
13	a4	202	CYC	C2C-C3C	5.14	1.68	1.54
13	Q6	201	CYC	C2C-C3C	5.14	1.68	1.54
13	F5	202	CYC	C2C-C3C	5.14	1.68	1.54
13	V3	202	CYC	C2C-C3C	5.14	1.68	1.54
13	J4	202	CYC	C2C-C3C	5.14	1.68	1.54
13	V5	202	CYC	C4B-C3B	-5.14	1.38	1.48
13	D6	201	CYC	C4B-C3B	-5.14	1.38	1.48
13	V6	202	CYC	C4B-C3B	-5.14	1.38	1.48
13	Q4	202	CYC	C2C-C3C	5.13	1.68	1.54
13	Q5	201	CYC	C2C-C3C	5.13	1.68	1.54
13	V4	202	CYC	C2C-C3C	5.13	1.68	1.54
13	X3	201	CYC	C4B-C3B	-5.13	1.38	1.48
13	J6	202	CYC	C2C-C3C	5.13	1.68	1.54
13	V2	201	CYC	C2C-C3C	5.13	1.68	1.54
13	g2	201	CYC	C4B-C3B	-5.13	1.38	1.48
13	P7	202	CYC	C2C-C3C	5.13	1.68	1.54
13	D5	201	CYC	C4B-C3B	-5.13	1.38	1.48
13	J6	201	CYC	C2C-C3C	5.13	1.68	1.54
13	T6	201	CYC	C2C-C3C	5.13	1.68	1.54
13	J1	202	CYC	C4B-C3B	-5.12	1.38	1.48
13	w2	201	CYC	C4B-C3B	-5.12	1.38	1.48
13	E1	201	CYC	C2C-C3C	5.12	1.68	1.54
13	42	302	CYC	C4B-C3B	-5.12	1.38	1.48
13	32	301	CYC	C2C-C3C	5.12	1.68	1.54
13	J4	201	CYC	C2C-C3C	5.12	1.68	1.54
13	J5	202	CYC	C2C-C3C	5.12	1.68	1.54
13	M6	201	CYC	C4B-C3B	-5.12	1.38	1.48
13	a3	201	CYC	C4B-C3B	-5.12	1.38	1.48
13	y2	201	CYC	C4B-C3B	-5.12	1.38	1.48
13	E3	201	CYC	C2C-C3C	5.12	1.68	1.54
13	E5	201	CYC	C2C-C3C	5.12	1.68	1.54
13	Q2	201	CYC	C4B-C3B	-5.12	1.38	1.48
13	M5	201	CYC	C4B-C3B	-5.11	1.38	1.48
13	F5	201	CYC	C2C-C3C	5.11	1.68	1.54
13	52	302	CYC	C4B-C3B	-5.11	1.38	1.48
13	Z4	301	CYC	C4B-C3B	-5.11	1.38	1.48
13	s2	201	CYC	C2C-C3C	5.11	1.68	1.54
13	E6	201	CYC	C2C-C3C	5.11	1.68	1.54
13	F6	201	CYC	C2C-C3C	5.11	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t2	201	CYC	C4B-C3B	-5.11	1.38	1.48
13	C6	202	CYC	C4B-C3B	-5.11	1.38	1.48
13	J4	202	CYC	C4B-C3B	-5.11	1.38	1.48
13	o2	801	CYC	C1A-C2A	-5.11	1.37	1.45
13	V1	201	CYC	C4B-C3B	-5.11	1.38	1.48
13	z2	201	CYC	C4B-C3B	-5.11	1.38	1.48
13	J1	201	CYC	C2C-C3C	5.10	1.68	1.54
13	C5	202	CYC	C4B-C3B	-5.10	1.38	1.48
13	J6	202	CYC	C4B-C3B	-5.10	1.38	1.48
13	J5	202	CYC	C4B-C3B	-5.10	1.38	1.48
13	V1	202	CYC	C2C-C3C	5.10	1.68	1.54
13	F1	201	CYC	C2C-C3C	5.10	1.68	1.54
13	F4	201	CYC	C2C-C3C	5.10	1.68	1.54
13	v2	201	CYC	C2C-C3C	5.09	1.68	1.54
13	a7	201	CYC	C4B-C3B	-5.09	1.38	1.48
13	R5	201	CYC	C4B-C3B	-5.09	1.38	1.48
13	V2	201	CYC	C4B-C3B	-5.09	1.38	1.48
13	a5	202	CYC	C4B-C3B	-5.09	1.38	1.48
13	A2	202	CYC	C4B-C3B	-5.09	1.38	1.48
13	T4	201	CYC	C2C-C3C	5.09	1.68	1.54
13	X7	201	CYC	C4B-C3B	-5.09	1.38	1.48
13	T3	201	CYC	C2C-C3C	5.09	1.68	1.54
13	a6	202	CYC	C4B-C3B	-5.09	1.38	1.48
13	x2	201	CYC	C2C-C3C	5.09	1.68	1.54
13	M4	201	CYC	C4B-C3B	-5.09	1.38	1.48
13	G2	201	CYC	C2C-C3C	5.08	1.68	1.54
13	X7	201	CYC	C2C-C3C	5.08	1.68	1.54
13	32	302	CYC	C4B-C3B	-5.08	1.38	1.48
13	E4	201	CYC	C4B-C3B	-5.08	1.38	1.48
13	n2	201	CYC	C1A-C2A	-5.08	1.37	1.45
13	D2	201	CYC	C2C-C3C	5.08	1.68	1.54
13	V3	202	CYC	C4B-C3B	-5.08	1.38	1.48
13	P5	202	CYC	C2C-C3C	5.08	1.68	1.54
13	o2	801	CYC	C2C-C3C	5.07	1.68	1.54
13	P4	201	CYC	C2C-C3C	5.07	1.68	1.54
13	R2	201	CYC	C2C-C3C	5.07	1.68	1.54
13	T2	201	CYC	C4B-C3B	-5.07	1.38	1.48
13	e2	201	CYC	C1A-C2A	-5.07	1.37	1.45
13	a6	202	CYC	C2C-C3C	5.07	1.68	1.54
13	V1	202	CYC	C4B-C3B	-5.07	1.38	1.48
13	X3	201	CYC	C2C-C3C	5.07	1.68	1.54
13	U2	201	CYC	C2C-C3C	5.07	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P5	201	CYC	C4B-C3B	-5.07	1.38	1.48
13	T7	201	CYC	C2C-C3C	5.07	1.68	1.54
13	p2	201	CYC	C1A-C2A	-5.07	1.37	1.45
13	D4	201	CYC	C4B-C3B	-5.07	1.38	1.48
13	V7	202	CYC	C4B-C3B	-5.07	1.38	1.48
13	M7	201	CYC	C4B-C3B	-5.07	1.38	1.48
13	P5	202	CYC	C4B-C3B	-5.06	1.38	1.48
13	R6	201	CYC	C4B-C3B	-5.06	1.38	1.48
13	a5	202	CYC	C2C-C3C	5.06	1.68	1.54
13	D3	201	CYC	C4B-C3B	-5.06	1.38	1.48
13	a4	202	CYC	C4B-C3B	-5.06	1.38	1.48
13	R1	201	CYC	C4B-C3B	-5.06	1.38	1.48
13	K6	201	CYC	C4B-C3B	-5.06	1.38	1.48
13	42	301	CYC	C2C-C3C	5.06	1.68	1.54
13	a1	202	CYC	C4B-C3B	-5.05	1.38	1.48
13	n2	201	CYC	C4B-C3B	-5.05	1.38	1.48
13	W5	201	CYC	C4B-C3B	-5.05	1.38	1.48
13	X1	201	CYC	C2C-C3C	5.05	1.68	1.54
13	E2	201	CYC	C2C-C3C	5.05	1.68	1.54
13	T5	201	CYC	C2C-C3C	5.05	1.68	1.54
13	X2	201	CYC	C4B-C3B	-5.05	1.38	1.48
13	P4	202	CYC	C4B-C3B	-5.05	1.38	1.48
13	R4	201	CYC	C4B-C3B	-5.05	1.38	1.48
13	G6	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	T1	201	CYC	C2C-C3C	5.04	1.68	1.54
13	A6	301	CYC	C2C-C3C	5.04	1.68	1.54
13	M3	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	D2	201	CYC	C1A-C2A	-5.04	1.37	1.45
13	P6	202	CYC	C2C-C3C	5.04	1.68	1.54
13	C2	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	J1	202	CYC	C2C-C3C	5.04	1.68	1.54
13	a1	202	CYC	C2C-C3C	5.04	1.68	1.54
13	C1	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	J1	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	P6	201	CYC	C4B-C3B	-5.04	1.38	1.48
13	G1	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	W2	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	L5	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	P1	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	k2	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	L4	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	S1	201	CYC	C4B-C3B	-5.03	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a3	202	CYC	C4B-C3B	-5.03	1.39	1.48
13	W1	201	CYC	C4B-C3B	-5.03	1.39	1.48
13	X2	201	CYC	C2C-C3C	5.03	1.68	1.54
13	L2	201	CYC	C4B-C3B	-5.02	1.39	1.48
13	m2	201	CYC	C4B-C3B	-5.02	1.39	1.48
13	Z3	301	CYC	C4B-C3B	-5.02	1.39	1.48
13	P7	201	CYC	C4B-C3B	-5.02	1.39	1.48
13	A1	301	CYC	C2C-C3C	5.02	1.68	1.54
13	T2	201	CYC	C2C-C3C	5.02	1.68	1.54
13	A1	301	CYC	C4B-C3B	-5.02	1.39	1.48
13	M2	201	CYC	C4B-C3B	-5.02	1.39	1.48
13	J6	201	CYC	C4B-C3B	-5.02	1.39	1.48
13	V4	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	F4	202	CYC	C4B-C3B	-5.01	1.39	1.48
13	e2	201	CYC	C2C-C3C	5.01	1.68	1.54
13	C3	202	CYC	C4B-C3B	-5.01	1.39	1.48
13	C4	202	CYC	C4B-C3B	-5.01	1.39	1.48
13	J4	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	U2	201	CYC	C1A-C2A	-5.01	1.37	1.45
13	D7	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	J5	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	R2	201	CYC	C1A-C2A	-5.01	1.37	1.45
13	L6	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	N5	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	V6	201	CYC	C4B-C3B	-5.01	1.39	1.48
13	T5	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	V5	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	s2	201	CYC	C1A-C2A	-5.00	1.37	1.45
13	F6	202	CYC	C4B-C3B	-5.00	1.39	1.48
13	l2	201	CYC	C1A-C2A	-5.00	1.37	1.45
13	K1	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	C5	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	Q1	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	S6	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	F5	202	CYC	C4B-C3B	-5.00	1.39	1.48
13	22	302	CYC	C4B-C3B	-5.00	1.39	1.48
13	T1	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	T6	201	CYC	C4B-C3B	-5.00	1.39	1.48
13	a7	202	CYC	C4B-C3B	-5.00	1.39	1.48
13	P6	202	CYC	C4B-C3B	-5.00	1.39	1.48
13	P1	202	CYC	C4B-C3B	-4.99	1.39	1.48
13	W6	201	CYC	C4B-C3B	-4.99	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C4	201	CYC	C4B-C3B	-4.99	1.39	1.48
13	G5	201	CYC	C4B-C3B	-4.99	1.39	1.48
13	C7	202	CYC	C4B-C3B	-4.99	1.39	1.48
13	52	301	CYC	C2C-C3C	4.99	1.68	1.54
13	C6	201	CYC	C4B-C3B	-4.99	1.39	1.48
13	h2	201	CYC	C1A-C2A	-4.98	1.37	1.45
13	d2	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	P3	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	A1	302	CYC	C1A-C2A	-4.98	1.37	1.45
13	J7	202	CYC	C4B-C3B	-4.98	1.39	1.48
13	F1	202	CYC	C4B-C3B	-4.98	1.39	1.48
13	N6	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	P1	202	CYC	C2C-C3C	4.98	1.67	1.54
13	B1	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	R3	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	A6	301	CYC	C4B-C3B	-4.98	1.39	1.48
13	R7	201	CYC	C4B-C3B	-4.98	1.39	1.48
13	E2	201	CYC	C1A-C2A	-4.98	1.38	1.45
13	E3	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	J3	202	CYC	C4B-C3B	-4.97	1.39	1.48
13	K3	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	S5	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	Z1	301	CYC	C1A-C2A	-4.97	1.38	1.45
13	x2	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	A2	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	F5	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	H1	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	c2	801	CYC	C4B-C3B	-4.97	1.39	1.48
13	H2	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	T7	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	F1	201	CYC	C4B-C3B	-4.97	1.39	1.48
13	U1	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	i2	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	W4	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	N4	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	G4	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	O2	201	CYC	C1A-C2A	-4.96	1.38	1.45
13	B6	201	CYC	C4B-C3B	-4.96	1.39	1.48
13	m2	201	CYC	C1A-C2A	-4.95	1.38	1.45
13	P4	201	CYC	C4B-C3B	-4.95	1.39	1.48
13	52	301	CYC	C4B-C3B	-4.95	1.39	1.48
13	L3	201	CYC	C4B-C3B	-4.95	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	201	CYC	C1A-C2A	-4.95	1.38	1.45
13	N1	201	CYC	C4B-C3B	-4.95	1.39	1.48
13	L1	201	CYC	C1A-C2A	-4.95	1.38	1.45
13	F3	202	CYC	C4B-C3B	-4.94	1.39	1.48
13	I3	201	CYC	C4B-C3B	-4.94	1.39	1.48
13	U5	201	CYC	C4B-C3B	-4.94	1.39	1.48
13	f2	201	CYC	C2C-C3C	4.94	1.67	1.54
13	K4	201	CYC	C4B-C3B	-4.94	1.39	1.48
13	F6	201	CYC	C4B-C3B	-4.94	1.39	1.48
13	Z5	301	CYC	C1A-C2A	-4.93	1.38	1.45
13	T5	202	CYC	C4B-C3B	-4.93	1.39	1.48
13	T4	201	CYC	C4B-C3B	-4.93	1.39	1.48
13	v2	201	CYC	C1A-C2A	-4.93	1.38	1.45
13	J3	201	CYC	C4B-C3B	-4.93	1.39	1.48
13	L7	201	CYC	C4B-C3B	-4.93	1.39	1.48
13	j2	201	CYC	C4B-C3B	-4.93	1.39	1.48
13	G3	201	CYC	C4B-C3B	-4.93	1.39	1.48
13	S3	201	CYC	C4B-C3B	-4.92	1.39	1.48
13	Z7	301	CYC	C4B-C3B	-4.92	1.39	1.48
13	K5	201	CYC	C4B-C3B	-4.92	1.39	1.48
13	P2	201	CYC	C1A-C2A	-4.92	1.38	1.45
13	a2	201	CYC	C4B-C3B	-4.92	1.39	1.48
13	K7	201	CYC	C4B-C3B	-4.92	1.39	1.48
13	H4	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	U4	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	B5	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	B4	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	N2	802	CYC	C2C-C3C	4.91	1.67	1.54
13	E7	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	T4	202	CYC	C4B-C3B	-4.91	1.39	1.48
13	z2	201	CYC	C1A-C2A	-4.91	1.38	1.45
13	V1	201	CYC	C1A-C2A	-4.91	1.38	1.45
13	W1	201	CYC	C1A-C2A	-4.91	1.38	1.45
13	S4	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	C3	201	CYC	C4B-C3B	-4.91	1.39	1.48
13	N2	801	CYC	C1A-C2A	-4.90	1.38	1.45
13	52	302	CYC	C1A-C2A	-4.90	1.38	1.45
13	A6	302	CYC	C1A-C2A	-4.90	1.38	1.45
13	42	302	CYC	C1A-C2A	-4.90	1.38	1.45
13	T3	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	I5	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	G7	201	CYC	C4B-C3B	-4.90	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T1	202	CYC	C4B-C3B	-4.90	1.39	1.48
13	A1	301	CYC	C1A-C2A	-4.90	1.38	1.45
13	F4	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	Q5	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	F7	202	CYC	C4B-C3B	-4.90	1.39	1.48
13	U7	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	F7	201	CYC	C4B-C3B	-4.90	1.39	1.48
13	A6	301	CYC	C1A-C2A	-4.89	1.38	1.45
13	Q2	201	CYC	C1A-C2A	-4.89	1.38	1.45
13	B2	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	H6	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	I7	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	S7	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	H5	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	L2	201	CYC	C1A-C2A	-4.89	1.38	1.45
13	J7	201	CYC	C4B-C3B	-4.89	1.39	1.48
13	g2	201	CYC	C1A-C2A	-4.89	1.38	1.45
13	U6	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	H3	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	I1	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	L6	201	CYC	C1A-C2A	-4.88	1.38	1.45
13	V3	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	U3	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	Q6	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	H7	201	CYC	C4B-C3B	-4.88	1.39	1.48
13	42	301	CYC	C4B-C3B	-4.87	1.39	1.48
13	V4	201	CYC	C1A-C2A	-4.87	1.38	1.45
13	N3	201	CYC	C4B-C3B	-4.87	1.39	1.48
13	G2	201	CYC	C1A-C2A	-4.87	1.38	1.45
13	X7	201	CYC	C1A-C2A	-4.87	1.38	1.45
13	T6	202	CYC	C4B-C3B	-4.87	1.39	1.48
13	Z6	301	CYC	C1A-C2A	-4.87	1.38	1.45
13	Q4	201	CYC	C4B-C3B	-4.87	1.39	1.48
13	B3	201	CYC	C4B-C3B	-4.86	1.39	1.48
13	w2	201	CYC	C1A-C2A	-4.86	1.38	1.45
13	B5	201	CYC	C1A-C2A	-4.86	1.38	1.45
13	X3	201	CYC	C1A-C2A	-4.85	1.38	1.45
13	P3	202	CYC	C4B-C3B	-4.85	1.39	1.48
13	F3	201	CYC	C4B-C3B	-4.85	1.39	1.48
13	V5	201	CYC	C1A-C2A	-4.85	1.38	1.45
13	32	301	CYC	C4B-C3B	-4.85	1.39	1.48
13	X6	201	CYC	C1A-C2A	-4.84	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N7	201	CYC	C4B-C3B	-4.84	1.39	1.48
13	X5	201	CYC	C1A-C2A	-4.84	1.38	1.45
13	C7	201	CYC	C4B-C3B	-4.84	1.39	1.48
13	B7	201	CYC	C4B-C3B	-4.84	1.39	1.48
13	W3	201	CYC	C4B-C3B	-4.83	1.39	1.48
13	W7	201	CYC	C4B-C3B	-4.83	1.39	1.48
13	y2	201	CYC	C1A-C2A	-4.83	1.38	1.45
13	V7	201	CYC	C4B-C3B	-4.83	1.39	1.48
13	r2	201	CYC	C1A-C2A	-4.83	1.38	1.45
13	t2	201	CYC	C1A-C2A	-4.83	1.38	1.45
13	J5	201	CYC	C1A-C2A	-4.83	1.38	1.45
13	B1	201	CYC	C1A-C2A	-4.83	1.38	1.45
13	J1	201	CYC	C1A-C2A	-4.82	1.38	1.45
13	M1	201	CYC	C1A-C2A	-4.82	1.38	1.45
13	P7	202	CYC	C4B-C3B	-4.82	1.39	1.48
13	W2	201	CYC	C1A-C2A	-4.82	1.38	1.45
13	F1	201	CYC	C1A-C2A	-4.82	1.38	1.45
13	M6	201	CYC	C1A-C2A	-4.82	1.38	1.45
13	I4	201	CYC	C4B-C3B	-4.82	1.39	1.48
13	Q3	201	CYC	C4B-C3B	-4.81	1.39	1.48
13	D4	201	CYC	C1A-C2A	-4.81	1.38	1.45
13	D6	201	CYC	C1A-C2A	-4.81	1.38	1.45
13	X1	201	CYC	C1A-C2A	-4.81	1.38	1.45
13	Z4	301	CYC	C1A-C2A	-4.81	1.38	1.45
13	a6	201	CYC	C1A-C2A	-4.81	1.38	1.45
13	N1	201	CYC	C1A-C2A	-4.80	1.38	1.45
13	22	301	CYC	C4B-C3B	-4.80	1.39	1.48
13	I6	201	CYC	C4B-C3B	-4.80	1.39	1.48
13	X4	201	CYC	C1A-C2A	-4.79	1.38	1.45
13	a5	201	CYC	C1A-C2A	-4.79	1.38	1.45
13	52	301	CYC	C1A-C2A	-4.79	1.38	1.45
13	Q7	201	CYC	C4B-C3B	-4.79	1.39	1.48
13	V3	201	CYC	C1A-C2A	-4.78	1.38	1.45
13	M5	201	CYC	C1A-C2A	-4.78	1.38	1.45
13	V7	201	CYC	C1A-C2A	-4.78	1.38	1.45
13	C1	201	CYC	C1A-C2A	-4.78	1.38	1.45
13	T3	202	CYC	C4B-C3B	-4.78	1.39	1.48
13	U1	201	CYC	C1A-C2A	-4.77	1.38	1.45
13	I6	201	CYC	C1A-C2A	-4.77	1.38	1.45
13	Q5	202	CYC	C1A-C2A	-4.77	1.38	1.45
13	J6	201	CYC	C1A-C2A	-4.77	1.38	1.45
13	Q1	202	CYC	C1A-C2A	-4.77	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N2	802	CYC	C1A-C2A	-4.77	1.38	1.45
13	N4	201	CYC	C1A-C2A	-4.76	1.38	1.45
13	Q4	202	CYC	C1A-C2A	-4.76	1.38	1.45
13	B2	202	CYC	C4B-C3B	-4.76	1.39	1.48
13	G5	201	CYC	C1A-C2A	-4.76	1.38	1.45
13	N6	201	CYC	C1A-C2A	-4.76	1.38	1.45
13	Z3	301	CYC	C1A-C2A	-4.75	1.38	1.45
13	42	301	CYC	C1A-C2A	-4.74	1.38	1.45
13	U5	201	CYC	C1A-C2A	-4.74	1.38	1.45
13	N5	201	CYC	C1A-C2A	-4.74	1.38	1.45
13	32	302	CYC	C1A-C2A	-4.74	1.38	1.45
13	a3	201	CYC	C1A-C2A	-4.74	1.38	1.45
13	K6	201	CYC	C1A-C2A	-4.74	1.38	1.45
13	Z7	301	CYC	C1A-C2A	-4.74	1.38	1.45
13	22	301	CYC	C1A-C2A	-4.73	1.38	1.45
13	22	302	CYC	C1A-C2A	-4.73	1.38	1.45
13	D1	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	F5	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	W6	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	X2	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	M4	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	W5	201	CYC	C1A-C2A	-4.73	1.38	1.45
13	I3	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	I4	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	W4	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	a7	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	J3	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	V6	201	CYC	C1A-C2A	-4.72	1.38	1.45
13	B4	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	G1	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	32	301	CYC	C1A-C2A	-4.71	1.38	1.45
13	T1	202	CYC	C1A-C2A	-4.71	1.38	1.45
13	K1	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	H1	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	J4	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	K5	201	CYC	C1A-C2A	-4.71	1.38	1.45
13	S2	201	CYC	C1A-C2A	-4.70	1.38	1.45
13	Q5	201	CYC	C1A-C2A	-4.70	1.38	1.45
13	T7	202	CYC	C4B-C3B	-4.70	1.39	1.48
13	S4	201	CYC	C1A-C2A	-4.70	1.38	1.45
13	I1	201	CYC	C1A-C2A	-4.70	1.38	1.45
13	V2	201	CYC	C1A-C2A	-4.69	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q1	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	Q6	202	CYC	C1A-C2A	-4.69	1.38	1.45
13	I5	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	G6	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	S1	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	K4	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	C6	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	Q4	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	D5	201	CYC	C1A-C2A	-4.69	1.38	1.45
13	F6	201	CYC	C1A-C2A	-4.68	1.38	1.45
13	P1	201	CYC	C1A-C2A	-4.68	1.38	1.45
13	L4	201	CYC	C1A-C2A	-4.68	1.38	1.45
13	S5	201	CYC	C1A-C2A	-4.67	1.38	1.45
13	C5	201	CYC	C1A-C2A	-4.67	1.38	1.45
13	F4	201	CYC	C1A-C2A	-4.67	1.38	1.45
13	P7	201	CYC	C1A-C2A	-4.66	1.38	1.45
13	J7	201	CYC	C1A-C2A	-4.66	1.38	1.45
13	H5	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	B6	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	J6	202	CYC	C1A-C2A	-4.65	1.38	1.45
13	G4	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	K3	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	P3	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	T6	202	CYC	C1A-C2A	-4.65	1.38	1.45
13	Q6	201	CYC	C1A-C2A	-4.65	1.38	1.45
13	U4	201	CYC	C1A-C2A	-4.64	1.38	1.45
13	I7	201	CYC	C1A-C2A	-4.64	1.38	1.45
13	P5	201	CYC	C1A-C2A	-4.64	1.38	1.45
13	T3	202	CYC	C1A-C2A	-4.64	1.38	1.45
13	T5	202	CYC	C1A-C2A	-4.64	1.38	1.45
13	N3	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	D7	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	P1	202	CYC	C1A-C2A	-4.63	1.38	1.45
13	S6	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	E1	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	L5	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	G7	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	N7	201	CYC	C1A-C2A	-4.63	1.38	1.45
13	P4	202	CYC	C1A-C2A	-4.63	1.38	1.45
13	J4	202	CYC	C1A-C2A	-4.62	1.38	1.45
13	a1	202	CYC	C1A-C2A	-4.62	1.38	1.45
13	J5	202	CYC	C1A-C2A	-4.62	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M3	201	CYC	C1A-C2A	-4.62	1.38	1.45
13	S3	201	CYC	C1A-C2A	-4.62	1.38	1.45
13	P6	202	CYC	C1A-C2A	-4.61	1.38	1.45
13	P6	201	CYC	C1A-C2A	-4.61	1.38	1.45
13	T4	202	CYC	C1A-C2A	-4.61	1.38	1.45
13	H6	201	CYC	C1A-C2A	-4.61	1.38	1.45
13	K7	201	CYC	C1A-C2A	-4.61	1.38	1.45
13	G3	201	CYC	C1A-C2A	-4.60	1.38	1.45
13	d2	201	CYC	C1A-C2A	-4.60	1.38	1.45
13	Q7	202	CYC	C1A-C2A	-4.60	1.38	1.45
13	E5	201	CYC	C1A-C2A	-4.59	1.38	1.45
13	H7	201	CYC	C1A-C2A	-4.59	1.38	1.45
13	P5	202	CYC	C1A-C2A	-4.59	1.38	1.45
13	T7	202	CYC	C1A-C2A	-4.59	1.38	1.45
13	a5	202	CYC	C1A-C2A	-4.59	1.38	1.45
13	U6	201	CYC	C1A-C2A	-4.59	1.38	1.45
13	A2	202	CYC	C1A-C2A	-4.58	1.38	1.45
13	F6	202	CYC	C1A-C2A	-4.58	1.38	1.45
13	x2	201	CYC	C1A-C2A	-4.58	1.38	1.45
13	C4	201	CYC	C1A-C2A	-4.58	1.38	1.45
13	B7	201	CYC	C1A-C2A	-4.57	1.38	1.45
13	M7	201	CYC	C1A-C2A	-4.57	1.38	1.45
13	F3	201	CYC	C1A-C2A	-4.57	1.38	1.45
13	Q3	202	CYC	C1A-C2A	-4.57	1.38	1.45
13	a4	202	CYC	C1A-C2A	-4.57	1.38	1.45
13	F5	202	CYC	C1A-C2A	-4.56	1.38	1.45
13	H3	201	CYC	C1A-C2A	-4.56	1.38	1.45
13	F1	202	CYC	C1A-C2A	-4.56	1.38	1.45
13	W3	201	CYC	C1A-C2A	-4.56	1.38	1.45
13	j2	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	V6	202	CYC	C1A-C2A	-4.55	1.38	1.45
13	J1	202	CYC	C1A-C2A	-4.55	1.38	1.45
13	C7	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	L7	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	S7	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	Q3	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	R1	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	C3	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	B3	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	R5	201	CYC	C1A-C2A	-4.55	1.38	1.45
13	a6	202	CYC	C1A-C2A	-4.55	1.38	1.45
13	L3	201	CYC	C1A-C2A	-4.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H4	201	CYC	C1A-C2A	-4.54	1.38	1.45
13	F7	201	CYC	C1A-C2A	-4.54	1.38	1.45
13	E4	201	CYC	C1A-C2A	-4.54	1.38	1.45
13	T2	201	CYC	C1A-C2A	-4.54	1.38	1.45
13	Q7	201	CYC	C1A-C2A	-4.53	1.38	1.45
13	W7	201	CYC	C1A-C2A	-4.53	1.38	1.45
13	a3	202	CYC	C1A-C2A	-4.52	1.38	1.45
13	T6	201	CYC	C1A-C2A	-4.52	1.38	1.45
13	U7	201	CYC	C1A-C2A	-4.52	1.38	1.45
13	U3	201	CYC	C1A-C2A	-4.51	1.38	1.45
13	D3	201	CYC	C1A-C2A	-4.51	1.38	1.45
13	V5	202	CYC	C1A-C2A	-4.51	1.38	1.45
13	V4	202	CYC	C1A-C2A	-4.50	1.38	1.45
13	R4	201	CYC	C1A-C2A	-4.50	1.38	1.45
13	A2	201	CYC	C1A-C2A	-4.50	1.38	1.45
13	E6	201	CYC	C1A-C2A	-4.49	1.38	1.45
13	R3	201	CYC	C1A-C2A	-4.48	1.38	1.45
13	P4	201	CYC	C1A-C2A	-4.48	1.38	1.45
13	i2	201	CYC	C1A-C2A	-4.48	1.38	1.45
13	F3	202	CYC	C1A-C2A	-4.48	1.38	1.45
13	P3	202	CYC	C1A-C2A	-4.47	1.38	1.45
13	C1	202	CYC	C1A-C2A	-4.47	1.38	1.45
13	B2	202	CYC	C1A-C2A	-4.47	1.38	1.45
13	R7	201	CYC	C1A-C2A	-4.47	1.38	1.45
13	R6	201	CYC	C1A-C2A	-4.47	1.38	1.45
13	C5	202	CYC	C1A-C2A	-4.46	1.38	1.45
13	C4	202	CYC	C1A-C2A	-4.46	1.38	1.45
13	B2	201	CYC	C1A-C2A	-4.46	1.38	1.45
13	T1	201	CYC	C1A-C2A	-4.45	1.38	1.45
13	P7	202	CYC	C1A-C2A	-4.45	1.38	1.45
13	a7	202	CYC	C1A-C2A	-4.45	1.38	1.45
13	J3	202	CYC	C1A-C2A	-4.45	1.38	1.45
13	F7	202	CYC	C1A-C2A	-4.45	1.38	1.45
13	V1	202	CYC	C1A-C2A	-4.45	1.38	1.45
13	J7	202	CYC	C1A-C2A	-4.44	1.38	1.45
13	T5	201	CYC	C1A-C2A	-4.44	1.38	1.45
13	T4	201	CYC	C1A-C2A	-4.44	1.38	1.45
13	F4	202	CYC	C1A-C2A	-4.44	1.38	1.45
13	C6	202	CYC	C1A-C2A	-4.41	1.38	1.45
13	a2	201	CYC	C1A-C2A	-4.40	1.38	1.45
13	k2	201	CYC	C1A-C2A	-4.40	1.38	1.45
13	F2	201	CYC	C1A-C2A	-4.39	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C2	201	CYC	C1A-C2A	-4.38	1.38	1.45
13	V7	202	CYC	C1A-C2A	-4.38	1.38	1.45
13	C7	202	CYC	C1A-C2A	-4.37	1.38	1.45
13	E3	201	CYC	C1A-C2A	-4.36	1.38	1.45
13	C3	202	CYC	C1A-C2A	-4.36	1.38	1.45
13	V3	202	CYC	C1A-C2A	-4.35	1.38	1.45
13	T3	201	CYC	C1A-C2A	-4.34	1.38	1.45
13	T7	201	CYC	C1A-C2A	-4.33	1.39	1.45
13	E7	201	CYC	C1A-C2A	-4.33	1.39	1.45
13	c2	801	CYC	C1A-C2A	-4.32	1.39	1.45
13	H2	201	CYC	C1A-C2A	-4.18	1.39	1.45
13	o2	801	CYC	C1B-NB	-3.88	1.31	1.37
13	G1	201	CYC	C1B-C2B	-3.82	1.38	1.45
13	m2	201	CYC	C1B-C2B	-3.81	1.38	1.45
13	X3	201	CYC	C1B-NB	-3.80	1.31	1.37
13	N6	201	CYC	C1B-C2B	-3.79	1.38	1.45
13	B1	201	CYC	C1B-C2B	-3.78	1.38	1.45
13	N5	201	CYC	C1B-C2B	-3.74	1.38	1.45
13	N4	201	CYC	C1B-C2B	-3.74	1.38	1.45
13	B6	201	CYC	C1B-C2B	-3.74	1.38	1.45
13	K1	201	CYC	C1B-C2B	-3.73	1.38	1.45
13	N1	201	CYC	C1B-C2B	-3.71	1.38	1.45
13	f2	201	CYC	C4D-ND	-3.71	1.31	1.37
13	G5	201	CYC	C1B-C2B	-3.71	1.38	1.45
13	I1	201	CYC	C1B-C2B	-3.70	1.38	1.45
13	f2	201	CYC	C1B-NB	-3.69	1.31	1.37
13	S2	201	CYC	C1B-NB	-3.69	1.31	1.37
13	X5	201	CYC	C1B-NB	-3.68	1.31	1.37
13	N2	802	CYC	C1B-C2B	-3.68	1.38	1.45
13	R2	201	CYC	C1B-C2B	-3.68	1.38	1.45
13	t2	201	CYC	C1B-C2B	-3.67	1.38	1.45
13	X4	201	CYC	C1B-NB	-3.67	1.31	1.37
13	N2	802	CYC	C1B-NB	-3.67	1.31	1.37
13	U2	201	CYC	C1B-NB	-3.67	1.31	1.37
13	B4	201	CYC	C1B-C2B	-3.67	1.38	1.45
13	X7	201	CYC	C1B-NB	-3.66	1.31	1.37
13	H1	201	CYC	C1B-C2B	-3.66	1.38	1.45
13	F4	201	CYC	C1B-C2B	-3.66	1.38	1.45
13	f2	201	CYC	C1B-C2B	-3.66	1.38	1.45
13	n2	201	CYC	C1B-NB	-3.65	1.31	1.37
13	o2	801	CYC	C4D-ND	-3.65	1.31	1.37
13	s2	201	CYC	C1B-NB	-3.65	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G6	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	B5	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	B3	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	R3	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	F5	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	p2	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	F3	201	CYC	C1B-C2B	-3.64	1.38	1.45
13	R1	201	CYC	C1B-C2B	-3.63	1.38	1.45
13	h2	201	CYC	C1B-NB	-3.63	1.31	1.37
13	H4	201	CYC	C1B-C2B	-3.63	1.38	1.45
13	U2	201	CYC	C4D-ND	-3.63	1.31	1.37
13	N3	201	CYC	C1B-C2B	-3.63	1.38	1.45
13	X1	201	CYC	C1B-NB	-3.62	1.31	1.37
13	g2	201	CYC	C1B-C2B	-3.62	1.38	1.45
13	k2	201	CYC	C1B-C2B	-3.62	1.38	1.45
13	B7	201	CYC	C1B-C2B	-3.62	1.38	1.45
13	T2	201	CYC	C1B-C2B	-3.61	1.38	1.45
13	R5	201	CYC	C1B-C2B	-3.61	1.38	1.45
13	B2	202	CYC	C1B-C2B	-3.61	1.38	1.45
13	h2	201	CYC	C1B-C2B	-3.61	1.38	1.45
13	S5	201	CYC	C1B-C2B	-3.61	1.38	1.45
13	Z1	301	CYC	C1B-NB	-3.60	1.31	1.37
13	v2	201	CYC	C1B-NB	-3.60	1.31	1.37
13	F6	202	CYC	C1B-C2B	-3.60	1.38	1.45
13	a6	202	CYC	C4D-ND	-3.60	1.31	1.37
13	G3	201	CYC	C1B-C2B	-3.60	1.38	1.45
13	E2	201	CYC	C1B-NB	-3.60	1.31	1.37
13	S2	201	CYC	C1B-C2B	-3.60	1.38	1.45
13	F6	201	CYC	C1B-C2B	-3.60	1.38	1.45
13	T1	202	CYC	C1B-C2B	-3.60	1.38	1.45
13	G4	201	CYC	C1B-C2B	-3.60	1.38	1.45
13	K7	201	CYC	C1B-C2B	-3.60	1.38	1.45
13	H6	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	U3	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	D1	201	CYC	C4D-ND	-3.59	1.31	1.37
13	F2	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	z2	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	D2	201	CYC	C1B-NB	-3.59	1.31	1.37
13	K5	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	F1	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	W6	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	N7	201	CYC	C1B-C2B	-3.59	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W3	201	CYC	C1B-C2B	-3.59	1.38	1.45
13	V2	201	CYC	C1B-C2B	-3.58	1.38	1.45
13	S1	201	CYC	C1B-C2B	-3.58	1.38	1.45
13	F1	202	CYC	C1B-C2B	-3.58	1.38	1.45
13	n2	201	CYC	C1B-C2B	-3.58	1.38	1.45
13	S4	201	CYC	C1B-C2B	-3.58	1.38	1.45
13	I6	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	O2	201	CYC	C1B-NB	-3.57	1.31	1.37
13	F5	202	CYC	C1B-C2B	-3.57	1.38	1.45
13	R6	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	Z6	301	CYC	C1B-NB	-3.57	1.31	1.37
13	t2	201	CYC	C4D-ND	-3.57	1.31	1.37
13	F4	202	CYC	C1B-C2B	-3.57	1.38	1.45
13	X6	201	CYC	C1B-NB	-3.57	1.31	1.37
13	W7	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	K3	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	H5	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	L1	201	CYC	C1B-NB	-3.57	1.31	1.37
13	Z5	301	CYC	C1B-NB	-3.57	1.31	1.37
13	l2	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	R4	201	CYC	C1B-C2B	-3.57	1.38	1.45
13	P2	201	CYC	C1B-C2B	-3.56	1.38	1.45
13	T4	202	CYC	C1B-C2B	-3.56	1.38	1.45
13	T5	202	CYC	C1B-C2B	-3.56	1.38	1.45
13	G2	201	CYC	C1B-NB	-3.56	1.31	1.37
13	t2	201	CYC	C1B-NB	-3.56	1.31	1.37
13	F3	202	CYC	C1B-C2B	-3.56	1.38	1.45
13	I5	201	CYC	C1B-C2B	-3.56	1.38	1.45
13	T6	202	CYC	C1B-C2B	-3.56	1.38	1.45
13	G7	201	CYC	C1B-C2B	-3.56	1.38	1.45
13	L7	201	CYC	C1B-C2B	-3.55	1.38	1.45
13	r2	201	CYC	C1B-NB	-3.55	1.31	1.37
13	H3	201	CYC	C1B-C2B	-3.55	1.38	1.45
13	L6	201	CYC	C1B-C2B	-3.55	1.38	1.45
13	L3	201	CYC	C1B-C2B	-3.55	1.38	1.45
13	s2	201	CYC	C1B-C2B	-3.55	1.38	1.45
13	L6	201	CYC	C1B-NB	-3.54	1.31	1.37
13	W1	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	S3	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	I3	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	R2	201	CYC	C1B-NB	-3.54	1.31	1.37
13	D2	201	CYC	C1B-C2B	-3.54	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	o2	801	CYC	C1B-C2B	-3.54	1.38	1.45
13	H7	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	R7	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	w2	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	V5	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	U1	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	I4	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	P1	202	CYC	C1B-C2B	-3.54	1.38	1.45
13	L2	201	CYC	C1B-C2B	-3.54	1.38	1.45
13	P2	201	CYC	C1B-NB	-3.53	1.31	1.37
13	U2	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	N2	802	CYC	C1A-NA	-3.53	1.31	1.38
13	F7	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	K6	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	W4	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	S6	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	e2	201	CYC	C1B-C2B	-3.53	1.38	1.45
13	p2	201	CYC	C1B-NB	-3.52	1.31	1.37
13	Z4	301	CYC	C1B-NB	-3.52	1.31	1.37
13	P1	202	CYC	C4D-ND	-3.52	1.31	1.37
13	v2	201	CYC	C1B-C2B	-3.52	1.38	1.45
13	D5	201	CYC	C4D-ND	-3.52	1.31	1.37
13	T4	201	CYC	C1B-C2B	-3.52	1.38	1.45
13	P1	201	CYC	C1B-C2B	-3.52	1.38	1.45
13	L5	201	CYC	C1B-C2B	-3.52	1.38	1.45
13	P4	202	CYC	C1B-NB	-3.52	1.31	1.37
13	o2	801	CYC	C1D-ND	-3.52	1.31	1.37
13	T7	202	CYC	C1B-C2B	-3.51	1.38	1.45
13	V1	201	CYC	C1B-C2B	-3.51	1.38	1.45
13	t2	201	CYC	C1A-NA	-3.51	1.31	1.38
13	S7	201	CYC	C1B-C2B	-3.51	1.38	1.45
13	F7	202	CYC	C1B-C2B	-3.51	1.38	1.45
13	C5	202	CYC	C1B-C2B	-3.51	1.38	1.45
13	a5	202	CYC	C4D-ND	-3.50	1.31	1.37
13	r2	201	CYC	C1B-C2B	-3.50	1.38	1.45
13	a1	202	CYC	C4D-ND	-3.50	1.31	1.37
13	I7	201	CYC	C1B-C2B	-3.50	1.38	1.45
13	a5	201	CYC	C1B-NB	-3.50	1.31	1.37
13	e2	201	CYC	C1B-NB	-3.50	1.31	1.37
13	w2	201	CYC	C1B-NB	-3.49	1.31	1.37
13	X2	201	CYC	C1B-NB	-3.49	1.31	1.37
13	y2	201	CYC	C1B-C2B	-3.49	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T3	202	CYC	C1B-C2B	-3.49	1.38	1.45
13	y2	201	CYC	C1B-NB	-3.49	1.31	1.37
13	C1	202	CYC	C1B-C2B	-3.49	1.38	1.45
13	P5	201	CYC	C1B-C2B	-3.49	1.38	1.45
13	J1	201	CYC	C1B-C2B	-3.49	1.38	1.45
13	M1	201	CYC	C4D-ND	-3.49	1.31	1.37
13	G2	201	CYC	C1B-C2B	-3.49	1.38	1.45
13	N2	801	CYC	C1B-C2B	-3.49	1.38	1.45
13	S2	201	CYC	C1A-NA	-3.49	1.31	1.38
13	P4	201	CYC	C1B-C2B	-3.49	1.38	1.45
13	a1	201	CYC	C1B-NB	-3.48	1.31	1.37
13	U6	201	CYC	C1B-C2B	-3.48	1.38	1.45
13	a1	201	CYC	C4D-ND	-3.48	1.31	1.37
13	a6	201	CYC	C1B-NB	-3.48	1.31	1.37
13	a1	202	CYC	C1B-C2B	-3.48	1.38	1.45
13	L5	201	CYC	C1B-NB	-3.48	1.31	1.37
13	P6	202	CYC	C1B-C2B	-3.48	1.38	1.45
13	M2	201	CYC	C1B-NB	-3.48	1.31	1.37
13	D7	201	CYC	C4D-ND	-3.48	1.31	1.37
13	P6	201	CYC	C1B-C2B	-3.48	1.38	1.45
13	V1	201	CYC	C1B-NB	-3.48	1.31	1.37
13	M6	201	CYC	C4D-ND	-3.48	1.31	1.37
13	P5	202	CYC	C4D-ND	-3.48	1.31	1.37
13	n2	201	CYC	C1A-NA	-3.48	1.31	1.38
13	z2	201	CYC	C1B-NB	-3.48	1.31	1.37
13	X2	201	CYC	C1B-C2B	-3.48	1.38	1.45
13	P2	201	CYC	C4D-ND	-3.48	1.31	1.37
13	U7	201	CYC	C1B-C2B	-3.48	1.38	1.45
13	V4	201	CYC	C1B-C2B	-3.48	1.38	1.45
13	g2	201	CYC	C1B-NB	-3.48	1.31	1.37
13	L4	201	CYC	C1B-NB	-3.47	1.31	1.37
13	P5	201	CYC	C1B-NB	-3.47	1.31	1.37
13	j2	201	CYC	C1B-C2B	-3.47	1.38	1.45
13	W5	201	CYC	C1B-C2B	-3.47	1.38	1.45
13	Z1	301	CYC	C4D-ND	-3.47	1.31	1.37
13	m2	201	CYC	C1B-NB	-3.47	1.31	1.37
13	P1	202	CYC	C1B-NB	-3.47	1.31	1.37
13	J6	201	CYC	C1B-C2B	-3.47	1.38	1.45
13	T3	201	CYC	C1B-C2B	-3.47	1.38	1.45
13	C6	202	CYC	C1B-C2B	-3.46	1.38	1.45
13	U4	201	CYC	C1B-C2B	-3.46	1.38	1.45
13	X2	201	CYC	C4D-ND	-3.46	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J7	201	CYC	C1B-C2B	-3.46	1.38	1.45
13	B5	201	CYC	C1B-NB	-3.46	1.31	1.37
13	J3	202	CYC	C1B-C2B	-3.46	1.38	1.45
13	M2	201	CYC	C1B-C2B	-3.46	1.38	1.45
13	U5	201	CYC	C1B-C2B	-3.46	1.38	1.45
13	T5	201	CYC	C1B-C2B	-3.45	1.38	1.45
13	V6	201	CYC	C1B-NB	-3.45	1.31	1.37
13	C4	202	CYC	C1B-C2B	-3.45	1.38	1.45
13	T6	201	CYC	C1B-C2B	-3.45	1.38	1.45
13	G1	201	CYC	C1B-NB	-3.45	1.31	1.37
13	E5	201	CYC	C1B-C2B	-3.45	1.38	1.45
13	E1	201	CYC	C1B-C2B	-3.45	1.38	1.45
13	E6	201	CYC	C1B-C2B	-3.45	1.38	1.45
13	P7	202	CYC	C1B-C2B	-3.45	1.38	1.45
13	L4	201	CYC	C1B-C2B	-3.44	1.38	1.45
13	S2	201	CYC	C4D-ND	-3.44	1.31	1.37
13	C6	201	CYC	C4D-ND	-3.44	1.31	1.37
13	T1	201	CYC	C1B-C2B	-3.44	1.38	1.45
13	P3	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	P5	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	D4	201	CYC	C4D-ND	-3.44	1.31	1.37
13	L3	201	CYC	C4D-ND	-3.44	1.31	1.37
13	V1	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	P4	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	N1	201	CYC	C1B-NB	-3.44	1.31	1.37
13	V6	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	J6	202	CYC	C4D-ND	-3.44	1.31	1.37
13	Q2	201	CYC	C1B-C2B	-3.44	1.38	1.45
13	V6	201	CYC	C1B-C2B	-3.44	1.38	1.45
13	i2	201	CYC	C4D-ND	-3.44	1.32	1.37
13	a5	202	CYC	C1B-C2B	-3.44	1.38	1.45
13	W1	201	CYC	C1B-NB	-3.44	1.32	1.37
13	a6	201	CYC	C4D-ND	-3.43	1.32	1.37
13	J5	202	CYC	C1B-C2B	-3.43	1.38	1.45
13	22	301	CYC	C1B-NB	-3.43	1.32	1.37
13	X3	201	CYC	C4D-ND	-3.43	1.32	1.37
13	O2	201	CYC	C1B-C2B	-3.43	1.39	1.45
13	C5	201	CYC	C1B-NB	-3.43	1.32	1.37
13	L2	201	CYC	C1B-NB	-3.43	1.32	1.37
13	42	301	CYC	C4D-ND	-3.43	1.32	1.37
13	N2	801	CYC	C1B-NB	-3.43	1.32	1.37
13	a4	202	CYC	C1B-C2B	-3.43	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	x2	201	CYC	C4D-ND	-3.43	1.32	1.37
13	a4	202	CYC	C4D-ND	-3.43	1.32	1.37
13	Z1	301	CYC	C1B-C2B	-3.43	1.39	1.45
13	a3	201	CYC	C1B-NB	-3.43	1.32	1.37
13	K5	201	CYC	C1B-NB	-3.43	1.32	1.37
13	E4	201	CYC	C1B-C2B	-3.43	1.39	1.45
13	L1	201	CYC	C1B-C2B	-3.43	1.39	1.45
13	T7	201	CYC	C1B-C2B	-3.42	1.39	1.45
13	U2	201	CYC	C1A-NA	-3.42	1.31	1.38
13	E1	201	CYC	C4D-ND	-3.42	1.32	1.37
13	L1	201	CYC	C4D-ND	-3.42	1.32	1.37
13	M4	201	CYC	C4D-ND	-3.42	1.32	1.37
13	H5	201	CYC	C1B-NB	-3.42	1.32	1.37
13	F1	201	CYC	C1B-NB	-3.42	1.32	1.37
13	J4	202	CYC	C1B-C2B	-3.42	1.39	1.45
13	T2	201	CYC	C1B-NB	-3.42	1.32	1.37
13	L6	201	CYC	C4D-ND	-3.42	1.32	1.37
13	P4	201	CYC	C4D-ND	-3.42	1.32	1.37
13	L7	201	CYC	C4D-ND	-3.42	1.32	1.37
13	Z3	301	CYC	C1B-NB	-3.42	1.32	1.37
13	J3	201	CYC	C1B-C2B	-3.42	1.39	1.45
13	v2	201	CYC	C1A-NA	-3.42	1.31	1.38
13	D6	201	CYC	C4D-ND	-3.42	1.32	1.37
13	T1	201	CYC	C4D-ND	-3.42	1.32	1.37
13	a3	202	CYC	C4D-ND	-3.42	1.32	1.37
13	G6	201	CYC	C1B-NB	-3.42	1.32	1.37
13	T2	201	CYC	C1A-NA	-3.42	1.31	1.38
13	a5	201	CYC	C4D-ND	-3.41	1.32	1.37
13	a2	201	CYC	C1B-C2B	-3.41	1.39	1.45
13	X6	201	CYC	C4D-ND	-3.41	1.32	1.37
13	T2	201	CYC	C4D-ND	-3.41	1.32	1.37
13	V3	201	CYC	C1B-C2B	-3.41	1.39	1.45
13	X7	201	CYC	C4D-ND	-3.41	1.32	1.37
13	L5	201	CYC	C1A-NA	-3.41	1.31	1.38
13	D4	201	CYC	C1B-C2B	-3.41	1.39	1.45
13	F2	201	CYC	C1B-NB	-3.41	1.32	1.37
13	J6	201	CYC	C1B-NB	-3.41	1.32	1.37
13	P6	202	CYC	C4D-ND	-3.41	1.32	1.37
13	a7	202	CYC	C4D-ND	-3.41	1.32	1.37
13	D1	201	CYC	C1B-C2B	-3.41	1.39	1.45
13	X5	201	CYC	C4D-ND	-3.41	1.32	1.37
13	E3	201	CYC	C1B-C2B	-3.41	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J7	202	CYC	C1B-C2B	-3.41	1.39	1.45
13	Z7	301	CYC	C1B-NB	-3.41	1.32	1.37
13	A6	301	CYC	C1B-NB	-3.41	1.32	1.37
13	E2	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	X1	201	CYC	C4D-ND	-3.40	1.32	1.37
13	o2	801	CYC	C1A-NA	-3.40	1.31	1.38
13	H2	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	W5	201	CYC	C1B-NB	-3.40	1.32	1.37
13	C2	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	52	301	CYC	C1B-NB	-3.40	1.32	1.37
13	K4	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	f2	201	CYC	C1A-NA	-3.40	1.31	1.38
13	a3	201	CYC	C4D-ND	-3.40	1.32	1.37
13	B1	201	CYC	C1B-NB	-3.40	1.32	1.37
13	F6	201	CYC	C1B-NB	-3.40	1.32	1.37
13	L5	201	CYC	C4D-ND	-3.40	1.32	1.37
13	c2	801	CYC	C1B-C2B	-3.40	1.39	1.45
13	V7	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	P2	201	CYC	C1A-NA	-3.40	1.31	1.38
13	D5	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	E7	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	V7	202	CYC	C1B-C2B	-3.40	1.39	1.45
13	H1	201	CYC	C1B-NB	-3.40	1.32	1.37
13	X4	201	CYC	C4D-ND	-3.40	1.32	1.37
13	J7	202	CYC	C4D-ND	-3.40	1.32	1.37
13	C6	201	CYC	C1B-C2B	-3.40	1.39	1.45
13	K1	201	CYC	C1B-NB	-3.39	1.32	1.37
13	M2	201	CYC	C4D-ND	-3.39	1.32	1.37
13	D6	201	CYC	C1B-NB	-3.39	1.32	1.37
13	a7	201	CYC	C1B-NB	-3.39	1.32	1.37
13	C1	201	CYC	C4D-ND	-3.39	1.32	1.37
13	J1	201	CYC	C1B-NB	-3.39	1.32	1.37
13	Z3	301	CYC	C4D-ND	-3.39	1.32	1.37
13	P6	201	CYC	C1B-NB	-3.39	1.32	1.37
13	L4	201	CYC	C1A-NA	-3.39	1.31	1.38
13	B4	201	CYC	C1B-NB	-3.39	1.32	1.37
13	V1	201	CYC	C4D-ND	-3.39	1.32	1.37
13	P4	201	CYC	C1B-NB	-3.39	1.32	1.37
13	y2	201	CYC	C1A-NA	-3.39	1.31	1.38
13	J4	201	CYC	C1B-C2B	-3.39	1.39	1.45
13	A2	202	CYC	C1B-C2B	-3.39	1.39	1.45
13	C4	201	CYC	C1B-C2B	-3.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e2	201	CYC	C1A-NA	-3.39	1.31	1.38
13	L4	201	CYC	C4D-ND	-3.39	1.32	1.37
13	z2	201	CYC	C1A-NA	-3.39	1.31	1.38
13	V4	202	CYC	C1B-C2B	-3.38	1.39	1.45
13	K6	201	CYC	C1B-NB	-3.38	1.32	1.37
13	B2	202	CYC	C4D-ND	-3.38	1.32	1.37
13	T6	201	CYC	C1B-NB	-3.38	1.32	1.37
13	V6	201	CYC	C4D-ND	-3.38	1.32	1.37
13	V3	202	CYC	C1B-C2B	-3.38	1.39	1.45
13	P3	201	CYC	C1B-NB	-3.38	1.32	1.37
13	Q1	201	CYC	C1B-C2B	-3.38	1.39	1.45
13	Z5	301	CYC	C1B-C2B	-3.38	1.39	1.45
13	n2	201	CYC	C4D-ND	-3.38	1.32	1.37
13	a3	202	CYC	C1B-C2B	-3.38	1.39	1.45
13	A6	301	CYC	C4D-ND	-3.38	1.32	1.37
13	32	302	CYC	C1B-C2B	-3.38	1.39	1.45
13	V2	201	CYC	C1B-NB	-3.38	1.32	1.37
13	P5	202	CYC	C1B-NB	-3.38	1.32	1.37
13	a7	202	CYC	C1B-C2B	-3.38	1.39	1.45
13	C1	201	CYC	C1B-NB	-3.38	1.32	1.37
13	L3	201	CYC	C1B-NB	-3.38	1.32	1.37
13	H6	201	CYC	C1B-NB	-3.38	1.32	1.37
13	P1	201	CYC	C1B-NB	-3.38	1.32	1.37
13	A1	301	CYC	C1B-NB	-3.38	1.32	1.37
13	T4	202	CYC	C1B-NB	-3.38	1.32	1.37
13	G5	201	CYC	C1B-NB	-3.38	1.32	1.37
13	M5	201	CYC	C4D-ND	-3.38	1.32	1.37
13	J5	201	CYC	C1B-C2B	-3.38	1.39	1.45
13	J4	202	CYC	C4D-ND	-3.37	1.32	1.37
13	V4	201	CYC	C1B-NB	-3.37	1.32	1.37
13	P3	202	CYC	C1B-NB	-3.37	1.32	1.37
13	P6	202	CYC	C1B-NB	-3.37	1.32	1.37
13	V5	202	CYC	C1B-C2B	-3.37	1.39	1.45
13	E4	201	CYC	C4D-ND	-3.37	1.32	1.37
13	H4	201	CYC	C1B-NB	-3.37	1.32	1.37
13	J6	202	CYC	C1B-C2B	-3.37	1.39	1.45
13	J5	202	CYC	C4D-ND	-3.37	1.32	1.37
13	P3	201	CYC	C1B-C2B	-3.37	1.39	1.45
13	N6	201	CYC	C1B-NB	-3.37	1.32	1.37
13	S1	201	CYC	C1B-NB	-3.37	1.32	1.37
13	L3	201	CYC	C1A-NA	-3.37	1.31	1.38
13	G4	201	CYC	C1B-NB	-3.37	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P7	201	CYC	C1B-C2B	-3.37	1.39	1.45
13	T4	201	CYC	C1B-NB	-3.37	1.32	1.37
13	C6	201	CYC	C1B-NB	-3.37	1.32	1.37
13	P7	201	CYC	C1B-NB	-3.37	1.32	1.37
13	42	301	CYC	C1B-NB	-3.37	1.32	1.37
13	Q6	201	CYC	C1B-C2B	-3.36	1.39	1.45
13	G2	201	CYC	C1A-NA	-3.36	1.31	1.38
13	T1	201	CYC	C1B-NB	-3.36	1.32	1.37
13	Z5	301	CYC	C4D-ND	-3.36	1.32	1.37
13	J6	202	CYC	C1B-NB	-3.36	1.32	1.37
13	h2	201	CYC	C1A-NA	-3.36	1.31	1.38
13	52	301	CYC	C4D-ND	-3.36	1.32	1.37
13	Q2	201	CYC	C1B-NB	-3.36	1.32	1.37
13	J1	201	CYC	C4D-ND	-3.36	1.32	1.37
13	B6	201	CYC	C1B-NB	-3.36	1.32	1.37
13	C1	201	CYC	C1B-C2B	-3.36	1.39	1.45
13	T6	202	CYC	C1B-NB	-3.36	1.32	1.37
13	E6	201	CYC	C4D-ND	-3.36	1.32	1.37
13	D1	201	CYC	C1B-NB	-3.36	1.32	1.37
13	M6	201	CYC	C1B-C2B	-3.36	1.39	1.45
13	J1	202	CYC	C1B-C2B	-3.36	1.39	1.45
13	C7	202	CYC	C1B-C2B	-3.36	1.39	1.45
13	T3	201	CYC	C1B-NB	-3.36	1.32	1.37
13	Z4	301	CYC	C4D-ND	-3.36	1.32	1.37
13	a6	202	CYC	C1B-C2B	-3.36	1.39	1.45
13	d2	201	CYC	C1B-C2B	-3.36	1.39	1.45
13	X4	201	CYC	C1A-NA	-3.35	1.31	1.38
13	32	301	CYC	C1B-NB	-3.35	1.32	1.37
13	C4	201	CYC	C1B-NB	-3.35	1.32	1.37
13	I6	201	CYC	C1B-NB	-3.35	1.32	1.37
13	x2	201	CYC	C1B-C2B	-3.35	1.39	1.45
13	l2	201	CYC	C1A-NA	-3.35	1.31	1.38
13	D5	201	CYC	C1B-NB	-3.35	1.32	1.37
13	T7	201	CYC	C1B-NB	-3.35	1.32	1.37
13	C3	202	CYC	C1B-C2B	-3.35	1.39	1.45
13	T5	202	CYC	C1B-NB	-3.35	1.32	1.37
13	a5	202	CYC	C1B-NB	-3.35	1.32	1.37
13	P7	202	CYC	C1B-NB	-3.35	1.32	1.37
13	C5	201	CYC	C1B-C2B	-3.35	1.39	1.45
13	s2	201	CYC	C4D-ND	-3.35	1.32	1.37
13	T6	201	CYC	C4D-ND	-3.35	1.32	1.37
13	l2	201	CYC	C4D-ND	-3.35	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	p2	201	CYC	C1A-NA	-3.35	1.31	1.38
13	Q5	201	CYC	C1B-C2B	-3.34	1.39	1.45
13	a6	202	CYC	C1B-NB	-3.34	1.32	1.37
13	C4	201	CYC	C4D-ND	-3.34	1.32	1.37
13	S5	201	CYC	C1B-NB	-3.34	1.32	1.37
13	C6	202	CYC	C1B-NB	-3.34	1.32	1.37
13	J5	202	CYC	C1B-NB	-3.34	1.32	1.37
13	E1	201	CYC	C1B-NB	-3.34	1.32	1.37
13	K3	201	CYC	C1B-NB	-3.34	1.32	1.37
13	N5	201	CYC	C1B-NB	-3.34	1.32	1.37
13	L7	201	CYC	C1A-NA	-3.34	1.31	1.38
13	r2	201	CYC	C1A-NA	-3.34	1.31	1.38
13	V5	201	CYC	C1B-NB	-3.34	1.32	1.37
13	Z6	301	CYC	C4D-ND	-3.34	1.32	1.37
13	D6	201	CYC	C1B-C2B	-3.34	1.39	1.45
13	22	301	CYC	C4D-ND	-3.34	1.32	1.37
13	J3	202	CYC	C4D-ND	-3.34	1.32	1.37
13	C7	201	CYC	C1B-C2B	-3.34	1.39	1.45
13	J4	201	CYC	C1B-NB	-3.34	1.32	1.37
13	L7	201	CYC	C1B-NB	-3.34	1.32	1.37
13	Q4	201	CYC	C1B-NB	-3.34	1.32	1.37
13	X6	201	CYC	C1A-NA	-3.34	1.31	1.38
13	B3	201	CYC	C1B-NB	-3.34	1.32	1.37
13	M2	201	CYC	C1A-NA	-3.34	1.31	1.38
13	W6	201	CYC	C1B-NB	-3.34	1.32	1.37
13	S6	201	CYC	C1B-NB	-3.34	1.32	1.37
13	C3	201	CYC	C1B-NB	-3.33	1.32	1.37
13	V4	201	CYC	C4D-ND	-3.33	1.32	1.37
13	22	302	CYC	C1B-C2B	-3.33	1.39	1.45
13	Q6	202	CYC	C1B-NB	-3.33	1.32	1.37
13	Q3	201	CYC	C1B-NB	-3.33	1.32	1.37
13	F2	201	CYC	C1A-NA	-3.33	1.31	1.38
13	J1	202	CYC	C4D-ND	-3.33	1.32	1.37
13	D4	201	CYC	C1B-NB	-3.33	1.32	1.37
13	l2	201	CYC	C1B-NB	-3.33	1.32	1.37
13	M3	201	CYC	C4D-ND	-3.33	1.32	1.37
13	E5	201	CYC	C1B-NB	-3.33	1.32	1.37
13	42	302	CYC	C1B-C2B	-3.33	1.39	1.45
13	R2	201	CYC	C4D-ND	-3.33	1.32	1.37
13	V2	201	CYC	C4D-ND	-3.33	1.32	1.37
13	V3	202	CYC	C4D-ND	-3.33	1.32	1.37
13	T1	202	CYC	C1B-NB	-3.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D3	201	CYC	C1B-C2B	-3.33	1.39	1.45
13	R1	201	CYC	C1B-NB	-3.33	1.32	1.37
13	52	302	CYC	C1B-C2B	-3.33	1.39	1.45
13	Q1	202	CYC	C1B-NB	-3.33	1.32	1.37
13	A2	202	CYC	C1B-NB	-3.33	1.32	1.37
13	I5	201	CYC	C1B-NB	-3.33	1.32	1.37
13	C7	202	CYC	C1B-NB	-3.33	1.32	1.37
13	L6	201	CYC	C1A-NA	-3.33	1.31	1.38
13	R5	201	CYC	C1B-NB	-3.33	1.32	1.37
13	a3	202	CYC	C1B-NB	-3.33	1.32	1.37
13	B2	201	CYC	C1B-C2B	-3.33	1.39	1.45
13	c2	801	CYC	C1B-NB	-3.32	1.32	1.37
13	A1	301	CYC	C4D-ND	-3.32	1.32	1.37
13	E4	201	CYC	C1B-NB	-3.32	1.32	1.37
13	M6	201	CYC	C1B-NB	-3.32	1.32	1.37
13	Q4	202	CYC	C1B-C2B	-3.32	1.39	1.45
13	W3	201	CYC	C1B-NB	-3.32	1.32	1.37
13	a1	202	CYC	C1B-NB	-3.32	1.32	1.37
13	a4	202	CYC	C1B-NB	-3.32	1.32	1.37
13	F6	202	CYC	C1B-NB	-3.32	1.32	1.37
13	S4	201	CYC	C1B-NB	-3.32	1.32	1.37
13	V5	201	CYC	C4D-ND	-3.32	1.32	1.37
13	T5	201	CYC	C1B-NB	-3.32	1.32	1.37
13	Q4	201	CYC	C1B-C2B	-3.32	1.39	1.45
13	A6	302	CYC	C1B-C2B	-3.32	1.39	1.45
13	M3	201	CYC	C1B-NB	-3.32	1.32	1.37
13	U6	201	CYC	C1B-NB	-3.32	1.32	1.37
13	I1	201	CYC	C1B-NB	-3.32	1.32	1.37
13	Q7	201	CYC	C1B-C2B	-3.32	1.39	1.45
13	J1	202	CYC	C1B-NB	-3.32	1.32	1.37
13	V6	202	CYC	C1B-NB	-3.32	1.32	1.37
13	a1	201	CYC	C1B-C2B	-3.32	1.39	1.45
13	Z4	301	CYC	C1B-C2B	-3.32	1.39	1.45
13	E2	201	CYC	C1A-NA	-3.32	1.31	1.38
13	V3	201	CYC	C1B-NB	-3.32	1.32	1.37
13	X1	201	CYC	C1A-NA	-3.32	1.31	1.38
13	Q1	201	CYC	C1B-NB	-3.32	1.32	1.37
13	G3	201	CYC	C1B-NB	-3.32	1.32	1.37
13	E6	201	CYC	C1B-NB	-3.32	1.32	1.37
13	F3	201	CYC	C1B-NB	-3.32	1.32	1.37
13	K4	201	CYC	C1B-NB	-3.31	1.32	1.37
13	C3	201	CYC	C1B-C2B	-3.31	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z6	301	CYC	C1B-C2B	-3.31	1.39	1.45
13	N2	801	CYC	C4D-ND	-3.31	1.32	1.37
13	N4	201	CYC	C1B-NB	-3.31	1.32	1.37
13	F5	201	CYC	C1B-NB	-3.31	1.32	1.37
13	Q3	201	CYC	C1B-C2B	-3.31	1.39	1.45
13	a7	201	CYC	C4D-ND	-3.31	1.32	1.37
13	I4	201	CYC	C1B-NB	-3.31	1.32	1.37
13	R3	201	CYC	C1B-NB	-3.31	1.32	1.37
13	J5	201	CYC	C4D-ND	-3.31	1.32	1.37
13	W7	201	CYC	C1B-NB	-3.31	1.32	1.37
13	C1	202	CYC	C1B-NB	-3.31	1.32	1.37
13	e2	201	CYC	C4D-ND	-3.31	1.32	1.37
13	W2	201	CYC	C1B-NB	-3.31	1.32	1.37
13	T3	201	CYC	C4D-ND	-3.31	1.32	1.37
13	M1	201	CYC	C1B-C2B	-3.31	1.39	1.45
13	F5	201	CYC	C1D-ND	-3.31	1.32	1.37
13	a6	202	CYC	C1D-ND	-3.31	1.32	1.37
13	U5	201	CYC	C1B-NB	-3.31	1.32	1.37
13	M7	201	CYC	C4D-ND	-3.31	1.32	1.37
13	E7	201	CYC	C1B-NB	-3.31	1.32	1.37
13	K7	201	CYC	C1B-NB	-3.31	1.32	1.37
13	g2	201	CYC	C1A-NA	-3.31	1.31	1.38
13	C3	202	CYC	C1B-NB	-3.31	1.32	1.37
13	U4	201	CYC	C1B-NB	-3.31	1.32	1.37
13	J4	202	CYC	C1B-NB	-3.31	1.32	1.37
13	C7	201	CYC	C1B-NB	-3.31	1.32	1.37
13	Q5	201	CYC	C1B-NB	-3.30	1.32	1.37
13	E3	201	CYC	C1B-NB	-3.30	1.32	1.37
13	N2	802	CYC	C1D-ND	-3.30	1.32	1.37
13	m2	201	CYC	C4D-ND	-3.30	1.32	1.37
13	X2	201	CYC	C1A-NA	-3.30	1.31	1.38
13	E5	201	CYC	C4D-ND	-3.30	1.32	1.37
13	V7	201	CYC	C4D-ND	-3.30	1.32	1.37
13	R2	201	CYC	C1A-NA	-3.30	1.31	1.38
13	H3	201	CYC	C1B-NB	-3.30	1.32	1.37
13	E2	201	CYC	C4D-ND	-3.30	1.32	1.37
13	N2	802	CYC	C4D-ND	-3.30	1.32	1.37
13	W2	201	CYC	C1B-C2B	-3.30	1.39	1.45
13	V7	201	CYC	C1B-NB	-3.30	1.32	1.37
13	a7	202	CYC	C1B-NB	-3.30	1.32	1.37
13	A6	301	CYC	C1A-NA	-3.30	1.31	1.38
13	E6	201	CYC	C1A-NA	-3.30	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R4	201	CYC	C1B-NB	-3.30	1.32	1.37
13	M1	201	CYC	C1B-NB	-3.30	1.32	1.37
13	F1	202	CYC	C1B-NB	-3.30	1.32	1.37
13	r2	201	CYC	C4D-ND	-3.30	1.32	1.37
13	32	301	CYC	C1A-NA	-3.30	1.31	1.38
13	Q7	201	CYC	C1B-NB	-3.30	1.32	1.37
13	A2	201	CYC	C1B-NB	-3.30	1.32	1.37
13	Q1	202	CYC	C1B-C2B	-3.29	1.39	1.45
13	M7	201	CYC	C1B-C2B	-3.29	1.39	1.45
13	D2	201	CYC	C1A-NA	-3.29	1.31	1.38
13	Q6	201	CYC	C1B-NB	-3.29	1.32	1.37
13	M7	201	CYC	C1B-NB	-3.29	1.32	1.37
13	k2	201	CYC	C1B-NB	-3.29	1.32	1.37
13	T5	201	CYC	C4D-ND	-3.29	1.32	1.37
13	R7	201	CYC	C1B-NB	-3.29	1.32	1.37
13	A2	201	CYC	C1B-C2B	-3.29	1.39	1.45
13	C7	201	CYC	C4D-ND	-3.29	1.32	1.37
13	Q6	202	CYC	C1B-C2B	-3.29	1.39	1.45
13	v2	201	CYC	C4D-ND	-3.29	1.32	1.37
13	F7	201	CYC	C1B-NB	-3.29	1.32	1.37
13	Q4	202	CYC	C1B-NB	-3.29	1.32	1.37
13	s2	201	CYC	C1A-NA	-3.29	1.31	1.38
13	Q5	202	CYC	C1B-NB	-3.29	1.32	1.37
13	l2	201	CYC	C1D-ND	-3.29	1.32	1.37
13	a3	202	CYC	C1D-ND	-3.29	1.32	1.37
13	U1	201	CYC	C1B-NB	-3.29	1.32	1.37
13	C3	201	CYC	C4D-ND	-3.29	1.32	1.37
13	Z5	301	CYC	C1A-NA	-3.29	1.31	1.38
13	L1	201	CYC	C1A-NA	-3.29	1.31	1.38
13	F4	201	CYC	C1B-NB	-3.29	1.32	1.37
13	K1	201	CYC	C1A-NA	-3.29	1.31	1.38
13	Q3	202	CYC	C1B-NB	-3.29	1.32	1.37
13	E7	201	CYC	C1D-ND	-3.29	1.32	1.37
13	x2	201	CYC	C1B-NB	-3.28	1.32	1.37
13	S3	201	CYC	C1B-NB	-3.28	1.32	1.37
13	A1	302	CYC	C1B-C2B	-3.28	1.39	1.45
13	32	301	CYC	C4D-ND	-3.28	1.32	1.37
13	C5	202	CYC	C1B-NB	-3.28	1.32	1.37
13	G7	201	CYC	C1B-NB	-3.28	1.32	1.37
13	X3	201	CYC	C1A-NA	-3.28	1.31	1.38
13	X5	201	CYC	C1A-NA	-3.28	1.31	1.38
13	T4	201	CYC	C4D-ND	-3.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m2	201	CYC	C1A-NA	-3.28	1.31	1.38
13	M4	201	CYC	C1B-NB	-3.28	1.32	1.37
13	C5	201	CYC	C4D-ND	-3.28	1.32	1.37
13	D7	201	CYC	C1B-NB	-3.28	1.32	1.37
13	Z1	301	CYC	C1A-NA	-3.28	1.31	1.38
13	V1	202	CYC	C1B-NB	-3.28	1.32	1.37
13	R6	201	CYC	C1B-NB	-3.28	1.32	1.37
13	a6	201	CYC	C1B-C2B	-3.28	1.39	1.45
13	i2	201	CYC	C1B-NB	-3.28	1.32	1.37
13	C4	202	CYC	C1B-NB	-3.28	1.32	1.37
13	J5	201	CYC	C1B-NB	-3.28	1.32	1.37
13	52	301	CYC	C1A-NA	-3.28	1.31	1.38
13	V7	202	CYC	C4D-ND	-3.28	1.32	1.37
13	I3	201	CYC	C1B-NB	-3.27	1.32	1.37
13	V1	202	CYC	C4D-ND	-3.27	1.32	1.37
13	d2	201	CYC	C1B-NB	-3.27	1.32	1.37
13	U7	201	CYC	C1B-NB	-3.27	1.32	1.37
13	E3	201	CYC	C4D-ND	-3.27	1.32	1.37
13	Z7	301	CYC	C1B-C2B	-3.27	1.39	1.45
13	W4	201	CYC	C1B-NB	-3.27	1.32	1.37
13	T7	202	CYC	C1B-NB	-3.27	1.32	1.37
13	Z3	301	CYC	C1B-C2B	-3.27	1.39	1.45
13	M5	201	CYC	C1B-C2B	-3.27	1.39	1.45
13	F4	202	CYC	C1B-NB	-3.27	1.32	1.37
13	J3	201	CYC	C1B-NB	-3.27	1.32	1.37
13	a7	202	CYC	C1D-ND	-3.27	1.32	1.37
13	F5	202	CYC	C1B-NB	-3.27	1.32	1.37
13	M5	201	CYC	C1B-NB	-3.27	1.32	1.37
13	B7	201	CYC	C1B-NB	-3.27	1.32	1.37
13	a2	201	CYC	C1B-NB	-3.27	1.32	1.37
13	H7	201	CYC	C1B-NB	-3.27	1.32	1.37
13	Q2	201	CYC	C1A-NA	-3.27	1.31	1.38
13	i2	201	CYC	C1B-C2B	-3.27	1.39	1.45
13	K5	201	CYC	C1A-NA	-3.27	1.31	1.38
13	a1	202	CYC	C1D-ND	-3.27	1.32	1.37
13	Q5	202	CYC	C1B-C2B	-3.26	1.39	1.45
13	N7	201	CYC	C1B-NB	-3.26	1.32	1.37
13	22	301	CYC	C1A-NA	-3.26	1.31	1.38
13	T3	202	CYC	C1B-NB	-3.26	1.32	1.37
13	A1	301	CYC	C1A-NA	-3.26	1.31	1.38
13	X7	201	CYC	C1A-NA	-3.26	1.31	1.38
13	J6	201	CYC	C4D-ND	-3.26	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M4	201	CYC	C1B-C2B	-3.26	1.39	1.45
13	a5	201	CYC	C1B-C2B	-3.26	1.39	1.45
13	T6	201	CYC	C1A-NA	-3.26	1.31	1.38
13	N5	201	CYC	C1A-NA	-3.26	1.31	1.38
13	J7	202	CYC	C1B-NB	-3.26	1.32	1.37
13	T7	201	CYC	C4D-ND	-3.26	1.32	1.37
13	V3	201	CYC	C4D-ND	-3.26	1.32	1.37
13	M3	201	CYC	C1B-C2B	-3.26	1.39	1.45
13	X6	201	CYC	C1B-C2B	-3.26	1.39	1.45
13	V5	202	CYC	C1B-NB	-3.25	1.32	1.37
13	Q3	202	CYC	C1B-C2B	-3.25	1.39	1.45
13	w2	201	CYC	C1A-NA	-3.25	1.31	1.38
13	N3	201	CYC	C1B-NB	-3.25	1.32	1.37
13	X3	201	CYC	C1B-C2B	-3.25	1.39	1.45
13	B2	201	CYC	C4D-ND	-3.25	1.32	1.37
13	F7	202	CYC	C1B-NB	-3.25	1.32	1.37
13	S7	201	CYC	C1B-NB	-3.25	1.32	1.37
13	G1	201	CYC	C1A-NA	-3.25	1.31	1.38
13	L2	201	CYC	C4D-ND	-3.25	1.32	1.37
13	F6	201	CYC	C1D-ND	-3.25	1.32	1.37
13	O2	201	CYC	C1A-NA	-3.25	1.31	1.38
13	Q7	202	CYC	C1B-NB	-3.25	1.32	1.37
13	N1	201	CYC	C1A-NA	-3.25	1.31	1.38
13	H5	201	CYC	C1A-NA	-3.25	1.31	1.38
13	A1	301	CYC	C1B-C2B	-3.25	1.39	1.45
13	a7	201	CYC	C1B-C2B	-3.25	1.39	1.45
13	N2	801	CYC	C1A-NA	-3.25	1.31	1.38
13	J3	202	CYC	C1B-NB	-3.25	1.32	1.37
13	N6	201	CYC	C1A-NA	-3.24	1.31	1.38
13	F1	201	CYC	C1D-ND	-3.24	1.32	1.37
13	J7	201	CYC	C1B-NB	-3.24	1.32	1.37
13	J4	201	CYC	C4D-ND	-3.24	1.32	1.37
13	V7	202	CYC	C1B-NB	-3.24	1.32	1.37
13	h2	201	CYC	C4D-ND	-3.24	1.32	1.37
13	D3	201	CYC	C4D-ND	-3.24	1.32	1.37
13	X7	201	CYC	C1B-C2B	-3.24	1.39	1.45
13	a5	202	CYC	C1D-ND	-3.24	1.32	1.37
13	T5	201	CYC	C1A-NA	-3.24	1.31	1.38
13	F2	201	CYC	C4D-ND	-3.24	1.32	1.37
13	Z7	301	CYC	C4D-ND	-3.24	1.32	1.37
13	T4	201	CYC	C1A-NA	-3.24	1.31	1.38
13	P3	202	CYC	C4D-ND	-3.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J6	202	CYC	C1D-ND	-3.23	1.32	1.37
13	E7	201	CYC	C4D-ND	-3.23	1.32	1.37
13	a5	201	CYC	C1A-NA	-3.23	1.31	1.38
13	V2	201	CYC	C1A-NA	-3.23	1.31	1.38
13	B2	201	CYC	C1B-NB	-3.23	1.32	1.37
13	T1	201	CYC	C1A-NA	-3.23	1.31	1.38
13	F5	201	CYC	C1A-NA	-3.23	1.31	1.38
13	V5	202	CYC	C4D-ND	-3.23	1.32	1.37
13	J7	201	CYC	C4D-ND	-3.23	1.32	1.37
13	Q7	202	CYC	C1B-C2B	-3.23	1.39	1.45
13	J3	201	CYC	C4D-ND	-3.23	1.32	1.37
13	D7	201	CYC	C1B-C2B	-3.23	1.39	1.45
13	V6	202	CYC	C4D-ND	-3.23	1.32	1.37
13	X1	201	CYC	C1B-C2B	-3.23	1.39	1.45
13	B1	201	CYC	C1A-NA	-3.22	1.31	1.38
13	F3	202	CYC	C1B-NB	-3.22	1.32	1.37
13	X5	201	CYC	C1B-C2B	-3.22	1.39	1.45
13	G4	201	CYC	C1A-NA	-3.22	1.31	1.38
13	32	301	CYC	C1B-C2B	-3.22	1.39	1.45
13	X4	201	CYC	C1B-C2B	-3.22	1.39	1.45
13	I7	201	CYC	C1B-NB	-3.22	1.32	1.37
13	H1	201	CYC	C1A-NA	-3.22	1.31	1.38
13	E2	201	CYC	C1D-ND	-3.22	1.32	1.37
13	Z4	301	CYC	C1A-NA	-3.22	1.31	1.38
13	J1	201	CYC	C1A-NA	-3.22	1.31	1.38
13	a4	202	CYC	C1D-ND	-3.21	1.32	1.37
13	B5	201	CYC	C1A-NA	-3.21	1.31	1.38
13	k2	201	CYC	C1D-ND	-3.21	1.32	1.37
13	U3	201	CYC	C1B-NB	-3.21	1.32	1.37
13	I1	201	CYC	C1A-NA	-3.21	1.31	1.38
13	e2	201	CYC	C1D-ND	-3.21	1.32	1.37
13	j2	201	CYC	C1B-NB	-3.21	1.32	1.37
13	V3	202	CYC	C1B-NB	-3.21	1.32	1.37
13	V4	202	CYC	C1B-NB	-3.21	1.32	1.37
13	a3	201	CYC	C1B-C2B	-3.21	1.39	1.45
13	Z3	301	CYC	C1D-ND	-3.21	1.32	1.37
13	A6	301	CYC	C1B-C2B	-3.21	1.39	1.45
13	H2	201	CYC	C1B-NB	-3.21	1.32	1.37
13	42	301	CYC	C1A-NA	-3.21	1.31	1.38
13	a5	202	CYC	C1A-NA	-3.21	1.31	1.38
13	B4	201	CYC	C1A-NA	-3.21	1.31	1.38
13	I6	201	CYC	C4D-ND	-3.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E3	201	CYC	C1D-ND	-3.20	1.32	1.37
13	D6	201	CYC	C1A-NA	-3.20	1.31	1.38
13	H6	201	CYC	C1A-NA	-3.20	1.31	1.38
13	a1	201	CYC	C1A-NA	-3.20	1.31	1.38
13	A1	302	CYC	C1A-NA	-3.20	1.31	1.38
13	V4	202	CYC	C4D-ND	-3.20	1.32	1.37
13	F4	201	CYC	C1D-ND	-3.20	1.32	1.37
13	P7	201	CYC	C4D-ND	-3.20	1.32	1.37
13	D3	201	CYC	C1B-NB	-3.20	1.32	1.37
13	a1	202	CYC	C1A-NA	-3.20	1.31	1.38
13	B6	201	CYC	C1A-NA	-3.20	1.31	1.38
13	G5	201	CYC	C1A-NA	-3.20	1.31	1.38
13	Z6	301	CYC	C1A-NA	-3.20	1.31	1.38
13	V1	202	CYC	C1A-NA	-3.20	1.31	1.38
13	p2	201	CYC	C4D-ND	-3.20	1.32	1.37
13	E4	201	CYC	C1D-ND	-3.20	1.32	1.37
13	W5	201	CYC	C1A-NA	-3.20	1.31	1.38
13	H4	201	CYC	C1A-NA	-3.19	1.31	1.38
13	a4	202	CYC	C1A-NA	-3.19	1.31	1.38
13	E7	201	CYC	C1A-NA	-3.19	1.31	1.38
13	Q7	201	CYC	C4D-ND	-3.19	1.32	1.37
13	52	302	CYC	C4D-ND	-3.19	1.32	1.37
13	C5	202	CYC	C1A-NA	-3.19	1.31	1.38
13	42	301	CYC	C1B-C2B	-3.19	1.39	1.45
13	T1	201	CYC	C1D-ND	-3.19	1.32	1.37
13	D1	201	CYC	C1D-ND	-3.19	1.32	1.37
13	A1	302	CYC	C4D-ND	-3.19	1.32	1.37
13	E6	201	CYC	C1D-ND	-3.19	1.32	1.37
13	E1	201	CYC	C1A-NA	-3.19	1.31	1.38
13	y2	201	CYC	C4D-ND	-3.19	1.32	1.37
13	a2	201	CYC	C1D-ND	-3.19	1.32	1.37
13	C5	201	CYC	C1A-NA	-3.19	1.31	1.38
13	E5	201	CYC	C1A-NA	-3.19	1.31	1.38
13	J6	201	CYC	C1A-NA	-3.19	1.31	1.38
13	E3	201	CYC	C1A-NA	-3.18	1.31	1.38
13	W6	201	CYC	C1A-NA	-3.18	1.31	1.38
13	E4	201	CYC	C1A-NA	-3.18	1.31	1.38
13	C1	202	CYC	C1A-NA	-3.18	1.31	1.38
13	D5	201	CYC	C1D-ND	-3.18	1.32	1.37
13	P6	201	CYC	C4D-ND	-3.18	1.32	1.37
13	U2	201	CYC	C1D-ND	-3.18	1.32	1.37
13	P7	202	CYC	C4D-ND	-3.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N4	201	CYC	C1A-NA	-3.18	1.31	1.38
13	F1	201	CYC	C1A-NA	-3.18	1.31	1.38
13	B2	202	CYC	C1B-NB	-3.18	1.32	1.37
13	C7	202	CYC	C1D-ND	-3.18	1.32	1.37
13	a6	202	CYC	C1A-NA	-3.17	1.31	1.38
13	E5	201	CYC	C1D-ND	-3.17	1.32	1.37
13	A1	302	CYC	C1B-NB	-3.17	1.32	1.37
13	P1	201	CYC	C4D-ND	-3.17	1.32	1.37
13	E1	201	CYC	C1D-ND	-3.17	1.32	1.37
13	C4	201	CYC	C1A-NA	-3.17	1.31	1.38
13	G6	201	CYC	C1A-NA	-3.17	1.31	1.38
13	D2	201	CYC	C4D-ND	-3.17	1.32	1.37
13	52	301	CYC	C1B-C2B	-3.17	1.39	1.45
13	s2	201	CYC	C1D-ND	-3.17	1.32	1.37
13	C3	201	CYC	C1A-NA	-3.17	1.31	1.38
13	F6	201	CYC	C1A-NA	-3.17	1.31	1.38
13	g2	201	CYC	C1D-ND	-3.17	1.32	1.37
13	22	301	CYC	C1B-C2B	-3.17	1.39	1.45
13	A2	201	CYC	C1A-NA	-3.16	1.31	1.38
13	w2	201	CYC	C4D-ND	-3.16	1.32	1.37
13	B1	201	CYC	C4D-ND	-3.16	1.32	1.37
13	H1	201	CYC	C4D-ND	-3.16	1.32	1.37
13	j2	201	CYC	C4D-ND	-3.16	1.32	1.37
13	C3	202	CYC	C1A-NA	-3.16	1.31	1.38
13	C6	201	CYC	C1A-NA	-3.16	1.31	1.38
13	Q3	201	CYC	C4D-ND	-3.16	1.32	1.37
13	Z7	301	CYC	C1D-ND	-3.16	1.32	1.37
13	Q4	201	CYC	C4D-ND	-3.16	1.32	1.37
13	L2	201	CYC	C1A-NA	-3.16	1.31	1.38
13	C2	201	CYC	C1B-NB	-3.16	1.32	1.37
13	I1	201	CYC	C4D-ND	-3.16	1.32	1.37
13	I4	201	CYC	C4D-ND	-3.16	1.32	1.37
13	W3	201	CYC	C4D-ND	-3.15	1.32	1.37
13	P3	201	CYC	C4D-ND	-3.15	1.32	1.37
13	I5	201	CYC	C1A-NA	-3.15	1.31	1.38
13	K3	201	CYC	C1A-NA	-3.15	1.31	1.38
13	z2	201	CYC	C4D-ND	-3.15	1.32	1.37
13	52	302	CYC	C1A-NA	-3.15	1.31	1.38
13	a3	202	CYC	C1A-NA	-3.15	1.31	1.38
13	W1	201	CYC	C1A-NA	-3.15	1.31	1.38
13	D1	201	CYC	C1A-NA	-3.15	1.31	1.38
13	A6	302	CYC	C1A-NA	-3.15	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T4	201	CYC	C1D-ND	-3.15	1.32	1.37
13	R1	201	CYC	C4D-ND	-3.15	1.32	1.37
13	22	302	CYC	C4D-ND	-3.15	1.32	1.37
13	A2	201	CYC	C1D-ND	-3.15	1.32	1.37
13	C1	201	CYC	C1A-NA	-3.15	1.31	1.38
13	f2	201	CYC	C1D-ND	-3.15	1.32	1.37
13	A2	202	CYC	C4D-ND	-3.14	1.32	1.37
13	C6	202	CYC	C1A-NA	-3.14	1.31	1.38
13	a6	201	CYC	C1A-NA	-3.14	1.31	1.38
13	X2	201	CYC	C1D-ND	-3.14	1.32	1.37
13	t2	201	CYC	C1D-ND	-3.14	1.32	1.37
13	A6	302	CYC	C4D-ND	-3.14	1.32	1.37
13	P5	201	CYC	C1A-NA	-3.14	1.31	1.38
13	G5	201	CYC	C4D-ND	-3.14	1.32	1.37
13	S1	201	CYC	C1A-NA	-3.14	1.31	1.38
13	C4	202	CYC	C1A-NA	-3.14	1.31	1.38
13	k2	201	CYC	C4D-ND	-3.14	1.32	1.37
13	F5	202	CYC	C1A-NA	-3.14	1.31	1.38
13	B2	201	CYC	C1A-NA	-3.14	1.31	1.38
13	F4	202	CYC	C1A-NA	-3.13	1.31	1.38
13	B2	202	CYC	C1D-ND	-3.13	1.32	1.37
13	g2	201	CYC	C4D-ND	-3.13	1.32	1.37
13	F4	201	CYC	C1A-NA	-3.13	1.31	1.38
13	U5	201	CYC	C1A-NA	-3.13	1.31	1.38
13	Q3	201	CYC	C1D-ND	-3.13	1.32	1.37
13	K6	201	CYC	C1A-NA	-3.13	1.31	1.38
13	C7	202	CYC	C1A-NA	-3.13	1.31	1.38
13	F1	201	CYC	C4D-ND	-3.13	1.32	1.37
13	G3	201	CYC	C1A-NA	-3.13	1.31	1.38
13	W4	201	CYC	C1A-NA	-3.13	1.31	1.38
13	F3	202	CYC	C4D-ND	-3.13	1.32	1.37
13	J7	202	CYC	C1D-ND	-3.13	1.32	1.37
13	F6	202	CYC	C1A-NA	-3.13	1.31	1.38
13	32	302	CYC	C4D-ND	-3.13	1.32	1.37
13	42	302	CYC	C1A-NA	-3.13	1.31	1.38
13	M6	201	CYC	C1A-NA	-3.13	1.31	1.38
13	V6	202	CYC	C1A-NA	-3.13	1.31	1.38
13	O2	201	CYC	C4D-ND	-3.13	1.32	1.37
13	V5	202	CYC	C1A-NA	-3.13	1.31	1.38
13	T5	201	CYC	C1D-ND	-3.13	1.32	1.37
13	a2	201	CYC	C1A-NA	-3.13	1.31	1.38
13	J3	202	CYC	C1A-NA	-3.13	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B6	201	CYC	C4D-ND	-3.13	1.32	1.37
13	T3	201	CYC	C1A-NA	-3.12	1.31	1.38
13	Z3	301	CYC	C1A-NA	-3.12	1.31	1.38
13	T7	201	CYC	C1A-NA	-3.12	1.31	1.38
13	W7	201	CYC	C4D-ND	-3.12	1.32	1.37
13	I6	201	CYC	C1A-NA	-3.12	1.31	1.38
13	A2	202	CYC	C1D-ND	-3.12	1.32	1.37
13	J3	202	CYC	C1D-ND	-3.12	1.32	1.37
13	Q7	201	CYC	C1D-ND	-3.12	1.32	1.37
13	T7	201	CYC	C1D-ND	-3.12	1.32	1.37
13	J1	202	CYC	C1A-NA	-3.12	1.32	1.38
13	N1	201	CYC	C4D-ND	-3.12	1.32	1.37
13	I4	201	CYC	C1A-NA	-3.12	1.32	1.38
13	V4	202	CYC	C1A-NA	-3.12	1.32	1.38
13	R5	201	CYC	C1A-NA	-3.12	1.32	1.38
13	W1	201	CYC	C4D-ND	-3.12	1.32	1.37
13	z2	201	CYC	C1D-ND	-3.12	1.32	1.37
13	22	302	CYC	C1B-NB	-3.12	1.32	1.37
13	i2	201	CYC	C1D-ND	-3.12	1.32	1.37
13	S4	201	CYC	C1A-NA	-3.12	1.32	1.38
13	y2	201	CYC	C1D-ND	-3.12	1.32	1.37
13	B3	201	CYC	C1A-NA	-3.11	1.32	1.38
13	U6	201	CYC	C1A-NA	-3.11	1.32	1.38
13	W2	201	CYC	C4D-ND	-3.11	1.32	1.37
13	B2	202	CYC	C4A-C3A	-3.11	1.39	1.45
13	S3	201	CYC	C1A-NA	-3.11	1.32	1.38
13	Z7	301	CYC	C1A-NA	-3.11	1.32	1.38
13	G2	201	CYC	C4D-ND	-3.11	1.32	1.37
13	F5	202	CYC	C4D-ND	-3.11	1.32	1.37
13	T6	202	CYC	C1A-NA	-3.11	1.32	1.38
13	a7	202	CYC	C1A-NA	-3.11	1.32	1.38
13	I5	201	CYC	C4D-ND	-3.11	1.32	1.37
13	D5	201	CYC	C1A-NA	-3.11	1.32	1.38
13	R1	201	CYC	C1A-NA	-3.11	1.32	1.38
13	R4	201	CYC	C1A-NA	-3.11	1.32	1.38
13	J5	201	CYC	C1A-NA	-3.11	1.32	1.38
13	J5	202	CYC	C1A-NA	-3.11	1.32	1.38
13	Q5	201	CYC	C4D-ND	-3.11	1.32	1.37
13	J4	202	CYC	C1D-ND	-3.11	1.32	1.37
13	Q6	201	CYC	C4D-ND	-3.11	1.32	1.37
13	T1	202	CYC	C1A-NA	-3.11	1.32	1.38
13	B4	201	CYC	C4D-ND	-3.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F5	202	CYC	C1D-ND	-3.11	1.32	1.37
13	A6	302	CYC	C1B-NB	-3.11	1.32	1.37
13	K7	201	CYC	C1A-NA	-3.11	1.32	1.38
13	B5	201	CYC	C4D-ND	-3.11	1.32	1.37
13	K4	201	CYC	C1A-NA	-3.11	1.32	1.38
13	M5	201	CYC	C1A-NA	-3.11	1.32	1.38
13	B7	201	CYC	C4D-ND	-3.11	1.32	1.37
13	J4	201	CYC	C1A-NA	-3.10	1.32	1.38
13	J7	202	CYC	C1A-NA	-3.10	1.32	1.38
13	J5	202	CYC	C1D-ND	-3.10	1.32	1.37
13	Q5	202	CYC	C4D-ND	-3.10	1.32	1.37
13	T5	202	CYC	C1A-NA	-3.10	1.32	1.38
13	J6	202	CYC	C1A-NA	-3.10	1.32	1.38
13	W3	201	CYC	C1A-NA	-3.10	1.32	1.38
13	S5	201	CYC	C1A-NA	-3.10	1.32	1.38
13	v2	201	CYC	C1D-ND	-3.10	1.32	1.37
13	C6	202	CYC	C1D-ND	-3.10	1.32	1.37
13	T6	201	CYC	C1D-ND	-3.10	1.32	1.37
13	F3	201	CYC	C1A-NA	-3.10	1.32	1.38
13	R4	201	CYC	C4D-ND	-3.10	1.32	1.37
13	P1	201	CYC	C1A-NA	-3.10	1.32	1.38
13	a2	201	CYC	C4D-ND	-3.10	1.32	1.37
13	R2	201	CYC	C1D-ND	-3.10	1.32	1.37
13	S7	201	CYC	C1A-NA	-3.10	1.32	1.38
13	R6	201	CYC	C1A-NA	-3.10	1.32	1.38
13	N6	201	CYC	C4D-ND	-3.10	1.32	1.37
13	K7	201	CYC	C4D-ND	-3.09	1.32	1.37
13	P4	202	CYC	C1A-NA	-3.09	1.32	1.38
13	F4	202	CYC	C4D-ND	-3.09	1.32	1.37
13	N3	201	CYC	C1A-NA	-3.09	1.32	1.38
13	B7	201	CYC	C1A-NA	-3.09	1.32	1.38
13	T2	201	CYC	C1D-ND	-3.09	1.32	1.37
13	T3	201	CYC	C1D-ND	-3.09	1.32	1.37
13	I3	201	CYC	C1A-NA	-3.09	1.32	1.38
13	R3	201	CYC	C1A-NA	-3.09	1.32	1.38
13	J7	201	CYC	C1A-NA	-3.09	1.32	1.38
13	W7	201	CYC	C1A-NA	-3.09	1.32	1.38
13	G6	201	CYC	C4D-ND	-3.09	1.32	1.37
13	J3	201	CYC	C1A-NA	-3.09	1.32	1.38
13	a7	201	CYC	C1A-NA	-3.09	1.32	1.38
13	P1	202	CYC	C1D-ND	-3.09	1.32	1.37
13	F1	202	CYC	C4D-ND	-3.09	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	52	302	CYC	C1B-NB	-3.09	1.32	1.37
13	n2	201	CYC	C1D-ND	-3.09	1.32	1.37
13	42	302	CYC	C1B-NB	-3.09	1.32	1.37
13	L3	201	CYC	C1D-ND	-3.09	1.32	1.37
13	P4	202	CYC	C4D-ND	-3.09	1.32	1.37
13	H2	201	CYC	C4A-C3A	-3.09	1.39	1.45
13	F7	201	CYC	C1D-ND	-3.09	1.32	1.37
13	F3	202	CYC	C1A-NA	-3.09	1.32	1.38
13	M2	201	CYC	C1D-ND	-3.09	1.32	1.37
13	F3	202	CYC	C1D-ND	-3.09	1.32	1.37
13	F6	201	CYC	C4D-ND	-3.09	1.32	1.37
13	F6	202	CYC	C4D-ND	-3.09	1.32	1.37
13	S6	201	CYC	C1A-NA	-3.09	1.32	1.38
13	C5	202	CYC	C1D-ND	-3.09	1.32	1.37
13	V4	202	CYC	C1D-ND	-3.09	1.32	1.37
13	Q1	201	CYC	C4D-ND	-3.08	1.32	1.37
13	H7	201	CYC	C4D-ND	-3.08	1.32	1.37
13	d2	201	CYC	C4D-ND	-3.08	1.32	1.37
13	F7	202	CYC	C4D-ND	-3.08	1.32	1.37
13	P3	201	CYC	C1A-NA	-3.08	1.32	1.38
13	x2	201	CYC	C1A-NA	-3.08	1.32	1.38
13	P7	201	CYC	C1A-NA	-3.08	1.32	1.38
13	a3	201	CYC	C1A-NA	-3.08	1.32	1.38
13	F5	201	CYC	C4D-ND	-3.08	1.32	1.37
13	M4	201	CYC	C1A-NA	-3.08	1.32	1.38
13	C2	201	CYC	C4D-ND	-3.08	1.32	1.37
13	U1	201	CYC	C1A-NA	-3.08	1.32	1.38
13	C2	201	CYC	C1D-ND	-3.08	1.32	1.37
13	D4	201	CYC	C1A-NA	-3.08	1.32	1.38
13	F3	201	CYC	C1D-ND	-3.08	1.32	1.37
13	N7	201	CYC	C4D-ND	-3.08	1.32	1.37
13	M1	201	CYC	C1A-NA	-3.08	1.32	1.38
13	J1	202	CYC	C1D-ND	-3.08	1.32	1.37
13	U4	201	CYC	C4D-ND	-3.08	1.32	1.37
13	k2	201	CYC	C1A-NA	-3.08	1.32	1.38
13	N3	201	CYC	C4D-ND	-3.08	1.32	1.37
13	C7	201	CYC	C1A-NA	-3.08	1.32	1.38
13	32	302	CYC	C1D-ND	-3.08	1.32	1.37
13	K5	201	CYC	C4D-ND	-3.08	1.32	1.37
13	W6	201	CYC	C4D-ND	-3.08	1.32	1.37
13	Q4	202	CYC	C4D-ND	-3.08	1.32	1.37
13	N5	201	CYC	C4D-ND	-3.08	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D4	201	CYC	C1D-ND	-3.07	1.32	1.37
13	F1	202	CYC	C1A-NA	-3.07	1.32	1.38
13	42	302	CYC	C4D-ND	-3.07	1.32	1.37
13	U3	201	CYC	C1A-NA	-3.07	1.32	1.38
13	Q1	202	CYC	C1A-NA	-3.07	1.32	1.38
13	Q5	202	CYC	C1A-NA	-3.07	1.32	1.38
13	K4	201	CYC	C4D-ND	-3.07	1.32	1.37
13	G7	201	CYC	C1A-NA	-3.07	1.32	1.38
13	R5	201	CYC	C4D-ND	-3.07	1.32	1.37
13	L7	201	CYC	C1D-ND	-3.07	1.32	1.37
13	V3	202	CYC	C1A-NA	-3.07	1.32	1.38
13	P6	202	CYC	C1D-ND	-3.07	1.32	1.37
13	G7	201	CYC	C4D-ND	-3.07	1.32	1.37
13	K1	201	CYC	C4D-ND	-3.07	1.32	1.37
13	H3	201	CYC	C4D-ND	-3.07	1.32	1.37
13	N4	201	CYC	C4D-ND	-3.07	1.32	1.37
13	Q4	202	CYC	C1A-NA	-3.06	1.32	1.38
13	F7	201	CYC	C1A-NA	-3.06	1.32	1.38
13	K3	201	CYC	C4D-ND	-3.06	1.32	1.37
13	F4	201	CYC	C4D-ND	-3.06	1.32	1.37
13	x2	201	CYC	C1D-ND	-3.06	1.32	1.37
13	W4	201	CYC	C4D-ND	-3.06	1.32	1.37
13	J4	202	CYC	C1A-NA	-3.06	1.32	1.38
13	F6	202	CYC	C1D-ND	-3.06	1.32	1.37
13	T4	202	CYC	C1A-NA	-3.06	1.32	1.38
13	F7	202	CYC	C1D-ND	-3.06	1.32	1.37
13	F7	202	CYC	C1A-NA	-3.06	1.32	1.38
13	G1	201	CYC	C4D-ND	-3.06	1.32	1.37
13	F2	201	CYC	C1D-ND	-3.06	1.32	1.37
13	V3	202	CYC	C1D-ND	-3.06	1.32	1.37
13	r2	201	CYC	C1D-ND	-3.06	1.32	1.37
13	U5	201	CYC	C4D-ND	-3.06	1.32	1.37
13	I7	201	CYC	C1A-NA	-3.06	1.32	1.38
13	P7	201	CYC	C1D-ND	-3.06	1.32	1.37
13	C3	202	CYC	C1D-ND	-3.06	1.32	1.37
13	R3	201	CYC	C4D-ND	-3.06	1.32	1.37
13	P5	201	CYC	C4D-ND	-3.06	1.32	1.37
13	N7	201	CYC	C1A-NA	-3.06	1.32	1.38
13	G4	201	CYC	C4D-ND	-3.06	1.32	1.37
13	Q1	201	CYC	C1A-NA	-3.06	1.32	1.38
13	I7	201	CYC	C4D-ND	-3.06	1.32	1.37
13	P6	201	CYC	C1A-NA	-3.05	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U7	201	CYC	C4D-ND	-3.05	1.32	1.37
13	32	302	CYC	C1A-NA	-3.05	1.32	1.38
13	j2	201	CYC	C1D-ND	-3.05	1.32	1.37
13	Q7	202	CYC	C4D-ND	-3.05	1.32	1.37
13	V1	201	CYC	C1A-NA	-3.05	1.32	1.38
13	22	302	CYC	C1A-NA	-3.05	1.32	1.38
13	C6	202	CYC	C4D-ND	-3.05	1.32	1.37
13	K6	201	CYC	C4D-ND	-3.05	1.32	1.37
13	i2	201	CYC	C1A-NA	-3.05	1.32	1.38
13	32	302	CYC	C1B-NB	-3.05	1.32	1.37
13	P3	202	CYC	C1D-ND	-3.05	1.32	1.37
13	Q6	202	CYC	C1A-NA	-3.05	1.32	1.38
13	J7	202	CYC	C4A-C3A	-3.05	1.39	1.45
13	H2	201	CYC	C4D-ND	-3.05	1.32	1.37
13	U4	201	CYC	C1A-NA	-3.05	1.32	1.38
13	U3	201	CYC	C4D-ND	-3.04	1.32	1.37
13	U1	201	CYC	C4D-ND	-3.04	1.32	1.37
13	C7	202	CYC	C4D-ND	-3.04	1.32	1.37
13	R7	201	CYC	C4D-ND	-3.04	1.32	1.37
13	22	302	CYC	C1D-ND	-3.04	1.32	1.37
13	B3	201	CYC	C4D-ND	-3.04	1.32	1.37
13	V7	202	CYC	C1A-NA	-3.04	1.32	1.38
13	D3	201	CYC	C1A-NA	-3.04	1.32	1.38
13	Q2	201	CYC	C4D-ND	-3.04	1.32	1.37
13	Q3	202	CYC	C4D-ND	-3.04	1.32	1.37
13	R7	201	CYC	C1A-NA	-3.04	1.32	1.38
13	F7	201	CYC	C4D-ND	-3.04	1.32	1.37
13	D7	201	CYC	C1D-ND	-3.04	1.32	1.37
13	H3	201	CYC	C1A-NA	-3.04	1.32	1.38
13	V5	201	CYC	C1A-NA	-3.04	1.32	1.38
13	T3	202	CYC	C1A-NA	-3.04	1.32	1.38
13	F1	202	CYC	C1D-ND	-3.04	1.32	1.37
13	V6	202	CYC	C1D-ND	-3.04	1.32	1.37
13	C3	202	CYC	C4D-ND	-3.04	1.32	1.37
13	C2	201	CYC	C1A-NA	-3.04	1.32	1.38
13	V7	202	CYC	C1D-ND	-3.04	1.32	1.37
13	F4	202	CYC	C1D-ND	-3.03	1.32	1.37
13	Q3	202	CYC	C1A-NA	-3.03	1.32	1.38
13	P3	201	CYC	C1D-ND	-3.03	1.32	1.37
13	W3	201	CYC	C1D-ND	-3.03	1.32	1.37
13	H6	201	CYC	C4D-ND	-3.03	1.32	1.37
13	I3	201	CYC	C4D-ND	-3.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a7	201	CYC	C1D-ND	-3.03	1.32	1.37
13	F3	201	CYC	C4D-ND	-3.03	1.32	1.37
13	P3	202	CYC	C4A-C3A	-3.03	1.39	1.45
13	R6	201	CYC	C4D-ND	-3.02	1.32	1.37
13	U6	201	CYC	C4D-ND	-3.02	1.32	1.37
13	B2	201	CYC	C1D-ND	-3.02	1.32	1.37
13	V5	202	CYC	C1D-ND	-3.02	1.32	1.37
13	P7	202	CYC	C4A-C3A	-3.02	1.39	1.45
13	L1	201	CYC	C1D-ND	-3.02	1.32	1.37
13	C1	202	CYC	C1D-ND	-3.02	1.32	1.37
13	Q6	201	CYC	C1A-NA	-3.02	1.32	1.38
13	B7	201	CYC	C1D-ND	-3.02	1.32	1.37
13	Q7	202	CYC	C1A-NA	-3.02	1.32	1.38
13	42	301	CYC	C1D-ND	-3.02	1.32	1.37
13	H5	201	CYC	C4D-ND	-3.02	1.32	1.37
13	D6	201	CYC	C1D-ND	-3.02	1.32	1.37
13	V4	201	CYC	C1A-NA	-3.02	1.32	1.38
13	A2	201	CYC	C4D-ND	-3.01	1.32	1.37
13	m2	201	CYC	C4A-C3A	-3.01	1.39	1.45
13	S1	201	CYC	C4D-ND	-3.01	1.32	1.37
13	H7	201	CYC	C1A-NA	-3.01	1.32	1.38
13	B2	202	CYC	C1A-NA	-3.01	1.32	1.38
13	W7	201	CYC	C1D-ND	-3.01	1.32	1.37
13	P2	201	CYC	C1D-ND	-3.01	1.32	1.37
13	K3	201	CYC	C1D-ND	-3.01	1.32	1.37
13	C4	202	CYC	C1D-ND	-3.01	1.32	1.37
13	W2	201	CYC	C1A-NA	-3.01	1.32	1.38
13	P7	202	CYC	C1D-ND	-3.01	1.32	1.37
13	U7	201	CYC	C1A-NA	-3.01	1.32	1.38
13	C5	202	CYC	C4D-ND	-3.01	1.32	1.37
13	P5	201	CYC	C1D-ND	-3.00	1.32	1.37
13	M4	201	CYC	C4A-C3A	-3.00	1.39	1.45
13	H2	201	CYC	C1D-ND	-3.00	1.32	1.37
13	P4	201	CYC	C1D-ND	-3.00	1.32	1.37
13	E7	201	CYC	C4A-C3A	-3.00	1.39	1.45
13	Q2	201	CYC	C1D-ND	-3.00	1.32	1.37
13	a3	201	CYC	C1D-ND	-3.00	1.32	1.37
13	V7	202	CYC	C4A-C3A	-3.00	1.39	1.45
13	Q6	202	CYC	C1D-ND	-3.00	1.32	1.37
13	Q5	201	CYC	C1A-NA	-3.00	1.32	1.38
13	Q7	202	CYC	C1D-ND	-3.00	1.32	1.37
13	L2	201	CYC	C1D-ND	-3.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E3	201	CYC	C4A-C3A	-3.00	1.39	1.45
13	J3	202	CYC	C4A-C3A	-3.00	1.39	1.45
13	C1	202	CYC	C4D-ND	-3.00	1.32	1.37
13	G3	201	CYC	C4D-ND	-3.00	1.32	1.37
13	Q6	202	CYC	C4D-ND	-3.00	1.32	1.37
13	C4	202	CYC	C4D-ND	-2.99	1.32	1.37
13	V1	202	CYC	C1D-ND	-2.99	1.32	1.37
13	A2	202	CYC	C1A-NA	-2.99	1.32	1.38
13	I4	201	CYC	C1D-ND	-2.99	1.32	1.37
13	T7	202	CYC	C1A-NA	-2.99	1.32	1.38
13	N2	801	CYC	C1D-ND	-2.99	1.32	1.37
13	C4	202	CYC	C4A-C3A	-2.99	1.39	1.45
13	D2	201	CYC	C1D-ND	-2.99	1.32	1.37
13	c2	801	CYC	C1A-NA	-2.99	1.32	1.38
13	P5	202	CYC	C1D-ND	-2.99	1.32	1.37
13	H4	201	CYC	C4D-ND	-2.99	1.32	1.37
13	V7	201	CYC	C1A-NA	-2.99	1.32	1.38
13	I6	201	CYC	C1D-ND	-2.98	1.32	1.37
13	U7	201	CYC	C1D-ND	-2.98	1.32	1.37
13	c2	801	CYC	C4A-C3A	-2.98	1.39	1.45
13	Q1	202	CYC	C4D-ND	-2.98	1.32	1.37
13	U3	201	CYC	C1D-ND	-2.98	1.32	1.37
13	S2	201	CYC	C1D-ND	-2.98	1.32	1.37
13	W5	201	CYC	C4D-ND	-2.98	1.32	1.37
13	T3	201	CYC	C4A-C3A	-2.98	1.39	1.45
13	w2	201	CYC	C1D-ND	-2.98	1.32	1.37
13	Q3	202	CYC	C1D-ND	-2.98	1.32	1.37
13	V6	201	CYC	C1A-NA	-2.98	1.32	1.38
13	P4	202	CYC	C1D-ND	-2.97	1.32	1.37
13	C5	202	CYC	C4A-C3A	-2.97	1.39	1.45
13	d2	201	CYC	C1D-ND	-2.97	1.32	1.37
13	h2	201	CYC	C1D-ND	-2.97	1.32	1.37
13	W2	201	CYC	C1D-ND	-2.97	1.32	1.37
13	I7	201	CYC	C1D-ND	-2.97	1.32	1.37
13	D3	201	CYC	C1D-ND	-2.97	1.32	1.37
13	P1	202	CYC	C4A-C3A	-2.97	1.39	1.45
13	Q4	201	CYC	C1D-ND	-2.97	1.32	1.37
13	Q4	201	CYC	C1A-NA	-2.97	1.32	1.38
13	X7	201	CYC	C1D-ND	-2.97	1.32	1.37
13	D7	201	CYC	C1A-NA	-2.97	1.32	1.38
13	T7	201	CYC	C4A-C3A	-2.96	1.39	1.45
13	S5	201	CYC	C4D-ND	-2.96	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R4	201	CYC	C4A-C3A	-2.96	1.39	1.45
13	V7	201	CYC	C1D-ND	-2.96	1.32	1.37
13	V3	201	CYC	C1A-NA	-2.96	1.32	1.38
13	T5	201	CYC	C4A-C3A	-2.96	1.39	1.45
13	U4	201	CYC	C1D-ND	-2.96	1.32	1.37
13	d2	201	CYC	C1A-NA	-2.96	1.32	1.38
13	H2	201	CYC	C1A-NA	-2.96	1.32	1.38
13	V3	202	CYC	C4A-C3A	-2.96	1.39	1.45
13	c2	801	CYC	C4D-ND	-2.96	1.32	1.37
13	R5	201	CYC	C4A-C3A	-2.96	1.39	1.45
13	j2	201	CYC	C1A-NA	-2.96	1.32	1.38
13	M3	201	CYC	C1A-NA	-2.96	1.32	1.38
13	S4	201	CYC	C4D-ND	-2.96	1.32	1.37
13	I1	201	CYC	C1D-ND	-2.95	1.32	1.37
13	A6	301	CYC	C1D-ND	-2.95	1.32	1.37
13	K7	201	CYC	C1D-ND	-2.95	1.32	1.37
13	G5	201	CYC	C1D-ND	-2.95	1.32	1.37
13	R7	201	CYC	C1D-ND	-2.95	1.32	1.37
13	R4	201	CYC	C1D-ND	-2.95	1.32	1.37
13	M5	201	CYC	C4A-C3A	-2.95	1.39	1.45
13	Q4	202	CYC	C1D-ND	-2.95	1.32	1.37
13	B3	201	CYC	C1D-ND	-2.95	1.32	1.37
13	B2	201	CYC	C4A-C3A	-2.95	1.39	1.45
13	E6	201	CYC	C4A-C3A	-2.95	1.39	1.45
13	S6	201	CYC	C4D-ND	-2.95	1.32	1.37
13	I3	201	CYC	C1D-ND	-2.95	1.32	1.37
13	C1	202	CYC	C4A-C3A	-2.95	1.39	1.45
13	V5	202	CYC	C4A-C3A	-2.95	1.39	1.45
13	R6	201	CYC	C1D-ND	-2.95	1.32	1.37
13	G6	201	CYC	C1D-ND	-2.94	1.32	1.37
13	T7	202	CYC	C4D-ND	-2.94	1.32	1.37
13	V1	201	CYC	C1D-ND	-2.94	1.32	1.37
13	P4	201	CYC	C4A-C3A	-2.94	1.39	1.45
13	C7	202	CYC	C4A-C3A	-2.94	1.39	1.45
13	T3	202	CYC	C4D-ND	-2.94	1.32	1.37
13	C6	202	CYC	C4A-C3A	-2.94	1.39	1.45
13	Z1	301	CYC	C1D-ND	-2.94	1.32	1.37
13	p2	201	CYC	C1D-ND	-2.94	1.32	1.37
13	P7	202	CYC	C1A-NA	-2.94	1.32	1.38
13	L4	201	CYC	C1D-ND	-2.94	1.32	1.37
13	R7	201	CYC	C4A-C3A	-2.94	1.39	1.45
13	X3	201	CYC	C1D-ND	-2.94	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T6	202	CYC	C4D-ND	-2.94	1.32	1.37
13	I5	201	CYC	C4A-C3A	-2.94	1.39	1.45
13	P6	202	CYC	C4A-C3A	-2.94	1.39	1.45
13	R1	201	CYC	C1D-ND	-2.94	1.32	1.37
13	22	301	CYC	C1D-ND	-2.94	1.32	1.37
13	m2	201	CYC	C1D-ND	-2.94	1.32	1.37
13	T1	201	CYC	C4A-C3A	-2.93	1.39	1.45
13	Q3	202	CYC	C4A-C3A	-2.93	1.39	1.45
13	M3	201	CYC	C4A-C3A	-2.93	1.39	1.45
13	Q7	202	CYC	C4A-C3A	-2.93	1.39	1.45
13	L6	201	CYC	C1D-ND	-2.93	1.32	1.37
13	C3	201	CYC	C4A-C3A	-2.93	1.39	1.45
13	B4	201	CYC	C1D-ND	-2.93	1.32	1.37
13	T5	202	CYC	C4D-ND	-2.93	1.32	1.37
13	T1	202	CYC	C4D-ND	-2.93	1.32	1.37
13	T4	201	CYC	C4A-C3A	-2.93	1.39	1.45
13	Q1	202	CYC	C1D-ND	-2.93	1.32	1.37
13	T6	201	CYC	C4A-C3A	-2.93	1.39	1.45
13	V6	202	CYC	C4A-C3A	-2.92	1.39	1.45
13	N4	201	CYC	C1D-ND	-2.92	1.32	1.37
13	G1	201	CYC	C4A-C3A	-2.92	1.39	1.45
13	P6	201	CYC	C1D-ND	-2.92	1.32	1.37
13	S3	201	CYC	C4D-ND	-2.92	1.32	1.37
13	V4	201	CYC	C1D-ND	-2.92	1.32	1.37
13	G4	201	CYC	C1D-ND	-2.92	1.32	1.37
13	N3	201	CYC	C1D-ND	-2.92	1.32	1.37
13	Q1	201	CYC	C1D-ND	-2.92	1.32	1.37
13	V4	202	CYC	C4A-C3A	-2.92	1.39	1.45
13	T4	202	CYC	C4D-ND	-2.92	1.32	1.37
13	C7	201	CYC	C4A-C3A	-2.92	1.39	1.45
13	S7	201	CYC	C4D-ND	-2.92	1.32	1.37
13	a7	202	CYC	C4A-C3A	-2.92	1.39	1.45
13	c2	801	CYC	C1D-ND	-2.92	1.32	1.37
13	M7	201	CYC	C1A-NA	-2.92	1.32	1.38
13	F7	201	CYC	C4A-C3A	-2.92	1.39	1.45
13	L5	201	CYC	C1D-ND	-2.92	1.32	1.37
13	V6	201	CYC	C1D-ND	-2.92	1.32	1.37
13	k2	201	CYC	C4A-C3A	-2.91	1.39	1.45
13	V1	202	CYC	C4A-C3A	-2.91	1.39	1.45
13	E5	201	CYC	C4A-C3A	-2.91	1.39	1.45
13	Q3	201	CYC	C1A-NA	-2.91	1.32	1.38
13	a6	201	CYC	C1D-ND	-2.91	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P5	202	CYC	C4A-C3A	-2.91	1.39	1.45
13	a1	201	CYC	C1D-ND	-2.91	1.32	1.37
13	I5	201	CYC	C1D-ND	-2.91	1.32	1.37
13	Q5	202	CYC	C1D-ND	-2.91	1.32	1.37
13	D3	201	CYC	C4A-C3A	-2.91	1.39	1.45
13	N7	201	CYC	C1D-ND	-2.91	1.32	1.37
13	R5	201	CYC	C1D-ND	-2.91	1.32	1.37
13	R3	201	CYC	C1D-ND	-2.91	1.32	1.37
13	E1	201	CYC	C4A-C3A	-2.91	1.39	1.45
13	R6	201	CYC	C4A-C3A	-2.90	1.39	1.45
13	G7	201	CYC	C1D-ND	-2.90	1.32	1.37
13	F5	201	CYC	C4A-C3A	-2.90	1.39	1.45
13	M3	201	CYC	C1D-ND	-2.90	1.32	1.37
13	C2	201	CYC	C4A-C3A	-2.90	1.39	1.45
13	J1	202	CYC	C4A-C3A	-2.90	1.39	1.45
13	52	301	CYC	C1D-ND	-2.90	1.32	1.37
13	Q6	201	CYC	C1D-ND	-2.90	1.32	1.37
13	P1	201	CYC	C1D-ND	-2.90	1.32	1.37
13	N5	201	CYC	C1D-ND	-2.90	1.32	1.37
13	X1	201	CYC	C1D-ND	-2.90	1.32	1.37
13	Q5	201	CYC	C1D-ND	-2.90	1.32	1.37
13	R3	201	CYC	C4A-C3A	-2.90	1.39	1.45
13	C6	201	CYC	C4A-C3A	-2.90	1.39	1.45
13	H7	201	CYC	C1D-ND	-2.89	1.32	1.37
13	W7	201	CYC	C4A-C3A	-2.89	1.39	1.45
13	X4	201	CYC	C1D-ND	-2.89	1.32	1.37
13	G6	201	CYC	C4A-C3A	-2.89	1.39	1.45
13	M7	201	CYC	C4A-C3A	-2.89	1.39	1.45
13	C3	202	CYC	C4A-C3A	-2.89	1.39	1.45
13	Q7	201	CYC	C1A-NA	-2.89	1.32	1.38
13	M5	201	CYC	C1D-ND	-2.89	1.32	1.37
13	U4	201	CYC	C4A-C3A	-2.89	1.39	1.45
13	R1	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	U5	201	CYC	C1D-ND	-2.88	1.32	1.37
13	E4	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	P3	202	CYC	C1A-NA	-2.88	1.32	1.38
13	i2	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	K4	201	CYC	C1D-ND	-2.88	1.32	1.37
13	F1	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	G1	201	CYC	C1D-ND	-2.88	1.32	1.37
13	X5	201	CYC	C1D-ND	-2.88	1.32	1.37
13	I1	201	CYC	C4A-C3A	-2.88	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V5	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	X6	201	CYC	C1D-ND	-2.88	1.32	1.37
13	G3	201	CYC	C1D-ND	-2.88	1.32	1.37
13	M1	201	CYC	C4A-C3A	-2.88	1.39	1.45
13	G5	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	V6	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	B5	201	CYC	C1D-ND	-2.87	1.32	1.37
13	H3	201	CYC	C1D-ND	-2.87	1.32	1.37
13	X5	201	CYC	C4B-NB	-2.87	1.31	1.38
13	K6	201	CYC	C1D-ND	-2.87	1.32	1.37
13	N6	201	CYC	C1D-ND	-2.87	1.32	1.37
13	M1	201	CYC	C1D-ND	-2.87	1.32	1.37
13	B6	201	CYC	C1D-ND	-2.87	1.32	1.37
13	U6	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	V1	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	F3	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	32	301	CYC	C1D-ND	-2.87	1.32	1.37
13	C1	201	CYC	C1D-ND	-2.87	1.32	1.37
13	C6	201	CYC	C1D-ND	-2.87	1.32	1.37
13	W3	201	CYC	C4A-C3A	-2.87	1.39	1.45
13	V2	201	CYC	C1D-ND	-2.87	1.32	1.37
13	M4	201	CYC	C1D-ND	-2.86	1.32	1.37
13	M6	201	CYC	C1D-ND	-2.86	1.32	1.37
13	U3	201	CYC	C4A-C3A	-2.86	1.39	1.45
13	Z6	301	CYC	C1D-ND	-2.86	1.32	1.37
13	H1	201	CYC	C4A-C3A	-2.86	1.39	1.45
13	V5	201	CYC	C1D-ND	-2.86	1.32	1.37
13	K5	201	CYC	C4A-C3A	-2.86	1.39	1.45
13	a5	201	CYC	C1D-ND	-2.86	1.32	1.37
13	J4	202	CYC	C4A-C3A	-2.86	1.39	1.45
13	X4	201	CYC	C4B-NB	-2.86	1.31	1.38
13	H1	201	CYC	C1D-ND	-2.86	1.32	1.37
13	G4	201	CYC	C4A-C3A	-2.86	1.39	1.45
13	C4	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	I6	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	N1	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	K4	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	U7	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	a3	202	CYC	C4A-C3A	-2.85	1.39	1.45
13	H4	201	CYC	C1D-ND	-2.85	1.33	1.37
13	W4	201	CYC	C1D-ND	-2.85	1.33	1.37
13	d2	201	CYC	C4A-C3A	-2.85	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P2	201	CYC	C4A-C3A	-2.85	1.39	1.45
13	O2	201	CYC	C1D-ND	-2.84	1.33	1.37
13	X1	201	CYC	C4B-NB	-2.84	1.31	1.38
13	K1	201	CYC	C1D-ND	-2.84	1.33	1.37
13	V3	201	CYC	C4A-C3A	-2.84	1.39	1.45
13	F4	201	CYC	C4A-C3A	-2.84	1.39	1.45
13	X3	201	CYC	C4B-NB	-2.84	1.31	1.38
13	F6	201	CYC	C4A-C3A	-2.84	1.39	1.45
13	M6	201	CYC	C4A-C3A	-2.84	1.39	1.45
13	G7	201	CYC	C4A-C3A	-2.84	1.39	1.45
13	G2	201	CYC	C1D-ND	-2.84	1.33	1.37
13	H6	201	CYC	C1D-ND	-2.84	1.33	1.37
13	Z4	301	CYC	C1D-ND	-2.83	1.33	1.37
13	U1	201	CYC	C1D-ND	-2.83	1.33	1.37
13	Z5	301	CYC	C1D-ND	-2.83	1.33	1.37
13	Q7	201	CYC	C4A-C3A	-2.83	1.39	1.45
13	B1	201	CYC	C1D-ND	-2.83	1.33	1.37
13	N1	201	CYC	C1D-ND	-2.83	1.33	1.37
13	H5	201	CYC	C4A-C3A	-2.83	1.39	1.45
13	T7	202	CYC	C1D-ND	-2.83	1.33	1.37
13	V4	201	CYC	C4A-C3A	-2.83	1.39	1.45
13	F7	202	CYC	C4A-C3A	-2.83	1.39	1.45
13	J7	201	CYC	C1D-ND	-2.83	1.33	1.37
13	B3	201	CYC	C4A-C3A	-2.83	1.39	1.45
13	A1	301	CYC	C1D-ND	-2.83	1.33	1.37
13	J4	201	CYC	C4A-C3A	-2.83	1.39	1.45
13	L2	201	CYC	C4A-C3A	-2.82	1.39	1.45
13	Q3	201	CYC	C4A-C3A	-2.82	1.39	1.45
13	H4	201	CYC	C4A-C3A	-2.82	1.39	1.45
13	T3	202	CYC	C1D-ND	-2.82	1.33	1.37
13	C7	201	CYC	C1D-ND	-2.82	1.33	1.37
13	a1	202	CYC	C4A-C3A	-2.81	1.39	1.45
13	J1	201	CYC	C4A-C3A	-2.81	1.39	1.45
13	V3	201	CYC	C1D-ND	-2.81	1.33	1.37
13	C3	201	CYC	C1D-ND	-2.81	1.33	1.37
13	J6	202	CYC	C4A-C3A	-2.81	1.39	1.45
13	U1	201	CYC	C4A-C3A	-2.81	1.39	1.45
13	o2	801	CYC	C4B-NB	-2.80	1.31	1.38
13	M7	201	CYC	C1D-ND	-2.80	1.33	1.37
13	J5	202	CYC	C4A-C3A	-2.80	1.39	1.45
13	A2	202	CYC	C4A-C3A	-2.80	1.39	1.45
13	W5	201	CYC	C4A-C3A	-2.80	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q6	201	CYC	C4A-C3A	-2.80	1.39	1.45
13	K5	201	CYC	C1D-ND	-2.80	1.33	1.37
13	J7	201	CYC	C4A-C3A	-2.80	1.39	1.45
13	D1	201	CYC	C4A-C3A	-2.80	1.39	1.45
13	Q5	201	CYC	C4A-C3A	-2.80	1.39	1.45
13	S7	201	CYC	C1D-ND	-2.80	1.33	1.37
13	I4	201	CYC	C4A-C3A	-2.80	1.39	1.45
13	T4	202	CYC	C1D-ND	-2.80	1.33	1.37
13	N3	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	B1	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	B4	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	T6	202	CYC	C1D-ND	-2.79	1.33	1.37
13	G3	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	J3	201	CYC	C1D-ND	-2.79	1.33	1.37
13	C1	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	H7	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	F1	202	CYC	C4A-C3A	-2.79	1.39	1.45
13	I3	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	V2	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	H6	201	CYC	C4A-C3A	-2.79	1.39	1.45
13	J1	201	CYC	C1D-ND	-2.79	1.33	1.37
13	K3	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	Q4	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	W6	201	CYC	C1D-ND	-2.78	1.33	1.37
13	W1	201	CYC	C1D-ND	-2.78	1.33	1.37
13	C5	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	U5	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	N5	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	N4	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	I7	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	U6	201	CYC	C1D-ND	-2.78	1.33	1.37
13	K1	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	F3	202	CYC	C4A-C3A	-2.78	1.39	1.45
13	B6	201	CYC	C4A-C3A	-2.78	1.39	1.45
13	C4	201	CYC	C1D-ND	-2.77	1.33	1.37
13	S4	201	CYC	C4A-C3A	-2.77	1.39	1.45
13	S4	201	CYC	C1D-ND	-2.77	1.33	1.37
13	D7	201	CYC	C4A-C3A	-2.77	1.39	1.45
13	N7	201	CYC	C4A-C3A	-2.77	1.39	1.45
13	T4	202	CYC	C4A-C3A	-2.77	1.39	1.45
13	F4	202	CYC	C4A-C3A	-2.77	1.39	1.45
13	B7	201	CYC	C4A-C3A	-2.77	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	42	302	CYC	C1D-ND	-2.77	1.33	1.37
13	S3	201	CYC	C1D-ND	-2.77	1.33	1.37
13	a2	201	CYC	C4A-C3A	-2.77	1.39	1.45
13	X6	201	CYC	C4B-NB	-2.76	1.31	1.38
13	T6	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	a5	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	H5	201	CYC	C1D-ND	-2.76	1.33	1.37
13	a6	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	X7	201	CYC	C4B-NB	-2.76	1.31	1.38
13	V7	201	CYC	C4A-C3A	-2.76	1.39	1.45
13	K6	201	CYC	C4A-C3A	-2.76	1.39	1.45
13	F5	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	J5	201	CYC	C1D-ND	-2.76	1.33	1.37
13	T3	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	J6	201	CYC	C1D-ND	-2.76	1.33	1.37
13	a4	202	CYC	C4A-C3A	-2.76	1.39	1.45
13	n2	201	CYC	C4B-NB	-2.76	1.31	1.38
13	H3	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	Q1	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	J6	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	S1	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	w2	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	N6	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	W1	201	CYC	C4A-C3A	-2.75	1.39	1.45
13	W5	201	CYC	C1D-ND	-2.75	1.33	1.37
13	S5	201	CYC	C1D-ND	-2.74	1.33	1.37
13	l2	201	CYC	C4A-C3A	-2.74	1.39	1.45
13	T1	202	CYC	C4A-C3A	-2.74	1.39	1.45
13	F6	202	CYC	C4A-C3A	-2.74	1.39	1.45
13	T2	201	CYC	C4A-C3A	-2.74	1.39	1.45
13	P4	201	CYC	C1A-NA	-2.74	1.32	1.38
13	W6	201	CYC	C4A-C3A	-2.74	1.39	1.45
13	S6	201	CYC	C4A-C3A	-2.74	1.39	1.45
13	T5	202	CYC	C1D-ND	-2.74	1.33	1.37
13	D5	201	CYC	C4A-C3A	-2.73	1.39	1.45
13	A1	302	CYC	C1D-ND	-2.73	1.33	1.37
13	Q6	202	CYC	C4A-C3A	-2.73	1.39	1.45
13	C5	201	CYC	C1D-ND	-2.73	1.33	1.37
13	B5	201	CYC	C4A-C3A	-2.73	1.39	1.45
13	a1	201	CYC	C4B-NB	-2.73	1.31	1.38
13	T7	202	CYC	C4A-C3A	-2.73	1.39	1.45
13	S3	201	CYC	C4A-C3A	-2.73	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S6	201	CYC	C1D-ND	-2.73	1.33	1.37
13	T5	202	CYC	C4A-C3A	-2.73	1.39	1.45
13	A6	302	CYC	C1D-ND	-2.73	1.33	1.37
13	W4	201	CYC	C4A-C3A	-2.72	1.39	1.45
13	h2	201	CYC	C4B-NB	-2.72	1.31	1.38
13	Q4	202	CYC	C4A-C3A	-2.72	1.39	1.45
13	Q1	202	CYC	C4A-C3A	-2.72	1.39	1.45
13	S1	201	CYC	C1D-ND	-2.72	1.33	1.37
13	K7	201	CYC	C4A-C3A	-2.72	1.39	1.45
13	S7	201	CYC	C4A-C3A	-2.72	1.39	1.45
13	J4	201	CYC	C1D-ND	-2.72	1.33	1.37
13	52	302	CYC	C1D-ND	-2.72	1.33	1.37
13	g2	201	CYC	C4A-C3A	-2.72	1.39	1.45
13	P5	202	CYC	C1A-NA	-2.72	1.32	1.38
13	S5	201	CYC	C4A-C3A	-2.72	1.39	1.45
13	T1	202	CYC	C1D-ND	-2.71	1.33	1.37
13	X2	201	CYC	C4A-C3A	-2.71	1.40	1.45
13	52	302	CYC	C4A-C3A	-2.70	1.40	1.45
13	v2	201	CYC	C4B-NB	-2.70	1.31	1.38
13	J3	201	CYC	C4A-C3A	-2.70	1.40	1.45
13	m2	201	CYC	C4B-NB	-2.70	1.31	1.38
13	z2	201	CYC	C4A-C3A	-2.69	1.40	1.45
13	L1	201	CYC	C4B-NB	-2.69	1.31	1.38
13	n2	201	CYC	C4A-C3A	-2.69	1.40	1.45
13	W1	201	CYC	C4B-NB	-2.69	1.31	1.38
13	J5	201	CYC	C4A-C3A	-2.69	1.40	1.45
13	x2	201	CYC	C4A-C3A	-2.68	1.40	1.45
13	a6	201	CYC	C4B-NB	-2.68	1.31	1.38
13	a5	201	CYC	C4B-NB	-2.68	1.31	1.38
13	Z5	301	CYC	C4B-NB	-2.68	1.31	1.38
13	P6	202	CYC	C1A-NA	-2.68	1.32	1.38
13	Z4	301	CYC	C4B-NB	-2.68	1.31	1.38
13	y2	201	CYC	C4A-C3A	-2.68	1.40	1.45
13	s2	201	CYC	C4B-NB	-2.67	1.31	1.38
13	N2	802	CYC	C4A-C3A	-2.67	1.40	1.45
13	S2	201	CYC	C4B-NB	-2.67	1.31	1.38
13	42	301	CYC	C4A-C3A	-2.67	1.40	1.45
13	Z7	301	CYC	C4A-C3A	-2.67	1.40	1.45
13	L2	201	CYC	C4B-NB	-2.67	1.31	1.38
13	e2	201	CYC	C4A-C3A	-2.67	1.40	1.45
13	t2	201	CYC	C4A-C3A	-2.67	1.40	1.45
13	O2	201	CYC	C4B-NB	-2.67	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f2	201	CYC	C4B-NB	-2.66	1.31	1.38
13	Q5	202	CYC	C4A-C3A	-2.66	1.40	1.45
13	Z1	301	CYC	C4B-NB	-2.66	1.31	1.38
13	52	301	CYC	C4A-C3A	-2.66	1.40	1.45
13	F2	201	CYC	C4A-C3A	-2.66	1.40	1.45
13	W2	201	CYC	C4A-C3A	-2.66	1.40	1.45
13	A2	201	CYC	C4A-C3A	-2.66	1.40	1.45
13	G2	201	CYC	C4B-NB	-2.66	1.31	1.38
13	M2	201	CYC	C4A-C3A	-2.65	1.40	1.45
13	L3	201	CYC	C4A-C3A	-2.65	1.40	1.45
13	a7	201	CYC	C4A-C3A	-2.65	1.40	1.45
13	S2	201	CYC	C4A-C3A	-2.65	1.40	1.45
13	A1	302	CYC	C4A-C3A	-2.65	1.40	1.45
13	y2	201	CYC	C4B-NB	-2.65	1.31	1.38
13	A6	301	CYC	C4A-C3A	-2.65	1.40	1.45
13	N2	802	CYC	C4B-NB	-2.65	1.31	1.38
13	F2	201	CYC	C4B-NB	-2.65	1.31	1.38
13	E2	201	CYC	C4B-NB	-2.65	1.31	1.38
13	C1	201	CYC	C4B-NB	-2.64	1.31	1.38
13	32	301	CYC	C4A-C3A	-2.64	1.40	1.45
13	V1	201	CYC	C4B-NB	-2.64	1.31	1.38
13	U2	201	CYC	C4B-NB	-2.64	1.31	1.38
13	p2	201	CYC	C4A-C3A	-2.63	1.40	1.45
13	N2	801	CYC	C4B-NB	-2.63	1.31	1.38
13	g2	201	CYC	C4B-NB	-2.63	1.31	1.38
13	s2	201	CYC	C4A-C3A	-2.63	1.40	1.45
13	W5	201	CYC	C4B-NB	-2.63	1.31	1.38
13	W6	201	CYC	C4B-NB	-2.63	1.31	1.38
13	22	301	CYC	C4A-C3A	-2.63	1.40	1.45
13	A6	302	CYC	C4A-C3A	-2.63	1.40	1.45
13	R2	201	CYC	C4B-NB	-2.63	1.31	1.38
13	Z6	301	CYC	C4B-NB	-2.62	1.31	1.38
13	M6	201	CYC	C4B-NB	-2.62	1.31	1.38
13	A1	301	CYC	C4A-C3A	-2.62	1.40	1.45
13	32	302	CYC	C4A-C3A	-2.62	1.40	1.45
13	P1	202	CYC	C4B-NB	-2.62	1.32	1.38
13	f2	201	CYC	C4A-C3A	-2.62	1.40	1.45
13	k2	201	CYC	C4B-NB	-2.62	1.32	1.38
13	D2	201	CYC	C4B-NB	-2.61	1.32	1.38
13	G1	201	CYC	C4B-NB	-2.61	1.32	1.38
13	M1	201	CYC	C4B-NB	-2.61	1.32	1.38
13	D4	201	CYC	C4A-C3A	-2.61	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t2	201	CYC	C4B-NB	-2.61	1.32	1.38
13	a7	201	CYC	C4B-NB	-2.61	1.32	1.38
13	L4	201	CYC	C4A-C3A	-2.61	1.40	1.45
13	P1	202	CYC	C1A-NA	-2.61	1.33	1.38
13	r2	201	CYC	C4A-C3A	-2.61	1.40	1.45
13	X2	201	CYC	C4B-NB	-2.61	1.32	1.38
13	L5	201	CYC	C4A-C3A	-2.61	1.40	1.45
13	Z3	301	CYC	C4B-NB	-2.61	1.32	1.38
13	L6	201	CYC	C4A-C3A	-2.61	1.40	1.45
13	P6	202	CYC	C4B-NB	-2.61	1.32	1.38
13	M2	201	CYC	C4B-NB	-2.60	1.32	1.38
13	w2	201	CYC	C4B-NB	-2.60	1.32	1.38
13	L7	201	CYC	C4A-C3A	-2.60	1.40	1.45
13	P2	201	CYC	C4B-NB	-2.60	1.32	1.38
13	e2	201	CYC	C4B-NB	-2.60	1.32	1.38
13	L6	201	CYC	C4B-NB	-2.60	1.32	1.38
13	U2	201	CYC	C4A-C3A	-2.60	1.40	1.45
13	j2	201	CYC	C4A-C3A	-2.60	1.40	1.45
13	K1	201	CYC	C4B-NB	-2.60	1.32	1.38
13	N1	201	CYC	C4B-NB	-2.60	1.32	1.38
13	V6	201	CYC	C4B-NB	-2.60	1.32	1.38
13	p2	201	CYC	C4B-NB	-2.60	1.32	1.38
13	O2	201	CYC	C4A-C3A	-2.60	1.40	1.45
13	a3	201	CYC	C4B-NB	-2.60	1.32	1.38
13	a6	201	CYC	C4A-C3A	-2.59	1.40	1.45
13	r2	201	CYC	C4B-NB	-2.59	1.32	1.38
13	P3	201	CYC	C4A-C3A	-2.59	1.40	1.45
13	G6	201	CYC	C4B-NB	-2.59	1.32	1.38
13	M4	201	CYC	C4B-NB	-2.59	1.32	1.38
13	Q2	201	CYC	C4A-C3A	-2.59	1.40	1.45
13	S5	201	CYC	C4B-NB	-2.59	1.32	1.38
13	F1	201	CYC	C4B-NB	-2.59	1.32	1.38
13	v2	201	CYC	C4A-C3A	-2.58	1.40	1.45
13	J1	201	CYC	C4B-NB	-2.58	1.32	1.38
13	A2	202	CYC	C4B-NB	-2.58	1.32	1.38
13	B5	201	CYC	C4B-NB	-2.58	1.32	1.38
13	M5	201	CYC	C4B-NB	-2.58	1.32	1.38
13	F4	201	CYC	C4B-NB	-2.58	1.32	1.38
13	42	302	CYC	C4A-C3A	-2.58	1.40	1.45
13	A1	301	CYC	C4B-NB	-2.58	1.32	1.38
13	K3	201	CYC	C4B-NB	-2.58	1.32	1.38
13	Z3	301	CYC	C4A-C3A	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a3	201	CYC	C4A-C3A	-2.58	1.40	1.45
13	H5	201	CYC	C4B-NB	-2.58	1.32	1.38
13	Z7	301	CYC	C4B-NB	-2.58	1.32	1.38
13	S1	201	CYC	C4B-NB	-2.58	1.32	1.38
13	C3	201	CYC	C4B-NB	-2.58	1.32	1.38
13	N6	201	CYC	C4B-NB	-2.57	1.32	1.38
13	U5	201	CYC	C4B-NB	-2.57	1.32	1.38
13	N2	801	CYC	C4A-C3A	-2.57	1.40	1.45
13	R2	201	CYC	C4A-C3A	-2.57	1.40	1.45
13	C6	201	CYC	C4B-NB	-2.57	1.32	1.38
13	52	301	CYC	C4B-NB	-2.57	1.32	1.38
13	L5	201	CYC	C4B-NB	-2.57	1.32	1.38
13	22	302	CYC	C4A-C3A	-2.56	1.40	1.45
13	T6	202	CYC	C4B-NB	-2.56	1.32	1.38
13	B1	201	CYC	C4B-NB	-2.56	1.32	1.38
13	N4	201	CYC	C4B-NB	-2.56	1.32	1.38
13	J6	202	CYC	C4B-NB	-2.56	1.32	1.38
13	P7	202	CYC	C4B-NB	-2.56	1.32	1.38
13	C5	201	CYC	C4B-NB	-2.56	1.32	1.38
13	P7	201	CYC	C4A-C3A	-2.56	1.40	1.45
13	T1	202	CYC	C4B-NB	-2.56	1.32	1.38
13	P5	201	CYC	C4B-NB	-2.56	1.32	1.38
13	B6	201	CYC	C4B-NB	-2.56	1.32	1.38
13	S4	201	CYC	C4B-NB	-2.56	1.32	1.38
13	P6	201	CYC	C4A-C3A	-2.56	1.40	1.45
13	K5	201	CYC	C4B-NB	-2.56	1.32	1.38
13	U4	201	CYC	C4B-NB	-2.55	1.32	1.38
13	L4	201	CYC	C4B-NB	-2.55	1.32	1.38
13	U1	201	CYC	C4B-NB	-2.55	1.32	1.38
13	R4	201	CYC	C4B-NB	-2.55	1.32	1.38
13	P4	201	CYC	C4B-NB	-2.55	1.32	1.38
13	T4	201	CYC	C4B-NB	-2.55	1.32	1.38
13	V5	201	CYC	C4B-NB	-2.55	1.32	1.38
13	D6	201	CYC	C4B-NB	-2.55	1.32	1.38
13	T5	202	CYC	C4B-NB	-2.55	1.32	1.38
13	K6	201	CYC	C4B-NB	-2.55	1.32	1.38
13	D2	201	CYC	C4A-C3A	-2.54	1.40	1.45
13	A6	301	CYC	C4B-NB	-2.54	1.32	1.38
13	D6	201	CYC	C4A-C3A	-2.54	1.40	1.45
13	D5	201	CYC	C4B-NB	-2.54	1.32	1.38
13	D1	201	CYC	C4B-NB	-2.54	1.32	1.38
13	F6	201	CYC	C4B-NB	-2.54	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J6	201	CYC	C4B-NB	-2.54	1.32	1.38
13	l2	201	CYC	C4B-NB	-2.54	1.32	1.38
13	i2	201	CYC	C4B-NB	-2.54	1.32	1.38
13	42	301	CYC	C4B-NB	-2.54	1.32	1.38
13	Q2	201	CYC	C4B-NB	-2.54	1.32	1.38
13	P3	202	CYC	C4B-NB	-2.54	1.32	1.38
13	T4	202	CYC	C4B-NB	-2.54	1.32	1.38
13	S6	201	CYC	C4B-NB	-2.54	1.32	1.38
13	X6	201	CYC	C4A-C3A	-2.54	1.40	1.45
13	j2	201	CYC	C4B-NB	-2.54	1.32	1.38
13	H6	201	CYC	C4B-NB	-2.54	1.32	1.38
13	M7	201	CYC	C4B-NB	-2.54	1.32	1.38
13	C7	201	CYC	C4B-NB	-2.54	1.32	1.38
13	R5	201	CYC	C4B-NB	-2.54	1.32	1.38
13	V4	201	CYC	C4B-NB	-2.54	1.32	1.38
13	G5	201	CYC	C4B-NB	-2.54	1.32	1.38
13	W4	201	CYC	C4B-NB	-2.53	1.32	1.38
13	R6	201	CYC	C4B-NB	-2.53	1.32	1.38
13	V3	201	CYC	C4B-NB	-2.53	1.32	1.38
13	J1	202	CYC	C4B-NB	-2.53	1.32	1.38
13	Q4	202	CYC	C4B-NB	-2.53	1.32	1.38
13	P5	202	CYC	C4B-NB	-2.53	1.32	1.38
13	D4	201	CYC	C4B-NB	-2.53	1.32	1.38
13	Q5	202	CYC	C4B-NB	-2.53	1.32	1.38
13	Q6	202	CYC	C4B-NB	-2.53	1.32	1.38
13	P4	202	CYC	C4B-NB	-2.53	1.32	1.38
13	X4	201	CYC	C4A-C3A	-2.53	1.40	1.45
13	H2	201	CYC	C4B-NB	-2.53	1.32	1.38
13	z2	201	CYC	C4B-NB	-2.53	1.32	1.38
13	U6	201	CYC	C4B-NB	-2.53	1.32	1.38
13	V7	201	CYC	C4B-NB	-2.52	1.32	1.38
13	E2	201	CYC	C4A-C3A	-2.52	1.40	1.45
13	T1	201	CYC	C4B-NB	-2.52	1.32	1.38
13	N5	201	CYC	C4B-NB	-2.52	1.32	1.38
13	R1	201	CYC	C4B-NB	-2.52	1.32	1.38
13	T5	201	CYC	C4B-NB	-2.52	1.32	1.38
13	W2	201	CYC	C4B-NB	-2.52	1.32	1.38
13	P1	201	CYC	C4A-C3A	-2.52	1.40	1.45
13	C1	202	CYC	C4B-NB	-2.52	1.32	1.38
13	x2	201	CYC	C4B-NB	-2.52	1.32	1.38
13	G4	201	CYC	C4B-NB	-2.52	1.32	1.38
13	Q5	201	CYC	C4B-NB	-2.52	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G7	201	CYC	C4B-NB	-2.52	1.32	1.38
13	Q7	201	CYC	C4B-NB	-2.52	1.32	1.38
13	a5	201	CYC	C4A-C3A	-2.52	1.40	1.45
13	I4	201	CYC	C4B-NB	-2.52	1.32	1.38
13	L1	201	CYC	C4A-C3A	-2.52	1.40	1.45
13	Q1	202	CYC	C4B-NB	-2.52	1.32	1.38
13	T6	201	CYC	C4B-NB	-2.52	1.32	1.38
13	K7	201	CYC	C4B-NB	-2.52	1.32	1.38
13	22	301	CYC	C4B-NB	-2.52	1.32	1.38
13	C6	202	CYC	C4B-NB	-2.52	1.32	1.38
13	J5	202	CYC	C4B-NB	-2.52	1.32	1.38
13	B4	201	CYC	C4B-NB	-2.52	1.32	1.38
13	C5	202	CYC	C4B-NB	-2.52	1.32	1.38
13	H1	201	CYC	C4B-NB	-2.51	1.32	1.38
13	J5	201	CYC	C4B-NB	-2.51	1.32	1.38
13	M3	201	CYC	C4B-NB	-2.51	1.32	1.38
13	D3	201	CYC	C4B-NB	-2.51	1.32	1.38
13	C3	202	CYC	C4B-NB	-2.51	1.32	1.38
13	C4	201	CYC	C4B-NB	-2.51	1.32	1.38
13	K4	201	CYC	C4B-NB	-2.51	1.32	1.38
13	J4	201	CYC	C4B-NB	-2.51	1.32	1.38
13	I6	201	CYC	C4B-NB	-2.51	1.32	1.38
13	A2	201	CYC	C4B-NB	-2.51	1.32	1.38
13	I5	201	CYC	C4B-NB	-2.51	1.32	1.38
13	E6	201	CYC	C4B-NB	-2.51	1.32	1.38
13	o2	801	CYC	C4A-C3A	-2.51	1.40	1.45
13	G2	201	CYC	C4A-C3A	-2.50	1.40	1.45
13	P4	202	CYC	C4A-C3A	-2.50	1.40	1.45
13	Q7	202	CYC	C4B-NB	-2.50	1.32	1.38
13	I3	201	CYC	C4B-NB	-2.50	1.32	1.38
13	I1	201	CYC	C4B-NB	-2.50	1.32	1.38
13	J4	202	CYC	C4B-NB	-2.50	1.32	1.38
13	Q6	201	CYC	C4B-NB	-2.50	1.32	1.38
13	E3	201	CYC	C4B-NB	-2.50	1.32	1.38
13	P6	201	CYC	C4B-NB	-2.50	1.32	1.38
13	C7	202	CYC	C4B-NB	-2.50	1.32	1.38
13	Z1	301	CYC	C4A-C3A	-2.50	1.40	1.45
13	P1	201	CYC	C4B-NB	-2.49	1.32	1.38
13	V1	202	CYC	C4B-NB	-2.49	1.32	1.38
13	32	301	CYC	C4B-NB	-2.49	1.32	1.38
13	Q4	201	CYC	C4B-NB	-2.49	1.32	1.38
13	Q1	201	CYC	C4B-NB	-2.49	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F3	201	CYC	C4B-NB	-2.49	1.32	1.38
13	a5	202	CYC	C4B-NB	-2.49	1.32	1.38
13	A1	302	CYC	C4B-NB	-2.49	1.32	1.38
13	E1	201	CYC	C4B-NB	-2.49	1.32	1.38
13	Q3	201	CYC	C4B-NB	-2.49	1.32	1.38
13	D7	201	CYC	C4B-NB	-2.49	1.32	1.38
13	I7	201	CYC	C4B-NB	-2.49	1.32	1.38
13	P7	201	CYC	C4B-NB	-2.49	1.32	1.38
13	X1	201	CYC	C4A-C3A	-2.49	1.40	1.45
13	H3	201	CYC	C4B-NB	-2.49	1.32	1.38
13	T3	201	CYC	C4B-NB	-2.49	1.32	1.38
13	N7	201	CYC	C4B-NB	-2.48	1.32	1.38
13	H4	201	CYC	C4B-NB	-2.48	1.32	1.38
13	Q3	202	CYC	C4B-NB	-2.48	1.32	1.38
13	a6	202	CYC	C4B-NB	-2.48	1.32	1.38
13	L7	201	CYC	C4B-NB	-2.48	1.32	1.38
13	E7	201	CYC	C4B-NB	-2.48	1.32	1.38
13	d2	201	CYC	C4B-NB	-2.48	1.32	1.38
13	a1	202	CYC	C4B-NB	-2.48	1.32	1.38
13	a1	201	CYC	C4A-C3A	-2.48	1.40	1.45
13	C4	202	CYC	C4B-NB	-2.48	1.32	1.38
13	V5	202	CYC	C4B-NB	-2.48	1.32	1.38
13	S7	201	CYC	C4B-NB	-2.47	1.32	1.38
13	Z6	301	CYC	C4A-C3A	-2.47	1.40	1.45
13	E5	201	CYC	C4B-NB	-2.47	1.32	1.38
13	F5	201	CYC	C4B-NB	-2.47	1.32	1.38
13	V2	201	CYC	C4B-NB	-2.47	1.32	1.38
13	a7	202	CYC	C4B-NB	-2.47	1.32	1.38
13	T7	201	CYC	C4B-NB	-2.47	1.32	1.38
13	R7	201	CYC	C4B-NB	-2.47	1.32	1.38
13	c2	801	CYC	C4B-NB	-2.47	1.32	1.38
13	a4	202	CYC	C4B-NB	-2.47	1.32	1.38
13	G3	201	CYC	C4B-NB	-2.47	1.32	1.38
13	W7	201	CYC	C4B-NB	-2.47	1.32	1.38
13	J3	201	CYC	C4B-NB	-2.47	1.32	1.38
13	V4	202	CYC	C4B-NB	-2.47	1.32	1.38
13	J7	201	CYC	C4B-NB	-2.47	1.32	1.38
13	Z4	301	CYC	C4A-C3A	-2.47	1.40	1.45
13	Z5	301	CYC	C4A-C3A	-2.46	1.40	1.45
13	B2	201	CYC	C4B-NB	-2.46	1.32	1.38
13	a2	201	CYC	C4B-NB	-2.46	1.32	1.38
13	R3	201	CYC	C4B-NB	-2.46	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S3	201	CYC	C4B-NB	-2.46	1.32	1.38
13	a3	202	CYC	C4B-NB	-2.46	1.32	1.38
13	U7	201	CYC	C4B-NB	-2.46	1.32	1.38
13	h2	201	CYC	C4A-C3A	-2.46	1.40	1.45
13	P5	201	CYC	C4A-C3A	-2.45	1.40	1.45
13	F1	202	CYC	C4B-NB	-2.45	1.32	1.38
13	V6	202	CYC	C4B-NB	-2.45	1.32	1.38
13	N3	201	CYC	C4B-NB	-2.45	1.32	1.38
13	X5	201	CYC	C4A-C3A	-2.45	1.40	1.45
13	F7	201	CYC	C4B-NB	-2.44	1.32	1.38
13	H7	201	CYC	C4B-NB	-2.44	1.32	1.38
13	V7	202	CYC	C4B-NB	-2.44	1.32	1.38
13	F6	202	CYC	C4B-NB	-2.44	1.32	1.38
13	T3	202	CYC	C4B-NB	-2.44	1.32	1.38
13	T2	201	CYC	C4B-NB	-2.44	1.32	1.38
13	V3	202	CYC	C4B-NB	-2.44	1.32	1.38
13	L3	201	CYC	C4B-NB	-2.44	1.32	1.38
13	U3	201	CYC	C4B-NB	-2.44	1.32	1.38
13	B7	201	CYC	C4B-NB	-2.44	1.32	1.38
13	f2	201	CYC	C4D-C3D	-2.44	1.37	1.42
13	P3	201	CYC	C4B-NB	-2.44	1.32	1.38
13	F5	202	CYC	C4B-NB	-2.44	1.32	1.38
13	F4	202	CYC	C4B-NB	-2.43	1.32	1.38
13	B3	201	CYC	C4B-NB	-2.43	1.32	1.38
13	P2	201	CYC	C4D-C3D	-2.43	1.37	1.42
13	T7	202	CYC	C4B-NB	-2.43	1.32	1.38
13	F7	202	CYC	C4B-NB	-2.43	1.32	1.38
13	E4	201	CYC	C4B-NB	-2.42	1.32	1.38
13	C2	201	CYC	C4B-NB	-2.42	1.32	1.38
13	W3	201	CYC	C4B-NB	-2.42	1.32	1.38
13	X3	201	CYC	C4A-C3A	-2.42	1.40	1.45
13	J3	202	CYC	C4B-NB	-2.41	1.32	1.38
13	J7	202	CYC	C4B-NB	-2.40	1.32	1.38
13	52	302	CYC	C4B-NB	-2.40	1.32	1.38
13	F3	202	CYC	C4B-NB	-2.40	1.32	1.38
13	X7	201	CYC	C4A-C3A	-2.40	1.40	1.45
13	Z1	301	CYC	C4D-C3D	-2.39	1.37	1.42
13	A6	302	CYC	C4B-NB	-2.39	1.32	1.38
13	42	302	CYC	C4B-NB	-2.37	1.32	1.38
13	32	302	CYC	C4B-NB	-2.36	1.32	1.38
13	22	302	CYC	C4B-NB	-2.36	1.32	1.38
13	M5	201	CYC	C4D-C3D	-2.36	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X6	201	CYC	C4D-C3D	-2.34	1.37	1.42
13	B2	202	CYC	C4B-NB	-2.33	1.32	1.38
13	X4	201	CYC	C4D-C3D	-2.33	1.37	1.42
13	Z5	301	CYC	C4D-C3D	-2.33	1.37	1.42
13	A1	301	CYC	C4D-C3D	-2.33	1.37	1.42
13	L1	201	CYC	C4D-C3D	-2.33	1.37	1.42
13	U2	201	CYC	C4D-C3D	-2.32	1.37	1.42
13	J6	201	CYC	C4D-C3D	-2.31	1.37	1.42
13	X1	201	CYC	C4D-C3D	-2.30	1.37	1.42
13	X5	201	CYC	C4D-C3D	-2.30	1.37	1.42
13	A6	301	CYC	C4D-C3D	-2.29	1.37	1.42
13	a6	201	CYC	C4D-C3D	-2.29	1.37	1.42
13	J1	201	CYC	C4D-C3D	-2.29	1.37	1.42
13	C1	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	M1	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	L6	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	L5	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	J3	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	M6	201	CYC	C4D-C3D	-2.28	1.37	1.42
13	a1	201	CYC	C4D-C3D	-2.27	1.37	1.42
13	C5	201	CYC	C4D-C3D	-2.26	1.37	1.42
13	p2	201	CYC	C4D-C3D	-2.26	1.37	1.42
13	Z6	301	CYC	C4D-C3D	-2.26	1.37	1.42
13	32	301	CYC	C4D-C3D	-2.26	1.37	1.42
13	X3	201	CYC	C4D-C3D	-2.26	1.37	1.42
13	M4	201	CYC	C4D-C3D	-2.26	1.37	1.42
13	J4	201	CYC	C4D-C3D	-2.25	1.37	1.42
13	t2	201	CYC	C4D-C3D	-2.25	1.37	1.42
13	A1	302	CYC	C4D-C3D	-2.25	1.37	1.42
13	C6	201	CYC	C4D-C3D	-2.24	1.37	1.42
13	J5	201	CYC	C4D-C3D	-2.23	1.37	1.42
13	52	301	CYC	C4D-C3D	-2.22	1.37	1.42
13	22	301	CYC	C4D-C3D	-2.21	1.37	1.42
13	J7	201	CYC	C4D-C3D	-2.21	1.37	1.42
13	G2	201	CYC	C4D-C3D	-2.20	1.37	1.42
13	Z4	301	CYC	C4D-C3D	-2.20	1.37	1.42
13	52	302	CYC	C4D-C3D	-2.20	1.37	1.42
13	X7	201	CYC	C4D-C3D	-2.19	1.37	1.42
13	a5	201	CYC	C4D-C3D	-2.19	1.37	1.42
13	C4	201	CYC	C4D-C3D	-2.19	1.38	1.42
13	V1	201	CYC	C4D-C3D	-2.19	1.38	1.42
13	X2	201	CYC	C4D-C3D	-2.18	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O2	201	CYC	C4D-C3D	-2.18	1.38	1.42
13	S2	201	CYC	C4D-C3D	-2.18	1.38	1.42
13	V5	201	CYC	C4D-C3D	-2.18	1.38	1.42
13	A6	302	CYC	C4D-C3D	-2.18	1.38	1.42
13	l2	201	CYC	C4D-C3D	-2.18	1.38	1.42
13	L4	201	CYC	C4D-C3D	-2.17	1.38	1.42
13	w2	201	CYC	C4D-C3D	-2.17	1.38	1.42
13	C3	201	CYC	C4D-C3D	-2.16	1.38	1.42
13	M3	201	CYC	C4D-C3D	-2.14	1.38	1.42
13	n2	201	CYC	C4D-C3D	-2.14	1.38	1.42
13	V2	201	CYC	C4D-C3D	-2.13	1.38	1.42
13	42	301	CYC	C4D-C3D	-2.13	1.38	1.42
13	e2	201	CYC	C4D-C3D	-2.12	1.38	1.42
13	m2	201	CYC	C4D-C3D	-2.12	1.38	1.42
13	C7	201	CYC	C4D-C3D	-2.11	1.38	1.42
13	N2	802	CYC	C4A-NA	-2.11	1.31	1.36
13	L7	201	CYC	C4D-C3D	-2.11	1.38	1.42
13	P4	201	CYC	C4D-C3D	-2.11	1.38	1.42
13	P6	202	CYC	C4D-C3D	-2.10	1.38	1.42
13	V4	201	CYC	C4D-C3D	-2.10	1.38	1.42
13	V6	201	CYC	C4D-C3D	-2.10	1.38	1.42
13	P1	202	CYC	C4D-C3D	-2.10	1.38	1.42
13	T2	201	CYC	C4D-C3D	-2.10	1.38	1.42
13	42	302	CYC	C4D-C3D	-2.10	1.38	1.42
13	x2	201	CYC	C4D-C3D	-2.09	1.38	1.42
13	N2	801	CYC	C4D-C3D	-2.09	1.38	1.42
13	g2	201	CYC	C4D-C3D	-2.09	1.38	1.42
13	L3	201	CYC	C4D-C3D	-2.09	1.38	1.42
13	N1	201	CYC	C4D-C3D	-2.08	1.38	1.42
13	s2	201	CYC	C4D-C3D	-2.08	1.38	1.42
13	h2	201	CYC	C4D-C3D	-2.08	1.38	1.42
13	v2	201	CYC	C4D-C3D	-2.08	1.38	1.42
13	a3	201	CYC	C4D-C3D	-2.08	1.38	1.42
13	P5	202	CYC	C4D-C3D	-2.08	1.38	1.42
13	U3	201	CYC	CAC-C3C	2.07	1.58	1.54
13	M7	201	CYC	C4D-C3D	-2.07	1.38	1.42
13	t2	201	CYC	C4A-NA	-2.07	1.31	1.36
13	B1	201	CYC	C4D-C3D	-2.07	1.38	1.42
13	M2	201	CYC	C4D-C3D	-2.07	1.38	1.42
13	a7	201	CYC	C4D-C3D	-2.07	1.38	1.42
13	V1	202	CYC	C4D-C3D	-2.06	1.38	1.42
13	K5	201	CYC	C4D-C3D	-2.06	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E7	201	CYC	C4A-NA	-2.06	1.31	1.36
13	R2	201	CYC	C4D-C3D	-2.06	1.38	1.42
13	B5	201	CYC	C4D-C3D	-2.06	1.38	1.42
13	K1	201	CYC	C4D-C3D	-2.05	1.38	1.42
13	E6	201	CYC	C4A-NA	-2.05	1.31	1.36
13	H6	201	CYC	C4D-C3D	-2.05	1.38	1.42
13	T5	201	CYC	C4A-NA	-2.04	1.32	1.36
13	L2	201	CYC	C4D-C3D	-2.04	1.38	1.42
13	G1	201	CYC	C4D-C3D	-2.04	1.38	1.42
13	V3	201	CYC	C4D-C3D	-2.04	1.38	1.42
13	E3	201	CYC	C4A-NA	-2.03	1.32	1.36
13	H1	201	CYC	C4D-C3D	-2.03	1.38	1.42
13	U1	201	CYC	C4D-C3D	-2.03	1.38	1.42
13	q2	201	CYC	C1B-C2B	-2.03	1.41	1.45
13	y2	201	CYC	C4D-C3D	-2.03	1.38	1.42
13	T2	201	CYC	C4A-NA	-2.03	1.32	1.36
13	L3	201	CYC	C4A-NA	-2.02	1.32	1.36
13	K6	201	CYC	C4D-C3D	-2.02	1.38	1.42
13	E2	201	CYC	C4D-C3D	-2.02	1.38	1.42
13	o2	801	CYC	C4D-C3D	-2.02	1.38	1.42
13	V5	202	CYC	C4D-C3D	-2.02	1.38	1.42
13	D6	201	CYC	C4D-C3D	-2.02	1.38	1.42
13	N6	201	CYC	C4D-C3D	-2.02	1.38	1.42
13	o2	801	CYC	C4A-NA	-2.01	1.32	1.36
13	W1	201	CYC	C4D-C3D	-2.01	1.38	1.42
13	F2	201	CYC	C4D-C3D	-2.01	1.38	1.42
13	V7	201	CYC	CAC-C3C	2.00	1.57	1.54
13	z2	201	CYC	C4D-C3D	-2.00	1.38	1.42

All (4018) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C1	202	CYC	OC-C1C-C2C	-22.95	107.93	126.17
13	C5	202	CYC	OC-C1C-C2C	-22.40	108.36	126.17
13	C6	202	CYC	OC-C1C-C2C	-22.30	108.44	126.17
13	C4	202	CYC	OC-C1C-C2C	-22.26	108.47	126.17
13	C3	202	CYC	OC-C1C-C2C	-21.72	108.90	126.17
13	C7	202	CYC	OC-C1C-C2C	-21.63	108.97	126.17
13	V6	201	CYC	OC-C1C-C2C	-21.58	109.01	126.17
13	V5	201	CYC	OC-C1C-C2C	-21.56	109.03	126.17
13	V4	201	CYC	OC-C1C-C2C	-21.55	109.03	126.17
13	a6	202	CYC	OC-C1C-C2C	-21.45	109.11	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W1	201	CYC	OC-C1C-C2C	-21.41	109.15	126.17
13	K6	201	CYC	OC-C1C-C2C	-21.40	109.15	126.17
13	B4	201	CYC	OC-C1C-C2C	-21.40	109.16	126.17
13	I3	201	CYC	OC-C1C-C2C	-21.38	109.17	126.17
13	T1	202	CYC	OC-C1C-C2C	-21.36	109.19	126.17
13	N6	201	CYC	OC-C1C-C2C	-21.28	109.25	126.17
13	B6	201	CYC	OC-C1C-C2C	-21.27	109.26	126.17
13	K1	201	CYC	OC-C1C-C2C	-21.23	109.29	126.17
13	T4	202	CYC	OC-C1C-C2C	-21.21	109.31	126.17
13	T6	202	CYC	OC-C1C-C2C	-21.21	109.31	126.17
13	V3	201	CYC	OC-C1C-C2C	-21.19	109.33	126.17
13	I5	201	CYC	OC-C1C-C2C	-21.17	109.34	126.17
13	G1	201	CYC	OC-C1C-C2C	-21.15	109.35	126.17
13	T5	202	CYC	OC-C1C-C2C	-21.13	109.37	126.17
13	B1	201	CYC	OC-C1C-C2C	-21.12	109.38	126.17
13	W6	201	CYC	OC-C1C-C2C	-21.12	109.38	126.17
13	I7	201	CYC	OC-C1C-C2C	-21.03	109.45	126.17
13	U5	201	CYC	OC-C1C-C2C	-21.01	109.47	126.17
13	52	302	CYC	OC-C1C-C2C	-21.01	109.47	126.17
13	H5	201	CYC	OC-C1C-C2C	-21.00	109.47	126.17
13	N1	201	CYC	OC-C1C-C2C	-21.00	109.47	126.17
13	a1	202	CYC	OC-C1C-C2C	-21.00	109.48	126.17
13	S2	201	CYC	OC-C1C-C2C	-20.97	109.50	126.17
13	T3	202	CYC	OC-C1C-C2C	-20.94	109.52	126.17
13	G3	201	CYC	OC-C1C-C2C	-20.92	109.54	126.17
13	G7	201	CYC	OC-C1C-C2C	-20.91	109.55	126.17
13	B5	201	CYC	OC-C1C-C2C	-20.91	109.55	126.17
13	I1	201	CYC	OC-C1C-C2C	-20.90	109.55	126.17
13	N7	201	CYC	OC-C1C-C2C	-20.88	109.57	126.17
13	L2	201	CYC	OC-C1C-C2C	-20.88	109.57	126.17
13	A1	302	CYC	OC-C1C-C2C	-20.86	109.59	126.17
13	U1	201	CYC	OC-C1C-C2C	-20.86	109.59	126.17
13	E1	201	CYC	OC-C1C-C2C	-20.85	109.59	126.17
13	K5	201	CYC	OC-C1C-C2C	-20.84	109.60	126.17
13	W2	201	CYC	OC-C1C-C2C	-20.84	109.60	126.17
13	U6	201	CYC	OC-C1C-C2C	-20.84	109.60	126.17
13	N3	201	CYC	OC-C1C-C2C	-20.83	109.61	126.17
13	H1	201	CYC	OC-C1C-C2C	-20.82	109.62	126.17
13	T7	202	CYC	OC-C1C-C2C	-20.79	109.64	126.17
13	K7	201	CYC	OC-C1C-C2C	-20.78	109.65	126.17
13	N5	201	CYC	OC-C1C-C2C	-20.76	109.67	126.17
13	V7	201	CYC	OC-C1C-C2C	-20.74	109.68	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F5	201	CYC	OC-C1C-C2C	-20.73	109.69	126.17
13	B7	201	CYC	OC-C1C-C2C	-20.73	109.69	126.17
13	I6	201	CYC	OC-C1C-C2C	-20.72	109.70	126.17
13	U7	201	CYC	OC-C1C-C2C	-20.71	109.70	126.17
13	T5	201	CYC	OC-C1C-C2C	-20.71	109.71	126.17
13	r2	201	CYC	OC-C1C-C2C	-20.71	109.71	126.17
13	V1	202	CYC	OC-C1C-C2C	-20.70	109.71	126.17
13	B3	201	CYC	OC-C1C-C2C	-20.70	109.72	126.17
13	V6	202	CYC	OC-C1C-C2C	-20.70	109.72	126.17
13	N2	801	CYC	OC-C1C-C2C	-20.69	109.72	126.17
13	W4	201	CYC	OC-C1C-C2C	-20.68	109.73	126.17
13	H6	201	CYC	OC-C1C-C2C	-20.68	109.73	126.17
13	E5	201	CYC	OC-C1C-C2C	-20.68	109.73	126.17
13	F4	201	CYC	OC-C1C-C2C	-20.66	109.75	126.17
13	F7	201	CYC	OC-C1C-C2C	-20.65	109.75	126.17
13	E4	201	CYC	OC-C1C-C2C	-20.64	109.76	126.17
13	J3	202	CYC	OC-C1C-C2C	-20.63	109.77	126.17
13	J5	202	CYC	OC-C1C-C2C	-20.63	109.77	126.17
13	E6	201	CYC	OC-C1C-C2C	-20.63	109.77	126.17
13	V2	201	CYC	OC-C1C-C2C	-20.62	109.78	126.17
13	H3	201	CYC	OC-C1C-C2C	-20.61	109.79	126.17
13	T4	201	CYC	OC-C1C-C2C	-20.61	109.79	126.17
13	H7	201	CYC	OC-C1C-C2C	-20.60	109.79	126.17
13	L1	201	CYC	OC-C1C-C2C	-20.60	109.80	126.17
13	J7	202	CYC	OC-C1C-C2C	-20.59	109.80	126.17
13	i2	201	CYC	OC-C1C-C2C	-20.59	109.81	126.17
13	F3	201	CYC	OC-C1C-C2C	-20.56	109.83	126.17
13	H4	201	CYC	OC-C1C-C2C	-20.56	109.83	126.17
13	Q3	202	CYC	OC-C1C-C2C	-20.56	109.83	126.17
13	J4	202	CYC	OC-C1C-C2C	-20.55	109.83	126.17
13	V7	202	CYC	OC-C1C-C2C	-20.55	109.83	126.17
13	J1	202	CYC	OC-C1C-C2C	-20.54	109.84	126.17
13	N4	201	CYC	OC-C1C-C2C	-20.54	109.84	126.17
13	F1	201	CYC	OC-C1C-C2C	-20.52	109.86	126.17
13	Q5	202	CYC	OC-C1C-C2C	-20.52	109.86	126.17
13	Q1	202	CYC	OC-C1C-C2C	-20.51	109.86	126.17
13	H2	201	CYC	OC-C1C-C2C	-20.50	109.87	126.17
13	X2	201	CYC	OC-C1C-C2C	-20.50	109.87	126.17
13	n2	201	CYC	OC-C1C-C2C	-20.50	109.88	126.17
13	T3	201	CYC	OC-C1C-C2C	-20.50	109.88	126.17
13	R1	201	CYC	OC-C1C-C2C	-20.48	109.89	126.17
13	D7	201	CYC	OC-C1C-C2C	-20.47	109.89	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L3	201	CYC	OC-C1C-C2C	-20.47	109.90	126.17
13	L7	201	CYC	OC-C1C-C2C	-20.47	109.90	126.17
13	a5	202	CYC	OC-C1C-C2C	-20.46	109.90	126.17
13	A6	302	CYC	OC-C1C-C2C	-20.46	109.90	126.17
13	J6	202	CYC	OC-C1C-C2C	-20.45	109.91	126.17
13	Q7	202	CYC	OC-C1C-C2C	-20.45	109.91	126.17
13	l2	201	CYC	OC-C1C-C2C	-20.43	109.93	126.17
13	a4	202	CYC	OC-C1C-C2C	-20.43	109.93	126.17
13	M5	201	CYC	OC-C1C-C2C	-20.43	109.93	126.17
13	m2	201	CYC	OC-C1C-C2C	-20.41	109.94	126.17
13	k2	201	CYC	OC-C1C-C2C	-20.39	109.96	126.17
13	V3	202	CYC	OC-C1C-C2C	-20.39	109.96	126.17
13	T7	201	CYC	OC-C1C-C2C	-20.38	109.97	126.17
13	T1	201	CYC	OC-C1C-C2C	-20.38	109.97	126.17
13	K4	201	CYC	OC-C1C-C2C	-20.38	109.97	126.17
13	J5	201	CYC	OC-C1C-C2C	-20.37	109.97	126.17
13	J1	201	CYC	OC-C1C-C2C	-20.37	109.97	126.17
13	P7	201	CYC	OC-C1C-C2C	-20.37	109.98	126.17
13	V5	202	CYC	OC-C1C-C2C	-20.35	109.99	126.17
13	A6	301	CYC	OC-C1C-C2C	-20.35	109.99	126.17
13	Q4	202	CYC	OC-C1C-C2C	-20.34	110.00	126.17
13	L5	201	CYC	OC-C1C-C2C	-20.34	110.00	126.17
13	M6	201	CYC	OC-C1C-C2C	-20.34	110.00	126.17
13	D3	201	CYC	OC-C1C-C2C	-20.33	110.01	126.17
13	V4	202	CYC	OC-C1C-C2C	-20.33	110.01	126.17
13	R6	201	CYC	OC-C1C-C2C	-20.32	110.01	126.17
13	o2	801	CYC	OC-C1C-C2C	-20.32	110.02	126.17
13	P2	201	CYC	OC-C1C-C2C	-20.32	110.02	126.17
13	E3	201	CYC	OC-C1C-C2C	-20.32	110.02	126.17
13	T6	201	CYC	OC-C1C-C2C	-20.32	110.02	126.17
13	W5	201	CYC	OC-C1C-C2C	-20.31	110.02	126.17
13	42	301	CYC	OC-C1C-C2C	-20.31	110.02	126.17
13	D4	201	CYC	OC-C1C-C2C	-20.31	110.02	126.17
13	J6	201	CYC	OC-C1C-C2C	-20.30	110.03	126.17
13	A2	202	CYC	OC-C1C-C2C	-20.30	110.04	126.17
13	G4	201	CYC	OC-C1C-C2C	-20.30	110.04	126.17
13	E7	201	CYC	OC-C1C-C2C	-20.28	110.05	126.17
13	52	301	CYC	OC-C1C-C2C	-20.28	110.05	126.17
13	P4	202	CYC	OC-C1C-C2C	-20.28	110.05	126.17
13	P3	201	CYC	OC-C1C-C2C	-20.28	110.05	126.17
13	J7	201	CYC	OC-C1C-C2C	-20.27	110.06	126.17
13	P5	201	CYC	OC-C1C-C2C	-20.27	110.06	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O2	201	CYC	OC-C1C-C2C	-20.26	110.06	126.17
13	Q6	202	CYC	OC-C1C-C2C	-20.26	110.06	126.17
13	J3	201	CYC	OC-C1C-C2C	-20.26	110.06	126.17
13	A1	301	CYC	OC-C1C-C2C	-20.25	110.07	126.17
13	V1	201	CYC	OC-C1C-C2C	-20.25	110.07	126.17
13	A2	201	CYC	OC-C1C-C2C	-20.25	110.07	126.17
13	y2	201	CYC	OC-C1C-C2C	-20.25	110.07	126.17
13	Q7	201	CYC	OC-C1C-C2C	-20.22	110.10	126.17
13	J4	201	CYC	OC-C1C-C2C	-20.22	110.10	126.17
13	U4	201	CYC	OC-C1C-C2C	-20.21	110.11	126.17
13	F7	202	CYC	OC-C1C-C2C	-20.21	110.11	126.17
13	Q3	201	CYC	OC-C1C-C2C	-20.20	110.11	126.17
13	I4	201	CYC	OC-C1C-C2C	-20.20	110.11	126.17
13	D6	201	CYC	OC-C1C-C2C	-20.20	110.11	126.17
13	W7	201	CYC	OC-C1C-C2C	-20.20	110.11	126.17
13	M4	201	CYC	OC-C1C-C2C	-20.19	110.12	126.17
13	P6	201	CYC	OC-C1C-C2C	-20.19	110.12	126.17
13	K3	201	CYC	OC-C1C-C2C	-20.19	110.12	126.17
13	F3	202	CYC	OC-C1C-C2C	-20.18	110.12	126.17
13	Q5	201	CYC	OC-C1C-C2C	-20.16	110.14	126.17
13	T2	201	CYC	OC-C1C-C2C	-20.16	110.14	126.17
13	Q1	201	CYC	OC-C1C-C2C	-20.16	110.15	126.17
13	R5	201	CYC	OC-C1C-C2C	-20.15	110.15	126.17
13	W3	201	CYC	OC-C1C-C2C	-20.15	110.15	126.17
13	Q2	201	CYC	OC-C1C-C2C	-20.14	110.16	126.17
13	M3	201	CYC	OC-C1C-C2C	-20.14	110.16	126.17
13	32	302	CYC	OC-C1C-C2C	-20.13	110.17	126.17
13	Q4	201	CYC	OC-C1C-C2C	-20.12	110.17	126.17
13	M7	201	CYC	OC-C1C-C2C	-20.12	110.17	126.17
13	P1	202	CYC	OC-C1C-C2C	-20.11	110.19	126.17
13	D1	201	CYC	OC-C1C-C2C	-20.10	110.19	126.17
13	L4	201	CYC	OC-C1C-C2C	-20.08	110.21	126.17
13	F6	202	CYC	OC-C1C-C2C	-20.08	110.21	126.17
13	D5	201	CYC	OC-C1C-C2C	-20.07	110.21	126.17
13	N2	802	CYC	OC-C1C-C2C	-20.07	110.22	126.17
13	F4	202	CYC	OC-C1C-C2C	-20.07	110.22	126.17
13	G6	201	CYC	OC-C1C-C2C	-20.05	110.23	126.17
13	P1	201	CYC	OC-C1C-C2C	-20.04	110.24	126.17
13	P3	202	CYC	OC-C1C-C2C	-20.03	110.25	126.17
13	p2	201	CYC	OC-C1C-C2C	-20.02	110.25	126.17
13	R4	201	CYC	OC-C1C-C2C	-20.02	110.25	126.17
13	F5	202	CYC	OC-C1C-C2C	-20.02	110.25	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	f2	201	CYC	OC-C1C-C2C	-20.01	110.26	126.17
13	a7	202	CYC	OC-C1C-C2C	-20.01	110.26	126.17
13	G5	201	CYC	OC-C1C-C2C	-20.01	110.26	126.17
13	P7	202	CYC	OC-C1C-C2C	-20.01	110.26	126.17
13	P6	202	CYC	OC-C1C-C2C	-19.98	110.29	126.17
13	M1	201	CYC	OC-C1C-C2C	-19.96	110.30	126.17
13	Q6	201	CYC	OC-C1C-C2C	-19.96	110.31	126.17
13	F2	201	CYC	OC-C1C-C2C	-19.94	110.32	126.17
13	d2	201	CYC	OC-C1C-C2C	-19.94	110.32	126.17
13	E2	201	CYC	OC-C1C-C2C	-19.93	110.33	126.17
13	a3	202	CYC	OC-C1C-C2C	-19.93	110.33	126.17
13	P4	201	CYC	OC-C1C-C2C	-19.93	110.33	126.17
13	x2	201	CYC	OC-C1C-C2C	-19.92	110.34	126.17
13	F1	202	CYC	OC-C1C-C2C	-19.91	110.34	126.17
13	22	301	CYC	OC-C1C-C2C	-19.91	110.34	126.17
13	P5	202	CYC	OC-C1C-C2C	-19.90	110.35	126.17
13	L6	201	CYC	OC-C1C-C2C	-19.88	110.37	126.17
13	22	302	CYC	OC-C1C-C2C	-19.85	110.39	126.17
13	s2	201	CYC	OC-C1C-C2C	-19.84	110.39	126.17
13	X7	201	CYC	OC-C1C-C2C	-19.84	110.40	126.17
13	v2	201	CYC	OC-C1C-C2C	-19.82	110.41	126.17
13	32	301	CYC	OC-C1C-C2C	-19.79	110.44	126.17
13	X3	201	CYC	OC-C1C-C2C	-19.78	110.44	126.17
13	a2	201	CYC	OC-C1C-C2C	-19.77	110.45	126.17
13	F6	201	CYC	OC-C1C-C2C	-19.73	110.48	126.17
13	G2	201	CYC	OC-C1C-C2C	-19.67	110.54	126.17
13	U3	201	CYC	OC-C1C-C2C	-19.63	110.56	126.17
13	R2	201	CYC	OC-C1C-C2C	-19.60	110.59	126.17
13	R7	201	CYC	OC-C1C-C2C	-19.59	110.60	126.17
13	R3	201	CYC	OC-C1C-C2C	-19.56	110.62	126.17
13	e2	201	CYC	OC-C1C-C2C	-19.45	110.71	126.17
13	w2	201	CYC	OC-C1C-C2C	-19.44	110.72	126.17
13	42	302	CYC	OC-C1C-C2C	-19.44	110.72	126.17
13	D2	201	CYC	OC-C1C-C2C	-19.43	110.73	126.17
13	S4	201	CYC	OC-C1C-C2C	-19.39	110.75	126.17
13	j2	201	CYC	OC-C1C-C2C	-19.37	110.77	126.17
13	B2	201	CYC	OC-C1C-C2C	-19.33	110.81	126.17
13	C2	201	CYC	OC-C1C-C2C	-19.19	110.92	126.17
13	S1	201	CYC	OC-C1C-C2C	-19.10	110.99	126.17
13	c2	801	CYC	OC-C1C-C2C	-19.07	111.01	126.17
13	S5	201	CYC	OC-C1C-C2C	-19.03	111.05	126.17
13	S6	201	CYC	OC-C1C-C2C	-19.00	111.07	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X1	201	CYC	OC-C1C-C2C	-18.97	111.09	126.17
13	S7	201	CYC	OC-C1C-C2C	-18.95	111.11	126.17
13	h2	201	CYC	OC-C1C-C2C	-18.92	111.13	126.17
13	S3	201	CYC	OC-C1C-C2C	-18.81	111.22	126.17
13	X6	201	CYC	OC-C1C-C2C	-18.76	111.25	126.17
13	Z7	301	CYC	OC-C1C-C2C	-18.76	111.25	126.17
13	Z3	301	CYC	OC-C1C-C2C	-18.53	111.44	126.17
13	t2	201	CYC	OC-C1C-C2C	-18.43	111.52	126.17
13	z2	201	CYC	OC-C1C-C2C	-18.43	111.52	126.17
13	U2	201	CYC	OC-C1C-C2C	-18.29	111.63	126.17
13	B2	202	CYC	OC-C1C-C2C	-18.27	111.65	126.17
13	X4	201	CYC	OC-C1C-C2C	-18.22	111.69	126.17
13	a1	201	CYC	OC-C1C-C2C	-18.20	111.70	126.17
13	M2	201	CYC	OC-C1C-C2C	-18.18	111.72	126.17
13	Z6	301	CYC	OC-C1C-C2C	-18.17	111.72	126.17
13	a6	201	CYC	OC-C1C-C2C	-18.13	111.76	126.17
13	a5	201	CYC	OC-C1C-C2C	-17.97	111.89	126.17
13	Z5	301	CYC	OC-C1C-C2C	-17.96	111.89	126.17
13	C1	201	CYC	OC-C1C-C2C	-17.96	111.89	126.17
13	X5	201	CYC	OC-C1C-C2C	-17.92	111.92	126.17
13	Z4	301	CYC	OC-C1C-C2C	-17.90	111.94	126.17
13	a3	201	CYC	OC-C1C-C2C	-17.89	111.94	126.17
13	Z1	301	CYC	OC-C1C-C2C	-17.88	111.96	126.17
13	a7	201	CYC	OC-C1C-C2C	-17.87	111.97	126.17
13	g2	201	CYC	OC-C1C-C2C	-17.85	111.98	126.17
13	C4	201	CYC	OC-C1C-C2C	-17.82	112.00	126.17
13	C6	201	CYC	OC-C1C-C2C	-17.82	112.01	126.17
13	C5	201	CYC	OC-C1C-C2C	-17.80	112.02	126.17
13	C7	201	CYC	OC-C1C-C2C	-17.69	112.11	126.17
13	C3	201	CYC	OC-C1C-C2C	-17.62	112.17	126.17
13	o2	801	CYC	OC-C1C-NC	-13.91	108.53	124.93
13	g2	201	CYC	OC-C1C-NC	-13.84	108.62	124.93
13	o2	801	CYC	CHD-C4C-NC	-13.72	108.51	125.63
13	A2	202	CYC	CHD-C4C-NC	-13.60	108.66	125.63
13	L1	201	CYC	OC-C1C-NC	-13.47	109.05	124.93
13	k2	201	CYC	CHD-C4C-NC	-13.43	108.87	125.63
13	W7	201	CYC	CHD-C4C-NC	-13.29	109.04	125.63
13	N2	802	CYC	CHD-C4C-NC	-13.25	109.09	125.63
13	W3	201	CYC	CHD-C4C-NC	-13.25	109.09	125.63
13	K3	201	CYC	CHD-C4C-NC	-13.25	109.10	125.63
13	V2	201	CYC	OC-C1C-NC	-13.24	109.32	124.93
13	K7	201	CYC	CHD-C4C-NC	-13.23	109.12	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P6	201	CYC	CHD-C4C-NC	-13.22	109.13	125.63
13	W6	201	CYC	CHD-C4C-NC	-13.22	109.13	125.63
13	H2	201	CYC	CHD-C4C-NC	-13.20	109.15	125.63
13	Q3	202	CYC	CHD-C4C-NC	-13.20	109.16	125.63
13	P5	201	CYC	CHD-C4C-NC	-13.20	109.16	125.63
13	w2	201	CYC	OC-C1C-NC	-13.19	109.38	124.93
13	P4	202	CYC	CHD-C4C-NC	-13.19	109.17	125.63
13	X6	201	CYC	OC-C1C-NC	-13.18	109.39	124.93
13	d2	201	CYC	CHD-C4C-NC	-13.18	109.17	125.63
13	U3	201	CYC	CHD-C4C-NC	-13.18	109.17	125.63
13	R1	201	CYC	CHD-C4C-NC	-13.17	109.19	125.63
13	N2	802	CYC	OC-C1C-NC	-13.17	109.41	124.93
13	U7	201	CYC	CHD-C4C-NC	-13.16	109.20	125.63
13	P1	201	CYC	CHD-C4C-NC	-13.15	109.22	125.63
13	G5	201	CYC	CHD-C4C-NC	-13.14	109.22	125.63
13	U3	201	CYC	OC-C1C-NC	-13.13	109.45	124.93
13	c2	801	CYC	CHD-C4C-NC	-13.12	109.25	125.63
13	F5	201	CYC	CHD-C4C-NC	-13.11	109.27	125.63
13	R5	201	CYC	CHD-C4C-NC	-13.09	109.28	125.63
13	F4	201	CYC	CHD-C4C-NC	-13.09	109.29	125.63
13	F3	202	CYC	CHD-C4C-NC	-13.08	109.30	125.63
13	Q2	201	CYC	CHD-C4C-NC	-13.08	109.30	125.63
13	U4	201	CYC	CHD-C4C-NC	-13.08	109.30	125.63
13	L6	201	CYC	OC-C1C-NC	-13.08	109.52	124.93
13	P7	201	CYC	CHD-C4C-NC	-13.07	109.31	125.63
13	F7	202	CYC	CHD-C4C-NC	-13.06	109.33	125.63
13	X1	201	CYC	OC-C1C-NC	-13.06	109.53	124.93
13	a6	201	CYC	OC-C1C-NC	-13.05	109.54	124.93
13	M1	201	CYC	OC-C1C-NC	-13.05	109.55	124.93
13	l2	201	CYC	OC-C1C-NC	-13.05	109.55	124.93
13	Q4	202	CYC	CHD-C4C-NC	-13.04	109.35	125.63
13	W4	201	CYC	CHD-C4C-NC	-13.04	109.36	125.63
13	N5	201	CYC	CHD-C4C-NC	-13.03	109.36	125.63
13	P3	201	CYC	CHD-C4C-NC	-13.03	109.36	125.63
13	N2	801	CYC	OC-C1C-NC	-13.03	109.57	124.93
13	F3	201	CYC	CHD-C4C-NC	-13.03	109.36	125.63
13	R4	201	CYC	CHD-C4C-NC	-13.03	109.37	125.63
13	C6	201	CYC	OC-C1C-NC	-13.02	109.58	124.93
13	I7	201	CYC	CHD-C4C-NC	-13.01	109.39	125.63
13	T7	202	CYC	CHD-C4C-NC	-12.99	109.41	125.63
13	Q6	202	CYC	CHD-C4C-NC	-12.99	109.41	125.63
13	J5	201	CYC	OC-C1C-NC	-12.99	109.61	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R6	201	CYC	CHD-C4C-NC	-12.99	109.42	125.63
13	F5	202	CYC	CHD-C4C-NC	-12.98	109.42	125.63
13	F7	201	CYC	CHD-C4C-NC	-12.98	109.43	125.63
13	J1	201	CYC	OC-C1C-NC	-12.98	109.63	124.93
13	Q1	202	CYC	CHD-C4C-NC	-12.98	109.43	125.63
13	E7	201	CYC	OC-C1C-NC	-12.98	109.63	124.93
13	V5	202	CYC	OC-C1C-NC	-12.97	109.64	124.93
13	M6	201	CYC	OC-C1C-NC	-12.97	109.64	124.93
13	P2	201	CYC	OC-C1C-NC	-12.97	109.64	124.93
13	P1	202	CYC	OC-C1C-NC	-12.96	109.65	124.93
13	A1	301	CYC	OC-C1C-NC	-12.95	109.66	124.93
13	G6	201	CYC	CHD-C4C-NC	-12.95	109.46	125.63
13	X7	201	CYC	OC-C1C-NC	-12.95	109.66	124.93
13	J6	201	CYC	OC-C1C-NC	-12.95	109.67	124.93
13	R7	201	CYC	CHD-C4C-NC	-12.95	109.47	125.63
13	J4	201	CYC	OC-C1C-NC	-12.94	109.67	124.93
13	I3	201	CYC	CHD-C4C-NC	-12.94	109.48	125.63
13	G4	201	CYC	CHD-C4C-NC	-12.94	109.48	125.63
13	Q7	202	CYC	CHD-C4C-NC	-12.93	109.48	125.63
13	W5	201	CYC	CHD-C4C-NC	-12.93	109.49	125.63
13	L5	201	CYC	OC-C1C-NC	-12.92	109.69	124.93
13	M4	201	CYC	OC-C1C-NC	-12.92	109.70	124.93
13	C6	202	CYC	OC-C1C-NC	-12.92	109.70	124.93
13	U6	201	CYC	CHD-C4C-NC	-12.92	109.50	125.63
13	X3	201	CYC	OC-C1C-NC	-12.91	109.71	124.93
13	I5	201	CYC	CHD-C4C-NC	-12.91	109.51	125.63
13	T3	202	CYC	CHD-C4C-NC	-12.91	109.52	125.63
13	Q5	202	CYC	CHD-C4C-NC	-12.91	109.52	125.63
13	J7	201	CYC	OC-C1C-NC	-12.91	109.71	124.93
13	K1	201	CYC	OC-C1C-NC	-12.91	109.72	124.93
13	I7	201	CYC	OC-C1C-NC	-12.90	109.72	124.93
13	x2	201	CYC	OC-C1C-NC	-12.90	109.72	124.93
13	J3	201	CYC	OC-C1C-NC	-12.90	109.73	124.93
13	F4	202	CYC	CHD-C4C-NC	-12.90	109.53	125.63
13	M5	201	CYC	OC-C1C-NC	-12.89	109.73	124.93
13	Z7	301	CYC	OC-C1C-NC	-12.89	109.74	124.93
13	P5	202	CYC	OC-C1C-NC	-12.89	109.74	124.93
13	T4	201	CYC	OC-C1C-NC	-12.88	109.74	124.93
13	L7	201	CYC	OC-C1C-NC	-12.88	109.74	124.93
13	K7	201	CYC	OC-C1C-NC	-12.88	109.75	124.93
13	X2	201	CYC	OC-C1C-NC	-12.88	109.75	124.93
13	C1	201	CYC	OC-C1C-NC	-12.88	109.75	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J4	202	CYC	OC-C1C-NC	-12.88	109.75	124.93
13	V7	202	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	L3	201	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	F2	201	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	Z5	301	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	a5	201	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	J5	202	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	P6	202	CYC	OC-C1C-NC	-12.87	109.76	124.93
13	D3	201	CYC	OC-C1C-NC	-12.86	109.77	124.93
13	R3	201	CYC	CHD-C4C-NC	-12.86	109.58	125.63
13	F6	201	CYC	CHD-C4C-NC	-12.86	109.58	125.63
13	F1	202	CYC	CHD-C4C-NC	-12.85	109.59	125.63
13	G3	201	CYC	CHD-C4C-NC	-12.85	109.60	125.63
13	G7	201	CYC	CHD-C4C-NC	-12.84	109.60	125.63
13	L4	201	CYC	OC-C1C-NC	-12.84	109.79	124.93
13	G2	201	CYC	CHD-C4C-NC	-12.84	109.60	125.63
13	Z3	301	CYC	OC-C1C-NC	-12.84	109.79	124.93
13	B7	201	CYC	OC-C1C-NC	-12.83	109.80	124.93
13	C7	201	CYC	OC-C1C-NC	-12.83	109.80	124.93
13	W1	201	CYC	CHD-C4C-NC	-12.83	109.61	125.63
13	M2	201	CYC	OC-C1C-NC	-12.83	109.81	124.93
13	U4	201	CYC	OC-C1C-NC	-12.83	109.81	124.93
13	m2	201	CYC	OC-C1C-NC	-12.83	109.81	124.93
13	N4	201	CYC	OC-C1C-NC	-12.82	109.81	124.93
13	R6	201	CYC	OC-C1C-NC	-12.82	109.81	124.93
13	P4	201	CYC	OC-C1C-NC	-12.82	109.81	124.93
13	Z6	301	CYC	OC-C1C-NC	-12.82	109.81	124.93
13	X4	201	CYC	OC-C1C-NC	-12.82	109.82	124.93
13	E3	201	CYC	OC-C1C-NC	-12.82	109.82	124.93
13	T5	201	CYC	OC-C1C-NC	-12.81	109.82	124.93
13	T4	202	CYC	CHD-C4C-NC	-12.81	109.63	125.63
13	a7	201	CYC	OC-C1C-NC	-12.81	109.82	124.93
13	A2	201	CYC	CHD-C4C-NC	-12.81	109.64	125.63
13	N1	201	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	P3	202	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	C3	202	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	r2	201	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	C7	202	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	J6	202	CYC	OC-C1C-NC	-12.81	109.83	124.93
13	K3	201	CYC	OC-C1C-NC	-12.80	109.84	124.93
13	N7	201	CYC	CHD-C4C-NC	-12.80	109.65	125.63
13	C2	201	CYC	OC-C1C-NC	-12.80	109.84	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X5	201	CYC	OC-C1C-NC	-12.80	109.84	124.93
13	N4	201	CYC	CHD-C4C-NC	-12.80	109.65	125.63
13	U7	201	CYC	OC-C1C-NC	-12.80	109.84	124.93
13	B3	201	CYC	OC-C1C-NC	-12.80	109.84	124.93
13	A6	301	CYC	OC-C1C-NC	-12.80	109.84	124.93
13	H7	201	CYC	CHD-C4C-NC	-12.80	109.66	125.63
13	V4	202	CYC	OC-C1C-NC	-12.79	109.85	124.93
13	V3	202	CYC	OC-C1C-NC	-12.79	109.85	124.93
13	a3	201	CYC	OC-C1C-NC	-12.79	109.85	124.93
13	K5	201	CYC	CHD-C4C-NC	-12.79	109.67	125.63
13	I3	201	CYC	OC-C1C-NC	-12.78	109.86	124.93
13	F6	202	CYC	CHD-C4C-NC	-12.78	109.68	125.63
13	U2	201	CYC	OC-C1C-NC	-12.78	109.87	124.93
13	C1	202	CYC	OC-C1C-NC	-12.78	109.87	124.93
13	Z1	301	CYC	OC-C1C-NC	-12.78	109.87	124.93
13	j2	201	CYC	OC-C1C-NC	-12.77	109.87	124.93
13	G3	201	CYC	OC-C1C-NC	-12.77	109.88	124.93
13	K4	201	CYC	OC-C1C-NC	-12.77	109.88	124.93
13	C5	202	CYC	OC-C1C-NC	-12.76	109.89	124.93
13	n2	201	CYC	OC-C1C-NC	-12.76	109.89	124.93
13	d2	201	CYC	OC-C1C-NC	-12.76	109.89	124.93
13	k2	201	CYC	OC-C1C-NC	-12.76	109.89	124.93
13	E4	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
13	B4	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
13	M3	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
13	E5	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
13	I5	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
13	F1	201	CYC	CHD-C4C-NC	-12.75	109.72	125.63
13	S2	201	CYC	OC-C1C-NC	-12.74	109.91	124.93
13	J3	202	CYC	OC-C1C-NC	-12.74	109.91	124.93
13	f2	201	CYC	OC-C1C-NC	-12.73	109.92	124.93
13	G4	201	CYC	OC-C1C-NC	-12.73	109.92	124.93
13	A2	201	CYC	OC-C1C-NC	-12.73	109.92	124.93
13	T7	201	CYC	OC-C1C-NC	-12.73	109.92	124.93
13	h2	201	CYC	CHD-C4C-NC	-12.72	109.75	125.63
13	32	301	CYC	OC-C1C-NC	-12.72	109.93	124.93
13	K4	201	CYC	CHD-C4C-NC	-12.72	109.76	125.63
13	V6	202	CYC	OC-C1C-NC	-12.72	109.94	124.93
13	T5	202	CYC	CHD-C4C-NC	-12.72	109.76	125.63
13	T2	201	CYC	OC-C1C-NC	-12.71	109.94	124.93
13	j2	201	CYC	CHD-C4C-NC	-12.71	109.76	125.63
13	C4	202	CYC	OC-C1C-NC	-12.71	109.95	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D7	201	CYC	OC-C1C-NC	-12.71	109.95	124.93
13	B7	201	CYC	CHD-C4C-NC	-12.70	109.77	125.63
13	G5	201	CYC	OC-C1C-NC	-12.70	109.96	124.93
13	N1	201	CYC	CHD-C4C-NC	-12.70	109.78	125.63
13	P7	201	CYC	OC-C1C-NC	-12.70	109.96	124.93
13	U1	201	CYC	CHD-C4C-NC	-12.70	109.78	125.63
13	N3	201	CYC	CHD-C4C-NC	-12.70	109.78	125.63
13	a1	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	T3	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	M7	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	E6	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	W7	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	G6	201	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	Q7	202	CYC	OC-C1C-NC	-12.69	109.97	124.93
13	T6	202	CYC	CHD-C4C-NC	-12.68	109.80	125.63
13	V1	202	CYC	OC-C1C-NC	-12.68	109.98	124.93
13	J7	202	CYC	OC-C1C-NC	-12.68	109.98	124.93
13	W3	201	CYC	OC-C1C-NC	-12.68	109.98	124.93
13	t2	201	CYC	OC-C1C-NC	-12.68	109.99	124.93
13	B3	201	CYC	CHD-C4C-NC	-12.67	109.81	125.63
13	D4	201	CYC	OC-C1C-NC	-12.67	109.99	124.93
13	Q2	201	CYC	OC-C1C-NC	-12.66	110.00	124.93
13	C4	201	CYC	OC-C1C-NC	-12.66	110.01	124.93
13	H3	201	CYC	CHD-C4C-NC	-12.66	109.83	125.63
13	P6	201	CYC	OC-C1C-NC	-12.65	110.01	124.93
13	z2	201	CYC	OC-C1C-NC	-12.65	110.02	124.93
13	D5	201	CYC	OC-C1C-NC	-12.64	110.03	124.93
13	D1	201	CYC	OC-C1C-NC	-12.64	110.03	124.93
13	p2	201	CYC	OC-C1C-NC	-12.64	110.03	124.93
13	J1	202	CYC	OC-C1C-NC	-12.63	110.04	124.93
13	H4	201	CYC	CHD-C4C-NC	-12.63	109.86	125.63
13	Q3	202	CYC	OC-C1C-NC	-12.63	110.04	124.93
13	D6	201	CYC	OC-C1C-NC	-12.63	110.04	124.93
13	22	301	CYC	OC-C1C-NC	-12.63	110.04	124.93
13	U5	201	CYC	CHD-C4C-NC	-12.62	109.87	125.63
13	P3	201	CYC	OC-C1C-NC	-12.62	110.05	124.93
13	T6	201	CYC	OC-C1C-NC	-12.62	110.05	124.93
13	K1	201	CYC	CHD-C4C-NC	-12.62	109.88	125.63
13	Z4	301	CYC	OC-C1C-NC	-12.61	110.06	124.93
13	Q4	202	CYC	OC-C1C-NC	-12.59	110.08	124.93
13	F6	202	CYC	OC-C1C-NC	-12.59	110.08	124.93
13	H1	201	CYC	CHD-C4C-NC	-12.59	109.91	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G7	201	CYC	OC-C1C-NC	-12.59	110.09	124.93
13	52	301	CYC	OC-C1C-NC	-12.59	110.09	124.93
13	A2	202	CYC	OC-C1C-NC	-12.59	110.09	124.93
13	E1	201	CYC	OC-C1C-NC	-12.59	110.09	124.93
13	F1	201	CYC	OC-C1C-NC	-12.58	110.09	124.93
13	P4	202	CYC	OC-C1C-NC	-12.58	110.10	124.93
13	42	301	CYC	OC-C1C-NC	-12.58	110.10	124.93
13	W2	201	CYC	CHD-C4C-NC	-12.58	109.93	125.63
13	N6	201	CYC	CHD-C4C-NC	-12.57	109.94	125.63
13	s2	201	CYC	CHD-C4C-NC	-12.57	109.94	125.63
13	F1	202	CYC	OC-C1C-NC	-12.57	110.12	124.93
13	I1	201	CYC	CHD-C4C-NC	-12.56	109.95	125.63
13	K6	201	CYC	OC-C1C-NC	-12.56	110.13	124.93
13	C5	201	CYC	OC-C1C-NC	-12.55	110.14	124.93
13	B6	201	CYC	CHD-C4C-NC	-12.55	109.97	125.63
13	H2	201	CYC	OC-C1C-NC	-12.54	110.14	124.93
13	Q6	201	CYC	OC-C1C-NC	-12.54	110.14	124.93
13	C2	201	CYC	CHD-C4C-NC	-12.54	109.98	125.63
13	D2	201	CYC	OC-C1C-NC	-12.54	110.15	124.93
13	Q5	202	CYC	OC-C1C-NC	-12.54	110.15	124.93
13	I4	201	CYC	OC-C1C-NC	-12.53	110.16	124.93
13	a2	201	CYC	CHD-C4C-NC	-12.53	109.99	125.63
13	I4	201	CYC	CHD-C4C-NC	-12.53	109.99	125.63
13	Q4	201	CYC	OC-C1C-NC	-12.52	110.17	124.93
13	a2	201	CYC	OC-C1C-NC	-12.52	110.17	124.93
13	Q1	202	CYC	OC-C1C-NC	-12.52	110.17	124.93
13	N7	201	CYC	OC-C1C-NC	-12.52	110.17	124.93
13	F3	202	CYC	OC-C1C-NC	-12.52	110.17	124.93
13	Q6	202	CYC	OC-C1C-NC	-12.51	110.18	124.93
13	W4	201	CYC	OC-C1C-NC	-12.51	110.18	124.93
13	F7	202	CYC	OC-C1C-NC	-12.51	110.18	124.93
13	r2	201	CYC	CHD-C4C-NC	-12.51	110.01	125.63
13	P7	202	CYC	OC-C1C-NC	-12.51	110.18	124.93
13	F5	201	CYC	OC-C1C-NC	-12.51	110.18	124.93
13	T1	201	CYC	OC-C1C-NC	-12.51	110.19	124.93
13	v2	201	CYC	OC-C1C-NC	-12.51	110.19	124.93
13	G1	201	CYC	OC-C1C-NC	-12.50	110.19	124.93
13	Q1	201	CYC	OC-C1C-NC	-12.50	110.19	124.93
13	K5	201	CYC	OC-C1C-NC	-12.50	110.20	124.93
13	B5	201	CYC	OC-C1C-NC	-12.49	110.20	124.93
13	y2	201	CYC	OC-C1C-NC	-12.49	110.21	124.93
13	N3	201	CYC	OC-C1C-NC	-12.49	110.21	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	32	302	CYC	OC-C1C-NC	-12.47	110.23	124.93
13	F4	202	CYC	OC-C1C-NC	-12.47	110.23	124.93
13	R5	201	CYC	OC-C1C-NC	-12.47	110.23	124.93
13	L2	201	CYC	OC-C1C-NC	-12.47	110.23	124.93
13	N6	201	CYC	OC-C1C-NC	-12.46	110.24	124.93
13	O2	201	CYC	OC-C1C-NC	-12.45	110.25	124.93
13	V3	201	CYC	OC-C1C-NC	-12.45	110.25	124.93
13	R7	201	CYC	OC-C1C-NC	-12.45	110.25	124.93
13	N5	201	CYC	OC-C1C-NC	-12.45	110.25	124.93
13	P5	201	CYC	OC-C1C-NC	-12.45	110.25	124.93
13	Q3	201	CYC	OC-C1C-NC	-12.45	110.26	124.93
13	I6	201	CYC	OC-C1C-NC	-12.45	110.26	124.93
13	Q7	201	CYC	OC-C1C-NC	-12.44	110.26	124.93
13	W5	201	CYC	OC-C1C-NC	-12.44	110.27	124.93
13	V5	201	CYC	OC-C1C-NC	-12.44	110.27	124.93
13	T1	202	CYC	CHD-C4C-NC	-12.43	110.11	125.63
13	R4	201	CYC	OC-C1C-NC	-12.43	110.27	124.93
13	U5	201	CYC	OC-C1C-NC	-12.43	110.28	124.93
13	B5	201	CYC	CHD-C4C-NC	-12.43	110.11	125.63
13	U6	201	CYC	OC-C1C-NC	-12.43	110.28	124.93
13	B6	201	CYC	OC-C1C-NC	-12.43	110.28	124.93
13	R1	201	CYC	OC-C1C-NC	-12.42	110.29	124.93
13	B4	201	CYC	CHD-C4C-NC	-12.42	110.13	125.63
13	22	302	CYC	OC-C1C-NC	-12.41	110.30	124.93
13	T3	202	CYC	OC-C1C-NC	-12.40	110.31	124.93
13	T6	202	CYC	OC-C1C-NC	-12.40	110.31	124.93
13	K6	201	CYC	CHD-C4C-NC	-12.40	110.16	125.63
13	V4	201	CYC	OC-C1C-NC	-12.40	110.32	124.93
13	R2	201	CYC	OC-C1C-NC	-12.39	110.32	124.93
13	F5	202	CYC	OC-C1C-NC	-12.38	110.33	124.93
13	F6	201	CYC	OC-C1C-NC	-12.38	110.33	124.93
13	a6	202	CYC	OC-C1C-NC	-12.38	110.33	124.93
13	U1	201	CYC	OC-C1C-NC	-12.38	110.33	124.93
13	T1	202	CYC	OC-C1C-NC	-12.38	110.34	124.93
13	T7	202	CYC	OC-C1C-NC	-12.37	110.34	124.93
13	H6	201	CYC	OC-C1C-NC	-12.37	110.34	124.93
13	C3	201	CYC	OC-C1C-NC	-12.37	110.35	124.93
13	F3	201	CYC	OC-C1C-NC	-12.37	110.35	124.93
13	F7	201	CYC	OC-C1C-NC	-12.36	110.36	124.93
13	H5	201	CYC	CHD-C4C-NC	-12.36	110.21	125.63
13	B1	201	CYC	CHD-C4C-NC	-12.36	110.21	125.63
13	V7	201	CYC	OC-C1C-NC	-12.35	110.37	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H6	201	CYC	CHD-C4C-NC	-12.35	110.21	125.63
13	F4	201	CYC	OC-C1C-NC	-12.35	110.37	124.93
13	P1	201	CYC	OC-C1C-NC	-12.35	110.37	124.93
13	a1	202	CYC	OC-C1C-NC	-12.34	110.38	124.93
13	B2	202	CYC	OC-C1C-NC	-12.33	110.40	124.93
13	M2	201	CYC	CHD-C4C-NC	-12.32	110.25	125.63
13	W6	201	CYC	OC-C1C-NC	-12.32	110.40	124.93
13	a7	202	CYC	OC-C1C-NC	-12.32	110.40	124.93
13	R2	201	CYC	CHD-C4C-NC	-12.32	110.25	125.63
13	x2	201	CYC	CHD-C4C-NC	-12.32	110.26	125.63
13	H5	201	CYC	OC-C1C-NC	-12.32	110.41	124.93
13	M4	201	CYC	CHD-C4C-NC	-12.31	110.26	125.63
13	R3	201	CYC	OC-C1C-NC	-12.31	110.42	124.93
13	I1	201	CYC	OC-C1C-NC	-12.31	110.42	124.93
13	E2	201	CYC	OC-C1C-NC	-12.31	110.42	124.93
13	e2	201	CYC	OC-C1C-NC	-12.31	110.42	124.93
13	g2	201	CYC	CHD-C4C-NC	-12.30	110.28	125.63
13	G2	201	CYC	OC-C1C-NC	-12.30	110.43	124.93
13	I6	201	CYC	CHD-C4C-NC	-12.30	110.28	125.63
13	T5	202	CYC	OC-C1C-NC	-12.29	110.44	124.93
13	D2	201	CYC	CHD-C4C-NC	-12.29	110.29	125.63
13	H4	201	CYC	OC-C1C-NC	-12.29	110.44	124.93
13	v2	201	CYC	CHD-C4C-NC	-12.28	110.30	125.63
13	G1	201	CYC	CHD-C4C-NC	-12.28	110.30	125.63
13	H3	201	CYC	OC-C1C-NC	-12.27	110.46	124.93
13	i2	201	CYC	OC-C1C-NC	-12.26	110.47	124.93
13	T4	202	CYC	OC-C1C-NC	-12.26	110.47	124.93
13	H7	201	CYC	OC-C1C-NC	-12.26	110.47	124.93
13	W2	201	CYC	OC-C1C-NC	-12.24	110.50	124.93
13	C7	202	CYC	CHD-C4C-NC	-12.24	110.36	125.63
13	s2	201	CYC	OC-C1C-NC	-12.22	110.52	124.93
13	H1	201	CYC	OC-C1C-NC	-12.22	110.53	124.93
13	S2	201	CYC	CHD-C4C-NC	-12.22	110.38	125.63
13	a3	202	CYC	OC-C1C-NC	-12.21	110.54	124.93
13	D6	201	CYC	CHD-C4C-NC	-12.21	110.39	125.63
13	W1	201	CYC	OC-C1C-NC	-12.20	110.55	124.93
13	e2	201	CYC	CHD-C4C-NC	-12.19	110.42	125.63
13	V6	201	CYC	OC-C1C-NC	-12.17	110.58	124.93
13	a5	202	CYC	OC-C1C-NC	-12.14	110.61	124.93
13	M1	201	CYC	CHD-C4C-NC	-12.12	110.50	125.63
13	P7	202	CYC	CHD-C4C-NC	-12.10	110.53	125.63
13	M5	201	CYC	CHD-C4C-NC	-12.10	110.53	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	h2	201	CYC	OC-C1C-NC	-12.07	110.69	124.93
13	Q7	201	CYC	CHD-C4C-NC	-12.07	110.57	125.63
13	52	301	CYC	CHD-C4C-NC	-12.06	110.58	125.63
13	Q5	201	CYC	OC-C1C-NC	-12.04	110.73	124.93
13	C3	202	CYC	CHD-C4C-NC	-12.04	110.60	125.63
13	B1	201	CYC	OC-C1C-NC	-12.03	110.75	124.93
13	a4	202	CYC	OC-C1C-NC	-12.03	110.75	124.93
13	32	302	CYC	CHD-C4C-NC	-12.01	110.64	125.63
13	P3	202	CYC	CHD-C4C-NC	-12.01	110.64	125.63
13	Q3	201	CYC	CHD-C4C-NC	-12.01	110.64	125.63
13	D7	201	CYC	CHD-C4C-NC	-12.00	110.65	125.63
13	J4	201	CYC	CHD-C4C-NC	-12.00	110.65	125.63
13	22	302	CYC	CHD-C4C-NC	-12.00	110.66	125.63
13	52	302	CYC	OC-C1C-NC	-11.97	110.81	124.93
13	E2	201	CYC	CHD-C4C-NC	-11.95	110.72	125.63
13	w2	201	CYC	CHD-C4C-NC	-11.93	110.74	125.63
13	z2	201	CYC	CHD-C4C-NC	-11.90	110.77	125.63
13	P4	201	CYC	CHD-C4C-NC	-11.88	110.80	125.63
13	A6	301	CYC	CHD-C4C-NC	-11.88	110.80	125.63
13	P6	202	CYC	CHD-C4C-NC	-11.88	110.80	125.63
13	n2	201	CYC	CHD-C4C-NC	-11.86	110.82	125.63
13	B2	201	CYC	OC-C1C-NC	-11.83	110.98	124.93
13	F2	201	CYC	CHD-C4C-NC	-11.82	110.88	125.63
13	D4	201	CYC	CHD-C4C-NC	-11.81	110.88	125.63
13	S1	201	CYC	CHD-C4C-NC	-11.81	110.89	125.63
13	y2	201	CYC	CHD-C4C-NC	-11.79	110.92	125.63
13	S4	201	CYC	CHD-C4C-NC	-11.77	110.94	125.63
13	A1	301	CYC	CHD-C4C-NC	-11.76	110.95	125.63
13	M6	201	CYC	CHD-C4C-NC	-11.76	110.96	125.63
13	42	302	CYC	OC-C1C-NC	-11.75	111.08	124.93
13	L2	201	CYC	CHD-C4C-NC	-11.75	110.97	125.63
13	m2	201	CYC	CHD-C4C-NC	-11.75	110.97	125.63
13	C4	202	CYC	CHD-C4C-NC	-11.71	111.02	125.63
13	C6	202	CYC	CHD-C4C-NC	-11.70	111.02	125.63
13	Z7	301	CYC	CHD-C4C-NC	-11.68	111.05	125.63
13	C1	202	CYC	CHD-C4C-NC	-11.67	111.06	125.63
13	M7	201	CYC	CHD-C4C-NC	-11.66	111.08	125.63
13	S6	201	CYC	CHD-C4C-NC	-11.64	111.09	125.63
13	Q4	201	CYC	CHD-C4C-NC	-11.64	111.11	125.63
13	J7	201	CYC	CHD-C4C-NC	-11.63	111.12	125.63
13	S5	201	CYC	CHD-C4C-NC	-11.62	111.13	125.63
13	l2	201	CYC	CHD-C4C-NC	-11.60	111.15	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M3	201	CYC	CHD-C4C-NC	-11.57	111.18	125.63
13	P5	202	CYC	CHD-C4C-NC	-11.53	111.23	125.63
13	J3	201	CYC	CHD-C4C-NC	-11.53	111.24	125.63
13	C5	202	CYC	CHD-C4C-NC	-11.50	111.28	125.63
13	Q6	201	CYC	CHD-C4C-NC	-11.48	111.29	125.63
13	J5	201	CYC	CHD-C4C-NC	-11.48	111.30	125.63
13	J1	201	CYC	CHD-C4C-NC	-11.46	111.32	125.63
13	A6	302	CYC	OC-C1C-NC	-11.46	111.42	124.93
13	22	301	CYC	CHD-C4C-NC	-11.44	111.34	125.63
13	V1	201	CYC	OC-C1C-NC	-11.44	111.44	124.93
13	S3	201	CYC	CHD-C4C-NC	-11.44	111.35	125.63
13	S7	201	CYC	CHD-C4C-NC	-11.40	111.40	125.63
13	42	301	CYC	CHD-C4C-NC	-11.40	111.41	125.63
13	B2	201	CYC	CHD-C4C-NC	-11.39	111.42	125.63
13	c2	801	CYC	OC-C1C-NC	-11.38	111.51	124.93
13	X2	201	CYC	CHD-C4C-NC	-11.37	111.44	125.63
13	O2	201	CYC	CHD-C4C-NC	-11.36	111.45	125.63
13	Z3	301	CYC	CHD-C4C-NC	-11.34	111.48	125.63
13	P1	202	CYC	CHD-C4C-NC	-11.34	111.48	125.63
13	Z1	301	CYC	C1C-NC-C4C	-11.33	99.20	113.41
13	32	301	CYC	CHD-C4C-NC	-11.32	111.50	125.63
13	V7	201	CYC	CHD-C4C-NC	-11.31	111.51	125.63
13	L3	201	CYC	CHD-C4C-NC	-11.30	111.52	125.63
13	a5	201	CYC	CHD-C4C-NC	-11.29	111.54	125.63
13	p2	201	CYC	CHD-C4C-NC	-11.28	111.55	125.63
13	L7	201	CYC	CHD-C4C-NC	-11.27	111.56	125.63
13	42	302	CYC	CHD-C4C-NC	-11.27	111.57	125.63
13	A1	302	CYC	OC-C1C-NC	-11.23	111.69	124.93
13	J6	201	CYC	CHD-C4C-NC	-11.19	111.66	125.63
13	Q1	201	CYC	CHD-C4C-NC	-11.18	111.67	125.63
13	J1	202	CYC	CHD-C4C-NC	-11.17	111.69	125.63
13	Q5	201	CYC	CHD-C4C-NC	-11.15	111.71	125.63
13	a1	201	CYC	CHD-C4C-NC	-11.14	111.73	125.63
13	V1	202	CYC	CHD-C4C-NC	-11.13	111.74	125.63
13	J5	202	CYC	CHD-C4C-NC	-11.13	111.74	125.63
13	Z4	301	CYC	C1C-NC-C4C	-11.12	99.47	113.41
13	Z6	301	CYC	C1C-NC-C4C	-11.11	99.48	113.41
13	X7	201	CYC	CHD-C4C-NC	-11.09	111.79	125.63
13	X3	201	CYC	CHD-C4C-NC	-11.08	111.80	125.63
13	a6	201	CYC	CHD-C4C-NC	-11.08	111.80	125.63
13	J7	202	CYC	CHD-C4C-NC	-11.06	111.82	125.63
13	a7	201	CYC	CHD-C4C-NC	-11.06	111.82	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J6	202	CYC	CHD-C4C-NC	-11.06	111.83	125.63
13	J4	202	CYC	CHD-C4C-NC	-11.04	111.85	125.63
13	L5	201	CYC	CHD-C4C-NC	-11.03	111.86	125.63
13	T5	201	CYC	CHD-C4C-NC	-11.02	111.88	125.63
13	T2	201	CYC	CHD-C4C-NC	-11.01	111.89	125.63
13	V4	202	CYC	CHD-C4C-NC	-10.99	111.91	125.63
13	C7	201	CYC	CHD-C4C-NC	-10.97	111.94	125.63
13	C3	201	CYC	CHD-C4C-NC	-10.96	111.94	125.63
13	L4	201	CYC	CHD-C4C-NC	-10.95	111.96	125.63
13	a3	201	CYC	CHD-C4C-NC	-10.93	111.99	125.63
13	i2	201	CYC	CHD-C4C-NC	-10.90	112.02	125.63
13	S1	201	CYC	OC-C1C-NC	-10.89	112.09	124.93
13	X4	201	CYC	CHD-C4C-NC	-10.89	112.04	125.63
13	V5	202	CYC	CHD-C4C-NC	-10.89	112.04	125.63
13	J3	202	CYC	CHD-C4C-NC	-10.84	112.10	125.63
13	L1	201	CYC	C1C-NC-C4C	-10.83	99.82	113.41
13	P2	201	CYC	CHD-C4C-NC	-10.83	112.11	125.63
13	S4	201	CYC	OC-C1C-NC	-10.83	112.17	124.93
13	X6	201	CYC	CHD-C4C-NC	-10.81	112.14	125.63
13	E6	201	CYC	CHD-C4C-NC	-10.81	112.14	125.63
13	E1	201	CYC	CHD-C4C-NC	-10.76	112.20	125.63
13	E5	201	CYC	CHD-C4C-NC	-10.75	112.21	125.63
13	S6	201	CYC	OC-C1C-NC	-10.75	112.26	124.93
13	Z5	301	CYC	C1C-NC-C4C	-10.75	99.93	113.41
13	E4	201	CYC	CHD-C4C-NC	-10.74	112.22	125.63
13	V7	202	CYC	CHD-C4C-NC	-10.74	112.23	125.63
13	T4	201	CYC	CHD-C4C-NC	-10.71	112.26	125.63
13	o2	801	CYC	C1D-CHD-C4C	-10.69	109.51	127.76
13	V3	202	CYC	CHD-C4C-NC	-10.68	112.30	125.63
13	C6	201	CYC	CHD-C4C-NC	-10.63	112.36	125.63
13	S5	201	CYC	OC-C1C-NC	-10.58	112.45	124.93
13	T6	201	CYC	CHD-C4C-NC	-10.58	112.43	125.63
13	S3	201	CYC	OC-C1C-NC	-10.57	112.47	124.93
13	V6	202	CYC	CHD-C4C-NC	-10.55	112.46	125.63
13	E3	201	CYC	CHD-C4C-NC	-10.55	112.46	125.63
13	T1	201	CYC	CHD-C4C-NC	-10.55	112.47	125.63
13	V2	201	CYC	CHD-C4C-NC	-10.53	112.49	125.63
13	V3	201	CYC	CHD-C4C-NC	-10.52	112.50	125.63
13	S7	201	CYC	OC-C1C-NC	-10.52	112.53	124.93
13	t2	201	CYC	CHD-C4C-NC	-10.52	112.50	125.63
13	V1	201	CYC	C1C-NC-C4C	-10.51	100.23	113.41
13	C3	201	CYC	C1C-NC-C4C	-10.50	100.23	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D3	201	CYC	CHD-C4C-NC	-10.50	112.52	125.63
13	E7	201	CYC	CHD-C4C-NC	-10.48	112.55	125.63
13	X1	201	CYC	CHD-C4C-NC	-10.46	112.58	125.63
13	X5	201	CYC	CHD-C4C-NC	-10.45	112.58	125.63
13	a1	201	CYC	C1C-NC-C4C	-10.44	100.31	113.41
13	52	302	CYC	CHD-C4C-NC	-10.44	112.60	125.63
13	H2	201	CYC	C1D-CHD-C4C	-10.37	110.05	127.76
13	A1	302	CYC	C1C-NC-C4C	-10.33	100.46	113.41
13	f2	201	CYC	CHD-C4C-NC	-10.29	112.79	125.63
13	C1	201	CYC	CHD-C4C-NC	-10.25	112.83	125.63
13	N2	801	CYC	CHD-C4C-NC	-10.24	112.85	125.63
13	N2	802	CYC	C1D-CHD-C4C	-10.23	110.30	127.76
13	C5	201	CYC	C1C-NC-C4C	-10.20	100.61	113.41
13	Q7	202	CYC	C1D-CHD-C4C	-10.19	110.37	127.76
13	A6	302	CYC	C1C-NC-C4C	-10.18	100.65	113.41
13	V6	201	CYC	CHD-C4C-NC	-10.16	112.95	125.63
13	Q3	202	CYC	C1D-CHD-C4C	-10.15	110.44	127.76
13	T7	201	CYC	CHD-C4C-NC	-10.15	112.96	125.63
13	A6	302	CYC	CHD-C4C-NC	-10.15	112.96	125.63
13	C4	201	CYC	CHD-C4C-NC	-10.14	112.97	125.63
13	C5	201	CYC	CHD-C4C-NC	-10.14	112.97	125.63
13	V4	201	CYC	CHD-C4C-NC	-10.14	112.97	125.63
13	E7	201	CYC	C4D-CHA-C1A	-10.12	106.13	128.22
13	D5	201	CYC	CHD-C4C-NC	-10.11	113.01	125.63
13	U2	201	CYC	CHD-C4C-NC	-10.11	113.02	125.63
13	L6	201	CYC	CHD-C4C-NC	-10.10	113.02	125.63
13	A2	202	CYC	C1D-CHD-C4C	-10.04	110.63	127.76
13	Q4	202	CYC	C1D-CHD-C4C	-10.02	110.65	127.76
13	a3	201	CYC	C1C-NC-C4C	-10.01	100.85	113.41
13	C6	201	CYC	C1C-NC-C4C	-9.99	100.88	113.41
13	V5	201	CYC	CHD-C4C-NC	-9.99	113.16	125.63
13	C1	201	CYC	C1C-NC-C4C	-9.98	100.89	113.41
13	L1	201	CYC	CHD-C4C-NC	-9.97	113.18	125.63
13	T3	201	CYC	CHD-C4C-NC	-9.97	113.19	125.63
13	A1	302	CYC	CHD-C4C-NC	-9.96	113.19	125.63
13	a7	201	CYC	C1C-NC-C4C	-9.95	100.93	113.41
13	D1	201	CYC	CHD-C4C-NC	-9.95	113.21	125.63
13	F3	202	CYC	C1D-CHD-C4C	-9.95	110.78	127.76
13	K7	201	CYC	C1D-CHD-C4C	-9.93	110.82	127.76
13	F7	202	CYC	C1D-CHD-C4C	-9.92	110.83	127.76
13	Q2	201	CYC	C1D-CHD-C4C	-9.89	110.89	127.76
13	Z6	301	CYC	CHD-C4C-NC	-9.88	113.29	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P7	201	CYC	C1D-CHD-C4C	-9.88	110.90	127.76
13	C4	201	CYC	C1C-NC-C4C	-9.88	101.02	113.41
13	Z4	301	CYC	CHD-C4C-NC	-9.86	113.32	125.63
13	a6	201	CYC	C1C-NC-C4C	-9.83	101.08	113.41
13	K3	201	CYC	C1D-CHD-C4C	-9.82	111.01	127.76
13	a5	201	CYC	C1C-NC-C4C	-9.80	101.12	113.41
13	Q6	202	CYC	C1D-CHD-C4C	-9.78	111.06	127.76
13	E3	201	CYC	C4D-CHA-C1A	-9.77	106.89	128.22
13	Z5	301	CYC	CHD-C4C-NC	-9.76	113.44	125.63
13	V1	201	CYC	CHD-C4C-NC	-9.75	113.46	125.63
13	X5	201	CYC	C1C-NC-C4C	-9.74	101.19	113.41
13	F5	202	CYC	C1D-CHD-C4C	-9.72	111.17	127.76
13	F4	202	CYC	C1D-CHD-C4C	-9.68	111.24	127.76
13	F6	202	CYC	C1D-CHD-C4C	-9.66	111.28	127.76
13	W7	201	CYC	C1D-CHD-C4C	-9.66	111.28	127.76
13	Z1	301	CYC	CHD-C4C-NC	-9.65	113.59	125.63
13	H7	201	CYC	C1D-CHD-C4C	-9.63	111.33	127.76
13	k2	201	CYC	C1D-CHD-C4C	-9.63	111.33	127.76
13	L6	201	CYC	C1C-NC-C4C	-9.62	101.34	113.41
13	D3	201	CYC	C1C-NC-C4C	-9.62	101.35	113.41
13	R1	201	CYC	C1D-CHD-C4C	-9.61	111.36	127.76
13	N7	201	CYC	C1D-CHD-C4C	-9.61	111.36	127.76
13	P3	201	CYC	C1D-CHD-C4C	-9.60	111.37	127.76
13	B2	202	CYC	CHD-C4C-NC	-9.58	113.68	125.63
13	Q1	202	CYC	C1D-CHD-C4C	-9.55	111.46	127.76
13	t2	201	CYC	C1C-NC-C4C	-9.53	101.45	113.41
13	Q5	202	CYC	C1D-CHD-C4C	-9.52	111.51	127.76
13	N2	801	CYC	C1C-NC-C4C	-9.52	101.47	113.41
13	U2	201	CYC	C1C-NC-C4C	-9.51	101.49	113.41
13	F1	202	CYC	C1D-CHD-C4C	-9.50	111.54	127.76
13	W3	201	CYC	C1D-CHD-C4C	-9.49	111.57	127.76
13	F6	201	CYC	C1D-CHD-C4C	-9.46	111.62	127.76
13	a1	202	CYC	C1C-NC-C4C	-9.45	101.55	113.41
13	R4	201	CYC	C1D-CHD-C4C	-9.45	111.64	127.76
13	U3	201	CYC	C1D-CHD-C4C	-9.43	111.66	127.76
13	G3	201	CYC	C1D-CHD-C4C	-9.42	111.69	127.76
13	R7	201	CYC	C1D-CHD-C4C	-9.41	111.70	127.76
13	B2	202	CYC	C1C-NC-C4C	-9.40	101.62	113.41
13	R5	201	CYC	C1D-CHD-C4C	-9.40	111.72	127.76
13	H3	201	CYC	C1D-CHD-C4C	-9.40	111.72	127.76
13	U7	201	CYC	C1D-CHD-C4C	-9.38	111.74	127.76
13	C2	201	CYC	C1D-CHD-C4C	-9.35	111.80	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T7	202	CYC	C1D-CHD-C4C	-9.33	111.84	127.76
13	R6	201	CYC	C1D-CHD-C4C	-9.32	111.85	127.76
13	A2	201	CYC	C1D-CHD-C4C	-9.31	111.87	127.76
13	V2	201	CYC	C1C-NC-C4C	-9.29	101.76	113.41
13	U4	201	CYC	C1D-CHD-C4C	-9.28	111.93	127.76
13	a6	202	CYC	C1C-NC-C4C	-9.27	101.78	113.41
13	52	302	CYC	C1C-NC-C4C	-9.27	101.78	113.41
13	T3	202	CYC	C1D-CHD-C4C	-9.27	111.94	127.76
13	N3	201	CYC	C1D-CHD-C4C	-9.26	111.96	127.76
13	D5	201	CYC	C1C-NC-C4C	-9.23	101.83	113.41
13	C7	201	CYC	C1C-NC-C4C	-9.23	101.84	113.41
13	W2	201	CYC	C1D-CHD-C4C	-9.22	112.02	127.76
13	G7	201	CYC	C1D-CHD-C4C	-9.21	112.03	127.76
13	o2	801	CYC	C2C-C1C-NC	-9.19	100.64	108.29
13	M2	201	CYC	C1C-NC-C4C	-9.19	101.89	113.41
13	a7	202	CYC	C1C-NC-C4C	-9.13	101.95	113.41
13	R3	201	CYC	C1D-CHD-C4C	-9.12	112.20	127.76
13	G2	201	CYC	C1D-CHD-C4C	-9.07	112.27	127.76
13	P4	202	CYC	C1D-CHD-C4C	-9.03	112.35	127.76
13	V4	202	CYC	C1D-CHD-C4C	-9.02	112.36	127.76
13	a4	202	CYC	C1C-NC-C4C	-9.01	102.11	113.41
13	a3	202	CYC	C1C-NC-C4C	-9.01	102.11	113.41
13	C7	202	CYC	C1D-CHD-C4C	-9.00	112.40	127.76
13	K1	201	CYC	C1D-CHD-C4C	-8.96	112.47	127.76
13	U1	201	CYC	C1D-CHD-C4C	-8.94	112.50	127.76
13	a7	202	CYC	C4D-CHA-C1A	-8.92	108.75	128.22
13	D1	201	CYC	C1C-NC-C4C	-8.91	102.23	113.41
13	a5	202	CYC	CHD-C4C-NC	-8.91	114.51	125.63
13	a5	202	CYC	C1C-NC-C4C	-8.90	102.25	113.41
13	c2	801	CYC	C1C-NC-C4C	-8.90	102.25	113.41
13	P5	201	CYC	C1D-CHD-C4C	-8.89	112.58	127.76
13	N4	201	CYC	C1D-CHD-C4C	-8.89	112.59	127.76
13	T7	201	CYC	C4D-CHA-C1A	-8.89	108.82	128.22
13	G5	201	CYC	C1D-CHD-C4C	-8.88	112.60	127.76
13	W1	201	CYC	C1D-CHD-C4C	-8.88	112.61	127.76
13	H6	201	CYC	C1D-CHD-C4C	-8.88	112.61	127.76
13	V5	202	CYC	C1D-CHD-C4C	-8.88	112.61	127.76
13	T4	201	CYC	C4D-CHA-C1A	-8.87	108.84	128.22
13	U5	201	CYC	C1D-CHD-C4C	-8.84	112.68	127.76
13	G4	201	CYC	C1D-CHD-C4C	-8.83	112.69	127.76
13	T4	201	CYC	C1D-CHD-C4C	-8.83	112.69	127.76
13	E1	201	CYC	C1C-NC-C4C	-8.82	102.34	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C3	202	CYC	C1D-CHD-C4C	-8.82	112.71	127.76
13	H1	201	CYC	C1D-CHD-C4C	-8.81	112.72	127.76
13	S2	201	CYC	C1C-NC-C4C	-8.81	102.36	113.41
13	a3	202	CYC	CHD-C4C-NC	-8.80	114.64	125.63
13	z2	201	CYC	C1C-NC-C4C	-8.79	102.38	113.41
13	V5	202	CYC	C1C-NC-C4C	-8.79	102.38	113.41
13	T4	202	CYC	C1D-CHD-C4C	-8.79	112.76	127.76
13	T3	201	CYC	C4D-CHA-C1A	-8.78	109.04	128.22
13	h2	201	CYC	C1D-CHD-C4C	-8.78	112.77	127.76
13	G6	201	CYC	C1D-CHD-C4C	-8.76	112.81	127.76
13	a7	202	CYC	CHD-C4C-NC	-8.76	114.70	125.63
13	T5	201	CYC	C1D-CHD-C4C	-8.75	112.82	127.76
13	d2	201	CYC	C1D-CHD-C4C	-8.75	112.83	127.76
13	H4	201	CYC	C1D-CHD-C4C	-8.75	112.83	127.76
13	P6	201	CYC	C1D-CHD-C4C	-8.75	112.83	127.76
13	D2	201	CYC	C1D-CHD-C4C	-8.74	112.85	127.76
13	V7	202	CYC	C1C-NC-C4C	-8.73	102.46	113.41
13	V6	201	CYC	C1C-NC-C4C	-8.72	102.48	113.41
13	K4	201	CYC	C1D-CHD-C4C	-8.70	112.90	127.76
13	V6	202	CYC	C1C-NC-C4C	-8.70	102.50	113.41
13	K6	201	CYC	C1D-CHD-C4C	-8.69	112.92	127.76
13	T6	202	CYC	C1D-CHD-C4C	-8.66	112.97	127.76
13	N1	201	CYC	C1D-CHD-C4C	-8.66	112.99	127.76
13	N6	201	CYC	C1D-CHD-C4C	-8.64	113.02	127.76
13	J6	202	CYC	C1C-NC-C4C	-8.63	102.59	113.41
13	E6	201	CYC	C4D-CHA-C1A	-8.62	109.40	128.22
13	E4	201	CYC	C1C-NC-C4C	-8.61	102.61	113.41
13	T5	201	CYC	C4D-CHA-C1A	-8.57	109.50	128.22
13	G1	201	CYC	C1D-CHD-C4C	-8.55	113.17	127.76
13	J4	202	CYC	C1C-NC-C4C	-8.55	102.69	113.41
13	T4	201	CYC	C1C-NC-C4C	-8.54	102.70	113.41
13	V1	202	CYC	C1D-CHD-C4C	-8.54	113.19	127.76
13	W6	201	CYC	C1D-CHD-C4C	-8.53	113.20	127.76
13	R2	201	CYC	C1D-CHD-C4C	-8.51	113.23	127.76
13	s2	201	CYC	C1D-CHD-C4C	-8.51	113.24	127.76
13	H5	201	CYC	C1D-CHD-C4C	-8.50	113.25	127.76
13	c2	801	CYC	C1D-CHD-C4C	-8.50	113.26	127.76
13	T1	202	CYC	C1D-CHD-C4C	-8.49	113.27	127.76
13	C6	202	CYC	C1D-CHD-C4C	-8.49	113.27	127.76
13	J5	202	CYC	C1C-NC-C4C	-8.48	102.77	113.41
13	T5	201	CYC	C1C-NC-C4C	-8.48	102.77	113.41
13	T5	202	CYC	C1D-CHD-C4C	-8.48	113.29	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	j2	201	CYC	C1D-CHD-C4C	-8.48	113.29	127.76
13	E5	201	CYC	C1C-NC-C4C	-8.47	102.78	113.41
13	C7	202	CYC	C4D-CHA-C1A	-8.45	109.77	128.22
13	a4	202	CYC	CHD-C4C-NC	-8.44	115.09	125.63
13	a3	202	CYC	C4D-CHA-C1A	-8.43	109.81	128.22
13	v2	201	CYC	C1D-CHD-C4C	-8.43	113.37	127.76
13	P1	201	CYC	C1D-CHD-C4C	-8.42	113.39	127.76
13	V6	202	CYC	C1D-CHD-C4C	-8.41	113.41	127.76
13	V7	202	CYC	C1D-CHD-C4C	-8.41	113.41	127.76
13	T3	201	CYC	C1C-NC-C4C	-8.41	102.86	113.41
13	a4	202	CYC	C4D-CHA-C1A	-8.41	109.86	128.22
13	C3	202	CYC	C4D-CHA-C1A	-8.39	109.89	128.22
13	W5	201	CYC	C1D-CHD-C4C	-8.39	113.44	127.76
13	a2	201	CYC	C1D-CHD-C4C	-8.39	113.44	127.76
13	F7	201	CYC	C1D-CHD-C4C	-8.38	113.45	127.76
13	T6	201	CYC	C1C-NC-C4C	-8.38	102.90	113.41
13	V4	202	CYC	C1C-NC-C4C	-8.37	102.91	113.41
13	E4	201	CYC	C4D-CHA-C1A	-8.37	109.95	128.22
13	V7	201	CYC	C1C-NC-C4C	-8.35	102.94	113.41
13	T7	201	CYC	C1C-NC-C4C	-8.35	102.94	113.41
13	e2	201	CYC	C1D-CHD-C4C	-8.35	113.51	127.76
13	V5	201	CYC	C1C-NC-C4C	-8.34	102.94	113.41
13	X4	201	CYC	C1C-NC-C4C	-8.34	102.95	113.41
13	E7	201	CYC	C1C-NC-C4C	-8.33	102.97	113.41
13	J3	202	CYC	C1C-NC-C4C	-8.32	102.98	113.41
13	E6	201	CYC	C1C-NC-C4C	-8.32	102.98	113.41
13	i2	201	CYC	C1C-NC-C4C	-8.30	103.00	113.41
13	f2	201	CYC	C1C-NC-C4C	-8.29	103.02	113.41
13	V3	202	CYC	C1C-NC-C4C	-8.27	103.03	113.41
13	F3	201	CYC	C1D-CHD-C4C	-8.27	113.65	127.76
13	F5	201	CYC	C1D-CHD-C4C	-8.25	113.69	127.76
13	T7	201	CYC	C1D-CHD-C4C	-8.24	113.70	127.76
13	V3	202	CYC	C1D-CHD-C4C	-8.24	113.70	127.76
13	T3	201	CYC	C1D-CHD-C4C	-8.20	113.76	127.76
13	a6	202	CYC	C4D-CHA-C1A	-8.20	110.31	128.22
13	42	302	CYC	C1C-NC-C4C	-8.20	103.13	113.41
13	T6	201	CYC	C4D-CHA-C1A	-8.19	110.33	128.22
13	T1	201	CYC	C1C-NC-C4C	-8.19	103.14	113.41
13	a5	202	CYC	C4D-CHA-C1A	-8.19	110.34	128.22
13	F4	201	CYC	C1D-CHD-C4C	-8.18	113.80	127.76
13	o2	801	CYC	C1C-NC-C4C	-8.18	103.15	113.41
13	E3	201	CYC	C1C-NC-C4C	-8.17	103.16	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J3	201	CYC	C1C-NC-C4C	-8.16	103.17	113.41
13	a6	202	CYC	CHD-C4C-NC	-8.16	115.44	125.63
13	E7	201	CYC	C1D-CHD-C4C	-8.16	113.84	127.76
13	D7	201	CYC	C1C-NC-C4C	-8.15	103.18	113.41
13	C1	202	CYC	C1D-CHD-C4C	-8.15	113.85	127.76
13	P2	201	CYC	C1C-NC-C4C	-8.15	103.19	113.41
13	V4	201	CYC	C1C-NC-C4C	-8.14	103.20	113.41
13	D3	201	CYC	C1D-CHD-C4C	-8.13	113.88	127.76
13	U6	201	CYC	C1D-CHD-C4C	-8.12	113.90	127.76
13	K6	201	CYC	C1C-NC-C4C	-8.12	103.23	113.41
13	a1	202	CYC	CHD-C4C-NC	-8.12	115.50	125.63
13	N3	201	CYC	C1C-NC-C4C	-8.11	103.23	113.41
13	L3	201	CYC	C1C-NC-C4C	-8.11	103.24	113.41
13	N6	201	CYC	C1C-NC-C4C	-8.10	103.25	113.41
13	V1	202	CYC	C1C-NC-C4C	-8.10	103.25	113.41
13	X6	201	CYC	C1C-NC-C4C	-8.10	103.25	113.41
13	W1	201	CYC	C1C-NC-C4C	-8.08	103.28	113.41
13	U7	201	CYC	C1C-NC-C4C	-8.07	103.28	113.41
13	J7	201	CYC	C1C-NC-C4C	-8.07	103.29	113.41
13	D4	201	CYC	C1C-NC-C4C	-8.06	103.30	113.41
13	F3	202	CYC	C4D-CHA-C1A	-8.05	110.64	128.22
13	J1	202	CYC	C1C-NC-C4C	-8.05	103.31	113.41
13	G1	201	CYC	C1C-NC-C4C	-8.05	103.32	113.41
13	W4	201	CYC	C1D-CHD-C4C	-8.04	114.05	127.76
13	k2	201	CYC	C1C-NC-C4C	-8.03	103.33	113.41
13	G7	201	CYC	C1C-NC-C4C	-8.02	103.35	113.41
13	E6	201	CYC	C1D-CHD-C4C	-8.02	114.07	127.76
13	N7	201	CYC	C1C-NC-C4C	-8.01	103.36	113.41
13	X1	201	CYC	C1C-NC-C4C	-8.00	103.37	113.41
13	J7	202	CYC	C4D-CHA-C1A	-8.00	110.74	128.22
13	U5	201	CYC	C1C-NC-C4C	-7.99	103.38	113.41
13	B2	202	CYC	C4D-CHA-C1A	-7.99	110.77	128.22
13	T6	201	CYC	C1D-CHD-C4C	-7.97	114.15	127.76
13	F7	202	CYC	C4D-CHA-C1A	-7.97	110.83	128.22
13	p2	201	CYC	C1C-NC-C4C	-7.95	103.44	113.41
13	T1	201	CYC	C4D-CHA-C1A	-7.95	110.86	128.22
13	J3	202	CYC	C4D-CHA-C1A	-7.94	110.88	128.22
13	z2	201	CYC	C1D-CHD-C4C	-7.93	114.22	127.76
13	L7	201	CYC	C1C-NC-C4C	-7.93	103.46	113.41
13	H6	201	CYC	C1C-NC-C4C	-7.92	103.47	113.41
13	C5	202	CYC	C1D-CHD-C4C	-7.92	114.25	127.76
13	V3	201	CYC	C1C-NC-C4C	-7.91	103.49	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H1	201	CYC	C1C-NC-C4C	-7.90	103.50	113.41
13	U1	201	CYC	C1C-NC-C4C	-7.90	103.50	113.41
13	I7	201	CYC	C1D-CHD-C4C	-7.89	114.30	127.76
13	H7	201	CYC	C1C-NC-C4C	-7.88	103.53	113.41
13	J7	202	CYC	C1C-NC-C4C	-7.87	103.54	113.41
13	Z3	301	CYC	C1C-NC-C4C	-7.87	103.54	113.41
13	H3	201	CYC	C1C-NC-C4C	-7.86	103.54	113.41
13	a1	202	CYC	C4D-CHA-C1A	-7.86	111.05	128.22
13	G3	201	CYC	C1C-NC-C4C	-7.84	103.57	113.41
13	i2	201	CYC	C4D-CHA-C1A	-7.82	111.15	128.22
13	K7	201	CYC	C1C-NC-C4C	-7.82	103.60	113.41
13	K5	201	CYC	C1D-CHD-C4C	-7.81	114.42	127.76
13	g2	201	CYC	C1D-CHD-C4C	-7.81	114.42	127.76
13	T1	201	CYC	C1D-CHD-C4C	-7.81	114.43	127.76
13	C4	202	CYC	C1D-CHD-C4C	-7.79	114.47	127.76
13	J6	201	CYC	C1C-NC-C4C	-7.79	103.64	113.41
13	W2	201	CYC	C1C-NC-C4C	-7.79	103.64	113.41
13	F5	202	CYC	C4D-CHA-C1A	-7.77	111.25	128.22
13	F1	201	CYC	C1D-CHD-C4C	-7.77	114.50	127.76
13	E3	201	CYC	C1D-CHD-C4C	-7.76	114.51	127.76
13	H5	201	CYC	C1C-NC-C4C	-7.76	103.67	113.41
13	B2	201	CYC	C4D-CHA-C1A	-7.75	111.29	128.22
13	H2	201	CYC	C1C-NC-C4C	-7.74	103.70	113.41
13	N1	201	CYC	C1C-NC-C4C	-7.72	103.72	113.41
13	r2	201	CYC	C1D-CHD-C4C	-7.72	114.59	127.76
13	K1	201	CYC	C1C-NC-C4C	-7.72	103.73	113.41
13	E2	201	CYC	C1D-CHD-C4C	-7.71	114.60	127.76
13	E5	201	CYC	C4D-CHA-C1A	-7.71	111.39	128.22
13	J5	201	CYC	C1C-NC-C4C	-7.69	103.77	113.41
13	P7	201	CYC	C1C-NC-C4C	-7.68	103.77	113.41
13	B2	201	CYC	C1D-CHD-C4C	-7.68	114.65	127.76
13	E4	201	CYC	C1D-CHD-C4C	-7.65	114.70	127.76
13	a2	201	CYC	C4D-CHA-C1A	-7.65	111.52	128.22
13	N5	201	CYC	C1D-CHD-C4C	-7.65	114.71	127.76
13	S5	201	CYC	C1C-NC-C4C	-7.64	103.82	113.41
13	I3	201	CYC	C1D-CHD-C4C	-7.64	114.73	127.76
13	P3	201	CYC	C1C-NC-C4C	-7.63	103.83	113.41
13	B7	201	CYC	C1D-CHD-C4C	-7.63	114.73	127.76
13	S7	201	CYC	C1C-NC-C4C	-7.61	103.86	113.41
13	L4	201	CYC	C1C-NC-C4C	-7.60	103.87	113.41
13	J1	201	CYC	C1C-NC-C4C	-7.60	103.88	113.41
13	V3	202	CYC	C4D-CHA-C1A	-7.59	111.64	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z7	301	CYC	C4D-CHA-C1A	-7.59	111.64	128.22
13	A1	302	CYC	C2C-C1C-NC	-7.56	102.00	108.29
13	L5	201	CYC	C1C-NC-C4C	-7.55	103.93	113.41
13	V2	201	CYC	C3C-C4C-NC	-7.55	98.22	107.94
13	E1	201	CYC	C4D-CHA-C1A	-7.54	111.76	128.22
13	22	302	CYC	C1D-CHD-C4C	-7.54	114.89	127.76
13	E5	201	CYC	C1D-CHD-C4C	-7.53	114.91	127.76
13	V7	202	CYC	C4D-CHA-C1A	-7.52	111.79	128.22
13	M6	201	CYC	C1C-NC-C4C	-7.51	103.98	113.41
13	S3	201	CYC	C1C-NC-C4C	-7.51	103.98	113.41
13	C2	201	CYC	C4D-CHA-C1A	-7.51	111.82	128.22
13	d2	201	CYC	C1C-NC-C4C	-7.50	104.00	113.41
13	Q7	201	CYC	C1D-CHD-C4C	-7.49	114.97	127.76
13	42	302	CYC	C2C-C1C-NC	-7.49	102.05	108.29
13	E1	201	CYC	C1D-CHD-C4C	-7.48	114.99	127.76
13	D6	201	CYC	C1C-NC-C4C	-7.47	104.04	113.41
13	F4	202	CYC	C4D-CHA-C1A	-7.46	111.93	128.22
13	M7	201	CYC	C1C-NC-C4C	-7.45	104.06	113.41
13	P7	202	CYC	C1B-CHB-C4A	-7.44	109.80	128.06
13	V4	202	CYC	C4D-CHA-C1A	-7.43	112.00	128.22
13	M3	201	CYC	C1C-NC-C4C	-7.42	104.10	113.41
13	V6	202	CYC	C4D-CHA-C1A	-7.42	112.02	128.22
13	K3	201	CYC	C1C-NC-C4C	-7.42	104.10	113.41
13	S7	201	CYC	C1D-CHD-C4C	-7.41	115.11	127.76
13	Q3	201	CYC	C1D-CHD-C4C	-7.40	115.12	127.76
13	I4	201	CYC	C1D-CHD-C4C	-7.40	115.13	127.76
13	V1	202	CYC	C4D-CHA-C1A	-7.39	112.08	128.22
13	k2	201	CYC	C1B-CHB-C4A	-7.39	109.91	128.06
13	P3	202	CYC	C1B-CHB-C4A	-7.39	109.91	128.06
13	32	302	CYC	C1D-CHD-C4C	-7.39	115.15	127.76
13	W7	201	CYC	C1C-NC-C4C	-7.39	104.14	113.41
13	Z3	301	CYC	C4D-CHA-C1A	-7.36	112.16	128.22
13	V5	202	CYC	C4D-CHA-C1A	-7.34	112.18	128.22
13	S1	201	CYC	C1C-NC-C4C	-7.34	104.20	113.41
13	F6	202	CYC	C4D-CHA-C1A	-7.34	112.19	128.22
13	M1	201	CYC	C1C-NC-C4C	-7.34	104.20	113.41
13	S7	201	CYC	C2C-C1C-NC	-7.34	102.18	108.29
13	V1	201	CYC	C2C-C1C-NC	-7.33	102.18	108.29
13	S6	201	CYC	C1C-NC-C4C	-7.33	104.22	113.41
13	a2	201	CYC	C1C-NC-C4C	-7.33	104.22	113.41
13	X3	201	CYC	C1C-NC-C4C	-7.33	104.22	113.41
13	B1	201	CYC	C1D-CHD-C4C	-7.33	115.26	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X7	201	CYC	C1C-NC-C4C	-7.32	104.22	113.41
13	R7	201	CYC	C1C-NC-C4C	-7.31	104.24	113.41
13	j2	201	CYC	C1C-NC-C4C	-7.30	104.25	113.41
13	P7	202	CYC	C1D-CHD-C4C	-7.28	115.33	127.76
13	S5	201	CYC	C2C-C1C-NC	-7.28	102.23	108.29
13	a7	202	CYC	C1D-CHD-C4C	-7.26	115.37	127.76
13	A6	302	CYC	C2C-C1C-NC	-7.24	102.26	108.29
13	B3	201	CYC	C1D-CHD-C4C	-7.24	115.40	127.76
13	P1	201	CYC	C1C-NC-C4C	-7.23	104.33	113.41
13	32	301	CYC	C1C-NC-C4C	-7.23	104.34	113.41
13	R3	201	CYC	C1C-NC-C4C	-7.23	104.34	113.41
13	S3	201	CYC	C2C-C1C-NC	-7.22	102.28	108.29
13	T2	201	CYC	C1C-NC-C4C	-7.21	104.37	113.41
13	O2	201	CYC	C1C-NC-C4C	-7.20	104.37	113.41
13	g2	201	CYC	C1C-NC-C4C	-7.20	104.38	113.41
13	S3	201	CYC	C1D-CHD-C4C	-7.18	115.50	127.76
13	I1	201	CYC	C1D-CHD-C4C	-7.18	115.50	127.76
13	I5	201	CYC	C1D-CHD-C4C	-7.18	115.51	127.76
13	B5	201	CYC	C1D-CHD-C4C	-7.18	115.51	127.76
13	W3	201	CYC	C1C-NC-C4C	-7.17	104.42	113.41
13	F1	202	CYC	C4D-CHA-C1A	-7.15	112.61	128.22
13	I6	201	CYC	C1D-CHD-C4C	-7.13	115.59	127.76
13	N2	801	CYC	C3C-C4C-NC	-7.12	98.78	107.94
13	C1	201	CYC	C3C-C4C-NC	-7.11	98.79	107.94
13	S4	201	CYC	C1C-NC-C4C	-7.10	104.50	113.41
13	a3	202	CYC	C1D-CHD-C4C	-7.10	115.65	127.76
13	P3	202	CYC	C4D-CHA-C1A	-7.09	112.73	128.22
13	F3	201	CYC	C1C-NC-C4C	-7.09	104.52	113.41
13	G6	201	CYC	C1C-NC-C4C	-7.09	104.52	113.41
13	F2	201	CYC	C1D-CHD-C4C	-7.08	115.67	127.76
13	P7	202	CYC	C4D-CHA-C1A	-7.07	112.78	128.22
13	F7	201	CYC	C1C-NC-C4C	-7.06	104.55	113.41
13	S1	201	CYC	C2C-C1C-NC	-7.05	102.41	108.29
13	M5	201	CYC	C1B-CHB-C4A	-7.05	110.74	128.06
13	J5	202	CYC	C1D-CHD-C4C	-7.05	115.73	127.76
13	B4	201	CYC	C1D-CHD-C4C	-7.05	115.73	127.76
13	y2	201	CYC	C1D-CHD-C4C	-7.04	115.74	127.76
13	C4	202	CYC	C4D-CHA-C1A	-7.04	112.84	128.22
13	S4	201	CYC	C1D-CHD-C4C	-7.04	115.74	127.76
13	C6	202	CYC	C4D-CHA-C1A	-7.04	112.84	128.22
13	e2	201	CYC	C1C-NC-C4C	-7.03	104.58	113.41
13	k2	201	CYC	C4D-CHA-C1A	-7.03	112.87	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A1	301	CYC	C1C-NC-C4C	-7.02	104.61	113.41
13	22	301	CYC	C1C-NC-C4C	-7.01	104.62	113.41
13	F4	201	CYC	C1C-NC-C4C	-7.00	104.63	113.41
13	M5	201	CYC	C1C-NC-C4C	-7.00	104.63	113.41
13	L7	201	CYC	C4D-CHA-C1A	-7.00	112.94	128.22
13	X2	201	CYC	C1C-NC-C4C	-6.99	104.64	113.41
13	U3	201	CYC	C1C-NC-C4C	-6.99	104.64	113.41
13	U4	201	CYC	C1C-NC-C4C	-6.99	104.64	113.41
13	R6	201	CYC	C1C-NC-C4C	-6.99	104.64	113.41
13	R1	201	CYC	C1C-NC-C4C	-6.99	104.64	113.41
13	H4	201	CYC	C1C-NC-C4C	-6.98	104.66	113.41
13	B6	201	CYC	C1D-CHD-C4C	-6.98	115.85	127.76
13	S6	201	CYC	C1D-CHD-C4C	-6.97	115.87	127.76
13	P5	202	CYC	C1C-NC-C4C	-6.97	104.67	113.41
13	h2	201	CYC	C1C-NC-C4C	-6.96	104.67	113.41
13	P1	202	CYC	C1C-NC-C4C	-6.96	104.68	113.41
13	Q4	201	CYC	C1D-CHD-C4C	-6.96	115.89	127.76
13	W6	201	CYC	C1C-NC-C4C	-6.95	104.69	113.41
13	C5	202	CYC	C4D-CHA-C1A	-6.95	113.04	128.22
13	L3	201	CYC	C4D-CHA-C1A	-6.93	113.08	128.22
13	M4	201	CYC	C1B-CHB-C4A	-6.92	111.06	128.06
13	S6	201	CYC	C2C-C1C-NC	-6.92	102.53	108.29
13	s2	201	CYC	C1C-NC-C4C	-6.92	104.73	113.41
13	N4	201	CYC	C1C-NC-C4C	-6.92	104.73	113.41
13	F1	201	CYC	C1C-NC-C4C	-6.91	104.74	113.41
13	E2	201	CYC	C1C-NC-C4C	-6.90	104.75	113.41
13	C2	201	CYC	C1C-NC-C4C	-6.90	104.76	113.41
13	M4	201	CYC	C1C-NC-C4C	-6.89	104.76	113.41
13	R5	201	CYC	C1C-NC-C4C	-6.89	104.76	113.41
13	F6	201	CYC	C1C-NC-C4C	-6.89	104.77	113.41
13	N2	802	CYC	C1C-NC-C4C	-6.89	104.77	113.41
13	R4	201	CYC	C1C-NC-C4C	-6.88	104.77	113.41
13	M7	201	CYC	C1B-CHB-C4A	-6.87	111.19	128.06
13	R2	201	CYC	C1C-NC-C4C	-6.86	104.80	113.41
13	I7	201	CYC	C1C-NC-C4C	-6.86	104.81	113.41
13	J6	202	CYC	C4D-CHA-C1A	-6.85	113.27	128.22
13	S5	201	CYC	C1D-CHD-C4C	-6.84	116.08	127.76
13	F5	201	CYC	C1C-NC-C4C	-6.84	104.83	113.41
13	C4	201	CYC	C3C-C4C-NC	-6.82	99.16	107.94
13	J4	201	CYC	C1C-NC-C4C	-6.80	104.88	113.41
13	P6	202	CYC	C1B-CHB-C4A	-6.80	111.37	128.06
13	A6	301	CYC	C1C-NC-C4C	-6.79	104.89	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J6	202	CYC	C1D-CHD-C4C	-6.79	116.17	127.76
13	U2	201	CYC	C4D-CHA-C1A	-6.79	113.39	128.22
13	Z7	301	CYC	C1C-NC-C4C	-6.79	104.90	113.41
13	B2	201	CYC	C1C-NC-C4C	-6.78	104.90	113.41
13	P1	202	CYC	C1B-CHB-C4A	-6.78	111.41	128.06
13	S4	201	CYC	C2C-C1C-NC	-6.77	102.65	108.29
13	J4	202	CYC	C1D-CHD-C4C	-6.76	116.22	127.76
13	H2	201	CYC	C4D-CHA-C1A	-6.76	113.46	128.22
13	G4	201	CYC	C1C-NC-C4C	-6.75	104.94	113.41
13	M1	201	CYC	C1B-CHB-C4A	-6.74	111.50	128.06
13	A2	201	CYC	C1C-NC-C4C	-6.73	104.97	113.41
13	J3	202	CYC	C1D-CHD-C4C	-6.72	116.28	127.76
13	M3	201	CYC	C1B-CHB-C4A	-6.72	111.55	128.06
13	W5	201	CYC	C1C-NC-C4C	-6.71	104.99	113.41
13	P5	201	CYC	C1C-NC-C4C	-6.71	104.99	113.41
13	Q1	201	CYC	C1D-CHD-C4C	-6.71	116.31	127.76
13	C5	201	CYC	C3C-C4C-NC	-6.69	99.32	107.94
13	F6	202	CYC	C1C-NC-C4C	-6.69	105.02	113.41
13	a2	201	CYC	C2C-C1C-NC	-6.69	102.72	108.29
13	V7	202	CYC	C1B-CHB-C4A	-6.67	111.67	128.06
13	P6	201	CYC	C1C-NC-C4C	-6.67	105.04	113.41
13	G5	201	CYC	C1C-NC-C4C	-6.67	105.05	113.41
13	P7	201	CYC	C4D-CHA-C1A	-6.66	113.68	128.22
13	Q5	201	CYC	C1D-CHD-C4C	-6.64	116.42	127.76
13	C7	201	CYC	C3C-C4C-NC	-6.64	99.39	107.94
13	i2	201	CYC	C1B-CHB-C4A	-6.64	111.75	128.06
13	Q6	201	CYC	C1D-CHD-C4C	-6.63	116.45	127.76
13	U6	201	CYC	C1C-NC-C4C	-6.62	105.11	113.41
13	J5	202	CYC	C4D-CHA-C1A	-6.62	113.77	128.22
13	D3	201	CYC	C4D-CHA-C1A	-6.60	113.80	128.22
13	42	301	CYC	C1C-NC-C4C	-6.58	105.15	113.41
13	W4	201	CYC	C1C-NC-C4C	-6.58	105.16	113.41
13	v2	201	CYC	C1C-NC-C4C	-6.56	105.18	113.41
13	N2	802	CYC	C4D-CHA-C1A	-6.56	113.90	128.22
13	J4	202	CYC	C4D-CHA-C1A	-6.56	113.90	128.22
13	P4	201	CYC	C1C-NC-C4C	-6.56	105.18	113.41
13	P4	202	CYC	C1C-NC-C4C	-6.55	105.19	113.41
13	F5	202	CYC	C1C-NC-C4C	-6.55	105.19	113.41
13	F1	202	CYC	C1C-NC-C4C	-6.55	105.20	113.41
13	C6	201	CYC	C3C-C4C-NC	-6.55	99.51	107.94
13	D2	201	CYC	C1C-NC-C4C	-6.54	105.20	113.41
13	C7	201	CYC	C1B-CHB-C4A	-6.53	112.02	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q7	201	CYC	C1B-CHB-C4A	-6.53	112.02	128.06
13	P3	201	CYC	C4D-CHA-C1A	-6.53	113.96	128.22
13	I3	201	CYC	C1C-NC-C4C	-6.53	105.22	113.41
13	A2	202	CYC	C1C-NC-C4C	-6.53	105.22	113.41
13	R7	201	CYC	C1B-CHB-C4A	-6.53	112.03	128.06
13	M2	201	CYC	C1D-CHD-C4C	-6.52	116.63	127.76
13	M6	201	CYC	C1B-CHB-C4A	-6.52	112.04	128.06
13	x2	201	CYC	C1C-NC-C4C	-6.52	105.23	113.41
13	L1	201	CYC	C3C-C4C-NC	-6.51	99.56	107.94
13	P4	201	CYC	C1B-CHB-C4A	-6.50	112.11	128.06
13	J1	202	CYC	C1D-CHD-C4C	-6.50	116.67	127.76
13	42	301	CYC	C4D-CHA-C1A	-6.50	114.04	128.22
13	w2	201	CYC	C1D-CHD-C4C	-6.49	116.68	127.76
13	Z4	301	CYC	C3C-C4C-NC	-6.49	99.59	107.94
13	N2	802	CYC	C2C-C1C-NC	-6.49	102.89	108.29
13	T2	201	CYC	C4D-CHA-C1A	-6.49	114.05	128.22
13	l2	201	CYC	C1D-CHD-C4C	-6.48	116.69	127.76
13	B5	201	CYC	C1C-NC-C4C	-6.48	105.28	113.41
13	C3	201	CYC	C1B-CHB-C4A	-6.47	112.16	128.06
13	p2	201	CYC	C2C-C1C-NC	-6.47	102.90	108.29
13	A2	201	CYC	C4D-CHA-C1A	-6.47	114.10	128.22
13	Z6	301	CYC	C3C-C4C-NC	-6.47	99.62	107.94
13	Q3	201	CYC	C1B-CHB-C4A	-6.47	112.18	128.06
13	Q7	202	CYC	C4D-CHA-C1A	-6.47	114.10	128.22
13	a4	202	CYC	C1D-CHD-C4C	-6.46	116.73	127.76
13	J7	202	CYC	C1D-CHD-C4C	-6.46	116.73	127.76
13	P3	202	CYC	C1D-CHD-C4C	-6.46	116.73	127.76
13	B1	201	CYC	C1C-NC-C4C	-6.46	105.30	113.41
13	P5	202	CYC	C1B-CHB-C4A	-6.46	112.19	128.06
13	Q3	202	CYC	C4D-CHA-C1A	-6.46	114.12	128.22
13	F3	202	CYC	C1C-NC-C4C	-6.46	105.31	113.41
13	22	301	CYC	C4D-CHA-C1A	-6.46	114.12	128.22
13	N5	201	CYC	C1C-NC-C4C	-6.45	105.31	113.41
13	P6	202	CYC	C1C-NC-C4C	-6.44	105.33	113.41
13	J1	202	CYC	C4D-CHA-C1A	-6.44	114.16	128.22
13	S1	201	CYC	C1D-CHD-C4C	-6.43	116.78	127.76
13	K4	201	CYC	C1C-NC-C4C	-6.42	105.35	113.41
13	A2	202	CYC	C4D-CHA-C1A	-6.42	114.20	128.22
13	22	302	CYC	C1C-NC-C4C	-6.42	105.36	113.41
13	C7	201	CYC	C4D-CHA-C1A	-6.41	114.22	128.22
13	F4	202	CYC	C1C-NC-C4C	-6.41	105.37	113.41
13	P6	202	CYC	C4D-CHA-C1A	-6.41	114.23	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J3	201	CYC	C1D-CHD-C4C	-6.41	116.83	127.76
13	F7	202	CYC	C1C-NC-C4C	-6.40	105.38	113.41
13	a7	201	CYC	C4D-CHA-C1A	-6.40	114.25	128.22
13	Q7	201	CYC	C1C-NC-C4C	-6.40	105.39	113.41
13	I4	201	CYC	C1C-NC-C4C	-6.39	105.39	113.41
13	Q6	201	CYC	C1C-NC-C4C	-6.39	105.39	113.41
13	Z1	301	CYC	C3C-C4C-NC	-6.39	99.71	107.94
13	52	301	CYC	C1C-NC-C4C	-6.39	105.39	113.41
13	t2	201	CYC	C4D-CHA-C1A	-6.39	114.28	128.22
13	j2	201	CYC	C4D-CHA-C1A	-6.38	114.28	128.22
13	Q5	201	CYC	C1C-NC-C4C	-6.38	105.40	113.41
13	P4	201	CYC	C4D-CHA-C1A	-6.38	114.29	128.22
13	d2	201	CYC	C4D-CHA-C1A	-6.37	114.30	128.22
13	32	302	CYC	C1C-NC-C4C	-6.36	105.43	113.41
13	o2	801	CYC	C4D-CHA-C1A	-6.36	114.33	128.22
13	y2	201	CYC	C1C-NC-C4C	-6.36	105.43	113.41
13	j2	201	CYC	C1B-CHB-C4A	-6.36	112.45	128.06
13	J7	201	CYC	C1D-CHD-C4C	-6.35	116.92	127.76
13	X7	201	CYC	C4D-CHA-C1A	-6.35	114.35	128.22
13	Q3	201	CYC	C1C-NC-C4C	-6.35	105.44	113.41
13	Z5	301	CYC	C3C-C4C-NC	-6.34	99.78	107.94
13	L2	201	CYC	C1D-CHD-C4C	-6.34	116.94	127.76
13	G2	201	CYC	C1C-NC-C4C	-6.34	105.46	113.41
13	Q4	201	CYC	C1C-NC-C4C	-6.34	105.46	113.41
13	H2	201	CYC	C1B-CHB-C4A	-6.34	112.49	128.06
13	f2	201	CYC	C4D-CHA-C1A	-6.32	114.41	128.22
13	V3	202	CYC	C1B-CHB-C4A	-6.32	112.55	128.06
13	T7	202	CYC	C1C-NC-C4C	-6.31	105.49	113.41
13	A6	301	CYC	C4D-CHA-C1A	-6.31	114.44	128.22
13	Q4	202	CYC	C1C-NC-C4C	-6.31	105.49	113.41
13	T6	202	CYC	C1C-NC-C4C	-6.31	105.49	113.41
13	C1	202	CYC	C4D-CHA-C1A	-6.31	114.45	128.22
13	X2	201	CYC	C4D-CHA-C1A	-6.31	114.45	128.22
13	D5	201	CYC	C4D-CHA-C1A	-6.30	114.45	128.22
13	c2	801	CYC	C4D-CHA-C1A	-6.30	114.46	128.22
13	S2	201	CYC	C4D-CHA-C1A	-6.30	114.46	128.22
13	T3	202	CYC	C1C-NC-C4C	-6.29	105.52	113.41
13	B2	202	CYC	C1D-CHD-C4C	-6.29	117.03	127.76
13	X3	201	CYC	C4D-CHA-C1A	-6.29	114.49	128.22
13	J7	201	CYC	C4D-CHA-C1A	-6.28	114.50	128.22
13	C3	201	CYC	C3C-C4C-NC	-6.27	99.87	107.94
13	Q5	202	CYC	C1C-NC-C4C	-6.26	105.56	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q1	201	CYC	C1C-NC-C4C	-6.25	105.56	113.41
13	f2	201	CYC	C1D-CHD-C4C	-6.23	117.12	127.76
13	L4	201	CYC	C4D-CHA-C1A	-6.23	114.61	128.22
13	Q6	202	CYC	C1C-NC-C4C	-6.23	105.59	113.41
13	L6	201	CYC	C4D-CHA-C1A	-6.22	114.63	128.22
13	D7	201	CYC	C4D-CHA-C1A	-6.21	114.65	128.22
13	a1	202	CYC	C3C-C4C-NC	-6.21	99.95	107.94
13	r2	201	CYC	C1C-NC-C4C	-6.20	105.63	113.41
13	M5	201	CYC	C1D-CHD-C4C	-6.20	117.17	127.76
13	M1	201	CYC	C1D-CHD-C4C	-6.20	117.18	127.76
13	Q7	202	CYC	C1C-NC-C4C	-6.19	105.64	113.41
13	m2	201	CYC	C1D-CHD-C4C	-6.19	117.20	127.76
13	B2	201	CYC	C1B-CHB-C4A	-6.19	112.86	128.06
13	Q1	202	CYC	C1C-NC-C4C	-6.18	105.65	113.41
13	L5	201	CYC	C4D-CHA-C1A	-6.18	114.73	128.22
13	X4	201	CYC	C4D-CHA-C1A	-6.17	114.75	128.22
13	a6	201	CYC	C3C-C4C-NC	-6.16	100.01	107.94
13	B3	201	CYC	C1C-NC-C4C	-6.16	105.69	113.41
13	I6	201	CYC	C1C-NC-C4C	-6.16	105.69	113.41
13	T4	202	CYC	C1C-NC-C4C	-6.15	105.69	113.41
13	Q2	201	CYC	C1C-NC-C4C	-6.15	105.70	113.41
13	P7	202	CYC	C1C-NC-C4C	-6.15	105.70	113.41
13	H7	201	CYC	C1B-CHB-C4A	-6.14	112.97	128.06
13	C3	201	CYC	C4D-CHA-C1A	-6.14	114.81	128.22
13	C6	201	CYC	C1B-CHB-C4A	-6.14	112.98	128.06
13	P2	201	CYC	C4D-CHA-C1A	-6.14	114.81	128.22
13	32	301	CYC	C4D-CHA-C1A	-6.13	114.82	128.22
13	a3	201	CYC	C4D-CHA-C1A	-6.13	114.83	128.22
13	I1	201	CYC	C1C-NC-C4C	-6.13	105.72	113.41
13	Q4	201	CYC	C1B-CHB-C4A	-6.13	113.00	128.06
13	J4	201	CYC	C1D-CHD-C4C	-6.13	117.30	127.76
13	V6	202	CYC	C1B-CHB-C4A	-6.11	113.06	128.06
13	52	302	CYC	C2C-C1C-NC	-6.10	103.21	108.29
13	T3	201	CYC	C1B-CHB-C4A	-6.10	113.08	128.06
13	n2	201	CYC	C1D-CHD-C4C	-6.10	117.36	127.76
13	p2	201	CYC	C1D-CHD-C4C	-6.10	117.36	127.76
13	P3	202	CYC	C1C-NC-C4C	-6.08	105.78	113.41
13	M4	201	CYC	C1D-CHD-C4C	-6.08	117.38	127.76
13	C3	202	CYC	C1C-NC-C4C	-6.08	105.79	113.41
13	K5	201	CYC	C1C-NC-C4C	-6.08	105.79	113.41
13	B7	201	CYC	C1C-NC-C4C	-6.08	105.79	113.41
13	M3	201	CYC	C1D-CHD-C4C	-6.07	117.41	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a5	202	CYC	C1D-CHD-C4C	-6.06	117.41	127.76
13	M7	201	CYC	C1D-CHD-C4C	-6.06	117.42	127.76
13	n2	201	CYC	C1C-NC-C4C	-6.06	105.81	113.41
13	A2	202	CYC	C1B-CHB-C4A	-6.06	113.18	128.06
13	L1	201	CYC	C4D-CHA-C1A	-6.05	115.01	128.22
13	T5	202	CYC	C1C-NC-C4C	-6.05	105.82	113.41
13	R4	201	CYC	C1B-CHB-C4A	-6.05	113.21	128.06
13	e2	201	CYC	C4D-CHA-C1A	-6.05	115.02	128.22
13	O2	201	CYC	C1D-CHD-C4C	-6.04	117.45	127.76
13	a1	202	CYC	C1D-CHD-C4C	-6.04	117.45	127.76
13	a6	202	CYC	C3C-C4C-NC	-6.04	100.17	107.94
13	B6	201	CYC	C1C-NC-C4C	-6.03	105.84	113.41
13	C4	202	CYC	C1C-NC-C4C	-6.03	105.84	113.41
13	V1	202	CYC	C1B-CHB-C4A	-6.03	113.25	128.06
13	P4	202	CYC	C4D-CHA-C1A	-6.03	115.06	128.22
13	Q6	202	CYC	C4D-CHA-C1A	-6.02	115.07	128.22
13	T1	202	CYC	C1C-NC-C4C	-6.01	105.87	113.41
13	C7	202	CYC	C1C-NC-C4C	-6.01	105.87	113.41
13	P5	202	CYC	C4D-CHA-C1A	-6.01	115.10	128.22
13	Z7	301	CYC	C1D-CHD-C4C	-6.01	117.51	127.76
13	J6	201	CYC	C1D-CHD-C4C	-6.00	117.52	127.76
13	x2	201	CYC	C4D-CHA-C1A	-6.00	115.11	128.22
13	U7	201	CYC	C1B-CHB-C4A	-6.00	113.33	128.06
13	C1	202	CYC	C1C-NC-C4C	-5.99	105.89	113.41
13	P5	201	CYC	C4D-CHA-C1A	-5.99	115.13	128.22
13	I7	201	CYC	C1B-CHB-C4A	-5.99	113.35	128.06
13	T2	201	CYC	C3C-C4C-NC	-5.99	100.23	107.94
13	s2	201	CYC	C4D-CHA-C1A	-5.98	115.15	128.22
13	U3	201	CYC	C1B-CHB-C4A	-5.98	113.37	128.06
13	C5	202	CYC	C1C-NC-C4C	-5.98	105.91	113.41
13	C6	202	CYC	C1C-NC-C4C	-5.98	105.91	113.41
13	E2	201	CYC	C4D-CHA-C1A	-5.98	115.17	128.22
13	w2	201	CYC	C1C-NC-C4C	-5.97	105.92	113.41
13	a1	201	CYC	C3C-C4C-NC	-5.97	100.25	107.94
13	V5	202	CYC	C1B-CHB-C4A	-5.97	113.40	128.06
13	R3	201	CYC	C1B-CHB-C4A	-5.96	113.41	128.06
13	J5	201	CYC	C1D-CHD-C4C	-5.95	117.61	127.76
13	V4	202	CYC	C1B-CHB-C4A	-5.93	113.49	128.06
13	D1	201	CYC	C4D-CHA-C1A	-5.93	115.27	128.22
13	Q2	201	CYC	C4D-CHA-C1A	-5.93	115.28	128.22
13	T7	201	CYC	C1B-CHB-C4A	-5.93	113.51	128.06
13	X4	201	CYC	C3C-C4C-NC	-5.92	100.31	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U4	201	CYC	C1B-CHB-C4A	-5.92	113.51	128.06
13	Q6	201	CYC	C1B-CHB-C4A	-5.92	113.51	128.06
13	z2	201	CYC	C4D-CHA-C1A	-5.92	115.29	128.22
13	a5	202	CYC	C3C-C4C-NC	-5.92	100.32	107.94
13	Q7	201	CYC	C4D-CHA-C1A	-5.92	115.30	128.22
13	R2	201	CYC	C4D-CHA-C1A	-5.91	115.31	128.22
13	M6	201	CYC	C1D-CHD-C4C	-5.91	117.68	127.76
13	a5	201	CYC	C3C-C4C-NC	-5.91	100.34	107.94
13	l2	201	CYC	C1C-NC-C4C	-5.89	106.02	113.41
13	Q3	202	CYC	C1C-NC-C4C	-5.89	106.02	113.41
13	D4	201	CYC	C4D-CHA-C1A	-5.89	115.36	128.22
13	v2	201	CYC	C4D-CHA-C1A	-5.88	115.39	128.22
13	D6	201	CYC	C4D-CHA-C1A	-5.87	115.40	128.22
13	c2	801	CYC	C1B-CHB-C4A	-5.87	113.64	128.06
13	R5	201	CYC	C1B-CHB-C4A	-5.87	113.64	128.06
13	L6	201	CYC	C3C-C4C-NC	-5.87	100.39	107.94
13	52	301	CYC	C4D-CHA-C1A	-5.86	115.42	128.22
13	h2	201	CYC	C2C-C1C-NC	-5.86	103.41	108.29
13	R7	201	CYC	C4D-CHA-C1A	-5.86	115.43	128.22
13	F3	201	CYC	C1B-CHB-C4A	-5.85	113.70	128.06
13	G7	201	CYC	C1B-CHB-C4A	-5.84	113.71	128.06
13	W7	201	CYC	C4D-CHA-C1A	-5.84	115.46	128.22
13	m2	201	CYC	C1C-NC-C4C	-5.84	106.09	113.41
13	P1	202	CYC	C4D-CHA-C1A	-5.83	115.48	128.22
13	W3	201	CYC	C4D-CHA-C1A	-5.83	115.48	128.22
13	Q3	201	CYC	C4D-CHA-C1A	-5.83	115.48	128.22
13	F7	202	CYC	C1B-CHB-C4A	-5.83	113.74	128.06
13	L2	201	CYC	C1C-NC-C4C	-5.83	106.10	113.41
13	C4	201	CYC	C1B-CHB-C4A	-5.82	113.76	128.06
13	M2	201	CYC	C2C-C1C-NC	-5.82	103.44	108.29
13	E7	201	CYC	C1B-CHB-C4A	-5.82	113.77	128.06
13	J3	201	CYC	C4D-CHA-C1A	-5.82	115.51	128.22
13	F2	201	CYC	C1C-NC-C4C	-5.82	106.11	113.41
13	J1	201	CYC	C1D-CHD-C4C	-5.81	117.85	127.76
13	X6	201	CYC	C4D-CHA-C1A	-5.81	115.54	128.22
13	U2	201	CYC	C3C-C4C-NC	-5.81	100.47	107.94
13	P1	201	CYC	C4D-CHA-C1A	-5.81	115.54	128.22
13	U2	201	CYC	C1D-CHD-C4C	-5.81	117.85	127.76
13	W7	201	CYC	C1B-CHB-C4A	-5.81	113.80	128.06
13	F7	201	CYC	C1B-CHB-C4A	-5.80	113.81	128.06
13	m2	201	CYC	C4D-CHA-C1A	-5.78	115.59	128.22
13	Q4	202	CYC	C4D-CHA-C1A	-5.77	115.61	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U7	201	CYC	C4D-CHA-C1A	-5.77	115.62	128.22
13	22	302	CYC	C4D-CHA-C1A	-5.76	115.64	128.22
13	X5	201	CYC	C3C-C4C-NC	-5.76	100.52	107.94
13	Q5	201	CYC	C1B-CHB-C4A	-5.76	113.91	128.06
13	A1	301	CYC	C3C-C4C-NC	-5.76	100.53	107.94
13	Z1	301	CYC	C4D-CHA-C1A	-5.75	115.66	128.22
13	P6	201	CYC	C4D-CHA-C1A	-5.74	115.68	128.22
13	R4	201	CYC	C4D-CHA-C1A	-5.74	115.68	128.22
13	X3	201	CYC	C1D-CHD-C4C	-5.74	117.97	127.76
13	F3	202	CYC	C1B-CHB-C4A	-5.73	113.98	128.06
13	Z5	301	CYC	C4D-CHA-C1A	-5.73	115.71	128.22
13	l2	201	CYC	C4D-CHA-C1A	-5.73	115.71	128.22
13	U3	201	CYC	C4D-CHA-C1A	-5.72	115.73	128.22
13	R3	201	CYC	C4D-CHA-C1A	-5.72	115.74	128.22
13	B4	201	CYC	C1C-NC-C4C	-5.71	106.25	113.41
13	w2	201	CYC	C4D-CHA-C1A	-5.70	115.78	128.22
13	C4	201	CYC	C4D-CHA-C1A	-5.70	115.78	128.22
13	B7	201	CYC	C4D-CHA-C1A	-5.70	115.78	128.22
13	X5	201	CYC	C4D-CHA-C1A	-5.70	115.78	128.22
13	V5	201	CYC	C3C-C4C-NC	-5.70	100.61	107.94
13	a3	201	CYC	C3C-C4C-NC	-5.69	100.61	107.94
13	V7	201	CYC	C1B-CHB-C4A	-5.69	114.08	128.06
13	C3	201	CYC	C2C-C1C-NC	-5.69	103.55	108.29
13	U5	201	CYC	C1B-CHB-C4A	-5.69	114.09	128.06
13	G7	201	CYC	C4D-CHA-C1A	-5.68	115.82	128.22
13	a7	201	CYC	C3C-C4C-NC	-5.68	100.63	107.94
13	N7	201	CYC	C4D-CHA-C1A	-5.68	115.83	128.22
13	V3	201	CYC	C1B-CHB-C4A	-5.67	114.13	128.06
13	F7	201	CYC	C4D-CHA-C1A	-5.67	115.84	128.22
13	H3	201	CYC	C1B-CHB-C4A	-5.66	114.15	128.06
13	K3	201	CYC	C4D-CHA-C1A	-5.66	115.86	128.22
13	C1	201	CYC	C4D-CHA-C1A	-5.66	115.86	128.22
13	K7	201	CYC	C1B-CHB-C4A	-5.66	114.17	128.06
13	a5	201	CYC	C4D-CHA-C1A	-5.65	115.87	128.22
13	C6	201	CYC	C4D-CHA-C1A	-5.65	115.88	128.22
13	32	302	CYC	C4D-CHA-C1A	-5.65	115.89	128.22
13	W3	201	CYC	C1B-CHB-C4A	-5.63	114.23	128.06
13	I3	201	CYC	C1B-CHB-C4A	-5.62	114.25	128.06
13	X5	201	CYC	C1D-CHD-C4C	-5.62	118.17	127.76
13	Z1	301	CYC	C2C-C1C-NC	-5.62	103.61	108.29
13	a4	202	CYC	C3C-C4C-NC	-5.61	100.71	107.94
13	Q1	202	CYC	C4D-CHA-C1A	-5.61	115.96	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V6	201	CYC	C3C-C4C-NC	-5.61	100.72	107.94
13	a3	201	CYC	C2C-C1C-NC	-5.61	103.61	108.29
13	a6	201	CYC	C4D-CHA-C1A	-5.61	115.98	128.22
13	X7	201	CYC	C1D-CHD-C4C	-5.61	118.19	127.76
13	a7	202	CYC	C3C-C4C-NC	-5.60	100.73	107.94
13	G3	201	CYC	C4D-CHA-C1A	-5.60	115.99	128.22
13	R5	201	CYC	C4D-CHA-C1A	-5.60	115.99	128.22
13	E3	201	CYC	C1B-CHB-C4A	-5.59	114.33	128.06
13	F2	201	CYC	C4D-CHA-C1A	-5.58	116.03	128.22
13	G3	201	CYC	C1B-CHB-C4A	-5.58	114.35	128.06
13	P2	201	CYC	C3C-C4C-NC	-5.58	100.75	107.94
13	K7	201	CYC	C4D-CHA-C1A	-5.58	116.03	128.22
13	V2	201	CYC	C4D-CHA-C1A	-5.58	116.05	128.22
13	L2	201	CYC	C4D-CHA-C1A	-5.57	116.06	128.22
13	P5	202	CYC	C3C-C4C-NC	-5.56	100.78	107.94
13	Z4	301	CYC	C4D-CHA-C1A	-5.55	116.09	128.22
13	C5	201	CYC	C4D-CHA-C1A	-5.55	116.09	128.22
13	Z6	301	CYC	C4D-CHA-C1A	-5.55	116.10	128.22
13	y2	201	CYC	C4D-CHA-C1A	-5.54	116.12	128.22
13	X2	201	CYC	C3C-C4C-NC	-5.54	100.81	107.94
13	r2	201	CYC	C4D-CHA-C1A	-5.54	116.13	128.22
13	N3	201	CYC	C4D-CHA-C1A	-5.54	116.13	128.22
13	d2	201	CYC	C1B-CHB-C4A	-5.54	114.46	128.06
13	R6	201	CYC	C4D-CHA-C1A	-5.53	116.14	128.22
13	J6	201	CYC	C4D-CHA-C1A	-5.53	116.15	128.22
13	N7	201	CYC	C1B-CHB-C4A	-5.53	114.49	128.06
13	Q5	202	CYC	C4D-CHA-C1A	-5.53	116.16	128.22
13	S6	201	CYC	C1B-CHB-C4A	-5.52	114.49	128.06
13	j2	201	CYC	C2C-C1C-NC	-5.52	103.69	108.29
13	K3	201	CYC	C1B-CHB-C4A	-5.52	114.51	128.06
13	I5	201	CYC	C1B-CHB-C4A	-5.51	114.52	128.06
13	x2	201	CYC	C1D-CHD-C4C	-5.51	118.35	127.76
13	F3	201	CYC	C4D-CHA-C1A	-5.51	116.19	128.22
13	X1	201	CYC	C4D-CHA-C1A	-5.51	116.19	128.22
13	V7	201	CYC	C4D-CHA-C1A	-5.51	116.19	128.22
13	B3	201	CYC	C4D-CHA-C1A	-5.50	116.20	128.22
13	M4	201	CYC	C4D-CHA-C1A	-5.50	116.20	128.22
13	M3	201	CYC	C4D-CHA-C1A	-5.50	116.20	128.22
13	M7	201	CYC	C4D-CHA-C1A	-5.50	116.20	128.22
13	A6	301	CYC	C3C-C4C-NC	-5.50	100.86	107.94
13	Z4	301	CYC	C2C-C1C-NC	-5.49	103.71	108.29
13	C7	202	CYC	C1B-CHB-C4A	-5.49	114.57	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F5	201	CYC	C4D-CHA-C1A	-5.49	116.23	128.22
13	F6	201	CYC	C4D-CHA-C1A	-5.49	116.24	128.22
13	J1	201	CYC	C4D-CHA-C1A	-5.49	116.24	128.22
13	U6	201	CYC	C1B-CHB-C4A	-5.49	114.59	128.06
13	I5	201	CYC	C1C-NC-C4C	-5.48	106.53	113.41
13	U4	201	CYC	C4D-CHA-C1A	-5.48	116.25	128.22
13	a3	202	CYC	C3C-C4C-NC	-5.48	100.89	107.94
13	I6	201	CYC	C4D-CHA-C1A	-5.48	116.26	128.22
13	C2	201	CYC	C1B-CHB-C4A	-5.48	114.61	128.06
13	N3	201	CYC	C1B-CHB-C4A	-5.48	114.61	128.06
13	Z3	301	CYC	C1D-CHD-C4C	-5.47	118.42	127.76
13	Q1	201	CYC	C1B-CHB-C4A	-5.47	114.62	128.06
13	I4	201	CYC	C4D-CHA-C1A	-5.47	116.27	128.22
13	t2	201	CYC	C1D-CHD-C4C	-5.47	118.42	127.76
13	M2	201	CYC	C4D-CHA-C1A	-5.47	116.27	128.22
13	a6	202	CYC	C1D-CHD-C4C	-5.47	118.43	127.76
13	V7	201	CYC	C1D-CHD-C4C	-5.47	118.43	127.76
13	42	302	CYC	C1D-CHD-C4C	-5.47	118.43	127.76
13	a7	201	CYC	C2C-C1C-NC	-5.46	103.74	108.29
13	Z6	301	CYC	C2C-C1C-NC	-5.46	103.74	108.29
13	I3	201	CYC	C4D-CHA-C1A	-5.45	116.33	128.22
13	N2	801	CYC	C4D-CHA-C1A	-5.44	116.33	128.22
13	Q7	202	CYC	C1B-CHB-C4A	-5.44	114.69	128.06
13	T4	201	CYC	C1B-CHB-C4A	-5.44	114.71	128.06
13	T4	202	CYC	C4D-CHA-C1A	-5.44	116.35	128.22
13	W2	201	CYC	C4D-CHA-C1A	-5.43	116.36	128.22
13	N2	801	CYC	C1D-CHD-C4C	-5.43	118.49	127.76
13	F4	201	CYC	C4D-CHA-C1A	-5.43	116.37	128.22
13	X6	201	CYC	C3C-C4C-NC	-5.43	100.96	107.94
13	J7	202	CYC	C1B-CHB-C4A	-5.42	114.75	128.06
13	R1	201	CYC	C4D-CHA-C1A	-5.42	116.39	128.22
13	M6	201	CYC	C4D-CHA-C1A	-5.42	116.39	128.22
13	i2	201	CYC	C1D-CHD-C4C	-5.40	118.54	127.76
13	I4	201	CYC	C1B-CHB-C4A	-5.40	114.79	128.06
13	O2	201	CYC	C2C-C1C-NC	-5.40	103.79	108.29
13	B2	202	CYC	C3C-C4C-NC	-5.39	101.00	107.94
13	C1	201	CYC	C1B-CHB-C4A	-5.39	114.82	128.06
13	A6	302	CYC	C1D-CHD-C4C	-5.39	118.56	127.76
13	X6	201	CYC	C1D-CHD-C4C	-5.39	118.56	127.76
13	X1	201	CYC	C1D-CHD-C4C	-5.39	118.57	127.76
13	V4	201	CYC	C3C-C4C-NC	-5.38	101.01	107.94
13	T7	202	CYC	C4D-CHA-C1A	-5.38	116.48	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I7	201	CYC	C4D-CHA-C1A	-5.38	116.48	128.22
13	B4	201	CYC	C4D-CHA-C1A	-5.37	116.48	128.22
13	P1	202	CYC	C3C-C4C-NC	-5.37	101.03	107.94
13	M5	201	CYC	C4D-CHA-C1A	-5.36	116.52	128.22
13	a1	201	CYC	C2C-C1C-NC	-5.35	103.83	108.29
13	e2	201	CYC	C2C-C1C-NC	-5.35	103.83	108.29
13	N5	201	CYC	C4D-CHA-C1A	-5.35	116.53	128.22
13	N4	201	CYC	C4D-CHA-C1A	-5.35	116.54	128.22
13	U1	201	CYC	C1B-CHB-C4A	-5.34	114.94	128.06
13	F1	202	CYC	C1B-CHB-C4A	-5.34	114.95	128.06
13	W1	201	CYC	C1B-CHB-C4A	-5.34	114.95	128.06
13	n2	201	CYC	C4D-CHA-C1A	-5.34	116.57	128.22
13	H5	201	CYC	C1B-CHB-C4A	-5.33	114.96	128.06
13	Q5	201	CYC	C2C-C1C-NC	-5.33	103.85	108.29
13	Q3	202	CYC	C1B-CHB-C4A	-5.33	114.98	128.06
13	S7	201	CYC	C1B-CHB-C4A	-5.32	114.99	128.06
13	F4	201	CYC	C1B-CHB-C4A	-5.32	114.99	128.06
13	J4	201	CYC	C4D-CHA-C1A	-5.31	116.62	128.22
13	F5	202	CYC	C2C-C1C-NC	-5.31	103.87	108.29
13	A1	301	CYC	C4D-CHA-C1A	-5.30	116.64	128.22
13	B7	201	CYC	C1B-CHB-C4A	-5.30	115.04	128.06
13	52	302	CYC	C1D-CHD-C4C	-5.29	118.73	127.76
13	T4	202	CYC	C1B-CHB-C4A	-5.29	115.07	128.06
13	T3	202	CYC	C4D-CHA-C1A	-5.28	116.68	128.22
13	g2	201	CYC	C4D-CHA-C1A	-5.27	116.70	128.22
13	N6	201	CYC	C4D-CHA-C1A	-5.27	116.70	128.22
13	T5	202	CYC	C1B-CHB-C4A	-5.27	115.11	128.06
13	W5	201	CYC	C1B-CHB-C4A	-5.27	115.11	128.06
13	X1	201	CYC	C3C-C4C-NC	-5.27	101.16	107.94
13	R6	201	CYC	C1B-CHB-C4A	-5.26	115.15	128.06
13	T5	201	CYC	C1B-CHB-C4A	-5.25	115.16	128.06
13	m2	201	CYC	C1B-CHB-C4A	-5.25	115.16	128.06
13	M1	201	CYC	C4D-CHA-C1A	-5.24	116.77	128.22
13	a1	201	CYC	C4D-CHA-C1A	-5.24	116.78	128.22
13	I1	201	CYC	C4D-CHA-C1A	-5.24	116.78	128.22
13	H7	201	CYC	C4D-CHA-C1A	-5.23	116.81	128.22
13	D3	201	CYC	C1B-CHB-C4A	-5.23	115.23	128.06
13	H4	201	CYC	C4D-CHA-C1A	-5.22	116.81	128.22
13	32	301	CYC	C3C-C4C-NC	-5.22	101.22	107.94
13	S4	201	CYC	C1B-CHB-C4A	-5.22	115.24	128.06
13	S5	201	CYC	C1B-CHB-C4A	-5.22	115.24	128.06
13	U5	201	CYC	C4D-CHA-C1A	-5.21	116.83	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P7	202	CYC	C2C-C1C-NC	-5.21	103.95	108.29
13	H6	201	CYC	C1B-CHB-C4A	-5.21	115.26	128.06
13	L3	201	CYC	C3C-C4C-NC	-5.21	101.24	107.94
13	V3	201	CYC	C3C-C4C-NC	-5.21	101.24	107.94
13	D5	201	CYC	C3C-C4C-NC	-5.20	101.25	107.94
13	W6	201	CYC	C1B-CHB-C4A	-5.20	115.29	128.06
13	T6	202	CYC	C4D-CHA-C1A	-5.20	116.87	128.22
13	a6	201	CYC	C2C-C1C-NC	-5.20	103.96	108.29
13	T5	202	CYC	C4D-CHA-C1A	-5.19	116.88	128.22
13	B6	201	CYC	C4D-CHA-C1A	-5.19	116.88	128.22
13	T7	202	CYC	C1B-CHB-C4A	-5.19	115.31	128.06
13	H4	201	CYC	C1B-CHB-C4A	-5.19	115.32	128.06
13	I6	201	CYC	C1B-CHB-C4A	-5.18	115.33	128.06
13	C3	201	CYC	C1D-CHD-C4C	-5.18	118.91	127.76
13	R1	201	CYC	C1B-CHB-C4A	-5.18	115.33	128.06
13	B3	201	CYC	C1B-CHB-C4A	-5.18	115.33	128.06
13	G4	201	CYC	C4D-CHA-C1A	-5.18	116.90	128.22
13	F1	201	CYC	C4D-CHA-C1A	-5.18	116.90	128.22
13	P6	202	CYC	C1D-CHD-C4C	-5.18	118.92	127.76
13	J7	201	CYC	C1B-CHB-C4A	-5.18	115.35	128.06
13	D2	201	CYC	C4D-CHA-C1A	-5.17	116.93	128.22
13	V1	201	CYC	C3C-C4C-NC	-5.17	101.29	107.94
13	z2	201	CYC	C2C-C1C-NC	-5.17	103.98	108.29
13	A1	302	CYC	C1D-CHD-C4C	-5.17	118.94	127.76
13	32	301	CYC	C1D-CHD-C4C	-5.16	118.95	127.76
13	K6	201	CYC	C1B-CHB-C4A	-5.16	115.39	128.06
13	H3	201	CYC	C4D-CHA-C1A	-5.16	116.96	128.22
13	K4	201	CYC	C1B-CHB-C4A	-5.15	115.41	128.06
13	V5	201	CYC	C4D-CHA-C1A	-5.15	116.97	128.22
13	F1	202	CYC	C2C-C1C-NC	-5.15	104.00	108.29
13	Z7	301	CYC	C2C-C3C-C4C	5.15	109.05	101.34
13	X4	201	CYC	C1D-CHD-C4C	-5.15	118.97	127.76
13	P4	201	CYC	C1D-CHD-C4C	-5.14	118.98	127.76
13	K1	201	CYC	C4D-CHA-C1A	-5.14	116.99	128.22
13	R2	201	CYC	C2C-C1C-NC	-5.14	104.01	108.29
13	C5	201	CYC	C1B-CHB-C4A	-5.13	115.45	128.06
13	Q4	201	CYC	C4D-CHA-C1A	-5.13	117.02	128.22
13	h2	201	CYC	C4D-CHA-C1A	-5.13	117.02	128.22
13	G5	201	CYC	C4D-CHA-C1A	-5.12	117.03	128.22
13	F4	202	CYC	C1B-CHB-C4A	-5.12	115.48	128.06
13	d2	201	CYC	C3C-C4C-NC	-5.12	101.35	107.94
13	S3	201	CYC	C1B-CHB-C4A	-5.12	115.49	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a7	202	CYC	C1B-CHB-C4A	-5.12	115.49	128.06
13	V3	201	CYC	C4D-CHA-C1A	-5.11	117.06	128.22
13	V4	201	CYC	C4D-CHA-C1A	-5.11	117.06	128.22
13	L7	201	CYC	C3C-C4C-NC	-5.11	101.36	107.94
13	U6	201	CYC	C4D-CHA-C1A	-5.11	117.06	128.22
13	G6	201	CYC	C1B-CHB-C4A	-5.11	115.52	128.06
13	I5	201	CYC	C4D-CHA-C1A	-5.10	117.08	128.22
13	V6	201	CYC	C4D-CHA-C1A	-5.10	117.08	128.22
13	F5	202	CYC	C1B-CHB-C4A	-5.09	115.55	128.06
13	I1	201	CYC	C1B-CHB-C4A	-5.09	115.57	128.06
13	H6	201	CYC	C4D-CHA-C1A	-5.08	117.12	128.22
13	22	301	CYC	C3C-C4C-NC	-5.08	101.40	107.94
13	W4	201	CYC	C4D-CHA-C1A	-5.08	117.14	128.22
13	D1	201	CYC	C3C-C4C-NC	-5.08	101.41	107.94
13	S1	201	CYC	C1B-CHB-C4A	-5.06	115.62	128.06
13	V7	201	CYC	C2C-C1C-NC	-5.06	104.07	108.29
13	42	301	CYC	C3C-C4C-NC	-5.06	101.42	107.94
13	22	301	CYC	C1D-CHD-C4C	-5.06	119.12	127.76
13	C6	201	CYC	C1D-CHD-C4C	-5.06	119.13	127.76
13	a7	201	CYC	C1D-CHD-C4C	-5.06	119.13	127.76
13	C3	202	CYC	C1B-CHB-C4A	-5.06	115.64	128.06
13	P5	201	CYC	C2C-C1C-NC	-5.05	104.08	108.29
13	T3	202	CYC	C1B-CHB-C4A	-5.05	115.65	128.06
13	A6	302	CYC	C3C-C4C-NC	-5.05	101.45	107.94
13	G2	201	CYC	C2C-C1C-NC	-5.04	104.09	108.29
13	F4	202	CYC	C2C-C1C-NC	-5.04	104.09	108.29
13	C7	201	CYC	C1D-CHD-C4C	-5.03	119.17	127.76
13	H1	201	CYC	C4D-CHA-C1A	-5.03	117.23	128.22
13	G6	201	CYC	C4D-CHA-C1A	-5.03	117.23	128.22
13	Q5	201	CYC	C4D-CHA-C1A	-5.03	117.23	128.22
13	E2	201	CYC	C2C-C1C-NC	-5.03	104.10	108.29
13	U1	201	CYC	C4D-CHA-C1A	-5.02	117.26	128.22
13	L6	201	CYC	C1D-CHD-C4C	-5.02	119.19	127.76
13	F1	201	CYC	C1B-CHB-C4A	-5.02	115.74	128.06
13	L2	201	CYC	C1B-CHB-C4A	-5.02	115.74	128.06
13	n2	201	CYC	CAB-C3B-C4B	5.01	129.12	121.37
13	W4	201	CYC	C1B-CHB-C4A	-5.01	115.76	128.06
13	a5	201	CYC	C2C-C1C-NC	-5.01	104.12	108.29
13	C4	202	CYC	C1B-CHB-C4A	-5.01	115.77	128.06
13	G5	201	CYC	C1B-CHB-C4A	-5.00	115.77	128.06
13	P5	202	CYC	C1D-CHD-C4C	-5.00	119.23	127.76
13	T1	202	CYC	C1B-CHB-C4A	-5.00	115.78	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B5	201	CYC	C4D-CHA-C1A	-5.00	117.31	128.22
13	L4	201	CYC	C3C-C4C-NC	-5.00	101.51	107.94
13	L1	201	CYC	C1D-CHD-C4C	-4.98	119.26	127.76
13	52	301	CYC	C1D-CHD-C4C	-4.98	119.27	127.76
13	A1	302	CYC	C3C-C4C-NC	-4.98	101.54	107.94
13	L5	201	CYC	C1D-CHD-C4C	-4.97	119.28	127.76
13	K5	201	CYC	C4D-CHA-C1A	-4.97	117.37	128.22
13	T6	202	CYC	C1B-CHB-C4A	-4.97	115.85	128.06
13	P4	201	CYC	C3C-C4C-NC	-4.97	101.55	107.94
13	a3	201	CYC	C1D-CHD-C4C	-4.96	119.29	127.76
13	L7	201	CYC	C1D-CHD-C4C	-4.96	119.29	127.76
13	C5	201	CYC	C2C-C1C-NC	-4.96	104.16	108.29
13	T1	202	CYC	C4D-CHA-C1A	-4.96	117.40	128.22
13	F6	202	CYC	C1B-CHB-C4A	-4.96	115.89	128.06
13	S7	201	CYC	C4D-CHA-C1A	-4.95	117.40	128.22
13	J3	202	CYC	C1B-CHB-C4A	-4.95	115.90	128.06
13	H5	201	CYC	C4D-CHA-C1A	-4.95	117.42	128.22
13	a1	201	CYC	C1D-CHD-C4C	-4.95	119.32	127.76
13	R7	201	CYC	C3C-C4C-NC	-4.94	101.58	107.94
13	52	302	CYC	C4D-CHA-C1A	-4.94	117.44	128.22
13	W6	201	CYC	C4D-CHA-C1A	-4.94	117.44	128.22
13	H1	201	CYC	C1B-CHB-C4A	-4.94	115.94	128.06
13	S3	201	CYC	C4D-CHA-C1A	-4.93	117.44	128.22
13	N6	201	CYC	C1B-CHB-C4A	-4.93	115.95	128.06
13	p2	201	CYC	C4D-CHA-C1A	-4.92	117.47	128.22
13	F6	202	CYC	C2C-C1C-NC	-4.92	104.19	108.29
13	N1	201	CYC	C4D-CHA-C1A	-4.92	117.48	128.22
13	L3	201	CYC	C1D-CHD-C4C	-4.91	119.37	127.76
13	G1	201	CYC	C4D-CHA-C1A	-4.91	117.49	128.22
13	L5	201	CYC	C3C-C4C-NC	-4.91	101.62	107.94
13	V4	201	CYC	C1B-CHB-C4A	-4.91	116.00	128.06
13	Q1	201	CYC	C4D-CHA-C1A	-4.91	117.50	128.22
13	Q6	201	CYC	C4D-CHA-C1A	-4.91	117.50	128.22
13	S4	201	CYC	C4D-CHA-C1A	-4.90	117.53	128.22
13	J5	201	CYC	C4D-CHA-C1A	-4.90	117.53	128.22
13	T1	201	CYC	C1B-CHB-C4A	-4.89	116.04	128.06
13	V5	201	CYC	C1B-CHB-C4A	-4.89	116.05	128.06
13	W5	201	CYC	C4D-CHA-C1A	-4.89	117.54	128.22
13	K4	201	CYC	C4D-CHA-C1A	-4.89	117.54	128.22
13	Z5	301	CYC	C2C-C1C-NC	-4.89	104.22	108.29
13	R3	201	CYC	C3C-C4C-NC	-4.88	101.66	107.94
13	G1	201	CYC	C1B-CHB-C4A	-4.87	116.09	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C2	201	CYC	C2C-C1C-NC	-4.87	104.23	108.29
13	B5	201	CYC	C1B-CHB-C4A	-4.87	116.10	128.06
13	A6	301	CYC	C1D-CHD-C4C	-4.86	119.47	127.76
13	K5	201	CYC	C1B-CHB-C4A	-4.86	116.13	128.06
13	w2	201	CYC	C2C-C3C-C4C	4.86	108.61	101.34
13	C5	202	CYC	C1B-CHB-C4A	-4.84	116.17	128.06
13	A1	301	CYC	C1D-CHD-C4C	-4.84	119.50	127.76
13	E7	201	CYC	C3C-C4C-NC	-4.83	101.72	107.94
13	F5	201	CYC	C1B-CHB-C4A	-4.81	116.23	128.06
13	B1	201	CYC	C4D-CHA-C1A	-4.81	117.71	128.22
13	P6	202	CYC	C3C-C4C-NC	-4.81	101.75	107.94
13	V1	201	CYC	C1D-CHD-C4C	-4.81	119.55	127.76
13	D5	201	CYC	C1D-CHD-C4C	-4.81	119.56	127.76
13	a5	201	CYC	C1D-CHD-C4C	-4.81	119.56	127.76
13	Z1	301	CYC	C1D-CHD-C4C	-4.80	119.58	127.76
13	T6	201	CYC	C1B-CHB-C4A	-4.80	116.28	128.06
13	V1	201	CYC	C4D-CHA-C1A	-4.79	117.75	128.22
13	J4	201	CYC	C1B-CHB-C4A	-4.79	116.29	128.06
13	42	302	CYC	C4D-CHA-C1A	-4.79	117.76	128.22
13	C4	201	CYC	C1D-CHD-C4C	-4.79	119.59	127.76
13	C1	201	CYC	C1D-CHD-C4C	-4.78	119.60	127.76
13	42	301	CYC	C1D-CHD-C4C	-4.78	119.60	127.76
13	X2	201	CYC	C1D-CHD-C4C	-4.77	119.62	127.76
13	P1	202	CYC	C1D-CHD-C4C	-4.77	119.62	127.76
13	Z6	301	CYC	C1D-CHD-C4C	-4.77	119.63	127.76
13	A1	302	CYC	C4D-CHA-C1A	-4.76	117.82	128.22
13	A6	302	CYC	C4D-CHA-C1A	-4.76	117.82	128.22
13	52	302	CYC	C3C-C4C-NC	-4.76	101.81	107.94
13	K6	201	CYC	C4D-CHA-C1A	-4.75	117.84	128.22
13	C6	202	CYC	C1B-CHB-C4A	-4.74	116.41	128.06
13	B1	201	CYC	C1B-CHB-C4A	-4.74	116.41	128.06
13	B5	201	CYC	C2C-C1C-NC	-4.74	104.34	108.29
13	V3	201	CYC	C1D-CHD-C4C	-4.74	119.68	127.76
13	O2	201	CYC	C4D-CHA-C1A	-4.74	117.88	128.22
13	V2	201	CYC	C1D-CHD-C4C	-4.73	119.70	127.76
13	C5	201	CYC	C1D-CHD-C4C	-4.72	119.70	127.76
13	W1	201	CYC	C4D-CHA-C1A	-4.72	117.91	128.22
13	E5	201	CYC	C3C-C4C-NC	-4.72	101.86	107.94
13	V6	201	CYC	C1B-CHB-C4A	-4.71	116.49	128.06
13	J3	201	CYC	C1B-CHB-C4A	-4.71	116.50	128.06
13	E4	201	CYC	C3C-C4C-NC	-4.70	101.89	107.94
13	S2	201	CYC	C1D-CHD-C4C	-4.70	119.75	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C5	201	CYC	CMD-C2D-C1D	4.69	132.44	125.62
13	A1	301	CYC	CMD-C2D-C1D	4.69	132.44	125.62
13	L4	201	CYC	C1D-CHD-C4C	-4.69	119.77	127.76
13	E1	201	CYC	C3C-C4C-NC	-4.68	101.91	107.94
13	P6	201	CYC	C2C-C3C-C4C	4.68	108.35	101.34
13	Z3	301	CYC	C2C-C3C-C4C	4.68	108.34	101.34
13	E3	201	CYC	C3C-C4C-NC	-4.67	101.92	107.94
13	E6	201	CYC	C1B-CHB-C4A	-4.67	116.58	128.06
13	G2	201	CYC	C4D-CHA-C1A	-4.67	118.02	128.22
13	B2	202	CYC	CAB-C3B-C4B	4.67	128.59	121.37
13	C1	201	CYC	CMD-C2D-C1D	4.66	132.39	125.62
13	I5	201	CYC	C2C-C3C-C4C	4.66	108.32	101.34
13	B4	201	CYC	C1B-CHB-C4A	-4.66	116.62	128.06
13	C6	201	CYC	CMD-C2D-C1D	4.65	132.38	125.62
13	s2	201	CYC	C2C-C1C-NC	-4.65	104.41	108.29
13	V6	201	CYC	C1D-CHD-C4C	-4.64	119.84	127.76
13	V5	201	CYC	C1D-CHD-C4C	-4.64	119.84	127.76
13	T7	202	CYC	CAB-C3B-C4B	4.64	128.55	121.37
13	B1	201	CYC	C2C-C1C-NC	-4.64	104.42	108.29
13	I1	201	CYC	C2C-C3C-C4C	4.64	108.29	101.34
13	V1	201	CYC	C1B-CHB-C4A	-4.63	116.68	128.06
13	P4	202	CYC	C2C-C3C-C4C	4.63	108.28	101.34
13	j2	201	CYC	C2C-C3C-C4C	4.63	108.28	101.34
13	T2	201	CYC	CAB-C3B-C4B	4.63	128.53	121.37
13	M1	201	CYC	CMD-C2D-C1D	4.63	132.35	125.62
13	H6	201	CYC	C3C-C4C-NC	-4.62	101.99	107.94
13	S1	201	CYC	C4D-CHA-C1A	-4.62	118.13	128.22
13	P2	201	CYC	C1D-CHD-C4C	-4.62	119.88	127.76
13	O2	201	CYC	C2C-C3C-C4C	4.62	108.26	101.34
13	S2	201	CYC	C2C-C1C-NC	-4.62	104.44	108.29
13	N4	201	CYC	C1B-CHB-C4A	-4.62	116.72	128.06
13	D6	201	CYC	C1D-CHD-C4C	-4.62	119.88	127.76
13	a1	201	CYC	CMD-C2D-C1D	4.62	132.33	125.62
13	q2	201	CYC	C1C-NC-C4C	-4.61	107.62	113.41
13	a6	201	CYC	C1D-CHD-C4C	-4.61	119.89	127.76
13	J3	201	CYC	CMD-C2D-C1D	4.61	132.32	125.62
13	f2	201	CYC	C3C-C4C-NC	-4.61	102.01	107.94
13	B5	201	CYC	C2C-C3C-C4C	4.60	108.23	101.34
13	N2	801	CYC	CMD-C2D-C1D	4.60	132.30	125.62
13	52	301	CYC	C3C-C4C-NC	-4.60	102.02	107.94
13	J5	201	CYC	CAB-C3B-C4B	4.60	128.48	121.37
13	I4	201	CYC	C2C-C3C-C4C	4.58	108.20	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	y2	201	CYC	C2C-C3C-C4C	4.58	108.20	101.34
13	B6	201	CYC	C1B-CHB-C4A	-4.58	116.82	128.06
13	C3	201	CYC	CMD-C2D-C1D	4.58	132.27	125.62
13	Z5	301	CYC	C1D-CHD-C4C	-4.57	119.96	127.76
13	J4	201	CYC	CMD-C2D-C1D	4.57	132.26	125.62
13	D1	201	CYC	C1D-CHD-C4C	-4.57	119.97	127.76
13	D3	201	CYC	C3C-C4C-NC	-4.56	102.06	107.94
13	F6	201	CYC	C1B-CHB-C4A	-4.56	116.85	128.06
13	G4	201	CYC	C1B-CHB-C4A	-4.56	116.85	128.06
13	C4	201	CYC	CMD-C2D-C1D	4.56	132.25	125.62
13	52	301	CYC	C2C-C1C-NC	-4.56	104.49	108.29
13	J6	201	CYC	CMD-C2D-C1D	4.56	132.24	125.62
13	Z3	301	CYC	C2C-C1C-NC	-4.55	104.50	108.29
13	S5	201	CYC	C4D-CHA-C1A	-4.55	118.29	128.22
13	Z4	301	CYC	C1D-CHD-C4C	-4.55	120.00	127.76
13	I6	201	CYC	C2C-C3C-C4C	4.54	108.14	101.34
13	X3	201	CYC	C2C-C1C-NC	-4.54	104.51	108.29
13	Q4	201	CYC	CAB-C3B-C4B	4.54	128.38	121.37
13	J1	201	CYC	C1B-CHB-C4A	-4.53	116.94	128.06
13	J1	201	CYC	CMD-C2D-C1D	4.53	132.20	125.62
13	D7	201	CYC	C1D-CHD-C4C	-4.52	120.04	127.76
13	F6	201	CYC	CAD-C3D-C4D	4.52	132.94	125.77
13	P1	201	CYC	C2C-C3C-C4C	4.51	108.10	101.34
13	J4	202	CYC	C3C-C4C-NC	-4.51	102.13	107.94
13	C4	201	CYC	C2C-C1C-NC	-4.51	104.53	108.29
13	P5	201	CYC	C2C-C3C-C4C	4.51	108.09	101.34
13	J3	201	CYC	CAB-C3B-C4B	4.50	128.33	121.37
13	J7	201	CYC	CMD-C2D-C1D	4.50	132.16	125.62
13	Q3	201	CYC	CAB-C3B-C4B	4.50	128.33	121.37
13	G1	201	CYC	C3C-C4C-NC	-4.50	102.15	107.94
13	Q7	201	CYC	CAB-C3B-C4B	4.49	128.32	121.37
13	V6	201	CYC	C2C-C1C-NC	-4.49	104.55	108.29
13	X5	201	CYC	CMD-C2D-C1D	4.49	132.15	125.62
13	a3	202	CYC	C1B-CHB-C4A	-4.49	117.04	128.06
13	I6	201	CYC	CAB-C3B-C4B	4.48	128.30	121.37
13	J6	201	CYC	CAB-C3B-C4B	4.47	128.29	121.37
13	32	301	CYC	CAB-C3B-C4B	4.47	128.29	121.37
13	J1	201	CYC	CAB-C3B-C4B	4.47	128.28	121.37
13	N1	201	CYC	CAB-C3B-C4B	4.47	128.28	121.37
13	t2	201	CYC	CAB-C3B-C4B	4.47	128.28	121.37
13	T3	202	CYC	CAB-C3B-C4B	4.46	128.28	121.37
13	C1	201	CYC	C2C-C1C-NC	-4.46	104.57	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S6	201	CYC	C4D-CHA-C1A	-4.46	118.47	128.22
13	I4	201	CYC	CAB-C3B-C4B	4.46	128.27	121.37
13	J4	201	CYC	CAB-C3B-C4B	4.46	128.26	121.37
13	Q6	201	CYC	CAB-C3B-C4B	4.46	128.26	121.37
13	T3	201	CYC	C3C-C4C-NC	-4.45	102.21	107.94
13	D4	201	CYC	C1D-CHD-C4C	-4.45	120.17	127.76
13	D2	201	CYC	CMA-C3A-C4A	4.45	132.01	125.10
13	J6	201	CYC	C1B-CHB-C4A	-4.45	117.14	128.06
13	K1	201	CYC	C1B-CHB-C4A	-4.44	117.14	128.06
13	p2	201	CYC	CAB-C3B-C4B	4.44	128.24	121.37
13	T2	201	CYC	C1D-CHD-C4C	-4.44	120.18	127.76
13	B4	201	CYC	C2C-C3C-C4C	4.44	107.99	101.34
13	J5	201	CYC	CMD-C2D-C1D	4.44	132.08	125.62
13	V4	201	CYC	C1D-CHD-C4C	-4.44	120.18	127.76
13	L2	201	CYC	CAB-C3B-C4B	4.44	128.24	121.37
13	M5	201	CYC	CMD-C2D-C1D	4.44	132.07	125.62
13	T1	201	CYC	CAB-C3B-C4B	4.44	128.23	121.37
13	P2	201	CYC	CAB-C3B-C4B	4.44	128.23	121.37
13	J7	201	CYC	CAB-C3B-C4B	4.44	128.23	121.37
13	C2	201	CYC	C2C-C3C-C4C	4.44	107.98	101.34
13	X7	201	CYC	C2C-C1C-NC	-4.43	104.60	108.29
13	z2	201	CYC	CAB-C3B-C4B	4.43	128.22	121.37
13	H1	201	CYC	C3C-C4C-NC	-4.43	102.24	107.94
13	p2	201	CYC	C2C-C3C-C4C	4.43	107.97	101.34
13	M4	201	CYC	CMD-C2D-C1D	4.42	132.05	125.62
13	B1	201	CYC	C2C-C3C-C4C	4.42	107.96	101.34
13	22	301	CYC	CAB-C3B-C4B	4.42	128.21	121.37
13	G7	201	CYC	C3C-C4C-NC	-4.42	102.25	107.94
13	Q5	201	CYC	CAB-C3B-C4B	4.42	128.21	121.37
13	F4	201	CYC	CAB-C3B-C4B	4.42	128.20	121.37
13	D7	201	CYC	C1B-CHB-C4A	-4.41	117.22	128.06
13	N5	201	CYC	C1B-CHB-C4A	-4.41	117.22	128.06
13	g2	201	CYC	CAB-C3B-C4B	4.41	128.19	121.37
13	M2	201	CYC	CAB-C3B-C4B	4.40	128.18	121.37
13	S1	201	CYC	C2C-C3C-C4C	4.40	107.94	101.34
13	X1	201	CYC	CMD-C2D-C1D	4.40	132.02	125.62
13	U6	201	CYC	CAB-C3B-C4B	4.40	128.18	121.37
13	T7	201	CYC	C3C-C4C-NC	-4.40	102.28	107.94
13	V1	202	CYC	CAB-C3B-C4B	4.40	128.17	121.37
13	A6	301	CYC	CMD-C2D-C1D	4.40	132.01	125.62
13	T6	201	CYC	CAB-C3B-C4B	4.39	128.16	121.37
13	42	301	CYC	CAB-C3B-C4B	4.39	128.16	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	v2	201	CYC	C2C-C1C-NC	-4.39	104.63	108.29
13	T4	201	CYC	C3C-C4C-NC	-4.39	102.29	107.94
13	Q4	201	CYC	C2C-C1C-NC	-4.38	104.64	108.29
13	L5	201	CYC	CAB-C3B-C4B	4.38	128.15	121.37
13	V6	201	CYC	CAB-C3B-C4B	4.38	128.15	121.37
13	a6	201	CYC	CMD-C2D-C1D	4.38	131.99	125.62
13	I1	201	CYC	CAB-C3B-C4B	4.38	128.15	121.37
13	B2	201	CYC	CAB-C3B-C4B	4.38	128.14	121.37
13	m2	201	CYC	CAB-C3B-C4B	4.38	128.14	121.37
13	V1	201	CYC	CAB-C3B-C4B	4.38	128.14	121.37
13	F3	201	CYC	C3C-C4C-NC	-4.37	102.31	107.94
13	H5	201	CYC	C3C-C4C-NC	-4.37	102.32	107.94
13	V6	202	CYC	CAB-C3B-C4B	4.37	128.12	121.37
13	M3	201	CYC	CMD-C2D-C1D	4.37	131.96	125.62
13	N1	201	CYC	C1B-CHB-C4A	-4.36	117.35	128.06
13	G3	201	CYC	C3C-C4C-NC	-4.36	102.33	107.94
13	V5	202	CYC	CAB-C3B-C4B	4.36	128.11	121.37
13	f2	201	CYC	CMD-C2D-C1D	4.35	131.95	125.62
13	a2	201	CYC	CAB-C3B-C4B	4.35	128.10	121.37
13	B3	201	CYC	CAB-C3B-C4B	4.35	128.10	121.37
13	S4	201	CYC	C2C-C3C-C4C	4.35	107.85	101.34
13	N5	201	CYC	CAB-C3B-C4B	4.35	128.09	121.37
13	Z7	301	CYC	CAB-C3B-C4B	4.35	128.09	121.37
13	S6	201	CYC	C2C-C3C-C4C	4.34	107.85	101.34
13	V7	201	CYC	CAB-C3B-C4B	4.34	128.09	121.37
13	V5	202	CYC	C3C-C4C-NC	-4.34	102.35	107.94
13	V5	201	CYC	C2C-C1C-NC	-4.34	104.67	108.29
13	L1	201	CYC	CMD-C2D-C1D	4.34	131.93	125.62
13	J5	202	CYC	C3C-C4C-NC	-4.34	102.36	107.94
13	42	302	CYC	C2C-C3C-C4C	4.34	107.83	101.34
13	Z1	301	CYC	CMD-C2D-C1D	4.33	131.92	125.62
13	z2	201	CYC	C2C-C3C-C4C	4.33	107.83	101.34
13	F7	201	CYC	C3C-C4C-NC	-4.33	102.37	107.94
13	P2	201	CYC	CMD-C2D-C1D	4.33	131.91	125.62
13	M6	201	CYC	CMD-C2D-C1D	4.33	131.91	125.62
13	V2	201	CYC	CAB-C3B-C4B	4.33	128.06	121.37
13	V3	201	CYC	CAB-C3B-C4B	4.33	128.06	121.37
13	X6	201	CYC	CMD-C2D-C1D	4.32	131.91	125.62
13	J6	202	CYC	C1B-CHB-C4A	-4.32	117.44	128.06
13	C6	201	CYC	CAB-C3B-C4B	4.32	128.05	121.37
13	S5	201	CYC	C2C-C3C-C4C	4.32	107.81	101.34
13	G6	201	CYC	CAB-C3B-C4B	4.32	128.05	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T5	201	CYC	C3C-C4C-NC	-4.32	102.38	107.94
13	F6	201	CYC	CAB-C3B-C4B	4.32	128.05	121.37
13	V2	201	CYC	CMD-C2D-C1D	4.32	131.89	125.62
13	T6	201	CYC	C3C-C4C-NC	-4.31	102.39	107.94
13	V5	201	CYC	CAB-C3B-C4B	4.31	128.04	121.37
13	V4	201	CYC	C2C-C1C-NC	-4.31	104.70	108.29
13	K7	201	CYC	C3C-C4C-NC	-4.31	102.39	107.94
13	F3	201	CYC	CAB-C3B-C4B	4.31	128.03	121.37
13	I5	201	CYC	CAB-C3B-C4B	4.31	128.03	121.37
13	M7	201	CYC	CMD-C2D-C1D	4.31	131.88	125.62
13	F3	202	CYC	C2C-C1C-NC	-4.30	104.70	108.29
13	C5	201	CYC	CAB-C3B-C4B	4.30	128.02	121.37
13	V4	202	CYC	CAB-C3B-C4B	4.30	128.02	121.37
13	C4	202	CYC	C2C-C3C-C4C	4.30	107.78	101.34
13	G4	201	CYC	CAB-C3B-C4B	4.29	128.01	121.37
13	32	301	CYC	CMD-C2D-C1D	4.29	131.86	125.62
13	N1	201	CYC	C3C-C4C-NC	-4.29	102.42	107.94
13	X3	201	CYC	CMA-C3A-C4A	4.29	131.76	125.10
13	D4	201	CYC	C3C-C4C-NC	-4.29	102.42	107.94
13	C7	201	CYC	CAB-C3B-C4B	4.28	127.99	121.37
13	E6	201	CYC	C3C-C4C-NC	-4.28	102.43	107.94
13	C7	201	CYC	CMD-C2D-C1D	4.28	131.84	125.62
13	E4	201	CYC	C1B-CHB-C4A	-4.28	117.56	128.06
13	K1	201	CYC	CAB-C3B-C4B	4.28	127.98	121.37
13	R2	201	CYC	CAB-C3B-C4B	4.27	127.98	121.37
13	T3	201	CYC	CAB-C3B-C4B	4.27	127.98	121.37
13	V7	202	CYC	CAB-C3B-C4B	4.27	127.98	121.37
13	B7	201	CYC	CAB-C3B-C4B	4.27	127.97	121.37
13	C6	201	CYC	C2C-C1C-NC	-4.26	104.74	108.29
13	J6	202	CYC	C3C-C4C-NC	-4.26	102.45	107.94
13	V3	202	CYC	CAB-C3B-C4B	4.26	127.96	121.37
13	S3	201	CYC	C2C-C3C-C4C	4.26	107.72	101.34
13	L6	201	CYC	CMD-C2D-C1D	4.26	131.81	125.62
13	N2	801	CYC	CAB-C3B-C4B	4.26	127.95	121.37
13	w2	201	CYC	CAB-C3B-C4B	4.26	127.95	121.37
13	V4	202	CYC	C3C-C4C-NC	-4.26	102.46	107.94
13	F5	201	CYC	CAD-C3D-C4D	4.25	132.52	125.77
13	F3	202	CYC	C2C-C3C-C4C	4.25	107.71	101.34
13	F7	202	CYC	C2C-C1C-NC	-4.25	104.75	108.29
13	B4	201	CYC	CAB-C3B-C4B	4.25	127.94	121.37
13	P1	201	CYC	C2C-C1C-NC	-4.25	104.75	108.29
13	M2	201	CYC	C2C-C3C-C4C	4.25	107.70	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X4	201	CYC	CMD-C2D-C1D	4.25	131.79	125.62
13	F7	202	CYC	C2C-C3C-C4C	4.24	107.69	101.34
13	x2	201	CYC	CAB-C3B-C4B	4.24	127.93	121.37
13	N2	802	CYC	CAB-C3B-C4B	4.24	127.92	121.37
13	N3	201	CYC	CAB-C3B-C4B	4.24	127.92	121.37
13	W7	201	CYC	CAB-C3B-C4B	4.24	127.92	121.37
13	J1	202	CYC	C3C-C4C-NC	-4.24	102.49	107.94
13	P3	201	CYC	C2C-C3C-C4C	4.23	107.68	101.34
13	K5	201	CYC	CAB-C3B-C4B	4.23	127.92	121.37
13	E1	201	CYC	C1B-CHB-C4A	-4.23	117.66	128.06
13	Z6	301	CYC	CMD-C2D-C1D	4.23	131.77	125.62
13	T5	201	CYC	CAB-C3B-C4B	4.23	127.92	121.37
13	L4	201	CYC	CAB-C3B-C4B	4.23	127.91	121.37
13	B6	201	CYC	C2C-C3C-C4C	4.23	107.67	101.34
13	L1	201	CYC	CMA-C3A-C4A	4.23	131.66	125.10
13	a5	201	CYC	CMD-C2D-C1D	4.23	131.76	125.62
13	o2	801	CYC	CMA-C3A-C4A	4.23	131.66	125.10
13	P7	201	CYC	C2C-C3C-C4C	4.22	107.66	101.34
13	F5	202	CYC	CAB-C3B-C4B	4.22	127.90	121.37
13	C4	201	CYC	CAB-C3B-C4B	4.22	127.90	121.37
13	J3	202	CYC	C3C-C4C-NC	-4.22	102.51	107.94
13	W1	201	CYC	C3C-C4C-NC	-4.22	102.51	107.94
13	L3	201	CYC	CAB-C3B-C4B	4.22	127.89	121.37
13	A1	301	CYC	CAB-C3B-C4B	4.22	127.89	121.37
13	H5	201	CYC	CAB-C3B-C4B	4.22	127.89	121.37
13	B2	202	CYC	C1B-CHB-C4A	-4.22	117.71	128.06
13	X7	201	CYC	CMA-C3A-C4A	4.21	131.65	125.10
13	T7	201	CYC	CAB-C3B-C4B	4.21	127.89	121.37
13	X5	201	CYC	CMA-C3A-C4A	4.21	131.64	125.10
13	V7	201	CYC	C3C-C4C-NC	-4.21	102.52	107.94
13	X3	201	CYC	CAB-C3B-C4B	4.21	127.89	121.37
13	T4	201	CYC	CAB-C3B-C4B	4.21	127.89	121.37
13	Q1	201	CYC	CAB-C3B-C4B	4.21	127.88	121.37
13	R1	201	CYC	C3C-C4C-NC	-4.21	102.52	107.94
13	D2	201	CYC	C3C-C4C-NC	-4.21	102.52	107.94
13	G1	201	CYC	CAB-C3B-C4B	4.21	127.87	121.37
13	a1	202	CYC	CAB-C3B-C4B	4.21	127.87	121.37
13	H1	201	CYC	CAB-C3B-C4B	4.20	127.87	121.37
13	Z5	301	CYC	CMD-C2D-C1D	4.20	131.72	125.62
13	F1	202	CYC	CAB-C3B-C4B	4.20	127.86	121.37
13	F5	201	CYC	CAB-C3B-C4B	4.20	127.86	121.37
13	I7	201	CYC	CAB-C3B-C4B	4.20	127.86	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L2	201	CYC	C2C-C3C-C4C	4.20	107.63	101.34
13	W3	201	CYC	CAB-C3B-C4B	4.20	127.86	121.37
13	B2	201	CYC	C2C-C1C-NC	-4.20	104.79	108.29
13	S1	201	CYC	CAB-C3B-C4B	4.20	127.86	121.37
13	P4	202	CYC	C2C-C1C-NC	-4.20	104.79	108.29
13	V4	201	CYC	CAB-C3B-C4B	4.19	127.85	121.37
13	Q6	202	CYC	C1B-CHB-C4A	-4.19	117.77	128.06
13	Q2	201	CYC	CAB-C3B-C4B	4.19	127.85	121.37
13	P1	202	CYC	CMD-C2D-C1D	4.19	131.70	125.62
13	m2	201	CYC	C2C-C3C-C4C	4.19	107.61	101.34
13	A6	301	CYC	CAB-C3B-C4B	4.19	127.84	121.37
13	H3	201	CYC	CAB-C3B-C4B	4.18	127.84	121.37
13	D7	201	CYC	CAB-C3B-C4B	4.18	127.84	121.37
13	S7	201	CYC	C2C-C3C-C4C	4.18	107.60	101.34
13	Q1	202	CYC	C2C-C1C-NC	-4.18	104.81	108.29
13	T6	202	CYC	CAB-C3B-C4B	4.18	127.83	121.37
13	C6	202	CYC	C2C-C3C-C4C	4.18	107.60	101.34
13	V3	201	CYC	C2C-C1C-NC	-4.18	104.81	108.29
13	U7	201	CYC	C3C-C4C-NC	-4.17	102.57	107.94
13	G3	201	CYC	CAB-C3B-C4B	4.17	127.82	121.37
13	N7	201	CYC	CAB-C3B-C4B	4.17	127.82	121.37
13	E5	201	CYC	C1B-CHB-C4A	-4.17	117.82	128.06
13	T1	202	CYC	CAB-C3B-C4B	4.17	127.82	121.37
13	Q5	202	CYC	C1B-CHB-C4A	-4.17	117.82	128.06
13	C5	202	CYC	C2C-C3C-C4C	4.17	107.58	101.34
13	F7	201	CYC	CAB-C3B-C4B	4.17	127.81	121.37
13	s2	201	CYC	CAB-C3B-C4B	4.17	127.81	121.37
13	C3	201	CYC	CAB-C3B-C4B	4.17	127.81	121.37
13	C4	202	CYC	CAB-C3B-C4B	4.16	127.81	121.37
13	T1	201	CYC	C3C-C4C-NC	-4.16	102.58	107.94
13	V3	202	CYC	C3C-C4C-NC	-4.16	102.58	107.94
13	52	301	CYC	CMD-C2D-C1D	4.16	131.66	125.62
13	22	301	CYC	CMD-C2D-C1D	4.16	131.66	125.62
13	S2	201	CYC	CAB-C3B-C4B	4.16	127.80	121.37
13	H4	201	CYC	CAB-C3B-C4B	4.15	127.79	121.37
13	N4	201	CYC	CAB-C3B-C4B	4.15	127.79	121.37
13	U5	201	CYC	C3C-C4C-NC	-4.15	102.60	107.94
13	L7	201	CYC	CAB-C3B-C4B	4.15	127.78	121.37
13	W7	201	CYC	C3C-C4C-NC	-4.15	102.60	107.94
13	F6	202	CYC	C2C-C3C-C4C	4.14	107.55	101.34
13	C7	201	CYC	C2C-C1C-NC	-4.14	104.84	108.29
13	F6	202	CYC	CAB-C3B-C4B	4.14	127.78	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	r2	201	CYC	CAB-C3B-C4B	4.14	127.78	121.37
13	U2	201	CYC	CAB-C3B-C4B	4.14	127.77	121.37
13	A2	201	CYC	CAB-C3B-C4B	4.14	127.77	121.37
13	p2	201	CYC	CMA-C3A-C4A	4.14	131.53	125.10
13	K3	201	CYC	C3C-C4C-NC	-4.14	102.61	107.94
13	J7	202	CYC	CAB-C3B-C4B	4.14	127.77	121.37
13	S2	201	CYC	C2C-C3C-C4C	4.14	107.53	101.34
13	O2	201	CYC	CAB-C3B-C4B	4.13	127.76	121.37
13	L6	201	CYC	CAB-C3B-C4B	4.13	127.76	121.37
13	V6	202	CYC	C3C-C4C-NC	-4.13	102.62	107.94
13	G7	201	CYC	CAB-C3B-C4B	4.13	127.76	121.37
13	B6	201	CYC	CAB-C3B-C4B	4.13	127.76	121.37
13	G6	201	CYC	C3C-C4C-NC	-4.13	102.63	107.94
13	T4	202	CYC	CAB-C3B-C4B	4.13	127.75	121.37
13	J5	202	CYC	C1B-CHB-C4A	-4.13	117.92	128.06
13	X7	201	CYC	CMD-C2D-C1D	4.13	131.62	125.62
13	A2	201	CYC	C3C-C4C-NC	-4.13	102.63	107.94
13	C1	201	CYC	CAB-C3B-C4B	4.12	127.75	121.37
13	U1	201	CYC	C3C-C4C-NC	-4.12	102.63	107.94
13	C1	202	CYC	C1B-CHB-C4A	-4.12	117.93	128.06
13	X1	201	CYC	CMA-C3A-C4A	4.12	131.50	125.10
13	X3	201	CYC	CMD-C2D-C1D	4.12	131.61	125.62
13	D4	201	CYC	CAB-C3B-C4B	4.12	127.74	121.37
13	H7	201	CYC	CAB-C3B-C4B	4.12	127.74	121.37
13	a5	202	CYC	CAB-C3B-C4B	4.12	127.74	121.37
13	J7	202	CYC	C3C-C4C-NC	-4.12	102.64	107.94
13	Z4	301	CYC	CMD-C2D-C1D	4.11	131.60	125.62
13	G2	201	CYC	CMA-C3A-C4A	4.11	131.49	125.10
13	P5	202	CYC	CMD-C2D-C1D	4.11	131.60	125.62
13	R4	201	CYC	C3C-C4C-NC	-4.11	102.65	107.94
13	U4	201	CYC	CAB-C3B-C4B	4.11	127.72	121.37
13	a3	201	CYC	CMD-C2D-C1D	4.11	131.59	125.62
13	J5	201	CYC	C1B-CHB-C4A	-4.10	117.98	128.06
13	U2	201	CYC	CMD-C2D-C1D	4.10	131.58	125.62
13	52	301	CYC	CAB-C3B-C4B	4.10	127.71	121.37
13	J3	202	CYC	CAB-C3B-C4B	4.10	127.70	121.37
13	W2	201	CYC	C2C-C3C-C4C	4.10	107.47	101.34
13	S3	201	CYC	CAB-C3B-C4B	4.09	127.70	121.37
13	P7	202	CYC	CAB-C3B-C4B	4.09	127.70	121.37
13	F4	202	CYC	CAB-C3B-C4B	4.09	127.70	121.37
13	T1	202	CYC	C2C-C3C-C4C	4.09	107.47	101.34
13	l2	201	CYC	CAB-C3B-C4B	4.09	127.70	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E7	201	CYC	CAB-C3B-C4B	4.09	127.70	121.37
13	i2	201	CYC	C3C-C4C-NC	-4.09	102.68	107.94
13	I3	201	CYC	CAB-C3B-C4B	4.09	127.69	121.37
13	C1	202	CYC	C2C-C3C-C4C	4.09	107.46	101.34
13	O2	201	CYC	CMA-C3A-C4A	4.09	131.45	125.10
13	R5	201	CYC	C3C-C4C-NC	-4.09	102.68	107.94
13	D3	201	CYC	CAB-C3B-C4B	4.09	127.69	121.37
13	W6	201	CYC	CAB-C3B-C4B	4.08	127.68	121.37
13	W2	201	CYC	CAB-C3B-C4B	4.08	127.68	121.37
13	B7	201	CYC	C2C-C3C-C4C	4.08	107.45	101.34
13	D1	201	CYC	CAB-C3B-C4B	4.08	127.68	121.37
13	J4	202	CYC	C1B-CHB-C4A	-4.08	118.04	128.06
13	Z3	301	CYC	CAB-C3B-C4B	4.08	127.67	121.37
13	N6	201	CYC	C3C-C4C-NC	-4.08	102.69	107.94
13	C7	202	CYC	CAB-C3B-C4B	4.07	127.67	121.37
13	a4	202	CYC	CAB-C3B-C4B	4.07	127.67	121.37
13	c2	801	CYC	C3C-C4C-NC	-4.07	102.70	107.94
13	f2	201	CYC	CMA-C3A-C4A	4.07	131.43	125.10
13	a7	202	CYC	CAB-C3B-C4B	4.07	127.67	121.37
13	F2	201	CYC	CAB-C3B-C4B	4.07	127.67	121.37
13	R6	201	CYC	C3C-C4C-NC	-4.07	102.70	107.94
13	W4	201	CYC	CAB-C3B-C4B	4.07	127.66	121.37
13	K1	201	CYC	C3C-C4C-NC	-4.06	102.71	107.94
13	S4	201	CYC	CAB-C3B-C4B	4.06	127.65	121.37
13	H4	201	CYC	C3C-C4C-NC	-4.06	102.71	107.94
13	x2	201	CYC	CMD-C2D-C1D	4.06	131.52	125.62
13	E3	201	CYC	CAB-C3B-C4B	4.06	127.65	121.37
13	F3	202	CYC	CAB-C3B-C4B	4.06	127.65	121.37
13	B5	201	CYC	CAB-C3B-C4B	4.06	127.65	121.37
13	S6	201	CYC	CAB-C3B-C4B	4.06	127.64	121.37
13	F2	201	CYC	C2C-C3C-C4C	4.05	107.41	101.34
13	X2	201	CYC	CAB-C3B-C4B	4.05	127.64	121.37
13	C5	202	CYC	CAB-C3B-C4B	4.05	127.64	121.37
13	I4	201	CYC	C2C-C1C-NC	-4.05	104.91	108.29
13	a3	202	CYC	CAB-C3B-C4B	4.05	127.64	121.37
13	w2	201	CYC	C1B-CHB-C4A	-4.05	118.11	128.06
13	F1	201	CYC	CAB-C3B-C4B	4.05	127.63	121.37
13	G5	201	CYC	CAB-C3B-C4B	4.05	127.63	121.37
13	g2	201	CYC	C2C-C3C-C4C	4.05	107.40	101.34
13	d2	201	CYC	CAB-C3B-C4B	4.05	127.63	121.37
13	J1	202	CYC	C1B-CHB-C4A	-4.05	118.12	128.06
13	a2	201	CYC	C2C-C3C-C4C	4.05	107.40	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N6	201	CYC	CAB-C3B-C4B	4.05	127.63	121.37
13	a6	202	CYC	CAB-C3B-C4B	4.04	127.62	121.37
13	22	302	CYC	CAB-C3B-C4B	4.04	127.62	121.37
13	U2	201	CYC	CMA-C3A-C4A	4.04	131.38	125.10
13	T5	202	CYC	CAB-C3B-C4B	4.04	127.62	121.37
13	t2	201	CYC	CMD-C2D-C1D	4.04	131.49	125.62
13	V7	202	CYC	C3C-C4C-NC	-4.04	102.74	107.94
13	e2	201	CYC	CMA-C3A-C4A	4.04	131.38	125.10
13	U3	201	CYC	CAB-C3B-C4B	4.04	127.62	121.37
13	P4	201	CYC	CAB-C3B-C4B	4.04	127.61	121.37
13	E2	201	CYC	CMA-C3A-C4A	4.03	131.37	125.10
13	Q4	202	CYC	C1B-CHB-C4A	-4.03	118.16	128.06
13	U1	201	CYC	CAB-C3B-C4B	4.03	127.61	121.37
13	a4	202	CYC	C1B-CHB-C4A	-4.03	118.16	128.06
13	H3	201	CYC	C3C-C4C-NC	-4.03	102.75	107.94
13	Z1	301	CYC	CAB-C3B-C4B	4.03	127.60	121.37
13	B3	201	CYC	C2C-C3C-C4C	4.03	107.37	101.34
13	R2	201	CYC	CMA-C3A-C4A	4.02	131.35	125.10
13	S7	201	CYC	CAB-C3B-C4B	4.02	127.59	121.37
13	F7	202	CYC	CAB-C3B-C4B	4.02	127.59	121.37
13	P6	201	CYC	C2C-C1C-NC	-4.02	104.94	108.29
13	e2	201	CYC	CAB-C3B-C4B	4.02	127.59	121.37
13	H6	201	CYC	CAB-C3B-C4B	4.02	127.59	121.37
13	B1	201	CYC	CAB-C3B-C4B	4.02	127.59	121.37
13	Z1	301	CYC	CMA-C3A-C4A	4.02	131.34	125.10
13	P3	202	CYC	CAB-C3B-C4B	4.02	127.58	121.37
13	D5	201	CYC	CAB-C3B-C4B	4.01	127.58	121.37
13	M3	201	CYC	C3C-C4C-NC	-4.01	102.78	107.94
13	k2	201	CYC	C3C-C4C-NC	-4.01	102.78	107.94
13	Z6	301	CYC	CMA-C3A-C4A	4.01	131.33	125.10
13	U5	201	CYC	CAB-C3B-C4B	4.01	127.57	121.37
13	32	302	CYC	CAB-C3B-C4B	4.01	127.57	121.37
13	Z5	301	CYC	CAB-C3B-C4B	4.01	127.57	121.37
13	J6	202	CYC	CAB-C3B-C4B	4.01	127.57	121.37
13	U7	201	CYC	CAB-C3B-C4B	4.01	127.57	121.37
13	C6	202	CYC	CAB-C3B-C4B	4.00	127.56	121.37
13	E4	201	CYC	CAB-C3B-C4B	4.00	127.56	121.37
13	J1	202	CYC	CAB-C3B-C4B	4.00	127.56	121.37
13	C3	202	CYC	CAB-C3B-C4B	4.00	127.56	121.37
13	l2	201	CYC	C2C-C3C-C4C	4.00	107.33	101.34
13	K4	201	CYC	CAB-C3B-C4B	4.00	127.55	121.37
13	W3	201	CYC	C3C-C4C-NC	-3.99	102.80	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S5	201	CYC	CAB-C3B-C4B	3.99	127.54	121.37
13	K6	201	CYC	C2C-C3C-C4C	3.99	107.32	101.34
13	H7	201	CYC	C3C-C4C-NC	-3.99	102.81	107.94
13	L4	201	CYC	CMD-C2D-C1D	3.99	131.42	125.62
13	T5	202	CYC	C2C-C3C-C4C	3.99	107.31	101.34
13	Z5	301	CYC	CMA-C3A-C4A	3.99	131.29	125.10
13	D6	201	CYC	CAB-C3B-C4B	3.98	127.53	121.37
13	K3	201	CYC	CAB-C3B-C4B	3.98	127.52	121.37
13	D2	201	CYC	C2C-C1C-NC	-3.98	104.98	108.29
13	P6	202	CYC	CMD-C2D-C1D	3.98	131.40	125.62
13	V1	202	CYC	C3C-C4C-NC	-3.97	102.83	107.94
13	L5	201	CYC	CMD-C2D-C1D	3.97	131.40	125.62
13	X7	201	CYC	CAB-C3B-C4B	3.95	127.49	121.37
13	I3	201	CYC	C2C-C3C-C4C	3.95	107.26	101.34
13	J4	202	CYC	CAB-C3B-C4B	3.95	127.48	121.37
13	E5	201	CYC	CAB-C3B-C4B	3.95	127.48	121.37
13	P4	201	CYC	CMD-C2D-C1D	3.95	131.36	125.62
13	a7	201	CYC	CAB-C3B-C4B	3.94	127.47	121.37
13	Z6	301	CYC	CAB-C3B-C4B	3.94	127.47	121.37
13	Z4	301	CYC	CAB-C3B-C4B	3.94	127.47	121.37
13	X7	201	CYC	C3C-C4C-NC	-3.94	102.87	107.94
13	52	302	CYC	CAB-C3B-C4B	3.94	127.46	121.37
13	J5	202	CYC	CAB-C3B-C4B	3.94	127.46	121.37
13	L7	201	CYC	CMD-C2D-C1D	3.94	131.34	125.62
13	22	302	CYC	C2C-C1C-NC	-3.94	105.01	108.29
13	N7	201	CYC	C3C-C4C-NC	-3.93	102.88	107.94
13	r2	201	CYC	CMA-C3A-C4A	3.93	131.21	125.10
13	P6	202	CYC	CAB-C3B-C4B	3.93	127.44	121.37
13	D2	201	CYC	CAB-C3B-C4B	3.93	127.44	121.37
13	E1	201	CYC	CAB-C3B-C4B	3.92	127.44	121.37
13	W1	201	CYC	CAB-C3B-C4B	3.92	127.43	121.37
13	E6	201	CYC	CAB-C3B-C4B	3.91	127.42	121.37
13	C1	202	CYC	CAB-C3B-C4B	3.91	127.42	121.37
13	C2	201	CYC	CAB-C3B-C4B	3.91	127.42	121.37
13	F4	201	CYC	C3C-C4C-NC	-3.91	102.91	107.94
13	r2	201	CYC	C2C-C3C-C4C	3.91	107.19	101.34
13	a3	201	CYC	CAB-C3B-C4B	3.91	127.41	121.37
13	Z7	301	CYC	C2C-C1C-NC	-3.90	105.04	108.29
13	D6	201	CYC	CMA-C3A-C4A	3.90	131.16	125.10
13	F6	201	CYC	C3C-C4C-NC	-3.90	102.92	107.94
13	Q2	201	CYC	C3C-C4C-NC	-3.89	102.93	107.94
13	J1	201	CYC	C3C-C4C-NC	-3.89	102.93	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N2	802	CYC	CMA-C3A-C4A	3.89	131.14	125.10
13	y2	201	CYC	CAB-C3B-C4B	3.89	127.39	121.37
13	E2	201	CYC	CAB-C3B-C4B	3.89	127.38	121.37
13	P5	202	CYC	CAB-C3B-C4B	3.89	127.38	121.37
13	C7	202	CYC	C2C-C3C-C4C	3.88	107.16	101.34
13	c2	801	CYC	C2C-C3C-C4C	3.88	107.15	101.34
13	K6	201	CYC	C3C-C4C-NC	-3.88	102.94	107.94
13	h2	201	CYC	CMA-C3A-C4A	3.88	131.13	125.10
13	G1	201	CYC	C2C-C3C-C4C	3.88	107.15	101.34
13	U4	201	CYC	C3C-C4C-NC	-3.88	102.95	107.94
13	a7	201	CYC	CMD-C2D-C1D	3.88	131.25	125.62
13	Q6	202	CYC	C2C-C1C-NC	-3.88	105.06	108.29
13	H5	201	CYC	C2C-C3C-C4C	3.87	107.14	101.34
13	F1	202	CYC	C2C-C3C-C4C	3.87	107.14	101.34
13	P1	202	CYC	CAB-C3B-C4B	3.87	127.35	121.37
13	42	302	CYC	CAB-C3B-C4B	3.87	127.35	121.37
13	L3	201	CYC	CMD-C2D-C1D	3.87	131.24	125.62
13	Z4	301	CYC	CMA-C3A-C4A	3.86	131.10	125.10
13	a4	201	CYC	C1D-CHD-C4C	3.86	134.35	127.76
13	M7	201	CYC	C3C-C4C-NC	-3.86	102.98	107.94
13	Q6	201	CYC	C2C-C1C-NC	-3.86	105.08	108.29
13	X6	201	CYC	CMA-C3A-C4A	3.85	131.09	125.10
13	a6	202	CYC	C1B-CHB-C4A	-3.85	118.60	128.06
13	H2	201	CYC	CAB-C3B-C4B	3.85	127.33	121.37
13	s2	201	CYC	CMA-C3A-C4A	3.85	131.08	125.10
13	a5	202	CYC	C1B-CHB-C4A	-3.85	118.60	128.06
13	X3	201	CYC	C3C-C4C-NC	-3.85	102.98	107.94
13	K7	201	CYC	CAB-C3B-C4B	3.85	127.32	121.37
13	N6	201	CYC	C2C-C3C-C4C	3.84	107.10	101.34
13	D7	201	CYC	C3C-C4C-NC	-3.84	102.99	107.94
13	o2	801	CYC	CHB-C4A-C3A	3.84	134.75	124.87
13	A1	301	CYC	C2C-C1C-NC	-3.84	105.09	108.29
13	U3	201	CYC	C3C-C4C-NC	-3.84	103.00	107.94
13	D7	201	CYC	C2C-C3C-C4C	3.84	107.09	101.34
13	J3	201	CYC	C3C-C4C-NC	-3.84	103.00	107.94
13	J7	201	CYC	C3C-C4C-NC	-3.83	103.01	107.94
13	Q5	202	CYC	C2C-C1C-NC	-3.83	105.10	108.29
13	W5	201	CYC	CAB-C3B-C4B	3.83	127.29	121.37
13	T4	202	CYC	C2C-C3C-C4C	3.83	107.07	101.34
13	P1	201	CYC	CAB-C3B-C4B	3.82	127.28	121.37
13	N3	201	CYC	C3C-C4C-NC	-3.82	103.02	107.94
13	V2	201	CYC	C1B-CHB-C4A	-3.82	118.69	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P6	201	CYC	CAB-C3B-C4B	3.82	127.27	121.37
13	P4	202	CYC	CAB-C3B-C4B	3.81	127.27	121.37
13	A1	302	CYC	CAB-C3B-C4B	3.81	127.27	121.37
13	G2	201	CYC	CAB-C3B-C4B	3.81	127.27	121.37
13	P3	201	CYC	CAB-C3B-C4B	3.81	127.27	121.37
13	J6	201	CYC	C3C-C4C-NC	-3.81	103.03	107.94
13	P3	201	CYC	C2C-C1C-NC	-3.81	105.11	108.29
13	T2	201	CYC	CMD-C2D-C1D	3.80	131.15	125.62
13	S2	201	CYC	CMD-C2D-C1D	3.80	131.14	125.62
13	X2	201	CYC	CMD-C2D-C1D	3.80	131.14	125.62
13	N3	201	CYC	C2C-C3C-C4C	3.80	107.03	101.34
13	52	302	CYC	C2C-C3C-C4C	3.80	107.03	101.34
13	Q1	201	CYC	C2C-C1C-NC	-3.79	105.13	108.29
13	w2	201	CYC	C2C-C1C-NC	-3.79	105.13	108.29
13	Q4	202	CYC	C2C-C1C-NC	-3.79	105.13	108.29
13	N2	801	CYC	CMA-C3A-C4A	3.79	130.99	125.10
13	B2	201	CYC	C3C-C4C-NC	-3.79	103.06	107.94
13	U2	201	CYC	CHB-C4A-C3A	3.79	134.61	124.87
13	H1	201	CYC	C2C-C3C-C4C	3.79	107.01	101.34
13	P3	202	CYC	C2C-C1C-NC	-3.79	105.13	108.29
13	N2	802	CYC	CHB-C4A-C3A	3.78	134.59	124.87
13	H2	201	CYC	C2C-C3C-C4C	3.78	107.01	101.34
13	f2	201	CYC	CAB-C3B-C4B	3.78	127.22	121.37
13	F2	201	CYC	CMA-C3A-C4A	3.78	130.97	125.10
13	P3	202	CYC	C3C-C4C-NC	-3.78	103.08	107.94
13	D6	201	CYC	C3C-C4C-NC	-3.78	103.08	107.94
13	C3	202	CYC	C2C-C3C-C4C	3.78	107.00	101.34
13	T6	202	CYC	C2C-C3C-C4C	3.78	107.00	101.34
13	x2	201	CYC	C1B-CHB-C4A	-3.78	118.79	128.06
13	j2	201	CYC	CAB-C3B-C4B	3.77	127.21	121.37
13	L1	201	CYC	CAB-C3B-C4B	3.77	127.21	121.37
13	U1	201	CYC	C2C-C3C-C4C	3.77	106.99	101.34
13	a5	202	CYC	C2C-C1C-NC	-3.77	105.15	108.29
13	G5	201	CYC	C3C-C4C-NC	-3.77	103.09	107.94
13	Z7	301	CYC	C1B-CHB-C4A	-3.77	118.80	128.06
13	M2	201	CYC	C3C-C4C-NC	-3.77	103.09	107.94
13	l2	201	CYC	CMA-C3A-C4A	3.77	130.95	125.10
13	i2	201	CYC	CMD-C2D-C1D	3.77	131.09	125.62
13	G2	201	CYC	C3C-C4C-NC	-3.76	103.10	107.94
13	a7	202	CYC	C2C-C1C-NC	-3.76	105.16	108.29
13	R3	201	CYC	C2C-C1C-NC	-3.75	105.16	108.29
13	L6	201	CYC	CMA-C3A-C4A	3.75	130.93	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I7	201	CYC	C2C-C3C-C4C	3.75	106.96	101.34
13	Z3	301	CYC	C3C-C4C-NC	-3.75	103.11	107.94
13	K6	201	CYC	CAB-C3B-C4B	3.75	127.17	121.37
13	g2	201	CYC	CMA-C3A-C4A	3.74	130.91	125.10
13	U5	201	CYC	C2C-C3C-C4C	3.74	106.94	101.34
13	a3	202	CYC	C2C-C1C-NC	-3.73	105.18	108.29
13	Q1	202	CYC	C1B-CHB-C4A	-3.73	118.89	128.06
13	c2	801	CYC	CAB-C3B-C4B	3.73	127.14	121.37
13	a1	202	CYC	C1B-CHB-C4A	-3.73	118.90	128.06
13	D6	201	CYC	C2C-C3C-C4C	3.72	106.92	101.34
13	P5	201	CYC	CAB-C3B-C4B	3.72	127.12	121.37
13	42	302	CYC	CMA-C3A-C4A	3.72	130.87	125.10
13	V2	201	CYC	C2C-C1C-NC	-3.71	105.19	108.29
13	A6	302	CYC	CAB-C3B-C4B	3.71	127.11	121.37
13	32	302	CYC	CMA-C3A-C4A	3.71	130.86	125.10
13	M6	201	CYC	C3C-C4C-NC	-3.71	103.17	107.94
13	F1	201	CYC	CAD-C3D-C4D	3.71	131.65	125.77
13	P4	201	CYC	C2C-C1C-NC	-3.70	105.20	108.29
13	32	301	CYC	C2C-C1C-NC	-3.70	105.20	108.29
13	A6	302	CYC	C2C-C3C-C4C	3.70	106.88	101.34
13	a5	201	CYC	CAB-C3B-C4B	3.70	127.09	121.37
13	V7	201	CYC	C2C-C3C-C4C	3.70	106.88	101.34
13	P5	201	CYC	CMA-C3A-C4A	3.69	130.83	125.10
13	P4	202	CYC	CMA-C3A-C4A	3.69	130.83	125.10
13	F4	202	CYC	C2C-C3C-C4C	3.67	106.84	101.34
13	A6	301	CYC	C2C-C1C-NC	-3.67	105.23	108.29
13	z2	201	CYC	CMA-C3A-C4A	3.67	130.79	125.10
13	F5	202	CYC	C2C-C3C-C4C	3.67	106.83	101.34
13	42	301	CYC	C2C-C1C-NC	-3.67	105.23	108.29
13	N1	201	CYC	C2C-C3C-C4C	3.66	106.82	101.34
13	32	302	CYC	C2C-C1C-NC	-3.66	105.24	108.29
13	K4	201	CYC	C2C-C3C-C4C	3.66	106.82	101.34
13	K1	201	CYC	C2C-C3C-C4C	3.66	106.82	101.34
13	g2	201	CYC	C3C-C4C-NC	-3.66	103.23	107.94
13	h2	201	CYC	CAB-C3B-C4B	3.66	127.03	121.37
13	P7	201	CYC	CAB-C3B-C4B	3.65	127.02	121.37
13	N7	201	CYC	C2C-C3C-C4C	3.65	106.81	101.34
13	D4	201	CYC	CMA-C3A-C4A	3.65	130.77	125.10
13	t2	201	CYC	C2C-C3C-C4C	3.65	106.80	101.34
13	F1	201	CYC	C3C-C4C-NC	-3.65	103.25	107.94
13	L1	201	CYC	C2C-C1C-NC	-3.65	105.25	108.29
13	N2	801	CYC	C2C-C1C-NC	-3.64	105.26	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	52	302	CYC	CMD-C2D-C1D	3.64	130.91	125.62
13	X6	201	CYC	CAB-C3B-C4B	3.64	126.99	121.37
13	J5	202	CYC	CMD-C2D-C1D	3.64	130.91	125.62
13	42	301	CYC	CMD-C2D-C1D	3.63	130.90	125.62
13	z2	201	CYC	C3C-C4C-NC	-3.63	103.27	107.94
13	G4	201	CYC	C3C-C4C-NC	-3.63	103.27	107.94
13	F6	201	CYC	C2C-C1C-NC	-3.63	105.27	108.29
13	22	302	CYC	CMA-C3A-C4A	3.63	130.73	125.10
13	N4	201	CYC	C2C-C3C-C4C	3.62	106.76	101.34
13	v2	201	CYC	CAB-C3B-C4B	3.62	126.97	121.37
13	I6	201	CYC	C2C-C1C-NC	-3.62	105.28	108.29
13	J6	202	CYC	CMD-C2D-C1D	3.62	130.88	125.62
13	A6	302	CYC	CMA-C3A-C4A	3.61	130.71	125.10
13	X4	201	CYC	CMA-C3A-C4A	3.61	130.71	125.10
13	t2	201	CYC	CHB-C4A-C3A	3.61	134.15	124.87
13	V4	201	CYC	CMD-C2D-C1D	3.61	130.86	125.62
13	P7	201	CYC	C1B-CHB-C4A	-3.60	119.21	128.06
13	A1	302	CYC	CMA-C3A-C4A	3.60	130.69	125.10
13	P6	202	CYC	C2C-C1C-NC	-3.60	105.29	108.29
13	P1	201	CYC	CMA-C3A-C4A	3.60	130.69	125.10
13	K5	201	CYC	C2C-C3C-C4C	3.59	106.72	101.34
13	S2	201	CYC	CHB-C4A-C3A	3.59	134.09	124.87
13	H3	201	CYC	C2C-C3C-C4C	3.58	106.70	101.34
13	W2	201	CYC	C1B-CHB-C4A	-3.58	119.27	128.06
13	V5	201	CYC	CMD-C2D-C1D	3.57	130.81	125.62
13	X4	201	CYC	CAB-C3B-C4B	3.57	126.89	121.37
13	L1	201	CYC	CHB-C4A-C3A	3.56	134.03	124.87
13	H6	201	CYC	C2C-C3C-C4C	3.56	106.68	101.34
13	a4	202	CYC	C2C-C1C-NC	-3.56	105.32	108.29
13	J4	202	CYC	CMD-C2D-C1D	3.56	130.80	125.62
13	X7	201	CYC	CHB-C4A-C3A	3.56	134.02	124.87
13	a1	202	CYC	C2C-C1C-NC	-3.56	105.32	108.29
13	J1	202	CYC	CMD-C2D-C1D	3.56	130.79	125.62
13	P1	202	CYC	C2C-C1C-NC	-3.56	105.32	108.29
13	A1	302	CYC	C2C-C3C-C4C	3.56	106.66	101.34
13	P7	201	CYC	C2C-C1C-NC	-3.55	105.33	108.29
13	P6	201	CYC	CMA-C3A-C4A	3.54	130.60	125.10
13	f2	201	CYC	CHB-C4A-C3A	3.54	133.97	124.87
13	n2	201	CYC	C2C-C3C-C4C	3.54	106.64	101.34
13	T2	201	CYC	C2C-C1C-NC	-3.54	105.34	108.29
13	W1	201	CYC	C2C-C3C-C4C	3.54	106.64	101.34
13	I1	201	CYC	C2C-C1C-NC	-3.53	105.34	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a1	201	CYC	CAB-C3B-C4B	3.53	126.83	121.37
13	a6	201	CYC	CAB-C3B-C4B	3.51	126.81	121.37
13	J5	201	CYC	C3C-C4C-NC	-3.51	103.42	107.94
13	a1	201	CYC	CMA-C3A-C4A	3.50	130.54	125.10
13	R2	201	CYC	CHB-C4A-C3A	3.50	133.87	124.87
13	T7	202	CYC	C2C-C3C-C4C	3.50	106.58	101.34
13	P5	202	CYC	C2C-C1C-NC	-3.49	105.38	108.29
13	R7	201	CYC	C2C-C1C-NC	-3.49	105.39	108.29
13	s2	201	CYC	CHB-C4A-C3A	3.48	133.81	124.87
13	H7	201	CYC	C2C-C3C-C4C	3.47	106.53	101.34
13	G1	201	CYC	C2C-C1C-NC	-3.46	105.40	108.29
13	t2	201	CYC	C2C-C1C-NC	-3.46	105.41	108.29
13	N4	201	CYC	C3C-C4C-NC	-3.46	103.49	107.94
13	H4	201	CYC	C2C-C3C-C4C	3.46	106.52	101.34
13	A2	202	CYC	C3C-C4C-NC	-3.45	103.50	107.94
13	22	301	CYC	C2C-C1C-NC	-3.44	105.42	108.29
13	Q3	202	CYC	C2C-C3C-C4C	3.44	106.49	101.34
13	M1	201	CYC	C3C-C4C-NC	-3.44	103.51	107.94
13	D4	201	CYC	CMD-C2D-C1D	3.43	130.61	125.62
13	X3	201	CYC	CHB-C4A-C3A	3.43	133.68	124.87
13	X2	201	CYC	C2C-C1C-NC	-3.43	105.43	108.29
13	V6	201	CYC	CMD-C2D-C1D	3.42	130.59	125.62
13	Q7	201	CYC	C2C-C1C-NC	-3.42	105.44	108.29
13	q2	201	CYC	CMB-C2B-C1B	3.42	128.31	124.16
13	Z5	301	CYC	CHB-C4A-C3A	3.41	133.64	124.87
13	J7	202	CYC	CMD-C2D-C1D	3.41	130.57	125.62
13	e2	201	CYC	CHB-C4A-C3A	3.41	133.63	124.87
13	V1	201	CYC	CMD-C2D-C1D	3.41	130.57	125.62
13	P3	201	CYC	C1B-CHB-C4A	-3.41	119.69	128.06
13	D7	201	CYC	C2C-C1C-NC	-3.40	105.45	108.29
13	G4	201	CYC	C2C-C3C-C4C	3.40	106.43	101.34
13	D4	201	CYC	C2C-C3C-C4C	3.40	106.43	101.34
13	D5	201	CYC	C1B-CHB-C4A	-3.40	119.72	128.06
13	v2	201	CYC	CHB-C4A-C3A	3.40	133.59	124.87
13	c2	801	CYC	C2C-C1C-NC	-3.40	105.46	108.29
13	D1	201	CYC	CMD-C2D-C1D	3.39	130.55	125.62
13	T2	201	CYC	CHB-C4A-C3A	3.39	133.58	124.87
13	W5	201	CYC	C3C-C4C-NC	-3.39	103.58	107.94
13	S2	201	CYC	CMA-C3A-C4A	3.39	130.36	125.10
13	D5	201	CYC	CMD-C2D-C1D	3.39	130.54	125.62
13	x2	201	CYC	C2C-C1C-NC	-3.38	105.47	108.29
13	D7	201	CYC	CMD-C2D-C1D	3.38	130.54	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	52	302	CYC	CMA-C3A-C4A	3.38	130.35	125.10
13	t2	201	CYC	CMA-C3A-C4A	3.38	130.35	125.10
13	F1	201	CYC	C2C-C1C-NC	-3.38	105.47	108.29
13	L4	201	CYC	CHB-C4A-C3A	3.38	133.54	124.87
13	Z1	301	CYC	CHB-C4A-C3A	3.37	133.54	124.87
13	A1	302	CYC	CMD-C2D-C1D	3.37	130.52	125.62
13	W6	201	CYC	C3C-C4C-NC	-3.37	103.60	107.94
13	F5	201	CYC	C3C-C4C-NC	-3.37	103.60	107.94
13	G5	201	CYC	C2C-C3C-C4C	3.37	106.39	101.34
13	A6	302	CYC	CMD-C2D-C1D	3.37	130.51	125.62
13	E2	201	CYC	CHB-C4A-C3A	3.37	133.52	124.87
13	X5	201	CYC	C2C-C1C-NC	-3.37	105.48	108.29
13	T3	202	CYC	C2C-C3C-C4C	3.36	106.38	101.34
13	L5	201	CYC	CMA-C3A-C4A	3.36	130.32	125.10
13	L4	201	CYC	CMA-C3A-C4A	3.36	130.31	125.10
13	L6	201	CYC	CHB-C4A-C3A	3.35	133.49	124.87
13	W1	201	CYC	CMA-C3A-C4A	3.35	130.31	125.10
13	v2	201	CYC	CMA-C3A-C4A	3.35	130.30	125.10
13	L5	201	CYC	CHB-C4A-C3A	3.35	133.48	124.87
13	v2	201	CYC	C2C-C3C-C4C	3.35	106.36	101.34
13	W2	201	CYC	CMA-C3A-C4A	3.35	130.30	125.10
13	a7	201	CYC	C1B-CHB-C4A	-3.35	119.84	128.06
13	z2	201	CYC	CHB-C4A-C3A	3.35	133.47	124.87
13	D6	201	CYC	CMD-C2D-C1D	3.34	130.48	125.62
13	h2	201	CYC	CHB-C4A-C3A	3.34	133.45	124.87
13	X1	201	CYC	CAB-C3B-C4B	3.34	126.53	121.37
13	Q1	202	CYC	CMA-C3A-C4A	3.33	130.28	125.10
13	M2	201	CYC	C1B-CHB-C4A	-3.33	119.88	128.06
13	Q5	202	CYC	CMA-C3A-C4A	3.33	130.27	125.10
13	L3	201	CYC	CHB-C4A-C3A	3.32	133.40	124.87
13	F5	201	CYC	C2C-C1C-NC	-3.32	105.52	108.29
13	G2	201	CYC	CHB-C4A-C3A	3.32	133.39	124.87
13	P7	201	CYC	CMA-C3A-C4A	3.32	130.25	125.10
13	V1	201	CYC	C2C-C3C-C4C	3.32	106.31	101.34
13	X4	201	CYC	C1B-CHB-C4A	-3.32	119.92	128.06
13	a6	202	CYC	C2C-C1C-NC	-3.31	105.53	108.29
13	B6	201	CYC	C2C-C1C-NC	-3.31	105.53	108.29
13	X4	201	CYC	C2C-C1C-NC	-3.30	105.54	108.29
13	P3	201	CYC	CMA-C3A-C4A	3.29	130.21	125.10
13	Z3	301	CYC	CMA-C3A-C4A	3.29	130.21	125.10
13	X1	201	CYC	C2C-C1C-NC	-3.29	105.55	108.29
13	f2	201	CYC	C2C-C1C-NC	-3.29	105.55	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D1	201	CYC	CMA-C3A-C4A	3.29	130.21	125.10
13	D2	201	CYC	CHB-C4A-C3A	3.28	133.30	124.87
13	Z4	301	CYC	CHB-C4A-C3A	3.28	133.30	124.87
13	G3	201	CYC	C2C-C3C-C4C	3.28	106.25	101.34
13	M4	201	CYC	C3C-C4C-NC	-3.28	103.72	107.94
13	J3	202	CYC	CMD-C2D-C1D	3.26	130.37	125.62
13	J4	201	CYC	C3C-C4C-NC	-3.26	103.75	107.94
13	y2	201	CYC	CMA-C3A-C4A	3.26	130.16	125.10
13	w2	201	CYC	CMA-C3A-C4A	3.25	130.15	125.10
13	F4	201	CYC	C2C-C1C-NC	-3.25	105.58	108.29
13	P2	201	CYC	CMA-C3A-C4A	3.25	130.14	125.10
13	U4	201	CYC	C2C-C3C-C4C	3.25	106.20	101.34
13	o2	801	CYC	C1A-NA-C4A	3.24	112.47	106.52
13	Z6	301	CYC	CHB-C4A-C3A	3.24	133.20	124.87
13	J5	201	CYC	CMA-C3A-C4A	3.24	130.13	125.10
13	I7	201	CYC	C3C-C4C-NC	-3.24	103.77	107.94
13	X5	201	CYC	CAB-C3B-C4B	3.24	126.38	121.37
13	J6	201	CYC	CMA-C3A-C4A	3.24	130.13	125.10
13	V3	201	CYC	C2C-C3C-C4C	3.24	106.19	101.34
13	n2	201	CYC	C1B-CHB-C4A	-3.23	120.12	128.06
13	U7	201	CYC	C2C-C3C-C4C	3.23	106.18	101.34
13	Q2	201	CYC	C2C-C1C-NC	-3.23	105.60	108.29
13	G7	201	CYC	C2C-C3C-C4C	3.23	106.17	101.34
13	G2	201	CYC	CHA-C4D-C3D	-3.22	120.30	127.22
13	F2	201	CYC	CHB-C4A-C3A	3.22	133.14	124.87
13	M1	201	CYC	CAB-C3B-C4B	3.21	126.34	121.37
13	K4	201	CYC	C3C-C4C-NC	-3.21	103.80	107.94
13	P5	201	CYC	C1B-CHB-C4A	-3.21	120.17	128.06
13	a7	201	CYC	C2C-C3C-C4C	3.21	106.14	101.34
13	Q2	201	CYC	C1B-CHB-C4A	-3.21	120.18	128.06
13	V1	201	CYC	CMA-C3A-C4A	3.21	130.08	125.10
13	V3	201	CYC	CMD-C2D-C1D	3.20	130.28	125.62
13	M5	201	CYC	C3C-C4C-NC	-3.20	103.82	107.94
13	X5	201	CYC	CHB-C4A-C3A	3.20	133.10	124.87
13	M6	201	CYC	CAB-C3B-C4B	3.20	126.32	121.37
13	A1	301	CYC	CMA-C3A-C4A	3.20	130.07	125.10
13	Q4	202	CYC	CMA-C3A-C4A	3.20	130.07	125.10
13	W6	201	CYC	CMA-C3A-C4A	3.20	130.06	125.10
13	X1	201	CYC	CHB-C4A-C3A	3.20	133.08	124.87
13	A2	202	CYC	CAB-C3B-C4B	3.19	126.30	121.37
13	B5	201	CYC	CMA-C3A-C4A	3.19	130.05	125.10
13	22	302	CYC	C3C-C4C-NC	-3.19	103.84	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H2	201	CYC	C3C-C4C-NC	-3.19	103.84	107.94
13	a3	201	CYC	C2C-C3C-C4C	3.18	106.11	101.34
13	D5	201	CYC	CMA-C3A-C4A	3.18	130.04	125.10
13	L5	201	CYC	C2C-C1C-NC	-3.18	105.64	108.29
13	o2	801	CYC	C2C-C3C-C4C	3.18	106.10	101.34
13	Q6	202	CYC	CAB-C3B-C4B	3.18	126.29	121.37
13	Q3	201	CYC	C2C-C1C-NC	-3.18	105.64	108.29
13	32	302	CYC	C3C-C4C-NC	-3.17	103.86	107.94
13	W2	201	CYC	C3C-C4C-NC	-3.17	103.86	107.94
13	i2	201	CYC	CAB-C3B-C4B	3.17	126.28	121.37
13	Q3	202	CYC	C2C-C1C-NC	-3.17	105.65	108.29
13	l2	201	CYC	CHB-C4A-C3A	3.17	133.01	124.87
13	N2	802	CYC	C1A-NA-C4A	3.17	112.33	106.52
13	a5	201	CYC	CMA-C3A-C4A	3.17	130.01	125.10
13	K6	201	CYC	CMA-C3A-C4A	3.16	130.01	125.10
13	a6	201	CYC	CMA-C3A-C4A	3.16	130.01	125.10
13	M3	201	CYC	CAB-C3B-C4B	3.16	126.26	121.37
13	L7	201	CYC	CHB-C4A-C3A	3.16	132.98	124.87
13	S2	201	CYC	C3C-C4C-NC	-3.15	103.88	107.94
13	p2	201	CYC	CHB-C4A-C3A	3.15	132.97	124.87
13	S2	201	CYC	C1A-NA-C4A	3.15	112.30	106.52
13	M7	201	CYC	CAB-C3B-C4B	3.14	126.23	121.37
13	L3	201	CYC	CMA-C3A-C4A	3.14	129.98	125.10
13	K7	201	CYC	C2C-C3C-C4C	3.14	106.05	101.34
13	B1	201	CYC	CMA-C3A-C4A	3.14	129.98	125.10
13	N2	801	CYC	CHB-C4A-C3A	3.14	132.94	124.87
13	U6	201	CYC	C3C-C4C-NC	-3.14	103.90	107.94
13	L7	201	CYC	CMA-C3A-C4A	3.14	129.97	125.10
13	m2	201	CYC	C2C-C1C-NC	-3.14	105.67	108.29
13	U2	201	CYC	C1A-NA-C4A	3.14	112.27	106.52
13	J1	201	CYC	CMA-C3A-C4A	3.13	129.96	125.10
13	Q7	202	CYC	C3C-C4C-NC	-3.13	103.91	107.94
13	Q4	202	CYC	CAB-C3B-C4B	3.13	126.21	121.37
13	U2	201	CYC	C2C-C1C-NC	-3.13	105.68	108.29
13	a6	201	CYC	C2C-C3C-C4C	3.13	106.02	101.34
13	y2	201	CYC	CHB-C4A-C3A	3.12	132.89	124.87
13	H1	201	CYC	C2C-C1C-NC	-3.12	105.69	108.29
13	M4	201	CYC	CAB-C3B-C4B	3.11	126.18	121.37
13	K6	201	CYC	C2C-C1C-NC	-3.11	105.70	108.29
13	T1	202	CYC	CMA-C3A-C4A	3.11	129.93	125.10
13	Q7	201	CYC	C3C-C4C-NC	-3.11	103.94	107.94
13	R2	201	CYC	C2C-C3C-C4C	3.11	105.99	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H5	201	CYC	C2C-C1C-NC	-3.10	105.70	108.29
13	Q5	202	CYC	CAB-C3B-C4B	3.10	126.17	121.37
13	Q3	201	CYC	C3C-C4C-NC	-3.10	103.95	107.94
13	P4	202	CYC	C1B-CHB-C4A	-3.10	120.44	128.06
13	R1	201	CYC	CAB-C3B-C4B	3.10	126.17	121.37
13	Q5	201	CYC	C2C-C3C-C4C	3.10	105.98	101.34
13	j2	201	CYC	CMA-C3A-C4A	3.09	129.91	125.10
13	R7	201	CYC	CAB-C3B-C4B	3.09	126.16	121.37
13	S5	201	CYC	CMA-C3A-C4A	3.09	129.90	125.10
13	X6	201	CYC	C2C-C1C-NC	-3.09	105.71	108.29
13	R4	201	CYC	CAB-C3B-C4B	3.09	126.14	121.37
13	A6	301	CYC	CMA-C3A-C4A	3.08	129.89	125.10
13	W4	201	CYC	CMA-C3A-C4A	3.08	129.89	125.10
13	R6	201	CYC	CAB-C3B-C4B	3.08	126.14	121.37
13	G6	201	CYC	C2C-C3C-C4C	3.08	105.95	101.34
13	M2	201	CYC	CMA-C3A-C4A	3.08	129.88	125.10
13	52	301	CYC	C1B-CHB-C4A	-3.08	120.50	128.06
13	X6	201	CYC	CHB-C4A-C3A	3.08	132.78	124.87
13	Q6	202	CYC	C3C-C4C-NC	-3.07	103.98	107.94
13	Q1	202	CYC	CAB-C3B-C4B	3.07	126.12	121.37
13	X7	201	CYC	C1A-NA-C4A	3.07	112.14	106.52
13	J3	201	CYC	CMA-C3A-C4A	3.07	129.86	125.10
13	R5	201	CYC	CAB-C3B-C4B	3.06	126.11	121.37
13	r2	201	CYC	CHB-C4A-C3A	3.06	132.74	124.87
13	32	301	CYC	CMA-C3A-C4A	3.06	129.85	125.10
13	X2	201	CYC	CMA-C3A-C4A	3.05	129.84	125.10
13	F5	201	CYC	CBD-CAD-C3D	3.05	120.97	112.53
13	F1	201	CYC	CMA-C3A-C4A	3.05	129.84	125.10
13	A2	201	CYC	C2C-C1C-NC	-3.05	105.75	108.29
13	N6	201	CYC	CMA-C3A-C4A	3.05	129.83	125.10
13	F6	201	CYC	CBD-CAD-C3D	3.05	120.96	112.53
13	M5	201	CYC	CAB-C3B-C4B	3.05	126.08	121.37
13	s2	201	CYC	C1A-NA-C4A	3.04	112.10	106.52
13	n2	201	CYC	CMA-C3A-C4A	3.04	129.82	125.10
13	o2	801	CYC	CAB-C3B-C4B	3.04	126.06	121.37
13	K3	201	CYC	C2C-C3C-C4C	3.04	105.89	101.34
13	Q3	202	CYC	CAB-C3B-C4B	3.03	126.06	121.37
13	Q7	202	CYC	CAB-C3B-C4B	3.03	126.06	121.37
13	F1	201	CYC	CBD-CAD-C3D	3.03	120.92	112.53
13	K1	201	CYC	CMA-C3A-C4A	3.03	129.81	125.10
13	D1	201	CYC	C1B-CHB-C4A	-3.03	120.62	128.06
13	P1	201	CYC	C1B-CHB-C4A	-3.03	120.62	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a5	202	CYC	CMD-C2D-C1D	3.03	130.02	125.62
13	J4	201	CYC	C2C-C1C-NC	-3.02	105.77	108.29
13	K7	201	CYC	CMA-C3A-C4A	3.02	129.79	125.10
13	F4	201	CYC	CAD-C3D-C4D	3.02	130.57	125.77
13	S6	201	CYC	CMA-C3A-C4A	3.02	129.79	125.10
13	V2	201	CYC	CMA-C3A-C4A	3.02	129.79	125.10
13	a3	201	CYC	CMA-C3A-C4A	3.01	129.78	125.10
13	S1	201	CYC	CMA-C3A-C4A	3.01	129.77	125.10
13	a5	201	CYC	C2C-C3C-C4C	3.01	105.84	101.34
13	Q6	202	CYC	CMA-C3A-C4A	3.01	129.77	125.10
13	N4	201	CYC	CMA-C3A-C4A	3.00	129.76	125.10
13	X3	201	CYC	C1A-NA-C4A	3.00	112.03	106.52
13	L5	201	CYC	C1A-NA-C4A	3.00	112.03	106.52
13	L3	201	CYC	C1A-NA-C4A	3.00	112.02	106.52
13	L4	201	CYC	C1A-NA-C4A	3.00	112.02	106.52
13	42	302	CYC	C3C-C4C-NC	-3.00	104.08	107.94
13	W5	201	CYC	CMA-C3A-C4A	2.99	129.75	125.10
13	L1	201	CYC	C1A-NA-C4A	2.99	112.01	106.52
13	Q2	201	CYC	CMA-C3A-C4A	2.99	129.75	125.10
13	R3	201	CYC	CAB-C3B-C4B	2.99	126.00	121.37
13	R4	201	CYC	C2C-C1C-NC	-2.99	105.80	108.29
13	Q6	201	CYC	C3C-C4C-NC	-2.99	104.09	107.94
13	T2	201	CYC	C1A-NA-C4A	2.99	112.00	106.52
13	E2	201	CYC	C1A-NA-C4A	2.99	112.00	106.52
13	22	301	CYC	CMA-C3A-C4A	2.98	129.73	125.10
13	F6	201	CYC	CMA-C3A-C4A	2.98	129.73	125.10
13	P3	202	CYC	CMD-C2D-C1D	2.98	129.96	125.62
13	L2	201	CYC	CMA-C3A-C4A	2.98	129.73	125.10
13	N1	201	CYC	CMA-C3A-C4A	2.98	129.73	125.10
13	L7	201	CYC	C1A-NA-C4A	2.98	111.99	106.52
13	Z7	301	CYC	CMA-C3A-C4A	2.98	129.72	125.10
13	V4	201	CYC	C2C-C3C-C4C	2.97	105.79	101.34
13	U5	201	CYC	C2C-C1C-NC	-2.97	105.81	108.29
13	N2	802	CYC	C3C-C4C-NC	-2.97	104.12	107.94
13	y2	201	CYC	C1A-NA-C4A	2.96	111.96	106.52
13	G1	201	CYC	CMA-C3A-C4A	2.96	129.70	125.10
13	P6	201	CYC	C1B-CHB-C4A	-2.96	120.78	128.06
13	x2	201	CYC	C2C-C3C-C4C	2.96	105.77	101.34
13	D4	201	CYC	C1B-CHB-C4A	-2.96	120.80	128.06
13	A2	201	CYC	C1A-NA-C4A	2.96	111.94	106.52
13	Z1	301	CYC	C1A-NA-C4A	2.95	111.94	106.52
13	S3	201	CYC	CMA-C3A-C4A	2.95	129.69	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N5	201	CYC	CMA-C3A-C4A	2.95	129.69	125.10
13	Q1	202	CYC	C2C-C3C-C4C	2.95	105.76	101.34
13	T5	202	CYC	CMA-C3A-C4A	2.95	129.68	125.10
13	W7	201	CYC	C2C-C3C-C4C	2.95	105.75	101.34
13	X1	201	CYC	C1A-NA-C4A	2.94	111.92	106.52
13	W3	201	CYC	C2C-C3C-C4C	2.94	105.75	101.34
13	t2	201	CYC	C1A-NA-C4A	2.94	111.92	106.52
13	L6	201	CYC	C1A-NA-C4A	2.94	111.92	106.52
13	52	301	CYC	CMA-C3A-C4A	2.94	129.67	125.10
13	k2	201	CYC	C2C-C3C-C4C	2.94	105.74	101.34
13	R2	201	CYC	C1A-NA-C4A	2.94	111.91	106.52
13	D6	201	CYC	CHB-C4A-C3A	2.94	132.43	124.87
13	V7	201	CYC	CMD-C2D-C1D	2.94	129.89	125.62
13	Q1	201	CYC	C2C-C3C-C4C	2.94	105.74	101.34
13	W4	201	CYC	C3C-C4C-NC	-2.94	104.16	107.94
13	Q4	202	CYC	OB-C4B-C3B	-2.94	124.94	128.03
13	N6	201	CYC	C2C-C1C-NC	-2.94	105.84	108.29
13	V7	201	CYC	CMA-C3A-C4A	2.94	129.66	125.10
13	B6	201	CYC	CMA-C3A-C4A	2.93	129.66	125.10
13	V6	201	CYC	CMA-C3A-C4A	2.93	129.66	125.10
13	v2	201	CYC	C1A-NA-C4A	2.93	111.90	106.52
13	N2	802	CYC	CHB-C4A-NA	-2.93	118.62	124.95
13	B4	201	CYC	CMA-C3A-C4A	2.93	129.65	125.10
13	Z3	301	CYC	C1B-CHB-C4A	-2.93	120.86	128.06
13	N3	201	CYC	C2C-C1C-NC	-2.93	105.85	108.29
13	a3	201	CYC	C1B-CHB-C4A	-2.93	120.87	128.06
13	T6	202	CYC	CMA-C3A-C4A	2.92	129.64	125.10
13	N5	201	CYC	C3C-C4C-NC	-2.92	104.18	107.94
13	Z5	301	CYC	C1A-NA-C4A	2.92	111.88	106.52
13	W5	201	CYC	C2C-C3C-C4C	2.92	105.71	101.34
13	Z4	301	CYC	C1A-NA-C4A	2.91	111.87	106.52
13	S7	201	CYC	CMA-C3A-C4A	2.91	129.62	125.10
13	a4	201	CYC	CMB-C2B-C1B	2.91	127.70	124.16
13	P2	201	CYC	CHB-C4A-C3A	2.91	132.35	124.87
13	A1	301	CYC	C1B-CHB-C4A	-2.91	120.91	128.06
13	I3	201	CYC	C3C-C4C-NC	-2.90	104.20	107.94
13	e2	201	CYC	C1A-NA-C4A	2.90	111.84	106.52
13	f2	201	CYC	C1A-NA-C4A	2.90	111.84	106.52
13	a6	202	CYC	CMA-C3A-C4A	2.89	129.59	125.10
13	42	301	CYC	CMA-C3A-C4A	2.89	129.59	125.10
13	X5	201	CYC	C1A-NA-C4A	2.88	111.81	106.52
13	H6	201	CYC	C2C-C1C-NC	-2.88	105.89	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z3	301	CYC	C1A-NA-C4A	2.88	111.81	106.52
13	l2	201	CYC	C1A-NA-C4A	2.88	111.81	106.52
13	p2	201	CYC	CHA-C4D-C3D	-2.88	121.02	127.22
13	K3	201	CYC	CMA-C3A-C4A	2.88	129.57	125.10
13	Q4	202	CYC	C3C-C4C-NC	-2.88	104.23	107.94
13	t2	201	CYC	CHB-C4A-NA	-2.88	118.74	124.95
13	42	301	CYC	C1B-CHB-C4A	-2.88	120.99	128.06
13	Z6	301	CYC	C1A-NA-C4A	2.88	111.80	106.52
13	Q1	201	CYC	C3C-C4C-NC	-2.88	104.24	107.94
13	J5	202	CYC	CMA-C3A-C4A	2.87	129.56	125.10
13	E2	201	CYC	C2C-C3C-C4C	2.87	105.64	101.34
13	V5	201	CYC	CMA-C3A-C4A	2.87	129.56	125.10
13	X6	201	CYC	C1A-NA-C4A	2.87	111.78	106.52
13	Q1	202	CYC	OB-C4B-C3B	-2.87	125.02	128.03
13	32	301	CYC	C1A-NA-C4A	2.87	111.78	106.52
13	U3	201	CYC	C2C-C3C-C4C	2.87	105.63	101.34
13	H5	201	CYC	CMA-C3A-C4A	2.86	129.54	125.10
13	Q3	202	CYC	OB-C4B-C3B	-2.86	125.03	128.03
13	L4	201	CYC	C2C-C1C-NC	-2.86	105.91	108.29
13	Q5	202	CYC	C3C-C4C-NC	-2.86	104.26	107.94
13	P4	202	CYC	CHB-C4A-C3A	2.86	132.22	124.87
13	H1	201	CYC	CMA-C3A-C4A	2.85	129.53	125.10
13	J4	201	CYC	CMA-C3A-C4A	2.85	129.53	125.10
13	s2	201	CYC	C2C-C3C-C4C	2.85	105.61	101.34
13	B2	202	CYC	C2C-C1C-NC	-2.85	105.91	108.29
13	42	301	CYC	C1A-NA-C4A	2.85	111.75	106.52
13	P5	201	CYC	CHB-C4A-C3A	2.85	132.19	124.87
13	F2	201	CYC	C1A-NA-C4A	2.85	111.75	106.52
13	22	301	CYC	C1A-NA-C4A	2.85	111.75	106.52
13	Q7	202	CYC	C2C-C1C-NC	-2.85	105.92	108.29
13	A2	201	CYC	CHB-C4A-C3A	2.85	132.19	124.87
13	V5	201	CYC	C2C-C3C-C4C	2.85	105.60	101.34
13	P1	201	CYC	CHB-C4A-C3A	2.84	132.17	124.87
13	F5	201	CYC	CMA-C3A-C4A	2.84	129.51	125.10
13	X4	201	CYC	C1A-NA-C4A	2.84	111.73	106.52
13	z2	201	CYC	C1A-NA-C4A	2.84	111.72	106.52
13	a7	201	CYC	CMA-C3A-C4A	2.84	129.50	125.10
13	P5	201	CYC	C1A-NA-C4A	2.84	111.72	106.52
13	G5	201	CYC	CMA-C3A-C4A	2.84	129.50	125.10
13	m2	201	CYC	CMA-C3A-C4A	2.83	129.50	125.10
13	V4	201	CYC	CMA-C3A-C4A	2.83	129.50	125.10
13	J6	202	CYC	CMA-C3A-C4A	2.83	129.50	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U2	201	CYC	CHB-C4A-NA	-2.83	118.84	124.95
13	O2	201	CYC	CHB-C4A-C3A	2.83	132.14	124.87
13	P1	201	CYC	C1A-NA-C4A	2.83	111.71	106.52
13	F4	201	CYC	CMA-C3A-C4A	2.83	129.49	125.10
13	P4	202	CYC	C1A-NA-C4A	2.83	111.70	106.52
13	W5	201	CYC	CMC-C2C-C1C	-2.82	106.31	112.40
13	D6	201	CYC	C1A-NA-C4A	2.82	111.70	106.52
13	T4	202	CYC	CMA-C3A-C4A	2.82	129.49	125.10
13	D4	201	CYC	C2C-C1C-NC	-2.82	105.94	108.29
13	x2	201	CYC	CMA-C3A-C4A	2.82	129.48	125.10
13	H4	201	CYC	CMA-C3A-C4A	2.82	129.48	125.10
13	P7	202	CYC	C3C-C4C-NC	-2.82	104.31	107.94
13	X2	201	CYC	CHB-C4A-C3A	2.82	132.11	124.87
13	P7	202	CYC	C2C-C3C-C4C	2.82	105.56	101.34
13	V3	201	CYC	CMA-C3A-C4A	2.82	129.47	125.10
13	G4	201	CYC	CMA-C3A-C4A	2.82	129.47	125.10
13	D2	201	CYC	C1A-NA-C4A	2.81	111.68	106.52
13	r2	201	CYC	C1A-NA-C4A	2.81	111.68	106.52
13	X4	201	CYC	CHB-C4A-C3A	2.81	132.10	124.87
13	A2	201	CYC	CMA-C3A-C4A	2.81	129.47	125.10
13	P3	201	CYC	C1A-NA-C4A	2.81	111.68	106.52
13	22	302	CYC	C1A-NA-C4A	2.81	111.68	106.52
13	X2	201	CYC	C1A-NA-C4A	2.81	111.68	106.52
13	q2	201	CYC	C1B-NB-C4B	-2.81	107.21	110.66
13	a6	201	CYC	C1B-CHB-C4A	-2.81	121.16	128.06
13	a6	202	CYC	CMD-C2D-C1D	2.81	129.70	125.62
13	M7	201	CYC	C2C-C1C-NC	-2.81	105.95	108.29
13	G6	201	CYC	CMA-C3A-C4A	2.80	129.46	125.10
13	A1	302	CYC	CHA-C4D-C3D	-2.80	121.20	127.22
13	O2	201	CYC	CHA-C4D-C3D	-2.80	121.20	127.22
13	N3	201	CYC	CMA-C3A-C4A	2.80	129.45	125.10
13	N2	801	CYC	C1A-NA-C4A	2.80	111.66	106.52
13	Q5	202	CYC	OB-C4B-C3B	-2.80	125.09	128.03
13	e2	201	CYC	C2C-C3C-C4C	2.80	105.53	101.34
13	p2	201	CYC	C3C-C4C-NC	-2.80	104.34	107.94
13	P6	201	CYC	C1A-NA-C4A	2.79	111.65	106.52
13	n2	201	CYC	C3C-C4C-NC	-2.79	104.35	107.94
13	Q4	201	CYC	C3C-C4C-NC	-2.79	104.35	107.94
13	S4	201	CYC	CMA-C3A-C4A	2.79	129.43	125.10
13	A6	301	CYC	C1B-CHB-C4A	-2.79	121.21	128.06
13	T2	201	CYC	CMA-C3A-C4A	2.79	129.43	125.10
13	a2	201	CYC	C1A-NA-C4A	2.79	111.63	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H6	201	CYC	CMA-C3A-C4A	2.78	129.42	125.10
13	I3	201	CYC	CMA-C3A-C4A	2.78	129.42	125.10
13	h2	201	CYC	C1A-NA-C4A	2.78	111.62	106.52
13	M3	201	CYC	C2C-C1C-NC	-2.78	105.97	108.29
13	L7	201	CYC	C2C-C1C-NC	-2.78	105.97	108.29
13	a1	202	CYC	CMD-C2D-C1D	2.78	129.66	125.62
13	V6	201	CYC	C2C-C3C-C4C	2.78	105.50	101.34
13	U1	201	CYC	C2C-C1C-NC	-2.78	105.98	108.29
13	a5	202	CYC	CMA-C3A-C4A	2.77	129.40	125.10
13	U1	201	CYC	CMA-C3A-C4A	2.77	129.40	125.10
13	22	301	CYC	C1B-CHB-C4A	-2.77	121.26	128.06
13	H3	201	CYC	CMA-C3A-C4A	2.77	129.40	125.10
13	A2	202	CYC	C2C-C1C-NC	-2.76	105.99	108.29
13	32	302	CYC	C1A-NA-C4A	2.76	111.59	106.52
13	K4	201	CYC	CMA-C3A-C4A	2.76	129.39	125.10
13	Q4	201	CYC	CMB-C2B-C1B	2.76	127.52	124.16
13	J4	202	CYC	CMA-C3A-C4A	2.76	129.38	125.10
13	P6	201	CYC	CHB-C4A-C3A	2.76	131.96	124.87
13	Z7	301	CYC	C1A-NA-C4A	2.76	111.58	106.52
13	Q7	202	CYC	C2C-C3C-C4C	2.76	105.47	101.34
13	P7	201	CYC	C1A-NA-C4A	2.76	111.58	106.52
13	D7	201	CYC	CMA-C3A-C4A	2.76	129.38	125.10
13	G2	201	CYC	C1A-NA-C4A	2.76	111.58	106.52
13	a1	202	CYC	CMA-C3A-C4A	2.75	129.38	125.10
13	32	301	CYC	CHB-C4A-C3A	2.75	131.95	124.87
13	H7	201	CYC	CMA-C3A-C4A	2.75	129.37	125.10
13	T7	201	CYC	C2C-C1C-NC	-2.75	106.00	108.29
13	a5	201	CYC	C1A-NA-C4A	2.75	111.56	106.52
13	g2	201	CYC	CHB-C4A-C3A	2.75	131.93	124.87
13	U5	201	CYC	CMA-C3A-C4A	2.75	129.37	125.10
13	N7	201	CYC	C2C-C1C-NC	-2.75	106.00	108.29
13	A6	301	CYC	C1A-NA-C4A	2.74	111.55	106.52
13	o2	801	CYC	CHB-C4A-NA	-2.74	119.03	124.95
13	D4	201	CYC	C1A-NA-C4A	2.74	111.55	106.52
13	J7	201	CYC	CMA-C3A-C4A	2.74	129.35	125.10
13	P2	201	CYC	C1A-NA-C4A	2.74	111.54	106.52
13	t2	201	CYC	C3C-C4C-NC	-2.74	104.42	107.94
13	p2	201	CYC	C1A-NA-C4A	2.73	111.53	106.52
13	52	301	CYC	C1A-NA-C4A	2.73	111.53	106.52
13	D6	201	CYC	C2C-C1C-NC	-2.73	106.01	108.29
13	C1	201	CYC	CMB-C2B-C1B	2.73	127.48	124.16
13	Q6	201	CYC	CMB-C2B-C1B	2.72	127.47	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a5	201	CYC	C1B-CHB-C4A	-2.72	121.38	128.06
13	x2	201	CYC	C1A-NA-C4A	2.72	111.51	106.52
13	Q6	202	CYC	OB-C4B-C3B	-2.72	125.17	128.03
13	Q7	202	CYC	OB-C4B-C3B	-2.72	125.17	128.03
13	22	302	CYC	CHB-C4A-C3A	2.72	131.85	124.87
13	Q4	201	CYC	C2C-C3C-C4C	2.72	105.41	101.34
13	a1	201	CYC	C2C-C3C-C4C	2.72	105.41	101.34
13	S2	201	CYC	CHB-C4A-NA	-2.71	119.09	124.95
13	a3	201	CYC	C1A-NA-C4A	2.71	111.50	106.52
13	L3	201	CYC	C2C-C1C-NC	-2.71	106.03	108.29
13	a5	201	CYC	CHB-C4A-C3A	2.71	131.84	124.87
13	a4	202	CYC	CMA-C3A-C4A	2.71	129.31	125.10
13	D1	201	CYC	C1A-NA-C4A	2.71	111.49	106.52
13	O2	201	CYC	C1A-NA-C4A	2.71	111.49	106.52
13	V3	202	CYC	CMD-C2D-C1D	2.70	129.55	125.62
13	N5	201	CYC	C2C-C3C-C4C	2.70	105.39	101.34
13	K5	201	CYC	CHA-C4D-C3D	-2.70	121.41	127.22
13	S1	201	CYC	CHA-C4D-C3D	-2.70	121.42	127.22
13	N2	801	CYC	CMD-C2D-C3D	-2.70	119.90	125.62
13	a1	201	CYC	C1A-NA-C4A	2.70	111.47	106.52
13	a1	201	CYC	CHB-C4A-C3A	2.70	131.80	124.87
13	I1	201	CYC	CMA-C3A-C4A	2.69	129.28	125.10
13	G3	201	CYC	CMA-C3A-C4A	2.69	129.28	125.10
13	I4	201	CYC	CMA-C3A-C4A	2.69	129.27	125.10
13	F6	202	CYC	CMA-C3A-C4A	2.69	129.27	125.10
13	I7	201	CYC	CMA-C3A-C4A	2.68	129.27	125.10
13	T4	201	CYC	C2C-C1C-NC	-2.68	106.05	108.29
13	N7	201	CYC	CMA-C3A-C4A	2.68	129.26	125.10
13	Q5	201	CYC	CMB-C2B-C1B	2.68	127.42	124.16
13	D4	201	CYC	CHB-C4A-C3A	2.68	131.75	124.87
13	P3	201	CYC	CHB-C4A-C3A	2.68	131.75	124.87
13	a1	201	CYC	C1B-CHB-C4A	-2.68	121.49	128.06
13	a7	201	CYC	C1A-NA-C4A	2.67	111.42	106.52
13	K1	201	CYC	CHA-C4D-C3D	-2.67	121.48	127.22
13	S5	201	CYC	CHA-C4D-C3D	-2.67	121.49	127.22
13	f2	201	CYC	CHB-C4A-NA	-2.67	119.20	124.95
13	22	301	CYC	CHB-C4A-C3A	2.67	131.72	124.87
13	32	302	CYC	CHB-C4A-C3A	2.66	131.72	124.87
13	K5	201	CYC	CMA-C3A-C4A	2.66	129.24	125.10
13	T3	202	CYC	CMA-C3A-C4A	2.66	129.23	125.10
13	S6	201	CYC	CHA-C4D-C3D	-2.66	121.50	127.22
13	J1	202	CYC	CMA-C3A-C4A	2.66	129.23	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	h2	201	CYC	C2C-C3C-C4C	2.66	105.32	101.34
13	D5	201	CYC	C1A-NA-C4A	2.66	111.39	106.52
13	Q5	202	CYC	C2C-C3C-C4C	2.65	105.31	101.34
13	l2	201	CYC	CHB-C1B-C2B	-2.65	121.68	126.97
13	T3	201	CYC	C2C-C1C-NC	-2.65	106.08	108.29
13	B1	201	CYC	CHA-C4D-C3D	-2.65	121.52	127.22
13	U1	201	CYC	CHA-C4D-C3D	-2.65	121.52	127.22
13	Q7	201	CYC	CMB-C2B-C1B	2.65	127.38	124.16
13	Q1	201	CYC	CMA-C3A-C4A	2.65	129.21	125.10
13	a6	201	CYC	C1A-NA-C4A	2.65	111.38	106.52
13	N2	802	CYC	CHB-C1B-C2B	-2.65	121.69	126.97
13	B2	201	CYC	CMD-C2D-C1D	2.64	129.46	125.62
13	42	302	CYC	CHA-C4D-C3D	-2.64	121.55	127.22
13	T1	201	CYC	C2C-C1C-NC	-2.64	106.09	108.29
13	T6	201	CYC	C2C-C1C-NC	-2.64	106.09	108.29
13	R2	201	CYC	CHB-C1B-C2B	-2.64	121.71	126.97
13	Q5	201	CYC	C3C-C4C-NC	-2.64	104.55	107.94
13	F1	202	CYC	CMA-C3A-C4A	2.64	129.19	125.10
13	A6	302	CYC	C1A-NA-C4A	2.63	111.35	106.52
13	B3	201	CYC	CMA-C3A-C4A	2.63	129.19	125.10
13	A6	302	CYC	CHB-C4A-C3A	2.63	131.63	124.87
13	a5	202	CYC	C1A-NA-C4A	2.63	111.34	106.52
13	A1	301	CYC	C1A-NA-C4A	2.63	111.34	106.52
13	52	302	CYC	C1A-NA-C4A	2.63	111.34	106.52
13	K6	201	CYC	CHA-C4D-C3D	-2.63	121.57	127.22
13	L2	201	CYC	C3C-C4C-NC	-2.63	104.56	107.94
13	42	302	CYC	CMD-C2D-C1D	2.63	129.44	125.62
13	f2	201	CYC	CHB-C1B-C2B	-2.63	121.73	126.97
13	P2	201	CYC	C2C-C1C-NC	-2.63	106.10	108.29
13	T7	202	CYC	CMA-C3A-C4A	2.62	129.18	125.10
13	a6	202	CYC	C1A-NA-C4A	2.62	111.33	106.52
13	T2	201	CYC	CHB-C4A-NA	-2.62	119.29	124.95
13	Q5	201	CYC	CMA-C3A-C4A	2.62	129.17	125.10
13	I6	201	CYC	CMA-C3A-C4A	2.62	129.17	125.10
13	N1	201	CYC	CHA-C4D-C3D	-2.62	121.58	127.22
13	X5	201	CYC	C1B-CHB-C4A	-2.62	121.62	128.06
13	X2	201	CYC	C1B-CHB-C4A	-2.62	121.62	128.06
13	Q2	201	CYC	C2C-C3C-C4C	2.62	105.26	101.34
13	G1	201	CYC	CHA-C4D-C3D	-2.62	121.59	127.22
13	H7	201	CYC	C2C-C1C-NC	-2.62	106.11	108.29
13	Q6	201	CYC	C2C-C3C-C4C	2.62	105.26	101.34
13	W2	201	CYC	C2C-C1C-NC	-2.62	106.11	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H3	201	CYC	C2C-C1C-NC	-2.62	106.11	108.29
13	V7	202	CYC	CMD-C2D-C1D	2.61	129.42	125.62
13	A6	301	CYC	CHB-C4A-C3A	2.61	131.59	124.87
13	T6	202	CYC	C3C-C4C-NC	-2.61	104.58	107.94
13	W4	201	CYC	C2C-C3C-C4C	2.61	105.25	101.34
13	L6	201	CYC	C2C-C1C-NC	-2.61	106.11	108.29
13	H2	201	CYC	C2C-C1C-NC	-2.61	106.11	108.29
13	42	302	CYC	C1A-NA-C4A	2.61	111.30	106.52
13	Q1	202	CYC	C3C-C4C-NC	-2.61	104.59	107.94
13	B7	201	CYC	CMA-C3A-C4A	2.61	129.15	125.10
13	G7	201	CYC	CMA-C3A-C4A	2.60	129.15	125.10
13	P7	201	CYC	CHB-C4A-C3A	2.60	131.56	124.87
13	Z3	301	CYC	CHB-C4A-C3A	2.60	131.56	124.87
13	Q4	202	CYC	C2C-C3C-C4C	2.60	105.24	101.34
13	a4	202	CYC	C1A-NA-C4A	2.60	111.28	106.52
13	H5	201	CYC	CHA-C4D-C3D	-2.60	121.64	127.22
13	F4	201	CYC	CBD-CAD-C3D	2.59	119.69	112.53
13	d2	201	CYC	C2C-C1C-NC	-2.59	106.13	108.29
13	W5	201	CYC	CHA-C4D-C3D	-2.59	121.65	127.22
13	t2	201	CYC	CHB-C1B-C2B	-2.59	121.81	126.97
13	H6	201	CYC	CHA-C4D-C3D	-2.59	121.66	127.22
13	C6	201	CYC	CMB-C2B-C1B	2.59	127.30	124.16
13	V2	201	CYC	C1A-NA-C4A	2.59	111.26	106.52
13	T5	201	CYC	C2C-C1C-NC	-2.58	106.14	108.29
13	A6	302	CYC	CHA-C4D-C3D	-2.58	121.67	127.22
13	42	302	CYC	CHB-C4A-C3A	2.58	131.50	124.87
13	a1	202	CYC	C1A-NA-C4A	2.57	111.23	106.52
13	N2	801	CYC	CBD-CAD-C3D	2.57	119.64	112.53
13	n2	201	CYC	C1A-NA-C4A	2.56	111.22	106.52
13	S4	201	CYC	CHA-C4D-C3D	-2.56	121.71	127.22
13	W2	201	CYC	C1A-NA-C4A	2.56	111.22	106.52
13	C5	201	CYC	C1A-NA-C4A	2.56	111.21	106.52
13	C3	201	CYC	CMB-C2B-C1B	2.56	127.27	124.16
13	W6	201	CYC	CMC-C2C-C1C	-2.56	106.89	112.40
13	F3	201	CYC	C2C-C1C-NC	-2.56	106.16	108.29
13	Q6	202	CYC	C2C-C3C-C4C	2.56	105.17	101.34
13	C4	201	CYC	CMB-C2B-C1B	2.56	127.27	124.16
13	W1	201	CYC	CHA-C4D-C3D	-2.55	121.73	127.22
13	W6	201	CYC	C2C-C3C-C4C	2.55	105.17	101.34
13	V1	202	CYC	CMD-C2D-C1D	2.55	129.33	125.62
13	a2	201	CYC	CHB-C4A-C3A	2.55	131.42	124.87
13	H1	201	CYC	CHA-C4D-C3D	-2.55	121.74	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R5	201	CYC	C2C-C1C-NC	-2.55	106.17	108.29
13	J1	202	CYC	C1A-NA-C4A	2.55	111.19	106.52
13	L1	201	CYC	CHB-C4A-NA	-2.55	119.46	124.95
13	J5	202	CYC	C1A-NA-C4A	2.54	111.19	106.52
13	X7	201	CYC	CHB-C4A-NA	-2.54	119.46	124.95
13	C3	201	CYC	C2C-C3C-C4C	2.54	105.15	101.34
13	R2	201	CYC	CHB-C4A-NA	-2.54	119.46	124.95
13	E5	201	CYC	C2C-C1C-NC	-2.54	106.17	108.29
13	C1	202	CYC	C1A-NA-C4A	2.54	111.18	106.52
13	A6	302	CYC	OB-C4B-C3B	-2.54	125.36	128.03
13	Q1	201	CYC	CMB-C2B-C1B	2.54	127.25	124.16
13	Q3	201	CYC	C2C-C3C-C4C	2.54	105.14	101.34
13	F5	202	CYC	CMA-C3A-C4A	2.54	129.04	125.10
13	A1	302	CYC	C1A-NA-C4A	2.54	111.18	106.52
13	E3	201	CYC	C2C-C1C-NC	-2.54	106.17	108.29
13	a4	202	CYC	CMD-C2D-C1D	2.54	129.31	125.62
13	E6	201	CYC	C1A-NA-C4A	2.54	111.17	106.52
13	D3	201	CYC	C2C-C1C-NC	-2.54	106.17	108.29
13	C6	201	CYC	C1A-NA-C4A	2.54	111.17	106.52
13	Q3	201	CYC	CMB-C2B-C1B	2.53	127.24	124.16
13	T6	201	CYC	C1A-NA-C4A	2.53	111.17	106.52
13	Q1	202	CYC	C1A-NA-C4A	2.53	111.17	106.52
13	52	302	CYC	CHB-C4A-C3A	2.53	131.38	124.87
13	C1	202	CYC	CMA-C3A-C4A	2.53	129.03	125.10
13	V5	202	CYC	CMD-C2D-C1D	2.53	129.30	125.62
13	C5	201	CYC	CMA-C3A-C4A	2.53	129.03	125.10
13	M4	201	CYC	C2C-C1C-NC	-2.53	106.18	108.29
13	j2	201	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	C4	201	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	M1	201	CYC	CMB-C2B-C1B	2.53	127.24	124.16
13	T1	201	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	B5	201	CYC	CHA-C4D-C3D	-2.53	121.78	127.22
13	T3	202	CYC	C3C-C4C-NC	-2.53	104.69	107.94
13	F6	201	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	C5	201	CYC	CMB-C2B-C1B	2.53	127.23	124.16
13	a3	202	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	J6	202	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	E7	201	CYC	C2C-C1C-NC	-2.53	106.18	108.29
13	Q1	201	CYC	C1A-NA-C4A	2.53	111.16	106.52
13	y2	201	CYC	C3C-C4C-NC	-2.53	104.69	107.94
13	B2	201	CYC	C1A-NA-C4A	2.53	111.15	106.52
13	Q6	202	CYC	C1A-NA-C4A	2.53	111.15	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	w2	201	CYC	C1A-NA-C4A	2.52	111.15	106.52
13	e2	201	CYC	CHB-C1B-C2B	-2.52	121.93	126.97
13	J5	201	CYC	C1A-NA-C4A	2.52	111.15	106.52
13	E4	201	CYC	C1A-NA-C4A	2.52	111.14	106.52
13	A1	302	CYC	CHB-C4A-C3A	2.52	131.34	124.87
13	a2	201	CYC	C1B-CHB-C4A	-2.52	121.87	128.06
13	A2	202	CYC	CMA-C3A-C4A	2.52	129.01	125.10
13	Z3	301	CYC	CMD-C2D-C1D	2.52	129.28	125.62
13	R1	201	CYC	C2C-C1C-NC	-2.52	106.19	108.29
13	E5	201	CYC	C1A-NA-C4A	2.51	111.13	106.52
13	Q6	201	CYC	CMA-C3A-C4A	2.51	129.00	125.10
13	F4	202	CYC	CMA-C3A-C4A	2.51	129.00	125.10
13	E1	201	CYC	C1A-NA-C4A	2.51	111.12	106.52
13	g2	201	CYC	C1A-NA-C4A	2.51	111.12	106.52
13	W4	201	CYC	CMC-C2C-C1C	-2.51	107.00	112.40
13	w2	201	CYC	CMB-C2B-C1B	2.51	127.21	124.16
13	D3	201	CYC	CMB-C2B-C1B	2.51	127.21	124.16
13	a3	201	CYC	CHB-C4A-C3A	2.51	131.31	124.87
13	C1	201	CYC	CMA-C3A-C4A	2.51	128.99	125.10
13	22	302	CYC	CHB-C1B-C2B	-2.51	121.97	126.97
13	n2	201	CYC	CHB-C4A-C3A	2.51	131.31	124.87
13	a6	201	CYC	CHB-C4A-C3A	2.51	131.31	124.87
13	32	302	CYC	C2C-C3C-C4C	2.50	105.09	101.34
13	z2	201	CYC	CHB-C4A-NA	-2.50	119.54	124.95
13	Q4	201	CYC	CMA-C3A-C4A	2.50	128.99	125.10
13	52	302	CYC	CHA-C4D-C3D	-2.50	121.84	127.22
13	v2	201	CYC	CHB-C4A-NA	-2.50	119.55	124.95
13	Q2	201	CYC	C1A-NA-C4A	2.50	111.11	106.52
13	p2	201	CYC	CMD-C2D-C1D	2.50	129.25	125.62
13	C1	201	CYC	C1A-NA-C4A	2.50	111.10	106.52
13	X6	201	CYC	C1B-CHB-C4A	-2.50	121.92	128.06
13	P3	202	CYC	C2C-C3C-C4C	2.50	105.08	101.34
13	n2	201	CYC	CHA-C4D-C3D	-2.50	121.85	127.22
13	W6	201	CYC	CHA-C4D-C3D	-2.50	121.85	127.22
13	32	301	CYC	C1B-CHB-C4A	-2.50	121.93	128.06
13	J4	201	CYC	CHA-C4D-C3D	-2.50	121.86	127.22
13	M2	201	CYC	C1A-NA-C4A	2.50	111.10	106.52
13	L3	201	CYC	CHB-C4A-NA	-2.49	119.57	124.95
13	42	301	CYC	CHB-C4A-C3A	2.49	131.28	124.87
13	E1	201	CYC	CMD-C2D-C1D	2.49	129.24	125.62
13	J4	202	CYC	C1A-NA-C4A	2.49	111.09	106.52
13	D6	201	CYC	C1B-CHB-C4A	-2.49	121.94	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L7	201	CYC	C1B-CHB-C4A	-2.49	121.94	128.06
13	C7	201	CYC	C1A-NA-C4A	2.49	111.09	106.52
13	L4	201	CYC	CHB-C4A-NA	-2.49	119.58	124.95
13	N2	802	CYC	C2C-C3C-C4C	2.49	105.06	101.34
13	D7	201	CYC	C1A-NA-C4A	2.49	111.08	106.52
13	F5	201	CYC	C1A-NA-C4A	2.49	111.08	106.52
13	U6	201	CYC	CHA-C4D-C3D	-2.49	121.88	127.22
13	E4	201	CYC	C2C-C1C-NC	-2.49	106.22	108.29
13	h2	201	CYC	CHA-C4D-C3D	-2.49	121.88	127.22
13	C3	201	CYC	C1A-NA-C4A	2.48	111.08	106.52
13	Q7	202	CYC	C3B-C4B-NB	2.48	108.75	106.77
13	C7	201	CYC	CMB-C2B-C1B	2.48	127.17	124.16
13	T4	202	CYC	C3C-C4C-NC	-2.48	104.75	107.94
13	T5	202	CYC	C3C-C4C-NC	-2.47	104.76	107.94
13	Q4	201	CYC	C1A-NA-C4A	2.47	111.06	106.52
13	g2	201	CYC	CHB-C1B-C2B	-2.47	122.04	126.97
13	E3	201	CYC	C1A-NA-C4A	2.47	111.06	106.52
13	T5	201	CYC	C1A-NA-C4A	2.47	111.06	106.52
13	U6	201	CYC	C2C-C3C-C4C	2.47	105.04	101.34
13	l2	201	CYC	OB-C4B-C3B	-2.47	125.44	128.03
13	F2	201	CYC	C2C-C1C-NC	-2.47	106.23	108.29
13	V5	202	CYC	CMB-C2B-C1B	2.47	127.16	124.16
13	X3	201	CYC	C1B-CHB-C4A	-2.47	122.00	128.06
13	T4	202	CYC	C1A-NA-C4A	2.47	111.04	106.52
13	W4	201	CYC	C1A-NA-C4A	2.47	111.04	106.52
13	A1	301	CYC	CHA-C4D-C3D	-2.47	121.92	127.22
13	s2	201	CYC	CHB-C4A-NA	-2.46	119.63	124.95
13	Q3	201	CYC	C1A-NA-C4A	2.46	111.03	106.52
13	Q7	201	CYC	C1A-NA-C4A	2.46	111.03	106.52
13	J6	201	CYC	C1A-NA-C4A	2.46	111.03	106.52
13	J5	201	CYC	CHA-C4D-C3D	-2.46	121.93	127.22
13	I5	201	CYC	CMA-C3A-C4A	2.46	128.91	125.10
13	J1	201	CYC	C1A-NA-C4A	2.45	111.02	106.52
13	T2	201	CYC	CHB-C1B-C2B	-2.45	122.08	126.97
13	T1	202	CYC	C1A-NA-C4A	2.45	111.02	106.52
13	T1	202	CYC	C3C-C4C-NC	-2.45	104.78	107.94
13	M5	201	CYC	C2C-C3C-C4C	2.45	105.01	101.34
13	J6	201	CYC	CHA-C4D-C3D	-2.45	121.95	127.22
13	V1	202	CYC	C2C-C1C-NC	-2.45	106.25	108.29
13	V4	202	CYC	CMB-C2B-C1B	2.45	127.14	124.16
13	U2	201	CYC	CHB-C1B-C2B	-2.45	122.08	126.97
13	e2	201	CYC	CHB-C4A-NA	-2.45	119.66	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q5	202	CYC	C1A-NA-C4A	2.45	111.01	106.52
13	L2	201	CYC	CMB-C2B-C1B	2.45	127.14	124.16
13	T7	202	CYC	C3C-C4C-NC	-2.45	104.79	107.94
13	D7	201	CYC	CMB-C2B-C1B	2.45	127.14	124.16
13	V6	201	CYC	C1A-NA-C4A	2.45	111.01	106.52
13	G5	201	CYC	CMC-C2C-C1C	-2.45	107.13	112.40
13	L5	201	CYC	CHB-C4A-NA	-2.45	119.67	124.95
13	F7	201	CYC	C2C-C1C-NC	-2.45	106.25	108.29
13	c2	801	CYC	C1A-NA-C4A	2.45	111.01	106.52
13	E1	201	CYC	C2C-C1C-NC	-2.44	106.25	108.29
13	m2	201	CYC	CHA-C4D-C3D	-2.44	121.97	127.22
13	G6	201	CYC	CHA-C4D-C3D	-2.44	121.97	127.22
13	a7	202	CYC	C1A-NA-C4A	2.44	111.00	106.52
13	T6	202	CYC	C1A-NA-C4A	2.44	111.00	106.52
13	Q7	201	CYC	C2C-C3C-C4C	2.44	104.99	101.34
13	T5	202	CYC	C1A-NA-C4A	2.44	111.00	106.52
13	Q1	202	CYC	C3B-C4B-NB	2.44	108.71	106.77
13	Q5	201	CYC	C1A-NA-C4A	2.44	110.99	106.52
13	Q4	202	CYC	C1A-NA-C4A	2.44	110.99	106.52
13	N5	201	CYC	C1A-NA-C4A	2.44	110.99	106.52
13	F1	201	CYC	C1A-NA-C4A	2.44	110.99	106.52
13	Q3	202	CYC	C3B-C4B-NB	2.43	108.71	106.77
13	Q4	202	CYC	C3B-C4B-NB	2.43	108.71	106.77
13	L6	201	CYC	CMC-C2C-C1C	-2.43	107.16	112.40
13	N2	801	CYC	CAD-C3D-C4D	2.43	129.63	125.77
13	X3	201	CYC	CHB-C4A-NA	-2.43	119.70	124.95
13	B3	201	CYC	C3C-C4C-NC	-2.43	104.81	107.94
13	M2	201	CYC	CHA-C1A-NA	2.43	129.70	124.60
13	G4	201	CYC	C1A-NA-C4A	2.43	110.97	106.52
13	r2	201	CYC	C3C-C4C-NC	-2.43	104.81	107.94
13	U3	201	CYC	CMA-C3A-C4A	2.43	128.87	125.10
13	M6	201	CYC	CMA-C3A-C4A	2.43	128.87	125.10
13	E1	201	CYC	CMA-C3A-C4A	2.43	128.87	125.10
13	U6	201	CYC	CMA-C3A-C4A	2.43	128.87	125.10
13	Q6	202	CYC	C3B-C4B-NB	2.43	108.70	106.77
13	X1	201	CYC	C1B-CHB-C4A	-2.43	122.10	128.06
13	O2	201	CYC	C3C-C4C-NC	-2.43	104.82	107.94
13	h2	201	CYC	C3C-C4C-NC	-2.43	104.82	107.94
13	Z7	301	CYC	C3C-C4C-NC	-2.43	104.82	107.94
13	C3	202	CYC	C1A-NA-C4A	2.43	110.97	106.52
13	B4	201	CYC	C1A-NA-C4A	2.42	110.97	106.52
13	A1	301	CYC	CHB-C4A-C3A	2.42	131.10	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q5	202	CYC	C3B-C4B-NB	2.42	108.70	106.77
13	R6	201	CYC	C2C-C3C-C4C	2.42	104.97	101.34
13	E7	201	CYC	C1A-NA-C4A	2.42	110.96	106.52
13	F2	201	CYC	CHB-C1B-C2B	-2.42	122.14	126.97
13	N6	201	CYC	CHA-C4D-C3D	-2.42	122.02	127.22
13	T1	202	CYC	CHA-C4D-C3D	-2.42	122.02	127.22
13	32	302	CYC	CHB-C1B-C2B	-2.42	122.14	126.97
13	C5	202	CYC	C1A-NA-C4A	2.42	110.95	106.52
13	W3	201	CYC	CMA-C3A-C4A	2.42	128.85	125.10
13	Q6	201	CYC	C1A-NA-C4A	2.42	110.95	106.52
13	M1	201	CYC	C2C-C1C-NC	-2.42	106.28	108.29
13	B2	202	CYC	CMD-C2D-C1D	2.42	129.13	125.62
13	J7	201	CYC	C2C-C1C-NC	-2.41	106.28	108.29
13	E5	201	CYC	OB-C4B-C3B	-2.41	125.50	128.03
13	a3	202	CYC	CMA-C3A-C4A	2.41	128.85	125.10
13	F6	202	CYC	C1A-NA-C4A	2.41	110.94	106.52
13	D3	201	CYC	CMA-C3A-C4A	2.41	128.84	125.10
13	22	302	CYC	C2C-C3C-C4C	2.41	104.95	101.34
13	K4	201	CYC	C1A-NA-C4A	2.41	110.94	106.52
13	52	302	CYC	CHB-C1B-C2B	-2.41	122.16	126.97
13	52	301	CYC	CHB-C4A-C3A	2.41	131.06	124.87
13	T3	202	CYC	C1A-NA-C4A	2.41	110.93	106.52
13	F4	202	CYC	C1A-NA-C4A	2.41	110.93	106.52
13	H4	201	CYC	C1A-NA-C4A	2.41	110.93	106.52
13	W5	201	CYC	C1A-NA-C4A	2.41	110.93	106.52
13	h2	201	CYC	CHB-C4A-NA	-2.41	119.76	124.95
13	C5	201	CYC	CMD-C2D-C3D	-2.41	120.52	125.62
13	K4	201	CYC	CHA-C4D-C3D	-2.40	122.05	127.22
13	F5	202	CYC	C1A-NA-C4A	2.40	110.93	106.52
13	k2	201	CYC	C2C-C1C-NC	-2.40	106.28	108.29
13	42	302	CYC	OB-C4B-C3B	-2.40	125.51	128.03
13	V1	201	CYC	CHA-C1A-NA	2.40	129.64	124.60
13	K1	201	CYC	C1A-NA-C4A	2.40	110.93	106.52
13	I6	201	CYC	C1A-NA-C4A	2.40	110.93	106.52
13	T4	201	CYC	C1A-NA-C4A	2.40	110.92	106.52
13	Z5	301	CYC	CHB-C4A-NA	-2.40	119.77	124.95
13	D3	201	CYC	C1A-NA-C4A	2.40	110.92	106.52
13	S2	201	CYC	CHB-C1B-C2B	-2.40	122.18	126.97
13	J3	201	CYC	C1A-NA-C4A	2.40	110.92	106.52
13	W7	201	CYC	CMA-C3A-C4A	2.40	128.82	125.10
13	M6	201	CYC	CMB-C2B-C1B	2.40	127.08	124.16
13	C6	202	CYC	C2C-C1C-NC	-2.40	106.29	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H4	201	CYC	CHA-C4D-C3D	-2.40	122.07	127.22
13	Q2	201	CYC	CHB-C4A-C3A	2.40	131.03	124.87
13	B7	201	CYC	C1A-NA-C4A	2.40	110.91	106.52
13	N4	201	CYC	C1A-NA-C4A	2.39	110.91	106.52
13	k2	201	CYC	CMA-C3A-C4A	2.39	128.81	125.10
13	S3	201	CYC	CHA-C4D-C3D	-2.39	122.08	127.22
13	M5	201	CYC	CHA-C4D-C3D	-2.39	122.09	127.22
13	T7	202	CYC	C1A-NA-C4A	2.39	110.90	106.52
13	z2	201	CYC	CHB-C1B-C2B	-2.39	122.21	126.97
13	E5	201	CYC	CMA-C3A-C4A	2.39	128.81	125.10
13	F7	201	CYC	CMA-C3A-C4A	2.39	128.81	125.10
13	C6	202	CYC	C1A-NA-C4A	2.39	110.89	106.52
13	V6	202	CYC	CMD-C2D-C1D	2.38	129.09	125.62
13	H5	201	CYC	C1A-NA-C4A	2.38	110.89	106.52
13	J7	201	CYC	C1A-NA-C4A	2.38	110.89	106.52
13	o2	801	CYC	C3C-C4C-NC	-2.38	104.87	107.94
13	W1	201	CYC	C1A-NA-C4A	2.38	110.89	106.52
13	R6	201	CYC	CMA-C3A-C4A	2.38	128.80	125.10
13	52	302	CYC	OB-C4B-C3B	-2.38	125.53	128.03
13	T7	201	CYC	C1A-NA-C4A	2.38	110.89	106.52
13	F3	202	CYC	CMA-C3A-C4A	2.38	128.80	125.10
13	L2	201	CYC	C1A-NA-C4A	2.38	110.89	106.52
13	G5	201	CYC	CHA-C4D-C3D	-2.38	122.10	127.22
13	J3	202	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	J4	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	A1	301	CYC	CMD-C2D-C3D	-2.38	120.58	125.62
13	D1	201	CYC	C2C-C1C-NC	-2.38	106.31	108.29
13	V1	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	S7	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	W3	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	K5	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	C4	202	CYC	C2C-C1C-NC	-2.38	106.31	108.29
13	L1	201	CYC	CMC-C2C-C1C	-2.38	107.28	112.40
13	W7	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	G5	201	CYC	C1A-NA-C4A	2.38	110.88	106.52
13	M1	201	CYC	CHA-C4D-C3D	-2.38	122.11	127.22
13	n2	201	CYC	CMC-C2C-C1C	-2.38	107.28	112.40
13	O2	201	CYC	CMD-C2D-C1D	2.37	129.07	125.62
13	E5	201	CYC	CMD-C2D-C1D	2.37	129.07	125.62
13	D5	201	CYC	C2C-C1C-NC	-2.37	106.31	108.29
13	P2	201	CYC	C1B-CHB-C4A	-2.37	122.23	128.06
13	G2	201	CYC	CHB-C4A-NA	-2.37	119.83	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A6	302	CYC	CHB-C1B-C2B	-2.37	122.24	126.97
13	V7	201	CYC	C1A-NA-C4A	2.37	110.87	106.52
13	J1	201	CYC	CHA-C4D-C3D	-2.37	122.12	127.22
13	U7	201	CYC	CMA-C3A-C4A	2.37	128.78	125.10
13	B3	201	CYC	C1A-NA-C4A	2.37	110.87	106.52
13	D1	201	CYC	CHD-C1D-ND	-2.37	119.93	125.29
13	U4	201	CYC	CMA-C3A-C4A	2.37	128.78	125.10
13	I4	201	CYC	C1A-NA-C4A	2.37	110.87	106.52
13	U5	201	CYC	C1A-NA-C4A	2.37	110.86	106.52
13	V4	201	CYC	C1A-NA-C4A	2.37	110.86	106.52
13	m2	201	CYC	C1A-NA-C4A	2.37	110.86	106.52
13	I1	201	CYC	C1A-NA-C4A	2.37	110.86	106.52
13	L6	201	CYC	CHB-C4A-NA	-2.36	119.85	124.95
13	C2	201	CYC	C1A-NA-C4A	2.36	110.86	106.52
13	V4	201	CYC	CHA-C1A-NA	2.36	129.56	124.60
13	J7	201	CYC	CMB-C2B-C1B	2.36	127.03	124.16
13	V5	201	CYC	C1A-NA-C4A	2.36	110.86	106.52
13	V3	202	CYC	C2C-C1C-NC	-2.36	106.32	108.29
13	L3	201	CYC	CHB-C1B-C2B	-2.36	122.26	126.97
13	C1	202	CYC	C2C-C1C-NC	-2.36	106.32	108.29
13	a2	201	CYC	CMA-C3A-C4A	2.36	128.76	125.10
13	M1	201	CYC	CMA-C3A-C4A	2.36	128.76	125.10
13	N5	201	CYC	CMC-C2C-C1C	-2.36	107.32	112.40
13	T7	201	CYC	C3B-C4B-NB	2.36	108.65	106.77
13	A2	202	CYC	C2C-C3C-C4C	2.36	104.87	101.34
13	F3	201	CYC	CMA-C3A-C4A	2.36	128.76	125.10
13	E4	201	CYC	OB-C4B-C3B	-2.36	125.56	128.03
13	R2	201	CYC	CHB-C1B-NB	2.36	131.08	126.06
13	A1	302	CYC	OB-C4B-C3B	-2.35	125.56	128.03
13	C1	201	CYC	CMD-C2D-C3D	-2.35	120.63	125.62
13	Q3	201	CYC	CMA-C3A-C4A	2.35	128.75	125.10
13	J3	201	CYC	CMD-C2D-C3D	-2.35	120.63	125.62
13	E6	201	CYC	OB-C4B-C3B	-2.35	125.56	128.03
13	N6	201	CYC	C1A-NA-C4A	2.35	110.83	106.52
13	C6	201	CYC	CMD-C2D-C3D	-2.35	120.64	125.62
13	K5	201	CYC	CMC-C2C-C1C	-2.35	107.33	112.40
13	F4	201	CYC	C1A-NA-C4A	2.35	110.83	106.52
13	V6	202	CYC	CMB-C2B-C1B	2.35	127.02	124.16
13	C4	202	CYC	C1A-NA-C4A	2.35	110.83	106.52
13	E2	201	CYC	CHB-C4A-NA	-2.35	119.88	124.95
13	Q3	202	CYC	C1A-NA-C4A	2.35	110.83	106.52
13	G1	201	CYC	C1A-NA-C4A	2.35	110.83	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	42	302	CYC	CHB-C1B-C2B	-2.35	122.29	126.97
13	L3	201	CYC	CHD-C1D-C2D	2.35	133.28	127.53
13	T3	201	CYC	C1A-NA-C4A	2.35	110.83	106.52
13	l2	201	CYC	CMC-C2C-C1C	-2.35	107.34	112.40
13	D5	201	CYC	CHD-C1D-ND	-2.35	119.99	125.29
13	E4	201	CYC	CMD-C2D-C1D	2.35	129.03	125.62
13	N1	201	CYC	C1A-NA-C4A	2.35	110.82	106.52
13	B6	201	CYC	C1A-NA-C4A	2.35	110.82	106.52
13	R6	201	CYC	C1A-NA-C4A	2.35	110.82	106.52
13	P1	202	CYC	CMA-C3A-C4A	2.34	128.74	125.10
13	D1	201	CYC	CHB-C4A-C3A	2.34	130.89	124.87
13	J7	202	CYC	C2C-C1C-NC	-2.34	106.33	108.29
13	D1	201	CYC	CHD-C1D-C2D	2.34	133.27	127.53
13	J4	202	CYC	C2C-C1C-NC	-2.34	106.34	108.29
13	K5	201	CYC	C3C-C4C-NC	-2.34	104.93	107.94
13	I5	201	CYC	C1A-NA-C4A	2.34	110.81	106.52
13	J3	201	CYC	C2C-C1C-NC	-2.34	106.34	108.29
13	C7	202	CYC	C1A-NA-C4A	2.34	110.81	106.52
13	E5	201	CYC	C3B-C4B-NB	2.34	108.63	106.77
13	V1	202	CYC	CMB-C2B-C1B	2.34	127.00	124.16
13	J3	202	CYC	C2C-C1C-NC	-2.33	106.34	108.29
13	F6	201	CYC	CAD-C3D-C2D	-2.33	121.84	127.07
13	M5	201	CYC	CMB-C2B-C1B	2.33	127.00	124.16
13	E1	201	CYC	OB-C4B-C3B	-2.33	125.58	128.03
13	m2	201	CYC	CMC-C2C-C1C	-2.33	107.38	112.40
13	G6	201	CYC	CMC-C2C-C1C	-2.33	107.38	112.40
13	J1	201	CYC	C2C-C1C-NC	-2.33	106.35	108.29
13	S3	201	CYC	C1A-NA-C4A	2.33	110.79	106.52
13	J5	201	CYC	CMB-C2B-C1B	2.33	126.99	124.16
13	F1	202	CYC	C1A-NA-C4A	2.33	110.79	106.52
13	G6	201	CYC	C1A-NA-C4A	2.33	110.79	106.52
13	M2	201	CYC	CHB-C4A-C3A	2.33	130.85	124.87
13	T3	201	CYC	C3B-C4B-NB	2.33	108.62	106.77
13	T6	201	CYC	CMD-C2D-C1D	2.33	129.00	125.62
13	v2	201	CYC	CHB-C1B-C2B	-2.33	122.33	126.97
13	G3	201	CYC	C1A-NA-C4A	2.33	110.79	106.52
13	F6	202	CYC	C3B-C4B-NB	2.33	108.62	106.77
13	C3	201	CYC	CMD-C2D-C3D	-2.33	120.69	125.62
13	a1	201	CYC	CHA-C4D-C3D	-2.32	122.22	127.22
13	P7	202	CYC	CMD-C2D-C1D	2.32	129.00	125.62
13	H6	201	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	C7	201	CYC	C2C-C3C-C4C	2.32	104.82	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K6	201	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	k2	201	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	W1	201	CYC	CHA-C1A-NA	2.32	129.47	124.60
13	I3	201	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	J7	202	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	K7	201	CYC	C1A-NA-C4A	2.32	110.78	106.52
13	R1	201	CYC	CMA-C3A-C4A	2.32	128.70	125.10
13	V6	202	CYC	C2C-C1C-NC	-2.32	106.36	108.29
13	Z1	301	CYC	CHB-C4A-NA	-2.32	119.94	124.95
13	H1	201	CYC	C1A-NA-C4A	2.32	110.77	106.52
13	E6	201	CYC	C3B-C4B-NB	2.32	108.61	106.77
13	42	302	CYC	CHA-C1A-NA	2.32	129.46	124.60
13	W6	201	CYC	C1A-NA-C4A	2.32	110.77	106.52
13	F3	202	CYC	C1A-NA-C4A	2.31	110.77	106.52
13	J5	202	CYC	C2C-C1C-NC	-2.31	106.36	108.29
13	G7	201	CYC	C2C-C1C-NC	-2.31	106.36	108.29
13	S1	201	CYC	C3C-C4C-NC	-2.31	104.96	107.94
13	L7	201	CYC	CHB-C4A-NA	-2.31	119.96	124.95
13	J1	202	CYC	C2C-C1C-NC	-2.31	106.36	108.29
13	J4	201	CYC	CMD-C2D-C3D	-2.31	120.72	125.62
13	E6	201	CYC	C2C-C1C-NC	-2.31	106.36	108.29
13	D2	201	CYC	CHB-C4A-NA	-2.31	119.97	124.95
13	S7	201	CYC	CHA-C4D-C3D	-2.31	122.26	127.22
13	J3	201	CYC	CHA-C4D-C3D	-2.31	122.26	127.22
13	B5	201	CYC	C1A-NA-C4A	2.31	110.75	106.52
13	V3	202	CYC	CMB-C2B-C1B	2.31	126.96	124.16
13	R2	201	CYC	C3C-C4C-NC	-2.31	104.97	107.94
13	N2	801	CYC	CHB-C1B-C2B	-2.31	122.37	126.97
13	G4	201	CYC	CHA-C4D-C3D	-2.31	122.26	127.22
13	R3	201	CYC	CMA-C3A-C4A	2.31	128.68	125.10
13	C4	201	CYC	CMA-C3A-C4A	2.31	128.68	125.10
13	L7	201	CYC	CHB-C1B-C2B	-2.31	122.37	126.97
13	r2	201	CYC	CHB-C1B-C2B	-2.30	122.37	126.97
13	U5	201	CYC	CHA-C4D-C3D	-2.30	122.27	127.22
13	G2	201	CYC	CHA-C4D-ND	2.30	130.50	125.29
13	E4	201	CYC	C3B-C4B-NB	2.30	108.60	106.77
13	w2	201	CYC	CHA-C4D-C3D	-2.30	122.27	127.22
13	R5	201	CYC	C3B-C4B-NB	2.30	108.60	106.77
13	I7	201	CYC	C1A-NA-C4A	2.30	110.74	106.52
13	N7	201	CYC	C1A-NA-C4A	2.30	110.74	106.52
13	P6	202	CYC	CMB-C2B-C1B	2.30	126.96	124.16
13	X1	201	CYC	CHA-C4D-C3D	-2.30	122.27	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D5	201	CYC	CHD-C1D-C2D	2.30	133.17	127.53
13	C4	201	CYC	CMD-C2D-C3D	-2.30	120.75	125.62
13	F2	201	CYC	CHB-C4A-NA	-2.30	119.99	124.95
13	R7	201	CYC	C3B-C4B-NB	2.30	108.60	106.77
13	C6	202	CYC	CMA-C3A-C4A	2.30	128.67	125.10
13	B7	201	CYC	C3C-C4C-NC	-2.30	104.98	107.94
13	J6	201	CYC	C2C-C1C-NC	-2.30	106.37	108.29
13	s2	201	CYC	C3C-C4C-NC	-2.30	104.98	107.94
13	S5	201	CYC	C3C-C4C-NC	-2.30	104.98	107.94
13	U4	201	CYC	CHA-C4D-C3D	-2.30	122.28	127.22
13	U6	201	CYC	C1A-NA-C4A	2.30	110.73	106.52
13	Q7	202	CYC	C1A-NA-C4A	2.30	110.73	106.52
13	R6	201	CYC	C3B-C4B-NB	2.30	108.60	106.77
13	J4	201	CYC	CMB-C2B-C1B	2.30	126.95	124.16
13	H3	201	CYC	C1A-NA-C4A	2.30	110.73	106.52
13	K3	201	CYC	C1A-NA-C4A	2.30	110.73	106.52
13	M4	201	CYC	C2C-C3C-C4C	2.29	104.78	101.34
13	Q7	202	CYC	CMA-C3A-C4A	2.29	128.66	125.10
13	V5	202	CYC	C2C-C1C-NC	-2.29	106.38	108.29
13	W1	201	CYC	C2C-C1C-NC	-2.29	106.38	108.29
13	R1	201	CYC	C1A-NA-C4A	2.29	110.72	106.52
13	a7	201	CYC	CHB-C4A-C3A	2.29	130.75	124.87
13	h2	201	CYC	CHB-C1B-C2B	-2.29	122.40	126.97
13	V2	201	CYC	CMB-C2B-C1B	2.29	126.94	124.16
13	K3	201	CYC	CHA-C4D-C3D	-2.29	122.30	127.22
13	T1	201	CYC	C3B-C4B-NB	2.29	108.59	106.77
13	G7	201	CYC	C1A-NA-C4A	2.29	110.71	106.52
13	M1	201	CYC	CHA-C1A-NA	2.29	129.40	124.60
13	P5	202	CYC	CMB-C2B-C1B	2.29	126.94	124.16
13	M6	201	CYC	C2C-C1C-NC	-2.28	106.38	108.29
13	F7	201	CYC	C1A-NA-C4A	2.28	110.71	106.52
13	T6	201	CYC	CMA-C3A-C4A	2.28	128.65	125.10
13	V3	201	CYC	C1A-NA-C4A	2.28	110.71	106.52
13	M5	201	CYC	C1A-NA-C4A	2.28	110.70	106.52
13	B2	202	CYC	CHB-C1B-C2B	-2.28	122.42	126.97
13	M2	201	CYC	CHA-C4D-C3D	-2.28	122.32	127.22
13	M6	201	CYC	C1A-NA-C4A	2.28	110.70	106.52
13	P4	201	CYC	CMB-C2B-C1B	2.28	126.93	124.16
13	M4	201	CYC	C1A-NA-C4A	2.28	110.70	106.52
13	L7	201	CYC	CHD-C1D-C2D	2.28	133.12	127.53
13	l2	201	CYC	CHB-C1B-NB	2.28	130.92	126.06
13	M1	201	CYC	CMD-C2D-C3D	-2.28	120.79	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N3	201	CYC	C1A-NA-C4A	2.28	110.70	106.52
13	C5	202	CYC	CMA-C3A-C4A	2.28	128.64	125.10
13	e2	201	CYC	OB-C4B-C3B	-2.28	125.64	128.03
13	T6	201	CYC	C3B-C4B-NB	2.28	108.58	106.77
13	C6	201	CYC	CMA-C3A-C4A	2.28	128.64	125.10
13	J6	202	CYC	C2C-C1C-NC	-2.28	106.39	108.29
13	E3	201	CYC	CMB-C2B-C1B	2.28	126.93	124.16
13	J3	201	CYC	CMB-C2B-C1B	2.28	126.93	124.16
13	B2	202	CYC	C1A-NA-C4A	2.28	110.69	106.52
13	d2	201	CYC	C1A-NA-C4A	2.28	110.69	106.52
13	m2	201	CYC	CMB-C2B-C1B	2.27	126.92	124.16
13	N5	201	CYC	CHA-C4D-C3D	-2.27	122.33	127.22
13	M4	201	CYC	CMB-C2B-C1B	2.27	126.92	124.16
13	a6	202	CYC	C3B-C4B-NB	2.27	108.58	106.77
13	D3	201	CYC	CMD-C2D-C1D	2.27	128.92	125.62
13	A1	302	CYC	CHB-C1B-C2B	-2.27	122.44	126.97
13	l2	201	CYC	CHA-C4D-C3D	-2.27	122.34	127.22
13	s2	201	CYC	C3B-C4B-NB	2.27	108.58	106.77
13	R4	201	CYC	C3B-C4B-NB	2.27	108.58	106.77
13	R1	201	CYC	C3B-C4B-NB	2.27	108.58	106.77
13	F5	202	CYC	C3B-C4B-NB	2.27	108.58	106.77
13	H7	201	CYC	C1A-NA-C4A	2.27	110.68	106.52
13	H3	201	CYC	CHA-C4D-C3D	-2.27	122.34	127.22
13	B6	201	CYC	CHA-C4D-C3D	-2.27	122.34	127.22
13	A1	302	CYC	CHA-C1A-NA	2.27	129.36	124.60
13	n2	201	CYC	CMB-C2B-C1B	2.27	126.92	124.16
13	K7	201	CYC	CHA-C4D-C3D	-2.27	122.35	127.22
13	A2	202	CYC	C1A-NA-C4A	2.27	110.68	106.52
13	T5	202	CYC	CHA-C4D-C3D	-2.27	122.35	127.22
13	V3	201	CYC	CHA-C1A-NA	2.27	129.36	124.60
13	J7	201	CYC	CMD-C2D-C3D	-2.27	120.82	125.62
13	V7	202	CYC	CMB-C2B-C1B	2.26	126.91	124.16
13	F7	202	CYC	C1A-NA-C4A	2.26	110.67	106.52
13	A1	301	CYC	CMB-C2B-C1B	2.26	126.91	124.16
13	V1	201	CYC	CHA-C4D-C3D	-2.26	122.36	127.22
13	U7	201	CYC	C1A-NA-C4A	2.26	110.67	106.52
13	a4	202	CYC	C3B-C4B-NB	2.26	108.57	106.77
13	B1	201	CYC	C1A-NA-C4A	2.26	110.67	106.52
13	J6	201	CYC	CMD-C2D-C3D	-2.26	120.83	125.62
13	U3	201	CYC	C1A-NA-C4A	2.26	110.67	106.52
13	S5	201	CYC	C1A-NA-C4A	2.26	110.67	106.52
13	M6	201	CYC	CHA-C4D-C3D	-2.26	122.36	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l2	201	CYC	C3C-C4C-NC	-2.26	105.03	107.94
13	M4	201	CYC	CHA-C4D-C3D	-2.26	122.36	127.22
13	T6	202	CYC	CHA-C4D-C3D	-2.26	122.36	127.22
13	n2	201	CYC	CHA-C1A-NA	2.26	129.34	124.60
13	P2	201	CYC	CHD-C1D-C2D	2.26	133.06	127.53
13	V4	202	CYC	C1A-NA-C4A	2.26	110.66	106.52
13	V4	202	CYC	CMD-C2D-C1D	2.26	128.90	125.62
13	V7	202	CYC	C2C-C1C-NC	-2.26	106.41	108.29
13	F3	201	CYC	C1A-NA-C4A	2.26	110.66	106.52
13	d2	201	CYC	CMA-C3A-C4A	2.26	128.60	125.10
13	V4	202	CYC	C2C-C1C-NC	-2.25	106.41	108.29
13	R1	201	CYC	OB-C4B-C3B	-2.25	125.66	128.03
13	J3	202	CYC	C3B-C4B-NB	2.25	108.56	106.77
13	D2	201	CYC	CHB-C1B-C2B	-2.25	122.48	126.97
13	R6	201	CYC	OB-C4B-C3B	-2.25	125.67	128.03
13	L1	201	CYC	CHD-C1D-C2D	2.25	133.05	127.53
13	E2	201	CYC	C3C-C4C-NC	-2.25	105.04	107.94
13	B2	201	CYC	CMB-C2B-C1B	2.25	126.90	124.16
13	Q1	201	CYC	CHA-C4D-C3D	-2.25	122.38	127.22
13	S1	201	CYC	C1A-NA-C4A	2.25	110.65	106.52
13	F5	201	CYC	C4D-C3D-C2D	-2.25	105.00	107.62
13	A2	201	CYC	C1B-CHB-C4A	-2.25	122.53	128.06
13	a1	201	CYC	CMD-C2D-C3D	-2.25	120.85	125.62
13	V1	202	CYC	C1A-NA-C4A	2.25	110.65	106.52
13	R2	201	CYC	C3B-C4B-NB	2.25	108.56	106.77
13	J7	202	CYC	C3B-C4B-NB	2.25	108.56	106.77
13	F7	202	CYC	CMA-C3A-C4A	2.25	128.59	125.10
13	a5	202	CYC	CHB-C4A-C3A	2.25	130.65	124.87
13	R4	201	CYC	C1A-NA-C4A	2.25	110.64	106.52
13	a7	202	CYC	C3B-C4B-NB	2.25	108.56	106.77
13	F3	201	CYC	CAD-C3D-C4D	2.25	129.34	125.77
13	J6	201	CYC	CMB-C2B-C1B	2.25	126.89	124.16
13	O2	201	CYC	C1B-CHB-C4A	-2.25	122.54	128.06
13	I1	201	CYC	CHA-C4D-C3D	-2.25	122.39	127.22
13	Q6	201	CYC	CHA-C4D-C3D	-2.25	122.39	127.22
13	M5	201	CYC	C2C-C1C-NC	-2.25	106.42	108.29
13	O2	201	CYC	CHA-C1A-NA	2.25	129.31	124.60
13	22	302	CYC	CHB-C1B-NB	2.24	130.85	126.06
13	U6	201	CYC	C2C-C1C-NC	-2.24	106.42	108.29
13	E3	201	CYC	C3B-C4B-NB	2.24	108.55	106.77
13	e2	201	CYC	CHB-C1B-NB	2.24	130.84	126.06
13	J3	202	CYC	OB-C4B-C3B	-2.24	125.68	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C5	202	CYC	C2C-C1C-NC	-2.24	106.42	108.29
13	H7	201	CYC	CHA-C4D-C3D	-2.24	122.41	127.22
13	G2	201	CYC	CHB-C1B-C2B	-2.24	122.50	126.97
13	I3	201	CYC	CHA-C4D-C3D	-2.24	122.41	127.22
13	R4	201	CYC	CMA-C3A-C4A	2.24	128.58	125.10
13	R5	201	CYC	CMA-C3A-C4A	2.24	128.57	125.10
13	S6	201	CYC	C1A-NA-C4A	2.24	110.62	106.52
13	I5	201	CYC	CHA-C4D-C3D	-2.24	122.41	127.22
13	v2	201	CYC	OB-C4B-C3B	-2.24	125.68	128.03
13	S4	201	CYC	C1A-NA-C4A	2.24	110.62	106.52
13	E7	201	CYC	CMB-C2B-C1B	2.24	126.88	124.16
13	V3	202	CYC	C1A-NA-C4A	2.24	110.62	106.52
13	V5	202	CYC	C1A-NA-C4A	2.24	110.62	106.52
13	F4	202	CYC	C3B-C4B-NB	2.24	108.55	106.77
13	T5	201	CYC	C3B-C4B-NB	2.24	108.55	106.77
13	M7	201	CYC	C1A-NA-C4A	2.23	110.62	106.52
13	Q7	201	CYC	CMA-C3A-C4A	2.23	128.57	125.10
13	V6	202	CYC	C1A-NA-C4A	2.23	110.62	106.52
13	T4	201	CYC	C3B-C4B-NB	2.23	108.55	106.77
13	L4	201	CYC	CHD-C1D-C2D	2.23	133.00	127.53
13	M3	201	CYC	OB-C4B-C3B	-2.23	125.69	128.03
13	Z4	301	CYC	C2C-C3C-C4C	2.23	104.68	101.34
13	V5	201	CYC	CHA-C1A-NA	2.23	129.29	124.60
13	52	302	CYC	CHA-C1A-NA	2.23	129.29	124.60
13	V7	201	CYC	CHA-C1A-NA	2.23	129.29	124.60
13	J1	201	CYC	CMD-C2D-C3D	-2.23	120.89	125.62
13	U1	201	CYC	C1A-NA-C4A	2.23	110.61	106.52
13	V6	201	CYC	CHA-C1A-NA	2.23	129.28	124.60
13	x2	201	CYC	CMB-C2B-C1B	2.23	126.87	124.16
13	Z4	301	CYC	CHB-C4A-NA	-2.23	120.14	124.95
13	A1	302	CYC	CHA-C4D-ND	2.23	130.32	125.29
13	V5	201	CYC	CHA-C4D-C3D	-2.23	122.43	127.22
13	k2	201	CYC	C3B-C4B-NB	2.23	108.54	106.77
13	M1	201	CYC	C1A-NA-C4A	2.23	110.60	106.52
13	A6	302	CYC	CHA-C1A-NA	2.23	129.27	124.60
13	C5	201	CYC	C2C-C3C-C4C	2.23	104.67	101.34
13	W4	201	CYC	CHA-C4D-C3D	-2.23	122.44	127.22
13	U4	201	CYC	C1A-NA-C4A	2.22	110.60	106.52
13	N4	201	CYC	CHA-C4D-C3D	-2.22	122.44	127.22
13	a5	202	CYC	OB-C4B-C3B	-2.22	125.69	128.03
13	R3	201	CYC	C3B-C4B-NB	2.22	108.54	106.77
13	c2	801	CYC	CMB-C2B-C1B	2.22	126.86	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K4	201	CYC	CMC-C2C-C1C	-2.22	107.61	112.40
13	F1	202	CYC	C3B-C4B-NB	2.22	108.54	106.77
13	s2	201	CYC	CHB-C1B-C2B	-2.22	122.54	126.97
13	X6	201	CYC	CHA-C4D-C3D	-2.22	122.45	127.22
13	y2	201	CYC	C1B-CHB-C4A	-2.22	122.61	128.06
13	R3	201	CYC	OB-C4B-C3B	-2.22	125.70	128.03
13	G6	201	CYC	C3B-C4B-NB	2.22	108.53	106.77
13	P2	201	CYC	CHB-C1B-C2B	-2.22	122.55	126.97
13	E5	201	CYC	CMB-C2B-C1B	2.22	126.86	124.16
13	V4	201	CYC	CHA-C4D-C3D	-2.22	122.45	127.22
13	a3	202	CYC	C3B-C4B-NB	2.22	108.53	106.77
13	M3	201	CYC	C1A-NA-C4A	2.22	110.58	106.52
13	V1	201	CYC	CMB-C2B-C1B	2.22	126.85	124.16
13	i2	201	CYC	C3B-C4B-NB	2.22	108.53	106.77
13	j2	201	CYC	O2A-CGA-CBA	2.21	121.00	114.00
13	E7	201	CYC	C3B-C4B-NB	2.21	108.53	106.77
13	a6	202	CYC	CHB-C4A-C3A	2.21	130.56	124.87
13	I7	201	CYC	CHA-C4D-C3D	-2.21	122.46	127.22
13	S6	201	CYC	CHA-C1A-NA	2.21	129.24	124.60
13	Z1	301	CYC	CHD-C1D-C2D	2.21	132.95	127.53
13	22	302	CYC	OB-C4B-C3B	-2.21	125.71	128.03
13	S2	201	CYC	CHD-C1D-C2D	2.21	132.95	127.53
13	J7	202	CYC	OB-C4B-C3B	-2.21	125.71	128.03
13	i2	201	CYC	C1A-NA-C4A	2.21	110.57	106.52
13	D7	201	CYC	CHD-C1D-ND	-2.21	120.30	125.29
13	e2	201	CYC	CHA-C4D-C3D	-2.21	122.47	127.22
13	R4	201	CYC	OB-C4B-C3B	-2.21	125.71	128.03
13	J5	201	CYC	CMD-C2D-C3D	-2.21	120.94	125.62
13	v2	201	CYC	C3C-C4C-NC	-2.21	105.10	107.94
13	V2	201	CYC	CHD-C1D-C2D	2.21	132.94	127.53
13	D7	201	CYC	CHD-C1D-C2D	2.21	132.94	127.53
13	E6	201	CYC	CMB-C2B-C1B	2.21	126.84	124.16
13	Q5	201	CYC	CHA-C4D-C3D	-2.21	122.48	127.22
13	X5	201	CYC	CHB-C4A-NA	-2.21	120.19	124.95
13	R3	201	CYC	CHA-C4D-C3D	-2.21	122.48	127.22
13	T1	201	CYC	CMA-C3A-C4A	2.21	128.53	125.10
13	M3	201	CYC	C3B-C4B-NB	2.20	108.52	106.77
13	Z7	301	CYC	CHB-C4A-C3A	2.20	130.53	124.87
13	f2	201	CYC	CHB-C1B-NB	2.20	130.76	126.06
13	a5	202	CYC	C3B-C4B-NB	2.20	108.52	106.77
13	V2	201	CYC	CMD-C2D-C3D	-2.20	120.96	125.62
13	V7	202	CYC	C1A-NA-C4A	2.20	110.56	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U7	201	CYC	C2C-C1C-NC	-2.20	106.46	108.29
13	Z6	301	CYC	CHB-C4A-NA	-2.20	120.21	124.95
13	Q5	202	CYC	CHA-C4D-C3D	-2.20	122.50	127.22
13	N1	201	CYC	C2C-C1C-NC	-2.20	106.46	108.29
13	N2	802	CYC	CHB-C1B-NB	2.20	130.74	126.06
13	J1	201	CYC	CMB-C2B-C1B	2.20	126.83	124.16
13	p2	201	CYC	CHB-C4A-NA	-2.20	120.21	124.95
13	R3	201	CYC	C1A-NA-C4A	2.19	110.54	106.52
13	F7	202	CYC	C3B-C4B-NB	2.19	108.52	106.77
13	C2	201	CYC	OB-C4B-C3B	-2.19	125.73	128.03
13	C2	201	CYC	CMB-C2B-C1B	2.19	126.83	124.16
13	Z5	301	CYC	CHD-C1D-C2D	2.19	132.90	127.53
13	I1	201	CYC	C3B-C4B-NB	2.19	108.51	106.77
13	E1	201	CYC	CMB-C2B-C1B	2.19	126.82	124.16
13	Q6	201	CYC	CHA-C1A-NA	2.19	129.20	124.60
13	a4	202	CYC	CHB-C4A-C3A	2.19	130.50	124.87
13	V3	201	CYC	CHA-C4D-C3D	-2.19	122.52	127.22
13	p2	201	CYC	CHA-C4D-ND	2.19	130.24	125.29
13	e2	201	CYC	C3C-C4C-NC	-2.19	105.12	107.94
13	N3	201	CYC	CHA-C4D-C3D	-2.19	122.52	127.22
13	R5	201	CYC	C1A-NA-C4A	2.19	110.53	106.52
13	32	302	CYC	OB-C4B-C3B	-2.19	125.73	128.03
13	x2	201	CYC	C3C-C4C-NC	-2.19	105.13	107.94
13	N2	801	CYC	CHB-C4A-NA	-2.18	120.23	124.95
13	d2	201	CYC	CMB-C2B-C1B	2.18	126.81	124.16
13	R7	201	CYC	OB-C4B-C3B	-2.18	125.74	128.03
13	D1	201	CYC	CMC-C2C-C1C	-2.18	107.70	112.40
13	Q3	202	CYC	CMA-C3A-C4A	2.18	128.49	125.10
13	V5	202	CYC	CMA-C3A-C4A	2.18	128.49	125.10
13	Q1	202	CYC	CHB-C4A-C3A	2.18	130.47	124.87
13	S3	201	CYC	C3C-C4C-NC	-2.18	105.13	107.94
13	P2	201	CYC	CMD-C2D-C3D	-2.18	121.00	125.62
13	i2	201	CYC	CHD-C1D-C2D	2.18	132.87	127.53
13	T1	201	CYC	CMB-C2B-C1B	2.18	126.81	124.16
13	J1	202	CYC	CMB-C2B-C1B	2.18	126.81	124.16
13	L2	201	CYC	CHA-C4D-C3D	-2.18	122.54	127.22
13	G2	201	CYC	C2C-C3C-C4C	2.18	104.60	101.34
13	H2	201	CYC	CMB-C2B-C1B	2.18	126.81	124.16
13	32	302	CYC	CHB-C1B-NB	2.18	130.70	126.06
13	C4	202	CYC	CMA-C3A-C4A	2.18	128.48	125.10
13	Q4	201	CYC	CHA-C1A-NA	2.18	129.17	124.60
13	k2	201	CYC	CAB-C3B-C4B	2.18	124.74	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R1	201	CYC	CHA-C4D-C3D	-2.18	122.54	127.22
13	F3	202	CYC	C3B-C4B-NB	2.18	108.50	106.77
13	W5	201	CYC	CMB-C2B-C1B	2.18	126.81	124.16
13	J5	201	CYC	CHA-C1A-NA	2.18	129.17	124.60
13	D4	201	CYC	CHD-C1D-ND	-2.18	120.38	125.29
13	F4	201	CYC	C3B-C4B-NB	2.18	108.50	106.77
13	L3	201	CYC	C1B-CHB-C4A	-2.18	122.72	128.06
13	52	301	CYC	CMB-C2B-C1B	2.17	126.80	124.16
13	F2	201	CYC	CHA-C4D-C3D	-2.17	122.55	127.22
13	f2	201	CYC	C3B-C4B-NB	2.17	108.50	106.77
13	C4	202	CYC	C3B-C4B-NB	2.17	108.50	106.77
13	D5	201	CYC	CHB-C4A-C3A	2.17	130.46	124.87
13	p2	201	CYC	CHA-C1A-NA	2.17	129.16	124.60
13	Z4	301	CYC	CHD-C1D-C2D	2.17	132.85	127.53
13	P1	202	CYC	CHA-C1A-NA	2.17	129.16	124.60
13	S2	201	CYC	O2A-CGA-CBA	2.17	120.86	114.00
13	x2	201	CYC	CHB-C4A-C3A	2.17	130.45	124.87
13	a6	201	CYC	CMD-C2D-C3D	-2.17	121.02	125.62
13	S5	201	CYC	CHA-C1A-NA	2.17	129.16	124.60
13	G3	201	CYC	CHA-C4D-C3D	-2.17	122.55	127.22
13	A6	301	CYC	CMD-C2D-C3D	-2.17	121.02	125.62
13	X5	201	CYC	CHA-C4D-C3D	-2.17	122.56	127.22
13	S4	201	CYC	C3C-C4C-NC	-2.17	105.15	107.94
13	P5	202	CYC	CMA-C3A-C4A	2.17	128.47	125.10
13	J6	202	CYC	CMB-C2B-C1B	2.17	126.80	124.16
13	Z5	301	CYC	CHA-C4D-C3D	-2.17	122.56	127.22
13	L3	201	CYC	CHD-C1D-ND	-2.17	120.39	125.29
13	P1	202	CYC	CMB-C2B-C1B	2.17	126.80	124.16
13	Q3	202	CYC	C3C-C4C-NC	-2.17	105.15	107.94
13	S6	201	CYC	C3C-C4C-NC	-2.17	105.15	107.94
13	C2	201	CYC	CMA-C3A-C4A	2.17	128.46	125.10
13	C5	202	CYC	C3B-C4B-NB	2.17	108.49	106.77
13	N7	201	CYC	C3B-C4B-NB	2.17	108.49	106.77
13	F1	201	CYC	C4D-C3D-C2D	-2.17	105.10	107.62
13	V7	201	CYC	CMB-C2B-C1B	2.16	126.79	124.16
13	G1	201	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	H2	201	CYC	C1A-NA-C4A	2.16	110.49	106.52
13	J1	202	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	G4	201	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	g2	201	CYC	C1B-CHB-C4A	-2.16	122.75	128.06
13	a1	201	CYC	CHA-C1A-NA	2.16	129.14	124.60
13	C6	201	CYC	CHD-C1D-C2D	2.16	132.83	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D5	201	CYC	CMB-C2B-C1B	2.16	126.79	124.16
13	V4	202	CYC	CMA-C3A-C4A	2.16	128.46	125.10
13	G4	201	CYC	CMC-C2C-C1C	-2.16	107.75	112.40
13	k2	201	CYC	OB-C4B-C3B	-2.16	125.76	128.03
13	C3	202	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	C6	202	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	M3	201	CYC	CMB-C2B-C1B	2.16	126.78	124.16
13	B3	201	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	N5	201	CYC	C3B-C4B-NB	2.16	108.49	106.77
13	D4	201	CYC	CHD-C1D-C2D	2.16	132.81	127.53
13	C5	202	CYC	CMB-C2B-C1B	2.16	126.78	124.16
13	E1	201	CYC	C3B-C4B-NB	2.16	108.48	106.77
13	F4	202	CYC	OB-C4B-C3B	-2.16	125.77	128.03
13	D5	201	CYC	CMC-C2C-C1C	-2.15	107.76	112.40
13	g2	201	CYC	CHA-C4D-C3D	-2.15	122.59	127.22
13	C4	202	CYC	OB-C4B-C3B	-2.15	125.77	128.03
13	F5	202	CYC	OB-C4B-C3B	-2.15	125.77	128.03
13	T2	201	CYC	CHD-C1D-C2D	2.15	132.81	127.53
13	Z1	301	CYC	C2C-C3C-C4C	2.15	104.56	101.34
13	y2	201	CYC	CHA-C4D-C3D	-2.15	122.59	127.22
13	a1	202	CYC	CHB-C4A-C3A	2.15	130.40	124.87
13	S7	201	CYC	C3C-C4C-NC	-2.15	105.17	107.94
13	a3	202	CYC	CMD-C2D-C1D	2.15	128.75	125.62
13	R5	201	CYC	CHA-C4D-C3D	-2.15	122.59	127.22
13	Z1	301	CYC	CHA-C4D-C3D	-2.15	122.59	127.22
13	Z6	301	CYC	CHA-C4D-C3D	-2.15	122.59	127.22
13	r2	201	CYC	CHB-C4A-NA	-2.15	120.31	124.95
13	X4	201	CYC	CHA-C4D-C3D	-2.15	122.60	127.22
13	Z6	301	CYC	C2C-C3C-C4C	2.15	104.56	101.34
13	C1	201	CYC	CHD-C1D-C2D	2.15	132.80	127.53
13	F5	201	CYC	C3B-C4B-NB	2.15	108.48	106.77
13	Q2	201	CYC	CMB-C2B-C1B	2.15	126.77	124.16
13	R7	201	CYC	CHA-C4D-C3D	-2.15	122.60	127.22
13	U2	201	CYC	CHD-C1D-C2D	2.15	132.79	127.53
13	G7	201	CYC	CHA-C4D-C3D	-2.15	122.61	127.22
13	B4	201	CYC	CHA-C4D-C3D	-2.15	122.61	127.22
13	D1	201	CYC	CMB-C2B-C1B	2.15	126.77	124.16
13	y2	201	CYC	CHB-C4A-NA	-2.15	120.32	124.95
13	K3	201	CYC	C3B-C4B-NB	2.14	108.48	106.77
13	F7	201	CYC	CAD-C3D-C4D	2.14	129.17	125.77
13	F7	202	CYC	OB-C4B-C3B	-2.14	125.78	128.03
13	N6	201	CYC	C3B-C4B-NB	2.14	108.47	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	p2	201	CYC	CHB-C1B-C2B	-2.14	122.69	126.97
13	U3	201	CYC	CMC-C2C-C1C	-2.14	107.78	112.40
13	L6	201	CYC	CHD-C1D-C2D	2.14	132.78	127.53
13	X1	201	CYC	CHB-C4A-NA	-2.14	120.33	124.95
13	K5	201	CYC	C3B-C4B-NB	2.14	108.47	106.77
13	K3	201	CYC	CMC-C2C-C1C	-2.14	107.79	112.40
13	V6	201	CYC	CMB-C2B-C1B	2.14	126.76	124.16
13	a1	202	CYC	C3B-C4B-NB	2.14	108.47	106.77
13	U2	201	CYC	C3B-C4B-NB	2.14	108.47	106.77
13	L1	201	CYC	CMD-C2D-C3D	-2.14	121.09	125.62
13	Z6	301	CYC	CHD-C1D-C2D	2.14	132.77	127.53
13	V4	202	CYC	OB-C4B-C3B	-2.14	125.79	128.03
13	a6	201	CYC	CMB-C2B-C1B	2.14	126.76	124.16
13	A6	301	CYC	CHD-C1D-C2D	2.14	132.76	127.53
13	K7	201	CYC	C3B-C4B-NB	2.13	108.47	106.77
13	g2	201	CYC	C2C-C1C-NC	-2.13	106.51	108.29
13	M6	201	CYC	CHA-C1A-NA	2.13	129.08	124.60
13	F1	202	CYC	OB-C4B-C3B	-2.13	125.79	128.03
13	I4	201	CYC	CHA-C4D-C3D	-2.13	122.63	127.22
13	M4	201	CYC	C3B-C4B-NB	2.13	108.47	106.77
13	X4	201	CYC	CMB-C2B-C1B	2.13	126.75	124.16
13	Q5	201	CYC	CHA-C1A-NA	2.13	129.08	124.60
13	C7	202	CYC	C3B-C4B-NB	2.13	108.47	106.77
13	C7	202	CYC	CMB-C2B-C1B	2.13	126.75	124.16
13	J5	201	CYC	C2C-C3C-C4C	2.13	104.53	101.34
13	S3	201	CYC	C3B-C4B-NB	2.13	108.47	106.77
13	I5	201	CYC	C3B-C4B-NB	2.13	108.47	106.77
13	i2	201	CYC	OB-C4B-C3B	-2.13	125.79	128.03
13	X7	201	CYC	CHD-C1D-C2D	2.13	132.75	127.53
13	U6	201	CYC	CMC-C2C-C1C	-2.13	107.81	112.40
13	X6	201	CYC	CHD-C1D-C2D	2.13	132.75	127.53
13	A1	302	CYC	CMB-C2B-C1B	2.13	126.75	124.16
13	g2	201	CYC	CHB-C1B-NB	2.13	130.60	126.06
13	a1	202	CYC	OB-C4B-C3B	-2.13	125.80	128.03
13	X5	201	CYC	CMB-C2B-C1B	2.13	126.74	124.16
13	a7	202	CYC	CMA-C3A-C4A	2.12	128.40	125.10
13	M3	201	CYC	CHA-C1A-NA	2.12	129.06	124.60
13	J7	202	CYC	CMB-C2B-C1B	2.12	126.74	124.16
13	X5	201	CYC	CMD-C2D-C3D	-2.12	121.12	125.62
13	Z5	301	CYC	C2C-C3C-C4C	2.12	104.52	101.34
13	w2	201	CYC	CMC-C2C-C1C	-2.12	107.83	112.40
13	C5	202	CYC	OB-C4B-C3B	-2.12	125.80	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M7	201	CYC	C3B-C4B-NB	2.12	108.46	106.77
13	I6	201	CYC	CHA-C4D-C3D	-2.12	122.66	127.22
13	F6	202	CYC	OB-C4B-C3B	-2.12	125.80	128.03
13	a4	202	CYC	OB-C4B-C3B	-2.12	125.81	128.03
13	A2	202	CYC	C3B-C4B-NB	2.12	108.45	106.77
13	R5	201	CYC	OB-C4B-C3B	-2.12	125.81	128.03
13	32	301	CYC	CMD-C2D-C3D	-2.12	121.13	125.62
13	B4	201	CYC	C3C-C4C-NC	-2.12	105.22	107.94
13	M7	201	CYC	CMB-C2B-C1B	2.12	126.73	124.16
13	C5	201	CYC	CHA-C4D-C3D	-2.12	122.67	127.22
13	K1	201	CYC	C3B-C4B-NB	2.12	108.45	106.77
13	G3	201	CYC	C3B-C4B-NB	2.12	108.45	106.77
13	j2	201	CYC	CMB-C2B-C1B	2.12	126.73	124.16
13	f2	201	CYC	OB-C4B-C3B	-2.12	125.81	128.03
13	C7	201	CYC	CMD-C2D-C3D	-2.12	121.14	125.62
13	U4	201	CYC	CMB-C2B-C1B	2.12	126.73	124.16
13	U4	201	CYC	CMC-C2C-C1C	-2.12	107.84	112.40
13	C1	202	CYC	CMB-C2B-C1B	2.12	126.73	124.16
13	G5	201	CYC	C3B-C4B-NB	2.11	108.45	106.77
13	R7	201	CYC	C1A-NA-C4A	2.11	110.40	106.52
13	X1	201	CYC	CMB-C2B-C1B	2.11	126.73	124.16
13	N1	201	CYC	C3B-C4B-NB	2.11	108.45	106.77
13	T1	201	CYC	CMD-C2D-C1D	2.11	128.69	125.62
13	F4	201	CYC	O2D-CGD-CBD	2.11	120.67	114.00
13	U2	201	CYC	CHD-C1D-ND	-2.11	120.52	125.29
13	C4	202	CYC	CMB-C2B-C1B	2.11	126.73	124.16
13	X6	201	CYC	CHB-C4A-NA	-2.11	120.39	124.95
13	Q1	201	CYC	CHA-C1A-NA	2.11	129.03	124.60
13	52	302	CYC	CHB-C1B-NB	2.11	130.56	126.06
13	L6	201	CYC	CMD-C2D-C3D	-2.11	121.15	125.62
13	T5	201	CYC	CMA-C3A-C4A	2.11	128.38	125.10
13	F3	202	CYC	OB-C4B-C3B	-2.11	125.82	128.03
13	W3	201	CYC	C3B-C4B-NB	2.11	108.45	106.77
13	O2	201	CYC	CHA-C4D-ND	2.11	130.05	125.29
13	P2	201	CYC	CMB-C2B-C1B	2.11	126.72	124.16
13	K5	201	CYC	CHA-C4D-ND	2.11	130.05	125.29
13	W7	201	CYC	C3B-C4B-NB	2.11	108.45	106.77
13	F7	202	CYC	CMB-C2B-C1B	2.11	126.72	124.16
13	h2	201	CYC	CHB-C1B-NB	2.11	130.55	126.06
13	H5	201	CYC	C3B-C4B-NB	2.11	108.44	106.77
13	V7	202	CYC	C3B-C4B-NB	2.11	108.44	106.77
13	F7	201	CYC	O2D-CGD-CBD	2.11	120.65	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N4	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	B7	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	M5	201	CYC	CMD-C2D-C3D	-2.10	121.16	125.62
13	X3	201	CYC	CMB-C2B-C1B	2.10	126.72	124.16
13	l2	201	CYC	CHB-C4A-NA	-2.10	120.41	124.95
13	V2	201	CYC	CHB-C4A-C3A	2.10	130.27	124.87
13	Z1	301	CYC	O2A-CGA-CBA	2.10	120.64	114.00
13	t2	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	S7	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	W2	201	CYC	CHB-C4A-C3A	2.10	130.27	124.87
13	L5	201	CYC	CHD-C1D-C2D	2.10	132.68	127.53
13	J4	202	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	F1	201	CYC	O2D-CGD-CBD	2.10	120.63	114.00
13	X3	201	CYC	CHD-C1D-C2D	2.10	132.67	127.53
13	r2	201	CYC	CMC-C2C-C1C	-2.10	107.88	112.40
13	E4	201	CYC	CMA-C3A-C4A	2.10	128.36	125.10
13	M7	201	CYC	CMD-C2D-C3D	-2.10	121.17	125.62
13	K6	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	v2	201	CYC	CHA-C4D-C3D	-2.10	122.71	127.22
13	T4	201	CYC	CMA-C3A-C4A	2.10	128.36	125.10
13	J5	201	CYC	C2C-C1C-NC	-2.10	106.54	108.29
13	B4	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	H1	201	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	J6	202	CYC	C3B-C4B-NB	2.10	108.44	106.77
13	a6	201	CYC	CHA-C4D-C3D	-2.10	122.72	127.22
13	S1	201	CYC	CHA-C4D-ND	2.10	130.02	125.29
13	R5	201	CYC	C2C-C3C-C4C	2.10	104.48	101.34
13	I4	201	CYC	C3B-C4B-NB	2.09	108.44	106.77
13	N1	201	CYC	CHA-C1A-NA	2.09	128.99	124.60
13	D7	201	CYC	C3B-C4B-NB	2.09	108.44	106.77
13	T2	201	CYC	CHB-C1B-NB	2.09	130.52	126.06
13	a5	202	CYC	CMB-C2B-C1B	2.09	126.70	124.16
13	V6	202	CYC	C2C-C3C-C4C	2.09	104.47	101.34
13	e2	201	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	B6	201	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	F6	201	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	E6	201	CYC	CMD-C2D-C1D	2.09	128.66	125.62
13	s2	201	CYC	CHA-C4D-C3D	-2.09	122.72	127.22
13	N7	201	CYC	CHA-C4D-C3D	-2.09	122.72	127.22
13	A6	302	CYC	CHB-C1B-NB	2.09	130.52	126.06
13	S4	201	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	a3	202	CYC	CMB-C2B-C1B	2.09	126.70	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L7	201	CYC	CHD-C1D-ND	-2.09	120.57	125.29
13	L2	201	CYC	CMC-C2C-C1C	-2.09	107.90	112.40
13	C3	202	CYC	CMB-C2B-C1B	2.09	126.70	124.16
13	S1	201	CYC	CHA-C1A-NA	2.09	128.98	124.60
13	U1	201	CYC	CHA-C1A-NA	2.09	128.98	124.60
13	32	301	CYC	CHD-C1D-C2D	2.09	132.65	127.53
13	M3	201	CYC	CMD-C2D-C3D	-2.09	121.19	125.62
13	X5	201	CYC	CHD-C1D-C2D	2.09	132.65	127.53
13	P1	201	CYC	C3C-C4C-NC	-2.09	105.25	107.94
13	P1	202	CYC	CHD-C1D-C2D	2.09	132.64	127.53
13	r2	201	CYC	O2A-CGA-CBA	2.09	120.59	114.00
13	D3	201	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	V5	202	CYC	C3B-C4B-NB	2.09	108.43	106.77
13	R7	201	CYC	CMA-C3A-C4A	2.09	128.34	125.10
13	D3	201	CYC	OB-C4B-C3B	-2.09	125.84	128.03
13	h2	201	CYC	CHA-C1A-NA	2.09	128.98	124.60
13	A1	302	CYC	C1B-CHB-C4A	-2.09	122.93	128.06
13	42	301	CYC	CMB-C2B-C1B	2.09	126.69	124.16
13	y2	201	CYC	O2D-CGD-CBD	2.09	120.59	114.00
13	v2	201	CYC	CHB-C1B-NB	2.09	130.51	126.06
13	M2	201	CYC	CMB-C2B-C1B	2.08	126.69	124.16
13	42	302	CYC	C1B-CHB-C4A	-2.08	122.94	128.06
13	M7	201	CYC	OB-C4B-C3B	-2.08	125.84	128.03
13	E4	201	CYC	CMB-C2B-C1B	2.08	126.69	124.16
13	J4	202	CYC	CMB-C2B-C1B	2.08	126.69	124.16
13	V3	202	CYC	C3B-C4B-NB	2.08	108.43	106.77
13	J7	201	CYC	CHA-C4D-C3D	-2.08	122.74	127.22
13	E2	201	CYC	CHB-C1B-C2B	-2.08	122.81	126.97
13	M4	201	CYC	CMD-C2D-C3D	-2.08	121.21	125.62
13	a7	202	CYC	CMD-C2D-C1D	2.08	128.65	125.62
13	42	302	CYC	CHB-C1B-NB	2.08	130.50	126.06
13	W2	201	CYC	CHA-C4D-C3D	-2.08	122.75	127.22
13	R4	201	CYC	CHA-C4D-C3D	-2.08	122.75	127.22
13	L6	201	CYC	CHB-C1B-C2B	-2.08	122.82	126.97
13	m2	201	CYC	C3C-C4C-NC	-2.08	105.26	107.94
13	C3	202	CYC	C3C-C4C-NC	-2.08	105.26	107.94
13	D2	201	CYC	CHA-C4D-C3D	-2.08	122.75	127.22
13	X1	201	CYC	CHD-C1D-C2D	2.08	132.63	127.53
13	M6	201	CYC	CMD-C2D-C3D	-2.08	121.21	125.62
13	M1	201	CYC	C3B-C4B-NB	2.08	108.42	106.77
13	V4	202	CYC	C3B-C4B-NB	2.08	108.42	106.77
13	C1	202	CYC	OB-C4B-C3B	-2.08	125.85	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R2	201	CYC	OB-C4B-C3B	-2.08	125.85	128.03
13	i2	201	CYC	CHD-C1D-ND	-2.08	120.59	125.29
13	L4	201	CYC	CHB-C1B-C2B	-2.08	122.82	126.97
13	W1	201	CYC	CMB-C2B-C1B	2.08	126.69	124.16
13	t2	201	CYC	CHD-C1D-C2D	2.08	132.62	127.53
13	M4	201	CYC	OB-C4B-C3B	-2.08	125.85	128.03
13	U3	201	CYC	C3B-C4B-NB	2.08	108.42	106.77
13	i2	201	CYC	C2C-C1C-NC	-2.08	106.56	108.29
13	M4	201	CYC	CMA-C3A-C4A	2.08	128.33	125.10
13	Q1	202	CYC	CHA-C4D-C3D	-2.08	122.75	127.22
13	H2	201	CYC	C3B-C4B-NB	2.08	108.42	106.77
13	H7	201	CYC	C3B-C4B-NB	2.08	108.42	106.77
13	F2	201	CYC	CMC-C2C-C1C	-2.08	107.93	112.40
13	a5	201	CYC	CMD-C2D-C3D	-2.08	121.22	125.62
13	U2	201	CYC	CHB-C1B-NB	2.08	130.49	126.06
13	P1	202	CYC	CHD-C1D-ND	-2.08	120.60	125.29
13	P2	201	CYC	CHA-C4D-C3D	-2.07	122.76	127.22
13	M6	201	CYC	OB-C4B-C3B	-2.07	125.85	128.03
13	Q5	202	CYC	CHA-C1A-NA	2.07	128.95	124.60
13	V6	202	CYC	CMA-C3A-C4A	2.07	128.32	125.10
13	P7	201	CYC	OB-C4B-C3B	-2.07	125.85	128.03
13	W2	201	CYC	CMB-C2B-C1B	2.07	126.68	124.16
13	I7	201	CYC	C3B-C4B-NB	2.07	108.42	106.77
13	U7	201	CYC	C3B-C4B-NB	2.07	108.42	106.77
13	T3	201	CYC	CMB-C2B-C1B	2.07	126.68	124.16
13	a1	201	CYC	CHD-C1D-C2D	2.07	132.60	127.53
13	G7	201	CYC	C3B-C4B-NB	2.07	108.42	106.77
13	T4	201	CYC	CMB-C2B-C1B	2.07	126.68	124.16
13	Z6	301	CYC	CMD-C2D-C3D	-2.07	121.23	125.62
13	V6	201	CYC	O2D-CGD-CBD	2.07	120.54	114.00
13	t2	201	CYC	CHD-C1D-ND	-2.07	120.61	125.29
13	a5	201	CYC	CHA-C4D-C3D	-2.07	122.77	127.22
13	a7	202	CYC	CMB-C2B-C1B	2.07	126.67	124.16
13	J1	201	CYC	C3B-C4B-NB	2.07	108.42	106.77
13	32	302	CYC	CHA-C1A-NA	2.07	128.94	124.60
13	Q4	202	CYC	CHA-C4D-C3D	-2.07	122.77	127.22
13	A6	302	CYC	CHA-C4D-ND	2.07	129.96	125.29
13	F4	201	CYC	C4D-C3D-C2D	-2.07	105.21	107.62
13	a6	202	CYC	OB-C4B-C3B	-2.07	125.86	128.03
13	A1	301	CYC	CHD-C1D-C2D	2.07	132.60	127.53
13	F2	201	CYC	CHB-C1B-NB	2.07	130.47	126.06
13	U1	201	CYC	C3B-C4B-NB	2.07	108.41	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P6	202	CYC	C2C-C3C-C4C	2.07	104.44	101.34
13	A6	301	CYC	CMB-C2B-C1B	2.07	126.67	124.16
13	J4	202	CYC	OB-C4B-C3B	-2.07	125.86	128.03
13	P3	202	CYC	CMB-C2B-C1B	2.07	126.67	124.16
13	Z7	301	CYC	CMB-C2B-C1B	2.07	126.67	124.16
13	M5	201	CYC	C3B-C4B-NB	2.07	108.41	106.77
13	J7	201	CYC	C3B-C4B-NB	2.07	108.41	106.77
13	U6	201	CYC	CMB-C2B-C1B	2.07	126.67	124.16
13	K1	201	CYC	C2C-C1C-NC	-2.07	106.57	108.29
13	F6	201	CYC	C4D-C3D-C2D	-2.06	105.22	107.62
13	H4	201	CYC	C3B-C4B-NB	2.06	108.41	106.77
13	U5	201	CYC	C3B-C4B-NB	2.06	108.41	106.77
13	C4	201	CYC	CHD-C1D-C2D	2.06	132.59	127.53
13	Q2	201	CYC	CHA-C4D-C3D	-2.06	122.79	127.22
13	D6	201	CYC	CHD-C1D-C2D	2.06	132.58	127.53
13	J5	202	CYC	C3B-C4B-NB	2.06	108.41	106.77
13	J5	202	CYC	CMB-C2B-C1B	2.06	126.67	124.16
13	W5	201	CYC	CHA-C1A-NA	2.06	128.93	124.60
13	C6	201	CYC	C2C-C3C-C4C	2.06	104.43	101.34
13	V6	202	CYC	C3B-C4B-NB	2.06	108.41	106.77
13	M3	201	CYC	CHA-C4D-C3D	-2.06	122.79	127.22
13	M1	201	CYC	OB-C4B-C3B	-2.06	125.87	128.03
13	R6	201	CYC	CHA-C4D-C3D	-2.06	122.79	127.22
13	W2	201	CYC	CHA-C1A-NA	2.06	128.92	124.60
13	Z7	301	CYC	CMD-C2D-C1D	2.06	128.61	125.62
13	G3	201	CYC	C2C-C1C-NC	-2.06	106.57	108.29
13	M7	201	CYC	CMA-C3A-C4A	2.06	128.29	125.10
13	M1	201	CYC	O2A-CGA-CBA	2.06	120.50	114.00
13	W4	201	CYC	C3B-C4B-NB	2.06	108.41	106.77
13	Z1	301	CYC	CMD-C2D-C3D	-2.05	121.27	125.62
13	I6	201	CYC	C3B-C4B-NB	2.05	108.40	106.77
13	w2	201	CYC	CHB-C4A-C3A	2.05	130.15	124.87
13	Z1	301	CYC	CHD-C1D-ND	-2.05	120.65	125.29
13	V3	201	CYC	CMB-C2B-C1B	2.05	126.66	124.16
13	C6	202	CYC	OB-C4B-C3B	-2.05	125.88	128.03
13	F5	201	CYC	CAD-C3D-C2D	-2.05	122.47	127.07
13	L3	201	CYC	C3B-C4B-NB	2.05	108.40	106.77
13	Z4	301	CYC	O2A-CGA-CBA	2.05	120.48	114.00
13	S6	201	CYC	CHA-C4D-ND	2.05	129.93	125.29
13	M7	201	CYC	CHA-C1A-NA	2.05	128.91	124.60
13	V1	202	CYC	C3B-C4B-NB	2.05	108.40	106.77
13	a1	201	CYC	CMB-C2B-C1B	2.05	126.65	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A6	302	CYC	CMB-C2B-C1B	2.05	126.65	124.16
13	Z4	301	CYC	CHA-C4D-C3D	-2.05	122.81	127.22
13	K1	201	CYC	CHA-C4D-ND	2.05	129.92	125.29
13	N2	801	CYC	CHD-C1D-C2D	2.05	132.55	127.53
13	22	301	CYC	CHD-C1D-C2D	2.05	132.55	127.53
13	D6	201	CYC	CHD-C1D-ND	-2.05	120.66	125.29
13	V1	202	CYC	CMA-C3A-C4A	2.05	128.28	125.10
13	I3	201	CYC	C3B-C4B-NB	2.05	108.40	106.77
13	X2	201	CYC	CHD-C1D-C2D	2.05	132.54	127.53
13	T6	201	CYC	CMB-C2B-C1B	2.05	126.65	124.16
13	T3	202	CYC	C3B-C4B-NB	2.05	108.40	106.77
13	T3	202	CYC	CHA-C4D-C3D	-2.05	122.82	127.22
13	T4	202	CYC	CHA-C4D-C3D	-2.05	122.82	127.22
13	F1	201	CYC	CHA-C1A-NA	2.05	128.89	124.60
13	C3	202	CYC	OB-C4B-C3B	-2.05	125.88	128.03
13	V7	202	CYC	OB-C4B-C3B	-2.05	125.88	128.03
13	H3	201	CYC	C3B-C4B-NB	2.04	108.40	106.77
13	Z6	301	CYC	O2A-CGA-CBA	2.04	120.46	114.00
13	B5	201	CYC	CHA-C1A-NA	2.04	128.89	124.60
13	N3	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	F5	202	CYC	CMB-C2B-C1B	2.04	126.64	124.16
13	X1	201	CYC	CMD-C2D-C3D	-2.04	121.29	125.62
13	a5	201	CYC	CMB-C2B-C1B	2.04	126.64	124.16
13	a7	201	CYC	CMB-C2B-C1B	2.04	126.64	124.16
13	W6	201	CYC	CHA-C1A-NA	2.04	128.88	124.60
13	X2	201	CYC	O2A-CGA-CBA	2.04	120.45	114.00
13	P6	202	CYC	CMA-C3A-C4A	2.04	128.27	125.10
13	L5	201	CYC	CHB-C1B-C2B	-2.04	122.90	126.97
13	z2	201	CYC	CHA-C4D-C3D	-2.04	122.83	127.22
13	T2	201	CYC	CHD-C1D-ND	-2.04	120.68	125.29
13	S5	201	CYC	CHA-C4D-ND	2.04	129.90	125.29
13	X4	201	CYC	CHD-C1D-C2D	2.04	132.53	127.53
13	A1	302	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	V6	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	T5	201	CYC	CMD-C2D-C1D	2.04	128.59	125.62
13	B1	201	CYC	CHA-C4D-ND	2.04	129.90	125.29
13	X6	201	CYC	CMB-C2B-C1B	2.04	126.64	124.16
13	V1	201	CYC	O2D-CGD-CBD	2.04	120.44	114.00
13	M5	201	CYC	OB-C4B-C3B	-2.04	125.89	128.03
13	S1	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	X2	201	CYC	CHD-C1D-ND	-2.04	120.69	125.29
13	52	302	CYC	C1B-CHB-C4A	-2.04	123.05	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B1	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	S5	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	D2	201	CYC	CHB-C1B-NB	2.04	130.40	126.06
13	x2	201	CYC	O2A-CGA-CBA	2.04	120.43	114.00
13	X6	201	CYC	CMD-C2D-C3D	-2.04	121.31	125.62
13	B2	202	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	S6	201	CYC	C3B-C4B-NB	2.04	108.39	106.77
13	T7	201	CYC	CMB-C2B-C1B	2.04	126.63	124.16
13	a4	202	CYC	CMB-C2B-C1B	2.03	126.63	124.16
13	W1	201	CYC	CMC-C2C-C1C	-2.03	108.02	112.40
13	T5	202	CYC	C3B-C4B-NB	2.03	108.39	106.77
13	x2	201	CYC	CHD-C1D-C2D	2.03	132.51	127.53
13	l2	201	CYC	O2D-CGD-CBD	2.03	120.43	114.00
13	A6	302	CYC	C1B-CHB-C4A	-2.03	123.06	128.06
13	22	302	CYC	CHA-C1A-NA	2.03	128.87	124.60
13	R2	201	CYC	CHA-C4D-C3D	-2.03	122.85	127.22
13	F3	201	CYC	O2D-CGD-CBD	2.03	120.42	114.00
13	P7	201	CYC	C3C-C4C-NC	-2.03	105.33	107.94
13	G1	201	CYC	CHA-C4D-ND	2.03	129.88	125.29
13	A2	201	CYC	C2C-C3C-C4C	2.03	104.38	101.34
13	P3	201	CYC	C3C-C4C-NC	-2.03	105.33	107.94
13	r2	201	CYC	CHA-C4D-C3D	-2.03	122.86	127.22
13	P5	202	CYC	CHA-C1A-NA	2.03	128.86	124.60
13	F3	202	CYC	CMB-C2B-C1B	2.03	126.63	124.16
13	x2	201	CYC	C3B-C4B-NB	2.03	108.38	106.77
13	J3	201	CYC	C3B-C4B-NB	2.03	108.38	106.77
13	T5	201	CYC	CMB-C2B-C1B	2.03	126.63	124.16
13	V1	201	CYC	C3B-C4B-NB	2.03	108.38	106.77
13	K6	201	CYC	CHA-C1A-NA	2.03	128.86	124.60
13	P2	201	CYC	CHB-C4A-NA	-2.03	120.58	124.95
13	42	302	CYC	CHA-C4D-ND	2.03	129.87	125.29
13	V3	202	CYC	OB-C4B-C3B	-2.03	125.90	128.03
13	K4	201	CYC	C3B-C4B-NB	2.03	108.38	106.77
13	a6	202	CYC	CMB-C2B-C1B	2.03	126.62	124.16
13	P1	201	CYC	CHB-C1B-C2B	-2.03	122.93	126.97
13	H5	201	CYC	CHA-C4D-ND	2.02	129.87	125.29
13	J6	201	CYC	C3B-C4B-NB	2.02	108.38	106.77
13	A1	301	CYC	CHA-C4D-ND	2.02	129.86	125.29
13	C3	202	CYC	CMA-C3A-C4A	2.02	128.24	125.10
13	P1	201	CYC	O2D-CGD-CBD	2.02	120.39	114.00
13	T1	202	CYC	CHA-C1A-NA	2.02	128.85	124.60
13	X7	201	CYC	CHD-C1D-ND	-2.02	120.72	125.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M6	201	CYC	O2A-CGA-CBA	2.02	120.39	114.00
13	E6	201	CYC	CMA-C3A-C4A	2.02	128.24	125.10
13	M6	201	CYC	C2C-C3C-C4C	2.02	104.37	101.34
13	B1	201	CYC	CHA-C1A-NA	2.02	128.84	124.60
13	32	302	CYC	C1B-CHB-C4A	-2.02	123.10	128.06
13	T6	202	CYC	CHA-C1A-NA	2.02	128.84	124.60
13	U4	201	CYC	C3B-C4B-NB	2.02	108.38	106.77
13	52	301	CYC	CHA-C4D-C3D	-2.02	122.88	127.22
13	T7	202	CYC	CHA-C4D-C3D	-2.02	122.88	127.22
13	N2	801	CYC	CHB-C1B-NB	2.02	130.36	126.06
13	a1	202	CYC	CHB-C1B-C2B	-2.02	122.95	126.97
13	V3	202	CYC	CMA-C3A-C4A	2.02	128.23	125.10
13	a3	201	CYC	CMB-C2B-C1B	2.02	126.61	124.16
13	U2	201	CYC	O2A-CGA-CBA	2.02	120.37	114.00
13	V6	202	CYC	OB-C4B-C3B	-2.01	125.92	128.03
13	S2	201	CYC	CHD-C1D-ND	-2.01	120.74	125.29
13	52	302	CYC	CMB-C2B-C1B	2.01	126.61	124.16
13	V4	201	CYC	CMB-C2B-C1B	2.01	126.61	124.16
13	V5	201	CYC	CMB-C2B-C1B	2.01	126.61	124.16
13	J4	201	CYC	C3B-C4B-NB	2.01	108.37	106.77
13	R1	201	CYC	C2C-C3C-C4C	2.01	104.35	101.34
13	F4	202	CYC	CMB-C2B-C1B	2.01	126.61	124.16
13	M3	201	CYC	CMA-C3A-C4A	2.01	128.22	125.10
13	X4	201	CYC	CMD-C2D-C3D	-2.01	121.36	125.62
13	P5	201	CYC	O2D-CGD-CBD	2.01	120.36	114.00
13	D4	201	CYC	CHA-C1A-NA	2.01	128.82	124.60
13	52	302	CYC	CHA-C4D-ND	2.01	129.84	125.29
13	V5	201	CYC	O2D-CGD-CBD	2.01	120.36	114.00
13	Z5	301	CYC	O2A-CGA-CBA	2.01	120.35	114.00
13	C4	201	CYC	C2C-C3C-C4C	2.01	104.35	101.34
13	J4	201	CYC	CHA-C4D-ND	2.01	129.83	125.29
13	C3	201	CYC	CMA-C3A-C4A	2.01	128.22	125.10
13	P4	201	CYC	CMA-C3A-C4A	2.01	128.22	125.10
13	J3	202	CYC	CMB-C2B-C1B	2.01	126.60	124.16
13	52	301	CYC	CMD-C2D-C3D	-2.01	121.36	125.62
13	L1	201	CYC	CHD-C1D-ND	-2.01	120.75	125.29
13	H4	201	CYC	CMC-C2C-C1C	-2.01	108.08	112.40
13	32	301	CYC	CHA-C4D-C3D	-2.01	122.91	127.22
13	L5	201	CYC	C3B-C4B-NB	2.01	108.37	106.77
13	H6	201	CYC	C3B-C4B-NB	2.01	108.37	106.77
13	T7	202	CYC	C3B-C4B-NB	2.01	108.37	106.77
13	P7	201	CYC	CMB-C2B-C1B	2.01	126.60	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F4	202	CYC	C3C-C4C-NC	-2.01	105.36	107.94
13	a1	201	CYC	CHD-C1D-ND	-2.01	120.76	125.29
13	K4	201	CYC	CHA-C1A-NA	2.01	128.81	124.60
13	D6	201	CYC	CMB-C2B-C1B	2.00	126.60	124.16
13	Z3	301	CYC	CMB-C2B-C1B	2.00	126.59	124.16
13	P5	202	CYC	CMD-C2D-C3D	-2.00	121.38	125.62
13	Q1	202	CYC	CMB-C2B-C1B	2.00	126.59	124.16
13	A2	201	CYC	CMB-C2B-C1B	2.00	126.59	124.16
13	W2	201	CYC	O2A-CGA-CBA	2.00	120.33	114.00
13	T4	202	CYC	C3B-C4B-NB	2.00	108.36	106.77
13	Z5	301	CYC	CMD-C2D-C3D	-2.00	121.38	125.62
13	l2	201	CYC	CMB-C2B-C1B	2.00	126.59	124.16
13	V5	201	CYC	O2A-CGA-CBA	2.00	120.33	114.00
13	D4	201	CYC	CMB-C2B-C1B	2.00	126.59	124.16
13	P6	201	CYC	O2D-CGD-CBD	2.00	120.32	114.00
13	H6	201	CYC	CHA-C4D-ND	2.00	129.81	125.29
13	M4	201	CYC	O2A-CGA-CBA	2.00	120.32	114.00
13	x2	201	CYC	CHD-C1D-ND	-2.00	120.77	125.29

There are no chirality outliers.

All (3423) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A1	301	CYC	NA-C4A-CHB-C1B
13	A1	301	CYC	C3A-C4A-CHB-C1B
13	A1	301	CYC	C4C-C3C-CAC-CBC
13	A1	301	CYC	NC-C4C-CHD-C1D
13	A1	302	CYC	NA-C4A-CHB-C1B
13	A1	302	CYC	C3A-C4A-CHB-C1B
13	A1	302	CYC	C2C-C3C-CAC-CBC
13	A1	302	CYC	C4C-C3C-CAC-CBC
13	A1	302	CYC	NC-C4C-CHD-C1D
13	B1	201	CYC	NA-C4A-CHB-C1B
13	B1	201	CYC	C3A-C4A-CHB-C1B
13	B1	201	CYC	C4C-C3C-CAC-CBC
13	B1	201	CYC	NC-C4C-CHD-C1D
13	C1	201	CYC	NA-C4A-CHB-C1B
13	C1	201	CYC	C3A-C4A-CHB-C1B
13	C1	201	CYC	C2C-C3C-CAC-CBC
13	C1	201	CYC	C4C-C3C-CAC-CBC
13	C1	201	CYC	NC-C4C-CHD-C1D
13	C1	202	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	C1	202	CYC	C2A-C1A-CHA-C4D
13	C1	202	CYC	ND-C4D-CHA-C1A
13	C1	202	CYC	C3D-C4D-CHA-C1A
13	C1	202	CYC	NA-C4A-CHB-C1B
13	C1	202	CYC	C3A-C4A-CHB-C1B
13	C1	202	CYC	C2C-C3C-CAC-CBC
13	C1	202	CYC	NC-C4C-CHD-C1D
13	C1	202	CYC	C3C-C4C-CHD-C1D
13	C1	202	CYC	ND-C1D-CHD-C4C
13	C1	202	CYC	C2D-C1D-CHD-C4C
13	D1	201	CYC	NA-C4A-CHB-C1B
13	D1	201	CYC	C3A-C4A-CHB-C1B
13	D1	201	CYC	C2C-C3C-CAC-CBC
13	D1	201	CYC	C4C-C3C-CAC-CBC
13	D1	201	CYC	NC-C4C-CHD-C1D
13	E1	201	CYC	NA-C1A-CHA-C4D
13	E1	201	CYC	C2A-C1A-CHA-C4D
13	E1	201	CYC	NA-C4A-CHB-C1B
13	E1	201	CYC	C3A-C4A-CHB-C1B
13	E1	201	CYC	C4C-C3C-CAC-CBC
13	E1	201	CYC	NC-C4C-CHD-C1D
13	E1	201	CYC	C3C-C4C-CHD-C1D
13	F1	201	CYC	NA-C4A-CHB-C1B
13	F1	201	CYC	C3A-C4A-CHB-C1B
13	F1	201	CYC	C2C-C3C-CAC-CBC
13	F1	201	CYC	C4C-C3C-CAC-CBC
13	F1	201	CYC	NC-C4C-CHD-C1D
13	F1	201	CYC	ND-C1D-CHD-C4C
13	F1	201	CYC	C2D-C1D-CHD-C4C
13	F1	202	CYC	NA-C1A-CHA-C4D
13	F1	202	CYC	C2A-C1A-CHA-C4D
13	F1	202	CYC	NA-C4A-CHB-C1B
13	F1	202	CYC	C3A-C4A-CHB-C1B
13	F1	202	CYC	C2C-C3C-CAC-CBC
13	F1	202	CYC	C4C-C3C-CAC-CBC
13	F1	202	CYC	NC-C4C-CHD-C1D
13	F1	202	CYC	ND-C1D-CHD-C4C
13	F1	202	CYC	C2D-C1D-CHD-C4C
13	G1	201	CYC	NA-C4A-CHB-C1B
13	G1	201	CYC	C3A-C4A-CHB-C1B
13	G1	201	CYC	C2C-C3C-CAC-CBC
13	G1	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	G1	201	CYC	NC-C4C-CHD-C1D
13	H1	201	CYC	NA-C4A-CHB-C1B
13	H1	201	CYC	C3A-C4A-CHB-C1B
13	H1	201	CYC	C2C-C3C-CAC-CBC
13	H1	201	CYC	C4C-C3C-CAC-CBC
13	H1	201	CYC	NC-C4C-CHD-C1D
13	I1	201	CYC	NA-C4A-CHB-C1B
13	I1	201	CYC	C3A-C4A-CHB-C1B
13	I1	201	CYC	C2C-C3C-CAC-CBC
13	I1	201	CYC	C4C-C3C-CAC-CBC
13	I1	201	CYC	NC-C4C-CHD-C1D
13	I1	201	CYC	C2D-C1D-CHD-C4C
13	J1	201	CYC	NA-C4A-CHB-C1B
13	J1	201	CYC	C3A-C4A-CHB-C1B
13	J1	201	CYC	C4C-C3C-CAC-CBC
13	J1	201	CYC	NC-C4C-CHD-C1D
13	J1	201	CYC	ND-C1D-CHD-C4C
13	J1	201	CYC	C2D-C1D-CHD-C4C
13	J1	202	CYC	NA-C4A-CHB-C1B
13	J1	202	CYC	C3A-C4A-CHB-C1B
13	J1	202	CYC	C2C-C3C-CAC-CBC
13	J1	202	CYC	C4C-C3C-CAC-CBC
13	J1	202	CYC	NC-C4C-CHD-C1D
13	J1	202	CYC	C3C-C4C-CHD-C1D
13	K1	201	CYC	NA-C4A-CHB-C1B
13	K1	201	CYC	C3A-C4A-CHB-C1B
13	K1	201	CYC	C2C-C3C-CAC-CBC
13	K1	201	CYC	C4C-C3C-CAC-CBC
13	K1	201	CYC	NC-C4C-CHD-C1D
13	K1	201	CYC	ND-C1D-CHD-C4C
13	K1	201	CYC	C2D-C1D-CHD-C4C
13	L1	201	CYC	C2C-C3C-CAC-CBC
13	L1	201	CYC	NC-C4C-CHD-C1D
13	M1	201	CYC	NA-C4A-CHB-C1B
13	M1	201	CYC	C3A-C4A-CHB-C1B
13	M1	201	CYC	NC-C4C-CHD-C1D
13	N1	201	CYC	NA-C4A-CHB-C1B
13	N1	201	CYC	C3A-C4A-CHB-C1B
13	N1	201	CYC	C2C-C3C-CAC-CBC
13	N1	201	CYC	C4C-C3C-CAC-CBC
13	N1	201	CYC	NC-C4C-CHD-C1D
13	N1	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	N1	201	CYC	C2D-C1D-CHD-C4C
13	P1	201	CYC	NA-C4A-CHB-C1B
13	P1	201	CYC	C2C-C3C-CAC-CBC
13	P1	201	CYC	C4C-C3C-CAC-CBC
13	P1	201	CYC	NC-C4C-CHD-C1D
13	P1	201	CYC	C3C-C4C-CHD-C1D
13	P1	202	CYC	NA-C4A-CHB-C1B
13	P1	202	CYC	C3A-C4A-CHB-C1B
13	P1	202	CYC	C4C-C3C-CAC-CBC
13	P1	202	CYC	NC-C4C-CHD-C1D
13	Q1	201	CYC	NA-C4A-CHB-C1B
13	Q1	201	CYC	C3A-C4A-CHB-C1B
13	Q1	201	CYC	C2C-C3C-CAC-CBC
13	Q1	201	CYC	C4C-C3C-CAC-CBC
13	Q1	201	CYC	NC-C4C-CHD-C1D
13	Q1	202	CYC	NA-C4A-CHB-C1B
13	Q1	202	CYC	C3A-C4A-CHB-C1B
13	Q1	202	CYC	C2C-C3C-CAC-CBC
13	Q1	202	CYC	C4C-C3C-CAC-CBC
13	Q1	202	CYC	NC-C4C-CHD-C1D
13	Q1	202	CYC	ND-C1D-CHD-C4C
13	Q1	202	CYC	C2D-C1D-CHD-C4C
13	R1	201	CYC	NA-C4A-CHB-C1B
13	R1	201	CYC	C3A-C4A-CHB-C1B
13	R1	201	CYC	C4C-C3C-CAC-CBC
13	R1	201	CYC	NC-C4C-CHD-C1D
13	R1	201	CYC	ND-C1D-CHD-C4C
13	R1	201	CYC	C2D-C1D-CHD-C4C
13	S1	201	CYC	NA-C4A-CHB-C1B
13	S1	201	CYC	C3A-C4A-CHB-C1B
13	S1	201	CYC	C2C-C3C-CAC-CBC
13	S1	201	CYC	C4C-C3C-CAC-CBC
13	S1	201	CYC	NC-C4C-CHD-C1D
13	T1	201	CYC	NA-C1A-CHA-C4D
13	T1	201	CYC	C2A-C1A-CHA-C4D
13	T1	201	CYC	ND-C4D-CHA-C1A
13	T1	201	CYC	C3D-C4D-CHA-C1A
13	T1	201	CYC	NA-C4A-CHB-C1B
13	T1	201	CYC	C3A-C4A-CHB-C1B
13	T1	201	CYC	C4C-C3C-CAC-CBC
13	T1	201	CYC	NC-C4C-CHD-C1D
13	T1	201	CYC	C3C-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	T1	202	CYC	NA-C4A-CHB-C1B
13	T1	202	CYC	C3A-C4A-CHB-C1B
13	T1	202	CYC	NC-C4C-CHD-C1D
13	T1	202	CYC	ND-C1D-CHD-C4C
13	T1	202	CYC	C2D-C1D-CHD-C4C
13	U1	201	CYC	NA-C4A-CHB-C1B
13	U1	201	CYC	C3A-C4A-CHB-C1B
13	U1	201	CYC	C2C-C3C-CAC-CBC
13	U1	201	CYC	C4C-C3C-CAC-CBC
13	U1	201	CYC	NC-C4C-CHD-C1D
13	U1	201	CYC	ND-C1D-CHD-C4C
13	U1	201	CYC	C2D-C1D-CHD-C4C
13	V1	201	CYC	NA-C4A-CHB-C1B
13	V1	201	CYC	C3A-C4A-CHB-C1B
13	V1	201	CYC	C2C-C3C-CAC-CBC
13	V1	201	CYC	C4C-C3C-CAC-CBC
13	V1	201	CYC	NC-C4C-CHD-C1D
13	V1	202	CYC	ND-C4D-CHA-C1A
13	V1	202	CYC	C3D-C4D-CHA-C1A
13	V1	202	CYC	NA-C4A-CHB-C1B
13	V1	202	CYC	C3A-C4A-CHB-C1B
13	V1	202	CYC	C4C-C3C-CAC-CBC
13	V1	202	CYC	NC-C4C-CHD-C1D
13	V1	202	CYC	C3C-C4C-CHD-C1D
13	W1	201	CYC	NA-C4A-CHB-C1B
13	W1	201	CYC	C3A-C4A-CHB-C1B
13	W1	201	CYC	C2C-C3C-CAC-CBC
13	W1	201	CYC	C4C-C3C-CAC-CBC
13	W1	201	CYC	NC-C4C-CHD-C1D
13	W1	201	CYC	ND-C1D-CHD-C4C
13	W1	201	CYC	C2D-C1D-CHD-C4C
13	X1	201	CYC	NA-C4A-CHB-C1B
13	X1	201	CYC	C2C-C3C-CAC-CBC
13	X1	201	CYC	NC-C4C-CHD-C1D
13	X1	201	CYC	ND-C1D-CHD-C4C
13	X1	201	CYC	C2D-C1D-CHD-C4C
13	Z1	301	CYC	C2C-C3C-CAC-CBC
13	Z1	301	CYC	C4C-C3C-CAC-CBC
13	Z1	301	CYC	NC-C4C-CHD-C1D
13	Z1	301	CYC	ND-C1D-CHD-C4C
13	Z1	301	CYC	C2D-C1D-CHD-C4C
13	a1	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	a1	201	CYC	C3A-C4A-CHB-C1B
13	a1	201	CYC	C2C-C3C-CAC-CBC
13	a1	201	CYC	C4C-C3C-CAC-CBC
13	a1	201	CYC	NC-C4C-CHD-C1D
13	a1	202	CYC	ND-C4D-CHA-C1A
13	a1	202	CYC	C3D-C4D-CHA-C1A
13	a1	202	CYC	NA-C4A-CHB-C1B
13	a1	202	CYC	C3A-C4A-CHB-C1B
13	a1	202	CYC	C2C-C3C-CAC-CBC
13	a1	202	CYC	NC-C4C-CHD-C1D
13	a1	202	CYC	C3C-C4C-CHD-C1D
13	22	301	CYC	NA-C4A-CHB-C1B
13	22	301	CYC	C3A-C4A-CHB-C1B
13	22	301	CYC	C2C-C3C-CAC-CBC
13	22	301	CYC	C4C-C3C-CAC-CBC
13	22	301	CYC	NC-C4C-CHD-C1D
13	22	302	CYC	NA-C4A-CHB-C1B
13	22	302	CYC	C3A-C4A-CHB-C1B
13	22	302	CYC	C2C-C3C-CAC-CBC
13	22	302	CYC	C4C-C3C-CAC-CBC
13	22	302	CYC	NC-C4C-CHD-C1D
13	22	302	CYC	C2D-C1D-CHD-C4C
13	32	301	CYC	NA-C4A-CHB-C1B
13	32	301	CYC	C3A-C4A-CHB-C1B
13	32	301	CYC	C2C-C3C-CAC-CBC
13	32	301	CYC	C4C-C3C-CAC-CBC
13	32	301	CYC	NC-C4C-CHD-C1D
13	32	302	CYC	NA-C4A-CHB-C1B
13	32	302	CYC	C3A-C4A-CHB-C1B
13	32	302	CYC	C2C-C3C-CAC-CBC
13	32	302	CYC	C4C-C3C-CAC-CBC
13	32	302	CYC	NC-C4C-CHD-C1D
13	32	302	CYC	C2D-C1D-CHD-C4C
13	42	301	CYC	NA-C4A-CHB-C1B
13	42	301	CYC	C3A-C4A-CHB-C1B
13	42	301	CYC	C2C-C3C-CAC-CBC
13	42	301	CYC	C4C-C3C-CAC-CBC
13	42	301	CYC	NC-C4C-CHD-C1D
13	42	302	CYC	NA-C4A-CHB-C1B
13	42	302	CYC	C3A-C4A-CHB-C1B
13	42	302	CYC	NC-C4C-CHD-C1D
13	52	301	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	52	301	CYC	C3A-C4A-CHB-C1B
13	52	301	CYC	C4C-C3C-CAC-CBC
13	52	301	CYC	NC-C4C-CHD-C1D
13	52	302	CYC	NA-C4A-CHB-C1B
13	52	302	CYC	C3A-C4A-CHB-C1B
13	52	302	CYC	NC-C4C-CHD-C1D
13	A2	201	CYC	NA-C4A-CHB-C1B
13	A2	201	CYC	C3A-C4A-CHB-C1B
13	A2	201	CYC	C4C-C3C-CAC-CBC
13	A2	201	CYC	NC-C4C-CHD-C1D
13	A2	201	CYC	ND-C1D-CHD-C4C
13	A2	201	CYC	C2D-C1D-CHD-C4C
13	A2	202	CYC	NA-C4A-CHB-C1B
13	A2	202	CYC	C3A-C4A-CHB-C1B
13	A2	202	CYC	C4C-C3C-CAC-CBC
13	A2	202	CYC	NC-C4C-CHD-C1D
13	A2	202	CYC	C3C-C4C-CHD-C1D
13	B2	201	CYC	NA-C1A-CHA-C4D
13	B2	201	CYC	C2A-C1A-CHA-C4D
13	B2	201	CYC	NA-C4A-CHB-C1B
13	B2	201	CYC	C3A-C4A-CHB-C1B
13	B2	201	CYC	C2C-C3C-CAC-CBC
13	B2	201	CYC	C4C-C3C-CAC-CBC
13	B2	201	CYC	NC-C4C-CHD-C1D
13	B2	201	CYC	C3C-C4C-CHD-C1D
13	B2	202	CYC	ND-C4D-CHA-C1A
13	B2	202	CYC	C3D-C4D-CHA-C1A
13	B2	202	CYC	NA-C4A-CHB-C1B
13	B2	202	CYC	C3A-C4A-CHB-C1B
13	B2	202	CYC	C4C-C3C-CAC-CBC
13	B2	202	CYC	NC-C4C-CHD-C1D
13	B2	202	CYC	C3C-C4C-CHD-C1D
13	C2	201	CYC	NA-C1A-CHA-C4D
13	C2	201	CYC	C2A-C1A-CHA-C4D
13	C2	201	CYC	NA-C4A-CHB-C1B
13	C2	201	CYC	C3A-C4A-CHB-C1B
13	C2	201	CYC	NC-C4C-CHD-C1D
13	C2	201	CYC	ND-C1D-CHD-C4C
13	C2	201	CYC	C2D-C1D-CHD-C4C
13	D2	201	CYC	C2C-C3C-CAC-CBC
13	D2	201	CYC	C4C-C3C-CAC-CBC
13	D2	201	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	E2	201	CYC	C2C-C3C-CAC-CBC
13	E2	201	CYC	C4C-C3C-CAC-CBC
13	E2	201	CYC	NC-C4C-CHD-C1D
13	E2	201	CYC	C2D-C1D-CHD-C4C
13	F2	201	CYC	NC-C4C-CHD-C1D
13	G2	201	CYC	C2C-C3C-CAC-CBC
13	G2	201	CYC	C4C-C3C-CAC-CBC
13	G2	201	CYC	NC-C4C-CHD-C1D
13	H2	201	CYC	NA-C4A-CHB-C1B
13	H2	201	CYC	C3A-C4A-CHB-C1B
13	H2	201	CYC	NC-C4C-CHD-C1D
13	H2	201	CYC	ND-C1D-CHD-C4C
13	H2	201	CYC	C2D-C1D-CHD-C4C
13	L2	201	CYC	NA-C4A-CHB-C1B
13	L2	201	CYC	C3A-C4A-CHB-C1B
13	L2	201	CYC	NC-C4C-CHD-C1D
13	M2	201	CYC	NA-C4A-CHB-C1B
13	M2	201	CYC	C3A-C4A-CHB-C1B
13	M2	201	CYC	NC-C4C-CHD-C1D
13	N2	801	CYC	NA-C4A-CHB-C1B
13	N2	801	CYC	C2C-C3C-CAC-CBC
13	N2	801	CYC	C4C-C3C-CAC-CBC
13	N2	801	CYC	NC-C4C-CHD-C1D
13	N2	802	CYC	C2C-C3C-CAC-CBC
13	N2	802	CYC	C4C-C3C-CAC-CBC
13	N2	802	CYC	NC-C4C-CHD-C1D
13	N2	802	CYC	C3C-C4C-CHD-C1D
13	O2	201	CYC	NA-C4A-CHB-C1B
13	O2	201	CYC	C3A-C4A-CHB-C1B
13	O2	201	CYC	NC-C4C-CHD-C1D
13	P2	201	CYC	NA-C4A-CHB-C1B
13	P2	201	CYC	C3A-C4A-CHB-C1B
13	P2	201	CYC	C4C-C3C-CAC-CBC
13	P2	201	CYC	NC-C4C-CHD-C1D
13	P2	201	CYC	ND-C1D-CHD-C4C
13	P2	201	CYC	C2D-C1D-CHD-C4C
13	Q2	201	CYC	ND-C4D-CHA-C1A
13	Q2	201	CYC	NA-C4A-CHB-C1B
13	Q2	201	CYC	C3A-C4A-CHB-C1B
13	Q2	201	CYC	C4C-C3C-CAC-CBC
13	Q2	201	CYC	NC-C4C-CHD-C1D
13	Q2	201	CYC	C3C-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	R2	201	CYC	C2C-C3C-CAC-CBC
13	R2	201	CYC	C4C-C3C-CAC-CBC
13	R2	201	CYC	NC-C4C-CHD-C1D
13	R2	201	CYC	ND-C1D-CHD-C4C
13	R2	201	CYC	C2D-C1D-CHD-C4C
13	S2	201	CYC	C4C-C3C-CAC-CBC
13	S2	201	CYC	NC-C4C-CHD-C1D
13	S2	201	CYC	ND-C1D-CHD-C4C
13	S2	201	CYC	C2D-C1D-CHD-C4C
13	T2	201	CYC	C4C-C3C-CAC-CBC
13	T2	201	CYC	NC-C4C-CHD-C1D
13	U2	201	CYC	C3A-C4A-CHB-C1B
13	U2	201	CYC	C2C-C3C-CAC-CBC
13	U2	201	CYC	C4C-C3C-CAC-CBC
13	U2	201	CYC	NC-C4C-CHD-C1D
13	U2	201	CYC	C3C-C4C-CHD-C1D
13	V2	201	CYC	NA-C4A-CHB-C1B
13	V2	201	CYC	C3A-C4A-CHB-C1B
13	V2	201	CYC	C4C-C3C-CAC-CBC
13	V2	201	CYC	NC-C4C-CHD-C1D
13	V2	201	CYC	C3C-C4C-CHD-C1D
13	W2	201	CYC	NA-C4A-CHB-C1B
13	W2	201	CYC	C3A-C4A-CHB-C1B
13	W2	201	CYC	NC-C4C-CHD-C1D
13	W2	201	CYC	ND-C1D-CHD-C4C
13	W2	201	CYC	C2D-C1D-CHD-C4C
13	X2	201	CYC	NA-C4A-CHB-C1B
13	X2	201	CYC	C3A-C4A-CHB-C1B
13	X2	201	CYC	C2B-C1B-CHB-C4A
13	X2	201	CYC	C4C-C3C-CAC-CBC
13	X2	201	CYC	NC-C4C-CHD-C1D
13	a2	201	CYC	NA-C1A-CHA-C4D
13	a2	201	CYC	NA-C4A-CHB-C1B
13	a2	201	CYC	C3A-C4A-CHB-C1B
13	a2	201	CYC	C2C-C3C-CAC-CBC
13	a2	201	CYC	C4C-C3C-CAC-CBC
13	a2	201	CYC	NC-C4C-CHD-C1D
13	c2	801	CYC	NA-C4A-CHB-C1B
13	c2	801	CYC	C3A-C4A-CHB-C1B
13	c2	801	CYC	C2C-C3C-CAC-CBC
13	c2	801	CYC	C4C-C3C-CAC-CBC
13	c2	801	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	c2	801	CYC	C3C-C4C-CHD-C1D
13	d2	201	CYC	NA-C4A-CHB-C1B
13	d2	201	CYC	C3A-C4A-CHB-C1B
13	d2	201	CYC	C2C-C3C-CAC-CBC
13	d2	201	CYC	C4C-C3C-CAC-CBC
13	d2	201	CYC	NC-C4C-CHD-C1D
13	d2	201	CYC	ND-C1D-CHD-C4C
13	d2	201	CYC	C2D-C1D-CHD-C4C
13	e2	201	CYC	C2C-C3C-CAC-CBC
13	e2	201	CYC	C4C-C3C-CAC-CBC
13	e2	201	CYC	NC-C4C-CHD-C1D
13	e2	201	CYC	ND-C1D-CHD-C4C
13	e2	201	CYC	C2D-C1D-CHD-C4C
13	f2	201	CYC	NC-C4C-CHD-C1D
13	g2	201	CYC	NA-C4A-CHB-C1B
13	g2	201	CYC	C3A-C4A-CHB-C1B
13	g2	201	CYC	NC-C4C-CHD-C1D
13	h2	201	CYC	C2C-C3C-CAC-CBC
13	h2	201	CYC	C4C-C3C-CAC-CBC
13	h2	201	CYC	NC-C4C-CHD-C1D
13	h2	201	CYC	ND-C1D-CHD-C4C
13	h2	201	CYC	C2D-C1D-CHD-C4C
13	i2	201	CYC	ND-C4D-CHA-C1A
13	i2	201	CYC	C3D-C4D-CHA-C1A
13	i2	201	CYC	NA-C4A-CHB-C1B
13	i2	201	CYC	C3A-C4A-CHB-C1B
13	i2	201	CYC	NC-C4C-CHD-C1D
13	j2	201	CYC	NA-C4A-CHB-C1B
13	j2	201	CYC	C3A-C4A-CHB-C1B
13	j2	201	CYC	NB-C1B-CHB-C4A
13	j2	201	CYC	C2B-C1B-CHB-C4A
13	j2	201	CYC	C2C-C3C-CAC-CBC
13	j2	201	CYC	C4C-C3C-CAC-CBC
13	j2	201	CYC	NC-C4C-CHD-C1D
13	k2	201	CYC	NA-C4A-CHB-C1B
13	k2	201	CYC	C3A-C4A-CHB-C1B
13	k2	201	CYC	C4B-C3B-CAB-CBB
13	k2	201	CYC	NC-C4C-CHD-C1D
13	k2	201	CYC	ND-C1D-CHD-C4C
13	k2	201	CYC	C2D-C1D-CHD-C4C
13	l2	201	CYC	NC-C4C-CHD-C1D
13	m2	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	m2	201	CYC	C3A-C4A-CHB-C1B
13	m2	201	CYC	C2A-CAA-CBA-CGA
13	m2	201	CYC	NC-C4C-CHD-C1D
13	n2	201	CYC	NA-C4A-CHB-C1B
13	n2	201	CYC	C3A-C4A-CHB-C1B
13	n2	201	CYC	NC-C4C-CHD-C1D
13	o2	801	CYC	NA-C4A-CHB-C1B
13	o2	801	CYC	C3A-C4A-CHB-C1B
13	o2	801	CYC	C2C-C3C-CAC-CBC
13	o2	801	CYC	C4C-C3C-CAC-CBC
13	o2	801	CYC	NC-C4C-CHD-C1D
13	o2	801	CYC	C3C-C4C-CHD-C1D
13	p2	201	CYC	NC-C4C-CHD-C1D
13	q2	201	CYC	NA-C4A-CHB-C1B
13	q2	201	CYC	C3A-C4A-CHB-C1B
13	q2	201	CYC	C2B-C1B-CHB-C4A
13	q2	201	CYC	C2C-C3C-CAC-CBC
13	q2	201	CYC	C4C-C3C-CAC-CBC
13	q2	201	CYC	NC-C4C-CHD-C1D
13	q2	201	CYC	C3C-C4C-CHD-C1D
13	r2	201	CYC	NC-C4C-CHD-C1D
13	r2	201	CYC	ND-C1D-CHD-C4C
13	r2	201	CYC	C2D-C1D-CHD-C4C
13	s2	201	CYC	C3A-C4A-CHB-C1B
13	s2	201	CYC	C4C-C3C-CAC-CBC
13	s2	201	CYC	NC-C4C-CHD-C1D
13	s2	201	CYC	ND-C1D-CHD-C4C
13	s2	201	CYC	C2D-C1D-CHD-C4C
13	t2	201	CYC	C3A-C4A-CHB-C1B
13	t2	201	CYC	C2C-C3C-CAC-CBC
13	t2	201	CYC	C4C-C3C-CAC-CBC
13	t2	201	CYC	NC-C4C-CHD-C1D
13	v2	201	CYC	C2C-C3C-CAC-CBC
13	v2	201	CYC	C4C-C3C-CAC-CBC
13	v2	201	CYC	NC-C4C-CHD-C1D
13	v2	201	CYC	ND-C1D-CHD-C4C
13	v2	201	CYC	C2D-C1D-CHD-C4C
13	w2	201	CYC	NA-C4A-CHB-C1B
13	w2	201	CYC	C3A-C4A-CHB-C1B
13	w2	201	CYC	NC-C4C-CHD-C1D
13	x2	201	CYC	NA-C4A-CHB-C1B
13	x2	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	x2	201	CYC	C2C-C3C-CAC-CBC
13	x2	201	CYC	C4C-C3C-CAC-CBC
13	x2	201	CYC	NC-C4C-CHD-C1D
13	y2	201	CYC	C2B-C1B-CHB-C4A
13	y2	201	CYC	NC-C4C-CHD-C1D
13	z2	201	CYC	C2A-CAA-CBA-CGA
13	z2	201	CYC	NC-C4C-CHD-C1D
13	B3	201	CYC	NA-C4A-CHB-C1B
13	B3	201	CYC	C3A-C4A-CHB-C1B
13	B3	201	CYC	NC-C4C-CHD-C1D
13	B3	201	CYC	ND-C1D-CHD-C4C
13	B3	201	CYC	C2D-C1D-CHD-C4C
13	C3	201	CYC	NA-C4A-CHB-C1B
13	C3	201	CYC	C3A-C4A-CHB-C1B
13	C3	201	CYC	C2C-C3C-CAC-CBC
13	C3	201	CYC	C4C-C3C-CAC-CBC
13	C3	201	CYC	NC-C4C-CHD-C1D
13	C3	202	CYC	NA-C1A-CHA-C4D
13	C3	202	CYC	C2A-C1A-CHA-C4D
13	C3	202	CYC	ND-C4D-CHA-C1A
13	C3	202	CYC	C3D-C4D-CHA-C1A
13	C3	202	CYC	NA-C4A-CHB-C1B
13	C3	202	CYC	C3A-C4A-CHB-C1B
13	C3	202	CYC	C2A-CAA-CBA-CGA
13	C3	202	CYC	NC-C4C-CHD-C1D
13	C3	202	CYC	C3C-C4C-CHD-C1D
13	C3	202	CYC	ND-C1D-CHD-C4C
13	C3	202	CYC	C2D-C1D-CHD-C4C
13	D3	201	CYC	NA-C4A-CHB-C1B
13	D3	201	CYC	C3A-C4A-CHB-C1B
13	D3	201	CYC	C2C-C3C-CAC-CBC
13	D3	201	CYC	C4C-C3C-CAC-CBC
13	D3	201	CYC	NC-C4C-CHD-C1D
13	D3	201	CYC	C3C-C4C-CHD-C1D
13	E3	201	CYC	NA-C1A-CHA-C4D
13	E3	201	CYC	C2A-C1A-CHA-C4D
13	E3	201	CYC	ND-C4D-CHA-C1A
13	E3	201	CYC	C3D-C4D-CHA-C1A
13	E3	201	CYC	NA-C4A-CHB-C1B
13	E3	201	CYC	C3A-C4A-CHB-C1B
13	E3	201	CYC	C2C-C3C-CAC-CBC
13	E3	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	E3	201	CYC	C3C-C4C-CHD-C1D
13	F3	201	CYC	NA-C4A-CHB-C1B
13	F3	201	CYC	C3A-C4A-CHB-C1B
13	F3	201	CYC	C4C-C3C-CAC-CBC
13	F3	201	CYC	NC-C4C-CHD-C1D
13	F3	201	CYC	ND-C1D-CHD-C4C
13	F3	201	CYC	C2D-C1D-CHD-C4C
13	F3	201	CYC	C4D-C3D-CAD-CBD
13	F3	202	CYC	NA-C1A-CHA-C4D
13	F3	202	CYC	C2A-C1A-CHA-C4D
13	F3	202	CYC	NA-C4A-CHB-C1B
13	F3	202	CYC	C3A-C4A-CHB-C1B
13	F3	202	CYC	C2C-C3C-CAC-CBC
13	F3	202	CYC	C4C-C3C-CAC-CBC
13	F3	202	CYC	NC-C4C-CHD-C1D
13	F3	202	CYC	ND-C1D-CHD-C4C
13	F3	202	CYC	C2D-C1D-CHD-C4C
13	G3	201	CYC	NA-C4A-CHB-C1B
13	G3	201	CYC	C3A-C4A-CHB-C1B
13	G3	201	CYC	C2C-C3C-CAC-CBC
13	G3	201	CYC	C4C-C3C-CAC-CBC
13	G3	201	CYC	NC-C4C-CHD-C1D
13	G3	201	CYC	ND-C1D-CHD-C4C
13	G3	201	CYC	C2D-C1D-CHD-C4C
13	H3	201	CYC	NA-C4A-CHB-C1B
13	H3	201	CYC	C3A-C4A-CHB-C1B
13	H3	201	CYC	C2C-C3C-CAC-CBC
13	H3	201	CYC	C4C-C3C-CAC-CBC
13	H3	201	CYC	NC-C4C-CHD-C1D
13	H3	201	CYC	ND-C1D-CHD-C4C
13	H3	201	CYC	C2D-C1D-CHD-C4C
13	I3	201	CYC	NA-C4A-CHB-C1B
13	I3	201	CYC	C3A-C4A-CHB-C1B
13	I3	201	CYC	NC-C4C-CHD-C1D
13	I3	201	CYC	ND-C1D-CHD-C4C
13	I3	201	CYC	C2D-C1D-CHD-C4C
13	J3	201	CYC	NA-C4A-CHB-C1B
13	J3	201	CYC	C3A-C4A-CHB-C1B
13	J3	201	CYC	NC-C4C-CHD-C1D
13	J3	201	CYC	ND-C1D-CHD-C4C
13	J3	201	CYC	C2D-C1D-CHD-C4C
13	J3	202	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	J3	202	CYC	C2A-C1A-CHA-C4D
13	J3	202	CYC	NA-C4A-CHB-C1B
13	J3	202	CYC	C3A-C4A-CHB-C1B
13	J3	202	CYC	C2C-C3C-CAC-CBC
13	J3	202	CYC	C4C-C3C-CAC-CBC
13	J3	202	CYC	NC-C4C-CHD-C1D
13	J3	202	CYC	C3C-C4C-CHD-C1D
13	K3	201	CYC	NA-C4A-CHB-C1B
13	K3	201	CYC	C3A-C4A-CHB-C1B
13	K3	201	CYC	C2C-C3C-CAC-CBC
13	K3	201	CYC	C4C-C3C-CAC-CBC
13	K3	201	CYC	NC-C4C-CHD-C1D
13	K3	201	CYC	ND-C1D-CHD-C4C
13	K3	201	CYC	C2D-C1D-CHD-C4C
13	L3	201	CYC	C4C-C3C-CAC-CBC
13	L3	201	CYC	NC-C4C-CHD-C1D
13	L3	201	CYC	ND-C1D-CHD-C4C
13	L3	201	CYC	C2D-C1D-CHD-C4C
13	M3	201	CYC	NA-C4A-CHB-C1B
13	M3	201	CYC	C3A-C4A-CHB-C1B
13	M3	201	CYC	C2C-C3C-CAC-CBC
13	M3	201	CYC	C4C-C3C-CAC-CBC
13	M3	201	CYC	NC-C4C-CHD-C1D
13	N3	201	CYC	NA-C4A-CHB-C1B
13	N3	201	CYC	C3A-C4A-CHB-C1B
13	N3	201	CYC	C2C-C3C-CAC-CBC
13	N3	201	CYC	C4C-C3C-CAC-CBC
13	N3	201	CYC	NC-C4C-CHD-C1D
13	N3	201	CYC	ND-C1D-CHD-C4C
13	N3	201	CYC	C2D-C1D-CHD-C4C
13	N3	201	CYC	C3D-CAD-CBD-CGD
13	P3	201	CYC	NA-C4A-CHB-C1B
13	P3	201	CYC	C3A-C4A-CHB-C1B
13	P3	201	CYC	C2C-C3C-CAC-CBC
13	P3	201	CYC	C4C-C3C-CAC-CBC
13	P3	201	CYC	NC-C4C-CHD-C1D
13	P3	201	CYC	C3C-C4C-CHD-C1D
13	P3	202	CYC	NA-C1A-CHA-C4D
13	P3	202	CYC	C2A-C1A-CHA-C4D
13	P3	202	CYC	NA-C4A-CHB-C1B
13	P3	202	CYC	C3A-C4A-CHB-C1B
13	P3	202	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	P3	202	CYC	C4C-C3C-CAC-CBC
13	P3	202	CYC	NC-C4C-CHD-C1D
13	P3	202	CYC	C3C-C4C-CHD-C1D
13	Q3	201	CYC	NA-C4A-CHB-C1B
13	Q3	201	CYC	C3A-C4A-CHB-C1B
13	Q3	201	CYC	C2C-C3C-CAC-CBC
13	Q3	201	CYC	C4C-C3C-CAC-CBC
13	Q3	201	CYC	NC-C4C-CHD-C1D
13	Q3	201	CYC	C2D-C1D-CHD-C4C
13	Q3	202	CYC	NA-C4A-CHB-C1B
13	Q3	202	CYC	C3A-C4A-CHB-C1B
13	Q3	202	CYC	C2C-C3C-CAC-CBC
13	Q3	202	CYC	C4C-C3C-CAC-CBC
13	Q3	202	CYC	NC-C4C-CHD-C1D
13	Q3	202	CYC	ND-C1D-CHD-C4C
13	Q3	202	CYC	C2D-C1D-CHD-C4C
13	R3	201	CYC	NA-C4A-CHB-C1B
13	R3	201	CYC	C3A-C4A-CHB-C1B
13	R3	201	CYC	C2C-C3C-CAC-CBC
13	R3	201	CYC	C4C-C3C-CAC-CBC
13	R3	201	CYC	NC-C4C-CHD-C1D
13	R3	201	CYC	ND-C1D-CHD-C4C
13	R3	201	CYC	C2D-C1D-CHD-C4C
13	S3	201	CYC	NA-C4A-CHB-C1B
13	S3	201	CYC	C3A-C4A-CHB-C1B
13	S3	201	CYC	C2C-C3C-CAC-CBC
13	S3	201	CYC	C4C-C3C-CAC-CBC
13	S3	201	CYC	NC-C4C-CHD-C1D
13	T3	201	CYC	NA-C1A-CHA-C4D
13	T3	201	CYC	C2A-C1A-CHA-C4D
13	T3	201	CYC	ND-C4D-CHA-C1A
13	T3	201	CYC	C3D-C4D-CHA-C1A
13	T3	201	CYC	NA-C4A-CHB-C1B
13	T3	201	CYC	C3A-C4A-CHB-C1B
13	T3	201	CYC	C4C-C3C-CAC-CBC
13	T3	201	CYC	NC-C4C-CHD-C1D
13	T3	201	CYC	C3C-C4C-CHD-C1D
13	T3	202	CYC	NA-C4A-CHB-C1B
13	T3	202	CYC	C3A-C4A-CHB-C1B
13	T3	202	CYC	NC-C4C-CHD-C1D
13	T3	202	CYC	ND-C1D-CHD-C4C
13	T3	202	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	U3	201	CYC	NA-C4A-CHB-C1B
13	U3	201	CYC	C3A-C4A-CHB-C1B
13	U3	201	CYC	C2C-C3C-CAC-CBC
13	U3	201	CYC	C4C-C3C-CAC-CBC
13	U3	201	CYC	NC-C4C-CHD-C1D
13	U3	201	CYC	ND-C1D-CHD-C4C
13	U3	201	CYC	C2D-C1D-CHD-C4C
13	V3	201	CYC	NA-C4A-CHB-C1B
13	V3	201	CYC	C3A-C4A-CHB-C1B
13	V3	201	CYC	C2C-C3C-CAC-CBC
13	V3	201	CYC	C4C-C3C-CAC-CBC
13	V3	201	CYC	NC-C4C-CHD-C1D
13	V3	202	CYC	ND-C4D-CHA-C1A
13	V3	202	CYC	C3D-C4D-CHA-C1A
13	V3	202	CYC	NA-C4A-CHB-C1B
13	V3	202	CYC	C3A-C4A-CHB-C1B
13	V3	202	CYC	C2A-CAA-CBA-CGA
13	V3	202	CYC	C4C-C3C-CAC-CBC
13	V3	202	CYC	NC-C4C-CHD-C1D
13	V3	202	CYC	C3C-C4C-CHD-C1D
13	W3	201	CYC	NA-C4A-CHB-C1B
13	W3	201	CYC	C3A-C4A-CHB-C1B
13	W3	201	CYC	C2A-CAA-CBA-CGA
13	W3	201	CYC	C2C-C3C-CAC-CBC
13	W3	201	CYC	C4C-C3C-CAC-CBC
13	W3	201	CYC	NC-C4C-CHD-C1D
13	W3	201	CYC	ND-C1D-CHD-C4C
13	W3	201	CYC	C2D-C1D-CHD-C4C
13	X3	201	CYC	NA-C4A-CHB-C1B
13	X3	201	CYC	NC-C4C-CHD-C1D
13	Z3	301	CYC	NA-C4A-CHB-C1B
13	Z3	301	CYC	C3A-C4A-CHB-C1B
13	Z3	301	CYC	C2C-C3C-CAC-CBC
13	Z3	301	CYC	NC-C4C-CHD-C1D
13	a3	201	CYC	NA-C4A-CHB-C1B
13	a3	201	CYC	C3A-C4A-CHB-C1B
13	a3	201	CYC	NC-C4C-CHD-C1D
13	a3	202	CYC	NA-C1A-CHA-C4D
13	a3	202	CYC	C2A-C1A-CHA-C4D
13	a3	202	CYC	ND-C4D-CHA-C1A
13	a3	202	CYC	C3D-C4D-CHA-C1A
13	a3	202	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	a3	202	CYC	C3A-C4A-CHB-C1B
13	a3	202	CYC	C2C-C3C-CAC-CBC
13	a3	202	CYC	C3C-C4C-CHD-C1D
13	B4	201	CYC	NA-C4A-CHB-C1B
13	B4	201	CYC	C3A-C4A-CHB-C1B
13	B4	201	CYC	C4C-C3C-CAC-CBC
13	B4	201	CYC	NC-C4C-CHD-C1D
13	B4	201	CYC	C2D-C1D-CHD-C4C
13	C4	201	CYC	NA-C4A-CHB-C1B
13	C4	201	CYC	C3A-C4A-CHB-C1B
13	C4	201	CYC	C2C-C3C-CAC-CBC
13	C4	201	CYC	C4C-C3C-CAC-CBC
13	C4	201	CYC	NC-C4C-CHD-C1D
13	C4	202	CYC	NA-C1A-CHA-C4D
13	C4	202	CYC	C2A-C1A-CHA-C4D
13	C4	202	CYC	ND-C4D-CHA-C1A
13	C4	202	CYC	C3D-C4D-CHA-C1A
13	C4	202	CYC	NA-C4A-CHB-C1B
13	C4	202	CYC	C3A-C4A-CHB-C1B
13	C4	202	CYC	C2A-CAA-CBA-CGA
13	C4	202	CYC	NC-C4C-CHD-C1D
13	C4	202	CYC	C3C-C4C-CHD-C1D
13	C4	202	CYC	ND-C1D-CHD-C4C
13	C4	202	CYC	C2D-C1D-CHD-C4C
13	D4	201	CYC	C2C-C3C-CAC-CBC
13	D4	201	CYC	C4C-C3C-CAC-CBC
13	D4	201	CYC	NC-C4C-CHD-C1D
13	E4	201	CYC	NA-C1A-CHA-C4D
13	E4	201	CYC	C2A-C1A-CHA-C4D
13	E4	201	CYC	ND-C4D-CHA-C1A
13	E4	201	CYC	C3D-C4D-CHA-C1A
13	E4	201	CYC	NA-C4A-CHB-C1B
13	E4	201	CYC	C3A-C4A-CHB-C1B
13	E4	201	CYC	C2A-CAA-CBA-CGA
13	E4	201	CYC	C2C-C3C-CAC-CBC
13	E4	201	CYC	C4C-C3C-CAC-CBC
13	E4	201	CYC	NC-C4C-CHD-C1D
13	E4	201	CYC	C3C-C4C-CHD-C1D
13	F4	201	CYC	NA-C4A-CHB-C1B
13	F4	201	CYC	C3A-C4A-CHB-C1B
13	F4	201	CYC	C2C-C3C-CAC-CBC
13	F4	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	F4	201	CYC	NC-C4C-CHD-C1D
13	F4	201	CYC	ND-C1D-CHD-C4C
13	F4	201	CYC	C2D-C1D-CHD-C4C
13	F4	201	CYC	C4D-C3D-CAD-CBD
13	F4	202	CYC	NA-C1A-CHA-C4D
13	F4	202	CYC	C2A-C1A-CHA-C4D
13	F4	202	CYC	NA-C4A-CHB-C1B
13	F4	202	CYC	C3A-C4A-CHB-C1B
13	F4	202	CYC	C2C-C3C-CAC-CBC
13	F4	202	CYC	C4C-C3C-CAC-CBC
13	F4	202	CYC	NC-C4C-CHD-C1D
13	F4	202	CYC	ND-C1D-CHD-C4C
13	F4	202	CYC	C2D-C1D-CHD-C4C
13	G4	201	CYC	NA-C4A-CHB-C1B
13	G4	201	CYC	C3A-C4A-CHB-C1B
13	G4	201	CYC	C2C-C3C-CAC-CBC
13	G4	201	CYC	C4C-C3C-CAC-CBC
13	G4	201	CYC	NC-C4C-CHD-C1D
13	G4	201	CYC	ND-C1D-CHD-C4C
13	G4	201	CYC	C2D-C1D-CHD-C4C
13	H4	201	CYC	NA-C4A-CHB-C1B
13	H4	201	CYC	C3A-C4A-CHB-C1B
13	H4	201	CYC	C2C-C3C-CAC-CBC
13	H4	201	CYC	C4C-C3C-CAC-CBC
13	H4	201	CYC	NC-C4C-CHD-C1D
13	H4	201	CYC	ND-C1D-CHD-C4C
13	H4	201	CYC	C2D-C1D-CHD-C4C
13	I4	201	CYC	NA-C4A-CHB-C1B
13	I4	201	CYC	C3A-C4A-CHB-C1B
13	I4	201	CYC	C4C-C3C-CAC-CBC
13	I4	201	CYC	NC-C4C-CHD-C1D
13	I4	201	CYC	ND-C1D-CHD-C4C
13	I4	201	CYC	C2D-C1D-CHD-C4C
13	J4	201	CYC	NA-C4A-CHB-C1B
13	J4	201	CYC	C3A-C4A-CHB-C1B
13	J4	201	CYC	C2C-C3C-CAC-CBC
13	J4	201	CYC	C4C-C3C-CAC-CBC
13	J4	201	CYC	NC-C4C-CHD-C1D
13	J4	202	CYC	NA-C4A-CHB-C1B
13	J4	202	CYC	C3A-C4A-CHB-C1B
13	J4	202	CYC	C2C-C3C-CAC-CBC
13	J4	202	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	J4	202	CYC	NC-C4C-CHD-C1D
13	J4	202	CYC	C3C-C4C-CHD-C1D
13	K4	201	CYC	NA-C4A-CHB-C1B
13	K4	201	CYC	C3A-C4A-CHB-C1B
13	K4	201	CYC	C2C-C3C-CAC-CBC
13	K4	201	CYC	C4C-C3C-CAC-CBC
13	K4	201	CYC	NC-C4C-CHD-C1D
13	K4	201	CYC	ND-C1D-CHD-C4C
13	K4	201	CYC	C2D-C1D-CHD-C4C
13	L4	201	CYC	NA-C4A-CHB-C1B
13	L4	201	CYC	C3A-C4A-CHB-C1B
13	L4	201	CYC	C4C-C3C-CAC-CBC
13	L4	201	CYC	NC-C4C-CHD-C1D
13	L4	201	CYC	ND-C1D-CHD-C4C
13	L4	201	CYC	C2D-C1D-CHD-C4C
13	M4	201	CYC	NA-C4A-CHB-C1B
13	M4	201	CYC	C3A-C4A-CHB-C1B
13	M4	201	CYC	C2C-C3C-CAC-CBC
13	M4	201	CYC	C4C-C3C-CAC-CBC
13	M4	201	CYC	NC-C4C-CHD-C1D
13	N4	201	CYC	NA-C4A-CHB-C1B
13	N4	201	CYC	C3A-C4A-CHB-C1B
13	N4	201	CYC	C2C-C3C-CAC-CBC
13	N4	201	CYC	C4C-C3C-CAC-CBC
13	N4	201	CYC	NC-C4C-CHD-C1D
13	N4	201	CYC	ND-C1D-CHD-C4C
13	N4	201	CYC	C2D-C1D-CHD-C4C
13	P4	201	CYC	NA-C1A-CHA-C4D
13	P4	201	CYC	C2A-C1A-CHA-C4D
13	P4	201	CYC	NA-C4A-CHB-C1B
13	P4	201	CYC	C3A-C4A-CHB-C1B
13	P4	201	CYC	C2C-C3C-CAC-CBC
13	P4	201	CYC	C4C-C3C-CAC-CBC
13	P4	201	CYC	NC-C4C-CHD-C1D
13	P4	202	CYC	C4C-C3C-CAC-CBC
13	P4	202	CYC	NC-C4C-CHD-C1D
13	P4	202	CYC	C3C-C4C-CHD-C1D
13	Q4	201	CYC	NA-C4A-CHB-C1B
13	Q4	201	CYC	C3A-C4A-CHB-C1B
13	Q4	201	CYC	C2C-C3C-CAC-CBC
13	Q4	201	CYC	C4C-C3C-CAC-CBC
13	Q4	201	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	Q4	202	CYC	NA-C4A-CHB-C1B
13	Q4	202	CYC	C3A-C4A-CHB-C1B
13	Q4	202	CYC	C2C-C3C-CAC-CBC
13	Q4	202	CYC	C4C-C3C-CAC-CBC
13	Q4	202	CYC	NC-C4C-CHD-C1D
13	Q4	202	CYC	ND-C1D-CHD-C4C
13	Q4	202	CYC	C2D-C1D-CHD-C4C
13	R4	201	CYC	NA-C4A-CHB-C1B
13	R4	201	CYC	C3A-C4A-CHB-C1B
13	R4	201	CYC	C2C-C3C-CAC-CBC
13	R4	201	CYC	C4C-C3C-CAC-CBC
13	R4	201	CYC	NC-C4C-CHD-C1D
13	R4	201	CYC	ND-C1D-CHD-C4C
13	R4	201	CYC	C2D-C1D-CHD-C4C
13	S4	201	CYC	NA-C4A-CHB-C1B
13	S4	201	CYC	C3A-C4A-CHB-C1B
13	S4	201	CYC	C2C-C3C-CAC-CBC
13	S4	201	CYC	C4C-C3C-CAC-CBC
13	S4	201	CYC	NC-C4C-CHD-C1D
13	T4	201	CYC	NA-C1A-CHA-C4D
13	T4	201	CYC	C2A-C1A-CHA-C4D
13	T4	201	CYC	ND-C4D-CHA-C1A
13	T4	201	CYC	C3D-C4D-CHA-C1A
13	T4	201	CYC	NA-C4A-CHB-C1B
13	T4	201	CYC	C3A-C4A-CHB-C1B
13	T4	201	CYC	C4C-C3C-CAC-CBC
13	T4	201	CYC	NC-C4C-CHD-C1D
13	T4	201	CYC	C3C-C4C-CHD-C1D
13	T4	202	CYC	NA-C4A-CHB-C1B
13	T4	202	CYC	C3A-C4A-CHB-C1B
13	T4	202	CYC	NC-C4C-CHD-C1D
13	T4	202	CYC	ND-C1D-CHD-C4C
13	T4	202	CYC	C2D-C1D-CHD-C4C
13	U4	201	CYC	NA-C4A-CHB-C1B
13	U4	201	CYC	C3A-C4A-CHB-C1B
13	U4	201	CYC	C2C-C3C-CAC-CBC
13	U4	201	CYC	C4C-C3C-CAC-CBC
13	U4	201	CYC	NC-C4C-CHD-C1D
13	U4	201	CYC	ND-C1D-CHD-C4C
13	U4	201	CYC	C2D-C1D-CHD-C4C
13	V4	201	CYC	NA-C4A-CHB-C1B
13	V4	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	V4	201	CYC	C2C-C3C-CAC-CBC
13	V4	201	CYC	C4C-C3C-CAC-CBC
13	V4	201	CYC	NC-C4C-CHD-C1D
13	V4	202	CYC	ND-C4D-CHA-C1A
13	V4	202	CYC	C3D-C4D-CHA-C1A
13	V4	202	CYC	NA-C4A-CHB-C1B
13	V4	202	CYC	C3A-C4A-CHB-C1B
13	V4	202	CYC	C2C-C3C-CAC-CBC
13	V4	202	CYC	C4C-C3C-CAC-CBC
13	V4	202	CYC	NC-C4C-CHD-C1D
13	V4	202	CYC	C3C-C4C-CHD-C1D
13	W4	201	CYC	NA-C4A-CHB-C1B
13	W4	201	CYC	C3A-C4A-CHB-C1B
13	W4	201	CYC	NC-C4C-CHD-C1D
13	W4	201	CYC	ND-C1D-CHD-C4C
13	W4	201	CYC	C2D-C1D-CHD-C4C
13	X4	201	CYC	NA-C4A-CHB-C1B
13	X4	201	CYC	C3A-C4A-CHB-C1B
13	X4	201	CYC	C2C-C3C-CAC-CBC
13	X4	201	CYC	C4C-C3C-CAC-CBC
13	X4	201	CYC	NC-C4C-CHD-C1D
13	Z4	301	CYC	C2C-C3C-CAC-CBC
13	Z4	301	CYC	C4C-C3C-CAC-CBC
13	Z4	301	CYC	NC-C4C-CHD-C1D
13	Z4	301	CYC	ND-C1D-CHD-C4C
13	Z4	301	CYC	C2D-C1D-CHD-C4C
13	a4	201	CYC	NA-C4A-CHB-C1B
13	a4	201	CYC	C3A-C4A-CHB-C1B
13	a4	202	CYC	NA-C1A-CHA-C4D
13	a4	202	CYC	ND-C4D-CHA-C1A
13	a4	202	CYC	C3D-C4D-CHA-C1A
13	a4	202	CYC	NA-C4A-CHB-C1B
13	a4	202	CYC	C3A-C4A-CHB-C1B
13	a4	202	CYC	C2C-C3C-CAC-CBC
13	a4	202	CYC	NC-C4C-CHD-C1D
13	a4	202	CYC	C3C-C4C-CHD-C1D
13	B5	201	CYC	NA-C4A-CHB-C1B
13	B5	201	CYC	C3A-C4A-CHB-C1B
13	B5	201	CYC	C4C-C3C-CAC-CBC
13	B5	201	CYC	NC-C4C-CHD-C1D
13	C5	201	CYC	NA-C4A-CHB-C1B
13	C5	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	C5	201	CYC	C2C-C3C-CAC-CBC
13	C5	201	CYC	C4C-C3C-CAC-CBC
13	C5	201	CYC	NC-C4C-CHD-C1D
13	C5	202	CYC	NA-C1A-CHA-C4D
13	C5	202	CYC	C2A-C1A-CHA-C4D
13	C5	202	CYC	ND-C4D-CHA-C1A
13	C5	202	CYC	C3D-C4D-CHA-C1A
13	C5	202	CYC	NA-C4A-CHB-C1B
13	C5	202	CYC	C3A-C4A-CHB-C1B
13	C5	202	CYC	NC-C4C-CHD-C1D
13	C5	202	CYC	C3C-C4C-CHD-C1D
13	C5	202	CYC	ND-C1D-CHD-C4C
13	C5	202	CYC	C2D-C1D-CHD-C4C
13	D5	201	CYC	NA-C4A-CHB-C1B
13	D5	201	CYC	C3A-C4A-CHB-C1B
13	D5	201	CYC	C2C-C3C-CAC-CBC
13	D5	201	CYC	C4C-C3C-CAC-CBC
13	D5	201	CYC	NC-C4C-CHD-C1D
13	E5	201	CYC	NA-C1A-CHA-C4D
13	E5	201	CYC	C2A-C1A-CHA-C4D
13	E5	201	CYC	NA-C4A-CHB-C1B
13	E5	201	CYC	C3A-C4A-CHB-C1B
13	E5	201	CYC	C4C-C3C-CAC-CBC
13	E5	201	CYC	NC-C4C-CHD-C1D
13	E5	201	CYC	C3C-C4C-CHD-C1D
13	F5	201	CYC	NA-C4A-CHB-C1B
13	F5	201	CYC	C3A-C4A-CHB-C1B
13	F5	201	CYC	C2C-C3C-CAC-CBC
13	F5	201	CYC	C4C-C3C-CAC-CBC
13	F5	201	CYC	NC-C4C-CHD-C1D
13	F5	201	CYC	ND-C1D-CHD-C4C
13	F5	201	CYC	C2D-C1D-CHD-C4C
13	F5	202	CYC	NA-C1A-CHA-C4D
13	F5	202	CYC	C2A-C1A-CHA-C4D
13	F5	202	CYC	NA-C4A-CHB-C1B
13	F5	202	CYC	C3A-C4A-CHB-C1B
13	F5	202	CYC	C2C-C3C-CAC-CBC
13	F5	202	CYC	C4C-C3C-CAC-CBC
13	F5	202	CYC	NC-C4C-CHD-C1D
13	F5	202	CYC	ND-C1D-CHD-C4C
13	F5	202	CYC	C2D-C1D-CHD-C4C
13	G5	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	G5	201	CYC	C3A-C4A-CHB-C1B
13	G5	201	CYC	C2C-C3C-CAC-CBC
13	G5	201	CYC	C4C-C3C-CAC-CBC
13	G5	201	CYC	NC-C4C-CHD-C1D
13	G5	201	CYC	ND-C1D-CHD-C4C
13	G5	201	CYC	C2D-C1D-CHD-C4C
13	H5	201	CYC	NA-C4A-CHB-C1B
13	H5	201	CYC	C3A-C4A-CHB-C1B
13	H5	201	CYC	C2C-C3C-CAC-CBC
13	H5	201	CYC	C4C-C3C-CAC-CBC
13	H5	201	CYC	NC-C4C-CHD-C1D
13	I5	201	CYC	NA-C4A-CHB-C1B
13	I5	201	CYC	C3A-C4A-CHB-C1B
13	I5	201	CYC	NC-C4C-CHD-C1D
13	I5	201	CYC	ND-C1D-CHD-C4C
13	I5	201	CYC	C2D-C1D-CHD-C4C
13	J5	201	CYC	NA-C4A-CHB-C1B
13	J5	201	CYC	C3A-C4A-CHB-C1B
13	J5	201	CYC	NC-C4C-CHD-C1D
13	J5	201	CYC	ND-C1D-CHD-C4C
13	J5	201	CYC	C2D-C1D-CHD-C4C
13	J5	202	CYC	NA-C4A-CHB-C1B
13	J5	202	CYC	C3A-C4A-CHB-C1B
13	J5	202	CYC	C2C-C3C-CAC-CBC
13	J5	202	CYC	C4C-C3C-CAC-CBC
13	J5	202	CYC	NC-C4C-CHD-C1D
13	J5	202	CYC	C3C-C4C-CHD-C1D
13	K5	201	CYC	NA-C4A-CHB-C1B
13	K5	201	CYC	C3A-C4A-CHB-C1B
13	K5	201	CYC	NC-C4C-CHD-C1D
13	K5	201	CYC	ND-C1D-CHD-C4C
13	K5	201	CYC	C2D-C1D-CHD-C4C
13	L5	201	CYC	NA-C4A-CHB-C1B
13	L5	201	CYC	C3A-C4A-CHB-C1B
13	L5	201	CYC	C2C-C3C-CAC-CBC
13	L5	201	CYC	C4C-C3C-CAC-CBC
13	L5	201	CYC	NC-C4C-CHD-C1D
13	M5	201	CYC	NA-C4A-CHB-C1B
13	M5	201	CYC	C3A-C4A-CHB-C1B
13	M5	201	CYC	NC-C4C-CHD-C1D
13	N5	201	CYC	NA-C4A-CHB-C1B
13	N5	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	N5	201	CYC	NC-C4C-CHD-C1D
13	N5	201	CYC	ND-C1D-CHD-C4C
13	N5	201	CYC	C2D-C1D-CHD-C4C
13	P5	201	CYC	C4C-C3C-CAC-CBC
13	P5	201	CYC	NC-C4C-CHD-C1D
13	P5	201	CYC	C3C-C4C-CHD-C1D
13	P5	201	CYC	C3D-CAD-CBD-CGD
13	P5	202	CYC	NA-C1A-CHA-C4D
13	P5	202	CYC	C2A-C1A-CHA-C4D
13	P5	202	CYC	NA-C4A-CHB-C1B
13	P5	202	CYC	C3A-C4A-CHB-C1B
13	P5	202	CYC	C2C-C3C-CAC-CBC
13	P5	202	CYC	C4C-C3C-CAC-CBC
13	P5	202	CYC	NC-C4C-CHD-C1D
13	Q5	201	CYC	NA-C4A-CHB-C1B
13	Q5	201	CYC	C3A-C4A-CHB-C1B
13	Q5	201	CYC	C2C-C3C-CAC-CBC
13	Q5	201	CYC	C4C-C3C-CAC-CBC
13	Q5	201	CYC	NC-C4C-CHD-C1D
13	Q5	202	CYC	NA-C4A-CHB-C1B
13	Q5	202	CYC	C3A-C4A-CHB-C1B
13	Q5	202	CYC	C2C-C3C-CAC-CBC
13	Q5	202	CYC	C4C-C3C-CAC-CBC
13	Q5	202	CYC	NC-C4C-CHD-C1D
13	Q5	202	CYC	ND-C1D-CHD-C4C
13	Q5	202	CYC	C2D-C1D-CHD-C4C
13	Q5	202	CYC	C3D-CAD-CBD-CGD
13	R5	201	CYC	NA-C4A-CHB-C1B
13	R5	201	CYC	C3A-C4A-CHB-C1B
13	R5	201	CYC	C4C-C3C-CAC-CBC
13	R5	201	CYC	NC-C4C-CHD-C1D
13	R5	201	CYC	ND-C1D-CHD-C4C
13	R5	201	CYC	C2D-C1D-CHD-C4C
13	S5	201	CYC	NA-C4A-CHB-C1B
13	S5	201	CYC	C3A-C4A-CHB-C1B
13	S5	201	CYC	C4C-C3C-CAC-CBC
13	S5	201	CYC	NC-C4C-CHD-C1D
13	T5	201	CYC	NA-C1A-CHA-C4D
13	T5	201	CYC	C2A-C1A-CHA-C4D
13	T5	201	CYC	ND-C4D-CHA-C1A
13	T5	201	CYC	C3D-C4D-CHA-C1A
13	T5	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	T5	201	CYC	C3A-C4A-CHB-C1B
13	T5	201	CYC	C4C-C3C-CAC-CBC
13	T5	201	CYC	NC-C4C-CHD-C1D
13	T5	201	CYC	C3C-C4C-CHD-C1D
13	T5	202	CYC	NA-C4A-CHB-C1B
13	T5	202	CYC	C3A-C4A-CHB-C1B
13	T5	202	CYC	NC-C4C-CHD-C1D
13	T5	202	CYC	ND-C1D-CHD-C4C
13	T5	202	CYC	C2D-C1D-CHD-C4C
13	U5	201	CYC	NA-C4A-CHB-C1B
13	U5	201	CYC	C3A-C4A-CHB-C1B
13	U5	201	CYC	C2C-C3C-CAC-CBC
13	U5	201	CYC	C4C-C3C-CAC-CBC
13	U5	201	CYC	NC-C4C-CHD-C1D
13	U5	201	CYC	ND-C1D-CHD-C4C
13	U5	201	CYC	C2D-C1D-CHD-C4C
13	V5	201	CYC	NA-C4A-CHB-C1B
13	V5	201	CYC	C3A-C4A-CHB-C1B
13	V5	201	CYC	C2C-C3C-CAC-CBC
13	V5	201	CYC	C4C-C3C-CAC-CBC
13	V5	201	CYC	NC-C4C-CHD-C1D
13	V5	202	CYC	ND-C4D-CHA-C1A
13	V5	202	CYC	C3D-C4D-CHA-C1A
13	V5	202	CYC	NA-C4A-CHB-C1B
13	V5	202	CYC	C3A-C4A-CHB-C1B
13	V5	202	CYC	C2C-C3C-CAC-CBC
13	V5	202	CYC	C4C-C3C-CAC-CBC
13	V5	202	CYC	NC-C4C-CHD-C1D
13	V5	202	CYC	C3C-C4C-CHD-C1D
13	W5	201	CYC	NA-C4A-CHB-C1B
13	W5	201	CYC	C3A-C4A-CHB-C1B
13	W5	201	CYC	NC-C4C-CHD-C1D
13	W5	201	CYC	ND-C1D-CHD-C4C
13	W5	201	CYC	C2D-C1D-CHD-C4C
13	X5	201	CYC	NA-C4A-CHB-C1B
13	X5	201	CYC	C2C-C3C-CAC-CBC
13	X5	201	CYC	C4C-C3C-CAC-CBC
13	X5	201	CYC	NC-C4C-CHD-C1D
13	X5	201	CYC	C2D-C1D-CHD-C4C
13	Z5	301	CYC	C2C-C3C-CAC-CBC
13	Z5	301	CYC	NC-C4C-CHD-C1D
13	Z5	301	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	Z5	301	CYC	C2D-C1D-CHD-C4C
13	a5	201	CYC	NA-C4A-CHB-C1B
13	a5	201	CYC	C3A-C4A-CHB-C1B
13	a5	201	CYC	C2C-C3C-CAC-CBC
13	a5	201	CYC	C4C-C3C-CAC-CBC
13	a5	201	CYC	NC-C4C-CHD-C1D
13	a5	202	CYC	ND-C4D-CHA-C1A
13	a5	202	CYC	C3D-C4D-CHA-C1A
13	a5	202	CYC	NA-C4A-CHB-C1B
13	a5	202	CYC	C3A-C4A-CHB-C1B
13	a5	202	CYC	NC-C4C-CHD-C1D
13	a5	202	CYC	C3C-C4C-CHD-C1D
13	A6	301	CYC	NA-C4A-CHB-C1B
13	A6	301	CYC	C3A-C4A-CHB-C1B
13	A6	301	CYC	C4C-C3C-CAC-CBC
13	A6	301	CYC	NC-C4C-CHD-C1D
13	A6	302	CYC	NA-C4A-CHB-C1B
13	A6	302	CYC	C3A-C4A-CHB-C1B
13	A6	302	CYC	C2C-C3C-CAC-CBC
13	A6	302	CYC	NC-C4C-CHD-C1D
13	B6	201	CYC	NA-C4A-CHB-C1B
13	B6	201	CYC	C3A-C4A-CHB-C1B
13	B6	201	CYC	C2C-C3C-CAC-CBC
13	B6	201	CYC	C4C-C3C-CAC-CBC
13	B6	201	CYC	NC-C4C-CHD-C1D
13	C6	201	CYC	NA-C4A-CHB-C1B
13	C6	201	CYC	C3A-C4A-CHB-C1B
13	C6	201	CYC	C2C-C3C-CAC-CBC
13	C6	201	CYC	C4C-C3C-CAC-CBC
13	C6	201	CYC	NC-C4C-CHD-C1D
13	C6	202	CYC	NA-C1A-CHA-C4D
13	C6	202	CYC	C2A-C1A-CHA-C4D
13	C6	202	CYC	ND-C4D-CHA-C1A
13	C6	202	CYC	C3D-C4D-CHA-C1A
13	C6	202	CYC	NA-C4A-CHB-C1B
13	C6	202	CYC	C3A-C4A-CHB-C1B
13	C6	202	CYC	NC-C4C-CHD-C1D
13	C6	202	CYC	C3C-C4C-CHD-C1D
13	C6	202	CYC	ND-C1D-CHD-C4C
13	C6	202	CYC	C2D-C1D-CHD-C4C
13	D6	201	CYC	C2C-C3C-CAC-CBC
13	D6	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	D6	201	CYC	NC-C4C-CHD-C1D
13	E6	201	CYC	NA-C1A-CHA-C4D
13	E6	201	CYC	C2A-C1A-CHA-C4D
13	E6	201	CYC	ND-C4D-CHA-C1A
13	E6	201	CYC	C3D-C4D-CHA-C1A
13	E6	201	CYC	NA-C4A-CHB-C1B
13	E6	201	CYC	C3A-C4A-CHB-C1B
13	E6	201	CYC	C4C-C3C-CAC-CBC
13	E6	201	CYC	NC-C4C-CHD-C1D
13	E6	201	CYC	C3C-C4C-CHD-C1D
13	F6	201	CYC	NA-C4A-CHB-C1B
13	F6	201	CYC	C3A-C4A-CHB-C1B
13	F6	201	CYC	C2C-C3C-CAC-CBC
13	F6	201	CYC	C4C-C3C-CAC-CBC
13	F6	201	CYC	NC-C4C-CHD-C1D
13	F6	201	CYC	ND-C1D-CHD-C4C
13	F6	201	CYC	C2D-C1D-CHD-C4C
13	F6	202	CYC	NA-C1A-CHA-C4D
13	F6	202	CYC	C2A-C1A-CHA-C4D
13	F6	202	CYC	NA-C4A-CHB-C1B
13	F6	202	CYC	C3A-C4A-CHB-C1B
13	F6	202	CYC	C2C-C3C-CAC-CBC
13	F6	202	CYC	C4C-C3C-CAC-CBC
13	F6	202	CYC	NC-C4C-CHD-C1D
13	F6	202	CYC	ND-C1D-CHD-C4C
13	F6	202	CYC	C2D-C1D-CHD-C4C
13	G6	201	CYC	NA-C4A-CHB-C1B
13	G6	201	CYC	C3A-C4A-CHB-C1B
13	G6	201	CYC	C2C-C3C-CAC-CBC
13	G6	201	CYC	C4C-C3C-CAC-CBC
13	G6	201	CYC	NC-C4C-CHD-C1D
13	G6	201	CYC	ND-C1D-CHD-C4C
13	G6	201	CYC	C2D-C1D-CHD-C4C
13	H6	201	CYC	NA-C4A-CHB-C1B
13	H6	201	CYC	C3A-C4A-CHB-C1B
13	H6	201	CYC	C2C-C3C-CAC-CBC
13	H6	201	CYC	C4C-C3C-CAC-CBC
13	H6	201	CYC	NC-C4C-CHD-C1D
13	I6	201	CYC	NA-C4A-CHB-C1B
13	I6	201	CYC	C3A-C4A-CHB-C1B
13	I6	201	CYC	C4C-C3C-CAC-CBC
13	I6	201	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	J6	201	CYC	NA-C4A-CHB-C1B
13	J6	201	CYC	C3A-C4A-CHB-C1B
13	J6	201	CYC	C4C-C3C-CAC-CBC
13	J6	201	CYC	NC-C4C-CHD-C1D
13	J6	201	CYC	ND-C1D-CHD-C4C
13	J6	201	CYC	C2D-C1D-CHD-C4C
13	J6	202	CYC	NA-C4A-CHB-C1B
13	J6	202	CYC	C3A-C4A-CHB-C1B
13	J6	202	CYC	C2C-C3C-CAC-CBC
13	J6	202	CYC	C4C-C3C-CAC-CBC
13	J6	202	CYC	NC-C4C-CHD-C1D
13	J6	202	CYC	C3C-C4C-CHD-C1D
13	K6	201	CYC	NA-C4A-CHB-C1B
13	K6	201	CYC	C3A-C4A-CHB-C1B
13	K6	201	CYC	C2C-C3C-CAC-CBC
13	K6	201	CYC	C4C-C3C-CAC-CBC
13	K6	201	CYC	NC-C4C-CHD-C1D
13	K6	201	CYC	C2D-C1D-CHD-C4C
13	L6	201	CYC	C3A-C4A-CHB-C1B
13	L6	201	CYC	NC-C4C-CHD-C1D
13	M6	201	CYC	NA-C4A-CHB-C1B
13	M6	201	CYC	C3A-C4A-CHB-C1B
13	M6	201	CYC	NC-C4C-CHD-C1D
13	N6	201	CYC	NA-C4A-CHB-C1B
13	N6	201	CYC	C3A-C4A-CHB-C1B
13	N6	201	CYC	C2C-C3C-CAC-CBC
13	N6	201	CYC	C4C-C3C-CAC-CBC
13	N6	201	CYC	NC-C4C-CHD-C1D
13	N6	201	CYC	ND-C1D-CHD-C4C
13	N6	201	CYC	C2D-C1D-CHD-C4C
13	P6	201	CYC	NA-C4A-CHB-C1B
13	P6	201	CYC	C4C-C3C-CAC-CBC
13	P6	201	CYC	NC-C4C-CHD-C1D
13	P6	201	CYC	C3C-C4C-CHD-C1D
13	P6	202	CYC	NA-C1A-CHA-C4D
13	P6	202	CYC	C2A-C1A-CHA-C4D
13	P6	202	CYC	NA-C4A-CHB-C1B
13	P6	202	CYC	C3A-C4A-CHB-C1B
13	P6	202	CYC	C2C-C3C-CAC-CBC
13	P6	202	CYC	C4C-C3C-CAC-CBC
13	P6	202	CYC	NC-C4C-CHD-C1D
13	Q6	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	Q6	201	CYC	C3A-C4A-CHB-C1B
13	Q6	201	CYC	C2C-C3C-CAC-CBC
13	Q6	201	CYC	C4C-C3C-CAC-CBC
13	Q6	201	CYC	NC-C4C-CHD-C1D
13	Q6	202	CYC	NA-C4A-CHB-C1B
13	Q6	202	CYC	C3A-C4A-CHB-C1B
13	Q6	202	CYC	C2C-C3C-CAC-CBC
13	Q6	202	CYC	C4C-C3C-CAC-CBC
13	Q6	202	CYC	NC-C4C-CHD-C1D
13	Q6	202	CYC	ND-C1D-CHD-C4C
13	Q6	202	CYC	C2D-C1D-CHD-C4C
13	R6	201	CYC	NA-C4A-CHB-C1B
13	R6	201	CYC	C3A-C4A-CHB-C1B
13	R6	201	CYC	C4C-C3C-CAC-CBC
13	R6	201	CYC	NC-C4C-CHD-C1D
13	R6	201	CYC	ND-C1D-CHD-C4C
13	R6	201	CYC	C2D-C1D-CHD-C4C
13	S6	201	CYC	NA-C4A-CHB-C1B
13	S6	201	CYC	C3A-C4A-CHB-C1B
13	S6	201	CYC	C2C-C3C-CAC-CBC
13	S6	201	CYC	C4C-C3C-CAC-CBC
13	S6	201	CYC	NC-C4C-CHD-C1D
13	T6	201	CYC	NA-C1A-CHA-C4D
13	T6	201	CYC	C2A-C1A-CHA-C4D
13	T6	201	CYC	ND-C4D-CHA-C1A
13	T6	201	CYC	C3D-C4D-CHA-C1A
13	T6	201	CYC	NA-C4A-CHB-C1B
13	T6	201	CYC	C3A-C4A-CHB-C1B
13	T6	201	CYC	C4C-C3C-CAC-CBC
13	T6	201	CYC	NC-C4C-CHD-C1D
13	T6	201	CYC	C3C-C4C-CHD-C1D
13	T6	202	CYC	NA-C4A-CHB-C1B
13	T6	202	CYC	C3A-C4A-CHB-C1B
13	T6	202	CYC	NC-C4C-CHD-C1D
13	T6	202	CYC	ND-C1D-CHD-C4C
13	T6	202	CYC	C2D-C1D-CHD-C4C
13	U6	201	CYC	NA-C4A-CHB-C1B
13	U6	201	CYC	C3A-C4A-CHB-C1B
13	U6	201	CYC	NC-C4C-CHD-C1D
13	U6	201	CYC	ND-C1D-CHD-C4C
13	U6	201	CYC	C2D-C1D-CHD-C4C
13	V6	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	V6	201	CYC	C3A-C4A-CHB-C1B
13	V6	201	CYC	C2C-C3C-CAC-CBC
13	V6	201	CYC	C4C-C3C-CAC-CBC
13	V6	201	CYC	NC-C4C-CHD-C1D
13	V6	202	CYC	ND-C4D-CHA-C1A
13	V6	202	CYC	C3D-C4D-CHA-C1A
13	V6	202	CYC	NA-C4A-CHB-C1B
13	V6	202	CYC	C3A-C4A-CHB-C1B
13	V6	202	CYC	C2C-C3C-CAC-CBC
13	V6	202	CYC	C4C-C3C-CAC-CBC
13	V6	202	CYC	NC-C4C-CHD-C1D
13	V6	202	CYC	C3C-C4C-CHD-C1D
13	W6	201	CYC	NA-C4A-CHB-C1B
13	W6	201	CYC	C3A-C4A-CHB-C1B
13	W6	201	CYC	NC-C4C-CHD-C1D
13	W6	201	CYC	ND-C1D-CHD-C4C
13	W6	201	CYC	C2D-C1D-CHD-C4C
13	X6	201	CYC	NA-C4A-CHB-C1B
13	X6	201	CYC	C3A-C4A-CHB-C1B
13	X6	201	CYC	C2C-C3C-CAC-CBC
13	X6	201	CYC	NC-C4C-CHD-C1D
13	X6	201	CYC	ND-C1D-CHD-C4C
13	X6	201	CYC	C2D-C1D-CHD-C4C
13	X6	201	CYC	C3D-CAD-CBD-CGD
13	Z6	301	CYC	C2C-C3C-CAC-CBC
13	Z6	301	CYC	C4C-C3C-CAC-CBC
13	Z6	301	CYC	NC-C4C-CHD-C1D
13	Z6	301	CYC	ND-C1D-CHD-C4C
13	Z6	301	CYC	C2D-C1D-CHD-C4C
13	a6	201	CYC	NA-C4A-CHB-C1B
13	a6	201	CYC	C3A-C4A-CHB-C1B
13	a6	201	CYC	C2C-C3C-CAC-CBC
13	a6	201	CYC	C4C-C3C-CAC-CBC
13	a6	201	CYC	NC-C4C-CHD-C1D
13	a6	202	CYC	ND-C4D-CHA-C1A
13	a6	202	CYC	C3D-C4D-CHA-C1A
13	a6	202	CYC	NA-C4A-CHB-C1B
13	a6	202	CYC	C3A-C4A-CHB-C1B
13	a6	202	CYC	NC-C4C-CHD-C1D
13	a6	202	CYC	C3C-C4C-CHD-C1D
13	B7	201	CYC	NA-C4A-CHB-C1B
13	B7	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	B7	201	CYC	C4C-C3C-CAC-CBC
13	B7	201	CYC	NC-C4C-CHD-C1D
13	B7	201	CYC	ND-C1D-CHD-C4C
13	B7	201	CYC	C2D-C1D-CHD-C4C
13	C7	201	CYC	NA-C4A-CHB-C1B
13	C7	201	CYC	C3A-C4A-CHB-C1B
13	C7	201	CYC	C2C-C3C-CAC-CBC
13	C7	201	CYC	C4C-C3C-CAC-CBC
13	C7	201	CYC	NC-C4C-CHD-C1D
13	C7	202	CYC	NA-C1A-CHA-C4D
13	C7	202	CYC	C2A-C1A-CHA-C4D
13	C7	202	CYC	ND-C4D-CHA-C1A
13	C7	202	CYC	C3D-C4D-CHA-C1A
13	C7	202	CYC	NA-C4A-CHB-C1B
13	C7	202	CYC	C3A-C4A-CHB-C1B
13	C7	202	CYC	NC-C4C-CHD-C1D
13	C7	202	CYC	C3C-C4C-CHD-C1D
13	C7	202	CYC	ND-C1D-CHD-C4C
13	C7	202	CYC	C2D-C1D-CHD-C4C
13	D7	201	CYC	NA-C4A-CHB-C1B
13	D7	201	CYC	C3A-C4A-CHB-C1B
13	D7	201	CYC	C2C-C3C-CAC-CBC
13	D7	201	CYC	C4C-C3C-CAC-CBC
13	D7	201	CYC	NC-C4C-CHD-C1D
13	E7	201	CYC	NA-C1A-CHA-C4D
13	E7	201	CYC	C2A-C1A-CHA-C4D
13	E7	201	CYC	ND-C4D-CHA-C1A
13	E7	201	CYC	C3D-C4D-CHA-C1A
13	E7	201	CYC	NA-C4A-CHB-C1B
13	E7	201	CYC	C3A-C4A-CHB-C1B
13	E7	201	CYC	C2C-C3C-CAC-CBC
13	E7	201	CYC	C4C-C3C-CAC-CBC
13	E7	201	CYC	C3C-C4C-CHD-C1D
13	F7	201	CYC	NA-C4A-CHB-C1B
13	F7	201	CYC	C3A-C4A-CHB-C1B
13	F7	201	CYC	C4C-C3C-CAC-CBC
13	F7	201	CYC	NC-C4C-CHD-C1D
13	F7	201	CYC	ND-C1D-CHD-C4C
13	F7	201	CYC	C2D-C1D-CHD-C4C
13	F7	202	CYC	NA-C1A-CHA-C4D
13	F7	202	CYC	C2A-C1A-CHA-C4D
13	F7	202	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	F7	202	CYC	C3A-C4A-CHB-C1B
13	F7	202	CYC	C2C-C3C-CAC-CBC
13	F7	202	CYC	C4C-C3C-CAC-CBC
13	F7	202	CYC	NC-C4C-CHD-C1D
13	F7	202	CYC	ND-C1D-CHD-C4C
13	F7	202	CYC	C2D-C1D-CHD-C4C
13	G7	201	CYC	NA-C4A-CHB-C1B
13	G7	201	CYC	C3A-C4A-CHB-C1B
13	G7	201	CYC	C2C-C3C-CAC-CBC
13	G7	201	CYC	C4C-C3C-CAC-CBC
13	G7	201	CYC	NC-C4C-CHD-C1D
13	G7	201	CYC	ND-C1D-CHD-C4C
13	G7	201	CYC	C2D-C1D-CHD-C4C
13	H7	201	CYC	NA-C4A-CHB-C1B
13	H7	201	CYC	C3A-C4A-CHB-C1B
13	H7	201	CYC	C2C-C3C-CAC-CBC
13	H7	201	CYC	C4C-C3C-CAC-CBC
13	H7	201	CYC	NC-C4C-CHD-C1D
13	H7	201	CYC	ND-C1D-CHD-C4C
13	H7	201	CYC	C2D-C1D-CHD-C4C
13	I7	201	CYC	NA-C4A-CHB-C1B
13	I7	201	CYC	C3A-C4A-CHB-C1B
13	I7	201	CYC	NC-C4C-CHD-C1D
13	I7	201	CYC	ND-C1D-CHD-C4C
13	I7	201	CYC	C2D-C1D-CHD-C4C
13	J7	201	CYC	NA-C4A-CHB-C1B
13	J7	201	CYC	C3A-C4A-CHB-C1B
13	J7	201	CYC	NC-C4C-CHD-C1D
13	J7	201	CYC	ND-C1D-CHD-C4C
13	J7	201	CYC	C2D-C1D-CHD-C4C
13	J7	202	CYC	NA-C1A-CHA-C4D
13	J7	202	CYC	C2A-C1A-CHA-C4D
13	J7	202	CYC	NA-C4A-CHB-C1B
13	J7	202	CYC	C3A-C4A-CHB-C1B
13	J7	202	CYC	C2C-C3C-CAC-CBC
13	J7	202	CYC	C4C-C3C-CAC-CBC
13	J7	202	CYC	NC-C4C-CHD-C1D
13	K7	201	CYC	NA-C4A-CHB-C1B
13	K7	201	CYC	C3A-C4A-CHB-C1B
13	K7	201	CYC	C2C-C3C-CAC-CBC
13	K7	201	CYC	C4C-C3C-CAC-CBC
13	K7	201	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
13	K7	201	CYC	ND-C1D-CHD-C4C
13	K7	201	CYC	C2D-C1D-CHD-C4C
13	L7	201	CYC	C2C-C3C-CAC-CBC
13	L7	201	CYC	C4C-C3C-CAC-CBC
13	L7	201	CYC	NC-C4C-CHD-C1D
13	L7	201	CYC	ND-C1D-CHD-C4C
13	L7	201	CYC	C2D-C1D-CHD-C4C
13	M7	201	CYC	NA-C4A-CHB-C1B
13	M7	201	CYC	C3A-C4A-CHB-C1B
13	M7	201	CYC	C2C-C3C-CAC-CBC
13	M7	201	CYC	C4C-C3C-CAC-CBC
13	M7	201	CYC	NC-C4C-CHD-C1D
13	N7	201	CYC	NA-C4A-CHB-C1B
13	N7	201	CYC	C3A-C4A-CHB-C1B
13	N7	201	CYC	C2C-C3C-CAC-CBC
13	N7	201	CYC	C4C-C3C-CAC-CBC
13	N7	201	CYC	NC-C4C-CHD-C1D
13	N7	201	CYC	ND-C1D-CHD-C4C
13	N7	201	CYC	C2D-C1D-CHD-C4C
13	P7	201	CYC	NA-C1A-CHA-C4D
13	P7	201	CYC	NA-C4A-CHB-C1B
13	P7	201	CYC	C2C-C3C-CAC-CBC
13	P7	201	CYC	C4C-C3C-CAC-CBC
13	P7	201	CYC	NC-C4C-CHD-C1D
13	P7	201	CYC	C3C-C4C-CHD-C1D
13	P7	202	CYC	NA-C1A-CHA-C4D
13	P7	202	CYC	C2A-C1A-CHA-C4D
13	P7	202	CYC	NA-C4A-CHB-C1B
13	P7	202	CYC	C3A-C4A-CHB-C1B
13	P7	202	CYC	C2C-C3C-CAC-CBC
13	P7	202	CYC	C4C-C3C-CAC-CBC
13	P7	202	CYC	NC-C4C-CHD-C1D
13	P7	202	CYC	C3C-C4C-CHD-C1D
13	Q7	201	CYC	NA-C4A-CHB-C1B
13	Q7	201	CYC	C3A-C4A-CHB-C1B
13	Q7	201	CYC	C2C-C3C-CAC-CBC
13	Q7	201	CYC	C4C-C3C-CAC-CBC
13	Q7	201	CYC	NC-C4C-CHD-C1D
13	Q7	201	CYC	C2D-C1D-CHD-C4C
13	Q7	202	CYC	NA-C4A-CHB-C1B
13	Q7	202	CYC	C3A-C4A-CHB-C1B
13	Q7	202	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	Q7	202	CYC	C4C-C3C-CAC-CBC
13	Q7	202	CYC	NC-C4C-CHD-C1D
13	Q7	202	CYC	ND-C1D-CHD-C4C
13	Q7	202	CYC	C2D-C1D-CHD-C4C
13	R7	201	CYC	NA-C4A-CHB-C1B
13	R7	201	CYC	C3A-C4A-CHB-C1B
13	R7	201	CYC	C2C-C3C-CAC-CBC
13	R7	201	CYC	C4C-C3C-CAC-CBC
13	R7	201	CYC	NC-C4C-CHD-C1D
13	R7	201	CYC	ND-C1D-CHD-C4C
13	R7	201	CYC	C2D-C1D-CHD-C4C
13	R7	201	CYC	C3D-CAD-CBD-CGD
13	S7	201	CYC	NA-C4A-CHB-C1B
13	S7	201	CYC	C3A-C4A-CHB-C1B
13	S7	201	CYC	C2C-C3C-CAC-CBC
13	S7	201	CYC	C4C-C3C-CAC-CBC
13	S7	201	CYC	NC-C4C-CHD-C1D
13	T7	201	CYC	NA-C1A-CHA-C4D
13	T7	201	CYC	C2A-C1A-CHA-C4D
13	T7	201	CYC	ND-C4D-CHA-C1A
13	T7	201	CYC	C3D-C4D-CHA-C1A
13	T7	201	CYC	NA-C4A-CHB-C1B
13	T7	201	CYC	C3A-C4A-CHB-C1B
13	T7	201	CYC	C4C-C3C-CAC-CBC
13	T7	201	CYC	NC-C4C-CHD-C1D
13	T7	201	CYC	C3C-C4C-CHD-C1D
13	T7	202	CYC	NA-C4A-CHB-C1B
13	T7	202	CYC	C3A-C4A-CHB-C1B
13	T7	202	CYC	NC-C4C-CHD-C1D
13	T7	202	CYC	ND-C1D-CHD-C4C
13	T7	202	CYC	C2D-C1D-CHD-C4C
13	U7	201	CYC	NA-C4A-CHB-C1B
13	U7	201	CYC	C3A-C4A-CHB-C1B
13	U7	201	CYC	C2C-C3C-CAC-CBC
13	U7	201	CYC	C4C-C3C-CAC-CBC
13	U7	201	CYC	NC-C4C-CHD-C1D
13	U7	201	CYC	ND-C1D-CHD-C4C
13	U7	201	CYC	C2D-C1D-CHD-C4C
13	V7	201	CYC	NA-C4A-CHB-C1B
13	V7	201	CYC	C3A-C4A-CHB-C1B
13	V7	201	CYC	C2C-C3C-CAC-CBC
13	V7	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	V7	201	CYC	NC-C4C-CHD-C1D
13	V7	202	CYC	ND-C4D-CHA-C1A
13	V7	202	CYC	C3D-C4D-CHA-C1A
13	V7	202	CYC	NA-C4A-CHB-C1B
13	V7	202	CYC	C3A-C4A-CHB-C1B
13	V7	202	CYC	C4C-C3C-CAC-CBC
13	V7	202	CYC	NC-C4C-CHD-C1D
13	V7	202	CYC	C3C-C4C-CHD-C1D
13	V7	202	CYC	C3D-CAD-CBD-CGD
13	W7	201	CYC	NA-C4A-CHB-C1B
13	W7	201	CYC	C3A-C4A-CHB-C1B
13	W7	201	CYC	C2C-C3C-CAC-CBC
13	W7	201	CYC	C4C-C3C-CAC-CBC
13	W7	201	CYC	NC-C4C-CHD-C1D
13	W7	201	CYC	ND-C1D-CHD-C4C
13	W7	201	CYC	C2D-C1D-CHD-C4C
13	X7	201	CYC	NC-C4C-CHD-C1D
13	Z7	301	CYC	NA-C1A-CHA-C4D
13	Z7	301	CYC	NA-C4A-CHB-C1B
13	Z7	301	CYC	C3A-C4A-CHB-C1B
13	Z7	301	CYC	C2C-C3C-CAC-CBC
13	Z7	301	CYC	NC-C4C-CHD-C1D
13	a7	201	CYC	NA-C4A-CHB-C1B
13	a7	201	CYC	C3A-C4A-CHB-C1B
13	a7	201	CYC	NC-C4C-CHD-C1D
13	a7	202	CYC	NA-C1A-CHA-C4D
13	a7	202	CYC	C2A-C1A-CHA-C4D
13	a7	202	CYC	ND-C4D-CHA-C1A
13	a7	202	CYC	C3D-C4D-CHA-C1A
13	a7	202	CYC	NA-C4A-CHB-C1B
13	a7	202	CYC	C3A-C4A-CHB-C1B
13	a7	202	CYC	C2C-C3C-CAC-CBC
13	a7	202	CYC	C3C-C4C-CHD-C1D
13	42	301	CYC	C2B-C3B-CAB-CBB
13	n2	201	CYC	C2B-C3B-CAB-CBB
13	A1	301	CYC	C2B-C3B-CAB-CBB
13	N1	201	CYC	C2B-C3B-CAB-CBB
13	22	301	CYC	C2B-C3B-CAB-CBB
13	32	301	CYC	C2B-C3B-CAB-CBB
13	52	301	CYC	C2B-C3B-CAB-CBB
13	Q3	201	CYC	C2B-C3B-CAB-CBB
13	X3	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	Q4	201	CYC	C2B-C3B-CAB-CBB
13	a4	201	CYC	C2B-C3B-CAB-CBB
13	A6	301	CYC	C2B-C3B-CAB-CBB
13	I6	201	CYC	C2B-C3B-CAB-CBB
13	T7	202	CYC	C2B-C3B-CAB-CBB
13	Z7	301	CYC	C2B-C3B-CAB-CBB
13	Z3	301	CYC	C2B-C3B-CAB-CBB
13	V7	201	CYC	C2B-C3B-CAB-CBB
13	V1	201	CYC	C2B-C3B-CAB-CBB
13	M2	201	CYC	C2B-C3B-CAB-CBB
13	T3	202	CYC	C2B-C3B-CAB-CBB
13	Q7	201	CYC	C2B-C3B-CAB-CBB
13	V3	201	CYC	C2B-C3B-CAB-CBB
13	N5	201	CYC	C2B-C3B-CAB-CBB
13	F4	201	CYC	C2B-C3B-CAB-CBB
13	I4	201	CYC	C2B-C3B-CAB-CBB
13	C5	201	CYC	C2B-C3B-CAB-CBB
13	L5	201	CYC	C2B-C3B-CAB-CBB
13	Q5	201	CYC	C2B-C3B-CAB-CBB
13	F6	201	CYC	C2B-C3B-CAB-CBB
13	J6	201	CYC	C2B-C3B-CAB-CBB
13	Q6	201	CYC	C2B-C3B-CAB-CBB
13	T6	202	CYC	C2B-C3B-CAB-CBB
13	V6	201	CYC	C2B-C3B-CAB-CBB
13	B2	201	CYC	C2B-C3B-CAB-CBB
13	J4	201	CYC	C2B-C3B-CAB-CBB
13	T6	201	CYC	C2B-C3B-CAB-CBB
13	a7	201	CYC	C2B-C3B-CAB-CBB
13	I1	201	CYC	C2B-C3B-CAB-CBB
13	K1	201	CYC	C2B-C3B-CAB-CBB
13	S1	201	CYC	C2B-C3B-CAB-CBB
13	Z1	301	CYC	C2B-C3B-CAB-CBB
13	O2	201	CYC	C2B-C3B-CAB-CBB
13	F3	201	CYC	C2B-C3B-CAB-CBB
13	V4	201	CYC	C2B-C3B-CAB-CBB
13	I5	201	CYC	C2B-C3B-CAB-CBB
13	J5	201	CYC	C2B-C3B-CAB-CBB
13	V5	201	CYC	C2B-C3B-CAB-CBB
13	U6	201	CYC	C2B-C3B-CAB-CBB
13	X7	201	CYC	C2B-C3B-CAB-CBB
13	F1	201	CYC	C2B-C3B-CAB-CBB
13	G1	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	J1	201	CYC	C2B-C3B-CAB-CBB
13	Q1	201	CYC	C2B-C3B-CAB-CBB
13	T1	201	CYC	C2B-C3B-CAB-CBB
13	T1	202	CYC	C2B-C3B-CAB-CBB
13	U1	201	CYC	C2B-C3B-CAB-CBB
13	L2	201	CYC	C2B-C3B-CAB-CBB
13	X2	201	CYC	C2B-C3B-CAB-CBB
13	p2	201	CYC	C2B-C3B-CAB-CBB
13	s2	201	CYC	C2B-C3B-CAB-CBB
13	B3	201	CYC	C2B-C3B-CAB-CBB
13	C3	201	CYC	C2B-C3B-CAB-CBB
13	G3	201	CYC	C2B-C3B-CAB-CBB
13	H3	201	CYC	C2B-C3B-CAB-CBB
13	I3	201	CYC	C2B-C3B-CAB-CBB
13	J3	201	CYC	C2B-C3B-CAB-CBB
13	P3	202	CYC	C2B-C3B-CAB-CBB
13	a3	201	CYC	C2B-C3B-CAB-CBB
13	B4	201	CYC	C2B-C3B-CAB-CBB
13	C4	201	CYC	C2B-C3B-CAB-CBB
13	G4	201	CYC	C2B-C3B-CAB-CBB
13	H4	201	CYC	C2B-C3B-CAB-CBB
13	L4	201	CYC	C2B-C3B-CAB-CBB
13	T4	202	CYC	C2B-C3B-CAB-CBB
13	Z4	301	CYC	C2B-C3B-CAB-CBB
13	B5	201	CYC	C2B-C3B-CAB-CBB
13	F5	201	CYC	C2B-C3B-CAB-CBB
13	H5	201	CYC	C2B-C3B-CAB-CBB
13	K5	201	CYC	C2B-C3B-CAB-CBB
13	Z5	301	CYC	C2B-C3B-CAB-CBB
13	a5	201	CYC	C2B-C3B-CAB-CBB
13	B6	201	CYC	C2B-C3B-CAB-CBB
13	C6	201	CYC	C2B-C3B-CAB-CBB
13	G6	201	CYC	C2B-C3B-CAB-CBB
13	L6	201	CYC	C2B-C3B-CAB-CBB
13	Z6	301	CYC	C2B-C3B-CAB-CBB
13	B7	201	CYC	C2B-C3B-CAB-CBB
13	C7	201	CYC	C2B-C3B-CAB-CBB
13	G7	201	CYC	C2B-C3B-CAB-CBB
13	I7	201	CYC	C2B-C3B-CAB-CBB
13	P7	202	CYC	C2B-C3B-CAB-CBB
13	H1	201	CYC	C2B-C3B-CAB-CBB
13	W1	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	P2	201	CYC	C2B-C3B-CAB-CBB
13	a2	201	CYC	C2B-C3B-CAB-CBB
13	N4	201	CYC	C2B-C3B-CAB-CBB
13	N6	201	CYC	C2B-C3B-CAB-CBB
13	G1	201	CYC	ND-C1D-CHD-C4C
13	H1	201	CYC	ND-C1D-CHD-C4C
13	I1	201	CYC	ND-C1D-CHD-C4C
13	J1	202	CYC	ND-C1D-CHD-C4C
13	L1	201	CYC	ND-C1D-CHD-C4C
13	M1	201	CYC	ND-C1D-CHD-C4C
13	22	302	CYC	ND-C1D-CHD-C4C
13	32	302	CYC	ND-C1D-CHD-C4C
13	42	301	CYC	ND-C1D-CHD-C4C
13	42	302	CYC	ND-C1D-CHD-C4C
13	A2	202	CYC	ND-C1D-CHD-C4C
13	D2	201	CYC	ND-C1D-CHD-C4C
13	E2	201	CYC	ND-C1D-CHD-C4C
13	N2	802	CYC	ND-C1D-CHD-C4C
13	g2	201	CYC	ND-C1D-CHD-C4C
13	p2	201	CYC	ND-C1D-CHD-C4C
13	q2	201	CYC	ND-C1D-CHD-C4C
13	z2	201	CYC	ND-C1D-CHD-C4C
13	J3	202	CYC	ND-C1D-CHD-C4C
13	Q3	201	CYC	ND-C1D-CHD-C4C
13	Z3	301	CYC	ND-C1D-CHD-C4C
13	a3	201	CYC	ND-C1D-CHD-C4C
13	B4	201	CYC	ND-C1D-CHD-C4C
13	J4	202	CYC	ND-C1D-CHD-C4C
13	Q4	201	CYC	ND-C1D-CHD-C4C
13	V4	201	CYC	ND-C1D-CHD-C4C
13	a4	201	CYC	ND-C1D-CHD-C4C
13	C5	201	CYC	ND-C1D-CHD-C4C
13	H5	201	CYC	ND-C1D-CHD-C4C
13	J5	202	CYC	ND-C1D-CHD-C4C
13	X5	201	CYC	ND-C1D-CHD-C4C
13	a5	202	CYC	ND-C1D-CHD-C4C
13	B6	201	CYC	ND-C1D-CHD-C4C
13	C6	201	CYC	ND-C1D-CHD-C4C
13	H6	201	CYC	ND-C1D-CHD-C4C
13	I6	201	CYC	ND-C1D-CHD-C4C
13	J6	202	CYC	ND-C1D-CHD-C4C
13	K6	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	L6	201	CYC	ND-C1D-CHD-C4C
13	P6	202	CYC	ND-C1D-CHD-C4C
13	Q6	201	CYC	ND-C1D-CHD-C4C
13	a6	202	CYC	ND-C1D-CHD-C4C
13	E7	201	CYC	ND-C1D-CHD-C4C
13	J7	202	CYC	ND-C1D-CHD-C4C
13	M7	201	CYC	ND-C1D-CHD-C4C
13	P7	202	CYC	ND-C1D-CHD-C4C
13	Q7	201	CYC	ND-C1D-CHD-C4C
13	S7	201	CYC	ND-C1D-CHD-C4C
13	a7	201	CYC	ND-C1D-CHD-C4C
13	A1	301	CYC	C2D-C1D-CHD-C4C
13	A1	302	CYC	C2D-C1D-CHD-C4C
13	B1	201	CYC	C2D-C1D-CHD-C4C
13	C1	201	CYC	C2D-C1D-CHD-C4C
13	D1	201	CYC	C2D-C1D-CHD-C4C
13	G1	201	CYC	C2D-C1D-CHD-C4C
13	H1	201	CYC	C2D-C1D-CHD-C4C
13	J1	202	CYC	C2D-C1D-CHD-C4C
13	L1	201	CYC	C2D-C1D-CHD-C4C
13	M1	201	CYC	C2D-C1D-CHD-C4C
13	Q1	201	CYC	C2D-C1D-CHD-C4C
13	V1	201	CYC	C2D-C1D-CHD-C4C
13	a1	201	CYC	C2D-C1D-CHD-C4C
13	a1	202	CYC	C2D-C1D-CHD-C4C
13	32	301	CYC	C2D-C1D-CHD-C4C
13	52	302	CYC	C2D-C1D-CHD-C4C
13	A2	202	CYC	C2D-C1D-CHD-C4C
13	D2	201	CYC	C2D-C1D-CHD-C4C
13	F2	201	CYC	C2D-C1D-CHD-C4C
13	N2	801	CYC	C2D-C1D-CHD-C4C
13	N2	802	CYC	C2D-C1D-CHD-C4C
13	V2	201	CYC	C2D-C1D-CHD-C4C
13	a2	201	CYC	C2D-C1D-CHD-C4C
13	g2	201	CYC	C2D-C1D-CHD-C4C
13	i2	201	CYC	C2D-C1D-CHD-C4C
13	l2	201	CYC	C2D-C1D-CHD-C4C
13	n2	201	CYC	C2D-C1D-CHD-C4C
13	t2	201	CYC	C2D-C1D-CHD-C4C
13	x2	201	CYC	C2D-C1D-CHD-C4C
13	y2	201	CYC	C2D-C1D-CHD-C4C
13	z2	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	J3	202	CYC	C2D-C1D-CHD-C4C
13	M3	201	CYC	C2D-C1D-CHD-C4C
13	S3	201	CYC	C2D-C1D-CHD-C4C
13	V3	201	CYC	C2D-C1D-CHD-C4C
13	X3	201	CYC	C2D-C1D-CHD-C4C
13	C4	201	CYC	C2D-C1D-CHD-C4C
13	J4	201	CYC	C2D-C1D-CHD-C4C
13	J4	202	CYC	C2D-C1D-CHD-C4C
13	Q4	201	CYC	C2D-C1D-CHD-C4C
13	V4	201	CYC	C2D-C1D-CHD-C4C
13	a4	202	CYC	C2D-C1D-CHD-C4C
13	C5	201	CYC	C2D-C1D-CHD-C4C
13	D5	201	CYC	C2D-C1D-CHD-C4C
13	H5	201	CYC	C2D-C1D-CHD-C4C
13	J5	202	CYC	C2D-C1D-CHD-C4C
13	L5	201	CYC	C2D-C1D-CHD-C4C
13	Q5	201	CYC	C2D-C1D-CHD-C4C
13	V5	201	CYC	C2D-C1D-CHD-C4C
13	a5	202	CYC	C2D-C1D-CHD-C4C
13	A6	302	CYC	C2D-C1D-CHD-C4C
13	B6	201	CYC	C2D-C1D-CHD-C4C
13	C6	201	CYC	C2D-C1D-CHD-C4C
13	H6	201	CYC	C2D-C1D-CHD-C4C
13	I6	201	CYC	C2D-C1D-CHD-C4C
13	L6	201	CYC	C2D-C1D-CHD-C4C
13	M6	201	CYC	C2D-C1D-CHD-C4C
13	Q6	201	CYC	C2D-C1D-CHD-C4C
13	V6	201	CYC	C2D-C1D-CHD-C4C
13	a6	202	CYC	C2D-C1D-CHD-C4C
13	M7	201	CYC	C2D-C1D-CHD-C4C
13	S7	201	CYC	C2D-C1D-CHD-C4C
13	X7	201	CYC	C2D-C1D-CHD-C4C
13	B1	201	CYC	C2B-C3B-CAB-CBB
13	F7	201	CYC	C2B-C3B-CAB-CBB
13	W7	201	CYC	C2B-C3B-CAB-CBB
13	X2	201	CYC	NB-C1B-CHB-C4A
13	22	302	CYC	C2B-C3B-CAB-CBB
13	32	302	CYC	C2B-C3B-CAB-CBB
13	U2	201	CYC	C2B-C3B-CAB-CBB
13	W2	201	CYC	C2B-C3B-CAB-CBB
13	m2	201	CYC	C2B-C3B-CAB-CBB
13	t2	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	N3	201	CYC	C2B-C3B-CAB-CBB
13	T3	201	CYC	C2B-C3B-CAB-CBB
13	W3	201	CYC	C2B-C3B-CAB-CBB
13	S4	201	CYC	C2B-C3B-CAB-CBB
13	T5	202	CYC	C2B-C3B-CAB-CBB
13	S6	201	CYC	C2B-C3B-CAB-CBB
13	H7	201	CYC	C2B-C3B-CAB-CBB
13	a4	201	CYC	C2B-C1B-CHB-C4A
13	C1	201	CYC	C2B-C3B-CAB-CBB
13	X4	201	CYC	C2B-C3B-CAB-CBB
13	S5	201	CYC	C2B-C3B-CAB-CBB
13	U5	201	CYC	C2B-C3B-CAB-CBB
13	W5	201	CYC	C2B-C3B-CAB-CBB
13	H6	201	CYC	C2B-C3B-CAB-CBB
13	L3	201	CYC	C2B-C3B-CAB-CBB
13	T4	201	CYC	C2B-C3B-CAB-CBB
13	W6	201	CYC	C2B-C3B-CAB-CBB
13	A1	302	CYC	C2B-C3B-CAB-CBB
13	V1	202	CYC	C2B-C3B-CAB-CBB
13	42	302	CYC	C2B-C3B-CAB-CBB
13	A2	201	CYC	C2B-C3B-CAB-CBB
13	Q2	201	CYC	C2B-C3B-CAB-CBB
13	T2	201	CYC	C2B-C3B-CAB-CBB
13	x2	201	CYC	C2B-C3B-CAB-CBB
13	D4	201	CYC	C2B-C3B-CAB-CBB
13	P4	201	CYC	C2B-C3B-CAB-CBB
13	U4	201	CYC	C2B-C3B-CAB-CBB
13	W4	201	CYC	C2B-C3B-CAB-CBB
13	T5	201	CYC	C2B-C3B-CAB-CBB
13	J7	201	CYC	C2B-C3B-CAB-CBB
13	N7	201	CYC	C2B-C3B-CAB-CBB
13	T7	201	CYC	C2B-C3B-CAB-CBB
13	d2	201	CYC	C2B-C3B-CAB-CBB
13	z2	201	CYC	C2B-C3B-CAB-CBB
13	J1	202	CYC	NA-C1A-CHA-C4D
13	P1	202	CYC	NA-C1A-CHA-C4D
13	a1	202	CYC	NA-C1A-CHA-C4D
13	B2	202	CYC	NA-C1A-CHA-C4D
13	d2	201	CYC	NA-C1A-CHA-C4D
13	i2	201	CYC	NA-C1A-CHA-C4D
13	C3	201	CYC	NA-C1A-CHA-C4D
13	D3	201	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	P3	201	CYC	NA-C1A-CHA-C4D
13	Z3	301	CYC	NA-C1A-CHA-C4D
13	J4	202	CYC	NA-C1A-CHA-C4D
13	P4	202	CYC	NA-C1A-CHA-C4D
13	J5	202	CYC	NA-C1A-CHA-C4D
13	a5	202	CYC	NA-C1A-CHA-C4D
13	J6	202	CYC	NA-C1A-CHA-C4D
13	P6	201	CYC	NA-C1A-CHA-C4D
13	a6	202	CYC	NA-C1A-CHA-C4D
13	C7	201	CYC	NA-C1A-CHA-C4D
13	a1	201	CYC	C2B-C3B-CAB-CBB
13	52	302	CYC	C2B-C3B-CAB-CBB
13	K3	201	CYC	C2B-C3B-CAB-CBB
13	S3	201	CYC	C2B-C3B-CAB-CBB
13	V5	202	CYC	C2B-C3B-CAB-CBB
13	V6	202	CYC	C2B-C3B-CAB-CBB
13	X6	201	CYC	C2B-C3B-CAB-CBB
13	a7	202	CYC	C2B-C3B-CAB-CBB
13	G2	201	CYC	C2B-C3B-CAB-CBB
13	Z7	301	CYC	C2A-C1A-CHA-C4D
13	D7	201	CYC	C2B-C3B-CAB-CBB
13	E2	201	CYC	C2B-C3B-CAB-CBB
13	P4	202	CYC	C2B-C3B-CAB-CBB
13	P5	202	CYC	C2B-C3B-CAB-CBB
13	A6	302	CYC	C2B-C3B-CAB-CBB
13	C7	202	CYC	C2B-C3B-CAB-CBB
13	F1	201	CYC	C4D-C3D-CAD-CBD
13	F5	201	CYC	C4D-C3D-CAD-CBD
13	F6	201	CYC	C4D-C3D-CAD-CBD
13	F2	201	CYC	NA-C4A-CHB-C1B
13	p2	201	CYC	NA-C4A-CHB-C1B
13	E1	201	CYC	C2A-CAA-CBA-CGA
13	Q1	202	CYC	C3D-CAD-CBD-CGD
13	V1	202	CYC	C2A-CAA-CBA-CGA
13	B2	201	CYC	C3D-CAD-CBD-CGD
13	D2	201	CYC	C2A-CAA-CBA-CGA
13	S2	201	CYC	C3D-CAD-CBD-CGD
13	W2	201	CYC	C2A-CAA-CBA-CGA
13	e2	201	CYC	C2A-CAA-CBA-CGA
13	e2	201	CYC	C3D-CAD-CBD-CGD
13	k2	201	CYC	C2A-CAA-CBA-CGA
13	B3	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
13	E3	201	CYC	C2A-CAA-CBA-CGA
13	R3	201	CYC	C3D-CAD-CBD-CGD
13	D4	201	CYC	C2A-CAA-CBA-CGA
13	Q4	202	CYC	C3D-CAD-CBD-CGD
13	R4	201	CYC	C3D-CAD-CBD-CGD
13	V5	202	CYC	C2A-CAA-CBA-CGA
13	E6	201	CYC	C2A-CAA-CBA-CGA
13	Q6	202	CYC	C3D-CAD-CBD-CGD
13	V6	202	CYC	C2A-CAA-CBA-CGA
13	B7	201	CYC	C3D-CAD-CBD-CGD
13	C7	202	CYC	C2A-CAA-CBA-CGA
13	E7	201	CYC	C2A-CAA-CBA-CGA
13	V7	202	CYC	C2A-CAA-CBA-CGA
13	F1	201	CYC	C2D-C3D-CAD-CBD
13	N2	802	CYC	C2B-C3B-CAB-CBB
13	S2	201	CYC	C2B-C3B-CAB-CBB
13	w2	201	CYC	C2B-C3B-CAB-CBB
13	U3	201	CYC	C2B-C3B-CAB-CBB
13	V3	202	CYC	C2B-C3B-CAB-CBB
13	a3	202	CYC	C2B-C3B-CAB-CBB
13	K4	201	CYC	C2B-C3B-CAB-CBB
13	D6	201	CYC	C2B-C3B-CAB-CBB
13	J6	202	CYC	C2B-C3B-CAB-CBB
13	P6	202	CYC	C2B-C3B-CAB-CBB
13	a6	201	CYC	C2B-C3B-CAB-CBB
13	K7	201	CYC	C2B-C3B-CAB-CBB
13	S7	201	CYC	C2B-C3B-CAB-CBB
13	V7	202	CYC	C2B-C3B-CAB-CBB
13	P1	201	CYC	C3A-C4A-CHB-C1B
13	X1	201	CYC	C3A-C4A-CHB-C1B
13	X3	201	CYC	C3A-C4A-CHB-C1B
13	P7	201	CYC	C3A-C4A-CHB-C1B
13	A1	301	CYC	ND-C1D-CHD-C4C
13	A1	302	CYC	ND-C1D-CHD-C4C
13	B1	201	CYC	ND-C1D-CHD-C4C
13	C1	201	CYC	ND-C1D-CHD-C4C
13	D1	201	CYC	ND-C1D-CHD-C4C
13	E1	201	CYC	ND-C4D-CHA-C1A
13	E1	201	CYC	ND-C1D-CHD-C4C
13	P1	201	CYC	ND-C1D-CHD-C4C
13	P1	202	CYC	ND-C1D-CHD-C4C
13	Q1	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	S1	201	CYC	ND-C1D-CHD-C4C
13	T1	201	CYC	ND-C1D-CHD-C4C
13	V1	201	CYC	ND-C1D-CHD-C4C
13	V1	202	CYC	ND-C1D-CHD-C4C
13	a1	201	CYC	ND-C1D-CHD-C4C
13	a1	202	CYC	ND-C1D-CHD-C4C
13	22	301	CYC	ND-C1D-CHD-C4C
13	32	301	CYC	ND-C1D-CHD-C4C
13	52	301	CYC	ND-C1D-CHD-C4C
13	52	302	CYC	ND-C1D-CHD-C4C
13	B2	201	CYC	ND-C1D-CHD-C4C
13	B2	202	CYC	ND-C1D-CHD-C4C
13	F2	201	CYC	ND-C1D-CHD-C4C
13	G2	201	CYC	ND-C1D-CHD-C4C
13	L2	201	CYC	ND-C1D-CHD-C4C
13	M2	201	CYC	ND-C1D-CHD-C4C
13	N2	801	CYC	ND-C1D-CHD-C4C
13	O2	201	CYC	ND-C1D-CHD-C4C
13	Q2	201	CYC	ND-C1D-CHD-C4C
13	T2	201	CYC	ND-C1D-CHD-C4C
13	U2	201	CYC	ND-C1D-CHD-C4C
13	V2	201	CYC	ND-C1D-CHD-C4C
13	a2	201	CYC	ND-C1D-CHD-C4C
13	c2	801	CYC	ND-C1D-CHD-C4C
13	f2	201	CYC	ND-C1D-CHD-C4C
13	i2	201	CYC	ND-C1D-CHD-C4C
13	j2	201	CYC	ND-C1D-CHD-C4C
13	l2	201	CYC	ND-C1D-CHD-C4C
13	m2	201	CYC	ND-C1D-CHD-C4C
13	n2	201	CYC	ND-C1D-CHD-C4C
13	o2	801	CYC	ND-C1D-CHD-C4C
13	t2	201	CYC	ND-C1D-CHD-C4C
13	w2	201	CYC	ND-C1D-CHD-C4C
13	x2	201	CYC	ND-C1D-CHD-C4C
13	y2	201	CYC	ND-C1D-CHD-C4C
13	C3	201	CYC	ND-C1D-CHD-C4C
13	D3	201	CYC	ND-C1D-CHD-C4C
13	E3	201	CYC	ND-C1D-CHD-C4C
13	M3	201	CYC	ND-C1D-CHD-C4C
13	P3	201	CYC	ND-C1D-CHD-C4C
13	P3	202	CYC	ND-C1D-CHD-C4C
13	S3	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	T3	201	CYC	ND-C1D-CHD-C4C
13	V3	201	CYC	ND-C1D-CHD-C4C
13	V3	202	CYC	ND-C1D-CHD-C4C
13	X3	201	CYC	ND-C1D-CHD-C4C
13	a3	202	CYC	ND-C1D-CHD-C4C
13	C4	201	CYC	ND-C1D-CHD-C4C
13	D4	201	CYC	ND-C1D-CHD-C4C
13	E4	201	CYC	ND-C1D-CHD-C4C
13	J4	201	CYC	ND-C1D-CHD-C4C
13	M4	201	CYC	ND-C1D-CHD-C4C
13	P4	201	CYC	ND-C1D-CHD-C4C
13	P4	202	CYC	ND-C1D-CHD-C4C
13	S4	201	CYC	ND-C1D-CHD-C4C
13	T4	201	CYC	ND-C1D-CHD-C4C
13	V4	202	CYC	ND-C1D-CHD-C4C
13	X4	201	CYC	ND-C1D-CHD-C4C
13	a4	202	CYC	ND-C1D-CHD-C4C
13	B5	201	CYC	ND-C1D-CHD-C4C
13	D5	201	CYC	ND-C1D-CHD-C4C
13	E5	201	CYC	ND-C4D-CHA-C1A
13	E5	201	CYC	ND-C1D-CHD-C4C
13	L5	201	CYC	ND-C1D-CHD-C4C
13	M5	201	CYC	ND-C1D-CHD-C4C
13	P5	201	CYC	ND-C1D-CHD-C4C
13	Q5	201	CYC	ND-C1D-CHD-C4C
13	S5	201	CYC	ND-C1D-CHD-C4C
13	T5	201	CYC	ND-C1D-CHD-C4C
13	V5	201	CYC	ND-C1D-CHD-C4C
13	V5	202	CYC	ND-C1D-CHD-C4C
13	a5	201	CYC	ND-C1D-CHD-C4C
13	A6	301	CYC	ND-C1D-CHD-C4C
13	A6	302	CYC	ND-C1D-CHD-C4C
13	D6	201	CYC	ND-C1D-CHD-C4C
13	E6	201	CYC	ND-C1D-CHD-C4C
13	M6	201	CYC	ND-C1D-CHD-C4C
13	P6	201	CYC	ND-C1D-CHD-C4C
13	S6	201	CYC	ND-C1D-CHD-C4C
13	T6	201	CYC	ND-C1D-CHD-C4C
13	V6	201	CYC	ND-C1D-CHD-C4C
13	V6	202	CYC	ND-C1D-CHD-C4C
13	a6	201	CYC	ND-C1D-CHD-C4C
13	D7	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	P7	201	CYC	ND-C1D-CHD-C4C
13	T7	201	CYC	ND-C1D-CHD-C4C
13	V7	201	CYC	ND-C1D-CHD-C4C
13	V7	202	CYC	ND-C1D-CHD-C4C
13	X7	201	CYC	ND-C1D-CHD-C4C
13	Z7	301	CYC	ND-C1D-CHD-C4C
13	a7	202	CYC	ND-C1D-CHD-C4C
13	P1	202	CYC	C2B-C3B-CAB-CBB
13	R2	201	CYC	C2B-C3B-CAB-CBB
13	y2	201	CYC	C2B-C3B-CAB-CBB
13	G5	201	CYC	C2B-C3B-CAB-CBB
13	P5	201	CYC	C2B-C3B-CAB-CBB
13	a5	202	CYC	C2B-C3B-CAB-CBB
13	E1	201	CYC	C2D-C1D-CHD-C4C
13	P1	201	CYC	C2D-C1D-CHD-C4C
13	P1	202	CYC	C2D-C1D-CHD-C4C
13	S1	201	CYC	C2D-C1D-CHD-C4C
13	T1	201	CYC	C2D-C1D-CHD-C4C
13	V1	202	CYC	C2D-C1D-CHD-C4C
13	22	301	CYC	C2D-C1D-CHD-C4C
13	42	301	CYC	C2D-C1D-CHD-C4C
13	52	301	CYC	C2D-C1D-CHD-C4C
13	B2	201	CYC	C2D-C1D-CHD-C4C
13	B2	202	CYC	C2D-C1D-CHD-C4C
13	G2	201	CYC	C2D-C1D-CHD-C4C
13	L2	201	CYC	C2D-C1D-CHD-C4C
13	M2	201	CYC	C2D-C1D-CHD-C4C
13	O2	201	CYC	C2D-C1D-CHD-C4C
13	Q2	201	CYC	C2D-C1D-CHD-C4C
13	T2	201	CYC	C2D-C1D-CHD-C4C
13	U2	201	CYC	C2D-C1D-CHD-C4C
13	X2	201	CYC	C2D-C1D-CHD-C4C
13	c2	801	CYC	C2D-C1D-CHD-C4C
13	f2	201	CYC	C2D-C1D-CHD-C4C
13	j2	201	CYC	C2D-C1D-CHD-C4C
13	m2	201	CYC	C2D-C1D-CHD-C4C
13	o2	801	CYC	C2D-C1D-CHD-C4C
13	q2	201	CYC	C2D-C1D-CHD-C4C
13	w2	201	CYC	C2D-C1D-CHD-C4C
13	C3	201	CYC	C2D-C1D-CHD-C4C
13	D3	201	CYC	C2D-C1D-CHD-C4C
13	E3	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	P3	201	CYC	C2D-C1D-CHD-C4C
13	P3	202	CYC	C2D-C1D-CHD-C4C
13	T3	201	CYC	C2D-C1D-CHD-C4C
13	V3	202	CYC	C2D-C1D-CHD-C4C
13	a3	201	CYC	C2D-C1D-CHD-C4C
13	a3	202	CYC	C2D-C1D-CHD-C4C
13	D4	201	CYC	C2D-C1D-CHD-C4C
13	E4	201	CYC	C2D-C1D-CHD-C4C
13	M4	201	CYC	C2D-C1D-CHD-C4C
13	P4	201	CYC	C2D-C1D-CHD-C4C
13	P4	202	CYC	C2D-C1D-CHD-C4C
13	S4	201	CYC	C2D-C1D-CHD-C4C
13	T4	201	CYC	C2D-C1D-CHD-C4C
13	V4	202	CYC	C2D-C1D-CHD-C4C
13	X4	201	CYC	C2D-C1D-CHD-C4C
13	a4	201	CYC	C2D-C1D-CHD-C4C
13	B5	201	CYC	C2D-C1D-CHD-C4C
13	E5	201	CYC	C2D-C1D-CHD-C4C
13	M5	201	CYC	C2D-C1D-CHD-C4C
13	P5	201	CYC	C2D-C1D-CHD-C4C
13	P5	202	CYC	C2D-C1D-CHD-C4C
13	S5	201	CYC	C2D-C1D-CHD-C4C
13	T5	201	CYC	C2D-C1D-CHD-C4C
13	V5	202	CYC	C2D-C1D-CHD-C4C
13	a5	201	CYC	C2D-C1D-CHD-C4C
13	A6	301	CYC	C2D-C1D-CHD-C4C
13	D6	201	CYC	C2D-C1D-CHD-C4C
13	E6	201	CYC	C2D-C1D-CHD-C4C
13	J6	202	CYC	C2D-C1D-CHD-C4C
13	P6	201	CYC	C2D-C1D-CHD-C4C
13	P6	202	CYC	C2D-C1D-CHD-C4C
13	S6	201	CYC	C2D-C1D-CHD-C4C
13	T6	201	CYC	C2D-C1D-CHD-C4C
13	V6	202	CYC	C2D-C1D-CHD-C4C
13	a6	201	CYC	C2D-C1D-CHD-C4C
13	D7	201	CYC	C2D-C1D-CHD-C4C
13	J7	202	CYC	C2D-C1D-CHD-C4C
13	P7	201	CYC	C2D-C1D-CHD-C4C
13	T7	201	CYC	C2D-C1D-CHD-C4C
13	V7	201	CYC	C2D-C1D-CHD-C4C
13	V7	202	CYC	C2D-C1D-CHD-C4C
13	Z7	301	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
13	a7	201	CYC	C2D-C1D-CHD-C4C
13	a7	202	CYC	C2D-C1D-CHD-C4C
13	L1	201	CYC	C2B-C3B-CAB-CBB
13	A2	201	CYC	NB-C1B-CHB-C4A
13	a2	201	CYC	NB-C1B-CHB-C4A
13	q2	201	CYC	NB-C1B-CHB-C4A
13	y2	201	CYC	NB-C1B-CHB-C4A
13	a4	201	CYC	NB-C1B-CHB-C4A
13	X5	201	CYC	NB-C1B-CHB-C4A
13	U7	201	CYC	C2B-C3B-CAB-CBB
13	P1	201	CYC	C2B-C3B-CAB-CBB
13	B2	202	CYC	C2B-C3B-CAB-CBB
13	h2	201	CYC	C2B-C3B-CAB-CBB
13	r2	201	CYC	C2B-C3B-CAB-CBB
13	a4	202	CYC	C2B-C3B-CAB-CBB
13	P6	201	CYC	C2B-C3B-CAB-CBB
13	E7	201	CYC	C2B-C3B-CAB-CBB
13	A2	201	CYC	C2B-C1B-CHB-C4A
13	a2	201	CYC	C2B-C1B-CHB-C4A
13	g2	201	CYC	C2B-C3B-CAB-CBB
13	a6	202	CYC	C2B-C3B-CAB-CBB
13	C3	202	CYC	C2B-C3B-CAB-CBB
13	F4	201	CYC	C2D-C3D-CAD-CBD
13	F5	201	CYC	C2D-C3D-CAD-CBD
13	F6	201	CYC	C2D-C3D-CAD-CBD
13	X2	201	CYC	ND-C1D-CHD-C4C
13	P5	202	CYC	ND-C1D-CHD-C4C
13	C7	201	CYC	ND-C1D-CHD-C4C
13	E3	201	CYC	C2B-C3B-CAB-CBB
13	D5	201	CYC	C2B-C3B-CAB-CBB
13	P1	201	CYC	NA-C1A-CHA-C4D
13	P5	201	CYC	NA-C1A-CHA-C4D
13	E1	201	CYC	C3D-C4D-CHA-C1A
13	42	302	CYC	C2D-C1D-CHD-C4C
13	Q2	201	CYC	C3D-C4D-CHA-C1A
13	p2	201	CYC	C2D-C1D-CHD-C4C
13	Z3	301	CYC	C2D-C1D-CHD-C4C
13	E5	201	CYC	C3D-C4D-CHA-C1A
13	C7	201	CYC	C2D-C1D-CHD-C4C
13	E7	201	CYC	C2D-C1D-CHD-C4C
13	P7	202	CYC	C2D-C1D-CHD-C4C
13	X1	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	k2	201	CYC	C2B-C3B-CAB-CBB
13	V4	202	CYC	C2B-C3B-CAB-CBB
13	L7	201	CYC	C2B-C3B-CAB-CBB
13	D2	201	CYC	C2B-C3B-CAB-CBB
13	A1	301	CYC	C4B-C3B-CAB-CBB
13	I1	201	CYC	C4B-C3B-CAB-CBB
13	K1	201	CYC	C4B-C3B-CAB-CBB
13	N1	201	CYC	C4B-C3B-CAB-CBB
13	S1	201	CYC	C4B-C3B-CAB-CBB
13	T1	201	CYC	C4B-C3B-CAB-CBB
13	V1	201	CYC	C4B-C3B-CAB-CBB
13	Z1	301	CYC	C4B-C3B-CAB-CBB
13	22	301	CYC	C4B-C3B-CAB-CBB
13	32	301	CYC	C4B-C3B-CAB-CBB
13	42	301	CYC	C4B-C3B-CAB-CBB
13	52	301	CYC	C4B-C3B-CAB-CBB
13	B2	201	CYC	C4B-C3B-CAB-CBB
13	L2	201	CYC	C4B-C3B-CAB-CBB
13	M2	201	CYC	C4B-C3B-CAB-CBB
13	O2	201	CYC	C4B-C3B-CAB-CBB
13	n2	201	CYC	C4B-C3B-CAB-CBB
13	F3	201	CYC	C4B-C3B-CAB-CBB
13	J3	201	CYC	C4B-C3B-CAB-CBB
13	Q3	201	CYC	C4B-C3B-CAB-CBB
13	T3	202	CYC	C4B-C3B-CAB-CBB
13	V3	201	CYC	C4B-C3B-CAB-CBB
13	X3	201	CYC	C4B-C3B-CAB-CBB
13	Z3	301	CYC	C4B-C3B-CAB-CBB
13	B4	201	CYC	C4B-C3B-CAB-CBB
13	F4	201	CYC	C4B-C3B-CAB-CBB
13	I4	201	CYC	C4B-C3B-CAB-CBB
13	J4	201	CYC	C4B-C3B-CAB-CBB
13	Q4	201	CYC	C4B-C3B-CAB-CBB
13	V4	201	CYC	C4B-C3B-CAB-CBB
13	a4	201	CYC	C4B-C3B-CAB-CBB
13	C5	201	CYC	C4B-C3B-CAB-CBB
13	I5	201	CYC	C4B-C3B-CAB-CBB
13	J5	201	CYC	C4B-C3B-CAB-CBB
13	L5	201	CYC	C4B-C3B-CAB-CBB
13	N5	201	CYC	C4B-C3B-CAB-CBB
13	Q5	201	CYC	C4B-C3B-CAB-CBB
13	V5	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	Z5	301	CYC	C4B-C3B-CAB-CBB
13	A6	301	CYC	C4B-C3B-CAB-CBB
13	F6	201	CYC	C4B-C3B-CAB-CBB
13	I6	201	CYC	C4B-C3B-CAB-CBB
13	J6	201	CYC	C4B-C3B-CAB-CBB
13	Q6	201	CYC	C4B-C3B-CAB-CBB
13	T6	201	CYC	C4B-C3B-CAB-CBB
13	T6	202	CYC	C4B-C3B-CAB-CBB
13	U6	201	CYC	C4B-C3B-CAB-CBB
13	V6	201	CYC	C4B-C3B-CAB-CBB
13	P7	202	CYC	C4B-C3B-CAB-CBB
13	Q7	201	CYC	C4B-C3B-CAB-CBB
13	T7	202	CYC	C4B-C3B-CAB-CBB
13	V7	201	CYC	C4B-C3B-CAB-CBB
13	X7	201	CYC	C4B-C3B-CAB-CBB
13	Z7	301	CYC	C4B-C3B-CAB-CBB
13	a7	201	CYC	C4B-C3B-CAB-CBB
13	a2	201	CYC	C2A-C1A-CHA-C4D
13	a4	202	CYC	C2A-C1A-CHA-C4D
13	P7	201	CYC	C2A-C1A-CHA-C4D
13	a1	202	CYC	C2B-C3B-CAB-CBB
13	C2	201	CYC	C2B-C3B-CAB-CBB
13	F3	202	CYC	C2B-C1B-CHB-C4A
13	V3	202	CYC	C2B-C1B-CHB-C4A
13	X4	201	CYC	C2B-C1B-CHB-C4A
13	X5	201	CYC	C2B-C1B-CHB-C4A
13	F6	202	CYC	C2B-C1B-CHB-C4A
13	X6	201	CYC	C2B-C1B-CHB-C4A
13	F7	202	CYC	C2B-C1B-CHB-C4A
13	H7	201	CYC	C2B-C1B-CHB-C4A
13	V7	202	CYC	C2B-C1B-CHB-C4A
13	a7	201	CYC	C2B-C1B-CHB-C4A
13	t2	201	CYC	NA-C4A-CHB-C1B
13	J1	202	CYC	C3D-CAD-CBD-CGD
13	X1	201	CYC	C3D-CAD-CBD-CGD
13	F2	201	CYC	C2A-CAA-CBA-CGA
13	N2	802	CYC	C2A-CAA-CBA-CGA
13	S2	201	CYC	C2A-CAA-CBA-CGA
13	j2	201	CYC	C3D-CAD-CBD-CGD
13	t2	201	CYC	C3D-CAD-CBD-CGD
13	C3	202	CYC	C3D-CAD-CBD-CGD
13	J3	202	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	J3	202	CYC	C3D-CAD-CBD-CGD
13	T3	202	CYC	C3D-CAD-CBD-CGD
13	V3	202	CYC	C3D-CAD-CBD-CGD
13	J4	202	CYC	C3D-CAD-CBD-CGD
13	V4	202	CYC	C2A-CAA-CBA-CGA
13	Z4	301	CYC	C3D-CAD-CBD-CGD
13	E5	201	CYC	C2A-CAA-CBA-CGA
13	J5	202	CYC	C3D-CAD-CBD-CGD
13	R5	201	CYC	C3D-CAD-CBD-CGD
13	X5	201	CYC	C3D-CAD-CBD-CGD
13	D6	201	CYC	C2A-CAA-CBA-CGA
13	J6	202	CYC	C3D-CAD-CBD-CGD
13	R6	201	CYC	C3D-CAD-CBD-CGD
13	C7	202	CYC	C3D-CAD-CBD-CGD
13	G7	201	CYC	C2A-CAA-CBA-CGA
13	J7	202	CYC	C2A-CAA-CBA-CGA
13	J7	202	CYC	C3D-CAD-CBD-CGD
13	N7	201	CYC	C3D-CAD-CBD-CGD
13	Q7	202	CYC	C3D-CAD-CBD-CGD
13	D1	201	CYC	C2B-C3B-CAB-CBB
13	D3	201	CYC	C2B-C3B-CAB-CBB
13	C4	202	CYC	C2B-C3B-CAB-CBB
13	e2	201	CYC	C2B-C3B-CAB-CBB
13	K6	201	CYC	C2B-C3B-CAB-CBB
13	L1	201	CYC	C3A-C4A-CHB-C1B
13	R2	201	CYC	C3A-C4A-CHB-C1B
13	S2	201	CYC	C3A-C4A-CHB-C1B
13	J5	202	CYC	C2B-C3B-CAB-CBB
13	D3	201	CYC	ND-C4D-CHA-C1A
13	Q7	202	CYC	ND-C4D-CHA-C1A
13	J1	202	CYC	C2B-C3B-CAB-CBB
13	C6	202	CYC	C2B-C3B-CAB-CBB
13	F1	202	CYC	NB-C1B-CHB-C4A
13	V1	202	CYC	NB-C1B-CHB-C4A
13	X1	201	CYC	NB-C1B-CHB-C4A
13	a1	201	CYC	NB-C1B-CHB-C4A
13	O2	201	CYC	NB-C1B-CHB-C4A
13	T2	201	CYC	NB-C1B-CHB-C4A
13	z2	201	CYC	NB-C1B-CHB-C4A
13	F3	202	CYC	NB-C1B-CHB-C4A
13	V3	202	CYC	NB-C1B-CHB-C4A
13	Z3	301	CYC	NB-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
13	a3	201	CYC	NB-C1B-CHB-C4A
13	F4	202	CYC	NB-C1B-CHB-C4A
13	L4	201	CYC	NB-C1B-CHB-C4A
13	X4	201	CYC	NB-C1B-CHB-C4A
13	L5	201	CYC	NB-C1B-CHB-C4A
13	F6	202	CYC	NB-C1B-CHB-C4A
13	V6	202	CYC	NB-C1B-CHB-C4A
13	X6	201	CYC	NB-C1B-CHB-C4A
13	a6	201	CYC	NB-C1B-CHB-C4A
13	F7	202	CYC	NB-C1B-CHB-C4A
13	H7	201	CYC	NB-C1B-CHB-C4A
13	S7	201	CYC	NB-C1B-CHB-C4A
13	V7	202	CYC	NB-C1B-CHB-C4A
13	a7	201	CYC	NB-C1B-CHB-C4A
13	H2	201	CYC	NA-C1A-CHA-C4D
13	V2	201	CYC	C2B-C3B-CAB-CBB
13	J4	202	CYC	C2B-C3B-CAB-CBB
13	F4	202	CYC	C2B-C1B-CHB-C4A
13	a6	201	CYC	C2B-C1B-CHB-C4A
13	P1	202	CYC	C2A-C1A-CHA-C4D
13	a1	202	CYC	C2A-C1A-CHA-C4D
13	d2	201	CYC	C2A-C1A-CHA-C4D
13	D3	201	CYC	C2A-C1A-CHA-C4D
13	v2	201	CYC	C2B-C3B-CAB-CBB
13	F7	201	CYC	C4D-C3D-CAD-CBD
13	L1	201	CYC	NA-C4A-CHB-C1B
13	Z1	301	CYC	NA-C4A-CHB-C1B
13	D2	201	CYC	NA-C4A-CHB-C1B
13	E2	201	CYC	NA-C4A-CHB-C1B
13	G2	201	CYC	NA-C4A-CHB-C1B
13	N2	802	CYC	NA-C4A-CHB-C1B
13	R2	201	CYC	NA-C4A-CHB-C1B
13	S2	201	CYC	NA-C4A-CHB-C1B
13	T2	201	CYC	NA-C4A-CHB-C1B
13	U2	201	CYC	NA-C4A-CHB-C1B
13	e2	201	CYC	NA-C4A-CHB-C1B
13	f2	201	CYC	NA-C4A-CHB-C1B
13	h2	201	CYC	NA-C4A-CHB-C1B
13	l2	201	CYC	NA-C4A-CHB-C1B
13	r2	201	CYC	NA-C4A-CHB-C1B
13	s2	201	CYC	NA-C4A-CHB-C1B
13	v2	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	y2	201	CYC	NA-C4A-CHB-C1B
13	z2	201	CYC	NA-C4A-CHB-C1B
13	L3	201	CYC	NA-C4A-CHB-C1B
13	D4	201	CYC	NA-C4A-CHB-C1B
13	P4	202	CYC	NA-C4A-CHB-C1B
13	Z4	301	CYC	NA-C4A-CHB-C1B
13	P5	201	CYC	NA-C4A-CHB-C1B
13	Z5	301	CYC	NA-C4A-CHB-C1B
13	D6	201	CYC	NA-C4A-CHB-C1B
13	L6	201	CYC	NA-C4A-CHB-C1B
13	Z6	301	CYC	NA-C4A-CHB-C1B
13	L7	201	CYC	NA-C4A-CHB-C1B
13	X7	201	CYC	NA-C4A-CHB-C1B
13	B2	201	CYC	C2A-CAA-CBA-CGA
13	i2	201	CYC	C3D-CAD-CBD-CGD
13	32	301	CYC	NB-C1B-CHB-C4A
13	V4	202	CYC	NB-C1B-CHB-C4A
13	P5	201	CYC	NB-C1B-CHB-C4A
13	V5	202	CYC	NB-C1B-CHB-C4A
13	a5	201	CYC	NB-C1B-CHB-C4A
13	F6	202	CYC	C2B-C3B-CAB-CBB
13	Z1	301	CYC	C3A-C4A-CHB-C1B
13	D2	201	CYC	C3A-C4A-CHB-C1B
13	E2	201	CYC	C3A-C4A-CHB-C1B
13	F2	201	CYC	C3A-C4A-CHB-C1B
13	G2	201	CYC	C3A-C4A-CHB-C1B
13	N2	801	CYC	C3A-C4A-CHB-C1B
13	N2	802	CYC	C3A-C4A-CHB-C1B
13	T2	201	CYC	C3A-C4A-CHB-C1B
13	e2	201	CYC	C3A-C4A-CHB-C1B
13	f2	201	CYC	C3A-C4A-CHB-C1B
13	h2	201	CYC	C3A-C4A-CHB-C1B
13	l2	201	CYC	C3A-C4A-CHB-C1B
13	p2	201	CYC	C3A-C4A-CHB-C1B
13	r2	201	CYC	C3A-C4A-CHB-C1B
13	v2	201	CYC	C3A-C4A-CHB-C1B
13	y2	201	CYC	C3A-C4A-CHB-C1B
13	z2	201	CYC	C3A-C4A-CHB-C1B
13	L3	201	CYC	C3A-C4A-CHB-C1B
13	D4	201	CYC	C3A-C4A-CHB-C1B
13	P4	202	CYC	C3A-C4A-CHB-C1B
13	Z4	301	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
13	P5	201	CYC	C3A-C4A-CHB-C1B
13	X5	201	CYC	C3A-C4A-CHB-C1B
13	Z5	301	CYC	C3A-C4A-CHB-C1B
13	D6	201	CYC	C3A-C4A-CHB-C1B
13	P6	201	CYC	C3A-C4A-CHB-C1B
13	Z6	301	CYC	C3A-C4A-CHB-C1B
13	L7	201	CYC	C3A-C4A-CHB-C1B
13	X7	201	CYC	C3A-C4A-CHB-C1B
13	V1	202	CYC	C2B-C1B-CHB-C4A
13	X1	201	CYC	C2B-C1B-CHB-C4A
13	S7	201	CYC	C2B-C1B-CHB-C4A
13	c2	801	CYC	C2B-C3B-CAB-CBB
13	f2	201	CYC	C2B-C3B-CAB-CBB
13	B1	201	CYC	C4B-C3B-CAB-CBB
13	C1	201	CYC	C4B-C3B-CAB-CBB
13	F1	201	CYC	C4B-C3B-CAB-CBB
13	G1	201	CYC	C4B-C3B-CAB-CBB
13	H1	201	CYC	C4B-C3B-CAB-CBB
13	J1	201	CYC	C4B-C3B-CAB-CBB
13	Q1	201	CYC	C4B-C3B-CAB-CBB
13	T1	202	CYC	C4B-C3B-CAB-CBB
13	U1	201	CYC	C4B-C3B-CAB-CBB
13	W1	201	CYC	C4B-C3B-CAB-CBB
13	22	302	CYC	C4B-C3B-CAB-CBB
13	32	302	CYC	C4B-C3B-CAB-CBB
13	P2	201	CYC	C4B-C3B-CAB-CBB
13	U2	201	CYC	C4B-C3B-CAB-CBB
13	W2	201	CYC	C4B-C3B-CAB-CBB
13	X2	201	CYC	C4B-C3B-CAB-CBB
13	a2	201	CYC	C4B-C3B-CAB-CBB
13	m2	201	CYC	C4B-C3B-CAB-CBB
13	p2	201	CYC	C4B-C3B-CAB-CBB
13	s2	201	CYC	C4B-C3B-CAB-CBB
13	t2	201	CYC	C4B-C3B-CAB-CBB
13	B3	201	CYC	C4B-C3B-CAB-CBB
13	C3	201	CYC	C4B-C3B-CAB-CBB
13	G3	201	CYC	C4B-C3B-CAB-CBB
13	H3	201	CYC	C4B-C3B-CAB-CBB
13	I3	201	CYC	C4B-C3B-CAB-CBB
13	N3	201	CYC	C4B-C3B-CAB-CBB
13	P3	202	CYC	C4B-C3B-CAB-CBB
13	T3	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	W3	201	CYC	C4B-C3B-CAB-CBB
13	a3	201	CYC	C4B-C3B-CAB-CBB
13	C4	201	CYC	C4B-C3B-CAB-CBB
13	G4	201	CYC	C4B-C3B-CAB-CBB
13	H4	201	CYC	C4B-C3B-CAB-CBB
13	L4	201	CYC	C4B-C3B-CAB-CBB
13	N4	201	CYC	C4B-C3B-CAB-CBB
13	S4	201	CYC	C4B-C3B-CAB-CBB
13	T4	201	CYC	C4B-C3B-CAB-CBB
13	T4	202	CYC	C4B-C3B-CAB-CBB
13	Z4	301	CYC	C4B-C3B-CAB-CBB
13	B5	201	CYC	C4B-C3B-CAB-CBB
13	F5	201	CYC	C4B-C3B-CAB-CBB
13	H5	201	CYC	C4B-C3B-CAB-CBB
13	K5	201	CYC	C4B-C3B-CAB-CBB
13	S5	201	CYC	C4B-C3B-CAB-CBB
13	T5	202	CYC	C4B-C3B-CAB-CBB
13	U5	201	CYC	C4B-C3B-CAB-CBB
13	W5	201	CYC	C4B-C3B-CAB-CBB
13	a5	201	CYC	C4B-C3B-CAB-CBB
13	B6	201	CYC	C4B-C3B-CAB-CBB
13	C6	201	CYC	C4B-C3B-CAB-CBB
13	G6	201	CYC	C4B-C3B-CAB-CBB
13	H6	201	CYC	C4B-C3B-CAB-CBB
13	L6	201	CYC	C4B-C3B-CAB-CBB
13	N6	201	CYC	C4B-C3B-CAB-CBB
13	S6	201	CYC	C4B-C3B-CAB-CBB
13	W6	201	CYC	C4B-C3B-CAB-CBB
13	Z6	301	CYC	C4B-C3B-CAB-CBB
13	B7	201	CYC	C4B-C3B-CAB-CBB
13	C7	201	CYC	C4B-C3B-CAB-CBB
13	F7	201	CYC	C4B-C3B-CAB-CBB
13	G7	201	CYC	C4B-C3B-CAB-CBB
13	H7	201	CYC	C4B-C3B-CAB-CBB
13	I7	201	CYC	C4B-C3B-CAB-CBB
13	W7	201	CYC	C4B-C3B-CAB-CBB
13	J1	202	CYC	C2A-C1A-CHA-C4D
13	B2	202	CYC	C2A-C1A-CHA-C4D
13	i2	201	CYC	C2A-C1A-CHA-C4D
13	C3	201	CYC	C2A-C1A-CHA-C4D
13	P3	201	CYC	C2A-C1A-CHA-C4D
13	Z3	301	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	J4	202	CYC	C2A-C1A-CHA-C4D
13	a5	202	CYC	C2A-C1A-CHA-C4D
13	J6	202	CYC	C2A-C1A-CHA-C4D
13	a6	202	CYC	C2A-C1A-CHA-C4D
13	C7	201	CYC	C2A-C1A-CHA-C4D
13	C1	202	CYC	C2B-C3B-CAB-CBB
13	F2	201	CYC	C2B-C3B-CAB-CBB
13	P3	201	CYC	C2B-C3B-CAB-CBB
13	E5	201	CYC	C2B-C3B-CAB-CBB
13	22	301	CYC	NB-C1B-CHB-C4A
13	42	301	CYC	NB-C1B-CHB-C4A
13	L3	201	CYC	NB-C1B-CHB-C4A
13	J3	202	CYC	C2B-C3B-CAB-CBB
13	A2	202	CYC	ND-C4D-CHA-C1A
13	H2	201	CYC	ND-C4D-CHA-C1A
13	Q3	202	CYC	ND-C4D-CHA-C1A
13	J7	202	CYC	ND-C4D-CHA-C1A
13	F1	202	CYC	C2B-C1B-CHB-C4A
13	P1	201	CYC	C3D-CAD-CBD-CGD
13	E2	201	CYC	C2A-CAA-CBA-CGA
13	s2	201	CYC	C2A-CAA-CBA-CGA
13	G3	201	CYC	C2A-CAA-CBA-CGA
13	G3	201	CYC	C3D-CAD-CBD-CGD
13	P4	202	CYC	C3D-CAD-CBD-CGD
13	a4	202	CYC	C2A-CAA-CBA-CGA
13	P6	201	CYC	C3D-CAD-CBD-CGD
13	T6	202	CYC	C3D-CAD-CBD-CGD
13	a6	202	CYC	C2A-CAA-CBA-CGA
13	D7	201	CYC	C2A-CAA-CBA-CGA
13	C5	202	CYC	C2B-C3B-CAB-CBB
13	J7	202	CYC	C2B-C3B-CAB-CBB
13	E4	201	CYC	C2B-C3B-CAB-CBB
13	A1	301	CYC	NB-C1B-CHB-C4A
13	52	301	CYC	NB-C1B-CHB-C4A
13	S3	201	CYC	NB-C1B-CHB-C4A
13	P4	202	CYC	NB-C1B-CHB-C4A
13	A6	301	CYC	NB-C1B-CHB-C4A
13	L7	201	CYC	NB-C1B-CHB-C4A
13	E1	201	CYC	C2B-C3B-CAB-CBB
13	P1	201	CYC	C2A-C1A-CHA-C4D
13	P4	202	CYC	C2A-C1A-CHA-C4D
13	J5	202	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	P5	201	CYC	C2A-C1A-CHA-C4D
13	P6	201	CYC	C2A-C1A-CHA-C4D
13	X5	201	CYC	C2B-C3B-CAB-CBB
13	D3	201	CYC	C3D-C4D-CHA-C1A
13	Q7	202	CYC	C3D-C4D-CHA-C1A
13	L4	201	CYC	C2B-C1B-CHB-C4A
13	L5	201	CYC	C2B-C1B-CHB-C4A
13	V6	202	CYC	C2B-C1B-CHB-C4A
13	E6	201	CYC	C2B-C3B-CAB-CBB
13	F3	201	CYC	C2D-C3D-CAD-CBD
13	F3	202	CYC	C2B-C3B-CAB-CBB
13	F7	202	CYC	C2B-C3B-CAB-CBB
13	H3	201	CYC	NB-C1B-CHB-C4A
13	F5	202	CYC	NB-C1B-CHB-C4A
13	K7	201	CYC	NB-C1B-CHB-C4A
13	52	301	CYC	NA-C1A-CHA-C4D
13	42	301	CYC	C2A-CAA-CBA-CGA
13	F2	201	CYC	C3D-CAD-CBD-CGD
13	f2	201	CYC	C3D-CAD-CBD-CGD
13	X4	201	CYC	C3D-CAD-CBD-CGD
13	K5	201	CYC	C3D-CAD-CBD-CGD
13	a5	202	CYC	C3D-CAD-CBD-CGD
13	G7	201	CYC	C3D-CAD-CBD-CGD
13	T7	202	CYC	C3D-CAD-CBD-CGD
13	J7	202	CYC	C3D-C4D-CHA-C1A
13	A1	302	CYC	C4B-C3B-CAB-CBB
13	V1	202	CYC	C4B-C3B-CAB-CBB
13	42	302	CYC	C4B-C3B-CAB-CBB
13	A2	201	CYC	C4B-C3B-CAB-CBB
13	Q2	201	CYC	C4B-C3B-CAB-CBB
13	T2	201	CYC	C4B-C3B-CAB-CBB
13	x2	201	CYC	C4B-C3B-CAB-CBB
13	L3	201	CYC	C4B-C3B-CAB-CBB
13	D4	201	CYC	C4B-C3B-CAB-CBB
13	P4	201	CYC	C4B-C3B-CAB-CBB
13	U4	201	CYC	C4B-C3B-CAB-CBB
13	W4	201	CYC	C4B-C3B-CAB-CBB
13	X4	201	CYC	C4B-C3B-CAB-CBB
13	T5	201	CYC	C4B-C3B-CAB-CBB
13	J7	201	CYC	C4B-C3B-CAB-CBB
13	N7	201	CYC	C4B-C3B-CAB-CBB
13	T7	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	H2	201	CYC	C2B-C3B-CAB-CBB
13	A1	301	CYC	C2C-C3C-CAC-CBC
13	B1	201	CYC	C2C-C3C-CAC-CBC
13	E1	201	CYC	C2C-C3C-CAC-CBC
13	J1	201	CYC	C2C-C3C-CAC-CBC
13	M1	201	CYC	C2C-C3C-CAC-CBC
13	P1	202	CYC	C2C-C3C-CAC-CBC
13	T1	201	CYC	C2C-C3C-CAC-CBC
13	V1	202	CYC	C2C-C3C-CAC-CBC
13	52	301	CYC	C2C-C3C-CAC-CBC
13	A2	201	CYC	C2C-C3C-CAC-CBC
13	A2	202	CYC	C2C-C3C-CAC-CBC
13	B2	202	CYC	C2C-C3C-CAC-CBC
13	Q2	201	CYC	C2C-C3C-CAC-CBC
13	S2	201	CYC	C2C-C3C-CAC-CBC
13	T2	201	CYC	C2C-C3C-CAC-CBC
13	V2	201	CYC	C2C-C3C-CAC-CBC
13	X2	201	CYC	C2C-C3C-CAC-CBC
13	s2	201	CYC	C2C-C3C-CAC-CBC
13	F3	201	CYC	C2C-C3C-CAC-CBC
13	L3	201	CYC	C2C-C3C-CAC-CBC
13	T3	201	CYC	C2C-C3C-CAC-CBC
13	V3	202	CYC	C2C-C3C-CAC-CBC
13	I4	201	CYC	C2C-C3C-CAC-CBC
13	L4	201	CYC	C2C-C3C-CAC-CBC
13	P4	202	CYC	C2C-C3C-CAC-CBC
13	T4	201	CYC	C2C-C3C-CAC-CBC
13	E5	201	CYC	C2C-C3C-CAC-CBC
13	P5	201	CYC	C2C-C3C-CAC-CBC
13	R5	201	CYC	C2C-C3C-CAC-CBC
13	S5	201	CYC	C2C-C3C-CAC-CBC
13	T5	201	CYC	C2C-C3C-CAC-CBC
13	W5	201	CYC	C2C-C3C-CAC-CBC
13	A6	301	CYC	C2C-C3C-CAC-CBC
13	E6	201	CYC	C2C-C3C-CAC-CBC
13	I6	201	CYC	C2C-C3C-CAC-CBC
13	J6	201	CYC	C2C-C3C-CAC-CBC
13	P6	201	CYC	C2C-C3C-CAC-CBC
13	T6	201	CYC	C2C-C3C-CAC-CBC
13	B7	201	CYC	C2C-C3C-CAC-CBC
13	F7	201	CYC	C2C-C3C-CAC-CBC
13	J7	201	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	T7	201	CYC	C2C-C3C-CAC-CBC
13	V7	202	CYC	C2C-C3C-CAC-CBC
13	X7	201	CYC	C2C-C3C-CAC-CBC
13	a7	201	CYC	C2C-C3C-CAC-CBC
13	A2	202	CYC	C3D-C4D-CHA-C1A
13	A6	301	CYC	NA-C1A-CHA-C4D
13	a1	201	CYC	C2B-C1B-CHB-C4A
13	O2	201	CYC	C2B-C1B-CHB-C4A
13	T2	201	CYC	C2B-C1B-CHB-C4A
13	z2	201	CYC	C2B-C1B-CHB-C4A
13	Z3	301	CYC	C2B-C1B-CHB-C4A
13	a3	201	CYC	C2B-C1B-CHB-C4A
13	P5	201	CYC	C2B-C1B-CHB-C4A
13	V5	202	CYC	C2B-C1B-CHB-C4A
13	a5	201	CYC	C2B-C1B-CHB-C4A
13	c2	801	CYC	C2A-CAA-CBA-CGA
13	Q3	202	CYC	C3D-CAD-CBD-CGD
13	P4	201	CYC	C2A-CAA-CBA-CGA
13	H2	201	CYC	C3D-C4D-CHA-C1A
13	Q3	202	CYC	C3D-C4D-CHA-C1A
13	Z7	301	CYC	NB-C1B-CHB-C4A
13	H2	201	CYC	C2A-C1A-CHA-C4D
13	V4	202	CYC	C2B-C1B-CHB-C4A
13	F5	202	CYC	C2B-C3B-CAB-CBB
13	J1	201	CYC	NA-C1A-CHA-C4D
13	V1	202	CYC	NA-C1A-CHA-C4D
13	42	301	CYC	NA-C1A-CHA-C4D
13	V3	202	CYC	NA-C1A-CHA-C4D
13	J4	201	CYC	NA-C1A-CHA-C4D
13	V4	202	CYC	NA-C1A-CHA-C4D
13	V6	202	CYC	NA-C1A-CHA-C4D
13	Q7	202	CYC	NA-C1A-CHA-C4D
13	V7	202	CYC	NA-C1A-CHA-C4D
13	a7	201	CYC	NA-C1A-CHA-C4D
13	t2	201	CYC	NB-C1B-CHB-C4A
13	R1	201	CYC	C3D-CAD-CBD-CGD
13	A2	202	CYC	C3D-CAD-CBD-CGD
13	B2	202	CYC	C2A-CAA-CBA-CGA
13	I3	201	CYC	C3D-CAD-CBD-CGD
13	V4	202	CYC	C3D-CAD-CBD-CGD
13	P5	202	CYC	C2A-CAA-CBA-CGA
13	F6	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
13	a1	201	CYC	C4B-C3B-CAB-CBB
13	52	302	CYC	C4B-C3B-CAB-CBB
13	G2	201	CYC	C4B-C3B-CAB-CBB
13	d2	201	CYC	C4B-C3B-CAB-CBB
13	z2	201	CYC	C4B-C3B-CAB-CBB
13	K3	201	CYC	C4B-C3B-CAB-CBB
13	S3	201	CYC	C4B-C3B-CAB-CBB
13	P5	202	CYC	C4B-C3B-CAB-CBB
13	V5	202	CYC	C4B-C3B-CAB-CBB
13	A6	302	CYC	C4B-C3B-CAB-CBB
13	V6	202	CYC	C4B-C3B-CAB-CBB
13	X6	201	CYC	C4B-C3B-CAB-CBB
13	C7	202	CYC	C4B-C3B-CAB-CBB
13	D7	201	CYC	C4B-C3B-CAB-CBB
13	a7	202	CYC	C4B-C3B-CAB-CBB
13	52	301	CYC	C2A-C1A-CHA-C4D
13	L6	201	CYC	NB-C1B-CHB-C4A
13	P6	201	CYC	NB-C1B-CHB-C4A
13	P7	201	CYC	NB-C1B-CHB-C4A
13	A1	301	CYC	NA-C1A-CHA-C4D
13	C1	201	CYC	NA-C1A-CHA-C4D
13	22	301	CYC	NA-C1A-CHA-C4D
13	C4	201	CYC	NA-C1A-CHA-C4D
13	C5	201	CYC	NA-C1A-CHA-C4D
13	V5	202	CYC	NA-C1A-CHA-C4D
13	J7	201	CYC	NA-C1A-CHA-C4D
13	J3	202	CYC	ND-C4D-CHA-C1A
13	22	301	CYC	C2B-C1B-CHB-C4A
13	32	301	CYC	C2B-C1B-CHB-C4A
13	42	301	CYC	C2B-C1B-CHB-C4A
13	H3	201	CYC	C2B-C1B-CHB-C4A
13	S3	201	CYC	C2B-C1B-CHB-C4A
13	P4	202	CYC	C2B-C1B-CHB-C4A
13	A1	301	CYC	C2A-CAA-CBA-CGA
13	C2	201	CYC	C3D-CAD-CBD-CGD
13	N3	201	CYC	C2A-CAA-CBA-CGA
13	T3	202	CYC	C2A-CAA-CBA-CGA
13	G4	201	CYC	C3D-CAD-CBD-CGD
13	D5	201	CYC	C2A-CAA-CBA-CGA
13	A6	301	CYC	C2A-CAA-CBA-CGA
13	G6	201	CYC	C3D-CAD-CBD-CGD
13	a6	202	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
13	H2	201	CYC	NB-C1B-CHB-C4A
13	p2	201	CYC	NB-C1B-CHB-C4A
13	B7	201	CYC	NB-C1B-CHB-C4A
13	Q7	201	CYC	NB-C1B-CHB-C4A
13	X7	201	CYC	NB-C1B-CHB-C4A
13	42	301	CYC	C2A-C1A-CHA-C4D
13	A6	301	CYC	C2A-C1A-CHA-C4D
13	d2	201	CYC	ND-C4D-CHA-C1A
13	c2	801	CYC	NA-C1A-CHA-C4D
13	52	301	CYC	C2B-C1B-CHB-C4A
13	K7	201	CYC	C2B-C1B-CHB-C4A
13	C1	202	CYC	C4C-C3C-CAC-CBC
13	L1	201	CYC	C4C-C3C-CAC-CBC
13	M1	201	CYC	C4C-C3C-CAC-CBC
13	M5	201	CYC	C4C-C3C-CAC-CBC
13	Z5	301	CYC	C4C-C3C-CAC-CBC
13	M6	201	CYC	C4C-C3C-CAC-CBC
13	X6	201	CYC	C4C-C3C-CAC-CBC
13	N2	801	CYC	C4D-C3D-CAD-CBD
13	F7	201	CYC	C2D-C3D-CAD-CBD
13	L1	201	CYC	C4B-C3B-CAB-CBB
13	P1	202	CYC	C4B-C3B-CAB-CBB
13	B2	202	CYC	C4B-C3B-CAB-CBB
13	E2	201	CYC	C4B-C3B-CAB-CBB
13	N2	802	CYC	C4B-C3B-CAB-CBB
13	R2	201	CYC	C4B-C3B-CAB-CBB
13	S2	201	CYC	C4B-C3B-CAB-CBB
13	h2	201	CYC	C4B-C3B-CAB-CBB
13	r2	201	CYC	C4B-C3B-CAB-CBB
13	w2	201	CYC	C4B-C3B-CAB-CBB
13	y2	201	CYC	C4B-C3B-CAB-CBB
13	R3	201	CYC	C4B-C3B-CAB-CBB
13	U3	201	CYC	C4B-C3B-CAB-CBB
13	V3	202	CYC	C4B-C3B-CAB-CBB
13	a3	202	CYC	C4B-C3B-CAB-CBB
13	K4	201	CYC	C4B-C3B-CAB-CBB
13	P4	202	CYC	C4B-C3B-CAB-CBB
13	G5	201	CYC	C4B-C3B-CAB-CBB
13	P5	201	CYC	C4B-C3B-CAB-CBB
13	a5	202	CYC	C4B-C3B-CAB-CBB
13	D6	201	CYC	C4B-C3B-CAB-CBB
13	J6	202	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	P6	202	CYC	C4B-C3B-CAB-CBB
13	a6	201	CYC	C4B-C3B-CAB-CBB
13	E7	201	CYC	C4B-C3B-CAB-CBB
13	K7	201	CYC	C4B-C3B-CAB-CBB
13	S7	201	CYC	C4B-C3B-CAB-CBB
13	U7	201	CYC	C4B-C3B-CAB-CBB
13	V7	202	CYC	C4B-C3B-CAB-CBB
13	V3	202	CYC	C2A-C1A-CHA-C4D
13	J3	202	CYC	C3D-C4D-CHA-C1A
13	H1	201	CYC	C2A-CAA-CBA-CGA
13	52	301	CYC	C2A-CAA-CBA-CGA
13	v2	201	CYC	C2A-CAA-CBA-CGA
13	V3	201	CYC	C2A-CAA-CBA-CGA
13	a3	201	CYC	C2A-CAA-CBA-CGA
13	V4	201	CYC	C2A-CAA-CBA-CGA
13	a4	201	CYC	C2A-CAA-CBA-CGA
13	a5	201	CYC	C2A-CAA-CBA-CGA
13	T6	201	CYC	C2A-CAA-CBA-CGA
13	V6	201	CYC	C2A-CAA-CBA-CGA
13	a7	201	CYC	C2A-CAA-CBA-CGA
13	F5	202	CYC	C2B-C1B-CHB-C4A
13	A6	301	CYC	C2B-C1B-CHB-C4A
13	k2	201	CYC	NA-C1A-CHA-C4D
13	Q3	202	CYC	NA-C1A-CHA-C4D
13	Q3	201	CYC	NB-C1B-CHB-C4A
13	D4	201	CYC	NB-C1B-CHB-C4A
13	Q4	201	CYC	NB-C1B-CHB-C4A
13	W4	201	CYC	NB-C1B-CHB-C4A
13	A1	301	CYC	C2B-C1B-CHB-C4A
13	L3	201	CYC	C2B-C1B-CHB-C4A
13	Q7	202	CYC	C2A-C1A-CHA-C4D
13	P1	201	CYC	C2A-CAA-CBA-CGA
13	V1	201	CYC	C2A-CAA-CBA-CGA
13	H2	201	CYC	C2A-CAA-CBA-CGA
13	P3	201	CYC	C2A-CAA-CBA-CGA
13	V5	201	CYC	C2A-CAA-CBA-CGA
13	a6	201	CYC	C2A-CAA-CBA-CGA
13	R3	201	CYC	C2B-C3B-CAB-CBB
13	D3	201	CYC	NB-C1B-CHB-C4A
13	P1	201	CYC	C4B-C3B-CAB-CBB
13	R1	201	CYC	C4B-C3B-CAB-CBB
13	X1	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	D2	201	CYC	C4B-C3B-CAB-CBB
13	g2	201	CYC	C4B-C3B-CAB-CBB
13	C3	202	CYC	C4B-C3B-CAB-CBB
13	E3	201	CYC	C4B-C3B-CAB-CBB
13	V4	202	CYC	C4B-C3B-CAB-CBB
13	a4	202	CYC	C4B-C3B-CAB-CBB
13	D5	201	CYC	C4B-C3B-CAB-CBB
13	R5	201	CYC	C4B-C3B-CAB-CBB
13	P6	201	CYC	C4B-C3B-CAB-CBB
13	R6	201	CYC	C4B-C3B-CAB-CBB
13	a6	202	CYC	C4B-C3B-CAB-CBB
13	L7	201	CYC	C4B-C3B-CAB-CBB
13	J1	201	CYC	C2A-C1A-CHA-C4D
13	V1	202	CYC	C2A-C1A-CHA-C4D
13	J4	201	CYC	C2A-C1A-CHA-C4D
13	V4	202	CYC	C2A-C1A-CHA-C4D
13	V6	202	CYC	C2A-C1A-CHA-C4D
13	V7	202	CYC	C2A-C1A-CHA-C4D
13	a7	201	CYC	C2A-C1A-CHA-C4D
13	R1	201	CYC	C2C-C3C-CAC-CBC
13	52	302	CYC	C2C-C3C-CAC-CBC
13	P2	201	CYC	C2C-C3C-CAC-CBC
13	a3	201	CYC	C2C-C3C-CAC-CBC
13	M5	201	CYC	C2C-C3C-CAC-CBC
13	M6	201	CYC	C2C-C3C-CAC-CBC
13	R6	201	CYC	C2C-C3C-CAC-CBC
13	a3	201	CYC	NA-C1A-CHA-C4D
13	G2	201	CYC	ND-C4D-CHA-C1A
13	K1	201	CYC	C3D-CAD-CBD-CGD
13	a2	201	CYC	C3D-CAD-CBD-CGD
13	g2	201	CYC	C3D-CAD-CBD-CGD
13	K4	201	CYC	C3D-CAD-CBD-CGD
13	C6	202	CYC	C3D-CAD-CBD-CGD
13	K6	201	CYC	C3D-CAD-CBD-CGD
13	q2	201	CYC	C2B-C3B-CAB-CBB
13	J7	202	CYC	C3C-C4C-CHD-C1D
13	A1	301	CYC	C2A-C1A-CHA-C4D
13	C1	201	CYC	C2A-C1A-CHA-C4D
13	22	301	CYC	C2A-C1A-CHA-C4D
13	k2	201	CYC	C2A-C1A-CHA-C4D
13	Q3	202	CYC	C2A-C1A-CHA-C4D
13	C4	201	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
13	C5	201	CYC	C2A-C1A-CHA-C4D
13	V5	202	CYC	C2A-C1A-CHA-C4D
13	L7	201	CYC	C2B-C1B-CHB-C4A
13	Z7	301	CYC	C2B-C1B-CHB-C4A
13	E3	201	CYC	NC-C4C-CHD-C1D
13	H1	201	CYC	NB-C1B-CHB-C4A
13	g2	201	CYC	NB-C1B-CHB-C4A
13	P3	201	CYC	NB-C1B-CHB-C4A
13	Q5	201	CYC	NB-C1B-CHB-C4A
13	P7	201	CYC	C2B-C3B-CAB-CBB
13	T1	202	CYC	C3D-CAD-CBD-CGD
13	K3	201	CYC	C3D-CAD-CBD-CGD
13	Q6	201	CYC	NB-C1B-CHB-C4A
13	a1	202	CYC	C4B-C3B-CAB-CBB
13	C2	201	CYC	C4B-C3B-CAB-CBB
13	D3	201	CYC	C4B-C3B-CAB-CBB
13	c2	801	CYC	C2A-C1A-CHA-C4D
13	J7	201	CYC	C2A-C1A-CHA-C4D
13	R5	201	CYC	C2B-C3B-CAB-CBB
13	d2	201	CYC	C3D-C4D-CHA-C1A
13	a1	202	CYC	C3D-CAD-CBD-CGD
13	A2	202	CYC	C2A-CAA-CBA-CGA
13	E2	201	CYC	C3D-CAD-CBD-CGD
13	P3	201	CYC	C3D-CAD-CBD-CGD
13	G5	201	CYC	C3D-CAD-CBD-CGD
13	N5	201	CYC	C3D-CAD-CBD-CGD
13	Q7	201	CYC	C2B-C1B-CHB-C4A
13	U5	201	CYC	NB-C1B-CHB-C4A
13	N2	801	CYC	C2D-C3D-CAD-CBD
13	Z7	301	CYC	ND-C4D-CHA-C1A
13	N3	201	CYC	NB-C1B-CHB-C4A
13	T4	202	CYC	NB-C1B-CHB-C4A
13	K6	201	CYC	NB-C1B-CHB-C4A
13	R6	201	CYC	C2B-C3B-CAB-CBB
13	R1	201	CYC	C2B-C3B-CAB-CBB
13	H1	201	CYC	C3D-CAD-CBD-CGD
13	I1	201	CYC	C3D-CAD-CBD-CGD
13	S1	201	CYC	C3D-CAD-CBD-CGD
13	N2	801	CYC	C2A-CAA-CBA-CGA
13	p2	201	CYC	C2A-CAA-CBA-CGA
13	S3	201	CYC	C3D-CAD-CBD-CGD
13	B4	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
13	N4	201	CYC	C3D-CAD-CBD-CGD
13	S4	201	CYC	C3D-CAD-CBD-CGD
13	L5	201	CYC	C3D-CAD-CBD-CGD
13	H6	201	CYC	C3D-CAD-CBD-CGD
13	I6	201	CYC	C3D-CAD-CBD-CGD
13	Q6	202	CYC	C2A-CAA-CBA-CGA
13	H7	201	CYC	C3D-CAD-CBD-CGD
13	52	302	CYC	CAA-CBA-CGA-O2A
13	a5	202	CYC	CAD-CBD-CGD-O2D
13	Q2	201	CYC	NA-C1A-CHA-C4D
13	j2	201	CYC	NA-C1A-CHA-C4D
13	a5	201	CYC	NA-C1A-CHA-C4D
13	a6	201	CYC	NA-C1A-CHA-C4D
13	w2	201	CYC	CAA-CBA-CGA-O2A
13	D1	201	CYC	C4B-C3B-CAB-CBB
13	e2	201	CYC	C4B-C3B-CAB-CBB
13	C4	202	CYC	C4B-C3B-CAB-CBB
13	K6	201	CYC	C4B-C3B-CAB-CBB
13	H2	201	CYC	C2B-C1B-CHB-C4A
13	P6	201	CYC	C2B-C1B-CHB-C4A
13	B7	201	CYC	C2B-C1B-CHB-C4A
13	P7	201	CYC	C2B-C1B-CHB-C4A
13	A6	302	CYC	CAA-CBA-CGA-O2A
13	L7	201	CYC	ND-C4D-CHA-C1A
13	D1	201	CYC	CAA-CBA-CGA-O2A
13	M1	201	CYC	CAA-CBA-CGA-O2A
13	52	302	CYC	CAA-CBA-CGA-O1A
13	F5	202	CYC	CAA-CBA-CGA-O2A
13	a6	202	CYC	CAD-CBD-CGD-O1D
13	Q3	201	CYC	C2B-C1B-CHB-C4A
13	f2	201	CYC	CAA-CBA-CGA-O2A
13	C3	201	CYC	CAA-CBA-CGA-O2A
13	C4	201	CYC	CAA-CBA-CGA-O1A
13	B6	201	CYC	CAA-CBA-CGA-O2A
13	M4	201	CYC	NA-C1A-CHA-C4D
13	F7	201	CYC	NA-C1A-CHA-C4D
13	G1	201	CYC	C3D-CAD-CBD-CGD
13	N2	802	CYC	C3D-CAD-CBD-CGD
13	l2	201	CYC	C2A-CAA-CBA-CGA
13	q2	201	CYC	C3D-CAD-CBD-CGD
13	D3	201	CYC	C2A-CAA-CBA-CGA
13	H3	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
13	L3	201	CYC	C3D-CAD-CBD-CGD
13	Q3	202	CYC	C2A-CAA-CBA-CGA
13	W3	201	CYC	C3D-CAD-CBD-CGD
13	L4	201	CYC	C3D-CAD-CBD-CGD
13	T5	202	CYC	C3D-CAD-CBD-CGD
13	B6	201	CYC	C3D-CAD-CBD-CGD
13	F6	201	CYC	C2A-CAA-CBA-CGA
13	J6	202	CYC	C2A-CAA-CBA-CGA
13	S6	201	CYC	C3D-CAD-CBD-CGD
13	I7	201	CYC	C3D-CAD-CBD-CGD
13	K7	201	CYC	C3D-CAD-CBD-CGD
13	F4	202	CYC	C2B-C3B-CAB-CBB
13	P1	202	CYC	CAA-CBA-CGA-O2A
13	f2	201	CYC	CAA-CBA-CGA-O1A
13	w2	201	CYC	CAA-CBA-CGA-O1A
13	T5	201	CYC	CAD-CBD-CGD-O2D
13	T1	201	CYC	CAD-CBD-CGD-O1D
13	a5	202	CYC	CAD-CBD-CGD-O1D
13	F6	202	CYC	CAA-CBA-CGA-O2A
13	T7	201	CYC	CAD-CBD-CGD-O2D
13	F1	202	CYC	CAA-CBA-CGA-O2A
13	a1	202	CYC	CAD-CBD-CGD-O1D
13	C2	201	CYC	CAA-CBA-CGA-O1A
13	k2	201	CYC	CAA-CBA-CGA-O1A
13	I1	201	CYC	CAA-CBA-CGA-O2A
13	Q1	201	CYC	CAA-CBA-CGA-O1A
13	Q1	201	CYC	CAA-CBA-CGA-O2A
13	S1	201	CYC	CAA-CBA-CGA-O2A
13	C2	201	CYC	CAA-CBA-CGA-O2A
13	I6	201	CYC	CAA-CBA-CGA-O2A
13	M6	201	CYC	CAA-CBA-CGA-O2A
13	N7	201	CYC	NB-C1B-CHB-C4A
13	T1	201	CYC	CAD-CBD-CGD-O2D
13	M2	201	CYC	CAA-CBA-CGA-O1A
13	C5	201	CYC	CAA-CBA-CGA-O1A
13	P5	202	CYC	CAA-CBA-CGA-O1A
13	A6	302	CYC	CAA-CBA-CGA-O1A
13	J1	201	CYC	CAA-CBA-CGA-O1A
13	N2	801	CYC	CAA-CBA-CGA-O1A
13	e2	201	CYC	CAD-CBD-CGD-O1D
13	P3	202	CYC	CAA-CBA-CGA-O2A
13	Q5	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	C7	201	CYC	CAA-CBA-CGA-O2A
13	a7	202	CYC	CAD-CBD-CGD-O1D
13	M2	201	CYC	CAA-CBA-CGA-O2A
13	M2	201	CYC	CAD-CBD-CGD-O2D
13	N2	801	CYC	CAA-CBA-CGA-O2A
13	S2	201	CYC	CAA-CBA-CGA-O1A
13	j2	201	CYC	CAA-CBA-CGA-O1A
13	P3	202	CYC	CAA-CBA-CGA-O1A
13	E4	201	CYC	CAD-CBD-CGD-O2D
13	Q4	201	CYC	CAA-CBA-CGA-O2A
13	X4	201	CYC	CAA-CBA-CGA-O1A
13	J6	201	CYC	CAA-CBA-CGA-O1A
13	J6	201	CYC	CAA-CBA-CGA-O2A
13	T7	202	CYC	CAA-CBA-CGA-O2A
13	X1	201	CYC	CAA-CBA-CGA-O1A
13	k2	201	CYC	CAA-CBA-CGA-O2A
13	Q3	201	CYC	CAA-CBA-CGA-O2A
13	Z3	301	CYC	CAA-CBA-CGA-O1A
13	a3	202	CYC	CAD-CBD-CGD-O1D
13	a4	202	CYC	CAD-CBD-CGD-O2D
13	C5	201	CYC	CAA-CBA-CGA-O2A
13	E5	201	CYC	CAD-CBD-CGD-O2D
13	P5	202	CYC	CAA-CBA-CGA-O2A
13	S6	201	CYC	CAA-CBA-CGA-O2A
13	U6	201	CYC	CAD-CBD-CGD-O2D
13	a6	202	CYC	CAD-CBD-CGD-O2D
13	C7	201	CYC	CAA-CBA-CGA-O1A
13	Q7	201	CYC	CAA-CBA-CGA-O2A
13	a7	202	CYC	CAD-CBD-CGD-O2D
13	B2	202	CYC	C3D-CAD-CBD-CGD
13	G2	201	CYC	C2A-CAA-CBA-CGA
13	L2	201	CYC	C2A-CAA-CBA-CGA
13	Q2	201	CYC	C3D-CAD-CBD-CGD
13	X3	201	CYC	C3D-CAD-CBD-CGD
13	T4	202	CYC	C3D-CAD-CBD-CGD
13	P5	201	CYC	C2A-CAA-CBA-CGA
13	S5	201	CYC	C3D-CAD-CBD-CGD
13	N6	201	CYC	C3D-CAD-CBD-CGD
13	P7	202	CYC	C3D-CAD-CBD-CGD
13	S7	201	CYC	C3D-CAD-CBD-CGD
13	W7	201	CYC	C3D-CAD-CBD-CGD
13	F1	202	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	C1	201	CYC	CAA-CBA-CGA-O2A
13	J1	201	CYC	CAA-CBA-CGA-O2A
13	L1	201	CYC	CAA-CBA-CGA-O2A
13	P1	202	CYC	CAA-CBA-CGA-O1A
13	a1	202	CYC	CAD-CBD-CGD-O2D
13	a2	201	CYC	CAD-CBD-CGD-O2D
13	t2	201	CYC	CAA-CBA-CGA-O1A
13	T3	201	CYC	CAD-CBD-CGD-O2D
13	V4	202	CYC	CAD-CBD-CGD-O1D
13	J5	202	CYC	CAA-CBA-CGA-O2A
13	T5	201	CYC	CAD-CBD-CGD-O1D
13	T5	202	CYC	CAA-CBA-CGA-O1A
13	V5	202	CYC	CAD-CBD-CGD-O1D
13	V5	202	CYC	CAD-CBD-CGD-O2D
13	a5	202	CYC	CAA-CBA-CGA-O2A
13	Q6	201	CYC	CAA-CBA-CGA-O1A
13	Z7	301	CYC	CAA-CBA-CGA-O1A
13	R4	201	CYC	C4B-C3B-CAB-CBB
13	R7	201	CYC	C4B-C3B-CAB-CBB
13	R4	201	CYC	C2B-C3B-CAB-CBB
13	C1	201	CYC	CAA-CBA-CGA-O1A
13	T3	202	CYC	CAA-CBA-CGA-O2A
13	a3	202	CYC	CAD-CBD-CGD-O2D
13	V4	202	CYC	CAD-CBD-CGD-O2D
13	T6	202	CYC	CAA-CBA-CGA-O1A
13	E7	201	CYC	CAD-CBD-CGD-O1D
13	E7	201	CYC	CAD-CBD-CGD-O2D
13	B5	201	CYC	C2C-C3C-CAC-CBC
13	Z1	301	CYC	CAA-CBA-CGA-O1A
13	S2	201	CYC	CAA-CBA-CGA-O2A
13	U2	201	CYC	CAA-CBA-CGA-O2A
13	V2	201	CYC	CAA-CBA-CGA-O1A
13	t2	201	CYC	CAA-CBA-CGA-O2A
13	X3	201	CYC	CAA-CBA-CGA-O1A
13	C4	201	CYC	CAA-CBA-CGA-O2A
13	E4	201	CYC	CAD-CBD-CGD-O1D
13	C6	201	CYC	CAA-CBA-CGA-O1A
13	X6	201	CYC	CAA-CBA-CGA-O1A
13	Q7	201	CYC	CAA-CBA-CGA-O1A
13	Q4	201	CYC	C2B-C1B-CHB-C4A
13	Q5	201	CYC	C2B-C1B-CHB-C4A
13	L6	201	CYC	C2B-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
13	T1	202	CYC	CAA-CBA-CGA-O1A
13	a2	201	CYC	CAD-CBD-CGD-O1D
13	e2	201	CYC	CAD-CBD-CGD-O2D
13	r2	201	CYC	CAA-CBA-CGA-O1A
13	Z6	301	CYC	CAD-CBD-CGD-O2D
13	X7	201	CYC	CAA-CBA-CGA-O1A
13	R7	201	CYC	C2B-C3B-CAB-CBB
13	J6	202	CYC	ND-C4D-CHA-C1A
13	U2	201	CYC	CAA-CBA-CGA-O1A
13	q2	201	CYC	CAD-CBD-CGD-O1D
13	E3	201	CYC	CAD-CBD-CGD-O2D
13	Q3	201	CYC	CAA-CBA-CGA-O1A
13	T4	202	CYC	CAA-CBA-CGA-O1A
13	H5	201	CYC	CAA-CBA-CGA-O2A
13	X5	201	CYC	CAA-CBA-CGA-O1A
13	P6	201	CYC	CAA-CBA-CGA-O2A
13	V6	201	CYC	CAA-CBA-CGA-O2A
13	I1	201	CYC	CAA-CBA-CGA-O1A
13	L1	201	CYC	CAA-CBA-CGA-O1A
13	g2	201	CYC	CAA-CBA-CGA-O2A
13	C3	201	CYC	CAA-CBA-CGA-O1A
13	T3	202	CYC	CAA-CBA-CGA-O1A
13	Q4	201	CYC	CAA-CBA-CGA-O1A
13	I6	201	CYC	CAA-CBA-CGA-O1A
13	M6	201	CYC	CAA-CBA-CGA-O1A
13	S6	201	CYC	CAA-CBA-CGA-O1A
13	E1	201	CYC	CAD-CBD-CGD-O2D
13	F1	202	CYC	CAA-CBA-CGA-O1A
13	S1	201	CYC	CAA-CBA-CGA-O1A
13	X1	201	CYC	CAA-CBA-CGA-O2A
13	M2	201	CYC	CAD-CBD-CGD-O1D
13	T3	201	CYC	CAD-CBD-CGD-O1D
13	F4	202	CYC	CAA-CBA-CGA-O2A
13	Z5	301	CYC	CAA-CBA-CGA-O1A
13	T7	201	CYC	CAD-CBD-CGD-O1D
13	W6	201	CYC	NB-C1B-CHB-C4A
13	W7	201	CYC	NB-C1B-CHB-C4A
13	T1	202	CYC	CAA-CBA-CGA-O2A
13	V1	202	CYC	CAD-CBD-CGD-O2D
13	X3	201	CYC	CAA-CBA-CGA-O2A
13	V4	201	CYC	CAA-CBA-CGA-O2A
13	F6	202	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	T6	202	CYC	CAA-CBA-CGA-O2A
13	Z6	301	CYC	CAD-CBD-CGD-O1D
13	C3	202	CYC	CAD-CBD-CGD-O2D
13	I3	201	CYC	CAA-CBA-CGA-O2A
13	F4	201	CYC	CAA-CBA-CGA-O2A
13	E5	201	CYC	CAD-CBD-CGD-O1D
13	S5	201	CYC	CAA-CBA-CGA-O2A
13	T5	202	CYC	CAA-CBA-CGA-O2A
13	I7	201	CYC	CAA-CBA-CGA-O2A
13	T7	202	CYC	CAA-CBA-CGA-O1A
13	X7	201	CYC	CAA-CBA-CGA-O2A
13	Q1	202	CYC	C2A-CAA-CBA-CGA
13	a1	202	CYC	C2A-CAA-CBA-CGA
13	U2	201	CYC	C3D-CAD-CBD-CGD
13	N4	201	CYC	C2A-CAA-CBA-CGA
13	W4	201	CYC	C3D-CAD-CBD-CGD
13	P6	201	CYC	C2A-CAA-CBA-CGA
13	Q7	202	CYC	C2A-CAA-CBA-CGA
13	a3	201	CYC	C2A-C1A-CHA-C4D
13	A1	302	CYC	CAA-CBA-CGA-O2A
13	J1	202	CYC	CAA-CBA-CGA-O2A
13	M1	201	CYC	CAA-CBA-CGA-O1A
13	Z1	301	CYC	CAA-CBA-CGA-O2A
13	q2	201	CYC	CAD-CBD-CGD-O2D
13	r2	201	CYC	CAA-CBA-CGA-O2A
13	F4	202	CYC	CAA-CBA-CGA-O1A
13	T4	202	CYC	CAA-CBA-CGA-O2A
13	a4	202	CYC	CAD-CBD-CGD-O1D
13	D5	201	CYC	CAA-CBA-CGA-O2A
13	F5	202	CYC	CAA-CBA-CGA-O1A
13	M5	201	CYC	CAA-CBA-CGA-O2A
13	S5	201	CYC	CAA-CBA-CGA-O1A
13	X5	201	CYC	CAA-CBA-CGA-O2A
13	a5	202	CYC	CAA-CBA-CGA-O1A
13	U6	201	CYC	CAD-CBD-CGD-O1D
13	X6	201	CYC	CAA-CBA-CGA-O2A
13	C7	202	CYC	CAD-CBD-CGD-O2D
13	B3	201	CYC	C4C-C3C-CAC-CBC
13	a3	202	CYC	C4C-C3C-CAC-CBC
13	J7	201	CYC	C4C-C3C-CAC-CBC
13	D1	201	CYC	CAA-CBA-CGA-O1A
13	V1	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	V1	202	CYC	CAD-CBD-CGD-O1D
13	q2	201	CYC	CAA-CBA-CGA-O2A
13	I3	201	CYC	CAA-CBA-CGA-O1A
13	F4	201	CYC	CAA-CBA-CGA-O1A
13	M4	201	CYC	CAA-CBA-CGA-O2A
13	M5	201	CYC	CAA-CBA-CGA-O1A
13	B6	201	CYC	CAA-CBA-CGA-O1A
13	I7	201	CYC	CAA-CBA-CGA-O1A
13	Z1	301	CYC	CAD-CBD-CGD-O2D
13	V2	201	CYC	CAA-CBA-CGA-O2A
13	Z3	301	CYC	CAA-CBA-CGA-O2A
13	P4	201	CYC	CAA-CBA-CGA-O2A
13	X4	201	CYC	CAA-CBA-CGA-O2A
13	J5	202	CYC	CAA-CBA-CGA-O1A
13	V5	201	CYC	CAA-CBA-CGA-O2A
13	Z5	301	CYC	CAA-CBA-CGA-O2A
13	L7	201	CYC	CAA-CBA-CGA-O1A
13	K3	201	CYC	NB-C1B-CHB-C4A
13	S6	201	CYC	NB-C1B-CHB-C4A
13	H2	201	CYC	CAA-CBA-CGA-O2A
13	j2	201	CYC	CAA-CBA-CGA-O2A
13	q2	201	CYC	CAA-CBA-CGA-O1A
13	G4	201	CYC	CAA-CBA-CGA-O2A
13	M4	201	CYC	CAA-CBA-CGA-O1A
13	a4	202	CYC	CAA-CBA-CGA-O2A
13	P5	201	CYC	CAA-CBA-CGA-O2A
13	Q6	201	CYC	CAA-CBA-CGA-O2A
13	L7	201	CYC	CAA-CBA-CGA-O2A
13	G1	201	CYC	CAA-CBA-CGA-O2A
13	J1	202	CYC	CAA-CBA-CGA-O1A
13	P1	201	CYC	CAA-CBA-CGA-O2A
13	H2	201	CYC	CAA-CBA-CGA-O1A
13	d2	201	CYC	CAA-CBA-CGA-O2A
13	D3	201	CYC	CAA-CBA-CGA-O1A
13	K3	201	CYC	CAA-CBA-CGA-O2A
13	I4	201	CYC	CAA-CBA-CGA-O2A
13	J4	202	CYC	CAA-CBA-CGA-O2A
13	N4	201	CYC	CAA-CBA-CGA-O1A
13	P4	202	CYC	CAD-CBD-CGD-O2D
13	U4	201	CYC	CAA-CBA-CGA-O2A
13	a4	201	CYC	CAA-CBA-CGA-O2A
13	D5	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	P5	201	CYC	CAD-CBD-CGD-O2D
13	C6	201	CYC	CAA-CBA-CGA-O2A
13	P6	201	CYC	CAA-CBA-CGA-O1A
13	T6	201	CYC	CAD-CBD-CGD-O2D
13	K7	201	CYC	CAA-CBA-CGA-O2A
13	P7	202	CYC	CAA-CBA-CGA-O2A
13	U7	201	CYC	CAD-CBD-CGD-O2D
13	t2	201	CYC	C2B-C1B-CHB-C4A
13	W4	201	CYC	C2B-C1B-CHB-C4A
13	F1	201	CYC	CAA-CBA-CGA-O1A
13	B2	201	CYC	CAA-CBA-CGA-O2A
13	d2	201	CYC	CAA-CBA-CGA-O1A
13	E3	201	CYC	CAD-CBD-CGD-O1D
13	W3	201	CYC	CAA-CBA-CGA-O1A
13	W3	201	CYC	CAA-CBA-CGA-O2A
13	G4	201	CYC	CAA-CBA-CGA-O1A
13	N4	201	CYC	CAA-CBA-CGA-O2A
13	T4	201	CYC	CAD-CBD-CGD-O1D
13	a4	202	CYC	CAA-CBA-CGA-O1A
13	H5	201	CYC	CAA-CBA-CGA-O1A
13	K5	201	CYC	CAA-CBA-CGA-O1A
13	L6	201	CYC	CAA-CBA-CGA-O2A
13	V6	202	CYC	CAD-CBD-CGD-O1D
13	V6	202	CYC	CAD-CBD-CGD-O2D
13	Z7	301	CYC	CAA-CBA-CGA-O2A
13	C1	202	CYC	CAA-CBA-CGA-O1A
13	A2	201	CYC	CAD-CBD-CGD-O2D
13	E4	201	CYC	CAA-CBA-CGA-O1A
13	J4	201	CYC	CAA-CBA-CGA-O1A
13	J4	201	CYC	CAA-CBA-CGA-O2A
13	P4	202	CYC	CAA-CBA-CGA-O1A
13	a4	201	CYC	CAD-CBD-CGD-O2D
13	Z5	301	CYC	CAD-CBD-CGD-O2D
13	R6	201	CYC	CAA-CBA-CGA-O1A
13	R7	201	CYC	CAA-CBA-CGA-O1A
13	J1	202	CYC	C4B-C3B-CAB-CBB
13	J5	202	CYC	C4B-C3B-CAB-CBB
13	Q7	202	CYC	C4B-C3B-CAB-CBB
13	K1	201	CYC	CAA-CBA-CGA-O1A
13	P1	201	CYC	CAA-CBA-CGA-O1A
13	A2	201	CYC	CAA-CBA-CGA-O2A
13	C2	201	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	C2	201	CYC	CAD-CBD-CGD-O2D
13	P2	201	CYC	CAA-CBA-CGA-O1A
13	Q2	201	CYC	CAD-CBD-CGD-O1D
13	l2	201	CYC	CAA-CBA-CGA-O1A
13	o2	801	CYC	CAA-CBA-CGA-O1A
13	V4	201	CYC	CAA-CBA-CGA-O1A
13	F5	202	CYC	CAD-CBD-CGD-O2D
13	G5	201	CYC	CAA-CBA-CGA-O1A
13	K5	201	CYC	CAA-CBA-CGA-O2A
13	N5	201	CYC	CAA-CBA-CGA-O2A
13	P5	201	CYC	CAA-CBA-CGA-O1A
13	Z6	301	CYC	CAA-CBA-CGA-O1A
13	U7	201	CYC	CAD-CBD-CGD-O1D
13	V7	201	CYC	CAA-CBA-CGA-O1A
13	V7	202	CYC	CAD-CBD-CGD-O1D
13	W7	201	CYC	CAA-CBA-CGA-O1A
13	Q7	202	CYC	C2B-C3B-CAB-CBB
13	Q2	201	CYC	C2A-C1A-CHA-C4D
13	A1	302	CYC	CAA-CBA-CGA-O1A
13	C1	202	CYC	CAA-CBA-CGA-O2A
13	E1	201	CYC	CAD-CBD-CGD-O1D
13	A2	201	CYC	CAD-CBD-CGD-O1D
13	B2	201	CYC	CAA-CBA-CGA-O1A
13	E2	201	CYC	CAA-CBA-CGA-O2A
13	D3	201	CYC	CAA-CBA-CGA-O2A
13	V3	201	CYC	CAA-CBA-CGA-O1A
13	E4	201	CYC	CAA-CBA-CGA-O2A
13	L4	201	CYC	CAA-CBA-CGA-O1A
13	P4	201	CYC	CAA-CBA-CGA-O1A
13	T4	201	CYC	CAD-CBD-CGD-O2D
13	E6	201	CYC	CAD-CBD-CGD-O2D
13	L6	201	CYC	CAA-CBA-CGA-O1A
13	P7	202	CYC	CAA-CBA-CGA-O1A
13	P1	201	CYC	NB-C1B-CHB-C4A
13	B3	201	CYC	NB-C1B-CHB-C4A
13	E7	201	CYC	NB-C1B-CHB-C4A
13	N1	201	CYC	C3D-CAD-CBD-CGD
13	22	302	CYC	C2A-CAA-CBA-CGA
13	H1	201	CYC	CAA-CBA-CGA-O1A
13	H1	201	CYC	CAA-CBA-CGA-O2A
13	V1	201	CYC	CAA-CBA-CGA-O1A
13	Q2	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	g2	201	CYC	CAA-CBA-CGA-O1A
13	o2	801	CYC	CAA-CBA-CGA-O2A
13	K3	201	CYC	CAA-CBA-CGA-O1A
13	V3	201	CYC	CAA-CBA-CGA-O2A
13	L4	201	CYC	CAA-CBA-CGA-O2A
13	P4	202	CYC	CAA-CBA-CGA-O2A
13	G5	201	CYC	CAA-CBA-CGA-O2A
13	R6	201	CYC	CAA-CBA-CGA-O2A
13	V6	201	CYC	CAA-CBA-CGA-O1A
13	V7	202	CYC	CAD-CBD-CGD-O2D
13	F1	201	CYC	CAA-CBA-CGA-O2A
13	K1	201	CYC	CAA-CBA-CGA-O2A
13	P2	201	CYC	CAA-CBA-CGA-O2A
13	l2	201	CYC	CAA-CBA-CGA-O2A
13	s2	201	CYC	CAA-CBA-CGA-O2A
13	G3	201	CYC	CAA-CBA-CGA-O2A
13	J3	202	CYC	CAD-CBD-CGD-O2D
13	V3	202	CYC	CAD-CBD-CGD-O2D
13	J4	202	CYC	CAA-CBA-CGA-O1A
13	R4	201	CYC	CAA-CBA-CGA-O2A
13	I5	201	CYC	CAA-CBA-CGA-O2A
13	K6	201	CYC	CAA-CBA-CGA-O2A
13	N6	201	CYC	CAA-CBA-CGA-O2A
13	F7	202	CYC	CAA-CBA-CGA-O2A
13	H7	201	CYC	CAA-CBA-CGA-O1A
13	H7	201	CYC	CAA-CBA-CGA-O2A
13	J7	201	CYC	CAA-CBA-CGA-O1A
13	J7	201	CYC	CAA-CBA-CGA-O2A
13	P7	201	CYC	CAA-CBA-CGA-O1A
13	V7	201	CYC	CAA-CBA-CGA-O2A
13	W7	201	CYC	CAA-CBA-CGA-O2A
13	U5	201	CYC	C2B-C1B-CHB-C4A
13	Q6	201	CYC	C2B-C1B-CHB-C4A
13	U1	201	CYC	CAD-CBD-CGD-O2D
13	W1	201	CYC	CAA-CBA-CGA-O2A
13	R2	201	CYC	CAA-CBA-CGA-O2A
13	R3	201	CYC	CAA-CBA-CGA-O1A
13	R3	201	CYC	CAA-CBA-CGA-O2A
13	Q5	201	CYC	CAA-CBA-CGA-O2A
13	V5	201	CYC	CAA-CBA-CGA-O1A
13	W5	201	CYC	CAA-CBA-CGA-O2A
13	D7	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	G7	201	CYC	CAA-CBA-CGA-O2A
13	P7	201	CYC	CAA-CBA-CGA-O2A
13	R7	201	CYC	CAA-CBA-CGA-O2A
13	s2	201	CYC	NA-C1A-CHA-C4D
13	V4	201	CYC	NA-C1A-CHA-C4D
13	G1	201	CYC	CAA-CBA-CGA-O1A
13	W1	201	CYC	CAA-CBA-CGA-O1A
13	22	301	CYC	CAA-CBA-CGA-O2A
13	J3	202	CYC	CAD-CBD-CGD-O1D
13	U4	201	CYC	CAA-CBA-CGA-O1A
13	P5	201	CYC	CAD-CBD-CGD-O1D
13	W5	201	CYC	CAA-CBA-CGA-O1A
13	Z1	301	CYC	CAD-CBD-CGD-O1D
13	I4	201	CYC	CAA-CBA-CGA-O1A
13	N5	201	CYC	CAA-CBA-CGA-O1A
13	D7	201	CYC	CAA-CBA-CGA-O1A
13	F7	202	CYC	CAA-CBA-CGA-O1A
13	R1	201	CYC	CAA-CBA-CGA-O2A
13	U1	201	CYC	CAD-CBD-CGD-O1D
13	C3	202	CYC	CAD-CBD-CGD-O1D
13	P4	202	CYC	CAD-CBD-CGD-O1D
13	R4	201	CYC	CAA-CBA-CGA-O1A
13	Z4	301	CYC	CAD-CBD-CGD-O1D
13	I5	201	CYC	CAA-CBA-CGA-O1A
13	N6	201	CYC	CAA-CBA-CGA-O1A
13	T6	201	CYC	CAD-CBD-CGD-O1D
13	J7	202	CYC	CAD-CBD-CGD-O2D
13	K7	201	CYC	CAA-CBA-CGA-O1A
13	R1	201	CYC	CAA-CBA-CGA-O1A
13	E2	201	CYC	CAA-CBA-CGA-O1A
13	R2	201	CYC	CAA-CBA-CGA-O1A
13	G3	201	CYC	CAA-CBA-CGA-O1A
13	V3	202	CYC	CAD-CBD-CGD-O1D
13	a4	201	CYC	CAA-CBA-CGA-O1A
13	C5	202	CYC	CAA-CBA-CGA-O1A
13	C5	202	CYC	CAA-CBA-CGA-O2A
13	G7	201	CYC	CAA-CBA-CGA-O1A
13	H1	201	CYC	C2B-C1B-CHB-C4A
13	D3	201	CYC	C2B-C1B-CHB-C4A
13	N3	201	CYC	C2B-C1B-CHB-C4A
13	T4	202	CYC	C2B-C1B-CHB-C4A
13	32	301	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	M3	201	CYC	CAA-CBA-CGA-O2A
13	E5	201	CYC	CAA-CBA-CGA-O2A
13	J5	201	CYC	CAA-CBA-CGA-O2A
13	R5	201	CYC	CAA-CBA-CGA-O2A
13	H6	201	CYC	CAA-CBA-CGA-O1A
13	H6	201	CYC	CAA-CBA-CGA-O2A
13	J6	202	CYC	CAA-CBA-CGA-O2A
13	J6	202	CYC	CAD-CBD-CGD-O2D
13	a6	202	CYC	CAA-CBA-CGA-O2A
13	B7	201	CYC	CAA-CBA-CGA-O2A
13	C7	202	CYC	CAD-CBD-CGD-O1D
13	J7	202	CYC	CAD-CBD-CGD-O1D
13	O2	201	CYC	C2A-CAA-CBA-CGA
13	d2	201	CYC	C3D-CAD-CBD-CGD
13	V5	202	CYC	C3D-CAD-CBD-CGD
13	P7	201	CYC	C2A-CAA-CBA-CGA
13	n2	201	CYC	CAA-CBA-CGA-O1A
13	S3	201	CYC	CAA-CBA-CGA-O2A
13	C4	202	CYC	CAA-CBA-CGA-O2A
13	R5	201	CYC	CAA-CBA-CGA-O1A
13	Z5	301	CYC	CAD-CBD-CGD-O1D
13	E6	201	CYC	CAD-CBD-CGD-O1D
13	K6	201	CYC	CAA-CBA-CGA-O1A
13	J7	202	CYC	CAA-CBA-CGA-O2A
13	U1	201	CYC	CAA-CBA-CGA-O1A
13	a1	202	CYC	CAA-CBA-CGA-O2A
13	22	301	CYC	CAA-CBA-CGA-O1A
13	32	301	CYC	CAA-CBA-CGA-O1A
13	42	302	CYC	CAA-CBA-CGA-O1A
13	J3	202	CYC	CAA-CBA-CGA-O2A
13	D4	201	CYC	CAA-CBA-CGA-O1A
13	Z4	301	CYC	CAD-CBD-CGD-O2D
13	B5	201	CYC	CAA-CBA-CGA-O2A
13	F5	201	CYC	CAA-CBA-CGA-O2A
13	J5	201	CYC	CAA-CBA-CGA-O1A
13	V6	202	CYC	CAA-CBA-CGA-O1A
13	W6	201	CYC	CAA-CBA-CGA-O1A
13	B7	201	CYC	CAA-CBA-CGA-O1A
13	E7	201	CYC	CAA-CBA-CGA-O2A
13	J7	202	CYC	CAA-CBA-CGA-O1A
13	N7	201	CYC	CAA-CBA-CGA-O2A
13	a7	202	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	J1	202	CYC	CAD-CBD-CGD-O1D
13	N1	201	CYC	CAA-CBA-CGA-O2A
13	V1	202	CYC	CAA-CBA-CGA-O1A
13	a1	202	CYC	CAA-CBA-CGA-O1A
13	22	302	CYC	CAA-CBA-CGA-O2A
13	32	302	CYC	CAA-CBA-CGA-O2A
13	P2	201	CYC	CAD-CBD-CGD-O1D
13	c2	801	CYC	CAA-CBA-CGA-O2A
13	s2	201	CYC	CAA-CBA-CGA-O1A
13	B3	201	CYC	CAA-CBA-CGA-O2A
13	L3	201	CYC	CAA-CBA-CGA-O1A
13	M3	201	CYC	CAA-CBA-CGA-O1A
13	P3	201	CYC	CAA-CBA-CGA-O2A
13	P3	201	CYC	CAD-CBD-CGD-O1D
13	S3	201	CYC	CAA-CBA-CGA-O1A
13	T3	201	CYC	CAA-CBA-CGA-O2A
13	V3	202	CYC	CAA-CBA-CGA-O1A
13	a3	202	CYC	CAA-CBA-CGA-O1A
13	B4	201	CYC	CAA-CBA-CGA-O2A
13	H4	201	CYC	CAA-CBA-CGA-O1A
13	J4	202	CYC	CAD-CBD-CGD-O1D
13	K4	201	CYC	CAA-CBA-CGA-O1A
13	S4	201	CYC	CAA-CBA-CGA-O2A
13	T4	201	CYC	CAA-CBA-CGA-O2A
13	V4	202	CYC	CAA-CBA-CGA-O1A
13	E5	201	CYC	CAA-CBA-CGA-O1A
13	F5	202	CYC	CAD-CBD-CGD-O1D
13	J5	202	CYC	CAD-CBD-CGD-O1D
13	J5	202	CYC	CAD-CBD-CGD-O2D
13	U5	201	CYC	CAA-CBA-CGA-O1A
13	V5	202	CYC	CAA-CBA-CGA-O2A
13	T6	201	CYC	CAA-CBA-CGA-O2A
13	P7	201	CYC	CAD-CBD-CGD-O2D
13	S7	201	CYC	CAA-CBA-CGA-O2A
13	V7	202	CYC	CAA-CBA-CGA-O1A
13	B1	201	CYC	CAA-CBA-CGA-O1A
13	B1	201	CYC	CAA-CBA-CGA-O2A
13	E1	201	CYC	CAA-CBA-CGA-O1A
13	N1	201	CYC	CAA-CBA-CGA-O1A
13	P1	201	CYC	CAD-CBD-CGD-O1D
13	P1	201	CYC	CAD-CBD-CGD-O2D
13	T1	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	T1	201	CYC	CAA-CBA-CGA-O2A
13	A2	201	CYC	CAA-CBA-CGA-O1A
13	F2	201	CYC	CAA-CBA-CGA-O1A
13	N2	802	CYC	CAA-CBA-CGA-O1A
13	N2	802	CYC	CAA-CBA-CGA-O2A
13	e2	201	CYC	CAA-CBA-CGA-O2A
13	x2	201	CYC	CAA-CBA-CGA-O1A
13	C3	202	CYC	CAA-CBA-CGA-O1A
13	E3	201	CYC	CAA-CBA-CGA-O1A
13	F3	201	CYC	CAA-CBA-CGA-O1A
13	F3	202	CYC	CAA-CBA-CGA-O2A
13	H3	201	CYC	CAA-CBA-CGA-O2A
13	J3	201	CYC	CAA-CBA-CGA-O1A
13	N3	201	CYC	CAA-CBA-CGA-O1A
13	U3	201	CYC	CAA-CBA-CGA-O1A
13	U3	201	CYC	CAD-CBD-CGD-O1D
13	V3	202	CYC	CAA-CBA-CGA-O2A
13	C4	202	CYC	CAA-CBA-CGA-O1A
13	D4	201	CYC	CAA-CBA-CGA-O2A
13	S4	201	CYC	CAA-CBA-CGA-O1A
13	V4	202	CYC	CAA-CBA-CGA-O2A
13	W4	201	CYC	CAA-CBA-CGA-O1A
13	L5	201	CYC	CAA-CBA-CGA-O2A
13	T5	201	CYC	CAA-CBA-CGA-O1A
13	C6	202	CYC	CAA-CBA-CGA-O1A
13	D6	201	CYC	CAA-CBA-CGA-O1A
13	E6	201	CYC	CAA-CBA-CGA-O1A
13	F6	201	CYC	CAA-CBA-CGA-O1A
13	G6	201	CYC	CAA-CBA-CGA-O2A
13	J6	202	CYC	CAA-CBA-CGA-O1A
13	P6	201	CYC	CAD-CBD-CGD-O1D
13	P6	202	CYC	CAA-CBA-CGA-O2A
13	U6	201	CYC	CAA-CBA-CGA-O1A
13	U6	201	CYC	CAA-CBA-CGA-O2A
13	C7	202	CYC	CAA-CBA-CGA-O1A
13	E7	201	CYC	CAA-CBA-CGA-O1A
13	F7	201	CYC	CAA-CBA-CGA-O1A
13	F7	201	CYC	CAA-CBA-CGA-O2A
13	M7	201	CYC	CAA-CBA-CGA-O1A
13	N7	201	CYC	CAA-CBA-CGA-O1A
13	S7	201	CYC	CAA-CBA-CGA-O1A
13	T7	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	U7	201	CYC	CAA-CBA-CGA-O1A
13	V7	202	CYC	CAA-CBA-CGA-O2A
13	E1	201	CYC	CAA-CBA-CGA-O2A
13	J1	202	CYC	CAD-CBD-CGD-O2D
13	42	302	CYC	CAA-CBA-CGA-O2A
13	F2	201	CYC	CAA-CBA-CGA-O2A
13	F3	201	CYC	CAA-CBA-CGA-O2A
13	J3	201	CYC	CAA-CBA-CGA-O2A
13	P3	201	CYC	CAD-CBD-CGD-O2D
13	U3	201	CYC	CAA-CBA-CGA-O2A
13	U3	201	CYC	CAD-CBD-CGD-O2D
13	a3	202	CYC	CAA-CBA-CGA-O2A
13	K4	201	CYC	CAA-CBA-CGA-O2A
13	B5	201	CYC	CAA-CBA-CGA-O1A
13	C6	202	CYC	CAA-CBA-CGA-O2A
13	E6	201	CYC	CAA-CBA-CGA-O2A
13	F6	201	CYC	CAA-CBA-CGA-O2A
13	J6	202	CYC	CAD-CBD-CGD-O1D
13	P6	202	CYC	CAA-CBA-CGA-O1A
13	V6	202	CYC	CAA-CBA-CGA-O2A
13	a6	202	CYC	CAA-CBA-CGA-O1A
13	C7	202	CYC	CAA-CBA-CGA-O2A
13	M7	201	CYC	CAA-CBA-CGA-O2A
13	T7	201	CYC	CAA-CBA-CGA-O2A
13	D4	201	CYC	C2B-C1B-CHB-C4A
13	X7	201	CYC	C2B-C1B-CHB-C4A
13	U1	201	CYC	CAA-CBA-CGA-O2A
13	V1	202	CYC	CAA-CBA-CGA-O2A
13	P2	201	CYC	CAD-CBD-CGD-O2D
13	W2	201	CYC	CAA-CBA-CGA-O2A
13	C3	202	CYC	CAA-CBA-CGA-O2A
13	E3	201	CYC	CAA-CBA-CGA-O2A
13	H3	201	CYC	CAA-CBA-CGA-O1A
13	J3	202	CYC	CAA-CBA-CGA-O1A
13	L3	201	CYC	CAA-CBA-CGA-O2A
13	N3	201	CYC	CAA-CBA-CGA-O2A
13	T3	201	CYC	CAA-CBA-CGA-O1A
13	H4	201	CYC	CAA-CBA-CGA-O2A
13	J4	202	CYC	CAD-CBD-CGD-O2D
13	U4	201	CYC	CAD-CBD-CGD-O2D
13	W4	201	CYC	CAA-CBA-CGA-O2A
13	a4	201	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	C5	202	CYC	CAD-CBD-CGD-O2D
13	F5	201	CYC	CAA-CBA-CGA-O1A
13	T5	201	CYC	CAA-CBA-CGA-O2A
13	U5	201	CYC	CAA-CBA-CGA-O2A
13	D6	201	CYC	CAA-CBA-CGA-O2A
13	D6	201	CYC	CAD-CBD-CGD-O2D
13	P6	201	CYC	CAD-CBD-CGD-O2D
13	U7	201	CYC	CAA-CBA-CGA-O2A
13	C6	202	CYC	C4B-C3B-CAB-CBB
13	D2	201	CYC	CAA-CBA-CGA-O2A
13	W6	201	CYC	CAA-CBA-CGA-O2A
13	22	302	CYC	CAA-CBA-CGA-O1A
13	32	302	CYC	CAA-CBA-CGA-O1A
13	c2	801	CYC	CAA-CBA-CGA-O1A
13	B3	201	CYC	CAA-CBA-CGA-O1A
13	F3	202	CYC	CAA-CBA-CGA-O1A
13	P3	201	CYC	CAA-CBA-CGA-O1A
13	B4	201	CYC	CAA-CBA-CGA-O1A
13	T4	201	CYC	CAA-CBA-CGA-O1A
13	L5	201	CYC	CAA-CBA-CGA-O1A
13	V5	202	CYC	CAA-CBA-CGA-O1A
13	G6	201	CYC	CAA-CBA-CGA-O1A
13	T6	201	CYC	CAA-CBA-CGA-O1A
13	P7	201	CYC	CAD-CBD-CGD-O1D
13	a7	202	CYC	CAA-CBA-CGA-O2A
13	U3	201	CYC	NB-C1B-CHB-C4A
13	I7	201	CYC	NB-C1B-CHB-C4A
13	M5	201	CYC	NA-C1A-CHA-C4D
13	H4	201	CYC	C3D-CAD-CBD-CGD
13	R4	201	CYC	C2A-CAA-CBA-CGA
13	H6	201	CYC	C2A-CAA-CBA-CGA
13	X7	201	CYC	C3D-CAD-CBD-CGD
13	a2	201	CYC	CAA-CBA-CGA-O2A
13	D7	201	CYC	CAD-CBD-CGD-O2D
13	G2	201	CYC	C3D-C4D-CHA-C1A
13	Z7	301	CYC	C3D-C4D-CHA-C1A
13	i2	201	CYC	CAD-CBD-CGD-O2D
13	v2	201	CYC	C3A-C2A-CAA-CBA
13	G2	201	CYC	CAD-CBD-CGD-O1D
13	G2	201	CYC	CAD-CBD-CGD-O2D
13	a5	201	CYC	C2A-C1A-CHA-C4D
13	X2	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	Z4	301	CYC	CAA-CBA-CGA-O1A
13	P3	201	CYC	C2B-C1B-CHB-C4A
13	32	301	CYC	NA-C1A-CHA-C4D
13	X4	201	CYC	NA-C1A-CHA-C4D
13	D5	201	CYC	NA-C1A-CHA-C4D
13	e2	201	CYC	CAA-CBA-CGA-O1A
13	Z4	301	CYC	CAA-CBA-CGA-O2A
13	D6	201	CYC	CAD-CBD-CGD-O1D
13	Z6	301	CYC	CAA-CBA-CGA-O2A
13	m2	201	CYC	CAD-CBD-CGD-O2D
13	Q5	202	CYC	CAA-CBA-CGA-O1A
13	R6	201	CYC	C2A-CAA-CBA-CGA
13	X2	201	CYC	CAA-CBA-CGA-O2A
13	y2	201	CYC	CAA-CBA-CGA-O1A
13	Q1	202	CYC	NB-C1B-CHB-C4A
13	Q3	202	CYC	C2B-C3B-CAB-CBB
13	C5	202	CYC	CAD-CBD-CGD-O1D
13	V2	201	CYC	C4B-C3B-CAB-CBB
13	v2	201	CYC	C4B-C3B-CAB-CBB
13	J4	202	CYC	C4B-C3B-CAB-CBB
13	y2	201	CYC	CAA-CBA-CGA-O2A
13	C4	202	CYC	CAD-CBD-CGD-O2D
13	U4	201	CYC	CAD-CBD-CGD-O1D
13	Q5	202	CYC	CAA-CBA-CGA-O2A
13	K6	201	CYC	C2B-C1B-CHB-C4A
13	N7	201	CYC	C2B-C1B-CHB-C4A
13	D2	201	CYC	CAA-CBA-CGA-O1A
13	W2	201	CYC	CAA-CBA-CGA-O1A
13	n2	201	CYC	CAA-CBA-CGA-O2A
13	J3	201	CYC	C2C-C3C-CAC-CBC
13	C6	202	CYC	C2C-C3C-CAC-CBC
13	D4	201	CYC	CAD-CBD-CGD-O2D
13	Q4	202	CYC	CAA-CBA-CGA-O1A
13	F3	201	CYC	NA-C1A-CHA-C4D
13	J6	201	CYC	NA-C1A-CHA-C4D
13	V6	201	CYC	NA-C1A-CHA-C4D
13	W3	201	CYC	NB-C1B-CHB-C4A
13	a2	201	CYC	CAA-CBA-CGA-O1A
13	v2	201	CYC	CAD-CBD-CGD-O2D
13	x2	201	CYC	CAA-CBA-CGA-O2A
13	i2	201	CYC	CAD-CBD-CGD-O1D
13	N5	201	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	F7	202	CYC	C2A-CAA-CBA-CGA
13	D7	201	CYC	CAD-CBD-CGD-O1D
13	p2	201	CYC	C2B-C1B-CHB-C4A
13	I1	201	CYC	CAD-CBD-CGD-O2D
13	P7	202	CYC	CAD-CBD-CGD-O2D
13	S2	201	CYC	CAD-CBD-CGD-O2D
13	D3	201	CYC	CAD-CBD-CGD-O2D
13	j2	201	CYC	CAD-CBD-CGD-O2D
13	J1	202	CYC	ND-C4D-CHA-C1A
13	J4	202	CYC	ND-C4D-CHA-C1A
13	Q3	202	CYC	CAA-CBA-CGA-O1A
13	C6	202	CYC	CAD-CBD-CGD-O2D
13	52	301	CYC	CAA-CBA-CGA-O2A
13	d2	201	CYC	CAD-CBD-CGD-O2D
13	K3	201	CYC	C2B-C1B-CHB-C4A
13	W7	201	CYC	C2B-C1B-CHB-C4A
13	B2	201	CYC	CAD-CBD-CGD-O2D
13	m2	201	CYC	CAD-CBD-CGD-O1D
13	C4	202	CYC	CAD-CBD-CGD-O1D
13	I4	201	CYC	CAD-CBD-CGD-O2D
13	E2	201	CYC	C3C-C4C-CHD-C1D
13	G2	201	CYC	C3C-C4C-CHD-C1D
13	j2	201	CYC	C3C-C4C-CHD-C1D
13	V7	201	CYC	C3C-C4C-CHD-C1D
13	W1	201	CYC	NB-C1B-CHB-C4A
13	T7	201	CYC	C2A-CAA-CBA-CGA
13	S2	201	CYC	CAD-CBD-CGD-O1D
13	j2	201	CYC	CAD-CBD-CGD-O1D
13	v2	201	CYC	CAA-CBA-CGA-O1A
13	I4	201	CYC	CAD-CBD-CGD-O1D
13	L7	201	CYC	C3D-C4D-CHA-C1A
13	D4	201	CYC	CAD-CBD-CGD-O1D
13	F6	201	CYC	CAD-CBD-CGD-O2D
13	F6	202	CYC	C4B-C3B-CAB-CBB
13	I1	201	CYC	CAD-CBD-CGD-O1D
13	d2	201	CYC	CAD-CBD-CGD-O1D
13	Q4	202	CYC	CAA-CBA-CGA-O2A
13	I5	201	CYC	CAD-CBD-CGD-O1D
13	I5	201	CYC	CAD-CBD-CGD-O2D
13	Q6	202	CYC	CAA-CBA-CGA-O2A
13	X2	201	CYC	NA-C1A-CHA-C4D
13	F1	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	B2	201	CYC	CAD-CBD-CGD-O1D
13	W6	201	CYC	C2B-C1B-CHB-C4A

There are no ring outliers.

252 monomers are involved in 1202 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U2	201	CYC	7	0
13	w2	201	CYC	3	0
13	P7	201	CYC	1	0
13	o2	801	CYC	8	0
13	S2	201	CYC	9	0
13	a2	201	CYC	7	0
13	I6	201	CYC	3	0
13	L1	201	CYC	5	0
13	F7	201	CYC	3	0
13	a5	201	CYC	5	0
13	A2	202	CYC	4	0
13	32	301	CYC	4	0
13	F6	202	CYC	4	0
13	v2	201	CYC	6	0
13	A2	201	CYC	6	0
13	M5	201	CYC	7	0
13	X4	201	CYC	8	0
13	Q5	202	CYC	5	0
13	S7	201	CYC	6	0
13	y2	201	CYC	6	0
13	W5	201	CYC	5	0
13	E4	201	CYC	4	0
13	C1	201	CYC	5	0
13	C5	202	CYC	7	0
13	Q6	201	CYC	7	0
13	T1	202	CYC	2	0
13	P3	201	CYC	1	0
13	B1	201	CYC	7	0
13	J3	201	CYC	2	0
13	C5	201	CYC	7	0
13	I7	201	CYC	2	0
13	V7	201	CYC	6	0
13	C3	202	CYC	4	0
13	Q3	202	CYC	3	0
13	V3	201	CYC	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T5	201	CYC	5	0
13	T6	202	CYC	1	0
13	T1	201	CYC	7	0
13	N2	801	CYC	3	0
13	a7	202	CYC	4	0
13	U3	201	CYC	1	0
13	J4	201	CYC	7	0
13	H5	201	CYC	3	0
13	Q3	201	CYC	8	0
13	P4	201	CYC	3	0
13	W6	201	CYC	3	0
13	A1	302	CYC	8	0
13	J6	202	CYC	2	0
13	V1	202	CYC	3	0
13	W1	201	CYC	6	0
13	A6	301	CYC	6	0
13	R1	201	CYC	4	0
13	H1	201	CYC	3	0
13	C3	201	CYC	4	0
13	J5	202	CYC	2	0
13	42	301	CYC	4	0
13	U5	201	CYC	4	0
13	C7	202	CYC	4	0
13	G6	201	CYC	2	0
13	R6	201	CYC	5	0
13	G7	201	CYC	1	0
13	T4	201	CYC	5	0
13	B4	201	CYC	5	0
13	x2	201	CYC	3	0
13	P7	202	CYC	1	0
13	N5	201	CYC	5	0
13	H6	201	CYC	1	0
13	F1	201	CYC	3	0
13	22	302	CYC	7	0
13	S5	201	CYC	7	0
13	X6	201	CYC	5	0
13	a6	201	CYC	8	0
13	W7	201	CYC	2	0
13	M7	201	CYC	6	0
13	U4	201	CYC	3	0
13	H4	201	CYC	3	0
13	X2	201	CYC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W3	201	CYC	3	0
13	H2	201	CYC	8	0
13	K7	201	CYC	2	0
13	K4	201	CYC	4	0
13	M2	201	CYC	8	0
13	R5	201	CYC	5	0
13	V5	201	CYC	5	0
13	W4	201	CYC	6	0
13	T3	201	CYC	6	0
13	f2	201	CYC	5	0
13	V4	202	CYC	4	0
13	L6	201	CYC	5	0
13	P3	202	CYC	3	0
13	Z4	301	CYC	5	0
13	J3	202	CYC	2	0
13	t2	201	CYC	2	0
13	D6	201	CYC	3	0
13	a3	202	CYC	5	0
13	B7	201	CYC	5	0
13	U6	201	CYC	3	0
13	T7	202	CYC	1	0
13	F3	201	CYC	3	0
13	Q4	201	CYC	6	0
13	g2	201	CYC	10	0
13	N3	201	CYC	4	0
13	I1	201	CYC	5	0
13	l2	201	CYC	8	0
13	K3	201	CYC	3	0
13	J1	201	CYC	5	0
13	p2	201	CYC	7	0
13	E2	201	CYC	7	0
13	K5	201	CYC	4	0
13	T2	201	CYC	5	0
13	N2	802	CYC	7	0
13	X7	201	CYC	9	0
13	B5	201	CYC	7	0
13	V1	201	CYC	8	0
13	S4	201	CYC	6	0
13	F3	202	CYC	4	0
13	Z7	301	CYC	7	0
13	I5	201	CYC	3	0
13	C4	202	CYC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N4	201	CYC	5	0
13	Z1	301	CYC	6	0
13	L2	201	CYC	7	0
13	B6	201	CYC	9	0
13	22	301	CYC	5	0
13	B3	201	CYC	5	0
13	P5	201	CYC	2	0
13	H7	201	CYC	1	0
13	Q7	202	CYC	4	0
13	S3	201	CYC	6	0
13	D3	201	CYC	3	0
13	a5	202	CYC	5	0
13	V2	201	CYC	2	0
13	G5	201	CYC	3	0
13	T3	202	CYC	1	0
13	F2	201	CYC	8	0
13	I3	201	CYC	4	0
13	D7	201	CYC	5	0
13	P1	201	CYC	2	0
13	M3	201	CYC	7	0
13	D2	201	CYC	8	0
13	P6	202	CYC	2	0
13	Q5	201	CYC	7	0
13	P2	201	CYC	3	0
13	B2	202	CYC	5	0
13	Q2	201	CYC	7	0
13	a4	201	CYC	7	0
13	E1	201	CYC	5	0
13	G1	201	CYC	4	0
13	a6	202	CYC	5	0
13	d2	201	CYC	6	0
13	R3	201	CYC	6	0
13	M6	201	CYC	7	0
13	A1	301	CYC	5	0
13	B2	201	CYC	3	0
13	D1	201	CYC	2	0
13	L7	201	CYC	4	0
13	L4	201	CYC	1	0
13	h2	201	CYC	9	0
13	F4	202	CYC	4	0
13	L5	201	CYC	5	0
13	J6	201	CYC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a1	202	CYC	6	0
13	S1	201	CYC	7	0
13	P6	201	CYC	2	0
13	C4	201	CYC	5	0
13	C7	201	CYC	4	0
13	L3	201	CYC	3	0
13	n2	201	CYC	7	0
13	E7	201	CYC	5	0
13	H3	201	CYC	1	0
13	J7	202	CYC	2	0
13	Q1	202	CYC	5	0
13	T4	202	CYC	2	0
13	V7	202	CYC	4	0
13	Q1	201	CYC	6	0
13	K6	201	CYC	5	0
13	V3	202	CYC	3	0
13	U1	201	CYC	2	0
13	N6	201	CYC	4	0
13	C6	201	CYC	5	0
13	C2	201	CYC	5	0
13	a1	201	CYC	3	0
13	q2	201	CYC	2	0
13	K1	201	CYC	4	0
13	k2	201	CYC	6	0
13	R2	201	CYC	9	0
13	G4	201	CYC	3	0
13	F7	202	CYC	4	0
13	D4	201	CYC	4	0
13	z2	201	CYC	6	0
13	Q4	202	CYC	5	0
13	R4	201	CYC	3	0
13	52	302	CYC	7	0
13	s2	201	CYC	9	0
13	52	301	CYC	6	0
13	F4	201	CYC	4	0
13	M4	201	CYC	4	0
13	T6	201	CYC	6	0
13	J1	202	CYC	2	0
13	E5	201	CYC	4	0
13	V6	202	CYC	4	0
13	a7	201	CYC	6	0
13	a3	201	CYC	7	0

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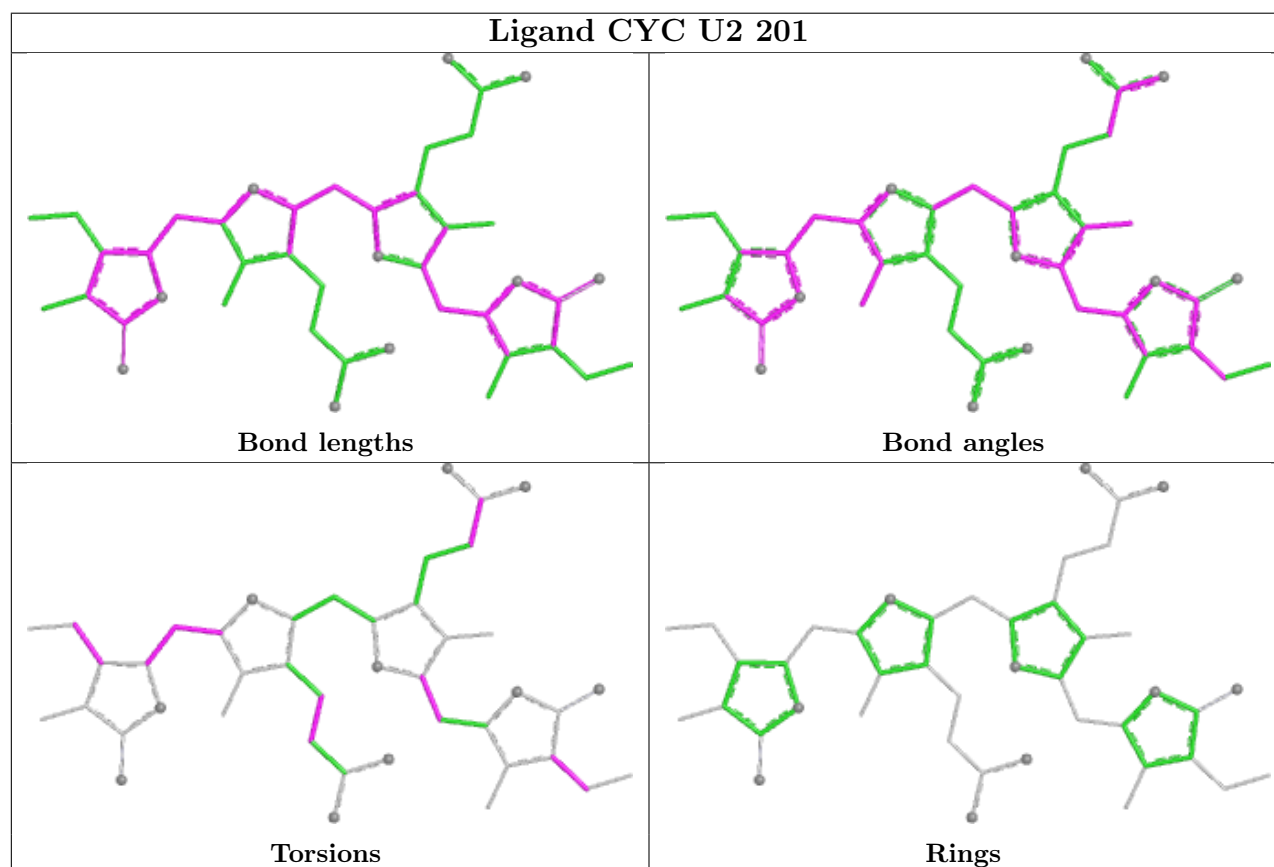
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	e2	201	CYC	8	0
13	V6	201	CYC	7	0
13	G3	201	CYC	2	0
13	F1	202	CYC	3	0
13	A6	302	CYC	8	0
13	S6	201	CYC	5	0
13	N1	201	CYC	5	0
13	F5	202	CYC	3	0
13	I4	201	CYC	3	0
13	Z5	301	CYC	5	0
13	M1	201	CYC	6	0
13	Q6	202	CYC	5	0
13	G2	201	CYC	8	0
13	X3	201	CYC	7	0
13	J5	201	CYC	2	0
13	Z6	301	CYC	4	0
13	J7	201	CYC	4	0
13	V4	201	CYC	6	0
13	U7	201	CYC	1	0
13	F5	201	CYC	4	0
13	a4	202	CYC	5	0
13	T5	202	CYC	3	0
13	32	302	CYC	8	0
13	c2	801	CYC	7	0
13	T7	201	CYC	7	0
13	P1	202	CYC	2	0
13	r2	201	CYC	6	0
13	F6	201	CYC	4	0
13	R7	201	CYC	3	0
13	j2	201	CYC	5	0
13	J4	202	CYC	3	0
13	X5	201	CYC	9	0
13	V5	202	CYC	3	0
13	P4	202	CYC	2	0
13	O2	201	CYC	5	0
13	E3	201	CYC	3	0
13	C1	202	CYC	8	0
13	N7	201	CYC	3	0
13	Q7	201	CYC	7	0
13	E6	201	CYC	5	0
13	i2	201	CYC	3	0
13	W2	201	CYC	7	0

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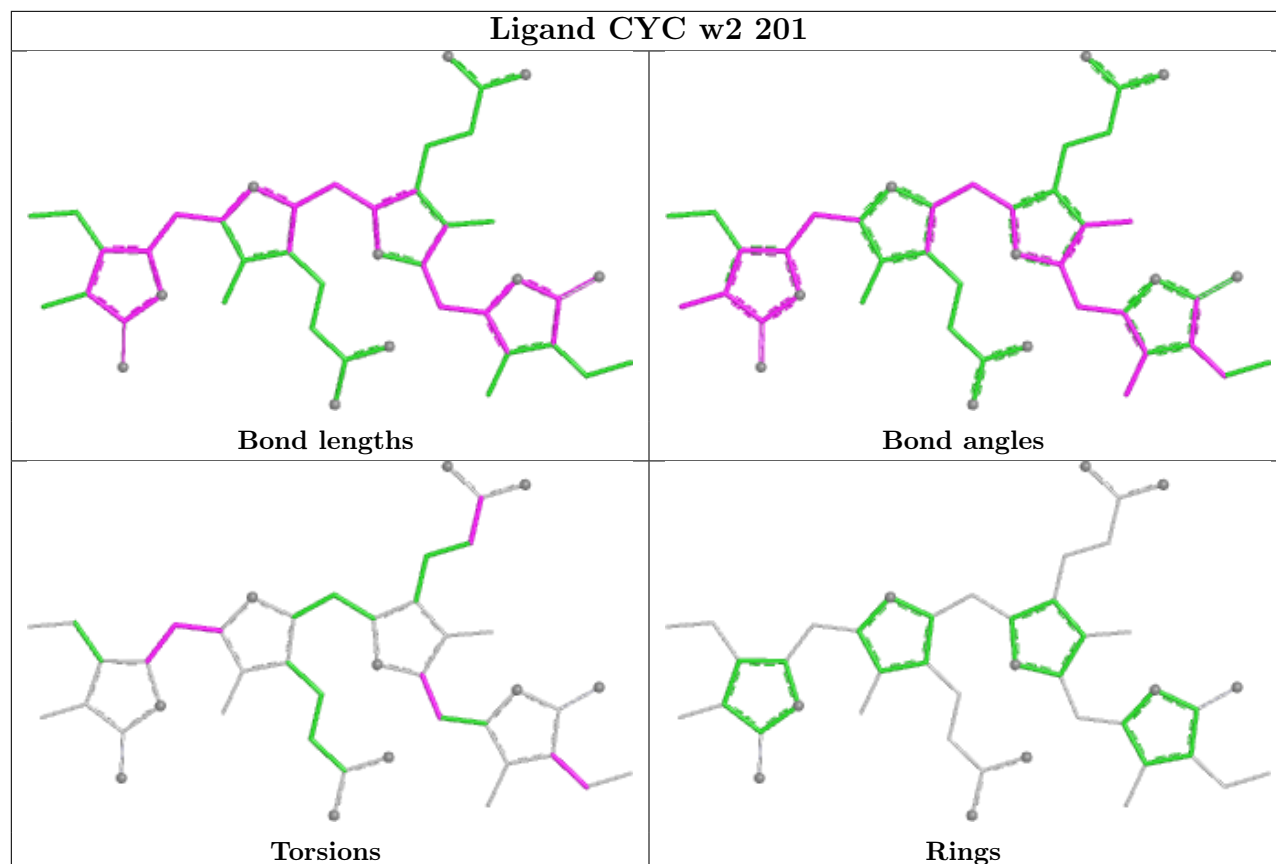
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D5	201	CYC	2	0
13	X1	201	CYC	9	0
13	P5	202	CYC	2	0
13	C6	202	CYC	6	0
13	m2	201	CYC	6	0
13	Z3	301	CYC	7	0
13	42	302	CYC	10	0

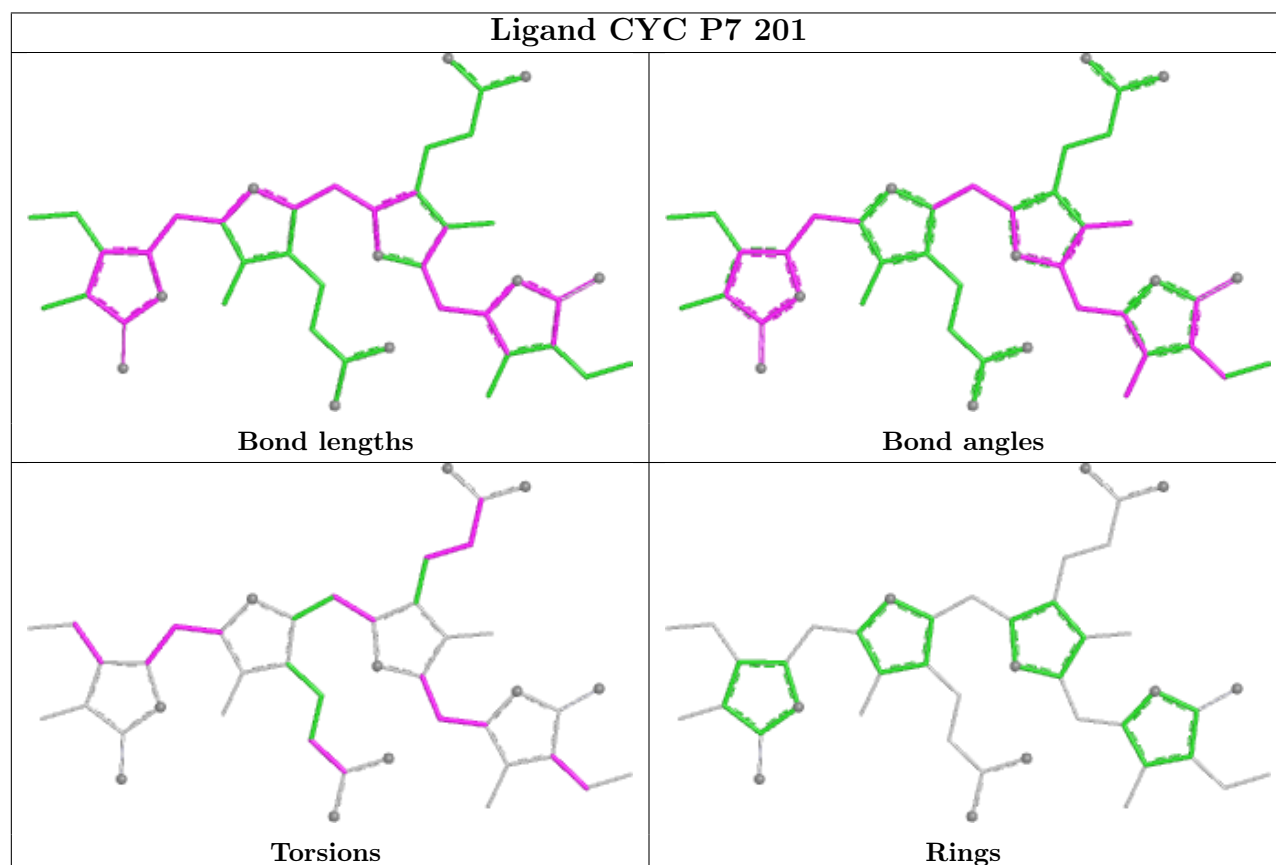
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

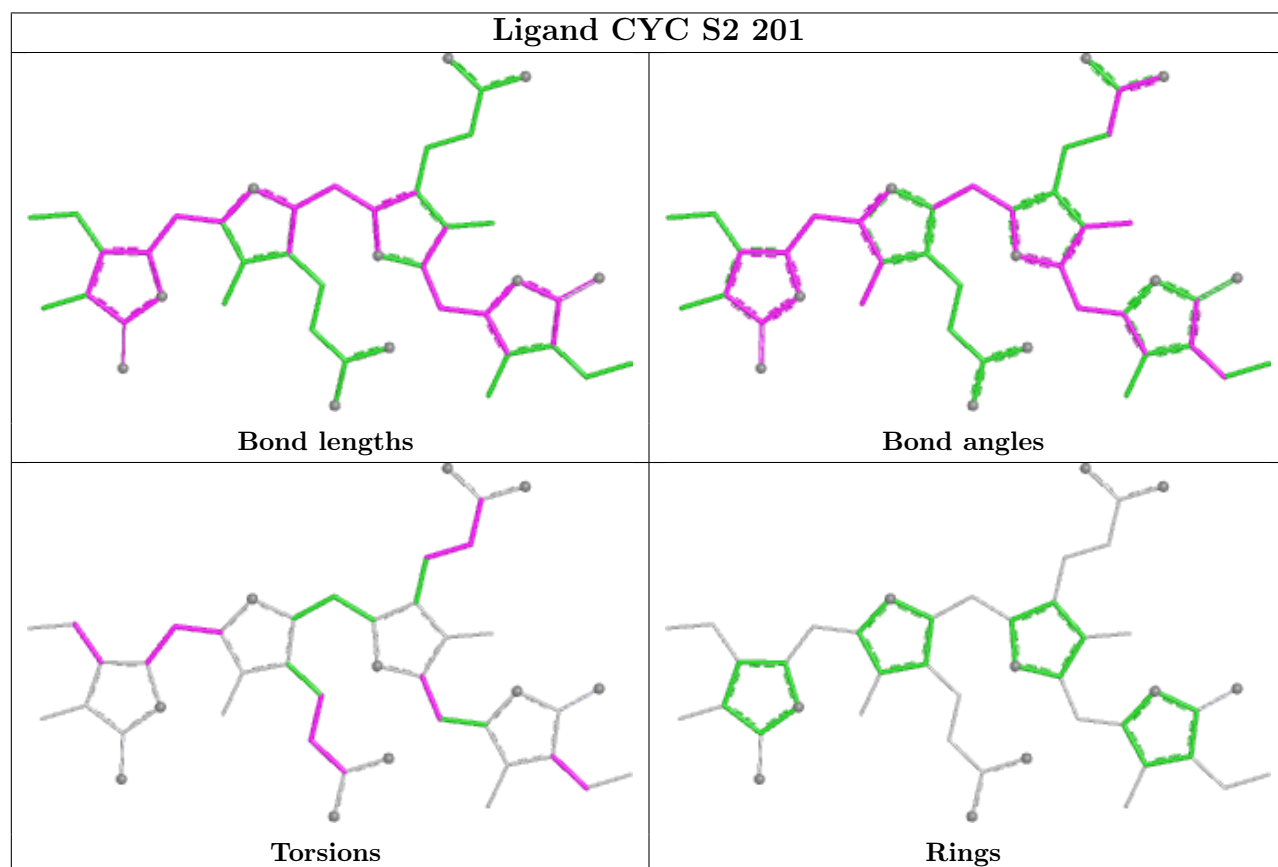
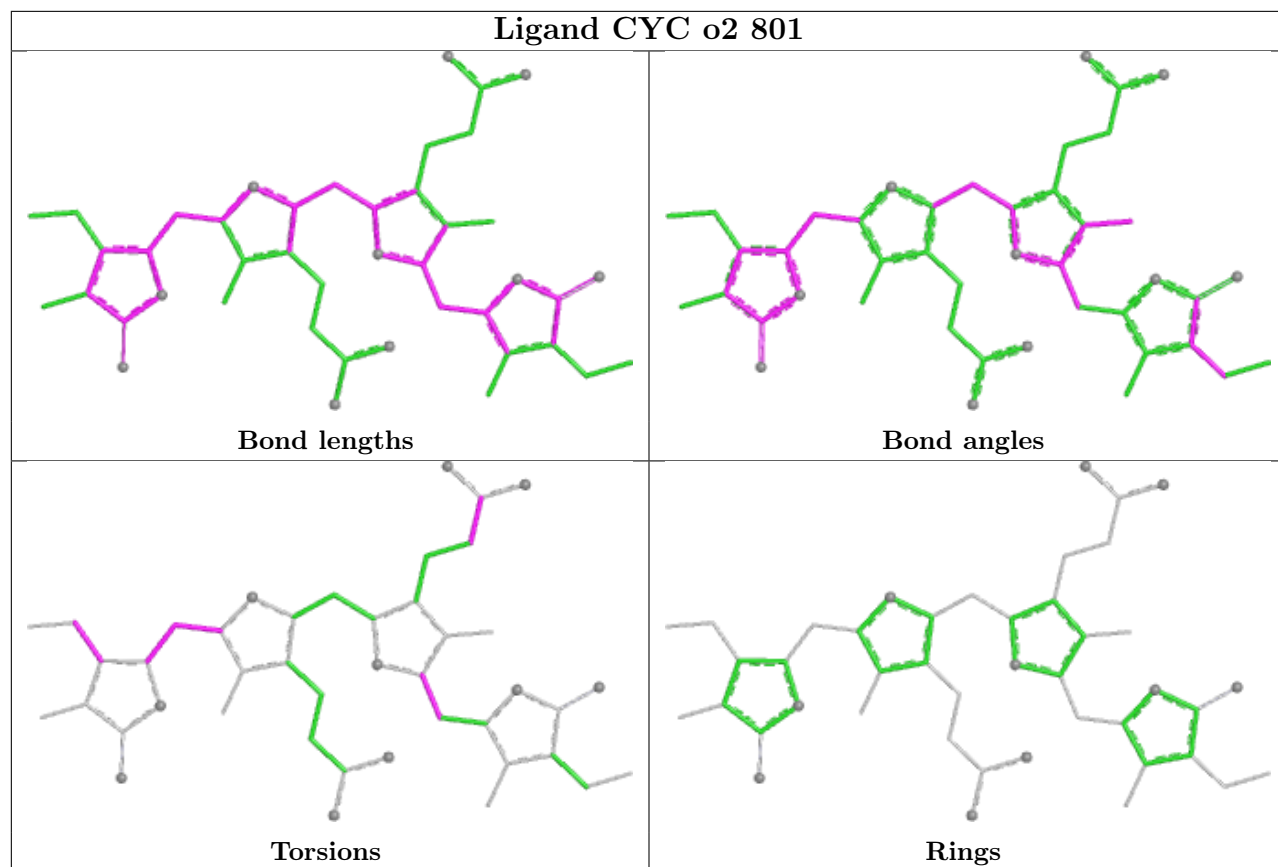


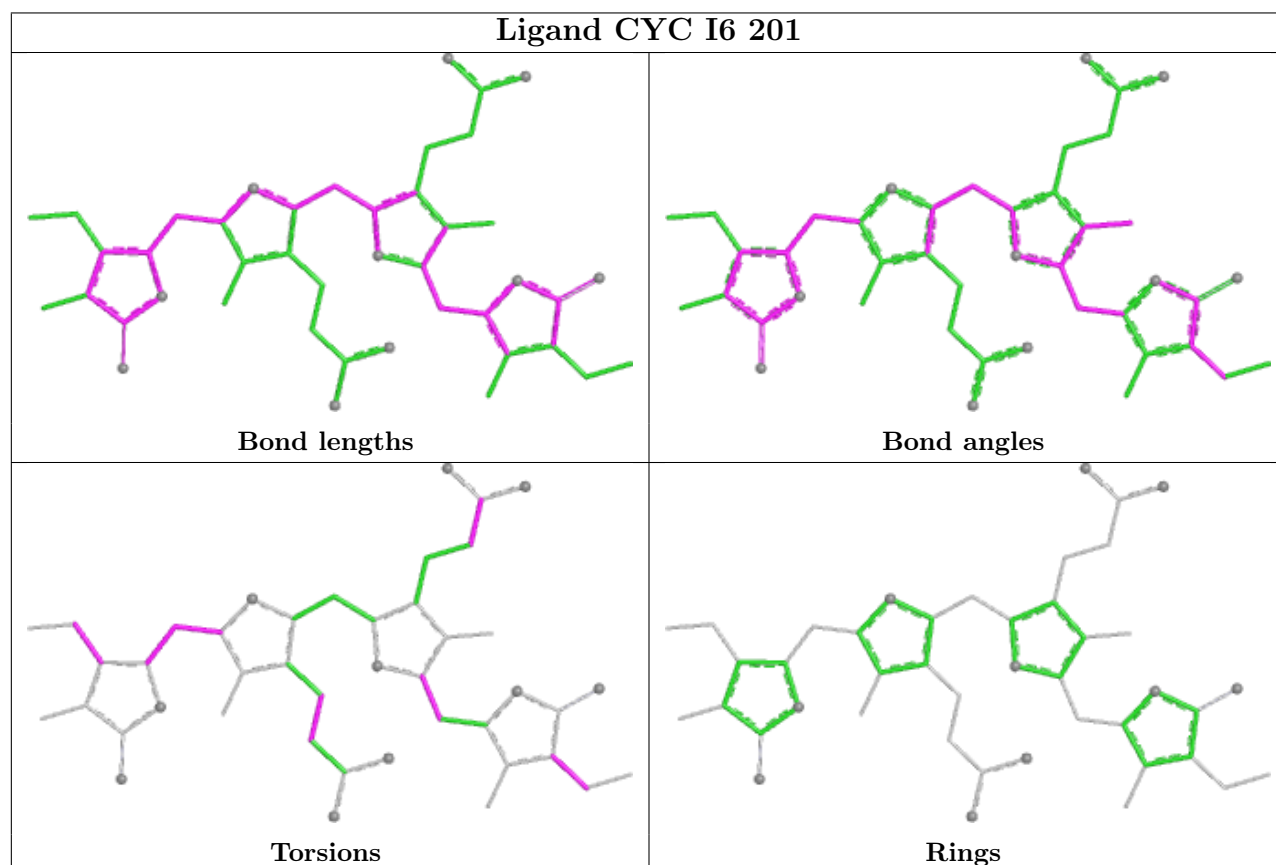
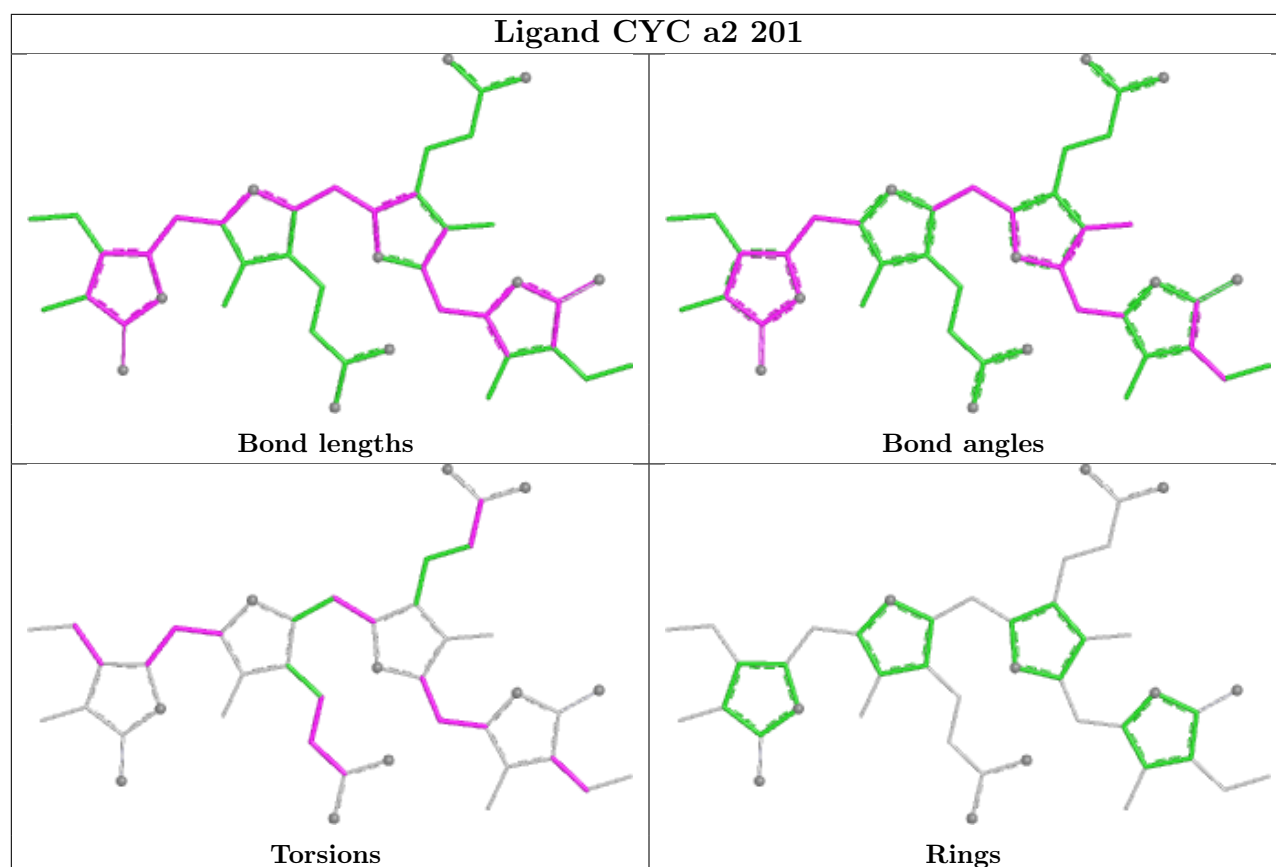
Ligand CYC w2 201



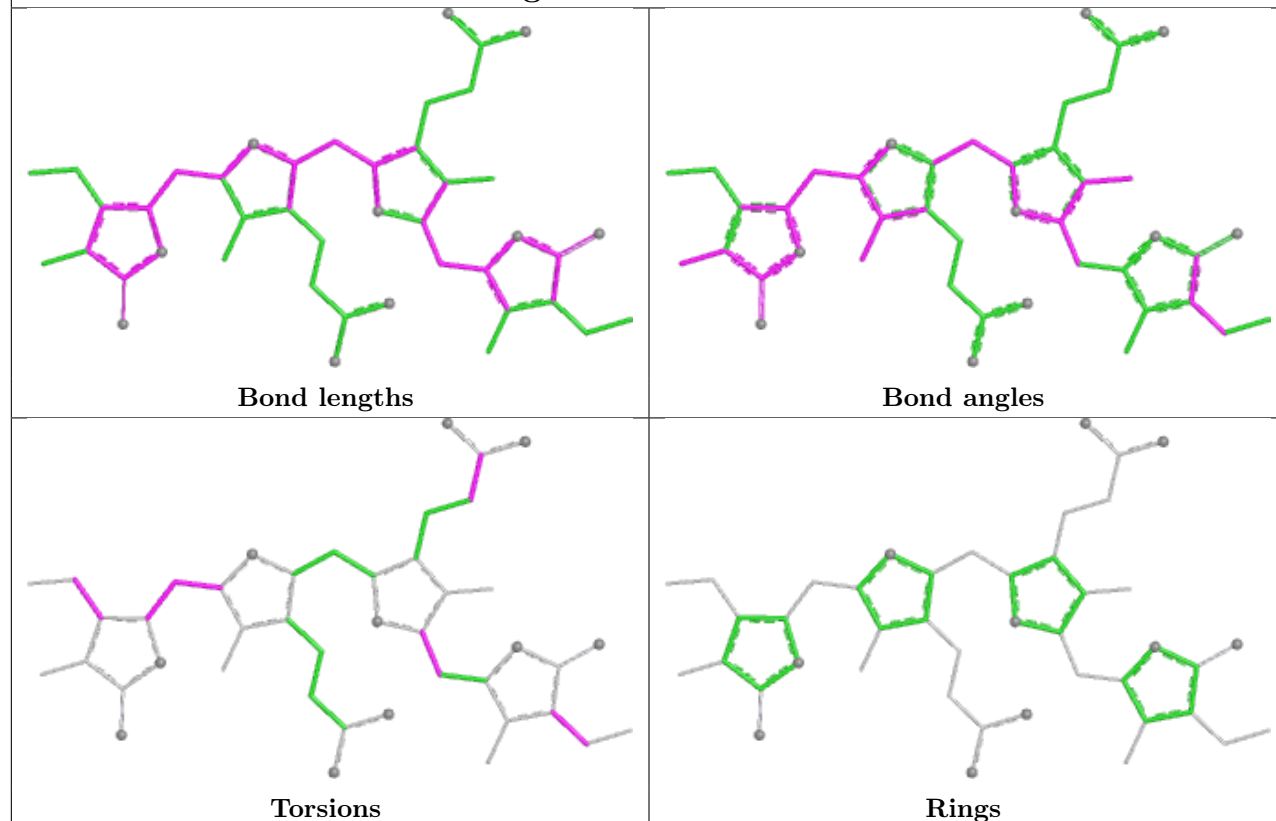
Ligand CYC P7 201



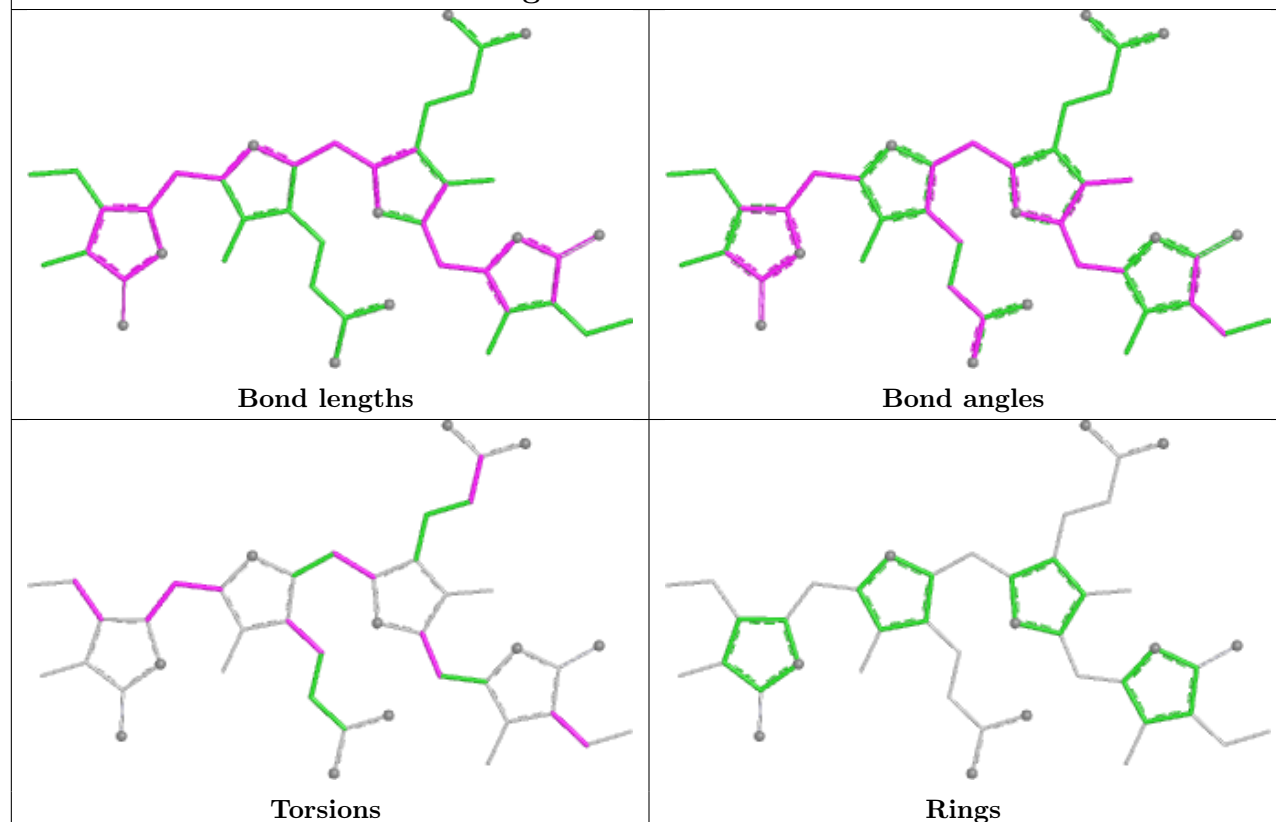


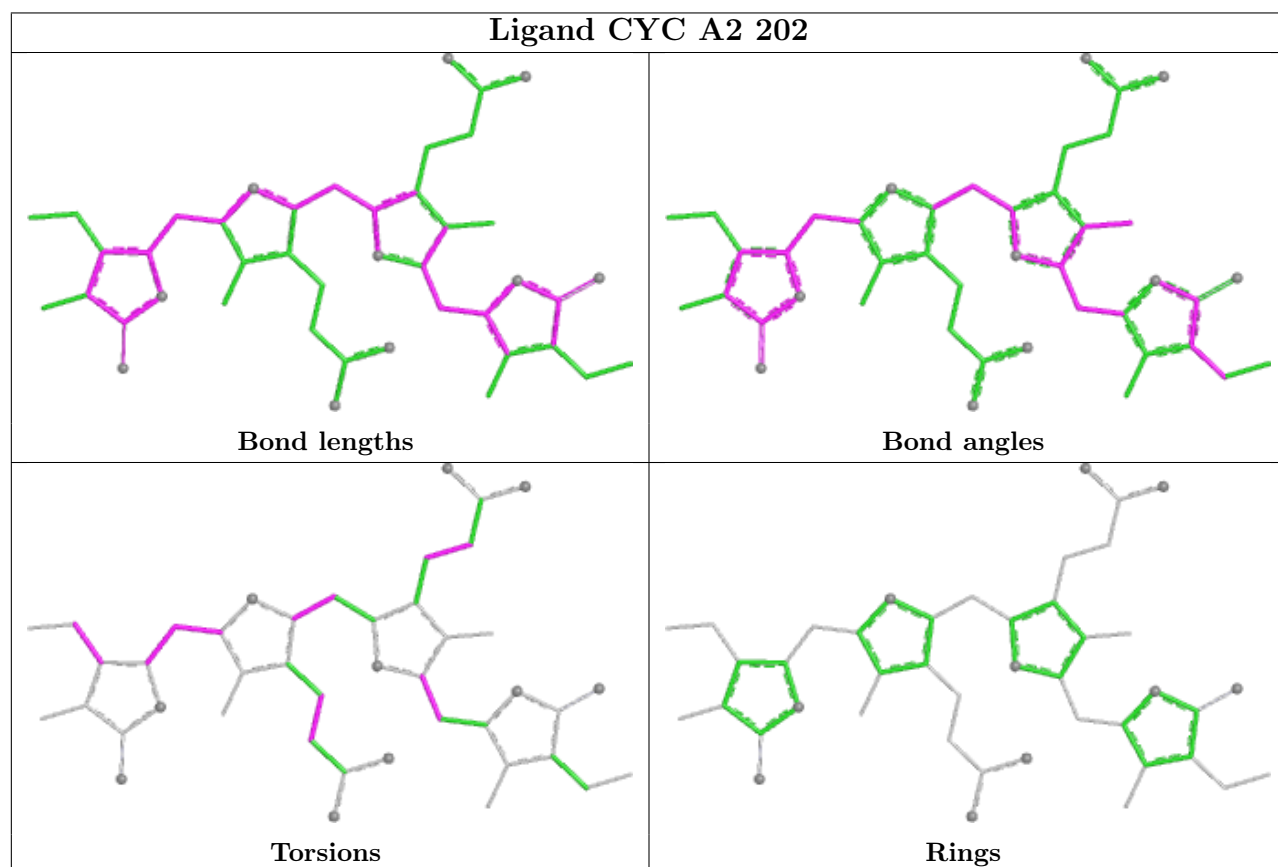
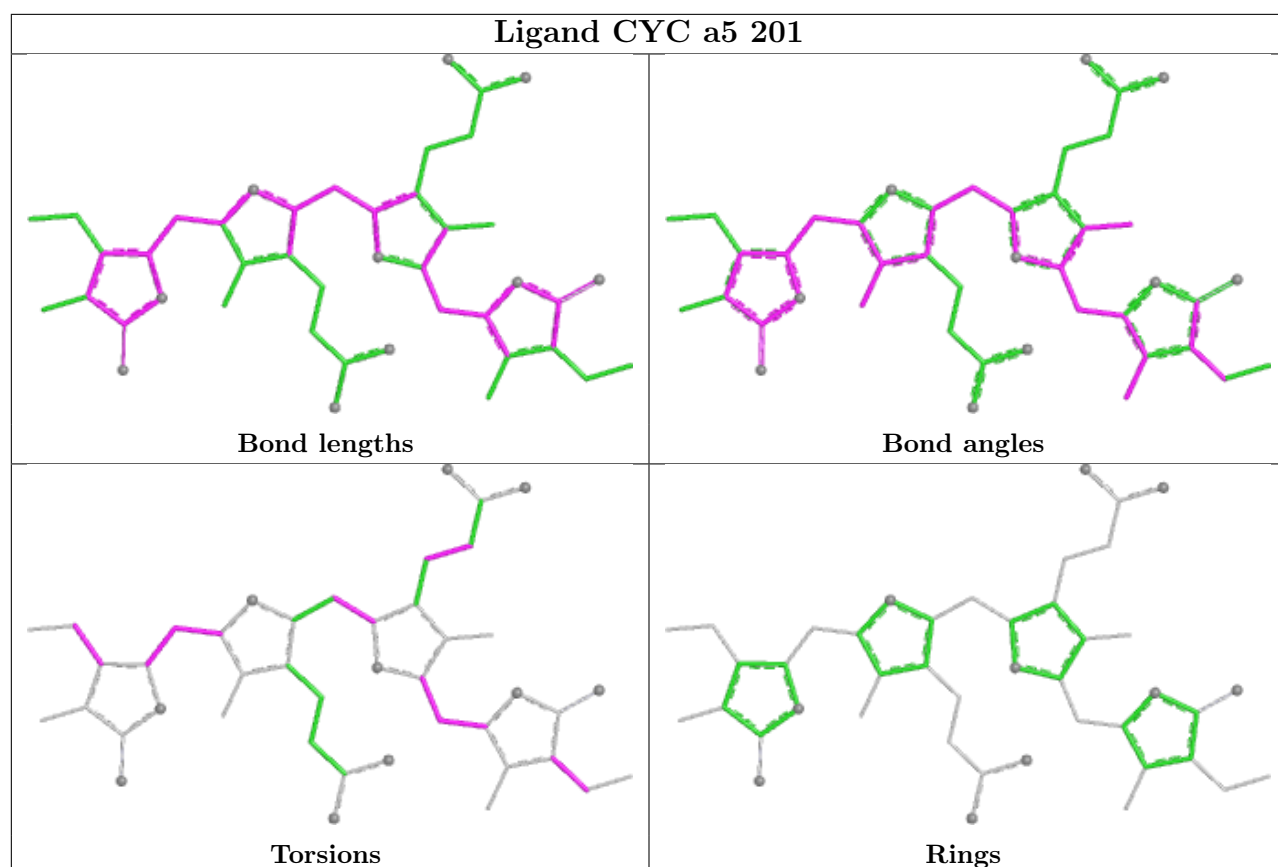


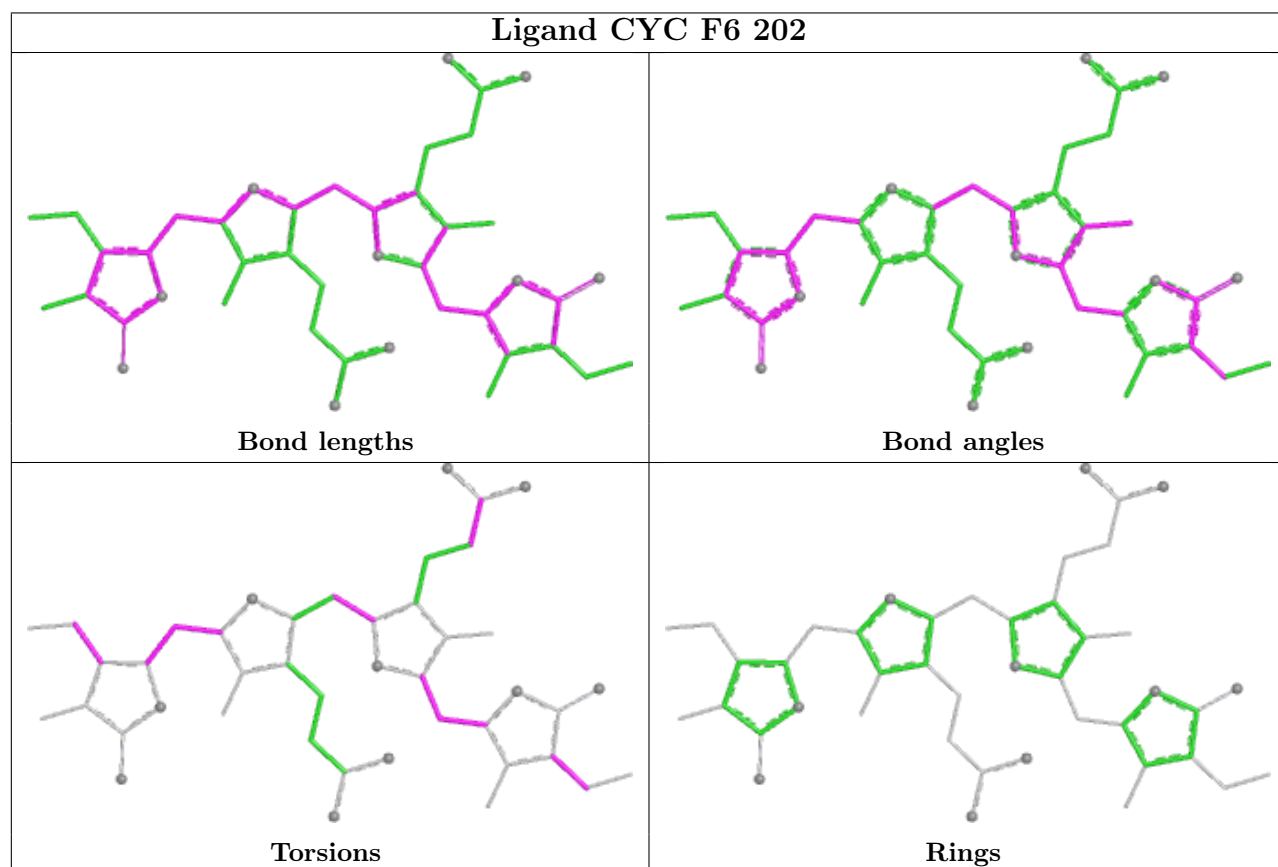
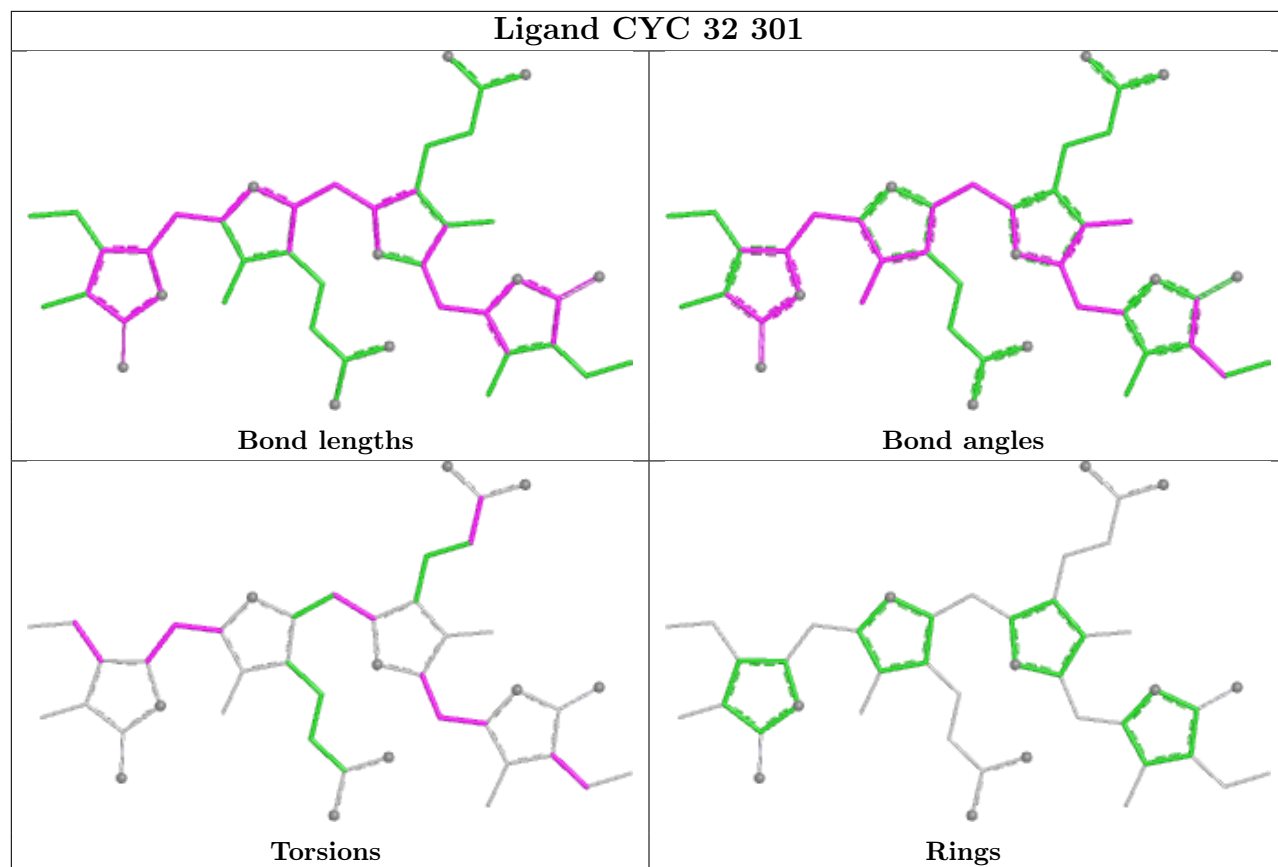
Ligand CYC L1 201

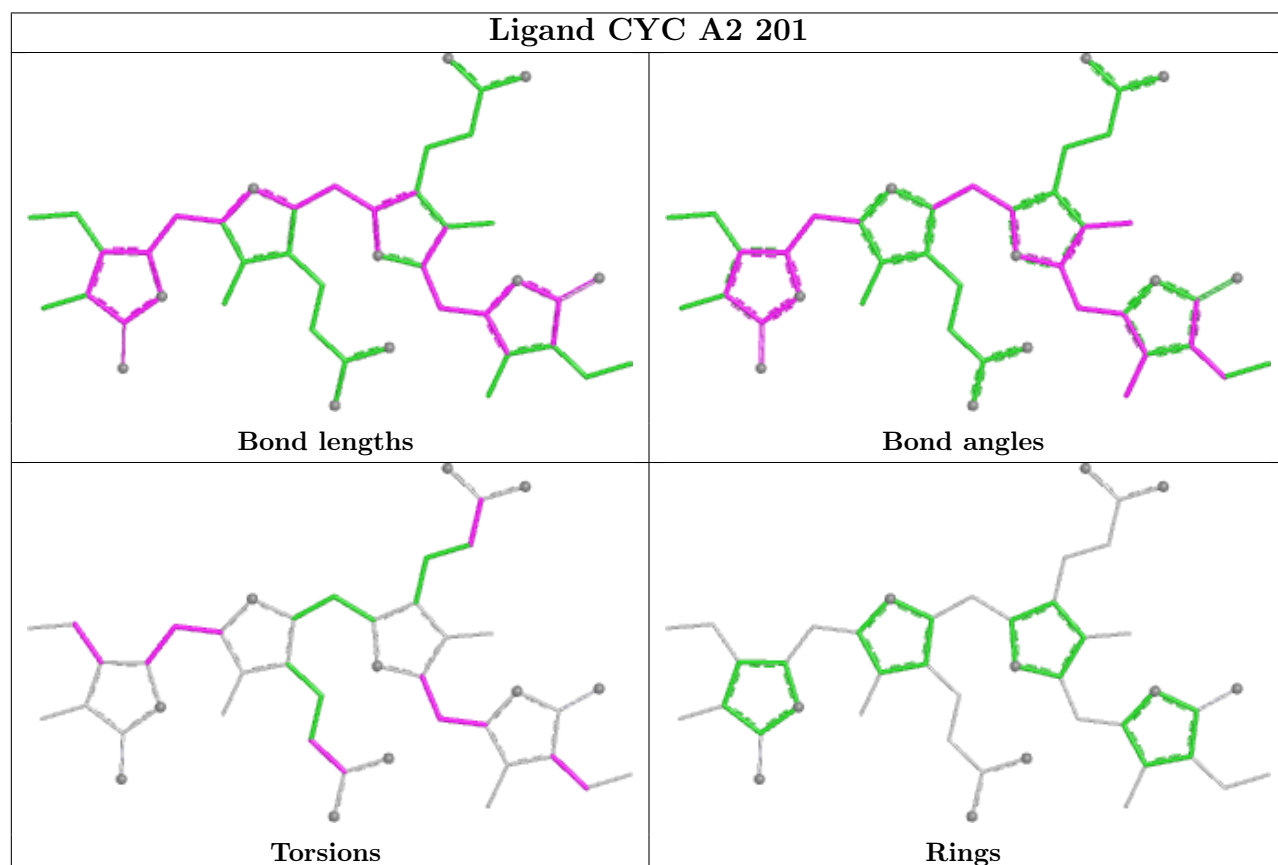
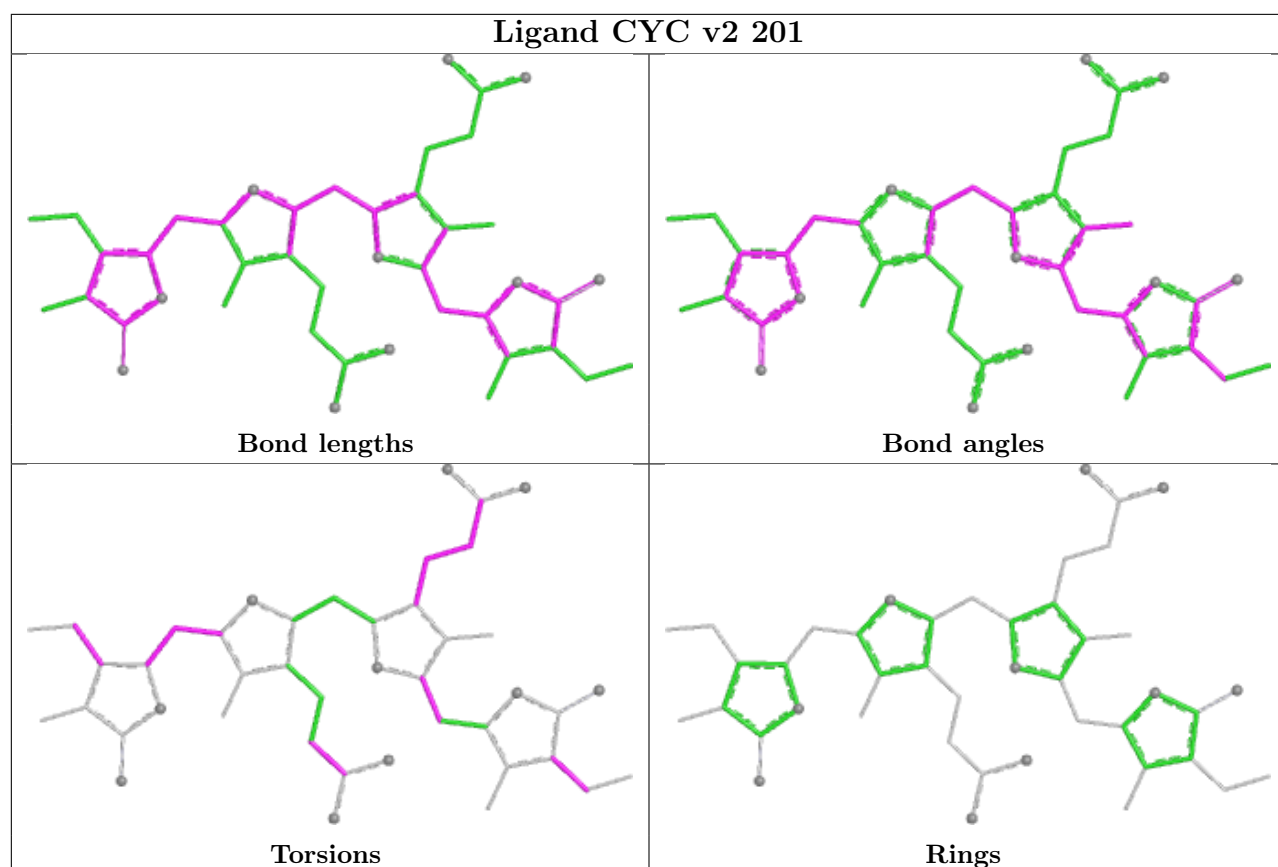


Ligand CYC F7 201

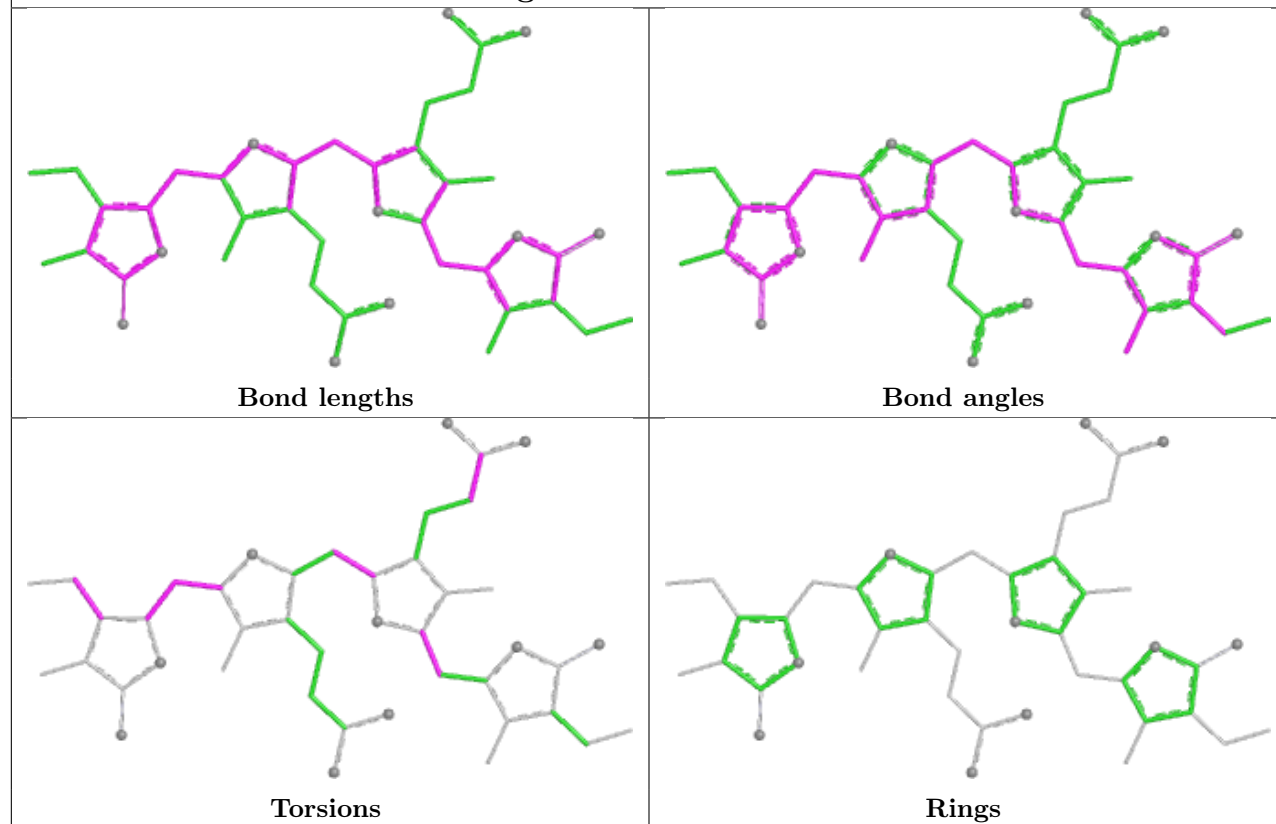




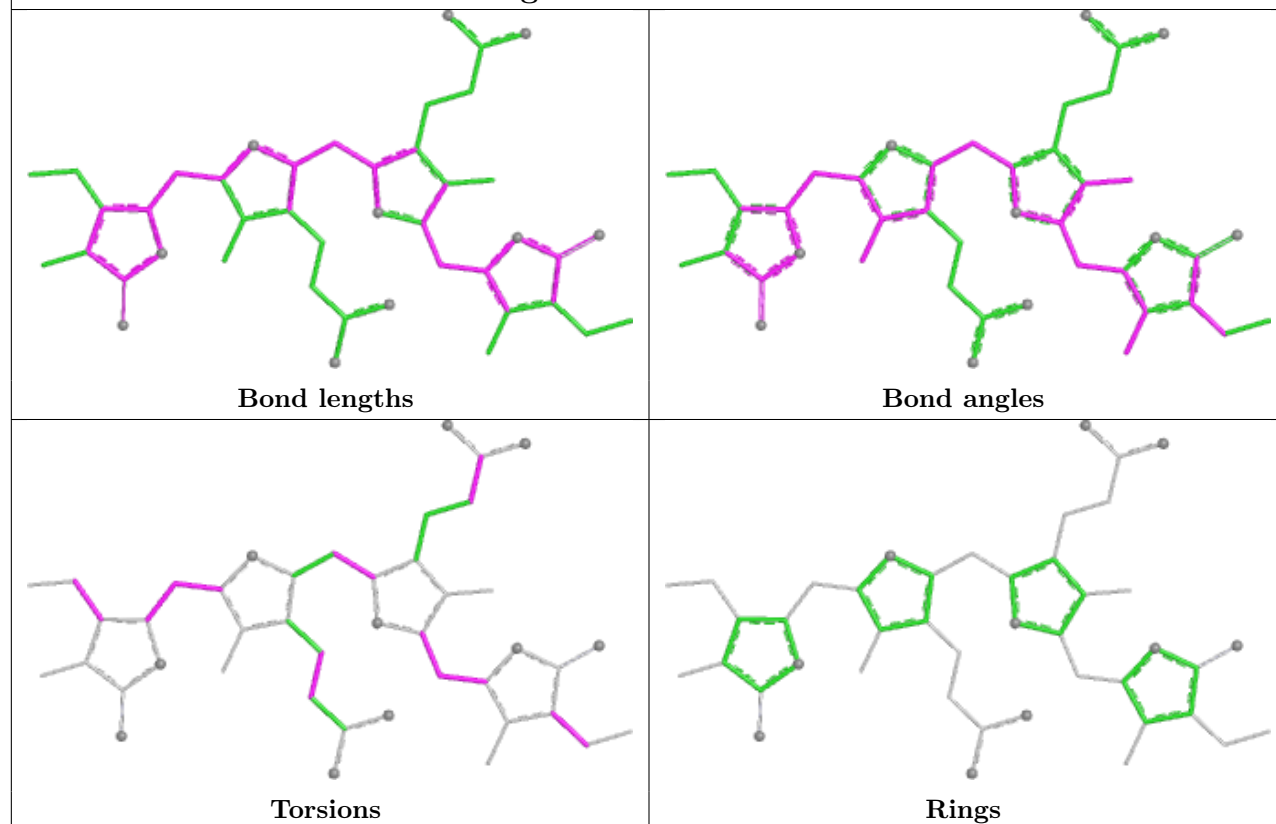




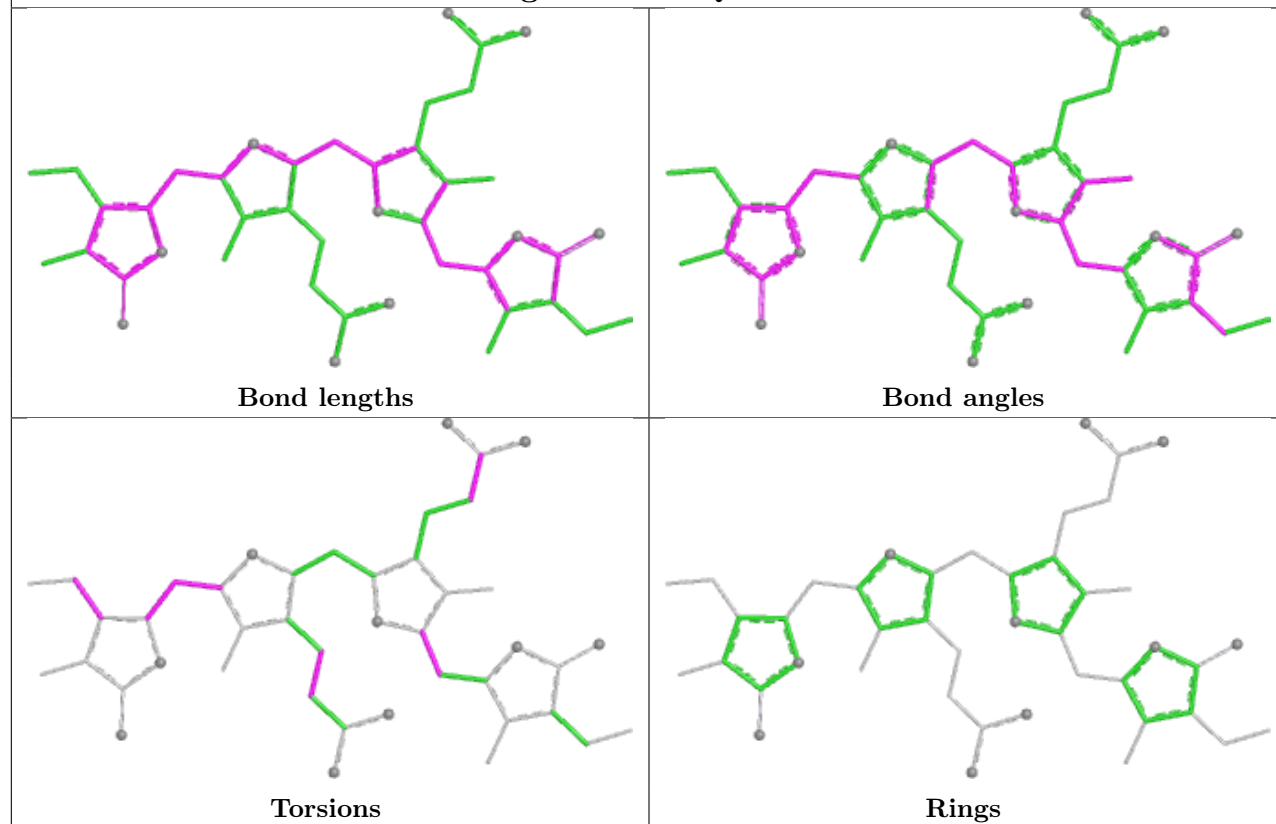
Ligand CYC M5 201



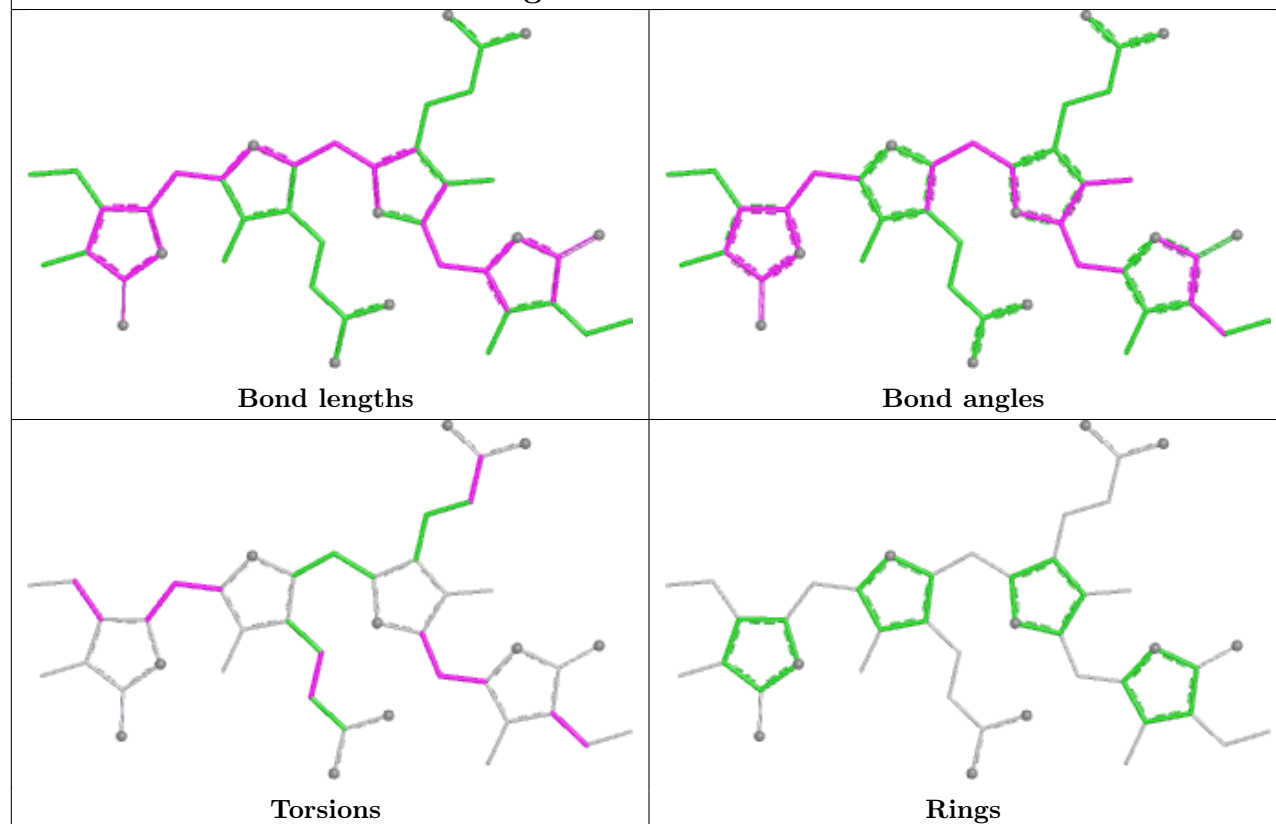
Ligand CYC X4 201

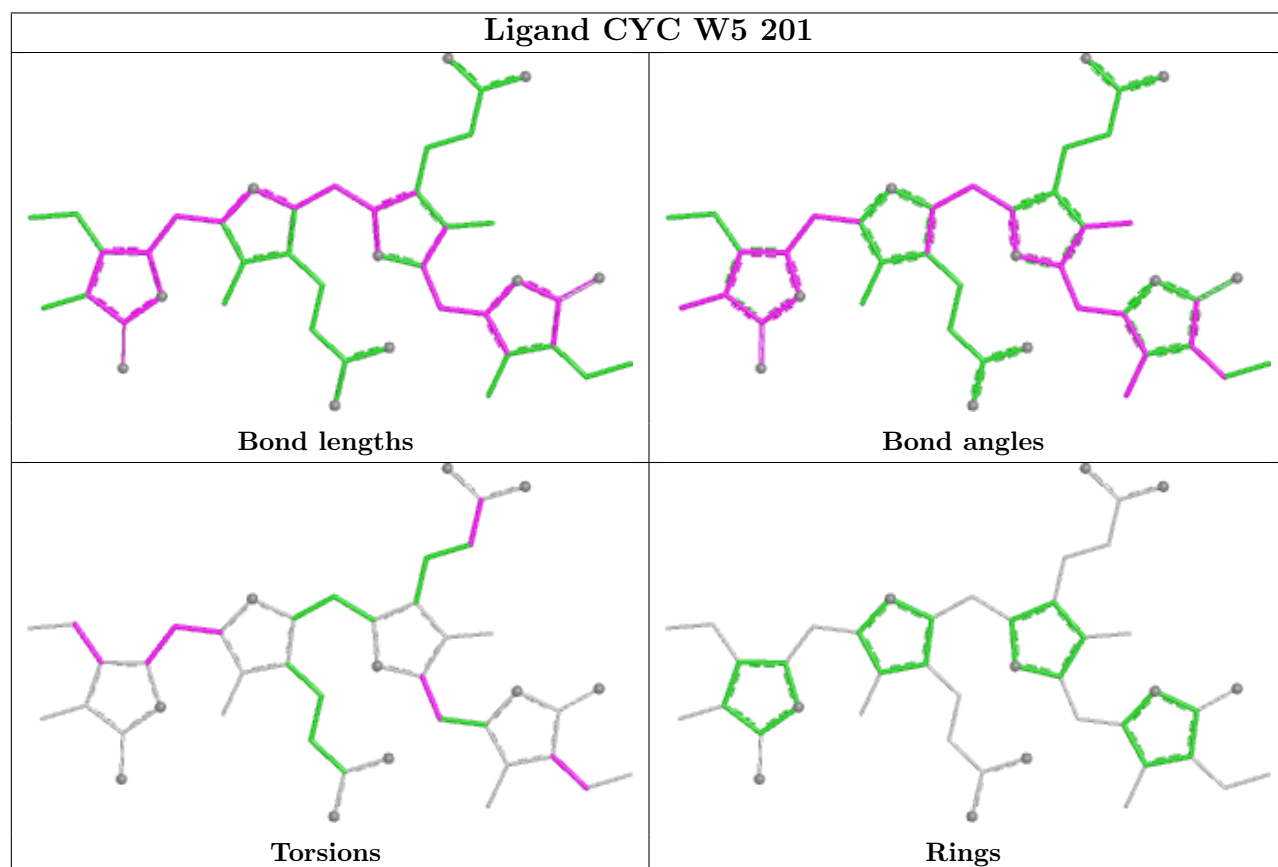
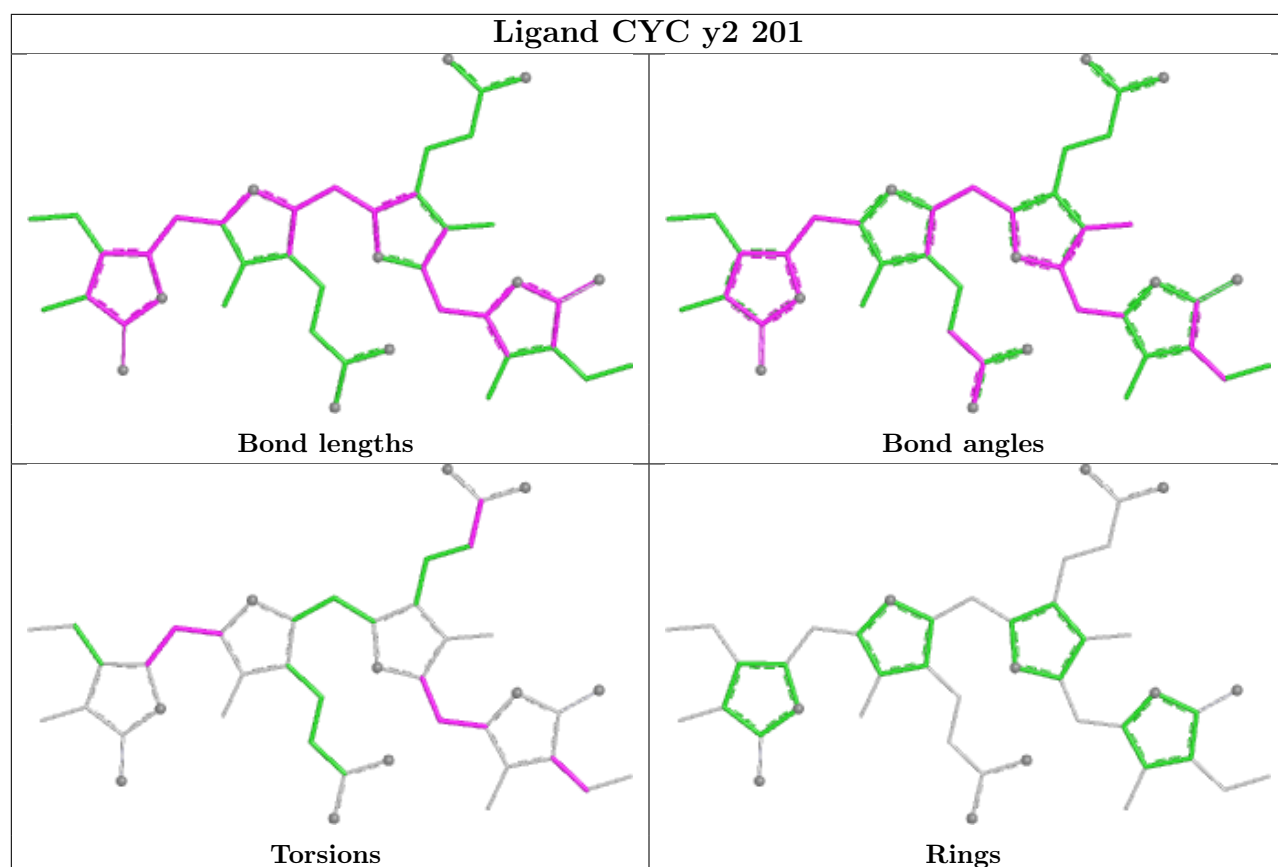


Ligand CYC Q5 202

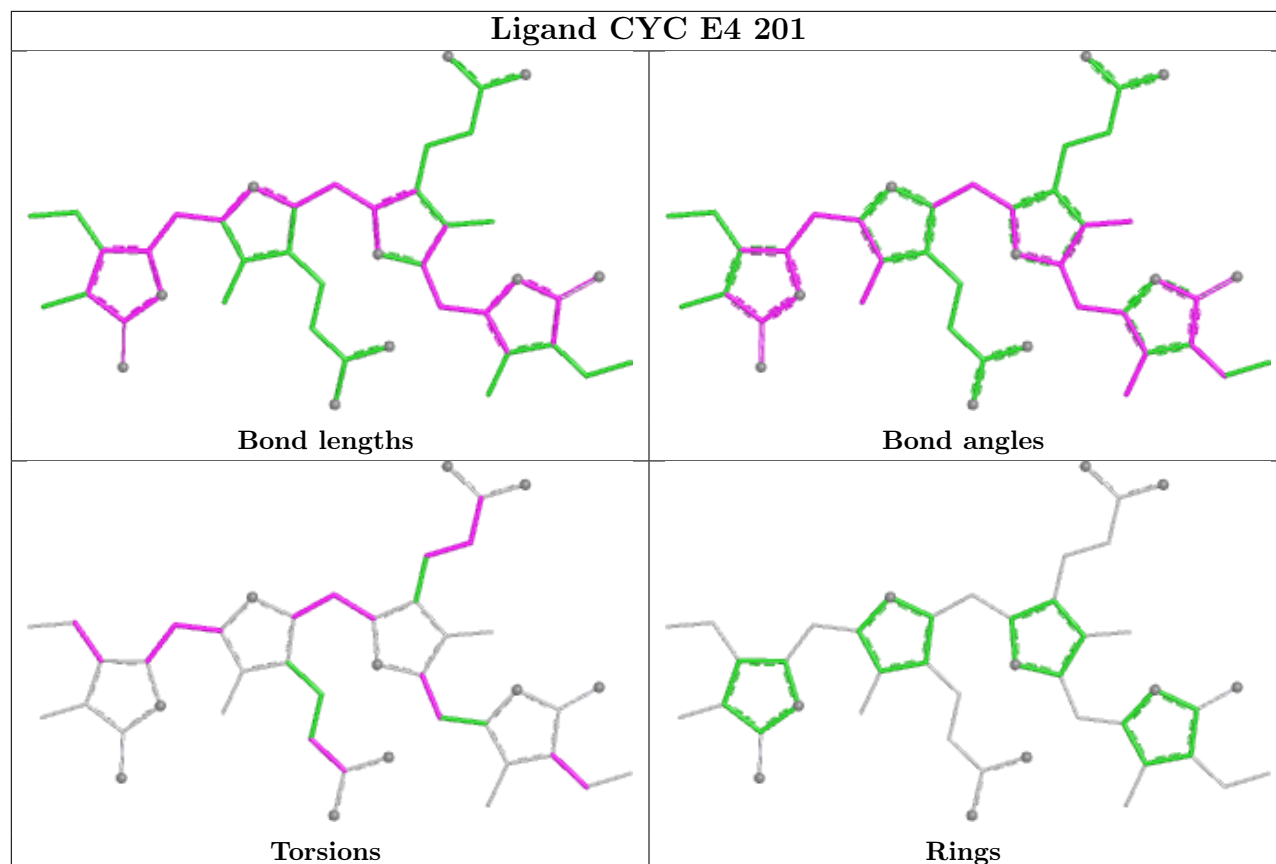


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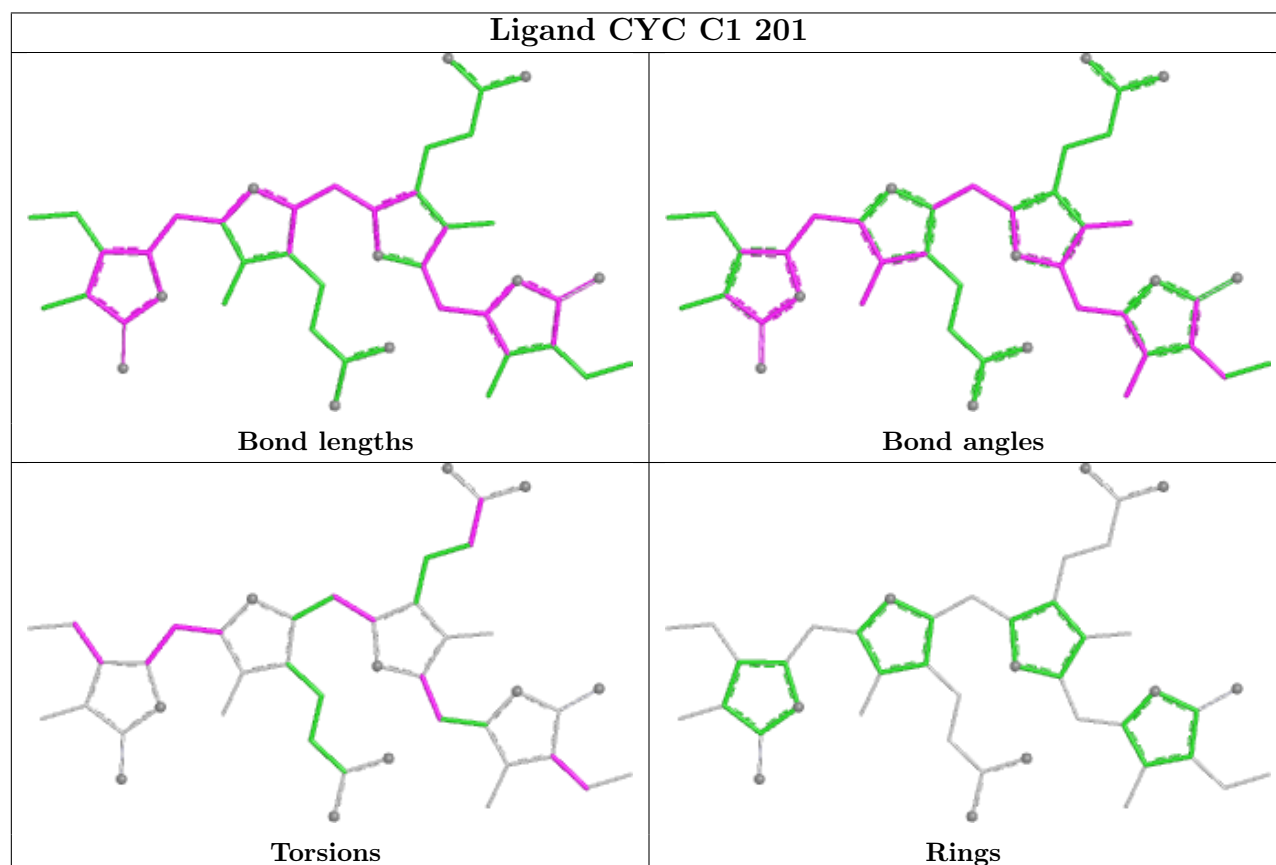




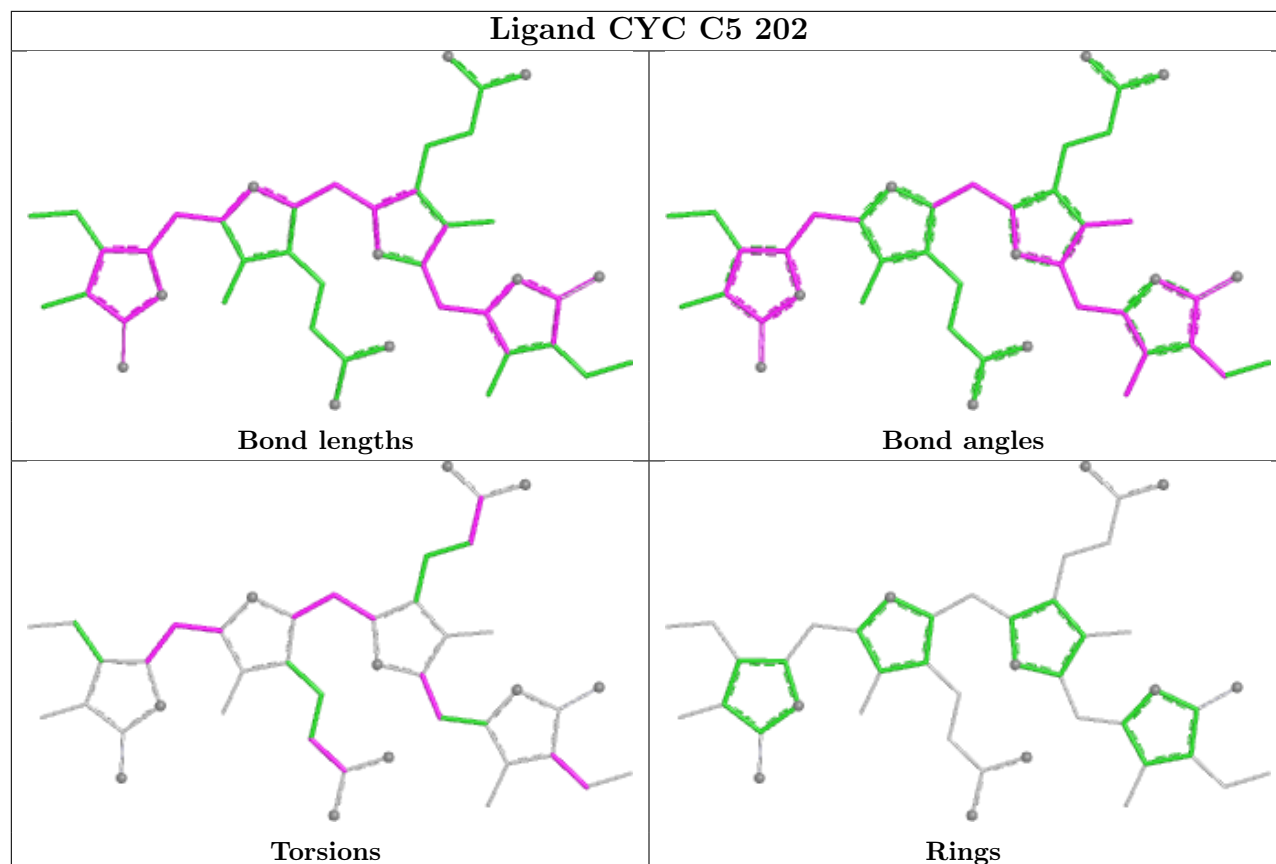
Ligand CYC E4 201



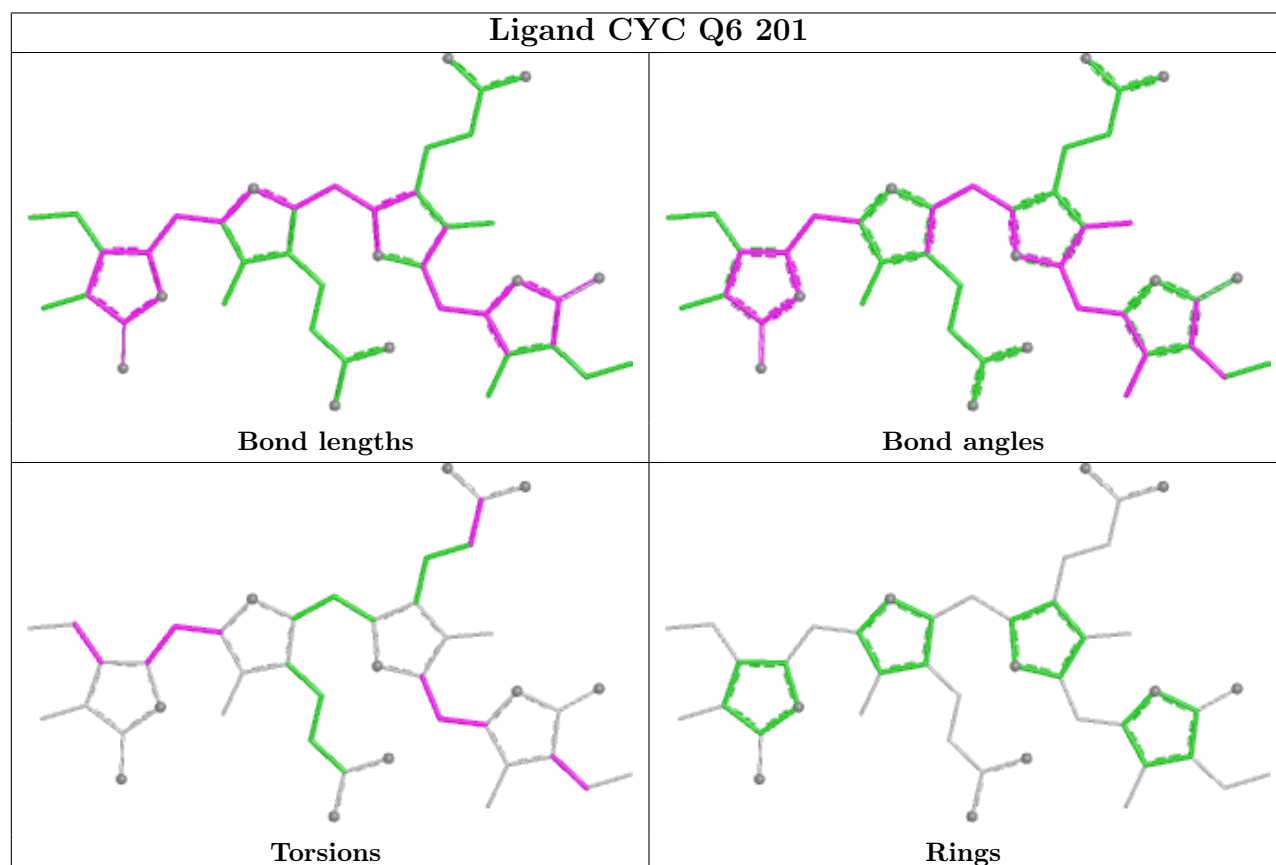
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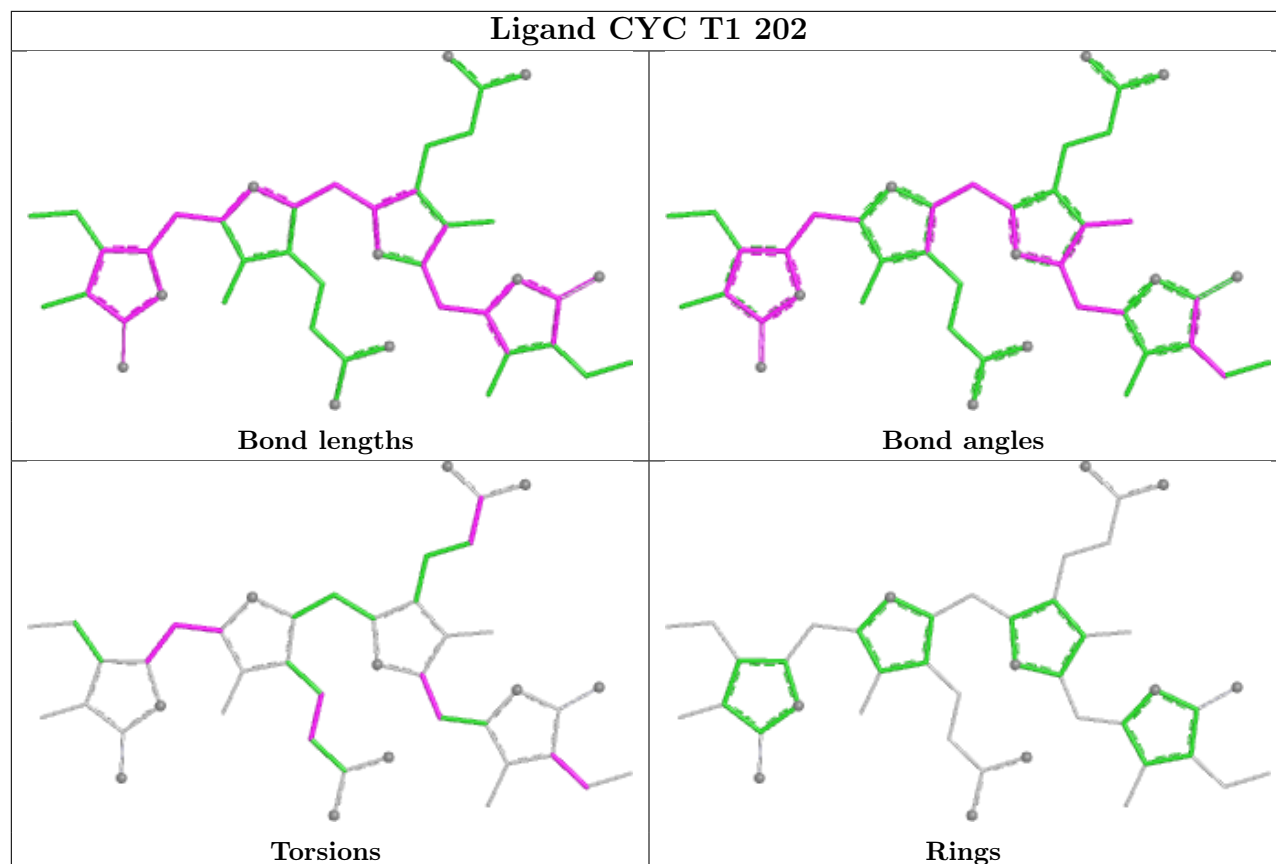
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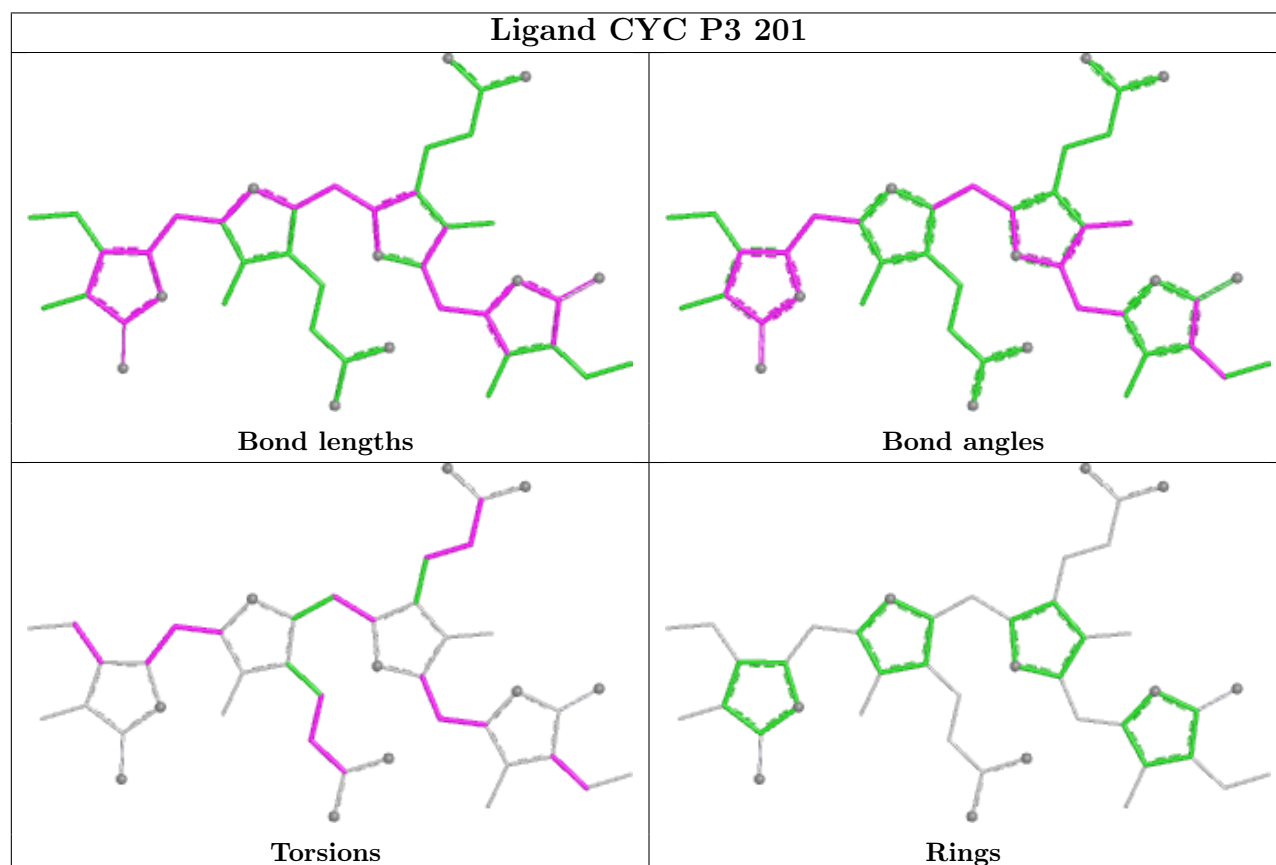
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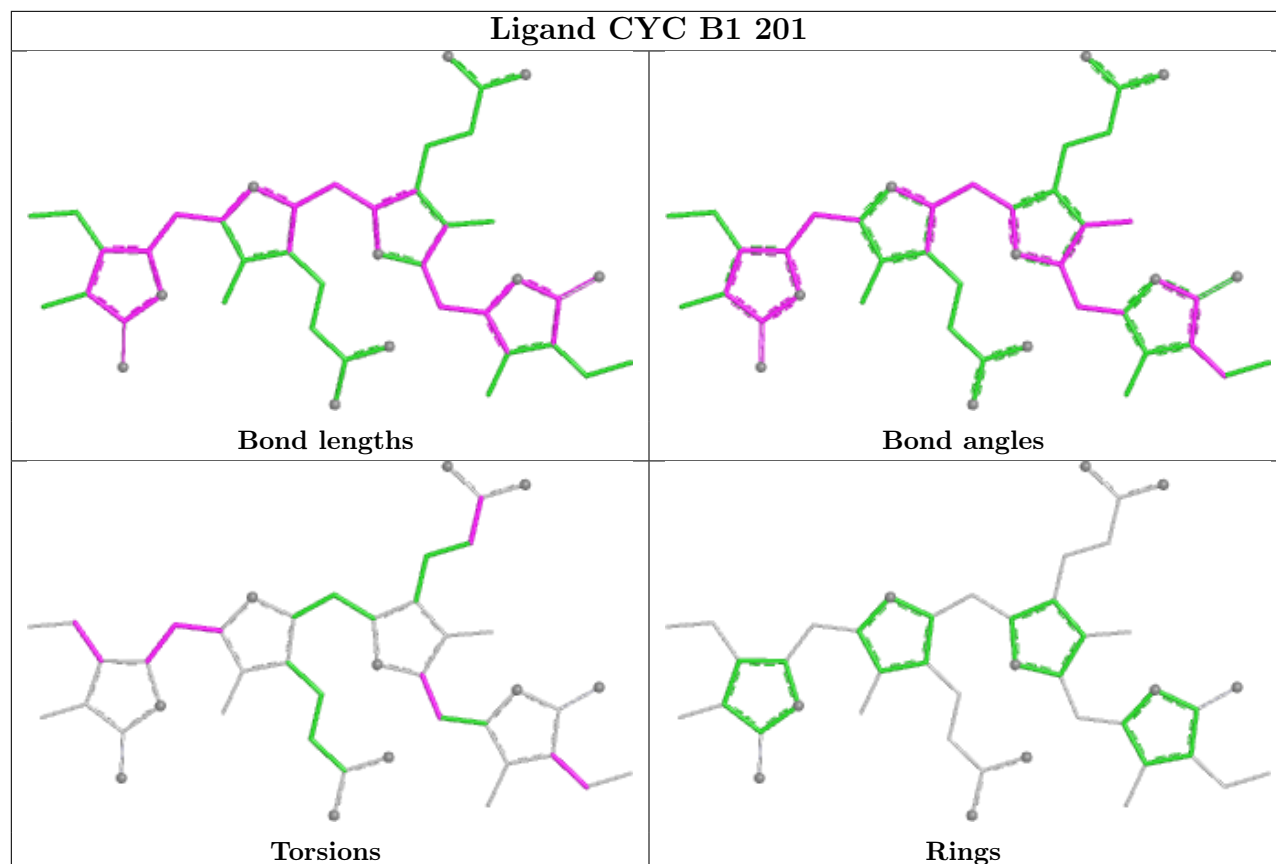
Ligand CYC T1 202



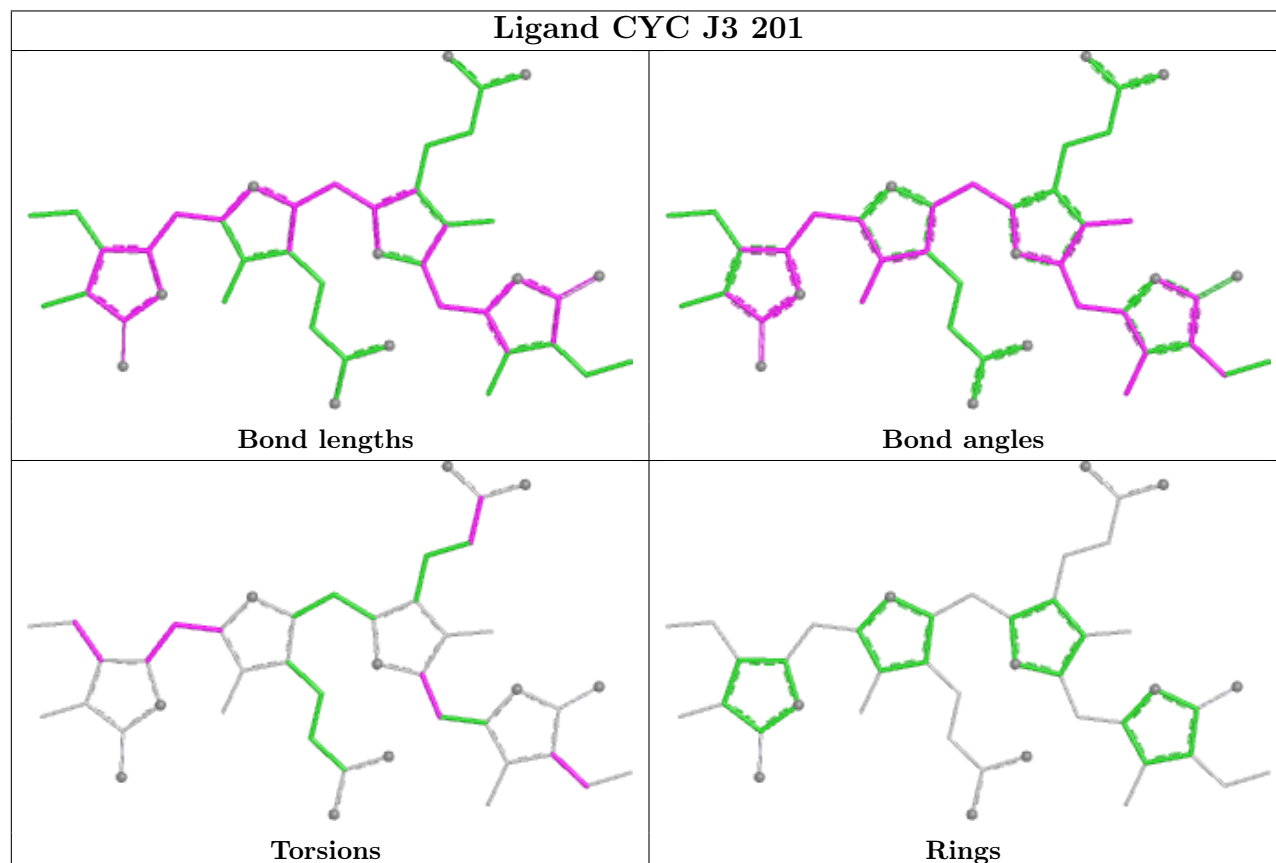
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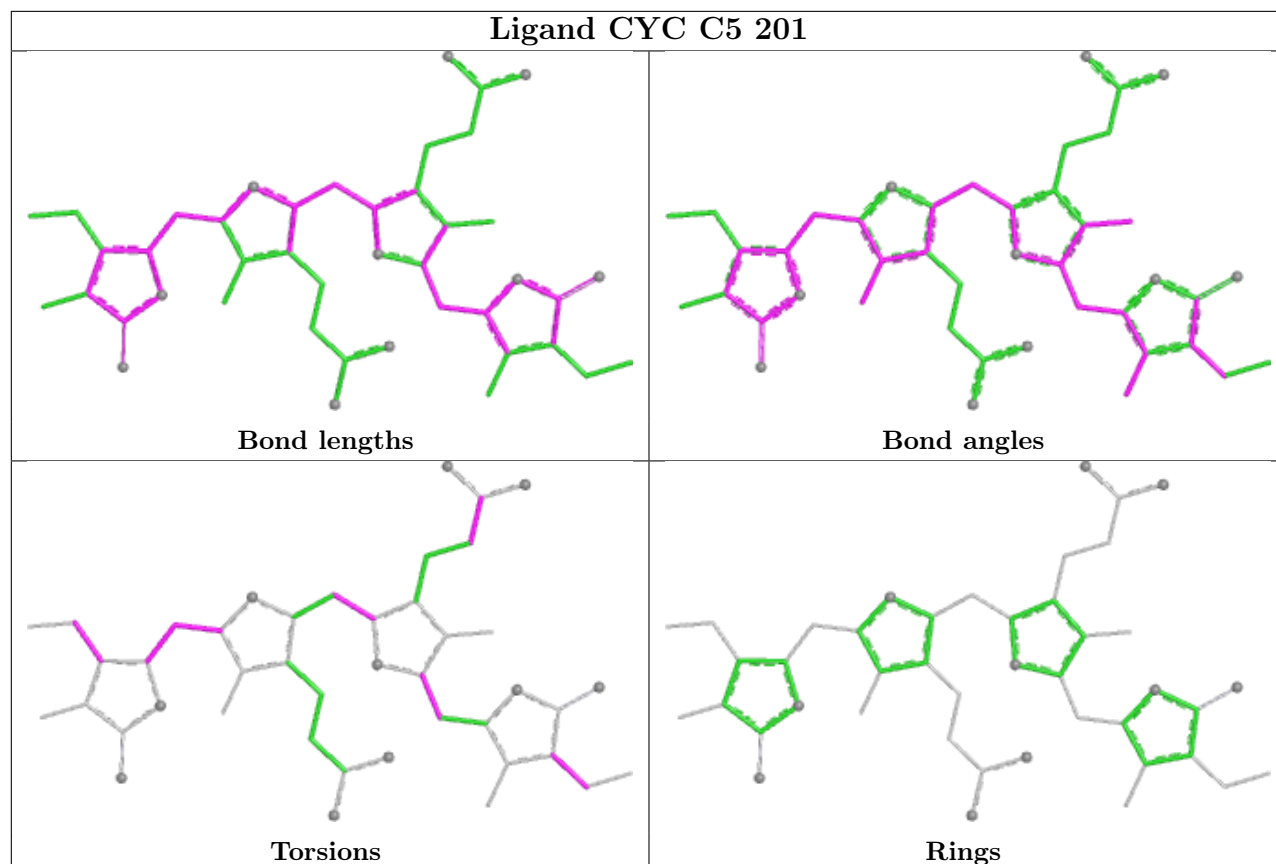
Ligand CYC B1 201



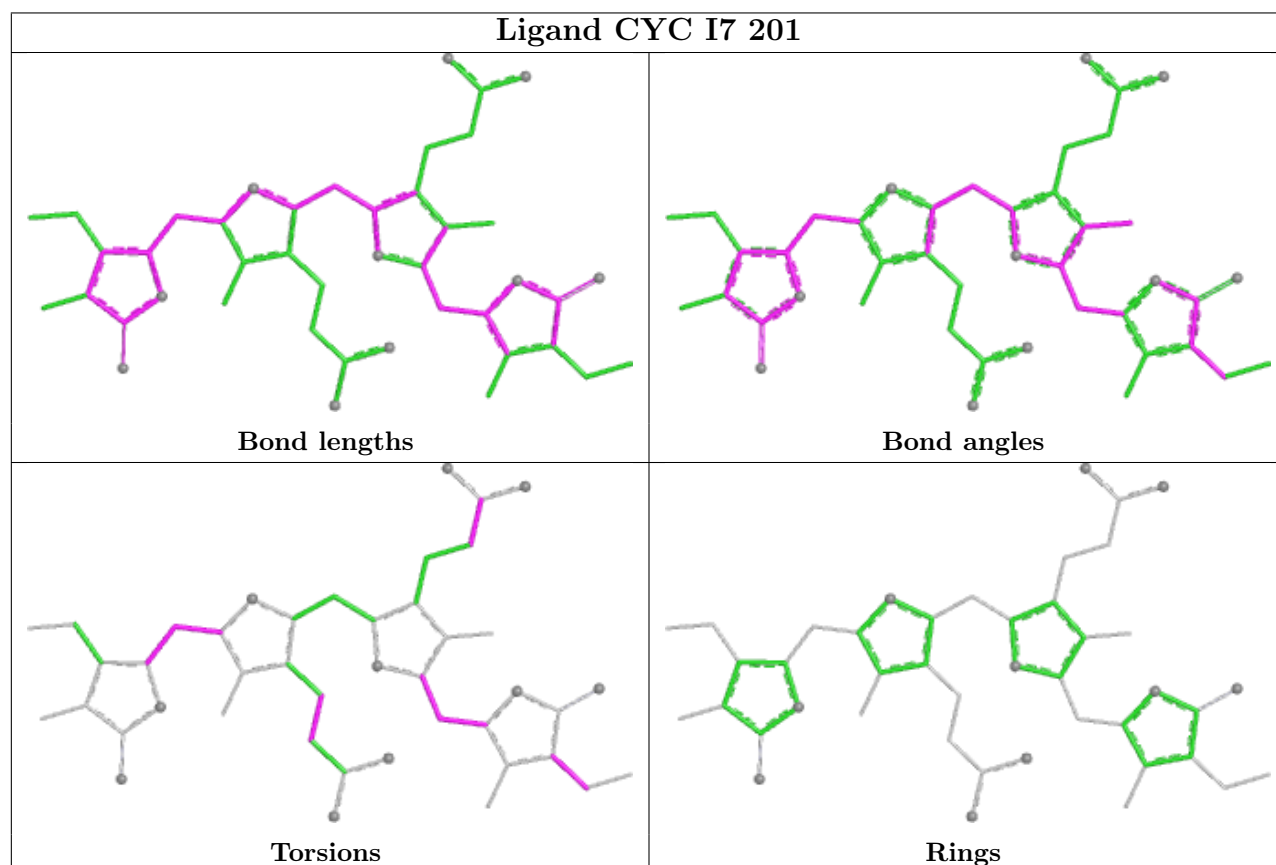
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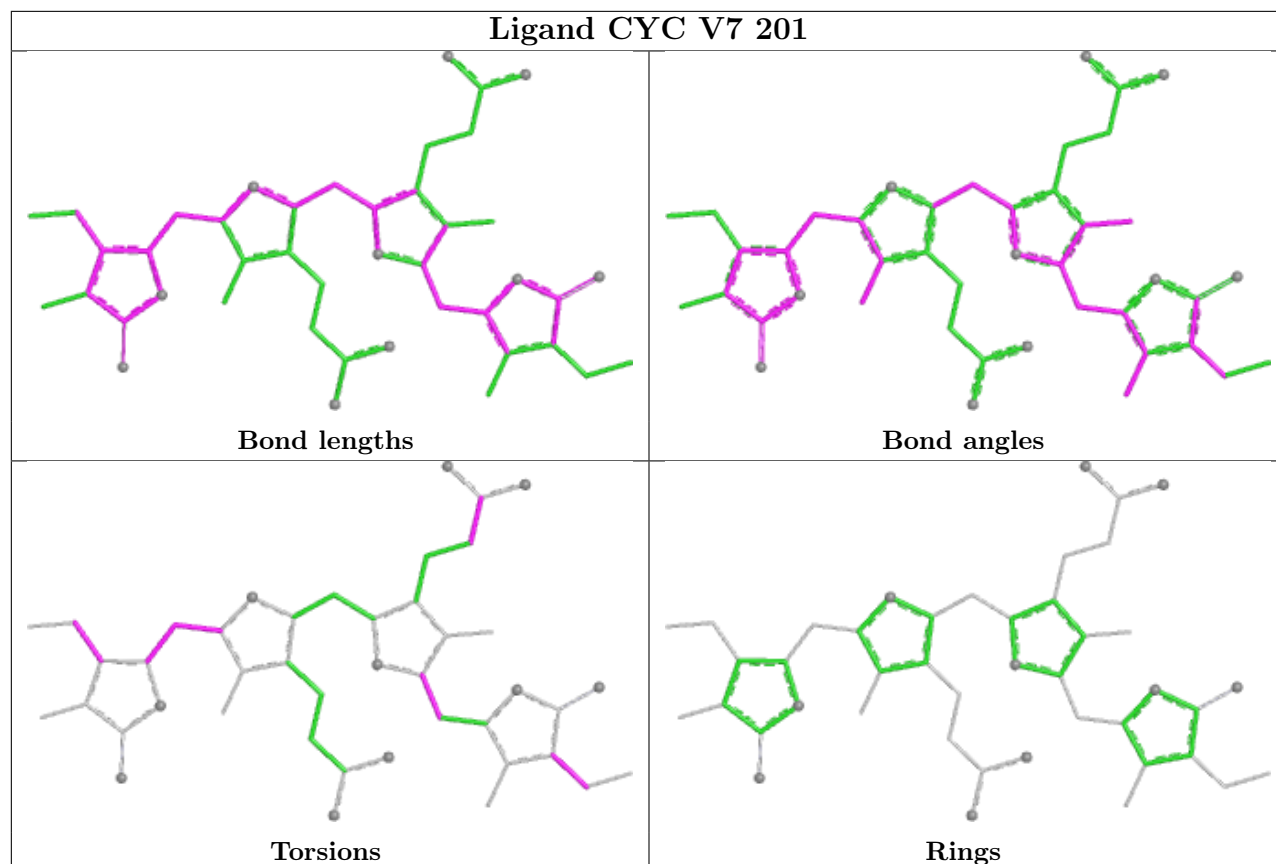
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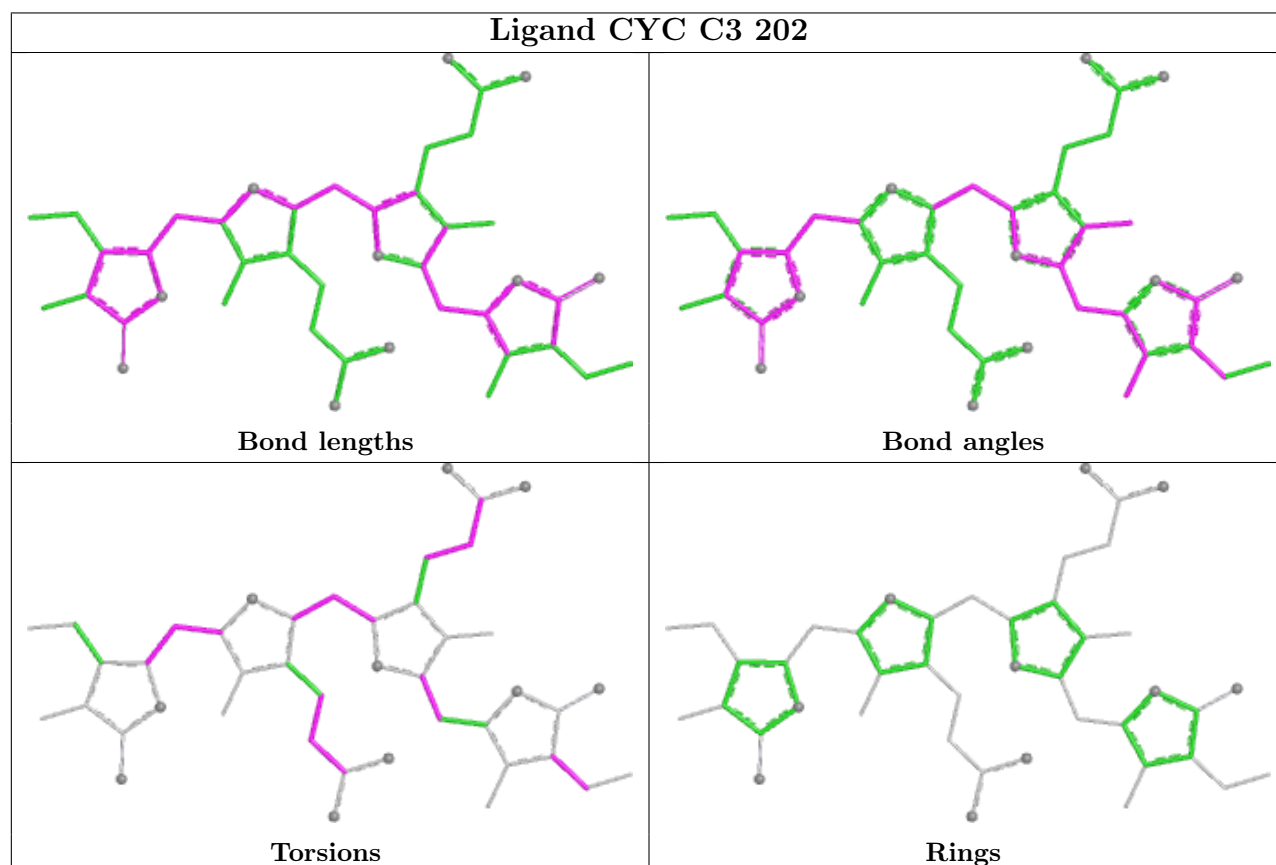
Ligand CYC I7 201



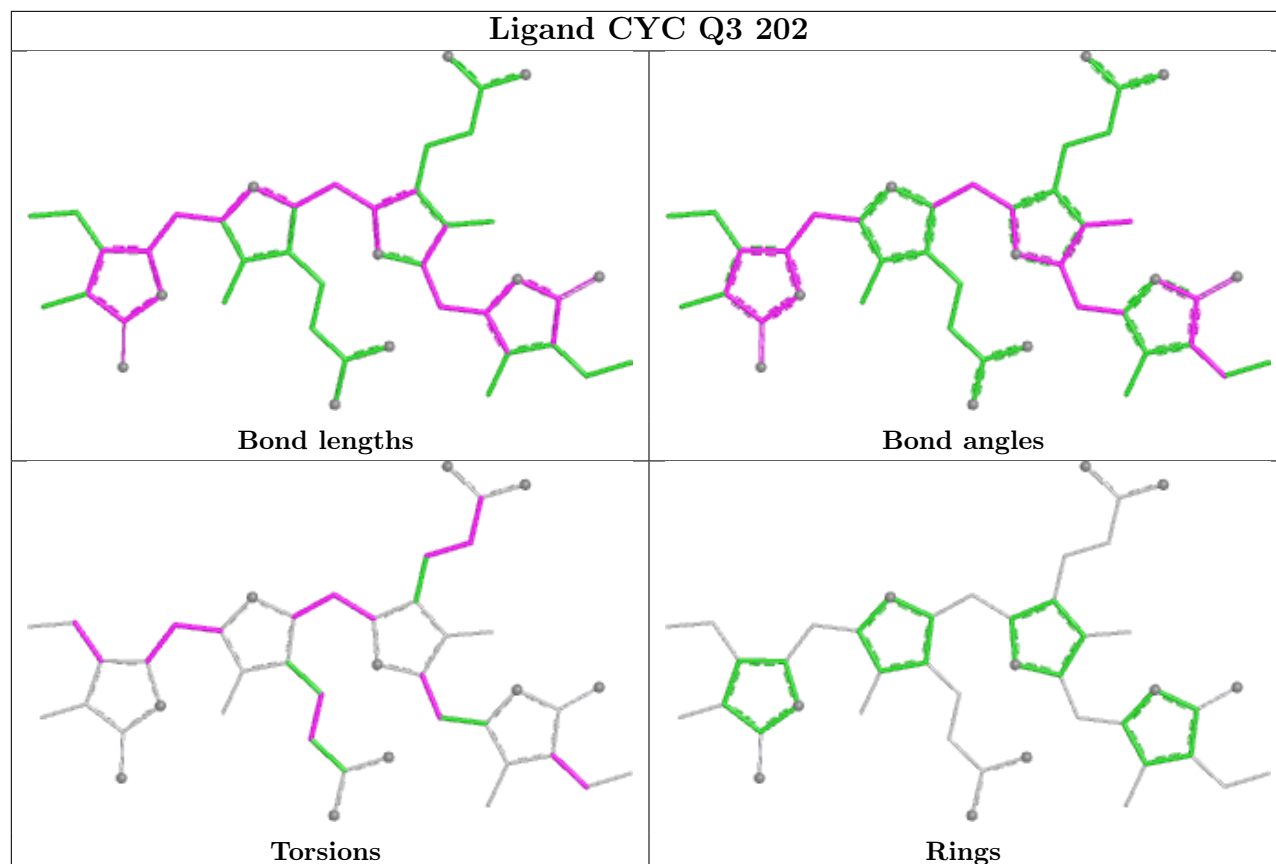
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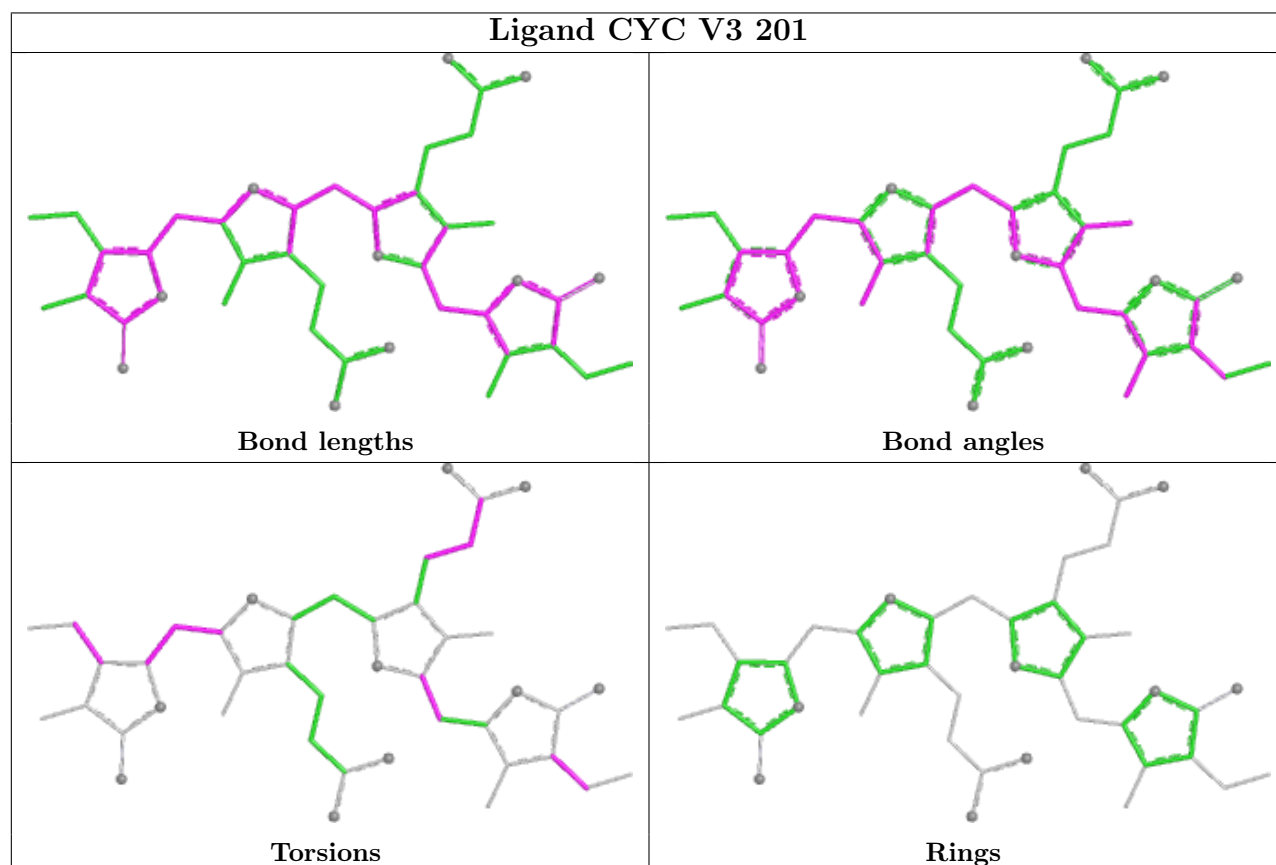
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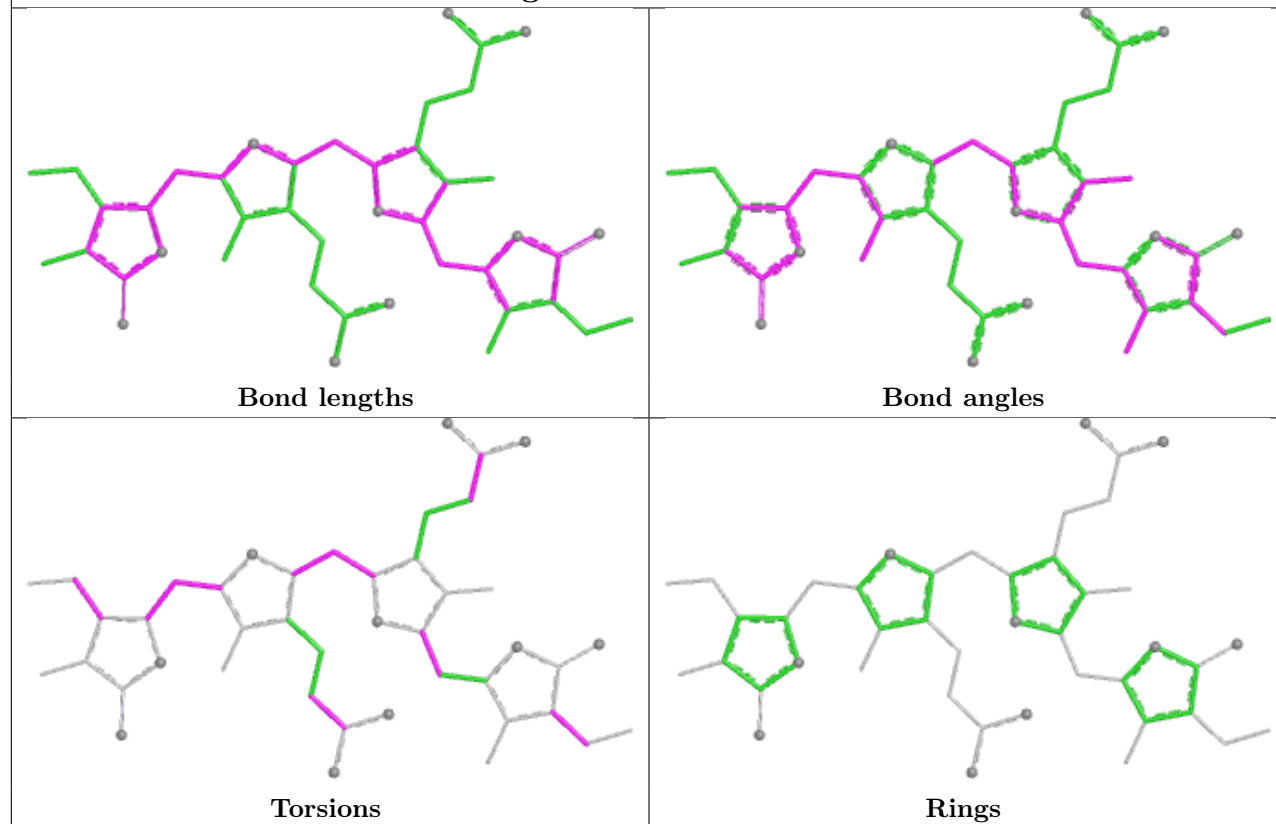
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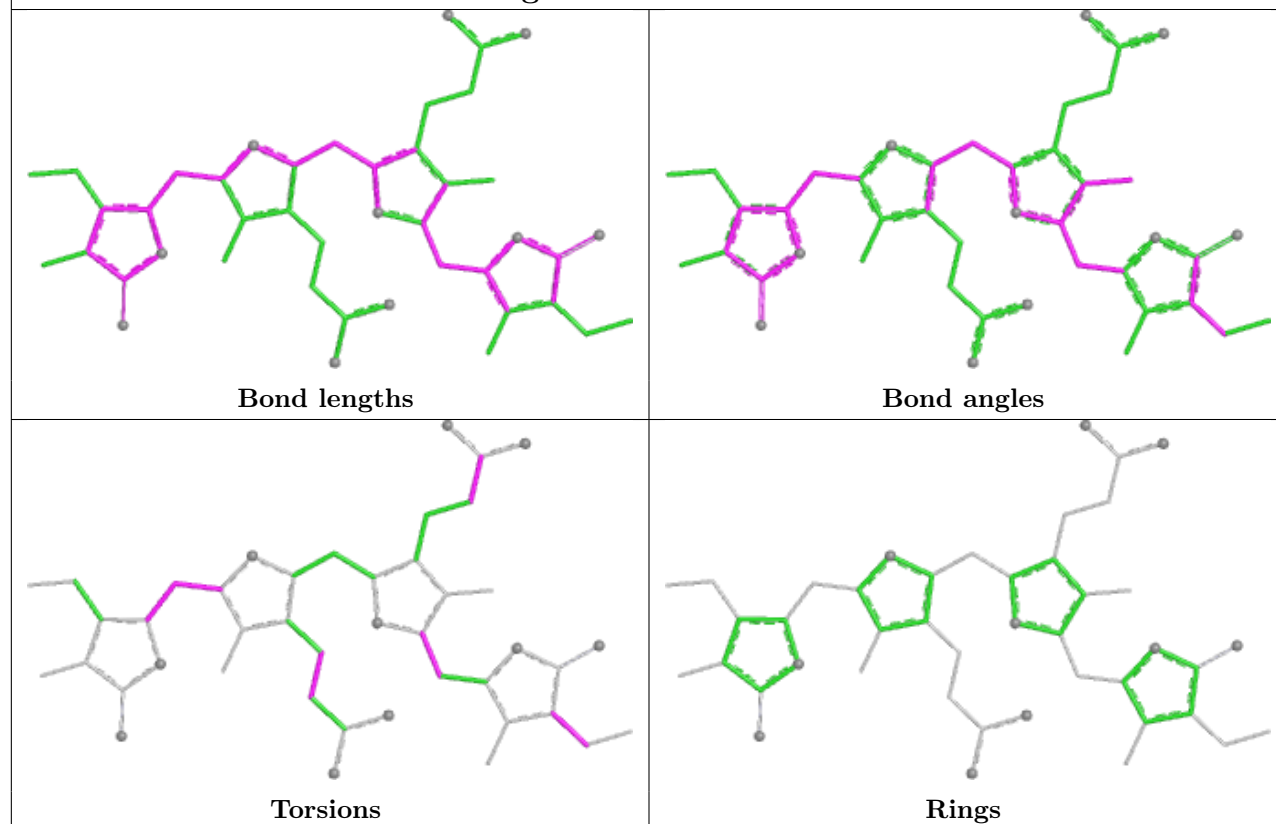
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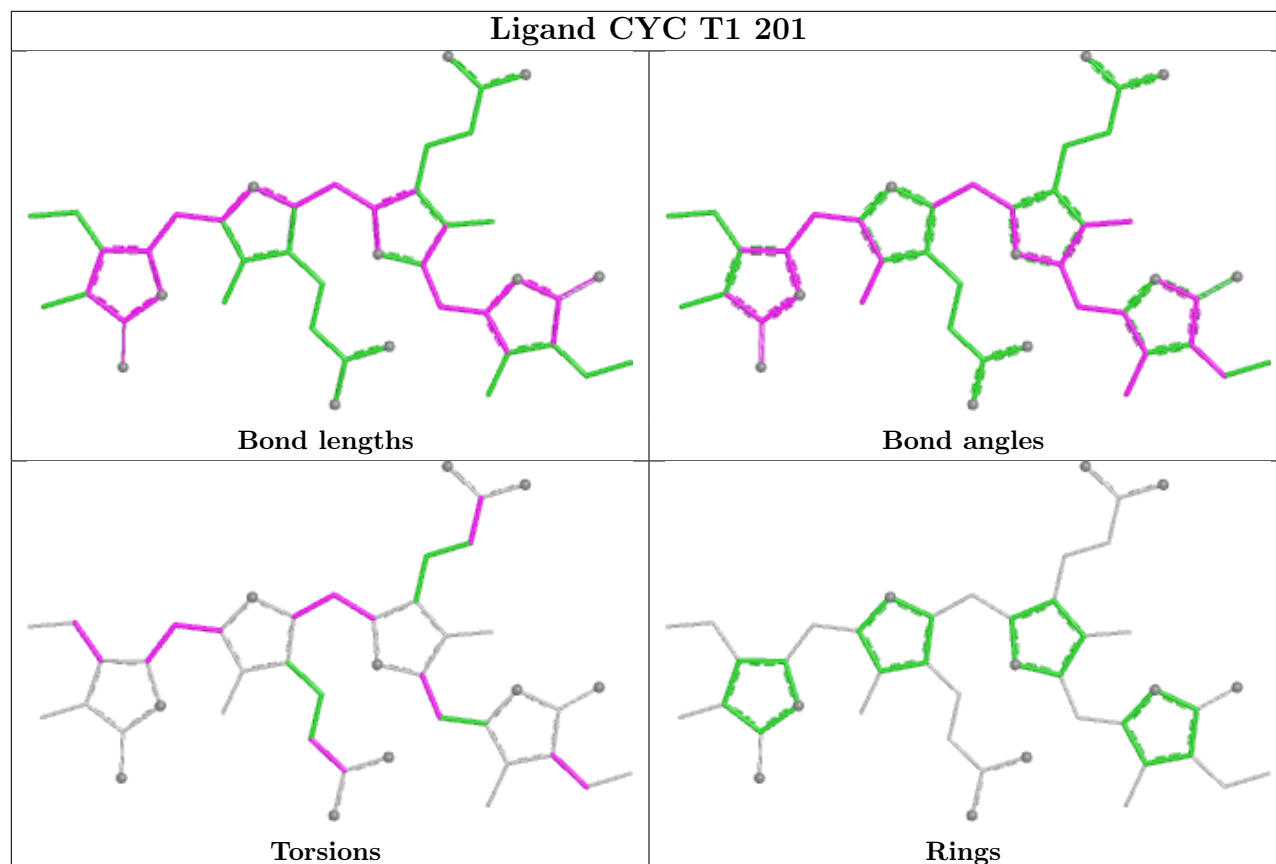
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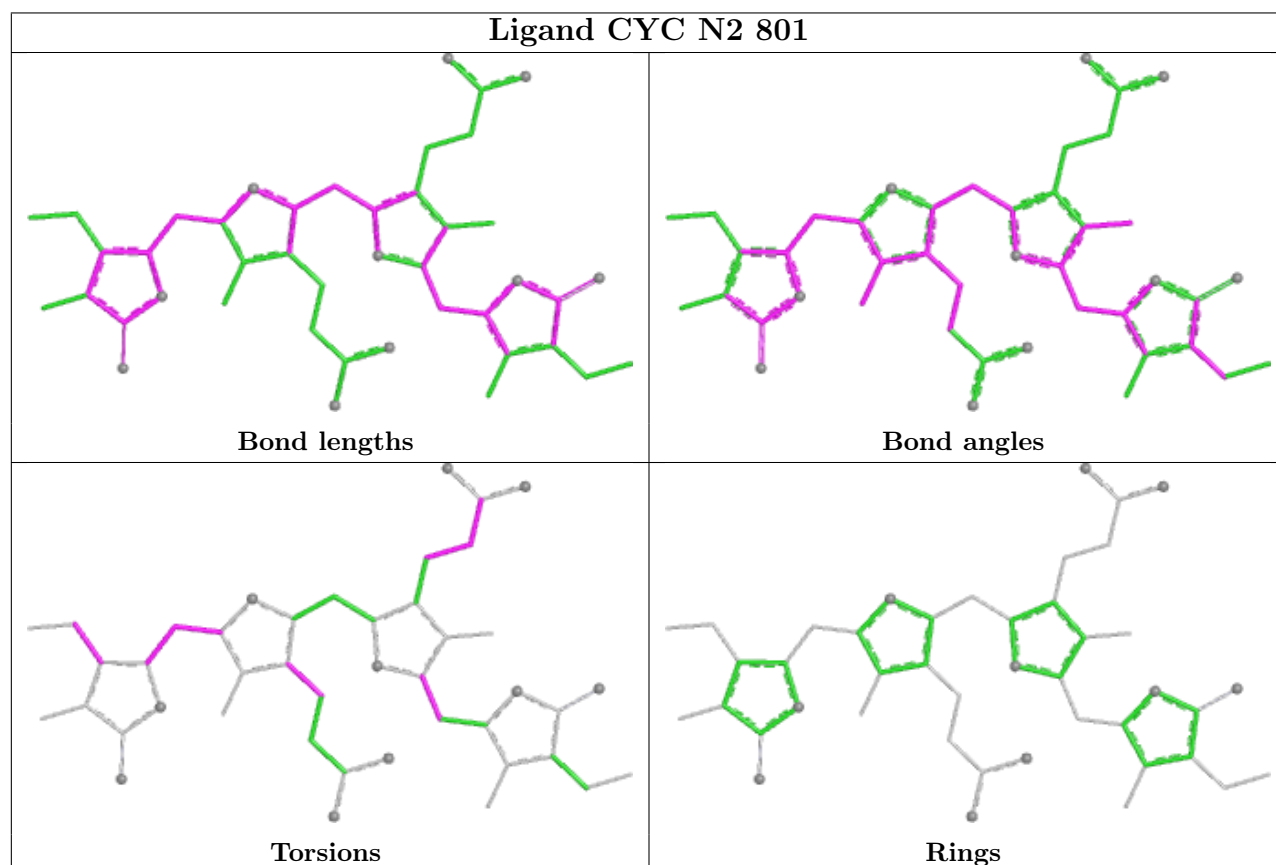
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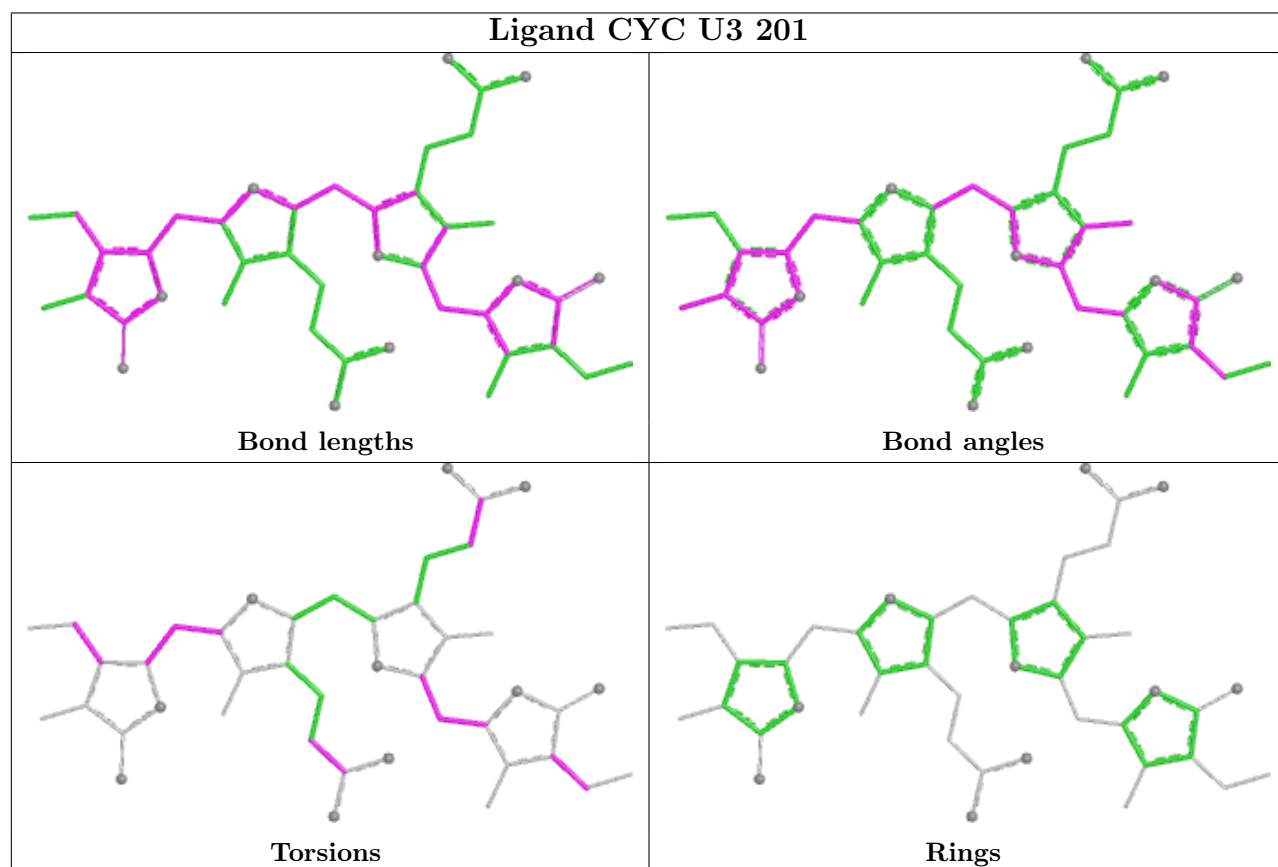
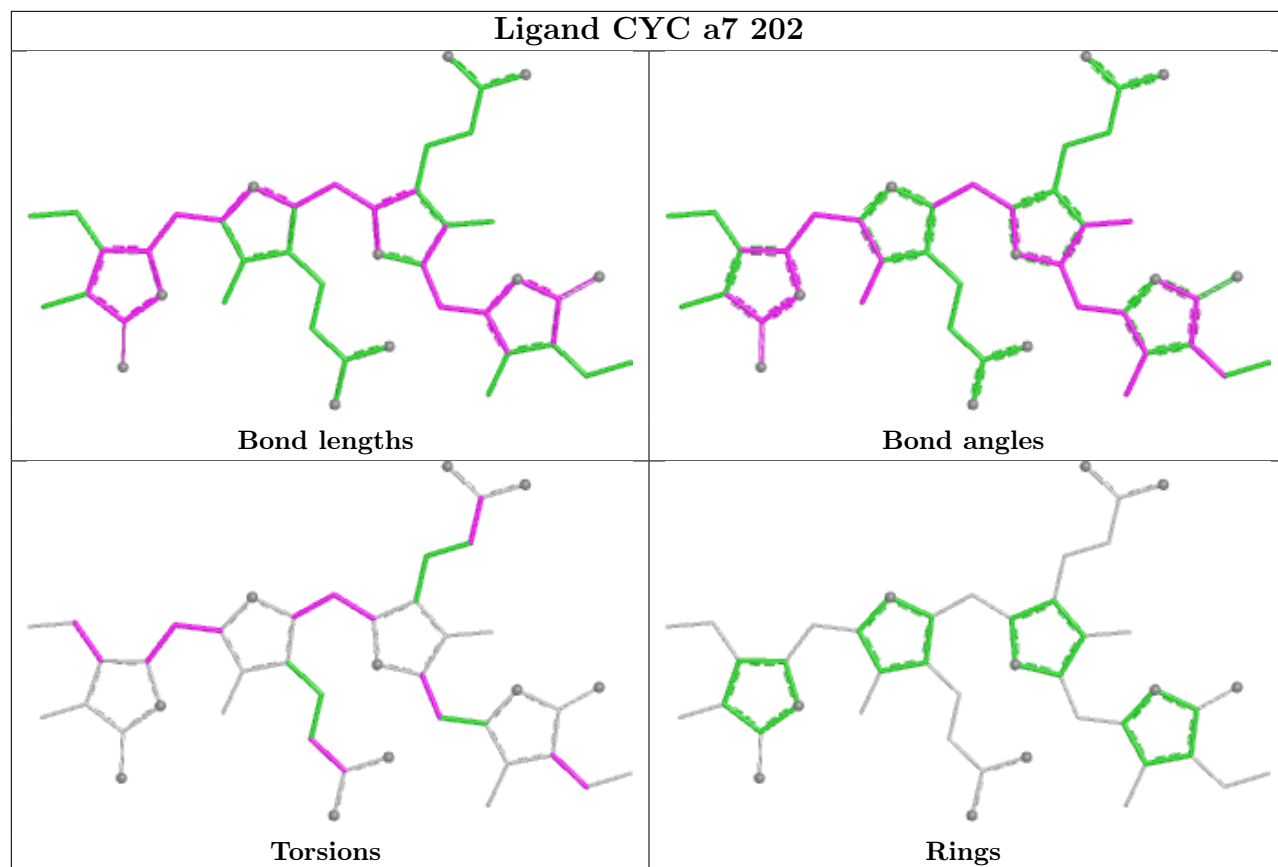


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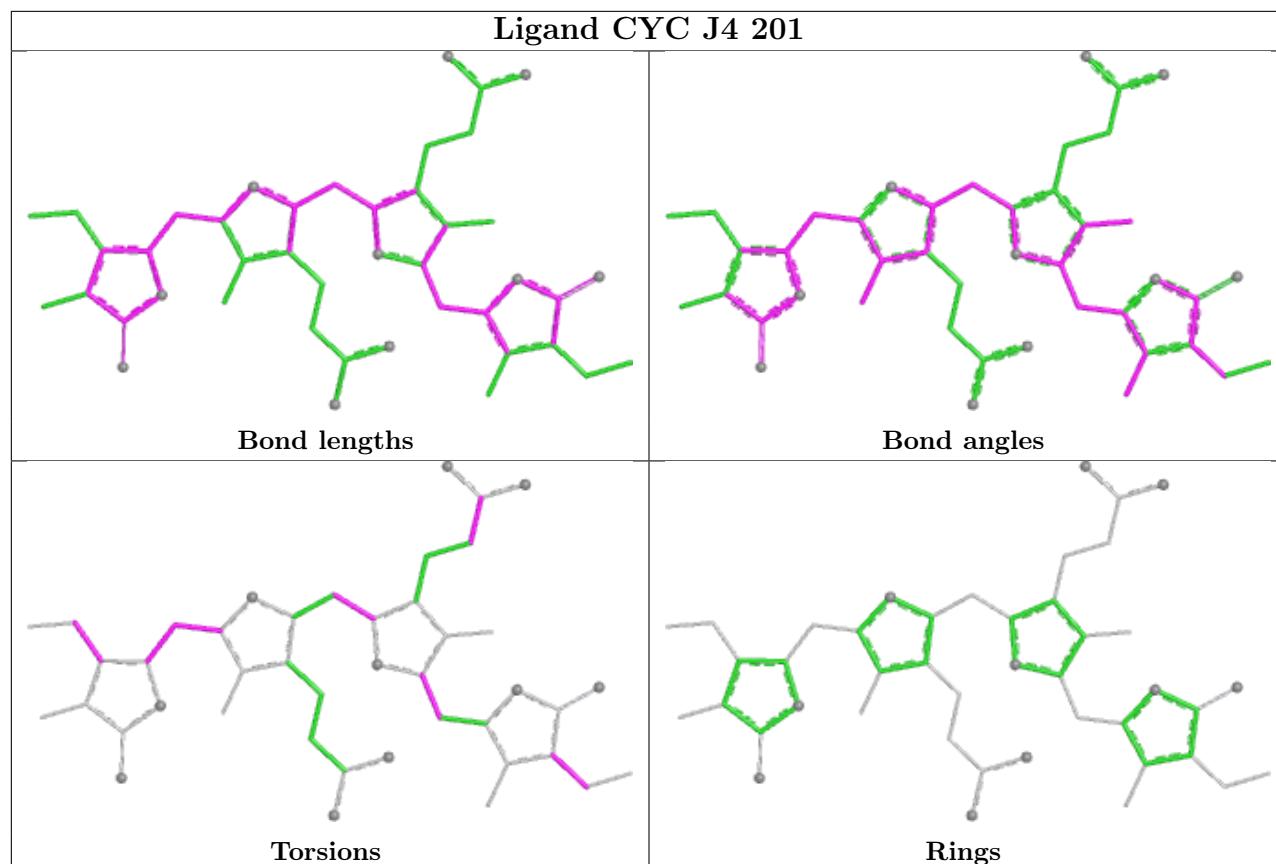


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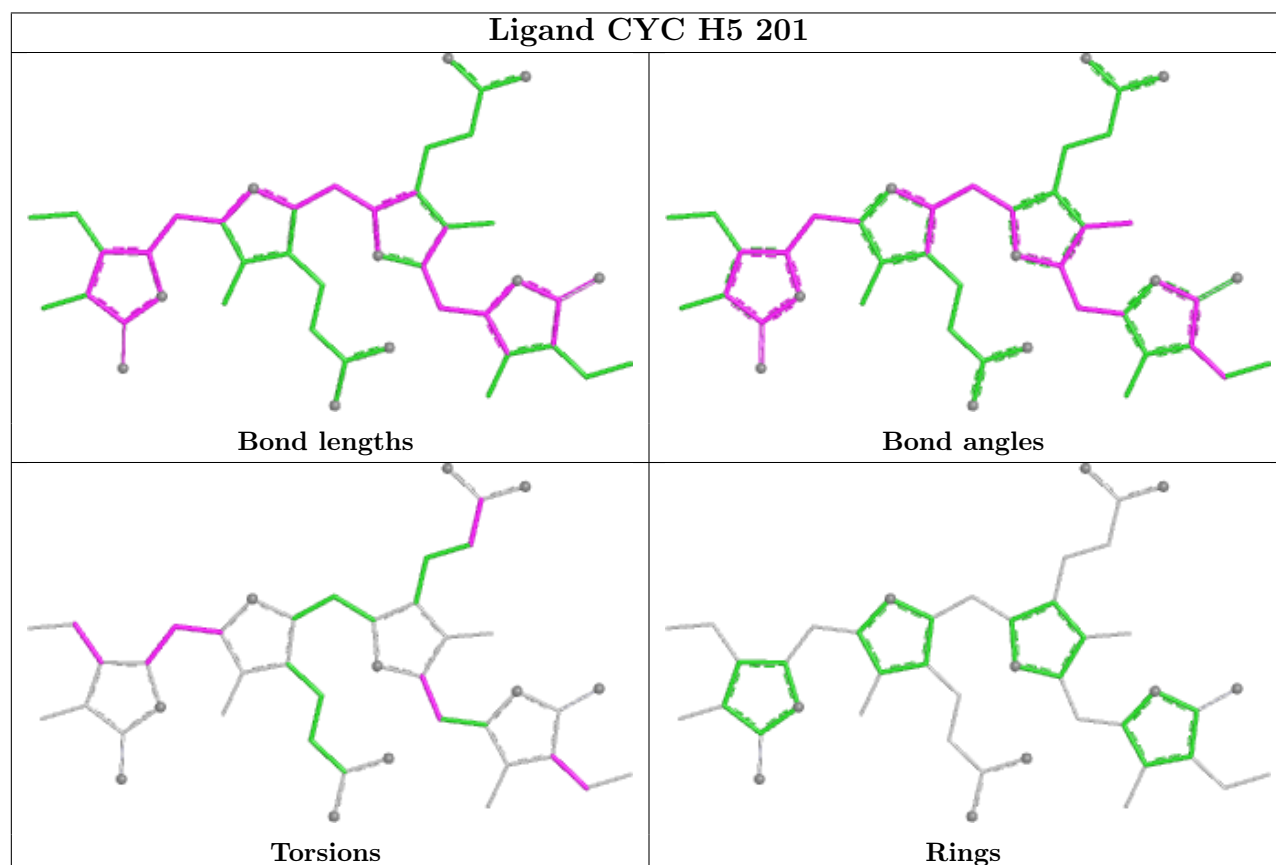




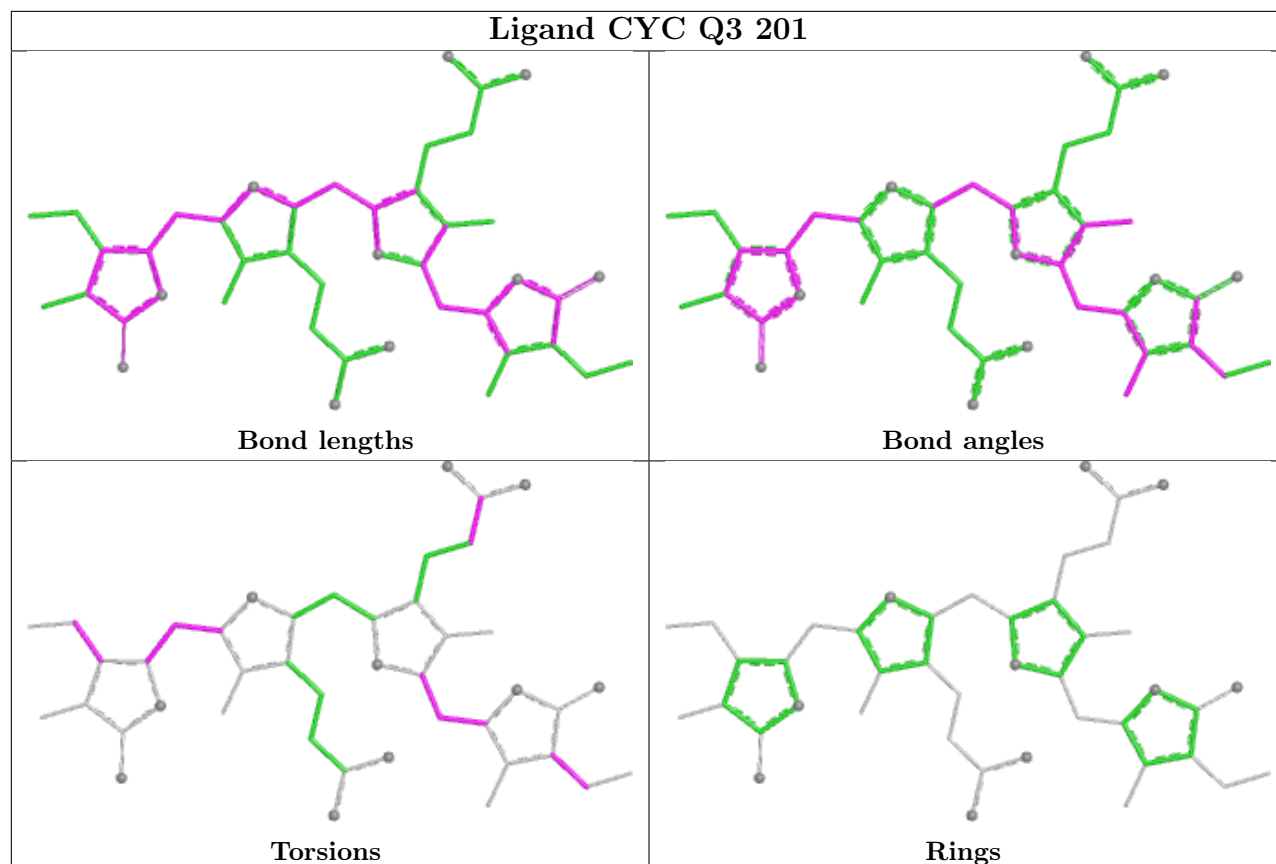
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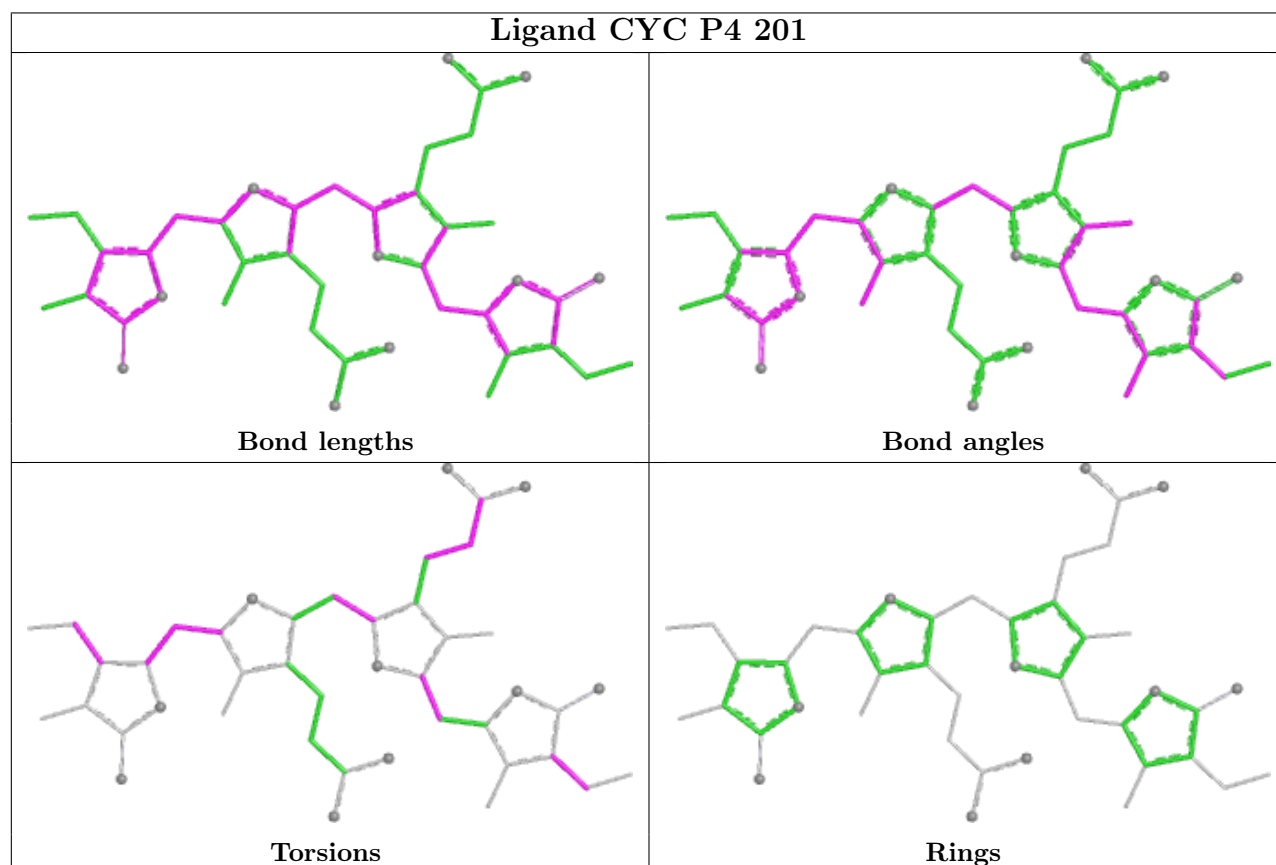
Ligand CYC H5 201



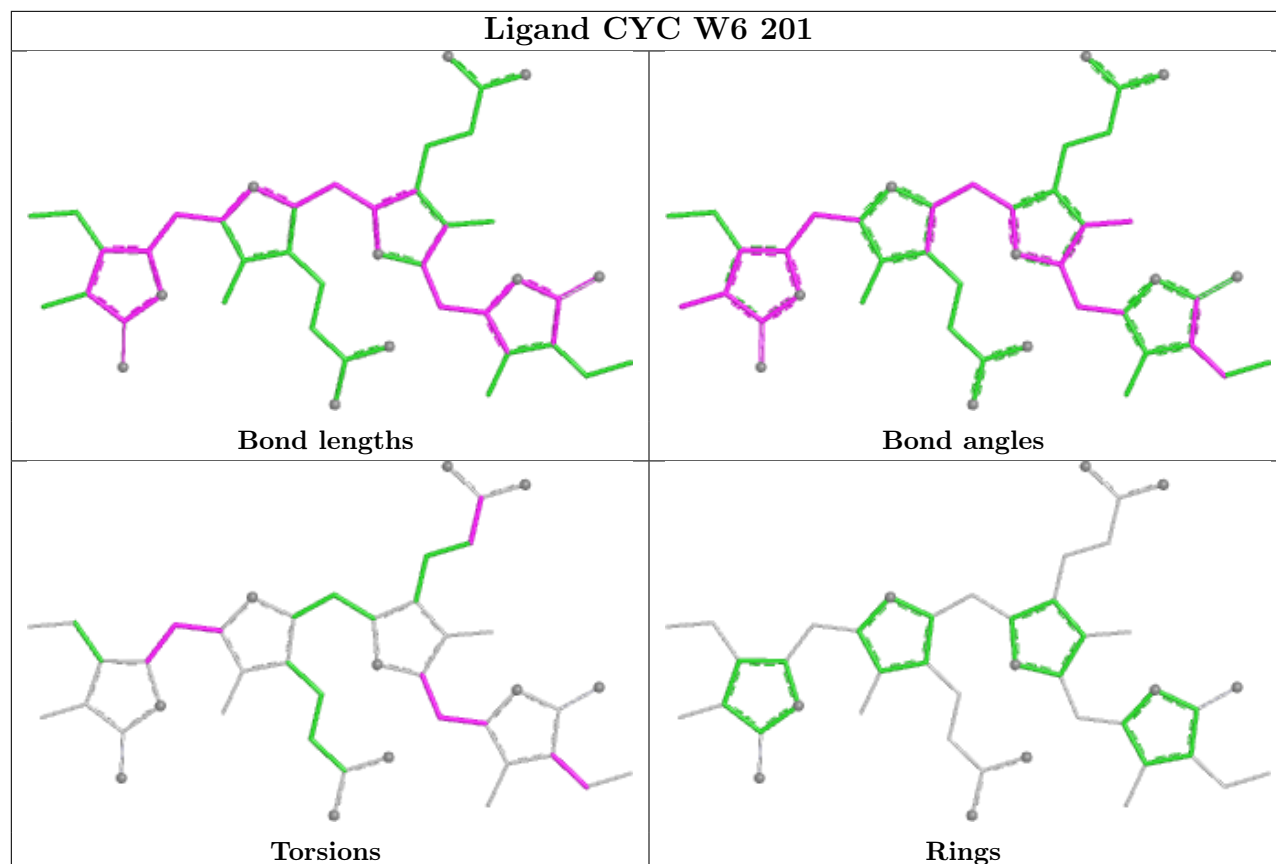
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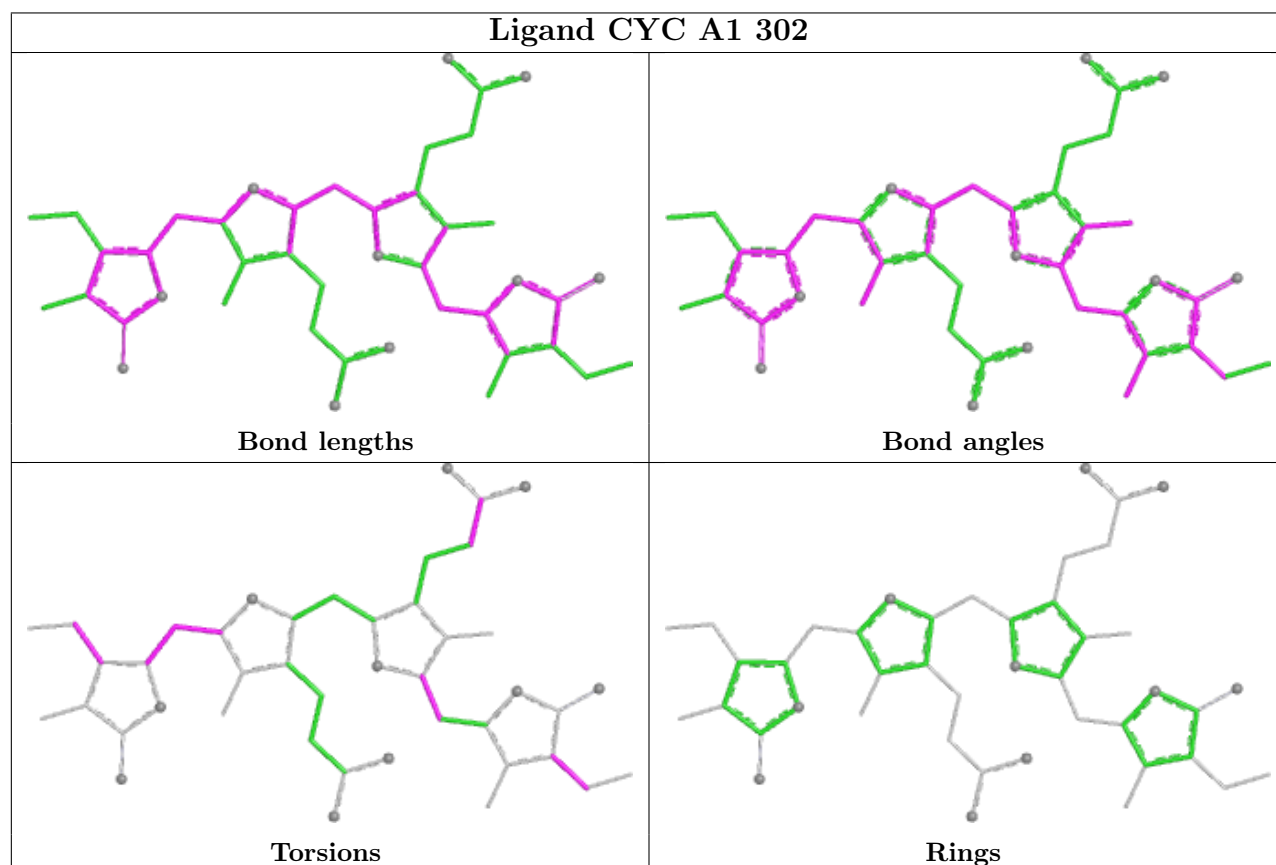
Ligand CYC P4 201



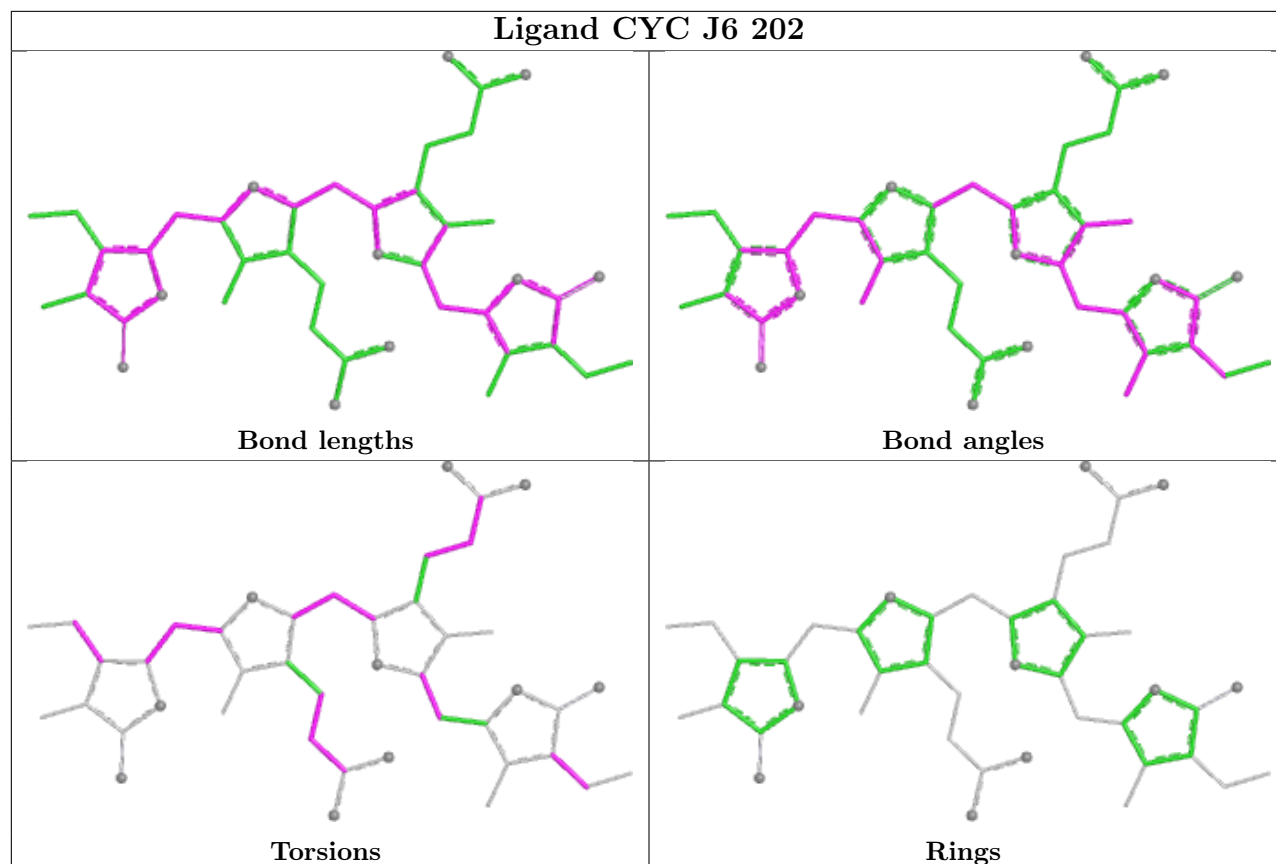
Ligand CYC W6 201



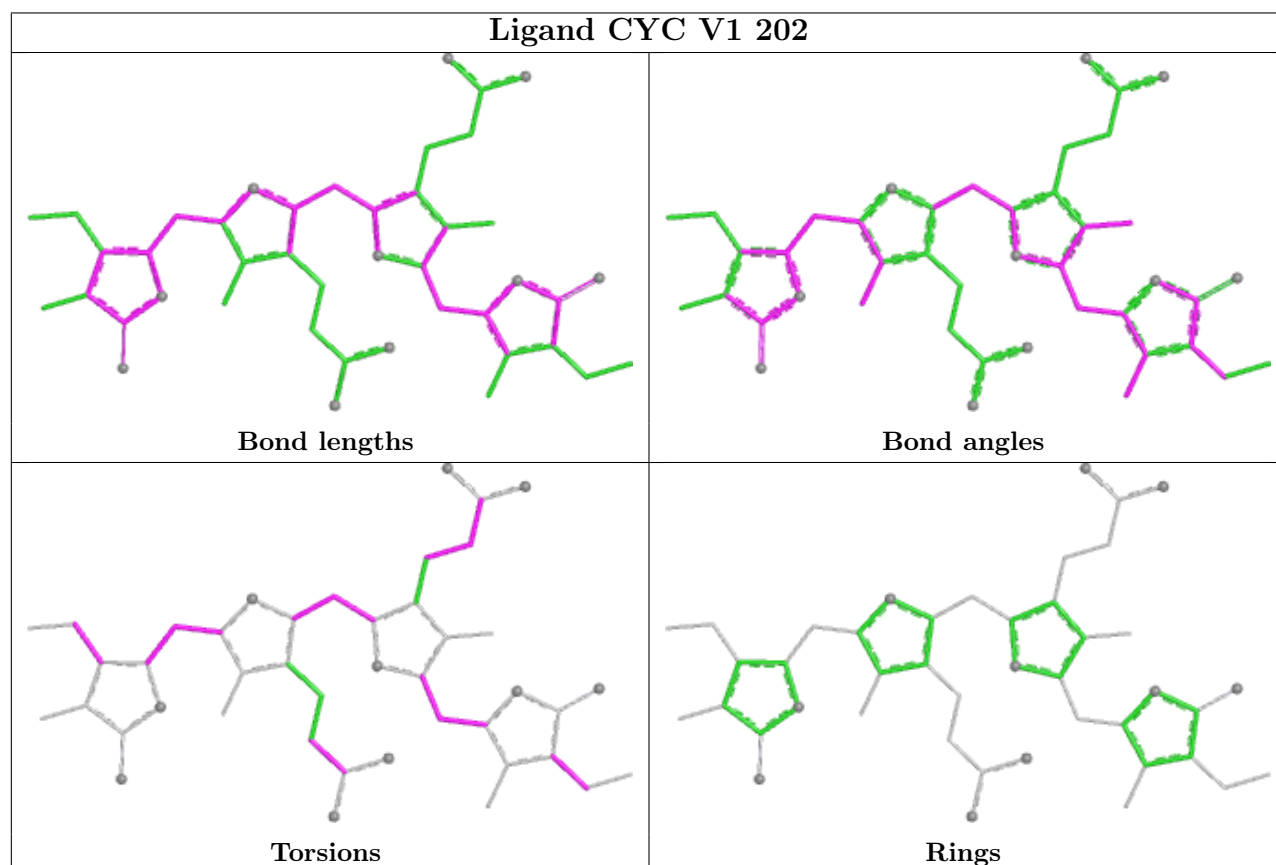
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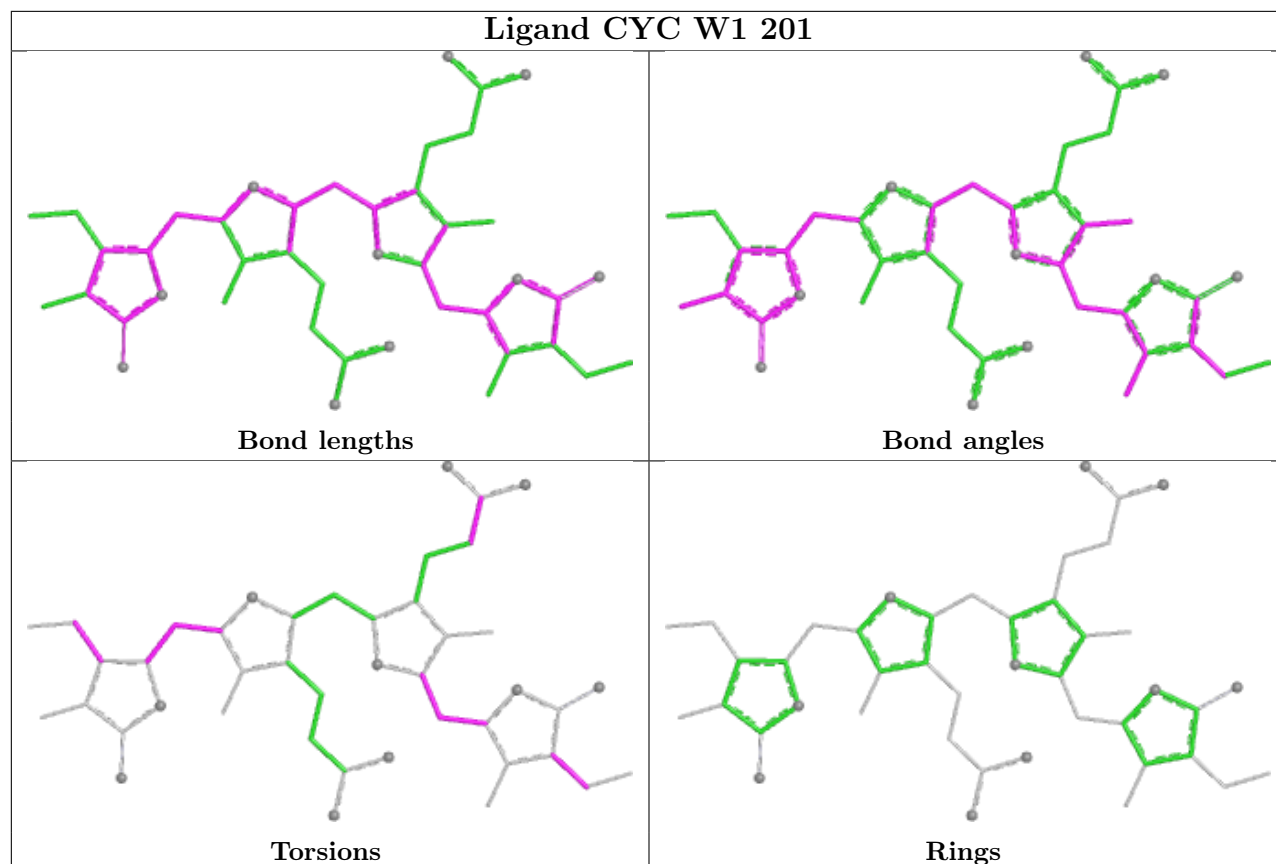
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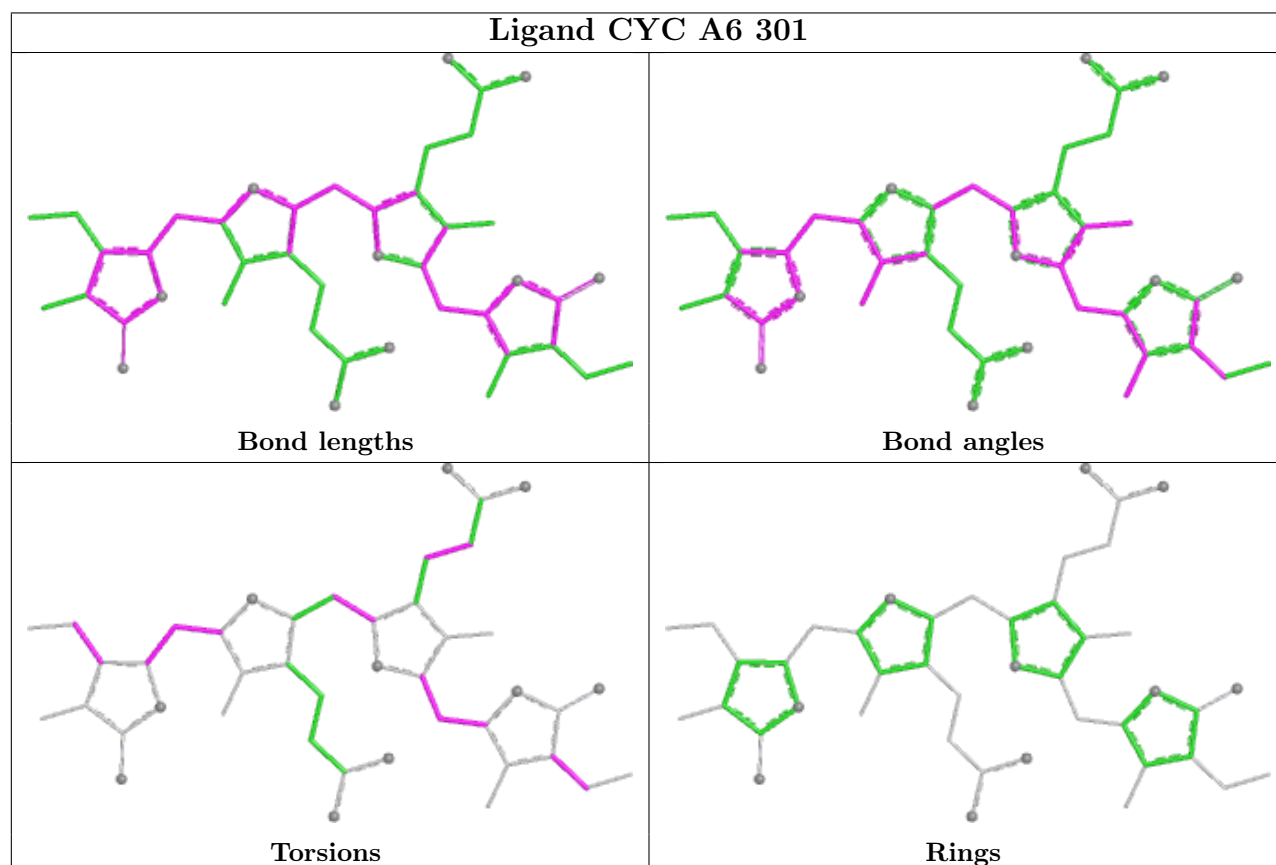
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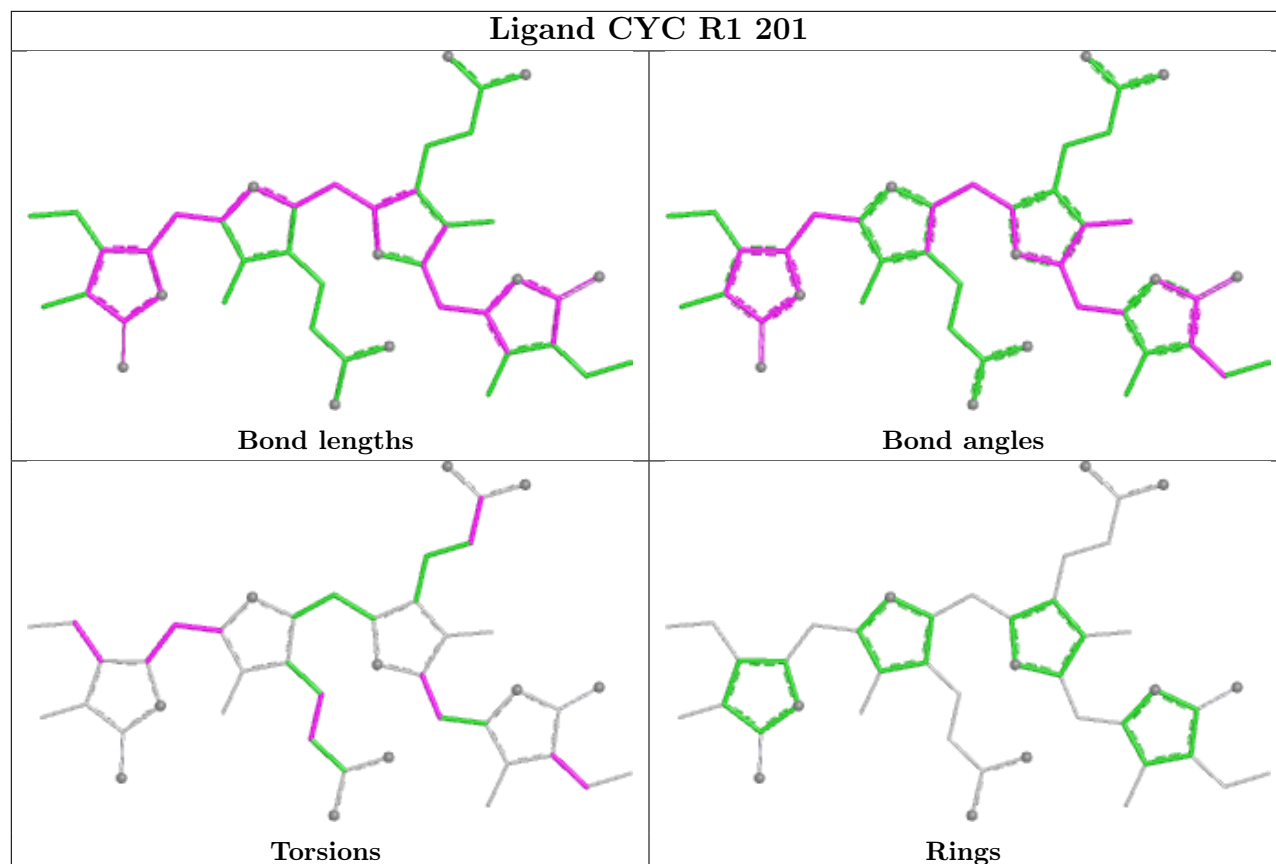
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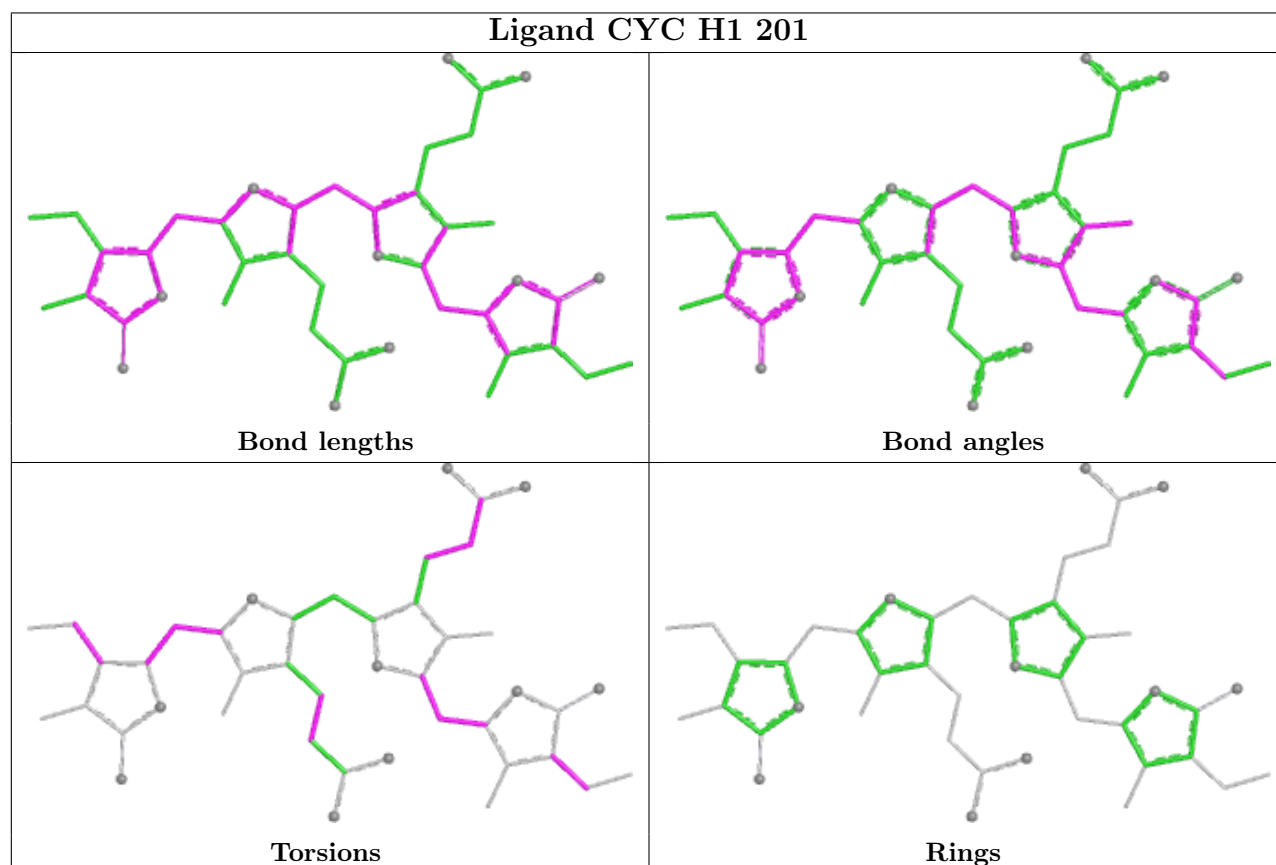
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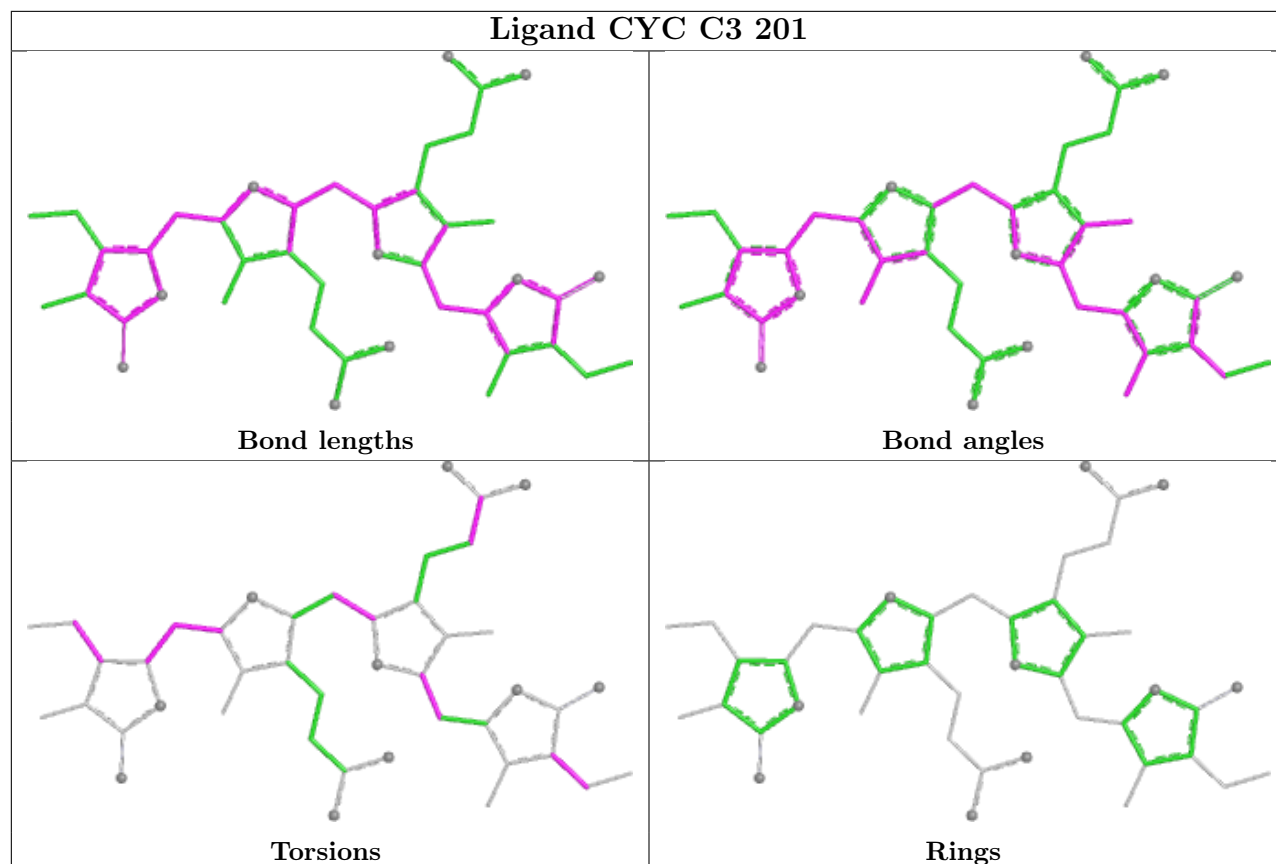
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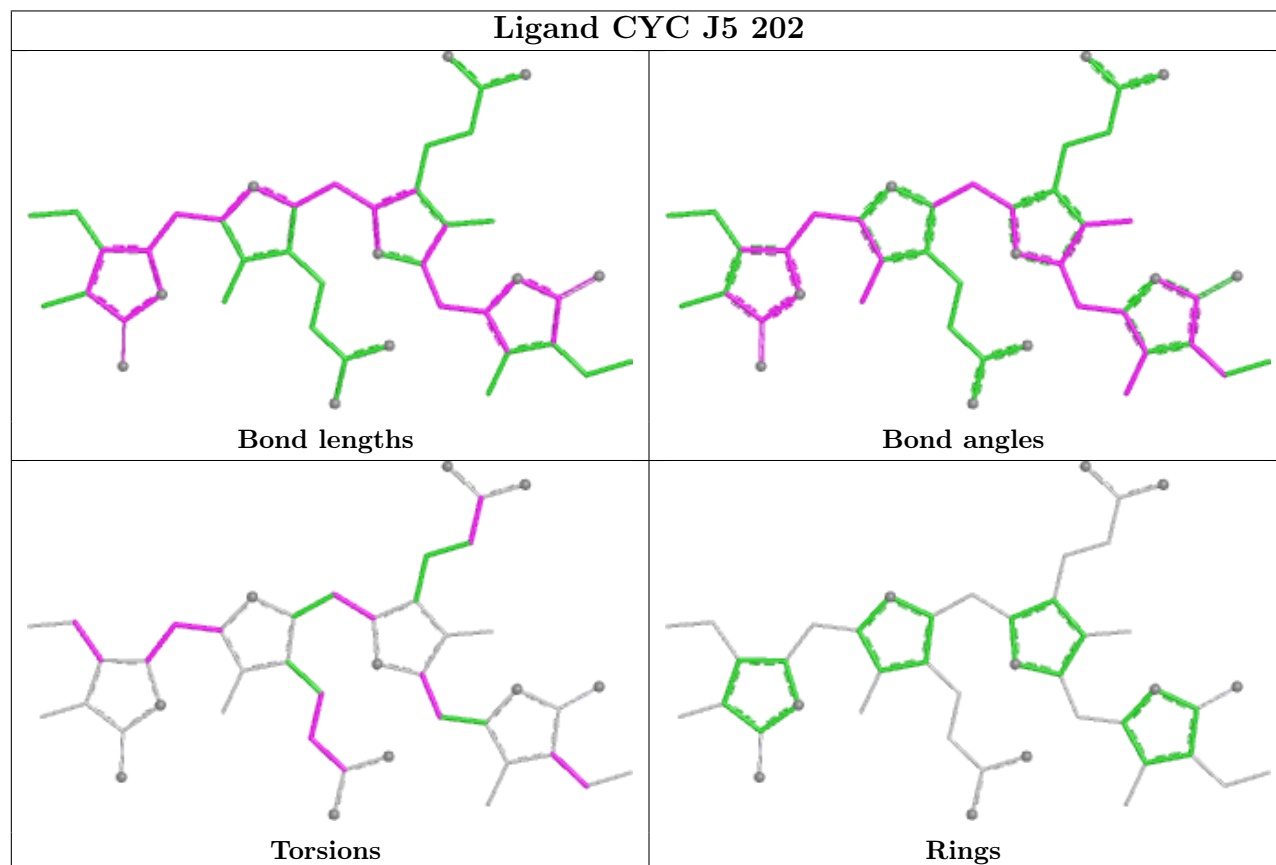
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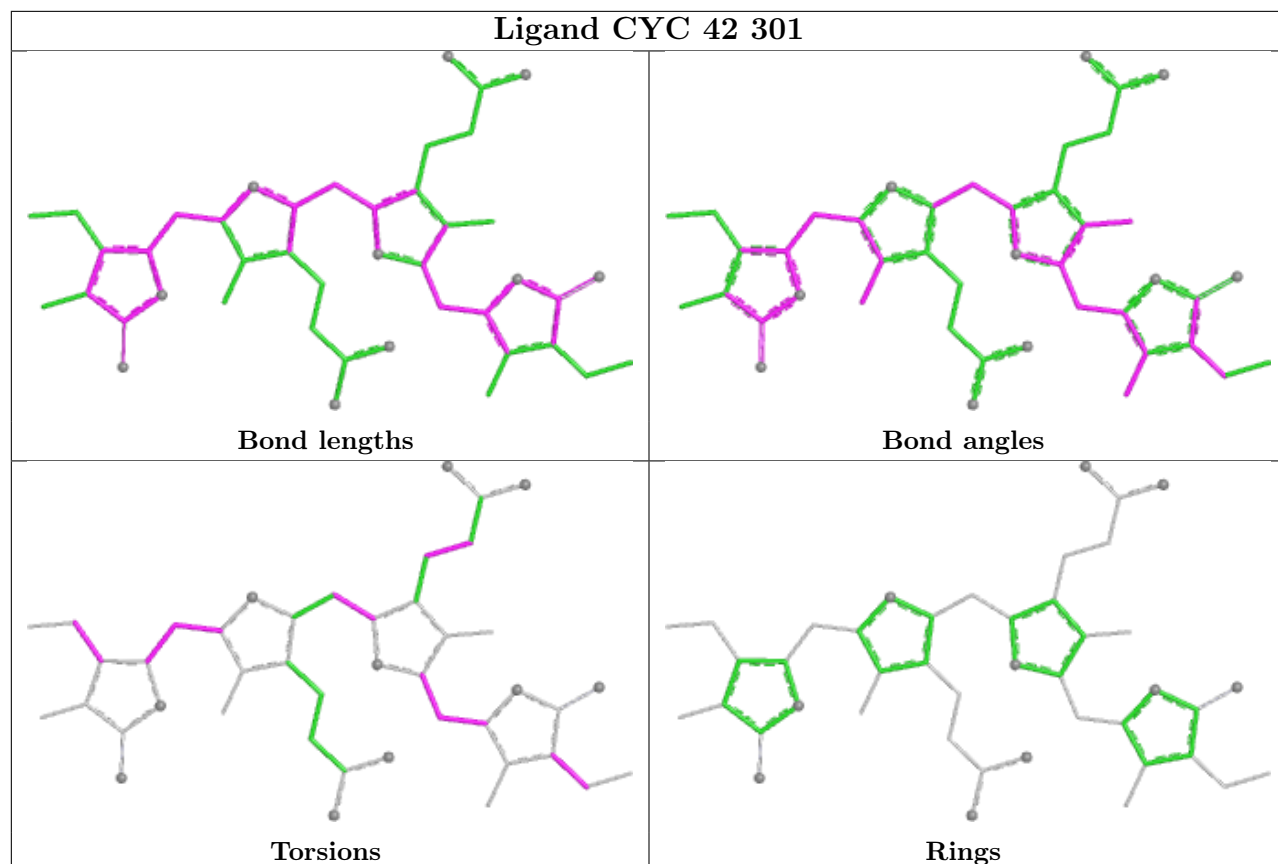
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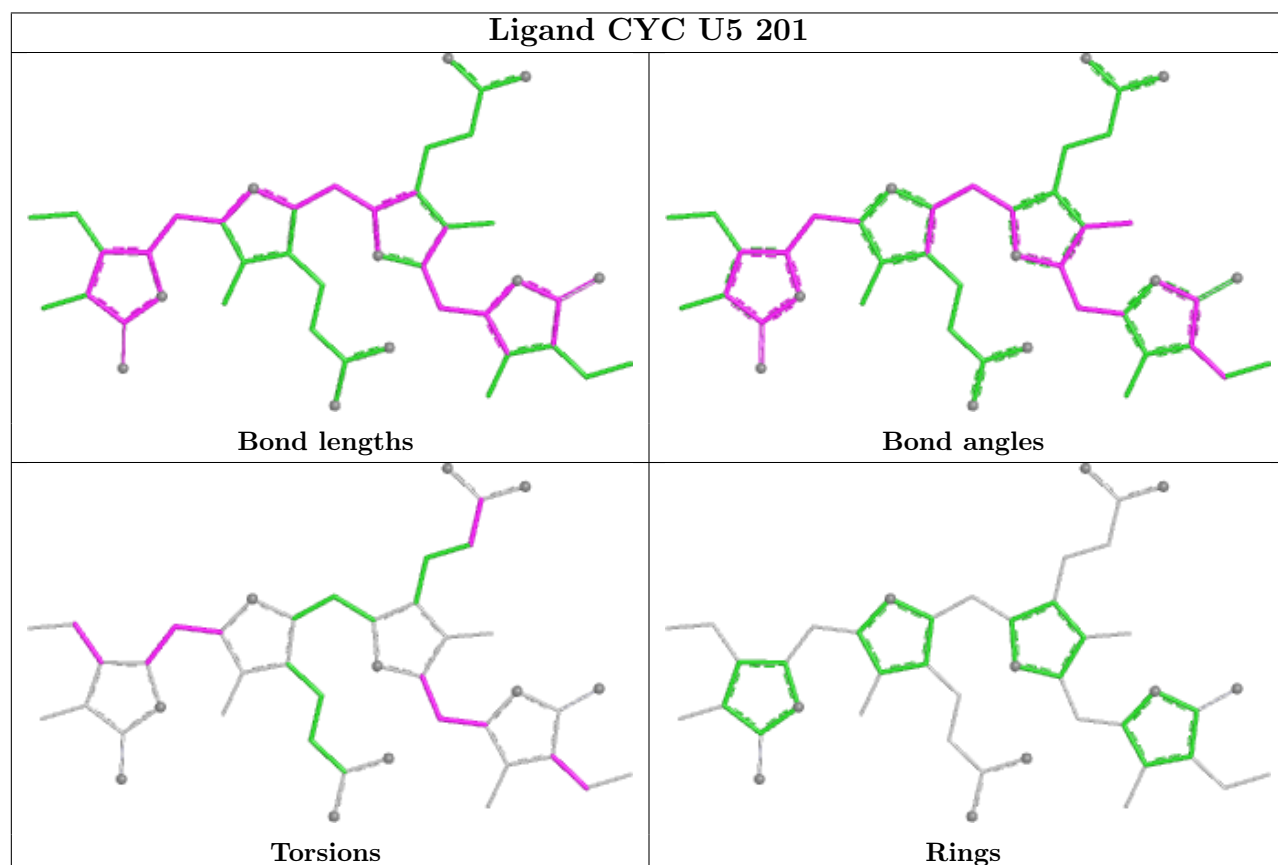
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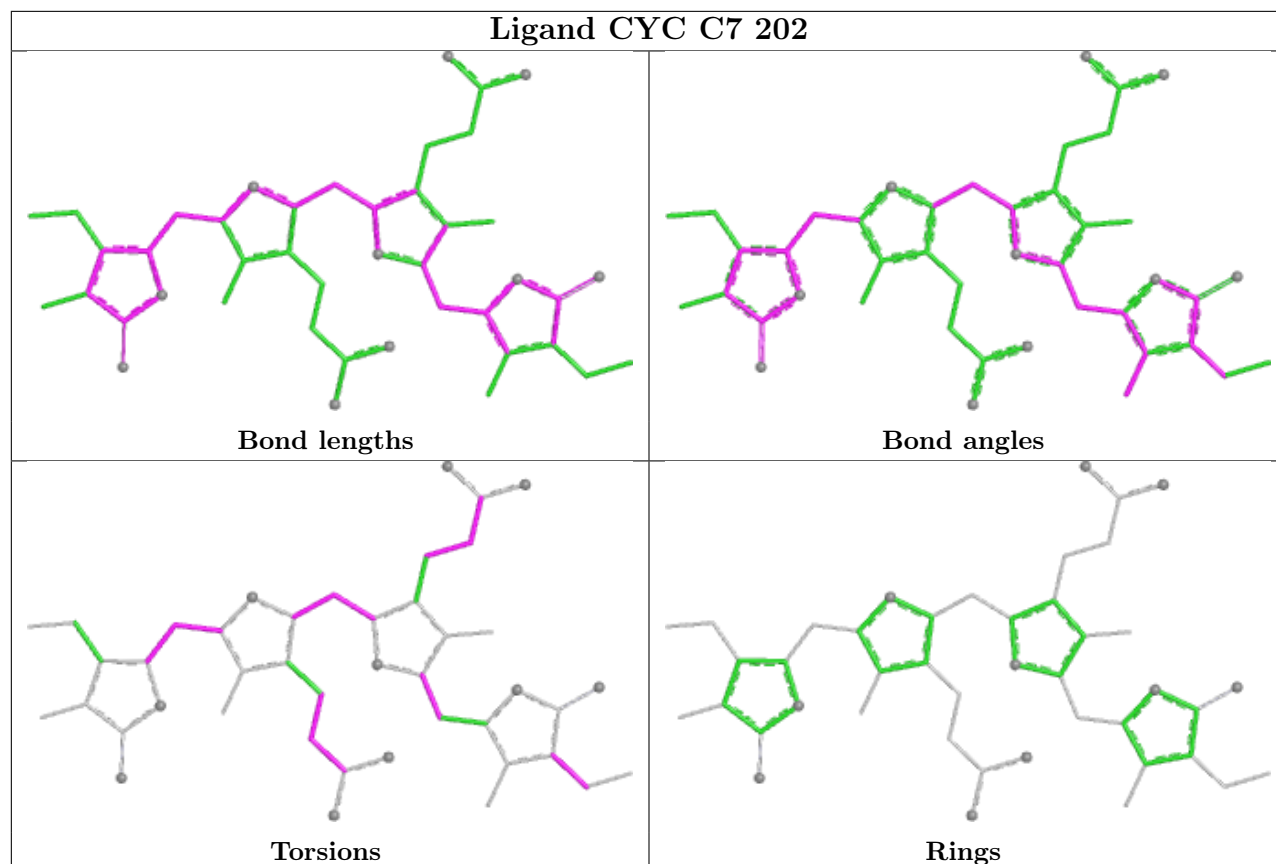
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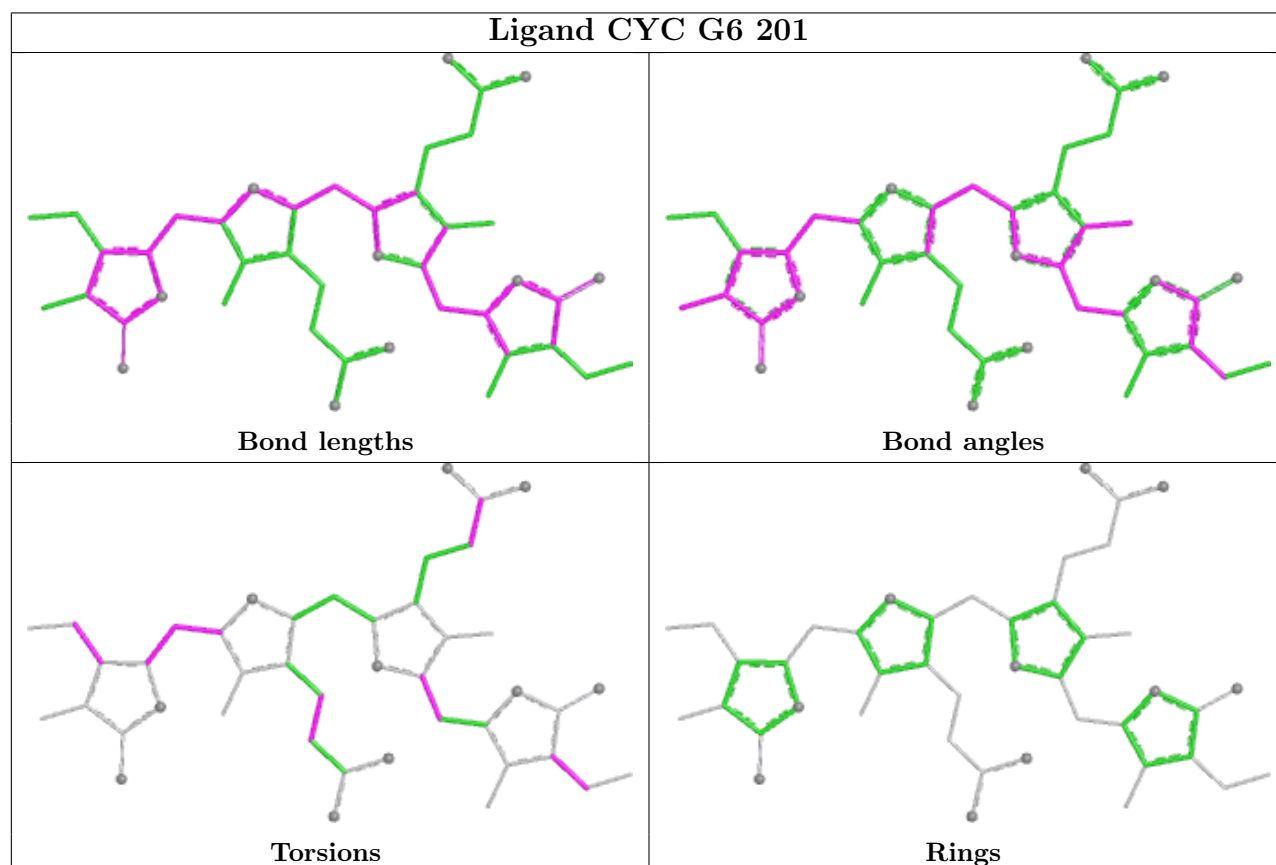
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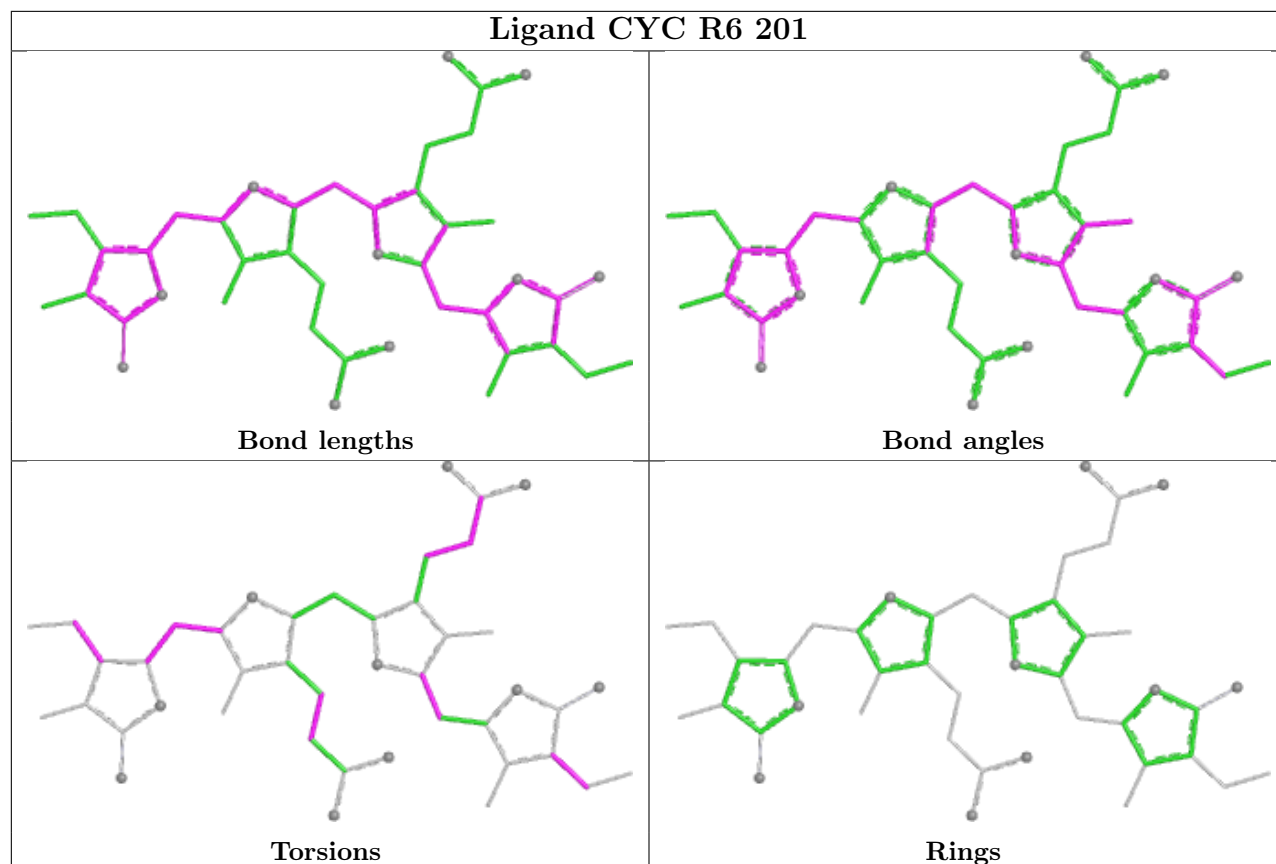
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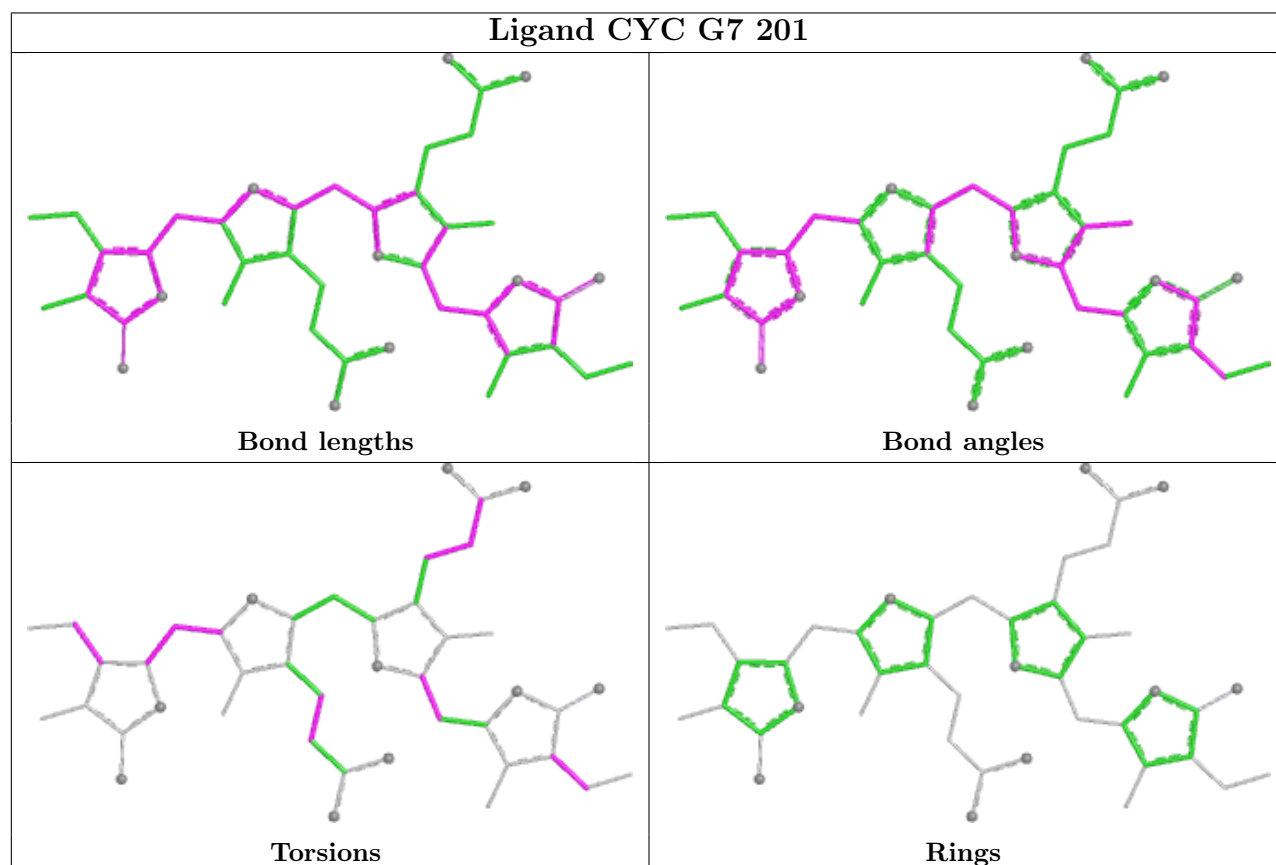
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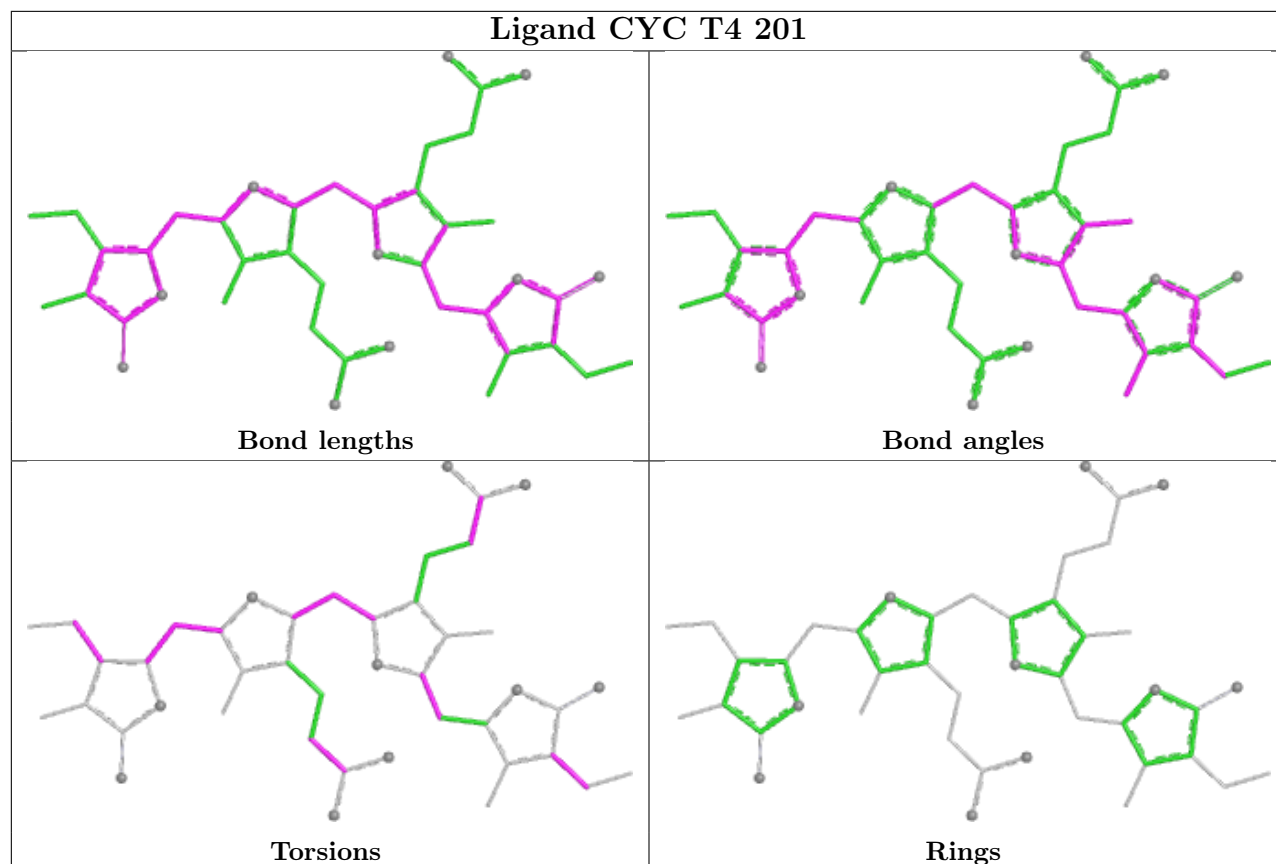
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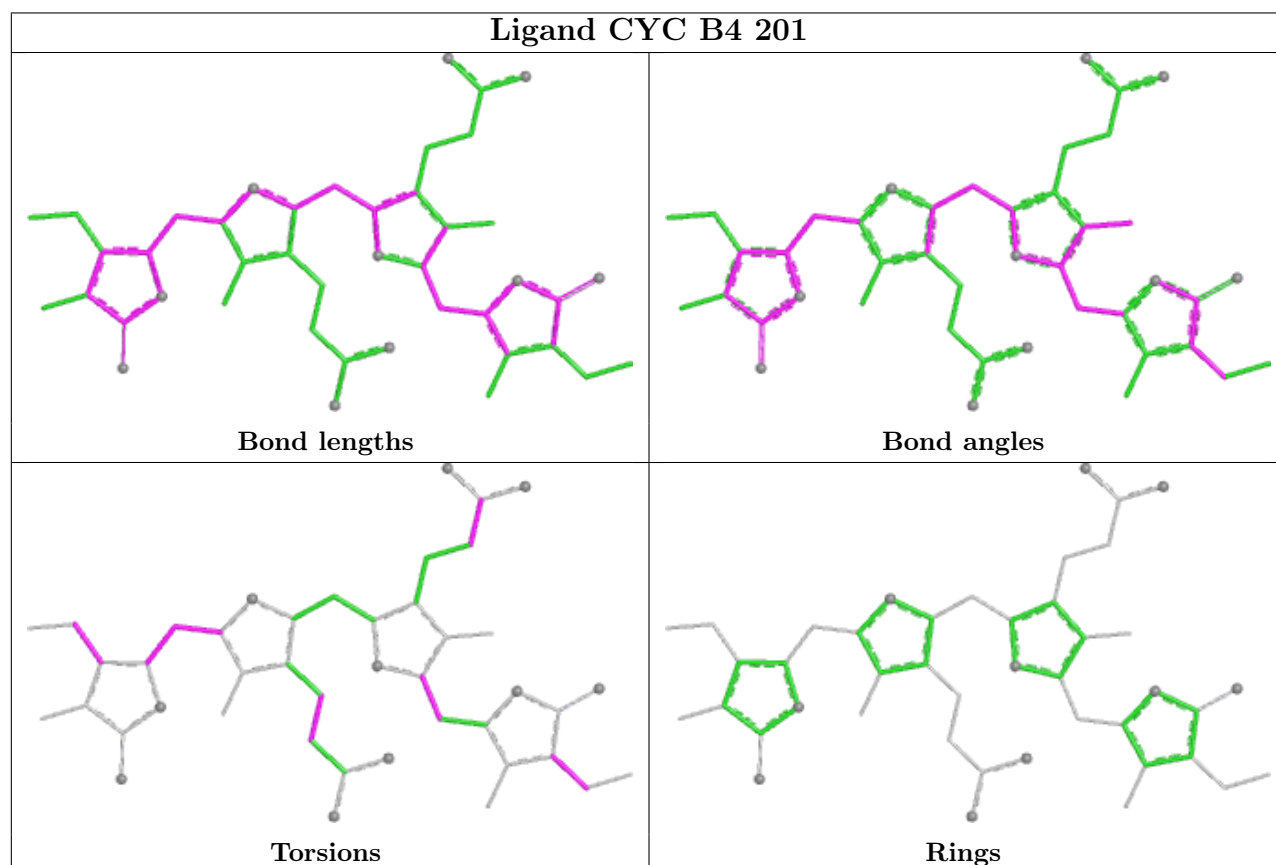
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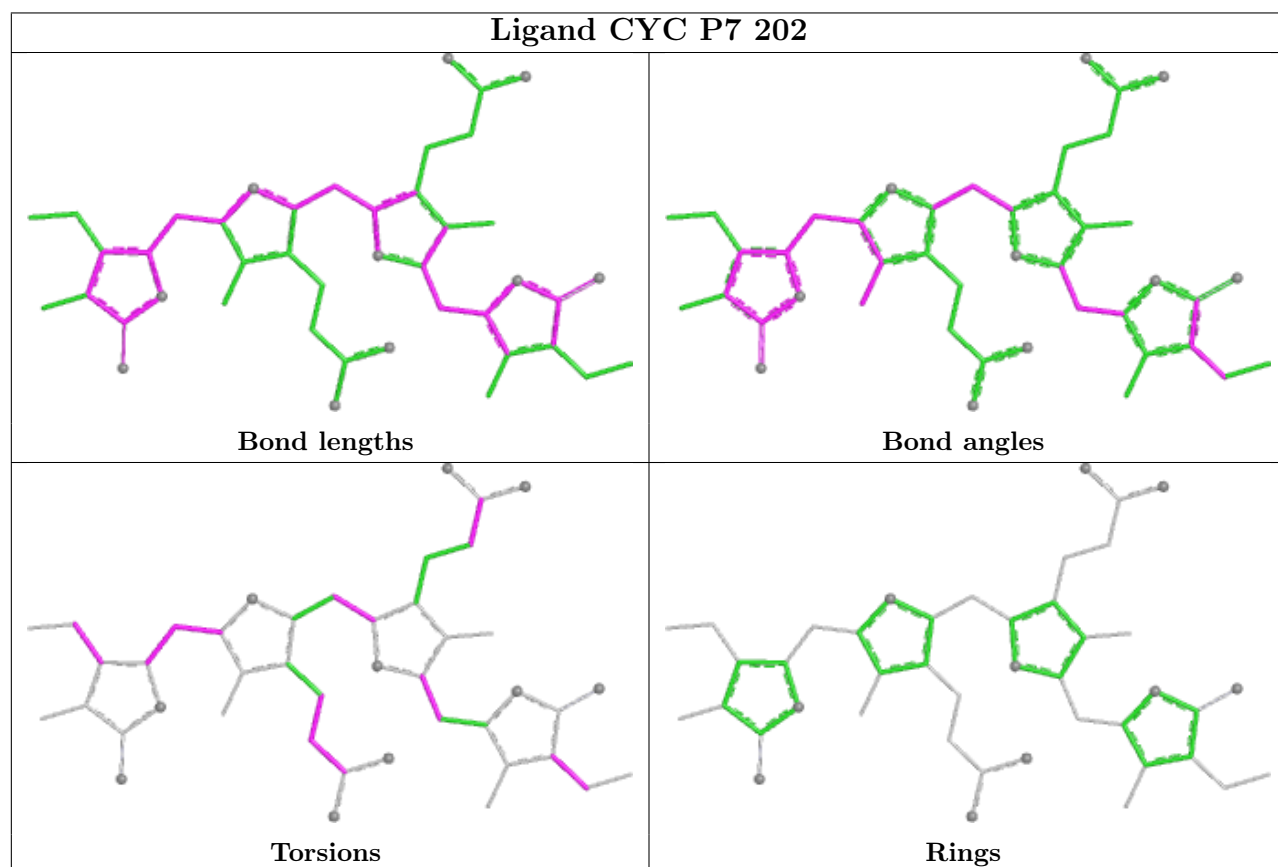
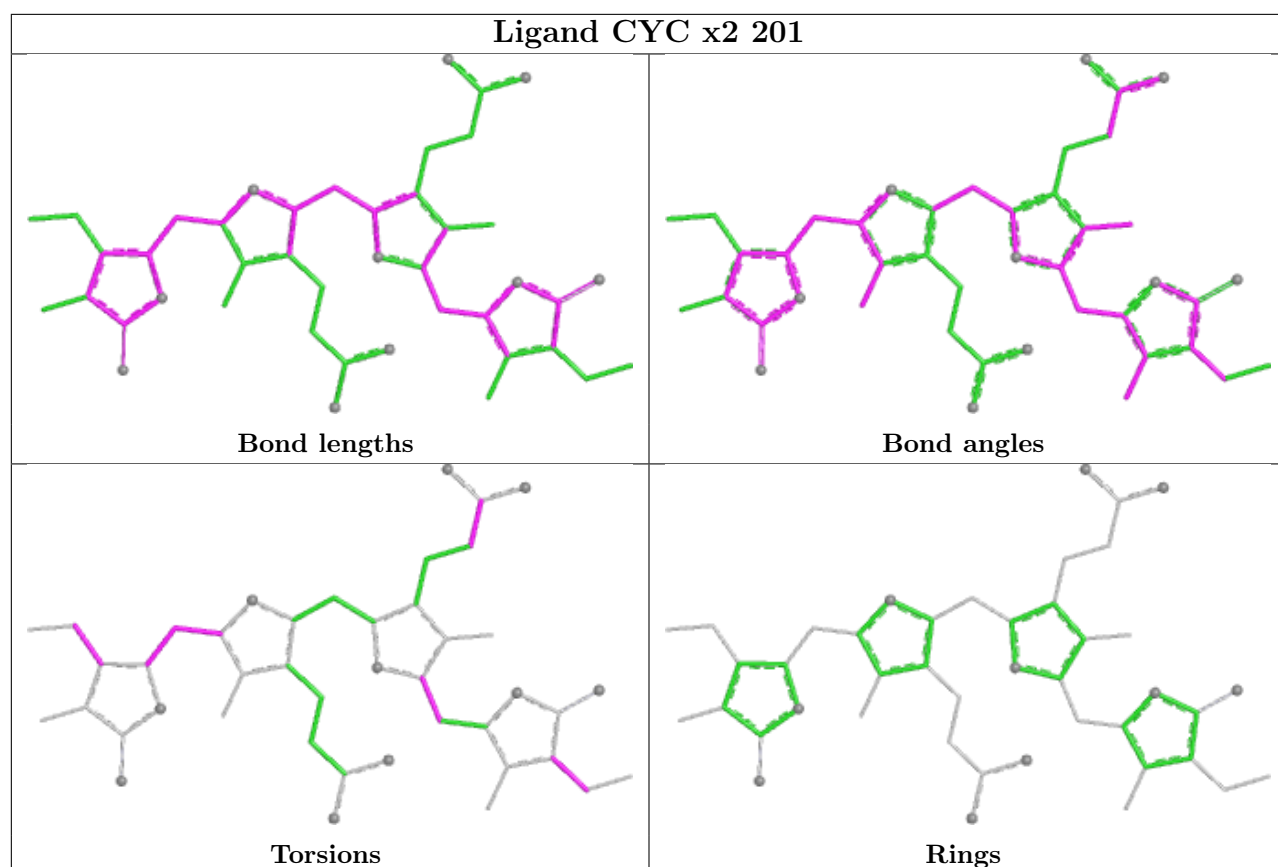


Ligand CYC T4 201

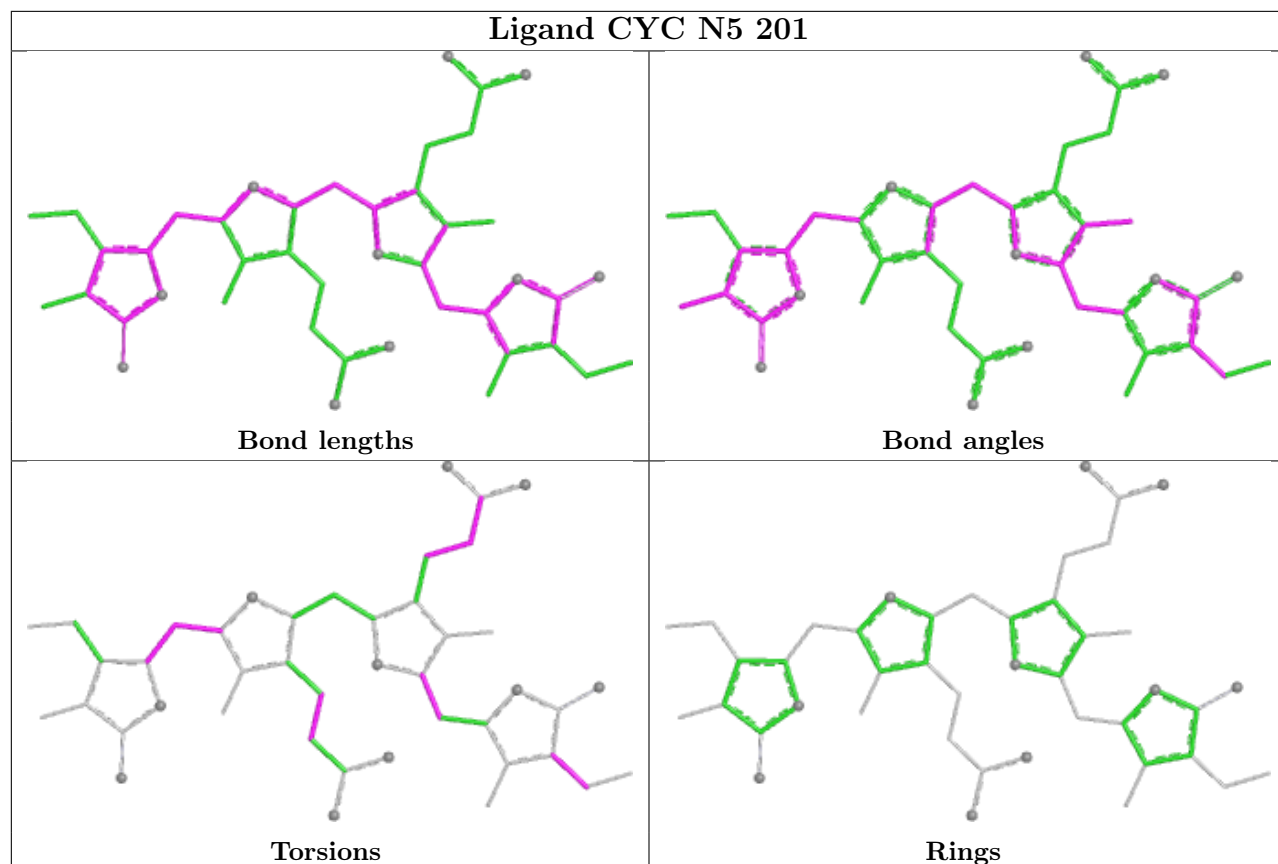


Ligand CYC B4 201

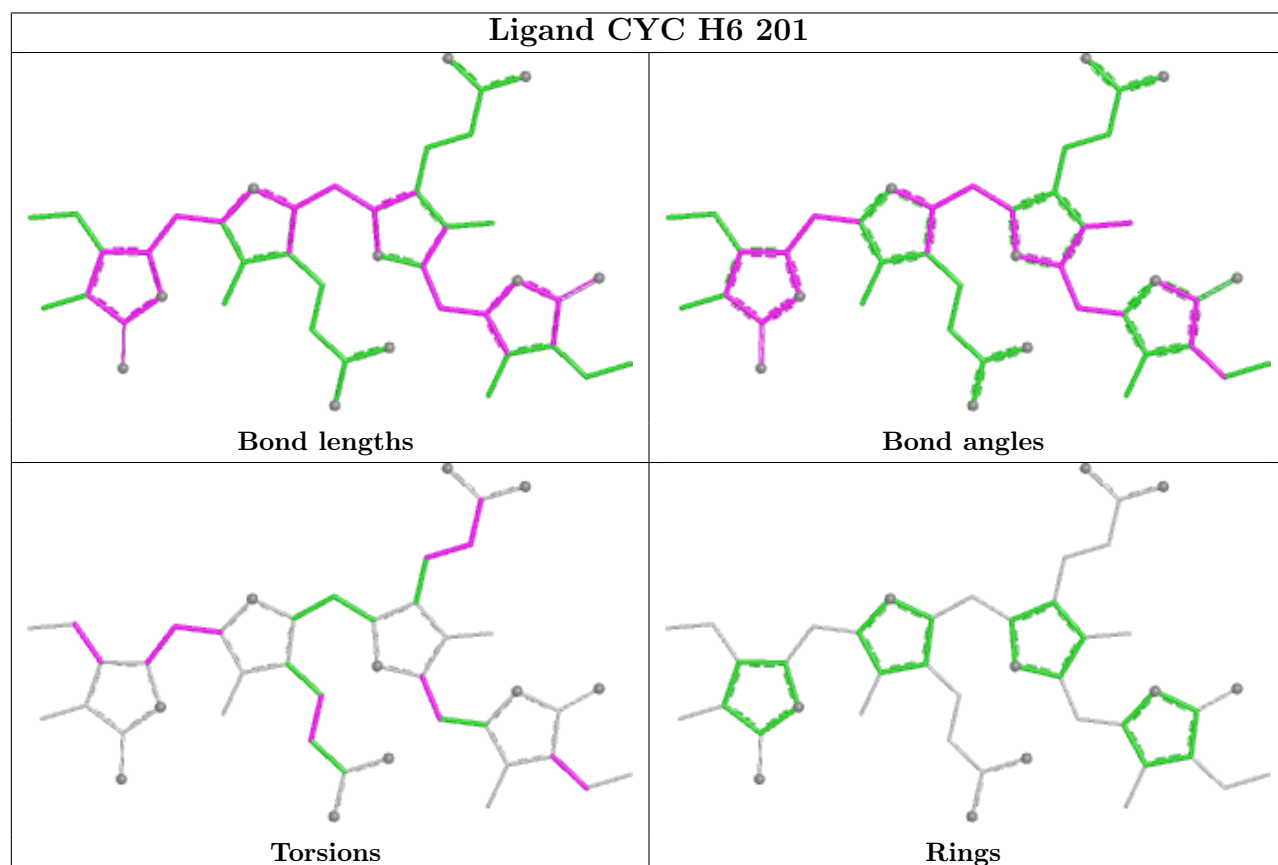




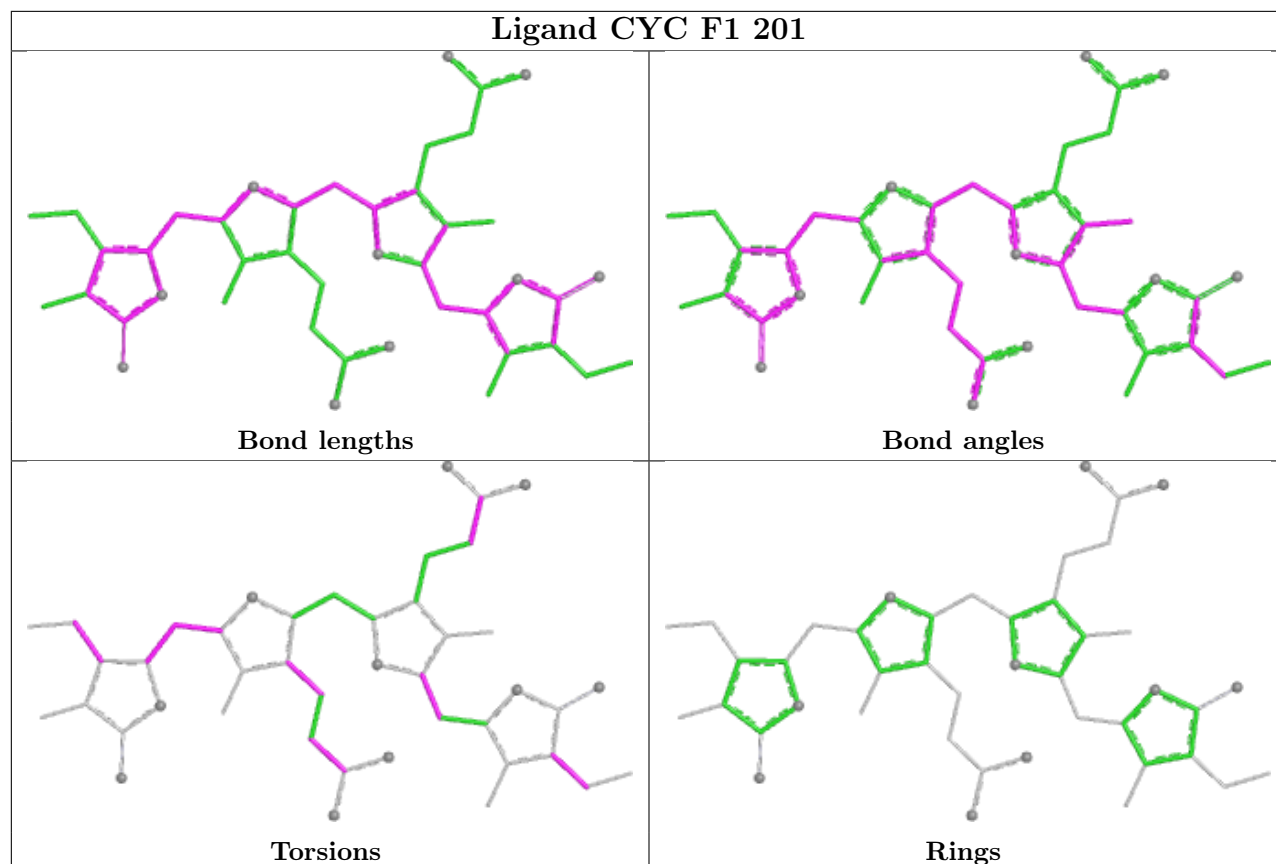
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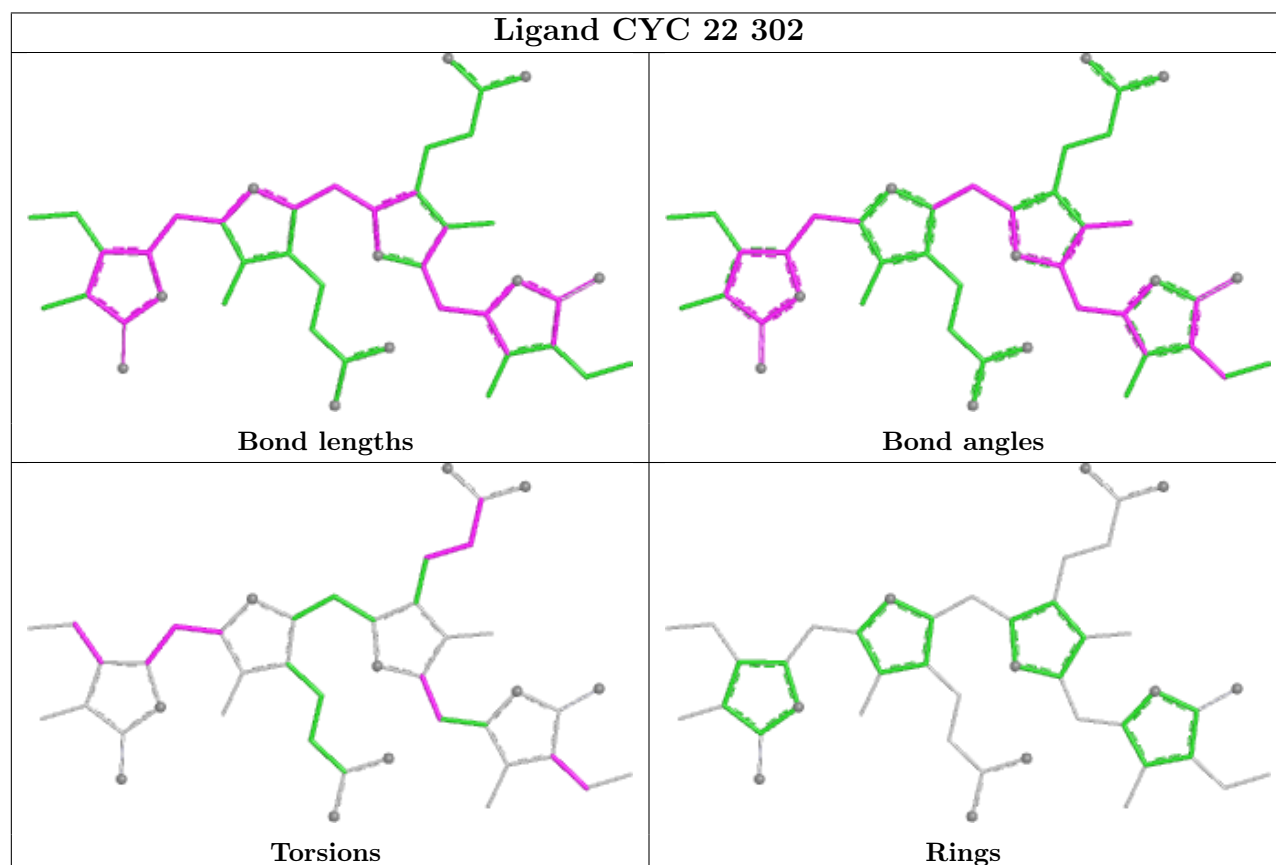
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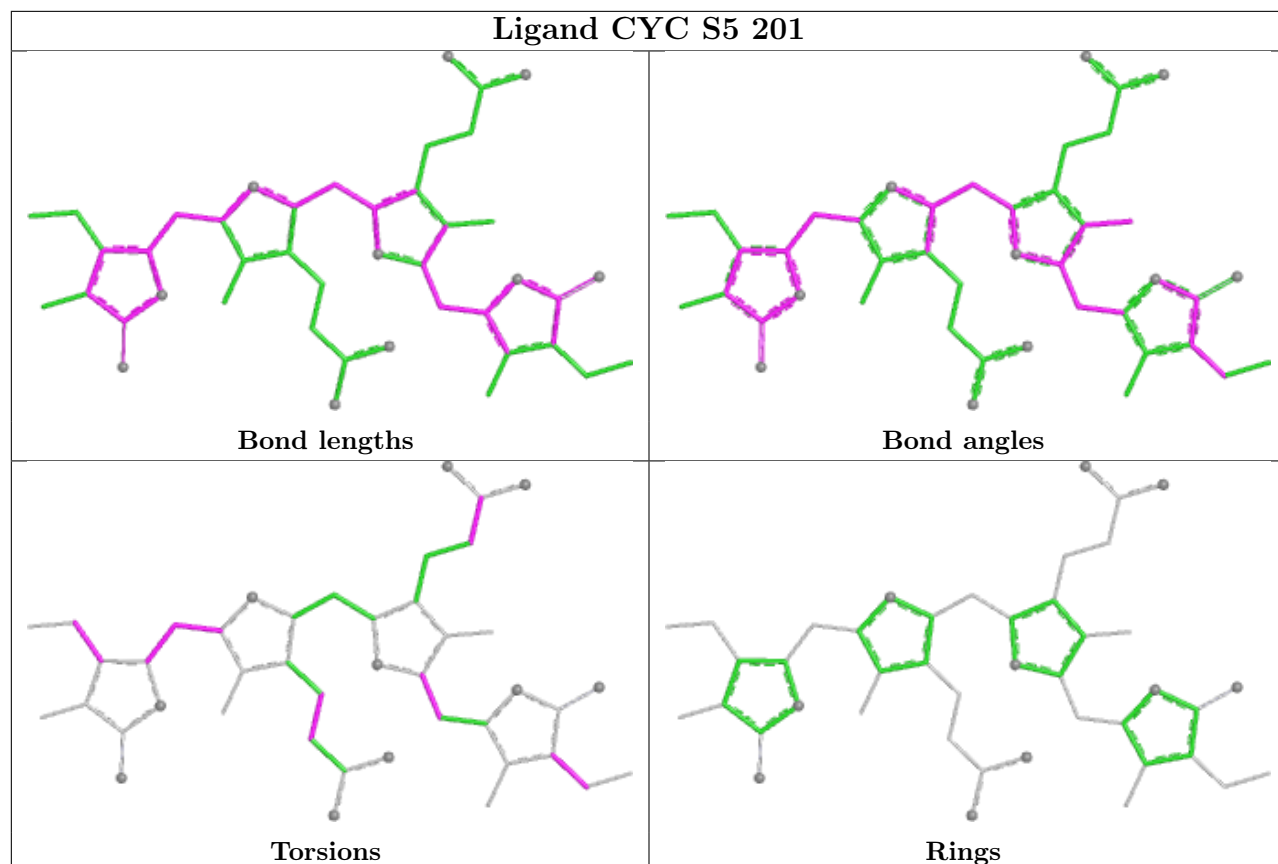
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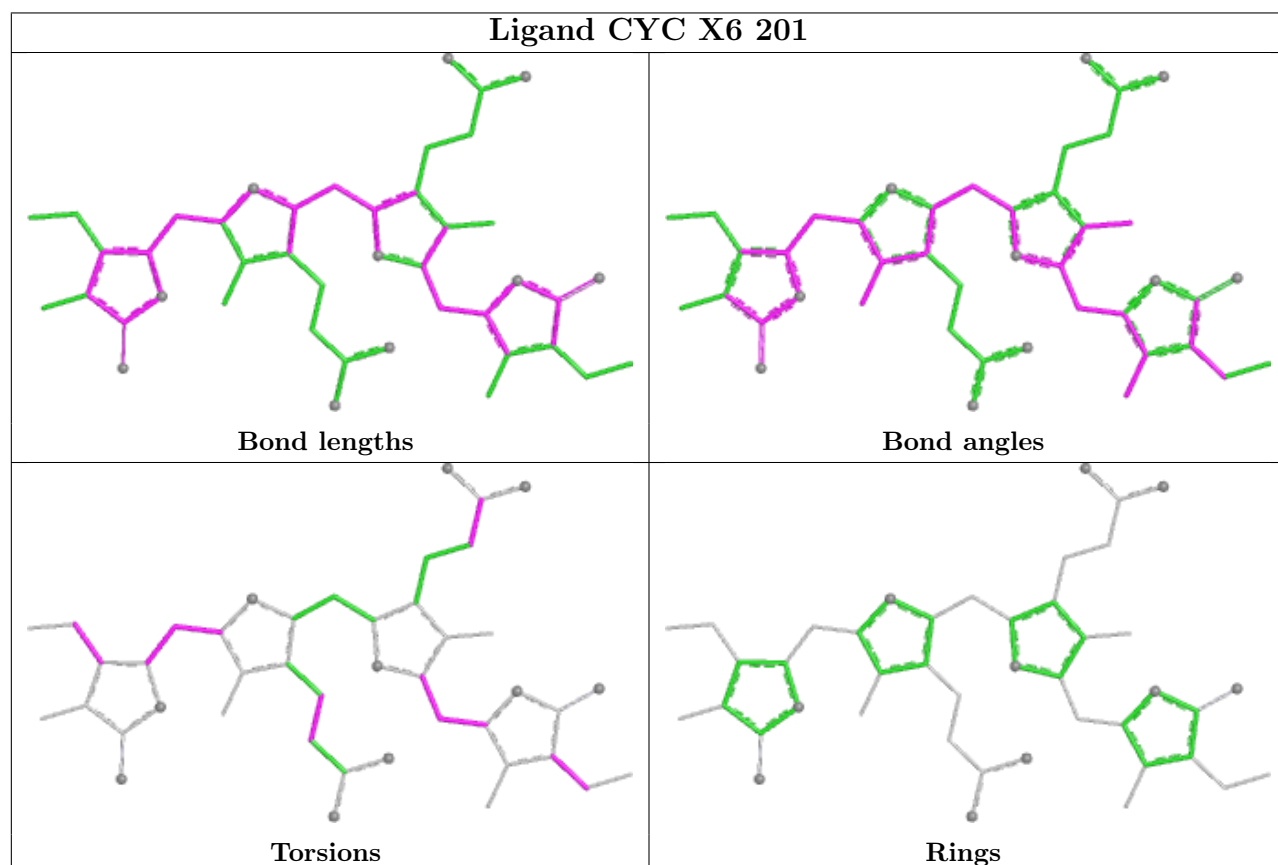
Ligand CYC 22 302

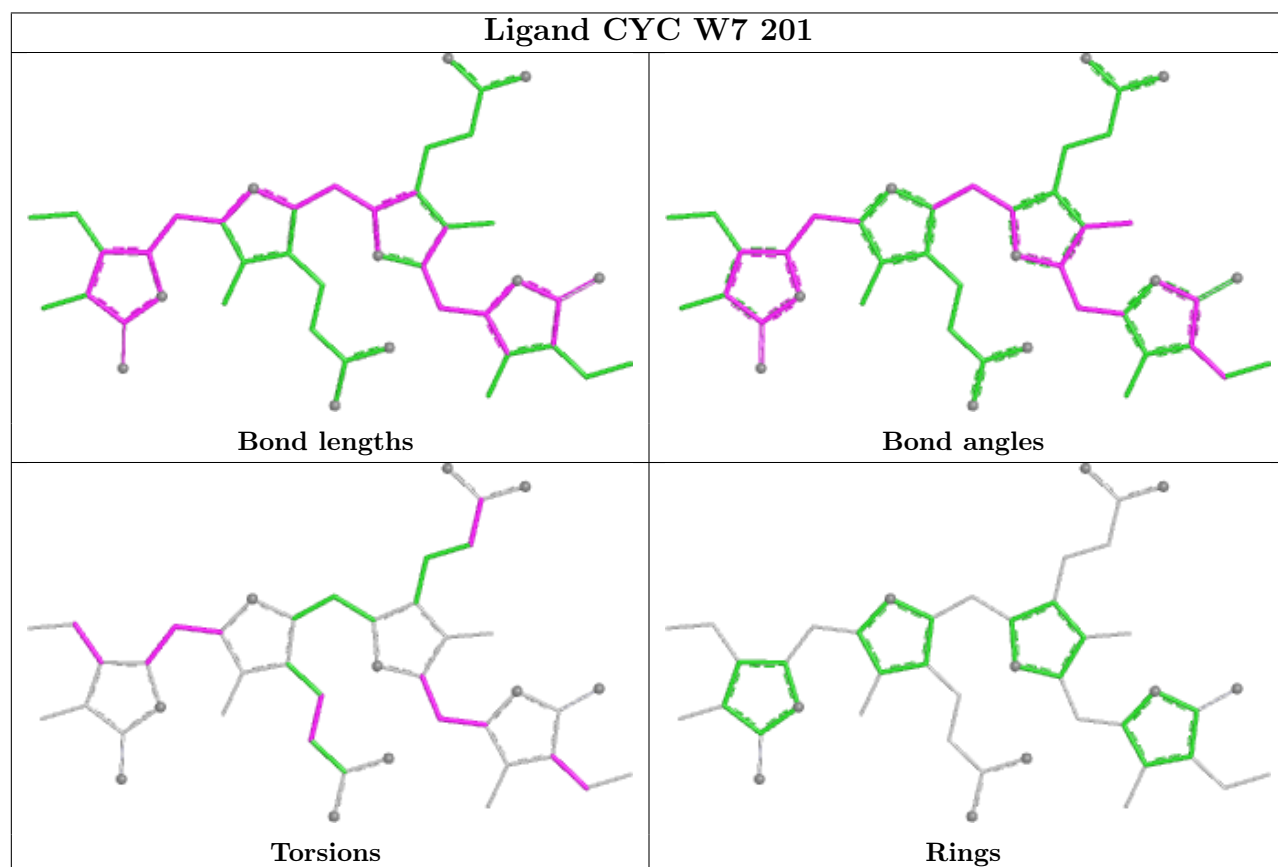
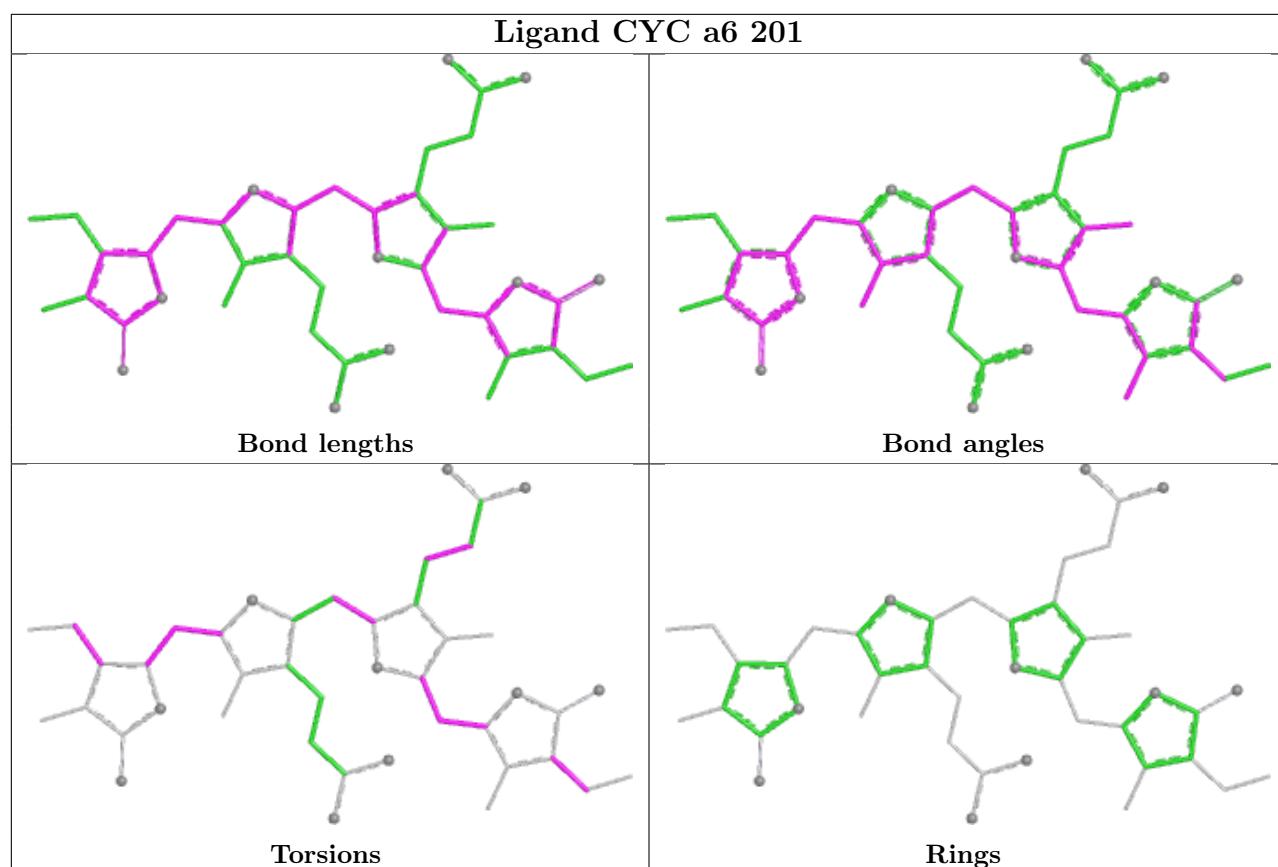


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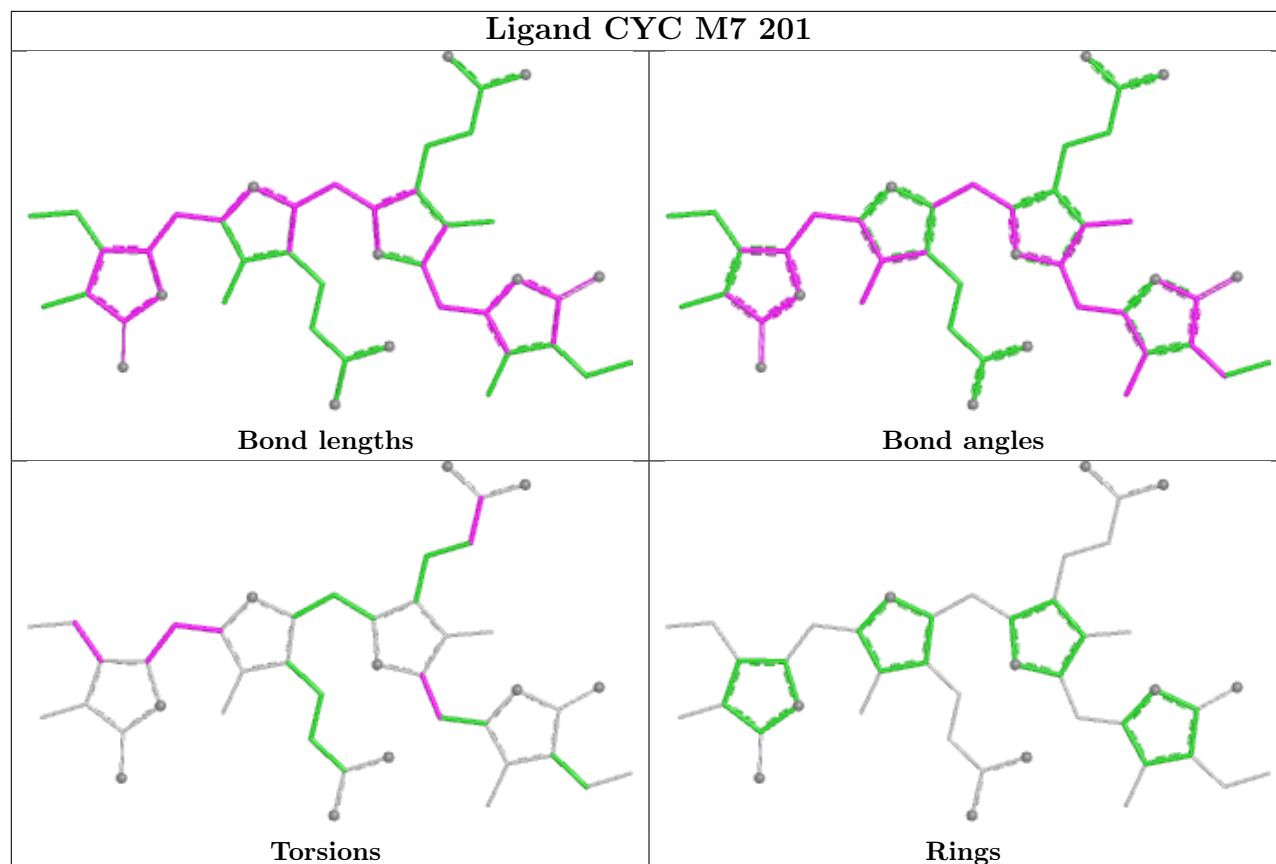


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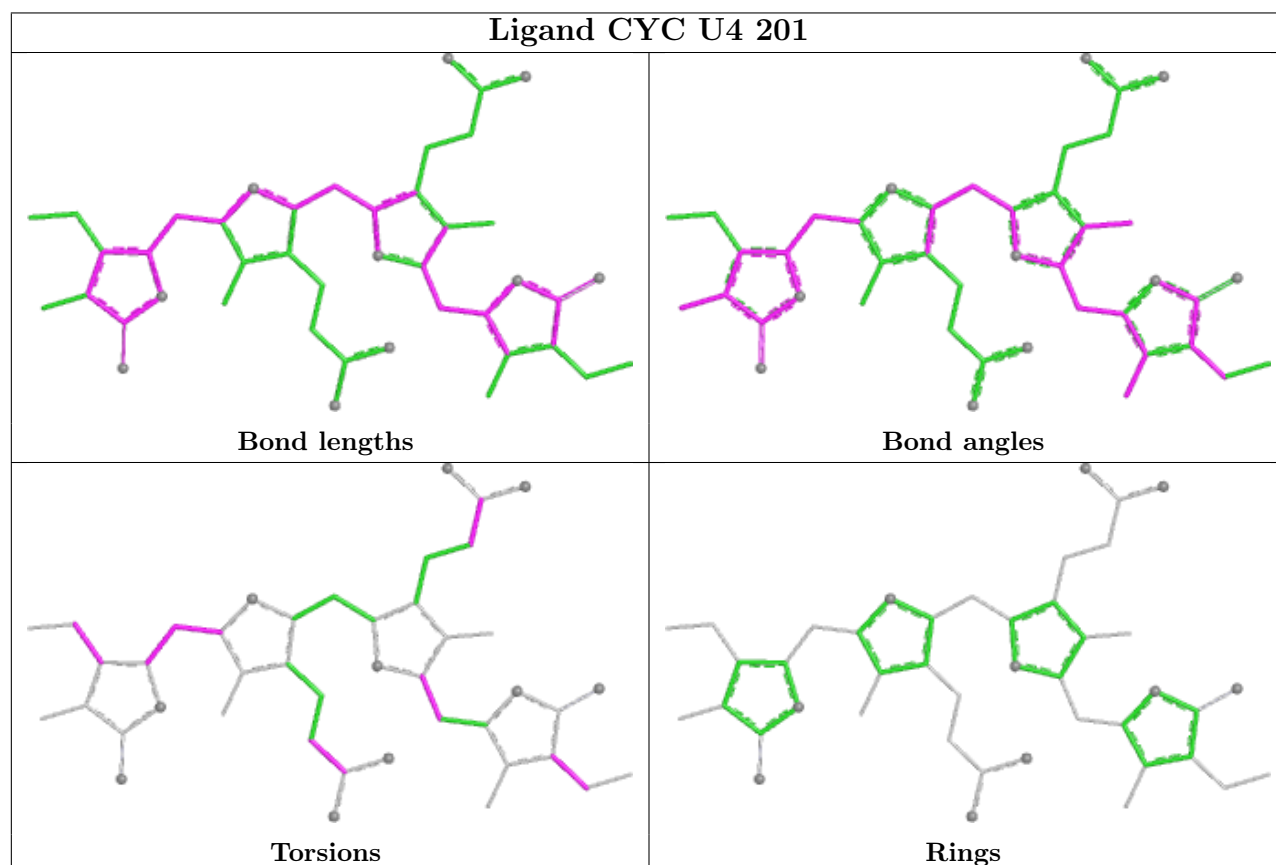




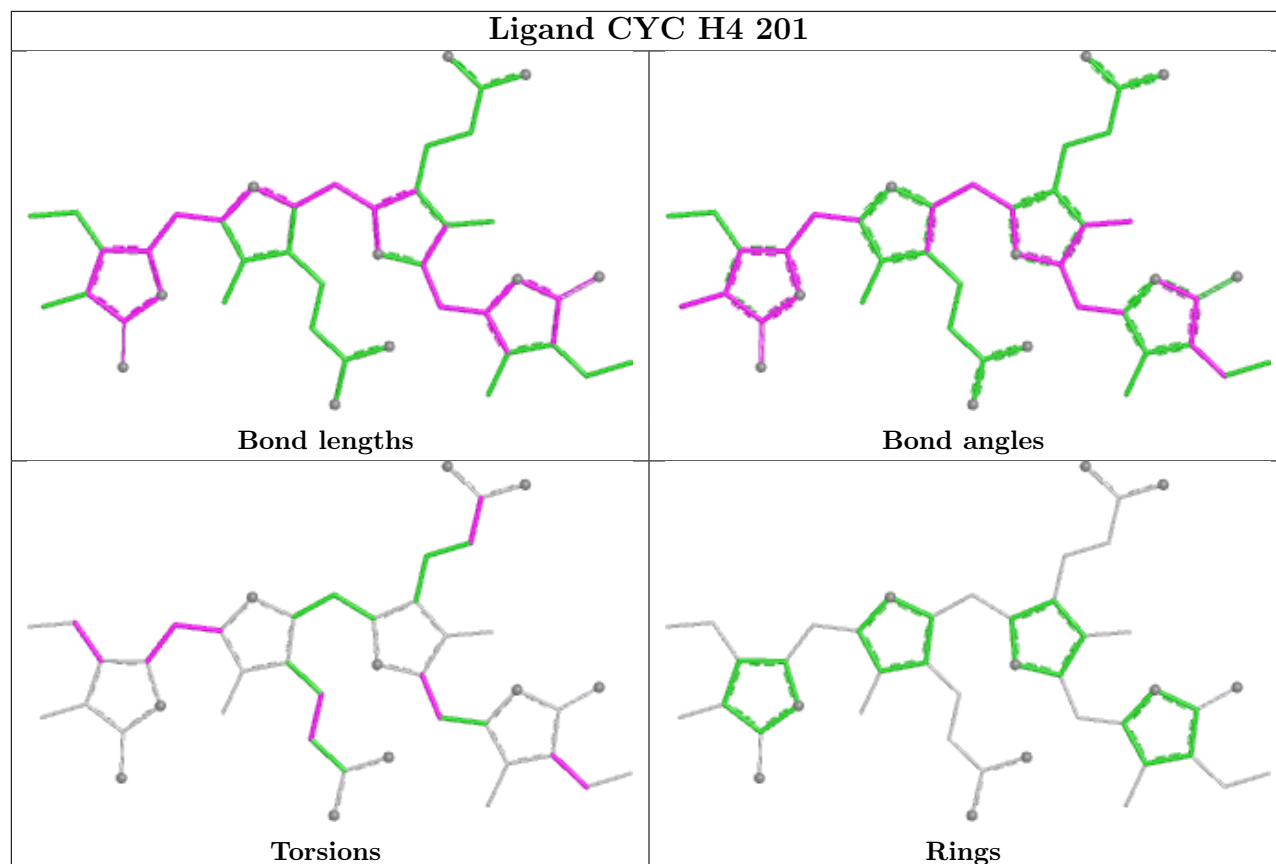
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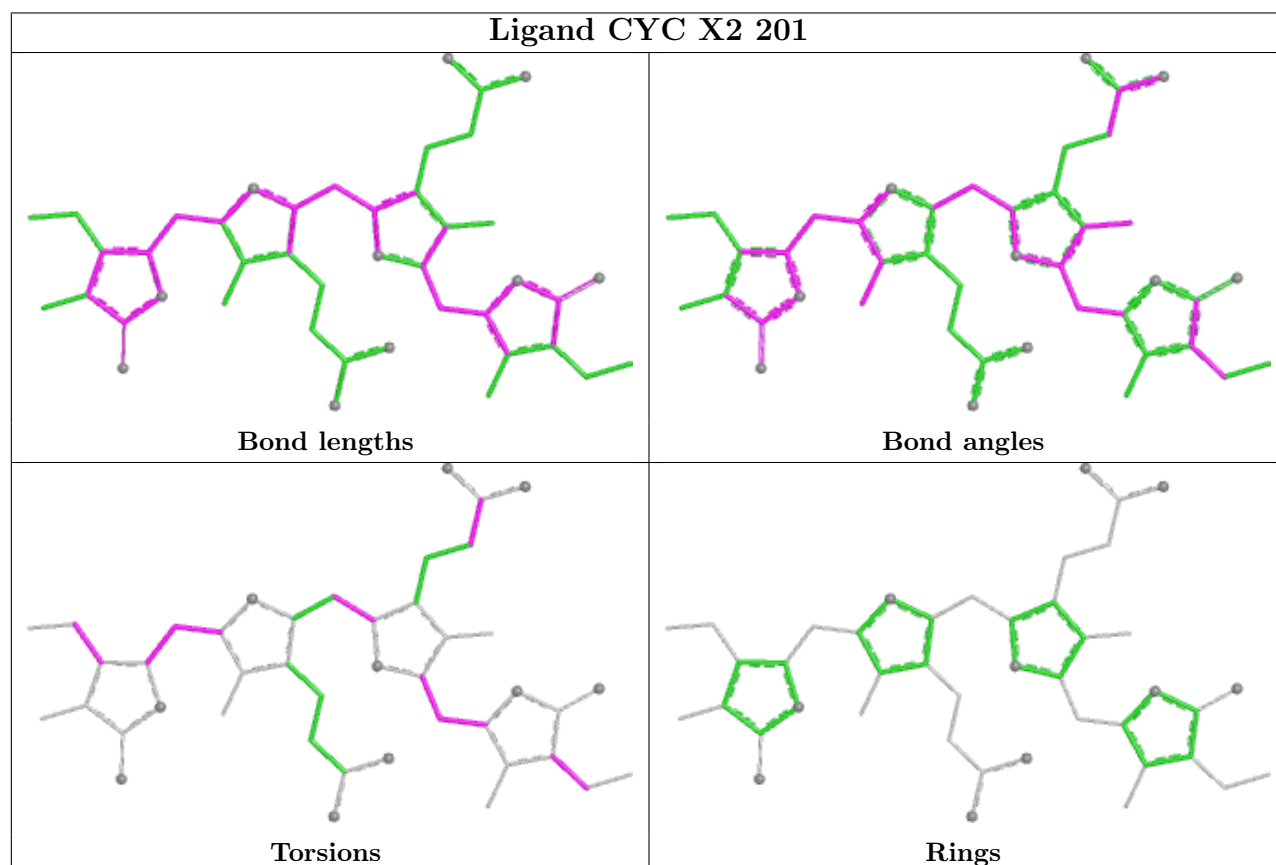
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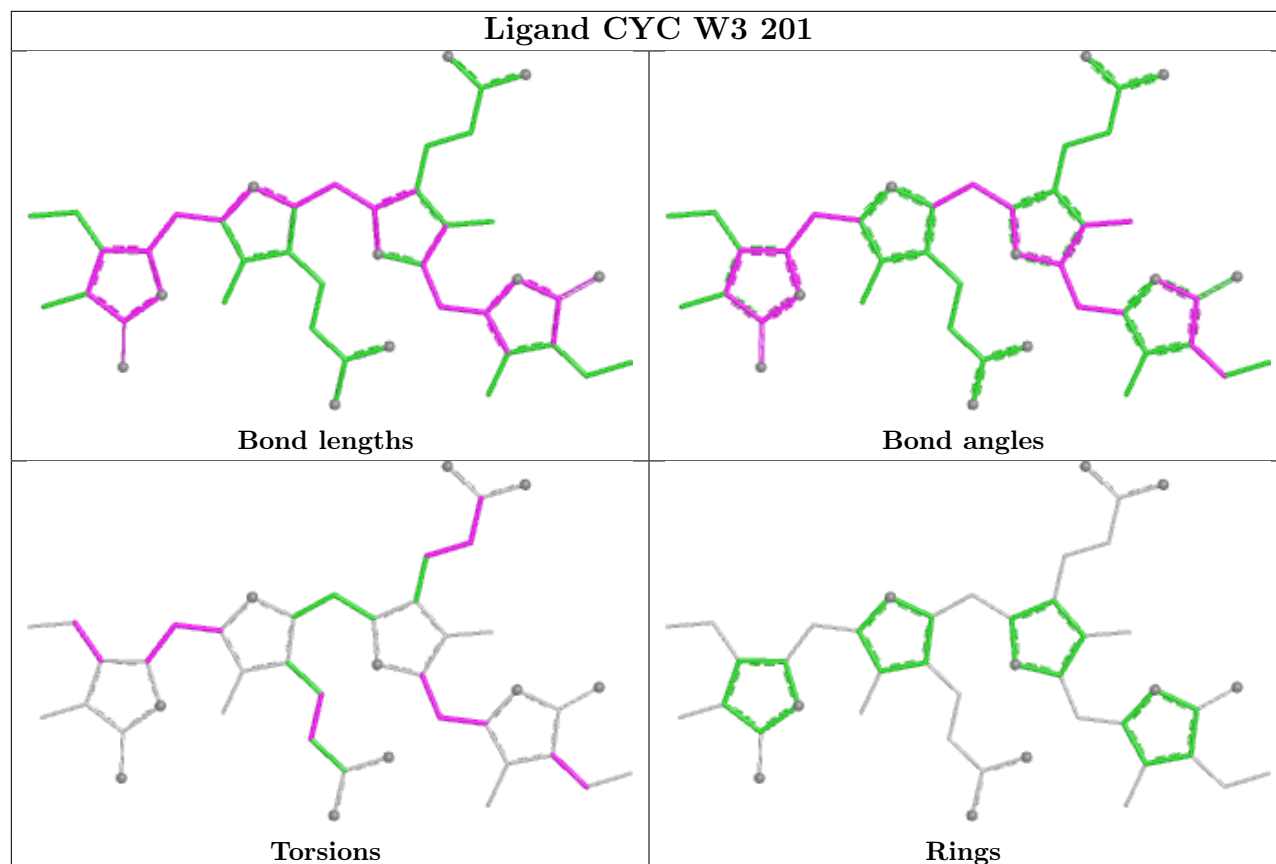
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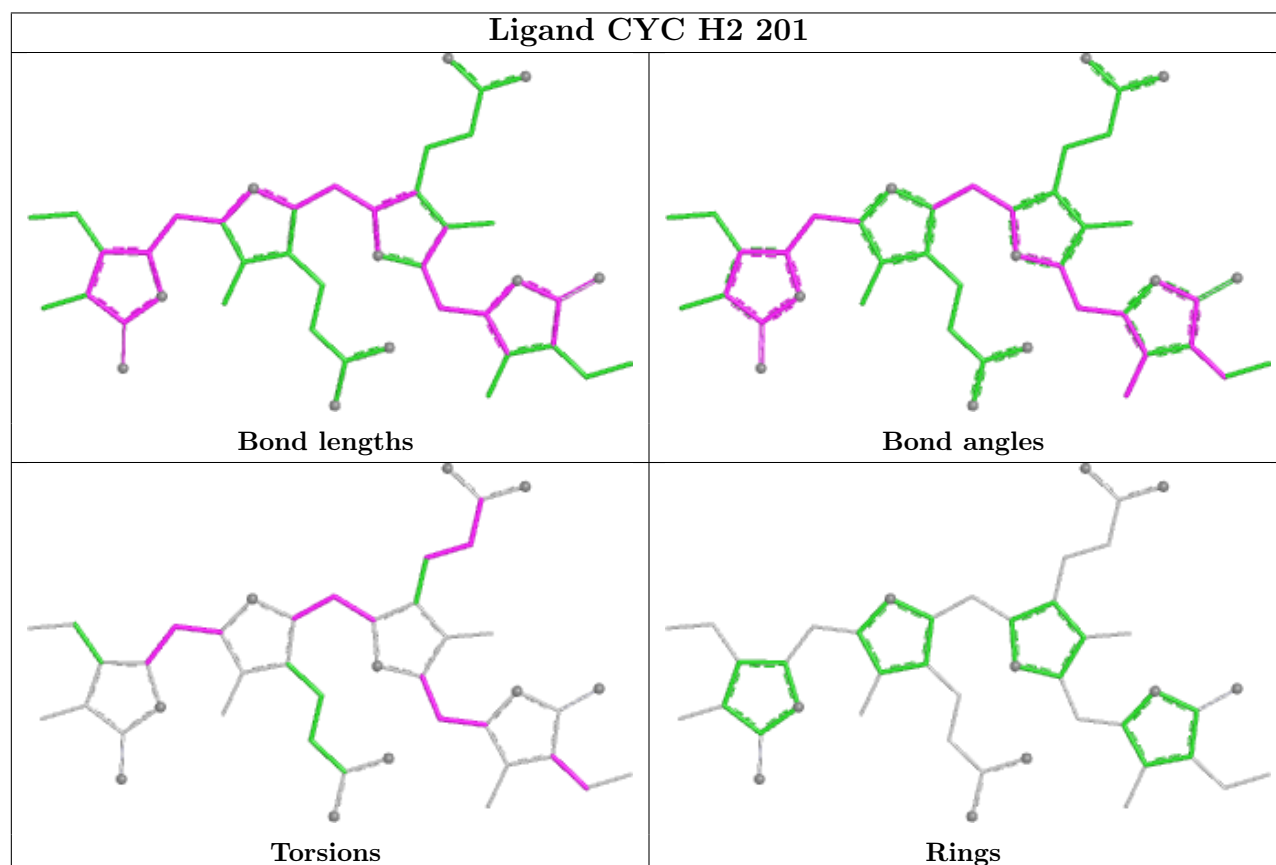
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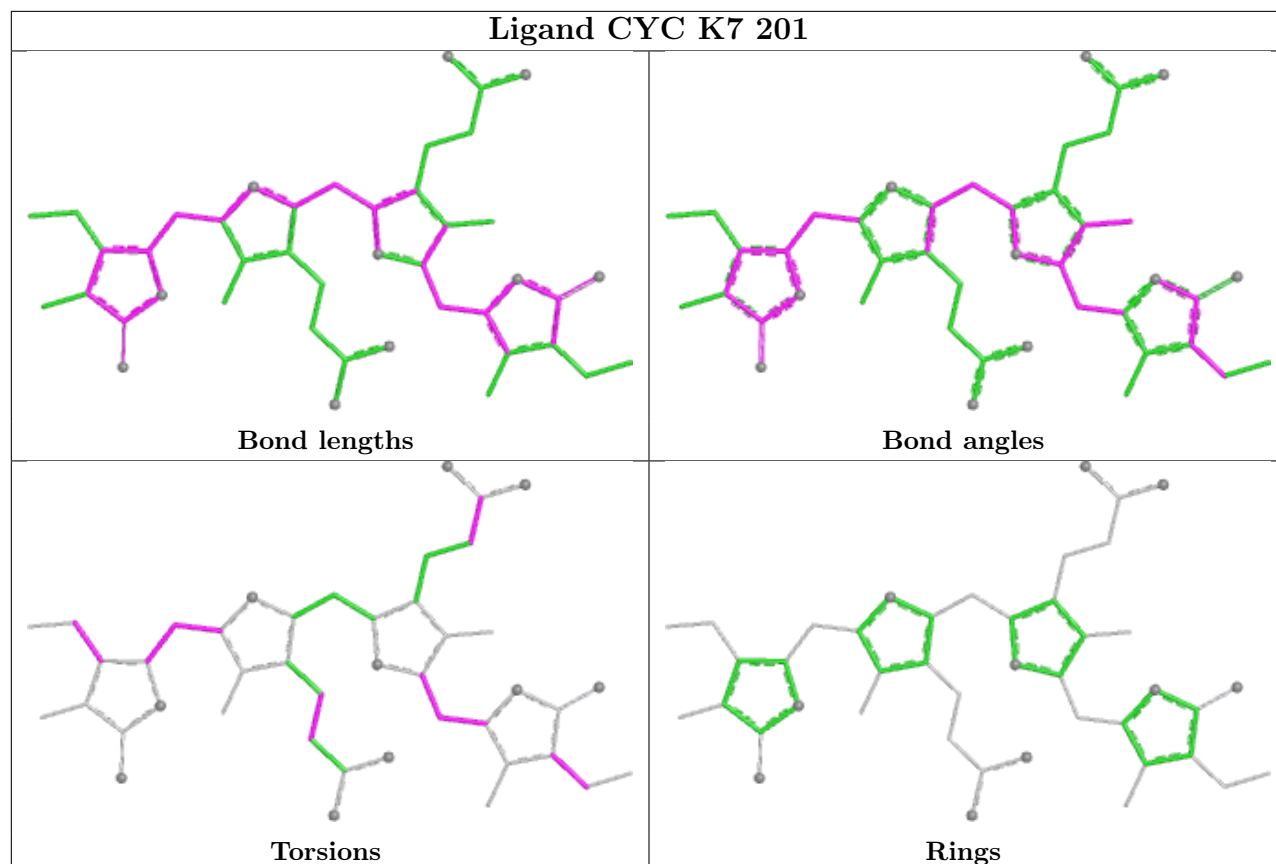
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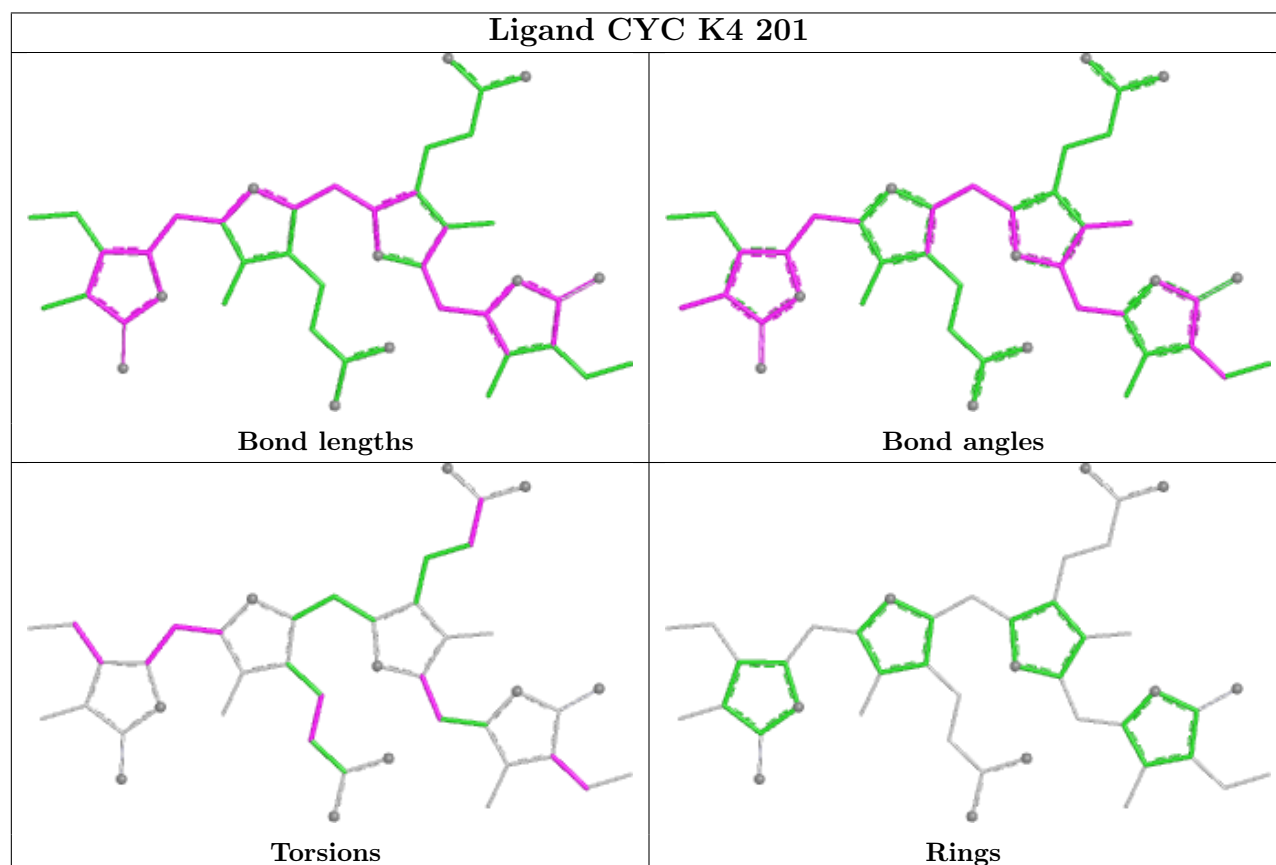
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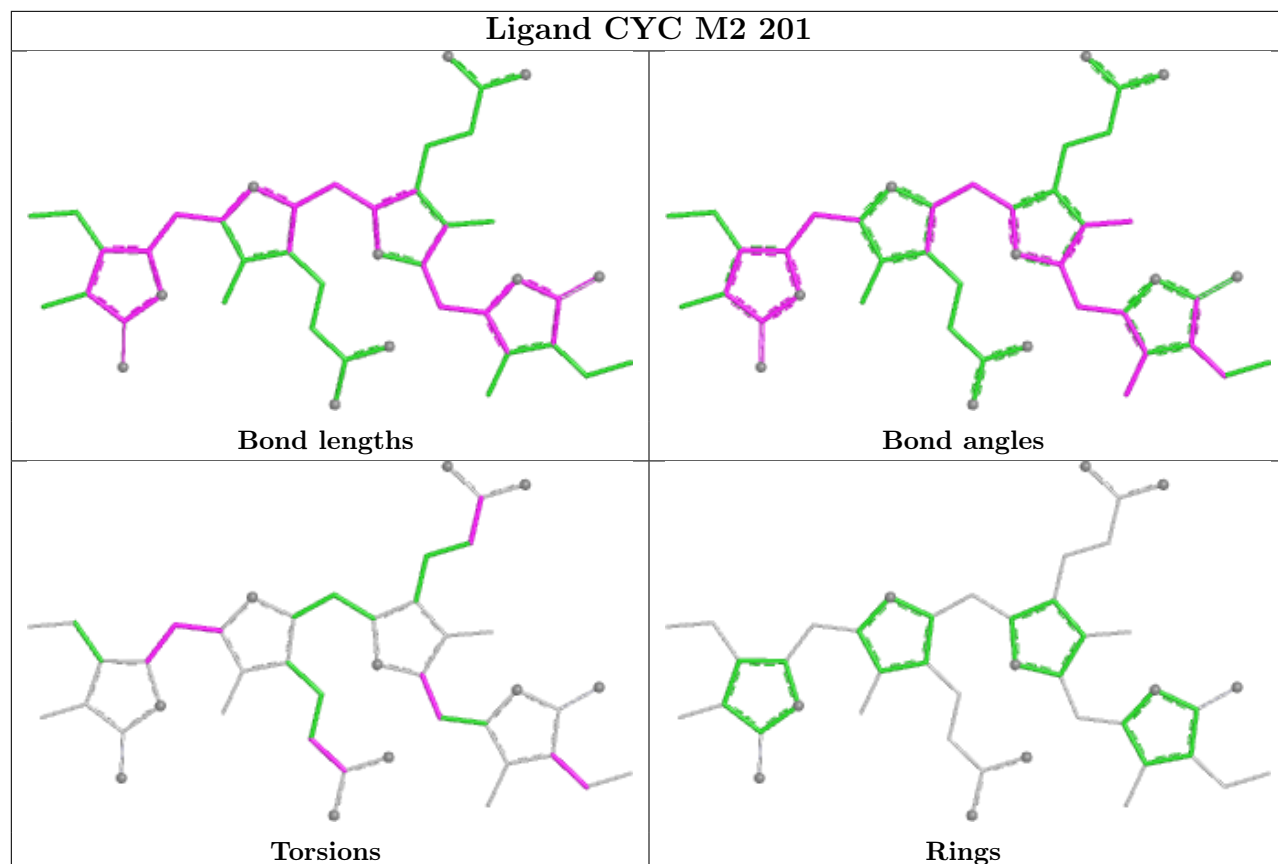
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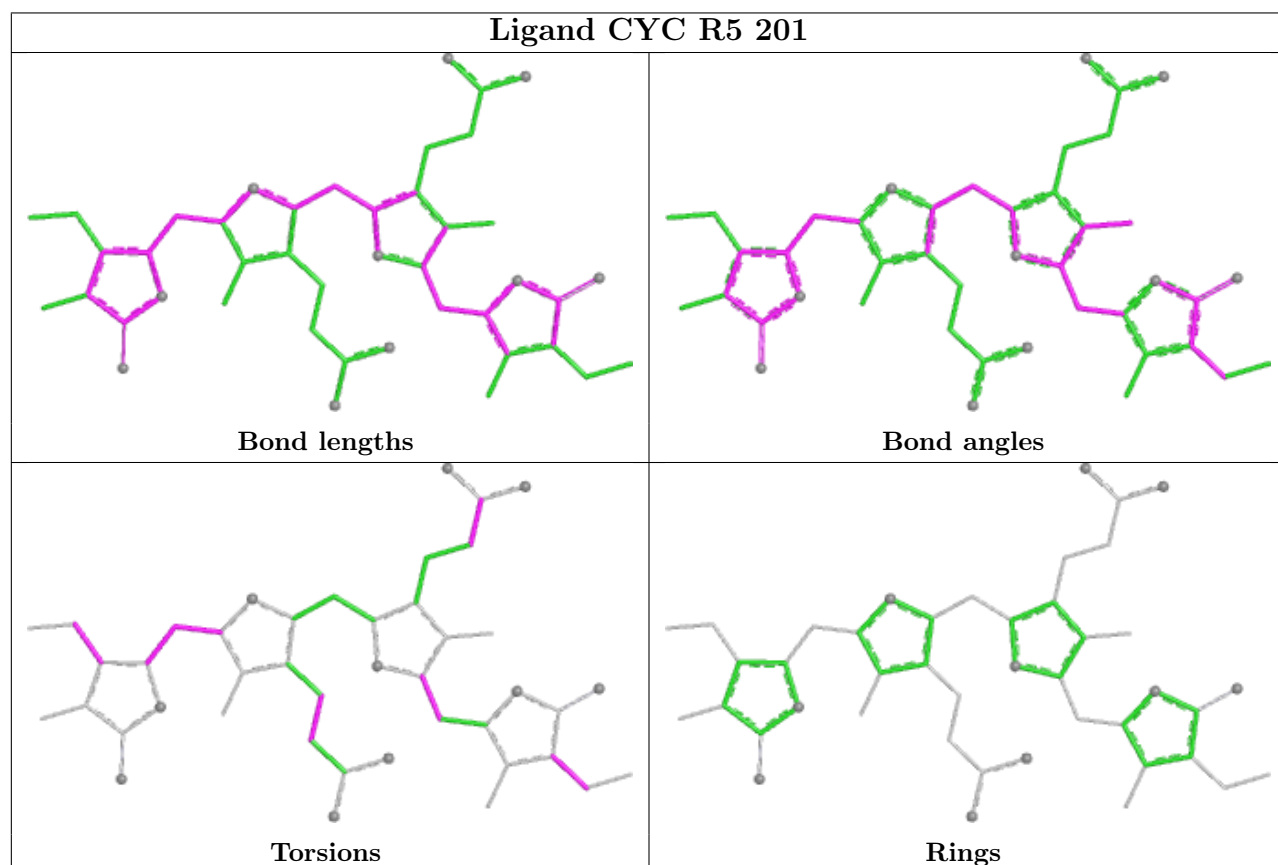
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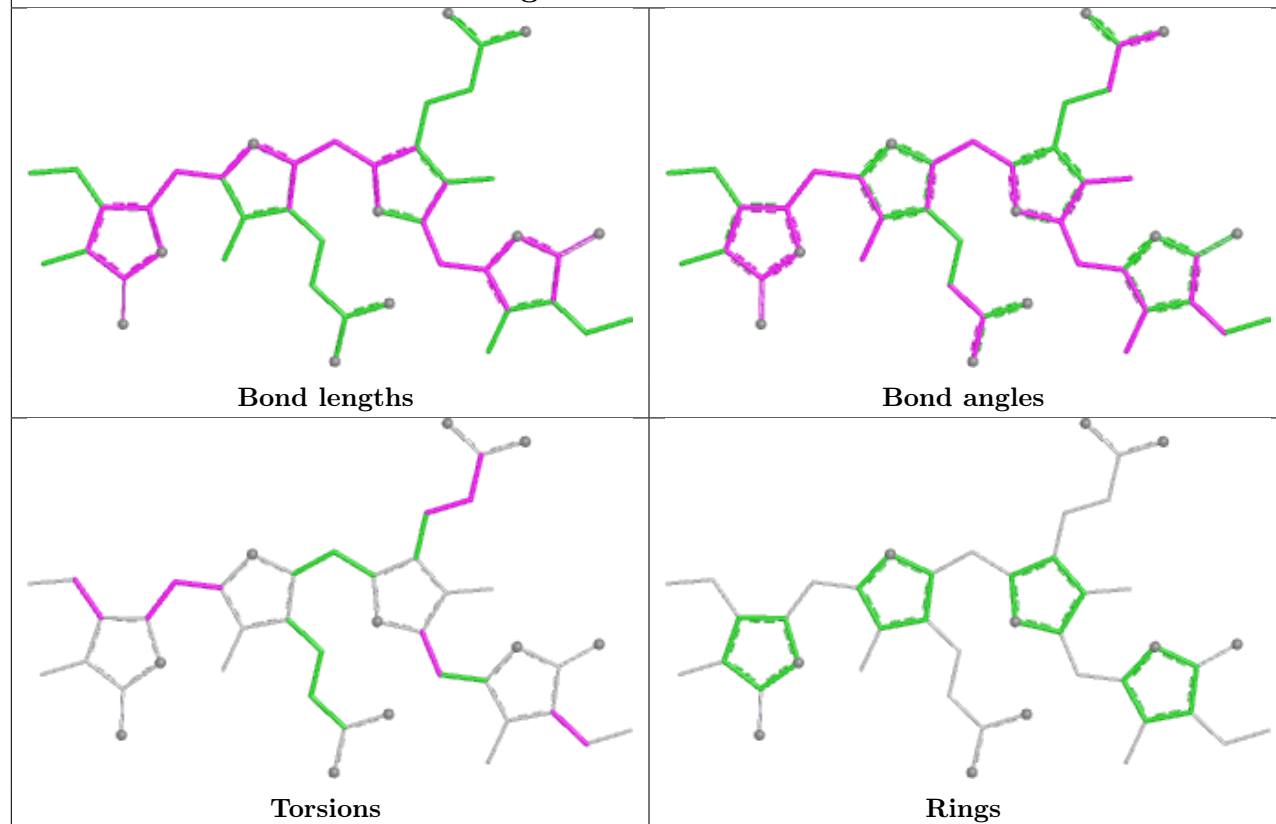
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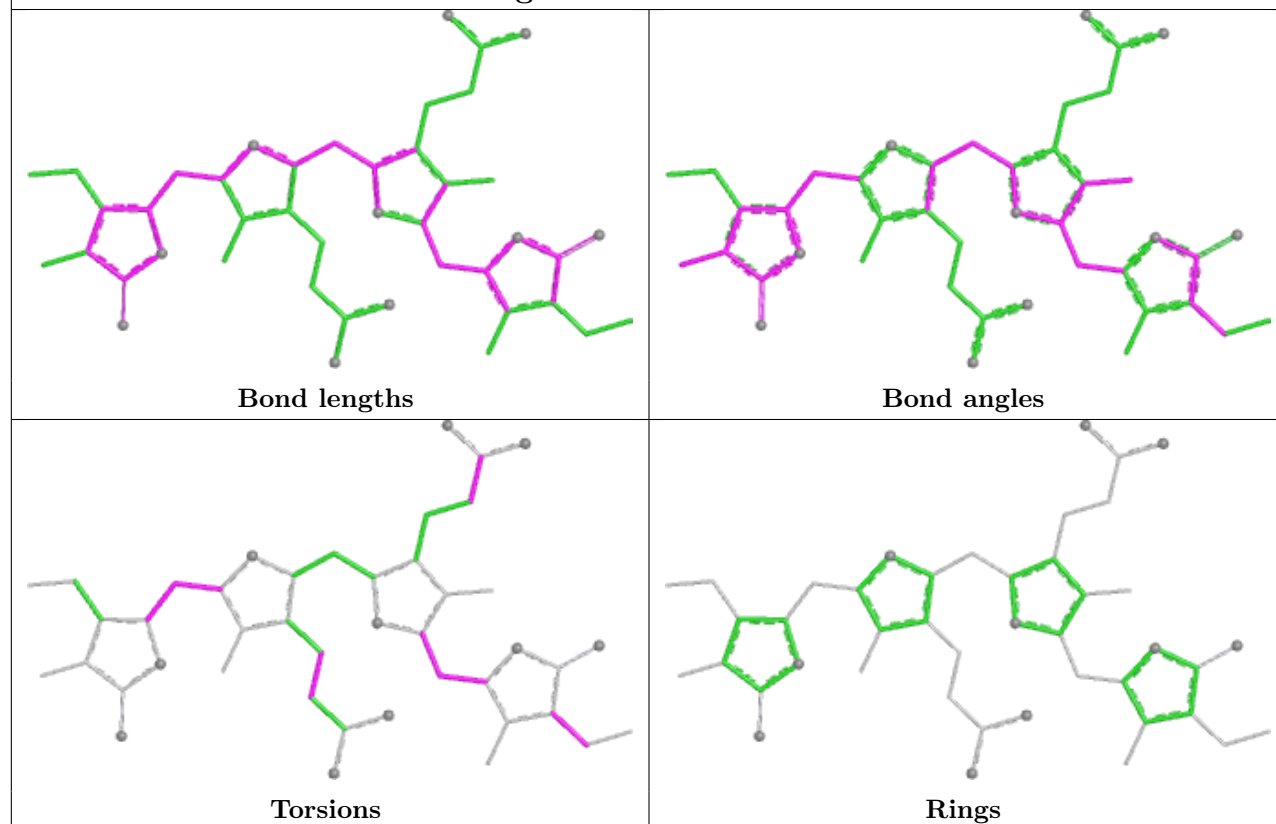
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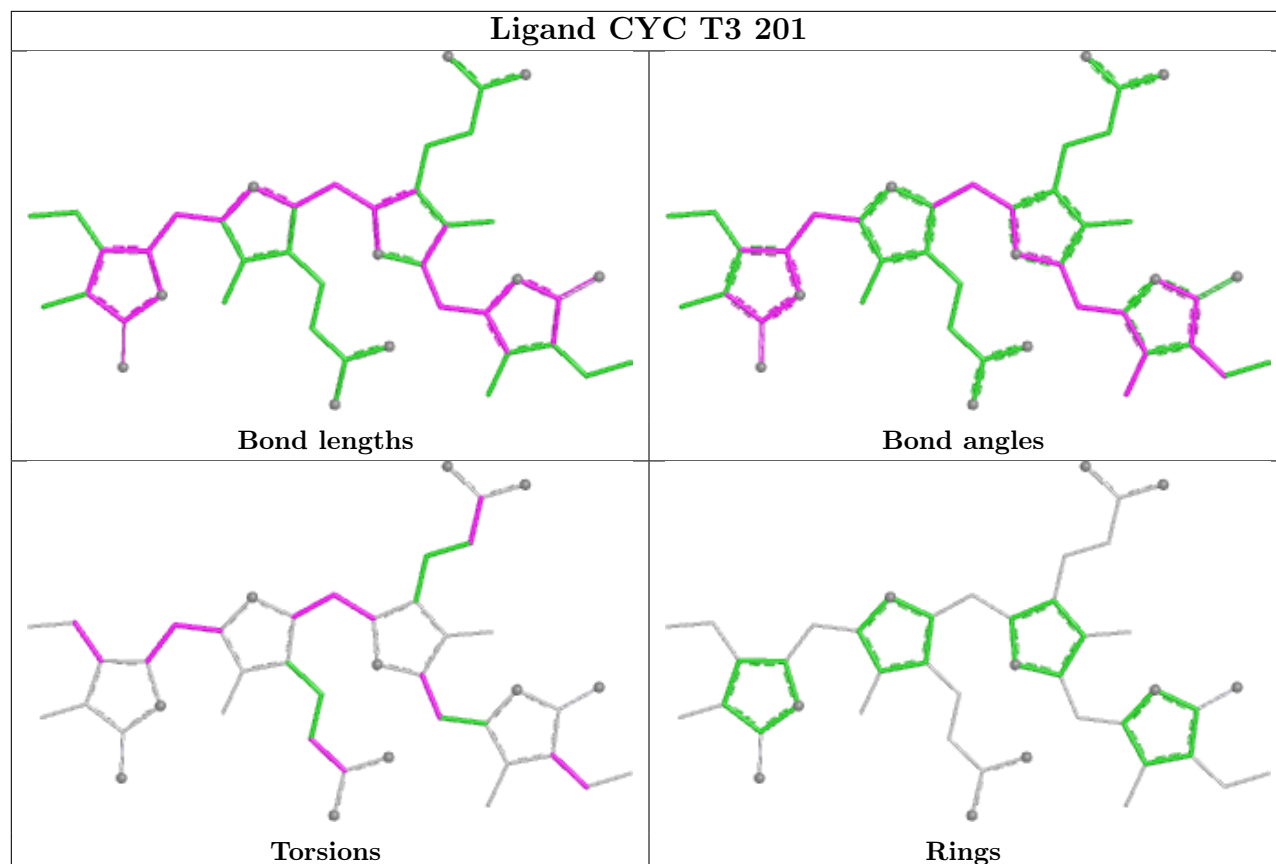
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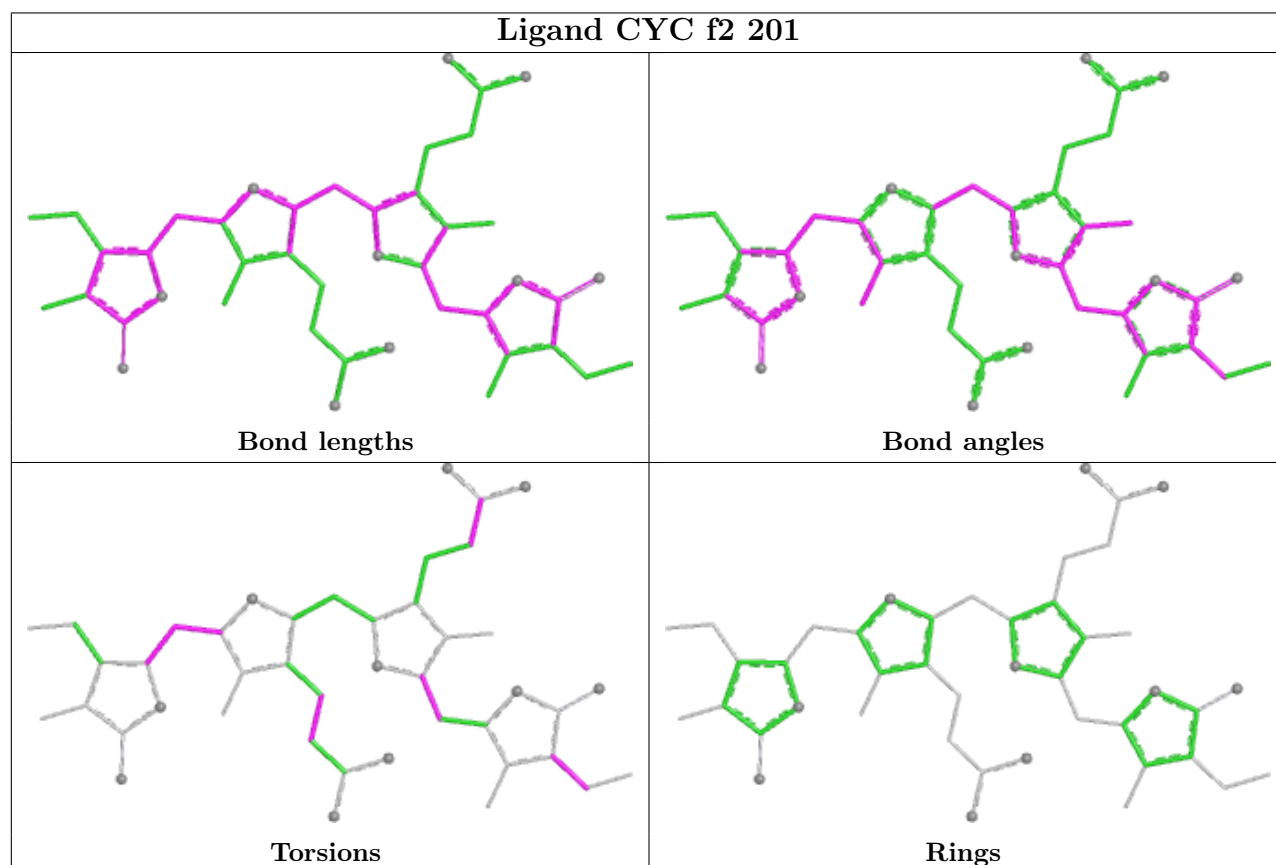
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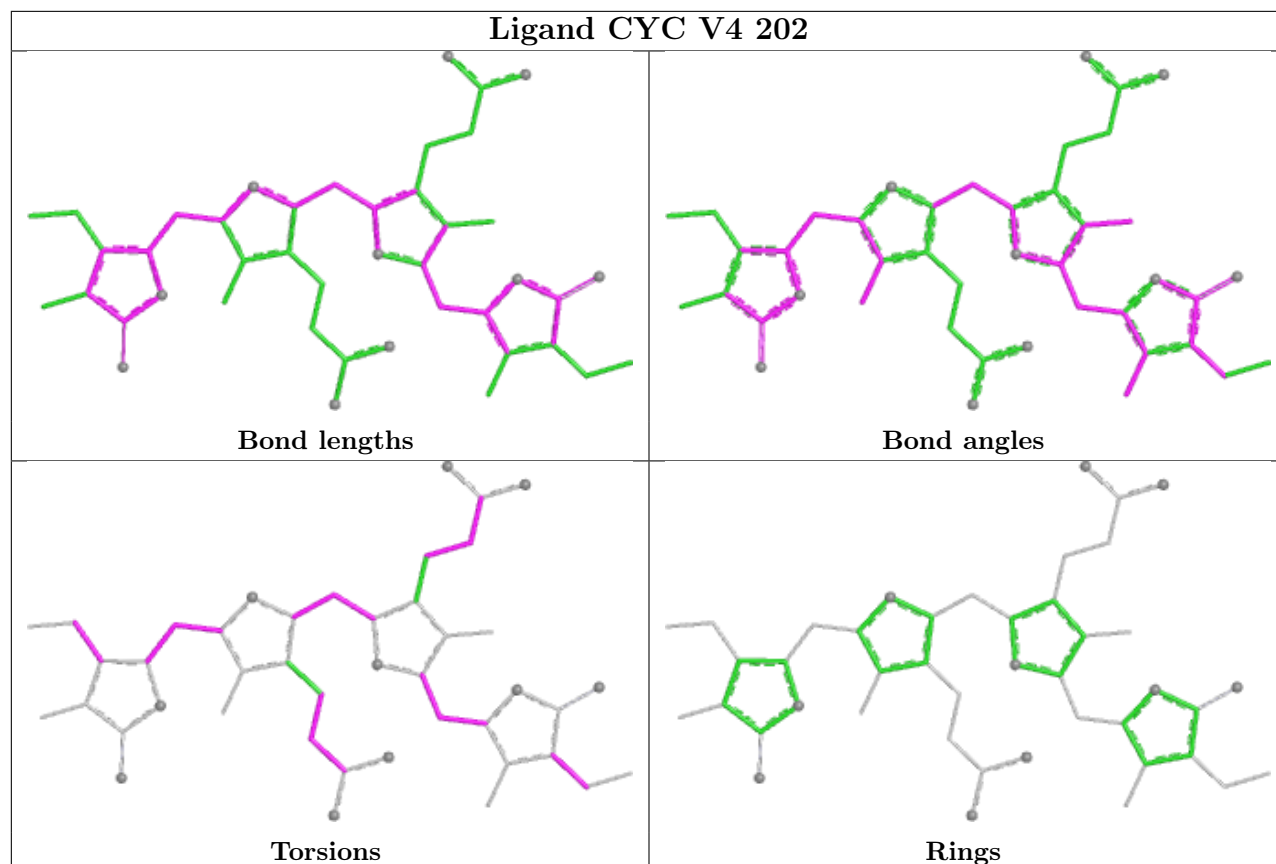
Ligand CYC T3 201



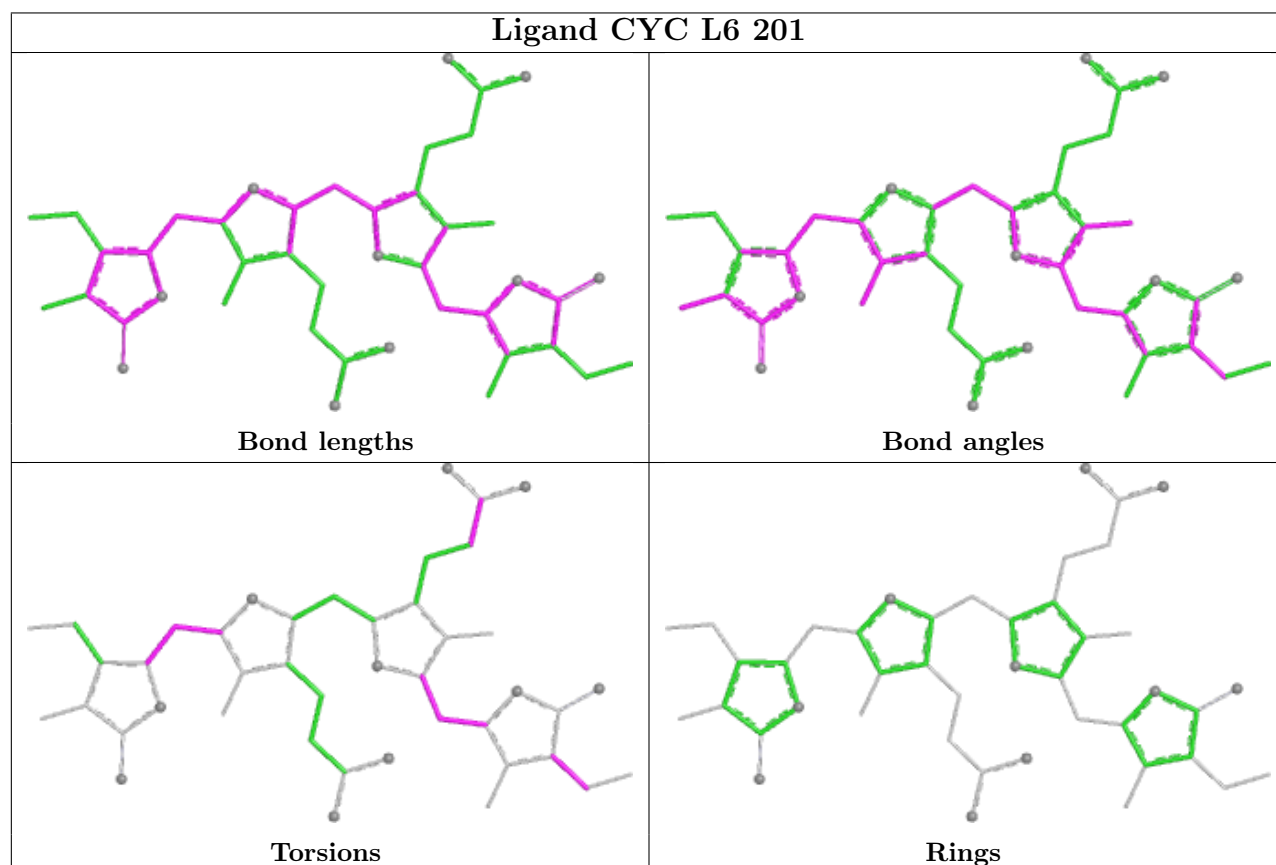
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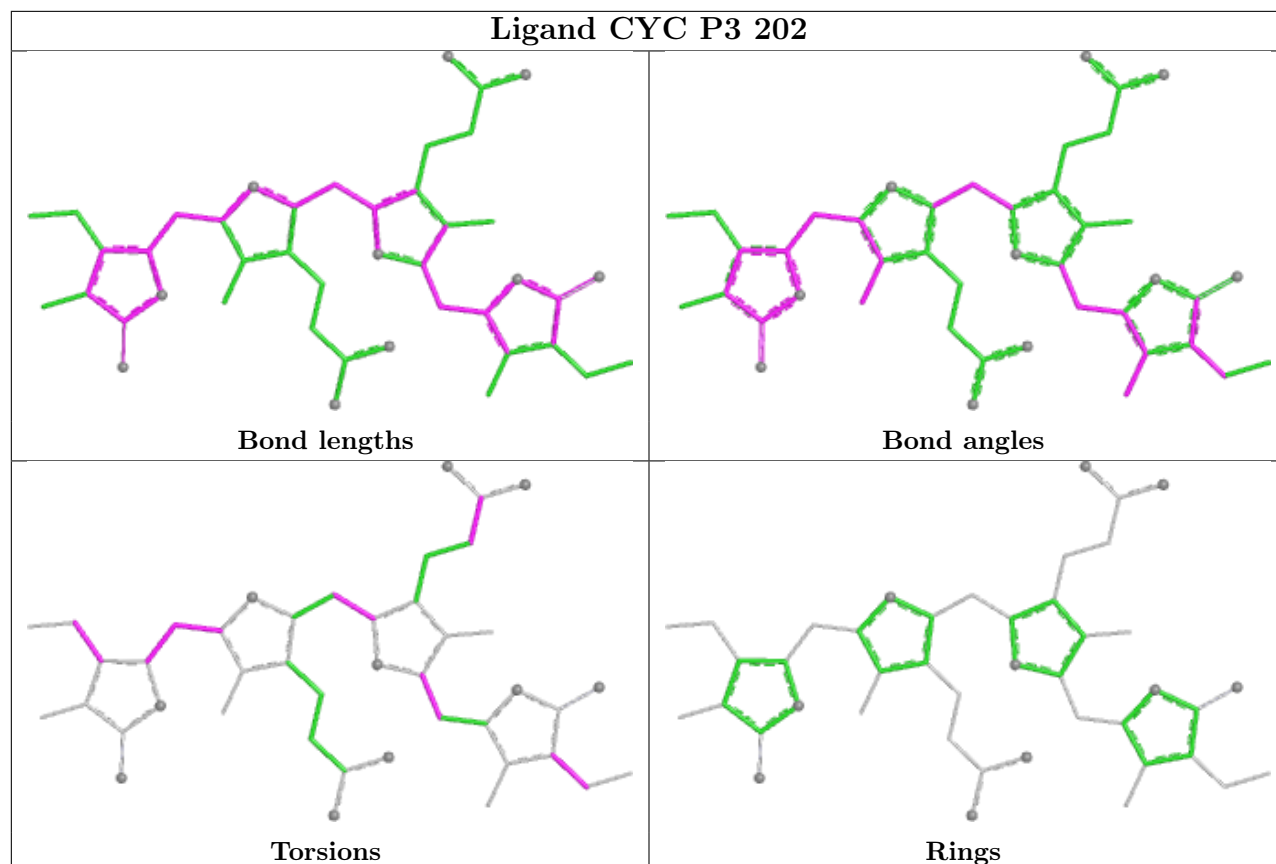
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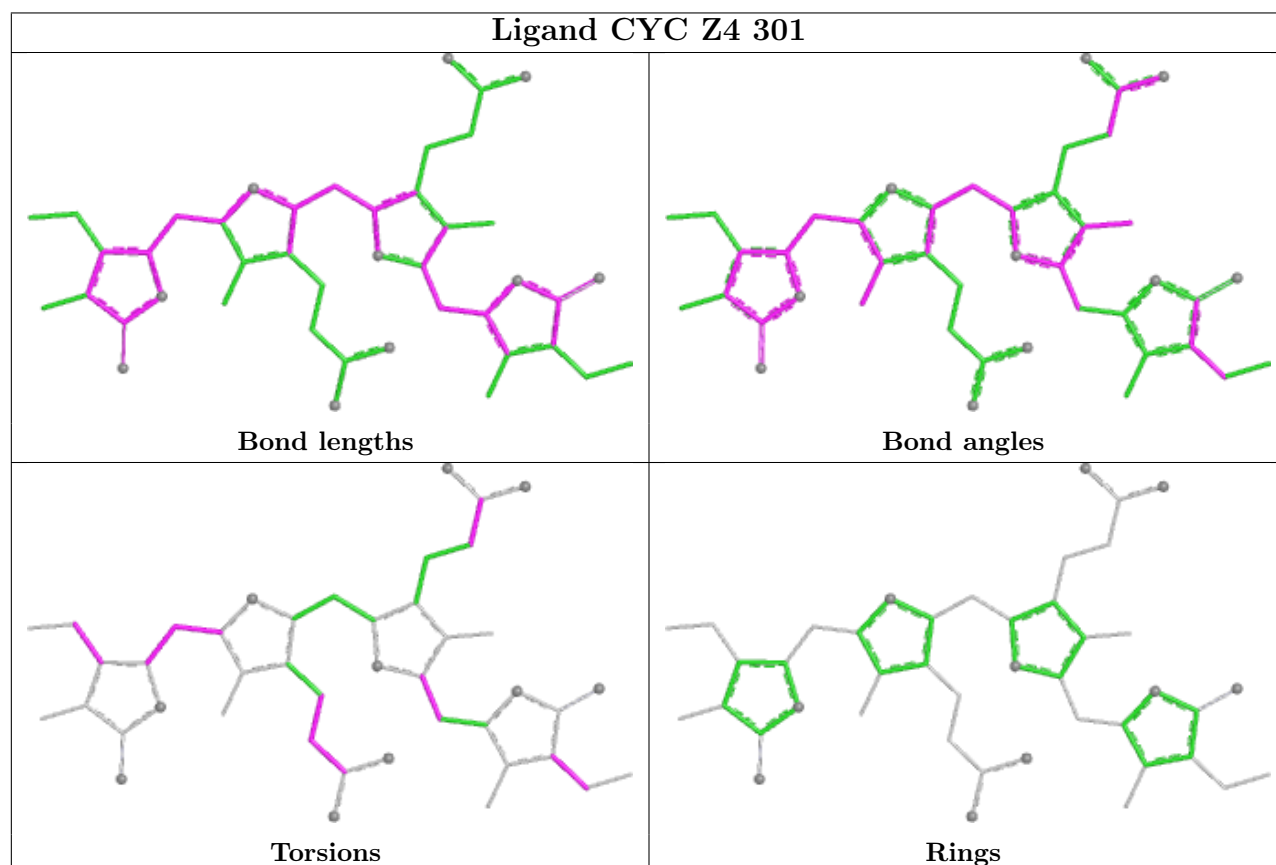
Ligand CYC L6 201

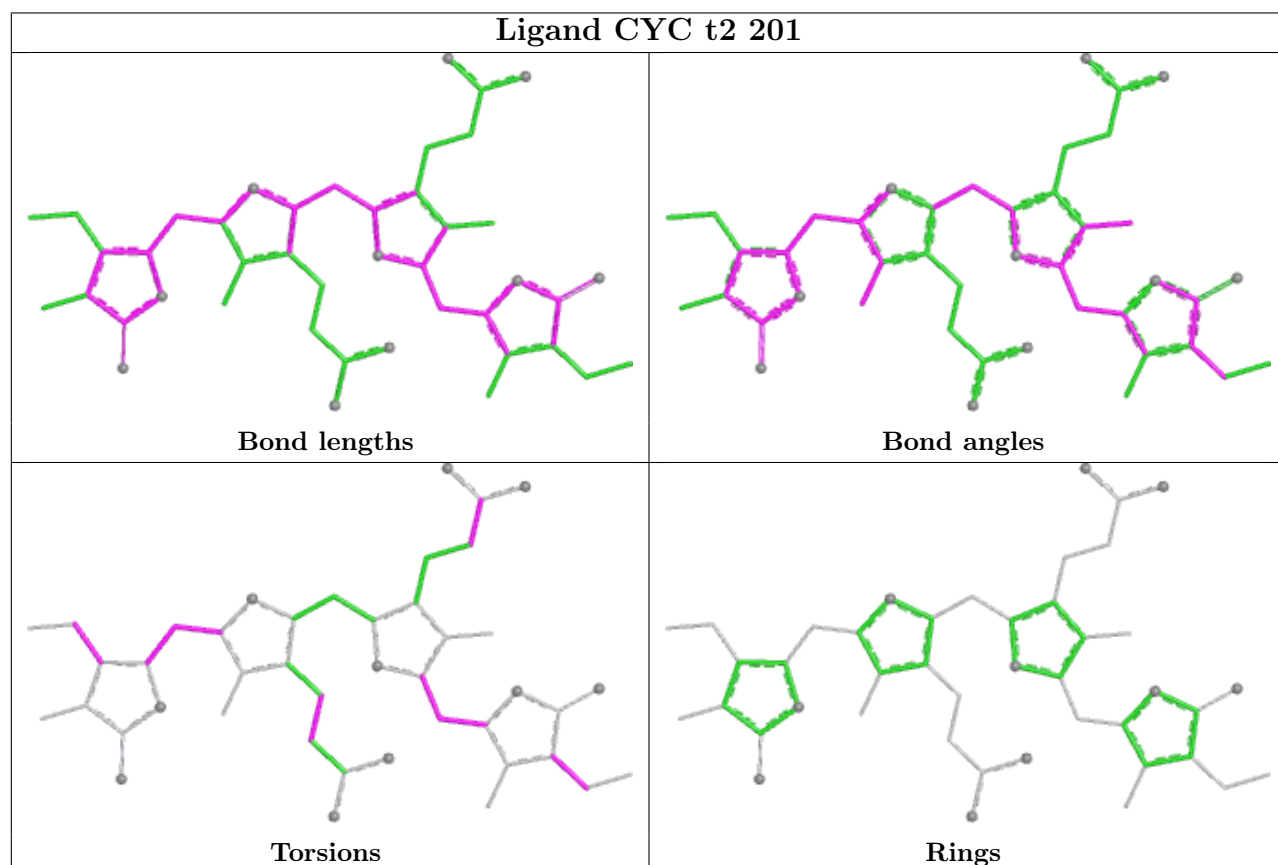
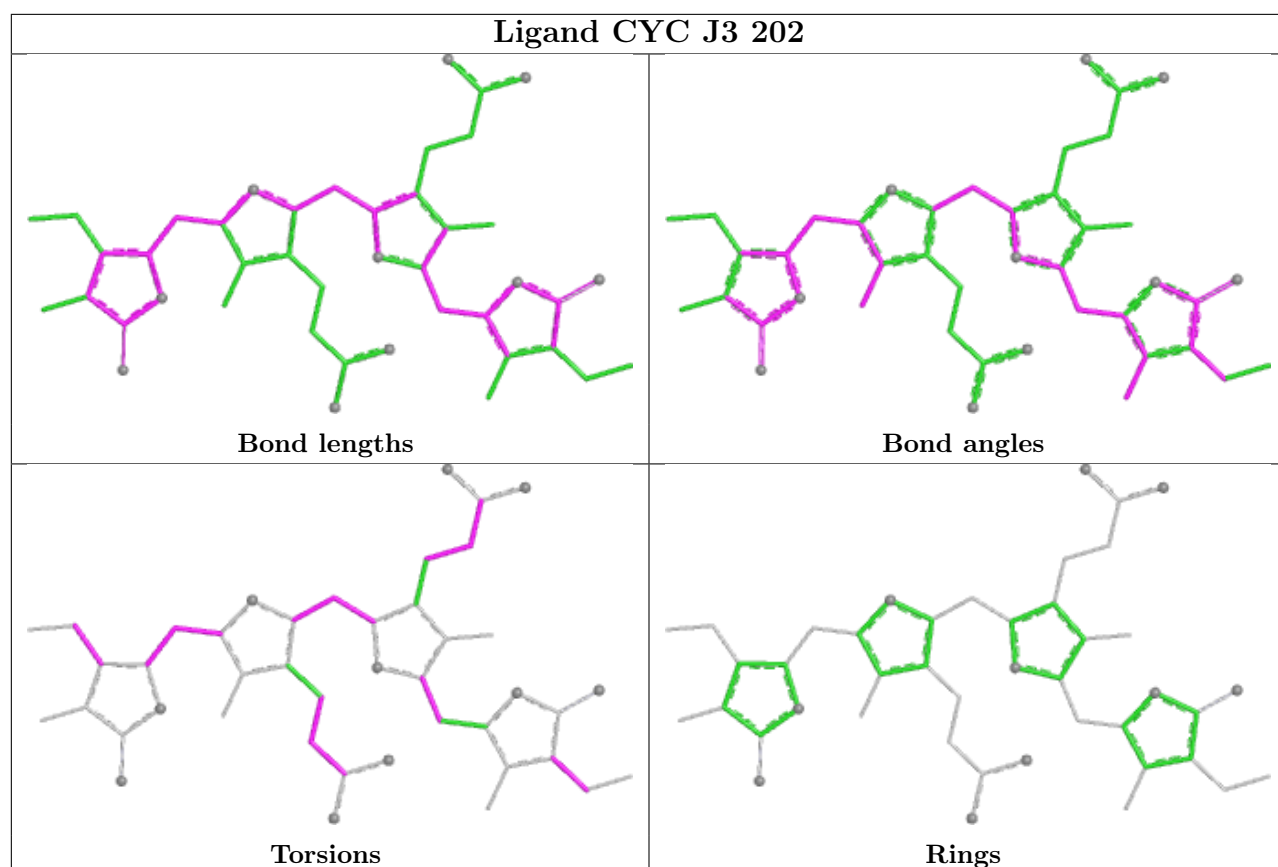


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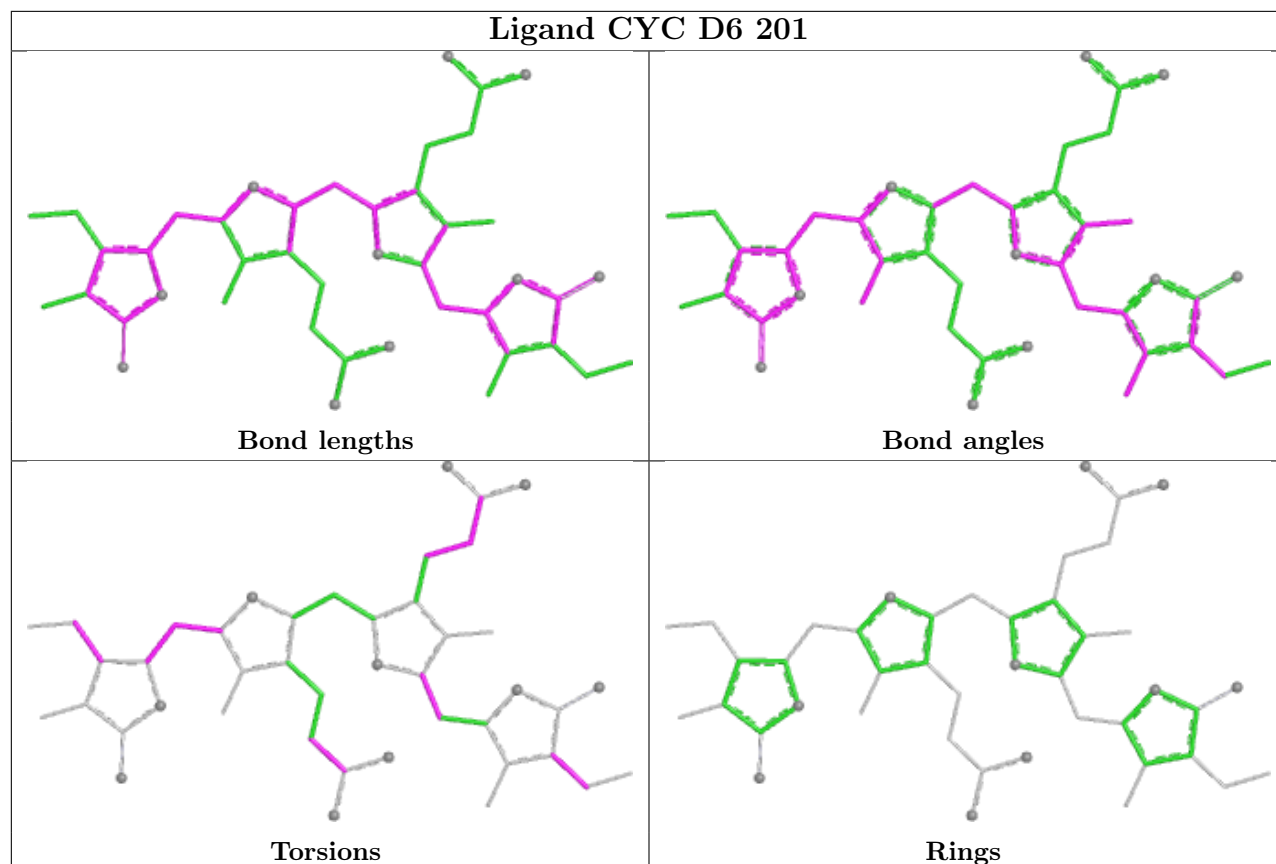


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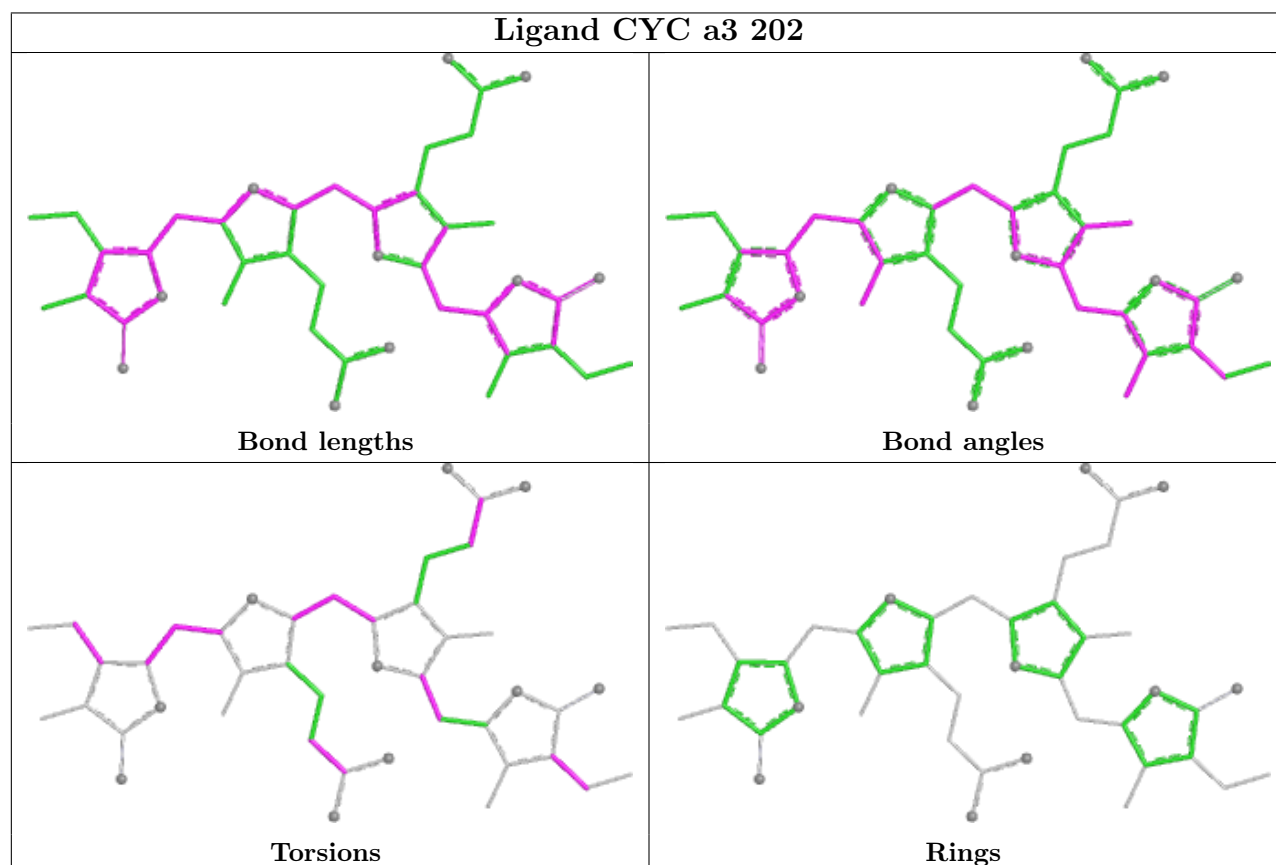




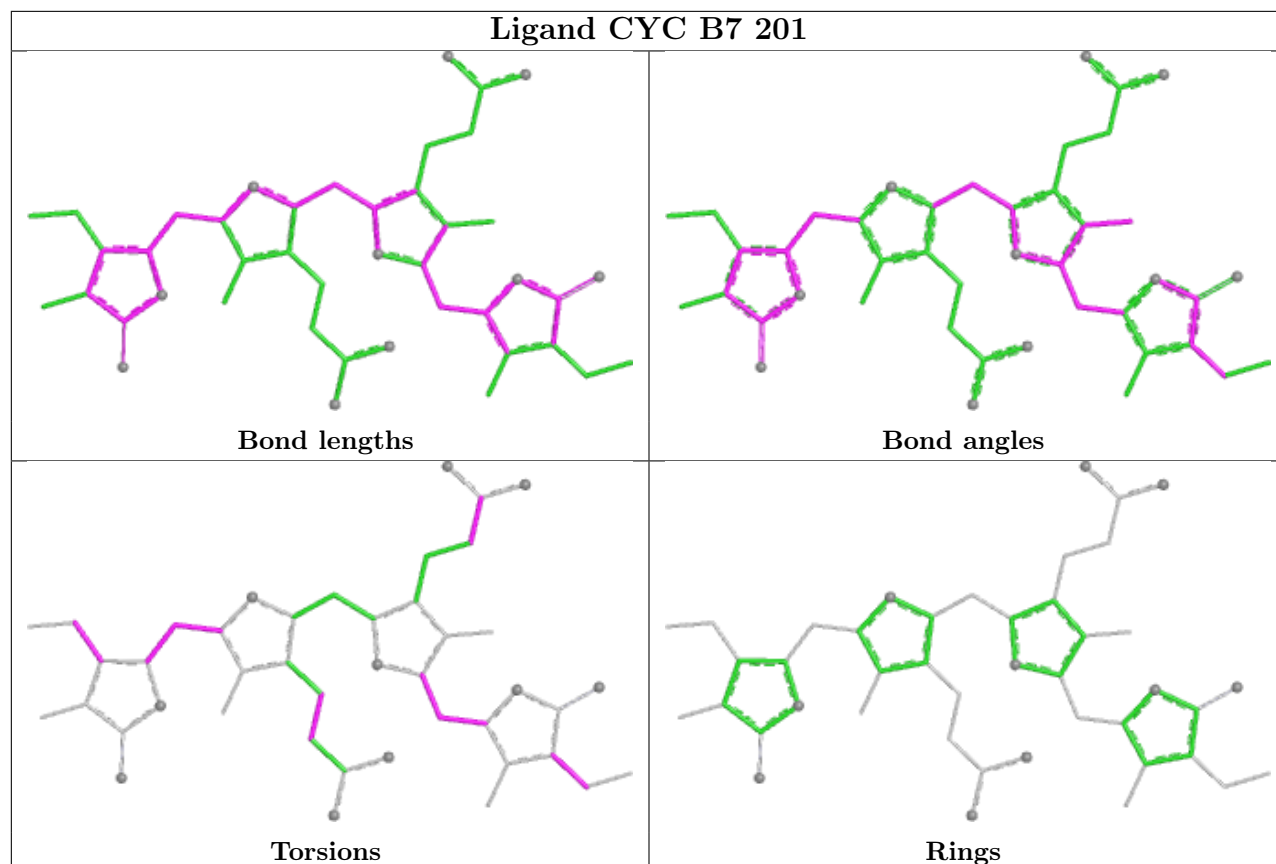
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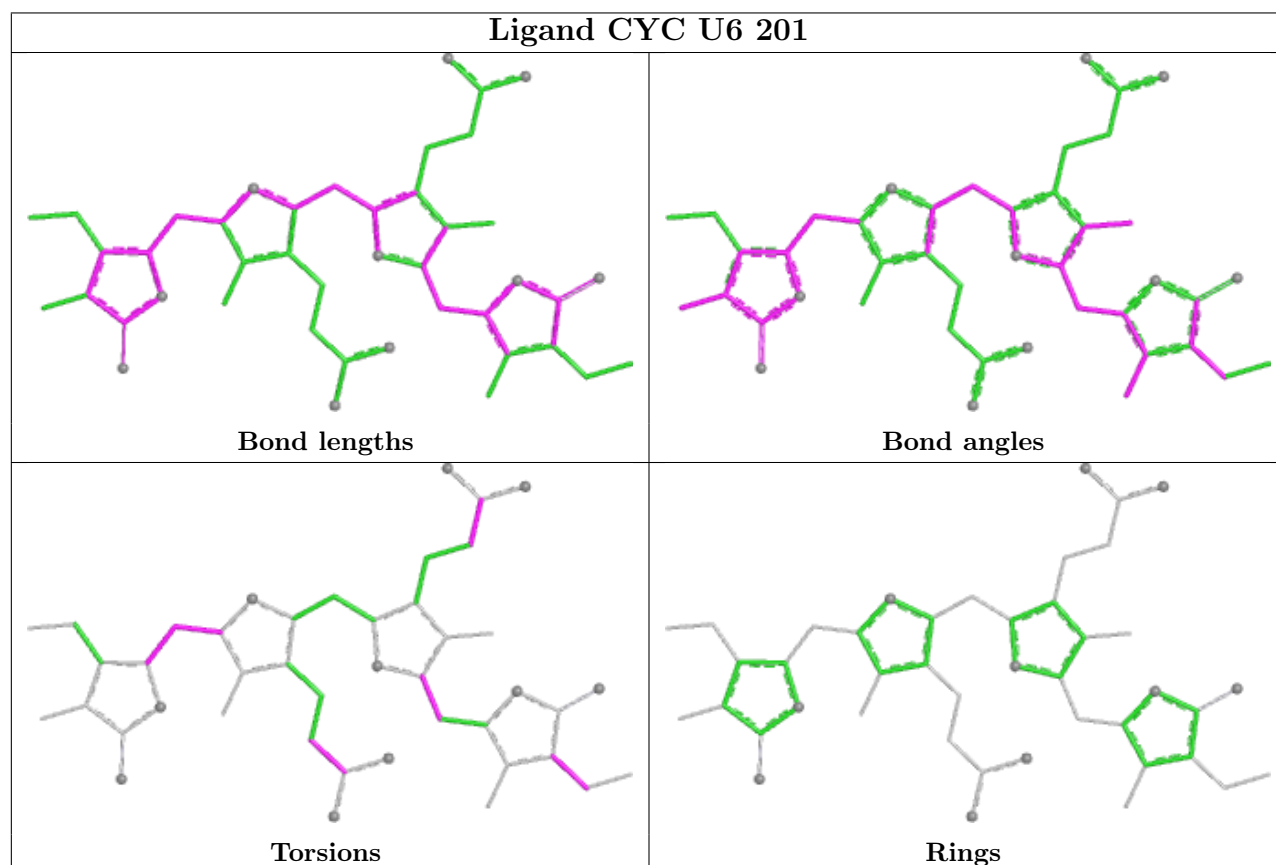
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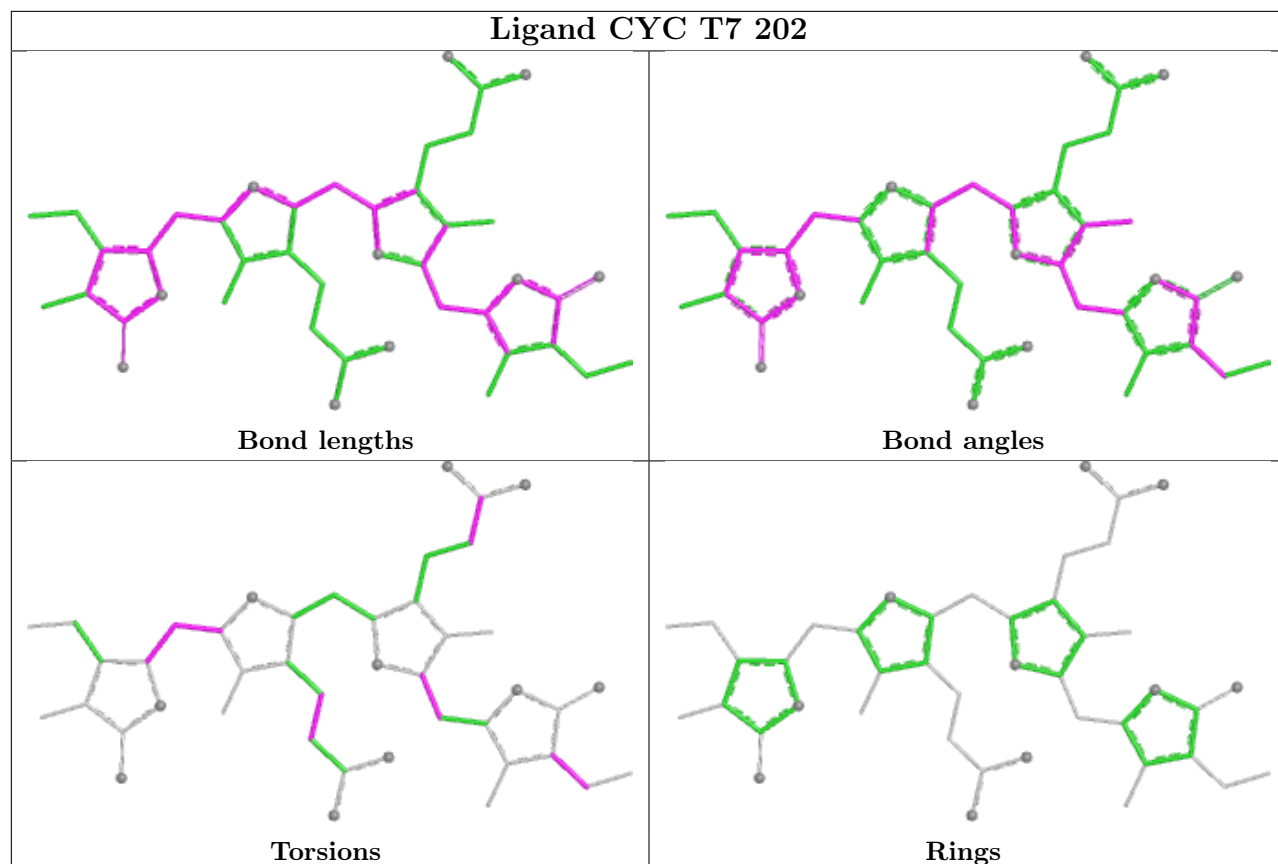
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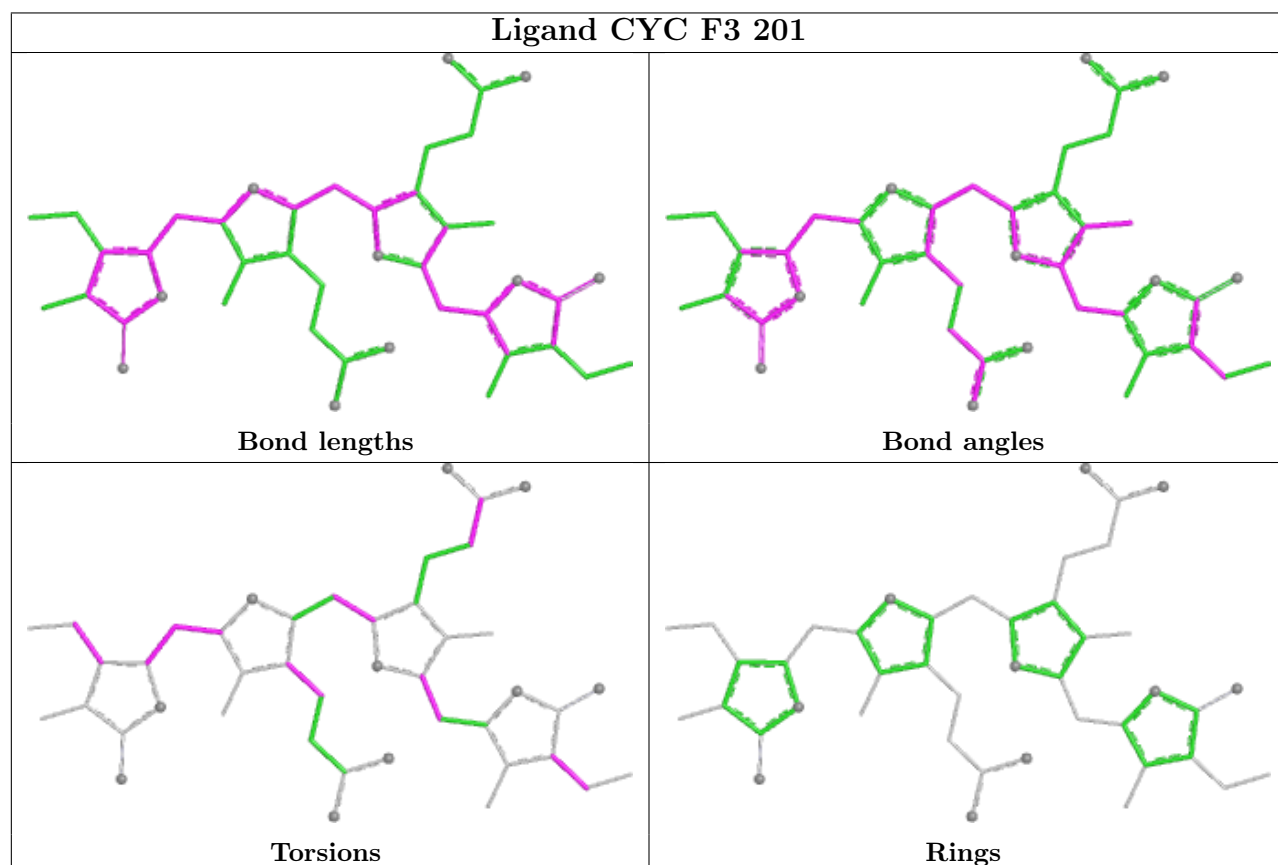
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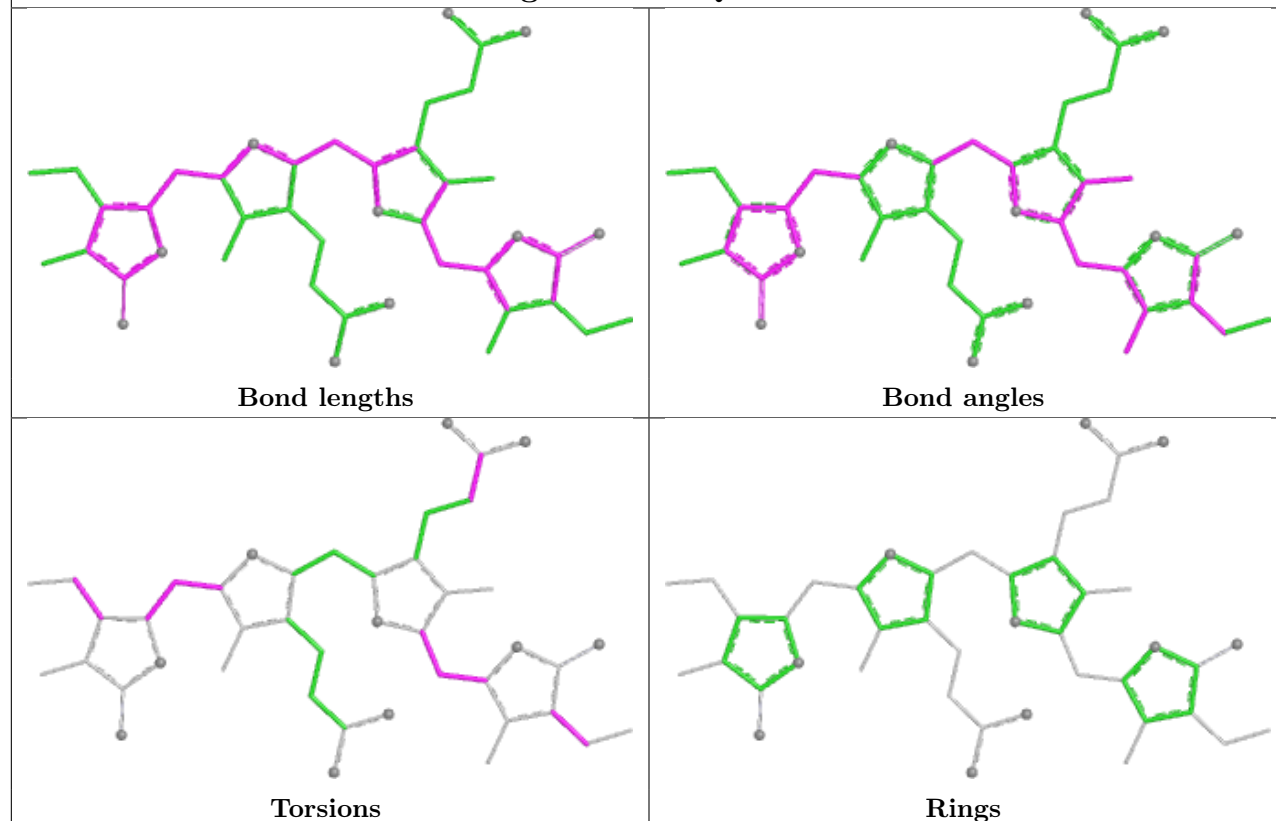
Ligand CYC T7 202



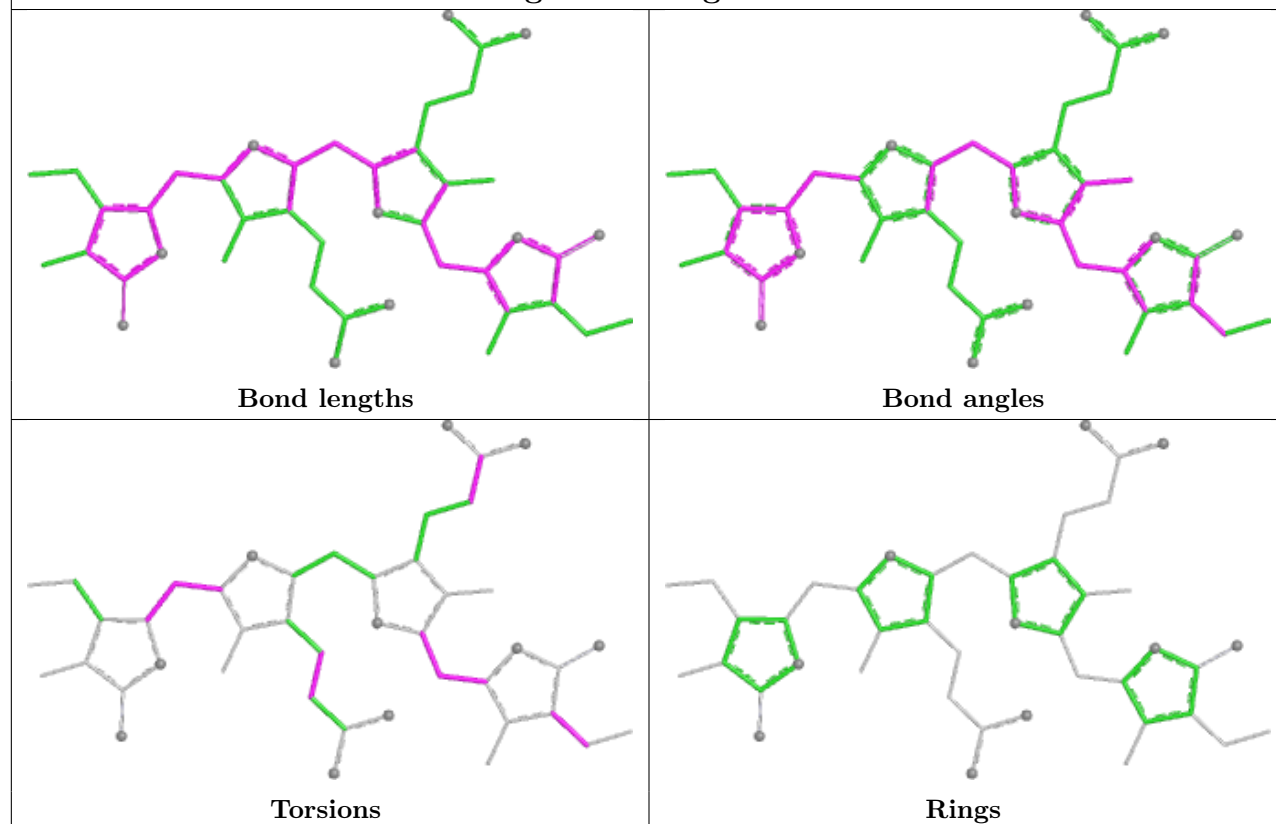
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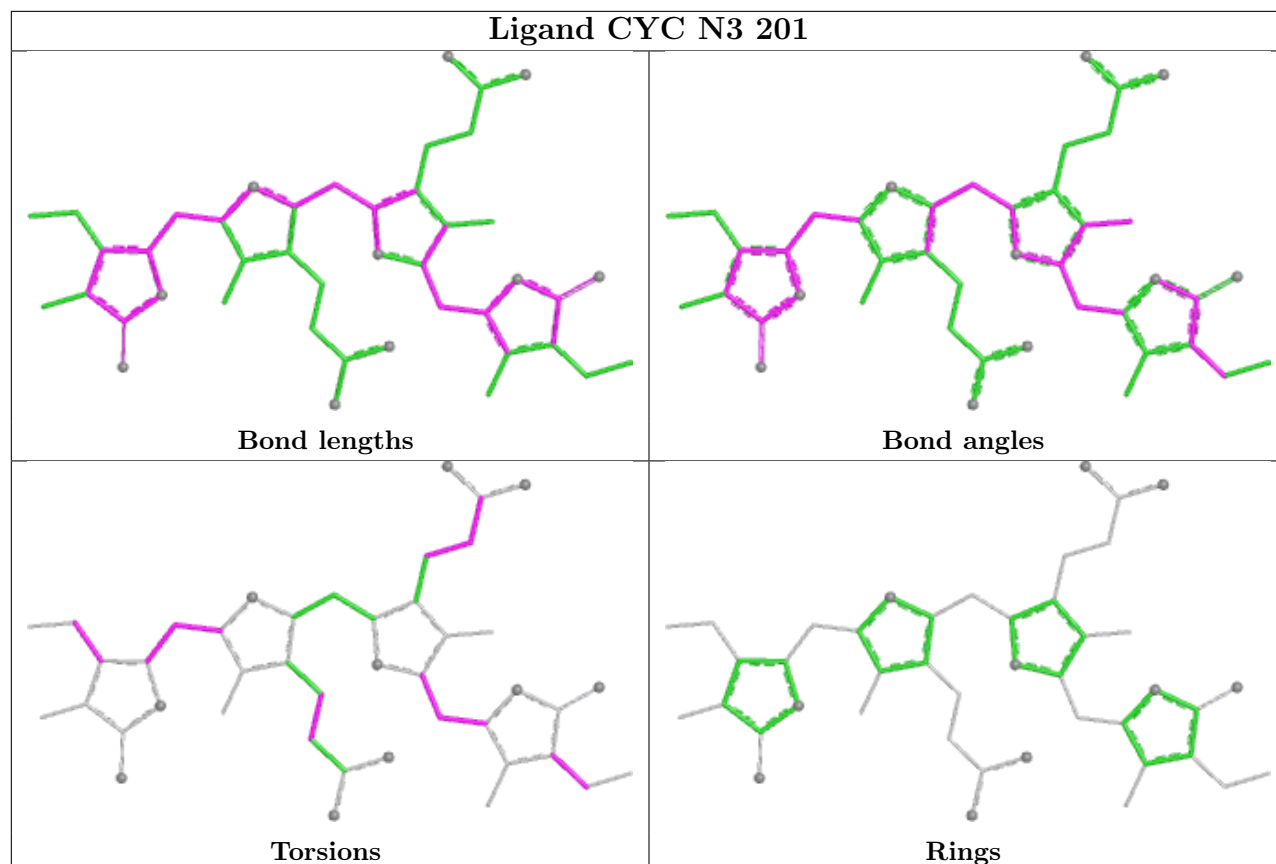
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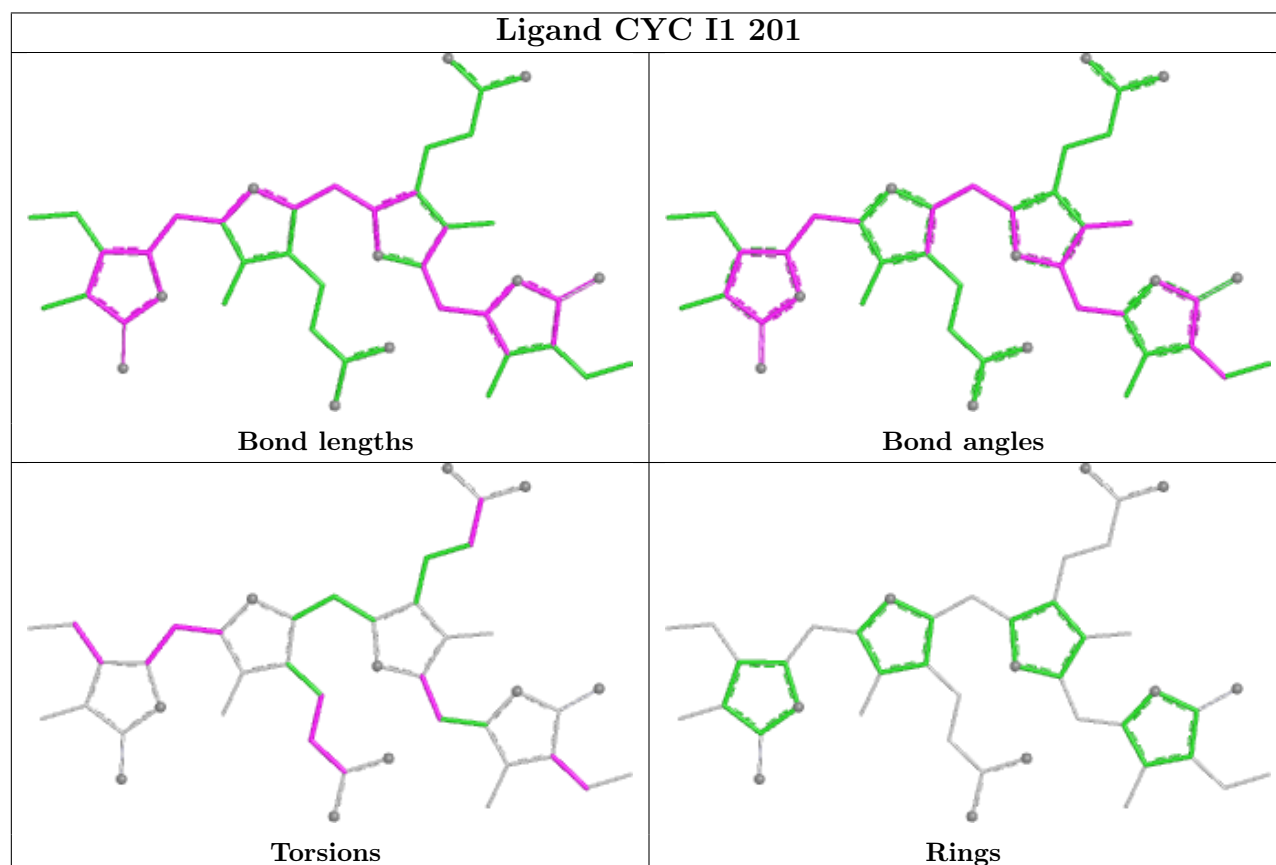
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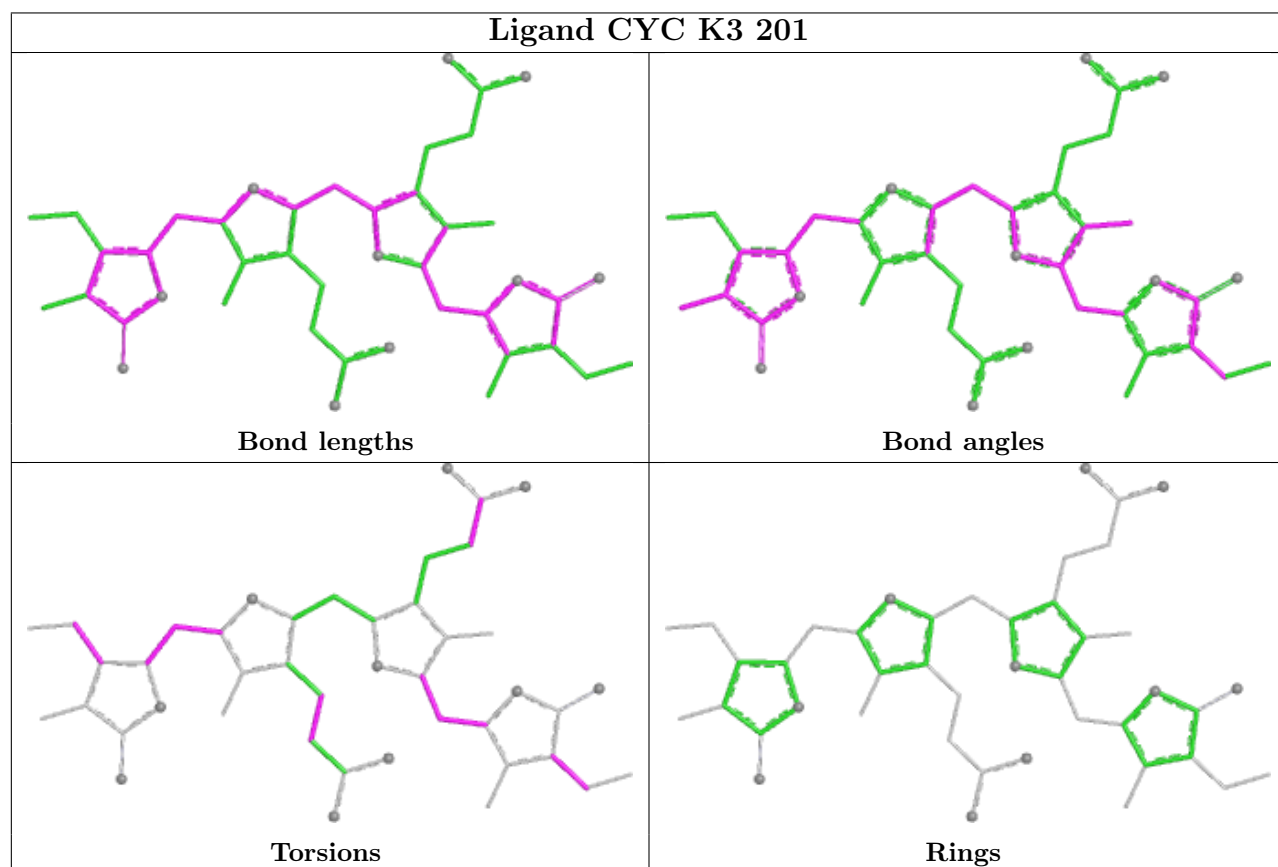
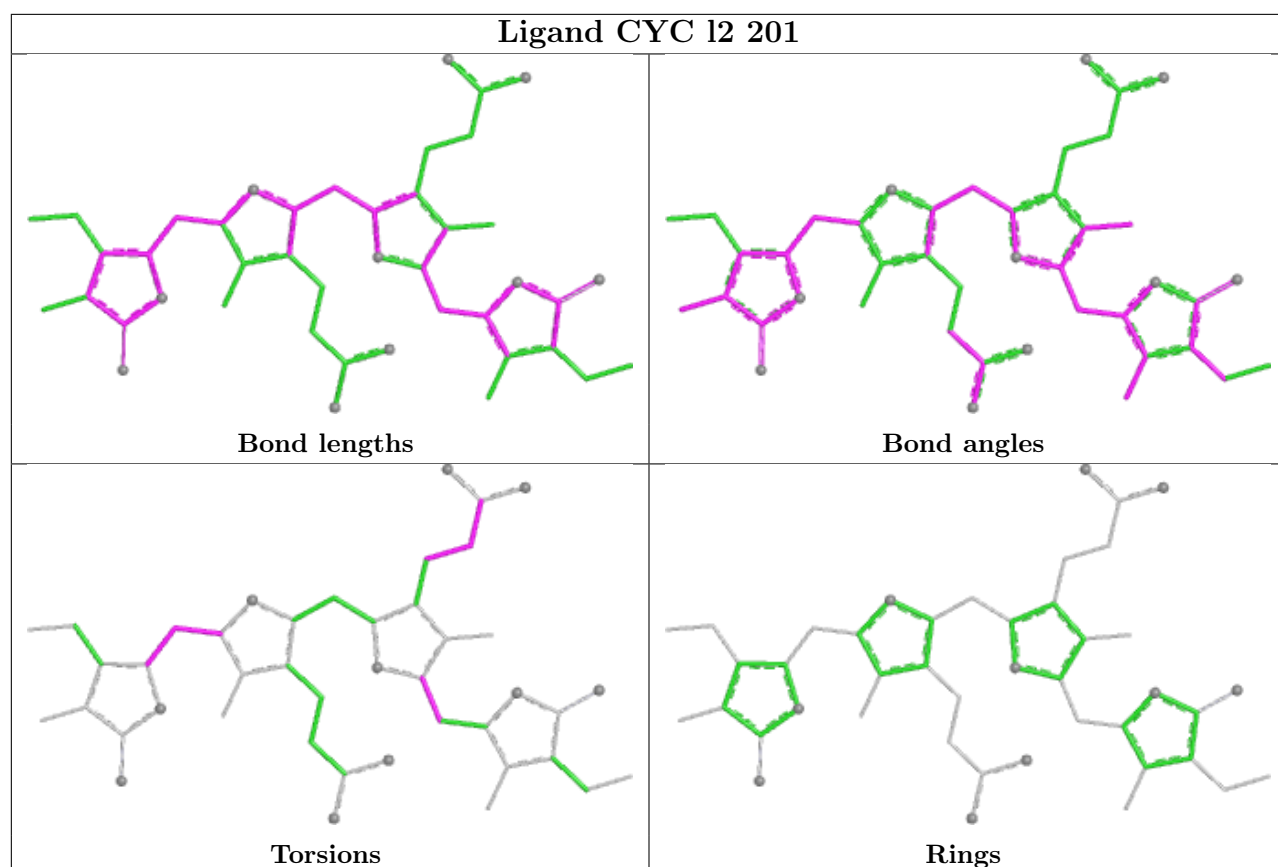


Ligand CYC N3 201

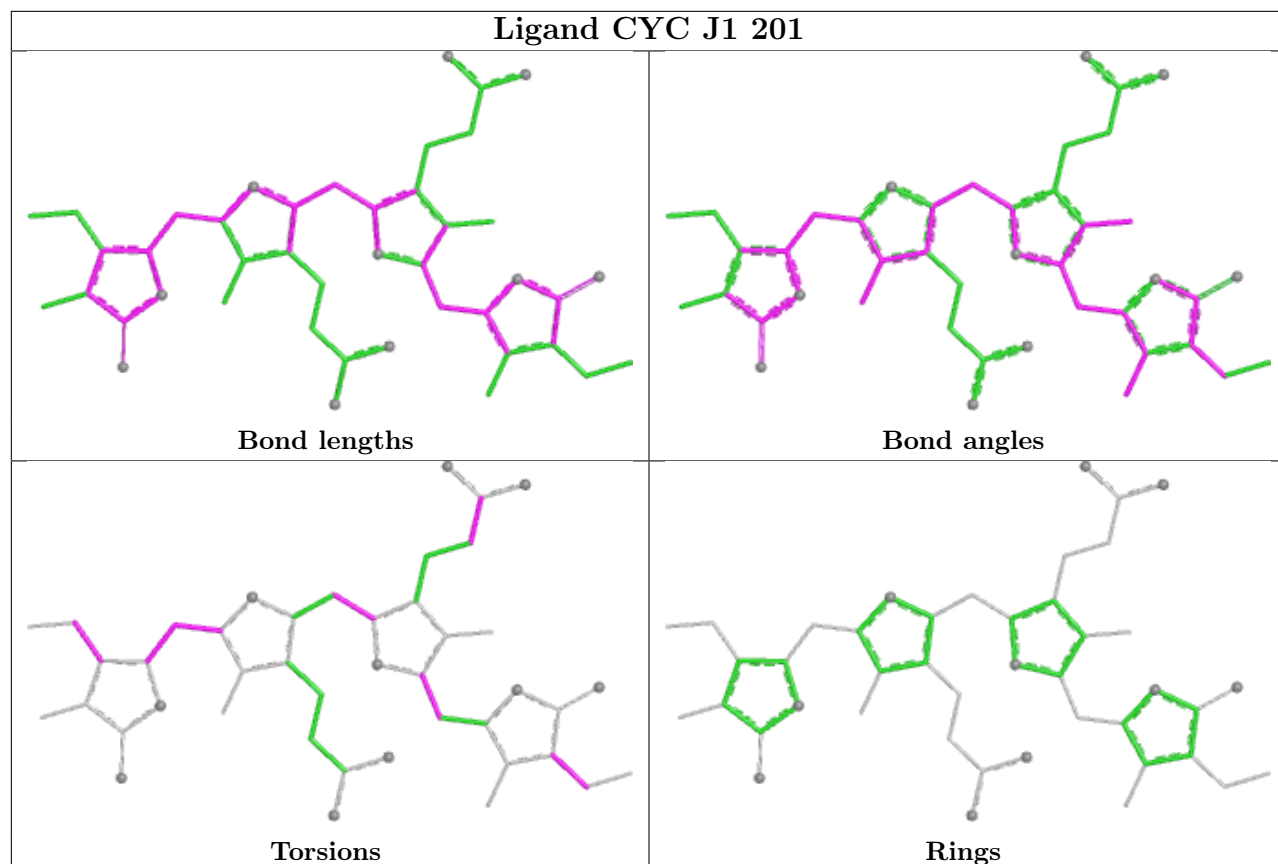


Ligand CYC I1 201

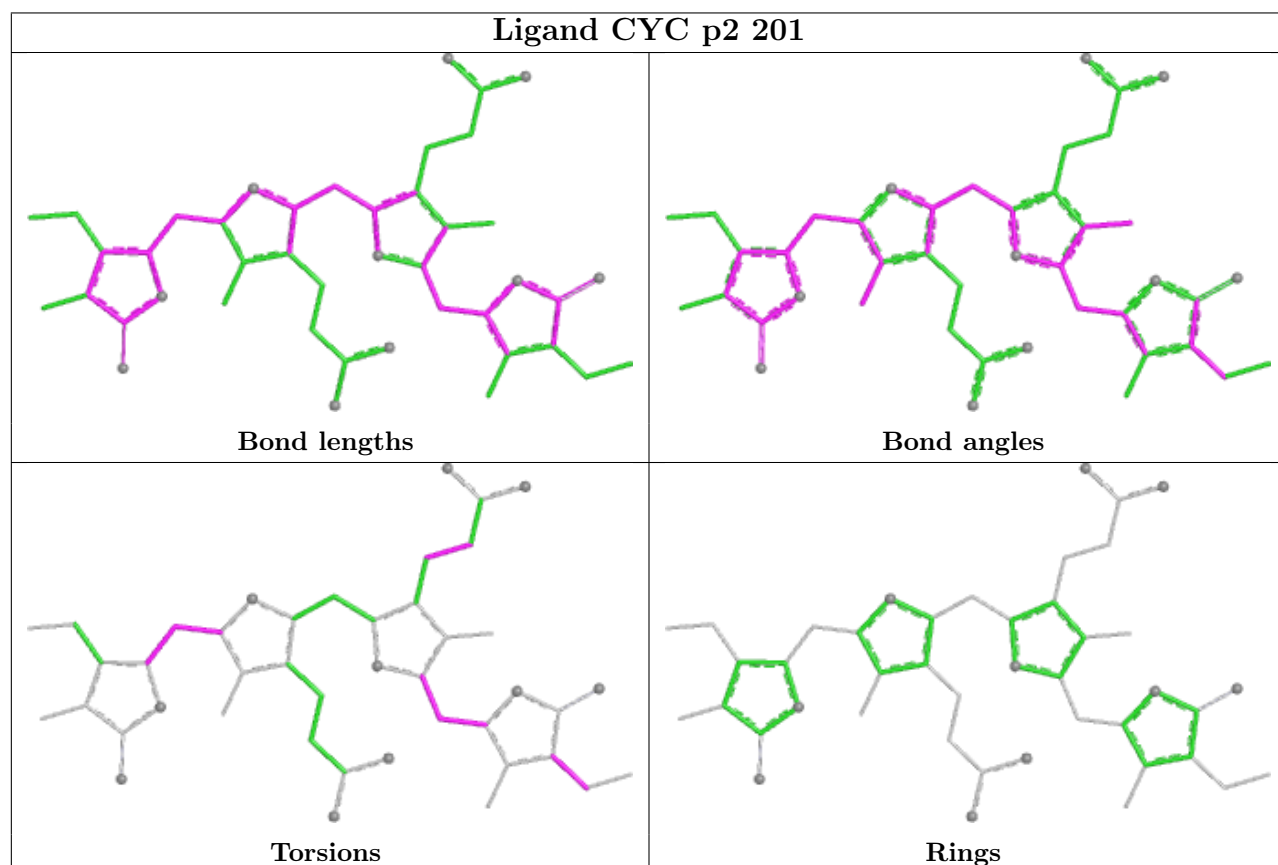




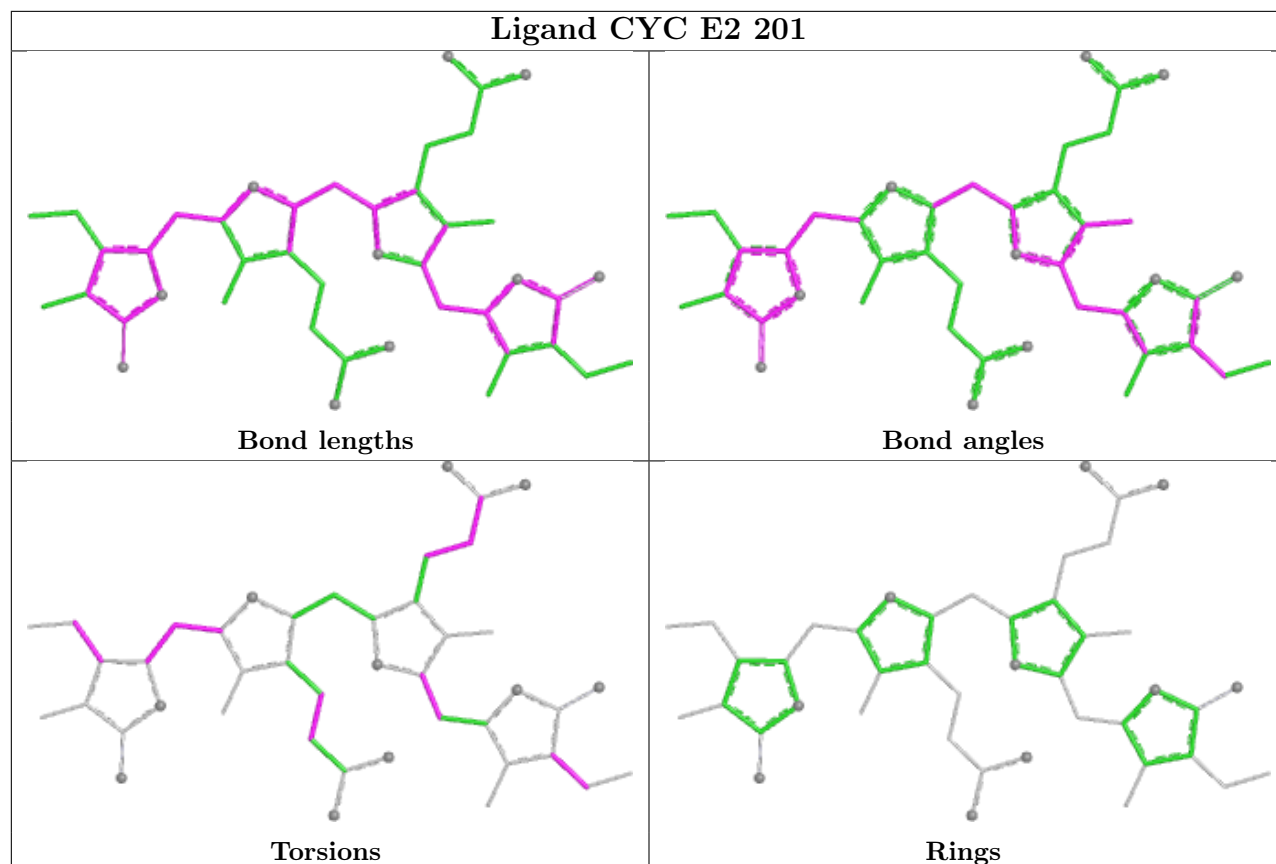
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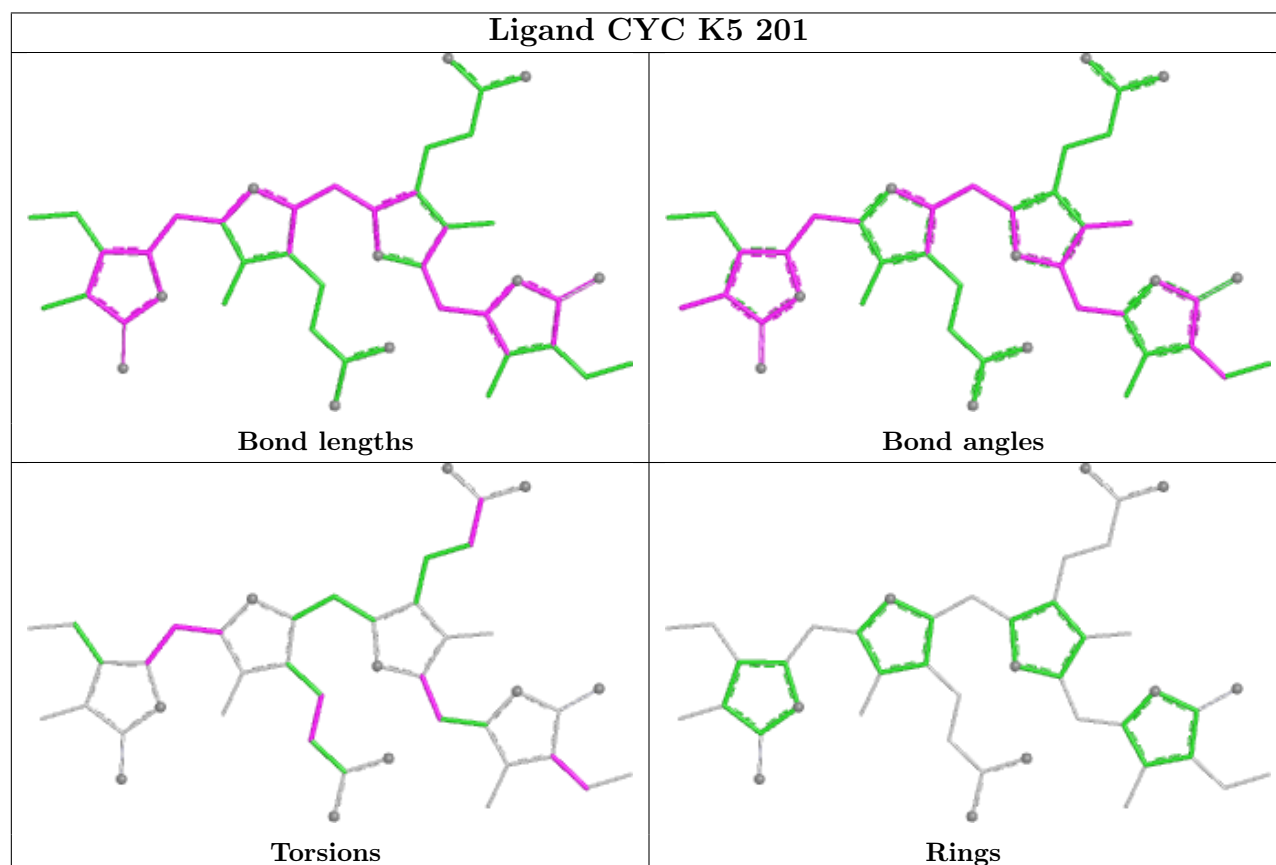
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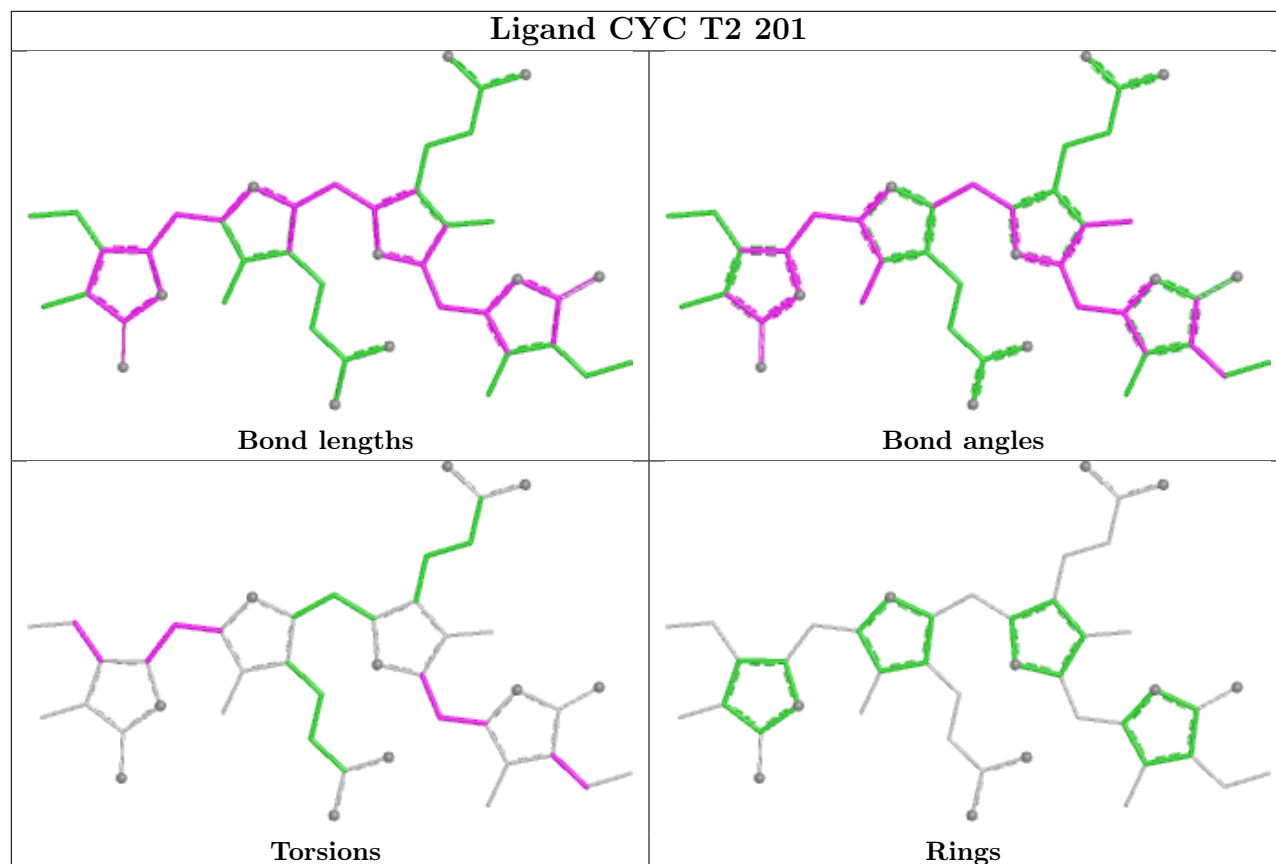
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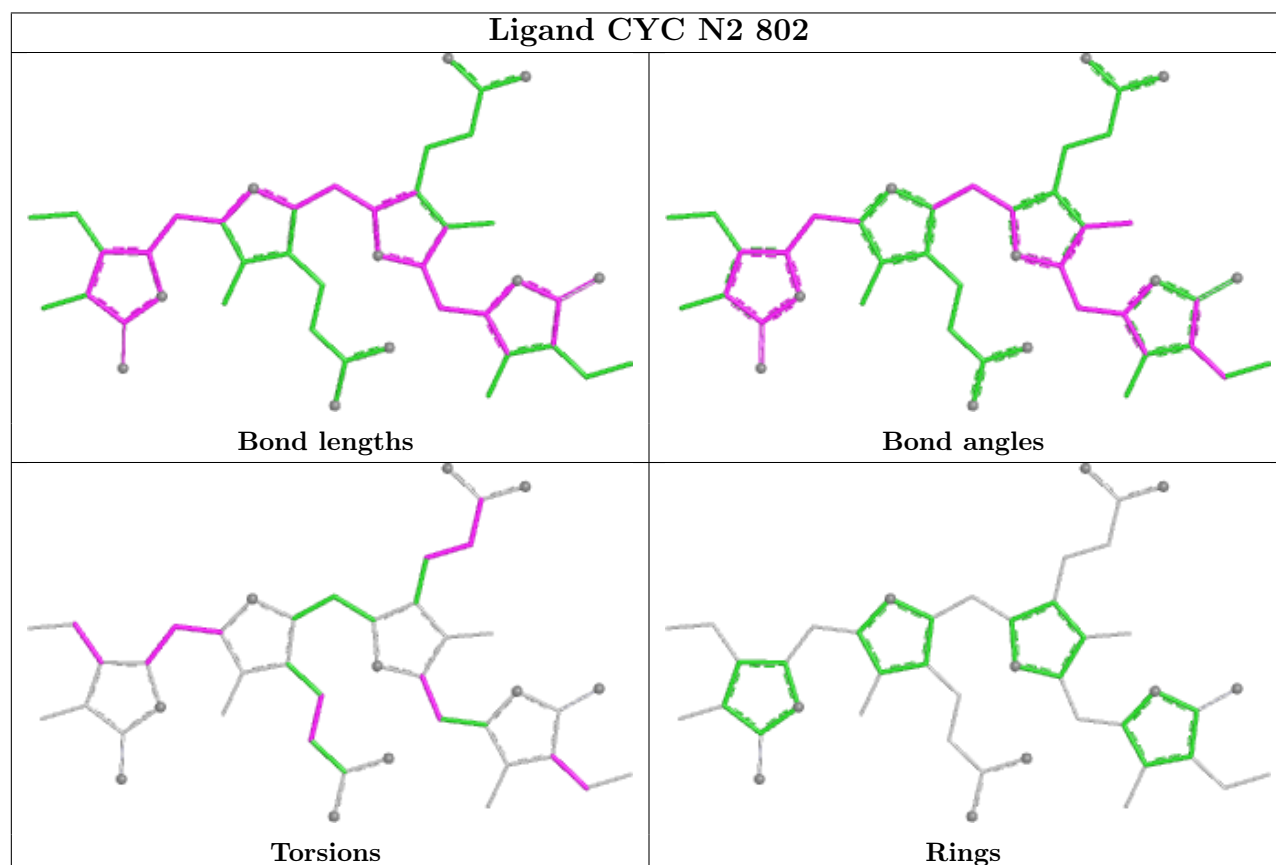
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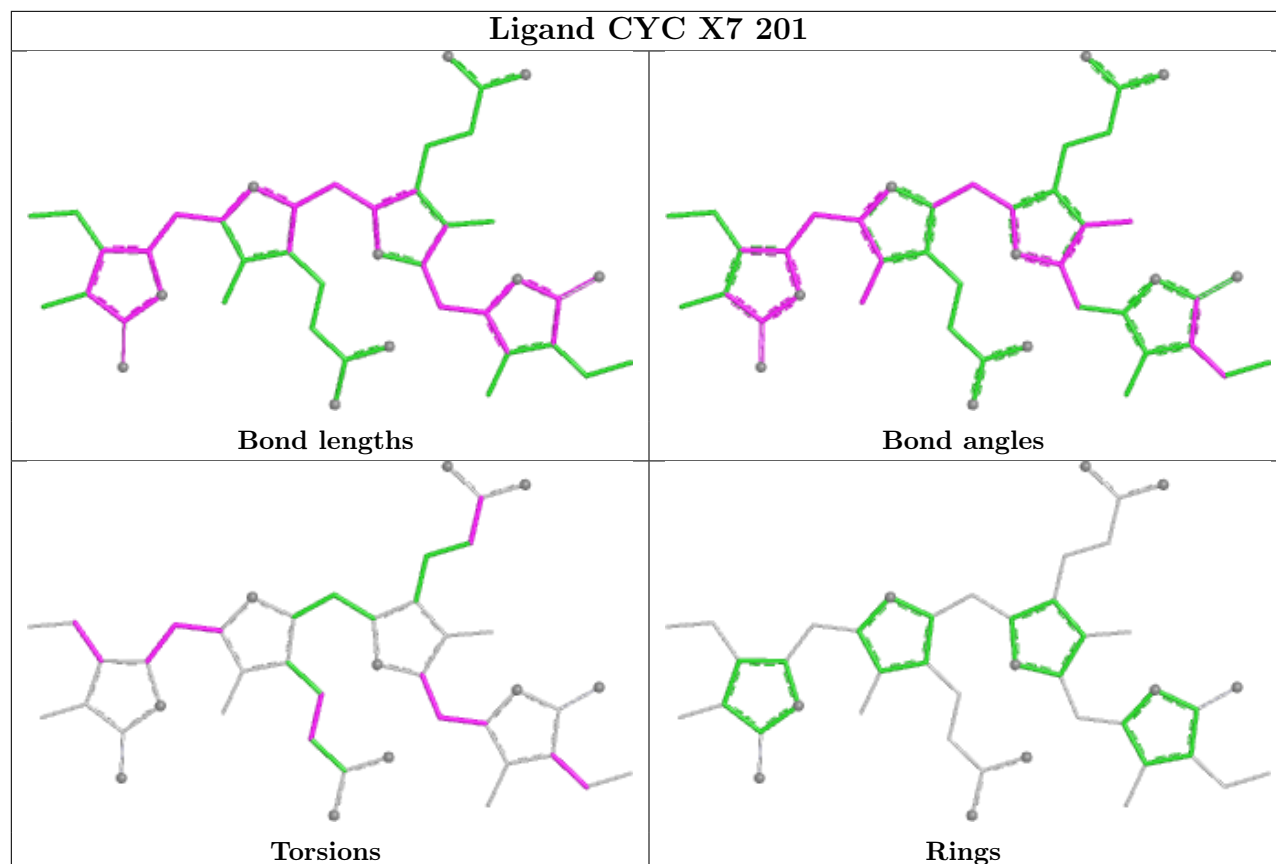
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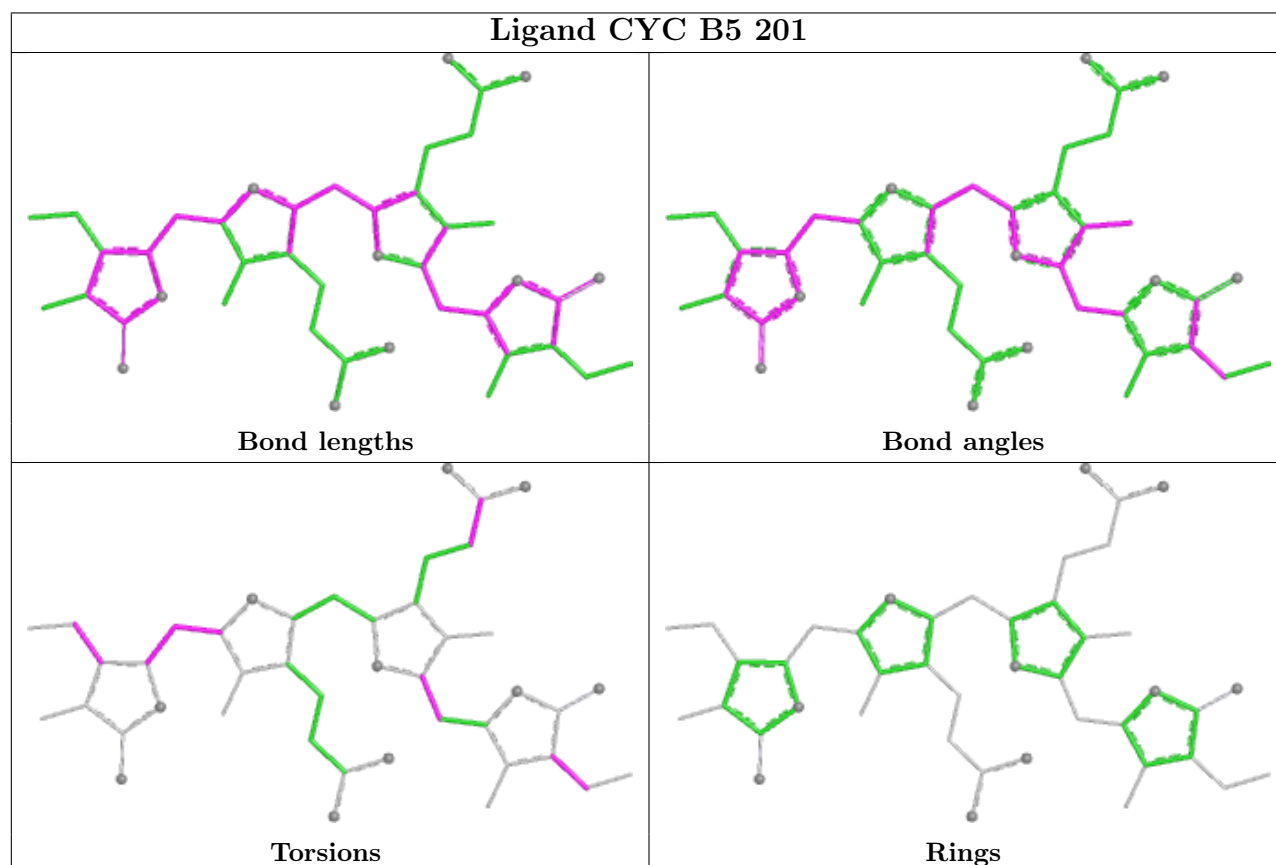
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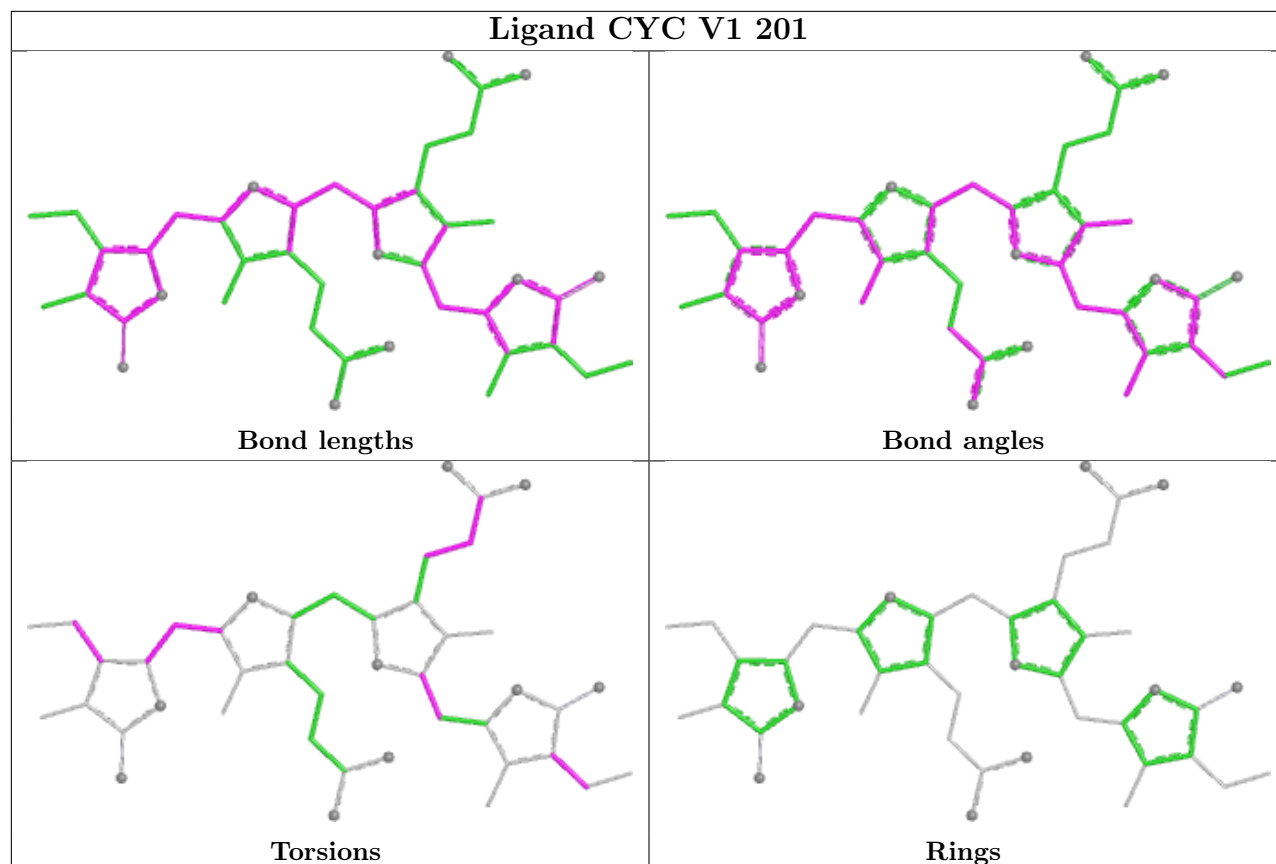
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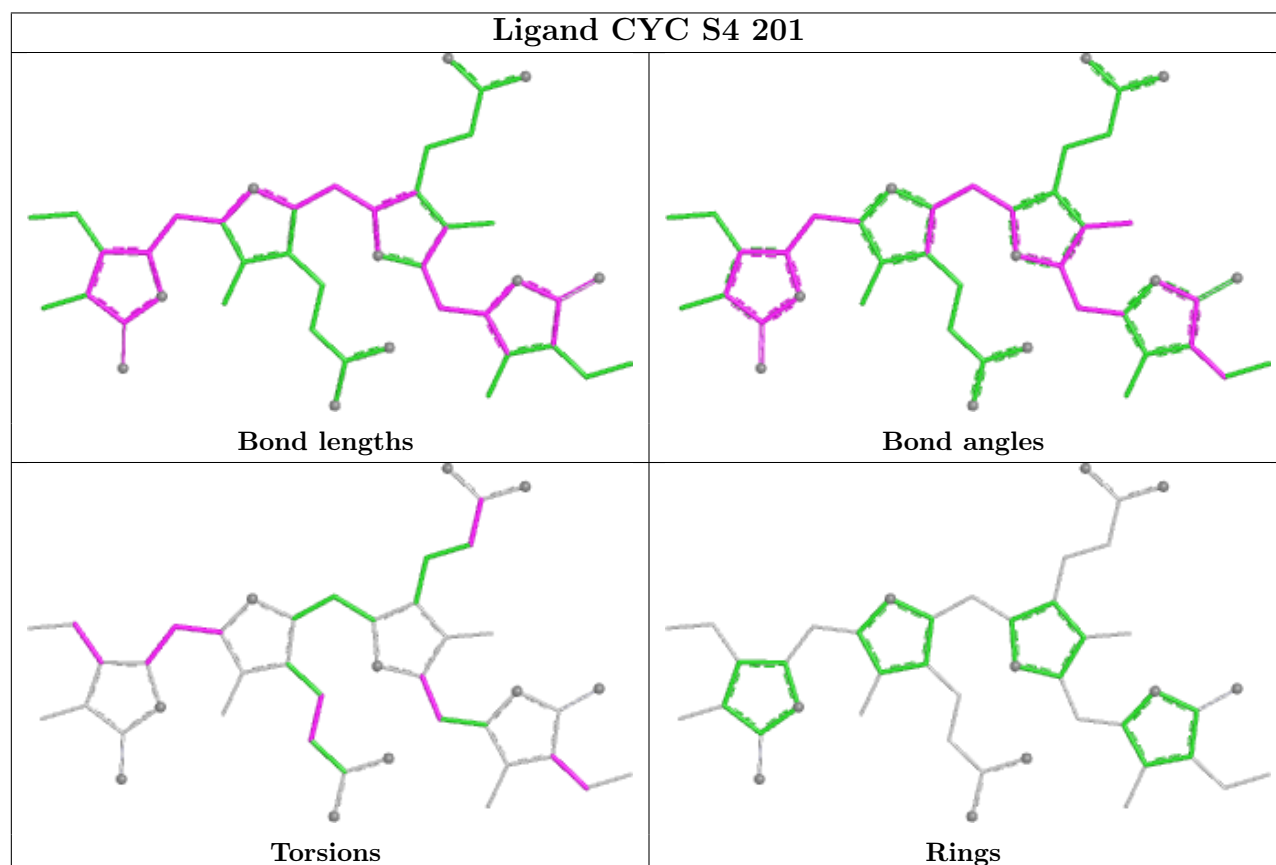
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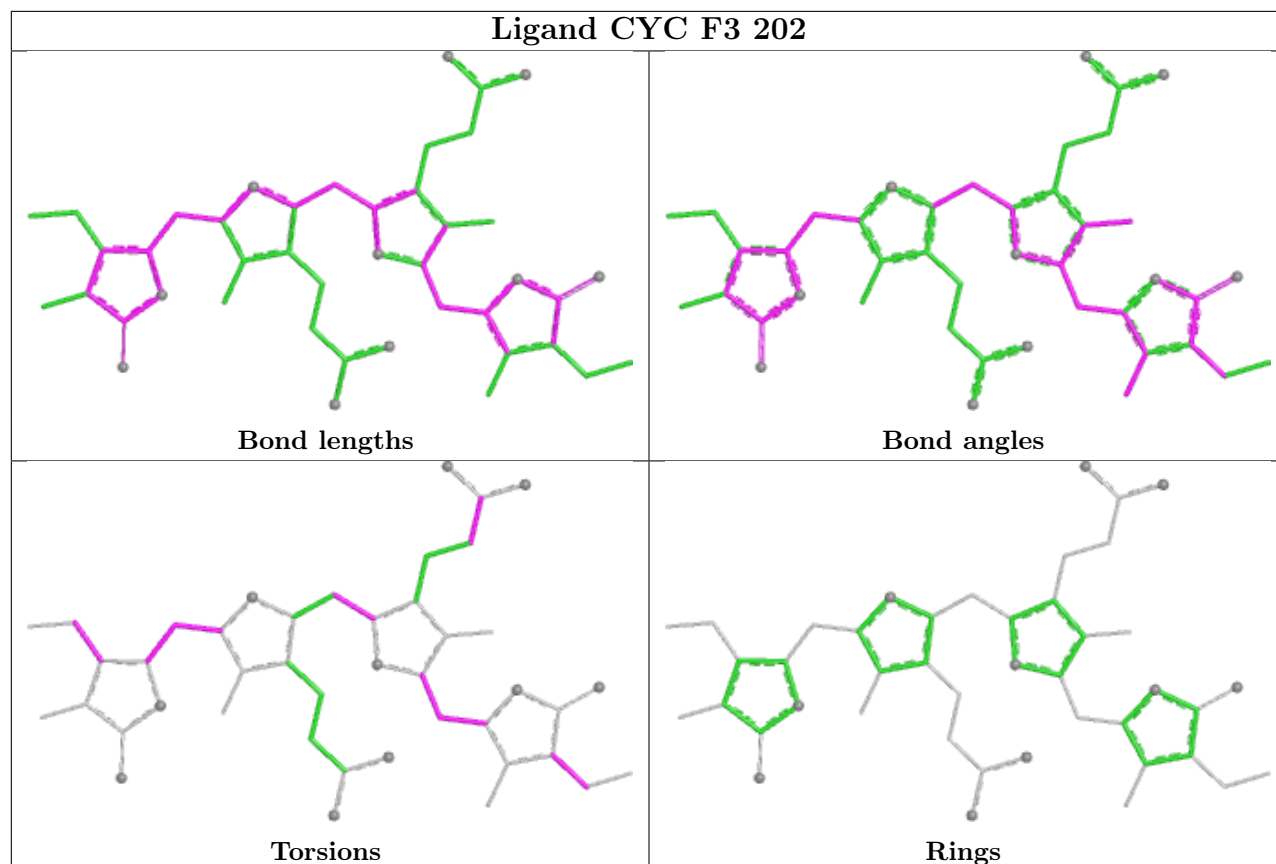
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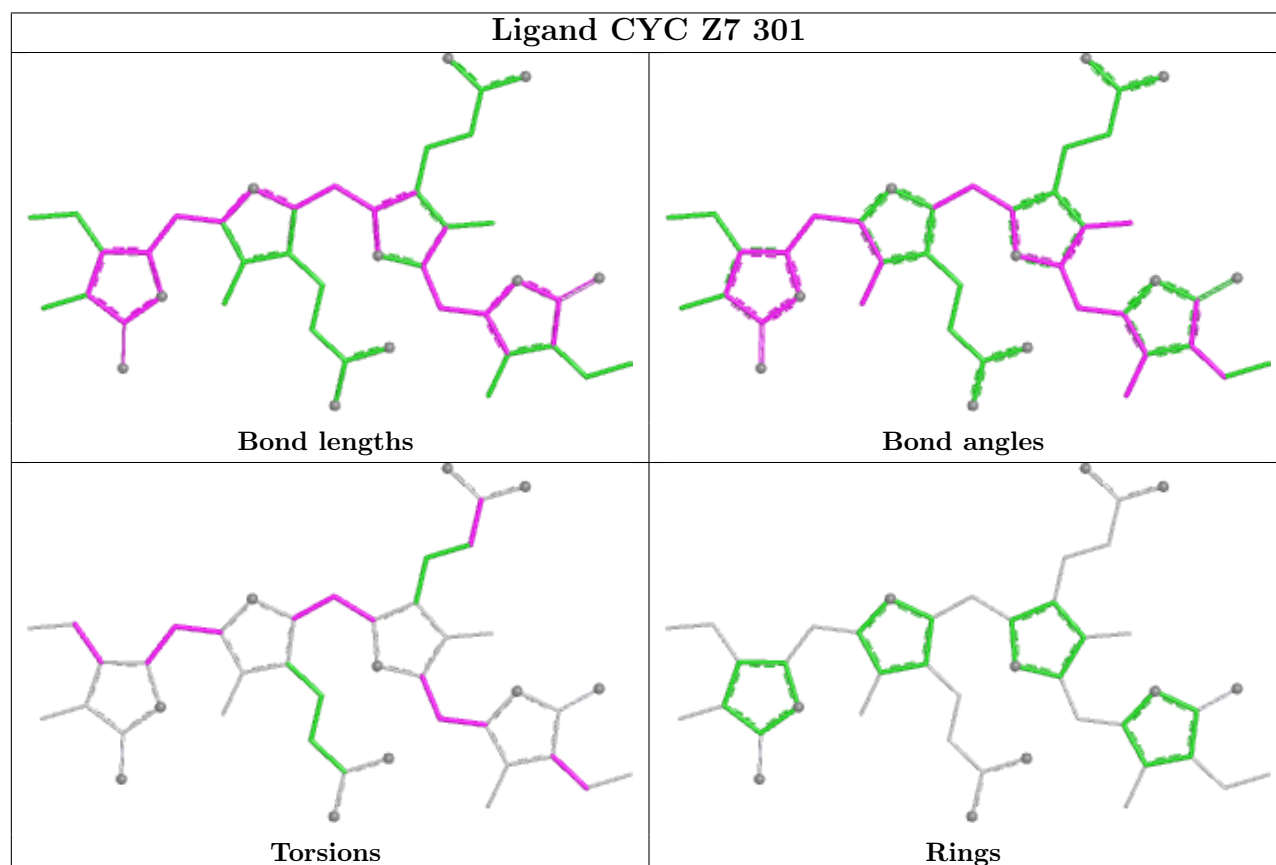
Ligand CYC S4 201

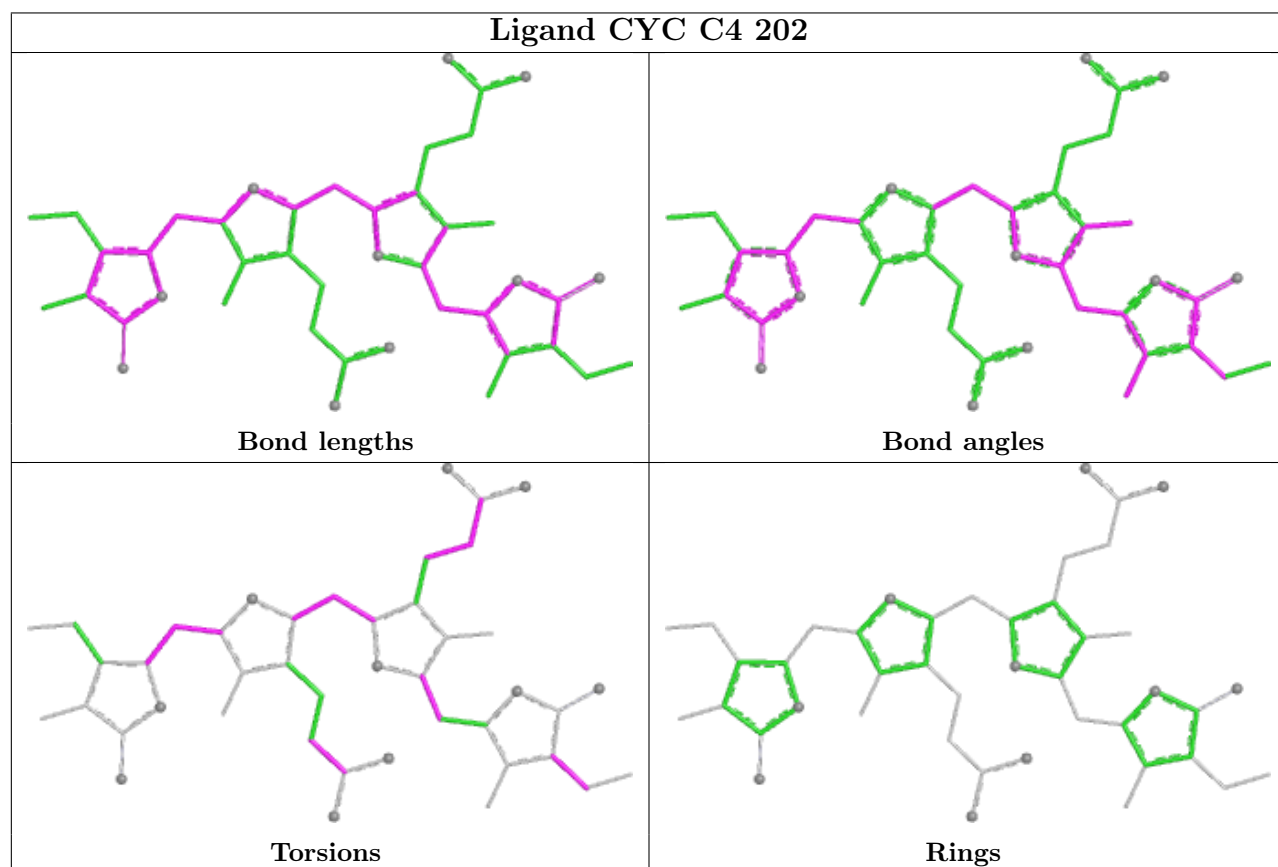
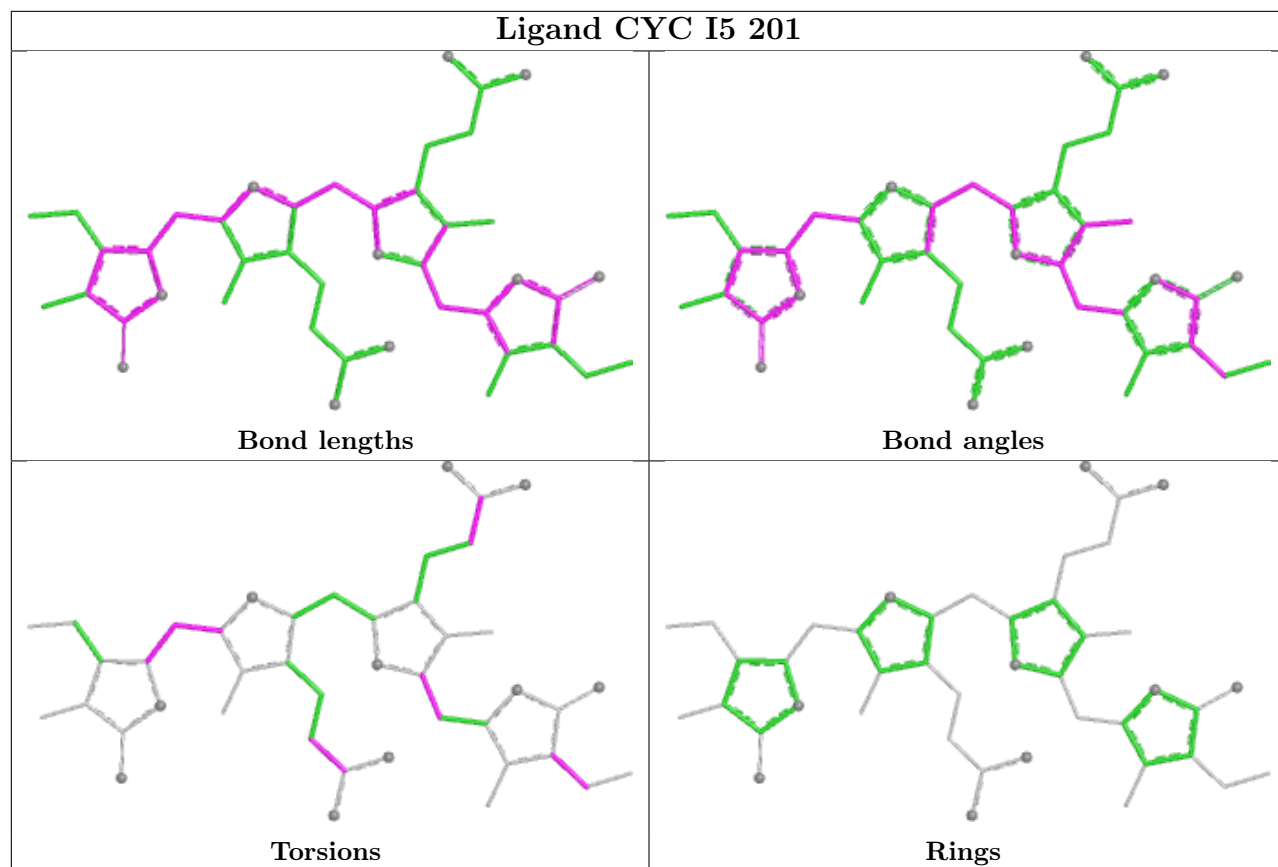


Ligand CYC F3 202

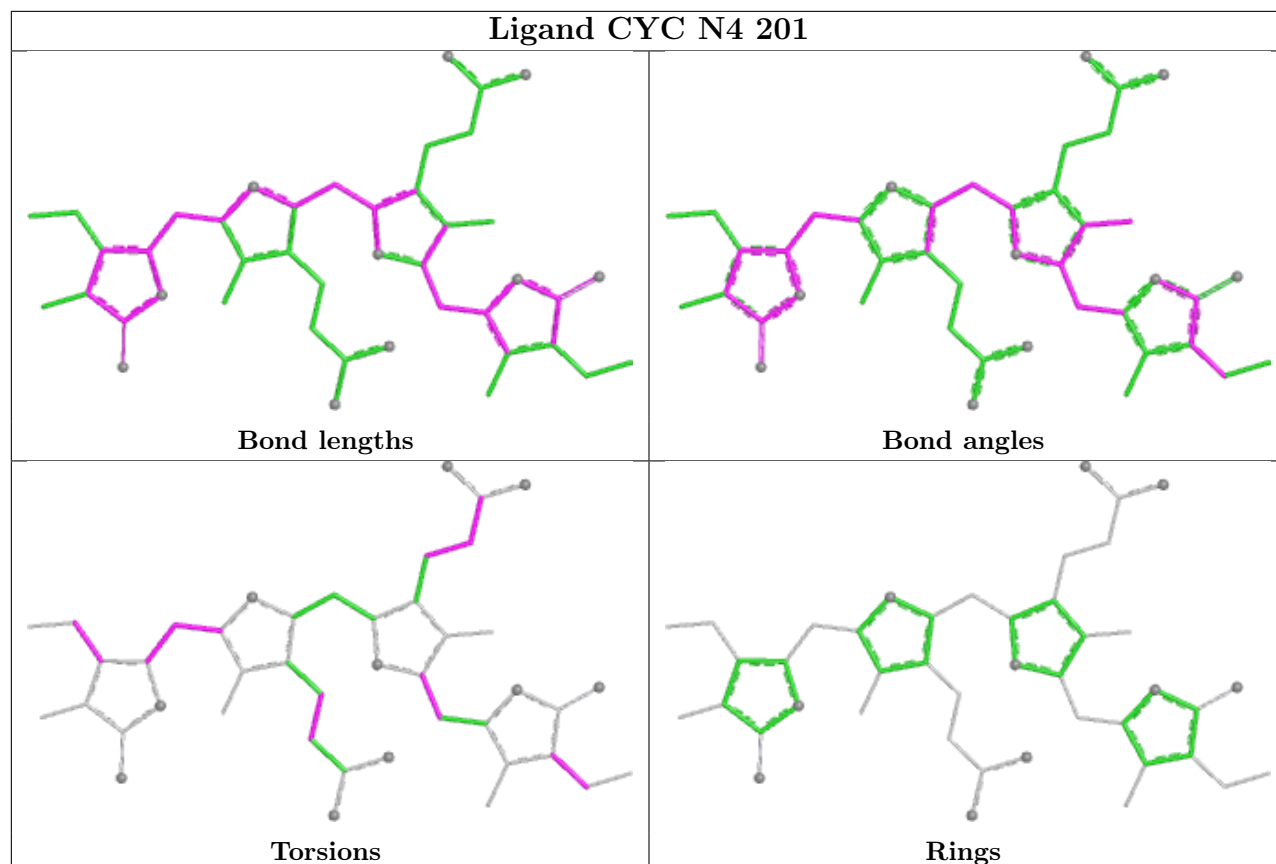


Ligand CYC Z7 301

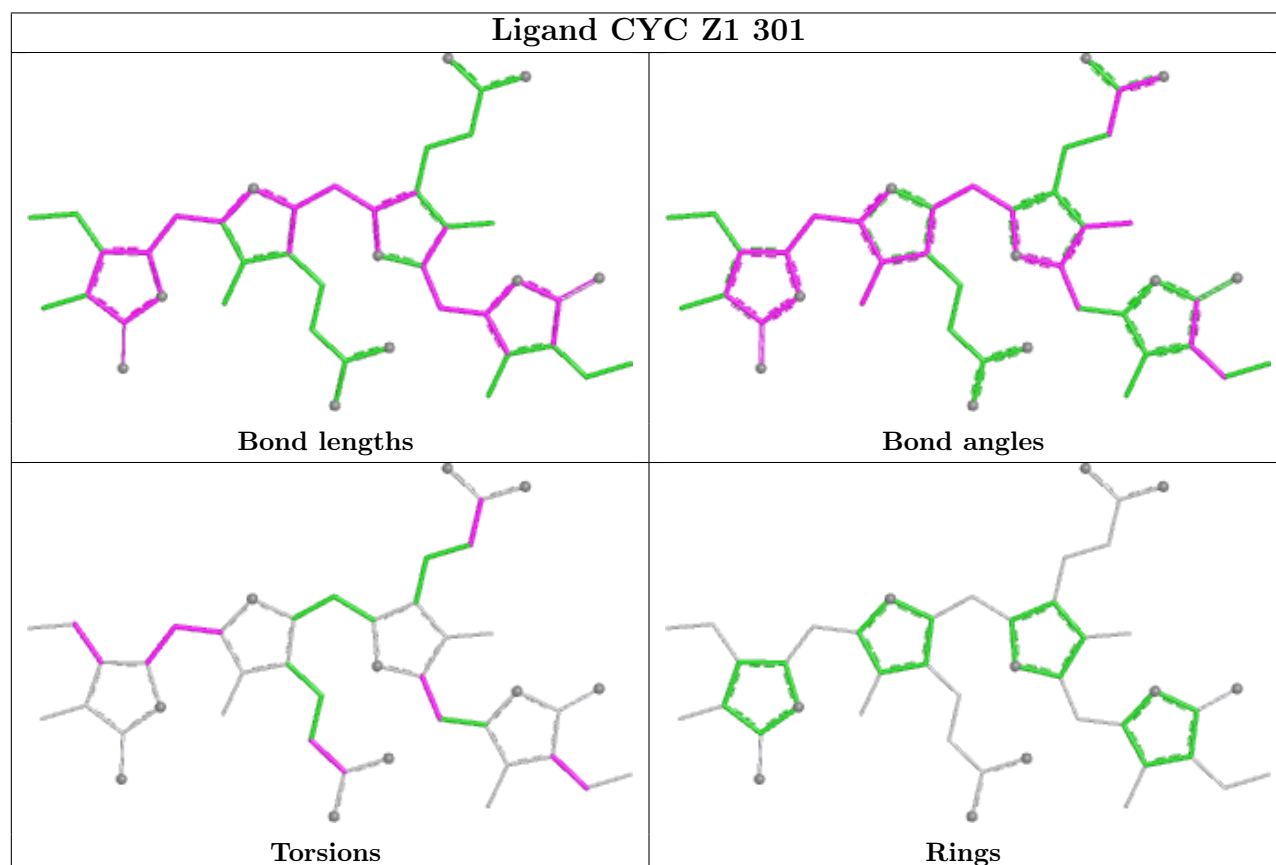




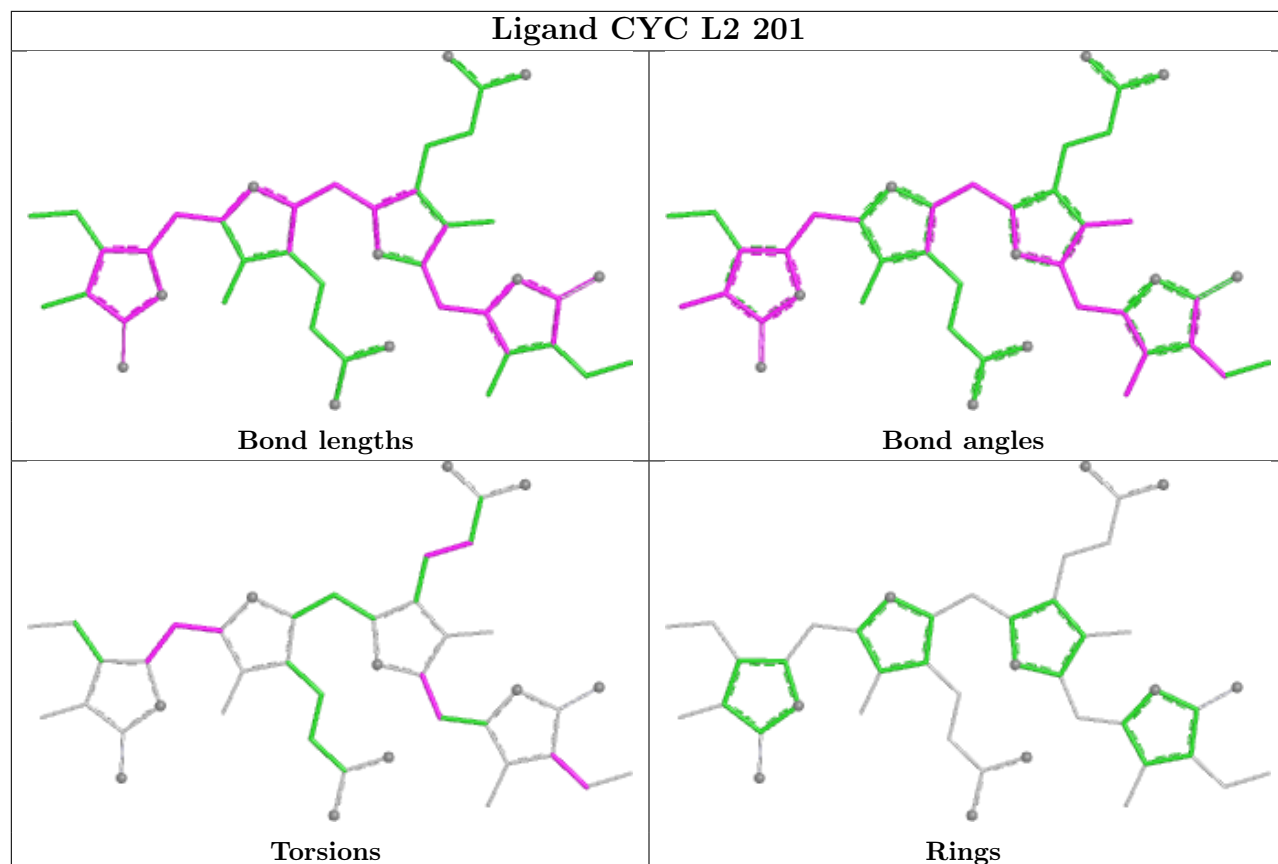
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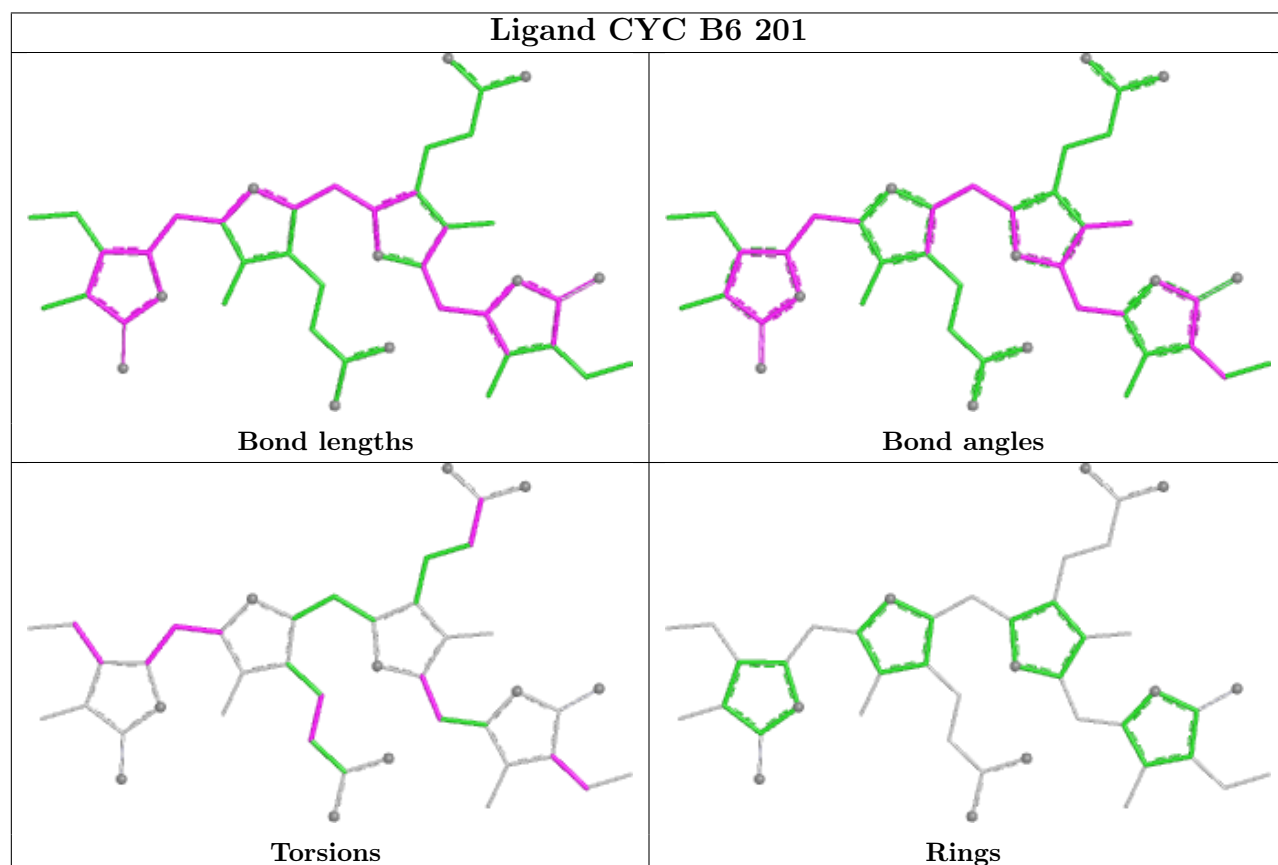
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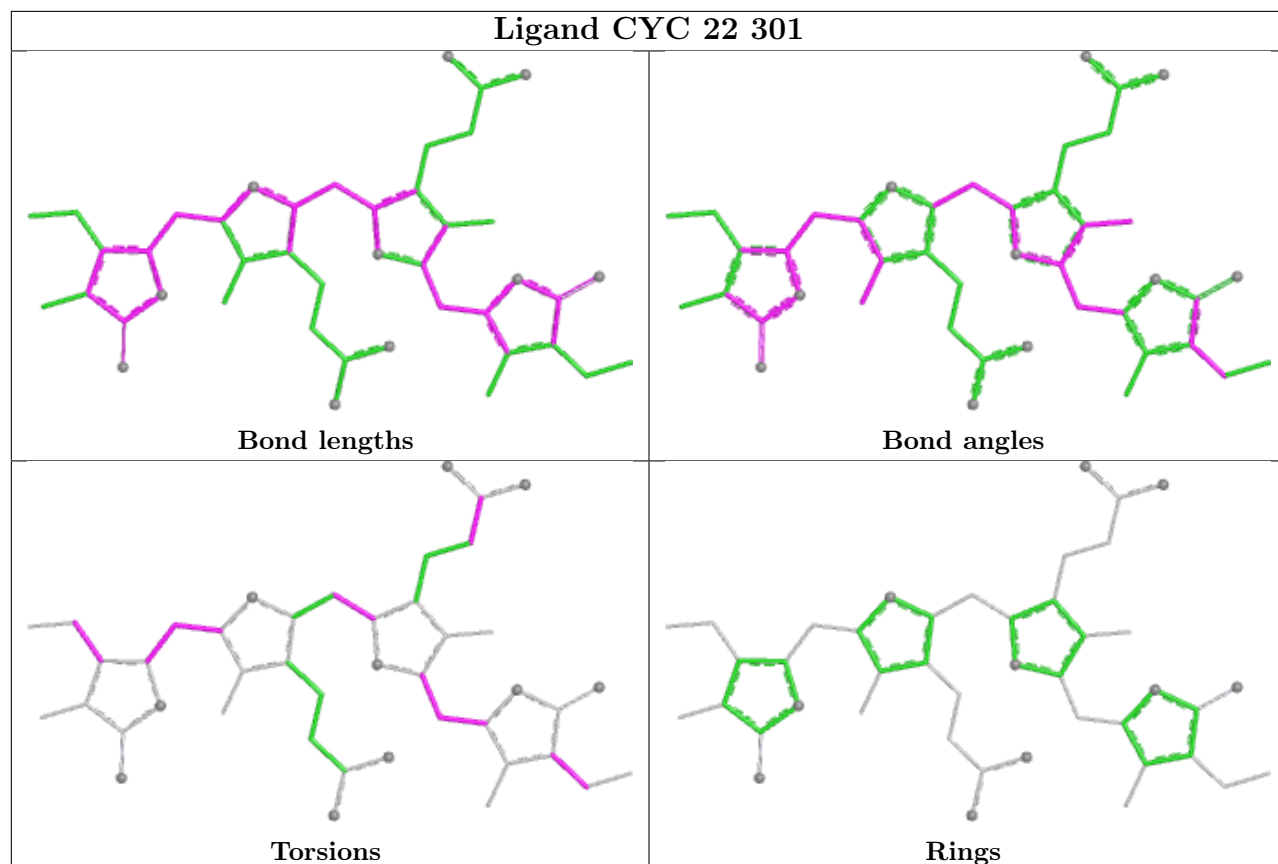
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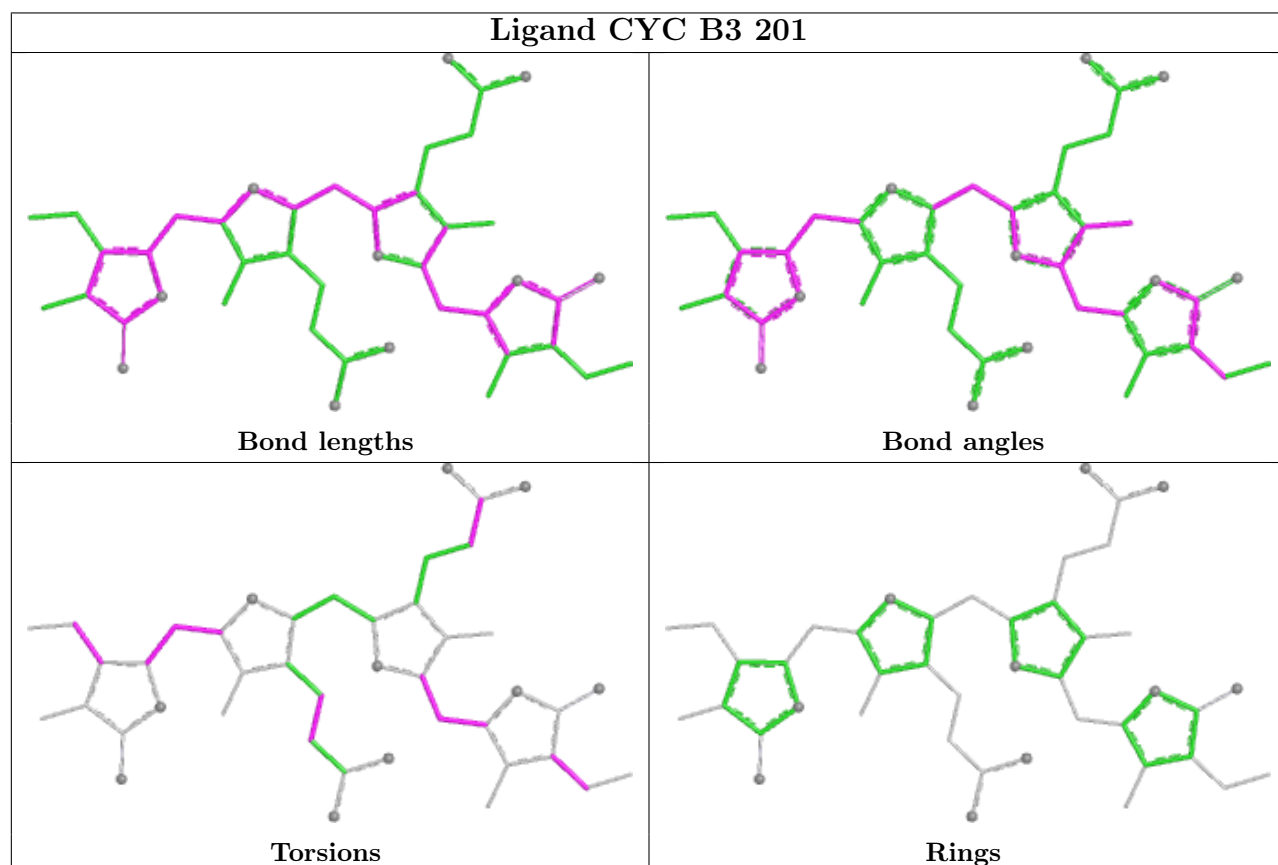
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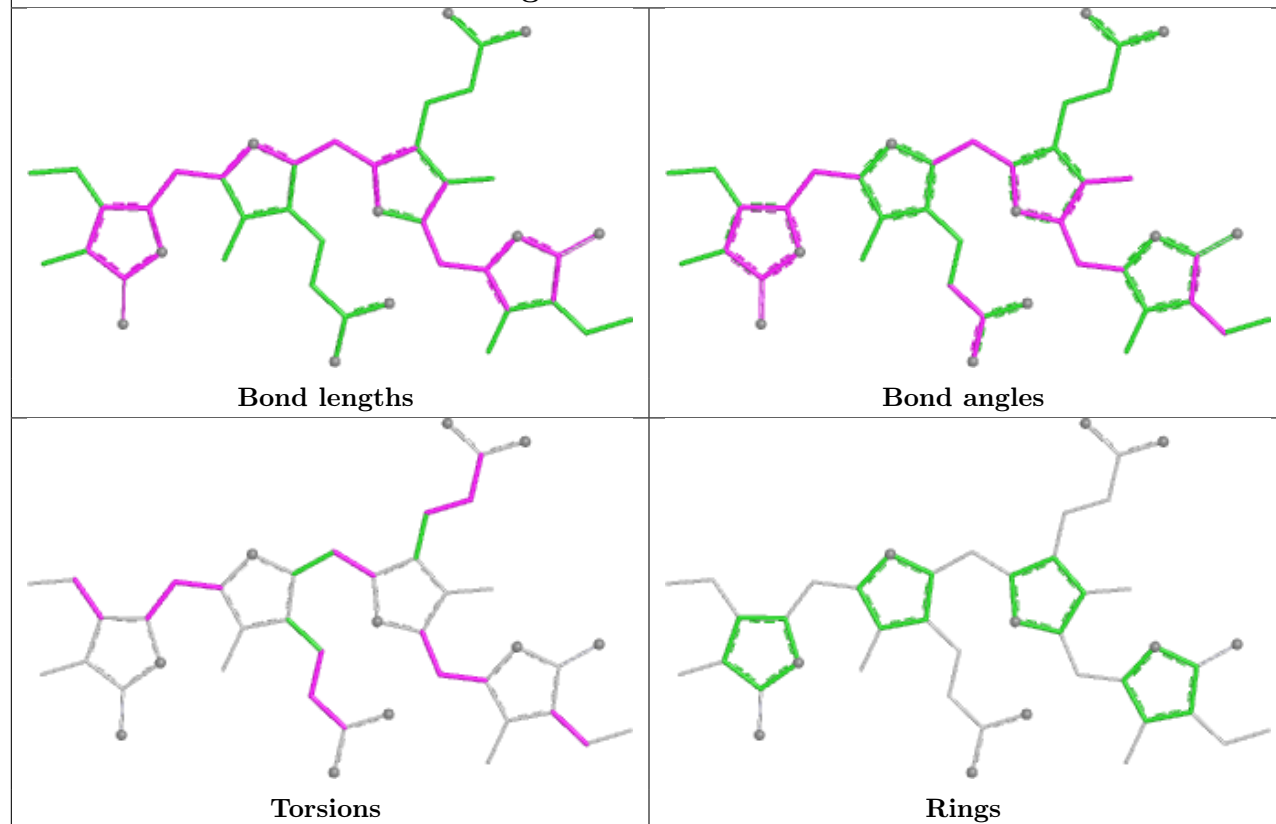
Ligand CYC 22 301



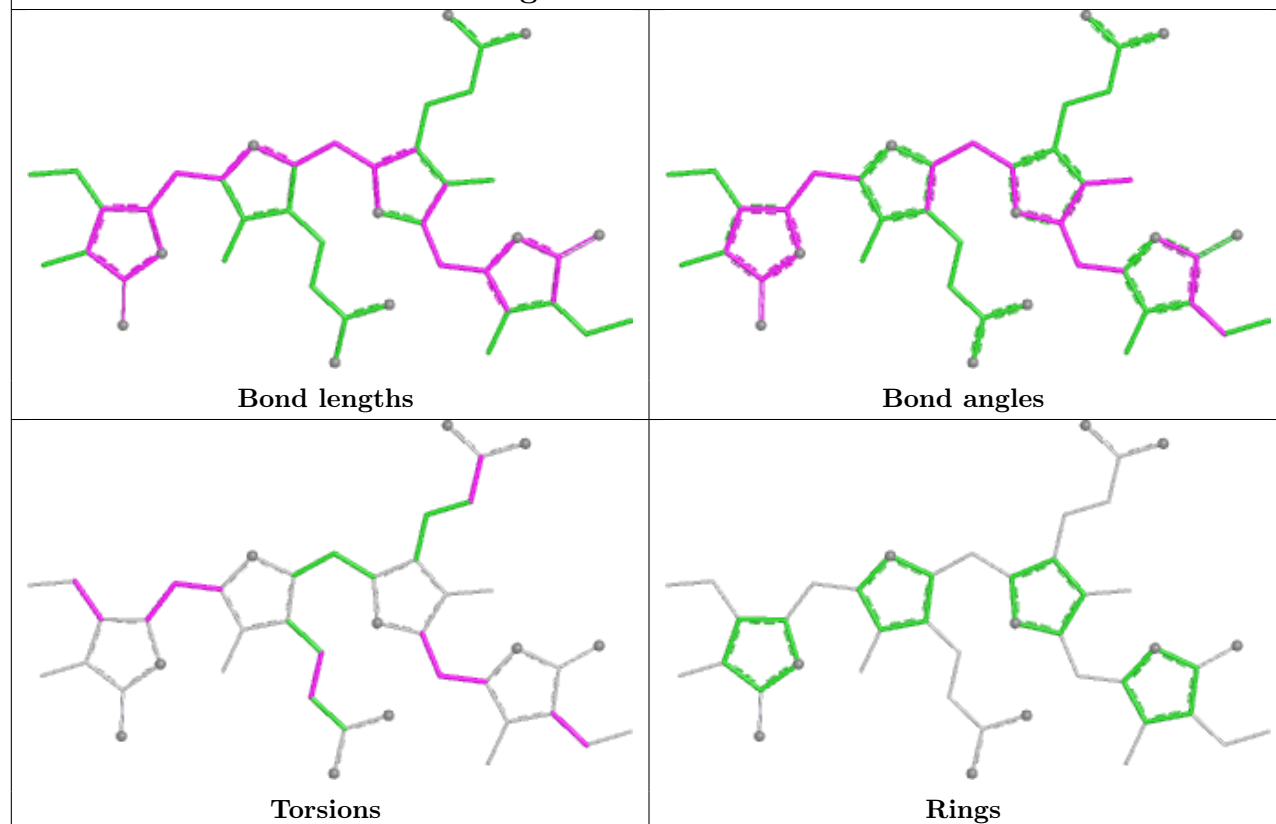
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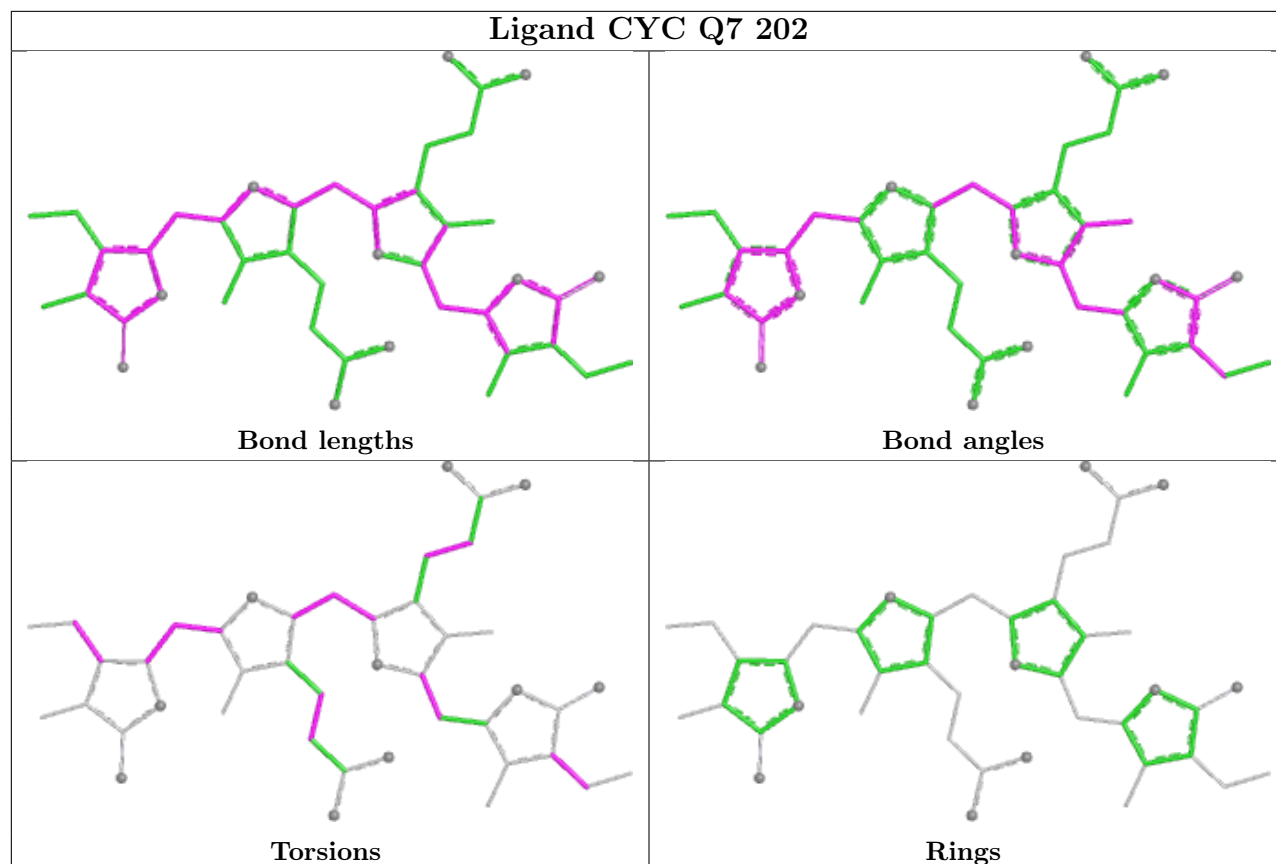
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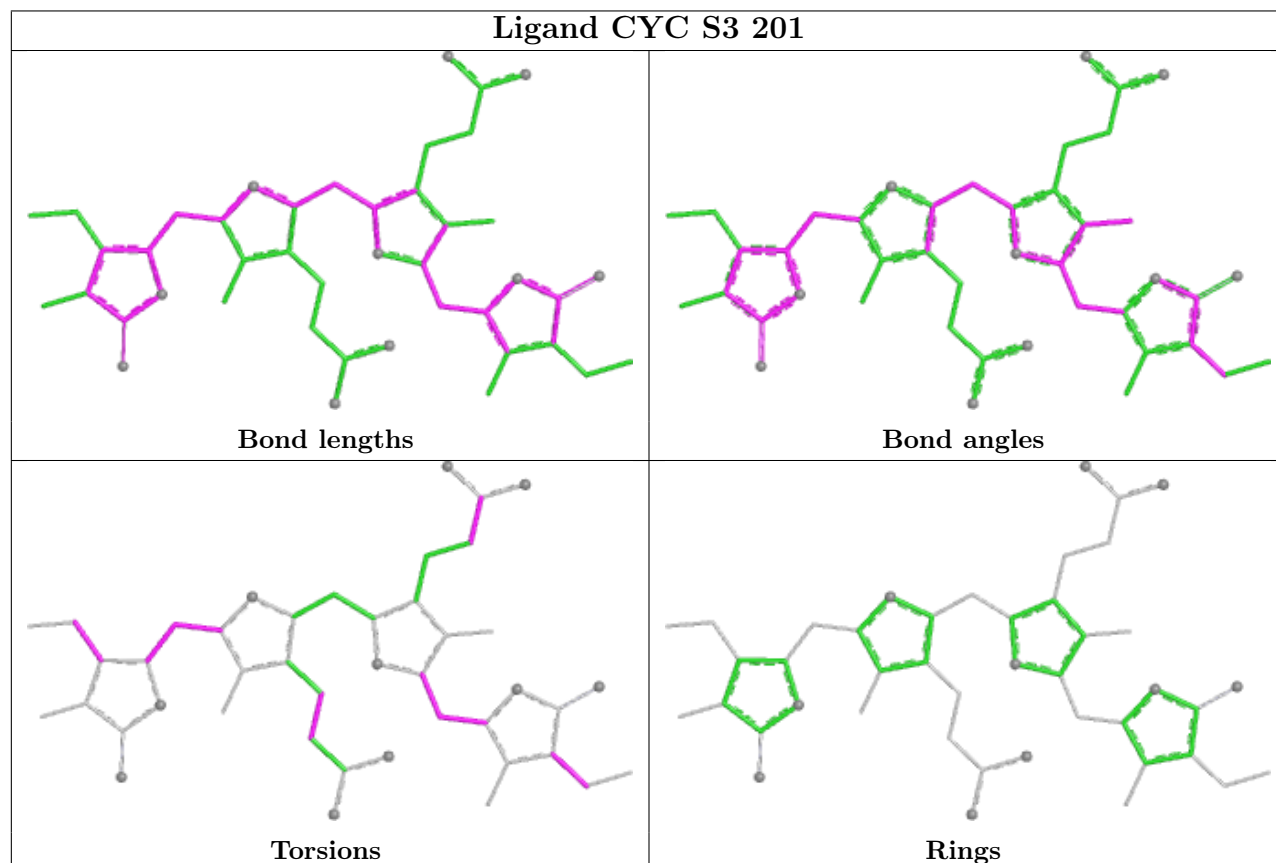
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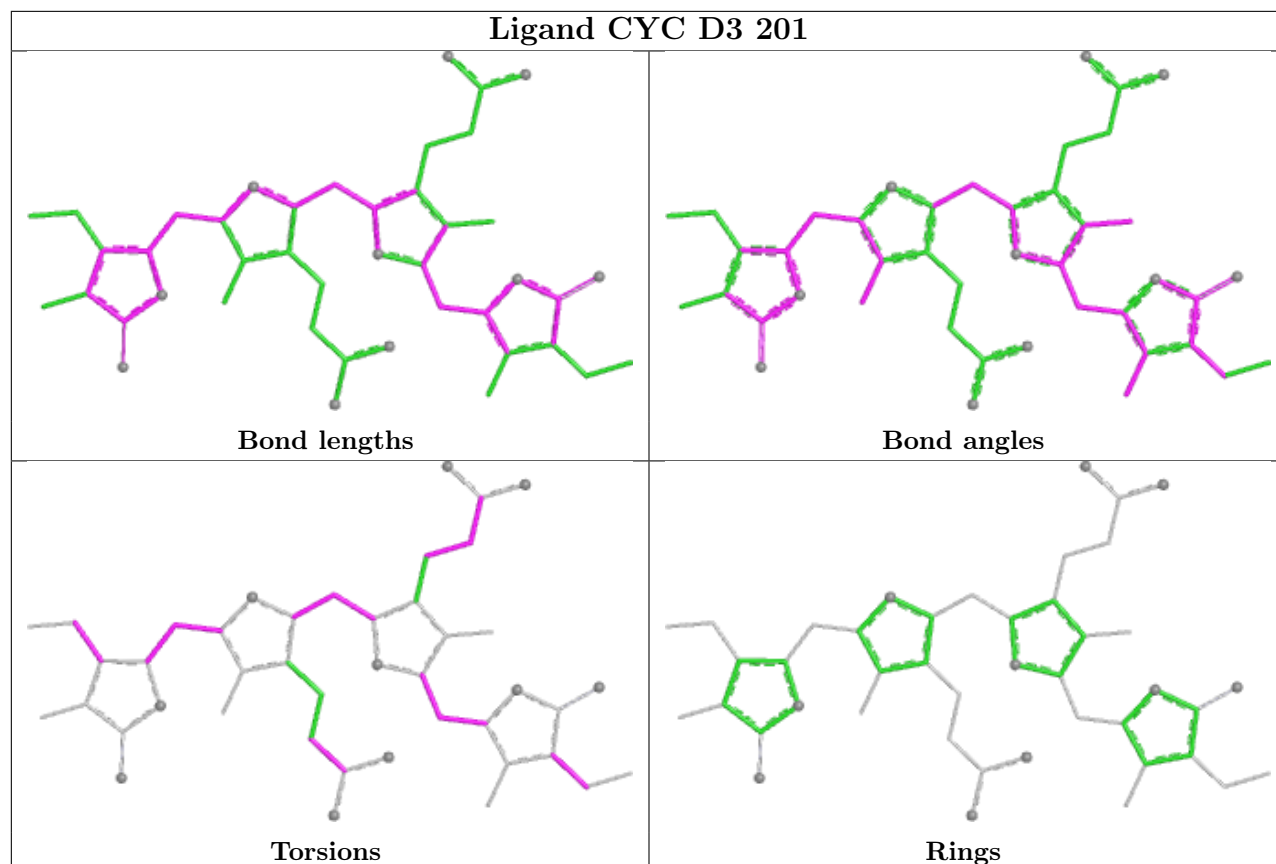
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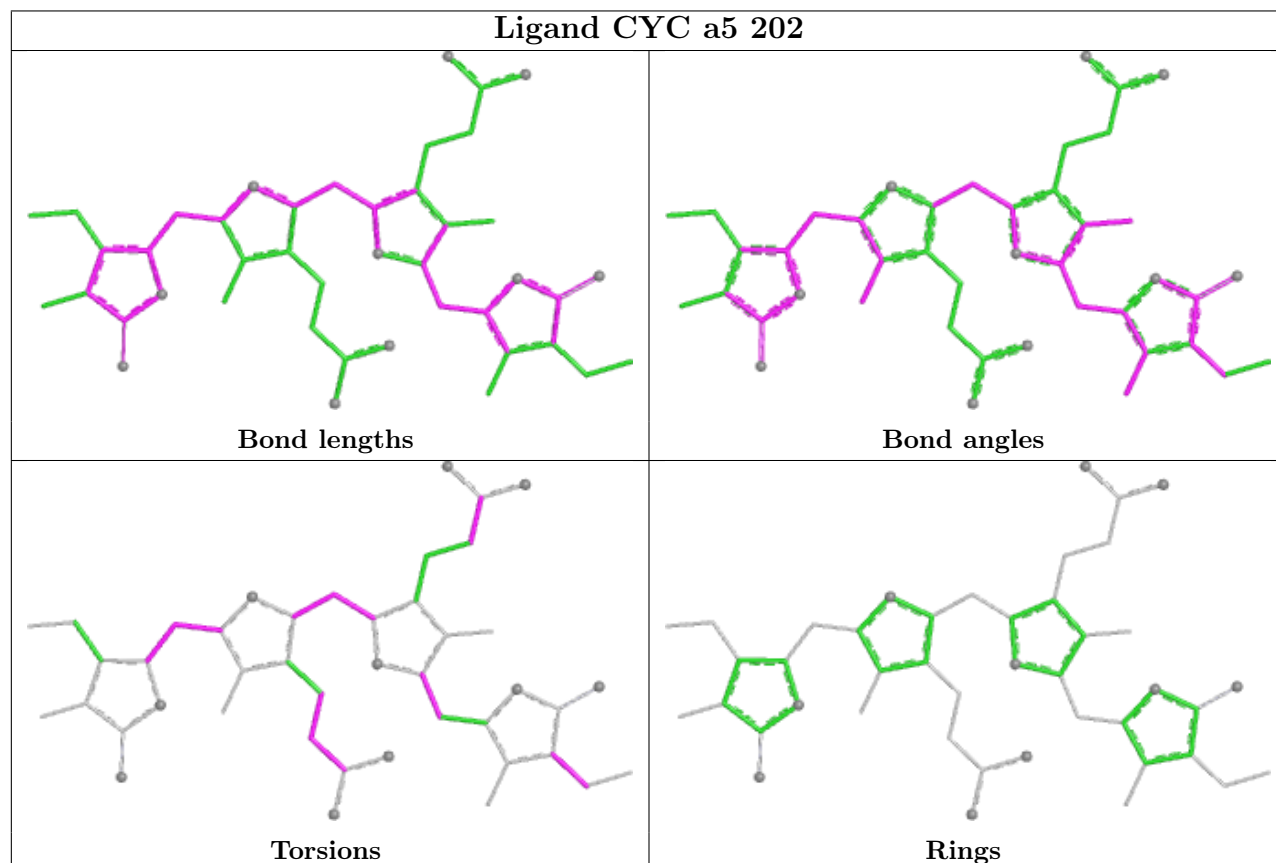
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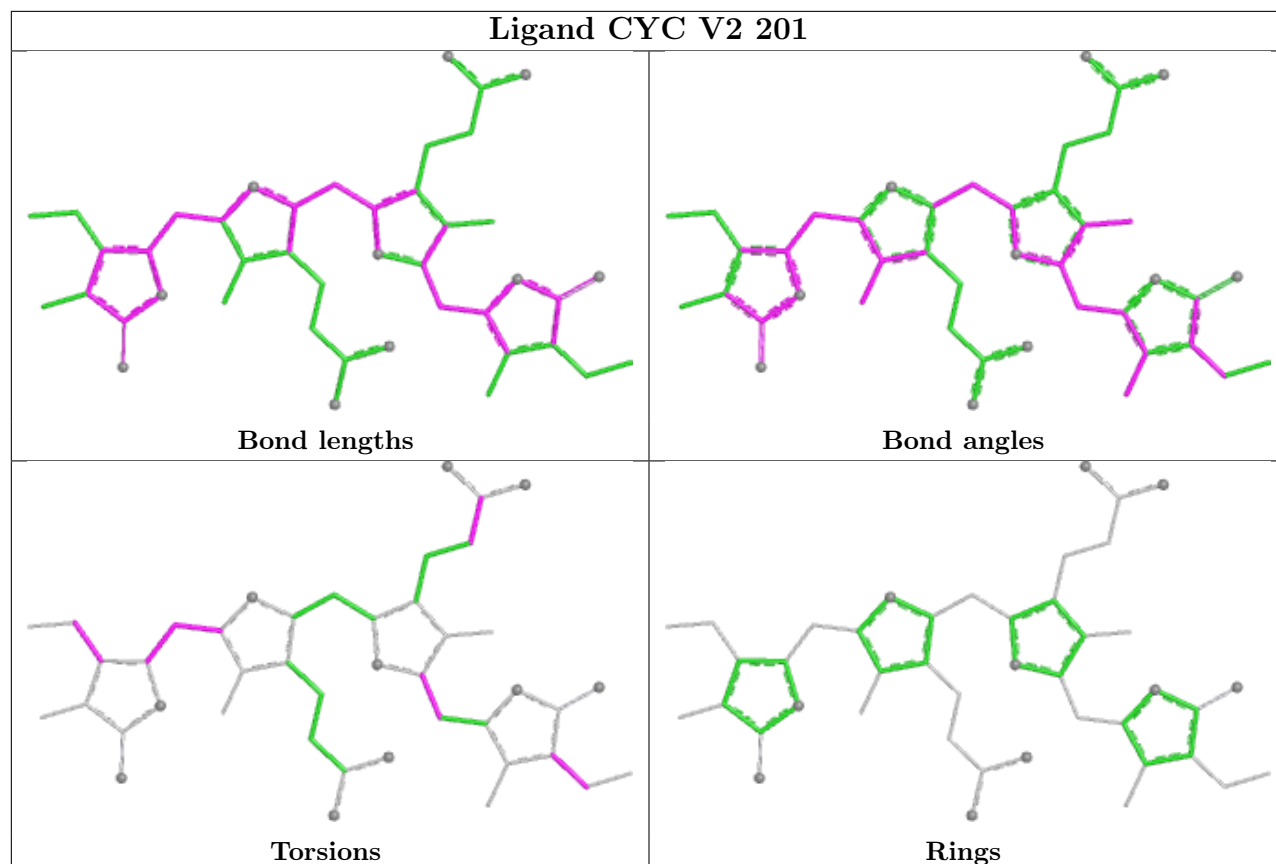
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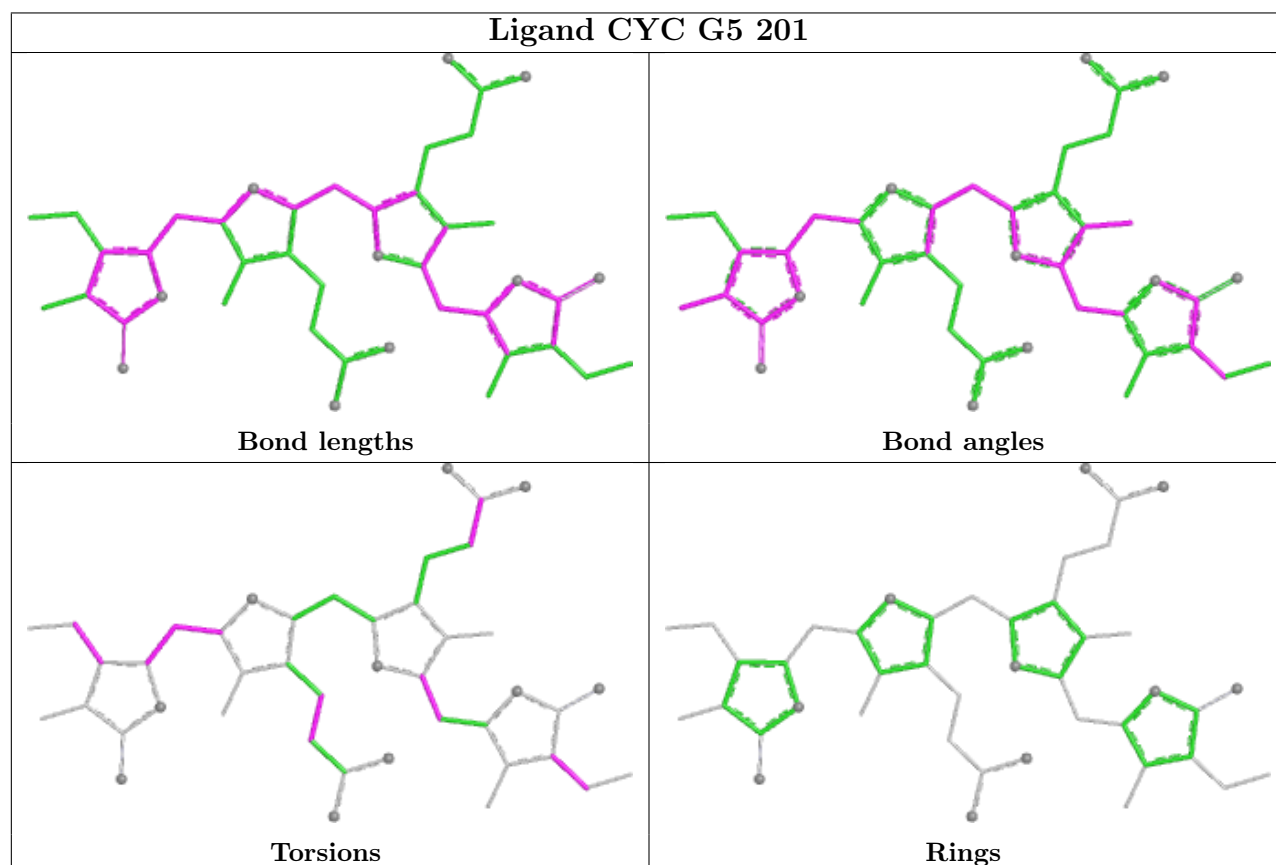
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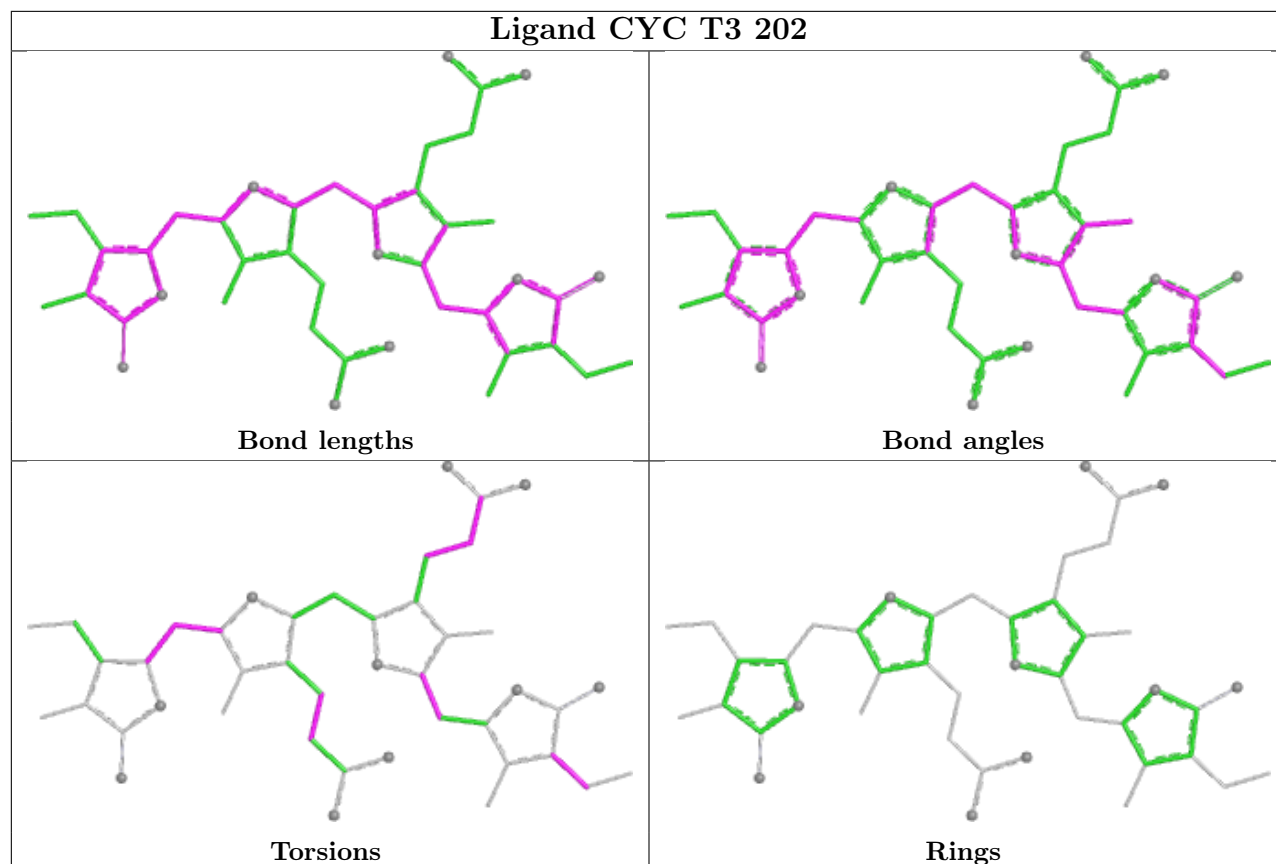
Ligand CYC V2 201



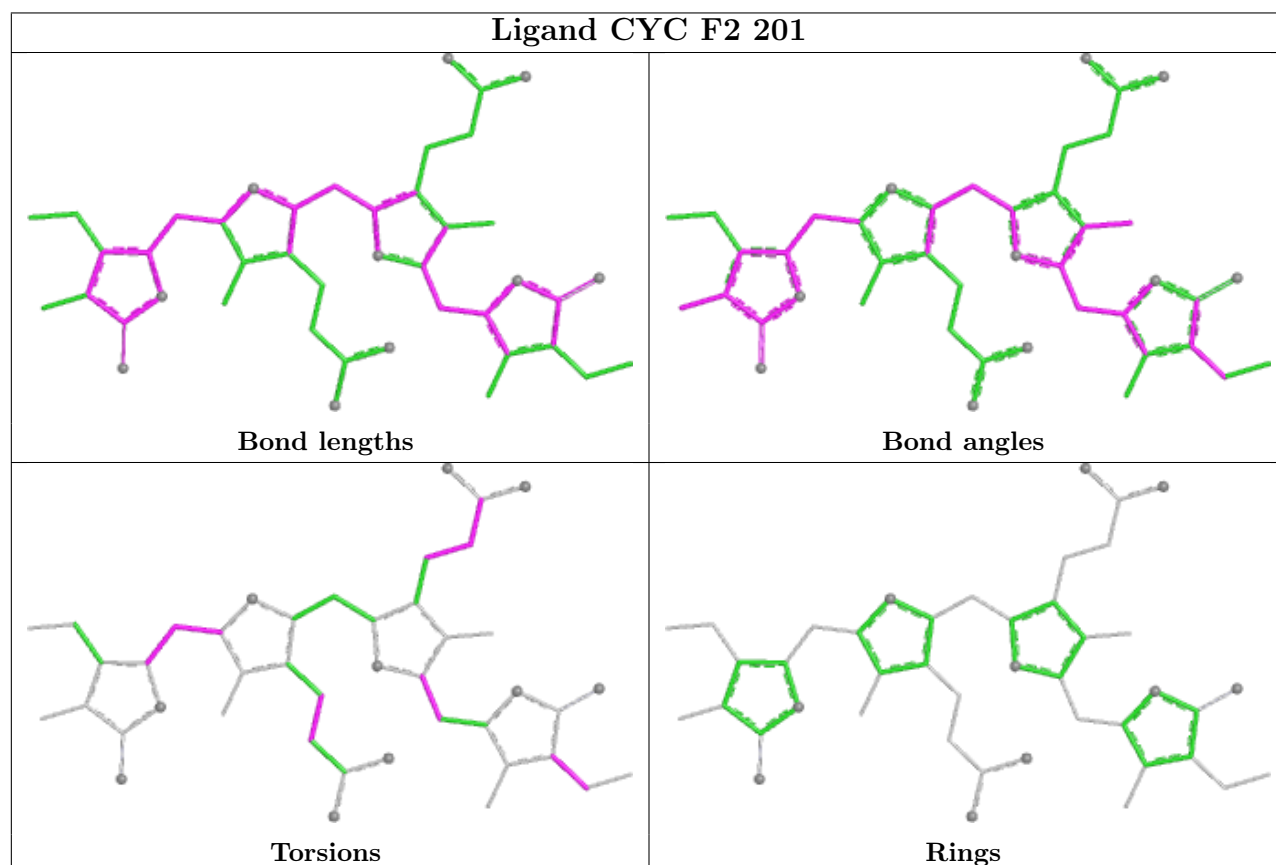
Ligand CYC G5 201

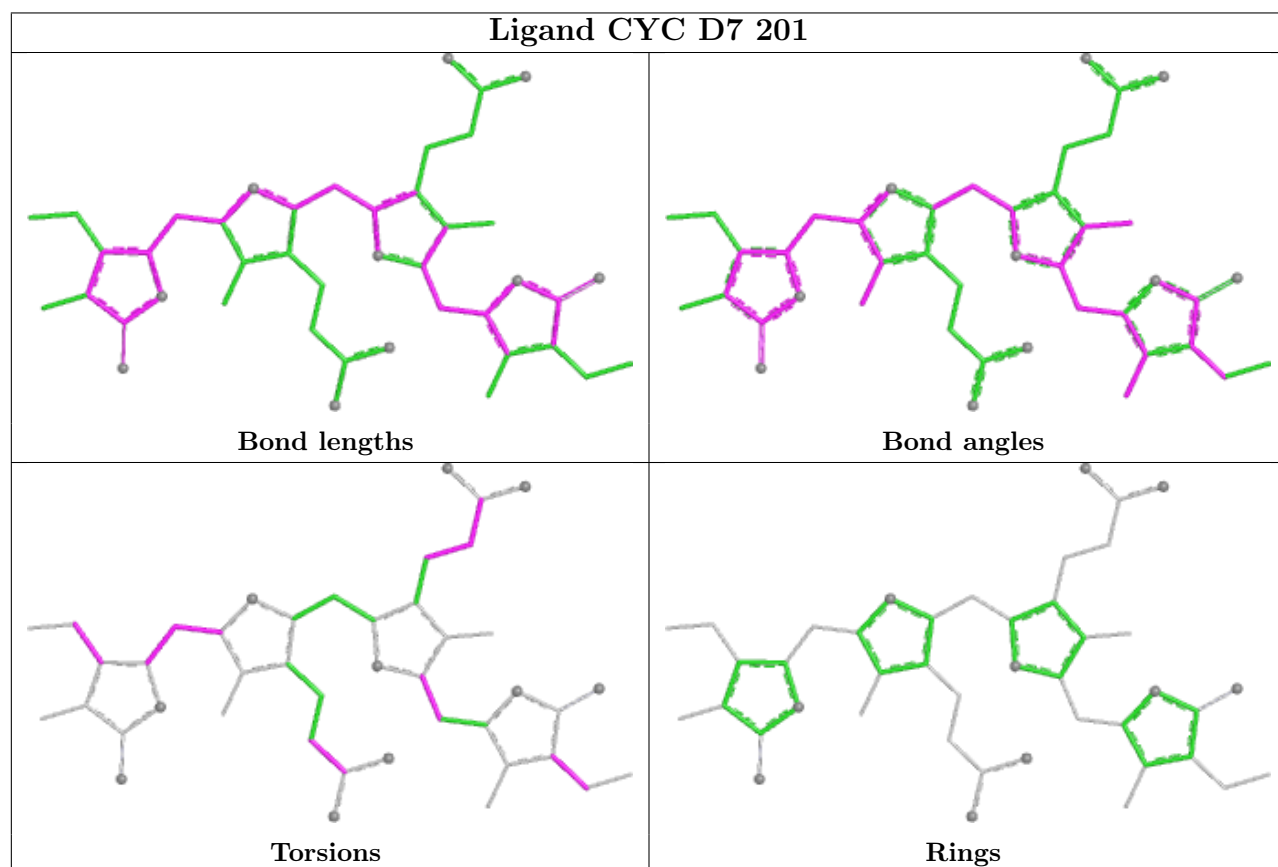
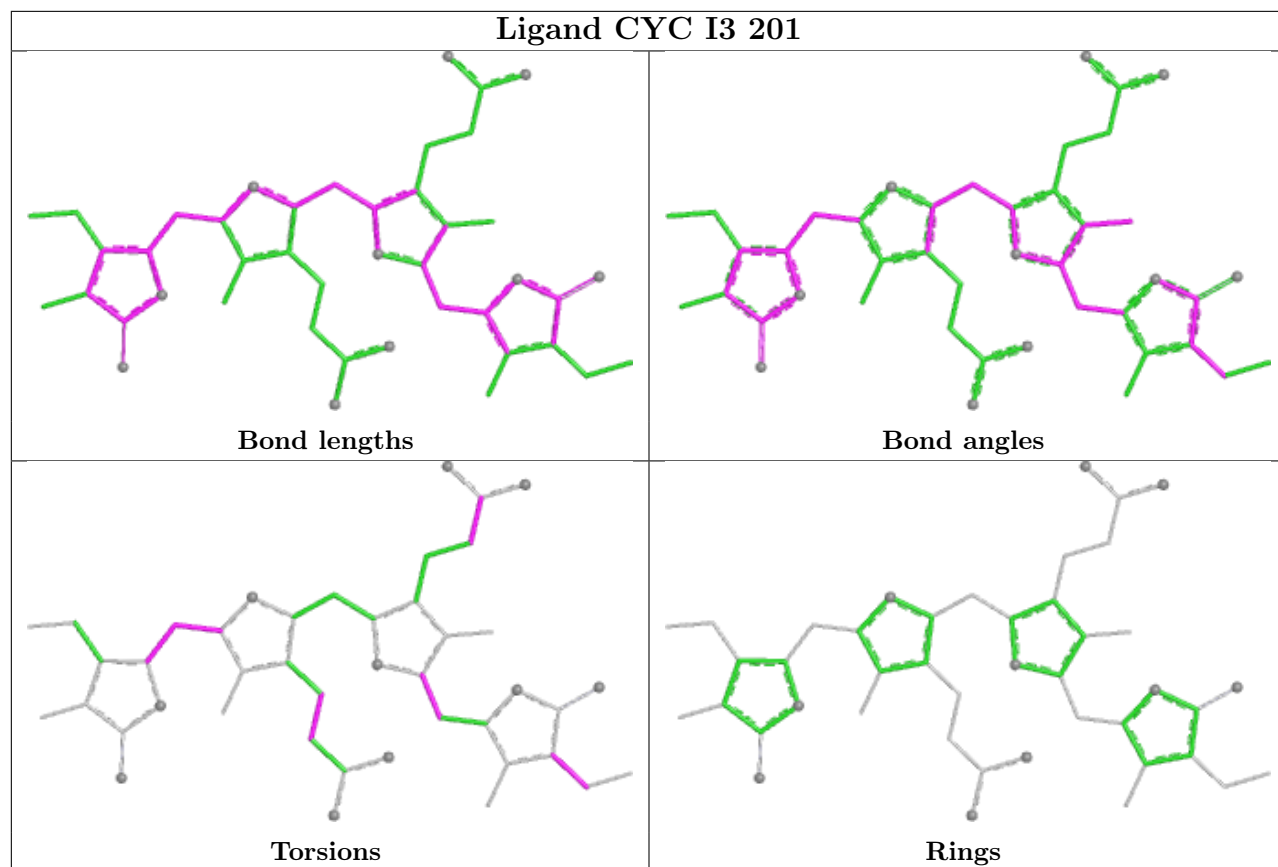


Ligand CYC T3 202

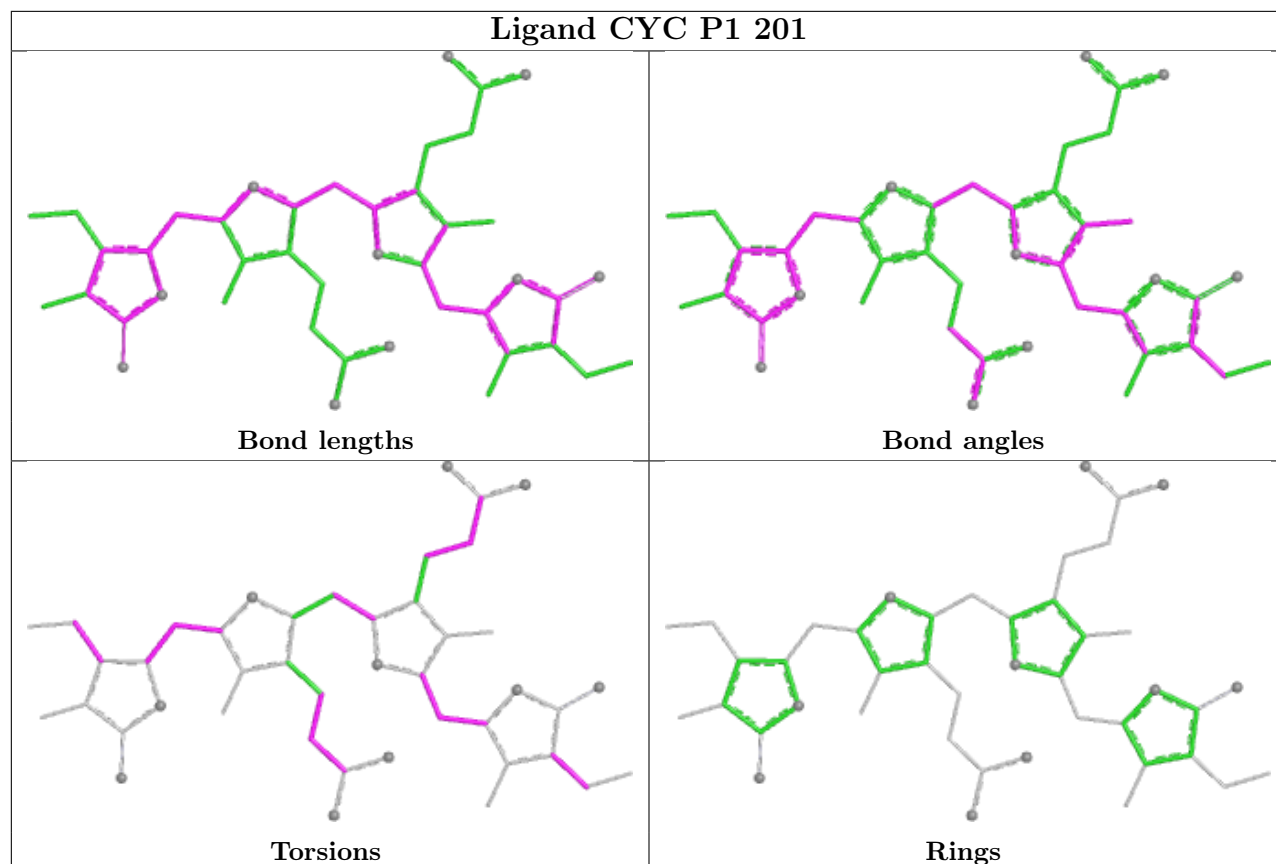


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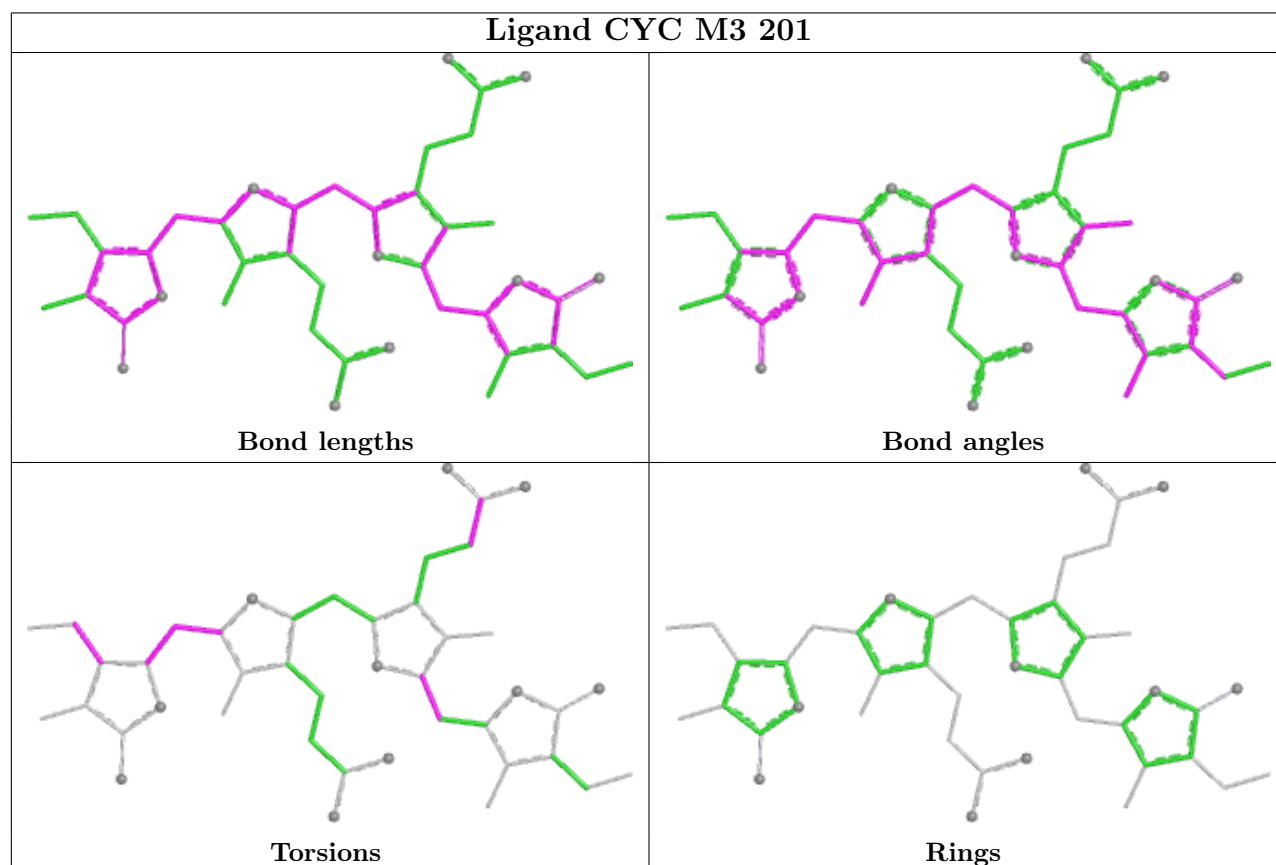




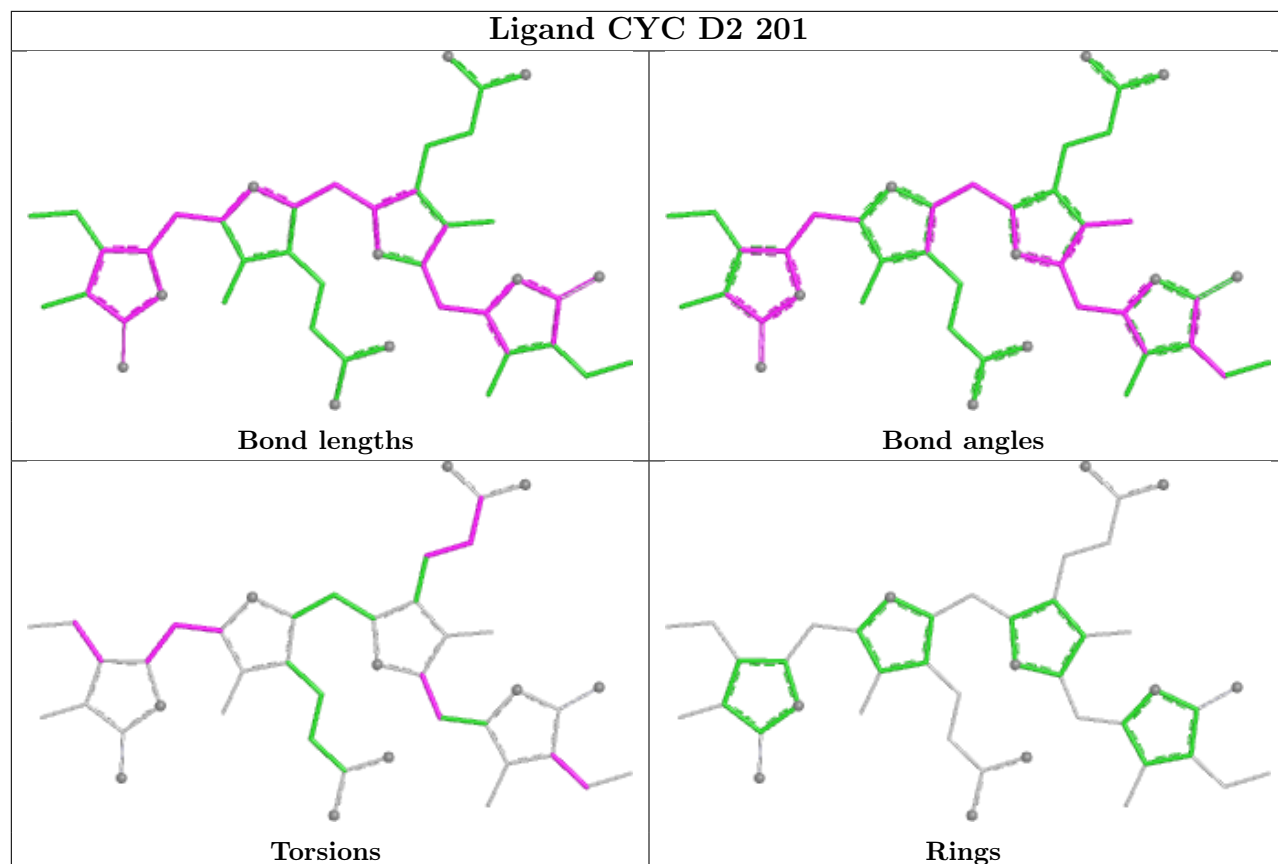
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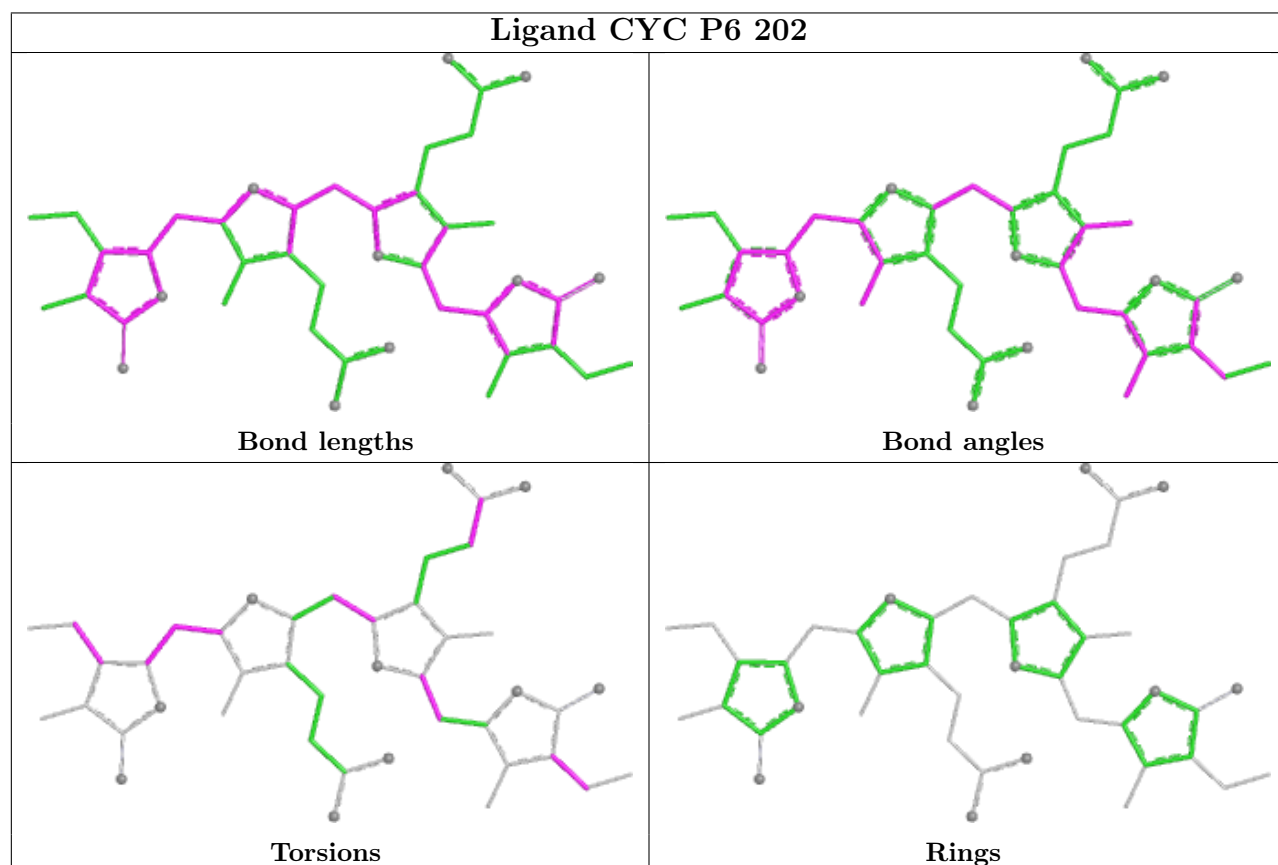
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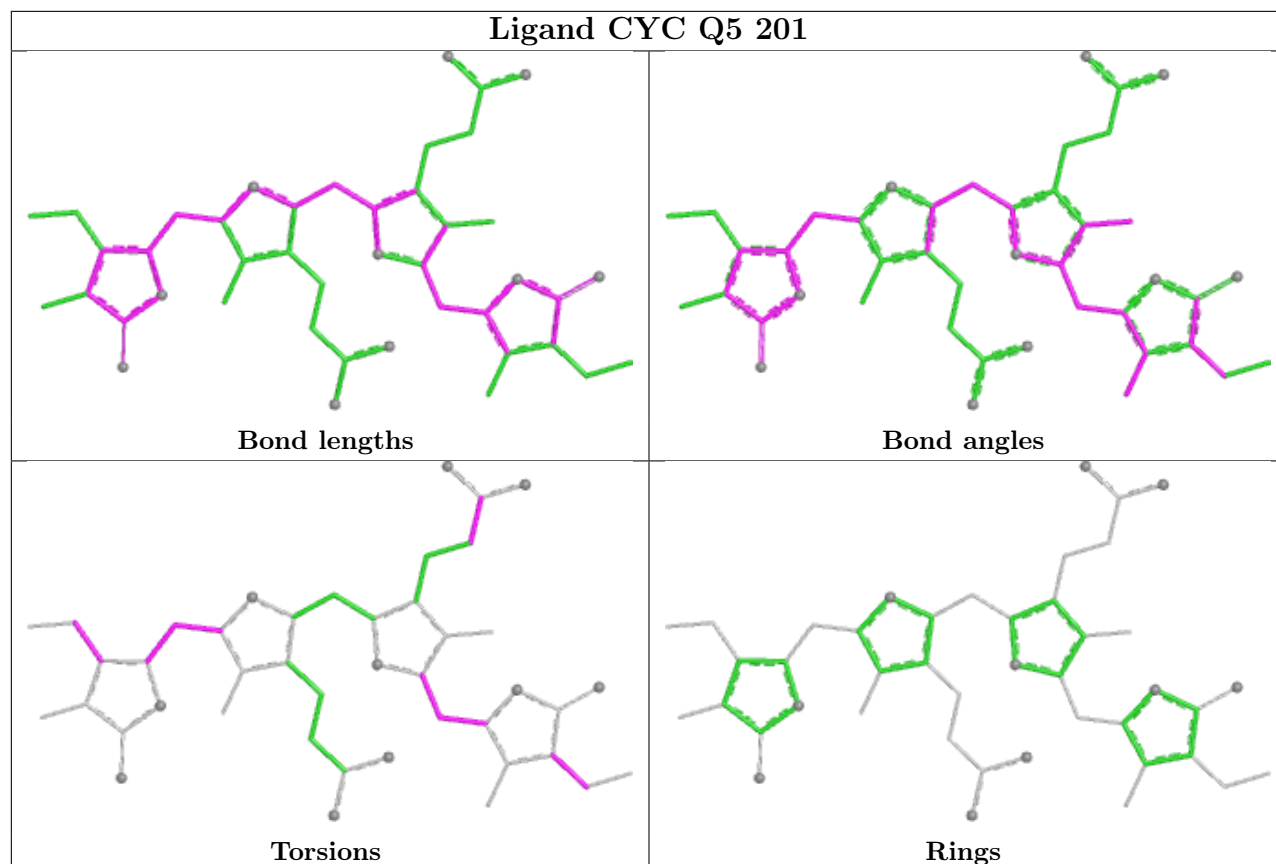
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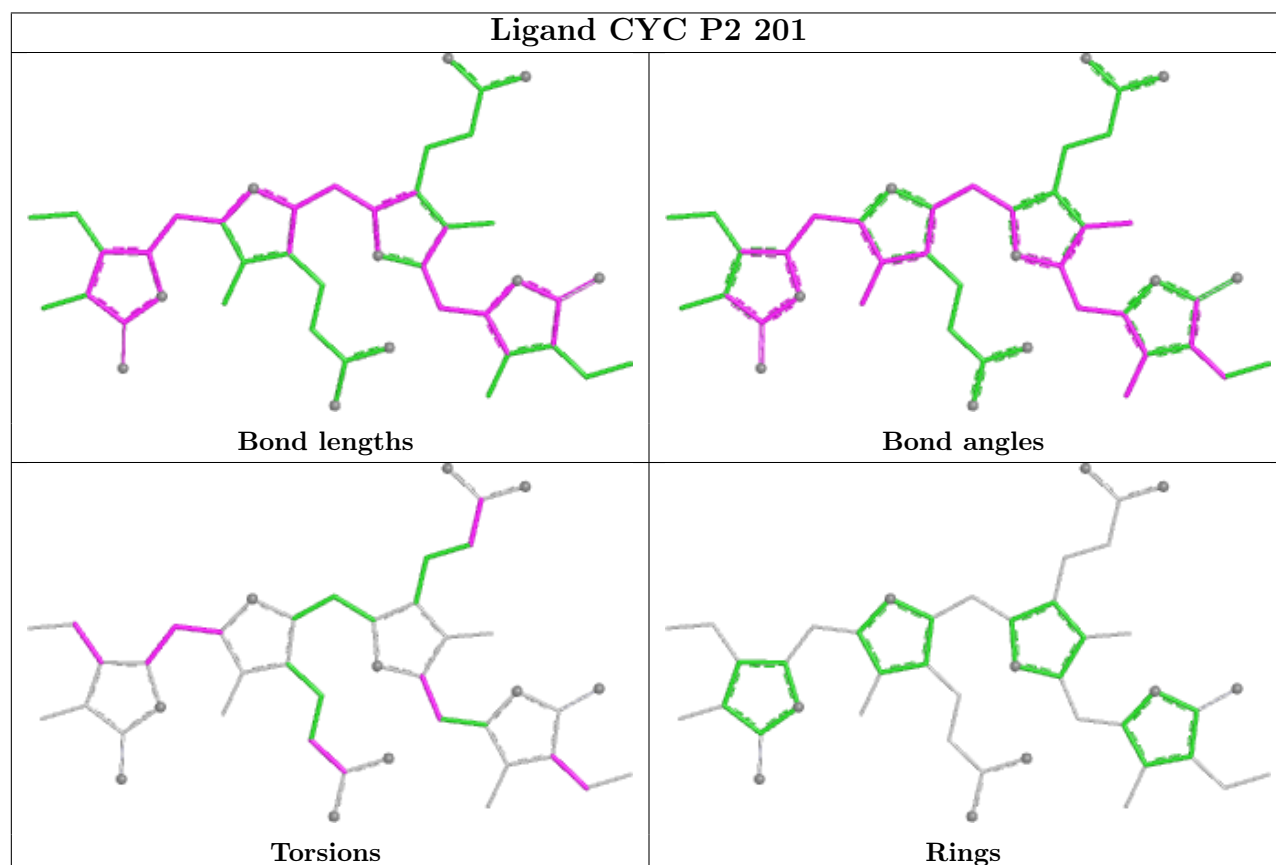
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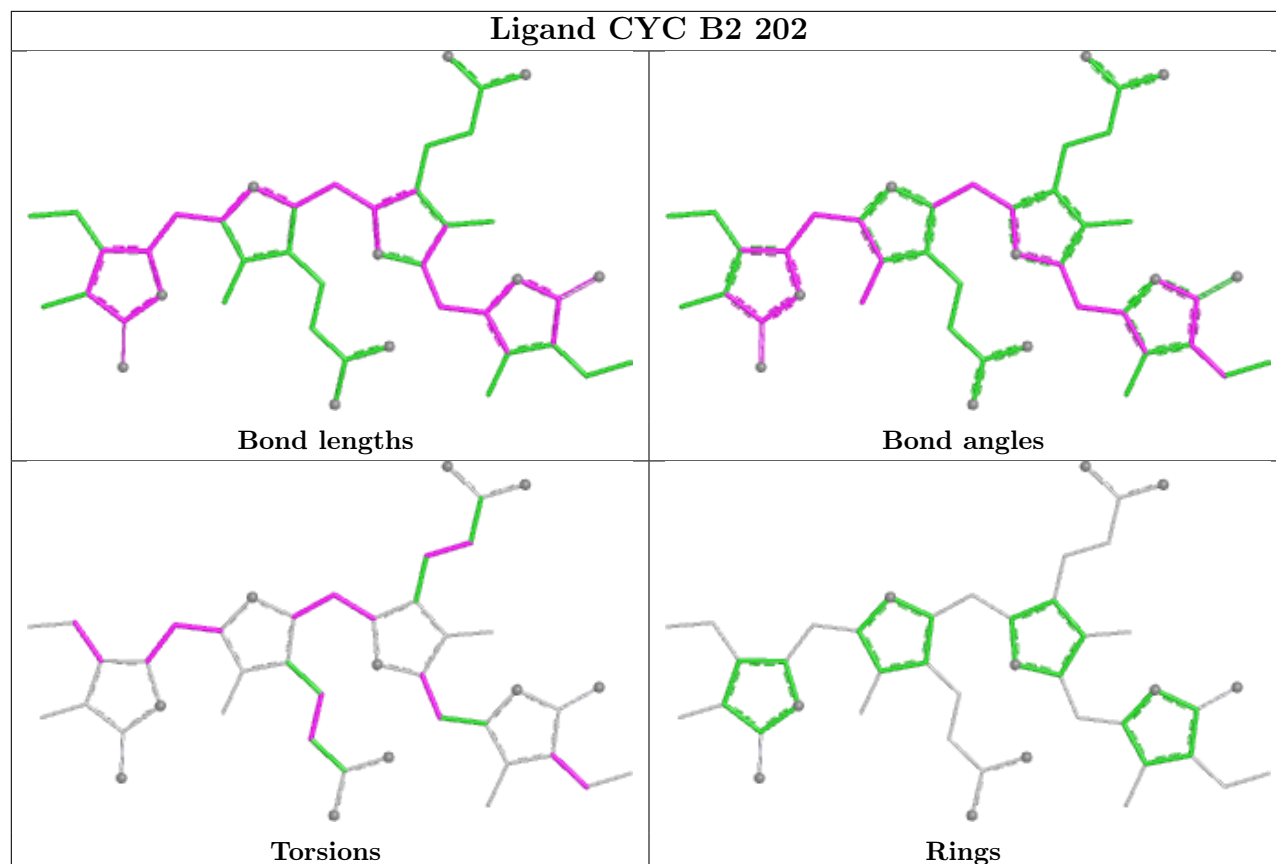
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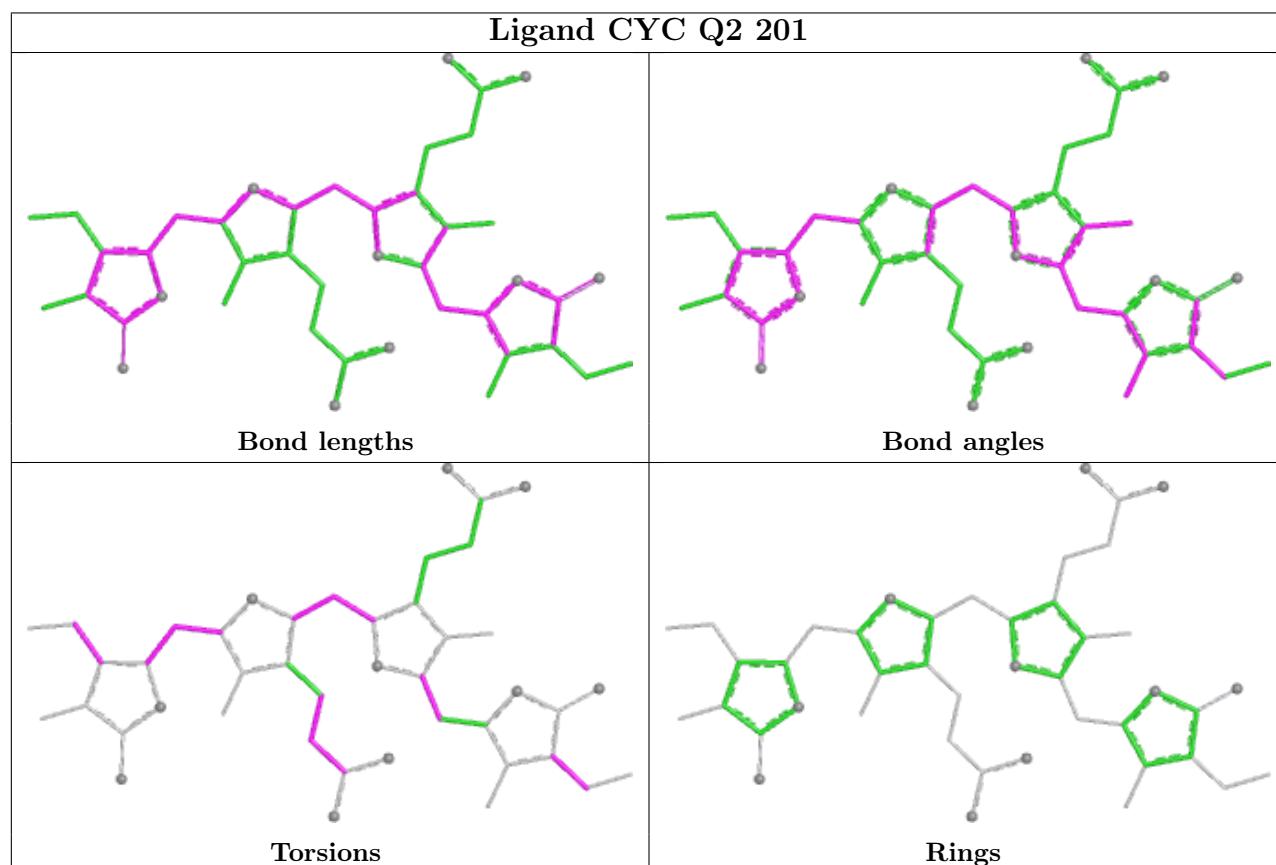
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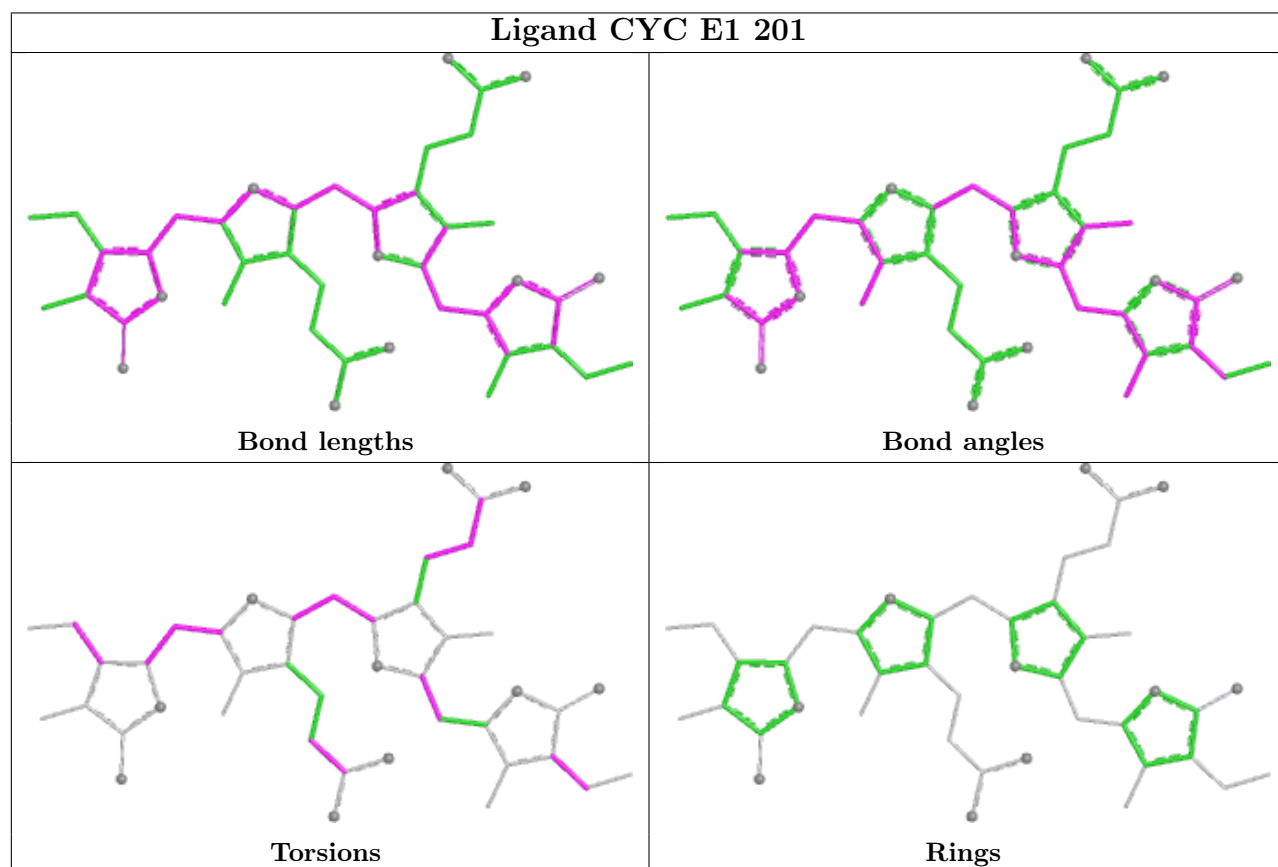
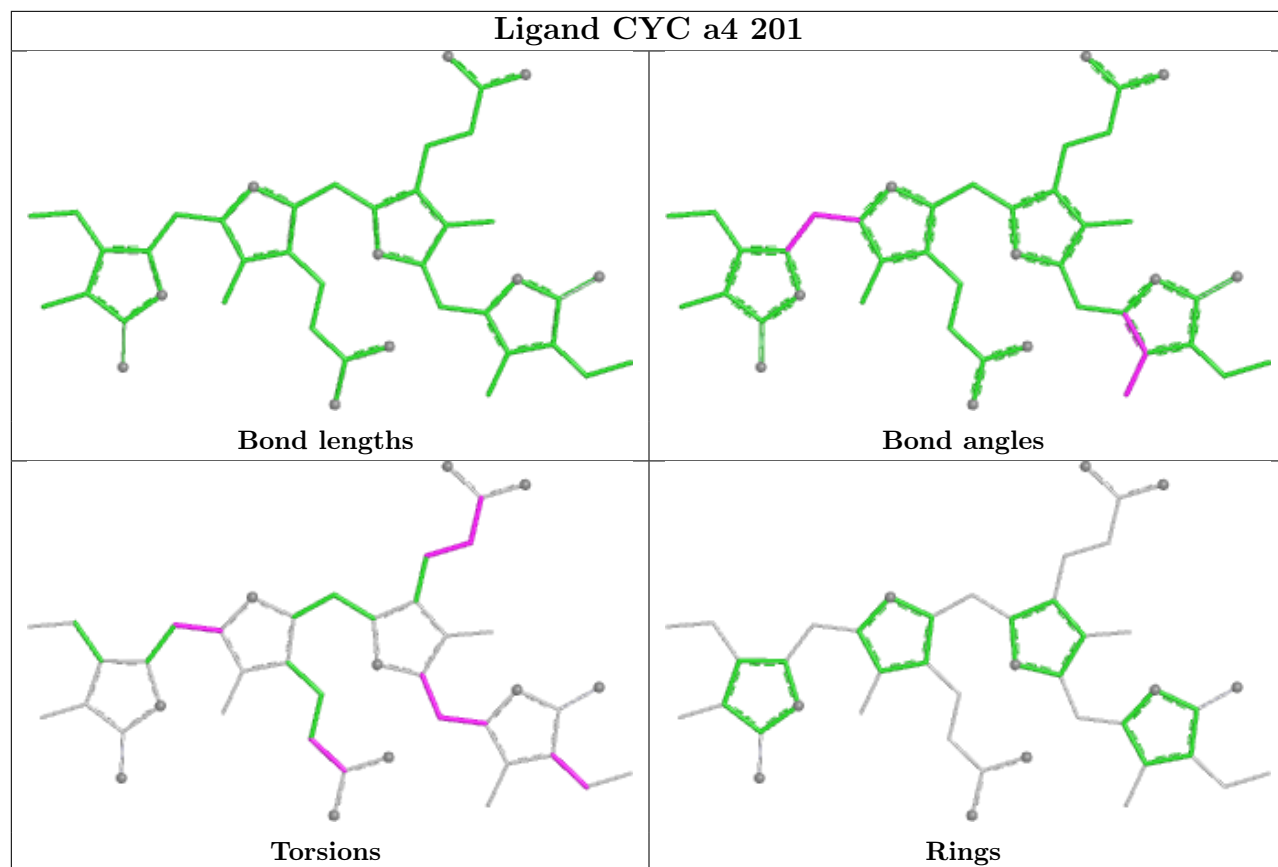


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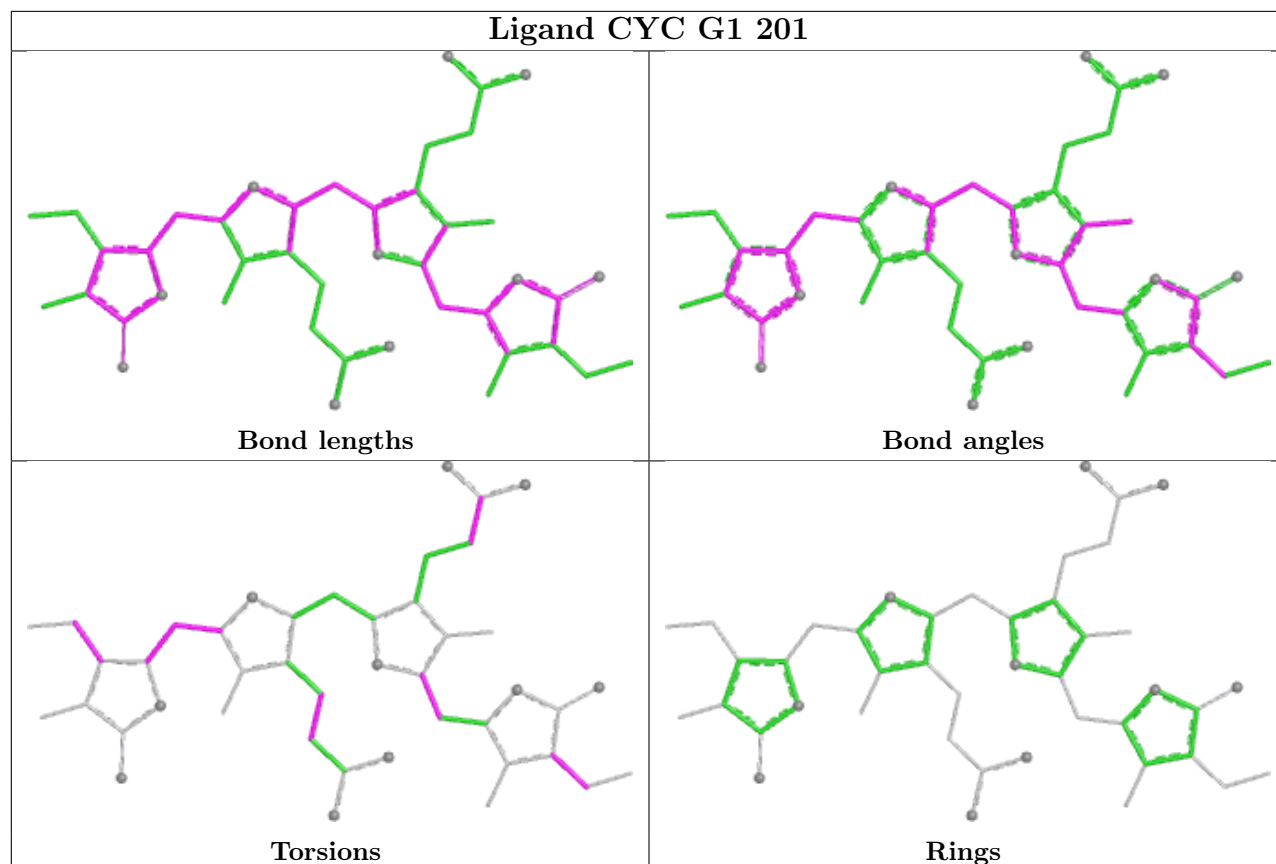


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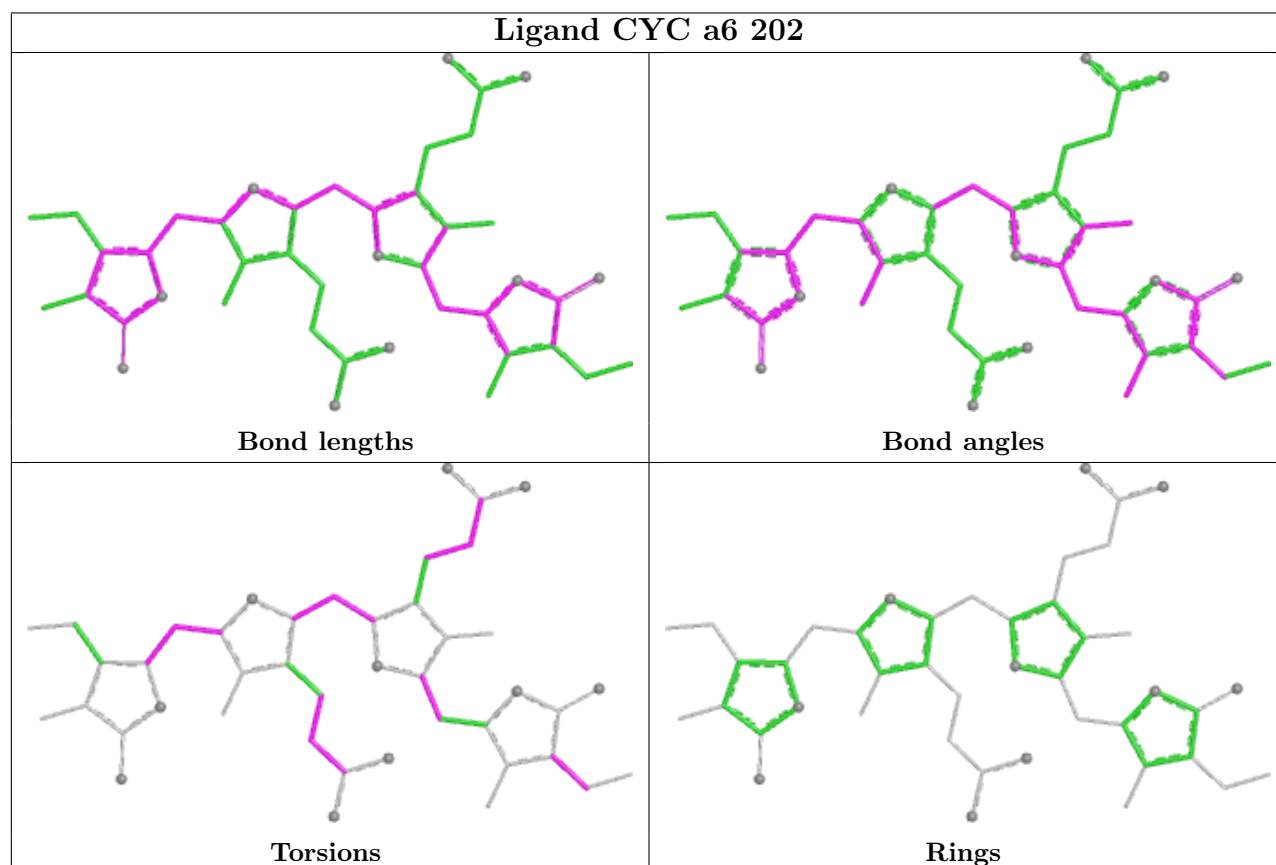




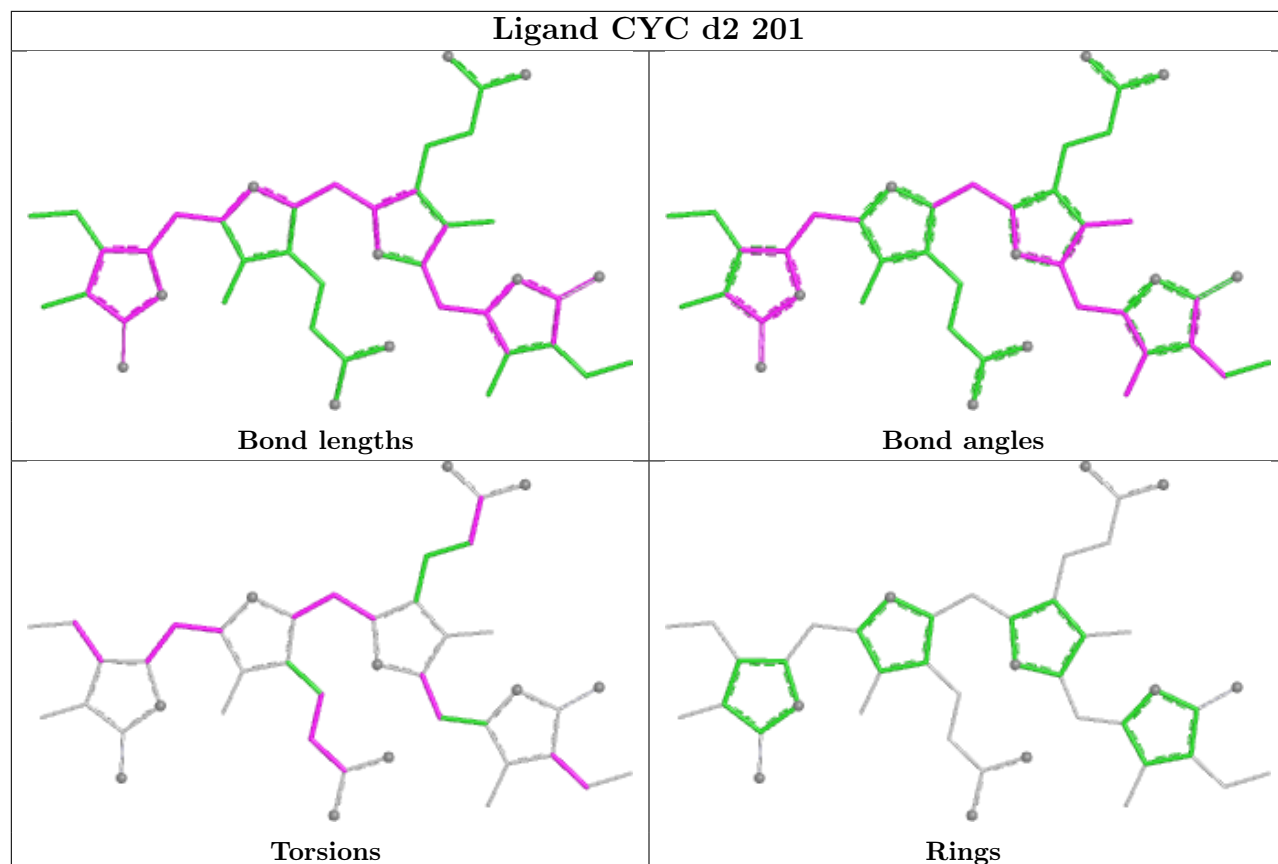
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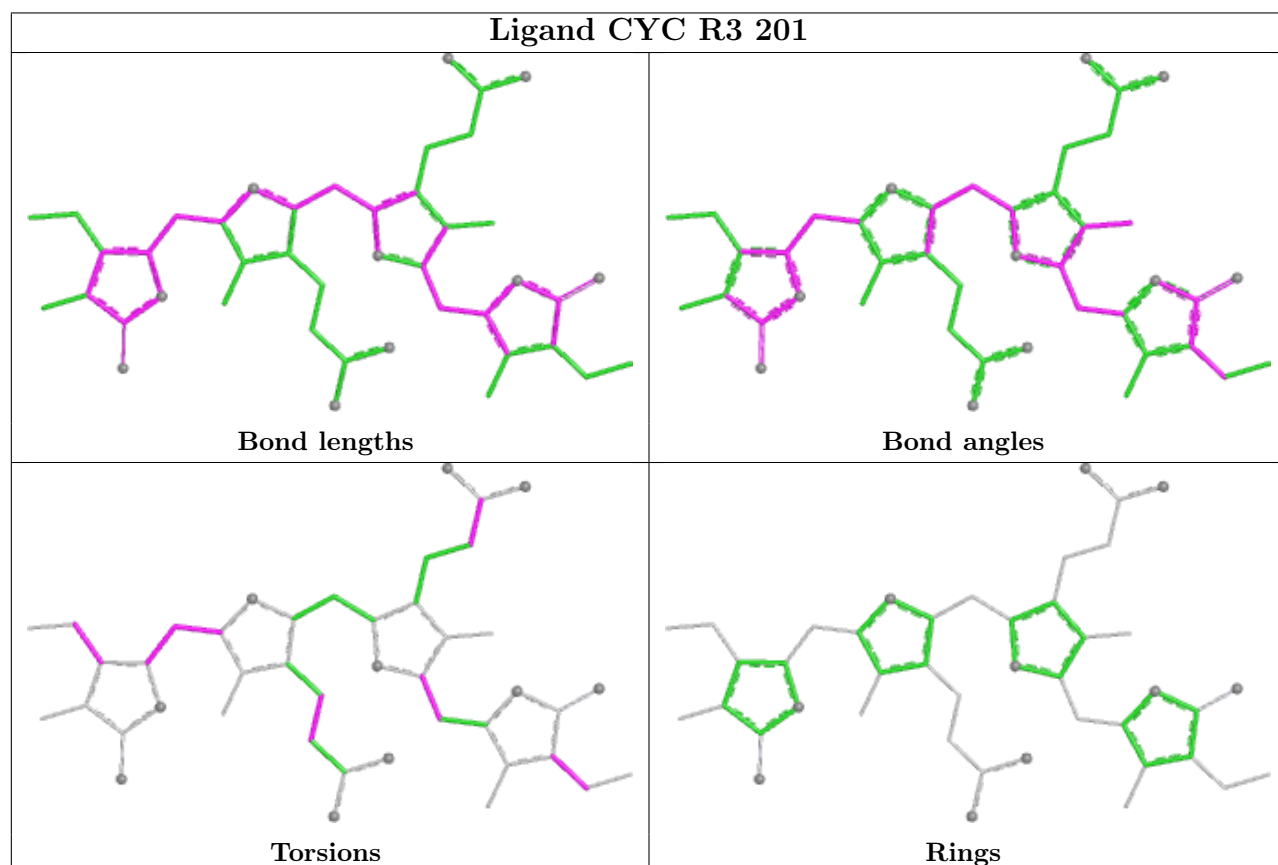
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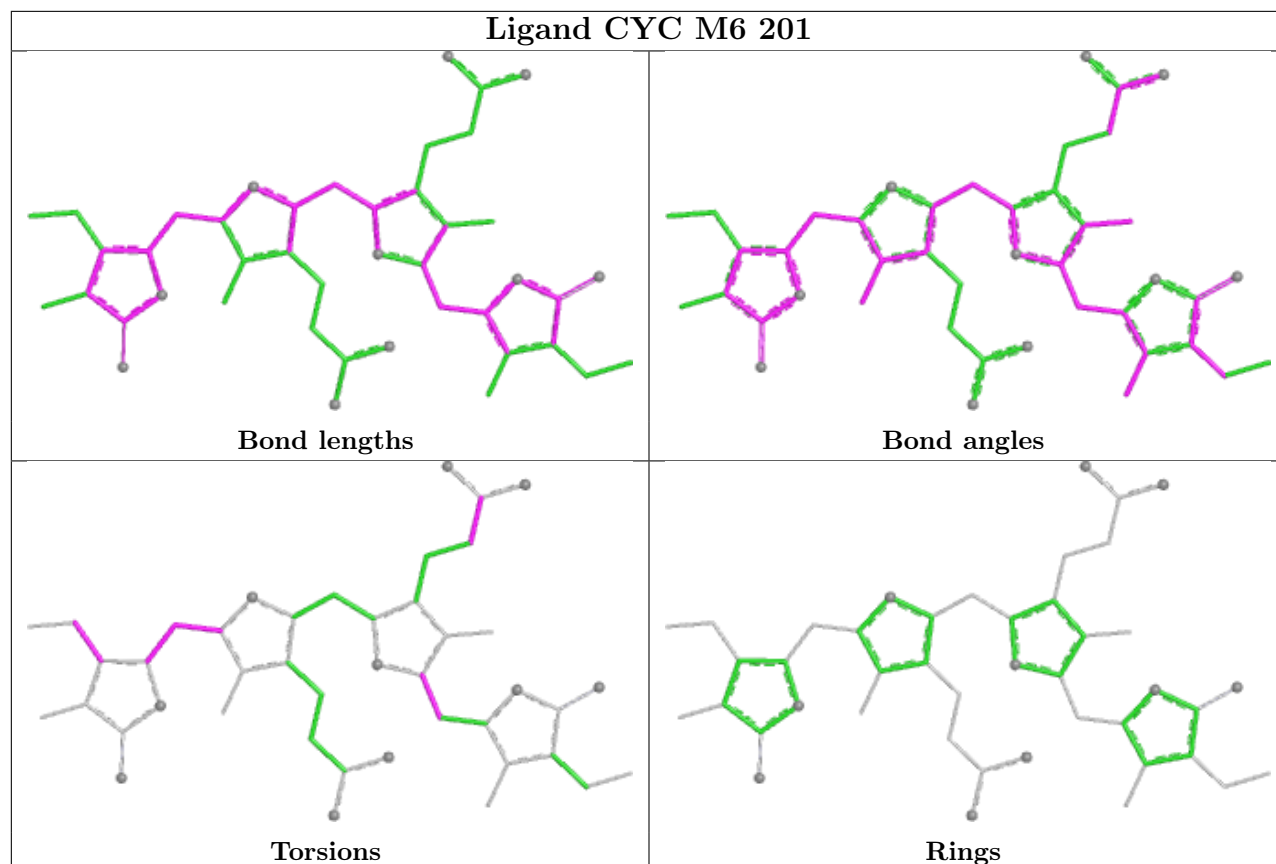
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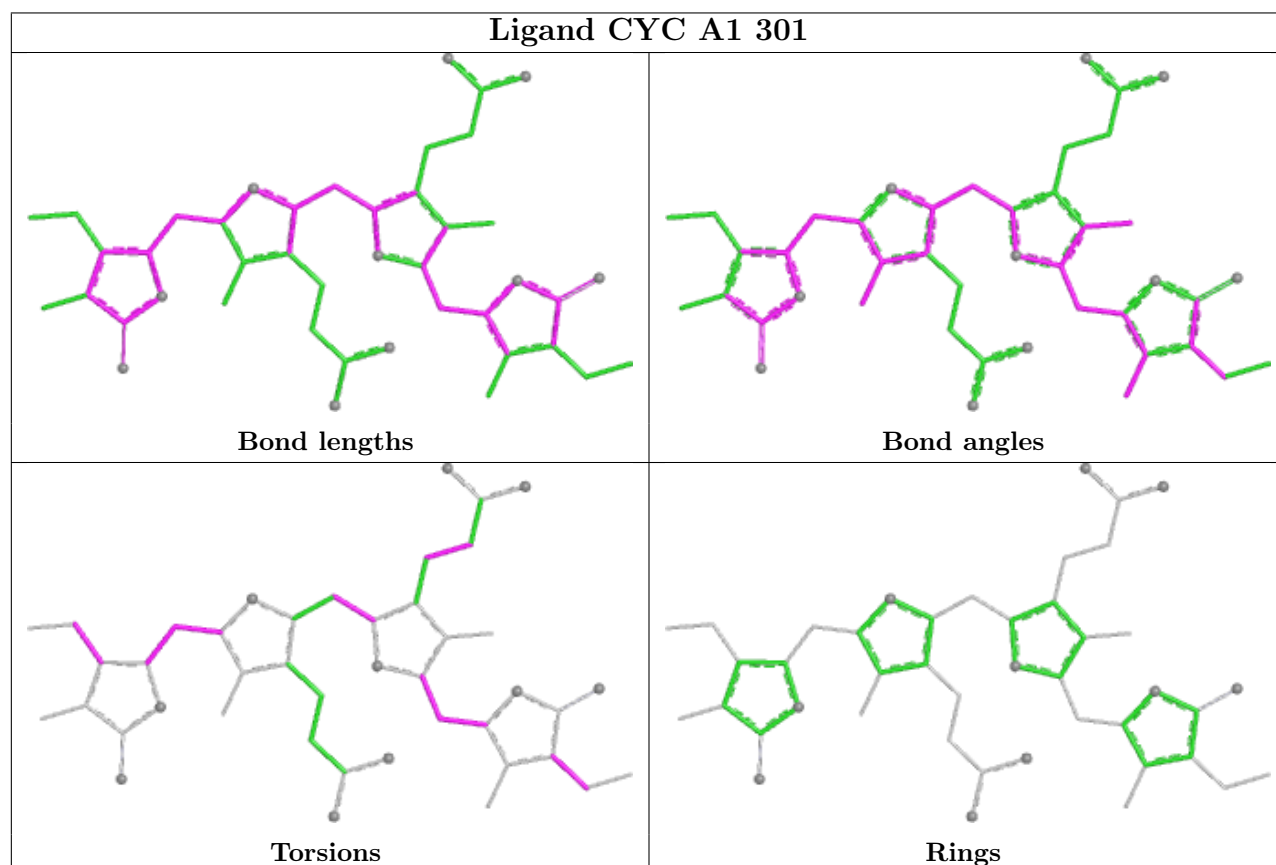
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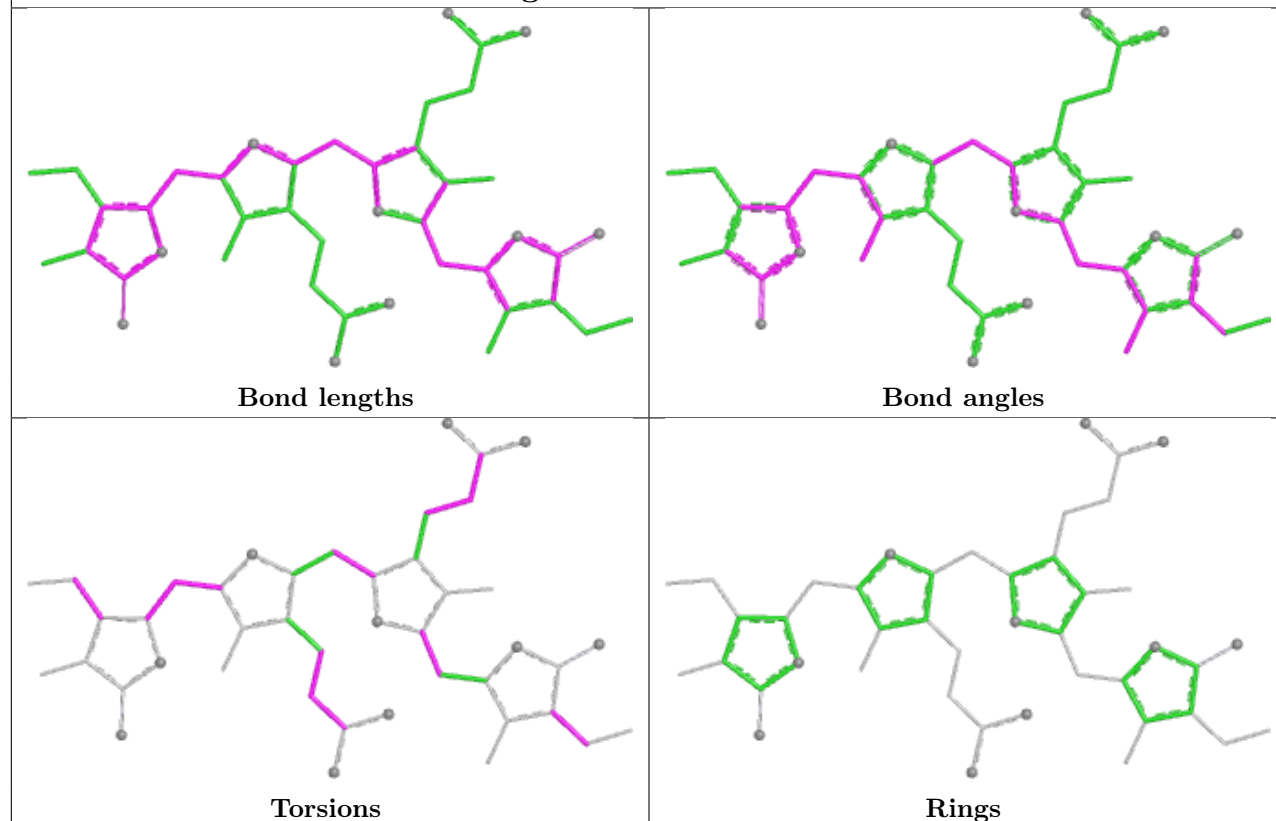
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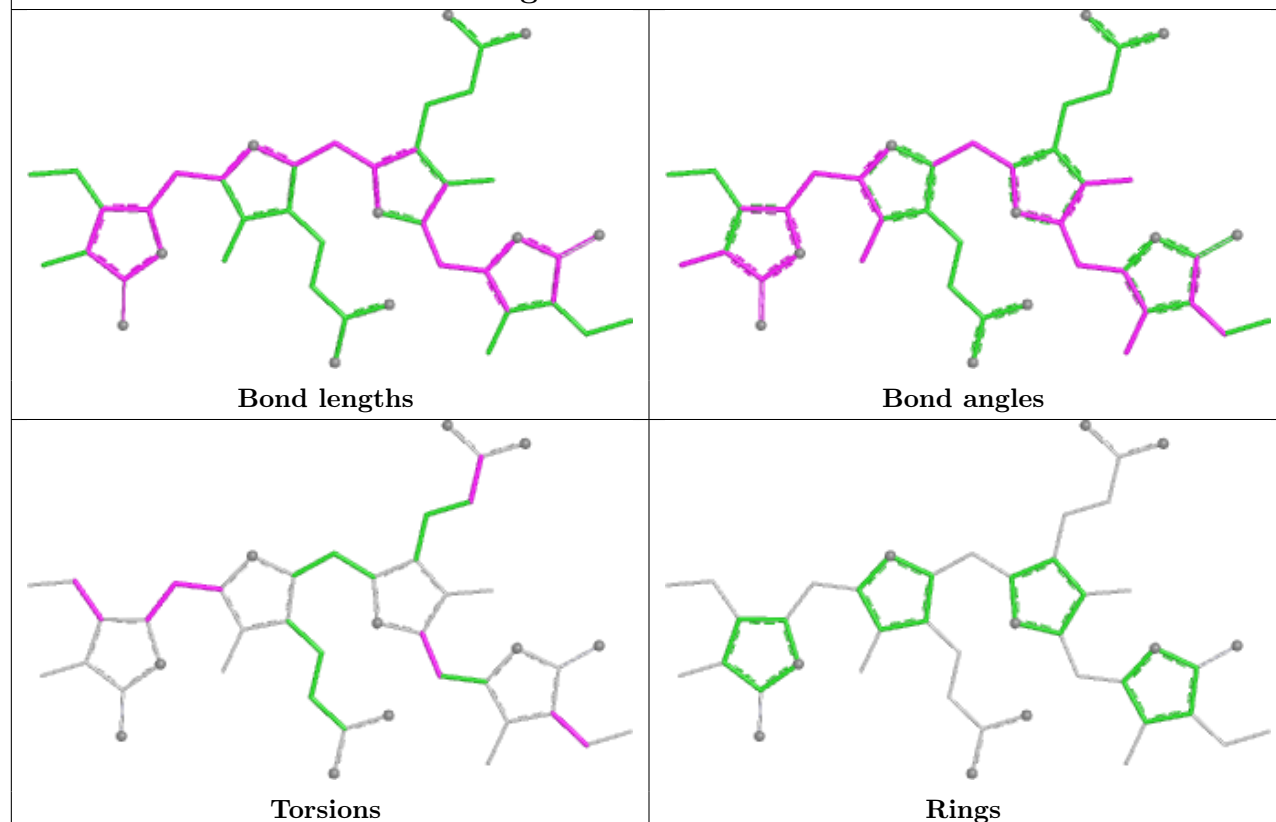
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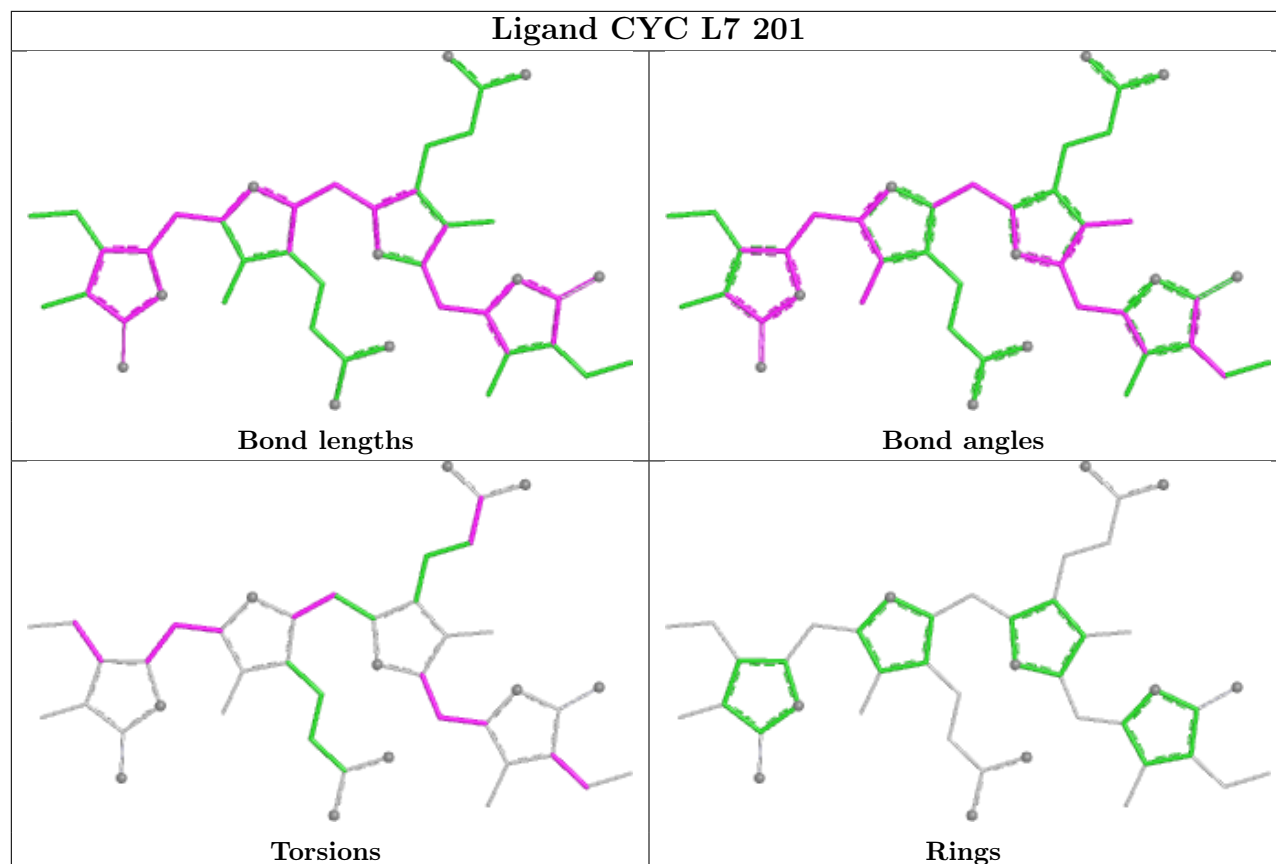
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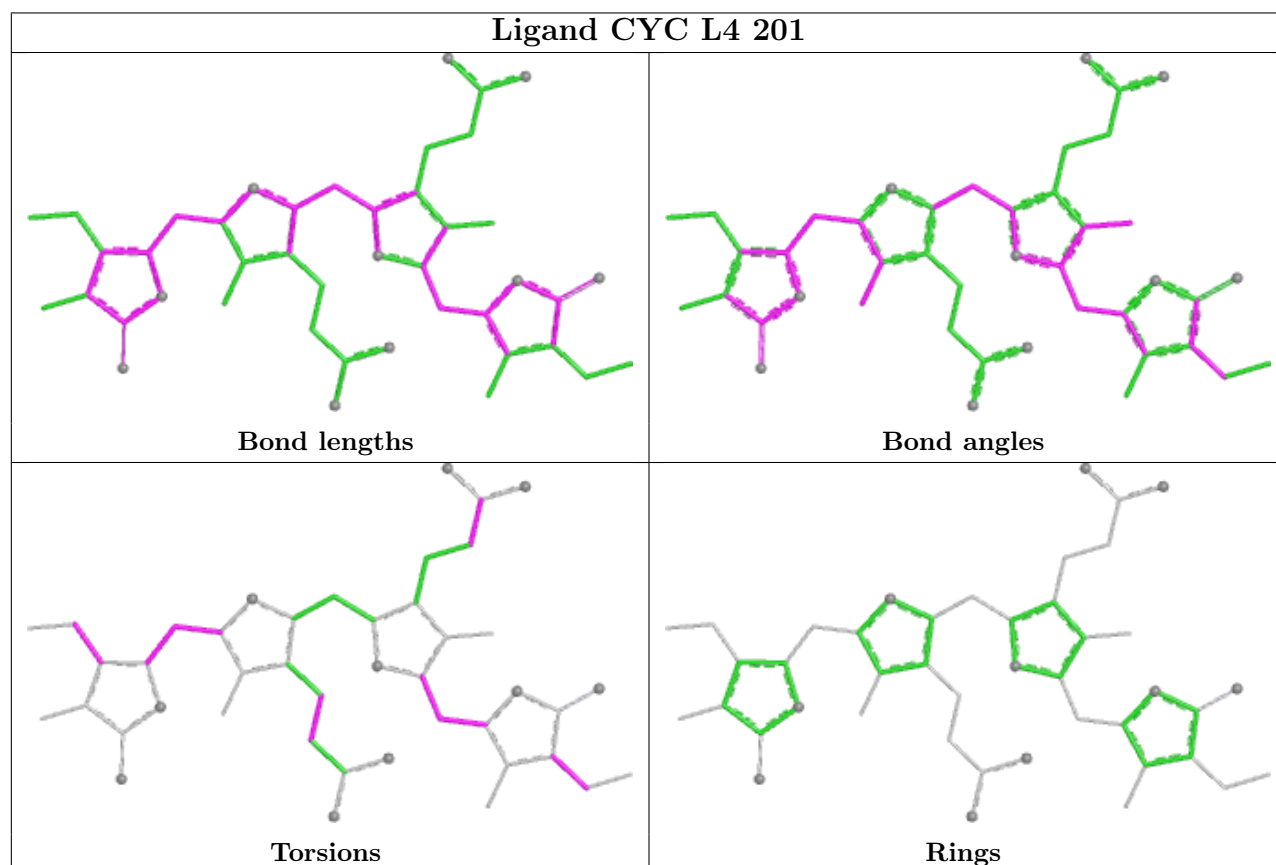
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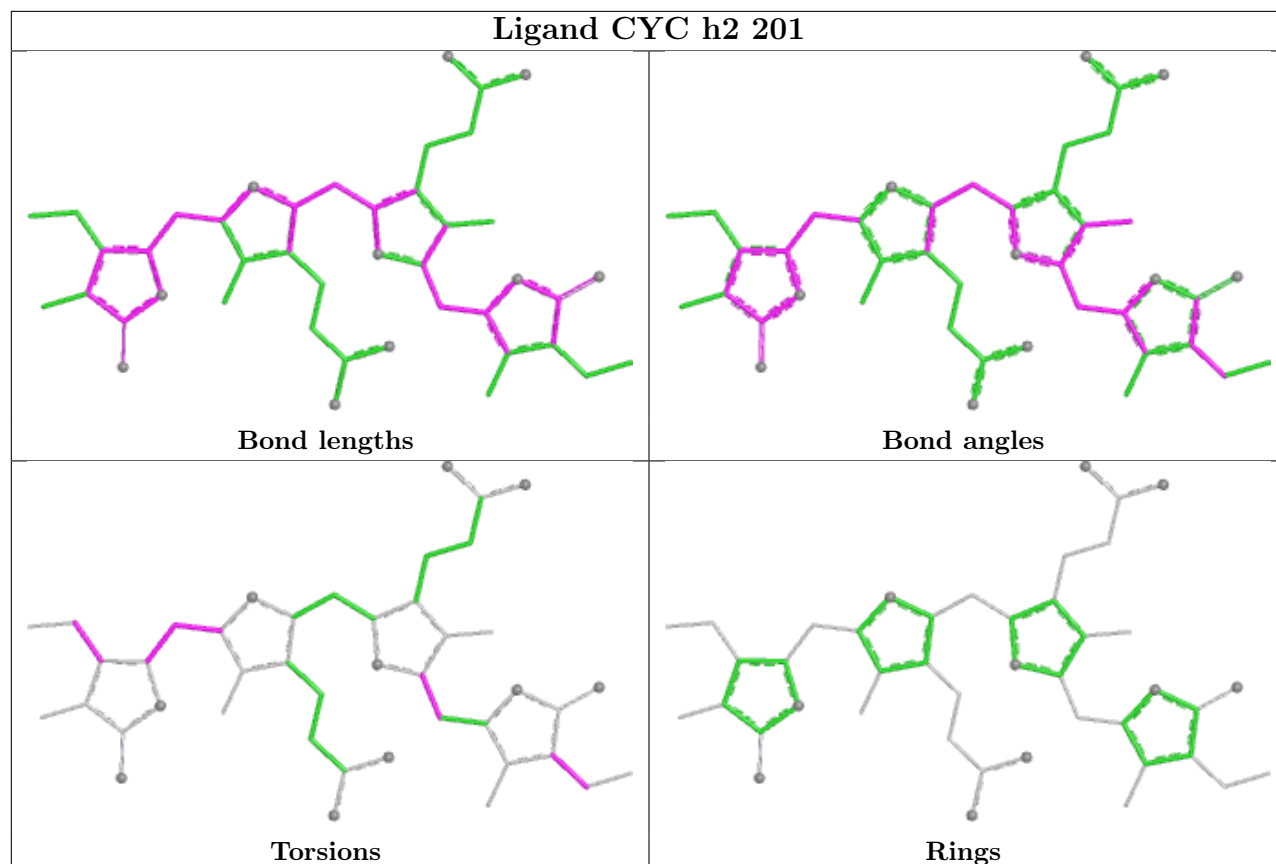
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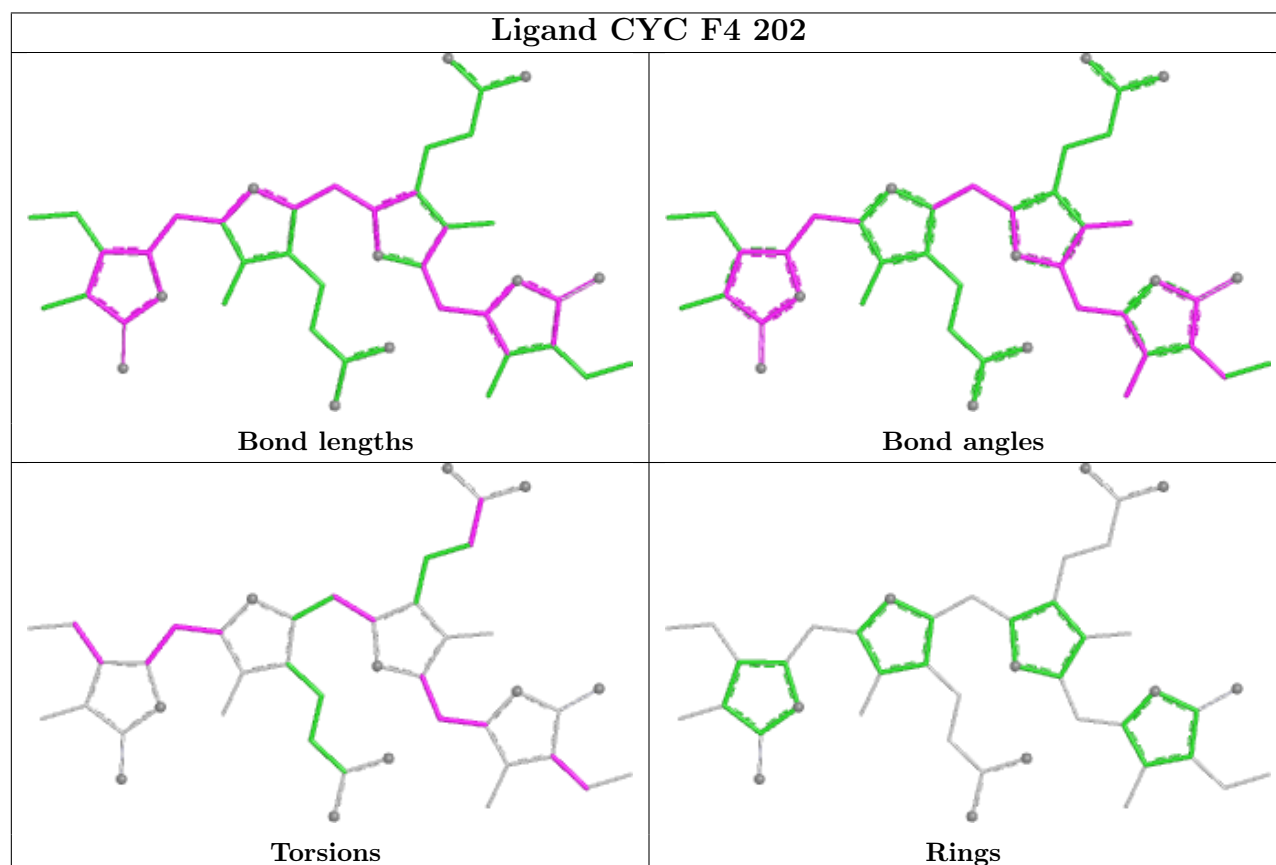
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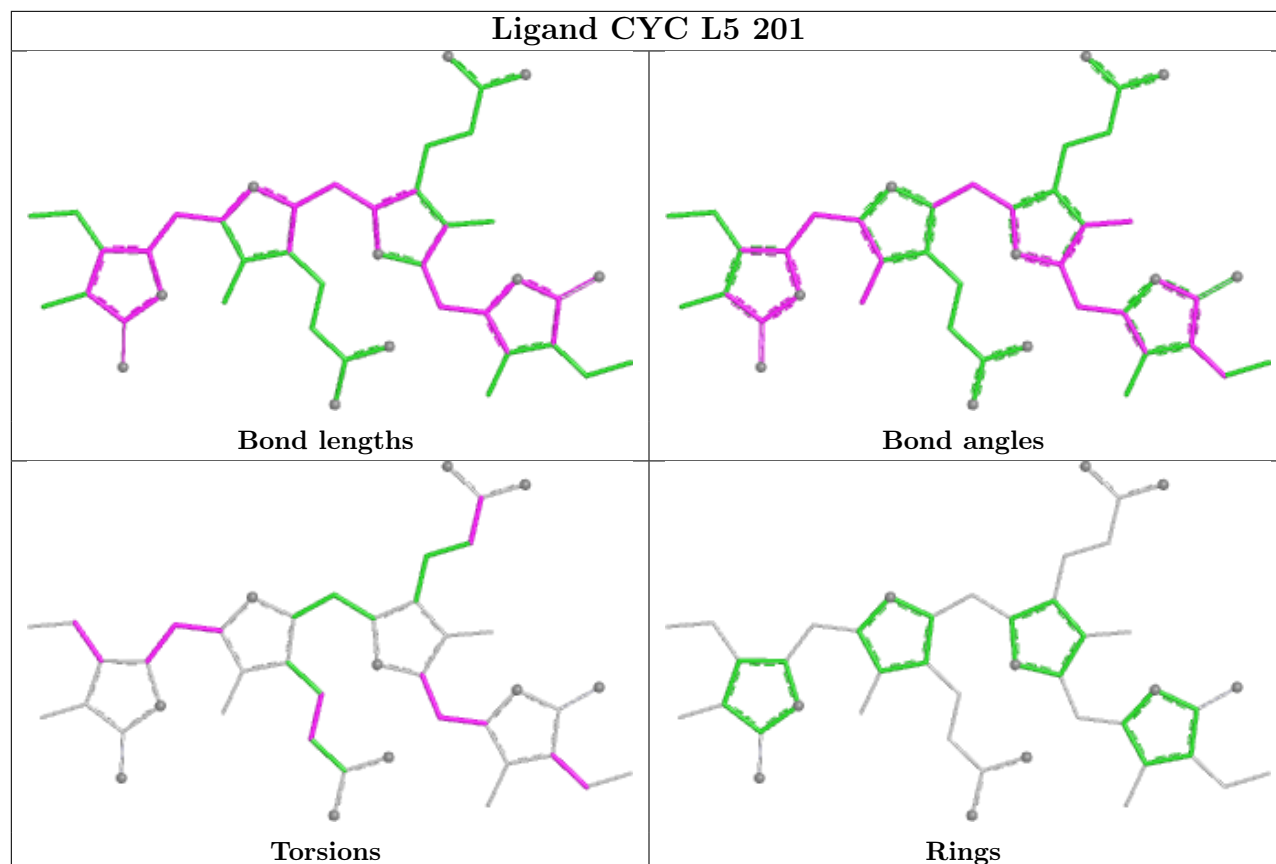
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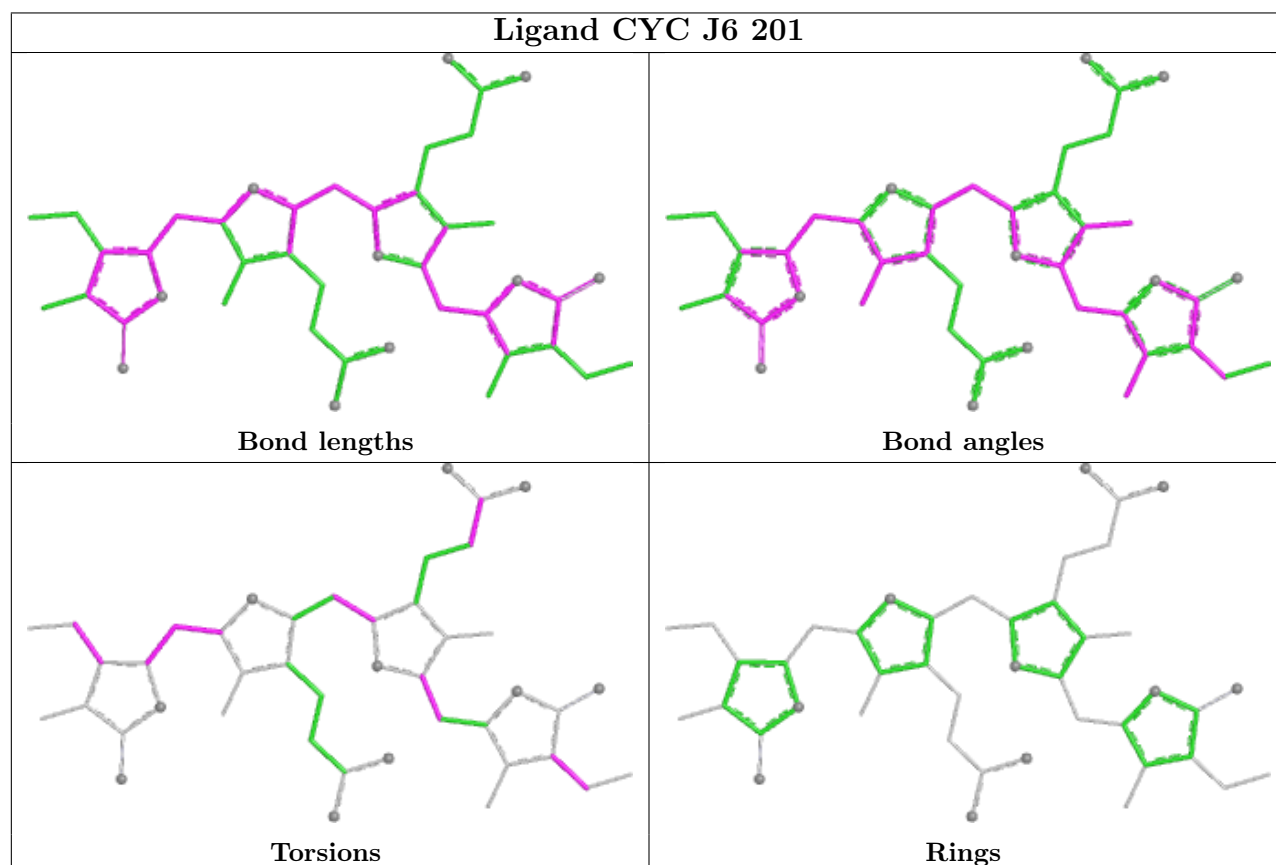
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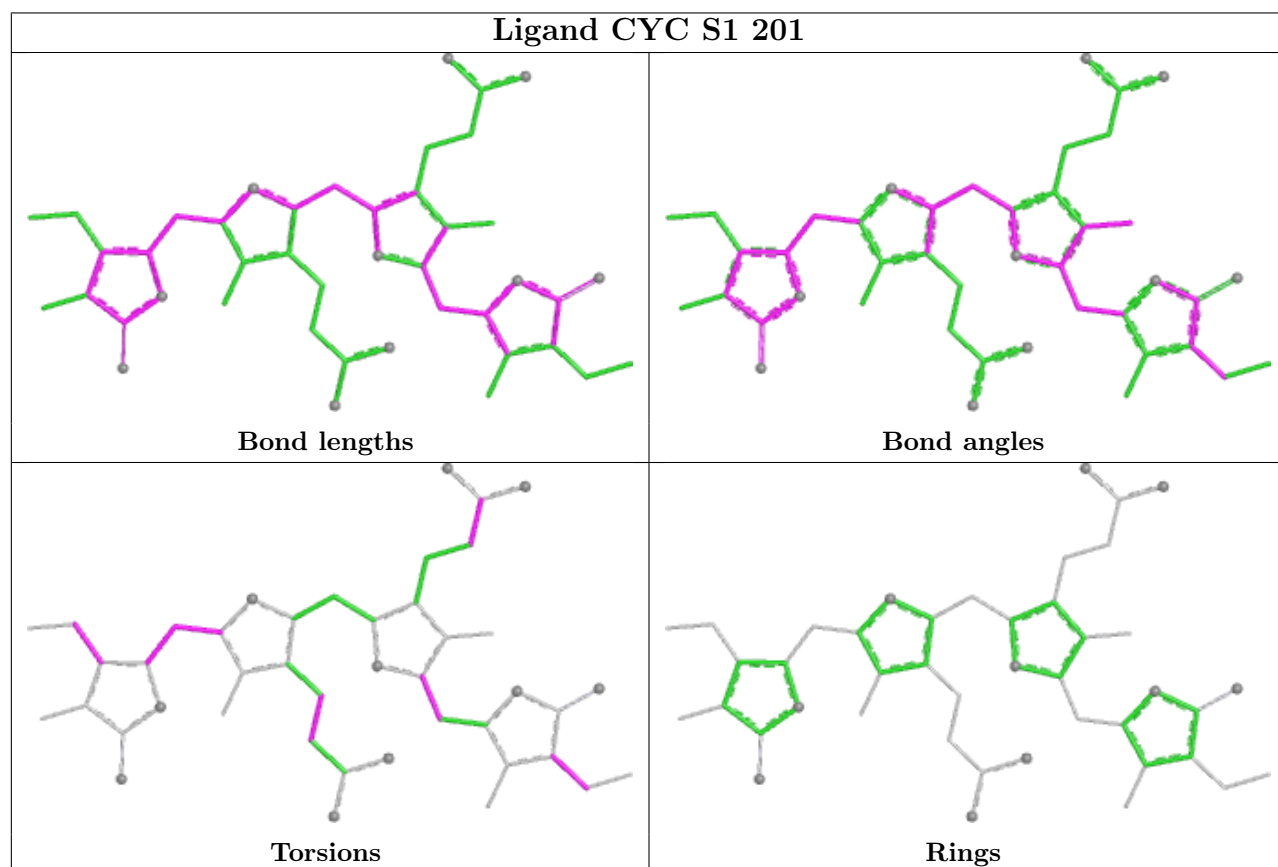
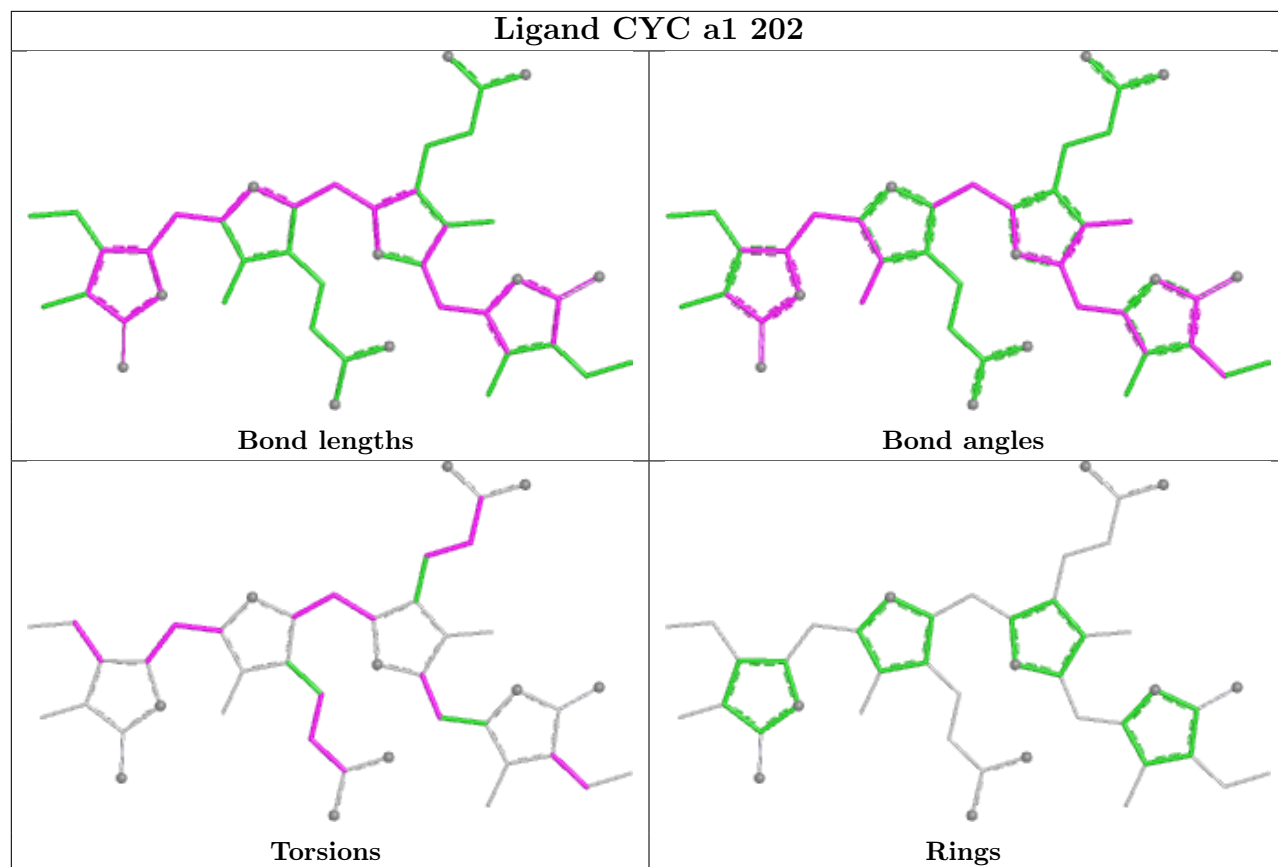


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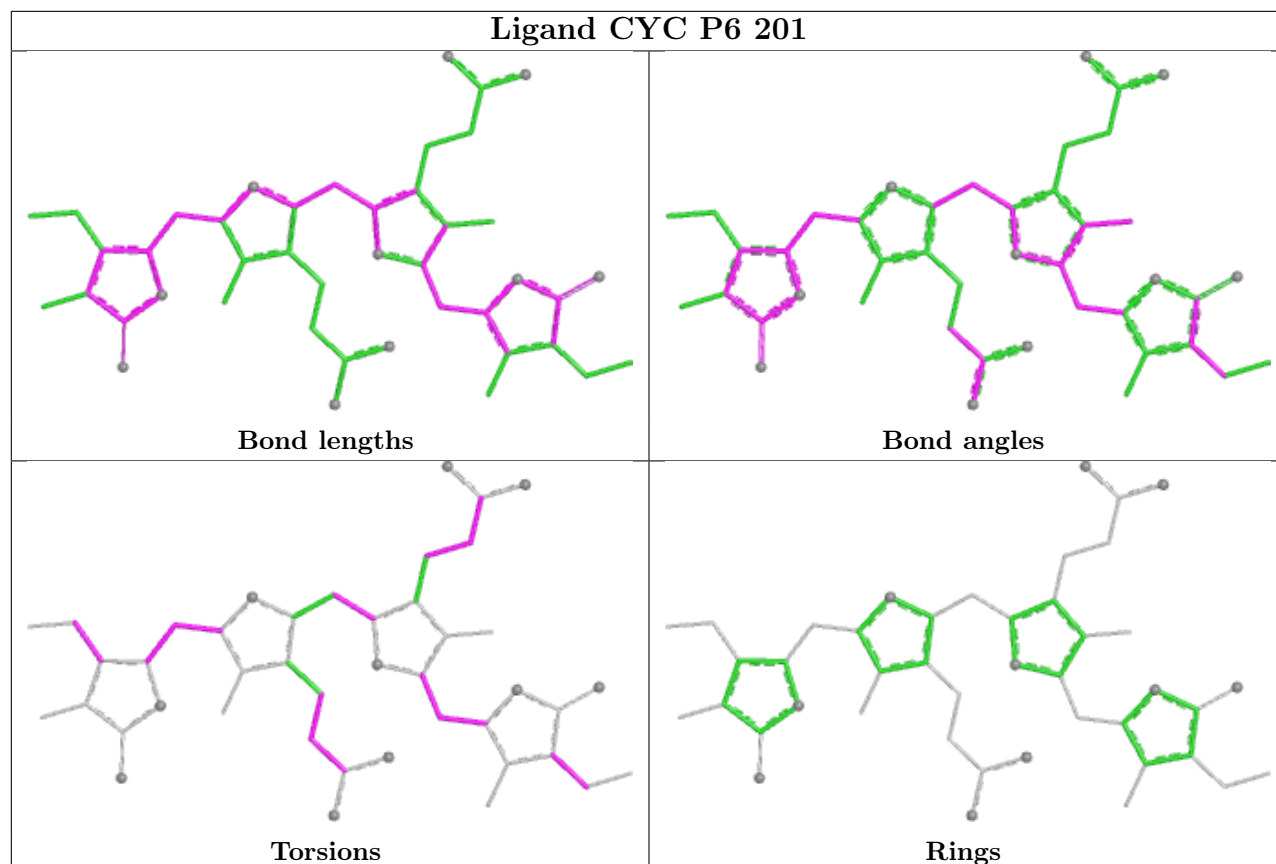


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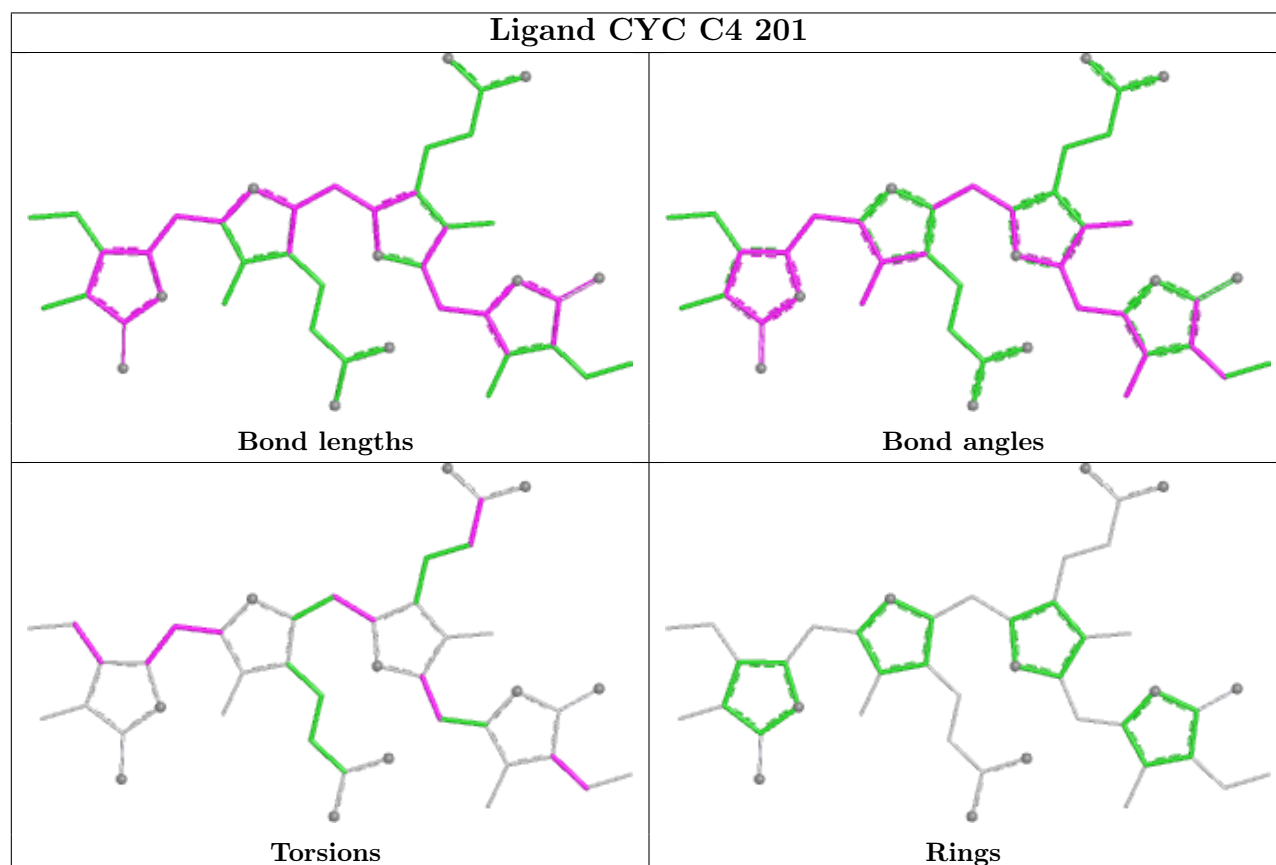




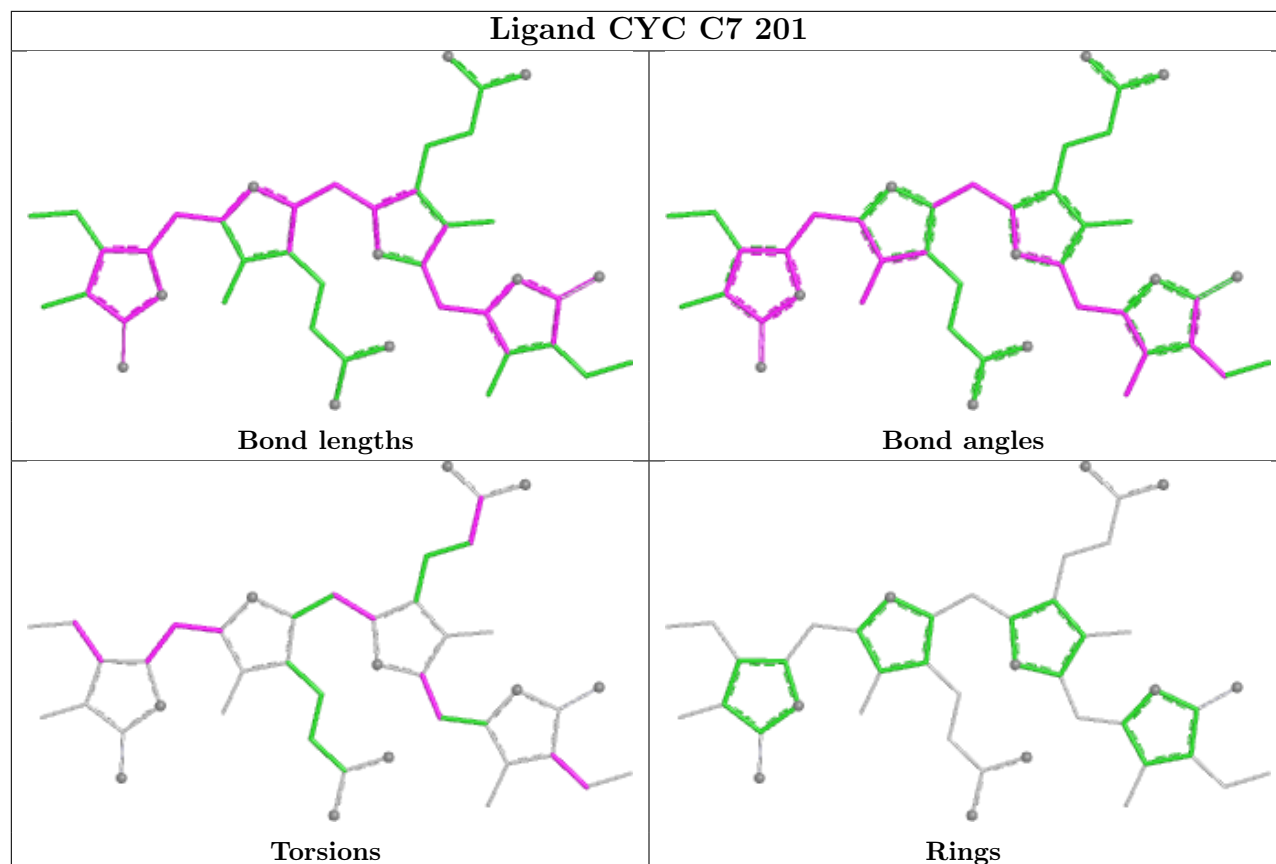
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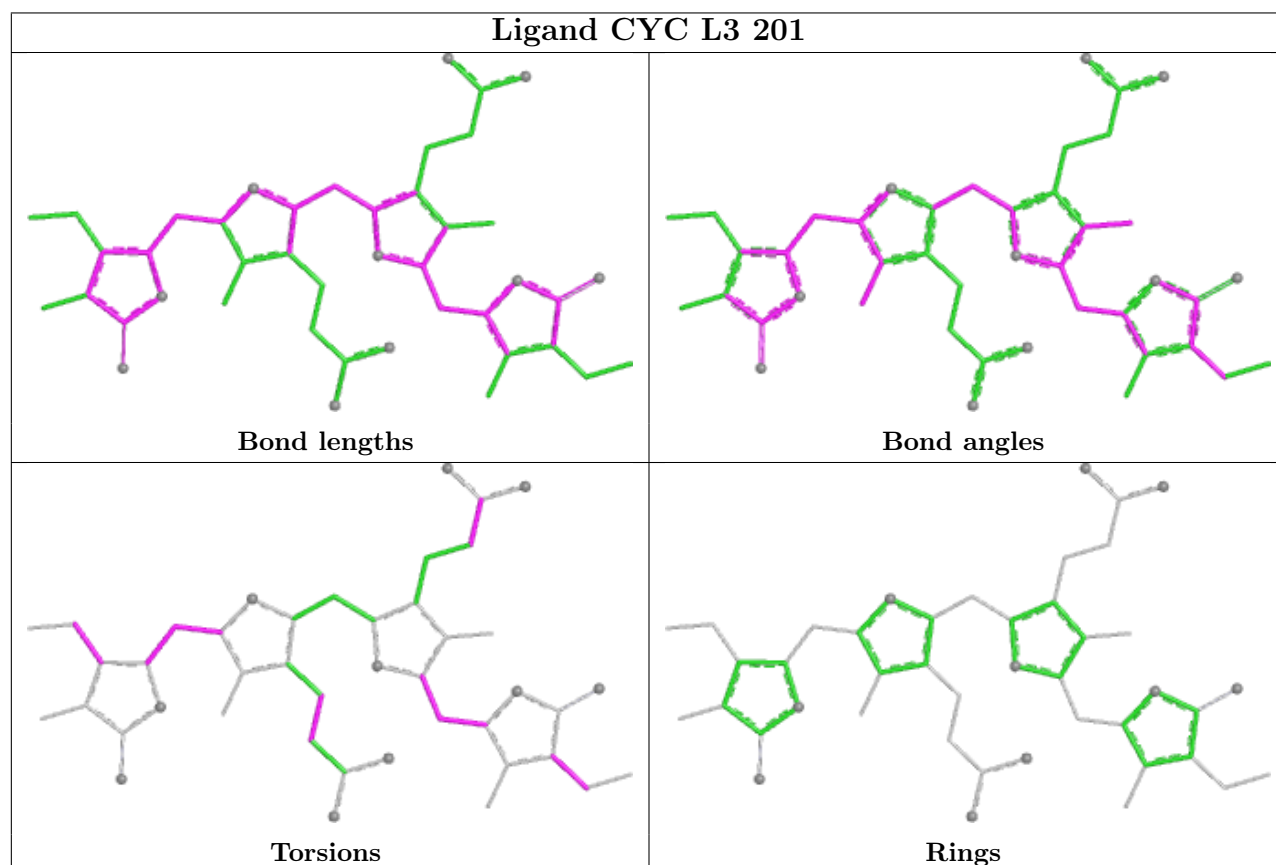
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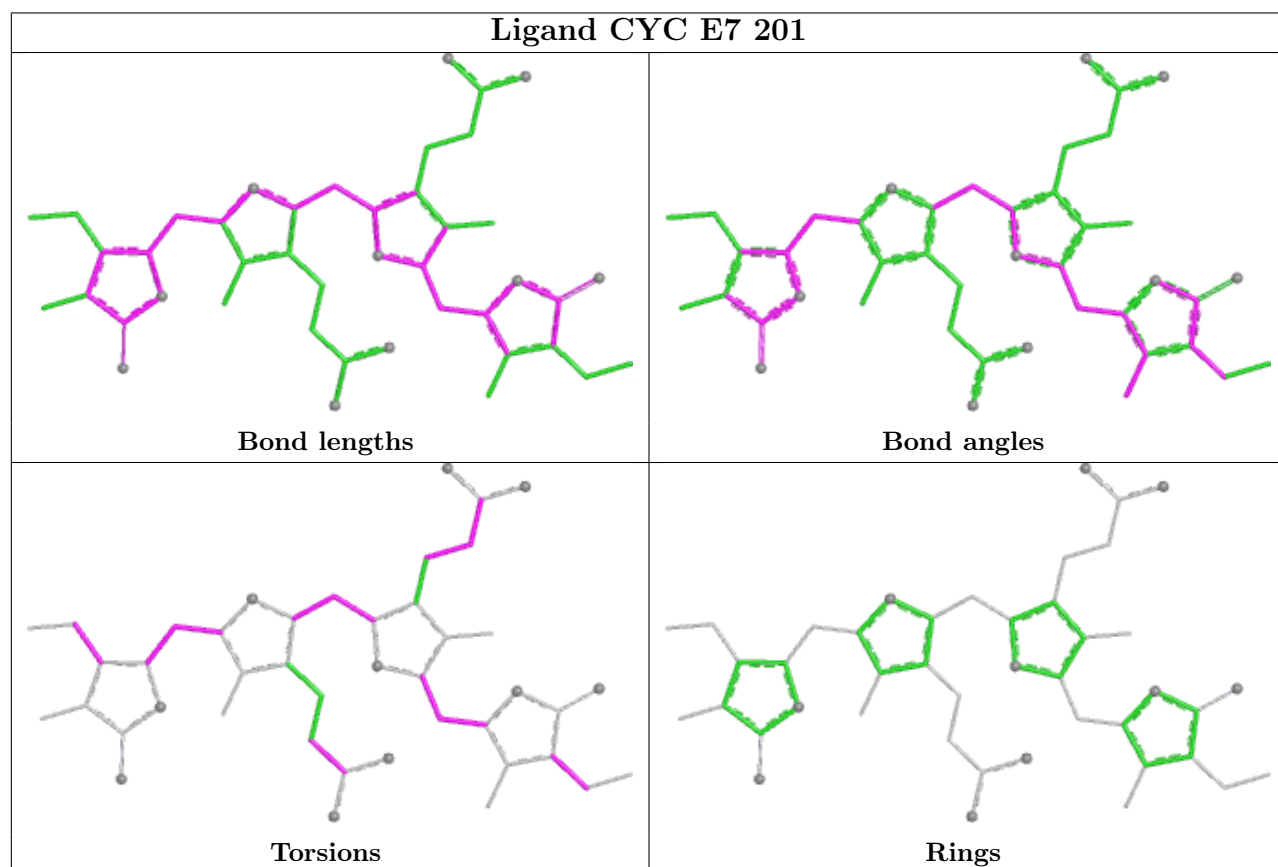
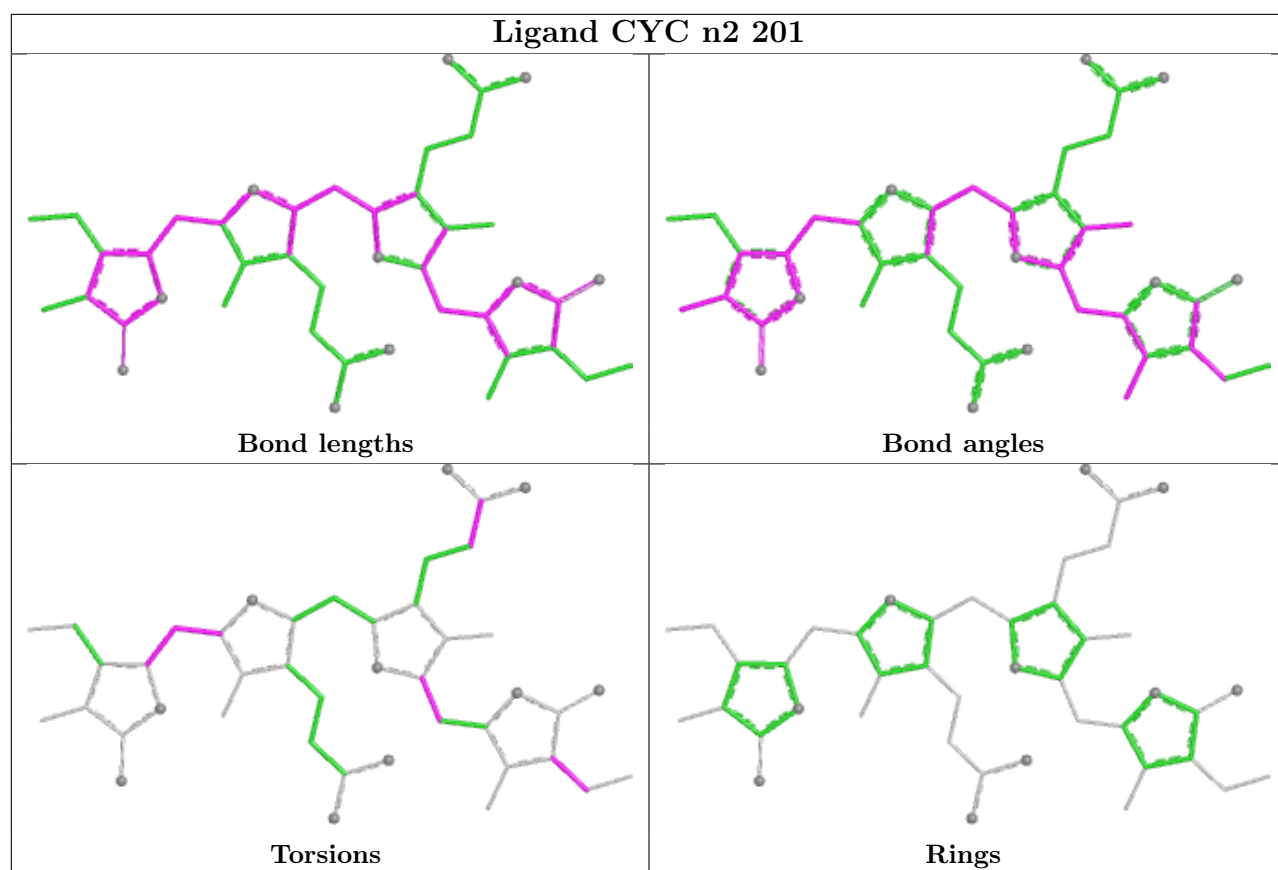


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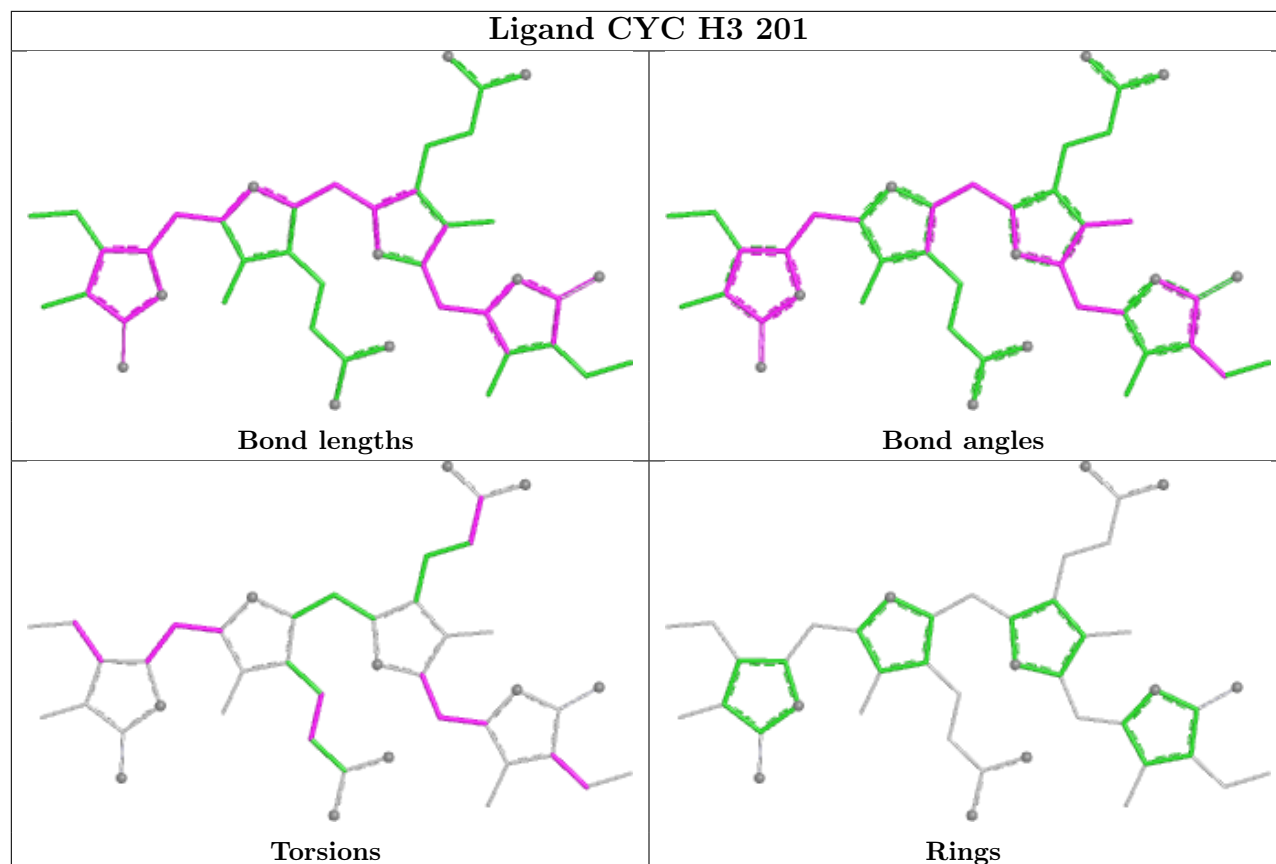


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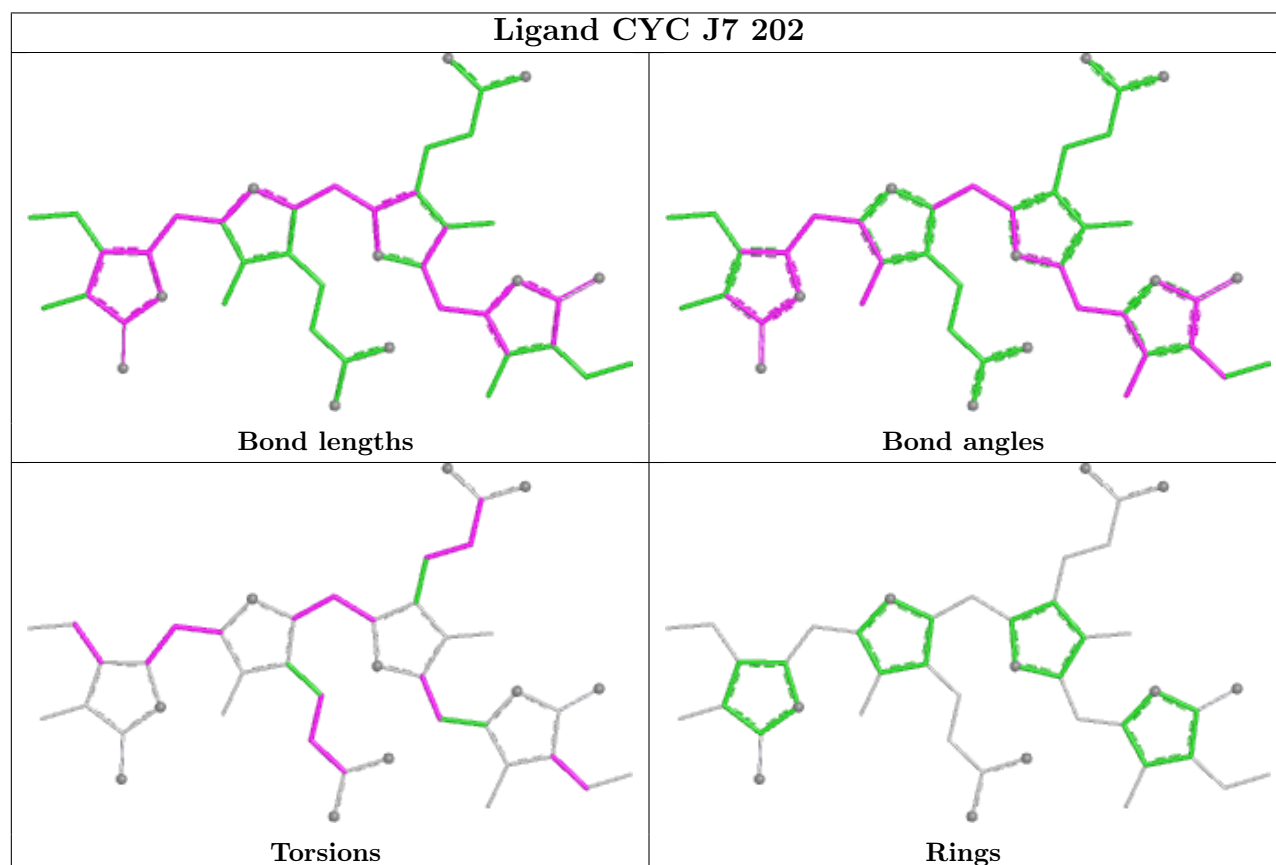




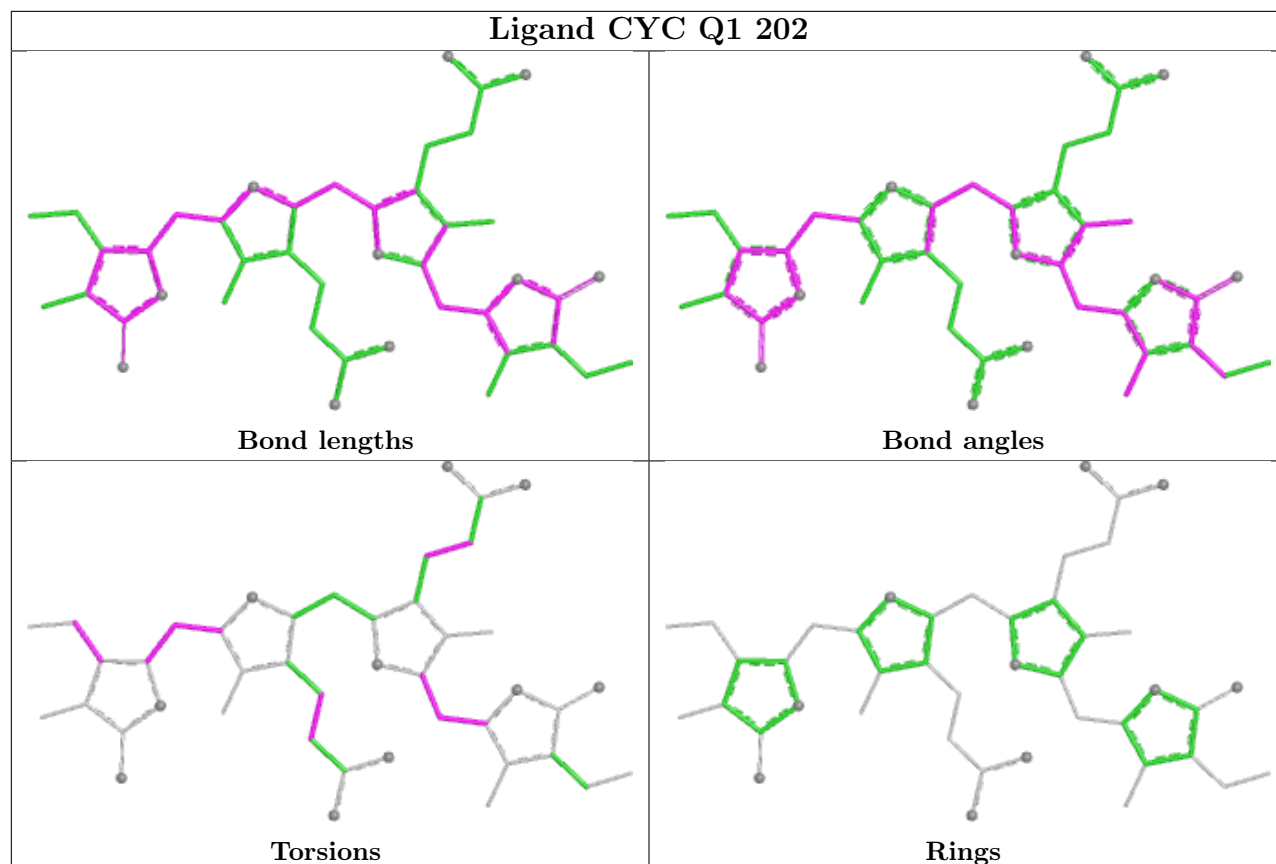
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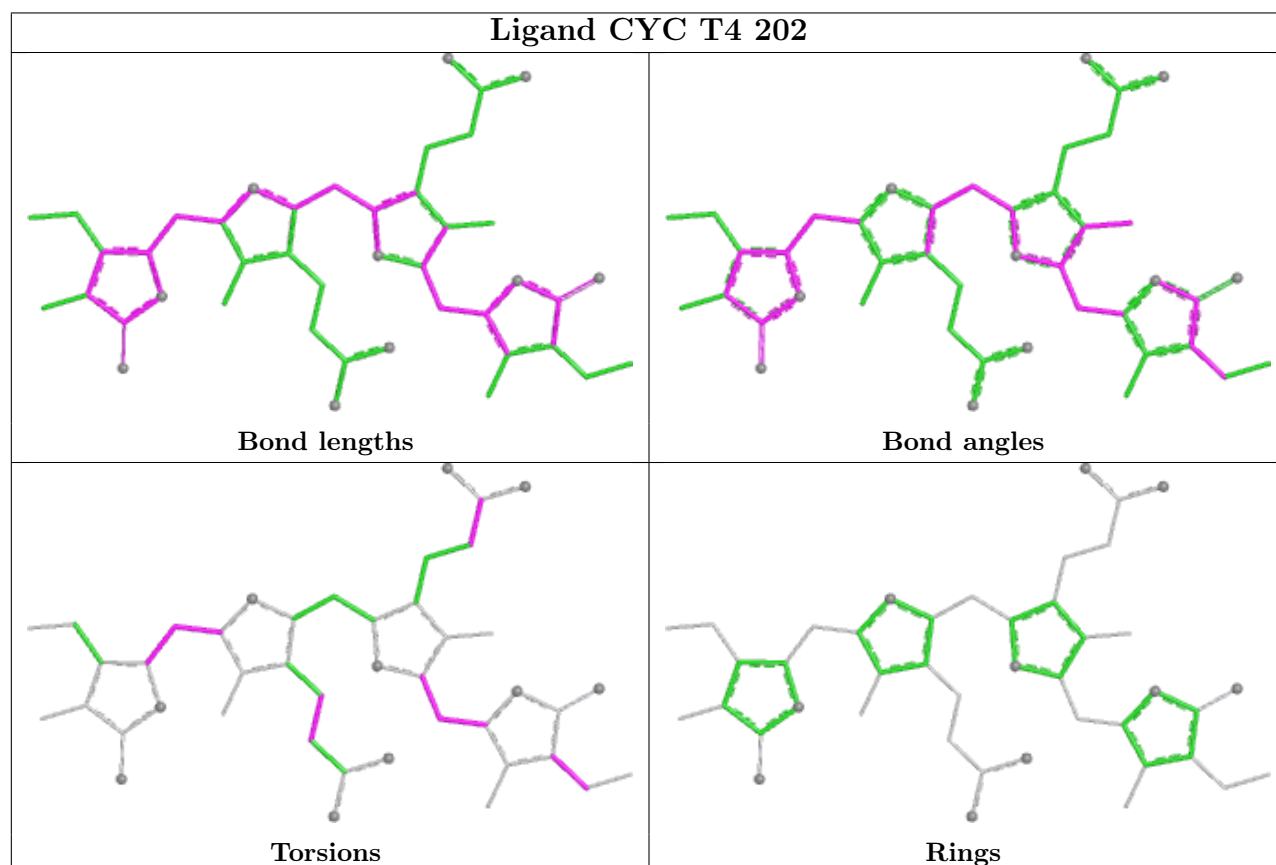
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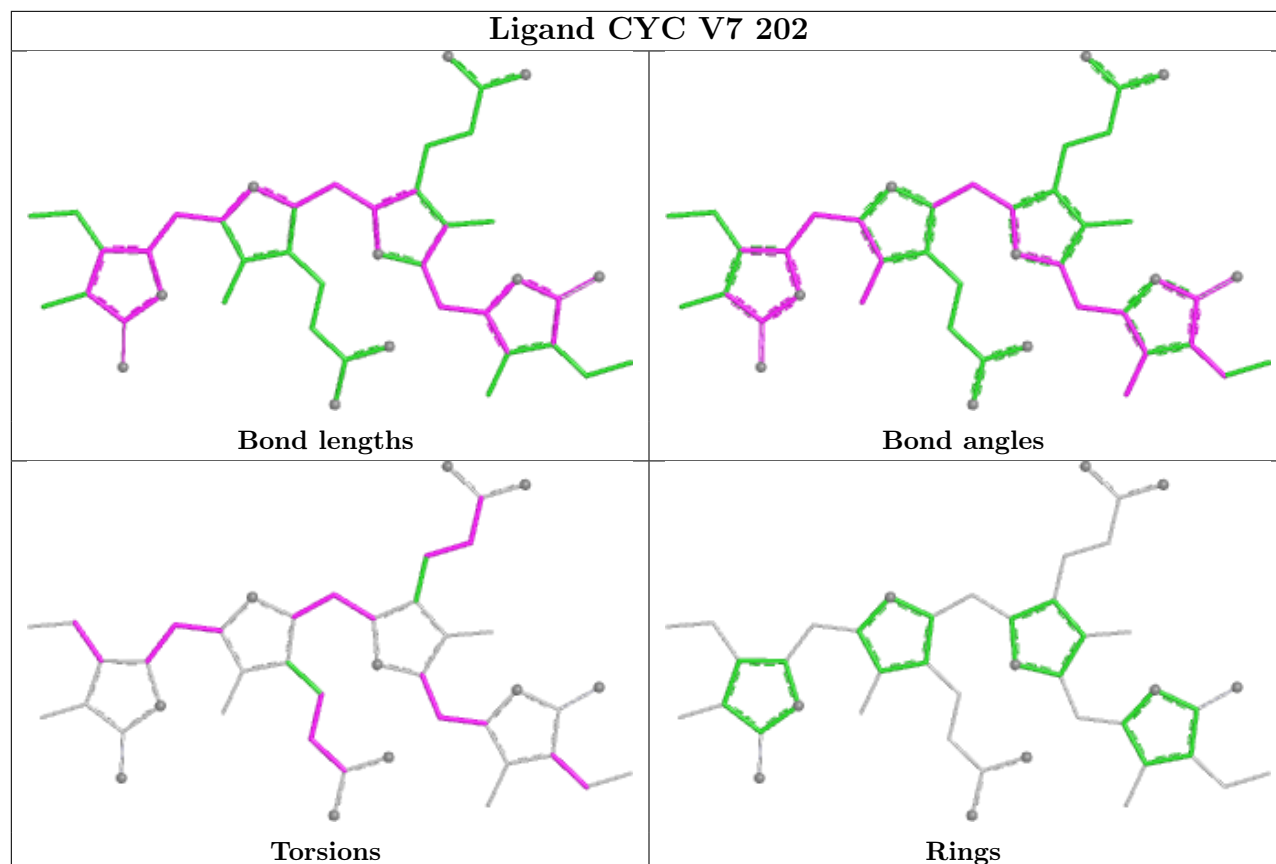
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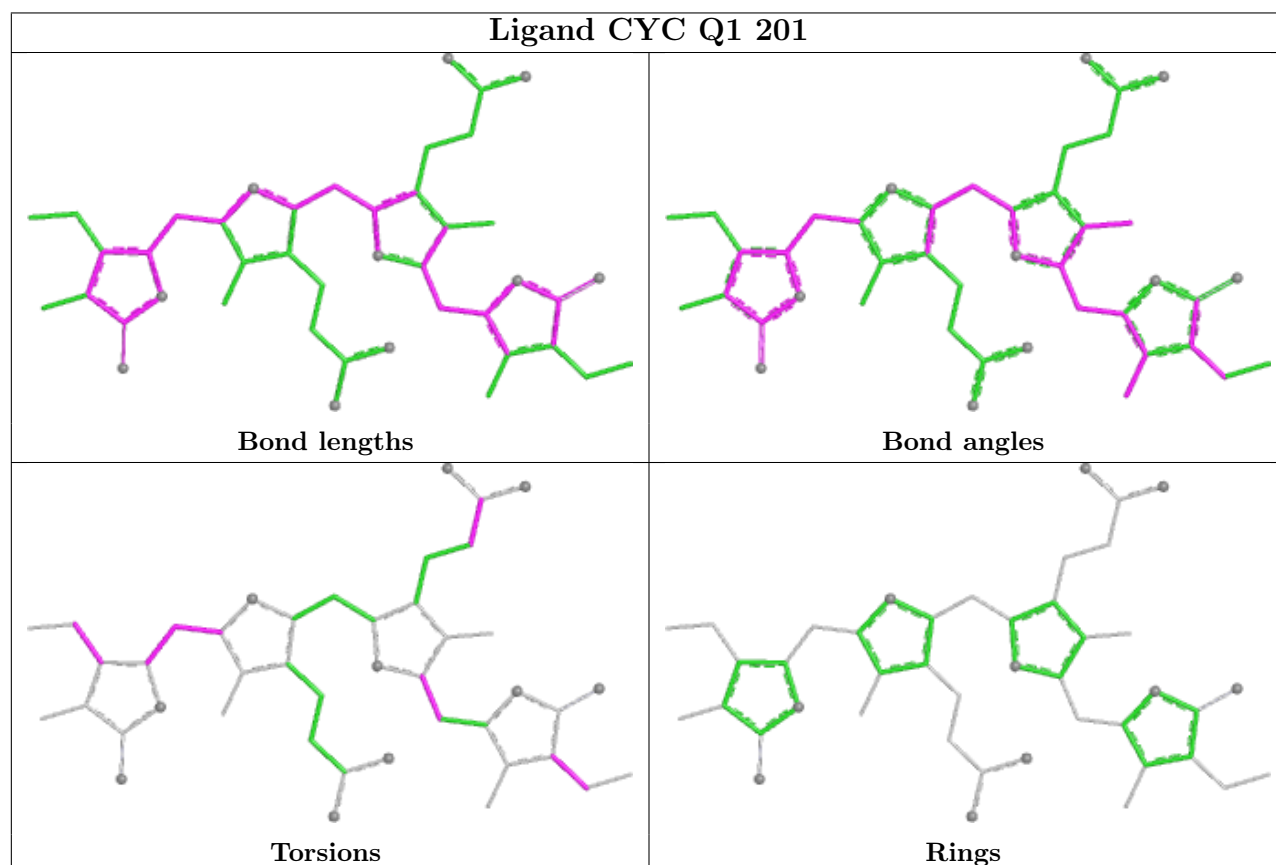
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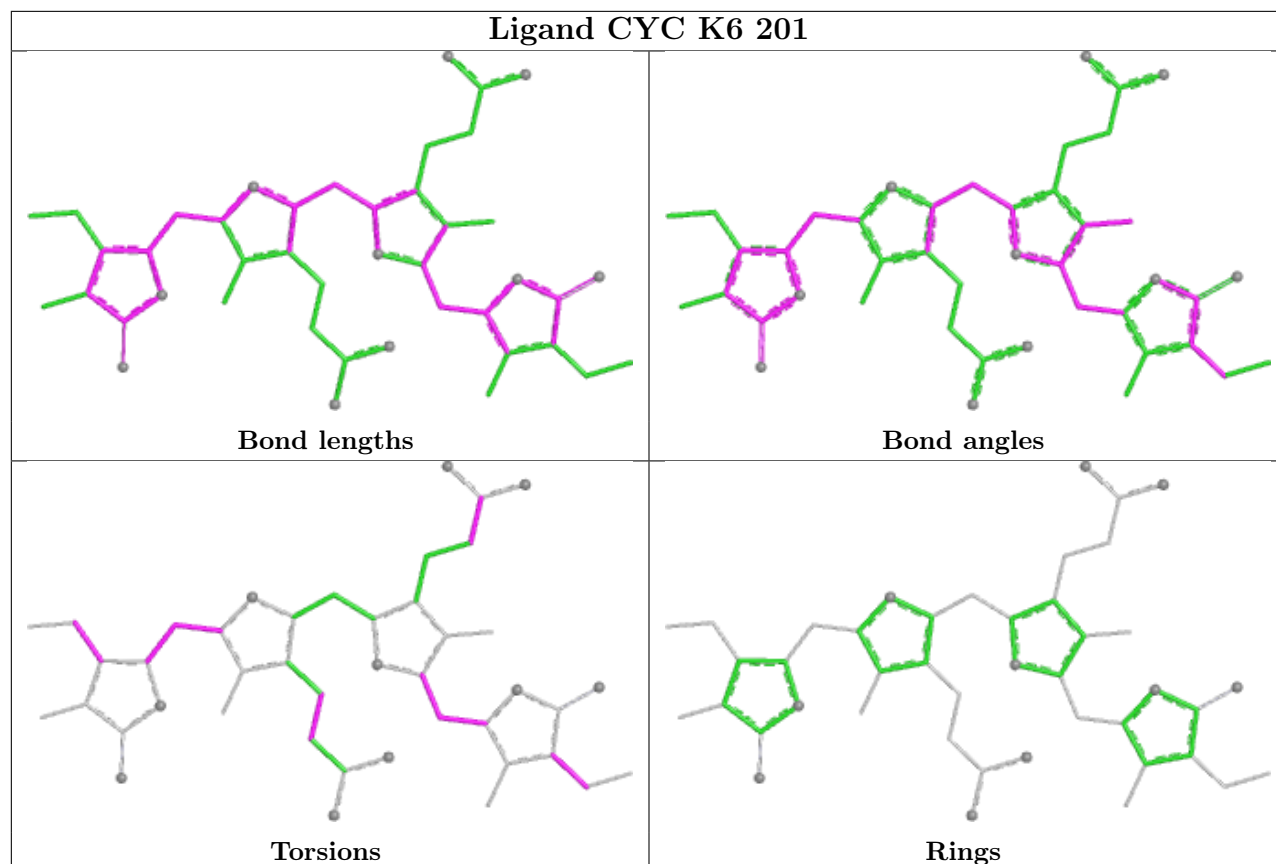
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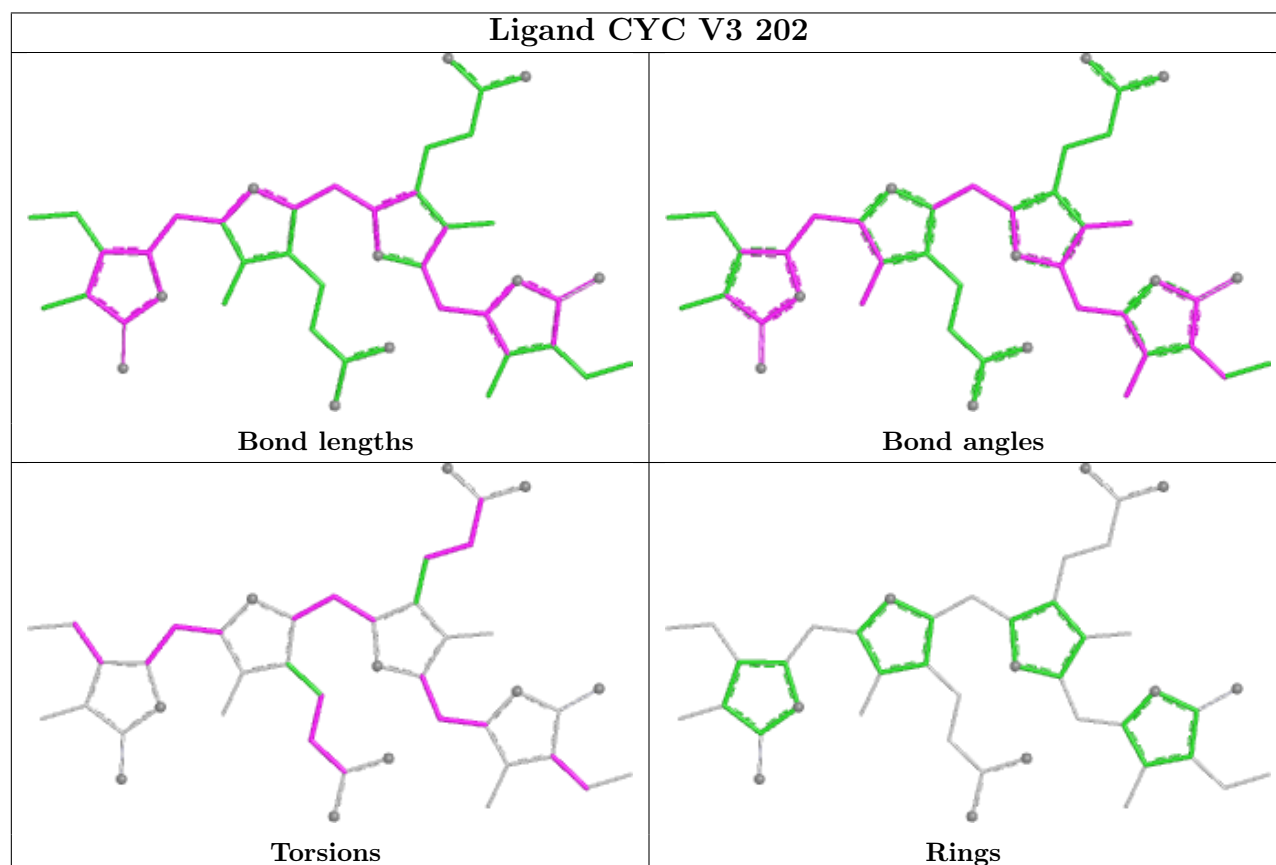
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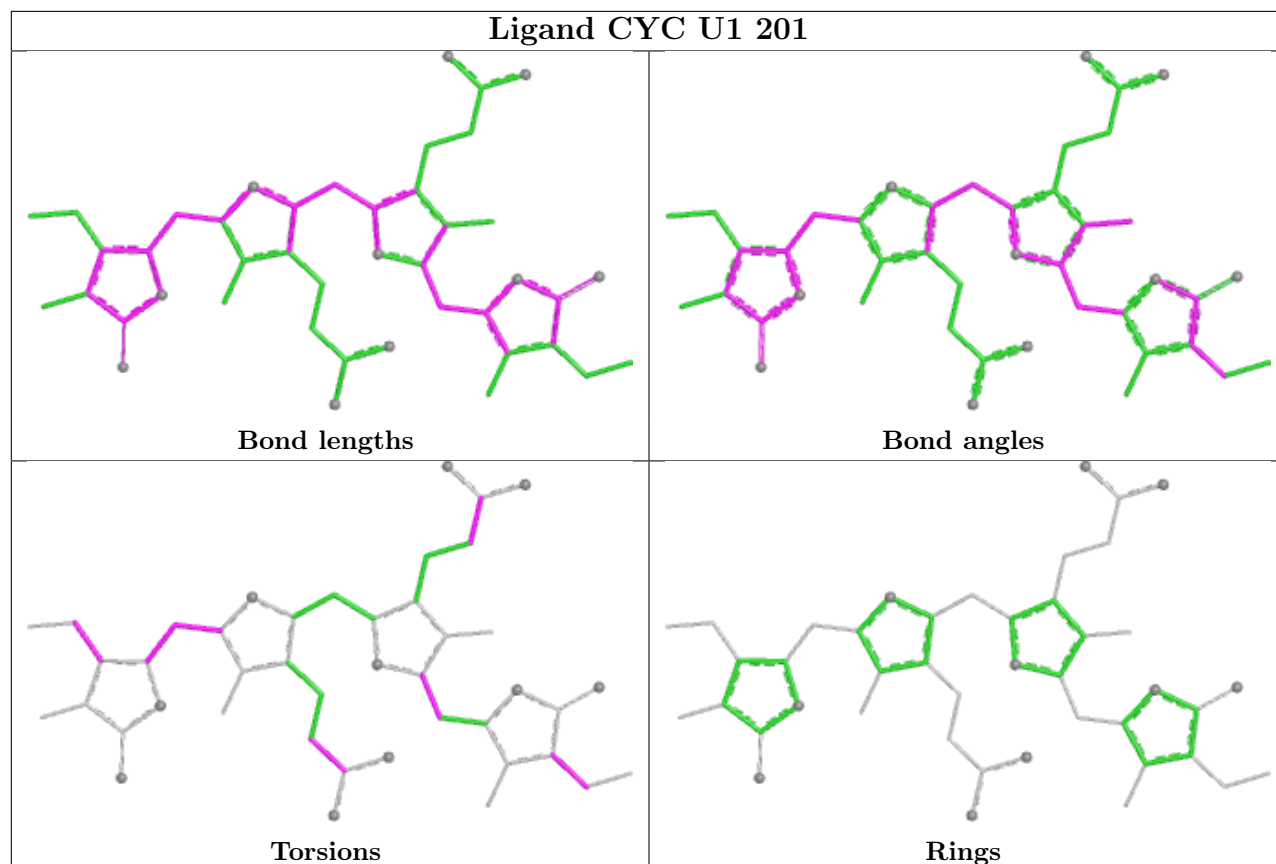
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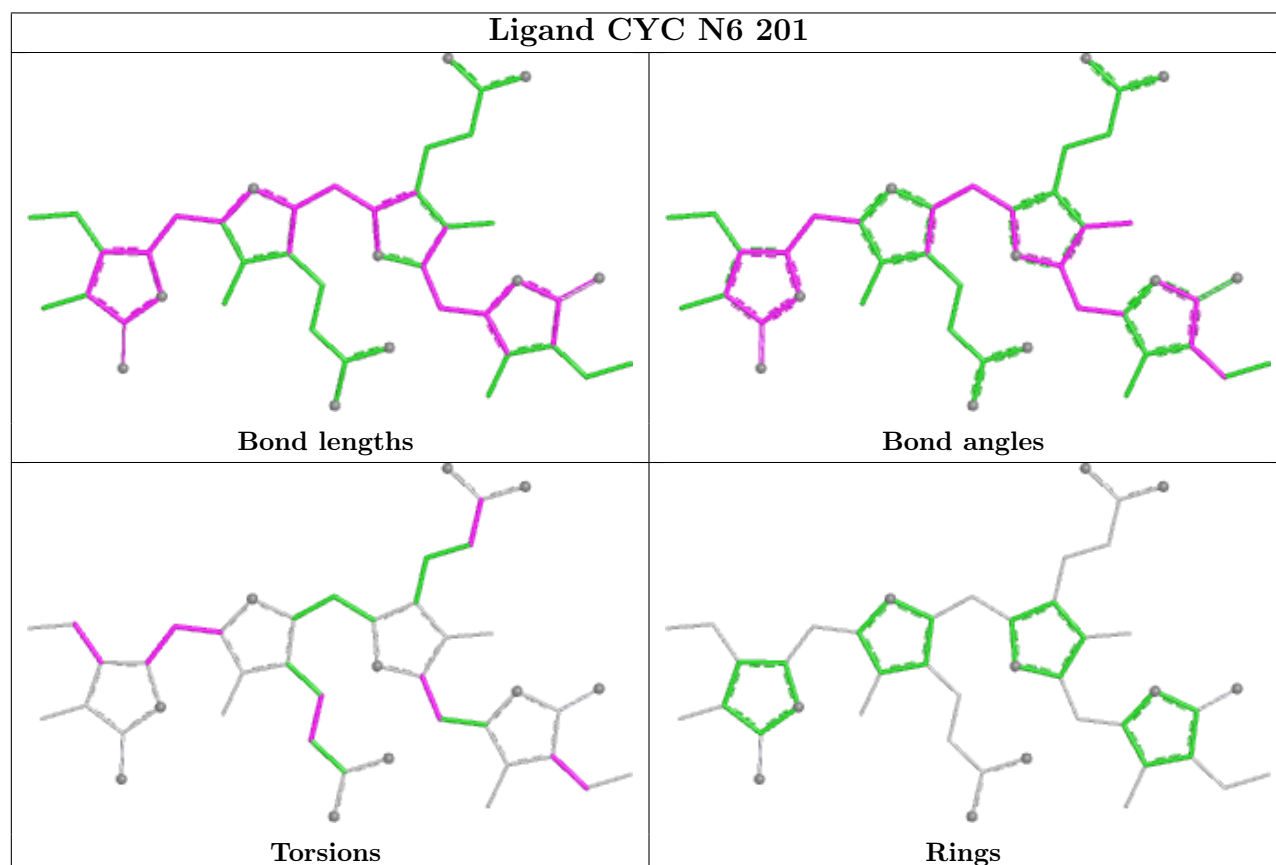
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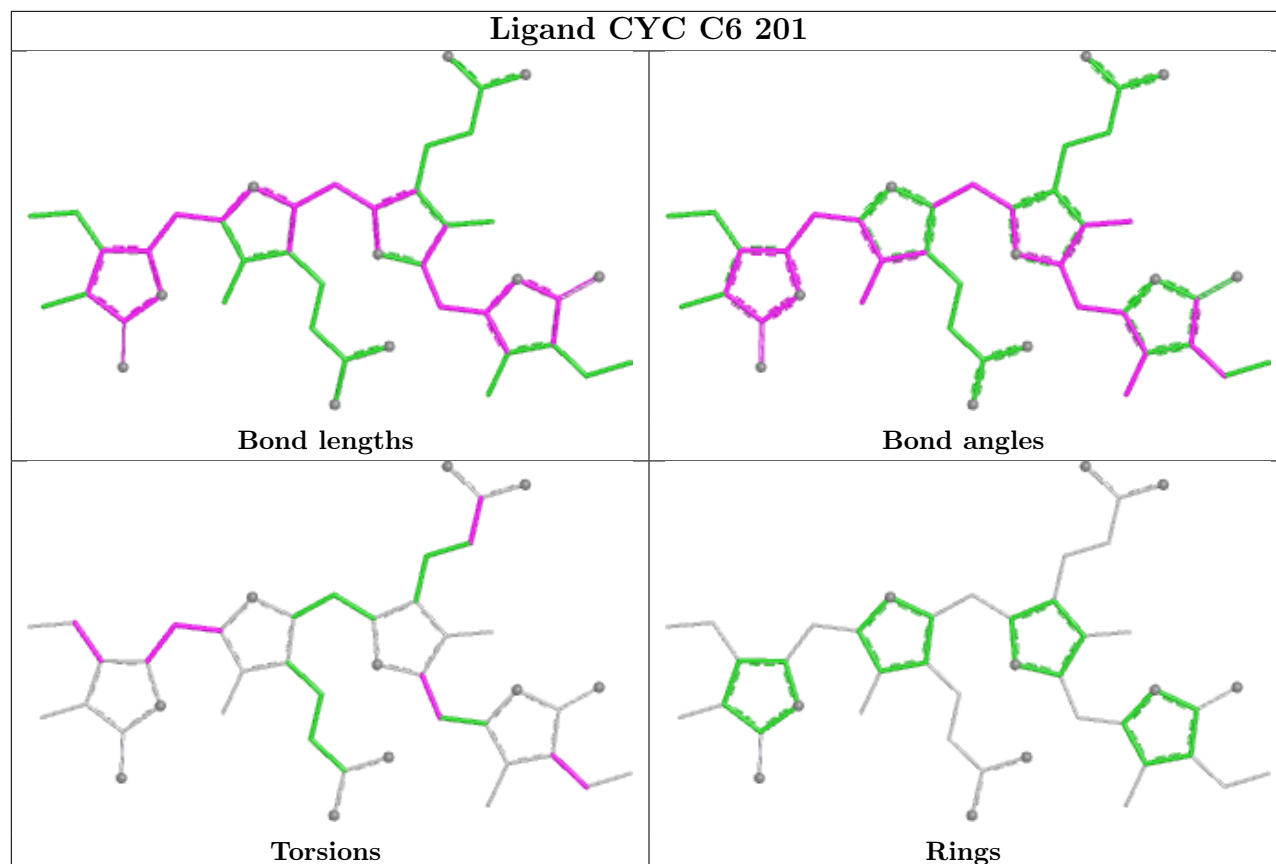
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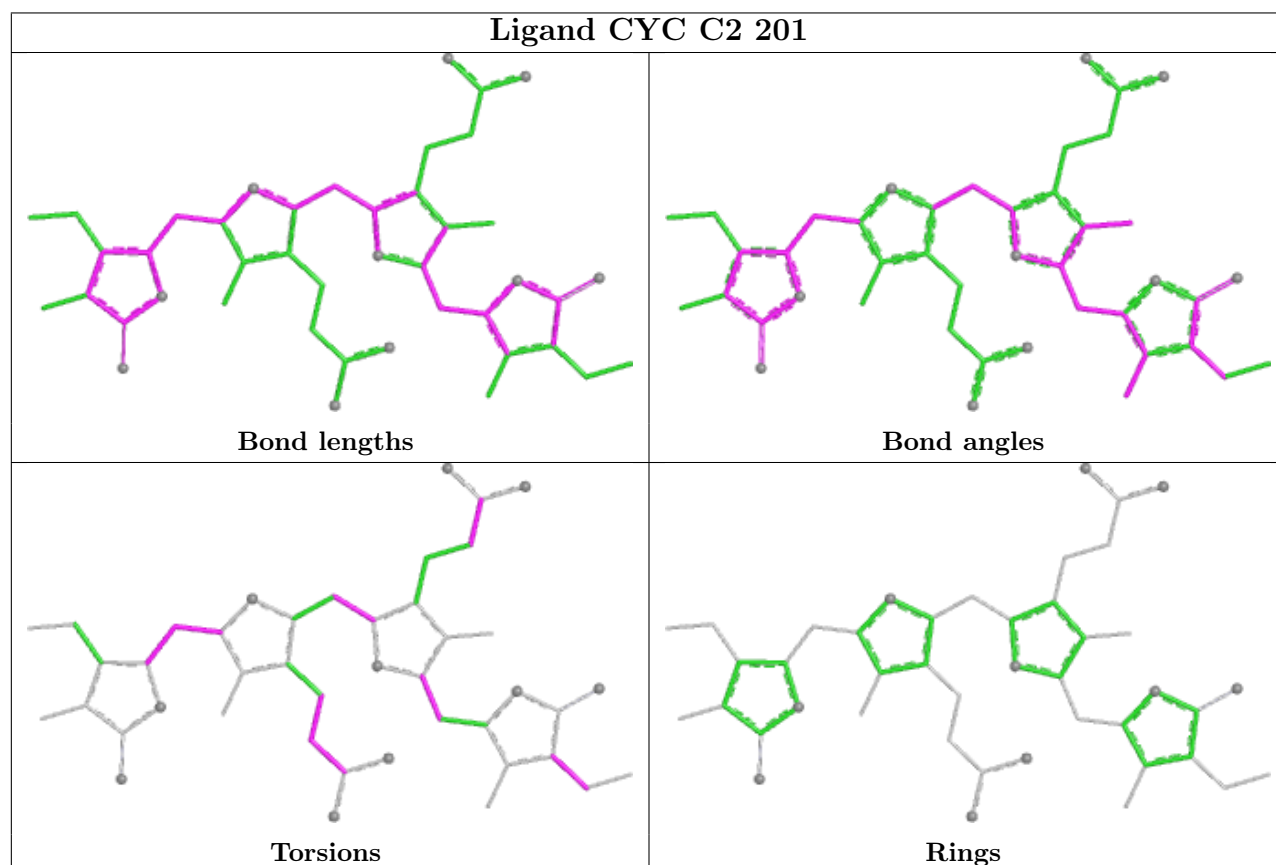
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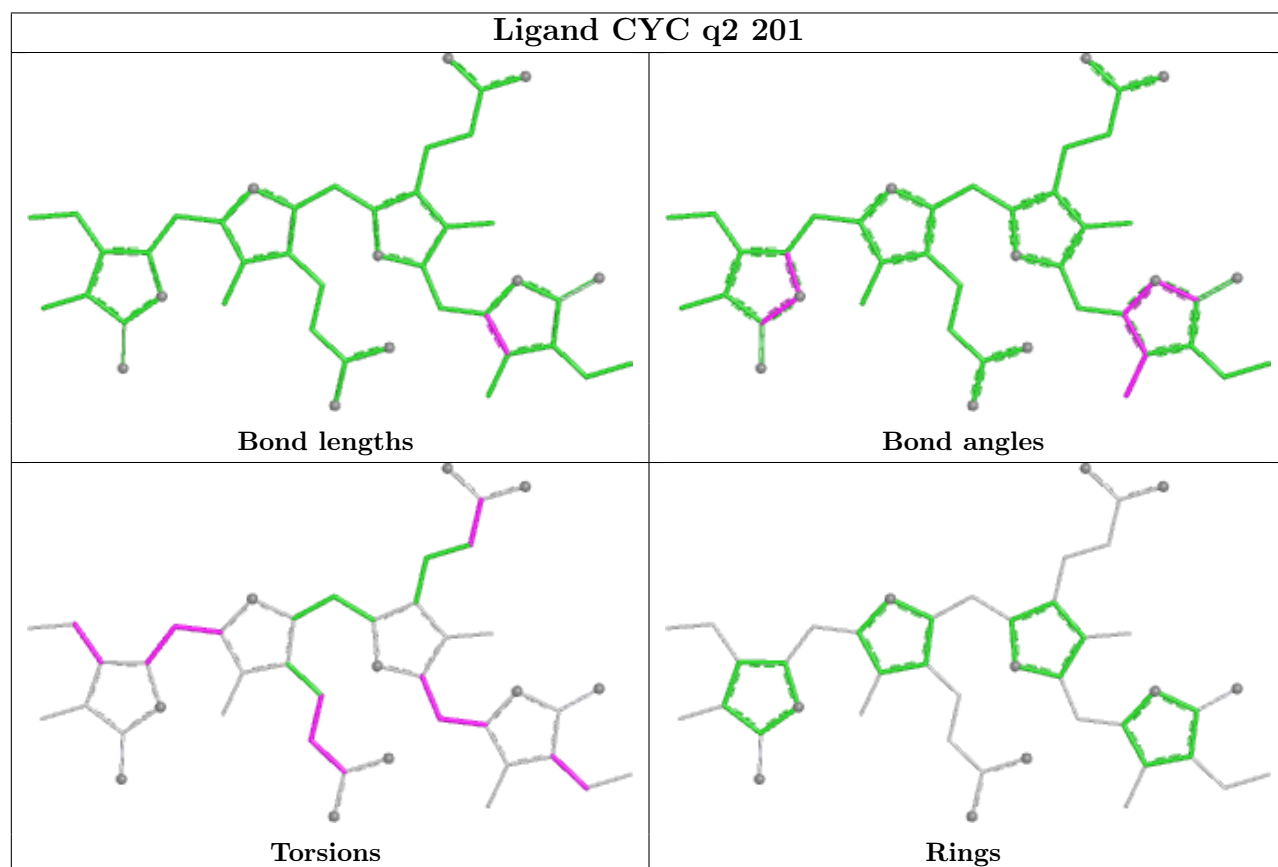
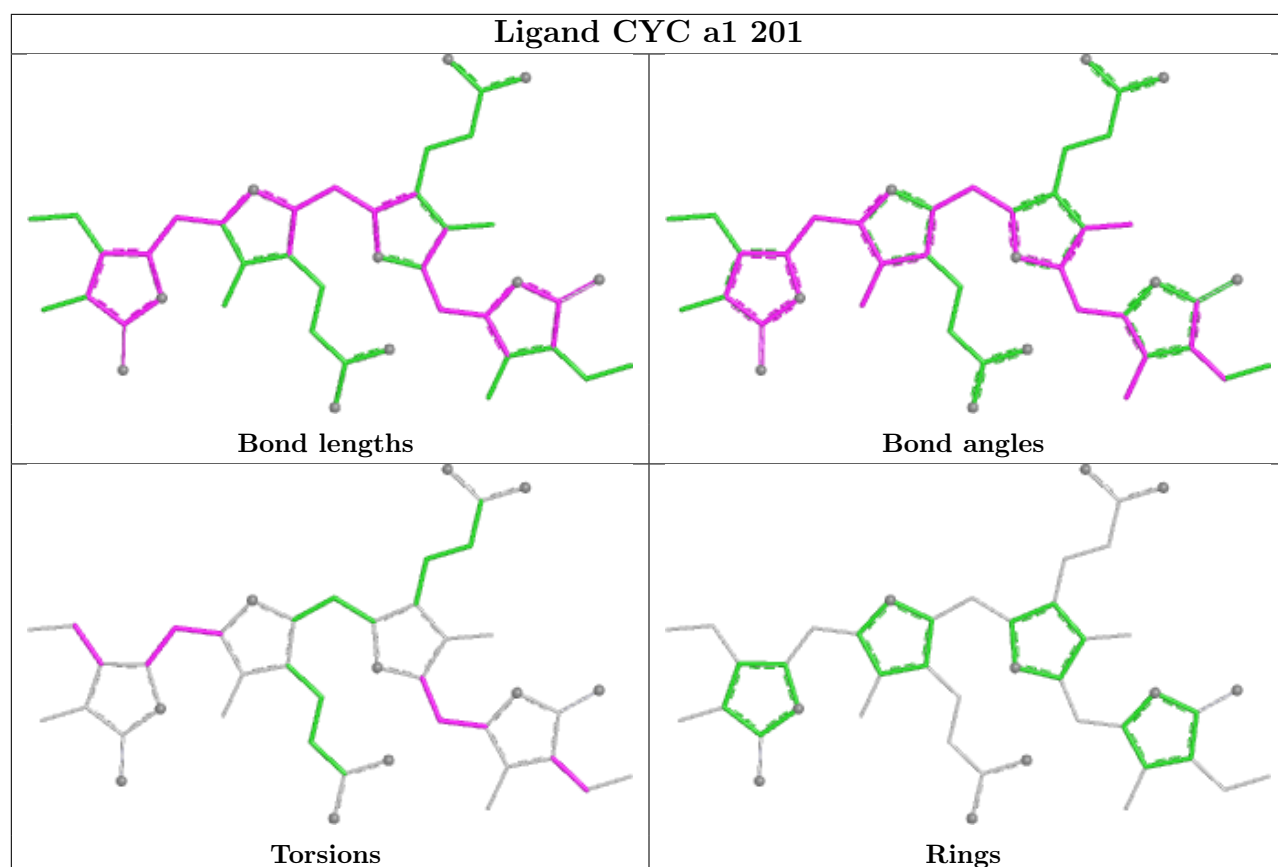


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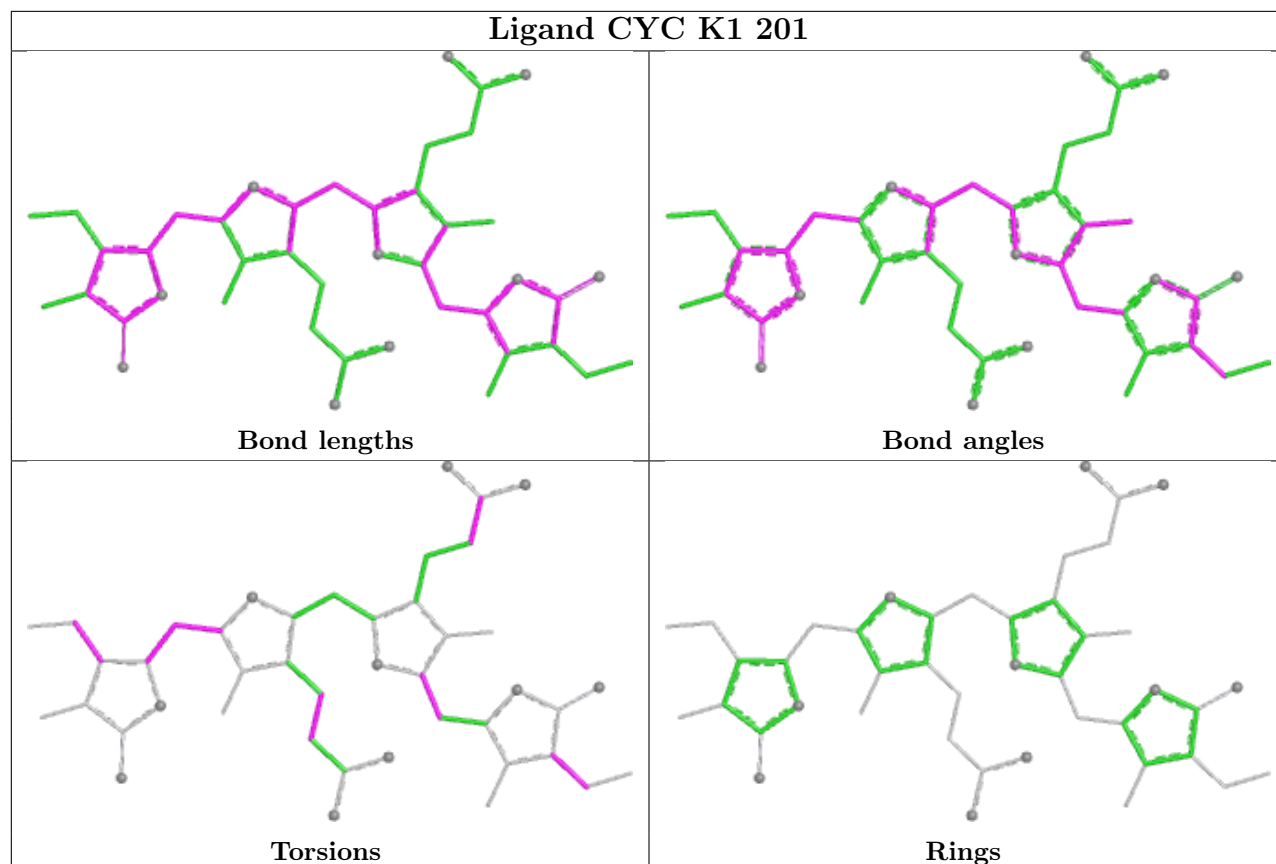


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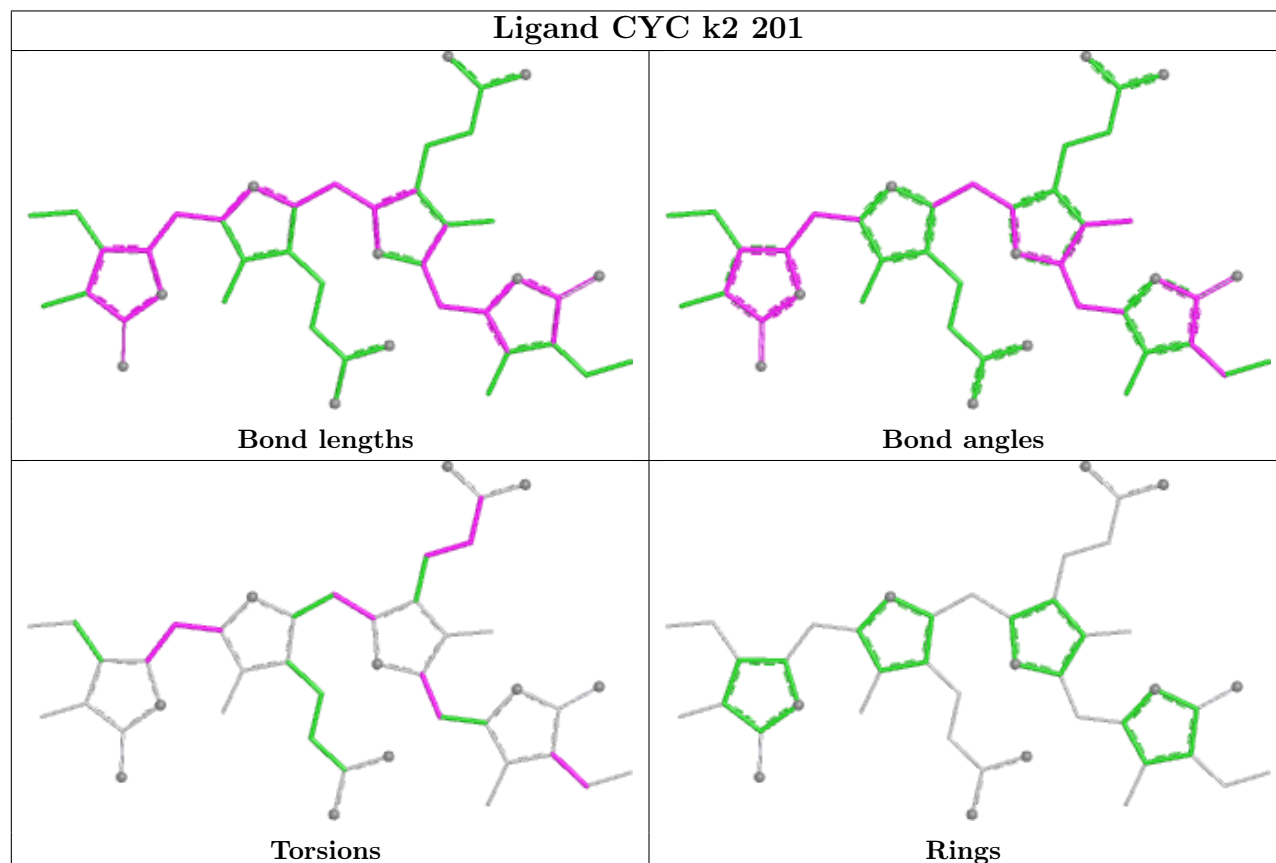




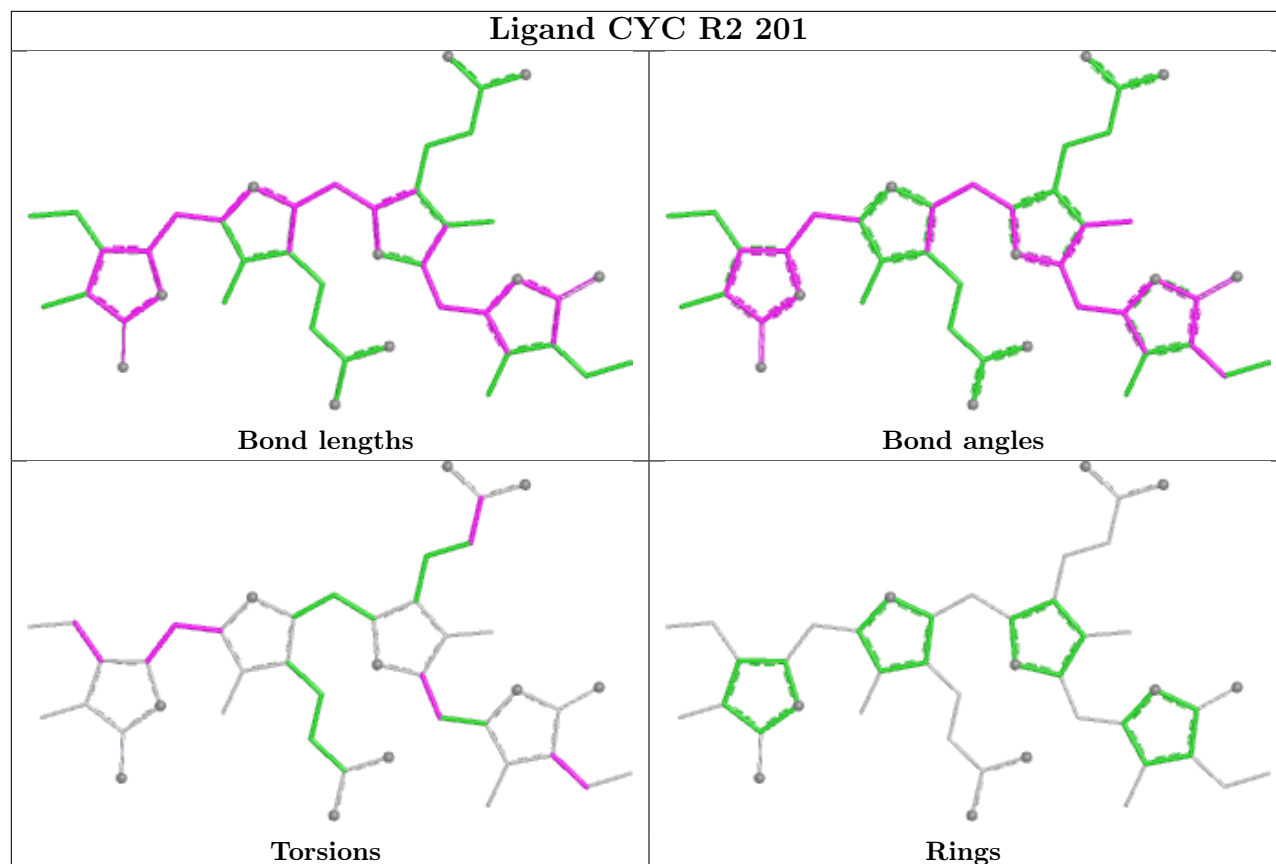
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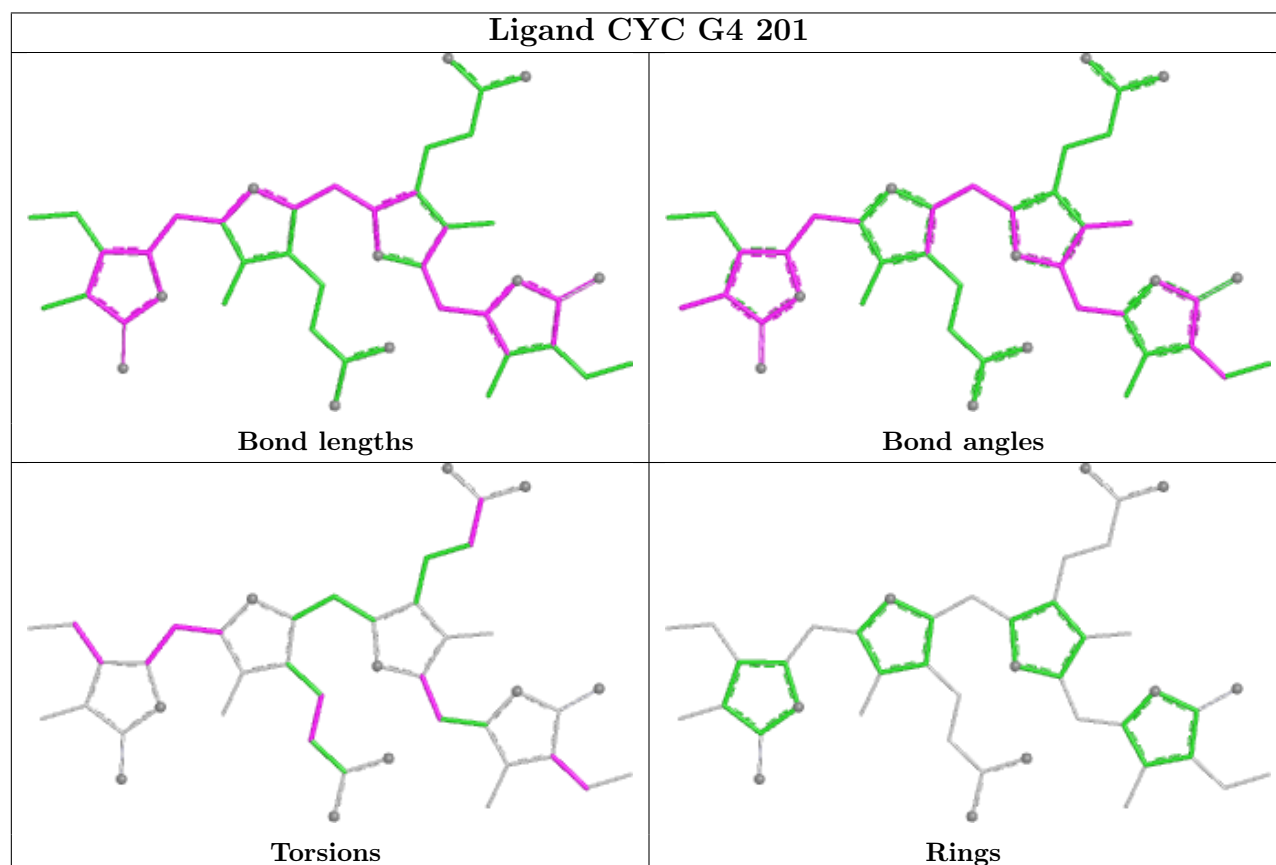
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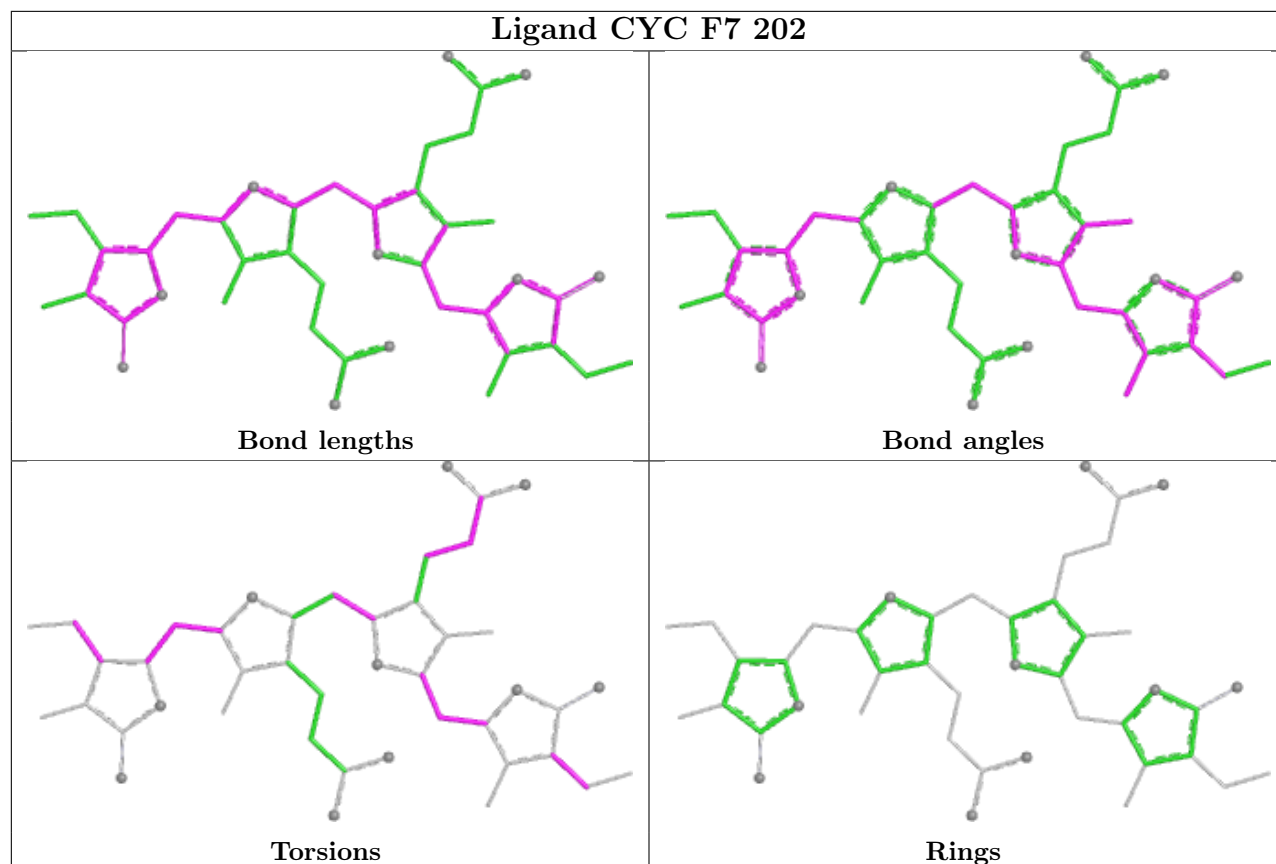
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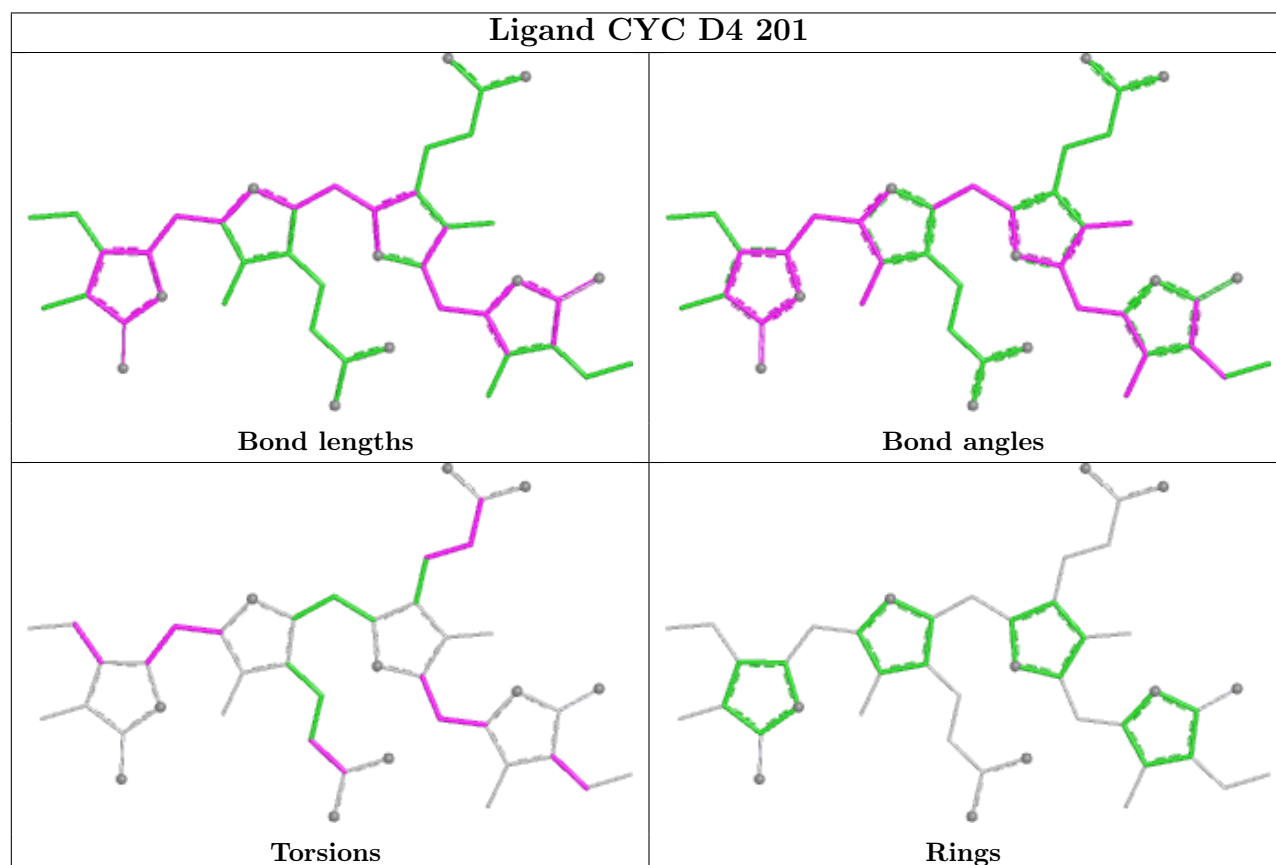
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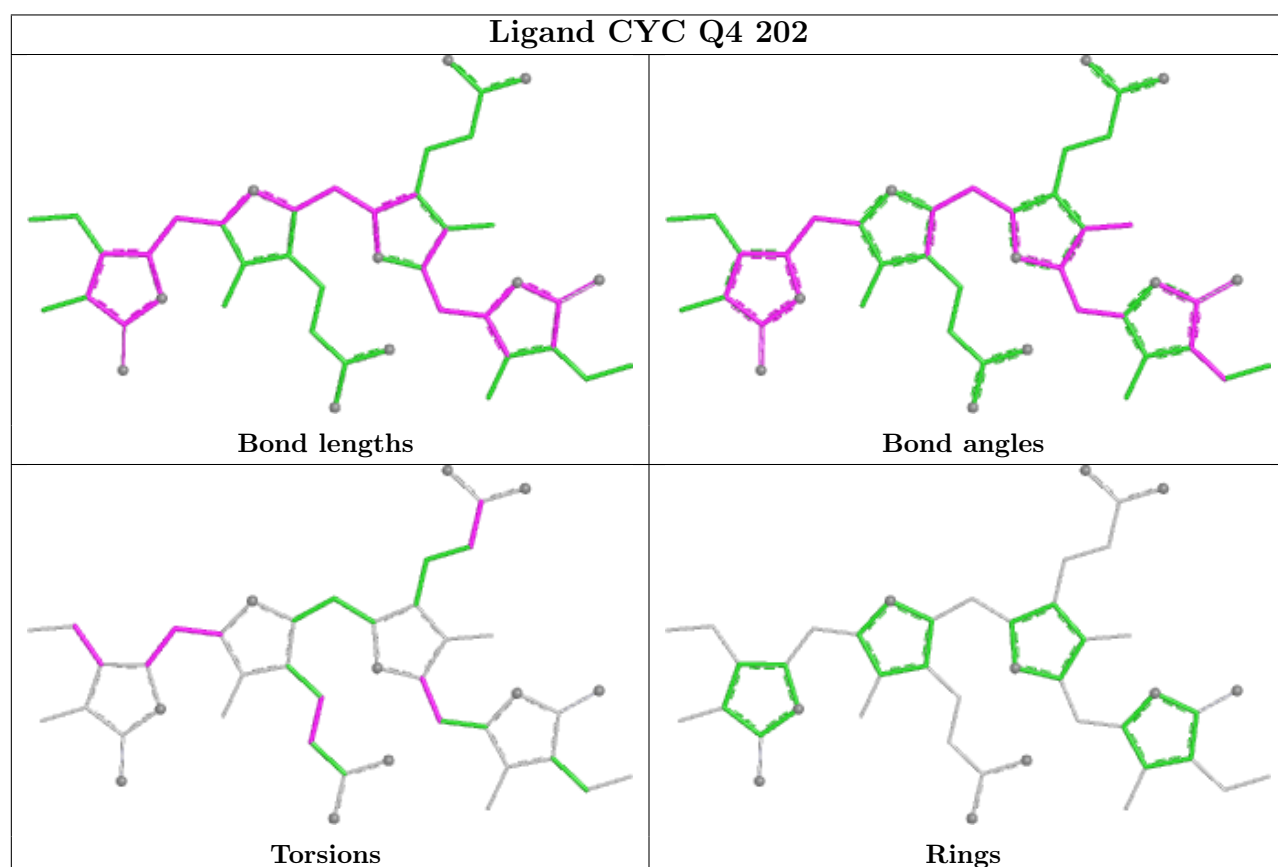
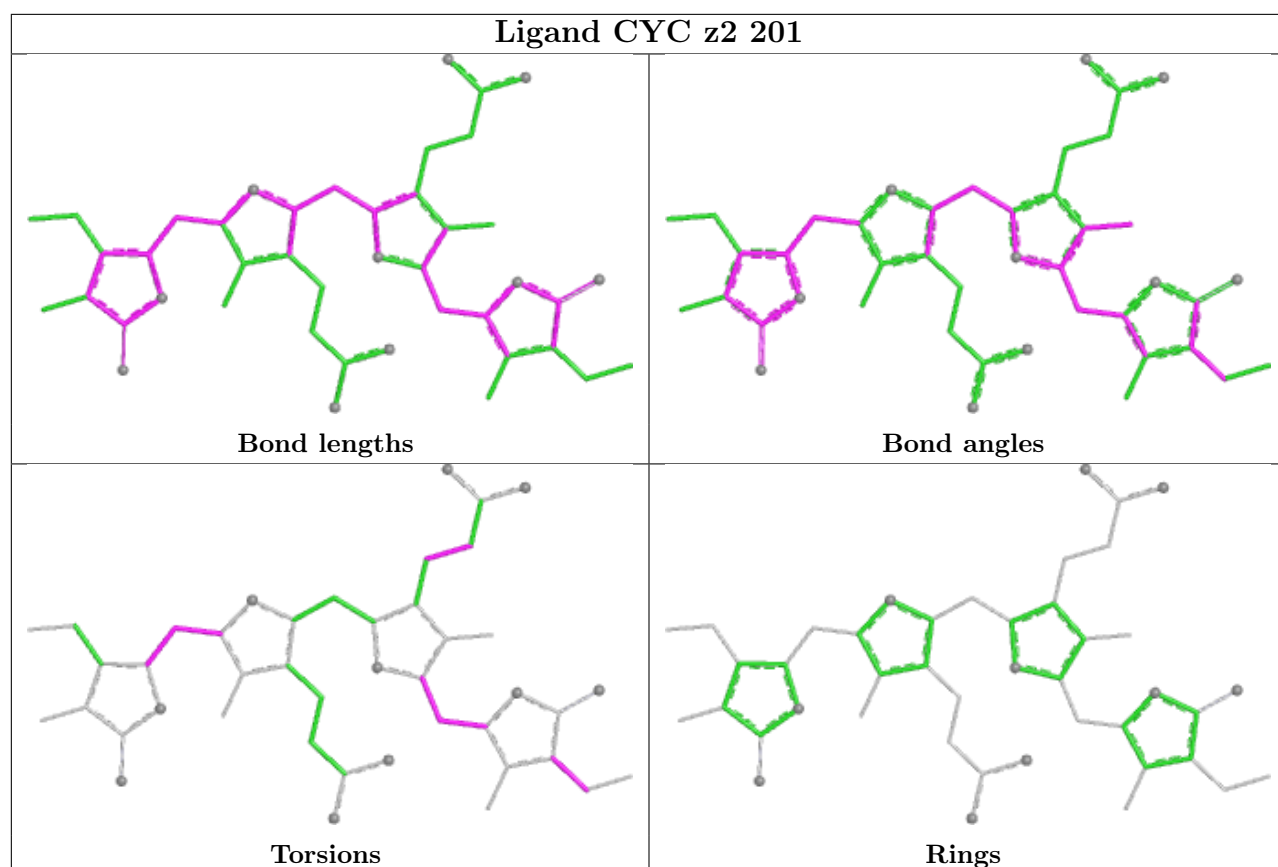


Ligand CYC F7 202

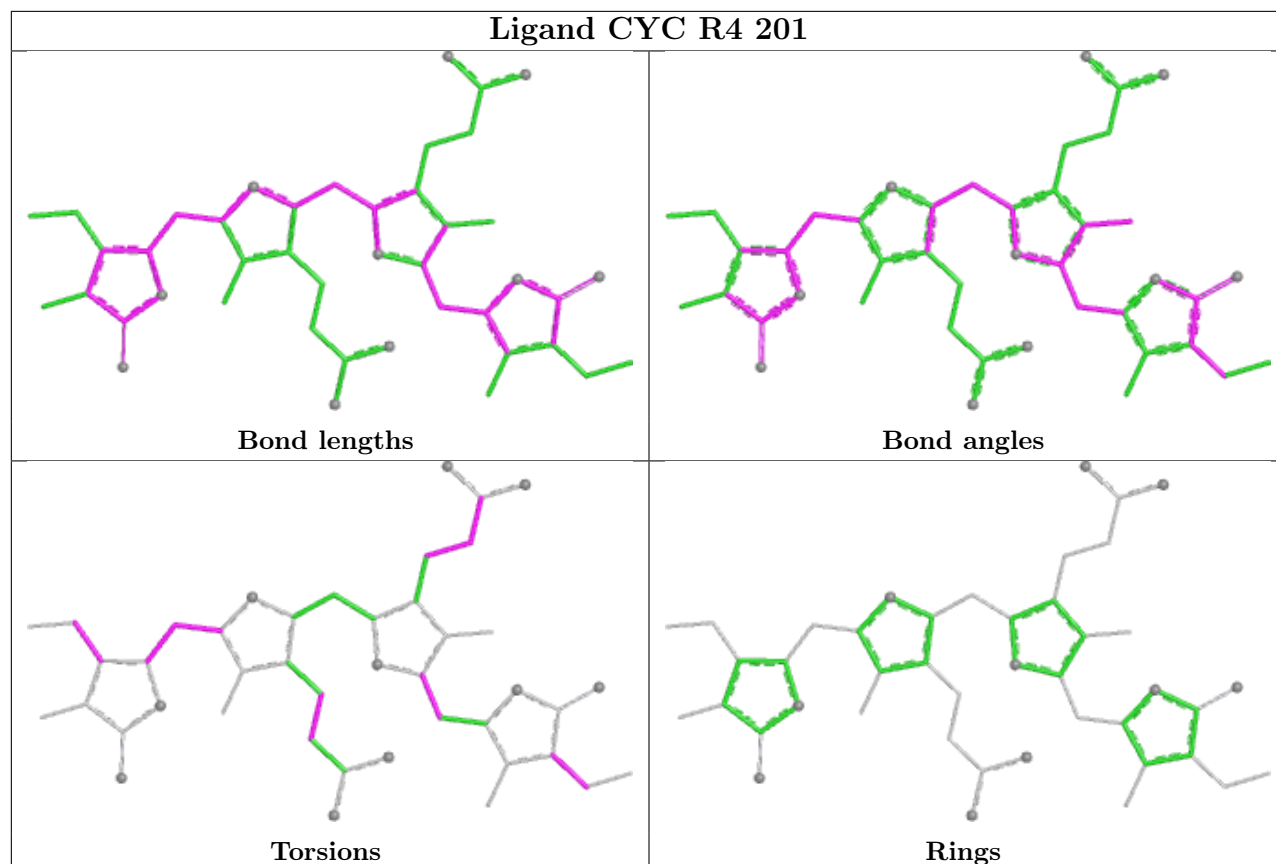


Ligand CYC D4 201

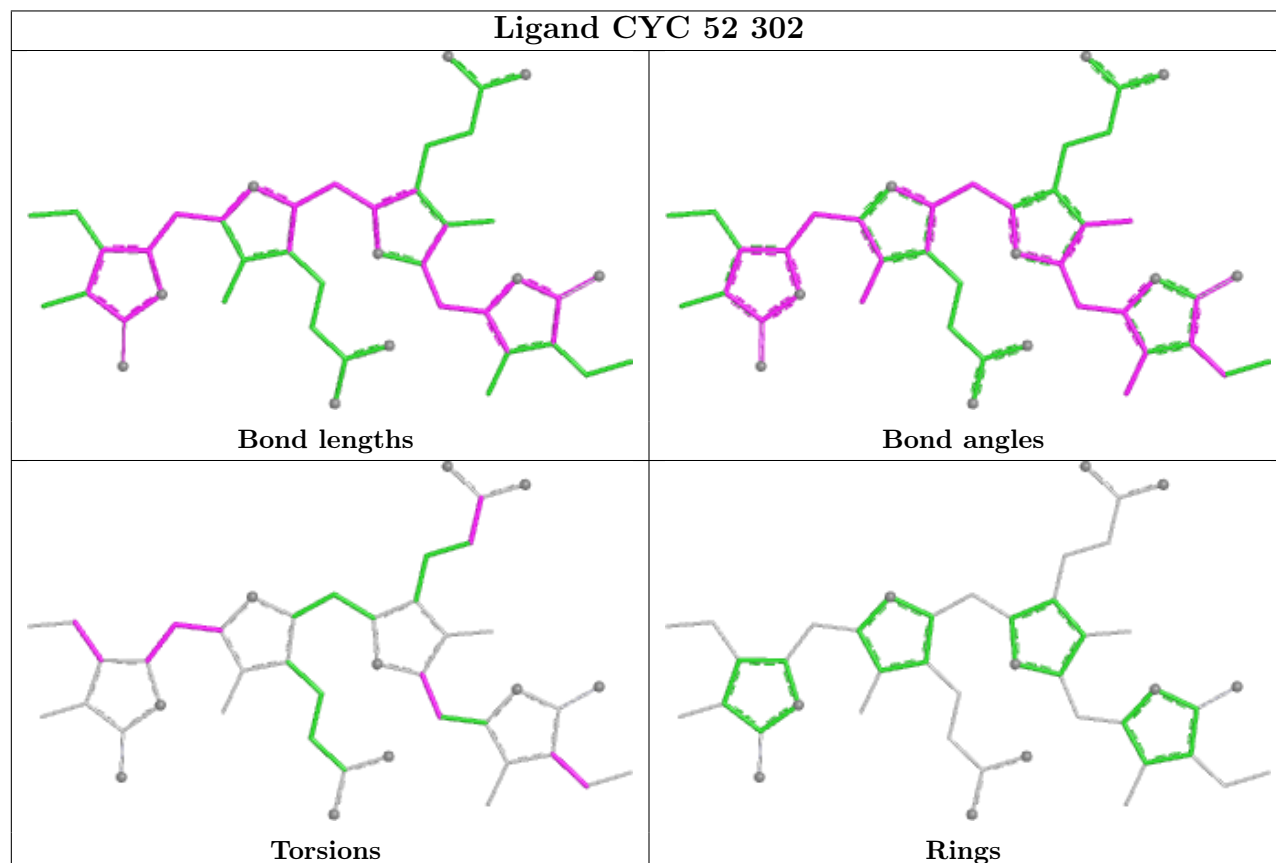


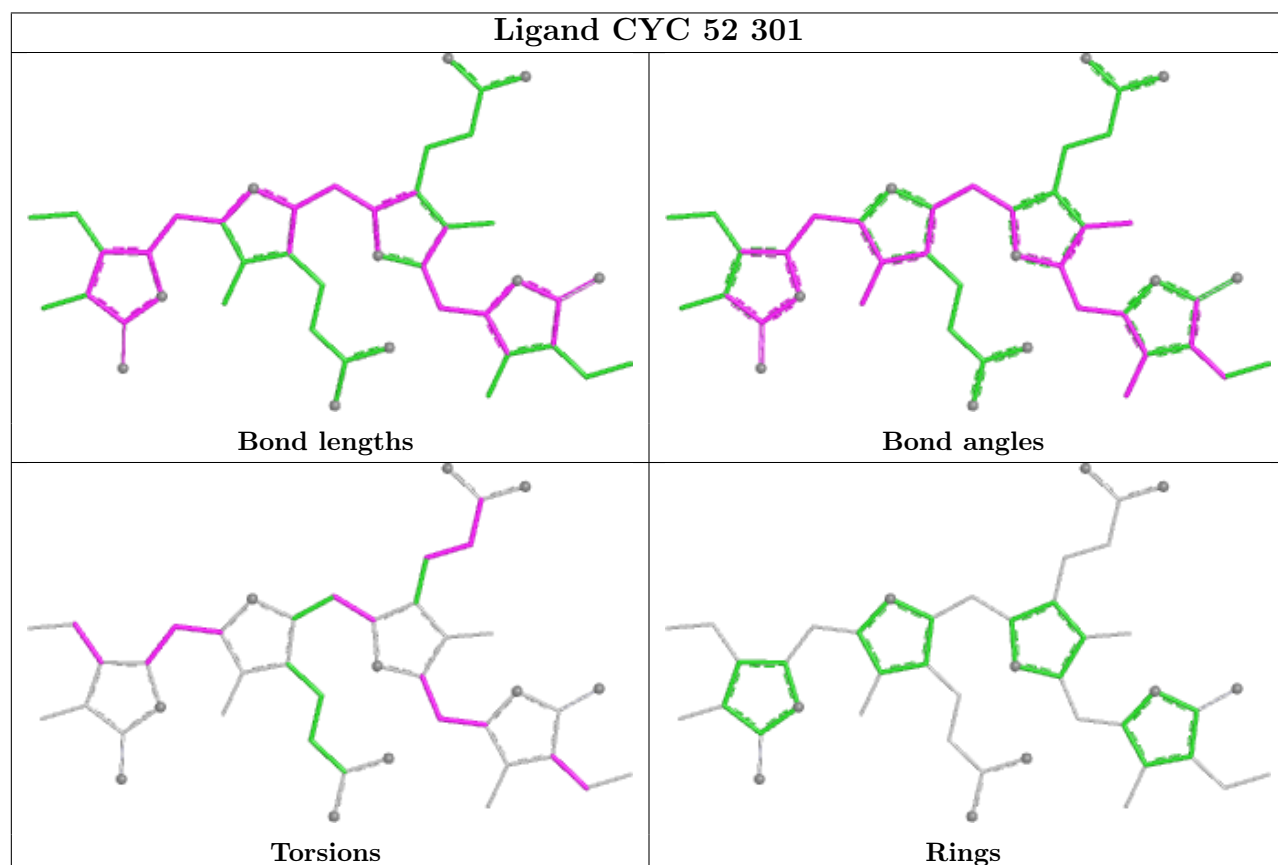
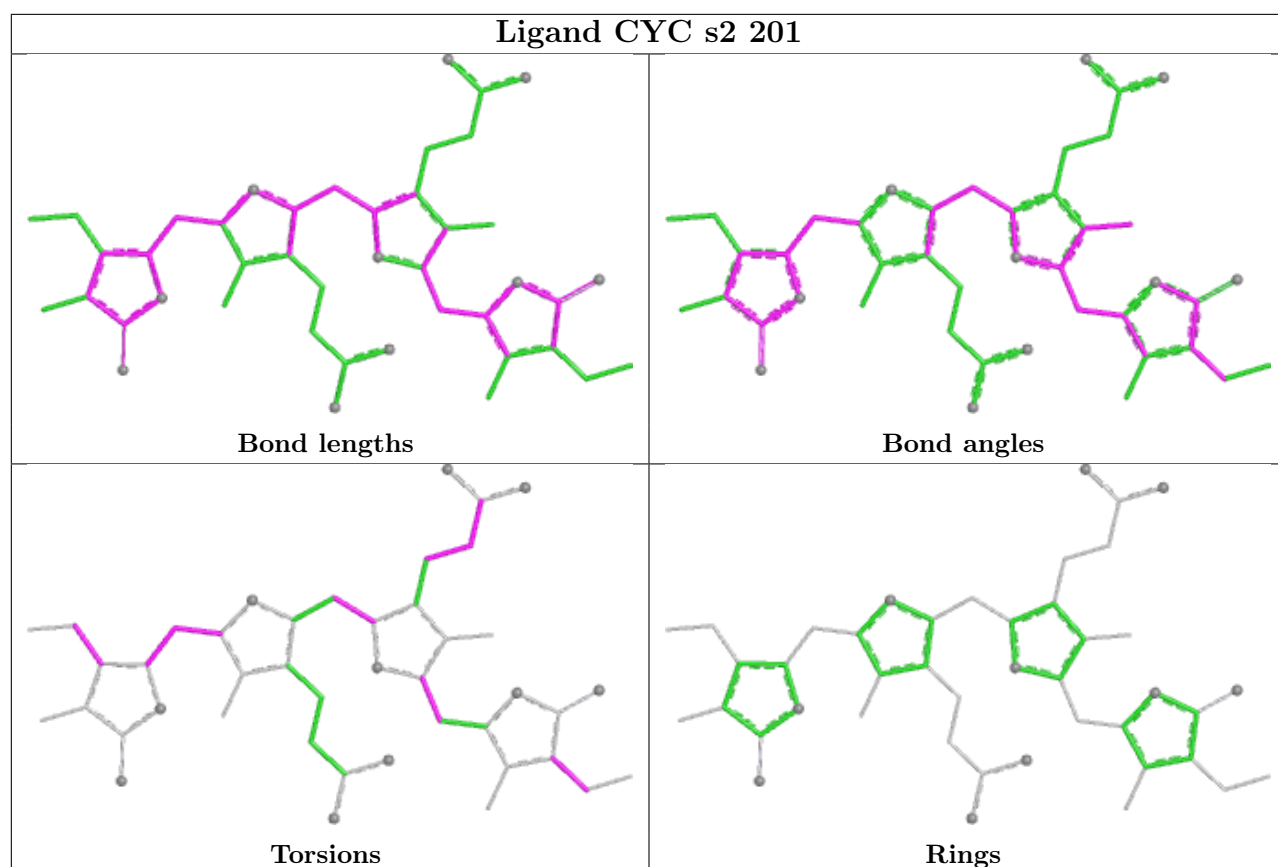


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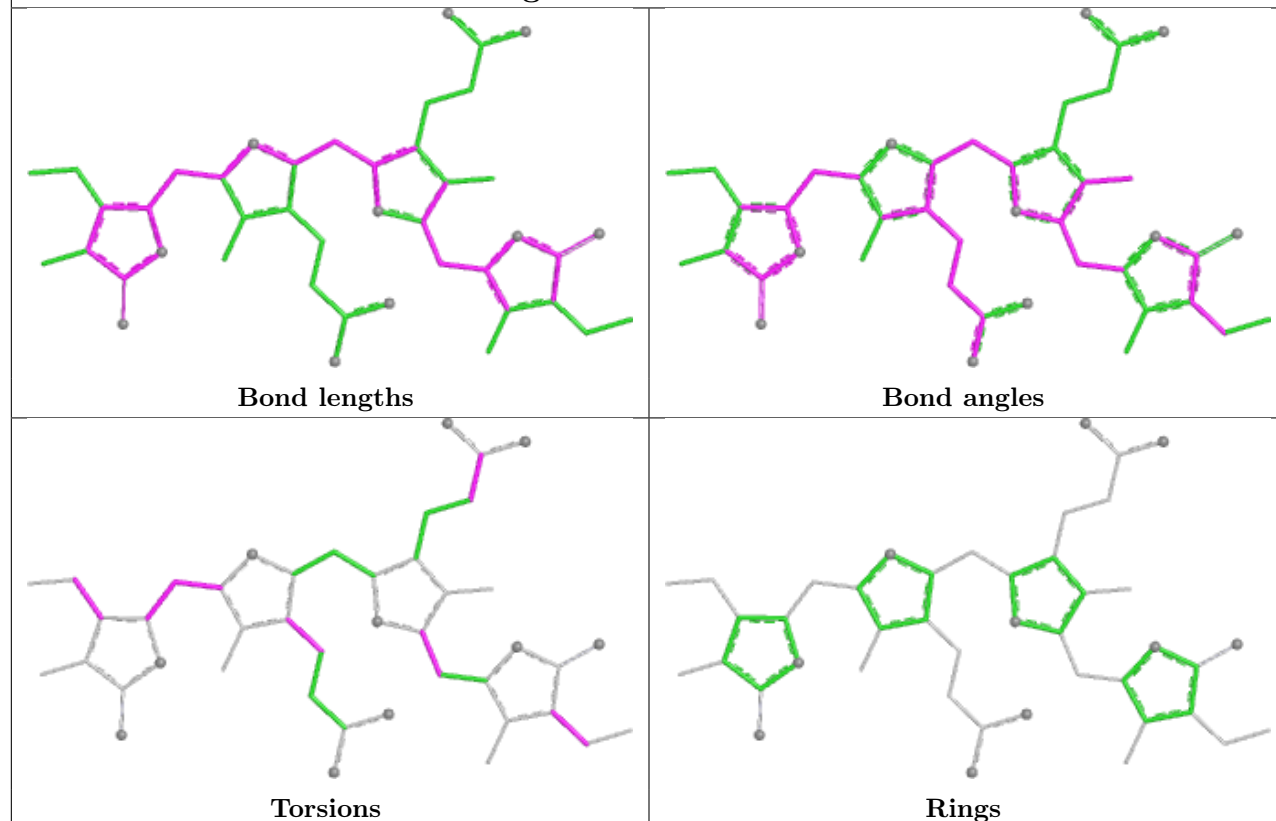


Ligand CYC 52 302

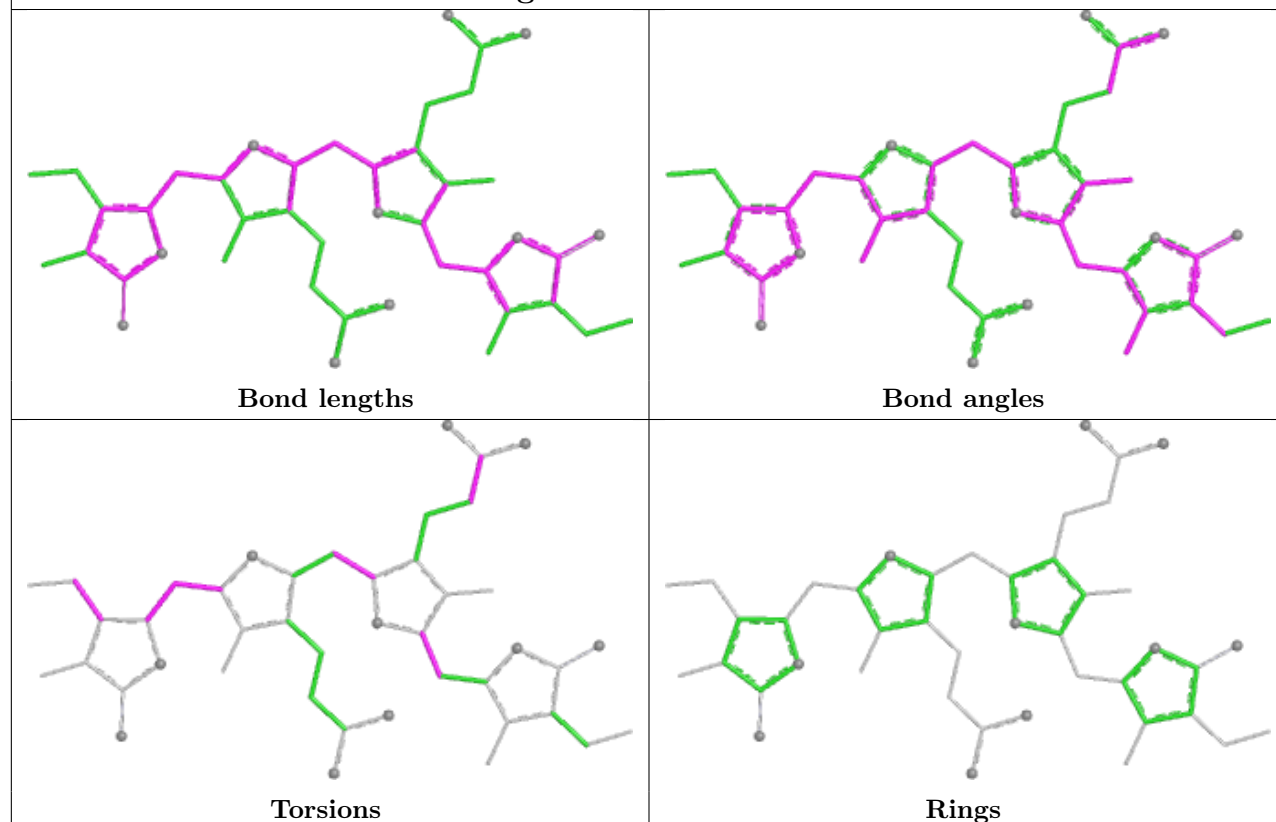




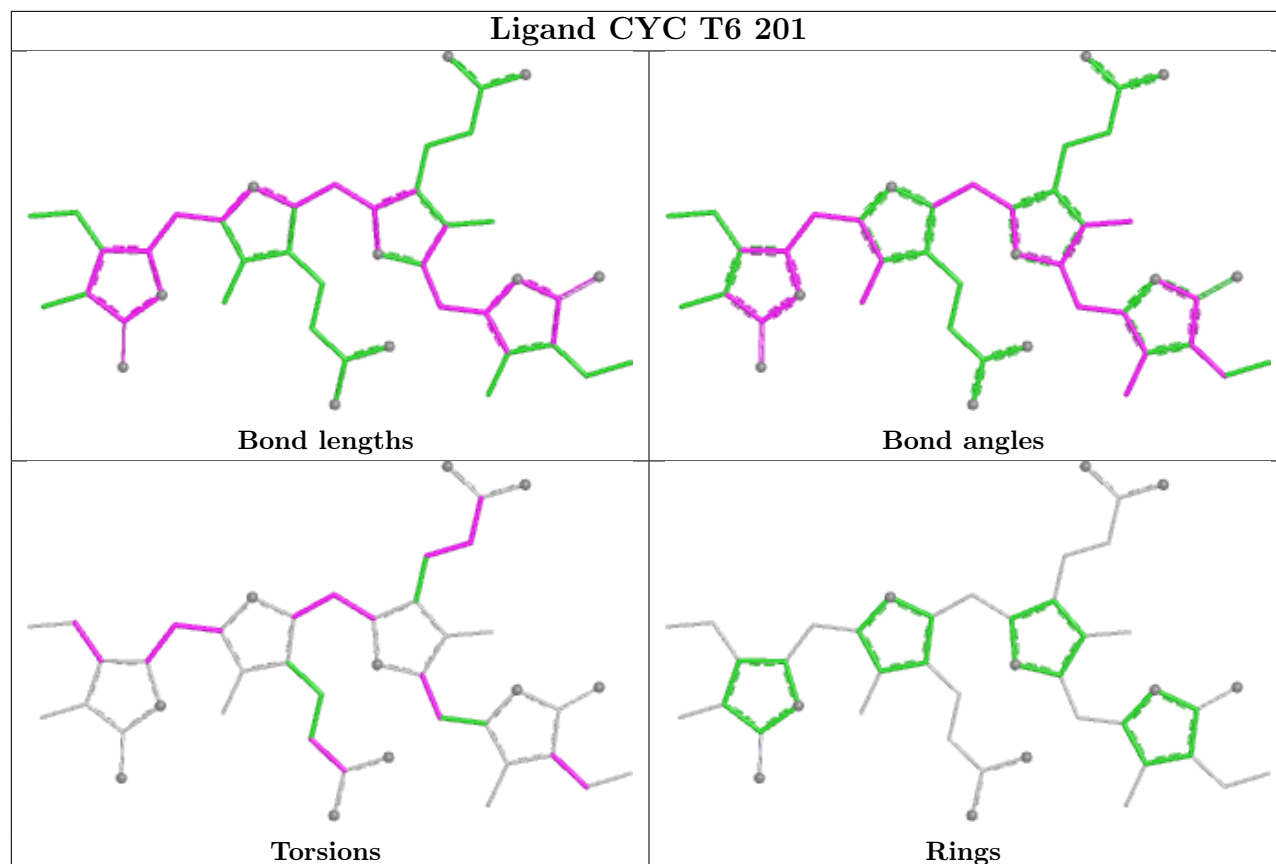
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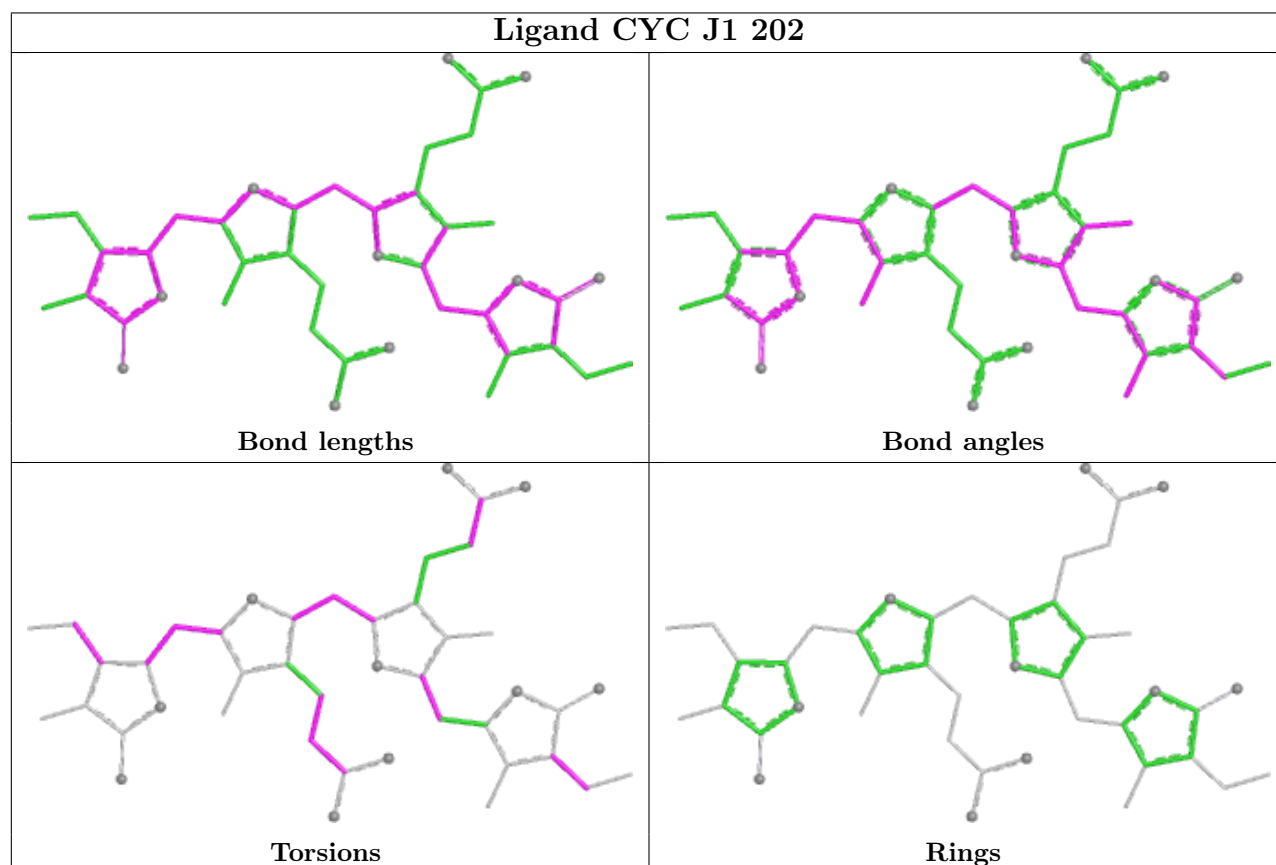
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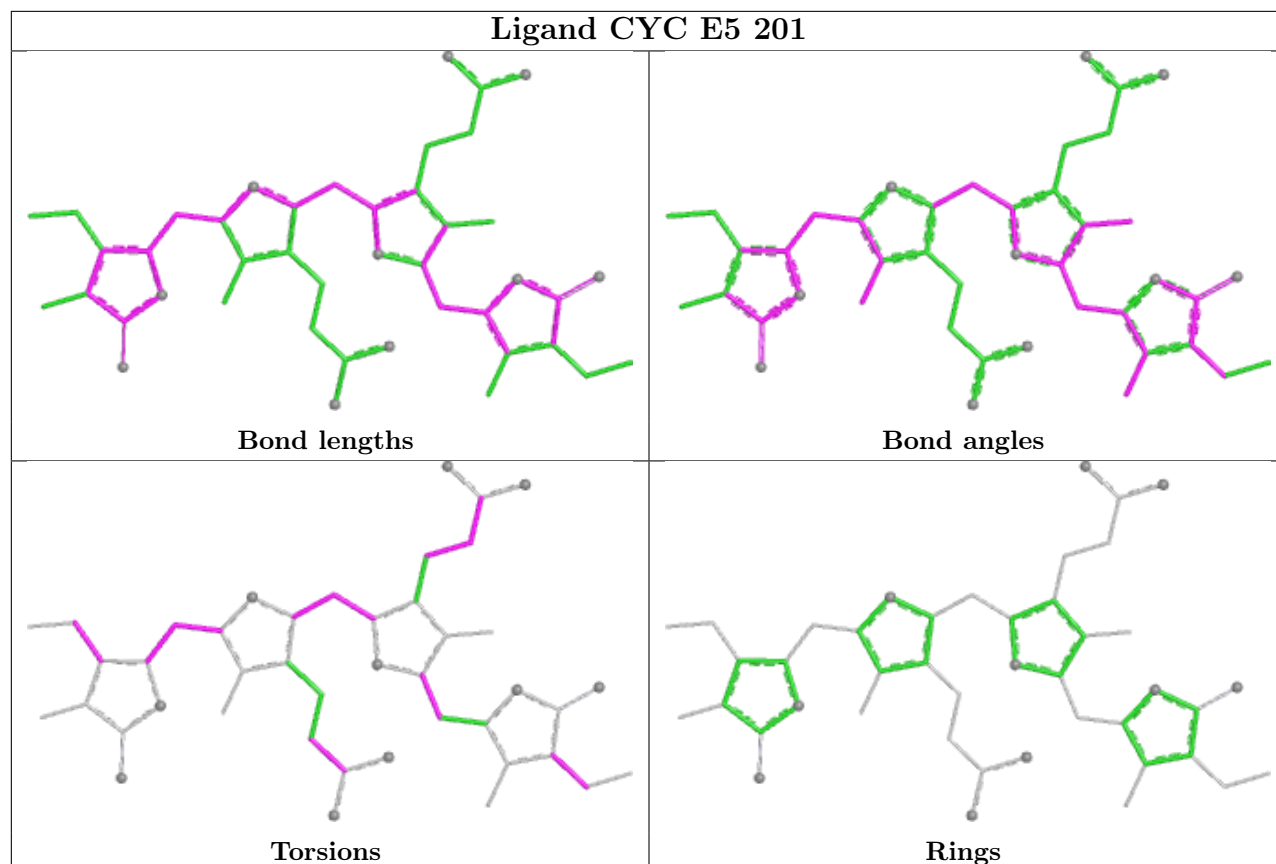
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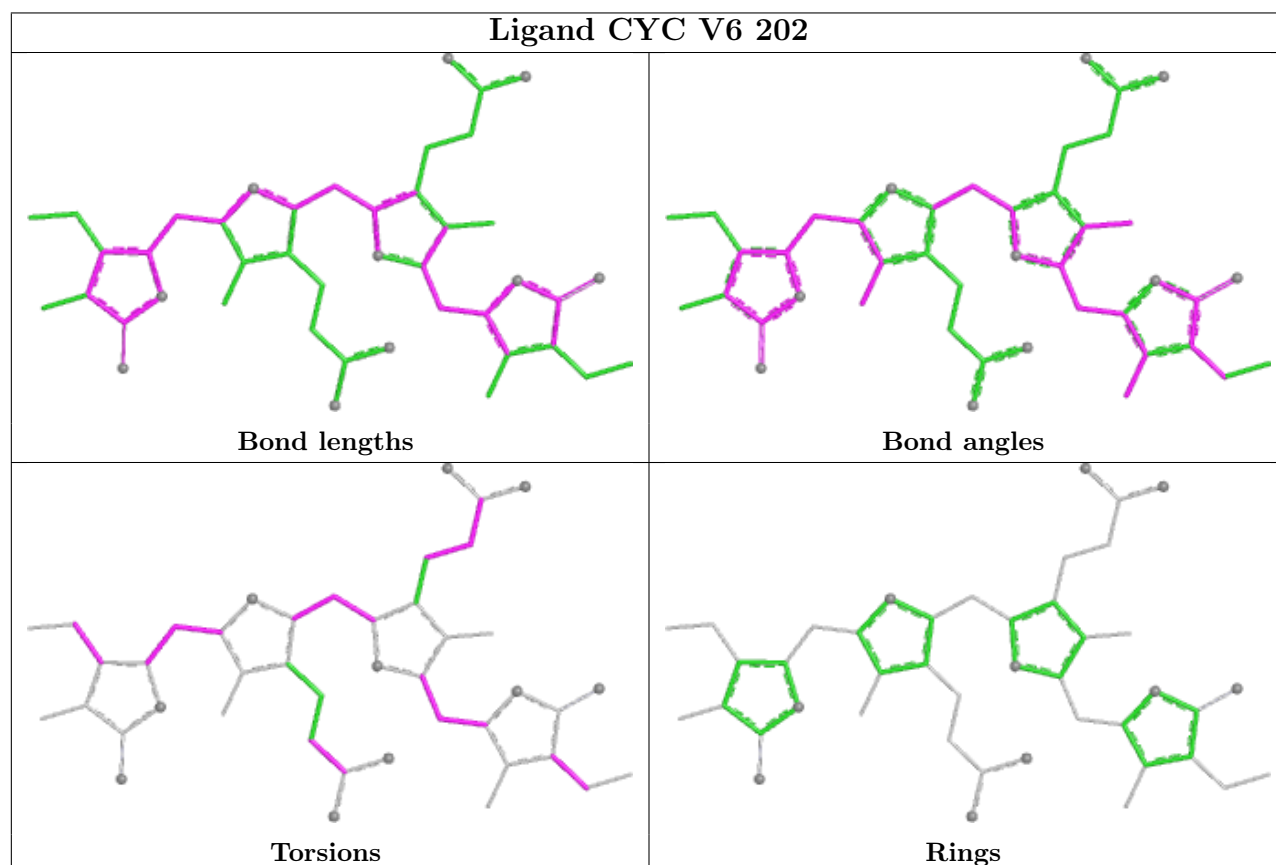
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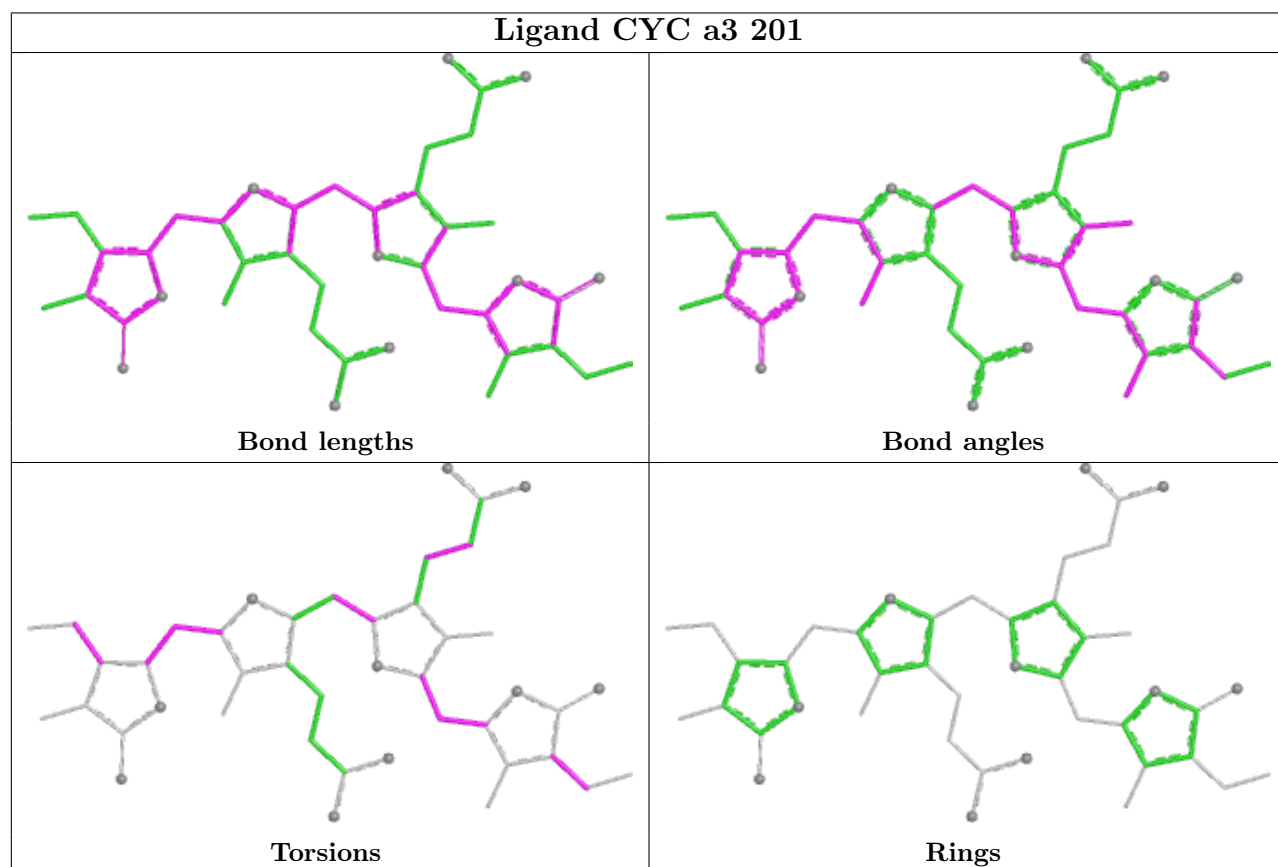
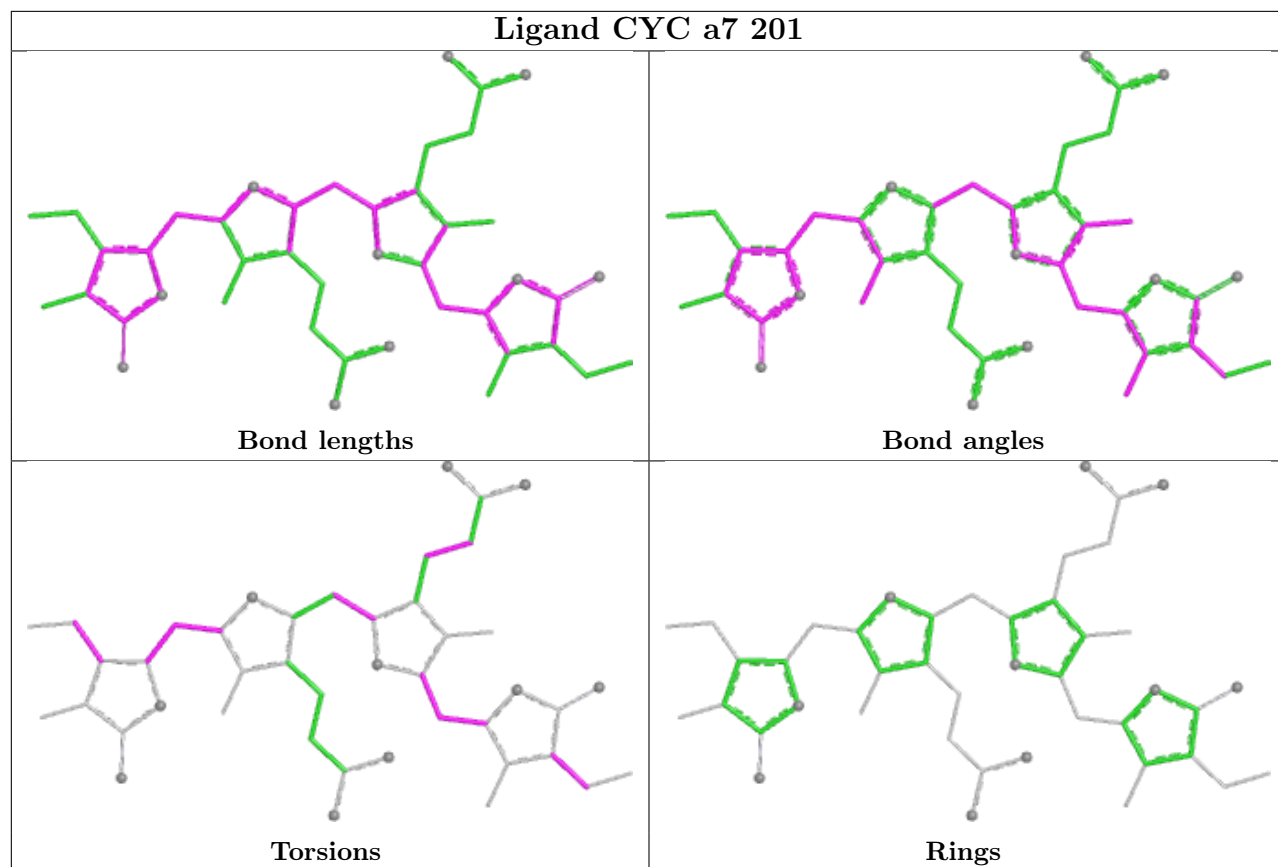


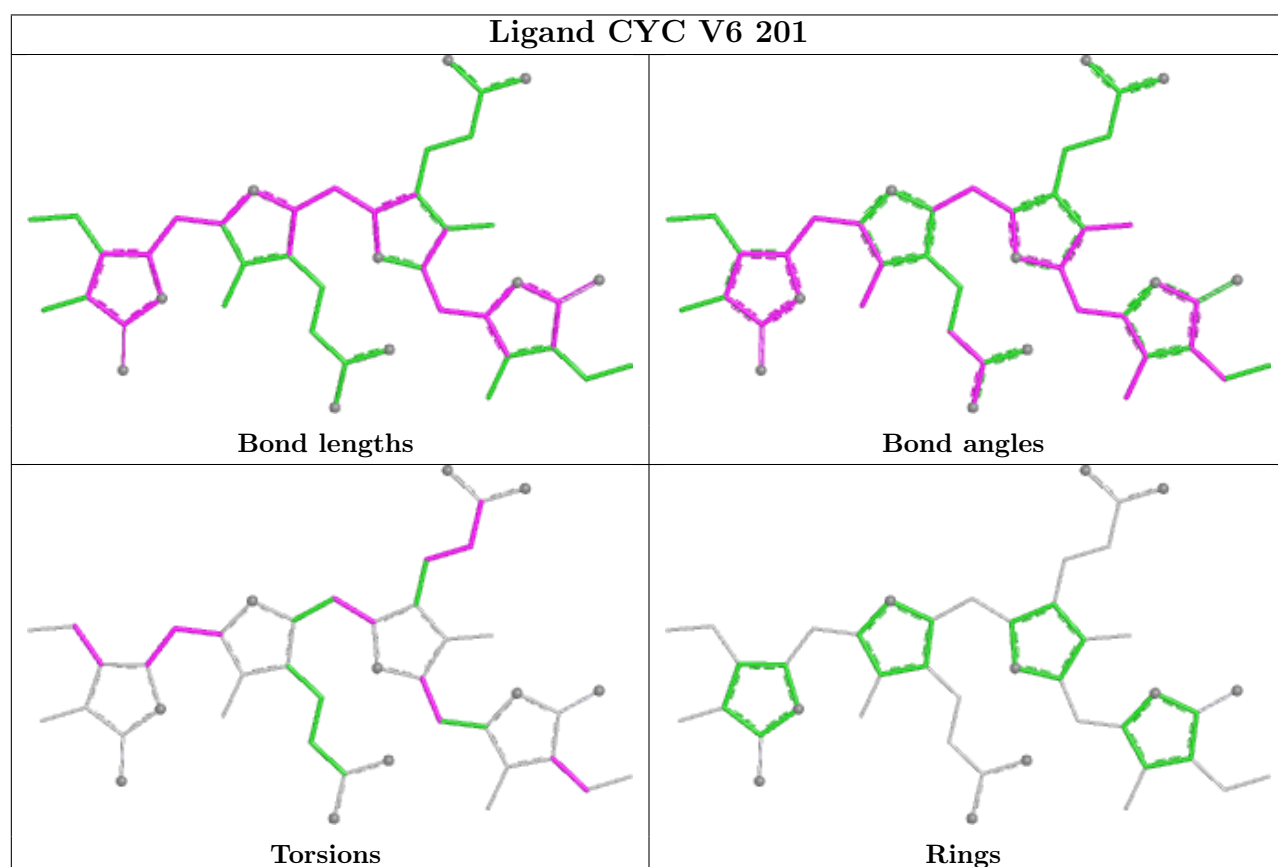
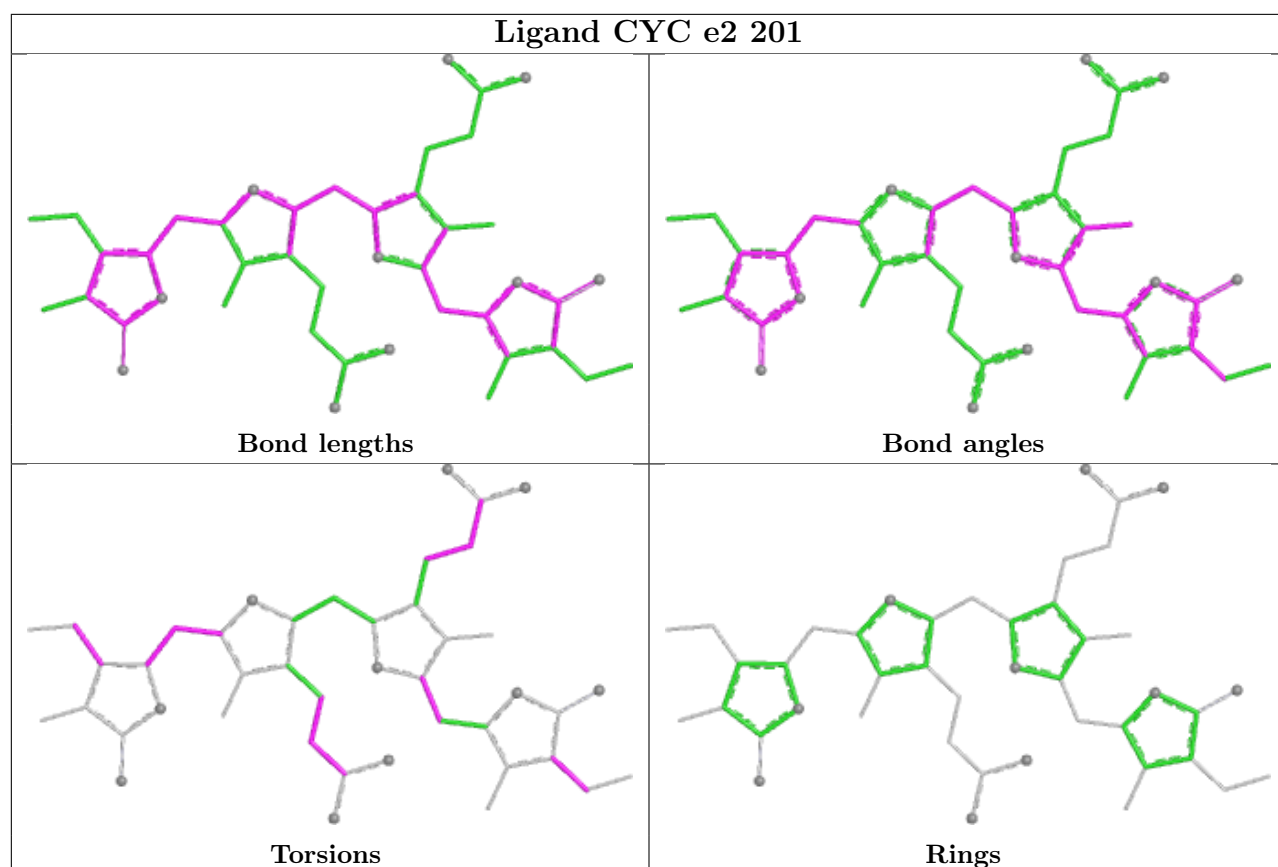
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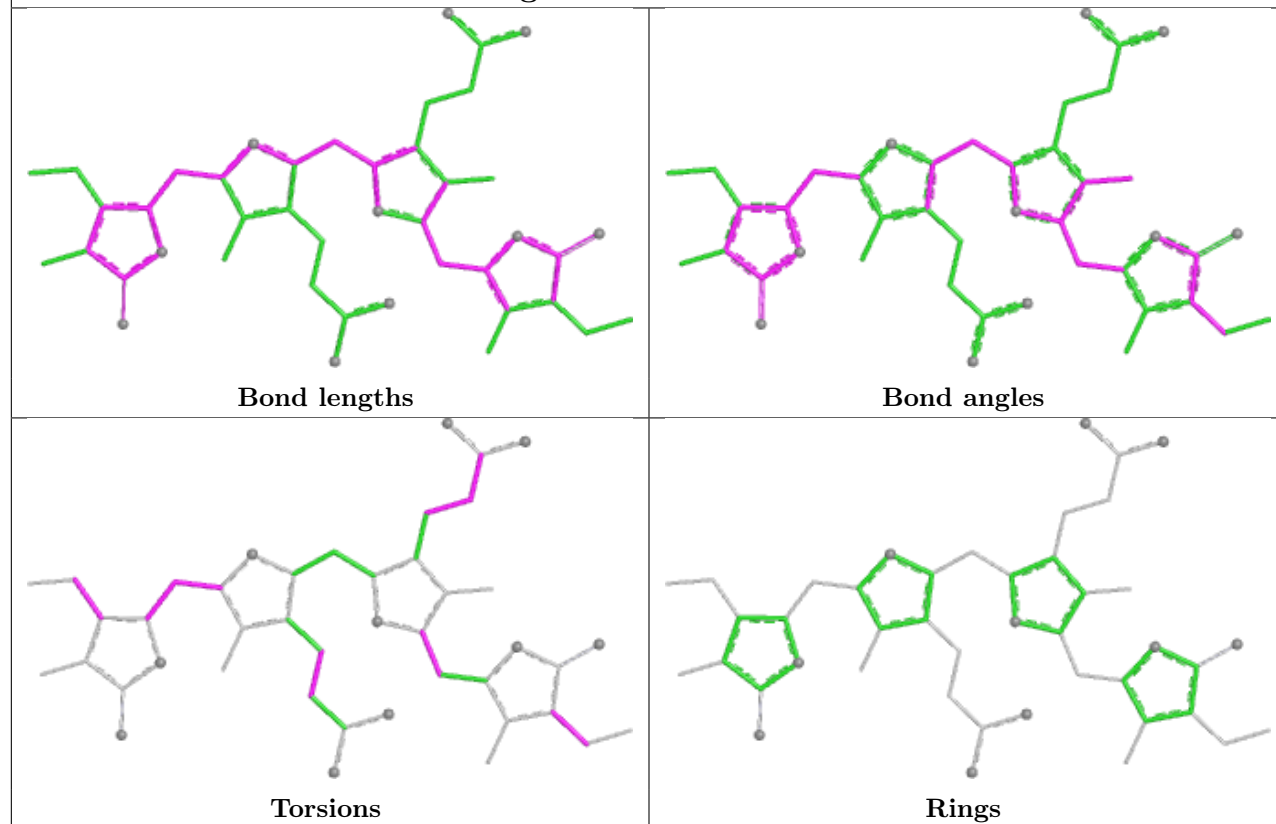
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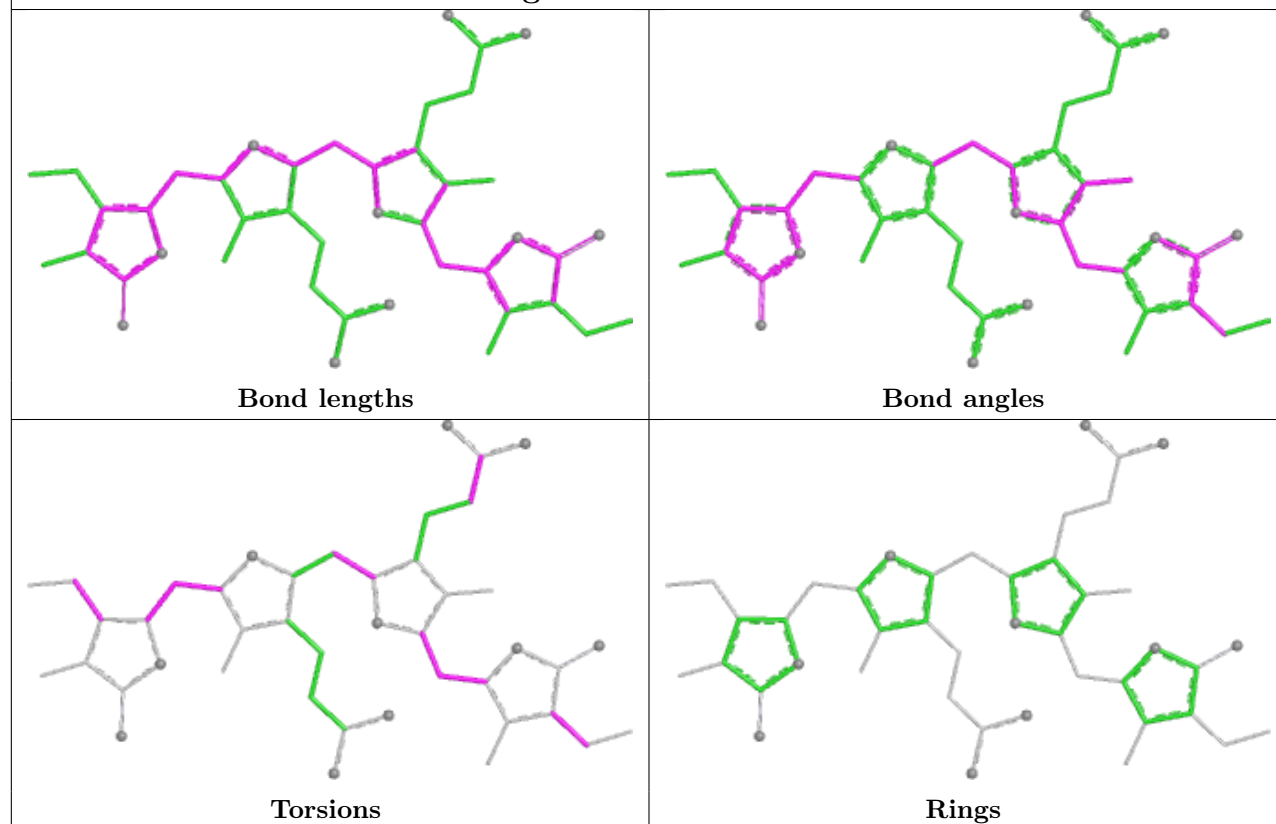




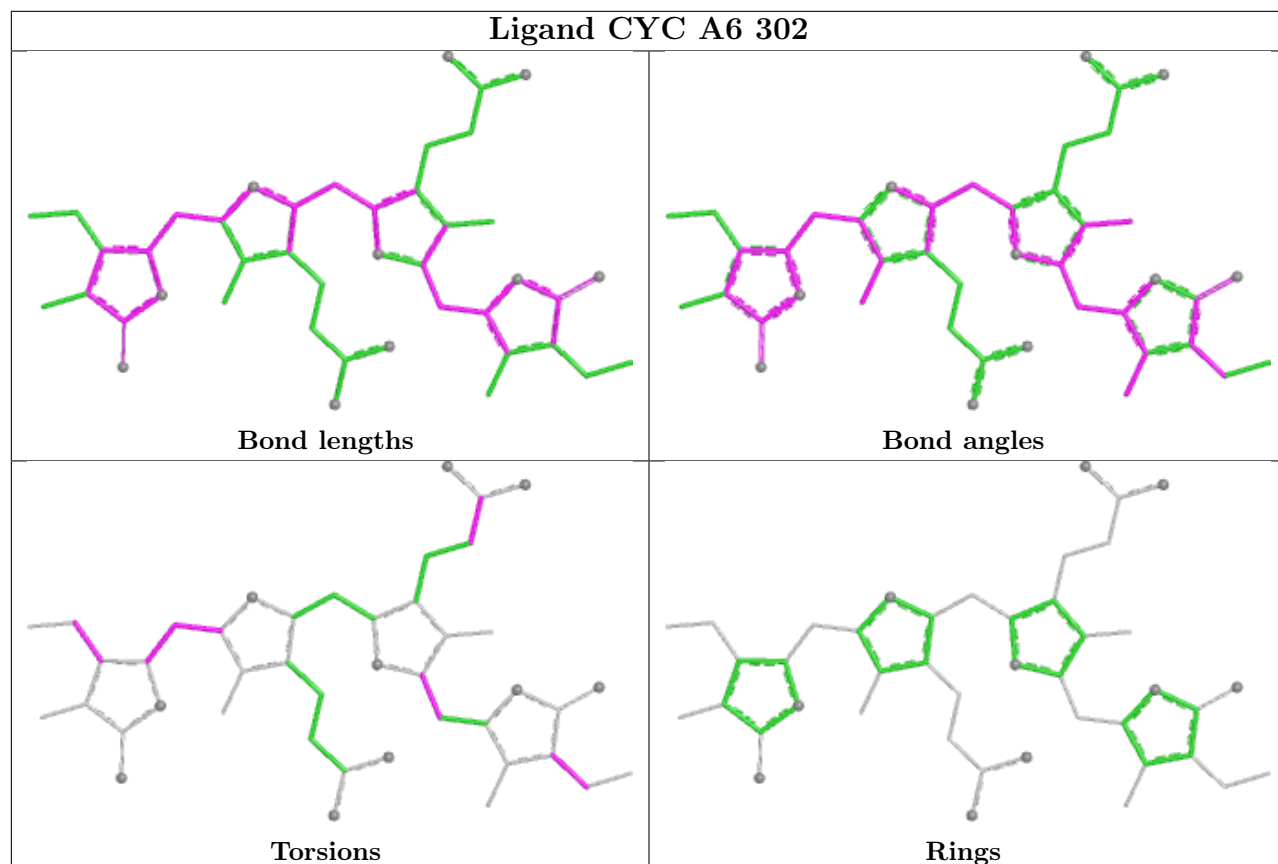
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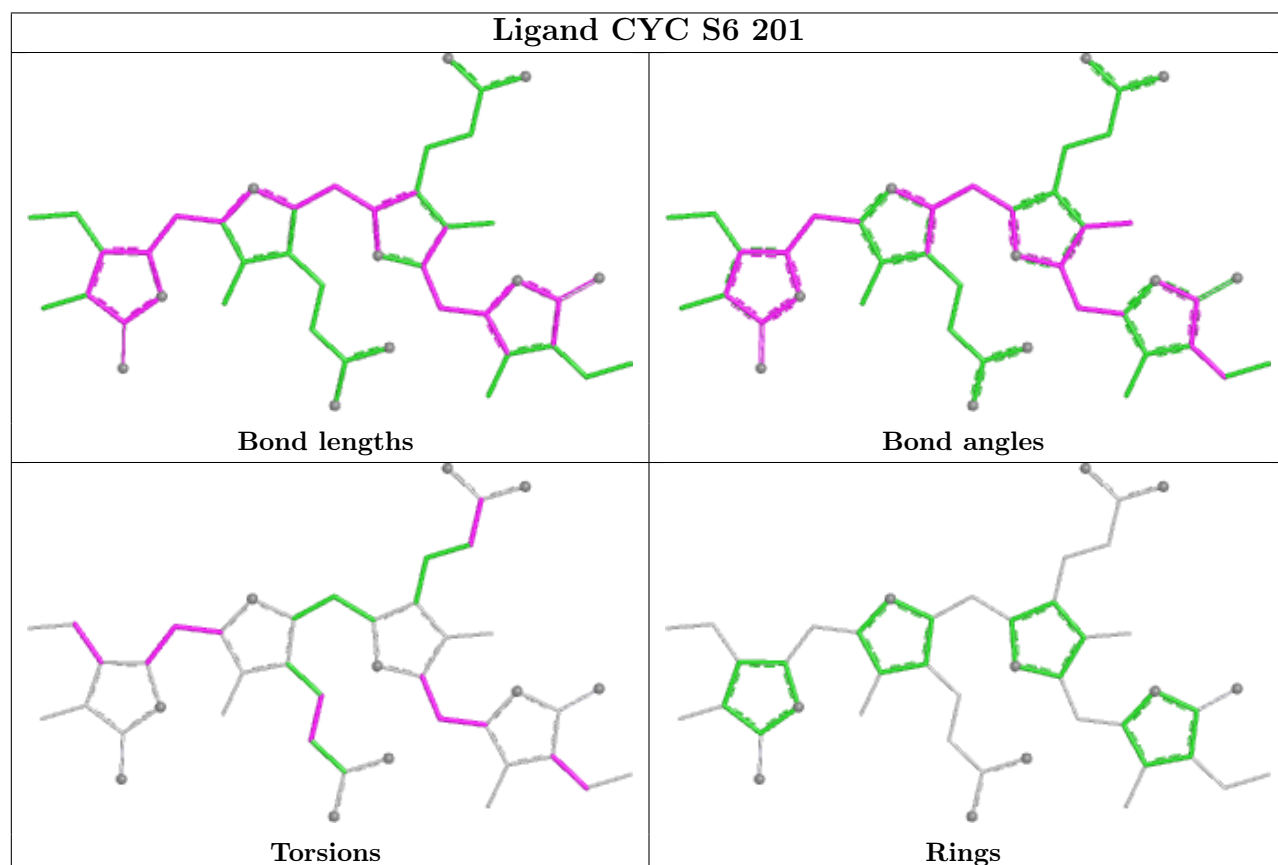
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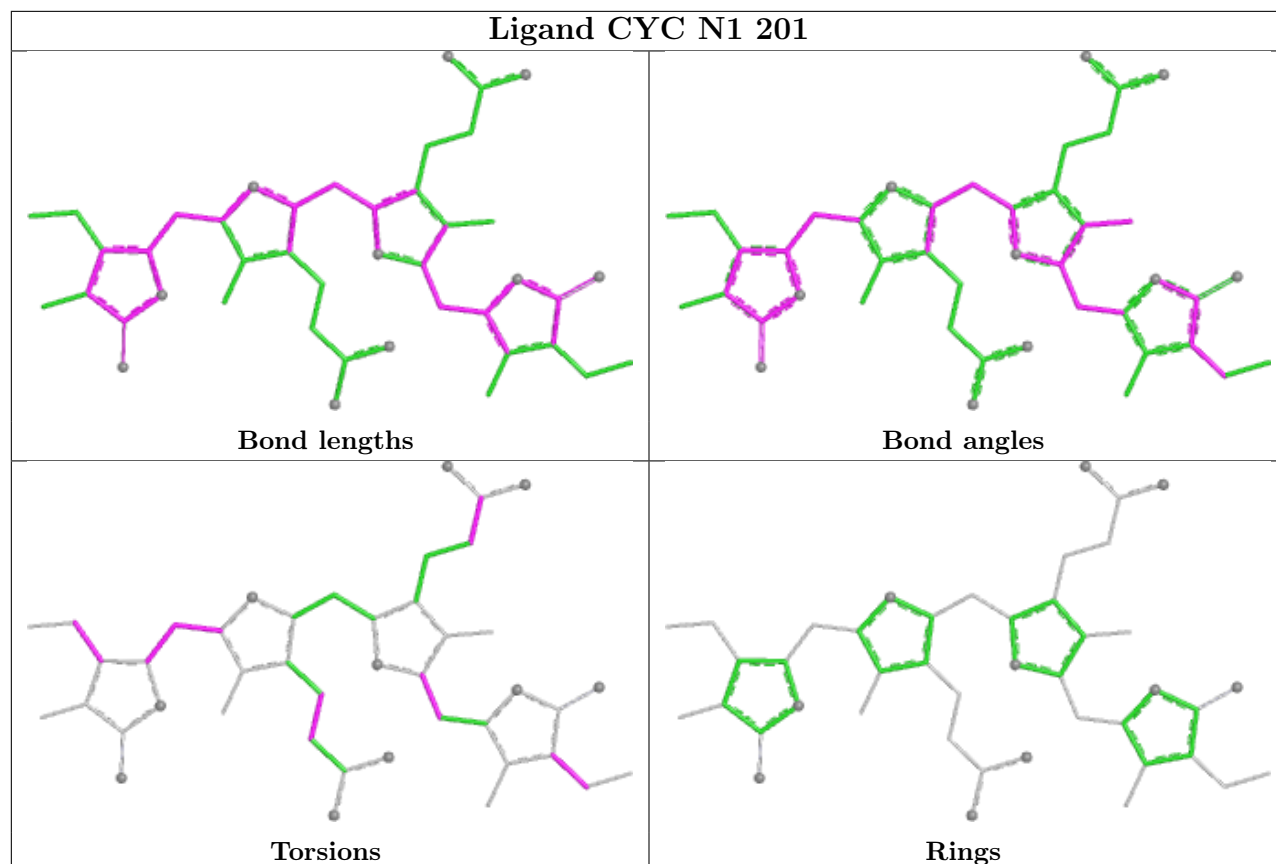
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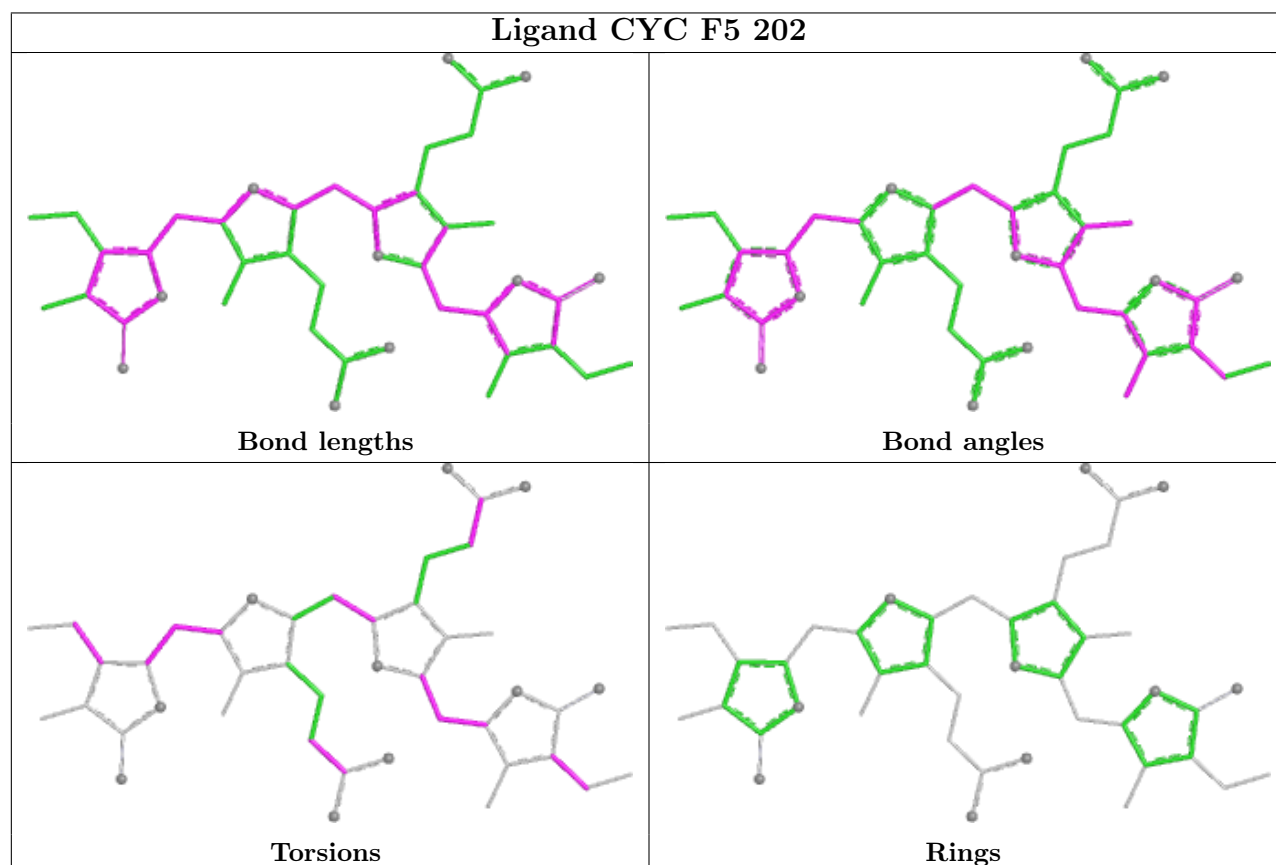
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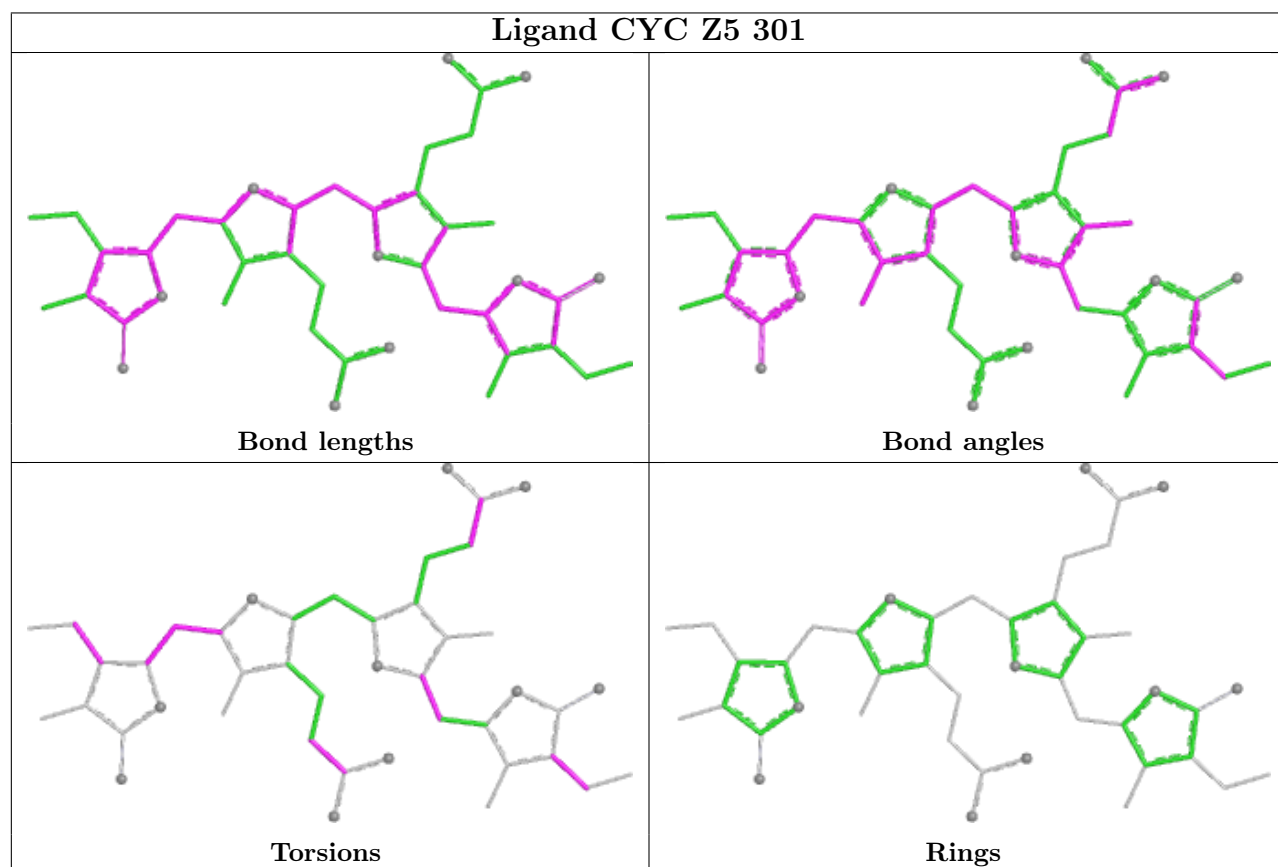
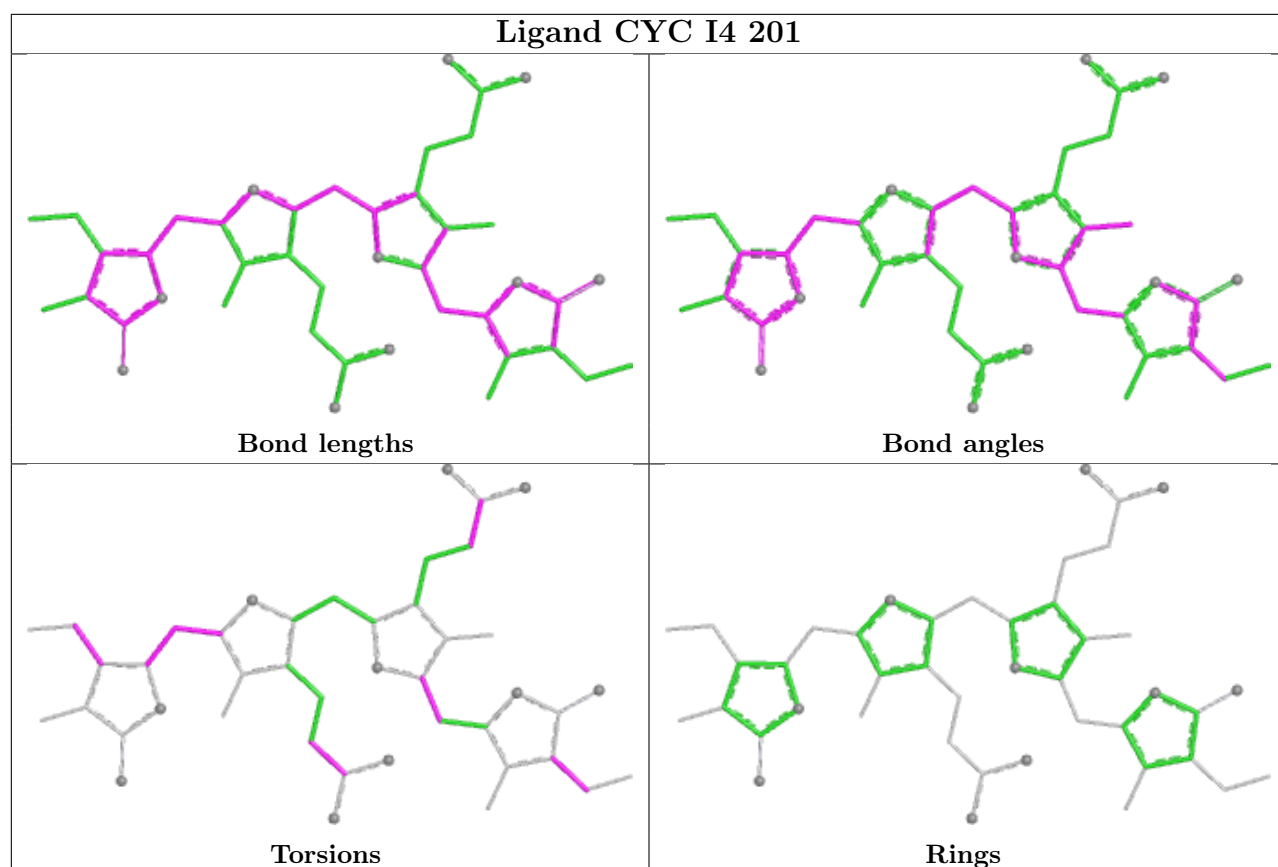


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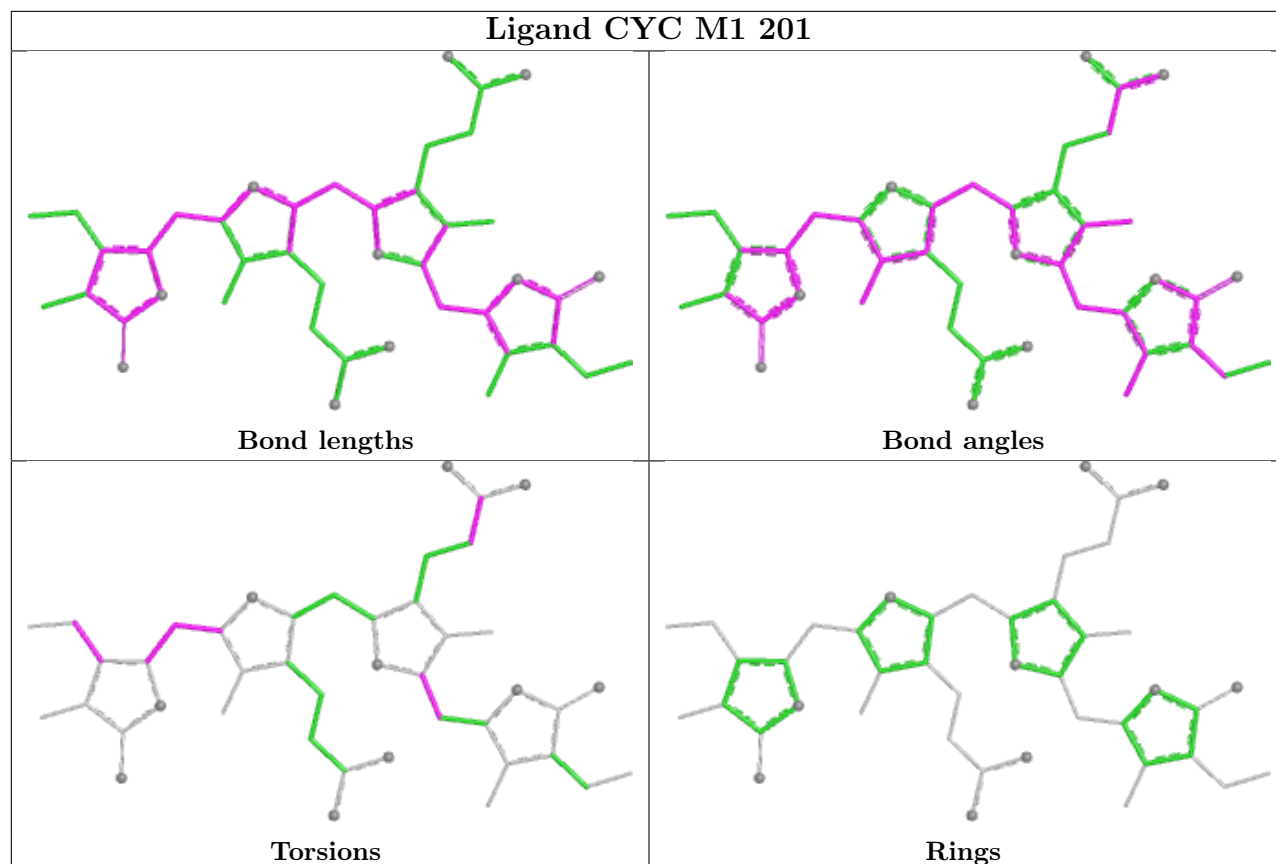


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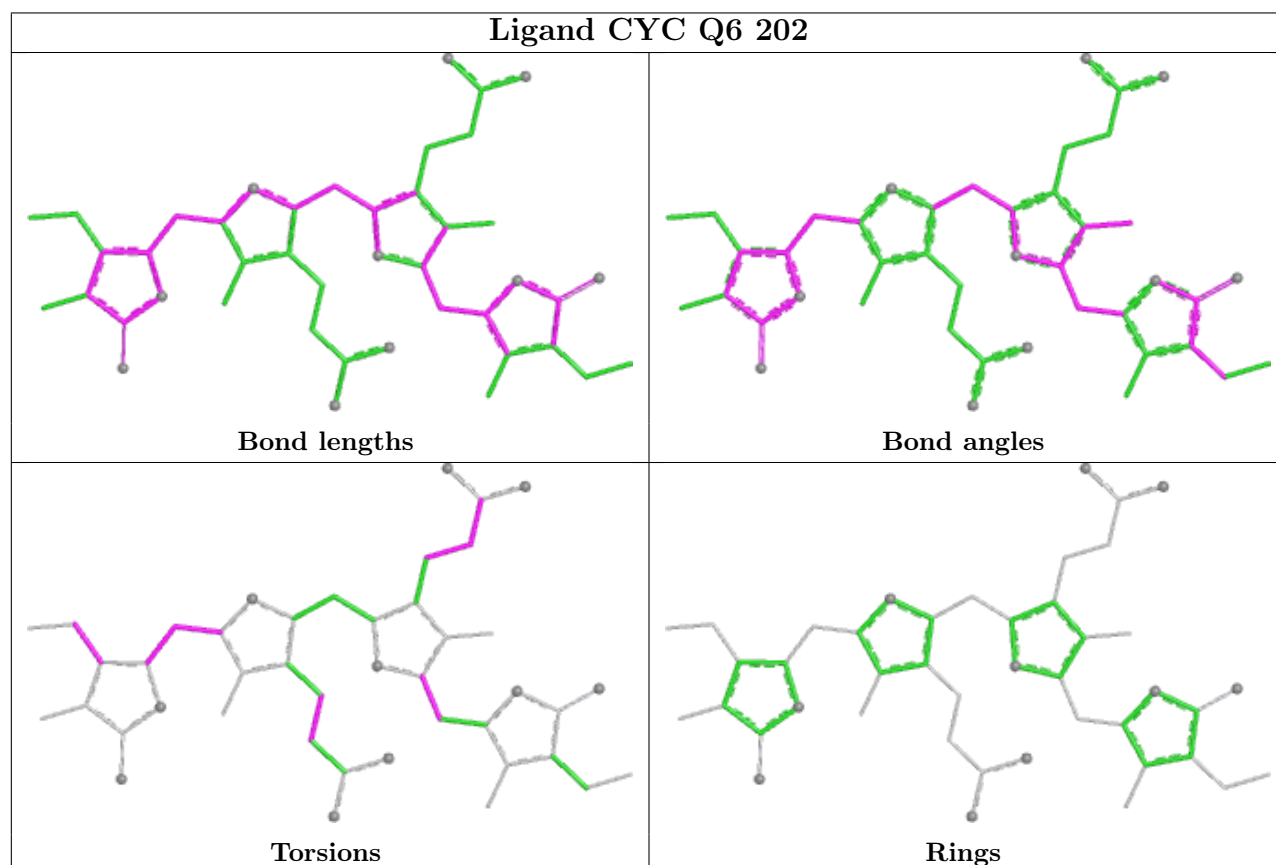




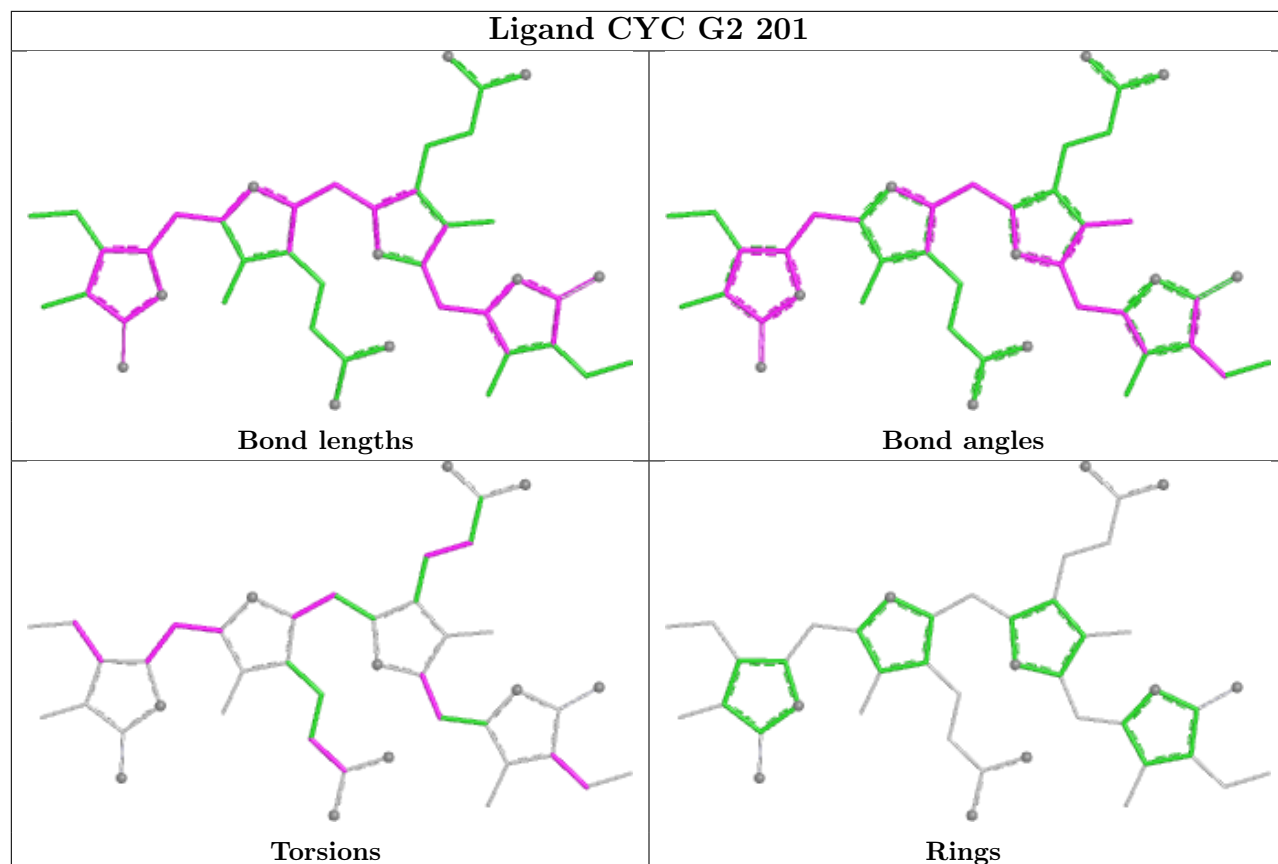
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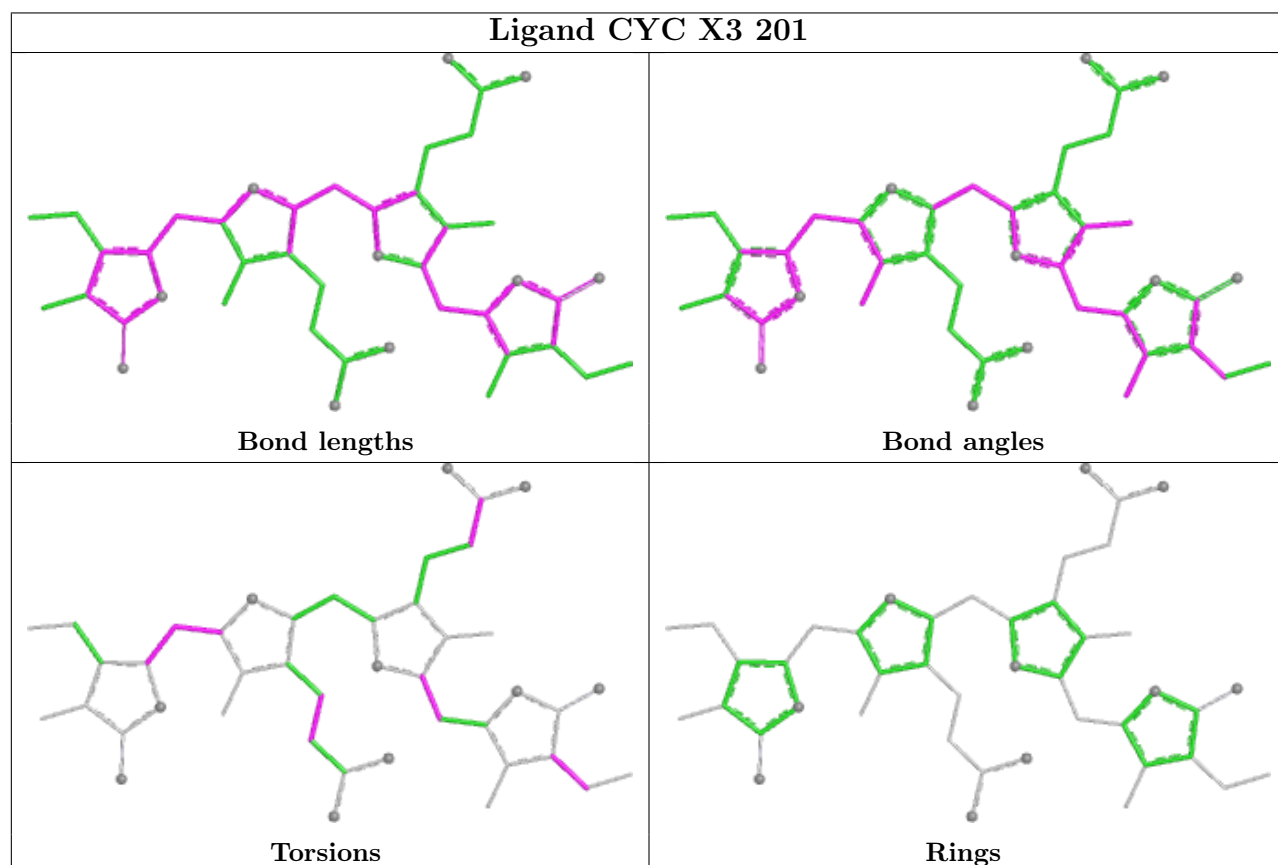
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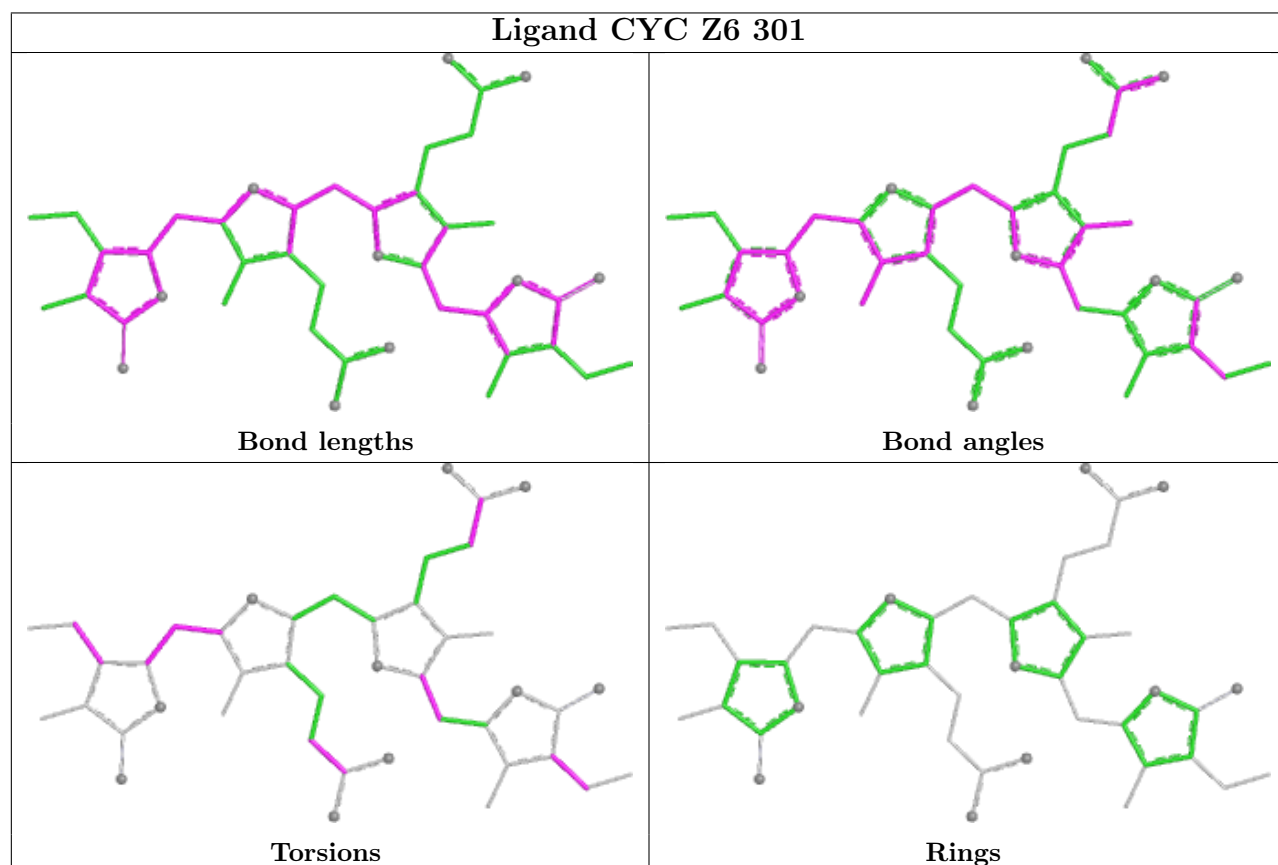
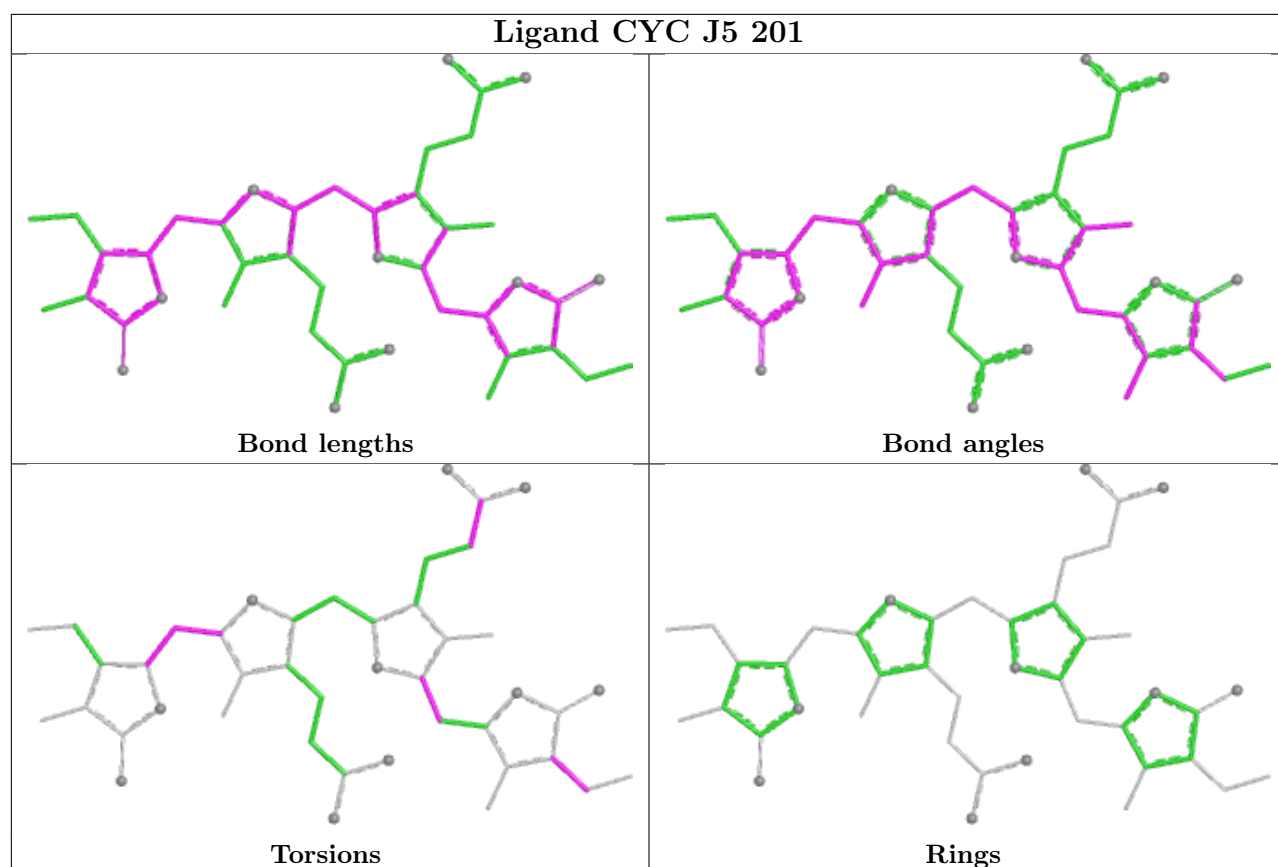


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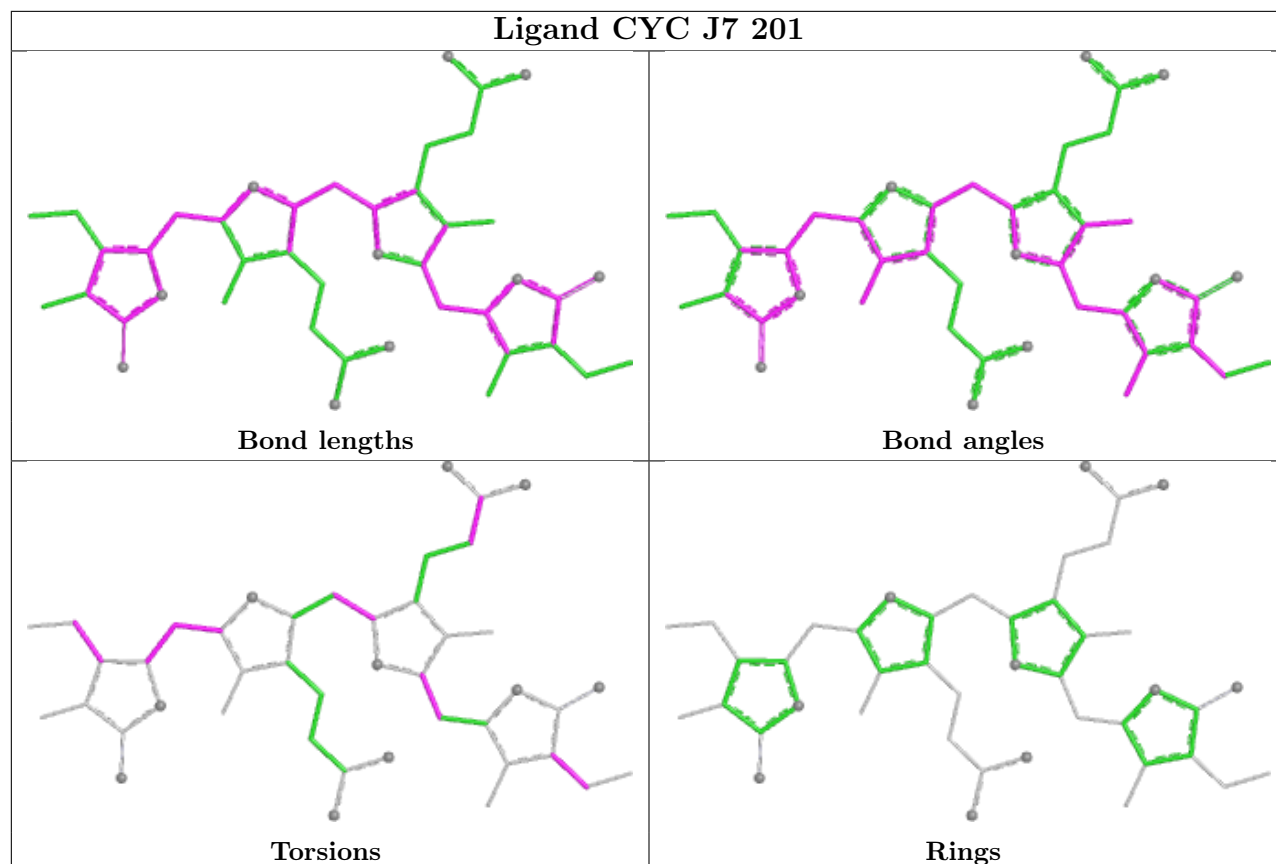


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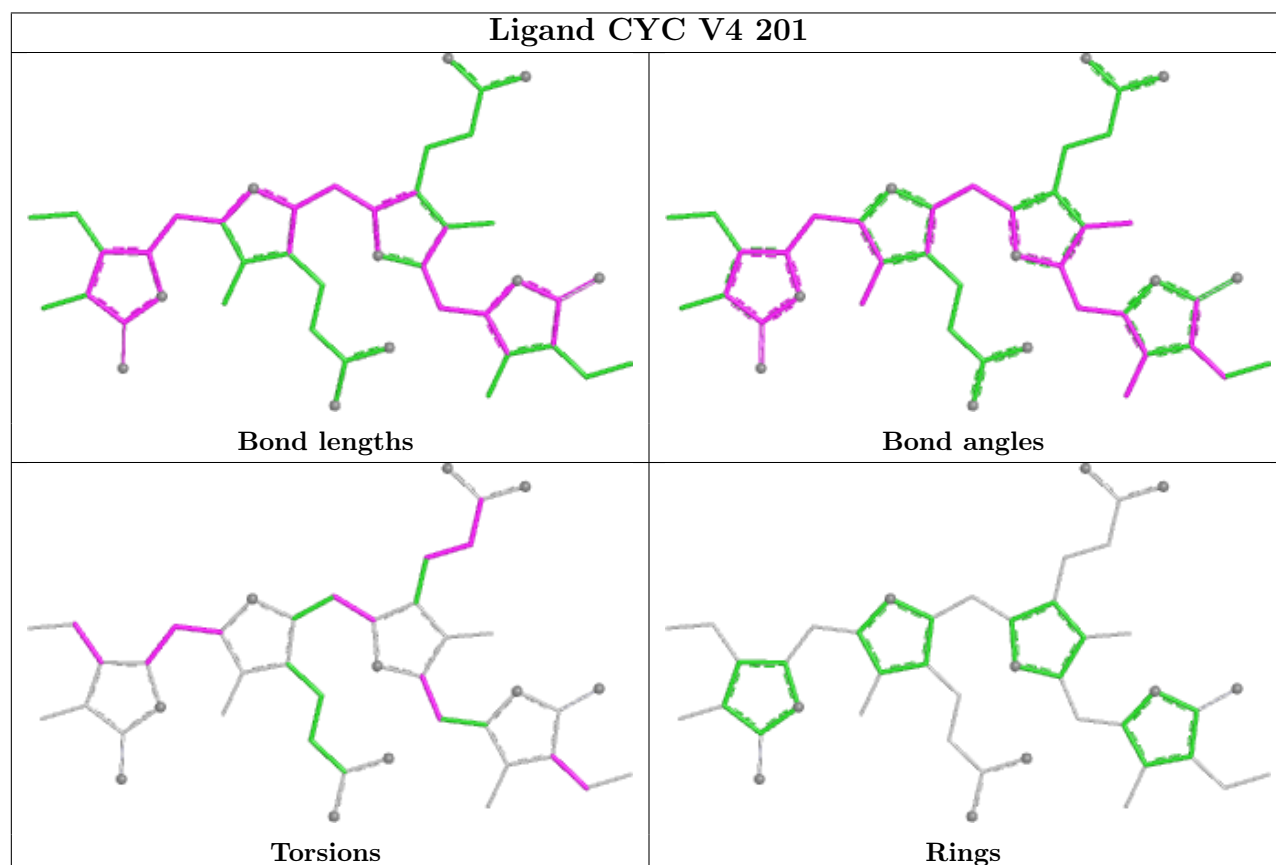




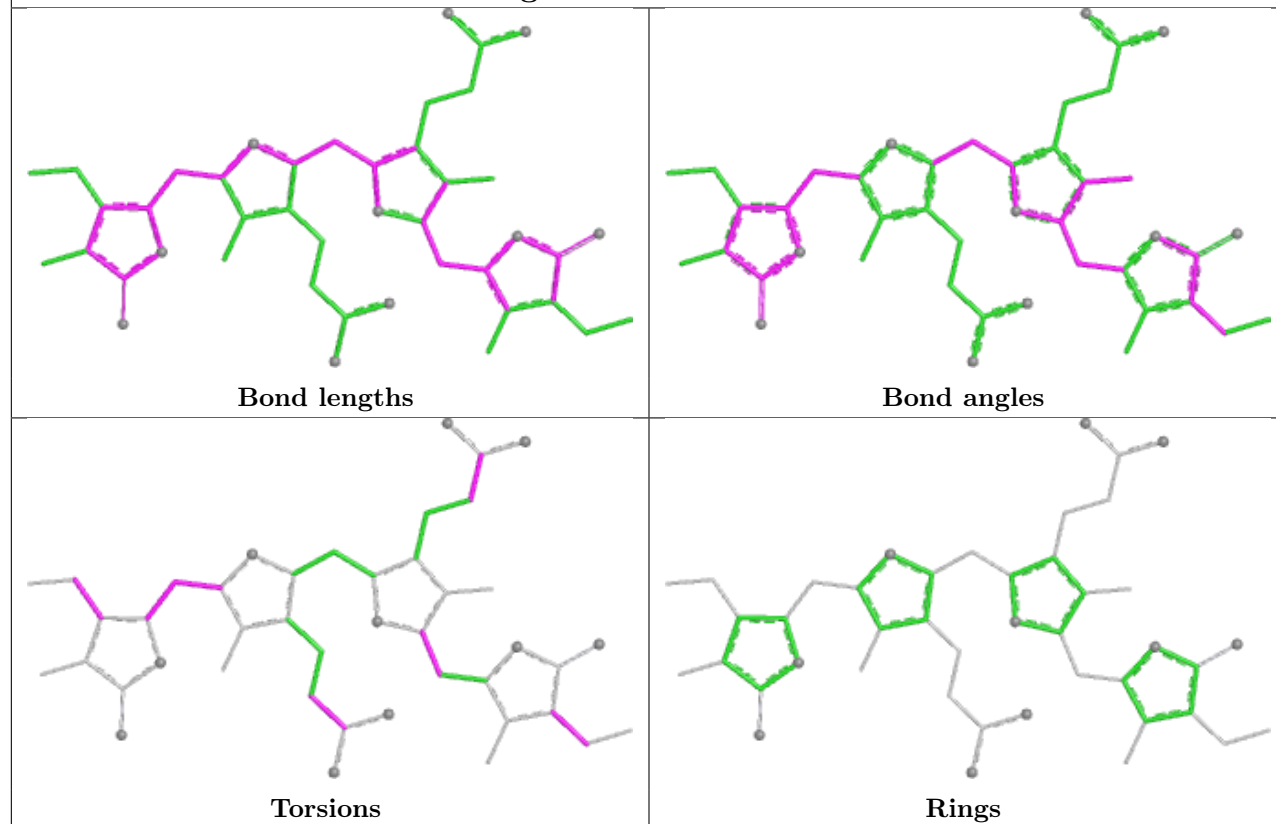
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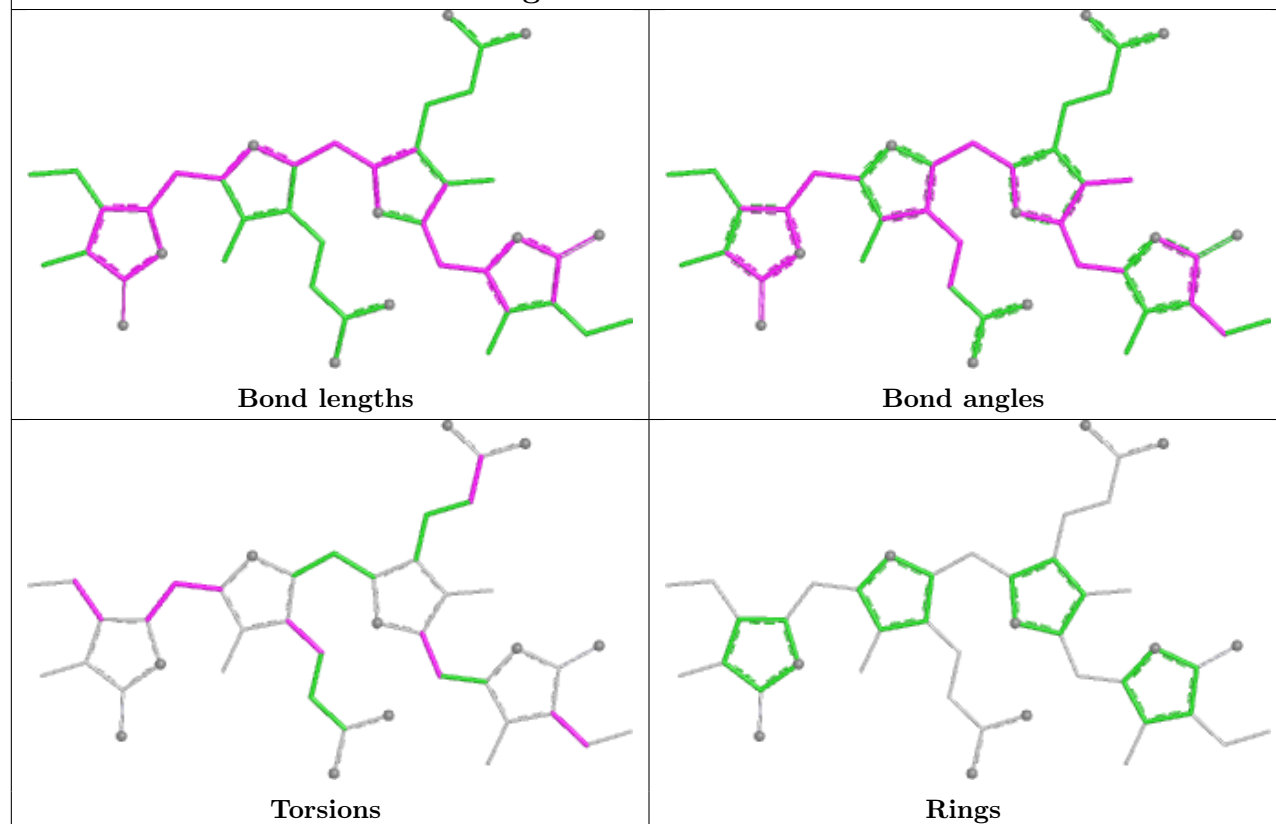
Ligand CYC V4 201

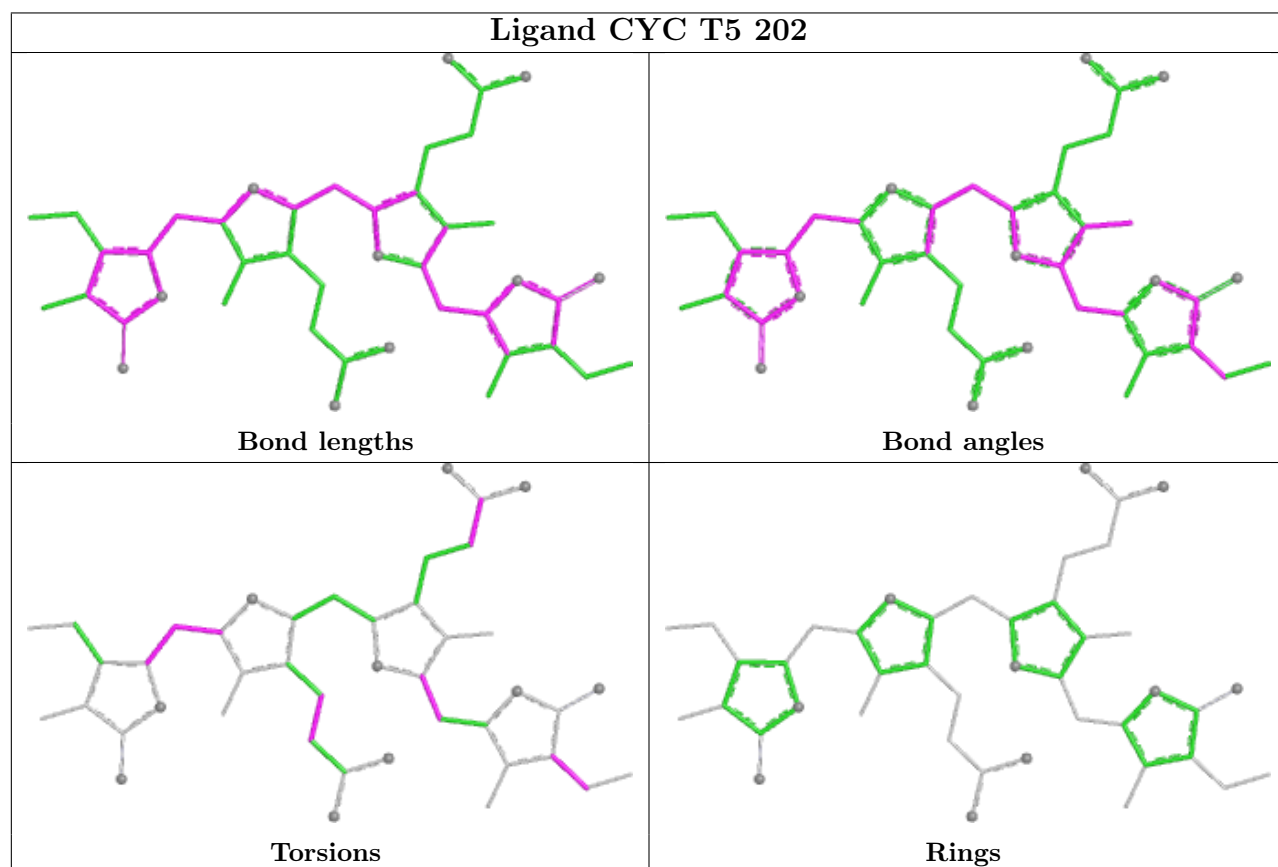
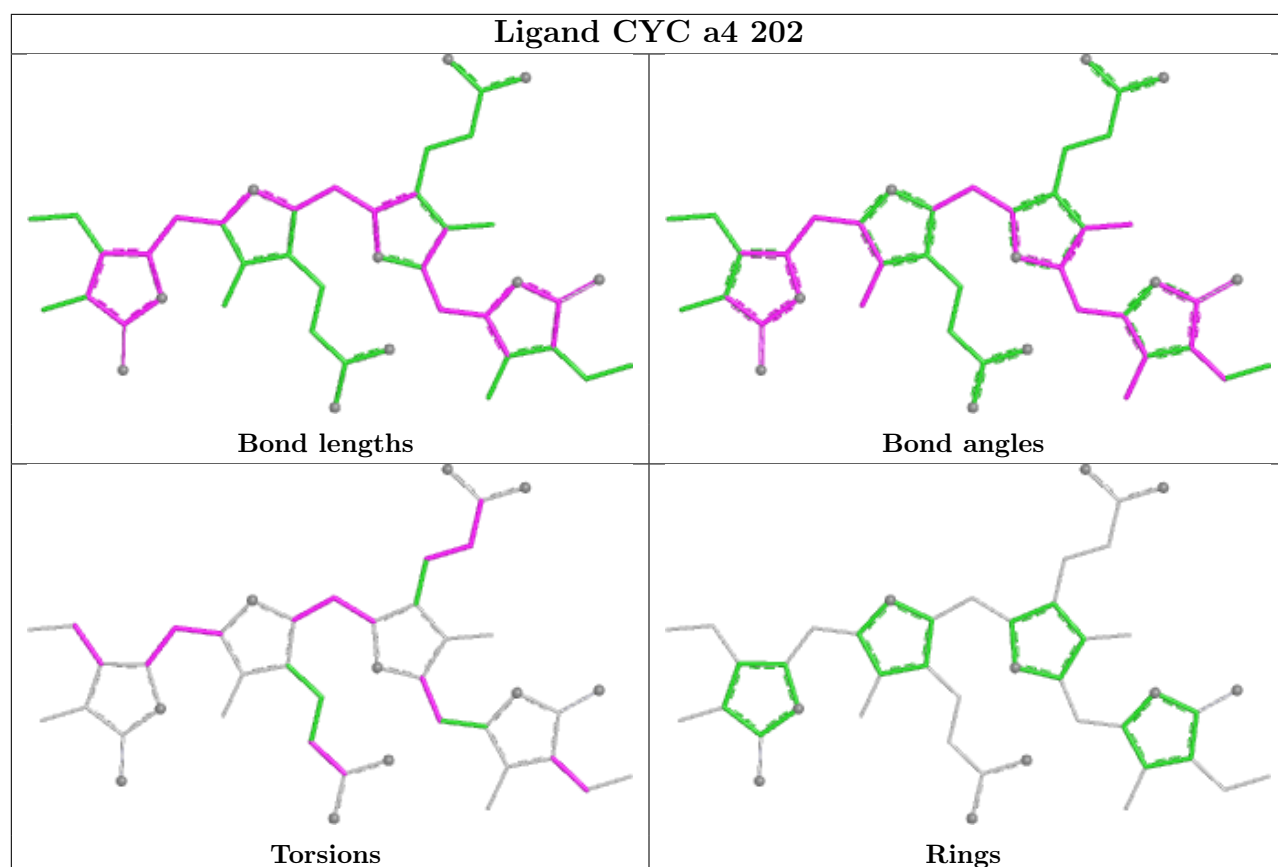


Ligand CYC U7 201

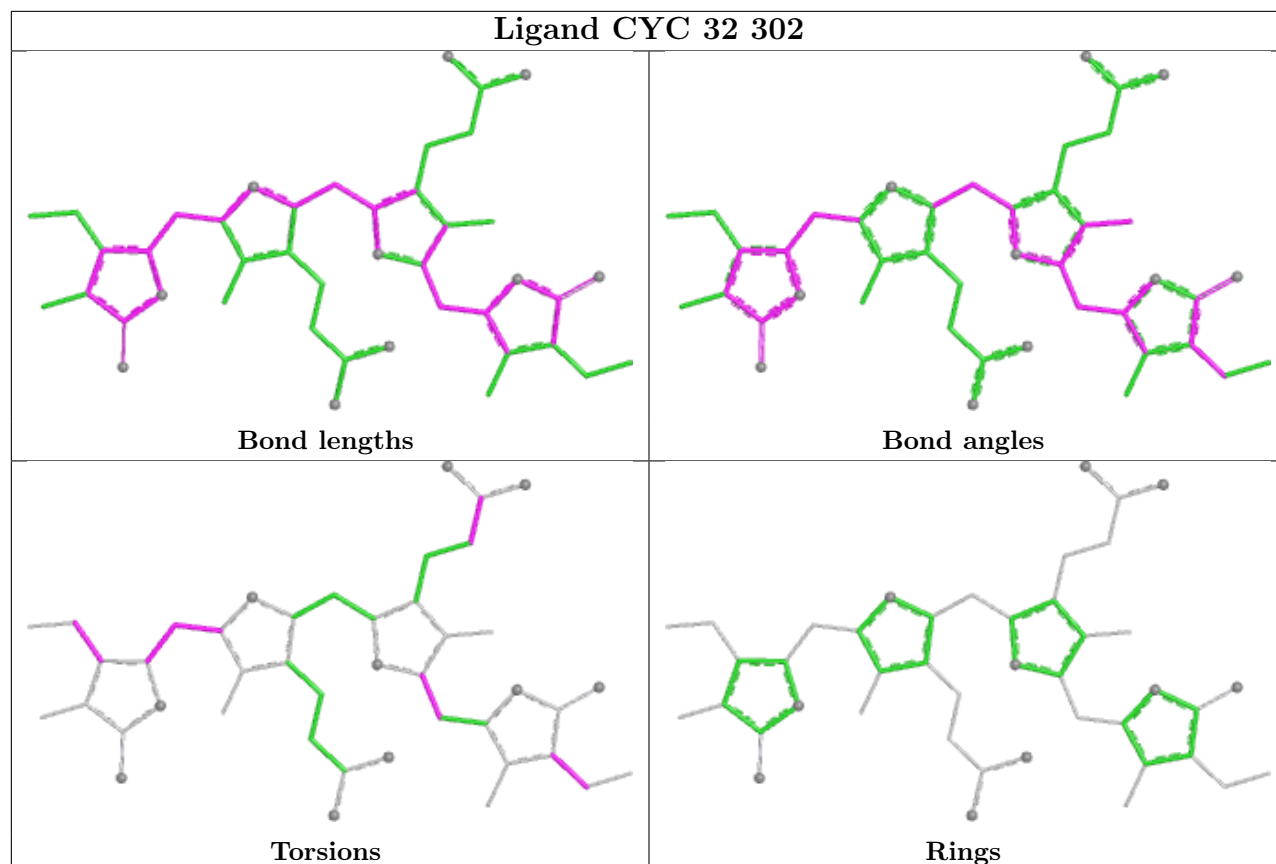


Ligand CYC F5 201

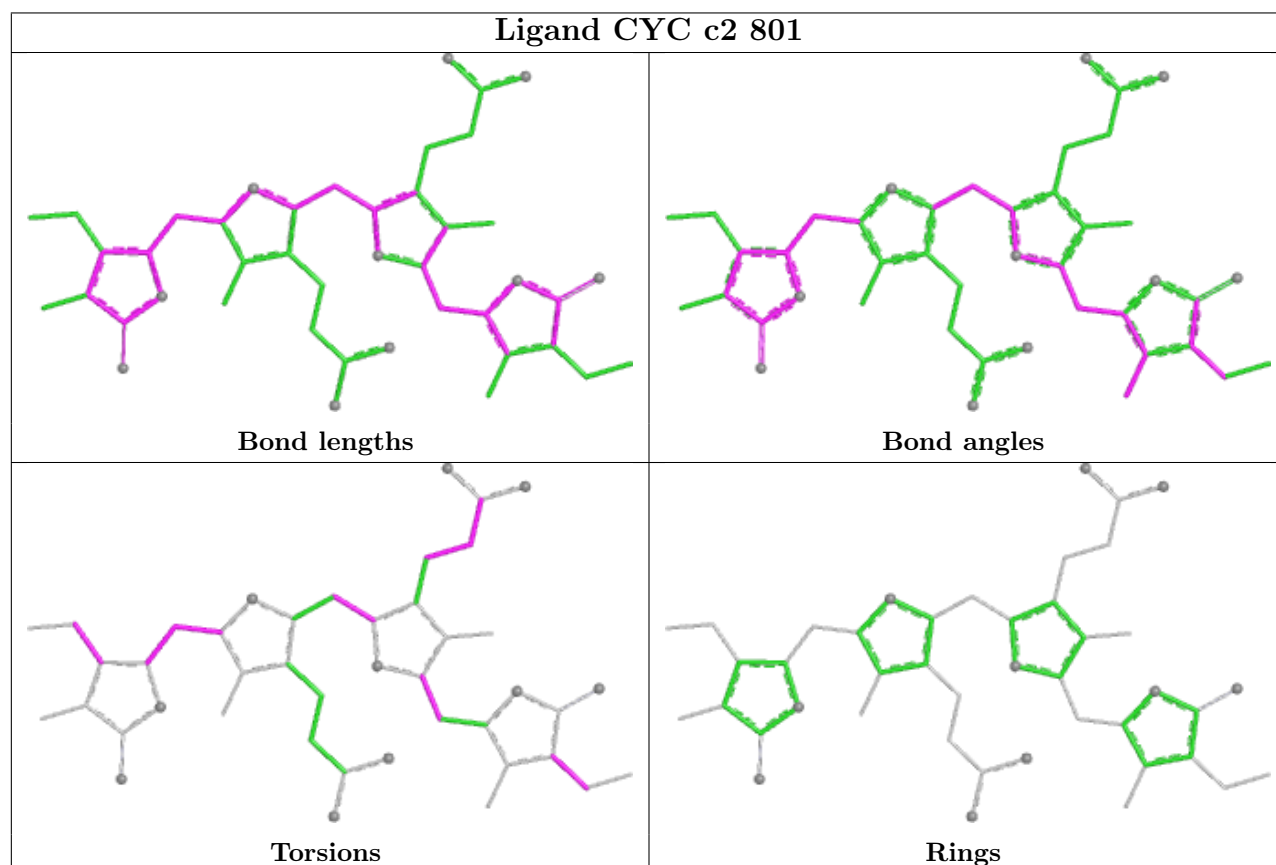




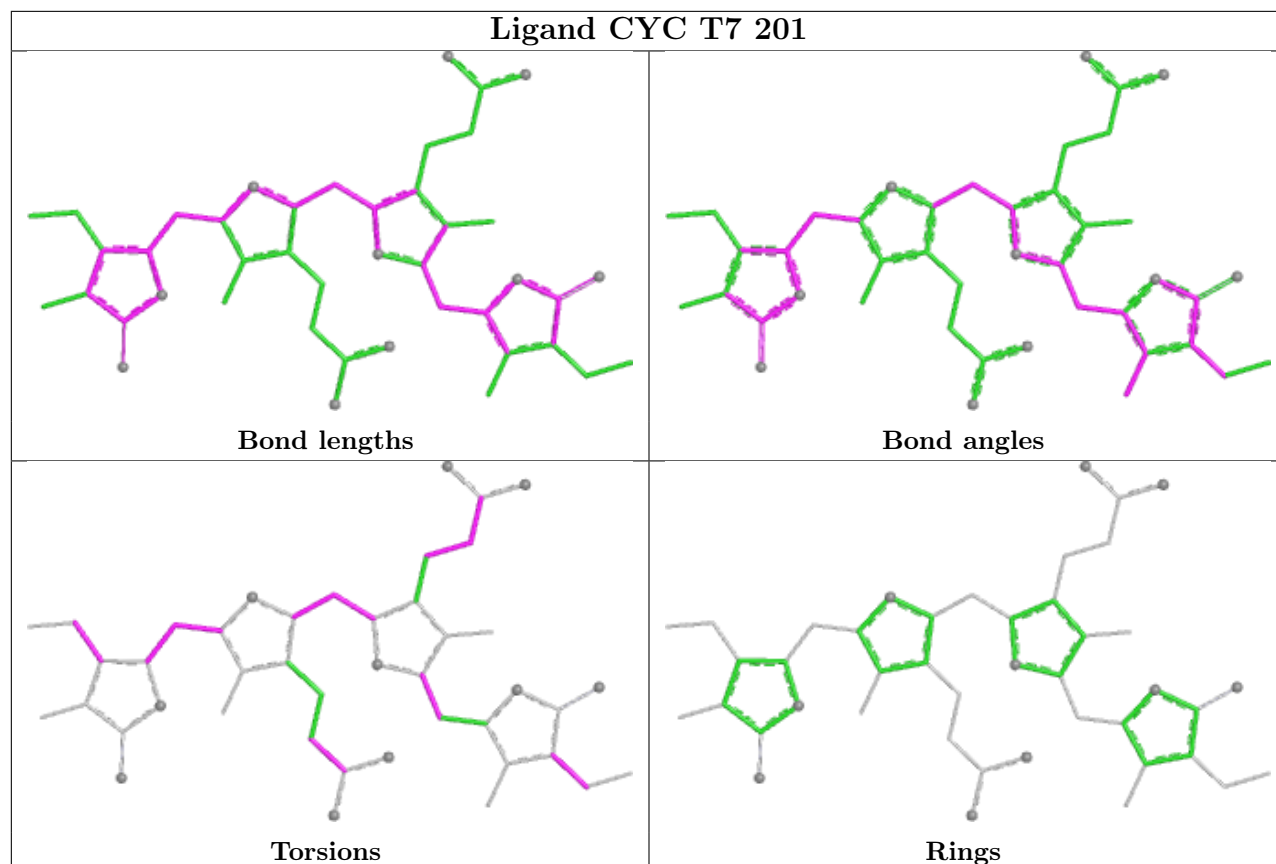
Ligand CYC 32 302



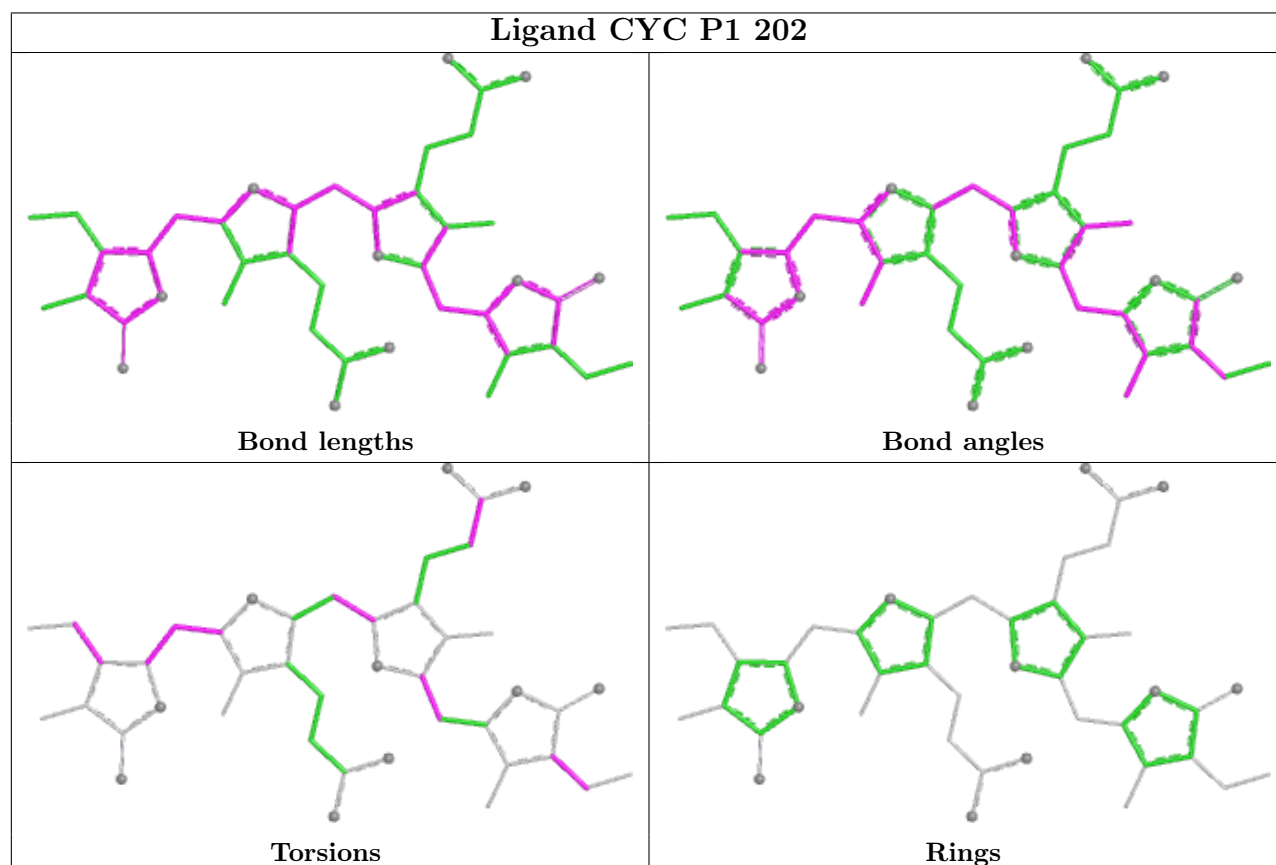
Ligand CYC c2 801

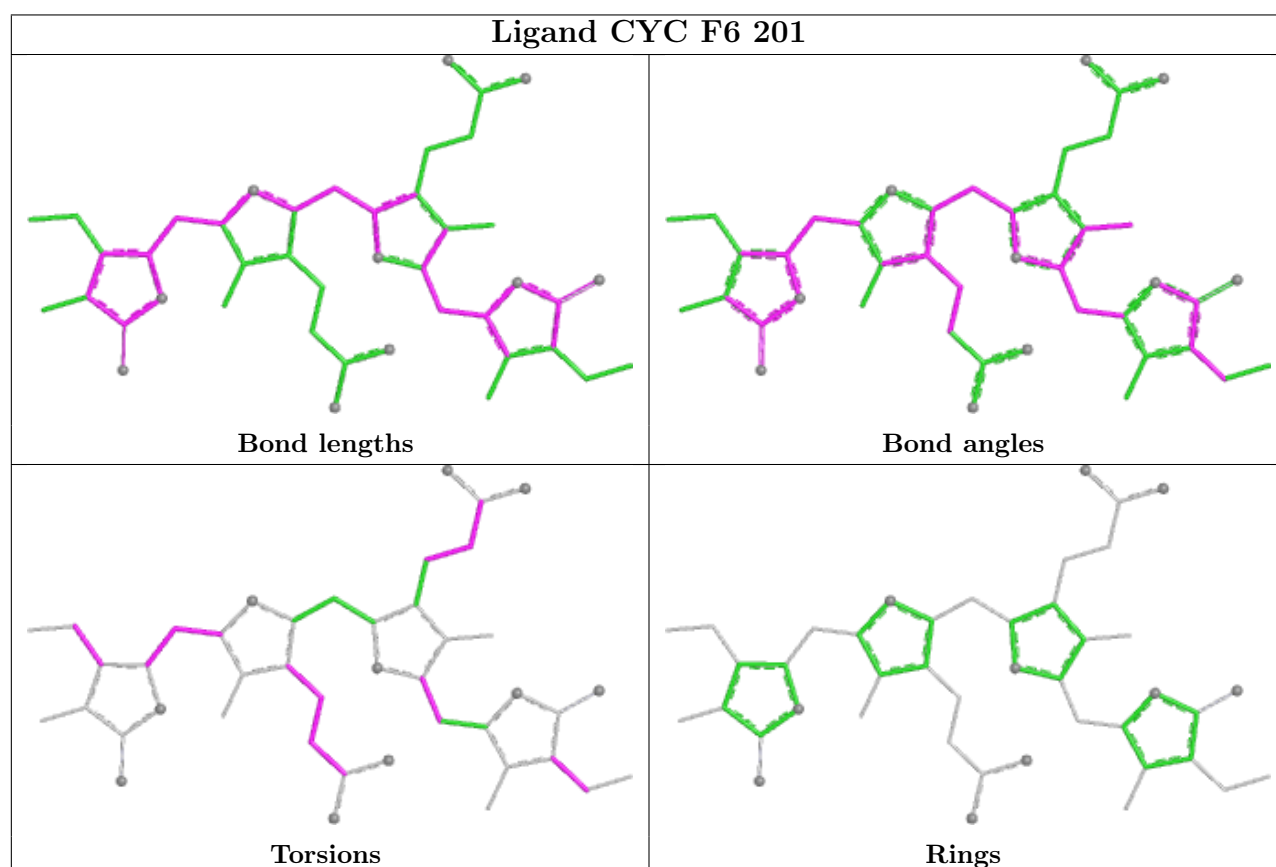
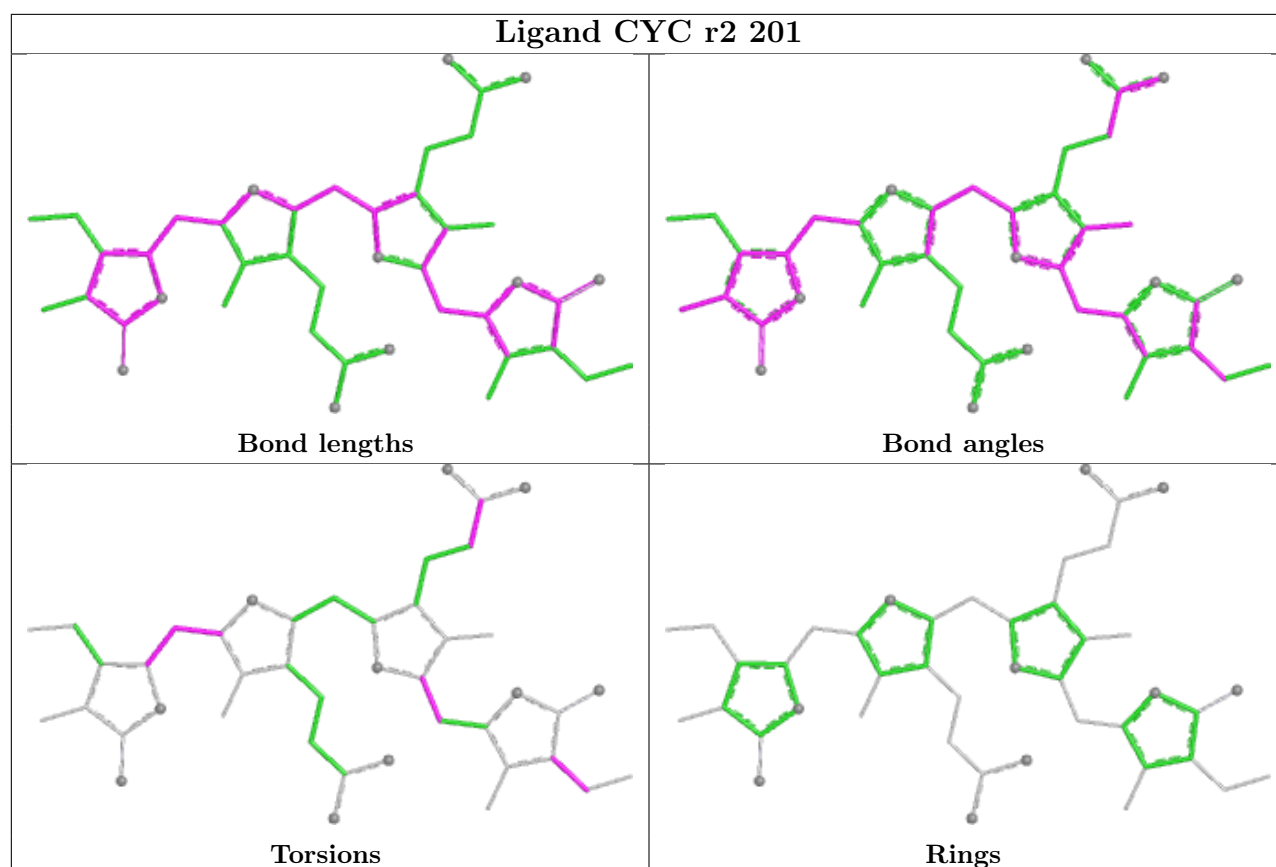


Ligand CYC T7 201

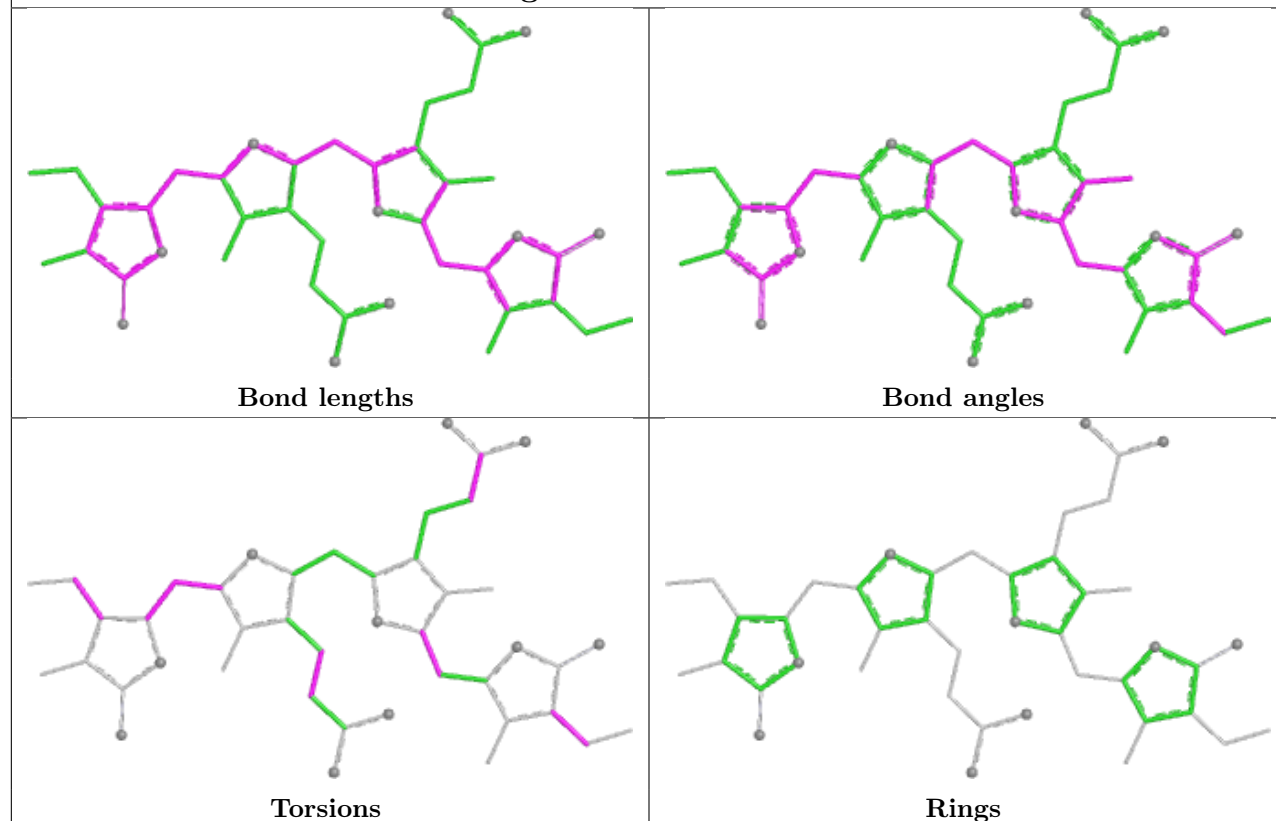


Ligand CYC P1 202

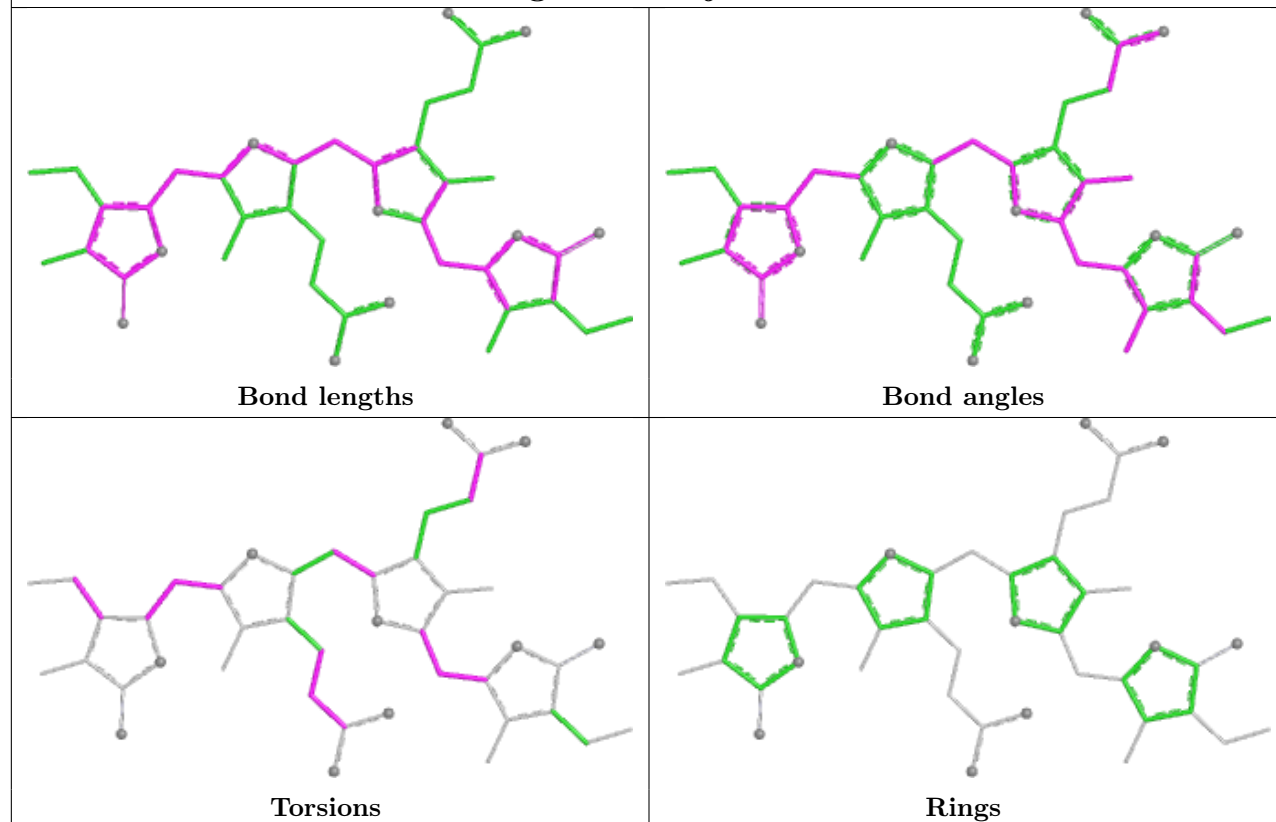




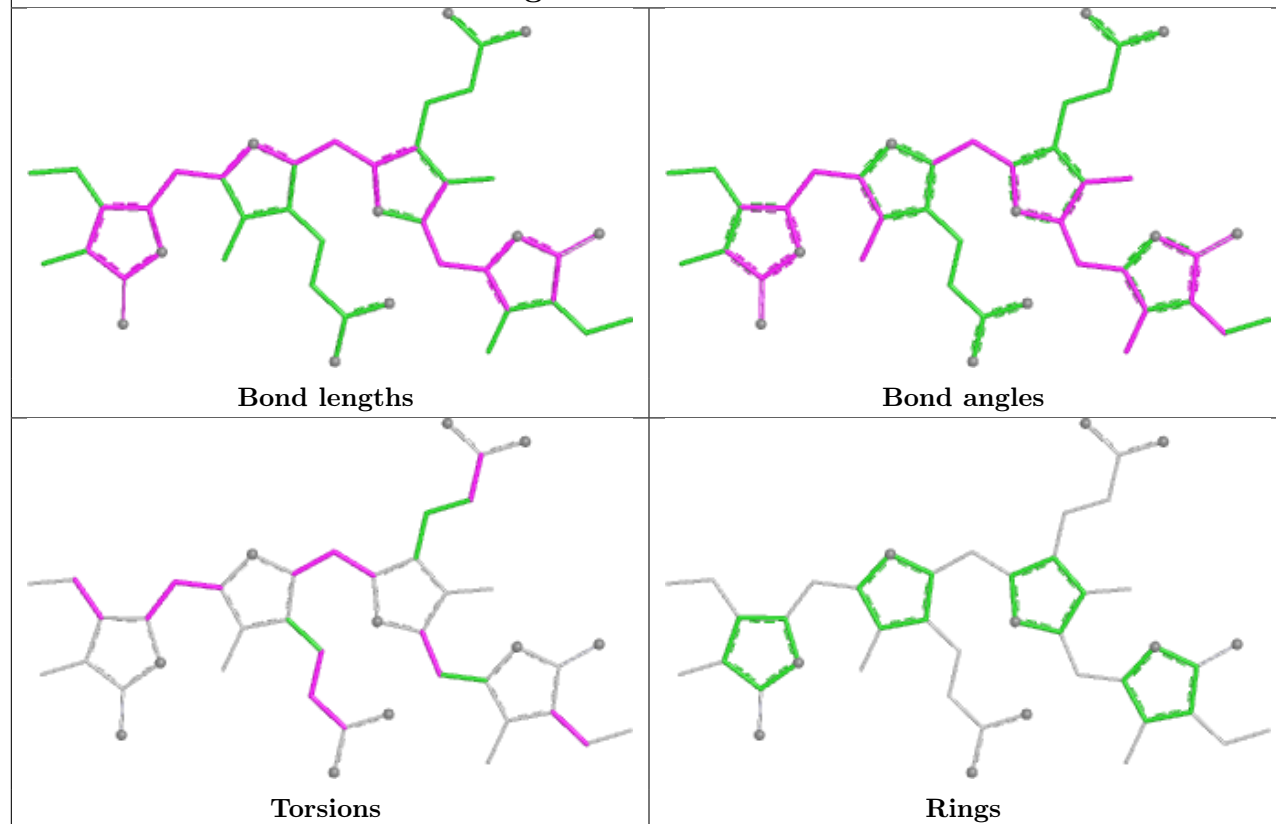
Ligand CYC R7 201



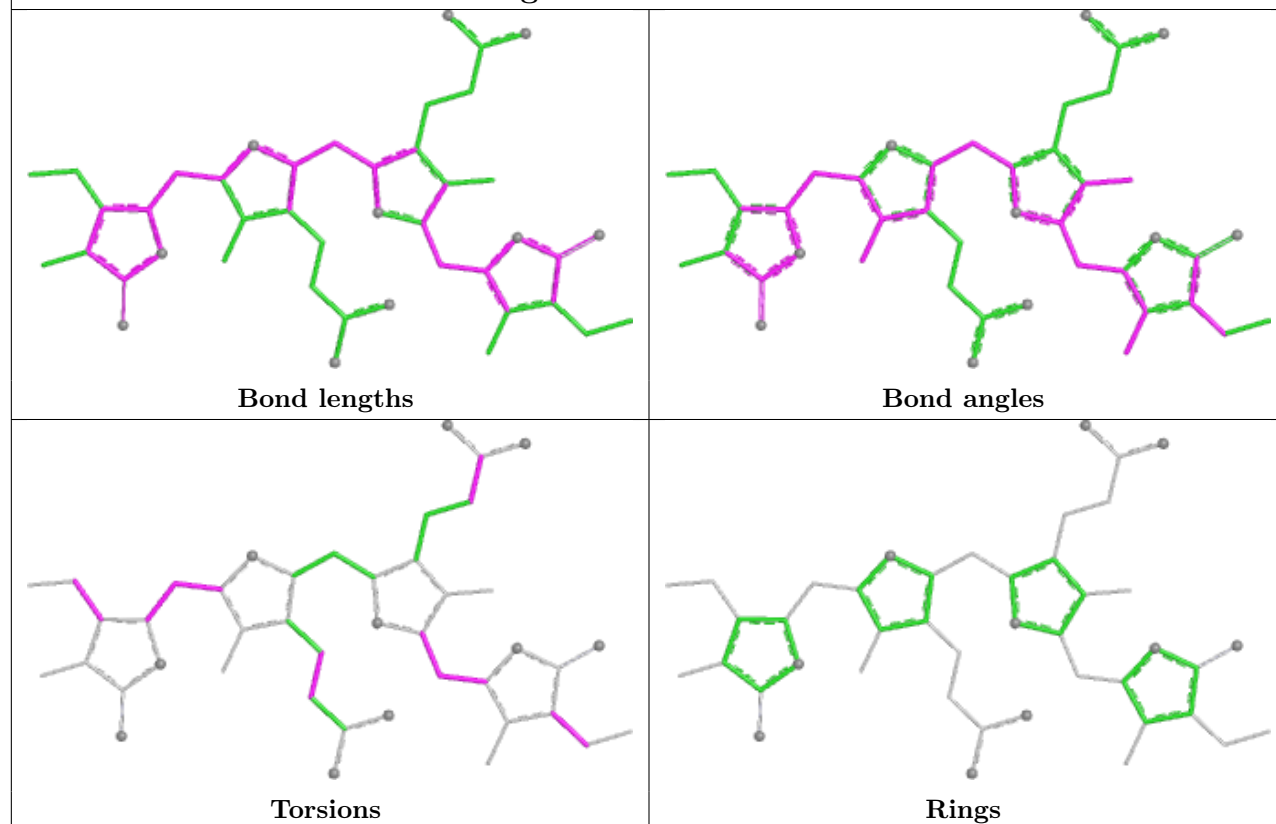
Ligand CYC j2 201



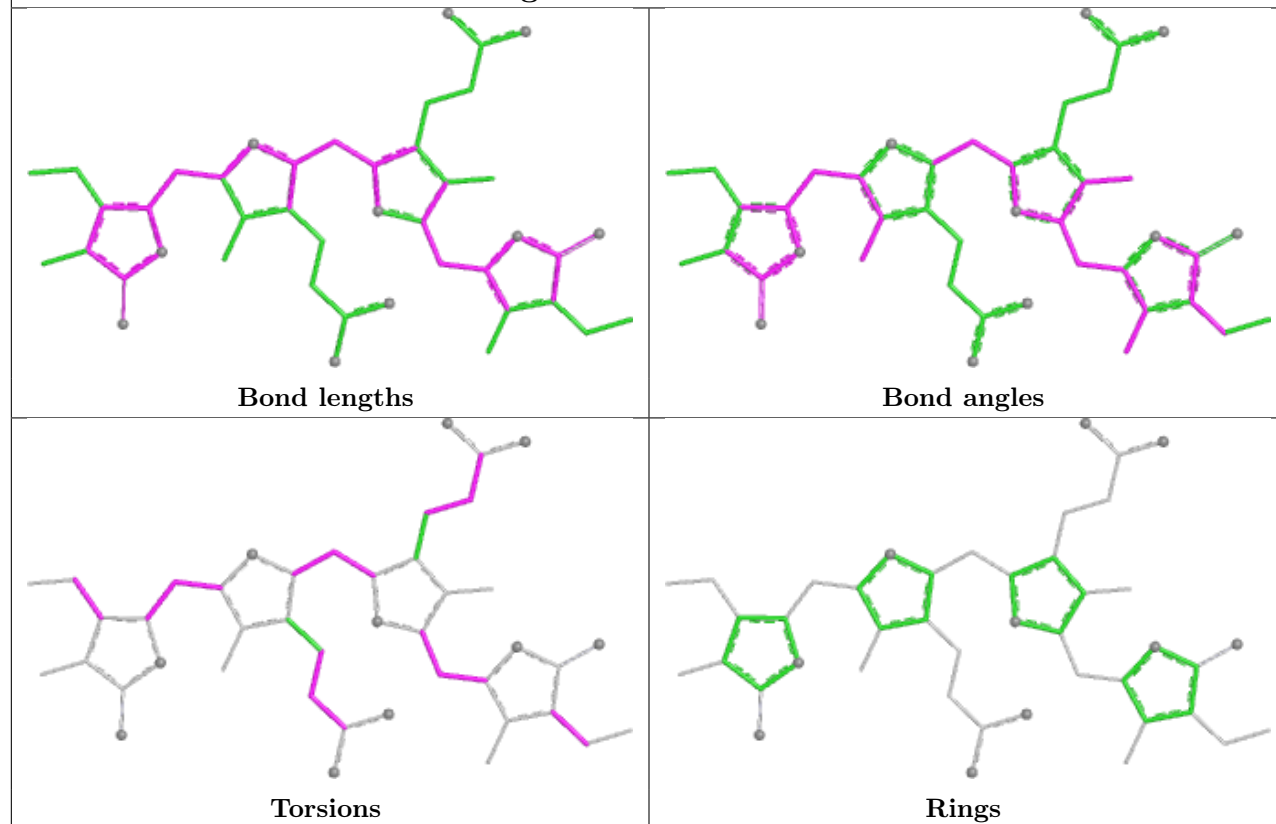
Ligand CYC J4 202



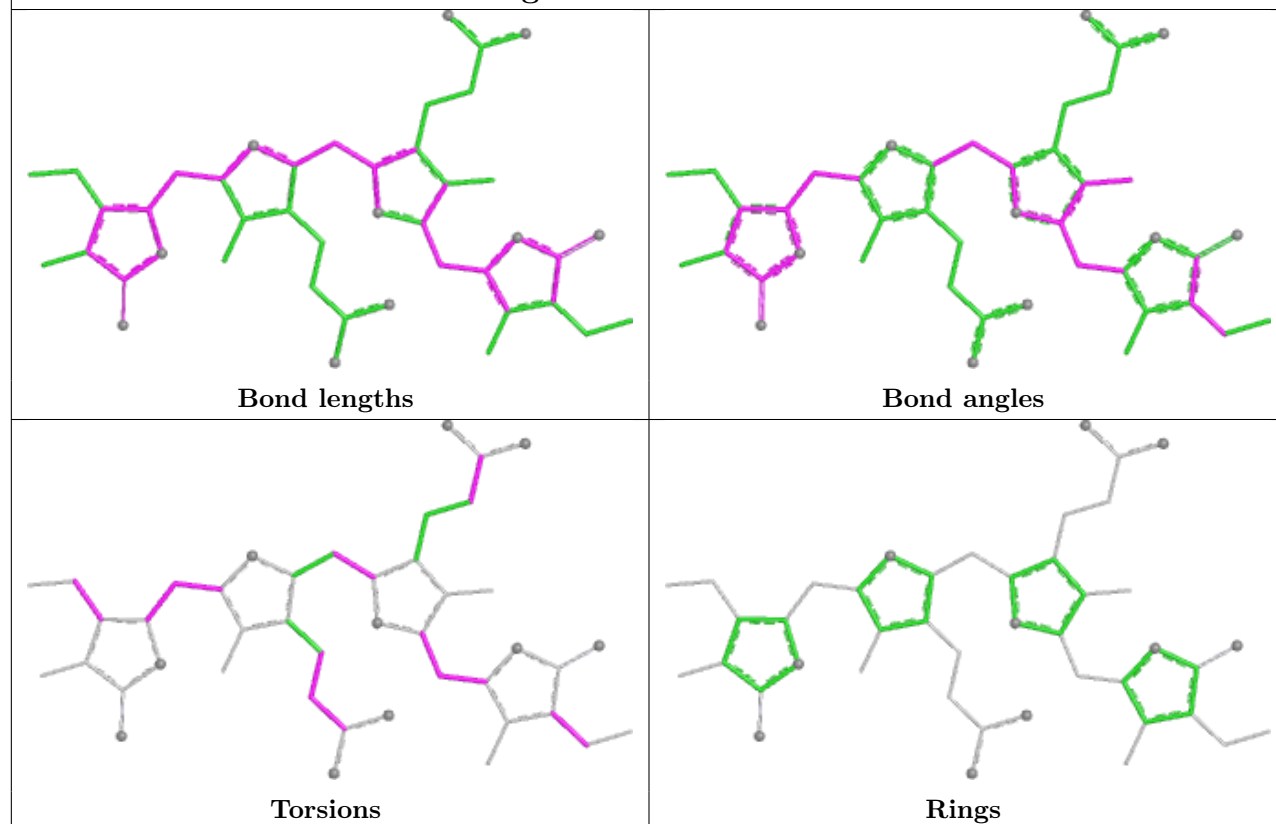
Ligand CYC X5 201



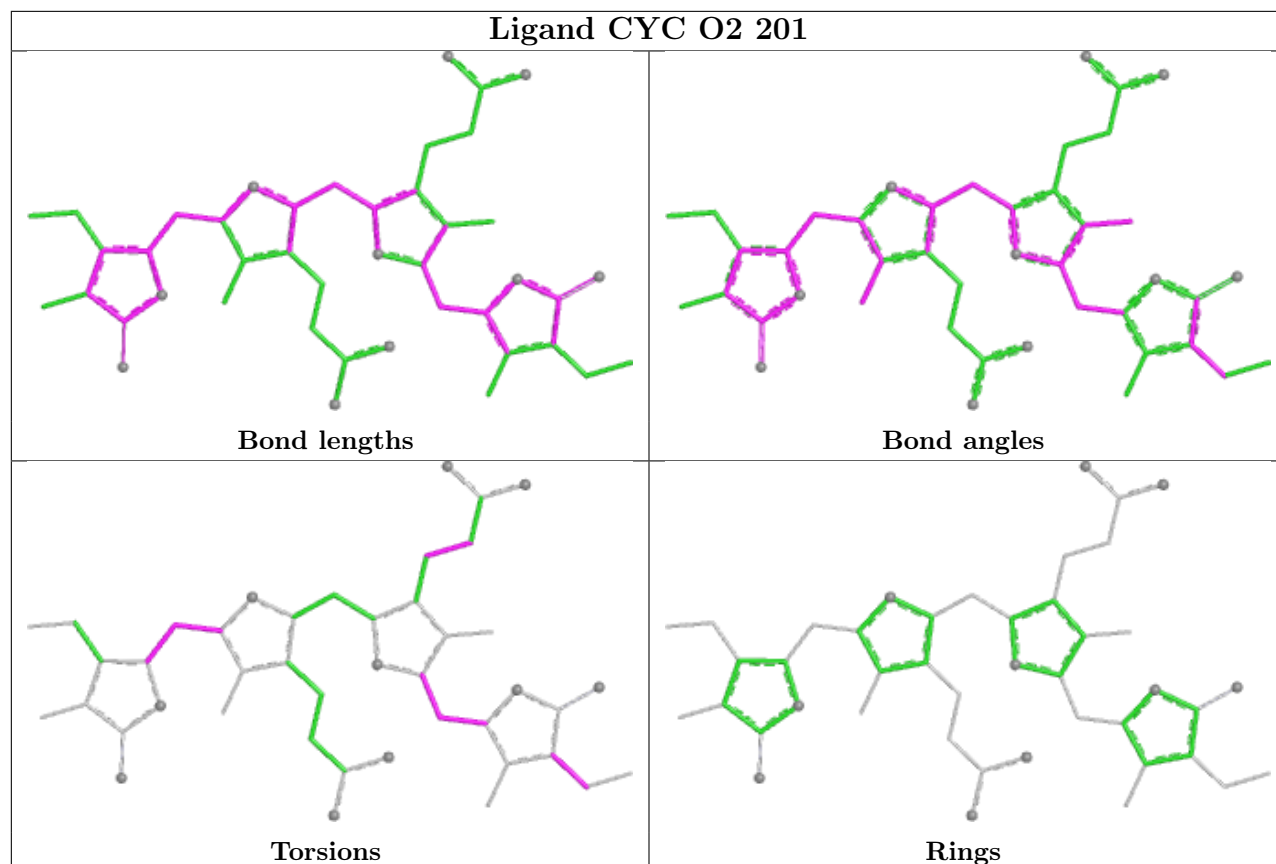
Ligand CYC V5 202



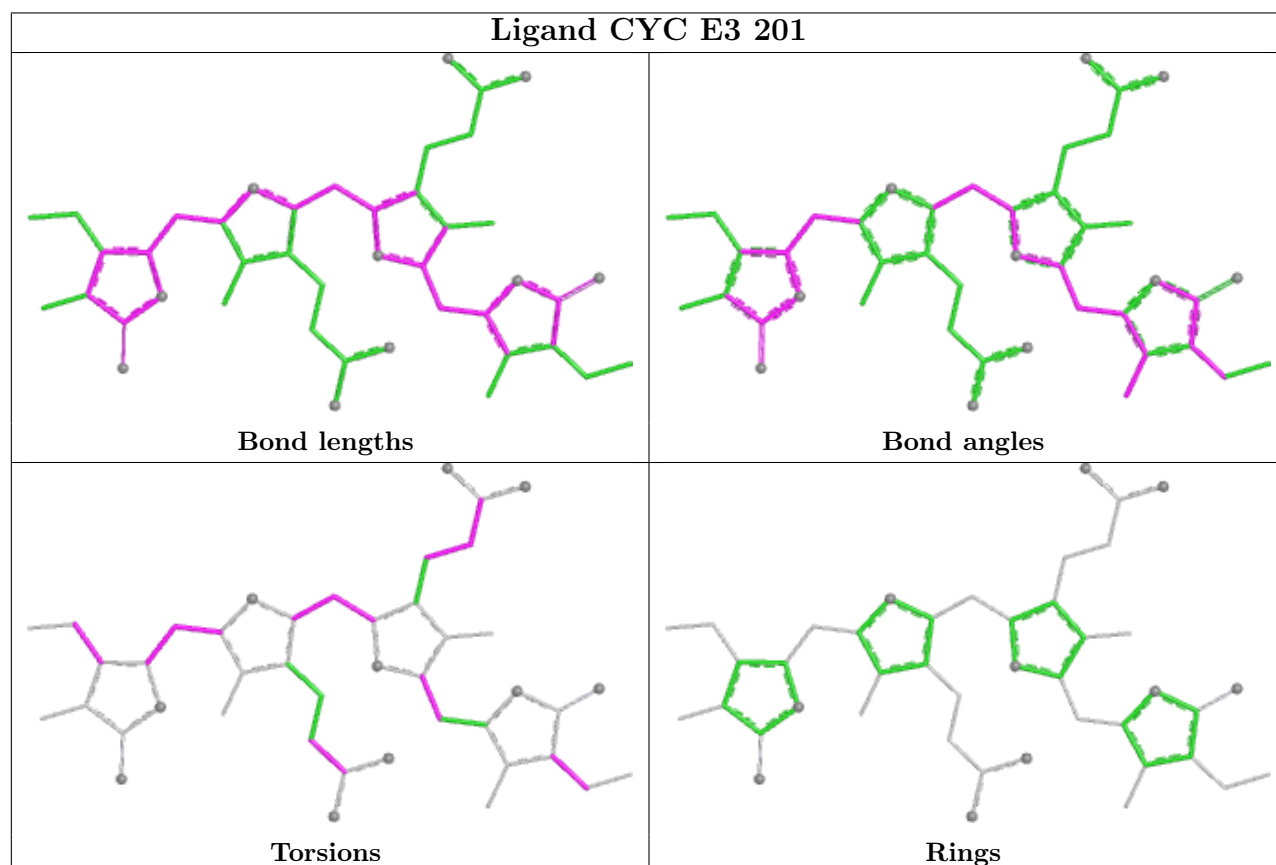
Ligand CYC P4 202



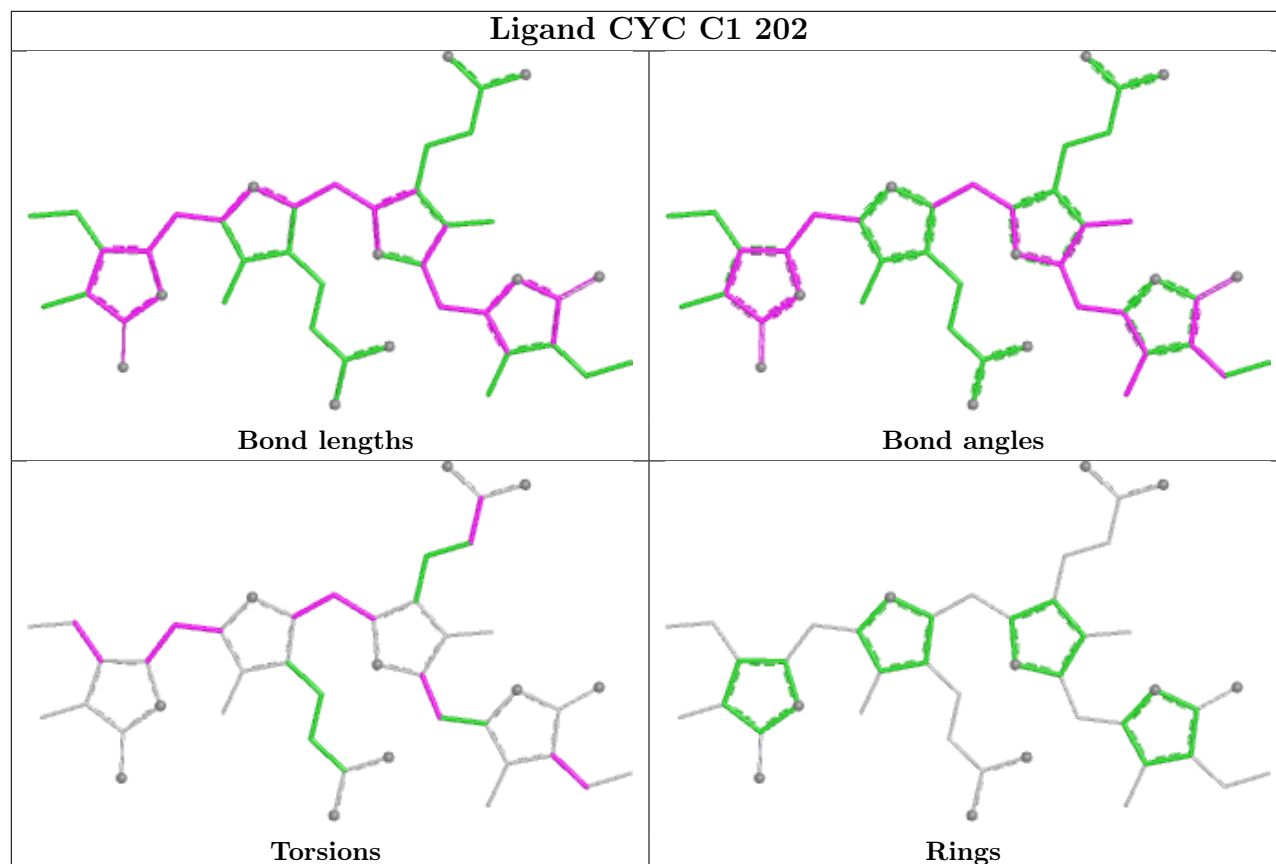
Ligand CYC O2 201



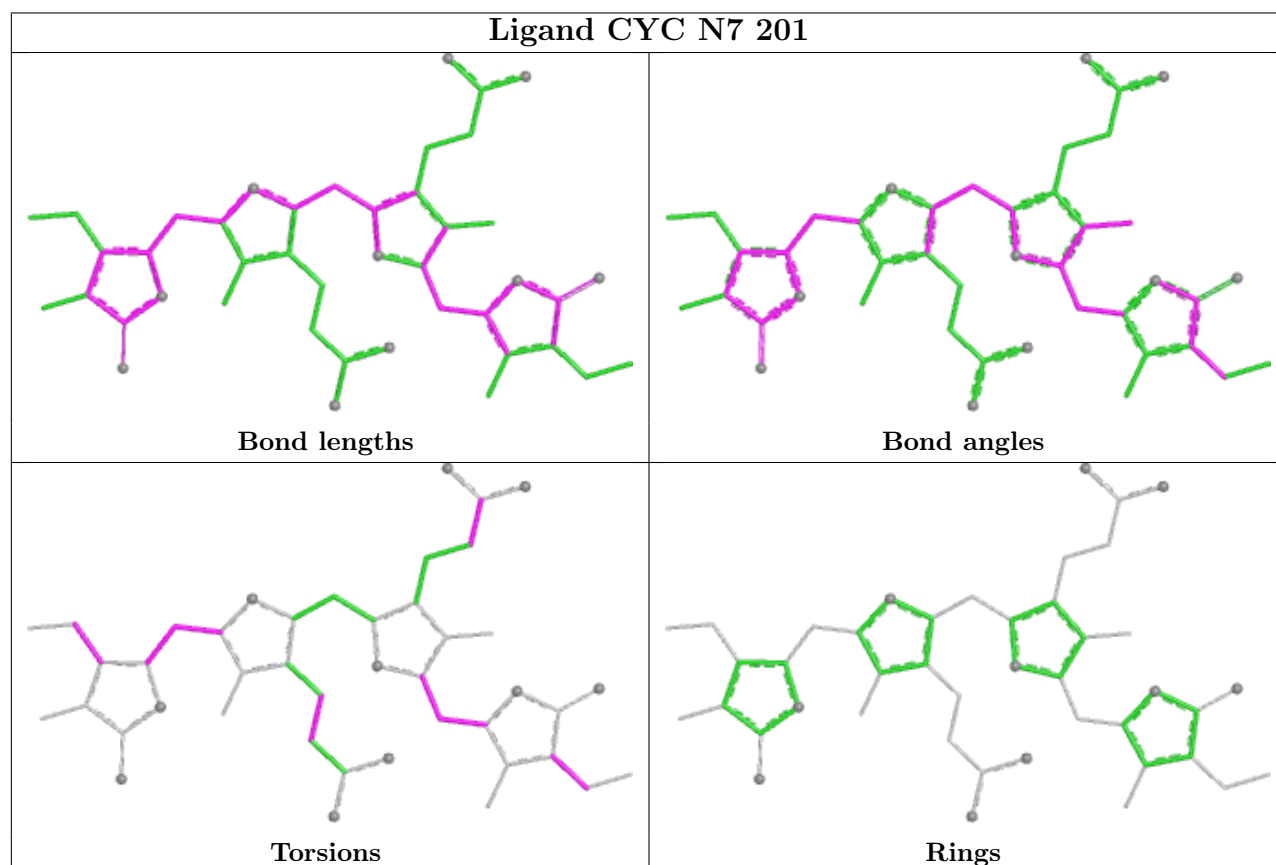
Ligand CYC E3 201



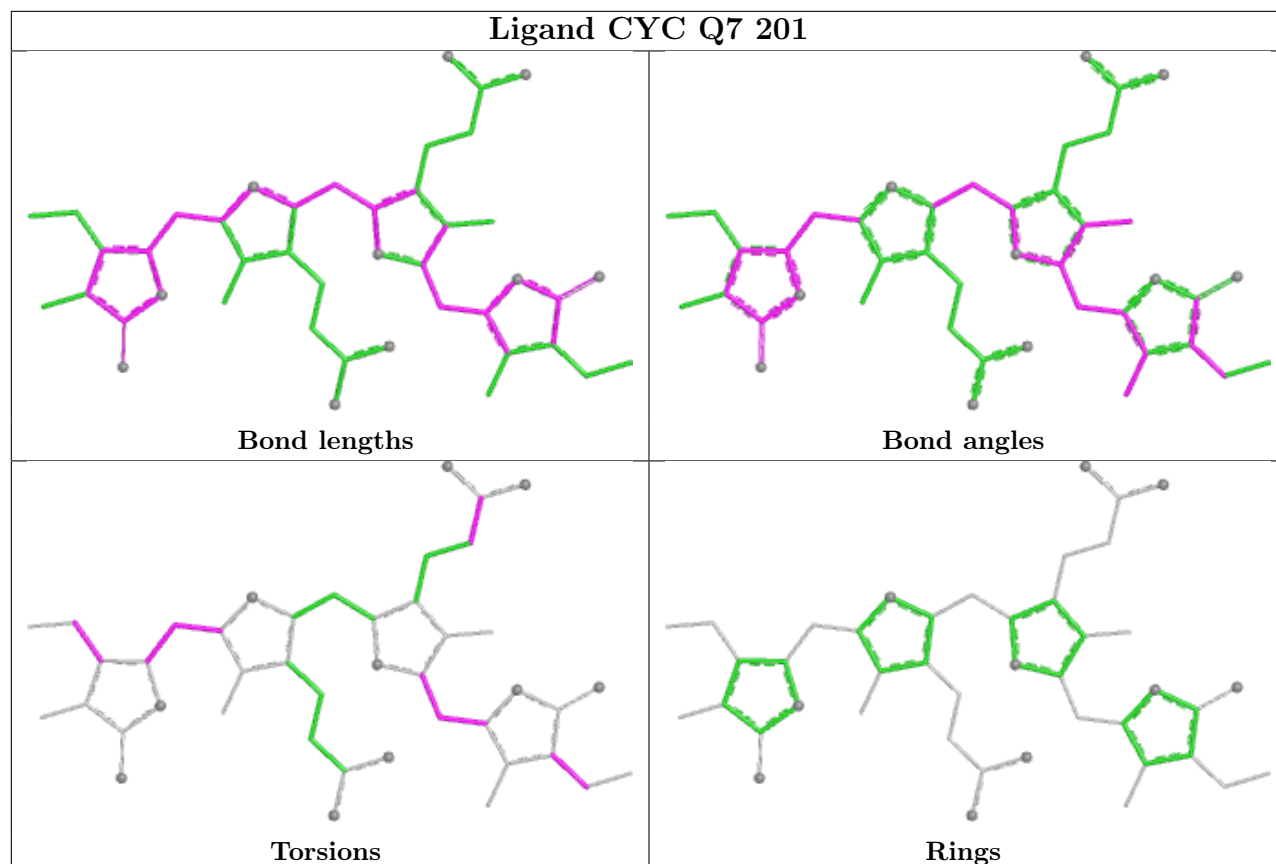
Ligand CYC C1 202



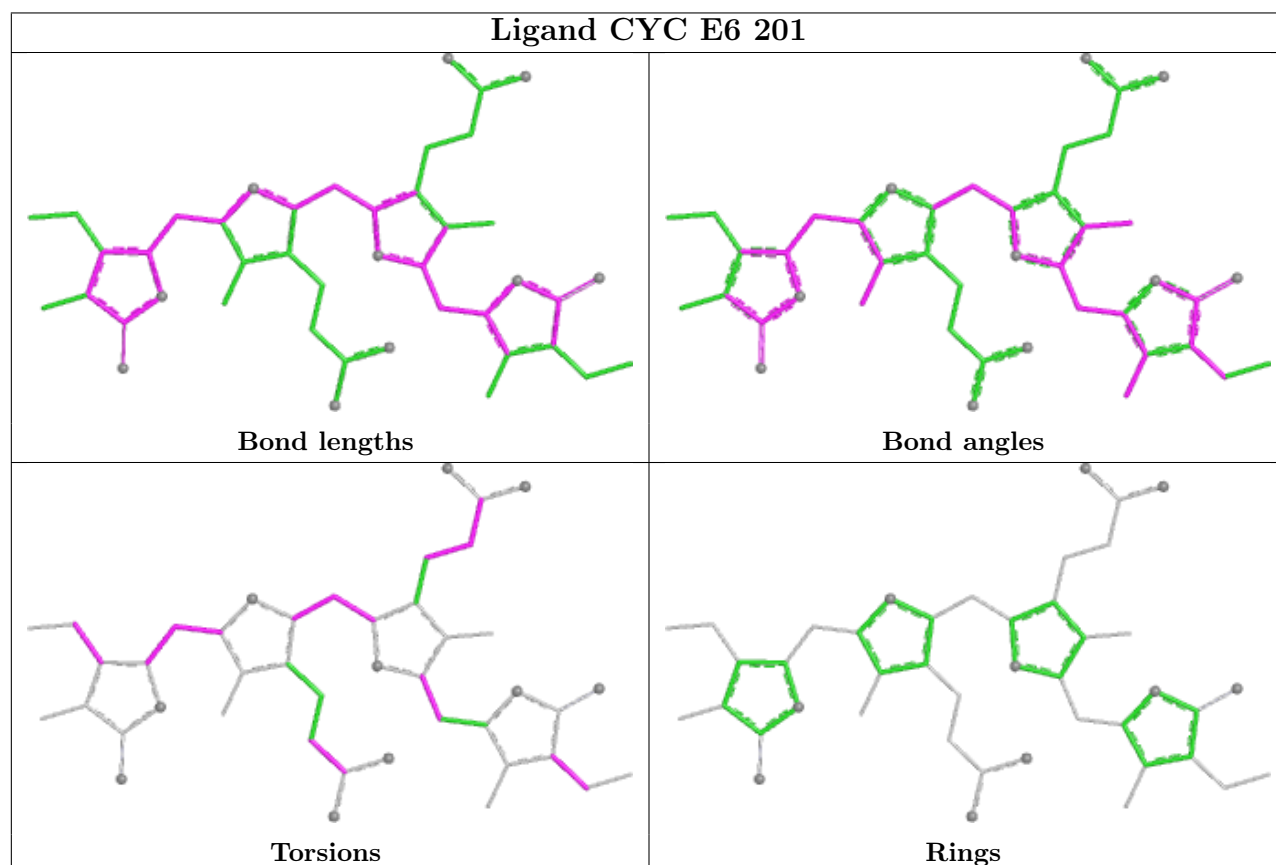
Ligand CYC N7 201

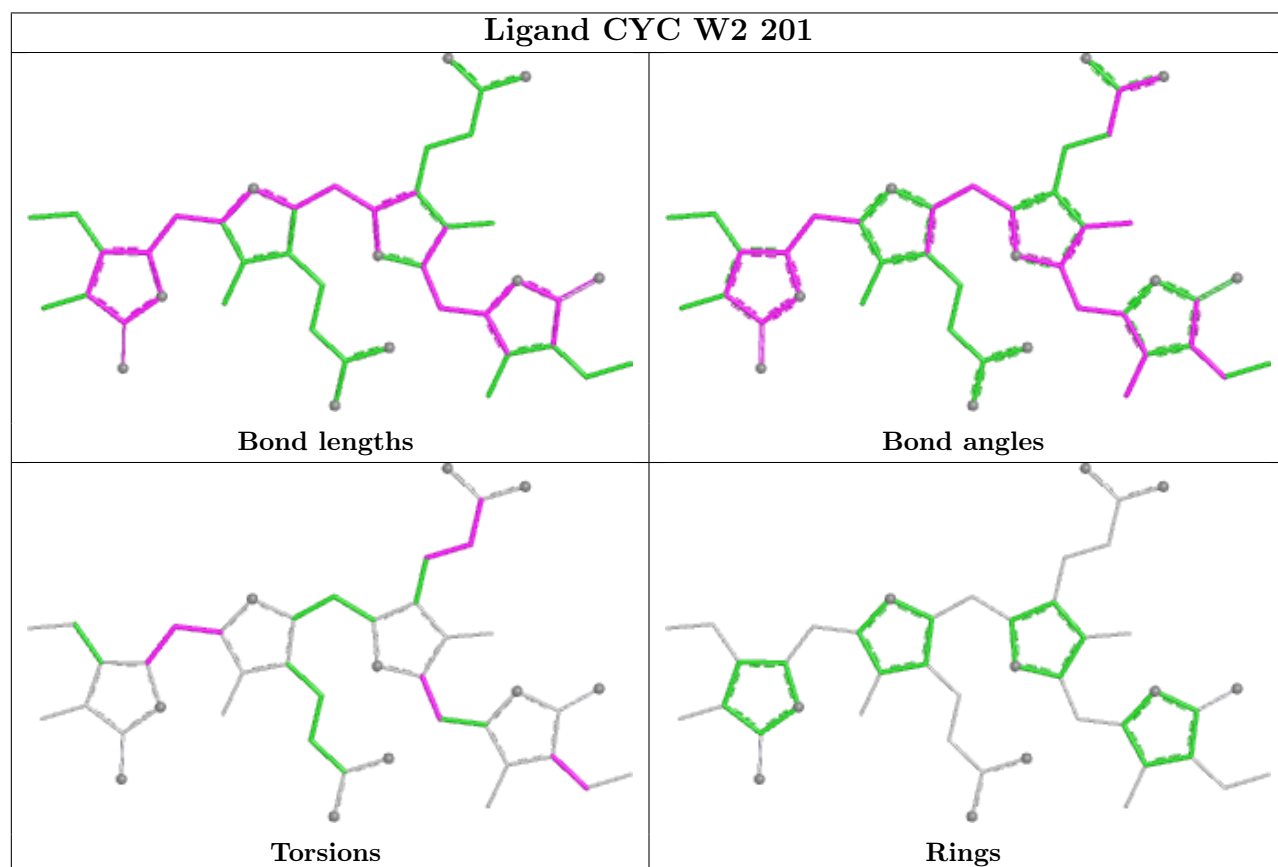
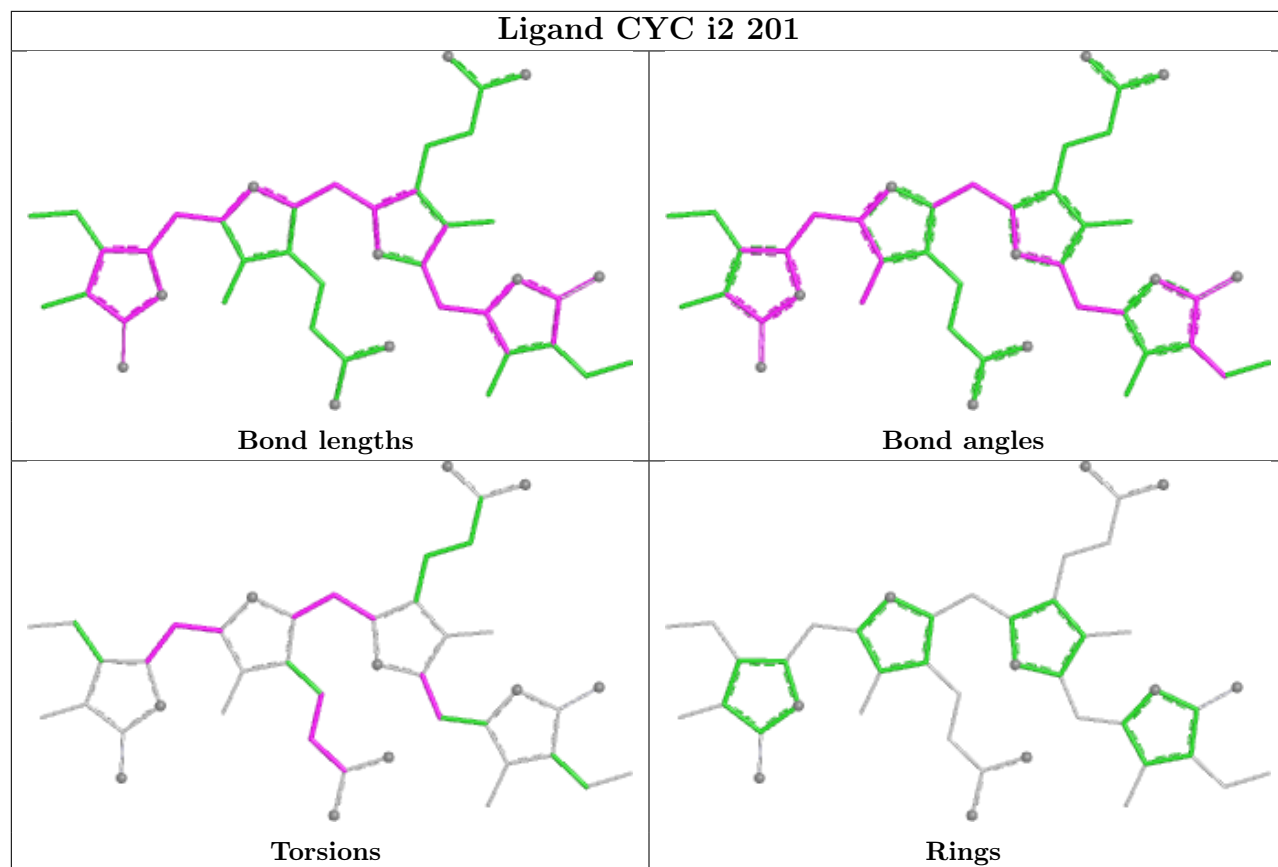


Ligand CYC Q7 201

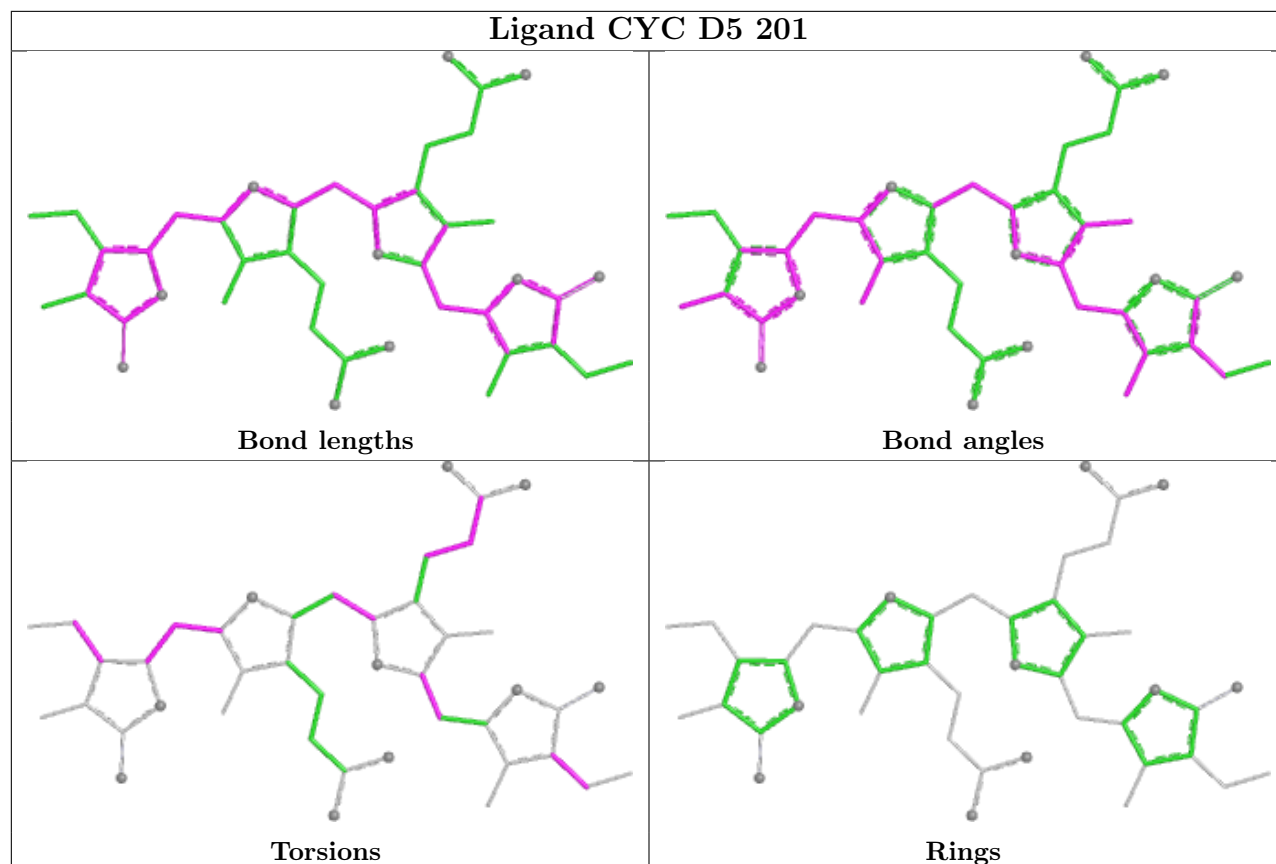


Ligand CYC E6 201

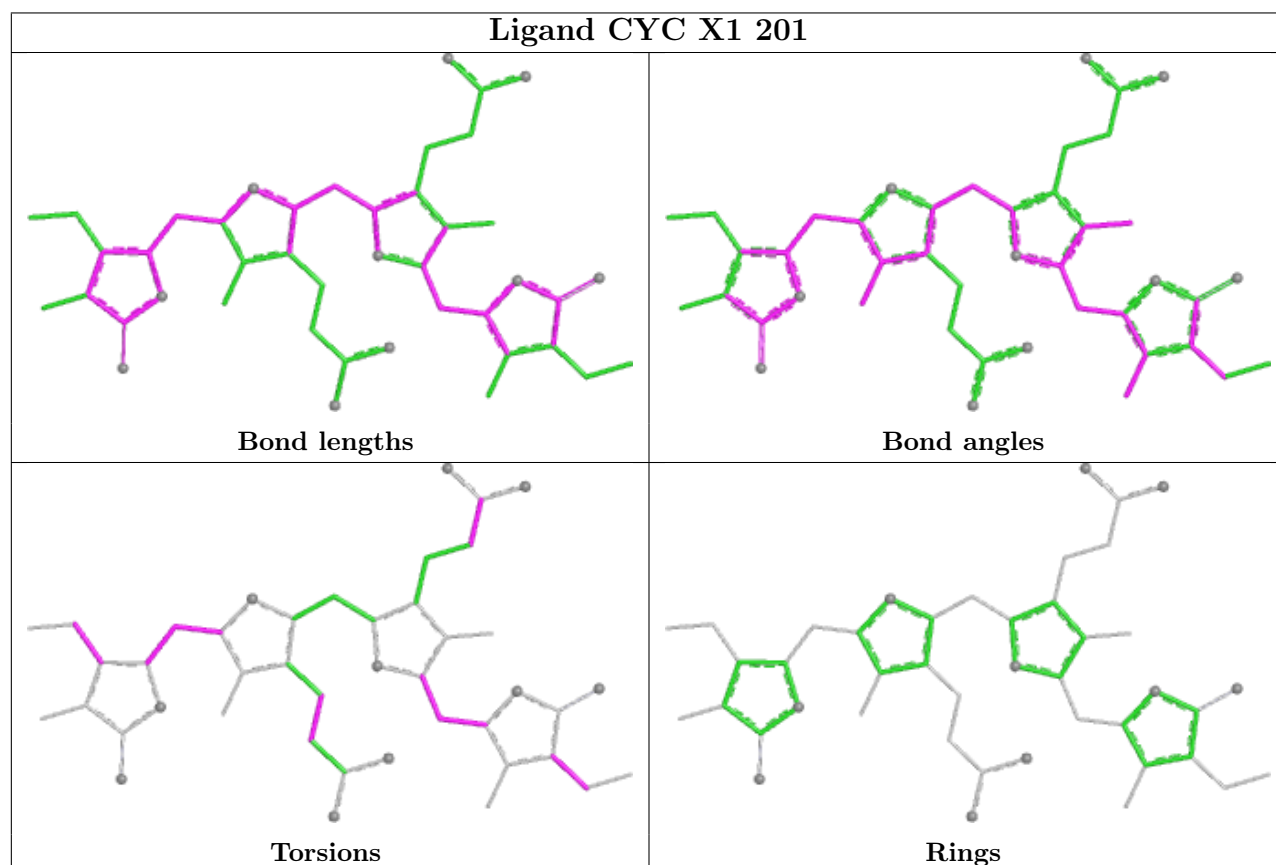




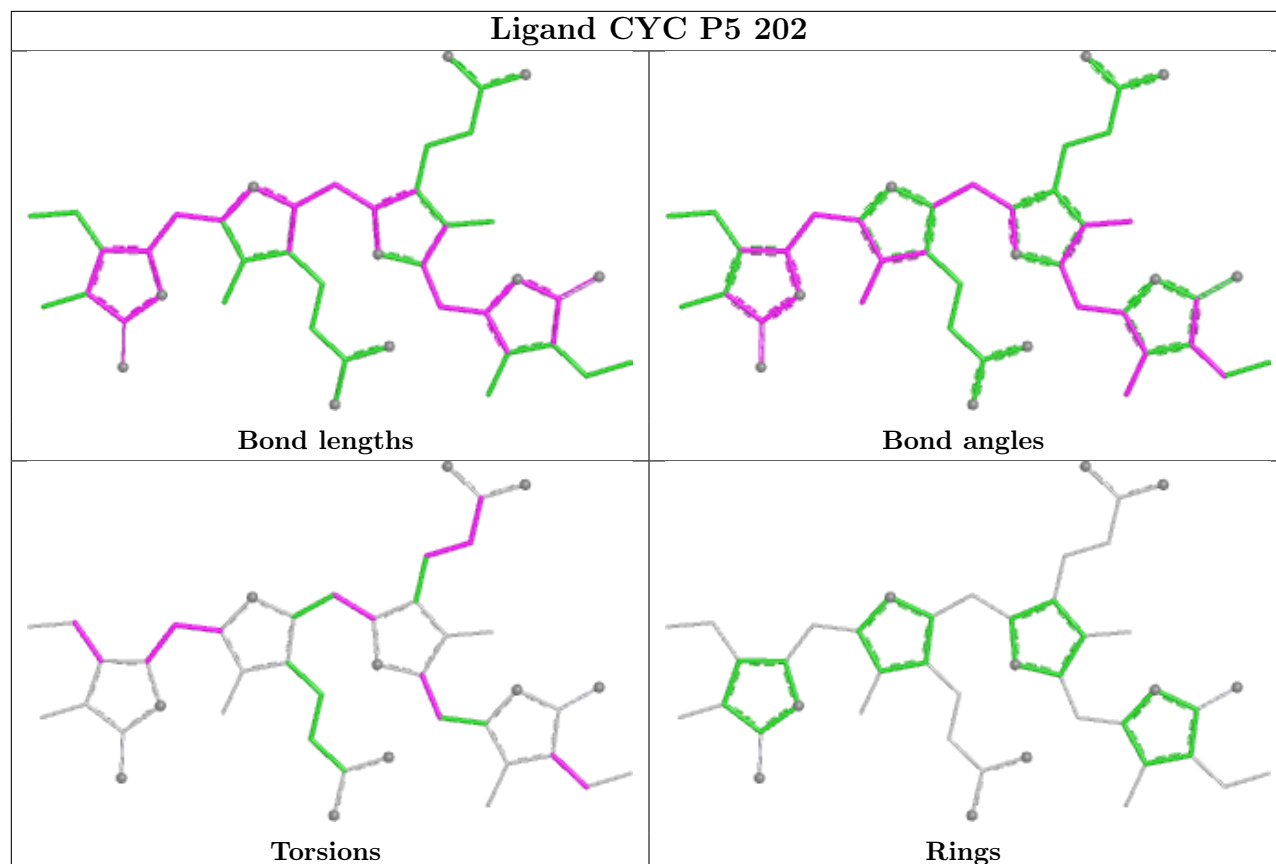
Ligand CYC D5 201



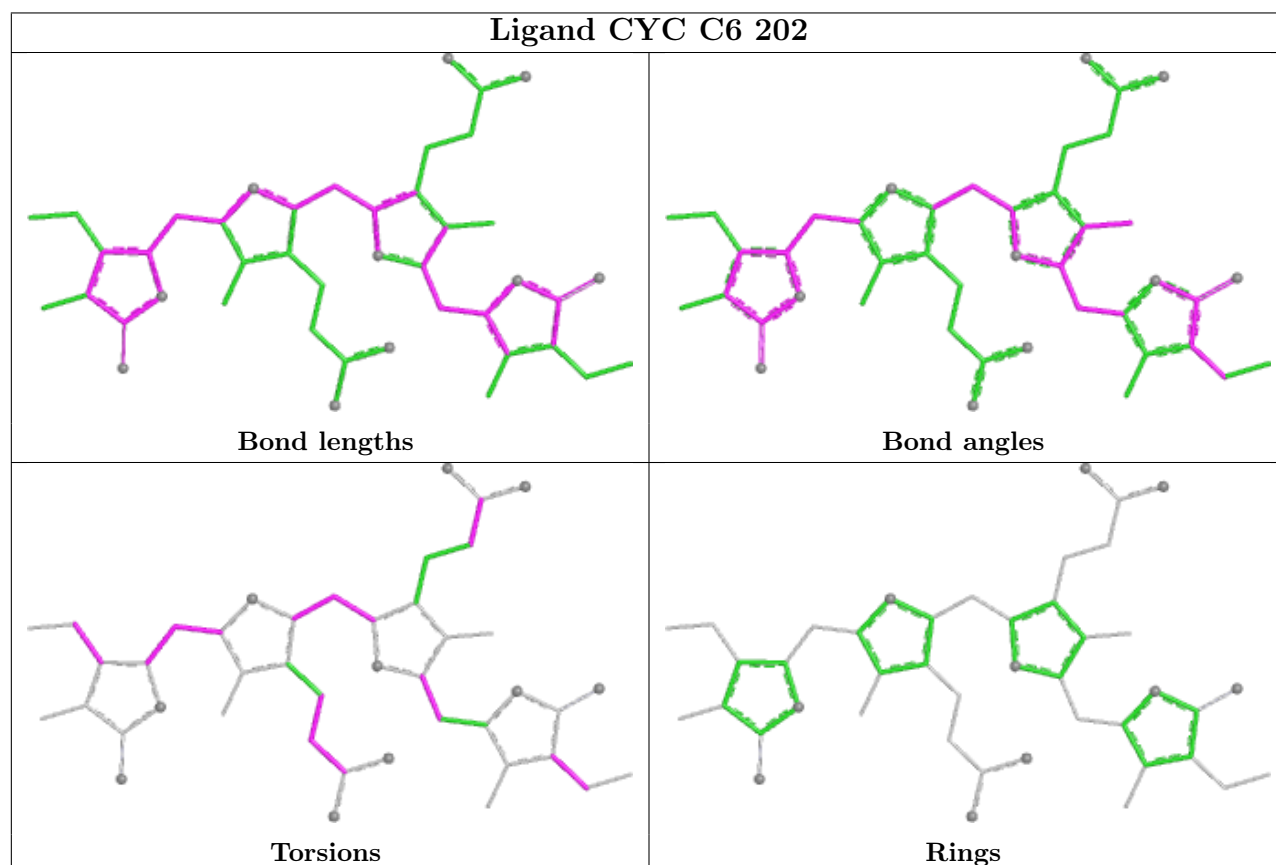
Ligand CYC X1 201



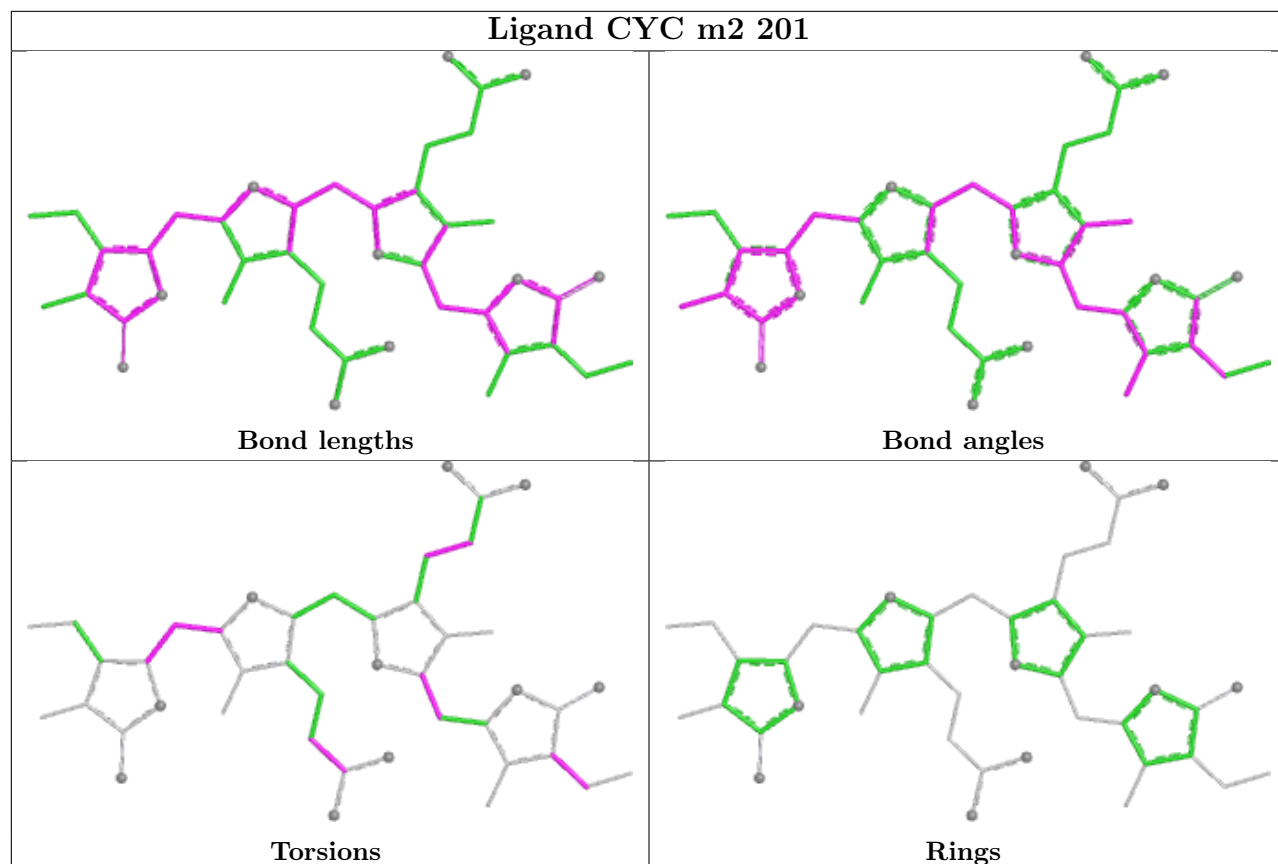
Ligand CYC P5 202



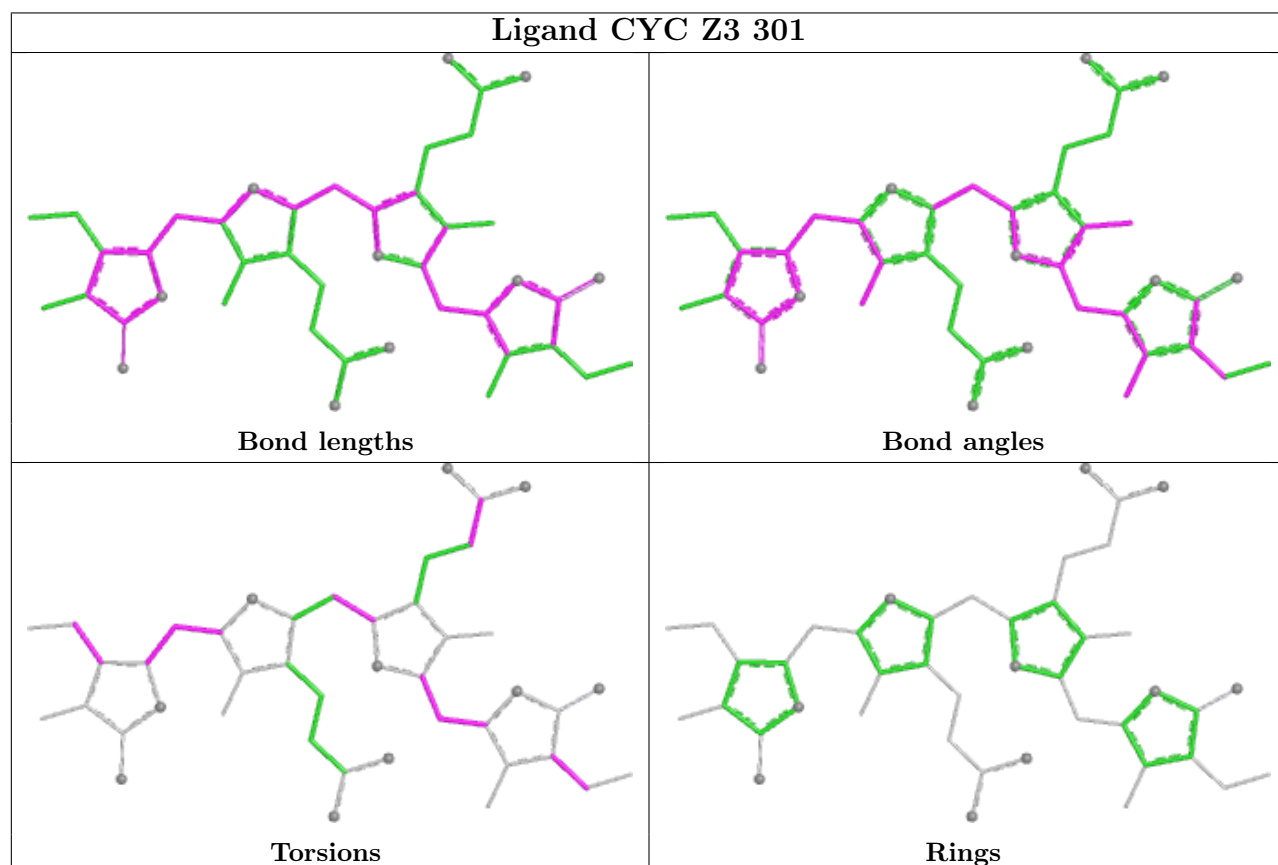
Ligand CYC C6 202

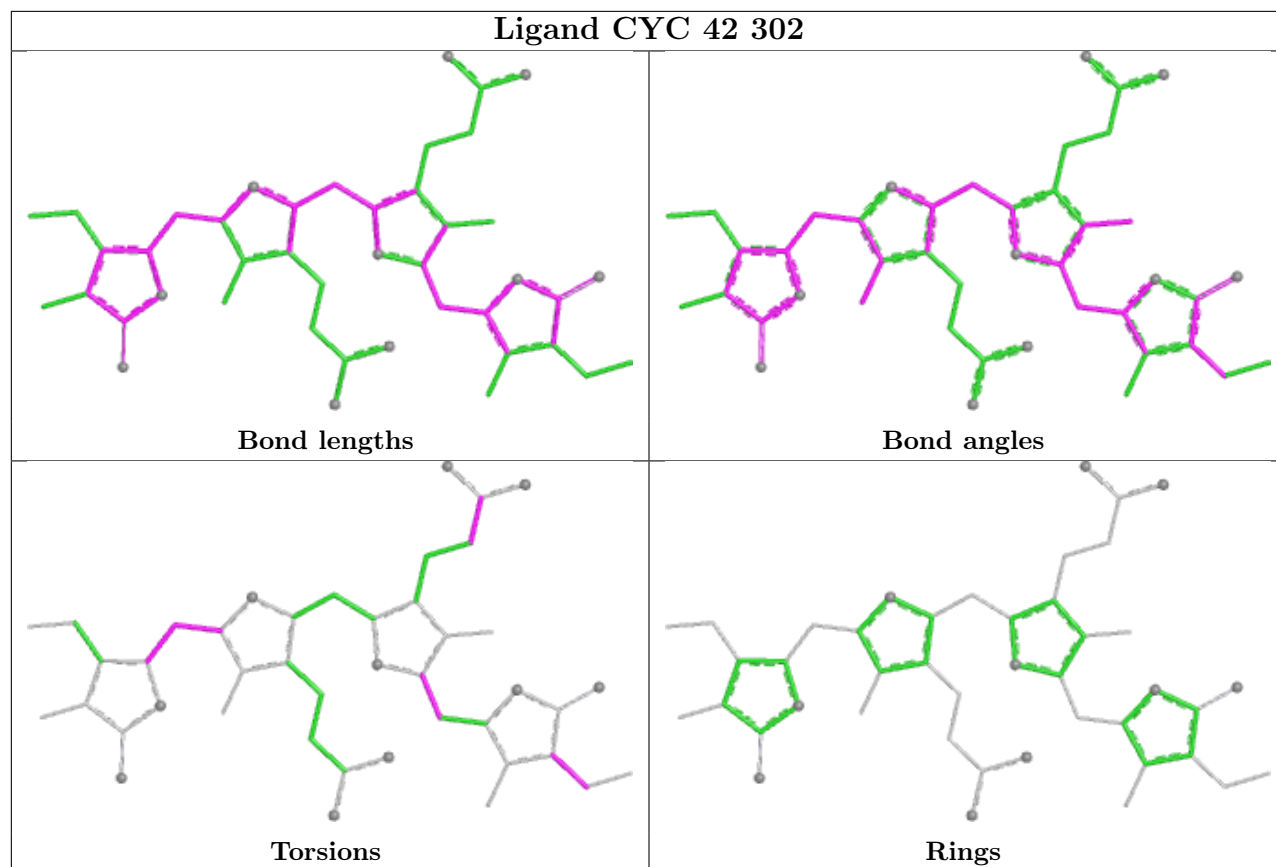


Ligand CYC m2 201



Ligand CYC Z3 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

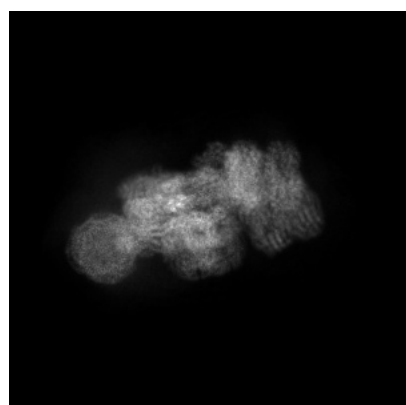
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65950. These allow visual inspection of the internal detail of the map and identification of artifacts.

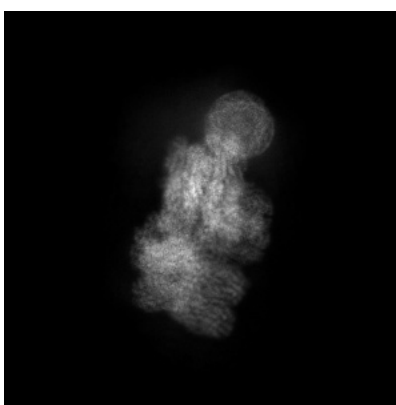
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

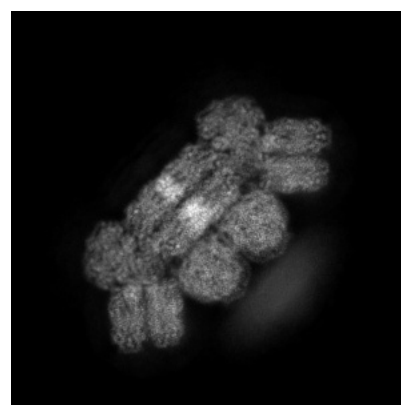
6.1.1 Primary map



X



Y

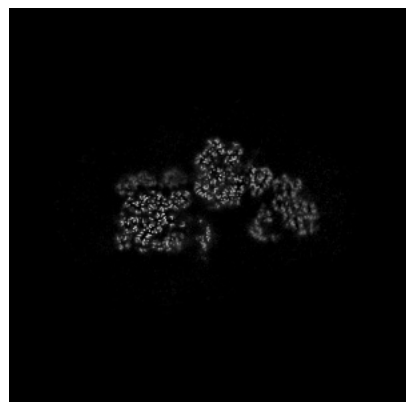


Z

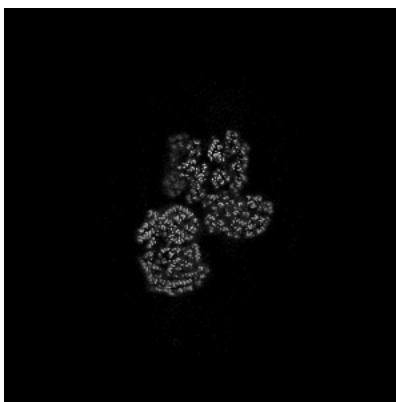
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

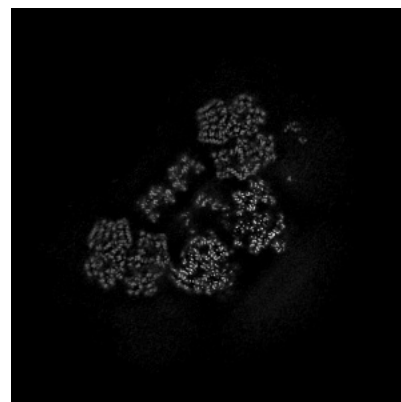
6.2.1 Primary map



X Index: 280



Y Index: 280

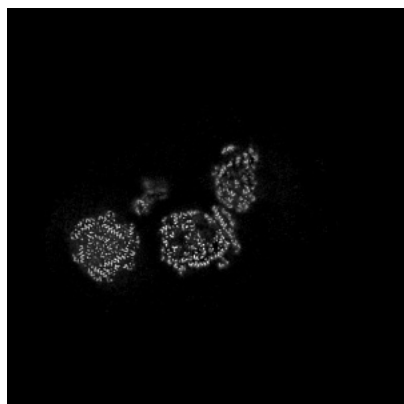


Z Index: 280

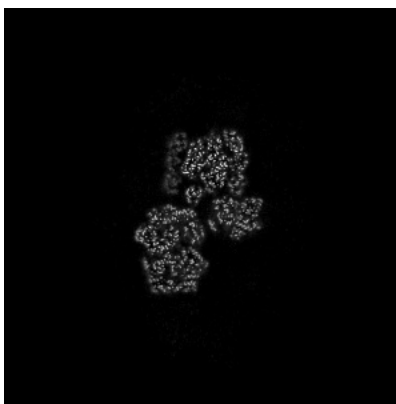
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

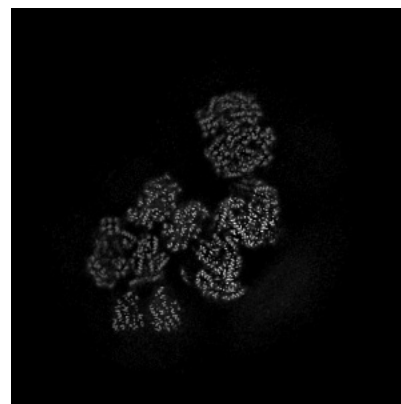
6.3.1 Primary map



X Index: 227



Y Index: 271



Z Index: 265

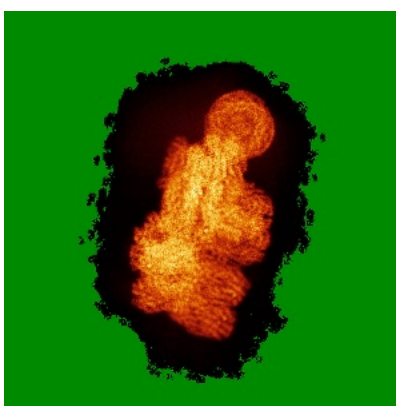
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

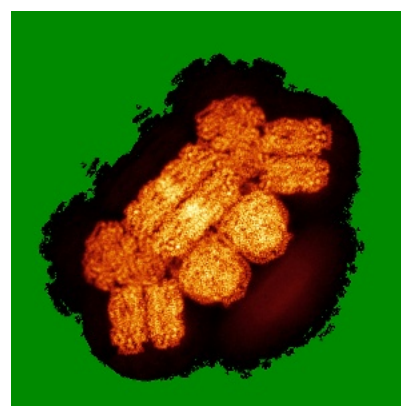
6.4.1 Primary map



X



Y

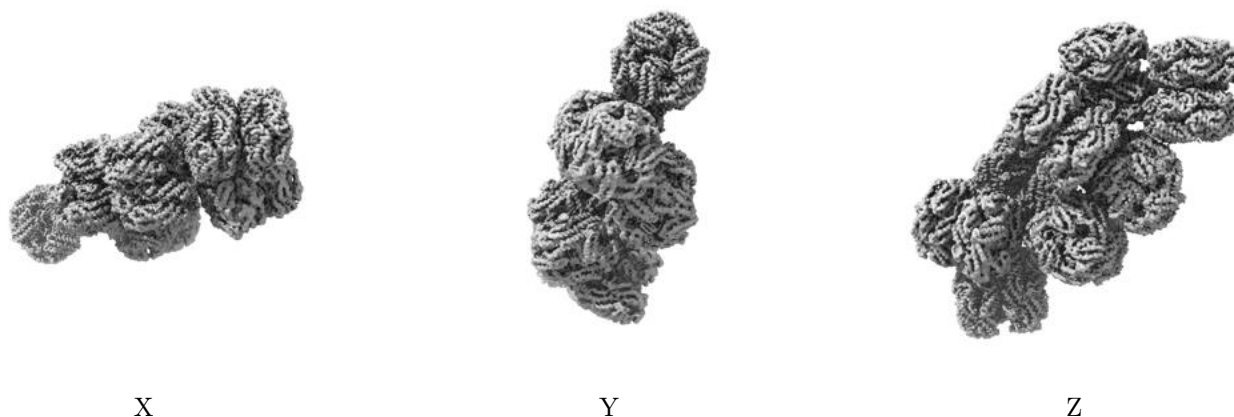


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

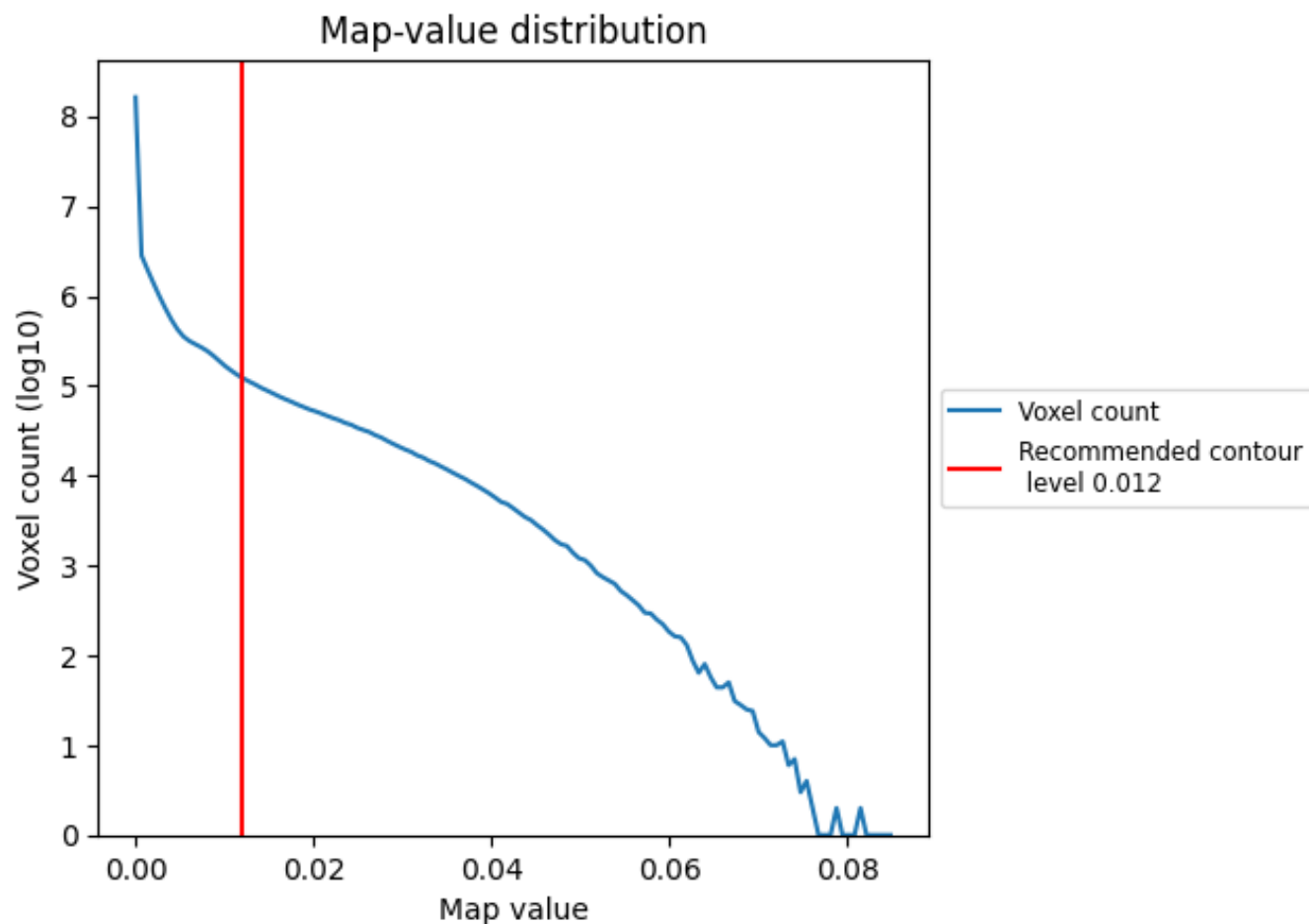
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

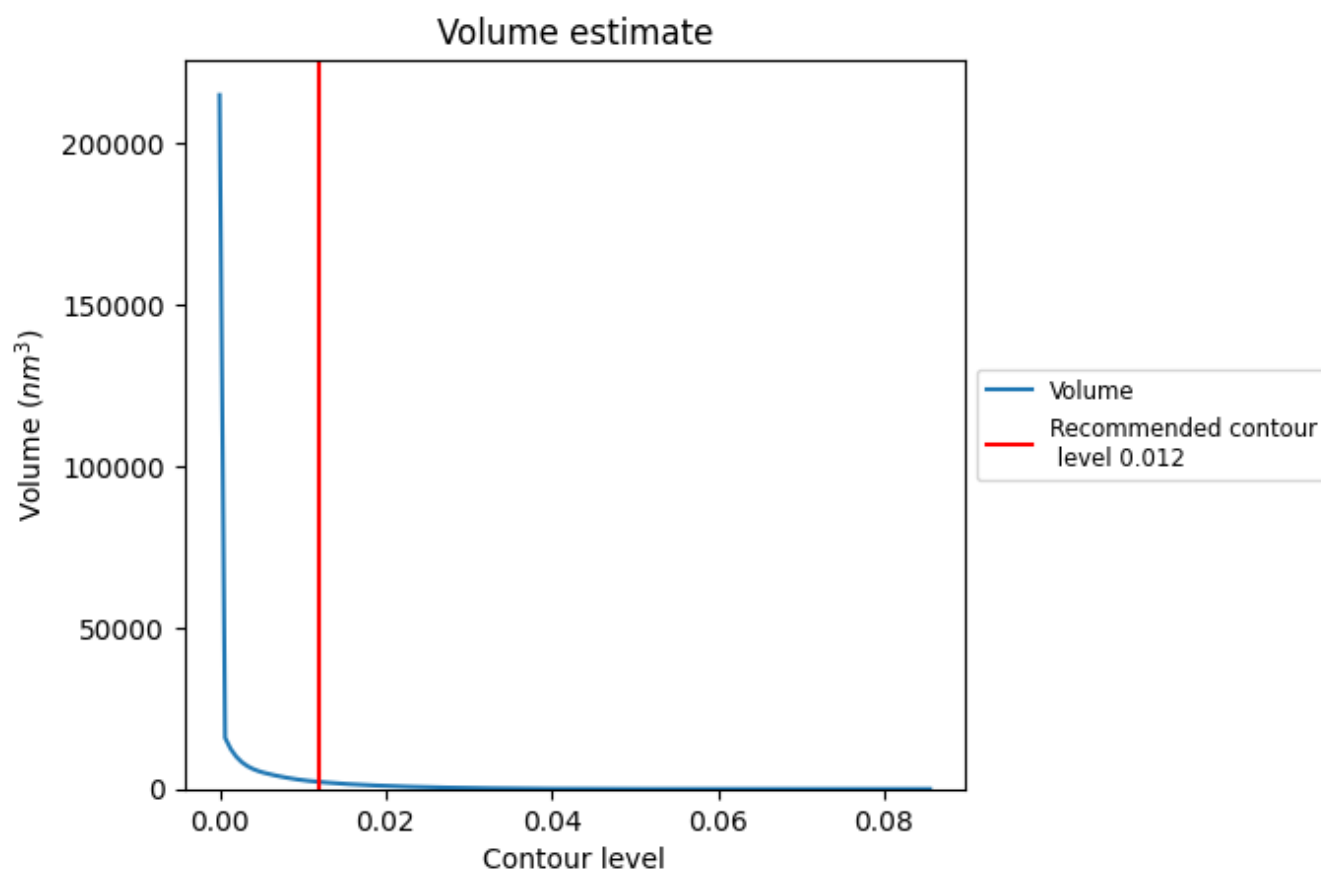
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

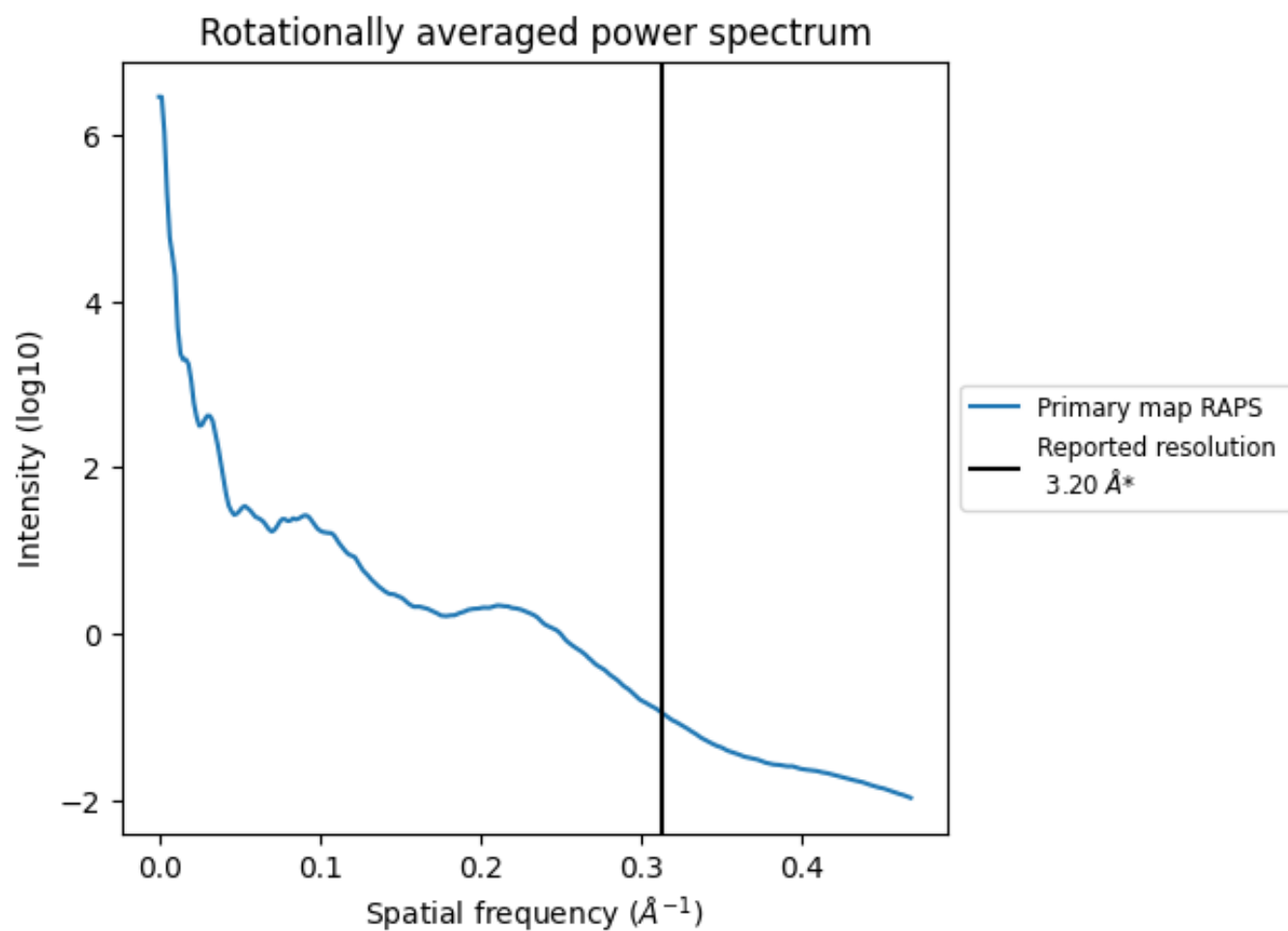
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2179 nm^3 ; this corresponds to an approximate mass of 1968 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

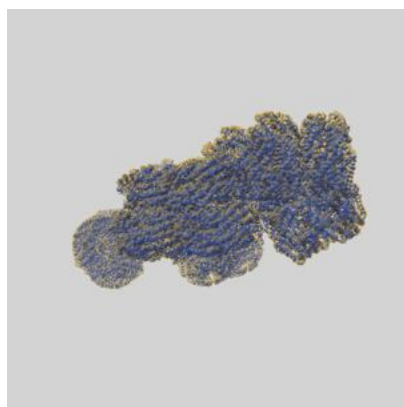
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

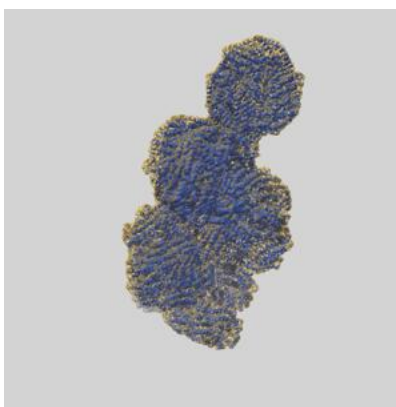
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65950 and PDB model 9WG7. Per-residue inclusion information can be found in section [3](#) on page [37](#).

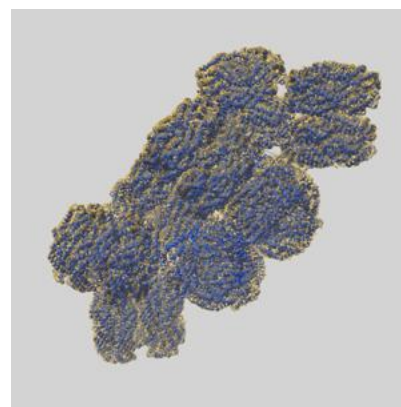
9.1 Map-model overlay [i](#)



X



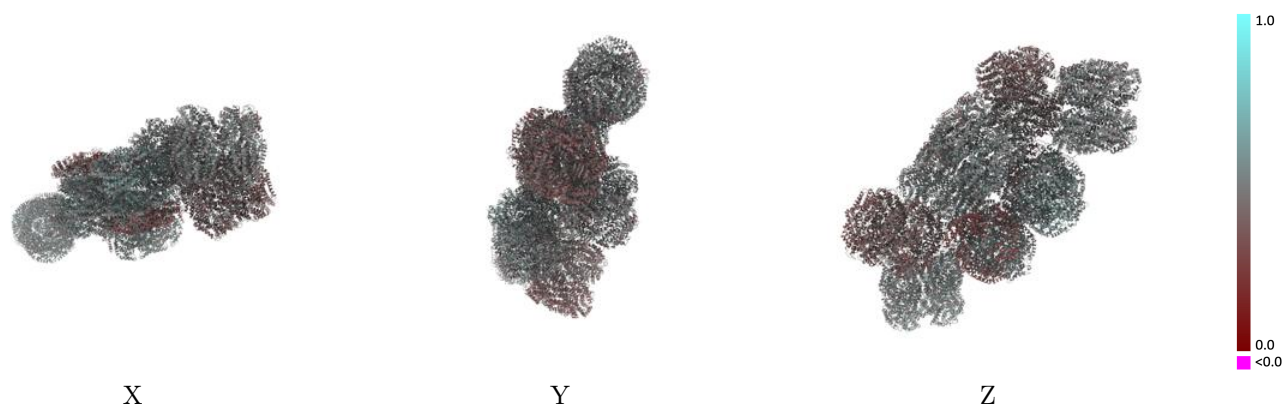
Y



Z

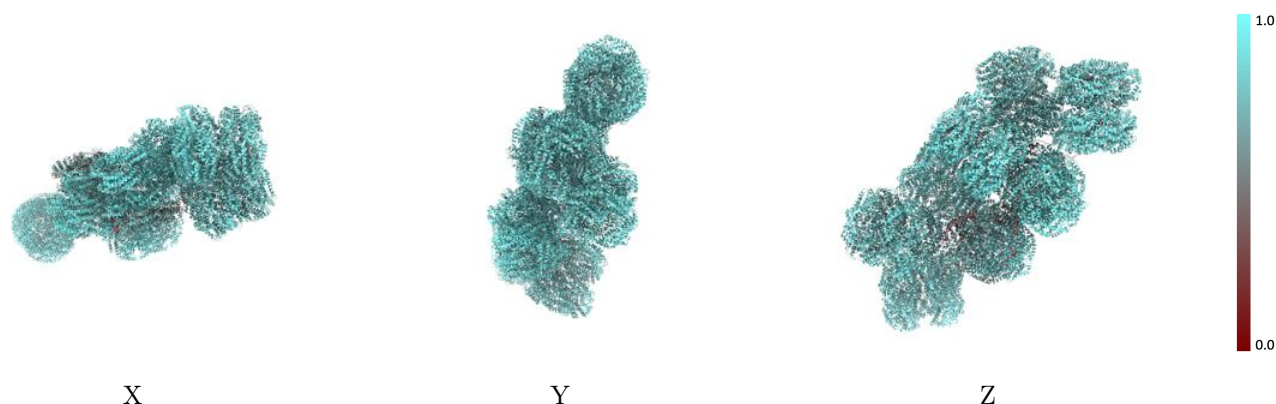
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



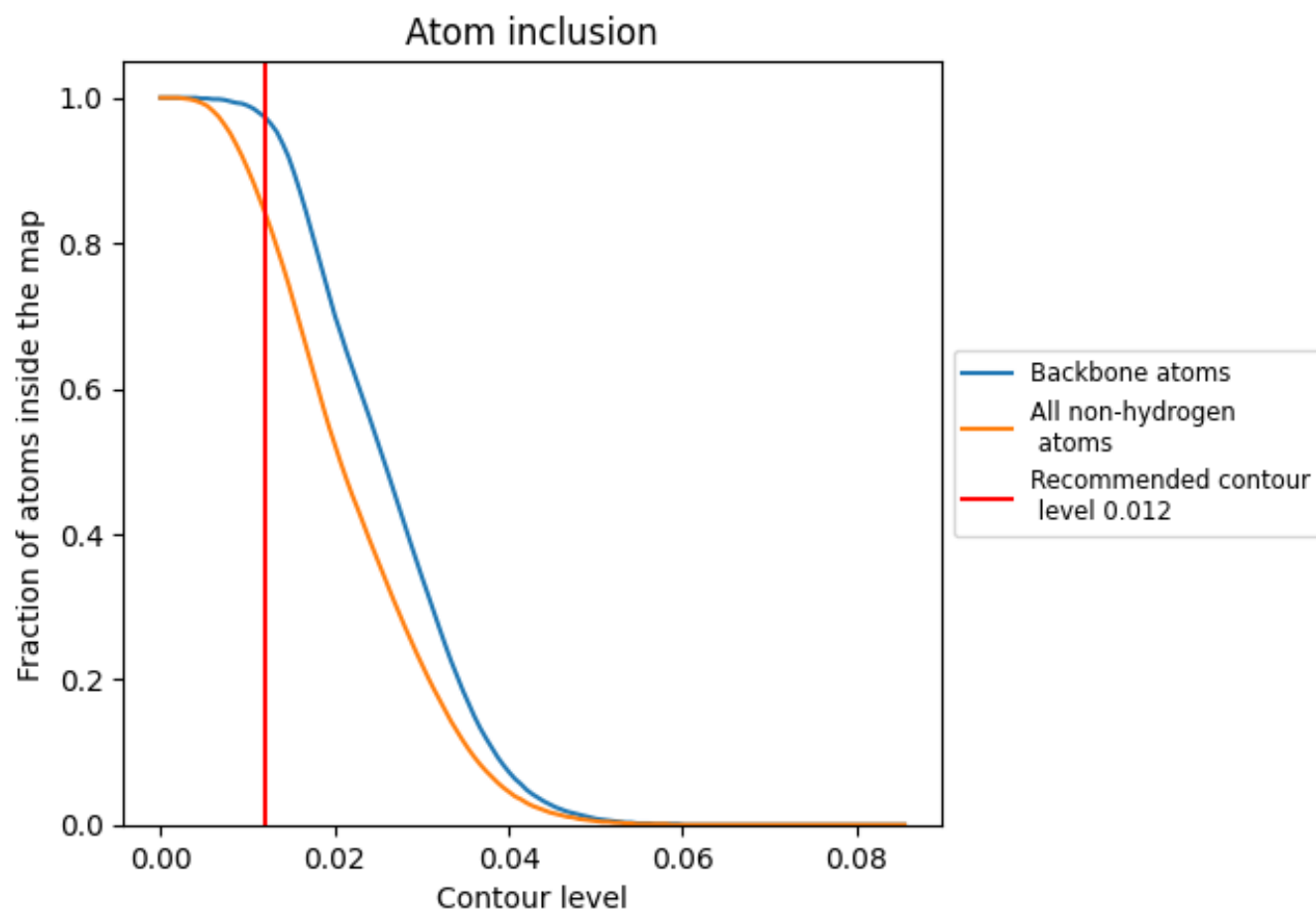
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.4720
02	 0.5310	 0.4130
12	 0.7850	 0.4980
22	 0.8050	 0.4420
32	 0.8250	 0.4640
42	 0.8300	 0.4900
52	 0.8400	 0.5060
A1	 0.9060	 0.5360
A2	 0.5960	 0.3470
A6	 0.8860	 0.5150
B1	 0.9410	 0.5320
B2	 0.6040	 0.3390
B3	 0.8460	 0.4210
B4	 0.8930	 0.5030
B5	 0.9110	 0.5240
B6	 0.9190	 0.5070
B7	 0.8260	 0.3960
C1	 0.9370	 0.5270
C2	 0.5610	 0.3040
C3	 0.8370	 0.4390
C4	 0.8740	 0.4930
C5	 0.8980	 0.5180
C6	 0.9100	 0.5060
C7	 0.8160	 0.4170
D1	 0.9420	 0.5190
D2	 0.8450	 0.4760
D3	 0.8230	 0.4140
D4	 0.8770	 0.4960
D5	 0.9020	 0.5180
D6	 0.9200	 0.5020
D7	 0.8000	 0.3900
E1	 0.9300	 0.5170
E2	 0.8730	 0.4970
E3	 0.8360	 0.4160
E4	 0.8700	 0.4840























































































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Chain	Atom inclusion	Q-score
E5	 0.9020	 0.5100
E6	 0.9050	 0.4950
E7	 0.8170	 0.3920
F1	 0.9390	 0.5210
F2	 0.8880	 0.5170
F3	 0.8280	 0.4210
F4	 0.8660	 0.4850
F5	 0.8970	 0.5080
F6	 0.9080	 0.5000
F7	 0.8140	 0.4010
G1	 0.9440	 0.5250
G2	 0.8570	 0.4770
G3	 0.8400	 0.4220
G4	 0.8830	 0.4950
G5	 0.9130	 0.5210
G6	 0.9170	 0.5050
G7	 0.8250	 0.3980
H1	 0.9420	 0.5230
H2	 0.4340	 0.3210
H3	 0.8520	 0.4170
H4	 0.8860	 0.4870
H5	 0.9180	 0.5130
H6	 0.9180	 0.5020
H7	 0.8400	 0.3990
I1	 0.9410	 0.5220
I2	 0.3770	 0.3150
I3	 0.8320	 0.4400
I4	 0.8800	 0.4900
I5	 0.9060	 0.5160
I6	 0.9200	 0.5030
I7	 0.8130	 0.4180
J1	 0.9250	 0.5270
J2	 0.5770	 0.3610
J3	 0.8150	 0.4430
J4	 0.8620	 0.5000
J5	 0.8920	 0.5160
J6	 0.9030	 0.5090
J7	 0.7950	 0.4230
K1	 0.9320	 0.5210
K2	 0.8970	 0.5210
K3	 0.8240	 0.4470
K4	 0.8690	 0.4810





















































































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Chain	Atom inclusion	Q-score
K5	 0.8980	 0.5030
K6	 0.9060	 0.4990
K7	 0.8050	 0.4250
L1	 0.9250	 0.5250
L2	 0.9190	 0.5360
L3	 0.8070	 0.4360
L4	 0.8480	 0.4900
L5	 0.8840	 0.5150
L6	 0.8900	 0.5030
L7	 0.7900	 0.4140
M1	 0.8880	 0.4870
M2	 0.9130	 0.5330
M3	 0.7840	 0.3800
M4	 0.7970	 0.4780
M5	 0.8300	 0.5010
M6	 0.8640	 0.4700
M7	 0.7610	 0.3640
N1	 0.9300	 0.5090
N2	 0.8730	 0.5330
N3	 0.8310	 0.4100
N4	 0.8570	 0.4930
N5	 0.8880	 0.5150
N6	 0.9050	 0.4900
N7	 0.8170	 0.3870
O1	 0.9210	 0.5140
O2	 0.9100	 0.5370
O3	 0.8030	 0.4210
O4	 0.8420	 0.4970
O5	 0.8760	 0.5130
O6	 0.8970	 0.4980
O7	 0.7730	 0.4000
P1	 0.8890	 0.4800
P2	 0.9100	 0.5340
P3	 0.7780	 0.3740
P4	 0.7940	 0.4690
P5	 0.8220	 0.4890
P6	 0.8560	 0.4590
P7	 0.7580	 0.3540
Q1	 0.8830	 0.4730
Q2	 0.8620	 0.4830
Q3	 0.7720	 0.3750
Q4	 0.7950	 0.4620





















































































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Chain	Atom inclusion	Q-score
Q5	 0.8260	 0.4860
Q6	 0.8520	 0.4550
Q7	 0.7560	 0.3550
R1	 0.9050	 0.4800
R2	 0.8730	 0.4980
R3	 0.7910	 0.3900
R4	 0.8120	 0.4720
R5	 0.8330	 0.4860
R6	 0.8810	 0.4600
R7	 0.7670	 0.3680
S1	 0.9000	 0.4820
S2	 0.8720	 0.5010
S3	 0.8060	 0.4060
S4	 0.8170	 0.4750
S5	 0.8460	 0.4950
S6	 0.8750	 0.4590
S7	 0.7810	 0.3870
T1	 0.9110	 0.4980
T2	 0.8790	 0.4910
T3	 0.7990	 0.3880
T4	 0.8260	 0.4860
T5	 0.8520	 0.5060
T6	 0.8830	 0.4760
T7	 0.7710	 0.3660
U1	 0.9140	 0.4990
U2	 0.8810	 0.5140
U3	 0.8190	 0.3930
U4	 0.8270	 0.4820
U5	 0.8530	 0.5070
U6	 0.8800	 0.4750
U7	 0.7980	 0.3700
V1	 0.9180	 0.5110
V2	 0.8710	 0.4890
V3	 0.8210	 0.4210
V4	 0.8410	 0.4930
V5	 0.8690	 0.5120
V6	 0.8810	 0.4920
V7	 0.8040	 0.4000
W1	 0.9280	 0.5130
W2	 0.7720	 0.4210
W3	 0.8000	 0.3890
W4	 0.8390	 0.4940





























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Chain	Atom inclusion	Q-score
W5	 0.8720	 0.5150
W6	 0.8950	 0.4880
W7	 0.7800	 0.3680
X1	 0.8860	 0.4950
X2	 0.8930	 0.5110
X3	 0.7830	 0.4140
X4	 0.8060	 0.4710
X5	 0.8360	 0.4930
X6	 0.8620	 0.4700
X7	 0.7630	 0.3940
Y1	 0.6700	 0.4390
Y2	 0.8860	 0.5340
Y3	 0.4900	 0.3410
Y4	 0.5330	 0.4380
Y5	 0.5850	 0.4540
Y6	 0.6110	 0.4220
Y7	 0.4400	 0.3290
Z1	 0.9280	 0.5460
Z2	 0.4970	 0.3960
Z3	 0.8160	 0.4600
Z4	 0.8450	 0.5160
Z5	 0.8790	 0.5390
Z6	 0.8920	 0.5220
Z7	 0.7950	 0.4390
a1	 0.9110	 0.5240
a2	 0.6450	 0.3750
a3	 0.8060	 0.4330
a4	 0.8550	 0.4750
a5	 0.8870	 0.5080
a6	 0.8950	 0.5000
a7	 0.7770	 0.4130
b2	 0.7190	 0.4840
c2	 0.6570	 0.3610
d2	 0.6200	 0.3320
e2	 0.8650	 0.4950
f2	 0.8920	 0.5210
g2	 0.9180	 0.5430
h2	 0.8870	 0.4960
i2	 0.4780	 0.3530
j2	 0.4440	 0.3480
k2	 0.6210	 0.3870
l2	 0.9180	 0.5460

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Chain	Atom inclusion	Q-score
m2	 0.9360	 0.5620
n2	 0.9380	 0.5590
o2	 0.8960	 0.5530
p2	 0.9300	 0.5570
q2	 0.9320	 0.5610
r2	 0.8910	 0.5080
s2	 0.9020	 0.5210
t2	 0.9030	 0.5270
u2	 0.9110	 0.5140
v2	 0.9040	 0.5310
w2	 0.9010	 0.5130
x2	 0.8040	 0.4420
y2	 0.9260	 0.5370
z2	 0.9130	 0.5530