



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 11:13 PM UTC

PDB ID : 9X6D / pdb_00009x6d
EMDB ID : EMD-66300
Title : The cryo-EM structure of phycobilisome rod from *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 : 2025-10-15
Resolution : 2.92 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:

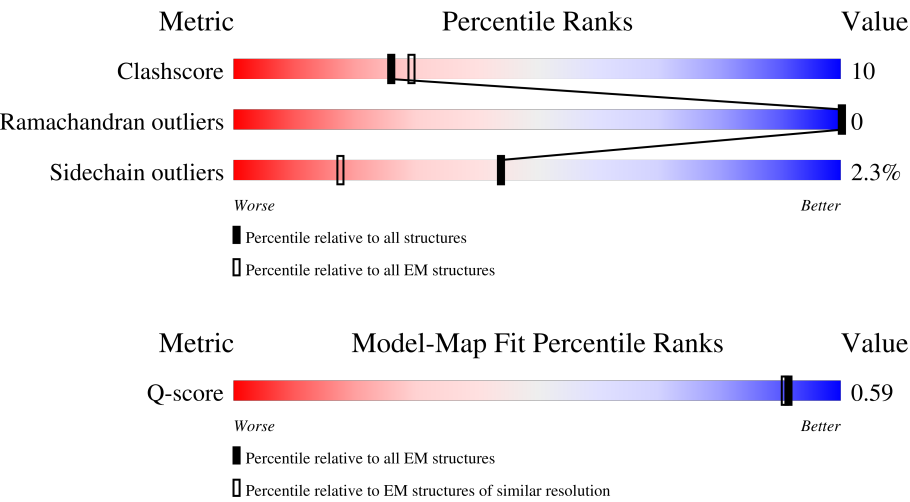
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.92 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	13007 (2.42 - 3.42)

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 <=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	A	250	<div><div>9%</div><div>56%</div><div>22%</div><div>•</div><div>22%</div></div>
2	B	163	<div><div>7%</div><div>78%</div><div>21%</div><div>••</div></div>
2	F	163	<div><div>10%</div><div>74%</div><div>25%</div><div>••</div></div>
2	G	163	<div><div>5%</div><div>78%</div><div>21%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	H	163	
2	I	163	
2	K	163	
2	N	163	
2	R	163	
2	S	163	
2	T	163	
2	U	163	
2	W	163	
3	C	173	
3	D	173	
3	E	173	
3	J	173	
3	L	173	
3	M	173	
3	O	173	
3	P	173	
3	Q	173	
3	V	173	
3	X	173	
3	a	173	
4	Y	273	
5	Z	289	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35641 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	A	196	Total	C	N	O	S	0	0
			1609	1029	280	299	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	F	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	G	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	H	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	I	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	K	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	N	163	Total	C	N	O	S	0	0
			1221	771	205	243	2		
2	R	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	S	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	T	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	U	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		
2	W	162	Total	C	N	O	S	0	0
			1213	766	204	242	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	D	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	E	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	J	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	L	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	M	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	O	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	P	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	Q	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	V	172	Total	C	N	O	S	0	0
			1272	788	228	250	6		
3	X	173	Total	C	N	O	S	0	0
			1280	793	229	251	7		
3	a	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	Y	57	Total	C	N	O	0	0
			457	279	94	84		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	288	Total	C	N	O	S	0	0
			2229	1397	400	429	3		

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆).



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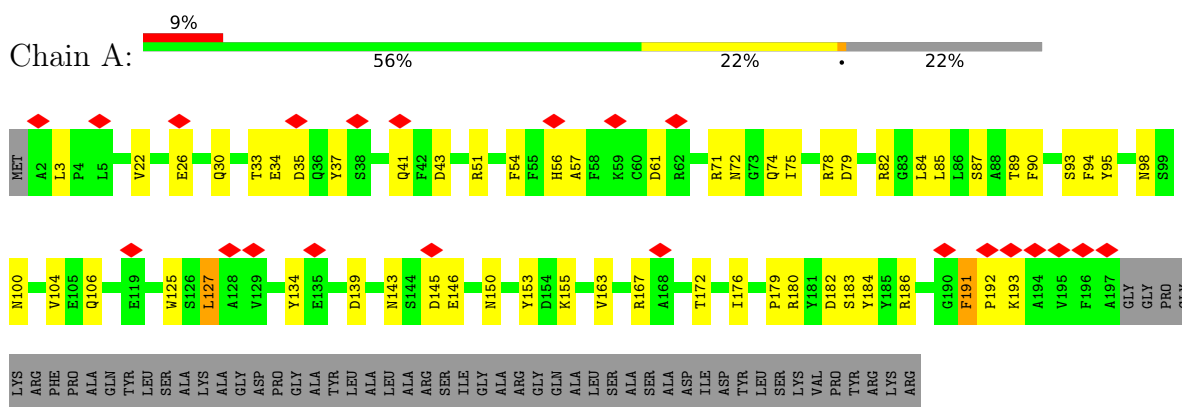
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Mol	Chain	Residues	Atoms				AltConf
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			43	33	4	6	
6	M	1	Total	C	N	O	0
			43	33	4	6	
6	N	1	Total	C	N	O	0
			43	33	4	6	
6	P	1	Total	C	N	O	0
			43	33	4	6	
6	Q	1	Total	C	N	O	0
			43	33	4	6	
6	Q	1	Total	C	N	O	0
			43	33	4	6	
6	R	1	Total	C	N	O	0
			43	33	4	6	
6	S	1	Total	C	N	O	0
			43	33	4	6	
6	T	1	Total	C	N	O	0
			43	33	4	6	
6	T	1	Total	C	N	O	0
			43	33	4	6	
6	U	1	Total	C	N	O	0
			43	33	4	6	
6	V	1	Total	C	N	O	0
			43	33	4	6	
6	V	1	Total	C	N	O	0
			43	33	4	6	
6	W	1	Total	C	N	O	0
			43	33	4	6	
6	X	1	Total	C	N	O	0
			43	33	4	6	
6	Y	1	Total	C	N	O	0
			43	33	4	6	
6	Z	1	Total	C	N	O	0
			43	33	4	6	
6	a	1	Total	C	N	O	0
			43	33	4	6	
6	a	1	Total	C	N	O	0
			43	33	4	6	

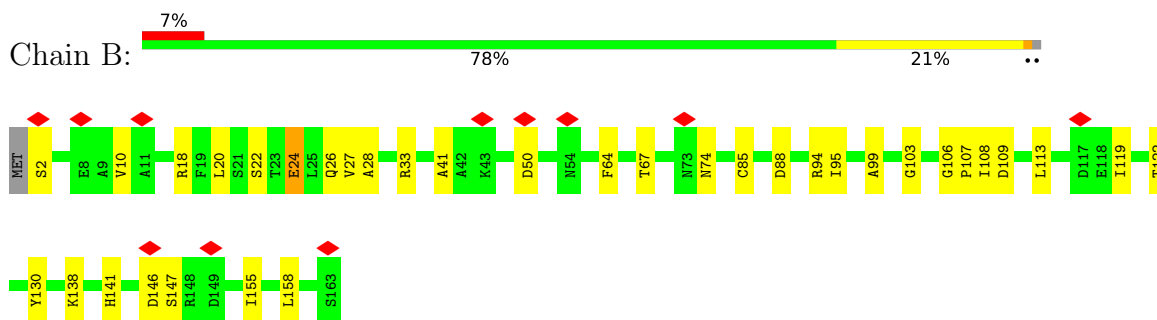
3 Residue-property plots

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.

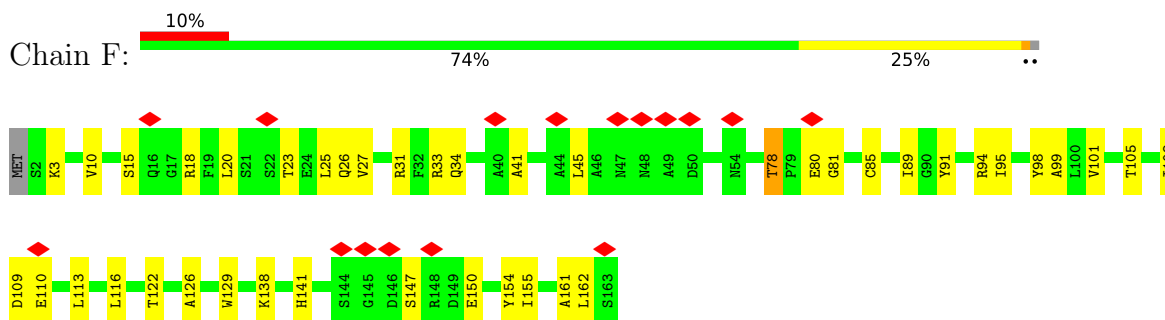
- Molecule 1: Phycobilisome rod-core linker polypeptide



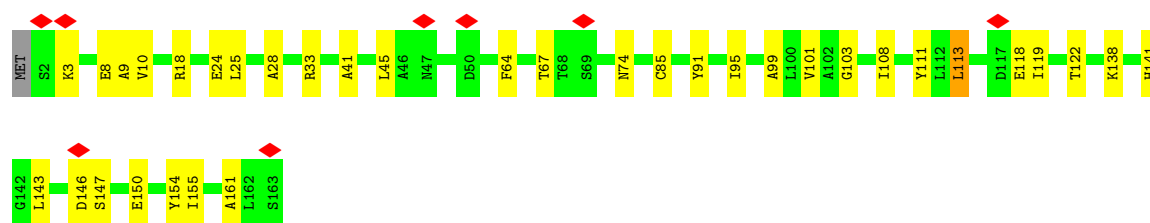
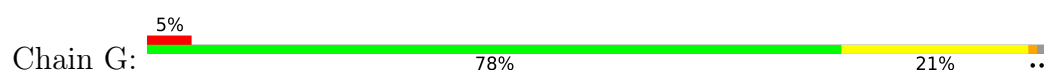
- Molecule 2: C-phycoerythrin alpha subunit



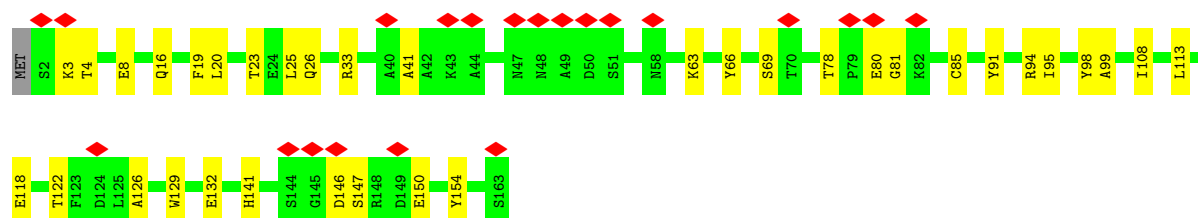
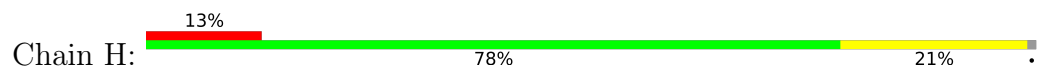
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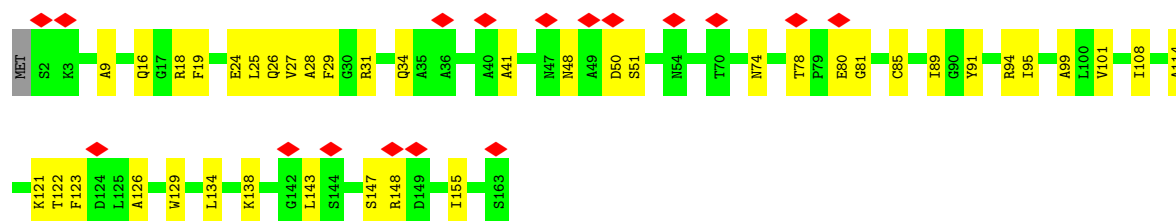
- Molecule 2: C-phycoerythrin alpha subunit



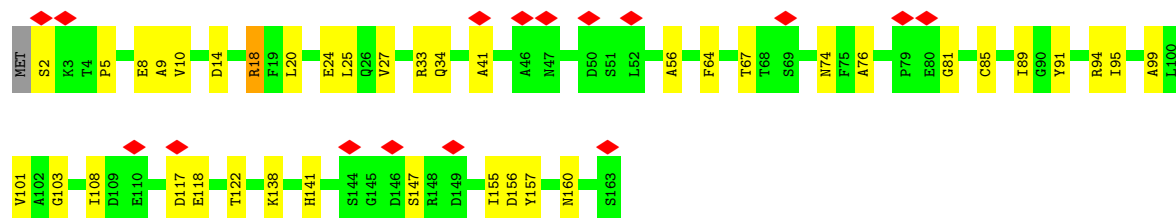
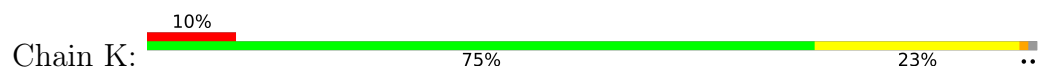
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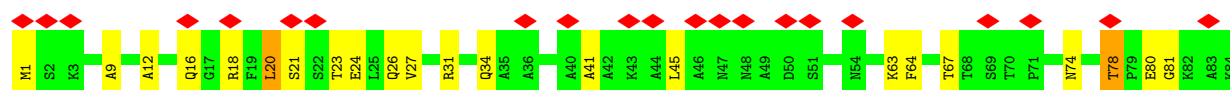
- Molecule 2: C-phycoerythrin alpha subunit

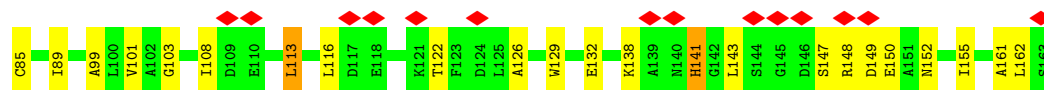


- Molecule 2: C-phycoerythrin alpha subunit

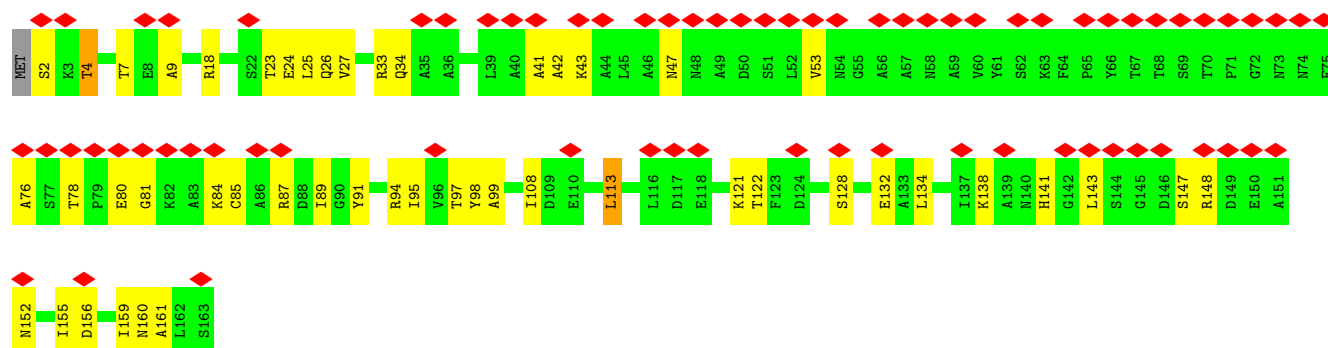


- Molecule 2: C-phycoerythrin alpha subunit

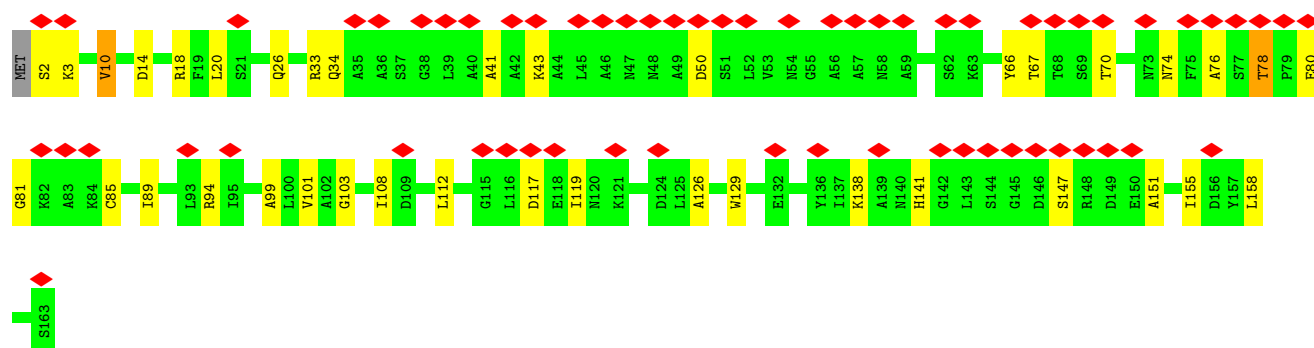
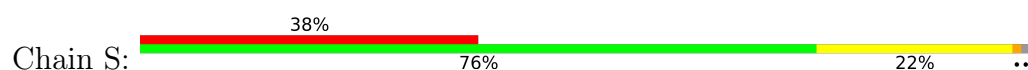




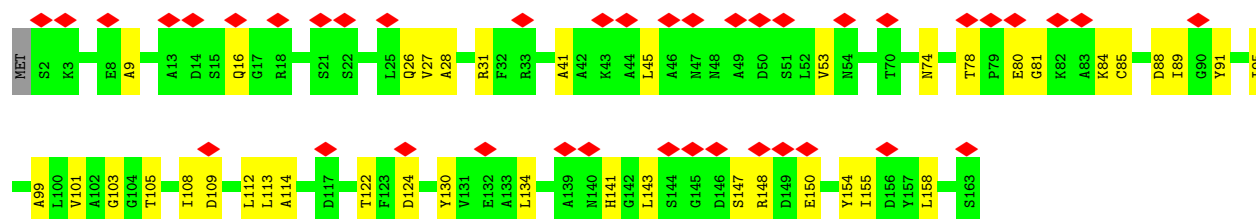
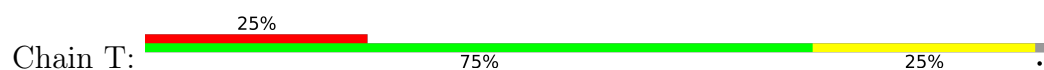
• Molecule 2: C-phycoerythrin alpha subunit



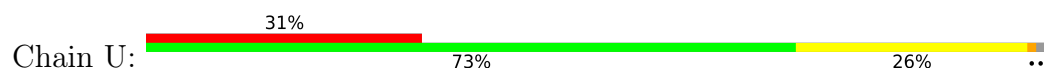
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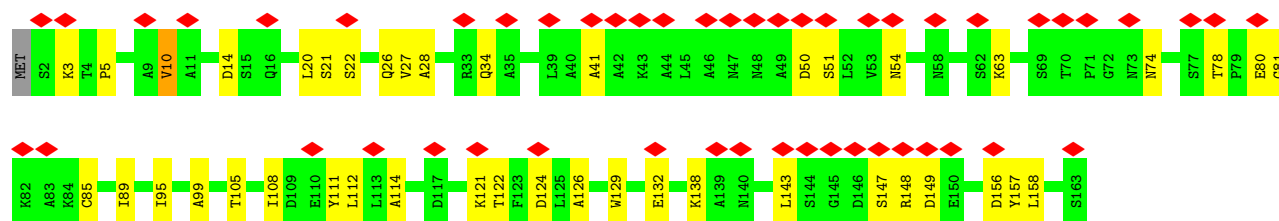


• Molecule 2: C-phycoerythrin alpha subunit

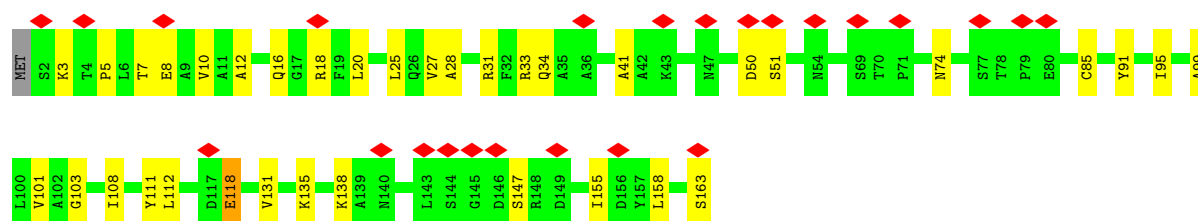
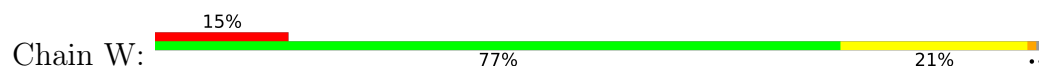


• Molecule 2: C-phycoerythrin alpha subunit

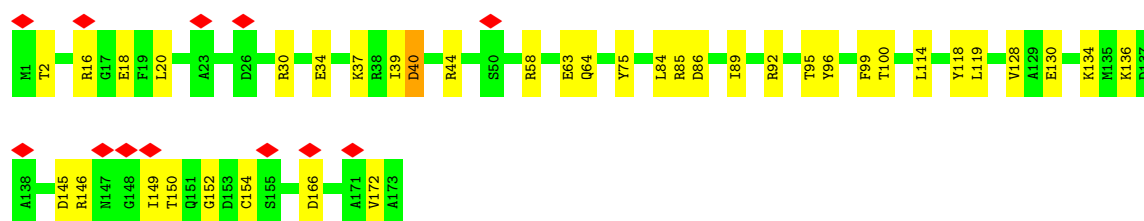
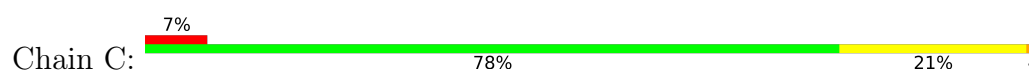




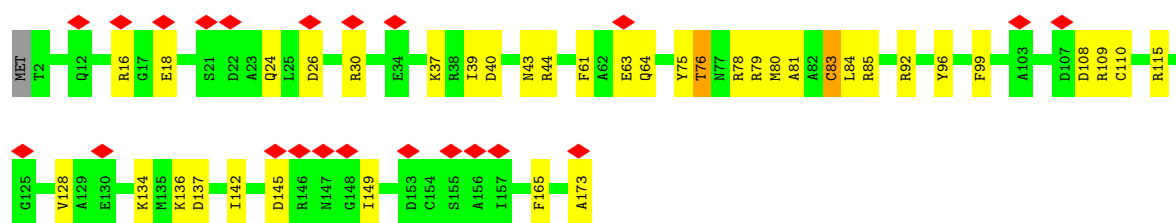
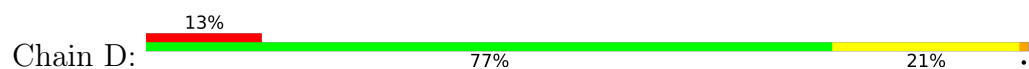
• Molecule 2: C-phycoerythrin alpha subunit



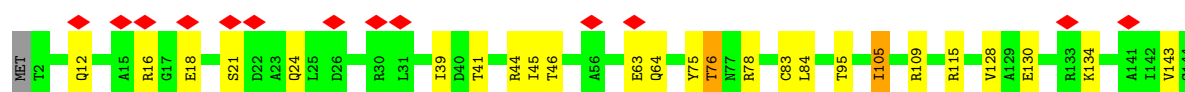
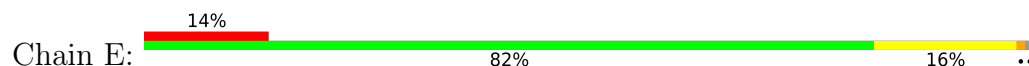
• Molecule 3: C-phycoerythrin beta subunit

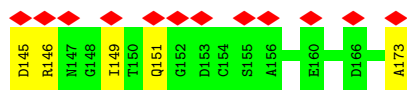


• Molecule 3: C-phycoerythrin beta subunit

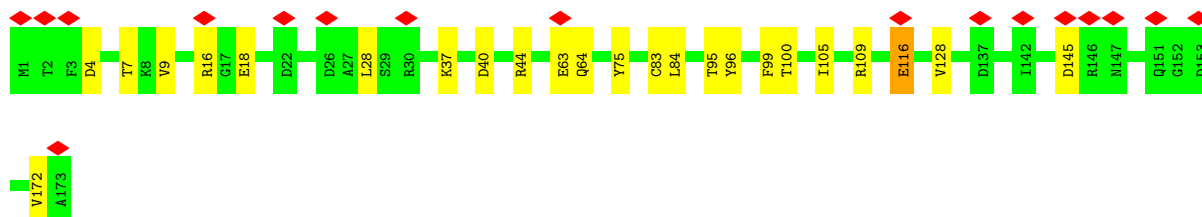
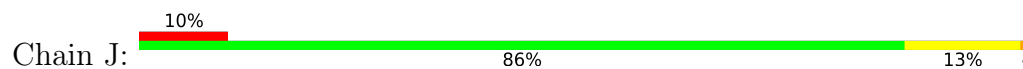


• Molecule 3: C-phycoerythrin beta subunit

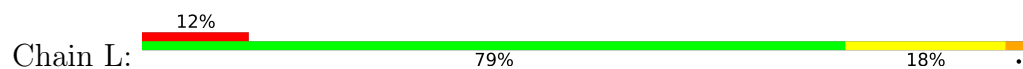




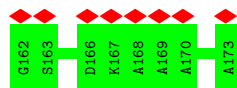
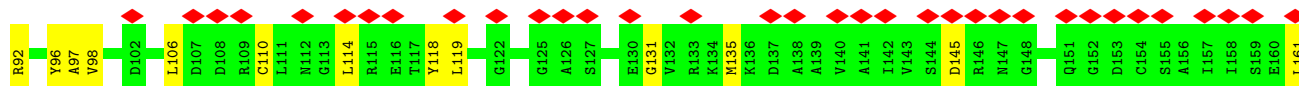
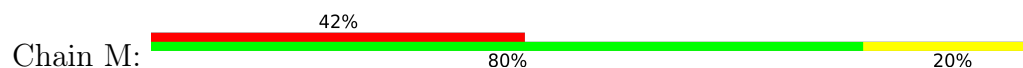
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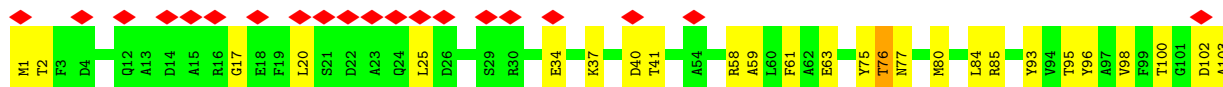
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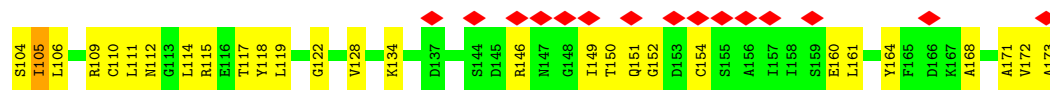


• Molecule 3: C-phycoerythrin beta subunit

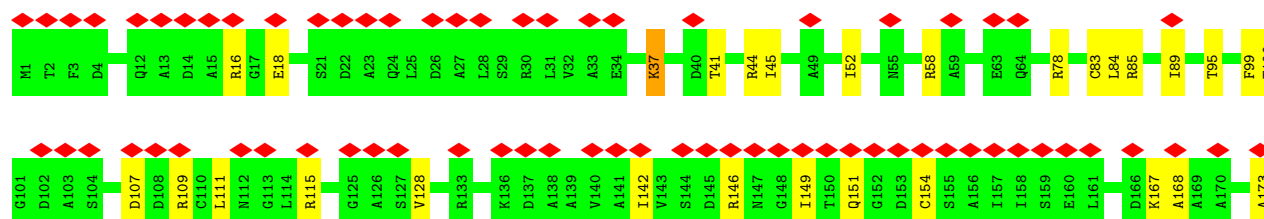
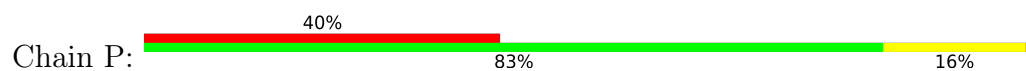


• Molecule 3: C-phycoerythrin beta subunit

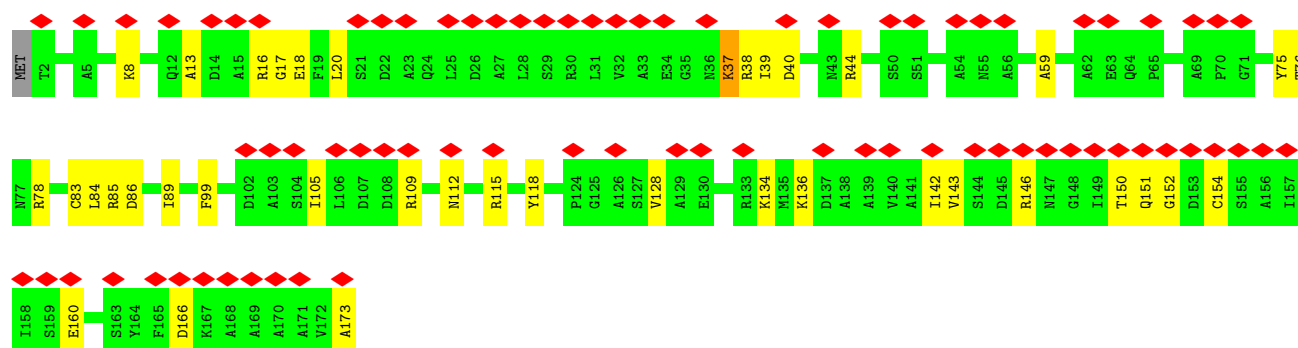
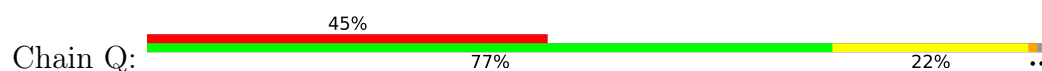




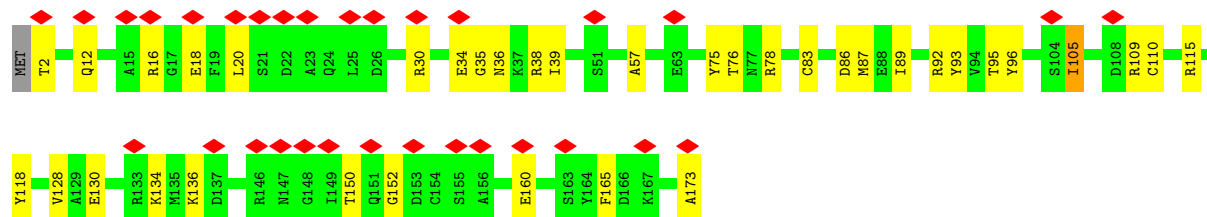
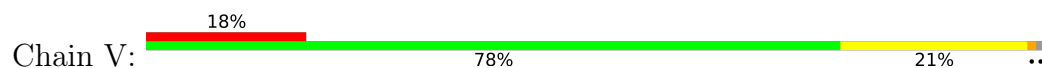
• Molecule 3: C-phycoerythrin beta subunit



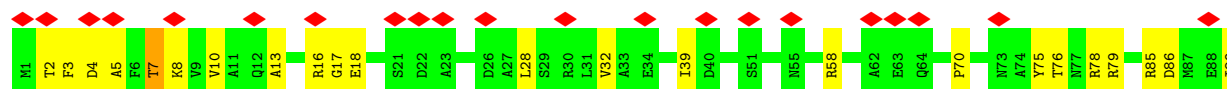
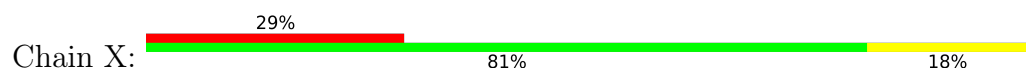
• Molecule 3: C-phycoerythrin beta subunit

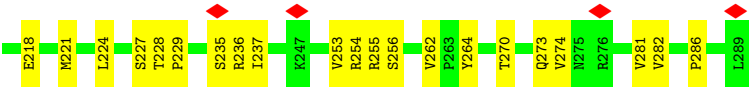


• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit





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	FSC 0.143 CUT-OFF	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	0.247	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.05	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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.25	0/1649	0.33	0/2235
2	B	0.23	0/1237	0.24	0/1681
2	F	0.22	0/1237	0.23	0/1681
2	G	0.22	0/1237	0.26	0/1681
2	H	0.22	0/1237	0.24	0/1681
2	I	0.22	0/1237	0.24	0/1681
2	K	0.22	0/1237	0.24	0/1681
2	N	0.21	0/1245	0.25	0/1691
2	R	0.19	0/1237	0.23	0/1681
2	S	0.19	0/1237	0.23	0/1681
2	T	0.20	0/1237	0.24	0/1681
2	U	0.19	0/1237	0.24	0/1681
2	W	0.21	0/1237	0.25	0/1681
3	C	0.23	0/1293	0.26	0/1748
3	D	0.22	0/1285	0.26	0/1738
3	E	0.22	0/1285	0.25	0/1738
3	J	0.22	0/1293	0.25	0/1748
3	L	0.23	0/1293	0.26	0/1748
3	M	0.18	0/1293	0.23	0/1748
3	O	0.21	0/1293	0.25	0/1748
3	P	0.18	0/1293	0.22	0/1748
3	Q	0.18	0/1285	0.24	0/1738
3	V	0.22	0/1285	0.25	0/1738
3	X	0.19	0/1293	0.26	0/1748
3	a	0.23	0/1285	0.26	0/1738
4	Y	0.12	0/462	0.23	0/621
5	Z	0.23	0/2272	0.29	0/3083
All	All	0.21	0/34711	0.25	0/47047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	1609	0	1561	42	0
2	B	1213	0	1180	29	0
2	F	1213	0	1181	29	0
2	G	1213	0	1180	22	0
2	H	1213	0	1180	23	0
2	I	1213	0	1180	33	0
2	K	1213	0	1180	30	0
2	N	1221	0	1192	39	0
2	R	1213	0	1181	39	0
2	S	1213	0	1180	34	0
2	T	1213	0	1177	30	0
2	U	1213	0	1180	35	0
2	W	1213	0	1180	31	0
3	C	1280	0	1283	29	0
3	D	1272	0	1270	35	0
3	E	1272	0	1270	28	0
3	J	1280	0	1280	19	0
3	L	1280	0	1285	31	0
3	M	1280	0	1283	27	0
3	O	1280	0	1285	43	0
3	P	1280	0	1282	21	0
3	Q	1272	0	1270	30	0
3	V	1272	0	1271	31	0
3	X	1280	0	1284	26	0
3	a	1272	0	1271	25	0
4	Y	457	0	462	15	0
5	Z	2229	0	2209	56	0
6	A	86	0	74	12	0
6	B	43	0	35	7	0
6	C	86	0	74	14	0
6	D	43	0	38	2	0
6	E	43	0	37	3	0
6	F	86	0	74	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	43	0	35	3	0
6	H	43	0	36	2	0
6	I	43	0	35	4	0
6	J	86	0	73	4	0
6	K	43	0	36	5	0
6	L	43	0	38	4	0
6	M	43	0	37	6	0
6	N	43	0	36	6	0
6	P	43	0	37	2	0
6	Q	86	0	76	10	0
6	R	43	0	38	5	0
6	S	43	0	35	6	0
6	T	86	0	73	8	0
6	U	43	0	36	4	0
6	V	86	0	72	11	0
6	W	43	0	36	5	0
6	X	43	0	37	8	0
6	Y	43	0	38	2	0
6	Z	43	0	38	5	0
6	a	86	0	75	9	0
All	All	35641	0	34986	717	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 10.

All (717) 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)
3:Q:83:CYS:HA	6:Q:201:CYC:HHD	1.61	0.82
3:V:109:ARG:HG2	5:Z:14:PRO:HG3	1.69	0.74
2:W:5:PRO:HG2	2:W:31:ARG:HD3	1.70	0.73
6:N:201:CYC:O2D	3:O:58:ARG:NH1	2.22	0.73
6:X:201:CYC:HMA3	6:X:201:CYC:HB	1.52	0.72
6:B:201:CYC:O2D	3:C:58:ARG:NH1	2.21	0.71
6:V:201:CYC:O1A	5:Z:180:ARG:NH2	2.22	0.71
2:R:156:ASP:O	2:R:160:ASN:ND2	2.24	0.70
2:S:41:ALA:HB2	2:S:147:SER:HB3	1.72	0.70
6:Z:301:CYC:HB	6:Z:301:CYC:HMA3	1.55	0.70
3:O:85:ARG:NH1	6:Z:301:CYC:O1A	2.25	0.70
2:H:95:ILE:HG22	2:H:108:ILE:HD13	1.75	0.69
2:W:138:LYS:HB2	2:W:155:ILE:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:ILE:HG21	6:C:202:CYC:HMC3	1.73	0.69
3:P:58:ARG:NH1	6:T:202:CYC:O2D	2.24	0.69
1:A:35:ASP:OD1	5:Z:254:ARG:NH1	2.25	0.69
3:C:16:ARG:NH1	3:C:18:GLU:OE2	2.26	0.68
3:L:16:ARG:NH1	3:L:18:GLU:OE2	2.26	0.68
3:P:115:ARG:NH1	3:P:173:ALA:O	2.26	0.68
3:V:16:ARG:NH1	3:V:18:GLU:OE2	2.26	0.68
1:A:100:ASN:ND2	3:D:109:ARG:O	2.26	0.67
3:E:12:GLN:NE2	3:E:24:GLN:OE1	2.28	0.67
3:D:26:ASP:OD2	3:D:30:ARG:NH1	2.28	0.66
5:Z:109:TYR:O	5:Z:167:ARG:NH1	2.28	0.66
2:R:78:THR:HG23	2:R:81:GLY:H	1.59	0.66
5:Z:138:GLU:OE2	5:Z:152:ARG:NH2	2.28	0.66
2:K:33:ARG:NH2	2:K:34:GLN:OE1	2.29	0.66
3:D:115:ARG:NH1	3:D:173:ALA:O	2.30	0.65
2:G:41:ALA:HB2	2:G:147:SER:HB3	1.76	0.65
1:A:72:ASN:OD1	1:A:74:GLN:NE2	2.29	0.65
3:J:9:VAL:HG11	3:J:28:LEU:HD11	1.76	0.65
2:I:95:ILE:HG22	2:I:108:ILE:HD13	1.78	0.65
3:E:12:GLN:OE1	3:E:16:ARG:NH1	2.30	0.65
3:J:75:TYR:O	6:K:201:CYC:OB	2.15	0.65
2:U:41:ALA:HB2	2:U:147:SER:HB3	1.79	0.65
1:A:98:ASN:O	3:D:109:ARG:NH1	2.30	0.65
2:F:95:ILE:HG22	2:F:108:ILE:HD13	1.79	0.65
2:I:48:ASN:OD1	2:I:51:SER:OG	2.15	0.65
2:W:74:ASN:HA	6:W:201:CYC:HBD2	1.79	0.65
3:X:3:PHE:HA	3:X:7:THR:HG23	1.79	0.65
2:B:138:LYS:HB2	2:B:155:ILE:HG21	1.79	0.64
3:Q:112:ASN:O	4:Y:261:HIS:NE2	2.29	0.64
3:E:115:ARG:NH1	3:E:173:ALA:O	2.30	0.64
2:N:103:GLY:O	2:U:26:GLN:NE2	2.29	0.64
2:S:103:GLY:O	2:T:26:GLN:NE2	2.31	0.64
3:M:1:MET:HG3	4:Y:218:ARG:HH21	1.61	0.64
3:P:16:ARG:NH1	3:P:18:GLU:OE2	2.30	0.64
2:K:41:ALA:HB2	2:K:147:SER:HB3	1.79	0.64
3:V:130:GLU:OE2	3:V:134:LYS:NZ	2.31	0.64
5:Z:102:HIS:NE2	5:Z:179:ASP:OD2	2.30	0.64
5:Z:10:LEU:HA	5:Z:205:PRO:HD2	1.80	0.63
2:N:101:VAL:HG21	3:V:20:LEU:HD12	1.79	0.63
4:Y:231:VAL:HG23	4:Y:234:ARG:HB2	1.79	0.63
1:A:93:SER:HB3	1:A:180:ARG:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:150:THR:O	6:Q:202:CYC:NC	2.30	0.63
2:S:138:LYS:HB2	2:S:155:ILE:HG21	1.81	0.63
5:Z:2:ALA:N	5:Z:155:GLU:OE1	2.32	0.63
6:G:201:CYC:OB	3:L:75:TYR:O	2.16	0.63
1:A:146:GLU:O	1:A:150:ASN:ND2	2.29	0.63
2:H:78:THR:HG23	2:H:81:GLY:H	1.63	0.63
2:N:63:LYS:HD2	2:N:132:GLU:HG3	1.81	0.63
2:U:149:ASP:HB3	6:V:202:CYC:HAB2	1.80	0.63
2:H:63:LYS:HG2	2:H:132:GLU:HG3	1.80	0.62
2:N:18:ARG:NH1	2:U:157:TYR:OH	2.32	0.62
3:X:78:ARG:NH2	6:X:201:CYC:O1D	2.31	0.62
1:A:176:ILE:O	3:a:117:THR:OG1	2.16	0.62
2:F:78:THR:HG23	2:F:81:GLY:H	1.63	0.62
1:A:51:ARG:NH2	2:F:15:SER:O	2.31	0.62
2:F:33:ARG:NH2	2:F:34:GLN:OE1	2.32	0.62
2:B:85:CYS:HA	6:B:201:CYC:HHD	1.81	0.62
3:E:95:THR:HG22	2:H:20:LEU:HD12	1.82	0.62
6:A:302:CYC:H3C	3:E:128:VAL:HG22	1.82	0.62
3:Q:128:VAL:HG22	6:Q:201:CYC:H3C	1.82	0.62
1:A:153:TYR:OH	5:Z:273:GLN:OE1	2.15	0.61
2:R:33:ARG:NH2	2:R:34:GLN:OE1	2.32	0.61
3:C:154:CYS:SG	6:C:202:CYC:OC	2.58	0.61
5:Z:49:ILE:HD12	5:Z:53:GLU:HG3	1.82	0.61
3:a:152:GLY:O	6:a:202:CYC:OC	2.17	0.61
2:G:3:LYS:HD2	2:H:16:GLN:HE22	1.65	0.61
2:B:41:ALA:HB2	2:B:147:SER:HB3	1.82	0.61
2:T:78:THR:HG23	2:T:81:GLY:H	1.65	0.61
3:E:84:LEU:HD13	2:F:122:THR:HG21	1.81	0.61
2:B:20:LEU:HD12	3:J:95:THR:HG22	1.83	0.61
3:E:130:GLU:OE2	3:E:134:LYS:NZ	2.33	0.61
3:L:83:CYS:SG	6:L:201:CYC:HAC2	2.41	0.61
2:S:78:THR:HG23	2:S:81:GLY:H	1.66	0.61
1:A:167:ARG:NH1	6:A:302:CYC:O2D	2.34	0.60
3:P:109:ARG:NH1	2:U:14:ASP:OD2	2.34	0.60
6:F:202:CYC:NC	3:L:150:THR:O	2.33	0.60
2:R:23:THR:HG21	2:W:8:GLU:HG3	1.82	0.60
2:N:26:GLN:HG2	2:U:34:GLN:HG3	1.83	0.60
2:N:18:ARG:NH2	2:U:105:THR:OG1	2.35	0.60
3:M:76:THR:HG22	3:M:78:ARG:H	1.65	0.60
5:Z:74:ARG:NH2	5:Z:135:ASP:OD1	2.35	0.60
2:I:94:ARG:NH2	3:a:75:TYR:OH	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:ARG:HH12	3:D:145:ASP:HB3	1.66	0.59
2:W:31:ARG:NH2	2:W:101:VAL:O	2.35	0.59
6:Z:301:CYC:HB	6:Z:301:CYC:CMA	2.14	0.59
1:A:37:TYR:HB3	1:A:41:GLN:HB2	1.82	0.59
2:G:85:CYS:HA	6:G:201:CYC:HHD	1.84	0.59
2:N:113:LEU:HD21	2:N:161:ALA:HB1	1.82	0.59
3:X:4:ASP:HA	3:X:100:THR:HB	1.84	0.59
3:a:146:ARG:NH1	3:a:152:GLY:O	2.35	0.59
1:A:30:GLN:OE1	1:A:155:LYS:NZ	2.35	0.59
5:Z:142:THR:OG1	5:Z:152:ARG:NH1	2.35	0.59
5:Z:142:THR:HG21	5:Z:152:ARG:HD2	1.85	0.59
6:a:201:CYC:NC	6:a:201:CYC:HMD1	2.17	0.59
3:Q:75:TYR:OH	2:R:94:ARG:NH2	2.30	0.59
3:Q:115:ARG:NH1	3:Q:173:ALA:O	2.36	0.59
2:U:78:THR:HG23	2:U:81:GLY:H	1.66	0.59
2:N:78:THR:HG23	2:N:81:GLY:H	1.67	0.59
1:A:106:GLN:NE2	1:A:179:PRO:O	2.36	0.59
3:V:38:ARG:NH2	3:V:160:GLU:OE1	2.36	0.59
3:O:95:THR:HG22	2:S:20:LEU:HD12	1.84	0.58
2:I:85:CYS:HA	6:I:201:CYC:HHD	1.83	0.58
2:W:85:CYS:HA	6:W:201:CYC:HHD	1.83	0.58
3:X:4:ASP:OD1	3:X:5:ALA:N	2.33	0.58
3:X:89:ILE:HG21	6:X:201:CYC:HAB1	1.85	0.58
2:K:85:CYS:HA	6:K:201:CYC:HHD	1.85	0.58
2:K:138:LYS:HB2	2:K:155:ILE:HG21	1.85	0.58
3:C:146:ARG:NH2	3:C:152:GLY:O	2.36	0.58
6:B:201:CYC:OB	3:C:75:TYR:O	2.20	0.58
3:C:130:GLU:OE2	3:C:134:LYS:NZ	2.36	0.58
6:a:201:CYC:CMA	6:a:201:CYC:HB	2.16	0.58
3:O:117:THR:HG23	5:Z:165:LEU:HD22	1.86	0.58
6:A:302:CYC:HHD	3:E:83:CYS:HA	1.85	0.58
2:S:3:LYS:HD3	2:T:16:GLN:HE22	1.67	0.58
3:D:16:ARG:NE	3:D:18:GLU:OE2	2.36	0.58
2:I:78:THR:HG23	2:I:81:GLY:H	1.69	0.57
3:O:96:TYR:OH	2:S:18:ARG:O	2.20	0.57
5:Z:201:PRO:HD3	5:Z:221:MET:HE1	1.86	0.57
2:I:121:LYS:NZ	2:K:117:ASP:OD1	2.36	0.57
2:N:41:ALA:HB2	2:N:147:SER:HB3	1.86	0.57
2:H:41:ALA:HB2	2:H:147:SER:HB3	1.86	0.57
2:R:134:LEU:HB2	2:R:159:ILE:HD11	1.85	0.57
2:W:41:ALA:HB2	2:W:147:SER:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:227:SER:HA	5:Z:237:ILE:HD11	1.86	0.57
3:J:75:TYR:OH	2:K:94:ARG:NH2	2.25	0.57
3:a:9:VAL:HG11	3:a:28:LEU:HD11	1.85	0.57
3:D:43:ASN:HB2	2:I:25:LEU:HD21	1.87	0.57
3:V:89:ILE:HG12	3:V:92:ARG:HH21	1.70	0.57
1:A:54:PHE:HE1	1:A:90:PHE:HB2	1.68	0.57
6:A:301:CYC:NC	6:A:301:CYC:HMD1	2.20	0.57
3:J:16:ARG:HG3	3:J:18:GLU:HG2	1.86	0.57
3:L:9:VAL:HG21	3:L:28:LEU:HD11	1.86	0.57
3:L:116:GLU:HG3	5:Z:212:VAL:HG22	1.87	0.57
2:R:26:GLN:NE2	2:W:103:GLY:O	2.37	0.56
2:K:9:ALA:HB1	2:K:24:GLU:HG3	1.86	0.56
2:N:149:ASP:HB3	6:P:201:CYC:H2C	1.85	0.56
2:F:85:CYS:HB2	6:F:201:CYC:H2C	1.86	0.56
3:P:85:ARG:NE	4:Y:238:ARG:HH21	2.03	0.56
2:W:33:ARG:NH2	2:W:34:GLN:OE1	2.38	0.56
6:a:202:CYC:HMA3	6:a:202:CYC:HB	1.70	0.56
6:a:202:CYC:HMA3	6:a:202:CYC:NB	2.20	0.56
2:N:1:MET:N	3:V:2:THR:OG1	2.36	0.56
3:D:149:ILE:HD13	6:D:201:CYC:H3C	1.87	0.56
3:Q:76:THR:HG22	3:Q:78:ARG:H	1.70	0.56
6:X:201:CYC:HB	6:X:201:CYC:CMA	2.18	0.56
2:S:94:ARG:NH2	3:X:75:TYR:OH	2.27	0.56
2:I:41:ALA:HB2	2:I:147:SER:HB3	1.87	0.56
5:Z:4:THR:OG1	6:Z:301:CYC:O1D	2.24	0.56
6:J:201:CYC:HMA3	5:Z:224:LEU:HD23	1.88	0.56
2:W:85:CYS:HA	6:W:201:CYC:HAC2	1.86	0.56
1:A:85:LEU:O	1:A:134:TYR:OH	2.21	0.55
3:M:63:GLU:HG3	3:M:64:GLN:HG3	1.89	0.55
6:M:201:CYC:HAA1	5:Z:64:ASN:HB2	1.87	0.55
1:A:95:TYR:O	3:D:109:ARG:NH1	2.40	0.55
3:M:89:ILE:HG12	3:M:92:ARG:HH21	1.71	0.55
3:D:39:ILE:HG23	2:I:25:LEU:HG	1.88	0.55
3:M:57:ALA:HB2	3:M:87:MET:HE1	1.88	0.55
2:G:113:LEU:HD11	2:G:161:ALA:HB1	1.89	0.55
3:M:44:ARG:NH2	3:M:145:ASP:O	2.40	0.55
3:O:34:GLU:HG3	3:O:37:LYS:HD2	1.88	0.55
2:R:78:THR:OG1	2:R:80:GLU:OE1	2.24	0.55
3:V:78:ARG:NH1	6:V:201:CYC:O1D	2.39	0.55
2:S:18:ARG:NH2	2:T:105:THR:OG1	2.39	0.55
3:a:115:ARG:NH1	3:a:173:ALA:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:HB1	1:A:61:ASP:HB2	1.88	0.55
2:N:85:CYS:HA	6:N:201:CYC:HHD	1.88	0.55
3:P:107:ASP:HA	3:P:111:LEU:HB2	1.88	0.55
3:a:21:SER:H	3:a:24:GLN:HE21	1.55	0.55
2:K:2:SER:O	3:L:1:MET:N	2.40	0.55
3:L:93:TYR:OH	5:Z:254:ARG:NH2	2.40	0.55
2:R:85:CYS:HA	6:R:201:CYC:HHD	1.88	0.55
1:A:56:HIS:O	1:A:56:HIS:ND1	2.40	0.55
2:B:22:SER:O	2:B:26:GLN:HG2	2.07	0.55
2:R:113:LEU:HD11	2:R:161:ALA:HB1	1.89	0.55
2:S:26:GLN:NE2	2:T:103:GLY:O	2.38	0.55
2:S:33:ARG:NH2	2:S:34:GLN:OE1	2.40	0.55
3:O:146:ARG:HD2	6:T:201:CYC:HMC2	1.87	0.54
2:I:16:GLN:OE1	2:I:18:ARG:NE	2.37	0.54
6:J:202:CYC:NB	6:J:202:CYC:HMA3	2.22	0.54
2:K:85:CYS:HA	6:K:201:CYC:HAC2	1.88	0.54
2:R:41:ALA:HB2	2:R:147:SER:HB3	1.89	0.54
2:G:74:ASN:HA	6:G:201:CYC:HBD2	1.90	0.54
6:C:201:CYC:O2D	5:Z:236:ARG:NH2	2.40	0.54
3:D:96:TYR:OH	2:I:18:ARG:O	2.20	0.54
2:F:41:ALA:HB2	2:F:147:SER:HB3	1.89	0.54
2:U:21:SER:OG	2:U:22:SER:N	2.40	0.54
2:S:74:ASN:HA	6:S:201:CYC:HBD2	1.90	0.54
3:a:114:LEU:HD23	3:a:172:VAL:HG12	1.88	0.54
1:A:26:GLU:OE2	3:a:2:THR:N	2.41	0.54
2:I:91:TYR:O	2:I:95:ILE:HG12	2.08	0.54
3:Q:83:CYS:SG	6:Q:201:CYC:HAC2	2.48	0.54
6:V:201:CYC:HC	6:V:201:CYC:HMD3	1.72	0.54
2:W:16:GLN:HG3	2:W:18:ARG:HG2	1.89	0.54
3:O:146:ARG:NE	3:O:151:GLN:OE1	2.38	0.54
3:E:18:GLU:O	2:H:98:TYR:OH	2.24	0.53
3:M:22:ASP:OD1	2:R:43:LYS:NZ	2.41	0.53
3:V:93:TYR:CG	3:V:110:CYS:HB2	2.43	0.53
3:Q:84:LEU:HD13	2:R:122:THR:HG21	1.91	0.53
3:V:115:ARG:HD2	5:Z:208:GLY:HA3	1.90	0.53
2:B:122:THR:HG21	3:C:84:LEU:HD13	1.91	0.53
5:Z:55:LEU:HD21	5:Z:79:SER:HB3	1.90	0.53
3:P:128:VAL:HG22	6:Y:301:CYC:H3C	1.89	0.53
2:T:78:THR:OG1	2:T:80:GLU:OE1	2.27	0.53
2:W:99:ALA:HB2	2:W:108:ILE:HG13	1.91	0.53
3:X:13:ALA:O	3:X:17:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:GLU:HG3	3:C:64:GLN:HG3	1.90	0.53
3:O:102:ASP:OD1	3:O:104:SER:N	2.41	0.53
3:P:111:LEU:HD21	3:P:168:ALA:HA	1.90	0.53
2:F:78:THR:OG1	2:F:80:GLU:OE1	2.27	0.52
2:T:74:ASN:ND2	2:T:124:ASP:OD2	2.42	0.52
2:I:31:ARG:NH2	2:I:101:VAL:O	2.42	0.52
2:U:78:THR:OG1	2:U:80:GLU:OE1	2.27	0.52
3:V:76:THR:HG22	3:V:78:ARG:H	1.74	0.52
1:A:191:PHE:O	1:A:193:LYS:N	2.42	0.52
2:G:8:GLU:HG3	2:H:23:THR:HG21	1.91	0.52
3:M:131:GLY:O	3:M:135:MET:HG3	2.10	0.52
5:Z:211:TYR:HB2	5:Z:282:VAL:HG21	1.90	0.52
2:U:85:CYS:HA	6:U:201:CYC:HAC2	1.92	0.52
6:A:302:CYC:O1A	3:E:78:ARG:NH2	2.39	0.52
6:J:202:CYC:HMA3	6:J:202:CYC:HB	1.73	0.52
6:N:201:CYC:OB	3:O:75:TYR:O	2.28	0.52
3:O:106:LEU:HG	3:O:111:LEU:HD22	1.90	0.52
3:a:44:ARG:HH12	3:a:145:ASP:HB3	1.75	0.52
6:A:301:CYC:HMD1	6:A:301:CYC:HC	1.75	0.52
2:I:122:THR:HG21	3:a:84:LEU:HD13	1.91	0.52
2:U:121:LYS:NZ	2:W:163:SER:OXT	2.42	0.52
3:Q:16:ARG:HG3	3:Q:18:GLU:HG2	1.92	0.52
6:A:301:CYC:H3C	3:D:128:VAL:HG22	1.92	0.51
2:B:33:ARG:NH1	2:B:146:ASP:OD2	2.43	0.51
2:B:64:PHE:O	2:B:67:THR:OG1	2.27	0.51
3:E:146:ARG:HB3	3:E:151:GLN:HE21	1.75	0.51
3:P:44:ARG:HH21	3:P:149:ILE:HB	1.74	0.51
3:V:76:THR:HG23	2:W:111:TYR:HA	1.92	0.51
2:W:20:LEU:HD12	3:X:95:THR:HG22	1.92	0.51
3:X:3:PHE:HB3	3:X:8:LYS:HB2	1.92	0.51
1:A:41:GLN:HG2	3:L:1:MET:HA	1.91	0.51
2:F:98:TYR:OH	3:a:18:GLU:O	2.28	0.51
3:O:25:LEU:HD22	2:S:43:LYS:HB2	1.92	0.51
3:P:37:LYS:HE2	3:P:154:CYS:HB3	1.91	0.51
3:Q:154:CYS:SG	6:Q:202:CYC:HAC2	2.51	0.51
2:R:138:LYS:HB2	2:R:155:ILE:HG21	1.93	0.51
2:F:20:LEU:HD12	3:a:95:THR:HG22	1.91	0.51
5:Z:41:ARG:NH2	5:Z:175:TYR:O	2.43	0.51
6:A:301:CYC:HAC2	3:D:83:CYS:SG	2.51	0.51
2:F:85:CYS:HA	6:F:201:CYC:HHD	1.92	0.51
2:F:99:ALA:HB2	2:F:108:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:63:GLU:HG3	3:J:64:GLN:HG3	1.93	0.51
2:R:121:LYS:NZ	2:S:117:ASP:OD1	2.44	0.51
2:S:18:ARG:NH1	2:T:109:ASP:OD2	2.43	0.51
2:U:85:CYS:HA	6:U:201:CYC:HHD	1.92	0.51
3:V:152:GLY:HA3	6:V:202:CYC:HMD2	1.93	0.51
2:K:85:CYS:O	2:K:89:ILE:HG12	2.11	0.51
2:B:74:ASN:HA	6:B:201:CYC:HBD2	1.93	0.51
2:W:10:VAL:HG21	3:X:100:THR:HG23	1.93	0.51
3:a:34:GLU:OE1	3:a:37:LYS:NZ	2.37	0.51
3:D:75:TYR:OH	2:H:94:ARG:NH2	2.31	0.51
3:Q:146:ARG:HB3	3:Q:151:GLN:HE22	1.76	0.51
3:X:16:ARG:NE	3:X:18:GLU:OE2	2.44	0.50
1:A:78:ARG:NH1	1:A:143:ASN:OD1	2.44	0.50
2:U:63:LYS:HD3	2:U:132:GLU:HG3	1.94	0.50
3:O:119:LEU:HD11	5:Z:286:PRO:HD2	1.94	0.50
3:Q:109:ARG:O	4:Y:261:HIS:ND1	2.45	0.50
2:R:128:SER:O	2:R:132:GLU:HG3	2.11	0.50
3:D:75:TYR:O	6:H:201:CYC:OB	2.30	0.50
3:M:80:MET:HE3	3:M:80:MET:O	2.12	0.50
2:N:1:MET:SD	3:V:2:THR:N	2.85	0.50
3:X:86:ASP:OD2	3:X:118:TYR:OH	2.27	0.50
4:Y:228:GLN:OE1	4:Y:266:ARG:NE	2.40	0.50
1:A:184:TYR:OH	3:D:108:ASP:OD1	2.23	0.50
3:M:76:THR:HG23	2:U:111:TYR:HA	1.92	0.50
2:S:67:THR:HG22	2:S:76:ALA:H	1.77	0.50
2:N:20:LEU:HD12	2:N:24:GLU:HG2	1.94	0.50
3:C:119:LEU:HD22	3:O:122:GLY:HA2	1.93	0.49
2:F:91:TYR:O	2:F:95:ILE:HG12	2.12	0.49
2:G:122:THR:HG21	3:L:84:LEU:HD13	1.93	0.49
2:F:26:GLN:NE2	2:K:103:GLY:O	2.43	0.49
3:V:30:ARG:O	3:V:34:GLU:HG2	2.11	0.49
5:Z:43:VAL:HA	5:Z:102:HIS:HB3	1.94	0.49
2:W:95:ILE:HG13	2:W:112:LEU:HD13	1.95	0.49
5:Z:262:VAL:HG11	5:Z:270:THR:HG21	1.93	0.49
2:B:99:ALA:HA	2:B:107:PRO:HG2	1.95	0.49
6:F:201:CYC:HHA	6:F:201:CYC:HBD2	1.95	0.49
2:G:103:GLY:O	2:H:26:GLN:NE2	2.44	0.49
2:N:9:ALA:HB1	2:N:24:GLU:HG3	1.94	0.49
3:O:146:ARG:HH21	3:O:151:GLN:HB3	1.76	0.49
2:R:85:CYS:HB2	6:R:201:CYC:H2C	1.93	0.49
3:a:146:ARG:HD3	6:a:202:CYC:HMC2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:85:CYS:HA	6:N:201:CYC:HAC2	1.95	0.49
2:H:33:ARG:NH1	2:H:146:ASP:OD2	2.45	0.49
4:Y:218:ARG:HG2	4:Y:250:TYR:HB3	1.94	0.49
3:E:146:ARG:HD2	3:E:151:GLN:HG3	1.95	0.49
2:G:9:ALA:HB1	2:G:24:GLU:HG3	1.94	0.49
2:K:20:LEU:HD12	3:L:95:THR:HG22	1.95	0.49
2:N:24:GLU:OE1	2:N:24:GLU:N	2.42	0.49
3:O:102:ASP:OD1	3:O:103:ALA:N	2.46	0.49
2:U:112:LEU:HD23	2:U:158:LEU:HD21	1.95	0.49
2:W:7:THR:HG23	3:X:2:THR:HB	1.95	0.49
3:J:128:VAL:HB	3:J:172:VAL:HG11	1.95	0.49
1:A:179:PRO:HB2	3:a:121:LEU:HD21	1.95	0.49
2:H:108:ILE:HG22	2:H:113:LEU:HG	1.95	0.49
2:N:31:ARG:NH2	2:N:101:VAL:O	2.46	0.48
2:B:109:ASP:HA	2:B:113:LEU:HB2	1.95	0.48
3:C:128:VAL:HG22	6:C:201:CYC:H3C	1.95	0.48
3:O:37:LYS:O	3:O:41:THR:HG23	2.13	0.48
1:A:3:LEU:HD21	3:D:81:ALA:HB3	1.95	0.48
3:L:63:GLU:HG3	3:L:64:GLN:HG3	1.96	0.48
2:T:41:ALA:HB2	2:T:147:SER:HB3	1.95	0.48
6:a:201:CYC:HB	6:a:201:CYC:HMA3	1.76	0.48
6:A:302:CYC:HMD3	6:A:302:CYC:HC	1.79	0.48
3:L:76:THR:HG22	3:L:78:ARG:H	1.78	0.48
3:P:44:ARG:HE	3:P:149:ILE:HD12	1.78	0.48
3:Q:13:ALA:O	3:Q:17:GLY:N	2.46	0.48
3:V:92:ARG:O	3:V:95:THR:OG1	2.24	0.48
2:W:112:LEU:HD12	6:W:201:CYC:HAB1	1.96	0.48
6:C:202:CYC:NB	6:C:202:CYC:HMA3	2.28	0.48
3:M:18:GLU:O	2:R:98:TYR:OH	2.31	0.48
2:R:42:ALA:HB1	2:R:97:THR:HG23	1.96	0.48
5:Z:211:TYR:OH	5:Z:218:GLU:OE1	2.29	0.48
3:E:75:TYR:O	6:F:201:CYC:OB	2.31	0.48
3:O:111:LEU:HG	3:O:171:ALA:HB3	1.95	0.48
6:P:201:CYC:HAC1	6:P:201:CYC:HHD	1.40	0.48
2:T:95:ILE:HG13	2:T:112:LEU:HD13	1.96	0.48
1:A:75:ILE:HB	1:A:79:ASP:HB2	1.95	0.48
3:C:44:ARG:NE	6:C:202:CYC:HMC1	2.29	0.48
3:E:44:ARG:HH12	3:E:145:ASP:HB3	1.79	0.48
3:L:34:GLU:HG3	3:L:37:LYS:HD2	1.95	0.48
3:O:17:GLY:HA3	3:X:70:PRO:HB3	1.96	0.48
4:Y:225:GLN:HG2	4:Y:245:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:TYR:O	2:H:95:ILE:HG12	2.13	0.48
2:N:12:ALA:O	2:N:16:GLN:HG2	2.14	0.48
3:V:57:ALA:HB2	3:V:87:MET:HE1	1.94	0.48
6:X:201:CYC:CGA	5:Z:115:ILE:HG12	2.44	0.48
3:D:80:MET:HE3	3:D:80:MET:O	2.14	0.48
3:J:116:GLU:N	3:J:116:GLU:OE1	2.44	0.48
2:R:143:LEU:C	2:R:148:ARG:HB2	2.39	0.48
2:U:74:ASN:HA	6:U:201:CYC:HBD2	1.95	0.48
3:X:91:LEU:HB2	3:X:135:MET:HE3	1.95	0.48
5:Z:85:LYS:HG3	5:Z:180:ARG:HD3	1.96	0.48
6:F:202:CYC:H3C	3:L:149:ILE:HD13	1.96	0.47
6:L:201:CYC:OB	5:Z:254:ARG:O	2.32	0.47
3:X:128:VAL:HG22	6:X:201:CYC:H3C	1.96	0.47
3:C:85:ARG:NH2	6:C:201:CYC:O2A	2.47	0.47
2:I:78:THR:OG1	2:I:80:GLU:OE1	2.31	0.47
3:M:44:ARG:HH21	3:M:145:ASP:HB3	1.78	0.47
2:R:53:VAL:HG23	2:R:89:ILE:HB	1.96	0.47
2:H:85:CYS:HA	6:H:201:CYC:HHD	1.97	0.47
3:Q:37:LYS:N	3:Q:37:LYS:HE2	2.29	0.47
2:B:18:ARG:O	3:J:96:TYR:OH	2.31	0.47
2:B:94:ARG:NH2	3:C:75:TYR:OH	2.30	0.47
2:N:74:ASN:HA	6:N:201:CYC:HBD2	1.96	0.47
2:N:122:THR:HG21	3:O:84:LEU:HD13	1.95	0.47
2:S:67:THR:HG21	6:S:201:CYC:HMC2	1.96	0.47
6:V:201:CYC:HC	6:V:201:CYC:CMD	2.28	0.47
1:A:84:LEU:O	1:A:87:SER:OG	2.25	0.47
6:E:201:CYC:HMA3	6:E:201:CYC:NB	2.29	0.47
2:N:45:LEU:HD21	2:N:141:HIS:HB2	1.96	0.47
2:S:99:ALA:HB2	2:S:108:ILE:HG13	1.96	0.47
3:C:154:CYS:SG	6:C:202:CYC:HAC2	2.55	0.47
3:E:105:ILE:HD12	3:E:109:ARG:HG3	1.95	0.47
3:Q:109:ARG:HA	4:Y:261:HIS:HB3	1.96	0.47
1:A:182:ASP:OD1	1:A:183:SER:N	2.43	0.47
2:F:45:LEU:HD21	2:F:141:HIS:HB2	1.96	0.47
2:N:99:ALA:HB2	2:N:108:ILE:HG13	1.97	0.47
3:P:95:THR:HG22	2:U:20:LEU:HD12	1.96	0.47
3:Q:86:ASP:OD2	3:Q:118:TYR:OH	2.27	0.47
3:a:30:ARG:O	3:a:34:GLU:HG2	2.15	0.47
2:K:156:ASP:O	2:K:160:ASN:ND2	2.33	0.47
2:N:85:CYS:O	2:N:89:ILE:HG12	2.15	0.47
3:M:84:LEU:HD13	2:U:122:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:34:GLN:HE21	2:N:150:GLU:HB2	1.80	0.47
3:O:112:ASN:O	5:Z:162:SER:OG	2.20	0.47
2:B:88:ASP:HB3	2:B:130:TYR:HE1	1.80	0.47
2:B:103:GLY:O	2:I:26:GLN:NE2	2.48	0.47
2:N:116:LEU:HD21	2:N:162:LEU:HD21	1.96	0.47
3:Q:99:PHE:CZ	2:T:28:ALA:HB2	2.50	0.47
6:S:201:CYC:O2D	3:X:58:ARG:NH1	2.47	0.47
3:V:128:VAL:HG22	6:V:201:CYC:H3C	1.95	0.47
6:E:201:CYC:HMA3	6:E:201:CYC:HB	1.79	0.46
6:I:201:CYC:OB	3:a:75:TYR:O	2.33	0.46
3:O:61:PHE:CE2	3:O:80:MET:HE1	2.49	0.46
3:O:109:ARG:NH1	2:S:14:ASP:OD2	2.48	0.46
3:O:154:CYS:SG	6:T:201:CYC:HAC1	2.55	0.46
2:U:99:ALA:HB2	2:U:108:ILE:HG13	1.96	0.46
2:K:14:ASP:OD1	3:L:93:TYR:OH	2.23	0.46
2:K:118:GLU:OE1	2:K:118:GLU:N	2.42	0.46
3:P:84:LEU:HD13	2:T:122:THR:HG21	1.97	0.46
1:A:26:GLU:HB3	1:A:163:VAL:HG21	1.96	0.46
2:G:64:PHE:O	2:G:67:THR:OG1	2.25	0.46
3:M:114:LEU:HD11	3:M:118:TYR:CZ	2.50	0.46
3:O:20:LEU:HD22	2:S:101:VAL:HG21	1.97	0.46
2:T:91:TYR:O	2:T:95:ILE:HG12	2.16	0.46
2:I:74:ASN:HA	6:I:201:CYC:HBD2	1.97	0.46
3:J:84:LEU:HD13	2:K:122:THR:HG21	1.97	0.46
2:N:78:THR:OG1	2:N:80:GLU:OE1	2.32	0.46
3:O:80:MET:HE3	3:O:80:MET:O	2.15	0.46
2:R:43:LYS:O	2:R:47:ASN:ND2	2.35	0.46
2:R:155:ILE:O	2:R:159:ILE:HG12	2.16	0.46
2:H:78:THR:OG1	2:H:80:GLU:OE1	2.32	0.46
2:R:9:ALA:HB1	2:R:24:GLU:HG3	1.96	0.46
2:R:99:ALA:HB2	2:R:108:ILE:HG13	1.96	0.46
2:T:31:ARG:NH2	2:T:101:VAL:O	2.48	0.46
5:Z:173:ARG:NH1	5:Z:203:VAL:O	2.34	0.46
2:F:18:ARG:NH2	2:K:157:TYR:OH	2.49	0.46
3:V:75:TYR:O	6:W:201:CYC:OB	2.33	0.46
1:A:3:LEU:HD22	3:D:78:ARG:HG2	1.97	0.46
2:F:113:LEU:HD11	2:F:161:ALA:HB1	1.98	0.46
2:G:150:GLU:HG2	2:G:154:TYR:CE2	2.51	0.46
6:M:201:CYC:NC	6:M:201:CYC:HMD1	2.31	0.46
2:S:85:CYS:HA	6:S:201:CYC:HHD	1.96	0.46
2:K:74:ASN:HA	6:K:201:CYC:HBD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:44:ARG:HD3	3:Q:143:VAL:HA	1.98	0.46
2:U:50:ASP:O	2:U:54:ASN:ND2	2.38	0.46
2:W:18:ARG:O	3:X:96:TYR:OH	2.27	0.46
3:C:37:LYS:HE2	6:C:202:CYC:HMD2	1.97	0.46
2:K:8:GLU:HG3	2:K:9:ALA:N	2.30	0.46
3:V:105:ILE:HD12	3:V:109:ARG:HD3	1.97	0.46
5:Z:235:SER:HB3	5:Z:264:TYR:HB3	1.98	0.46
3:J:4:ASP:N	3:J:7:THR:OG1	2.46	0.45
3:O:2:THR:HG21	3:O:105:ILE:HA	1.96	0.45
3:P:52:ILE:HD11	3:P:142:ILE:HD12	1.98	0.45
2:W:12:ALA:O	2:W:16:GLN:HG2	2.16	0.45
4:Y:252:LYS:NZ	5:Z:70:ARG:HH22	2.13	0.45
2:G:138:LYS:HB2	2:G:155:ILE:HG21	1.98	0.45
3:O:100:THR:HG23	2:S:10:VAL:HG21	1.99	0.45
1:A:43:ASP:OD1	1:A:71:ARG:NH2	2.35	0.45
2:B:27:VAL:HG22	2:I:27:VAL:HG22	1.98	0.45
2:G:111:TYR:HA	3:L:76:THR:HG23	1.96	0.45
3:O:149:ILE:HD13	6:T:201:CYC:H3C	1.98	0.45
2:T:85:CYS:HA	6:T:202:CYC:HHD	1.98	0.45
3:X:7:THR:HA	3:X:10:VAL:HB	1.98	0.45
2:R:84:LYS:NZ	6:R:201:CYC:O1A	2.44	0.45
3:a:154:CYS:SG	6:a:202:CYC:HBC2	2.56	0.45
3:D:16:ARG:HH22	3:D:24:GLN:HE22	1.62	0.45
3:E:146:ARG:O	3:E:151:GLN:NE2	2.50	0.45
2:T:109:ASP:HA	2:T:113:LEU:HB2	1.98	0.45
2:T:150:GLU:HG2	2:T:154:TYR:CE2	2.52	0.45
3:V:150:THR:O	6:V:202:CYC:NC	2.42	0.45
2:W:112:LEU:HD23	2:W:158:LEU:HD21	1.98	0.45
5:Z:40:TYR:OH	5:Z:59:GLU:OE2	2.32	0.45
3:C:30:ARG:O	3:C:34:GLU:HG2	2.17	0.45
3:M:87:MET:HE2	6:M:201:CYC:HBC1	1.99	0.45
2:N:126:ALA:HB3	2:N:129:TRP:CE2	2.51	0.45
2:W:131:VAL:HG12	2:W:135:LYS:HE2	1.98	0.45
2:F:25:LEU:HD22	3:a:39:ILE:HG23	1.99	0.45
6:F:202:CYC:HHD	6:F:202:CYC:HAC1	1.57	0.45
2:I:85:CYS:HA	6:I:201:CYC:HAC1	1.84	0.45
6:A:302:CYC:HC	6:A:302:CYC:CMD	2.30	0.45
3:M:78:ARG:NH1	6:M:201:CYC:O1D	2.47	0.45
3:L:98:VAL:HG21	3:L:161:LEU:HD13	1.99	0.45
3:M:39:ILE:HG23	2:R:25:LEU:HD22	1.98	0.45
3:Q:128:VAL:HG13	6:Q:201:CYC:HBC3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:85:CYS:O	2:S:89:ILE:HG12	2.16	0.45
3:C:92:ARG:O	3:C:95:THR:OG1	2.29	0.44
2:K:5:PRO:HA	2:K:8:GLU:HG2	1.98	0.44
6:U:201:CYC:HAC2	6:U:201:CYC:HHD	1.56	0.44
2:B:85:CYS:HA	6:B:201:CYC:HAC1	1.81	0.44
2:B:108:ILE:HG22	2:B:113:LEU:HG	1.98	0.44
3:J:44:ARG:NH1	3:J:145:ASP:O	2.27	0.44
3:P:99:PHE:CZ	2:U:28:ALA:HB2	2.52	0.44
3:Q:142:ILE:HG13	3:Q:143:VAL:N	2.32	0.44
2:R:91:TYR:O	2:R:95:ILE:HG12	2.17	0.44
3:V:115:ARG:NH2	3:V:173:ALA:O	2.49	0.44
6:V:201:CYC:HHD	6:V:201:CYC:HAC2	1.42	0.44
2:U:74:ASN:ND2	2:U:124:ASP:OD2	2.50	0.44
2:W:50:ASP:OD1	2:W:51:SER:N	2.50	0.44
3:X:79:ARG:HD2	6:X:201:CYC:HBD2	1.99	0.44
1:A:180:ARG:HG3	6:a:201:CYC:HBA2	2.00	0.44
3:D:44:ARG:HE	3:D:149:ILE:HD12	1.83	0.44
3:L:67:LEU:HD21	6:L:201:CYC:HMC2	1.99	0.44
2:R:80:GLU:O	2:R:84:LYS:HG2	2.17	0.44
2:G:91:TYR:O	2:G:95:ILE:HG12	2.18	0.44
2:U:85:CYS:O	2:U:89:ILE:HG12	2.17	0.44
2:B:2:SER:HB3	2:B:106:GLY:HA3	1.99	0.44
3:E:21:SER:H	3:E:24:GLN:NE2	2.15	0.44
2:F:101:VAL:HG21	3:a:20:LEU:HD13	2.00	0.44
3:J:4:ASP:H	3:J:7:THR:HG1	1.66	0.44
3:J:37:LYS:N	3:J:37:LYS:HE2	2.33	0.44
2:T:74:ASN:HA	6:T:202:CYC:HBD2	1.98	0.44
2:T:95:ILE:HG22	2:T:108:ILE:HG12	1.99	0.44
3:D:37:LYS:HE2	3:D:37:LYS:N	2.32	0.44
2:G:45:LEU:HD21	2:G:141:HIS:HB2	2.00	0.44
2:I:50:ASP:OD1	2:I:50:ASP:N	2.50	0.44
2:S:85:CYS:HA	6:S:201:CYC:HAC1	1.71	0.44
2:T:99:ALA:HB2	2:T:108:ILE:HG13	1.99	0.44
3:X:76:THR:HG23	3:X:79:ARG:H	1.83	0.44
5:Z:36:ILE:HD13	5:Z:59:GLU:HG2	2.00	0.44
1:A:104:VAL:HG11	1:A:125:TRP:HB2	2.00	0.44
3:E:39:ILE:HG23	2:H:25:LEU:HD22	1.99	0.44
3:E:75:TYR:OH	2:F:94:ARG:NH2	2.32	0.44
3:O:160:GLU:HG2	3:O:164:TYR:CE2	2.53	0.44
3:C:96:TYR:OH	2:G:18:ARG:O	2.33	0.44
3:D:99:PHE:CZ	2:I:28:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:59:ALA:HB3	3:O:134:LYS:HD3	2.00	0.44
2:R:76:ALA:HA	2:R:81:GLY:HA3	2.00	0.44
3:E:63:GLU:HG3	3:E:64:GLN:HG3	2.00	0.43
2:F:27:VAL:HG13	2:K:27:VAL:HG22	1.99	0.43
2:F:138:LYS:HB2	2:F:155:ILE:HG21	2.00	0.43
3:O:61:PHE:CZ	3:O:80:MET:HE1	2.53	0.43
2:W:28:ALA:HB2	3:X:99:PHE:CZ	2.53	0.43
2:B:50:ASP:OD1	2:B:50:ASP:N	2.49	0.43
2:I:85:CYS:O	2:I:89:ILE:HG12	2.17	0.43
3:M:97:ALA:HB2	3:M:106:LEU:HB2	2.01	0.43
5:Z:10:LEU:HD13	5:Z:169:PHE:CE2	2.53	0.43
2:B:26:GLN:HE22	2:I:34:GLN:HG2	1.83	0.43
3:E:41:THR:O	3:E:45:ILE:HG12	2.18	0.43
2:H:3:LYS:HD2	2:H:8:GLU:OE2	2.18	0.43
3:O:1:MET:SD	2:S:2:SER:N	2.91	0.43
2:R:134:LEU:HB3	2:R:155:ILE:HG23	2.01	0.43
2:U:126:ALA:HB3	2:U:129:TRP:CE2	2.52	0.43
3:a:2:THR:HG23	3:a:105:ILE:HB	2.00	0.43
2:B:28:ALA:HB2	3:J:99:PHE:CE1	2.54	0.43
2:G:99:ALA:HB2	2:G:108:ILE:HG13	2.00	0.43
3:O:111:LEU:HD21	3:O:168:ALA:HA	1.99	0.43
3:Q:59:ALA:HB3	3:Q:134:LYS:HD3	2.01	0.43
3:Q:152:GLY:O	6:Q:202:CYC:OC	2.36	0.43
3:J:83:CYS:HA	6:J:201:CYC:HAC1	1.50	0.43
3:O:93:TYR:CG	3:O:110:CYS:HB2	2.53	0.43
2:R:4:THR:HG23	2:R:7:THR:HB	1.99	0.43
4:Y:235:THR:HB	5:Z:141:GLU:O	2.19	0.43
2:F:85:CYS:O	2:F:89:ILE:HG12	2.18	0.43
2:F:105:THR:OG1	2:K:18:ARG:NH2	2.49	0.43
2:K:2:SER:N	3:L:1:MET:H2	2.17	0.43
2:K:56:ALA:HB3	2:K:89:ILE:HG21	2.01	0.43
3:P:89:ILE:HD13	6:Y:301:CYC:HBB3	2.01	0.43
3:C:114:LEU:HD13	6:C:201:CYC:HMB2	2.00	0.43
6:K:201:CYC:HHD	6:K:201:CYC:HAC2	1.57	0.43
3:P:100:THR:HG23	2:U:10:VAL:HG21	2.01	0.43
5:Z:3:ILE:HD11	5:Z:165:LEU:HD11	2.01	0.43
5:Z:40:TYR:O	5:Z:44:LEU:HB2	2.19	0.43
2:B:95:ILE:HG22	2:B:108:ILE:HG12	2.00	0.43
3:C:86:ASP:OD2	3:C:118:TYR:OH	2.20	0.43
3:E:44:ARG:HE	3:E:149:ILE:HD12	1.84	0.43
2:K:76:ALA:HA	2:K:81:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:78:THR:OG1	2:S:80:GLU:OE1	2.36	0.43
2:N:64:PHE:O	2:N:67:THR:OG1	2.30	0.43
2:T:134:LEU:HB3	2:T:155:ILE:HG23	2.01	0.43
4:Y:238:ARG:NH1	4:Y:240:ARG:HH21	2.17	0.43
3:E:44:ARG:HD3	3:E:143:VAL:HA	2.01	0.42
2:H:150:GLU:HG2	2:H:154:TYR:CE2	2.54	0.42
2:N:18:ARG:NH2	2:N:21:SER:OG	2.51	0.42
3:P:146:ARG:NE	3:P:151:GLN:OE1	2.46	0.42
6:A:302:CYC:HAC2	3:E:83:CYS:HA	2.00	0.42
2:F:150:GLU:HG2	2:F:154:TYR:CE2	2.54	0.42
2:N:143:LEU:C	2:N:148:ARG:HB2	2.44	0.42
2:W:118:GLU:OE1	2:W:118:GLU:N	2.52	0.42
3:a:136:LYS:HB2	3:a:165:PHE:HB3	2.01	0.42
2:I:143:LEU:C	2:I:148:ARG:HB2	2.43	0.42
3:X:28:LEU:O	3:X:32:VAL:HG23	2.18	0.42
1:A:75:ILE:HG21	5:Z:229:PRO:HB2	2.01	0.42
3:D:134:LYS:HA	3:D:137:ASP:OD2	2.19	0.42
3:E:21:SER:H	3:E:24:GLN:HE21	1.66	0.42
2:F:116:LEU:HD21	2:F:162:LEU:HD21	2.01	0.42
2:S:151:ALA:O	2:S:155:ILE:HG12	2.19	0.42
3:X:109:ARG:NH1	5:Z:90:ASN:O	2.48	0.42
4:Y:234:ARG:HD2	4:Y:239:ILE:HG13	2.01	0.42
1:A:22:VAL:HB	2:F:109:ASP:HB3	2.00	0.42
3:M:89:ILE:HG21	6:M:201:CYC:HAB2	2.01	0.42
3:V:83:CYS:HA	6:V:201:CYC:HHD	2.01	0.42
6:B:201:CYC:HHD	6:B:201:CYC:HAC1	1.60	0.42
6:C:202:CYC:HMA3	6:C:202:CYC:HB	1.84	0.42
3:D:61:PHE:CE2	3:D:80:MET:HE1	2.54	0.42
3:L:40:ASP:CG	3:L:149:ILE:HD11	2.45	0.42
2:N:18:ARG:O	3:V:96:TYR:OH	2.35	0.42
3:O:128:VAL:HG22	6:Z:301:CYC:H3C	2.02	0.42
2:S:76:ALA:HA	2:S:81:GLY:HA3	2.01	0.42
2:U:22:SER:O	2:U:26:GLN:HG2	2.19	0.42
4:Y:248:VAL:HG21	4:Y:256:THR:HG21	2.01	0.42
1:A:145:ASP:N	1:A:145:ASP:OD1	2.52	0.42
3:C:20:LEU:HD22	2:G:101:VAL:HG21	2.01	0.42
3:O:76:THR:OG1	3:O:77:ASN:N	2.52	0.42
3:V:86:ASP:OD1	5:Z:48:TYR:OH	2.30	0.42
6:X:201:CYC:HMA2	5:Z:118:LEU:HD22	2.02	0.42
2:B:85:CYS:CA	6:B:201:CYC:HHD	2.50	0.42
6:C:202:CYC:HBC2	6:C:202:CYC:H2C	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:ARG:NH1	3:D:142:ILE:O	2.53	0.42
2:H:99:ALA:HB2	2:H:108:ILE:HG12	2.01	0.42
2:K:99:ALA:HB2	2:K:108:ILE:HG13	2.02	0.42
2:W:95:ILE:HG22	2:W:108:ILE:HG12	2.01	0.42
2:I:99:ALA:HB2	2:I:108:ILE:HG12	2.01	0.42
2:K:101:VAL:HG21	3:L:20:LEU:HD12	2.00	0.42
3:L:129:ALA:HB2	3:L:173:ALA:HB2	2.02	0.42
2:N:113:LEU:HA	2:N:113:LEU:HD23	1.79	0.42
2:N:138:LYS:HB2	2:N:155:ILE:HG21	2.01	0.42
2:R:27:VAL:HG22	2:W:27:VAL:HG13	2.02	0.42
2:R:132:GLU:HG3	2:R:132:GLU:H	1.71	0.42
2:U:95:ILE:HG22	2:U:108:ILE:HG12	2.01	0.42
3:D:76:THR:HG23	3:D:79:ARG:HG3	2.01	0.42
3:D:84:LEU:HD13	2:H:122:THR:HG21	2.02	0.42
2:S:66:TYR:O	2:S:70:THR:OG1	2.35	0.42
4:Y:234:ARG:NH1	4:Y:238:ARG:HG3	2.35	0.42
1:A:82:ARG:NE	1:A:139:ASP:OD1	2.44	0.41
2:F:126:ALA:HB3	2:F:129:TRP:CE2	2.55	0.41
2:T:9:ALA:HB2	2:T:27:VAL:HG11	2.01	0.41
1:A:34:GLU:OE1	5:Z:255:ARG:NE	2.49	0.41
2:B:20:LEU:HA	2:B:24:GLU:HG3	2.01	0.41
2:I:134:LEU:HB3	2:I:155:ILE:HG23	2.02	0.41
3:C:145:ASP:O	6:C:202:CYC:HMC2	2.20	0.41
2:G:33:ARG:NH1	2:G:146:ASP:OD2	2.51	0.41
3:L:25:LEU:HD13	3:L:25:LEU:HA	1.88	0.41
2:R:141:HIS:NE2	2:R:152:ASN:OD1	2.39	0.41
2:S:85:CYS:CA	6:S:201:CYC:HHD	2.51	0.41
3:V:83:CYS:HA	6:V:201:CYC:HAC2	2.02	0.41
1:A:94:PHE:O	1:A:98:ASN:ND2	2.53	0.41
2:F:31:ARG:NH2	2:F:101:VAL:O	2.53	0.41
2:H:126:ALA:HB3	2:H:129:TRP:CE2	2.56	0.41
2:K:91:TYR:O	2:K:95:ILE:HG12	2.21	0.41
3:M:28:LEU:O	3:M:32:VAL:HG23	2.21	0.41
2:N:1:MET:H3	3:V:2:THR:N	2.18	0.41
3:Q:38:ARG:HH12	3:Q:160:GLU:CD	2.28	0.41
3:Q:154:CYS:SG	6:Q:202:CYC:H2C	2.60	0.41
2:T:45:LEU:HD21	2:T:141:HIS:HB2	2.02	0.41
3:V:136:LYS:HB2	3:V:165:PHE:CG	2.56	0.41
5:Z:142:THR:HG21	5:Z:152:ARG:CD	2.50	0.41
2:B:10:VAL:HG21	3:J:100:THR:HG23	2.02	0.41
3:D:61:PHE:CZ	3:D:80:MET:HE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149:ILE:HD13	6:E:201:CYC:H3C	2.01	0.41
2:N:27:VAL:HG22	2:U:27:VAL:HG22	2.01	0.41
3:Q:20:LEU:HD22	2:T:101:VAL:HG21	2.02	0.41
2:T:85:CYS:O	2:T:89:ILE:HG12	2.20	0.41
5:Z:69:VAL:HB	5:Z:146:SER:HA	2.01	0.41
1:A:127:LEU:HD12	3:D:85:ARG:NE	2.36	0.41
3:C:100:THR:HG23	2:G:10:VAL:HG21	2.02	0.41
3:D:63:GLU:HG3	3:D:64:GLN:HG3	2.03	0.41
2:I:114:ALA:HB1	3:a:78:ARG:HD3	2.03	0.41
2:I:126:ALA:HB3	2:I:129:TRP:CE2	2.56	0.41
3:O:152:GLY:HA3	6:T:201:CYC:HMD2	2.01	0.41
3:Q:89:ILE:HD13	6:Q:201:CYC:HBB3	2.03	0.41
2:R:85:CYS:HA	6:R:201:CYC:HAC2	2.02	0.41
2:T:143:LEU:C	2:T:148:ARG:HB3	2.45	0.41
3:V:35:GLY:O	3:V:39:ILE:HG13	2.21	0.41
5:Z:274:VAL:HG11	5:Z:281:VAL:HG23	2.02	0.41
3:L:114:LEU:HD13	3:L:172:VAL:HG23	2.03	0.41
3:M:4:ASP:OD1	3:M:7:THR:OG1	2.35	0.41
3:Q:136:LYS:NZ	3:Q:166:ASP:OD1	2.42	0.41
2:T:88:ASP:HB3	2:T:130:TYR:HE1	1.85	0.41
3:L:114:LEU:HA	3:L:114:LEU:HD23	1.88	0.41
3:M:83:CYS:HA	6:M:201:CYC:HAC1	1.42	0.41
3:M:98:VAL:HG21	3:M:161:LEU:HD13	2.03	0.41
3:P:107:ASP:OD1	3:P:167:LYS:HD3	2.21	0.41
2:T:53:VAL:HG13	2:T:89:ILE:HB	2.03	0.41
2:U:138:LYS:NZ	2:U:156:ASP:OD1	2.29	0.41
2:W:3:LYS:HD3	2:W:3:LYS:HA	1.60	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.94	0.41
3:C:89:ILE:HG12	3:C:92:ARG:HH21	1.85	0.41
3:C:99:PHE:CZ	2:G:28:ALA:HB2	2.56	0.41
2:K:64:PHE:O	2:K:67:THR:OG1	2.27	0.41
3:M:96:TYR:OH	2:R:18:ARG:O	2.35	0.41
6:N:201:CYC:HHH	6:N:201:CYC:HAC2	1.59	0.41
3:O:118:TYR:HE2	3:O:128:VAL:HG11	1.86	0.41
2:S:158:LEU:HD23	2:S:158:LEU:HA	1.89	0.41
3:V:12:GLN:O	3:V:16:ARG:HG3	2.21	0.41
2:W:91:TYR:O	2:W:95:ILE:HG12	2.21	0.41
5:Z:94:ARG:HD3	5:Z:188:SER:HA	2.03	0.41
1:A:186:ARG:NH1	1:A:192:PRO:HG3	2.36	0.41
1:A:191:PHE:HD1	1:A:191:PHE:HA	1.69	0.41
2:I:138:LYS:HB2	2:I:155:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:76:THR:HG22	3:L:78:ARG:N	2.35	0.41
3:P:41:THR:O	3:P:45:ILE:HG12	2.21	0.41
2:S:50:ASP:OD1	2:S:50:ASP:N	2.53	0.41
2:S:112:LEU:HD23	2:S:158:LEU:HD21	2.02	0.41
2:T:158:LEU:HD23	2:T:158:LEU:HA	1.94	0.41
3:X:85:ARG:NH1	5:Z:119:ASP:OD1	2.49	0.41
6:A:301:CYC:HAB2	3:D:110:CYS:HA	2.03	0.40
2:B:24:GLU:H	2:B:24:GLU:HG2	1.63	0.40
2:B:33:ARG:HE	2:B:33:ARG:HB3	1.76	0.40
3:C:136:LYS:NZ	3:C:166:ASP:OD1	2.45	0.40
2:I:123:PHE:HE2	3:a:84:LEU:HD11	1.86	0.40
3:J:109:ARG:HD3	5:Z:228:THR:OG1	2.20	0.40
6:L:201:CYC:HMA1	6:L:201:CYC:NB	2.35	0.40
2:N:16:GLN:OE1	2:U:3:LYS:HE3	2.21	0.40
2:N:141:HIS:NE2	2:N:152:ASN:OD1	2.42	0.40
3:O:115:ARG:NE	3:O:173:ALA:O	2.50	0.40
3:Q:85:ARG:NH2	6:Q:201:CYC:O2A	2.49	0.40
6:T:201:CYC:HMA3	6:T:201:CYC:NB	2.36	0.40
3:C:39:ILE:HG23	2:G:25:LEU:HG	2.03	0.40
3:D:92:ARG:HG2	2:I:19:PHE:CZ	2.56	0.40
3:D:136:LYS:HB2	3:D:165:PHE:HB3	2.03	0.40
6:D:201:CYC:HMA1	2:I:29:PHE:CZ	2.56	0.40
2:I:9:ALA:HB1	2:I:24:GLU:HG3	2.04	0.40
3:M:78:ARG:HB2	2:U:114:ALA:HB3	2.03	0.40
3:O:98:VAL:HG21	3:O:161:LEU:HD13	2.02	0.40
3:O:114:LEU:HD23	3:O:172:VAL:HG12	2.03	0.40
2:S:126:ALA:HB3	2:S:129:TRP:CE2	2.56	0.40
5:Z:140:LEU:HD13	5:Z:140:LEU:HA	1.94	0.40
3:C:40:ASP:HB3	6:C:202:CYC:HAC1	2.03	0.40
3:E:76:THR:HG22	3:E:78:ARG:H	1.86	0.40
3:M:1:MET:HA	2:R:2:SER:HB2	2.02	0.40
3:M:91:LEU:HB2	3:M:135:MET:CE	2.51	0.40
3:E:46:THR:HG23	2:H:19:PHE:HB3	2.04	0.40
3:J:16:ARG:NH1	3:O:63:GLU:OE2	2.47	0.40
2:K:25:LEU:HD22	3:L:39:ILE:HG23	2.02	0.40
3:L:23:ALA:HA	3:L:26:ASP:OD2	2.21	0.40
3:L:117:THR:HG23	5:Z:256:SER:HB2	2.03	0.40
3:P:78:ARG:HB2	2:T:114:ALA:HB3	2.03	0.40
3:Q:8:LYS:HD3	3:Q:8:LYS:HA	1.93	0.40
2:R:87:ARG:NH2	6:R:201:CYC:O2A	2.54	0.40
2:U:50:ASP:OD1	2:U:51:SER:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:86:ASP:OD2	3:V:118:TYR:OH	2.27	0.40
2:W:25:LEU:HD22	3:X:39:ILE:HG23	2.03	0.40
3:D:40:ASP:CG	3:D:149:ILE:HD11	2.46	0.40
2:H:66:TYR:HA	2:H:69:SER:OG	2.22	0.40
3:L:44:ARG:HD3	3:L:143:VAL:HA	2.03	0.40
2:N:23:THR:HA	2:U:5:PRO:HG3	2.03	0.40
2:U:143:LEU:C	2:U:148:ARG:HB2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	194/250 (78%)	182 (94%)	12 (6%)	0	100	100
2	B	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	F	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	G	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	I	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	K	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	N	161/163 (99%)	158 (98%)	3 (2%)	0	100	100
2	R	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	S	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	T	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	U	160/163 (98%)	160 (100%)	0	0	100	100
2	W	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
3	C	171/173 (99%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	E	170/173 (98%)	170 (100%)	0	0	100	100
3	J	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	L	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	M	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
3	O	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
3	P	171/173 (99%)	171 (100%)	0	0	100	100
3	Q	170/173 (98%)	170 (100%)	0	0	100	100
3	V	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	X	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	a	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
4	Y	55/273 (20%)	52 (94%)	3 (6%)	0	100	100
5	Z	286/289 (99%)	277 (97%)	9 (3%)	0	100	100
All	All	4503/4844 (93%)	4428 (98%)	75 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	171/208 (82%)	166 (97%)	5 (3%)	37	69
2	B	122/123 (99%)	119 (98%)	3 (2%)	42	73
2	F	122/123 (99%)	117 (96%)	5 (4%)	27	60
2	G	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	H	122/123 (99%)	119 (98%)	3 (2%)	42	73
2	I	122/123 (99%)	122 (100%)	0	100	100
2	K	122/123 (99%)	119 (98%)	3 (2%)	42	73
2	N	123/123 (100%)	119 (97%)	4 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	122/123 (99%)	120 (98%)	2 (2%)	55	81
2	S	122/123 (99%)	118 (97%)	4 (3%)	33	65
2	T	122/123 (99%)	121 (99%)	1 (1%)	73	89
2	U	122/123 (99%)	121 (99%)	1 (1%)	73	89
2	W	122/123 (99%)	121 (99%)	1 (1%)	73	89
3	C	129/129 (100%)	125 (97%)	4 (3%)	35	67
3	D	128/129 (99%)	126 (98%)	2 (2%)	55	81
3	E	128/129 (99%)	126 (98%)	2 (2%)	55	81
3	J	129/129 (100%)	126 (98%)	3 (2%)	44	74
3	L	129/129 (100%)	122 (95%)	7 (5%)	20	49
3	M	129/129 (100%)	126 (98%)	3 (2%)	44	74
3	O	129/129 (100%)	125 (97%)	4 (3%)	35	67
3	P	129/129 (100%)	127 (98%)	2 (2%)	55	81
3	Q	128/129 (99%)	124 (97%)	4 (3%)	35	67
3	V	128/129 (99%)	126 (98%)	2 (2%)	55	81
3	X	129/129 (100%)	127 (98%)	2 (2%)	55	81
3	a	128/129 (99%)	125 (98%)	3 (2%)	44	74
4	Y	49/221 (22%)	45 (92%)	4 (8%)	10	31
5	Z	239/240 (100%)	236 (99%)	3 (1%)	61	84
All	All	3467/3693 (94%)	3386 (98%)	81 (2%)	44	74

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	89	THR
1	A	127	LEU
1	A	172	THR
1	A	191	PHE
2	B	24	GLU
2	B	119	ILE
2	B	141	HIS
3	C	2	THR
3	C	40	ASP
3	C	150	THR

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Mol	Chain	Res	Type
3	C	172	VAL
3	D	76	THR
3	D	83	CYS
3	E	76	THR
3	E	105	ILE
2	F	3	LYS
2	F	10	VAL
2	F	23	THR
2	F	78	THR
2	F	110	GLU
2	G	113	LEU
2	G	118	GLU
2	G	119	ILE
2	G	143	LEU
2	H	4	THR
2	H	118	GLU
2	H	141	HIS
3	J	40	ASP
3	J	105	ILE
3	J	116	GLU
2	K	10	VAL
2	K	18	ARG
2	K	141	HIS
3	L	9	VAL
3	L	25	LEU
3	L	40	ASP
3	L	67	LEU
3	L	87	MET
3	L	105	ILE
3	L	114	LEU
3	M	40	ASP
3	M	110	CYS
3	M	119	LEU
2	N	20	LEU
2	N	78	THR
2	N	113	LEU
2	N	141	HIS
3	O	40	ASP
3	O	76	THR
3	O	105	ILE
3	O	150	THR
3	P	37	LYS

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Mol	Chain	Res	Type
3	P	83	CYS
3	Q	37	LYS
3	Q	39	ILE
3	Q	40	ASP
3	Q	105	ILE
2	R	4	THR
2	R	113	LEU
2	S	10	VAL
2	S	78	THR
2	S	119	ILE
2	S	141	HIS
2	T	84	LYS
2	U	10	VAL
3	V	36	ASN
3	V	105	ILE
2	W	118	GLU
3	X	7	THR
3	X	172	VAL
4	Y	228	GLN
4	Y	231	VAL
4	Y	240	ARG
4	Y	271	THR
5	Z	141	GLU
5	Z	207	VAL
5	Z	253	VAL
3	a	40	ASP
3	a	83	CYS
3	a	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	74	GLN
3	D	43	ASN
3	D	48	ASN
2	G	160	ASN
2	I	140	ASN
2	K	140	ASN
3	L	43	ASN
3	P	24	GLN
2	S	54	ASN

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Mol	Chain	Res	Type
2	S	160	ASN
4	Y	254	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 ⓘ

34 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
6	CYC	Q	201	-	46,46,46	6.37	23 (50%)	63,67,67	3.93	16 (25%)
6	CYC	Y	301	-	46,46,46	6.36	23 (50%)	63,67,67	3.97	17 (26%)
6	CYC	T	202	2	46,46,46	6.35	22 (47%)	63,67,67	4.09	13 (20%)
6	CYC	S	201	2	46,46,46	6.37	23 (50%)	63,67,67	3.87	16 (25%)
6	CYC	C	202	-	46,46,46	6.39	22 (47%)	63,67,67	4.22	15 (23%)
6	CYC	K	201	2	46,46,46	6.32	23 (50%)	63,67,67	4.07	16 (25%)
6	CYC	N	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.05	15 (23%)
6	CYC	C	201	3	46,46,46	6.26	23 (50%)	63,67,67	3.97	17 (26%)
6	CYC	E	201	-	46,46,46	6.32	23 (50%)	63,67,67	4.10	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	X	201	3	46,46,46	6.30	23 (50%)	63,67,67	3.91	20 (31%)
6	CYC	F	202	-	46,46,46	6.37	22 (47%)	63,67,67	4.09	15 (23%)
6	CYC	Z	301	-	46,46,46	6.28	23 (50%)	63,67,67	4.01	20 (31%)
6	CYC	H	201	2	46,46,46	6.30	23 (50%)	63,67,67	4.15	15 (23%)
6	CYC	J	201	3	46,46,46	6.32	23 (50%)	63,67,67	4.09	18 (28%)
6	CYC	Q	202	-	46,46,46	6.37	22 (47%)	63,67,67	4.06	16 (25%)
6	CYC	a	201	-	46,46,46	6.28	23 (50%)	63,67,67	4.02	21 (33%)
6	CYC	F	201	-	46,46,46	6.36	22 (47%)	63,67,67	4.11	19 (30%)
6	CYC	A	301	-	46,46,46	6.36	23 (50%)	63,67,67	4.06	18 (28%)
6	CYC	P	201	-	46,46,46	6.35	22 (47%)	63,67,67	4.08	15 (23%)
6	CYC	U	201	2	46,46,46	6.30	23 (50%)	63,67,67	4.05	16 (25%)
6	CYC	J	202	3	46,46,46	6.32	22 (47%)	63,67,67	4.06	16 (25%)
6	CYC	B	201	2	46,46,46	6.37	23 (50%)	63,67,67	4.11	16 (25%)
6	CYC	G	201	2	46,46,46	6.31	23 (50%)	63,67,67	4.10	16 (25%)
6	CYC	V	202	3	46,46,46	6.33	24 (52%)	63,67,67	4.10	15 (23%)
6	CYC	T	201	-	46,46,46	6.32	24 (52%)	63,67,67	4.14	15 (23%)
6	CYC	W	201	2	46,46,46	6.35	23 (50%)	63,67,67	4.07	15 (23%)
6	CYC	I	201	2	46,46,46	6.36	23 (50%)	63,67,67	4.07	14 (22%)
6	CYC	M	201	3	46,46,46	6.36	23 (50%)	63,67,67	4.02	21 (33%)
6	CYC	a	202	-	46,46,46	6.35	23 (50%)	63,67,67	3.93	16 (25%)
6	CYC	D	201	-	46,46,46	6.31	23 (50%)	63,67,67	3.92	20 (31%)
6	CYC	R	201	-	46,46,46	6.36	23 (50%)	63,67,67	4.07	15 (23%)
6	CYC	A	302	-	46,46,46	6.37	23 (50%)	63,67,67	3.97	24 (38%)
6	CYC	V	201	3	46,46,46	6.37	23 (50%)	63,67,67	4.00	19 (30%)
6	CYC	L	201	-	46,46,46	6.34	24 (52%)	63,67,67	4.01	19 (30%)

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
6	CYC	Q	201	-	-	13/26/74/74	0/4/4/4
6	CYC	Y	301	-	-	14/26/74/74	0/4/4/4
6	CYC	T	202	2	-	11/26/74/74	0/4/4/4
6	CYC	S	201	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	C	202	-	-	17/26/74/74	0/4/4/4
6	CYC	K	201	2	-	11/26/74/74	0/4/4/4
6	CYC	N	201	2	-	11/26/74/74	0/4/4/4
6	CYC	C	201	3	-	12/26/74/74	0/4/4/4
6	CYC	E	201	-	-	18/26/74/74	0/4/4/4
6	CYC	X	201	3	-	14/26/74/74	0/4/4/4
6	CYC	F	202	-	-	13/26/74/74	0/4/4/4
6	CYC	Z	301	-	-	13/26/74/74	0/4/4/4
6	CYC	H	201	2	-	13/26/74/74	0/4/4/4
6	CYC	J	201	3	-	11/26/74/74	0/4/4/4
6	CYC	Q	202	-	-	11/26/74/74	0/4/4/4
6	CYC	a	201	-	-	13/26/74/74	0/4/4/4
6	CYC	F	201	-	-	14/26/74/74	0/4/4/4
6	CYC	A	301	-	-	14/26/74/74	0/4/4/4
6	CYC	P	201	-	-	20/26/74/74	0/4/4/4
6	CYC	U	201	2	-	13/26/74/74	0/4/4/4
6	CYC	J	202	3	-	16/26/74/74	0/4/4/4
6	CYC	B	201	2	-	12/26/74/74	0/4/4/4
6	CYC	G	201	2	-	12/26/74/74	0/4/4/4
6	CYC	V	202	3	-	21/26/74/74	0/4/4/4
6	CYC	T	201	-	-	18/26/74/74	0/4/4/4
6	CYC	W	201	2	-	9/26/74/74	0/4/4/4
6	CYC	I	201	2	-	14/26/74/74	0/4/4/4
6	CYC	M	201	3	-	9/26/74/74	0/4/4/4
6	CYC	a	202	-	-	17/26/74/74	0/4/4/4
6	CYC	D	201	-	-	11/26/74/74	0/4/4/4
6	CYC	R	201	-	-	12/26/74/74	0/4/4/4
6	CYC	A	302	-	-	9/26/74/74	0/4/4/4
6	CYC	V	201	3	-	12/26/74/74	0/4/4/4
6	CYC	L	201	-	-	13/26/74/74	0/4/4/4

All (778) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	CYC	C2C-C1C	-26.46	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	CYC	C2C-C1C	-26.41	1.28	1.52
6	V	201	CYC	C2C-C1C	-26.36	1.28	1.52
6	C	202	CYC	C2C-C1C	-26.20	1.28	1.52
6	I	201	CYC	C2C-C1C	-26.14	1.28	1.52
6	F	202	CYC	C2C-C1C	-26.05	1.28	1.52
6	S	201	CYC	C2C-C1C	-26.00	1.28	1.52
6	F	201	CYC	C2C-C1C	-25.87	1.29	1.52
6	Q	201	CYC	C2C-C1C	-25.86	1.29	1.52
6	P	201	CYC	C2C-C1C	-25.82	1.29	1.52
6	W	201	CYC	C2C-C1C	-25.75	1.29	1.52
6	A	301	CYC	C2C-C1C	-25.69	1.29	1.52
6	R	201	CYC	C2C-C1C	-25.63	1.29	1.52
6	Y	301	CYC	C2C-C1C	-25.62	1.29	1.52
6	M	201	CYC	C2C-C1C	-25.61	1.29	1.52
6	K	201	CYC	C2C-C1C	-25.57	1.29	1.52
6	T	202	CYC	C2C-C1C	-25.56	1.29	1.52
6	Q	202	CYC	C2C-C1C	-25.56	1.29	1.52
6	G	201	CYC	C2C-C1C	-25.56	1.29	1.52
6	N	201	CYC	C2C-C1C	-25.43	1.29	1.52
6	L	201	CYC	C2C-C1C	-25.38	1.29	1.52
6	J	201	CYC	C2C-C1C	-25.31	1.29	1.52
6	H	201	CYC	C2C-C1C	-25.28	1.29	1.52
6	U	201	CYC	C2C-C1C	-25.28	1.29	1.52
6	T	201	CYC	C2C-C1C	-25.09	1.29	1.52
6	V	202	CYC	C2C-C1C	-25.06	1.29	1.52
6	J	202	CYC	C2C-C1C	-25.04	1.29	1.52
6	E	201	CYC	C2C-C1C	-25.03	1.29	1.52
6	a	201	CYC	C2C-C1C	-25.01	1.29	1.52
6	a	202	CYC	C2C-C1C	-24.96	1.29	1.52
6	D	201	CYC	C2C-C1C	-24.85	1.29	1.52
6	Z	301	CYC	C2C-C1C	-24.84	1.30	1.52
6	C	201	CYC	C2C-C1C	-24.72	1.30	1.52
6	X	201	CYC	C2C-C1C	-24.64	1.30	1.52
6	a	202	CYC	C1C-NC	16.59	1.59	1.37
6	T	201	CYC	C1C-NC	16.26	1.59	1.37
6	R	201	CYC	C1C-NC	16.26	1.59	1.37
6	V	202	CYC	C1C-NC	16.24	1.59	1.37
6	Q	202	CYC	C1C-NC	16.15	1.58	1.37
6	E	201	CYC	C1C-NC	16.11	1.58	1.37
6	J	202	CYC	C1C-NC	16.07	1.58	1.37
6	Q	201	CYC	C1C-NC	16.05	1.58	1.37
6	D	201	CYC	C1C-NC	16.04	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	201	CYC	C1C-NC	16.03	1.58	1.37
6	F	201	CYC	C1C-NC	16.02	1.58	1.37
6	T	202	CYC	C1C-NC	16.01	1.58	1.37
6	W	201	CYC	C1C-NC	16.00	1.58	1.37
6	G	201	CYC	C1C-NC	15.97	1.58	1.37
6	X	201	CYC	C1C-NC	15.95	1.58	1.37
6	M	201	CYC	C1C-NC	15.94	1.58	1.37
6	N	201	CYC	C1C-NC	15.93	1.58	1.37
6	H	201	CYC	C1C-NC	15.92	1.58	1.37
6	F	202	CYC	C1C-NC	15.91	1.58	1.37
6	Y	301	CYC	C1C-NC	15.91	1.58	1.37
6	K	201	CYC	C1C-NC	15.90	1.58	1.37
6	L	201	CYC	C1C-NC	15.86	1.58	1.37
6	I	201	CYC	C1C-NC	15.81	1.58	1.37
6	C	202	CYC	C1C-NC	15.81	1.58	1.37
6	A	301	CYC	C1C-NC	15.80	1.58	1.37
6	J	201	CYC	C1C-NC	15.77	1.58	1.37
6	S	201	CYC	C1C-NC	15.75	1.58	1.37
6	B	201	CYC	C1C-NC	15.68	1.58	1.37
6	P	201	CYC	C1C-NC	15.54	1.58	1.37
6	C	201	CYC	C1C-NC	15.53	1.58	1.37
6	Z	301	CYC	C1C-NC	15.41	1.57	1.37
6	a	201	CYC	C1C-NC	15.35	1.57	1.37
6	V	201	CYC	C1C-NC	15.26	1.57	1.37
6	A	302	CYC	C1C-NC	15.19	1.57	1.37
6	A	302	CYC	CHD-C4C	13.16	1.58	1.36
6	V	201	CYC	CHD-C4C	13.11	1.58	1.36
6	T	202	CYC	CHD-C4C	13.10	1.58	1.36
6	P	201	CYC	CHD-C4C	13.09	1.58	1.36
6	S	201	CYC	CHD-C4C	13.03	1.58	1.36
6	C	202	CYC	CHD-C4C	13.02	1.58	1.36
6	F	202	CYC	CHD-C4C	13.01	1.57	1.36
6	V	202	CYC	CHD-C4C	12.99	1.57	1.36
6	Q	202	CYC	CHD-C4C	12.97	1.57	1.36
6	I	201	CYC	CHD-C4C	12.96	1.57	1.36
6	a	202	CYC	CHD-C4C	12.94	1.57	1.36
6	W	201	CYC	CHD-C4C	12.93	1.57	1.36
6	Z	301	CYC	CHD-C4C	12.92	1.57	1.36
6	T	201	CYC	CHD-C4C	12.91	1.57	1.36
6	N	201	CYC	CHD-C4C	12.91	1.57	1.36
6	U	201	CYC	CHD-C4C	12.89	1.57	1.36
6	X	201	CYC	CHD-C4C	12.87	1.57	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	201	CYC	CHD-C4C	12.87	1.57	1.36
6	B	201	CYC	CHD-C4C	12.86	1.57	1.36
6	Q	201	CYC	CHD-C4C	12.85	1.57	1.36
6	H	201	CYC	CHD-C4C	12.85	1.57	1.36
6	L	201	CYC	CHD-C4C	12.84	1.57	1.36
6	M	201	CYC	CHD-C4C	12.83	1.57	1.36
6	E	201	CYC	CHD-C4C	12.83	1.57	1.36
6	K	201	CYC	CHD-C4C	12.81	1.57	1.36
6	J	201	CYC	CHD-C4C	12.81	1.57	1.36
6	C	201	CYC	CHD-C4C	12.80	1.57	1.36
6	A	301	CYC	CHD-C4C	12.77	1.57	1.36
6	a	201	CYC	CHD-C4C	12.76	1.57	1.36
6	J	202	CYC	CHD-C4C	12.75	1.57	1.36
6	Y	301	CYC	CHD-C4C	12.73	1.57	1.36
6	G	201	CYC	CHD-C4C	12.72	1.57	1.36
6	F	201	CYC	CHD-C4C	12.70	1.57	1.36
6	D	201	CYC	CHD-C4C	12.68	1.57	1.36
6	C	202	CYC	C4C-NC	11.30	1.59	1.37
6	S	201	CYC	C4C-NC	11.07	1.58	1.37
6	F	202	CYC	C4C-NC	11.04	1.58	1.37
6	Q	202	CYC	C4C-NC	11.04	1.58	1.37
6	Q	201	CYC	C4C-NC	11.00	1.58	1.37
6	P	201	CYC	C4C-NC	10.96	1.58	1.37
6	a	202	CYC	C4C-NC	10.94	1.58	1.37
6	S	201	CYC	OC-C1C	10.94	1.44	1.23
6	F	201	CYC	C4C-NC	10.88	1.58	1.37
6	I	201	CYC	C4C-NC	10.88	1.58	1.37
6	Y	301	CYC	C4C-NC	10.87	1.58	1.37
6	R	201	CYC	C4C-NC	10.86	1.58	1.37
6	T	202	CYC	C4C-NC	10.86	1.58	1.37
6	M	201	CYC	C4C-NC	10.86	1.58	1.37
6	B	201	CYC	C4C-NC	10.82	1.58	1.37
6	A	302	CYC	C4C-NC	10.81	1.58	1.37
6	V	202	CYC	C4C-NC	10.81	1.58	1.37
6	Q	202	CYC	OC-C1C	10.78	1.44	1.23
6	T	201	CYC	C4C-NC	10.76	1.58	1.37
6	J	202	CYC	OC-C1C	10.75	1.44	1.23
6	U	201	CYC	C4C-NC	10.74	1.58	1.37
6	T	201	CYC	OC-C1C	10.73	1.44	1.23
6	Y	301	CYC	OC-C1C	10.73	1.44	1.23
6	D	201	CYC	OC-C1C	10.73	1.44	1.23
6	X	201	CYC	C4C-NC	10.73	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	201	CYC	OC-C1C	10.72	1.44	1.23
6	a	201	CYC	OC-C1C	10.72	1.44	1.23
6	H	201	CYC	C4C-NC	10.72	1.58	1.37
6	X	201	CYC	OC-C1C	10.72	1.44	1.23
6	E	201	CYC	OC-C1C	10.71	1.44	1.23
6	A	301	CYC	C4C-NC	10.70	1.58	1.37
6	F	202	CYC	OC-C1C	10.70	1.43	1.23
6	P	201	CYC	OC-C1C	10.69	1.43	1.23
6	a	202	CYC	OC-C1C	10.69	1.43	1.23
6	W	201	CYC	C4C-NC	10.69	1.58	1.37
6	V	202	CYC	OC-C1C	10.69	1.43	1.23
6	Z	301	CYC	OC-C1C	10.69	1.43	1.23
6	J	202	CYC	C4C-NC	10.68	1.58	1.37
6	E	201	CYC	C4C-NC	10.68	1.58	1.37
6	C	201	CYC	OC-C1C	10.67	1.43	1.23
6	G	201	CYC	C4C-NC	10.66	1.58	1.37
6	K	201	CYC	C4C-NC	10.66	1.58	1.37
6	Q	201	CYC	OC-C1C	10.66	1.43	1.23
6	V	201	CYC	C4C-NC	10.65	1.58	1.37
6	D	201	CYC	C4C-NC	10.65	1.58	1.37
6	L	201	CYC	C4C-NC	10.63	1.57	1.37
6	T	202	CYC	OC-C1C	10.62	1.43	1.23
6	N	201	CYC	C4C-NC	10.61	1.57	1.37
6	J	201	CYC	OC-C1C	10.61	1.43	1.23
6	J	201	CYC	C4C-NC	10.61	1.57	1.37
6	H	201	CYC	OC-C1C	10.61	1.43	1.23
6	R	201	CYC	OC-C1C	10.61	1.43	1.23
6	I	201	CYC	OC-C1C	10.58	1.43	1.23
6	N	201	CYC	OC-C1C	10.56	1.43	1.23
6	U	201	CYC	OC-C1C	10.56	1.43	1.23
6	V	201	CYC	OC-C1C	10.55	1.43	1.23
6	A	302	CYC	OC-C1C	10.54	1.43	1.23
6	A	301	CYC	OC-C1C	10.54	1.43	1.23
6	B	201	CYC	OC-C1C	10.53	1.43	1.23
6	C	202	CYC	OC-C1C	10.53	1.43	1.23
6	F	201	CYC	OC-C1C	10.51	1.43	1.23
6	L	201	CYC	OC-C1C	10.51	1.43	1.23
6	W	201	CYC	OC-C1C	10.50	1.43	1.23
6	C	201	CYC	C4C-NC	10.49	1.57	1.37
6	K	201	CYC	OC-C1C	10.47	1.43	1.23
6	G	201	CYC	OC-C1C	10.44	1.43	1.23
6	a	201	CYC	C4C-NC	10.42	1.57	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	301	CYC	C4C-NC	10.39	1.57	1.37
6	a	202	CYC	C3C-C4C	-10.34	1.28	1.50
6	E	201	CYC	C3C-C4C	-10.27	1.29	1.50
6	J	201	CYC	C3C-C4C	-10.23	1.29	1.50
6	X	201	CYC	C3C-C4C	-10.22	1.29	1.50
6	T	201	CYC	C3C-C4C	-10.21	1.29	1.50
6	J	202	CYC	C3C-C4C	-10.20	1.29	1.50
6	V	202	CYC	C3C-C4C	-10.16	1.29	1.50
6	D	201	CYC	C3C-C4C	-10.15	1.29	1.50
6	C	201	CYC	C3C-C4C	-10.15	1.29	1.50
6	Y	301	CYC	C3C-C4C	-10.13	1.29	1.50
6	A	301	CYC	C3C-C4C	-10.10	1.29	1.50
6	L	201	CYC	C3C-C4C	-10.09	1.29	1.50
6	M	201	CYC	C3C-C4C	-10.02	1.29	1.50
6	a	201	CYC	C3C-C4C	-9.99	1.29	1.50
6	Z	301	CYC	C3C-C4C	-9.98	1.29	1.50
6	R	201	CYC	C3C-C4C	-9.69	1.30	1.50
6	F	201	CYC	C3C-C4C	-9.60	1.30	1.50
6	Q	202	CYC	C3C-C4C	-9.51	1.30	1.50
6	H	201	CYC	C3C-C4C	-9.48	1.30	1.50
6	G	201	CYC	C3C-C4C	-9.47	1.30	1.50
6	K	201	CYC	C3C-C4C	-9.41	1.30	1.50
6	N	201	CYC	C3C-C4C	-9.40	1.30	1.50
6	W	201	CYC	C3C-C4C	-9.40	1.30	1.50
6	C	202	CYC	C3C-C4C	-9.37	1.30	1.50
6	U	201	CYC	C3C-C4C	-9.36	1.30	1.50
6	Q	201	CYC	C3C-C4C	-9.36	1.30	1.50
6	T	202	CYC	C3C-C4C	-9.30	1.31	1.50
6	F	202	CYC	C3C-C4C	-9.17	1.31	1.50
6	P	201	CYC	C3C-C4C	-9.15	1.31	1.50
6	B	201	CYC	C3C-C4C	-9.11	1.31	1.50
6	I	201	CYC	C3C-C4C	-9.07	1.31	1.50
6	V	201	CYC	C3C-C4C	-9.03	1.31	1.50
6	S	201	CYC	C3C-C4C	-9.01	1.31	1.50
6	A	301	CYC	OB-C4B	8.93	1.40	1.23
6	A	302	CYC	C3C-C4C	-8.93	1.31	1.50
6	Q	201	CYC	OB-C4B	8.89	1.40	1.23
6	P	201	CYC	OB-C4B	8.88	1.40	1.23
6	Y	301	CYC	OB-C4B	8.85	1.40	1.23
6	Z	301	CYC	OB-C4B	8.84	1.40	1.23
6	T	202	CYC	OB-C4B	8.82	1.40	1.23
6	R	201	CYC	OB-C4B	8.82	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	CYC	OB-C4B	8.82	1.40	1.23
6	W	201	CYC	OB-C4B	8.82	1.40	1.23
6	U	201	CYC	OB-C4B	8.81	1.40	1.23
6	I	201	CYC	OB-C4B	8.81	1.40	1.23
6	a	202	CYC	OB-C4B	8.81	1.40	1.23
6	F	202	CYC	OB-C4B	8.80	1.40	1.23
6	V	201	CYC	OB-C4B	8.79	1.40	1.23
6	H	201	CYC	OB-C4B	8.79	1.40	1.23
6	F	201	CYC	OB-C4B	8.79	1.40	1.23
6	N	201	CYC	OB-C4B	8.79	1.40	1.23
6	S	201	CYC	OB-C4B	8.78	1.40	1.23
6	V	202	CYC	OB-C4B	8.78	1.40	1.23
6	Q	202	CYC	OB-C4B	8.77	1.40	1.23
6	A	302	CYC	OB-C4B	8.77	1.40	1.23
6	M	201	CYC	OB-C4B	8.76	1.40	1.23
6	a	201	CYC	OB-C4B	8.76	1.40	1.23
6	C	202	CYC	OB-C4B	8.75	1.40	1.23
6	D	201	CYC	OB-C4B	8.74	1.40	1.23
6	B	201	CYC	OB-C4B	8.73	1.40	1.23
6	E	201	CYC	OB-C4B	8.73	1.40	1.23
6	K	201	CYC	OB-C4B	8.72	1.40	1.23
6	J	201	CYC	OB-C4B	8.71	1.40	1.23
6	T	201	CYC	OB-C4B	8.71	1.40	1.23
6	L	201	CYC	OB-C4B	8.71	1.40	1.23
6	J	202	CYC	OB-C4B	8.69	1.40	1.23
6	G	201	CYC	OB-C4B	8.67	1.40	1.23
6	X	201	CYC	OB-C4B	8.58	1.39	1.23
6	Q	201	CYC	CHA-C1A	7.77	1.53	1.38
6	Y	301	CYC	CHA-C1A	7.74	1.53	1.38
6	T	202	CYC	CHA-C1A	7.74	1.53	1.38
6	V	201	CYC	CHA-C1A	7.68	1.53	1.38
6	P	201	CYC	CHA-C1A	7.65	1.53	1.38
6	D	201	CYC	CHA-C1A	7.64	1.53	1.38
6	F	201	CYC	CHA-C1A	7.62	1.53	1.38
6	C	202	CYC	CHA-C1A	7.61	1.53	1.38
6	Q	202	CYC	CHA-C1A	7.60	1.53	1.38
6	M	201	CYC	CHA-C1A	7.59	1.53	1.38
6	J	202	CYC	CHA-C1A	7.58	1.53	1.38
6	L	201	CYC	CHA-C1A	7.56	1.53	1.38
6	C	201	CYC	CHA-C1A	7.55	1.53	1.38
6	U	201	CYC	CHA-C1A	7.55	1.52	1.38
6	F	202	CYC	CHA-C1A	7.54	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	201	CYC	CHA-C1A	7.53	1.52	1.38
6	X	201	CYC	CHA-C1A	7.53	1.52	1.38
6	J	201	CYC	CHA-C1A	7.52	1.52	1.38
6	R	201	CYC	CHA-C1A	7.51	1.52	1.38
6	S	201	CYC	CHA-C1A	7.50	1.52	1.38
6	V	202	CYC	CHA-C1A	7.49	1.52	1.38
6	W	201	CYC	CHA-C1A	7.49	1.52	1.38
6	K	201	CYC	CHA-C1A	7.48	1.52	1.38
6	a	201	CYC	CHA-C1A	7.48	1.52	1.38
6	G	201	CYC	CHA-C1A	7.48	1.52	1.38
6	A	301	CYC	CHA-C1A	7.47	1.52	1.38
6	I	201	CYC	CHA-C1A	7.47	1.52	1.38
6	Z	301	CYC	CHA-C1A	7.46	1.52	1.38
6	a	202	CYC	CHA-C1A	7.46	1.52	1.38
6	H	201	CYC	CHA-C1A	7.46	1.52	1.38
6	N	201	CYC	CHA-C1A	7.44	1.52	1.38
6	A	302	CYC	CHA-C1A	7.44	1.52	1.38
6	T	201	CYC	CHA-C1A	7.42	1.52	1.38
6	B	201	CYC	CHA-C1A	7.38	1.52	1.38
6	A	301	CYC	CHB-C1B	6.83	1.54	1.37
6	A	302	CYC	CHB-C1B	6.78	1.54	1.37
6	a	201	CYC	CHB-C1B	6.70	1.53	1.37
6	Z	301	CYC	CHB-C1B	6.66	1.53	1.37
6	V	202	CYC	CHB-C1B	6.66	1.53	1.37
6	J	202	CYC	CHB-C1B	6.64	1.53	1.37
6	Q	202	CYC	CHB-C1B	6.62	1.53	1.37
6	Q	201	CYC	CHB-C1B	6.60	1.53	1.37
6	X	201	CYC	CHB-C1B	6.59	1.53	1.37
6	M	201	CYC	CHB-C1B	6.56	1.53	1.37
6	C	202	CYC	CHB-C1B	6.55	1.53	1.37
6	J	201	CYC	CHB-C1B	6.55	1.53	1.37
6	V	201	CYC	CHB-C1B	6.54	1.53	1.37
6	Y	301	CYC	CHB-C1B	6.53	1.53	1.37
6	C	201	CYC	CHB-C1B	6.53	1.53	1.37
6	D	201	CYC	CHB-C1B	6.52	1.53	1.37
6	a	202	CYC	CHB-C1B	6.52	1.53	1.37
6	S	201	CYC	CHB-C1B	6.49	1.53	1.37
6	E	201	CYC	CHB-C1B	6.48	1.53	1.37
6	W	201	CYC	CHB-C1B	6.48	1.53	1.37
6	N	201	CYC	CHB-C1B	6.47	1.53	1.37
6	F	201	CYC	CHB-C1B	6.46	1.53	1.37
6	G	201	CYC	CHB-C1B	6.46	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	201	CYC	CHB-C1B	6.44	1.53	1.37
6	K	201	CYC	CHB-C1B	6.44	1.53	1.37
6	U	201	CYC	CHB-C1B	6.44	1.53	1.37
6	L	201	CYC	CHB-C1B	6.43	1.53	1.37
6	T	201	CYC	CHB-C1B	6.43	1.53	1.37
6	H	201	CYC	CHB-C1B	6.42	1.53	1.37
6	I	201	CYC	CHB-C1B	6.42	1.53	1.37
6	B	201	CYC	CHB-C1B	6.41	1.53	1.37
6	R	201	CYC	CHB-C1B	6.41	1.53	1.37
6	T	202	CYC	CHB-C1B	6.40	1.53	1.37
6	F	202	CYC	CHB-C1B	6.40	1.53	1.37
6	X	201	CYC	CHD-C1D	6.39	1.54	1.40
6	L	201	CYC	CHD-C1D	6.38	1.54	1.40
6	Z	301	CYC	CHD-C1D	6.38	1.54	1.40
6	C	201	CYC	CHD-C1D	6.36	1.54	1.40
6	J	201	CYC	CHD-C1D	6.33	1.54	1.40
6	M	201	CYC	CHD-C1D	6.31	1.54	1.40
6	A	301	CYC	CHD-C1D	6.30	1.54	1.40
6	a	201	CYC	CHD-C1D	6.30	1.54	1.40
6	Y	301	CYC	CHD-C1D	6.24	1.54	1.40
6	D	201	CYC	CHD-C1D	6.19	1.54	1.40
6	J	202	CYC	CHD-C1D	6.17	1.54	1.40
6	V	202	CYC	CHD-C1D	6.08	1.54	1.40
6	V	201	CYC	CHD-C1D	6.08	1.54	1.40
6	E	201	CYC	CHD-C1D	6.04	1.54	1.40
6	T	201	CYC	CHD-C1D	6.02	1.54	1.40
6	A	302	CYC	CHD-C1D	6.01	1.54	1.40
6	T	202	CYC	CHD-C1D	5.98	1.53	1.40
6	W	201	CYC	CHD-C1D	5.95	1.53	1.40
6	a	202	CYC	CHD-C1D	5.95	1.53	1.40
6	H	201	CYC	CHD-C1D	5.92	1.53	1.40
6	U	201	CYC	CHD-C1D	5.91	1.53	1.40
6	N	201	CYC	CHD-C1D	5.91	1.53	1.40
6	T	202	CYC	CHA-C4D	5.90	1.53	1.40
6	F	201	CYC	CHD-C1D	5.89	1.53	1.40
6	R	201	CYC	CHD-C1D	5.89	1.53	1.40
6	F	202	CYC	CHD-C1D	5.87	1.53	1.40
6	Q	202	CYC	CHD-C1D	5.86	1.53	1.40
6	K	201	CYC	CHD-C1D	5.85	1.53	1.40
6	S	201	CYC	CHD-C1D	5.85	1.53	1.40
6	X	201	CYC	CHB-C4A	5.84	1.54	1.40
6	Z	301	CYC	CHB-C4A	5.84	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	201	CYC	CHD-C1D	5.84	1.53	1.40
6	a	201	CYC	CHB-C4A	5.83	1.54	1.40
6	F	201	CYC	CHA-C4D	5.83	1.53	1.40
6	P	201	CYC	CHD-C1D	5.82	1.53	1.40
6	P	201	CYC	CHA-C4D	5.82	1.53	1.40
6	F	202	CYC	CHA-C4D	5.82	1.53	1.40
6	Q	201	CYC	CHB-C4A	5.82	1.54	1.40
6	G	201	CYC	CHD-C1D	5.81	1.53	1.40
6	C	202	CYC	CHA-C4D	5.80	1.53	1.40
6	Q	202	CYC	CHA-C4D	5.80	1.53	1.40
6	S	201	CYC	CHA-C4D	5.79	1.53	1.40
6	K	201	CYC	CHA-C4D	5.77	1.53	1.40
6	I	201	CYC	CHA-C4D	5.76	1.53	1.40
6	U	201	CYC	CHA-C4D	5.76	1.53	1.40
6	Q	201	CYC	CHD-C1D	5.76	1.53	1.40
6	W	201	CYC	CHA-C4D	5.76	1.53	1.40
6	A	301	CYC	CHB-C4A	5.75	1.53	1.40
6	R	201	CYC	CHA-C4D	5.74	1.53	1.40
6	B	201	CYC	CHD-C1D	5.74	1.53	1.40
6	C	201	CYC	CHB-C4A	5.74	1.53	1.40
6	P	201	CYC	CHB-C4A	5.74	1.53	1.40
6	L	201	CYC	CHA-C4D	5.74	1.53	1.40
6	G	201	CYC	CHA-C4D	5.72	1.53	1.40
6	A	302	CYC	CHB-C4A	5.72	1.53	1.40
6	C	201	CYC	CHA-C4D	5.71	1.53	1.40
6	H	201	CYC	CHA-C4D	5.71	1.53	1.40
6	Q	201	CYC	CHA-C4D	5.70	1.53	1.40
6	J	201	CYC	CHB-C4A	5.69	1.53	1.40
6	V	201	CYC	CHB-C4A	5.69	1.53	1.40
6	L	201	CYC	CHB-C4A	5.69	1.53	1.40
6	N	201	CYC	CHA-C4D	5.68	1.53	1.40
6	Q	202	CYC	CHB-C4A	5.68	1.53	1.40
6	B	201	CYC	CHA-C4D	5.67	1.53	1.40
6	W	201	CYC	CHB-C4A	5.67	1.53	1.40
6	J	202	CYC	CHB-C4A	5.66	1.53	1.40
6	D	201	CYC	CHB-C4A	5.65	1.53	1.40
6	Y	301	CYC	CHB-C4A	5.64	1.53	1.40
6	J	202	CYC	CHA-C4D	5.64	1.53	1.40
6	M	201	CYC	CHB-C4A	5.63	1.53	1.40
6	T	201	CYC	CHA-C4D	5.62	1.53	1.40
6	T	202	CYC	CHB-C4A	5.62	1.53	1.40
6	C	202	CYC	CHD-C1D	5.62	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	202	CYC	CHA-C4D	5.61	1.53	1.40
6	X	201	CYC	CHA-C4D	5.59	1.53	1.40
6	A	302	CYC	CHA-C4D	5.58	1.53	1.40
6	M	201	CYC	CHA-C4D	5.58	1.53	1.40
6	V	201	CYC	CHA-C4D	5.58	1.53	1.40
6	J	201	CYC	CHA-C4D	5.58	1.53	1.40
6	E	201	CYC	CHA-C4D	5.58	1.53	1.40
6	Y	301	CYC	CHA-C4D	5.58	1.53	1.40
6	F	201	CYC	CHB-C4A	5.57	1.53	1.40
6	F	202	CYC	CHB-C4A	5.57	1.53	1.40
6	a	202	CYC	CHB-C4A	5.57	1.53	1.40
6	B	201	CYC	CHB-C4A	5.57	1.53	1.40
6	A	301	CYC	CHA-C4D	5.56	1.52	1.40
6	Z	301	CYC	CHA-C4D	5.56	1.52	1.40
6	S	201	CYC	CHB-C4A	5.56	1.53	1.40
6	D	201	CYC	CHA-C4D	5.55	1.52	1.40
6	C	202	CYC	CHB-C4A	5.55	1.53	1.40
6	H	201	CYC	CHB-C4A	5.54	1.53	1.40
6	a	202	CYC	CHA-C4D	5.53	1.52	1.40
6	a	201	CYC	CHA-C4D	5.52	1.52	1.40
6	N	201	CYC	CHB-C4A	5.51	1.53	1.40
6	U	201	CYC	CHB-C4A	5.50	1.53	1.40
6	G	201	CYC	CHB-C4A	5.50	1.53	1.40
6	E	201	CYC	CHB-C4A	5.49	1.53	1.40
6	K	201	CYC	CHB-C4A	5.49	1.53	1.40
6	I	201	CYC	CHB-C4A	5.47	1.53	1.40
6	R	201	CYC	CHB-C4A	5.42	1.53	1.40
6	T	201	CYC	CHB-C4A	5.41	1.53	1.40
6	X	201	CYC	C4B-C3B	-5.38	1.38	1.48
6	U	201	CYC	C2C-C3C	5.38	1.69	1.54
6	Q	202	CYC	C4B-C3B	-5.37	1.38	1.48
6	P	201	CYC	C2C-C3C	5.37	1.69	1.54
6	H	201	CYC	C2C-C3C	5.37	1.69	1.54
6	A	302	CYC	C2C-C3C	5.37	1.69	1.54
6	Z	301	CYC	C2C-C3C	5.35	1.69	1.54
6	V	201	CYC	C2C-C3C	5.34	1.68	1.54
6	W	201	CYC	C2C-C3C	5.34	1.68	1.54
6	D	201	CYC	C2C-C3C	5.34	1.68	1.54
6	V	202	CYC	CHB-C4A	5.32	1.52	1.40
6	A	302	CYC	C4B-C3B	-5.32	1.38	1.48
6	N	201	CYC	C2C-C3C	5.32	1.68	1.54
6	K	201	CYC	C2C-C3C	5.31	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	201	CYC	C4B-C3B	-5.31	1.38	1.48
6	T	202	CYC	C2C-C3C	5.30	1.68	1.54
6	Z	301	CYC	C4B-C3B	-5.29	1.38	1.48
6	a	201	CYC	C2C-C3C	5.28	1.68	1.54
6	L	201	CYC	C4B-C3B	-5.27	1.38	1.48
6	G	201	CYC	C2C-C3C	5.26	1.68	1.54
6	D	201	CYC	C4B-C3B	-5.25	1.38	1.48
6	a	202	CYC	C4B-C3B	-5.24	1.38	1.48
6	E	201	CYC	C4B-C3B	-5.22	1.38	1.48
6	J	202	CYC	C4B-C3B	-5.22	1.38	1.48
6	C	202	CYC	C4B-C3B	-5.22	1.38	1.48
6	S	201	CYC	C2C-C3C	5.20	1.68	1.54
6	M	201	CYC	C4B-C3B	-5.20	1.38	1.48
6	A	302	CYC	C1A-C2A	-5.19	1.37	1.45
6	Q	202	CYC	C2C-C3C	5.19	1.68	1.54
6	a	201	CYC	C1A-C2A	-5.18	1.37	1.45
6	I	201	CYC	C2C-C3C	5.17	1.68	1.54
6	C	201	CYC	C2C-C3C	5.16	1.68	1.54
6	V	202	CYC	C4B-C3B	-5.15	1.38	1.48
6	C	202	CYC	C2C-C3C	5.14	1.68	1.54
6	R	201	CYC	C4B-C3B	-5.14	1.38	1.48
6	F	202	CYC	C2C-C3C	5.14	1.68	1.54
6	T	201	CYC	C4B-C3B	-5.13	1.38	1.48
6	R	201	CYC	C2C-C3C	5.12	1.68	1.54
6	J	201	CYC	C4B-C3B	-5.12	1.38	1.48
6	F	201	CYC	C4B-C3B	-5.11	1.38	1.48
6	X	201	CYC	C2C-C3C	5.10	1.68	1.54
6	P	201	CYC	C4B-C3B	-5.10	1.38	1.48
6	G	201	CYC	C4B-C3B	-5.09	1.38	1.48
6	Y	301	CYC	C4B-C3B	-5.09	1.38	1.48
6	L	201	CYC	C2C-C3C	5.09	1.68	1.54
6	Z	301	CYC	C1A-C2A	-5.09	1.37	1.45
6	A	301	CYC	C4B-C3B	-5.09	1.38	1.48
6	W	201	CYC	C4B-C3B	-5.09	1.38	1.48
6	C	201	CYC	C4B-C3B	-5.09	1.38	1.48
6	V	201	CYC	C4B-C3B	-5.09	1.38	1.48
6	S	201	CYC	C4B-C3B	-5.08	1.38	1.48
6	F	202	CYC	C4B-C3B	-5.08	1.38	1.48
6	B	201	CYC	C4B-C3B	-5.07	1.38	1.48
6	B	201	CYC	C2C-C3C	5.07	1.68	1.54
6	J	201	CYC	C2C-C3C	5.07	1.68	1.54
6	E	201	CYC	C2C-C3C	5.07	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	CYC	C1A-C2A	-5.07	1.37	1.45
6	K	201	CYC	C4B-C3B	-5.06	1.38	1.48
6	M	201	CYC	C2C-C3C	5.05	1.68	1.54
6	V	202	CYC	C2C-C3C	5.04	1.68	1.54
6	F	201	CYC	C2C-C3C	5.04	1.68	1.54
6	Q	201	CYC	C2C-C3C	5.04	1.68	1.54
6	J	202	CYC	C2C-C3C	5.03	1.68	1.54
6	B	201	CYC	C1A-C2A	-5.01	1.37	1.45
6	A	301	CYC	C2C-C3C	5.00	1.68	1.54
6	T	202	CYC	C4B-C3B	-4.99	1.39	1.48
6	H	201	CYC	C4B-C3B	-4.99	1.39	1.48
6	W	201	CYC	C1A-C2A	-4.99	1.37	1.45
6	N	201	CYC	C4B-C3B	-4.98	1.39	1.48
6	I	201	CYC	C4B-C3B	-4.97	1.39	1.48
6	X	201	CYC	C1A-C2A	-4.96	1.38	1.45
6	a	202	CYC	C2C-C3C	4.96	1.67	1.54
6	T	201	CYC	C2C-C3C	4.95	1.67	1.54
6	U	201	CYC	C4B-C3B	-4.95	1.39	1.48
6	Q	201	CYC	C4B-C3B	-4.94	1.39	1.48
6	F	201	CYC	C1A-C2A	-4.93	1.38	1.45
6	V	201	CYC	C1A-C2A	-4.92	1.38	1.45
6	M	201	CYC	C1A-C2A	-4.92	1.38	1.45
6	L	201	CYC	C1A-C2A	-4.91	1.38	1.45
6	N	201	CYC	C1A-C2A	-4.91	1.38	1.45
6	Y	301	CYC	C2C-C3C	4.91	1.67	1.54
6	H	201	CYC	C1A-C2A	-4.88	1.38	1.45
6	K	201	CYC	C1A-C2A	-4.87	1.38	1.45
6	C	201	CYC	C1A-C2A	-4.87	1.38	1.45
6	J	201	CYC	C1A-C2A	-4.86	1.38	1.45
6	G	201	CYC	C1A-C2A	-4.86	1.38	1.45
6	I	201	CYC	C1A-C2A	-4.84	1.38	1.45
6	D	201	CYC	C1A-C2A	-4.83	1.38	1.45
6	S	201	CYC	C1A-C2A	-4.83	1.38	1.45
6	Q	201	CYC	C1A-C2A	-4.83	1.38	1.45
6	T	202	CYC	C1A-C2A	-4.83	1.38	1.45
6	J	202	CYC	C1A-C2A	-4.80	1.38	1.45
6	Y	301	CYC	C1A-C2A	-4.79	1.38	1.45
6	U	201	CYC	C1A-C2A	-4.78	1.38	1.45
6	P	201	CYC	C1A-C2A	-4.77	1.38	1.45
6	E	201	CYC	C1A-C2A	-4.76	1.38	1.45
6	a	202	CYC	C1A-C2A	-4.74	1.38	1.45
6	R	201	CYC	C1A-C2A	-4.73	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	202	CYC	C1A-C2A	-4.67	1.38	1.45
6	F	202	CYC	C1A-C2A	-4.66	1.38	1.45
6	C	202	CYC	C1A-C2A	-4.62	1.38	1.45
6	V	202	CYC	C1A-C2A	-4.58	1.38	1.45
6	T	201	CYC	C1A-C2A	-4.57	1.38	1.45
6	N	201	CYC	C1B-C2B	-3.88	1.38	1.45
6	G	201	CYC	C1B-C2B	-3.85	1.38	1.45
6	I	201	CYC	C1B-C2B	-3.83	1.38	1.45
6	B	201	CYC	C1B-C2B	-3.82	1.38	1.45
6	X	201	CYC	C1B-NB	-3.79	1.31	1.37
6	Z	301	CYC	C1B-NB	-3.79	1.31	1.37
6	K	201	CYC	C1B-C2B	-3.79	1.38	1.45
6	S	201	CYC	C1B-C2B	-3.77	1.38	1.45
6	F	201	CYC	C1B-C2B	-3.76	1.38	1.45
6	H	201	CYC	C1B-C2B	-3.76	1.38	1.45
6	L	201	CYC	C1B-NB	-3.73	1.31	1.37
6	W	201	CYC	C1B-C2B	-3.72	1.38	1.45
6	T	202	CYC	C1B-C2B	-3.71	1.38	1.45
6	V	201	CYC	C1B-C2B	-3.70	1.38	1.45
6	D	201	CYC	C4D-ND	-3.69	1.31	1.37
6	F	202	CYC	C1B-C2B	-3.68	1.38	1.45
6	R	201	CYC	C1B-C2B	-3.68	1.38	1.45
6	a	201	CYC	C1B-NB	-3.67	1.31	1.37
6	P	201	CYC	C1B-NB	-3.64	1.31	1.37
6	U	201	CYC	C1B-C2B	-3.64	1.38	1.45
6	L	201	CYC	C1B-C2B	-3.64	1.38	1.45
6	C	202	CYC	C1B-C2B	-3.62	1.38	1.45
6	P	201	CYC	C1B-C2B	-3.62	1.38	1.45
6	Y	301	CYC	C4D-ND	-3.61	1.31	1.37
6	a	202	CYC	C4D-ND	-3.61	1.31	1.37
6	a	201	CYC	C4D-ND	-3.61	1.31	1.37
6	J	201	CYC	C1B-C2B	-3.59	1.38	1.45
6	T	201	CYC	C1B-C2B	-3.59	1.38	1.45
6	Y	301	CYC	C1B-C2B	-3.59	1.38	1.45
6	B	201	CYC	C1B-NB	-3.58	1.31	1.37
6	C	201	CYC	C4D-ND	-3.58	1.31	1.37
6	L	201	CYC	C4D-ND	-3.58	1.31	1.37
6	E	201	CYC	C4D-ND	-3.58	1.31	1.37
6	Z	301	CYC	C4D-ND	-3.57	1.31	1.37
6	K	201	CYC	C1B-NB	-3.57	1.31	1.37
6	W	201	CYC	C1B-NB	-3.57	1.31	1.37
6	a	202	CYC	C1B-C2B	-3.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	201	CYC	C4D-ND	-3.55	1.31	1.37
6	D	201	CYC	C1B-C2B	-3.53	1.38	1.45
6	J	201	CYC	C1B-NB	-3.52	1.31	1.37
6	A	301	CYC	C4D-ND	-3.52	1.31	1.37
6	G	201	CYC	C1B-NB	-3.52	1.31	1.37
6	C	201	CYC	C1B-NB	-3.52	1.31	1.37
6	R	201	CYC	C1B-NB	-3.52	1.31	1.37
6	V	201	CYC	C1B-NB	-3.52	1.31	1.37
6	E	201	CYC	C1B-C2B	-3.52	1.38	1.45
6	F	201	CYC	C1B-NB	-3.51	1.31	1.37
6	M	201	CYC	C4D-ND	-3.51	1.31	1.37
6	N	201	CYC	C1B-NB	-3.50	1.31	1.37
6	Z	301	CYC	C1B-C2B	-3.50	1.38	1.45
6	V	202	CYC	C1B-C2B	-3.50	1.38	1.45
6	L	201	CYC	C1A-NA	-3.49	1.31	1.38
6	I	201	CYC	C1B-NB	-3.49	1.31	1.37
6	C	201	CYC	C1B-C2B	-3.48	1.38	1.45
6	Q	201	CYC	C1B-C2B	-3.48	1.38	1.45
6	J	202	CYC	C1B-NB	-3.48	1.31	1.37
6	U	201	CYC	C1B-NB	-3.47	1.31	1.37
6	J	201	CYC	C4D-ND	-3.47	1.31	1.37
6	S	201	CYC	C1B-NB	-3.47	1.31	1.37
6	J	202	CYC	C1B-C2B	-3.47	1.38	1.45
6	A	301	CYC	C1B-NB	-3.46	1.31	1.37
6	J	202	CYC	C4D-ND	-3.46	1.31	1.37
6	D	201	CYC	C1B-NB	-3.46	1.31	1.37
6	T	202	CYC	C1B-NB	-3.45	1.31	1.37
6	Q	201	CYC	C1B-NB	-3.45	1.31	1.37
6	Q	202	CYC	C1B-NB	-3.44	1.31	1.37
6	Y	301	CYC	C1B-NB	-3.44	1.31	1.37
6	Q	202	CYC	C1B-C2B	-3.44	1.38	1.45
6	K	201	CYC	C1A-NA	-3.43	1.31	1.38
6	a	201	CYC	C1B-C2B	-3.43	1.39	1.45
6	A	302	CYC	C1B-C2B	-3.42	1.39	1.45
6	a	202	CYC	C1B-NB	-3.42	1.32	1.37
6	E	201	CYC	C1B-NB	-3.42	1.32	1.37
6	H	201	CYC	C1B-NB	-3.41	1.32	1.37
6	F	202	CYC	C1B-NB	-3.40	1.32	1.37
6	C	202	CYC	C1B-NB	-3.40	1.32	1.37
6	A	301	CYC	C1A-NA	-3.39	1.31	1.38
6	X	201	CYC	C1A-NA	-3.39	1.31	1.38
6	T	201	CYC	C4D-ND	-3.38	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	201	CYC	C1B-NB	-3.38	1.32	1.37
6	V	201	CYC	C4D-ND	-3.38	1.32	1.37
6	T	201	CYC	C1B-NB	-3.38	1.32	1.37
6	E	201	CYC	C1D-ND	-3.37	1.32	1.37
6	G	201	CYC	C1A-NA	-3.37	1.31	1.38
6	N	201	CYC	C1A-NA	-3.37	1.31	1.38
6	a	202	CYC	C1D-ND	-3.36	1.32	1.37
6	T	201	CYC	C1A-NA	-3.36	1.31	1.38
6	I	201	CYC	C1A-NA	-3.35	1.31	1.38
6	M	201	CYC	C1B-C2B	-3.35	1.39	1.45
6	Z	301	CYC	C1A-NA	-3.34	1.31	1.38
6	H	201	CYC	C1A-NA	-3.33	1.31	1.38
6	W	201	CYC	C1A-NA	-3.33	1.31	1.38
6	V	202	CYC	C1B-NB	-3.33	1.32	1.37
6	A	301	CYC	C1B-C2B	-3.32	1.39	1.45
6	a	201	CYC	C1A-NA	-3.32	1.31	1.38
6	B	201	CYC	C1A-NA	-3.32	1.31	1.38
6	X	201	CYC	C1B-C2B	-3.32	1.39	1.45
6	B	201	CYC	C4D-ND	-3.31	1.32	1.37
6	J	201	CYC	C1A-NA	-3.30	1.31	1.38
6	a	202	CYC	C1A-NA	-3.30	1.31	1.38
6	F	201	CYC	C1A-NA	-3.30	1.31	1.38
6	A	302	CYC	C1A-NA	-3.28	1.31	1.38
6	D	201	CYC	C1D-ND	-3.28	1.32	1.37
6	V	202	CYC	C1A-NA	-3.27	1.31	1.38
6	F	201	CYC	C1D-ND	-3.27	1.32	1.37
6	V	202	CYC	C4D-ND	-3.26	1.32	1.37
6	E	201	CYC	C1A-NA	-3.26	1.31	1.38
6	C	202	CYC	C1A-NA	-3.25	1.31	1.38
6	C	201	CYC	C1A-NA	-3.25	1.31	1.38
6	U	201	CYC	C1A-NA	-3.24	1.31	1.38
6	Q	201	CYC	C4D-ND	-3.23	1.32	1.37
6	A	302	CYC	C4D-ND	-3.22	1.32	1.37
6	D	201	CYC	C1A-NA	-3.20	1.31	1.38
6	S	201	CYC	C1A-NA	-3.20	1.31	1.38
6	M	201	CYC	C1A-NA	-3.19	1.31	1.38
6	R	201	CYC	C1A-NA	-3.19	1.31	1.38
6	I	201	CYC	C4D-ND	-3.18	1.32	1.37
6	P	201	CYC	C1A-NA	-3.18	1.31	1.38
6	Q	202	CYC	C1A-NA	-3.18	1.31	1.38
6	Y	301	CYC	C1D-ND	-3.17	1.32	1.37
6	J	202	CYC	C1A-NA	-3.17	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	201	CYC	C4D-ND	-3.17	1.32	1.37
6	J	202	CYC	C1D-ND	-3.17	1.32	1.37
6	F	202	CYC	C1A-NA	-3.17	1.31	1.38
6	A	302	CYC	C1B-NB	-3.16	1.32	1.37
6	R	201	CYC	C4D-ND	-3.16	1.32	1.37
6	G	201	CYC	C4D-ND	-3.16	1.32	1.37
6	T	202	CYC	C1A-NA	-3.15	1.31	1.38
6	H	201	CYC	C4D-ND	-3.15	1.32	1.37
6	K	201	CYC	C4D-ND	-3.15	1.32	1.37
6	N	201	CYC	C4D-ND	-3.14	1.32	1.37
6	V	201	CYC	C1A-NA	-3.13	1.31	1.38
6	W	201	CYC	C4D-ND	-3.13	1.32	1.37
6	F	201	CYC	C4D-ND	-3.12	1.32	1.37
6	T	201	CYC	C1D-ND	-3.12	1.32	1.37
6	L	201	CYC	C1D-ND	-3.11	1.32	1.37
6	C	202	CYC	C1D-ND	-3.11	1.32	1.37
6	F	202	CYC	C1D-ND	-3.11	1.32	1.37
6	Q	202	CYC	C4D-ND	-3.08	1.32	1.37
6	F	202	CYC	C4D-ND	-3.07	1.32	1.37
6	C	202	CYC	C4D-ND	-3.07	1.32	1.37
6	Q	201	CYC	C1A-NA	-3.07	1.32	1.38
6	C	202	CYC	C4A-C3A	-3.07	1.39	1.45
6	S	201	CYC	C4D-ND	-3.06	1.32	1.37
6	U	201	CYC	C4D-ND	-3.06	1.32	1.37
6	V	202	CYC	C1D-ND	-3.06	1.32	1.37
6	V	202	CYC	C4A-C3A	-3.03	1.39	1.45
6	Q	201	CYC	C1D-ND	-3.02	1.32	1.37
6	T	201	CYC	C4A-C3A	-3.02	1.39	1.45
6	a	201	CYC	C1D-ND	-3.02	1.32	1.37
6	Z	301	CYC	C1D-ND	-3.01	1.32	1.37
6	R	201	CYC	C4A-C3A	-3.00	1.39	1.45
6	V	201	CYC	C1D-ND	-2.99	1.32	1.37
6	B	201	CYC	C1D-ND	-2.98	1.32	1.37
6	E	201	CYC	C4A-C3A	-2.98	1.39	1.45
6	A	301	CYC	C1D-ND	-2.97	1.32	1.37
6	V	201	CYC	C4A-C3A	-2.96	1.39	1.45
6	U	201	CYC	C4A-C3A	-2.95	1.39	1.45
6	Y	301	CYC	C4A-C3A	-2.95	1.39	1.45
6	I	201	CYC	C1D-ND	-2.94	1.32	1.37
6	Q	202	CYC	C1D-ND	-2.94	1.32	1.37
6	M	201	CYC	C4A-C3A	-2.94	1.39	1.45
6	H	201	CYC	C1D-ND	-2.94	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	202	CYC	C4D-ND	-2.94	1.32	1.37
6	X	201	CYC	C1D-ND	-2.93	1.32	1.37
6	X	201	CYC	C4B-NB	-2.93	1.31	1.38
6	C	201	CYC	C1D-ND	-2.93	1.32	1.37
6	P	201	CYC	C1D-ND	-2.93	1.32	1.37
6	G	201	CYC	C4A-C3A	-2.92	1.39	1.45
6	R	201	CYC	C1D-ND	-2.92	1.32	1.37
6	J	202	CYC	C4A-C3A	-2.91	1.39	1.45
6	I	201	CYC	C4A-C3A	-2.91	1.39	1.45
6	N	201	CYC	C1D-ND	-2.91	1.32	1.37
6	F	201	CYC	C4A-C3A	-2.89	1.39	1.45
6	K	201	CYC	C1D-ND	-2.89	1.32	1.37
6	M	201	CYC	C1D-ND	-2.89	1.32	1.37
6	G	201	CYC	C1D-ND	-2.89	1.32	1.37
6	N	201	CYC	C4A-C3A	-2.89	1.39	1.45
6	H	201	CYC	C4A-C3A	-2.88	1.39	1.45
6	J	201	CYC	C1D-ND	-2.88	1.32	1.37
6	K	201	CYC	C4A-C3A	-2.86	1.39	1.45
6	C	201	CYC	C4A-C3A	-2.85	1.39	1.45
6	a	201	CYC	C4B-NB	-2.85	1.31	1.38
6	T	202	CYC	C4A-C3A	-2.84	1.39	1.45
6	A	302	CYC	C1D-ND	-2.84	1.33	1.37
6	D	201	CYC	C4A-C3A	-2.84	1.39	1.45
6	U	201	CYC	C1D-ND	-2.83	1.33	1.37
6	B	201	CYC	C4A-C3A	-2.83	1.39	1.45
6	J	201	CYC	C4A-C3A	-2.82	1.39	1.45
6	a	202	CYC	C4A-C3A	-2.82	1.39	1.45
6	Q	201	CYC	C4A-C3A	-2.81	1.39	1.45
6	W	201	CYC	C1D-ND	-2.81	1.33	1.37
6	W	201	CYC	C4A-C3A	-2.81	1.39	1.45
6	S	201	CYC	C4A-C3A	-2.79	1.39	1.45
6	S	201	CYC	C1D-ND	-2.77	1.33	1.37
6	Z	301	CYC	C4B-NB	-2.76	1.31	1.38
6	A	302	CYC	C4A-C3A	-2.76	1.39	1.45
6	Q	202	CYC	C4A-C3A	-2.76	1.39	1.45
6	F	202	CYC	C4A-C3A	-2.75	1.39	1.45
6	A	301	CYC	C4A-C3A	-2.74	1.39	1.45
6	T	202	CYC	C1D-ND	-2.74	1.33	1.37
6	W	201	CYC	C4B-NB	-2.72	1.31	1.38
6	L	201	CYC	C4A-C3A	-2.70	1.40	1.45
6	L	201	CYC	C4B-NB	-2.69	1.31	1.38
6	M	201	CYC	C4B-NB	-2.69	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	CYC	C4B-NB	-2.68	1.31	1.38
6	B	201	CYC	C4B-NB	-2.68	1.31	1.38
6	V	201	CYC	C4B-NB	-2.67	1.31	1.38
6	U	201	CYC	C4B-NB	-2.65	1.31	1.38
6	P	201	CYC	C4B-NB	-2.65	1.31	1.38
6	R	201	CYC	C4B-NB	-2.64	1.31	1.38
6	K	201	CYC	C4B-NB	-2.64	1.31	1.38
6	G	201	CYC	C4B-NB	-2.64	1.31	1.38
6	S	201	CYC	C4B-NB	-2.63	1.31	1.38
6	Y	301	CYC	C4B-NB	-2.62	1.31	1.38
6	A	301	CYC	C4B-NB	-2.61	1.32	1.38
6	J	201	CYC	C4B-NB	-2.61	1.32	1.38
6	T	202	CYC	C4B-NB	-2.61	1.32	1.38
6	C	201	CYC	C4B-NB	-2.60	1.32	1.38
6	N	201	CYC	C4B-NB	-2.60	1.32	1.38
6	H	201	CYC	C4B-NB	-2.60	1.32	1.38
6	Y	301	CYC	C1A-NA	-2.59	1.33	1.38
6	P	201	CYC	C4A-C3A	-2.59	1.40	1.45
6	a	201	CYC	C4A-C3A	-2.59	1.40	1.45
6	I	201	CYC	C4B-NB	-2.58	1.32	1.38
6	X	201	CYC	C4A-C3A	-2.58	1.40	1.45
6	Q	202	CYC	C4B-NB	-2.56	1.32	1.38
6	E	201	CYC	C4B-NB	-2.56	1.32	1.38
6	D	201	CYC	C4B-NB	-2.55	1.32	1.38
6	J	202	CYC	C4B-NB	-2.55	1.32	1.38
6	Z	301	CYC	C4A-C3A	-2.54	1.40	1.45
6	T	201	CYC	C4B-NB	-2.54	1.32	1.38
6	a	202	CYC	C4B-NB	-2.52	1.32	1.38
6	A	302	CYC	C4B-NB	-2.51	1.32	1.38
6	Z	301	CYC	C4D-C3D	-2.51	1.37	1.42
6	Q	201	CYC	C4B-NB	-2.50	1.32	1.38
6	C	202	CYC	C4B-NB	-2.50	1.32	1.38
6	V	202	CYC	C4B-NB	-2.49	1.32	1.38
6	F	202	CYC	C4B-NB	-2.49	1.32	1.38
6	X	201	CYC	C4D-C3D	-2.45	1.37	1.42
6	a	201	CYC	C4D-C3D	-2.41	1.37	1.42
6	L	201	CYC	C4D-C3D	-2.41	1.37	1.42
6	M	201	CYC	C4D-C3D	-2.39	1.37	1.42
6	J	201	CYC	C4D-C3D	-2.38	1.37	1.42
6	A	301	CYC	C4D-C3D	-2.38	1.37	1.42
6	C	201	CYC	C4D-C3D	-2.34	1.37	1.42
6	A	302	CYC	C4D-C3D	-2.34	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	301	CYC	C4D-C3D	-2.17	1.38	1.42
6	V	201	CYC	C4D-C3D	-2.17	1.38	1.42
6	H	201	CYC	C4D-C3D	-2.16	1.38	1.42
6	B	201	CYC	C4D-C3D	-2.16	1.38	1.42
6	K	201	CYC	C4D-C3D	-2.14	1.38	1.42
6	U	201	CYC	C4D-C3D	-2.11	1.38	1.42
6	N	201	CYC	C4D-C3D	-2.11	1.38	1.42
6	I	201	CYC	C4D-C3D	-2.10	1.38	1.42
6	V	202	CYC	C4D-C3D	-2.10	1.38	1.42
6	T	201	CYC	C4A-NA	-2.10	1.31	1.36
6	W	201	CYC	C4D-C3D	-2.09	1.38	1.42
6	a	202	CYC	C4D-C3D	-2.07	1.38	1.42
6	R	201	CYC	C4D-C3D	-2.06	1.38	1.42
6	G	201	CYC	C4D-C3D	-2.05	1.38	1.42
6	V	202	CYC	C4A-NA	-2.05	1.32	1.36
6	T	201	CYC	C4D-C3D	-2.04	1.38	1.42
6	E	201	CYC	C4A-NA	-2.03	1.32	1.36
6	D	201	CYC	C4D-C3D	-2.01	1.38	1.42
6	S	201	CYC	C4D-C3D	-2.01	1.38	1.42
6	Q	201	CYC	C4D-C3D	-2.01	1.38	1.42
6	L	201	CYC	C4A-NA	-2.01	1.32	1.36

All (575) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	202	CYC	OC-C1C-C2C	-23.26	107.68	126.17
6	B	201	CYC	OC-C1C-C2C	-22.04	108.64	126.17
6	T	202	CYC	OC-C1C-C2C	-21.45	109.12	126.17
6	I	201	CYC	OC-C1C-C2C	-21.34	109.20	126.17
6	H	201	CYC	OC-C1C-C2C	-21.16	109.35	126.17
6	T	201	CYC	OC-C1C-C2C	-21.00	109.47	126.17
6	E	201	CYC	OC-C1C-C2C	-20.79	109.64	126.17
6	F	201	CYC	OC-C1C-C2C	-20.78	109.65	126.17
6	W	201	CYC	OC-C1C-C2C	-20.76	109.66	126.17
6	J	201	CYC	OC-C1C-C2C	-20.75	109.67	126.17
6	A	301	CYC	OC-C1C-C2C	-20.70	109.71	126.17
6	J	202	CYC	OC-C1C-C2C	-20.70	109.71	126.17
6	Q	202	CYC	OC-C1C-C2C	-20.57	109.81	126.17
6	M	201	CYC	OC-C1C-C2C	-20.48	109.89	126.17
6	G	201	CYC	OC-C1C-C2C	-20.47	109.90	126.17
6	Q	201	CYC	OC-C1C-C2C	-20.41	109.95	126.17
6	K	201	CYC	OC-C1C-C2C	-20.40	109.95	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	201	CYC	OC-C1C-C2C	-20.40	109.95	126.17
6	V	202	CYC	OC-C1C-C2C	-20.31	110.02	126.17
6	R	201	CYC	OC-C1C-C2C	-20.29	110.04	126.17
6	U	201	CYC	OC-C1C-C2C	-20.29	110.04	126.17
6	N	201	CYC	OC-C1C-C2C	-20.26	110.06	126.17
6	P	201	CYC	OC-C1C-C2C	-20.26	110.07	126.17
6	L	201	CYC	OC-C1C-C2C	-20.23	110.09	126.17
6	a	202	CYC	OC-C1C-C2C	-20.13	110.17	126.17
6	D	201	CYC	OC-C1C-C2C	-19.89	110.36	126.17
6	Y	301	CYC	OC-C1C-C2C	-19.88	110.37	126.17
6	F	202	CYC	OC-C1C-C2C	-19.84	110.40	126.17
6	A	302	CYC	OC-C1C-C2C	-19.58	110.61	126.17
6	S	201	CYC	OC-C1C-C2C	-19.24	110.87	126.17
6	X	201	CYC	OC-C1C-C2C	-18.88	111.16	126.17
6	C	201	CYC	OC-C1C-C2C	-18.59	111.39	126.17
6	a	201	CYC	OC-C1C-C2C	-18.57	111.41	126.17
6	Z	301	CYC	OC-C1C-C2C	-18.13	111.76	126.17
6	J	201	CYC	OC-C1C-NC	-13.55	108.95	124.93
6	X	201	CYC	OC-C1C-NC	-13.39	109.14	124.93
6	C	201	CYC	OC-C1C-NC	-13.33	109.22	124.93
6	G	201	CYC	OC-C1C-NC	-13.31	109.24	124.93
6	P	201	CYC	CHD-C4C-NC	-13.26	109.08	125.63
6	L	201	CYC	OC-C1C-NC	-13.23	109.33	124.93
6	W	201	CYC	CHD-C4C-NC	-13.21	109.14	125.63
6	A	301	CYC	OC-C1C-NC	-13.21	109.36	124.93
6	Z	301	CYC	OC-C1C-NC	-13.20	109.37	124.93
6	K	201	CYC	OC-C1C-NC	-13.15	109.42	124.93
6	R	201	CYC	CHD-C4C-NC	-13.13	109.24	125.63
6	U	201	CYC	CHD-C4C-NC	-13.11	109.27	125.63
6	N	201	CYC	CHD-C4C-NC	-13.11	109.27	125.63
6	Y	301	CYC	OC-C1C-NC	-13.09	109.50	124.93
6	a	201	CYC	OC-C1C-NC	-13.01	109.59	124.93
6	V	202	CYC	OC-C1C-NC	-13.00	109.60	124.93
6	J	202	CYC	OC-C1C-NC	-12.95	109.66	124.93
6	N	201	CYC	OC-C1C-NC	-12.92	109.69	124.93
6	G	201	CYC	CHD-C4C-NC	-12.92	109.50	125.63
6	I	201	CYC	CHD-C4C-NC	-12.86	109.57	125.63
6	Q	202	CYC	CHD-C4C-NC	-12.86	109.58	125.63
6	F	201	CYC	CHD-C4C-NC	-12.85	109.59	125.63
6	K	201	CYC	CHD-C4C-NC	-12.85	109.60	125.63
6	T	201	CYC	OC-C1C-NC	-12.83	109.80	124.93
6	C	202	CYC	OC-C1C-NC	-12.83	109.81	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	201	CYC	OC-C1C-NC	-12.75	109.90	124.93
6	M	201	CYC	OC-C1C-NC	-12.73	109.92	124.93
6	U	201	CYC	OC-C1C-NC	-12.72	109.93	124.93
6	H	201	CYC	OC-C1C-NC	-12.71	109.95	124.93
6	H	201	CYC	CHD-C4C-NC	-12.69	109.79	125.63
6	T	202	CYC	CHD-C4C-NC	-12.66	109.82	125.63
6	F	201	CYC	OC-C1C-NC	-12.61	110.06	124.93
6	I	201	CYC	OC-C1C-NC	-12.57	110.11	124.93
6	D	201	CYC	OC-C1C-NC	-12.54	110.14	124.93
6	R	201	CYC	OC-C1C-NC	-12.54	110.14	124.93
6	B	201	CYC	CHD-C4C-NC	-12.53	109.99	125.63
6	T	202	CYC	OC-C1C-NC	-12.52	110.18	124.93
6	Q	202	CYC	OC-C1C-NC	-12.51	110.18	124.93
6	P	201	CYC	OC-C1C-NC	-12.49	110.21	124.93
6	Q	201	CYC	OC-C1C-NC	-12.47	110.23	124.93
6	B	201	CYC	OC-C1C-NC	-12.42	110.28	124.93
6	W	201	CYC	OC-C1C-NC	-12.39	110.32	124.93
6	F	202	CYC	OC-C1C-NC	-12.36	110.36	124.93
6	F	202	CYC	CHD-C4C-NC	-12.27	110.31	125.63
6	V	201	CYC	OC-C1C-NC	-12.15	110.61	124.93
6	M	201	CYC	CHD-C4C-NC	-12.13	110.49	125.63
6	S	201	CYC	CHD-C4C-NC	-12.00	110.66	125.63
6	A	301	CYC	CHD-C4C-NC	-11.96	110.70	125.63
6	a	202	CYC	OC-C1C-NC	-11.74	111.09	124.93
6	A	302	CYC	OC-C1C-NC	-11.60	111.26	124.93
6	Y	301	CYC	CHD-C4C-NC	-11.56	111.20	125.63
6	J	202	CYC	CHD-C4C-NC	-11.50	111.27	125.63
6	J	201	CYC	CHD-C4C-NC	-11.50	111.28	125.63
6	Z	301	CYC	C1C-NC-C4C	-11.38	99.14	113.41
6	C	202	CYC	CHD-C4C-NC	-11.33	111.48	125.63
6	a	201	CYC	CHD-C4C-NC	-11.31	111.51	125.63
6	Q	201	CYC	CHD-C4C-NC	-11.28	111.55	125.63
6	V	202	CYC	CHD-C4C-NC	-11.21	111.64	125.63
6	E	201	CYC	CHD-C4C-NC	-11.00	111.90	125.63
6	T	201	CYC	CHD-C4C-NC	-10.93	111.98	125.63
6	S	201	CYC	OC-C1C-NC	-10.93	112.04	124.93
6	L	201	CYC	CHD-C4C-NC	-10.87	112.06	125.63
6	X	201	CYC	CHD-C4C-NC	-10.83	112.11	125.63
6	A	302	CYC	CHD-C4C-NC	-10.57	112.44	125.63
6	a	201	CYC	C1C-NC-C4C	-10.45	100.30	113.41
6	C	201	CYC	CHD-C4C-NC	-10.34	112.73	125.63
6	D	201	CYC	CHD-C4C-NC	-10.02	113.12	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	301	CYC	CHD-C4C-NC	-9.85	113.33	125.63
6	V	201	CYC	CHD-C4C-NC	-9.84	113.35	125.63
6	C	201	CYC	C1C-NC-C4C	-9.46	101.54	113.41
6	Q	202	CYC	C1D-CHD-C4C	-9.34	111.82	127.76
6	R	201	CYC	C1D-CHD-C4C	-9.22	112.02	127.76
6	F	202	CYC	C1D-CHD-C4C	-9.17	112.11	127.76
6	a	202	CYC	C1C-NC-C4C	-9.10	102.00	113.41
6	A	302	CYC	C1C-NC-C4C	-9.04	102.07	113.41
6	V	201	CYC	C1C-NC-C4C	-9.02	102.10	113.41
6	D	201	CYC	C1C-NC-C4C	-8.91	102.24	113.41
6	E	201	CYC	C1C-NC-C4C	-8.89	102.26	113.41
6	V	202	CYC	C1D-CHD-C4C	-8.86	112.64	127.76
6	A	302	CYC	C2C-C1C-NC	-8.69	101.05	108.29
6	T	201	CYC	C1D-CHD-C4C	-8.66	112.98	127.76
6	G	201	CYC	C1D-CHD-C4C	-8.61	113.06	127.76
6	K	201	CYC	C1D-CHD-C4C	-8.59	113.09	127.76
6	H	201	CYC	C1D-CHD-C4C	-8.56	113.14	127.76
6	T	201	CYC	C1C-NC-C4C	-8.53	102.70	113.41
6	C	202	CYC	C1D-CHD-C4C	-8.50	113.26	127.76
6	J	202	CYC	C1C-NC-C4C	-8.44	102.82	113.41
6	U	201	CYC	C1D-CHD-C4C	-8.39	113.44	127.76
6	T	202	CYC	C1D-CHD-C4C	-8.34	113.53	127.76
6	T	201	CYC	C4D-CHA-C1A	-8.33	110.02	128.22
6	W	201	CYC	C1D-CHD-C4C	-8.24	113.70	127.76
6	N	201	CYC	C1D-CHD-C4C	-8.15	113.86	127.76
6	V	202	CYC	C1C-NC-C4C	-8.10	103.25	113.41
6	a	202	CYC	C4D-CHA-C1A	-8.08	110.58	128.22
6	P	201	CYC	C1D-CHD-C4C	-8.06	114.00	127.76
6	X	201	CYC	C1C-NC-C4C	-8.03	103.34	113.41
6	J	201	CYC	C1C-NC-C4C	-8.01	103.36	113.41
6	L	201	CYC	C1C-NC-C4C	-8.00	103.38	113.41
6	a	202	CYC	CHD-C4C-NC	-8.00	115.65	125.63
6	F	201	CYC	C1D-CHD-C4C	-7.94	114.20	127.76
6	E	201	CYC	C1D-CHD-C4C	-7.89	114.30	127.76
6	E	201	CYC	C4D-CHA-C1A	-7.73	111.35	128.22
6	V	201	CYC	C2C-C1C-NC	-7.59	101.97	108.29
6	V	202	CYC	C4D-CHA-C1A	-7.49	111.86	128.22
6	H	201	CYC	C1C-NC-C4C	-7.47	104.05	113.41
6	S	201	CYC	C1C-NC-C4C	-7.36	104.18	113.41
6	F	202	CYC	C4D-CHA-C1A	-7.34	112.19	128.22
6	A	301	CYC	C1C-NC-C4C	-7.17	104.41	113.41
6	F	202	CYC	C1C-NC-C4C	-7.08	104.53	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	201	CYC	C1D-CHD-C4C	-7.06	115.72	127.76
6	R	201	CYC	C1C-NC-C4C	-6.97	104.67	113.41
6	C	201	CYC	C3C-C4C-NC	-6.95	98.99	107.94
6	B	201	CYC	C1D-CHD-C4C	-6.93	115.93	127.76
6	M	201	CYC	C1B-CHB-C4A	-6.83	111.30	128.06
6	S	201	CYC	C2C-C1C-NC	-6.78	102.64	108.29
6	P	201	CYC	C1C-NC-C4C	-6.71	104.99	113.41
6	Q	201	CYC	C1D-CHD-C4C	-6.70	116.32	127.76
6	Y	301	CYC	C1C-NC-C4C	-6.68	105.03	113.41
6	F	201	CYC	C1C-NC-C4C	-6.67	105.05	113.41
6	J	202	CYC	C1D-CHD-C4C	-6.67	116.39	127.76
6	M	201	CYC	C1C-NC-C4C	-6.65	105.07	113.41
6	N	201	CYC	C1C-NC-C4C	-6.64	105.08	113.41
6	W	201	CYC	C1C-NC-C4C	-6.62	105.11	113.41
6	G	201	CYC	C1C-NC-C4C	-6.60	105.13	113.41
6	U	201	CYC	C1C-NC-C4C	-6.57	105.16	113.41
6	K	201	CYC	C1C-NC-C4C	-6.57	105.17	113.41
6	a	202	CYC	C1D-CHD-C4C	-6.55	116.58	127.76
6	C	202	CYC	C4D-CHA-C1A	-6.53	113.97	128.22
6	Z	301	CYC	C3C-C4C-NC	-6.52	99.55	107.94
6	Y	301	CYC	C1B-CHB-C4A	-6.42	112.30	128.06
6	V	202	CYC	C1B-CHB-C4A	-6.41	112.33	128.06
6	Q	201	CYC	C1C-NC-C4C	-6.34	105.45	113.41
6	S	201	CYC	C1D-CHD-C4C	-6.32	116.97	127.76
6	C	202	CYC	C1C-NC-C4C	-6.26	105.55	113.41
6	J	202	CYC	C4D-CHA-C1A	-6.25	114.57	128.22
6	Q	202	CYC	C1C-NC-C4C	-6.23	105.59	113.41
6	J	201	CYC	C1D-CHD-C4C	-6.22	117.15	127.76
6	L	201	CYC	C4D-CHA-C1A	-6.18	114.74	128.22
6	B	201	CYC	C1C-NC-C4C	-6.17	105.67	113.41
6	Y	301	CYC	C4D-CHA-C1A	-6.12	114.86	128.22
6	a	201	CYC	C3C-C4C-NC	-6.11	100.07	107.94
6	D	201	CYC	C4D-CHA-C1A	-6.07	114.96	128.22
6	R	201	CYC	C1B-CHB-C4A	-6.05	113.21	128.06
6	F	202	CYC	C2C-C1C-NC	-6.05	103.25	108.29
6	T	202	CYC	C1C-NC-C4C	-5.99	105.90	113.41
6	M	201	CYC	C1D-CHD-C4C	-5.92	117.66	127.76
6	Z	301	CYC	C4D-CHA-C1A	-5.89	115.36	128.22
6	P	201	CYC	C4D-CHA-C1A	-5.88	115.38	128.22
6	a	202	CYC	C3C-C4C-NC	-5.84	100.42	107.94
6	A	301	CYC	C4D-CHA-C1A	-5.77	115.62	128.22
6	I	201	CYC	C1C-NC-C4C	-5.75	106.20	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	201	CYC	C4D-CHA-C1A	-5.72	115.74	128.22
6	C	201	CYC	C4D-CHA-C1A	-5.70	115.77	128.22
6	a	201	CYC	C4D-CHA-C1A	-5.65	115.89	128.22
6	Q	202	CYC	C4D-CHA-C1A	-5.60	116.00	128.22
6	Q	201	CYC	C1B-CHB-C4A	-5.59	114.33	128.06
6	U	201	CYC	C1B-CHB-C4A	-5.52	114.51	128.06
6	J	201	CYC	C4D-CHA-C1A	-5.48	116.25	128.22
6	A	301	CYC	C3C-C4C-NC	-5.45	100.93	107.94
6	F	202	CYC	C1B-CHB-C4A	-5.41	114.76	128.06
6	X	201	CYC	C3C-C4C-NC	-5.38	101.02	107.94
6	I	201	CYC	C4D-CHA-C1A	-5.37	116.50	128.22
6	Z	301	CYC	C2C-C1C-NC	-5.37	103.82	108.29
6	R	201	CYC	C4D-CHA-C1A	-5.32	116.60	128.22
6	U	201	CYC	C4D-CHA-C1A	-5.31	116.62	128.22
6	B	201	CYC	C4D-CHA-C1A	-5.30	116.65	128.22
6	I	201	CYC	C1B-CHB-C4A	-5.28	115.09	128.06
6	T	202	CYC	C4D-CHA-C1A	-5.21	116.84	128.22
6	N	201	CYC	C4D-CHA-C1A	-5.21	116.85	128.22
6	T	201	CYC	C1B-CHB-C4A	-5.20	115.28	128.06
6	X	201	CYC	C1D-CHD-C4C	-5.20	118.89	127.76
6	T	202	CYC	C1B-CHB-C4A	-5.19	115.31	128.06
6	S	201	CYC	C1B-CHB-C4A	-5.18	115.33	128.06
6	H	201	CYC	C4D-CHA-C1A	-5.17	116.92	128.22
6	M	201	CYC	C4D-CHA-C1A	-5.17	116.94	128.22
6	H	201	CYC	C1B-CHB-C4A	-5.15	115.41	128.06
6	F	201	CYC	C4D-CHA-C1A	-5.12	117.04	128.22
6	L	201	CYC	C3C-C4C-NC	-5.11	101.36	107.94
6	a	201	CYC	C2C-C1C-NC	-5.07	104.06	108.29
6	D	201	CYC	C1D-CHD-C4C	-5.07	119.12	127.76
6	A	301	CYC	C1D-CHD-C4C	-5.05	119.13	127.76
6	L	201	CYC	C1D-CHD-C4C	-5.05	119.14	127.76
6	Q	201	CYC	C4D-CHA-C1A	-5.05	117.19	128.22
6	C	201	CYC	C1B-CHB-C4A	-5.04	115.69	128.06
6	K	201	CYC	C4D-CHA-C1A	-5.03	117.24	128.22
6	D	201	CYC	C3C-C4C-NC	-4.98	101.53	107.94
6	W	201	CYC	C1B-CHB-C4A	-4.97	115.85	128.06
6	a	201	CYC	C1D-CHD-C4C	-4.97	119.28	127.76
6	F	201	CYC	C1B-CHB-C4A	-4.96	115.87	128.06
6	Y	301	CYC	C3C-C4C-NC	-4.96	101.56	107.94
6	V	201	CYC	C4D-CHA-C1A	-4.94	117.43	128.22
6	A	302	CYC	C1D-CHD-C4C	-4.91	119.39	127.76
6	G	201	CYC	C4D-CHA-C1A	-4.90	117.52	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	CYC	CMD-C2D-C1D	4.88	132.71	125.62
6	S	201	CYC	C4D-CHA-C1A	-4.85	117.63	128.22
6	Q	201	CYC	CAB-C3B-C4B	4.82	128.83	121.37
6	Y	301	CYC	C1D-CHD-C4C	-4.82	119.53	127.76
6	C	201	CYC	C1D-CHD-C4C	-4.81	119.55	127.76
6	N	201	CYC	CAB-C3B-C4B	4.80	128.79	121.37
6	W	201	CYC	C4D-CHA-C1A	-4.78	117.78	128.22
6	P	201	CYC	C2C-C1C-NC	-4.76	104.32	108.29
6	V	201	CYC	CAB-C3B-C4B	4.76	128.73	121.37
6	J	201	CYC	CMD-C2D-C1D	4.72	132.48	125.62
6	a	202	CYC	C2C-C1C-NC	-4.72	104.36	108.29
6	a	201	CYC	CMD-C2D-C1D	4.70	132.45	125.62
6	Z	301	CYC	C1D-CHD-C4C	-4.69	119.76	127.76
6	P	201	CYC	C2C-C3C-C4C	4.67	108.33	101.34
6	I	201	CYC	C2C-C3C-C4C	4.64	108.29	101.34
6	I	201	CYC	CAB-C3B-C4B	4.63	128.54	121.37
6	M	201	CYC	CMD-C2D-C1D	4.62	132.34	125.62
6	A	302	CYC	C4D-CHA-C1A	-4.62	118.13	128.22
6	A	301	CYC	CMD-C2D-C1D	4.62	132.33	125.62
6	K	201	CYC	CAB-C3B-C4B	4.59	128.47	121.37
6	G	201	CYC	CAB-C3B-C4B	4.57	128.44	121.37
6	J	201	CYC	CAB-C3B-C4B	4.56	128.43	121.37
6	V	202	CYC	CAB-C3B-C4B	4.56	128.41	121.37
6	X	201	CYC	CMD-C2D-C1D	4.55	132.23	125.62
6	E	201	CYC	C3C-C4C-NC	-4.53	102.11	107.94
6	B	201	CYC	C1B-CHB-C4A	-4.52	116.96	128.06
6	C	201	CYC	CAB-C3B-C4B	4.47	128.29	121.37
6	T	201	CYC	C3C-C4C-NC	-4.43	102.24	107.94
6	Z	301	CYC	CMD-C2D-C1D	4.42	132.04	125.62
6	B	201	CYC	C2C-C3C-C4C	4.41	107.94	101.34
6	N	201	CYC	C1B-CHB-C4A	-4.40	117.25	128.06
6	C	202	CYC	C1B-CHB-C4A	-4.37	117.31	128.06
6	S	201	CYC	C2C-C3C-C4C	4.37	107.88	101.34
6	G	201	CYC	C1B-CHB-C4A	-4.36	117.34	128.06
6	U	201	CYC	CAB-C3B-C4B	4.34	128.09	121.37
6	K	201	CYC	C1B-CHB-C4A	-4.33	117.42	128.06
6	L	201	CYC	CMD-C2D-C1D	4.33	131.91	125.62
6	J	202	CYC	C3C-C4C-NC	-4.33	102.37	107.94
6	F	201	CYC	CAD-C3D-C4D	4.32	132.63	125.77
6	V	201	CYC	C1B-CHB-C4A	-4.32	117.44	128.06
6	H	201	CYC	CAB-C3B-C4B	4.31	128.03	121.37
6	Y	301	CYC	CMD-C2D-C1D	4.29	131.85	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	201	CYC	CAB-C3B-C4B	4.28	127.99	121.37
6	B	201	CYC	CAB-C3B-C4B	4.26	127.96	121.37
6	R	201	CYC	C3C-C4C-NC	-4.23	102.49	107.94
6	T	202	CYC	CAB-C3B-C4B	4.23	127.92	121.37
6	Q	201	CYC	C2C-C1C-NC	-4.23	104.76	108.29
6	V	202	CYC	C3C-C4C-NC	-4.23	102.49	107.94
6	Z	301	CYC	CAB-C3B-C4B	4.23	127.91	121.37
6	C	202	CYC	CAB-C3B-C4B	4.22	127.90	121.37
6	E	201	CYC	C1B-CHB-C4A	-4.21	117.73	128.06
6	S	201	CYC	CAB-C3B-C4B	4.20	127.86	121.37
6	Y	301	CYC	C2C-C1C-NC	-4.20	104.79	108.29
6	F	201	CYC	CAB-C3B-C4B	4.18	127.83	121.37
6	H	201	CYC	C3C-C4C-NC	-4.18	102.56	107.94
6	V	201	CYC	C2C-C3C-C4C	4.18	107.59	101.34
6	T	201	CYC	CAB-C3B-C4B	4.17	127.81	121.37
6	D	201	CYC	CAB-C3B-C4B	4.16	127.81	121.37
6	A	301	CYC	CAB-C3B-C4B	4.16	127.80	121.37
6	E	201	CYC	CAB-C3B-C4B	4.14	127.78	121.37
6	V	201	CYC	C1D-CHD-C4C	-4.14	120.70	127.76
6	A	302	CYC	C2C-C3C-C4C	4.13	107.52	101.34
6	F	202	CYC	CAB-C3B-C4B	4.12	127.74	121.37
6	X	201	CYC	CMA-C3A-C4A	4.12	131.50	125.10
6	a	202	CYC	CAB-C3B-C4B	4.11	127.72	121.37
6	F	202	CYC	C2C-C3C-C4C	4.08	107.45	101.34
6	J	202	CYC	C1B-CHB-C4A	-4.07	118.06	128.06
6	Q	202	CYC	C1B-CHB-C4A	-4.07	118.07	128.06
6	T	202	CYC	C2C-C3C-C4C	4.07	107.43	101.34
6	J	201	CYC	C1B-CHB-C4A	-4.04	118.14	128.06
6	J	202	CYC	CAB-C3B-C4B	4.03	127.61	121.37
6	L	201	CYC	CAB-C3B-C4B	4.02	127.59	121.37
6	G	201	CYC	C3C-C4C-NC	-4.01	102.78	107.94
6	Z	301	CYC	CMA-C3A-C4A	3.96	131.25	125.10
6	Y	301	CYC	CAB-C3B-C4B	3.91	127.42	121.37
6	C	202	CYC	C2C-C3C-C4C	3.91	107.20	101.34
6	J	202	CYC	CMD-C2D-C1D	3.89	131.27	125.62
6	a	202	CYC	C1B-CHB-C4A	-3.86	118.57	128.06
6	H	201	CYC	C2C-C3C-C4C	3.86	107.12	101.34
6	J	201	CYC	C3C-C4C-NC	-3.82	103.02	107.94
6	P	201	CYC	CAB-C3B-C4B	3.81	127.27	121.37
6	a	201	CYC	CAB-C3B-C4B	3.81	127.27	121.37
6	C	201	CYC	C2C-C1C-NC	-3.80	105.12	108.29
6	L	201	CYC	CMA-C3A-C4A	3.80	131.00	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	302	CYC	CAB-C3B-C4B	3.79	127.23	121.37
6	Q	202	CYC	C2C-C1C-NC	-3.77	105.15	108.29
6	P	201	CYC	CMA-C3A-C4A	3.77	130.95	125.10
6	V	201	CYC	C3C-C4C-NC	-3.69	103.20	107.94
6	K	201	CYC	C2C-C3C-C4C	3.67	106.83	101.34
6	M	201	CYC	C2C-C1C-NC	-3.66	105.24	108.29
6	A	302	CYC	CMA-C3A-C4A	3.65	130.77	125.10
6	D	201	CYC	CMD-C2D-C1D	3.63	130.90	125.62
6	U	201	CYC	C2C-C3C-C4C	3.62	106.77	101.34
6	A	301	CYC	C2C-C1C-NC	-3.59	105.30	108.29
6	F	201	CYC	C3C-C4C-NC	-3.55	103.37	107.94
6	P	201	CYC	C1B-CHB-C4A	-3.51	119.45	128.06
6	F	201	CYC	C2C-C1C-NC	-3.51	105.37	108.29
6	X	201	CYC	CAB-C3B-C4B	3.49	126.77	121.37
6	G	201	CYC	C2C-C3C-C4C	3.48	106.55	101.34
6	L	201	CYC	CHB-C4A-C3A	3.45	133.73	124.87
6	a	201	CYC	CMA-C3A-C4A	3.43	130.43	125.10
6	W	201	CYC	CMA-C3A-C4A	3.43	130.42	125.10
6	Z	301	CYC	CHB-C4A-C3A	3.41	133.64	124.87
6	B	201	CYC	C2C-C1C-NC	-3.40	105.46	108.29
6	B	201	CYC	CMA-C3A-C4A	3.37	130.33	125.10
6	J	201	CYC	CMA-C3A-C4A	3.36	130.31	125.10
6	N	201	CYC	C2C-C3C-C4C	3.34	106.34	101.34
6	D	201	CYC	C1B-CHB-C4A	-3.33	119.89	128.06
6	D	201	CYC	CMA-C3A-C4A	3.32	130.26	125.10
6	N	201	CYC	C3C-C4C-NC	-3.28	103.72	107.94
6	A	302	CYC	C3C-C4C-NC	-3.26	103.74	107.94
6	S	201	CYC	CMA-C3A-C4A	3.26	130.16	125.10
6	A	301	CYC	CMA-C3A-C4A	3.24	130.12	125.10
6	V	201	CYC	CMD-C2D-C1D	3.22	130.30	125.62
6	W	201	CYC	C3C-C4C-NC	-3.21	103.80	107.94
6	F	201	CYC	CMA-C3A-C4A	3.19	130.05	125.10
6	F	201	CYC	CBD-CAD-C3D	3.19	121.34	112.53
6	T	202	CYC	CMA-C3A-C4A	3.19	130.05	125.10
6	X	201	CYC	CHB-C4A-C3A	3.18	133.04	124.87
6	G	201	CYC	CMA-C3A-C4A	3.17	130.02	125.10
6	Q	201	CYC	C2C-C3C-C4C	3.17	106.08	101.34
6	M	201	CYC	CAB-C3B-C4B	3.16	126.26	121.37
6	V	201	CYC	CMA-C3A-C4A	3.14	129.97	125.10
6	Q	202	CYC	CMA-C3A-C4A	3.12	129.95	125.10
6	K	201	CYC	CMA-C3A-C4A	3.09	129.90	125.10
6	X	201	CYC	C2C-C1C-NC	-3.09	105.72	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	201	CYC	C2C-C3C-C4C	3.08	105.95	101.34
6	H	201	CYC	CMA-C3A-C4A	3.07	129.87	125.10
6	N	201	CYC	CMA-C3A-C4A	3.07	129.86	125.10
6	L	201	CYC	C2C-C1C-NC	-3.06	105.74	108.29
6	U	201	CYC	C3C-C4C-NC	-2.99	104.09	107.94
6	A	302	CYC	CHA-C4D-C3D	-2.99	120.80	127.22
6	A	302	CYC	CMD-C2D-C1D	2.98	129.95	125.62
6	R	201	CYC	C2C-C1C-NC	-2.96	105.82	108.29
6	a	202	CYC	CMA-C3A-C4A	2.94	129.66	125.10
6	J	202	CYC	CMA-C3A-C4A	2.94	129.66	125.10
6	C	202	CYC	C2C-C1C-NC	-2.94	105.84	108.29
6	T	201	CYC	C2C-C1C-NC	-2.93	105.84	108.29
6	a	202	CYC	CMD-C2D-C1D	2.93	129.88	125.62
6	Q	202	CYC	CAB-C3B-C4B	2.93	125.89	121.37
6	R	201	CYC	CAB-C3B-C4B	2.92	125.88	121.37
6	V	202	CYC	C2C-C1C-NC	-2.91	105.86	108.29
6	K	201	CYC	C3C-C4C-NC	-2.91	104.20	107.94
6	W	201	CYC	CMC-C2C-C1C	-2.91	106.14	112.40
6	X	201	CYC	C1A-NA-C4A	2.89	111.82	106.52
6	K	201	CYC	CMC-C2C-C1C	-2.87	106.21	112.40
6	Q	202	CYC	OB-C4B-C3B	-2.87	125.02	128.03
6	L	201	CYC	C1A-NA-C4A	2.86	111.76	106.52
6	C	201	CYC	CMA-C3A-C4A	2.82	129.49	125.10
6	I	201	CYC	CMA-C3A-C4A	2.82	129.48	125.10
6	Z	301	CYC	C1A-NA-C4A	2.81	111.67	106.52
6	M	201	CYC	C3C-C4C-NC	-2.80	104.34	107.94
6	P	201	CYC	CHB-C4A-C3A	2.79	132.05	124.87
6	a	201	CYC	C1B-CHB-C4A	-2.79	121.21	128.06
6	Q	202	CYC	C2C-C3C-C4C	2.75	105.47	101.34
6	N	201	CYC	CMC-C2C-C1C	-2.75	106.48	112.40
6	a	201	CYC	CHB-C4A-C3A	2.75	131.93	124.87
6	K	201	CYC	CHA-C4D-C3D	-2.73	121.34	127.22
6	A	301	CYC	C1B-CHB-C4A	-2.70	121.42	128.06
6	F	202	CYC	CMA-C3A-C4A	2.70	129.29	125.10
6	Q	202	CYC	C3C-C4C-NC	-2.69	104.47	107.94
6	P	201	CYC	C1A-NA-C4A	2.69	111.46	106.52
6	Q	201	CYC	C3C-C4C-NC	-2.67	104.50	107.94
6	G	201	CYC	CHA-C4D-C3D	-2.67	121.48	127.22
6	U	201	CYC	CHA-C4D-C3D	-2.66	121.49	127.22
6	U	201	CYC	CMC-C2C-C1C	-2.66	106.66	112.40
6	S	201	CYC	CHA-C4D-C3D	-2.66	121.50	127.22
6	a	201	CYC	C2C-C3C-C4C	2.65	105.31	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	202	CYC	CMD-C2D-C1D	2.65	129.47	125.62
6	Q	201	CYC	CMA-C3A-C4A	2.62	129.17	125.10
6	L	201	CYC	CHB-C4A-NA	-2.62	119.30	124.95
6	X	201	CYC	C1B-CHB-C4A	-2.61	121.64	128.06
6	W	201	CYC	CHA-C4D-C3D	-2.60	121.62	127.22
6	I	201	CYC	C2C-C1C-NC	-2.59	106.13	108.29
6	Q	202	CYC	C3B-C4B-NB	2.58	108.83	106.77
6	Q	201	CYC	CMB-C2B-C1B	2.58	127.29	124.16
6	a	201	CYC	C1A-NA-C4A	2.55	111.20	106.52
6	A	301	CYC	CHB-C4A-C3A	2.55	131.42	124.87
6	C	201	CYC	CMB-C2B-C1B	2.55	127.26	124.16
6	A	302	CYC	CHA-C1A-NA	2.54	129.94	124.60
6	D	201	CYC	CMC-C2C-C1C	-2.54	106.93	112.40
6	N	201	CYC	CHA-C4D-C3D	-2.53	121.78	127.22
6	A	301	CYC	C1A-NA-C4A	2.53	111.16	106.52
6	E	201	CYC	C2C-C1C-NC	-2.52	106.19	108.29
6	E	201	CYC	CMD-C2D-C1D	2.52	129.28	125.62
6	a	202	CYC	C1A-NA-C4A	2.51	111.12	106.52
6	B	201	CYC	CHA-C4D-C3D	-2.51	121.83	127.22
6	H	201	CYC	CHA-C4D-C3D	-2.50	121.85	127.22
6	T	202	CYC	C3C-C4C-NC	-2.49	104.73	107.94
6	R	201	CYC	CHA-C4D-C3D	-2.49	121.87	127.22
6	A	302	CYC	OB-C4B-C3B	-2.49	125.42	128.03
6	C	201	CYC	C1A-NA-C4A	2.49	111.08	106.52
6	D	201	CYC	C1A-NA-C4A	2.49	111.08	106.52
6	C	202	CYC	CMA-C3A-C4A	2.48	128.96	125.10
6	J	201	CYC	C1A-NA-C4A	2.47	111.06	106.52
6	A	302	CYC	CHB-C4A-C3A	2.47	131.22	124.87
6	I	201	CYC	CHA-C4D-C3D	-2.45	121.95	127.22
6	Q	201	CYC	C1A-NA-C4A	2.45	111.00	106.52
6	U	201	CYC	CMA-C3A-C4A	2.44	128.90	125.10
6	Z	301	CYC	CHB-C4A-NA	-2.44	119.68	124.95
6	E	201	CYC	C1A-NA-C4A	2.44	110.99	106.52
6	M	201	CYC	CHA-C4D-C3D	-2.43	122.00	127.22
6	Q	202	CYC	C1A-NA-C4A	2.42	110.97	106.52
6	A	302	CYC	C1A-NA-C4A	2.42	110.95	106.52
6	D	201	CYC	CHD-C1D-ND	-2.41	119.83	125.29
6	A	302	CYC	CHB-C1B-C2B	-2.41	122.16	126.97
6	J	202	CYC	C1A-NA-C4A	2.41	110.94	106.52
6	F	201	CYC	C1A-NA-C4A	2.41	110.94	106.52
6	M	201	CYC	CMB-C2B-C1B	2.41	127.09	124.16
6	C	201	CYC	CMD-C2D-C3D	-2.41	120.51	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	201	CYC	CHA-C4D-C3D	-2.40	122.05	127.22
6	T	201	CYC	C1A-NA-C4A	2.40	110.93	106.52
6	G	201	CYC	C3B-C4B-NB	2.40	108.68	106.77
6	T	202	CYC	C1A-NA-C4A	2.40	110.92	106.52
6	J	202	CYC	C2C-C1C-NC	-2.40	106.29	108.29
6	W	201	CYC	C1A-NA-C4A	2.40	110.91	106.52
6	V	201	CYC	C1A-NA-C4A	2.39	110.90	106.52
6	R	201	CYC	CMA-C3A-C4A	2.39	128.81	125.10
6	G	201	CYC	CMC-C2C-C1C	-2.38	107.26	112.40
6	C	202	CYC	C1A-NA-C4A	2.38	110.89	106.52
6	J	201	CYC	C2C-C1C-NC	-2.38	106.31	108.29
6	V	201	CYC	CHA-C1A-NA	2.37	129.57	124.60
6	K	201	CYC	C1A-NA-C4A	2.37	110.86	106.52
6	V	202	CYC	CMB-C2B-C1B	2.36	127.03	124.16
6	G	201	CYC	C1A-NA-C4A	2.36	110.84	106.52
6	T	202	CYC	CHA-C4D-C3D	-2.35	122.16	127.22
6	X	201	CYC	CHA-C4D-C3D	-2.35	122.17	127.22
6	K	201	CYC	C3B-C4B-NB	2.34	108.64	106.77
6	Z	301	CYC	CHA-C4D-C3D	-2.34	122.19	127.22
6	a	201	CYC	CHA-C4D-C3D	-2.33	122.21	127.22
6	N	201	CYC	C1A-NA-C4A	2.33	110.79	106.52
6	E	201	CYC	CMA-C3A-C4A	2.33	128.72	125.10
6	a	201	CYC	CMD-C2D-C3D	-2.32	120.70	125.62
6	E	201	CYC	OB-C4B-C3B	-2.32	125.59	128.03
6	H	201	CYC	C2C-C1C-NC	-2.31	106.36	108.29
6	I	201	CYC	C1A-NA-C4A	2.31	110.75	106.52
6	J	201	CYC	CMD-C2D-C3D	-2.30	120.74	125.62
6	M	201	CYC	CMA-C3A-C4A	2.30	128.67	125.10
6	B	201	CYC	C1A-NA-C4A	2.30	110.73	106.52
6	A	301	CYC	CMD-C2D-C3D	-2.29	120.76	125.62
6	M	201	CYC	C1A-NA-C4A	2.29	110.71	106.52
6	E	201	CYC	CMB-C2B-C1B	2.29	126.94	124.16
6	H	201	CYC	C1A-NA-C4A	2.28	110.71	106.52
6	A	302	CYC	CHA-C4D-ND	2.27	130.43	125.29
6	D	201	CYC	CHD-C1D-C2D	2.27	133.09	127.53
6	T	201	CYC	C3B-C4B-NB	2.27	108.58	106.77
6	F	201	CYC	C4D-C3D-C2D	-2.26	104.99	107.62
6	Y	301	CYC	CMA-C3A-C4A	2.26	128.61	125.10
6	U	201	CYC	C1A-NA-C4A	2.26	110.66	106.52
6	E	201	CYC	C3B-C4B-NB	2.25	108.56	106.77
6	N	201	CYC	C3B-C4B-NB	2.25	108.56	106.77
6	Y	301	CYC	CMB-C2B-C1B	2.24	126.88	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	201	CYC	CMB-C2B-C1B	2.24	126.88	124.16
6	D	201	CYC	CHB-C4A-C3A	2.23	130.61	124.87
6	L	201	CYC	CHB-C1B-C2B	-2.23	122.52	126.97
6	F	202	CYC	C1A-NA-C4A	2.23	110.61	106.52
6	H	201	CYC	C3B-C4B-NB	2.23	108.54	106.77
6	Z	301	CYC	CHD-C1D-C2D	2.23	132.99	127.53
6	Q	201	CYC	CHA-C4D-C3D	-2.23	122.43	127.22
6	a	202	CYC	C3B-C4B-NB	2.23	108.54	106.77
6	Y	301	CYC	CHA-C1A-NA	2.22	129.26	124.60
6	a	202	CYC	OB-C4B-C3B	-2.22	125.70	128.03
6	D	201	CYC	CMB-C2B-C1B	2.22	126.86	124.16
6	F	202	CYC	OB-C4B-C3B	-2.22	125.70	128.03
6	F	201	CYC	C3B-C4B-NB	2.21	108.53	106.77
6	B	201	CYC	C3B-C4B-NB	2.21	108.53	106.77
6	M	201	CYC	CMD-C2D-C3D	-2.21	120.94	125.62
6	D	201	CYC	C2C-C1C-NC	-2.21	106.45	108.29
6	S	201	CYC	C1A-NA-C4A	2.20	110.56	106.52
6	I	201	CYC	C3B-C4B-NB	2.20	108.52	106.77
6	A	301	CYC	CHA-C4D-C3D	-2.20	122.49	127.22
6	F	202	CYC	CMB-C2B-C1B	2.20	126.84	124.16
6	F	202	CYC	C3B-C4B-NB	2.20	108.52	106.77
6	A	302	CYC	C1B-CHB-C4A	-2.20	122.66	128.06
6	Q	201	CYC	CHA-C1A-NA	2.20	129.21	124.60
6	D	201	CYC	OB-C4B-C3B	-2.20	125.72	128.03
6	C	201	CYC	CHD-C1D-C2D	2.19	132.90	127.53
6	C	202	CYC	C3B-C4B-NB	2.19	108.51	106.77
6	J	201	CYC	CHB-C4A-C3A	2.19	130.49	124.87
6	a	202	CYC	CHB-C4A-C3A	2.19	130.49	124.87
6	J	202	CYC	CMB-C2B-C1B	2.19	126.82	124.16
6	V	201	CYC	CHA-C4D-C3D	-2.19	122.52	127.22
6	S	201	CYC	C3C-C4C-NC	-2.18	105.14	107.94
6	X	201	CYC	CHB-C4A-NA	-2.18	120.25	124.95
6	A	301	CYC	CMB-C2B-C1B	2.16	126.79	124.16
6	Z	301	CYC	O2A-CGA-CBA	2.15	120.81	114.00
6	X	201	CYC	CHD-C1D-C2D	2.15	132.79	127.53
6	D	201	CYC	C3B-C4B-NB	2.15	108.48	106.77
6	L	201	CYC	CHD-C1D-C2D	2.15	132.79	127.53
6	Z	301	CYC	CHD-C1D-ND	-2.14	120.46	125.29
6	F	201	CYC	C2C-C3C-C4C	2.14	104.54	101.34
6	T	201	CYC	CMD-C2D-C1D	2.14	128.72	125.62
6	T	201	CYC	CMA-C3A-C4A	2.13	128.41	125.10
6	R	201	CYC	C3B-C4B-NB	2.13	108.47	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	201	CYC	CMD-C2D-C3D	-2.13	121.11	125.62
6	M	201	CYC	C3B-C4B-NB	2.13	108.46	106.77
6	S	201	CYC	C3B-C4B-NB	2.13	108.46	106.77
6	Q	202	CYC	CHA-C4D-C3D	-2.13	122.64	127.22
6	M	201	CYC	OB-C4B-C3B	-2.13	125.80	128.03
6	M	201	CYC	CHA-C1A-NA	2.12	129.06	124.60
6	P	201	CYC	C3B-C4B-NB	2.12	108.46	106.77
6	M	201	CYC	C2C-C3C-C4C	2.12	104.52	101.34
6	W	201	CYC	CHA-C1A-NA	2.12	129.05	124.60
6	V	201	CYC	C3B-C4B-NB	2.12	108.45	106.77
6	T	201	CYC	OB-C4B-C3B	-2.12	125.81	128.03
6	a	201	CYC	CHD-C1D-C2D	2.11	132.70	127.53
6	V	202	CYC	C1A-NA-C4A	2.11	110.39	106.52
6	A	302	CYC	CHB-C1B-NB	2.10	130.55	126.06
6	A	302	CYC	C3B-C4B-NB	2.10	108.44	106.77
6	C	202	CYC	OB-C4B-C3B	-2.10	125.83	128.03
6	K	201	CYC	CHA-C4D-ND	2.10	130.02	125.29
6	F	201	CYC	CAD-C3D-C2D	-2.10	122.37	127.07
6	R	201	CYC	C1A-NA-C4A	2.08	110.33	106.52
6	V	202	CYC	CMA-C3A-C4A	2.07	128.32	125.10
6	L	201	CYC	C3B-C4B-NB	2.07	108.42	106.77
6	U	201	CYC	C3B-C4B-NB	2.07	108.41	106.77
6	C	202	CYC	CMB-C2B-C1B	2.06	126.67	124.16
6	J	202	CYC	C3B-C4B-NB	2.06	108.41	106.77
6	J	201	CYC	CMB-C2B-C1B	2.06	126.66	124.16
6	S	201	CYC	CHA-C1A-NA	2.06	128.92	124.60
6	J	201	CYC	C3B-C4B-NB	2.06	108.41	106.77
6	A	301	CYC	CHD-C1D-C2D	2.05	132.55	127.53
6	L	201	CYC	CMD-C2D-C3D	-2.05	121.28	125.62
6	C	201	CYC	CHD-C1D-ND	-2.04	120.67	125.29
6	A	302	CYC	CMB-C2B-C1B	2.04	126.64	124.16
6	X	201	CYC	CHD-C1D-ND	-2.04	120.68	125.29
6	V	202	CYC	C3B-C4B-NB	2.04	108.39	106.77
6	a	201	CYC	CHD-C1D-ND	-2.04	120.68	125.29
6	Y	301	CYC	CHD-C1D-C2D	2.03	132.51	127.53
6	Z	301	CYC	CMB-C2B-C1B	2.03	126.63	124.16
6	M	201	CYC	O2A-CGA-CBA	2.03	120.40	114.00
6	B	201	CYC	CMC-C2C-C1C	-2.03	108.03	112.40
6	a	201	CYC	CHA-C1A-NA	2.03	128.85	124.60
6	F	201	CYC	CHA-C1A-NA	2.02	128.85	124.60
6	Z	301	CYC	CMD-C2D-C3D	-2.02	121.33	125.62
6	J	202	CYC	OB-C4B-C3B	-2.02	125.91	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	201	CYC	CHA-C4D-ND	2.02	129.86	125.29
6	Y	301	CYC	CMD-C2D-C3D	-2.02	121.35	125.62
6	V	201	CYC	O2A-CGA-CBA	2.02	120.37	114.00
6	V	201	CYC	O2D-CGD-CBD	2.02	120.37	114.00
6	P	201	CYC	O2D-CGD-CBD	2.01	120.37	114.00
6	L	201	CYC	CHD-C1D-ND	-2.01	120.74	125.29
6	a	201	CYC	CMB-C2B-C1B	2.01	126.60	124.16
6	B	201	CYC	CHA-C1A-NA	2.01	128.81	124.60
6	A	302	CYC	CMC-C2C-C1C	-2.00	108.08	112.40
6	U	201	CYC	CHA-C4D-ND	2.00	129.82	125.29
6	R	201	CYC	OB-C4B-C3B	-2.00	125.93	128.03
6	Y	301	CYC	CHD-C1D-ND	-2.00	120.77	125.29

There are no chirality outliers.

All (452) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	CYC	NA-C4A-CHB-C1B
6	A	301	CYC	C3A-C4A-CHB-C1B
6	A	301	CYC	C2C-C3C-CAC-CBC
6	A	301	CYC	C4C-C3C-CAC-CBC
6	A	301	CYC	NC-C4C-CHD-C1D
6	A	302	CYC	NA-C4A-CHB-C1B
6	A	302	CYC	C3A-C4A-CHB-C1B
6	A	302	CYC	NC-C4C-CHD-C1D
6	B	201	CYC	NA-C4A-CHB-C1B
6	B	201	CYC	C3A-C4A-CHB-C1B
6	B	201	CYC	C2C-C3C-CAC-CBC
6	B	201	CYC	C4C-C3C-CAC-CBC
6	B	201	CYC	NC-C4C-CHD-C1D
6	C	201	CYC	NA-C4A-CHB-C1B
6	C	201	CYC	C3A-C4A-CHB-C1B
6	C	201	CYC	C2C-C3C-CAC-CBC
6	C	201	CYC	C4C-C3C-CAC-CBC
6	C	201	CYC	NC-C4C-CHD-C1D
6	C	202	CYC	NA-C1A-CHA-C4D
6	C	202	CYC	C2A-C1A-CHA-C4D
6	C	202	CYC	ND-C4D-CHA-C1A
6	C	202	CYC	C3D-C4D-CHA-C1A
6	C	202	CYC	NA-C4A-CHB-C1B
6	C	202	CYC	C3A-C4A-CHB-C1B
6	C	202	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	C	202	CYC	C4C-C3C-CAC-CBC
6	C	202	CYC	NC-C4C-CHD-C1D
6	C	202	CYC	C3C-C4C-CHD-C1D
6	C	202	CYC	ND-C1D-CHD-C4C
6	C	202	CYC	C2D-C1D-CHD-C4C
6	D	201	CYC	NA-C4A-CHB-C1B
6	D	201	CYC	C3A-C4A-CHB-C1B
6	D	201	CYC	C2C-C3C-CAC-CBC
6	D	201	CYC	C4C-C3C-CAC-CBC
6	D	201	CYC	NC-C4C-CHD-C1D
6	E	201	CYC	NA-C1A-CHA-C4D
6	E	201	CYC	C2A-C1A-CHA-C4D
6	E	201	CYC	ND-C4D-CHA-C1A
6	E	201	CYC	NA-C4A-CHB-C1B
6	E	201	CYC	C3A-C4A-CHB-C1B
6	E	201	CYC	C4C-C3C-CAC-CBC
6	E	201	CYC	NC-C4C-CHD-C1D
6	E	201	CYC	C3C-C4C-CHD-C1D
6	F	201	CYC	NA-C4A-CHB-C1B
6	F	201	CYC	C3A-C4A-CHB-C1B
6	F	201	CYC	C2C-C3C-CAC-CBC
6	F	201	CYC	C4C-C3C-CAC-CBC
6	F	201	CYC	NC-C4C-CHD-C1D
6	F	201	CYC	ND-C1D-CHD-C4C
6	F	201	CYC	C2D-C1D-CHD-C4C
6	F	202	CYC	NA-C1A-CHA-C4D
6	F	202	CYC	C2A-C1A-CHA-C4D
6	F	202	CYC	NA-C4A-CHB-C1B
6	F	202	CYC	C3A-C4A-CHB-C1B
6	F	202	CYC	C2C-C3C-CAC-CBC
6	F	202	CYC	C4C-C3C-CAC-CBC
6	F	202	CYC	NC-C4C-CHD-C1D
6	F	202	CYC	ND-C1D-CHD-C4C
6	F	202	CYC	C2D-C1D-CHD-C4C
6	G	201	CYC	NA-C4A-CHB-C1B
6	G	201	CYC	C3A-C4A-CHB-C1B
6	G	201	CYC	C2C-C3C-CAC-CBC
6	G	201	CYC	C4C-C3C-CAC-CBC
6	G	201	CYC	NC-C4C-CHD-C1D
6	G	201	CYC	ND-C1D-CHD-C4C
6	G	201	CYC	C2D-C1D-CHD-C4C
6	H	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	H	201	CYC	C3A-C4A-CHB-C1B
6	H	201	CYC	C2C-C3C-CAC-CBC
6	H	201	CYC	C4C-C3C-CAC-CBC
6	H	201	CYC	NC-C4C-CHD-C1D
6	H	201	CYC	C2D-C1D-CHD-C4C
6	I	201	CYC	NA-C4A-CHB-C1B
6	I	201	CYC	C3A-C4A-CHB-C1B
6	I	201	CYC	C4C-C3C-CAC-CBC
6	I	201	CYC	NC-C4C-CHD-C1D
6	I	201	CYC	C2D-C1D-CHD-C4C
6	J	201	CYC	NA-C4A-CHB-C1B
6	J	201	CYC	C3A-C4A-CHB-C1B
6	J	201	CYC	NC-C4C-CHD-C1D
6	J	201	CYC	ND-C1D-CHD-C4C
6	J	201	CYC	C2D-C1D-CHD-C4C
6	J	202	CYC	NA-C4A-CHB-C1B
6	J	202	CYC	C3A-C4A-CHB-C1B
6	J	202	CYC	C2C-C3C-CAC-CBC
6	J	202	CYC	C4C-C3C-CAC-CBC
6	J	202	CYC	NC-C4C-CHD-C1D
6	K	201	CYC	NA-C4A-CHB-C1B
6	K	201	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	C2C-C3C-CAC-CBC
6	K	201	CYC	NC-C4C-CHD-C1D
6	K	201	CYC	ND-C1D-CHD-C4C
6	K	201	CYC	C2D-C1D-CHD-C4C
6	L	201	CYC	NA-C4A-CHB-C1B
6	L	201	CYC	C3A-C4A-CHB-C1B
6	L	201	CYC	NC-C4C-CHD-C1D
6	M	201	CYC	NA-C4A-CHB-C1B
6	M	201	CYC	C3A-C4A-CHB-C1B
6	M	201	CYC	C2C-C3C-CAC-CBC
6	M	201	CYC	C4C-C3C-CAC-CBC
6	M	201	CYC	NC-C4C-CHD-C1D
6	N	201	CYC	NA-C4A-CHB-C1B
6	N	201	CYC	C3A-C4A-CHB-C1B
6	N	201	CYC	C2C-C3C-CAC-CBC
6	N	201	CYC	NC-C4C-CHD-C1D
6	N	201	CYC	ND-C1D-CHD-C4C
6	N	201	CYC	C2D-C1D-CHD-C4C
6	P	201	CYC	NA-C4A-CHB-C1B
6	P	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	P	201	CYC	NC-C4C-CHD-C1D
6	P	201	CYC	C3C-C4C-CHD-C1D
6	Q	201	CYC	NA-C4A-CHB-C1B
6	Q	201	CYC	C3A-C4A-CHB-C1B
6	Q	201	CYC	C2C-C3C-CAC-CBC
6	Q	201	CYC	C4C-C3C-CAC-CBC
6	Q	201	CYC	NC-C4C-CHD-C1D
6	Q	202	CYC	NA-C4A-CHB-C1B
6	Q	202	CYC	C3A-C4A-CHB-C1B
6	Q	202	CYC	C2C-C3C-CAC-CBC
6	Q	202	CYC	C4C-C3C-CAC-CBC
6	Q	202	CYC	NC-C4C-CHD-C1D
6	Q	202	CYC	ND-C1D-CHD-C4C
6	Q	202	CYC	C2D-C1D-CHD-C4C
6	R	201	CYC	NA-C4A-CHB-C1B
6	R	201	CYC	C3A-C4A-CHB-C1B
6	R	201	CYC	C4C-C3C-CAC-CBC
6	R	201	CYC	NC-C4C-CHD-C1D
6	R	201	CYC	ND-C1D-CHD-C4C
6	R	201	CYC	C2D-C1D-CHD-C4C
6	S	201	CYC	NA-C4A-CHB-C1B
6	S	201	CYC	C3A-C4A-CHB-C1B
6	S	201	CYC	C4C-C3C-CAC-CBC
6	S	201	CYC	NC-C4C-CHD-C1D
6	T	201	CYC	NA-C1A-CHA-C4D
6	T	201	CYC	C2A-C1A-CHA-C4D
6	T	201	CYC	ND-C4D-CHA-C1A
6	T	201	CYC	C3D-C4D-CHA-C1A
6	T	201	CYC	NA-C4A-CHB-C1B
6	T	201	CYC	C3A-C4A-CHB-C1B
6	T	201	CYC	C4C-C3C-CAC-CBC
6	T	201	CYC	NC-C4C-CHD-C1D
6	T	201	CYC	C3C-C4C-CHD-C1D
6	T	202	CYC	NA-C4A-CHB-C1B
6	T	202	CYC	C3A-C4A-CHB-C1B
6	T	202	CYC	NC-C4C-CHD-C1D
6	T	202	CYC	ND-C1D-CHD-C4C
6	T	202	CYC	C2D-C1D-CHD-C4C
6	U	201	CYC	NA-C4A-CHB-C1B
6	U	201	CYC	C3A-C4A-CHB-C1B
6	U	201	CYC	C2C-C3C-CAC-CBC
6	U	201	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
6	U	201	CYC	ND-C1D-CHD-C4C
6	U	201	CYC	C2D-C1D-CHD-C4C
6	V	201	CYC	NA-C4A-CHB-C1B
6	V	201	CYC	C3A-C4A-CHB-C1B
6	V	201	CYC	C2C-C3C-CAC-CBC
6	V	201	CYC	C4C-C3C-CAC-CBC
6	V	201	CYC	NC-C4C-CHD-C1D
6	V	202	CYC	ND-C4D-CHA-C1A
6	V	202	CYC	C3D-C4D-CHA-C1A
6	V	202	CYC	NA-C4A-CHB-C1B
6	V	202	CYC	C3A-C4A-CHB-C1B
6	V	202	CYC	C2C-C3C-CAC-CBC
6	V	202	CYC	C4C-C3C-CAC-CBC
6	V	202	CYC	NC-C4C-CHD-C1D
6	V	202	CYC	C3C-C4C-CHD-C1D
6	W	201	CYC	NA-C4A-CHB-C1B
6	W	201	CYC	C3A-C4A-CHB-C1B
6	W	201	CYC	NC-C4C-CHD-C1D
6	W	201	CYC	ND-C1D-CHD-C4C
6	W	201	CYC	C2D-C1D-CHD-C4C
6	X	201	CYC	NA-C4A-CHB-C1B
6	X	201	CYC	C3A-C4A-CHB-C1B
6	X	201	CYC	C2C-C3C-CAC-CBC
6	X	201	CYC	NC-C4C-CHD-C1D
6	X	201	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	C2D-C1D-CHD-C4C
6	Y	301	CYC	NA-C4A-CHB-C1B
6	Y	301	CYC	C3A-C4A-CHB-C1B
6	Y	301	CYC	C2C-C3C-CAC-CBC
6	Y	301	CYC	C4C-C3C-CAC-CBC
6	Y	301	CYC	NC-C4C-CHD-C1D
6	Z	301	CYC	C2C-C3C-CAC-CBC
6	Z	301	CYC	C4C-C3C-CAC-CBC
6	Z	301	CYC	NC-C4C-CHD-C1D
6	Z	301	CYC	ND-C1D-CHD-C4C
6	Z	301	CYC	C2D-C1D-CHD-C4C
6	a	201	CYC	NA-C4A-CHB-C1B
6	a	201	CYC	C3A-C4A-CHB-C1B
6	a	201	CYC	C2C-C3C-CAC-CBC
6	a	201	CYC	C4C-C3C-CAC-CBC
6	a	201	CYC	NC-C4C-CHD-C1D
6	a	202	CYC	ND-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
6	a	202	CYC	C3D-C4D-CHA-C1A
6	a	202	CYC	NA-C4A-CHB-C1B
6	a	202	CYC	C3A-C4A-CHB-C1B
6	a	202	CYC	NC-C4C-CHD-C1D
6	a	202	CYC	C3C-C4C-CHD-C1D
6	N	201	CYC	C2B-C3B-CAB-CBB
6	Q	201	CYC	C2B-C3B-CAB-CBB
6	V	201	CYC	C2B-C3B-CAB-CBB
6	A	301	CYC	C2B-C3B-CAB-CBB
6	J	201	CYC	C2B-C3B-CAB-CBB
6	K	201	CYC	C2B-C3B-CAB-CBB
6	C	201	CYC	C2B-C3B-CAB-CBB
6	I	201	CYC	C2B-C3B-CAB-CBB
6	G	201	CYC	C2B-C3B-CAB-CBB
6	Z	301	CYC	C2B-C3B-CAB-CBB
6	U	201	CYC	C2B-C3B-CAB-CBB
6	W	201	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	C2B-C3B-CAB-CBB
6	F	201	CYC	C2B-C3B-CAB-CBB
6	S	201	CYC	C2B-C3B-CAB-CBB
6	T	202	CYC	C2B-C3B-CAB-CBB
6	a	201	CYC	C2B-C3B-CAB-CBB
6	A	302	CYC	ND-C1D-CHD-C4C
6	C	201	CYC	ND-C1D-CHD-C4C
6	H	201	CYC	ND-C1D-CHD-C4C
6	I	201	CYC	ND-C1D-CHD-C4C
6	J	202	CYC	ND-C1D-CHD-C4C
6	B	201	CYC	C2D-C1D-CHD-C4C
6	C	201	CYC	C2D-C1D-CHD-C4C
6	D	201	CYC	C2D-C1D-CHD-C4C
6	E	201	CYC	C3D-C4D-CHA-C1A
6	E	201	CYC	C2D-C1D-CHD-C4C
6	L	201	CYC	C2D-C1D-CHD-C4C
6	M	201	CYC	C2D-C1D-CHD-C4C
6	Q	201	CYC	C2D-C1D-CHD-C4C
6	a	201	CYC	C2D-C1D-CHD-C4C
6	a	202	CYC	C2D-C1D-CHD-C4C
6	H	201	CYC	C2B-C3B-CAB-CBB
6	P	201	CYC	C2B-C3B-CAB-CBB
6	A	302	CYC	C2B-C3B-CAB-CBB
6	Y	301	CYC	NA-C1A-CHA-C4D
6	a	202	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	V	202	CYC	C2B-C3B-CAB-CBB
6	Y	301	CYC	C2B-C3B-CAB-CBB
6	F	201	CYC	C4D-C3D-CAD-CBD
6	P	201	CYC	C3D-CAD-CBD-CGD
6	Q	202	CYC	C3D-CAD-CBD-CGD
6	V	202	CYC	C2A-CAA-CBA-CGA
6	P	201	CYC	C3A-C4A-CHB-C1B
6	A	301	CYC	ND-C1D-CHD-C4C
6	B	201	CYC	ND-C1D-CHD-C4C
6	D	201	CYC	ND-C1D-CHD-C4C
6	E	201	CYC	ND-C1D-CHD-C4C
6	L	201	CYC	ND-C1D-CHD-C4C
6	M	201	CYC	ND-C1D-CHD-C4C
6	P	201	CYC	ND-C1D-CHD-C4C
6	Q	201	CYC	ND-C1D-CHD-C4C
6	S	201	CYC	ND-C1D-CHD-C4C
6	T	201	CYC	ND-C1D-CHD-C4C
6	V	201	CYC	ND-C1D-CHD-C4C
6	V	202	CYC	ND-C1D-CHD-C4C
6	Y	301	CYC	ND-C1D-CHD-C4C
6	a	201	CYC	ND-C1D-CHD-C4C
6	a	202	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	C2B-C3B-CAB-CBB
6	A	301	CYC	C2D-C1D-CHD-C4C
6	J	202	CYC	C2D-C1D-CHD-C4C
6	P	201	CYC	C2D-C1D-CHD-C4C
6	S	201	CYC	C2D-C1D-CHD-C4C
6	T	201	CYC	C2D-C1D-CHD-C4C
6	V	201	CYC	C2D-C1D-CHD-C4C
6	V	202	CYC	C2D-C1D-CHD-C4C
6	Y	301	CYC	C2D-C1D-CHD-C4C
6	F	201	CYC	C2D-C3D-CAD-CBD
6	A	302	CYC	C2D-C1D-CHD-C4C
6	L	201	CYC	C2B-C3B-CAB-CBB
6	A	301	CYC	C4B-C3B-CAB-CBB
6	C	201	CYC	C4B-C3B-CAB-CBB
6	G	201	CYC	C4B-C3B-CAB-CBB
6	I	201	CYC	C4B-C3B-CAB-CBB
6	J	201	CYC	C4B-C3B-CAB-CBB
6	K	201	CYC	C4B-C3B-CAB-CBB
6	N	201	CYC	C4B-C3B-CAB-CBB
6	Q	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	U	201	CYC	C4B-C3B-CAB-CBB
6	V	201	CYC	C4B-C3B-CAB-CBB
6	W	201	CYC	C4B-C3B-CAB-CBB
6	Z	301	CYC	C4B-C3B-CAB-CBB
6	T	201	CYC	C2B-C3B-CAB-CBB
6	E	201	CYC	C2A-CAA-CBA-CGA
6	J	202	CYC	C3D-CAD-CBD-CGD
6	X	201	CYC	C3D-CAD-CBD-CGD
6	V	202	CYC	NB-C1B-CHB-C4A
6	X	201	CYC	NB-C1B-CHB-C4A
6	Y	301	CYC	C2A-C1A-CHA-C4D
6	a	202	CYC	C2A-C1A-CHA-C4D
6	Z	301	CYC	NA-C4A-CHB-C1B
6	F	202	CYC	NB-C1B-CHB-C4A
6	C	202	CYC	C2B-C3B-CAB-CBB
6	a	202	CYC	C2B-C3B-CAB-CBB
6	Z	301	CYC	C3A-C4A-CHB-C1B
6	V	202	CYC	C2B-C1B-CHB-C4A
6	X	201	CYC	C2B-C1B-CHB-C4A
6	E	201	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	C4B-C3B-CAB-CBB
6	F	201	CYC	C4B-C3B-CAB-CBB
6	H	201	CYC	C4B-C3B-CAB-CBB
6	P	201	CYC	C4B-C3B-CAB-CBB
6	S	201	CYC	C4B-C3B-CAB-CBB
6	T	202	CYC	C4B-C3B-CAB-CBB
6	a	201	CYC	C4B-C3B-CAB-CBB
6	D	201	CYC	C2B-C3B-CAB-CBB
6	J	202	CYC	C2B-C3B-CAB-CBB
6	K	201	CYC	C3D-CAD-CBD-CGD
6	J	202	CYC	NA-C1A-CHA-C4D
6	F	202	CYC	C2B-C1B-CHB-C4A
6	a	201	CYC	NB-C1B-CHB-C4A
6	P	201	CYC	NA-C1A-CHA-C4D
6	R	201	CYC	C3D-CAD-CBD-CGD
6	A	302	CYC	C4B-C3B-CAB-CBB
6	E	201	CYC	C2C-C3C-CAC-CBC
6	J	201	CYC	C2C-C3C-CAC-CBC
6	P	201	CYC	C2C-C3C-CAC-CBC
6	R	201	CYC	C2C-C3C-CAC-CBC
6	T	201	CYC	C2C-C3C-CAC-CBC
6	V	202	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	A	301	CYC	NB-C1B-CHB-C4A
6	V	202	CYC	C4B-C3B-CAB-CBB
6	Y	301	CYC	C4B-C3B-CAB-CBB
6	J	202	CYC	C2A-C1A-CHA-C4D
6	L	201	CYC	NB-C1B-CHB-C4A
6	P	201	CYC	NB-C1B-CHB-C4A
6	A	301	CYC	NA-C1A-CHA-C4D
6	P	201	CYC	C2A-C1A-CHA-C4D
6	X	201	CYC	C4C-C3C-CAC-CBC
6	T	201	CYC	C4B-C3B-CAB-CBB
6	X	201	CYC	C4B-C3B-CAB-CBB
6	A	301	CYC	C2A-CAA-CBA-CGA
6	H	201	CYC	C3D-CAD-CBD-CGD
6	P	201	CYC	C2A-CAA-CBA-CGA
6	U	201	CYC	C3D-CAD-CBD-CGD
6	V	201	CYC	C2A-CAA-CBA-CGA
6	L	201	CYC	C4B-C3B-CAB-CBB
6	R	201	CYC	C4B-C3B-CAB-CBB
6	V	202	CYC	C2A-C1A-CHA-C4D
6	I	201	CYC	C2C-C3C-CAC-CBC
6	L	201	CYC	C2C-C3C-CAC-CBC
6	A	301	CYC	C2A-C1A-CHA-C4D
6	a	201	CYC	C2B-C1B-CHB-C4A
6	a	201	CYC	C2A-CAA-CBA-CGA
6	R	201	CYC	C2B-C3B-CAB-CBB
6	D	201	CYC	C2A-CAA-CBA-CGA
6	V	202	CYC	CAD-CBD-CGD-O2D
6	I	201	CYC	C3D-CAD-CBD-CGD
6	N	201	CYC	C3D-CAD-CBD-CGD
6	T	202	CYC	C3D-CAD-CBD-CGD
6	C	201	CYC	NA-C1A-CHA-C4D
6	J	201	CYC	CAA-CBA-CGA-O1A
6	V	202	CYC	CAD-CBD-CGD-O1D
6	G	201	CYC	C3D-CAD-CBD-CGD
6	D	201	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAD-CBD-CGD-O2D
6	Z	301	CYC	CAA-CBA-CGA-O1A
6	C	201	CYC	CAA-CBA-CGA-O2A
6	F	202	CYC	CAA-CBA-CGA-O2A
6	I	201	CYC	CAA-CBA-CGA-O2A
6	T	202	CYC	CAA-CBA-CGA-O1A
6	L	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	A	301	CYC	C2B-C1B-CHB-C4A
6	P	201	CYC	C2B-C1B-CHB-C4A
6	J	202	CYC	CAA-CBA-CGA-O2A
6	P	201	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAD-CBD-CGD-O1D
6	L	201	CYC	CAA-CBA-CGA-O1A
6	X	201	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	C3D-CAD-CBD-CGD
6	L	201	CYC	C3D-CAD-CBD-CGD
6	a	202	CYC	C3D-CAD-CBD-CGD
6	J	201	CYC	CAA-CBA-CGA-O2A
6	Q	201	CYC	CAA-CBA-CGA-O1A
6	W	201	CYC	CAA-CBA-CGA-O2A
6	F	202	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	CAA-CBA-CGA-O1A
6	J	202	CYC	CAA-CBA-CGA-O1A
6	U	201	CYC	CAD-CBD-CGD-O2D
6	M	201	CYC	CAA-CBA-CGA-O2A
6	X	201	CYC	CAA-CBA-CGA-O2A
6	C	201	CYC	CAA-CBA-CGA-O1A
6	Y	301	CYC	C2A-CAA-CBA-CGA
6	D	201	CYC	CAA-CBA-CGA-O1A
6	Q	201	CYC	CAA-CBA-CGA-O2A
6	Z	301	CYC	CAD-CBD-CGD-O2D
6	J	201	CYC	C4C-C3C-CAC-CBC
6	A	302	CYC	CAA-CBA-CGA-O2A
6	M	201	CYC	CAA-CBA-CGA-O1A
6	H	201	CYC	CAA-CBA-CGA-O2A
6	Z	301	CYC	CAA-CBA-CGA-O2A
6	a	202	CYC	CAA-CBA-CGA-O2A
6	Q	201	CYC	NB-C1B-CHB-C4A
6	P	201	CYC	CAD-CBD-CGD-O2D
6	T	202	CYC	CAA-CBA-CGA-O2A
6	B	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O2A
6	a	202	CYC	CAA-CBA-CGA-O1A
6	J	202	CYC	CAD-CBD-CGD-O2D
6	U	201	CYC	CAD-CBD-CGD-O1D
6	C	202	CYC	CAA-CBA-CGA-O2A
6	E	201	CYC	CAA-CBA-CGA-O1A
6	H	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	B	201	CYC	CAA-CBA-CGA-O2A
6	C	202	CYC	CAA-CBA-CGA-O1A
6	J	202	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAA-CBA-CGA-O1A
6	E	201	CYC	CAD-CBD-CGD-O2D
6	F	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	CAD-CBD-CGD-O1D
6	Z	301	CYC	CAD-CBD-CGD-O1D
6	S	201	CYC	C3D-CAD-CBD-CGD
6	E	201	CYC	CAA-CBA-CGA-O2A
6	V	201	CYC	CAA-CBA-CGA-O2A
6	G	201	CYC	CAA-CBA-CGA-O1A
6	G	201	CYC	CAA-CBA-CGA-O2A
6	N	201	CYC	CAA-CBA-CGA-O2A
6	V	202	CYC	CAA-CBA-CGA-O2A
6	F	201	CYC	CAA-CBA-CGA-O2A
6	Q	202	CYC	NA-C1A-CHA-C4D
6	a	202	CYC	CAD-CBD-CGD-O2D
6	N	201	CYC	CAA-CBA-CGA-O1A
6	V	202	CYC	CAA-CBA-CGA-O1A
6	L	201	CYC	C2B-C1B-CHB-C4A
6	S	201	CYC	CAA-CBA-CGA-O1A
6	S	201	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAA-CBA-CGA-O2A
6	E	201	CYC	CAD-CBD-CGD-O1D
6	Y	301	CYC	CAA-CBA-CGA-O2A
6	A	302	CYC	CAA-CBA-CGA-O1A
6	V	201	CYC	CAA-CBA-CGA-O1A
6	a	202	CYC	CAD-CBD-CGD-O1D
6	R	201	CYC	CAA-CBA-CGA-O1A
6	R	201	CYC	CAA-CBA-CGA-O2A
6	U	201	CYC	CAA-CBA-CGA-O1A
6	U	201	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAA-CBA-CGA-O1A
6	Y	301	CYC	CAA-CBA-CGA-O1A
6	C	202	CYC	CAD-CBD-CGD-O2D
6	Q	202	CYC	CAA-CBA-CGA-O1A
6	a	201	CYC	CAD-CBD-CGD-O2D
6	F	201	CYC	CAD-CBD-CGD-O2D
6	I	201	CYC	CAD-CBD-CGD-O2D
6	Q	202	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	J	202	CYC	C3C-C4C-CHD-C1D
6	H	201	CYC	NB-C1B-CHB-C4A
6	T	202	CYC	NB-C1B-CHB-C4A
6	C	202	CYC	C4B-C3B-CAB-CBB
6	a	202	CYC	C4B-C3B-CAB-CBB
6	I	201	CYC	CAD-CBD-CGD-O1D
6	Q	201	CYC	C2B-C1B-CHB-C4A

There are no ring outliers.

34 monomers are involved in 154 short contacts:

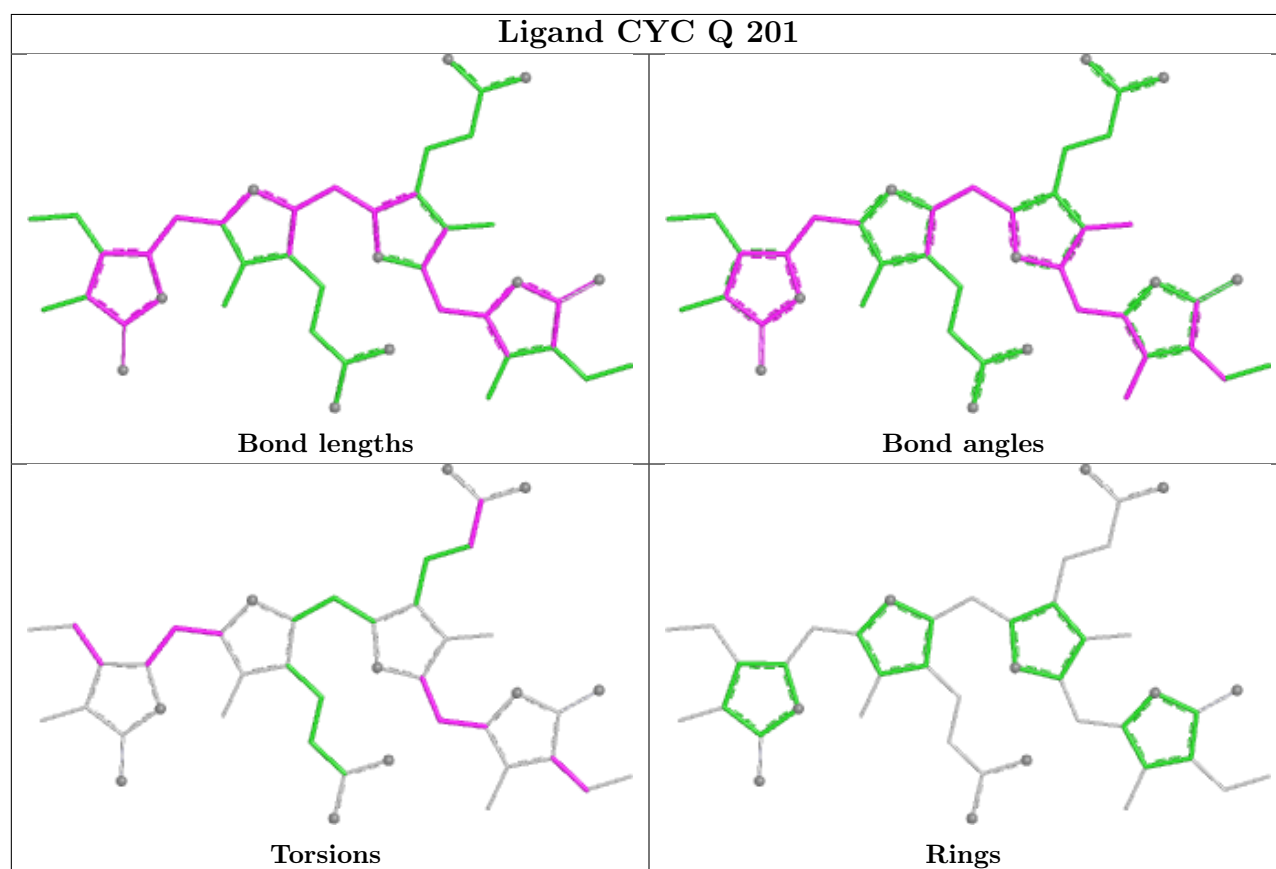
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	201	CYC	6	0
6	Y	301	CYC	2	0
6	T	202	CYC	3	0
6	S	201	CYC	6	0
6	C	202	CYC	10	0
6	K	201	CYC	5	0
6	N	201	CYC	6	0
6	C	201	CYC	4	0
6	E	201	CYC	3	0
6	X	201	CYC	8	0
6	F	202	CYC	3	0
6	Z	301	CYC	5	0
6	H	201	CYC	2	0
6	J	201	CYC	2	0
6	Q	202	CYC	4	0
6	a	201	CYC	4	0
6	F	201	CYC	4	0
6	A	301	CYC	5	0
6	P	201	CYC	2	0
6	U	201	CYC	4	0
6	J	202	CYC	2	0
6	B	201	CYC	7	0
6	G	201	CYC	3	0
6	V	202	CYC	3	0
6	T	201	CYC	5	0
6	W	201	CYC	5	0
6	I	201	CYC	4	0
6	M	201	CYC	6	0
6	a	202	CYC	5	0
6	D	201	CYC	2	0

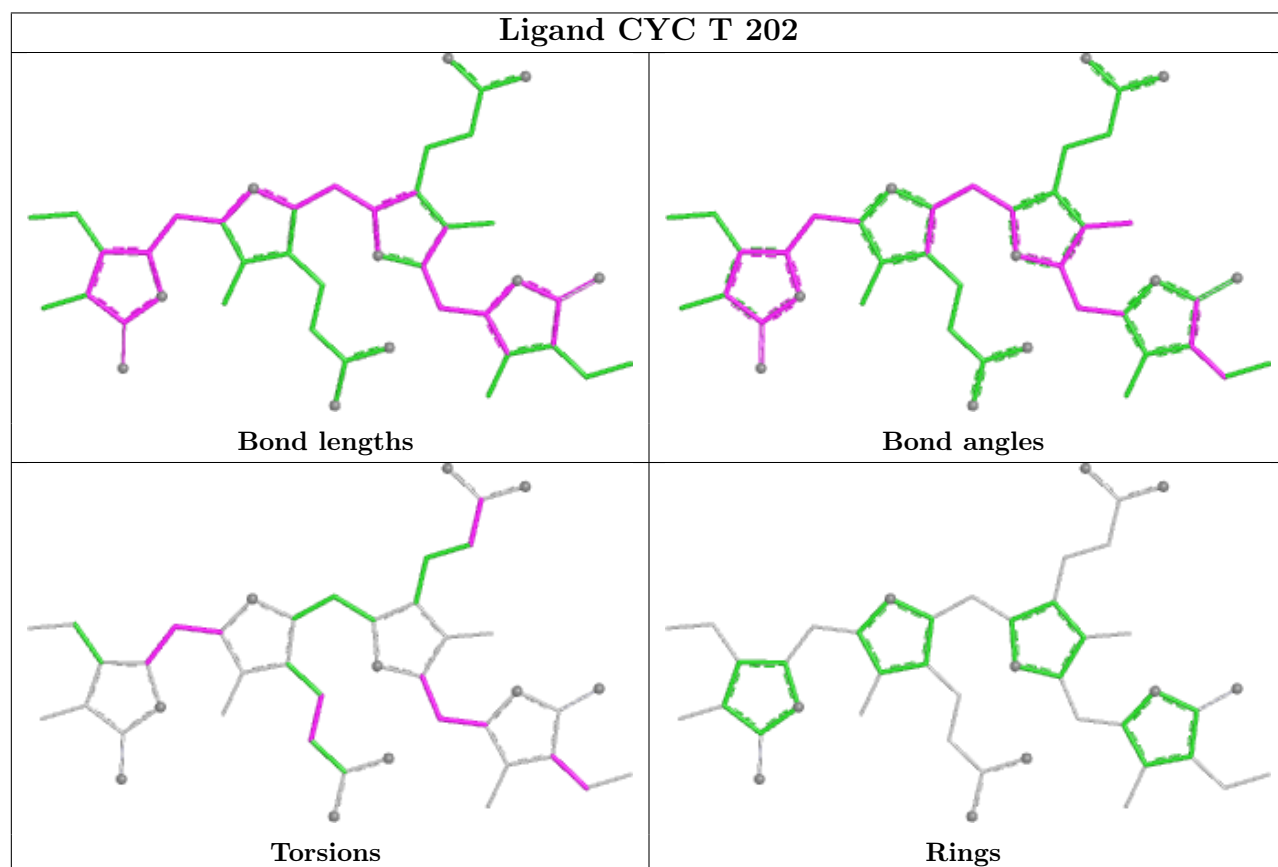
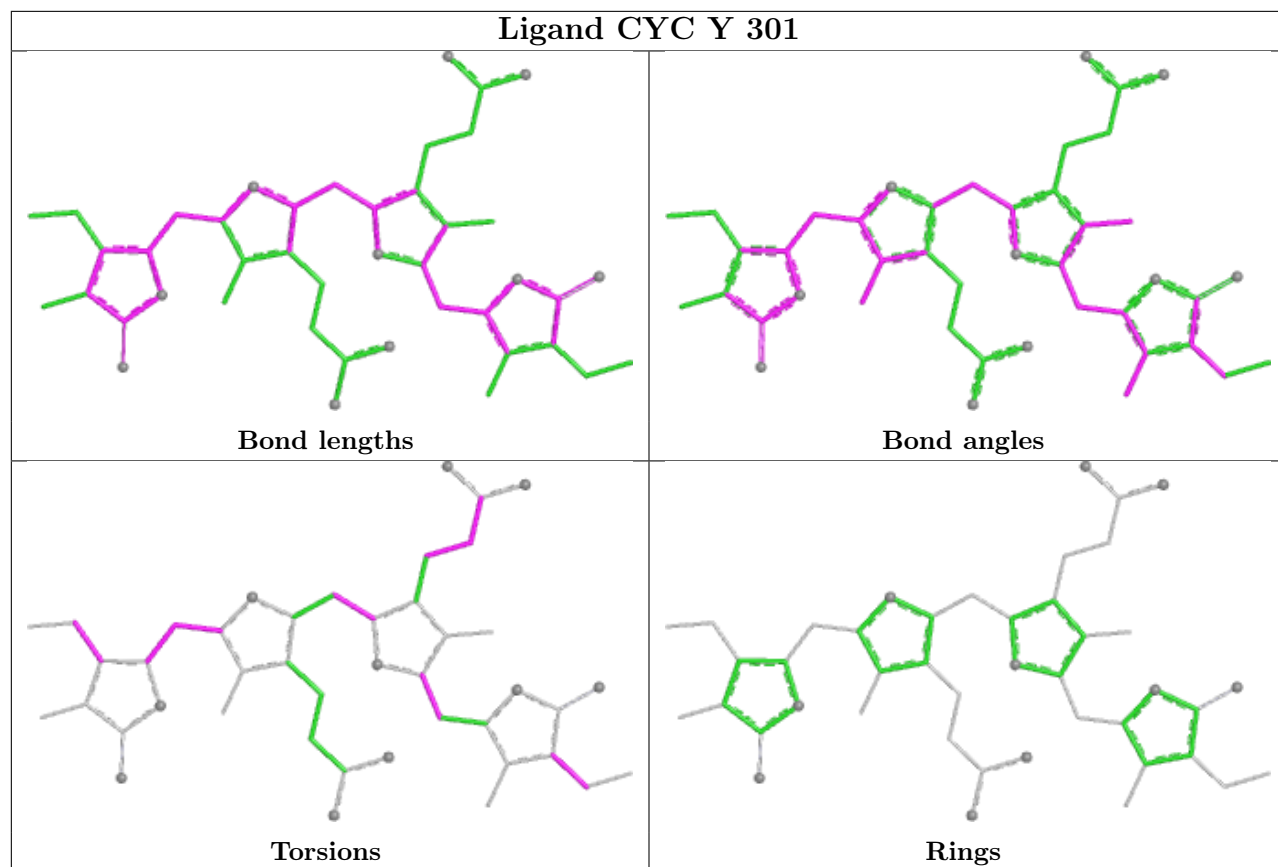
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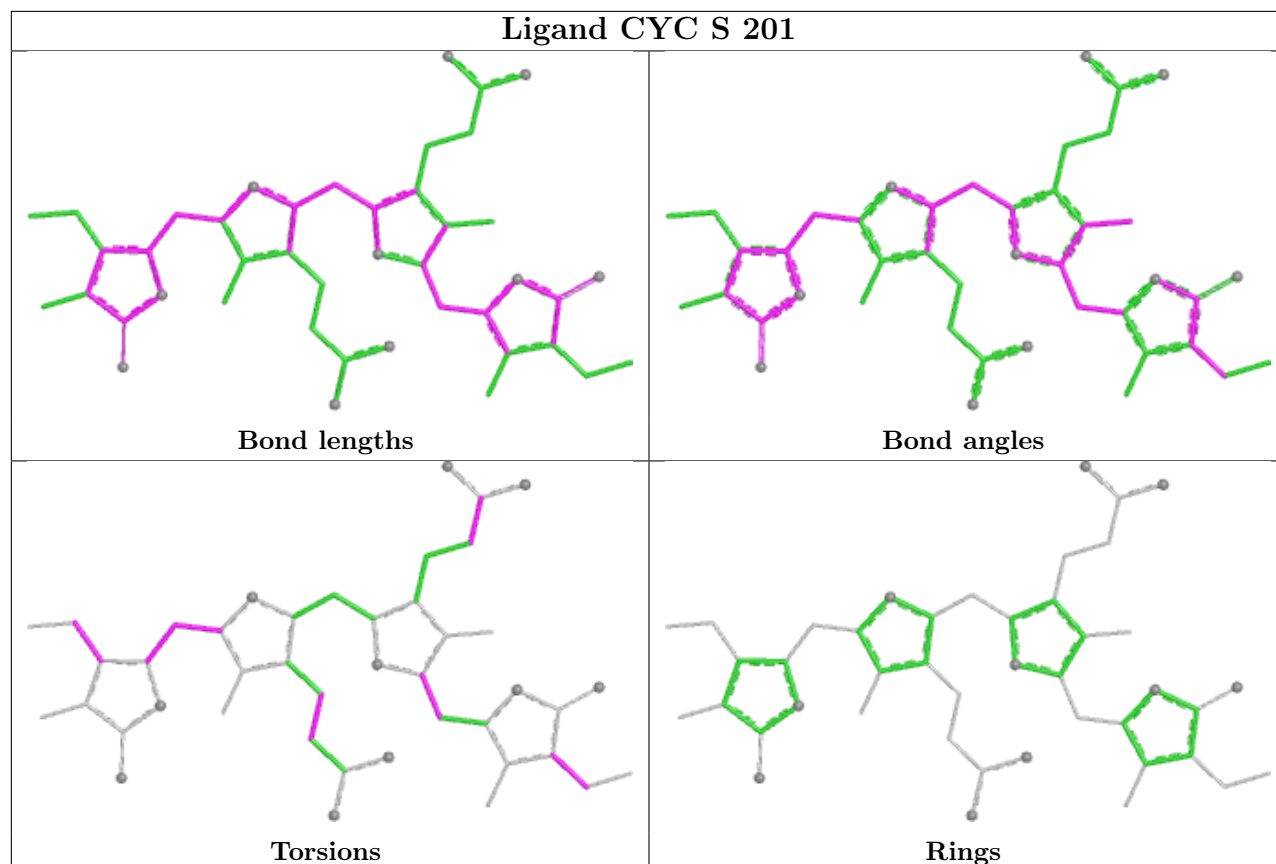
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	201	CYC	5	0
6	A	302	CYC	7	0
6	V	201	CYC	8	0
6	L	201	CYC	4	0

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.

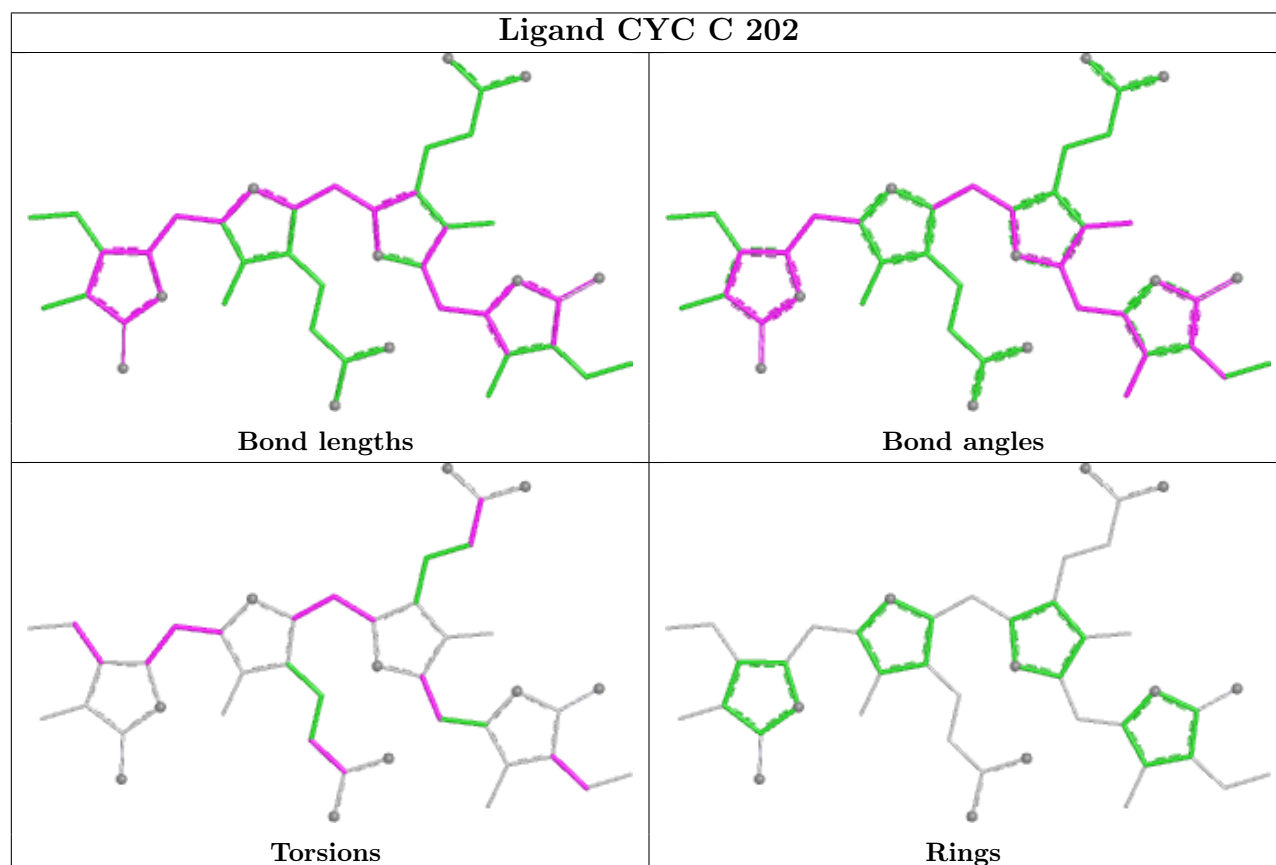


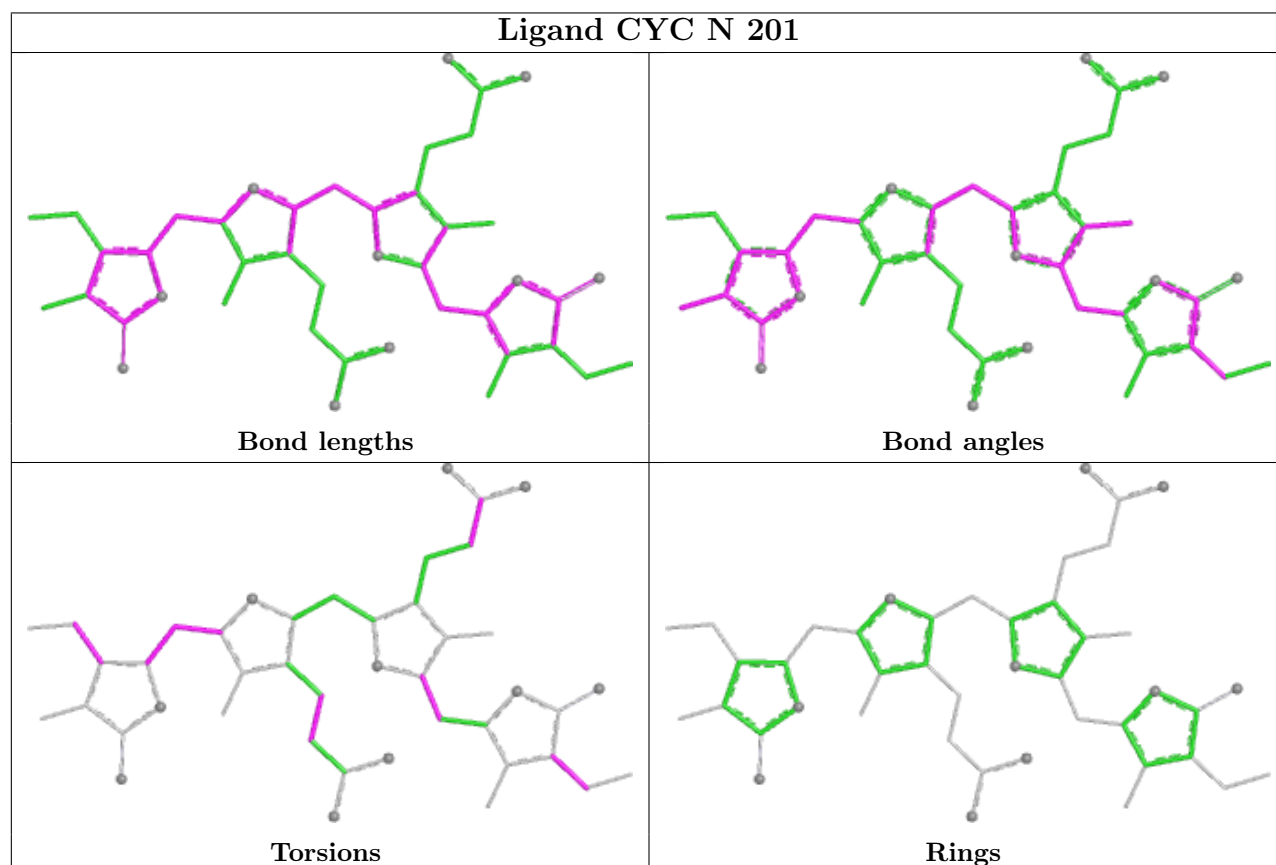
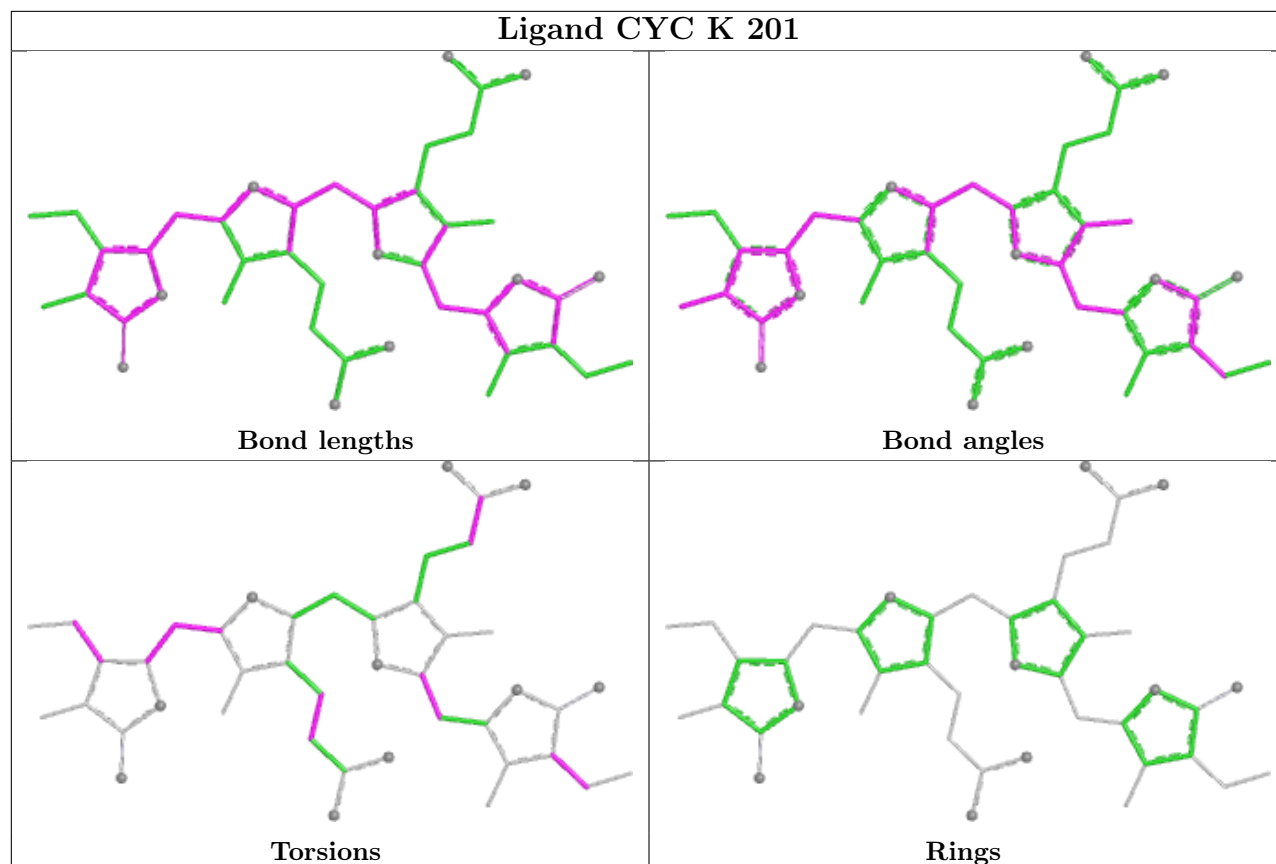


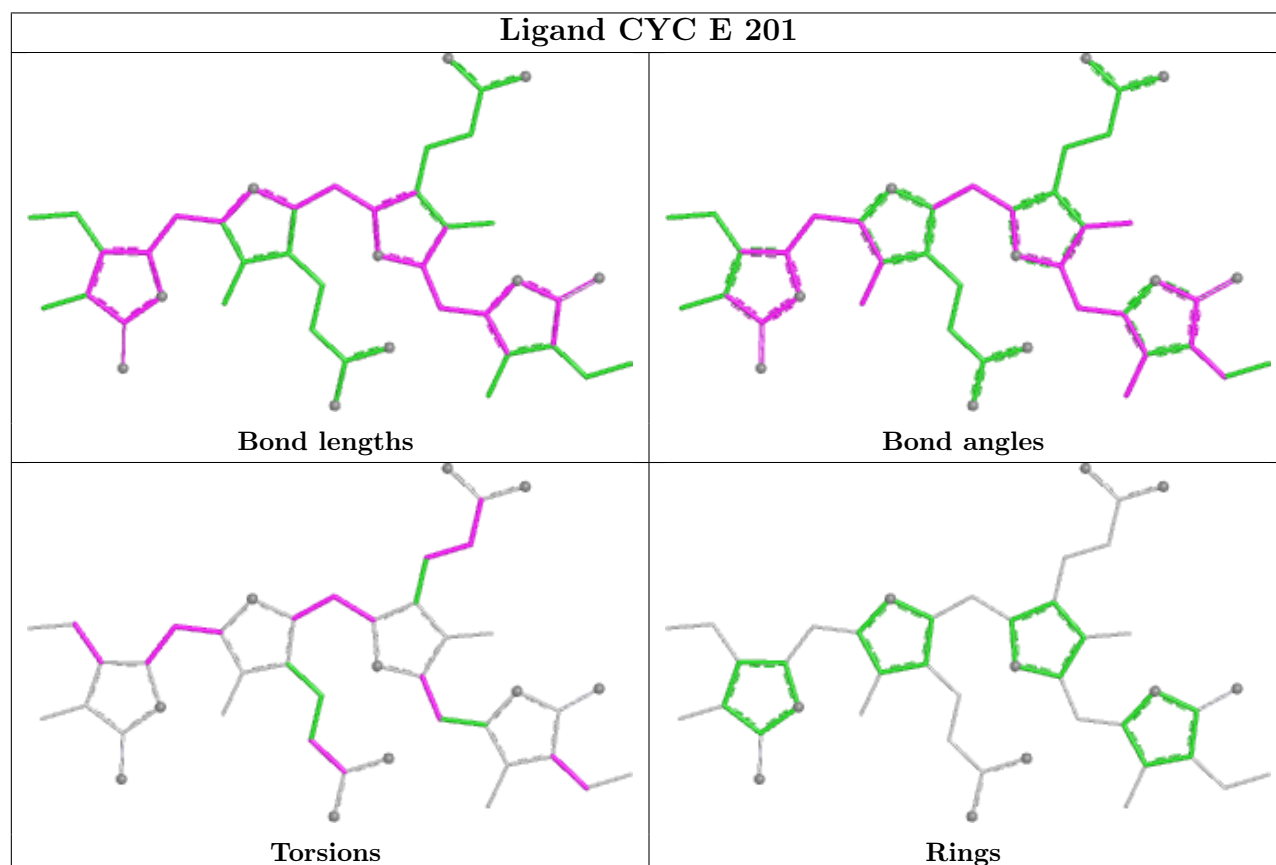
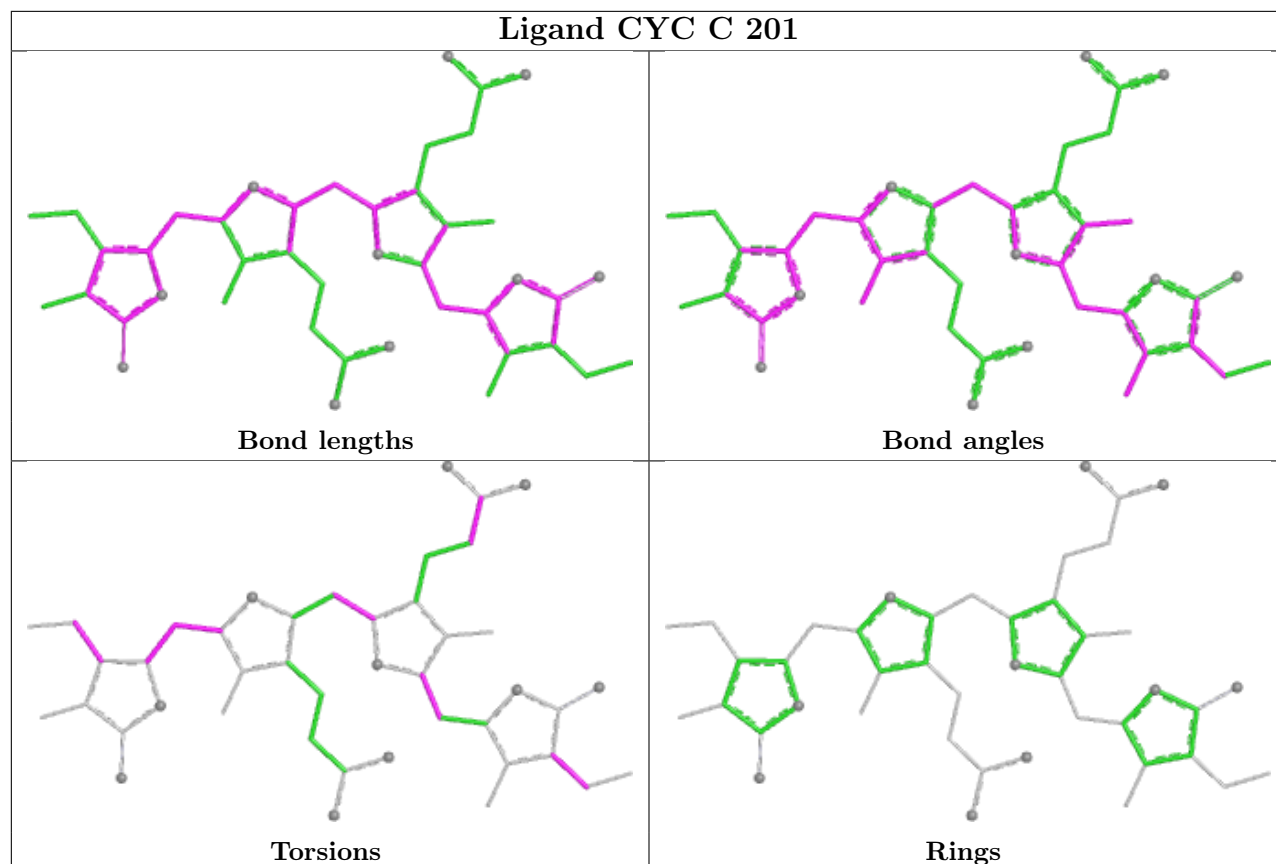
Ligand CYC S 201

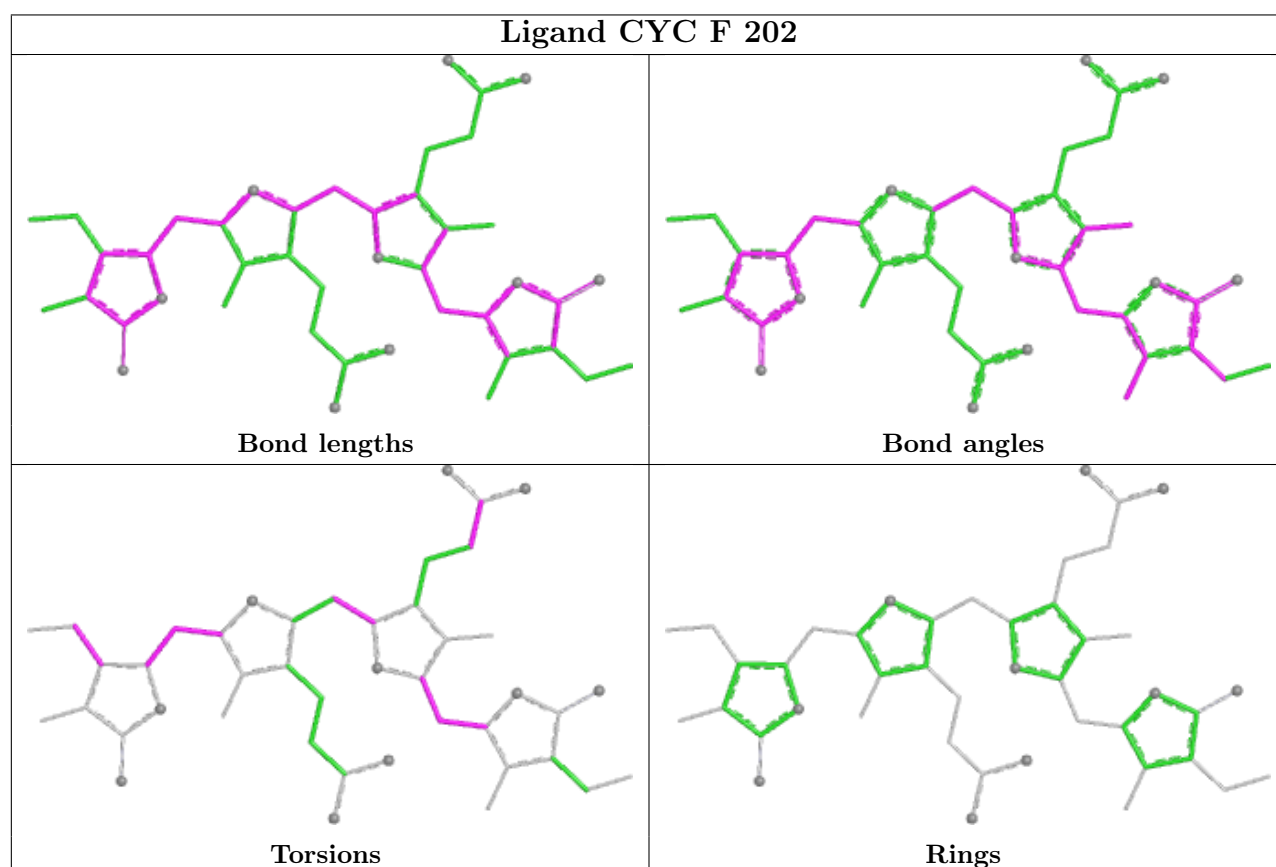
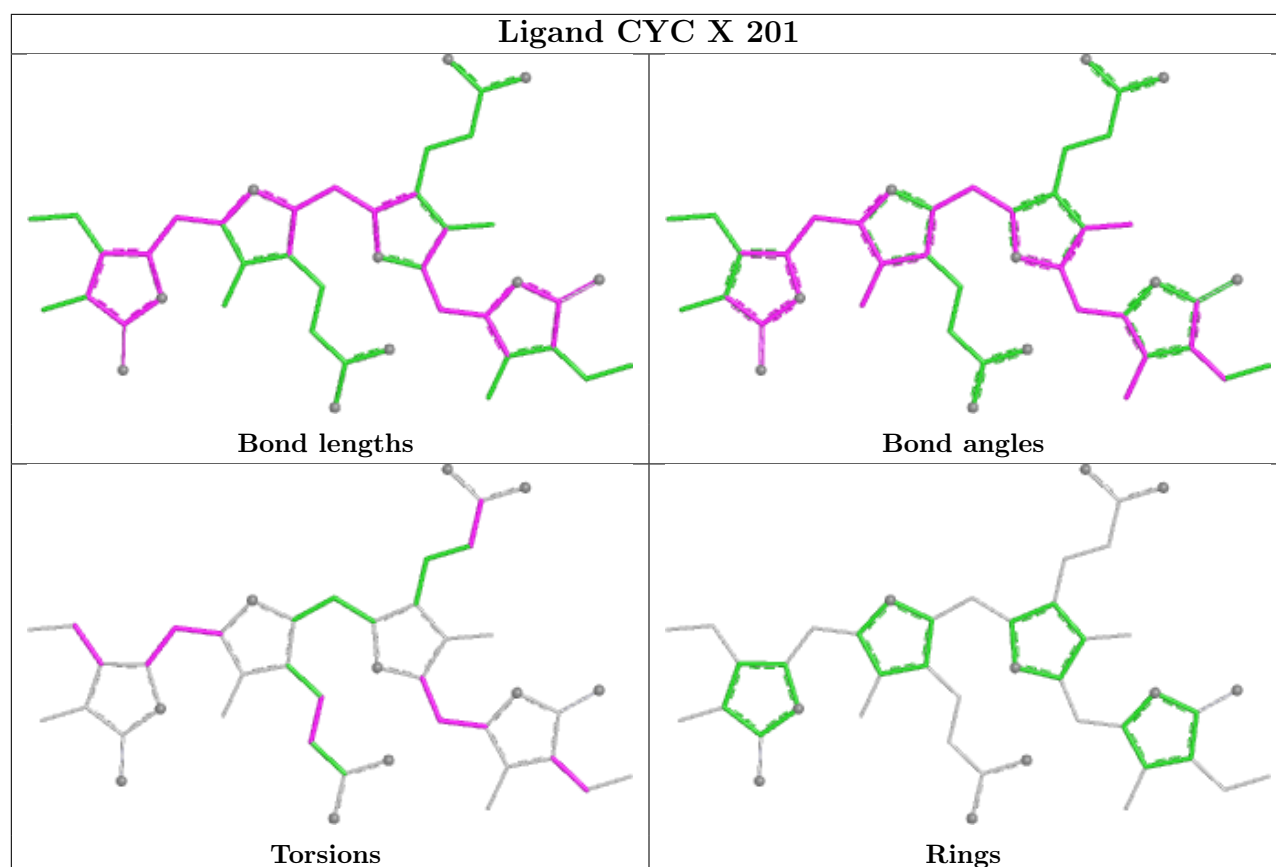


Ligand CYC C 202

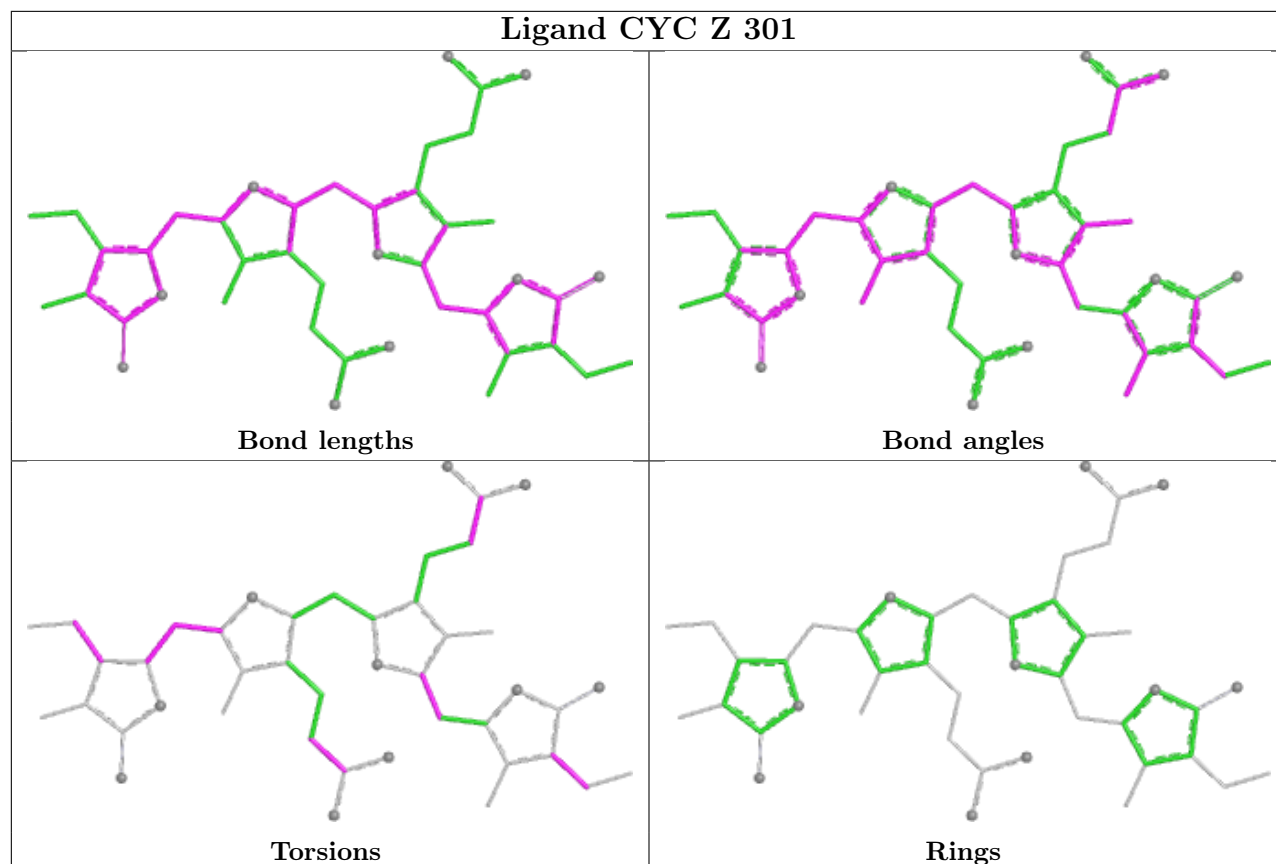




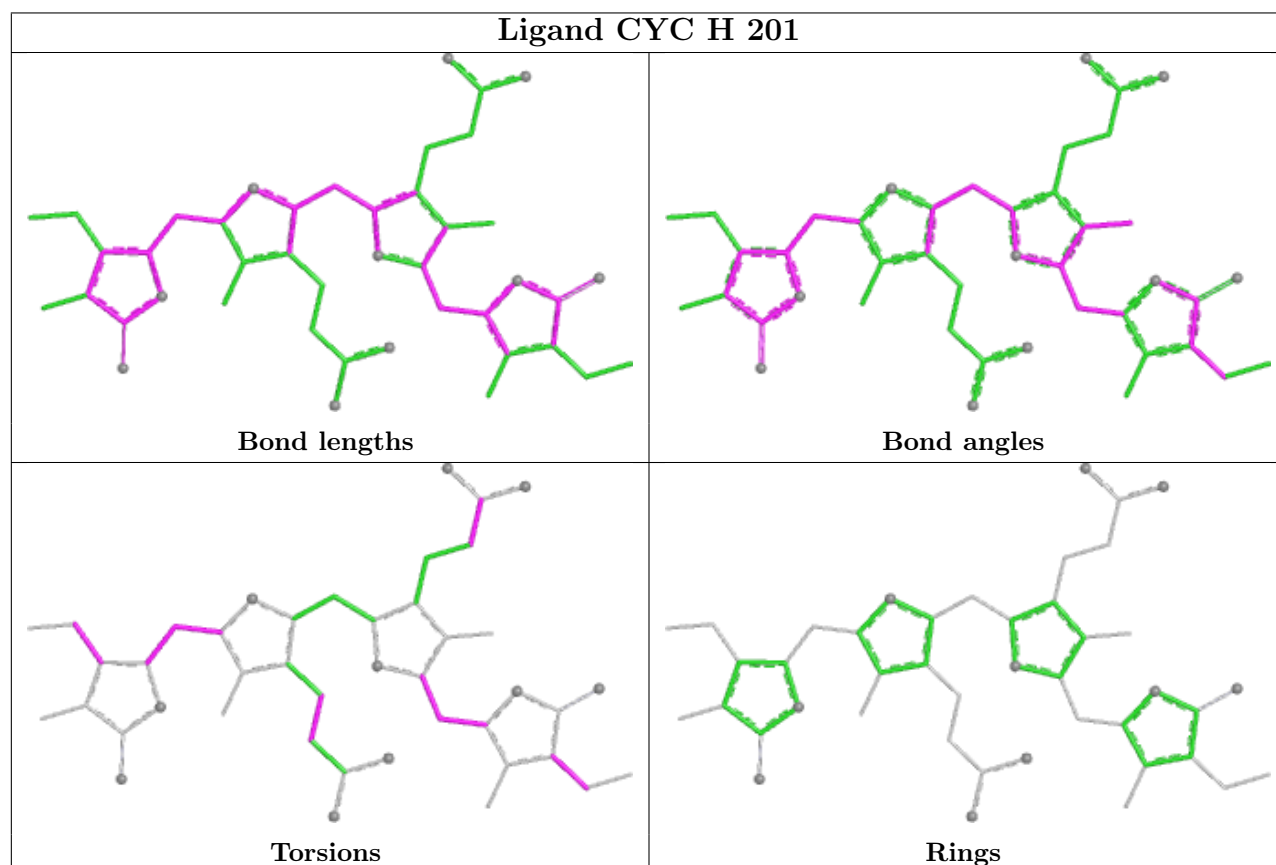




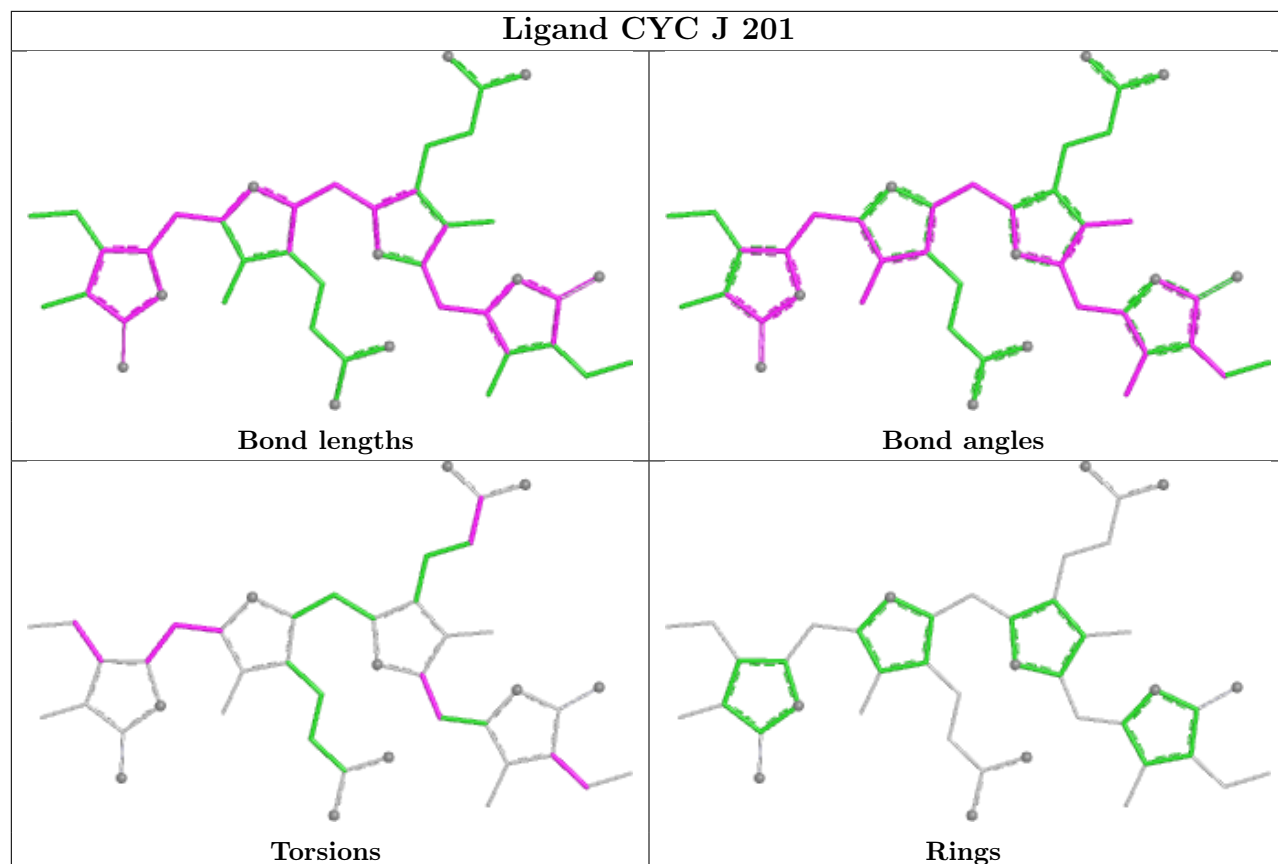
Ligand CYC Z 301



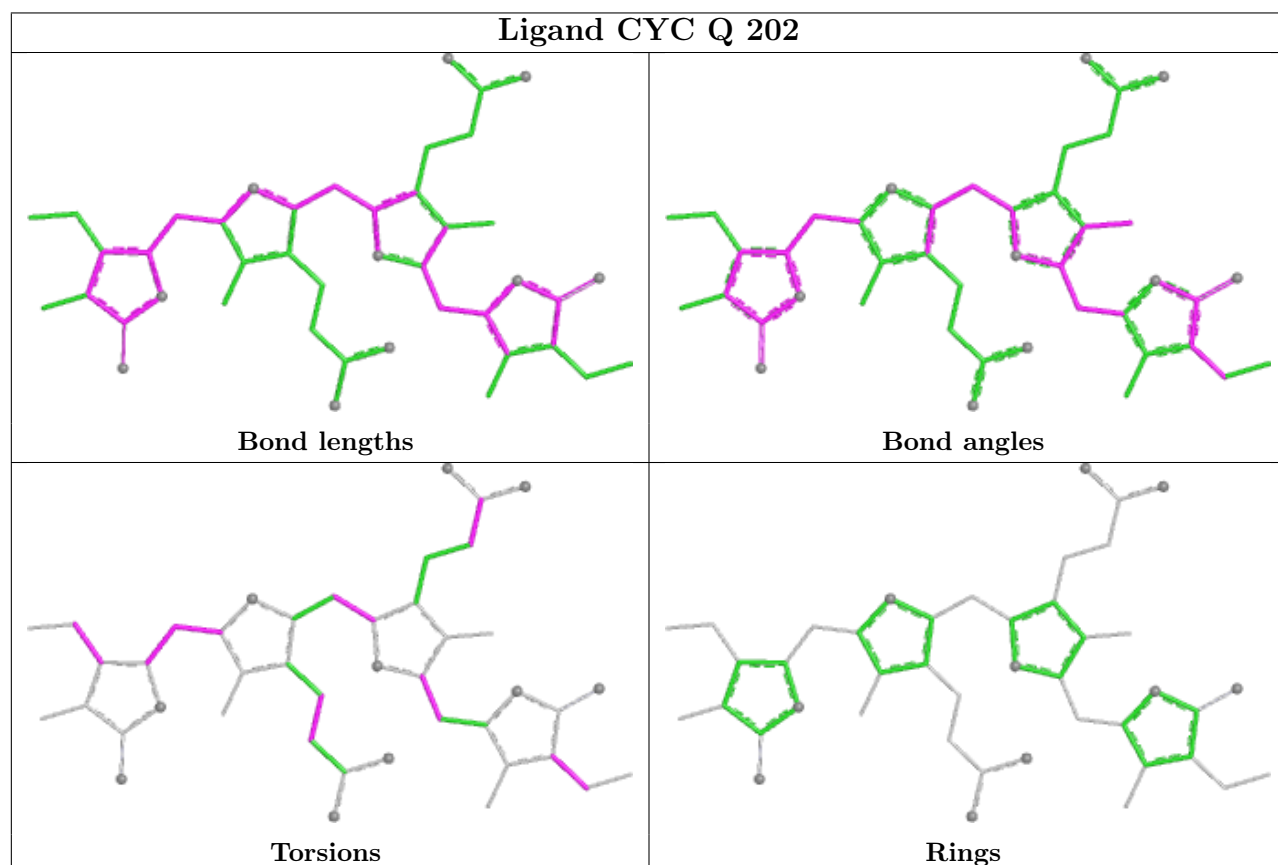
Ligand CYC H 201



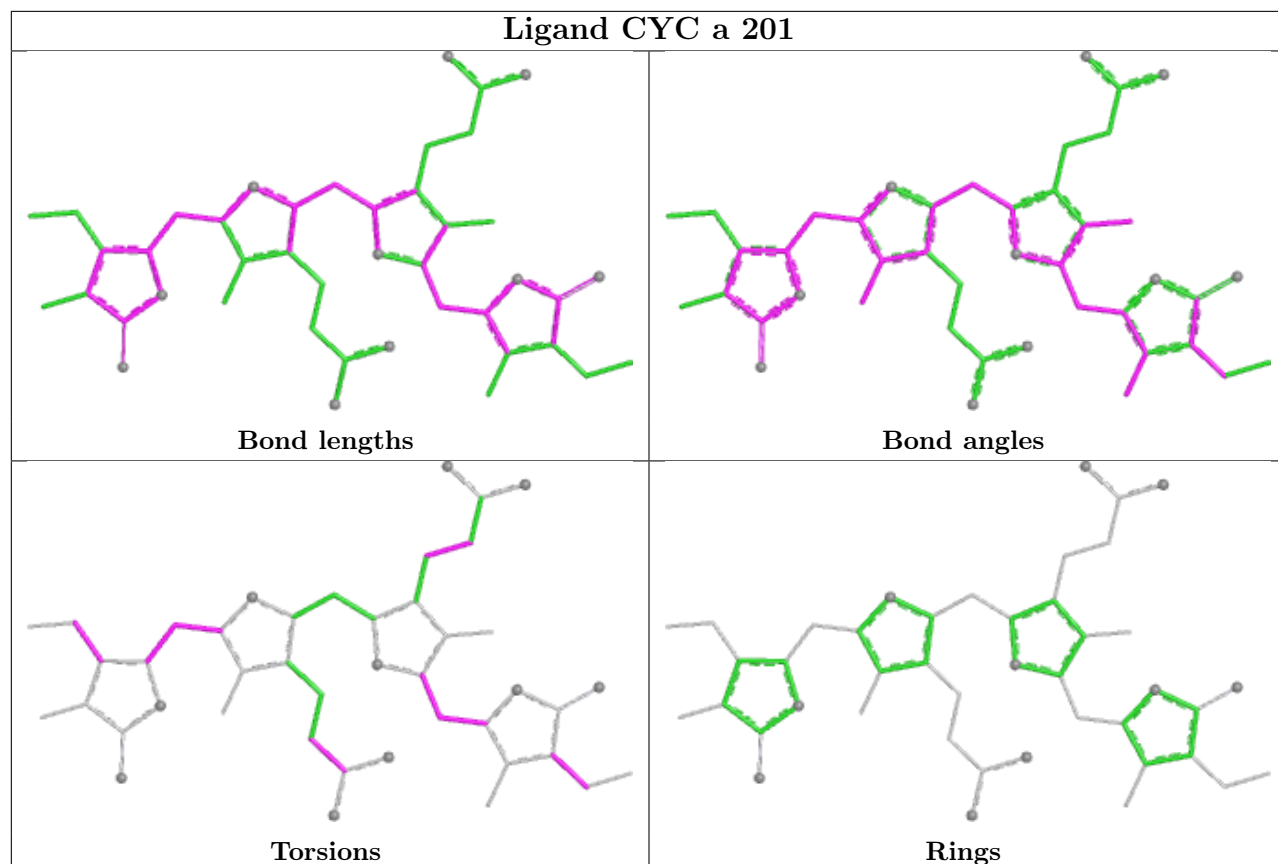
Ligand CYC J 201



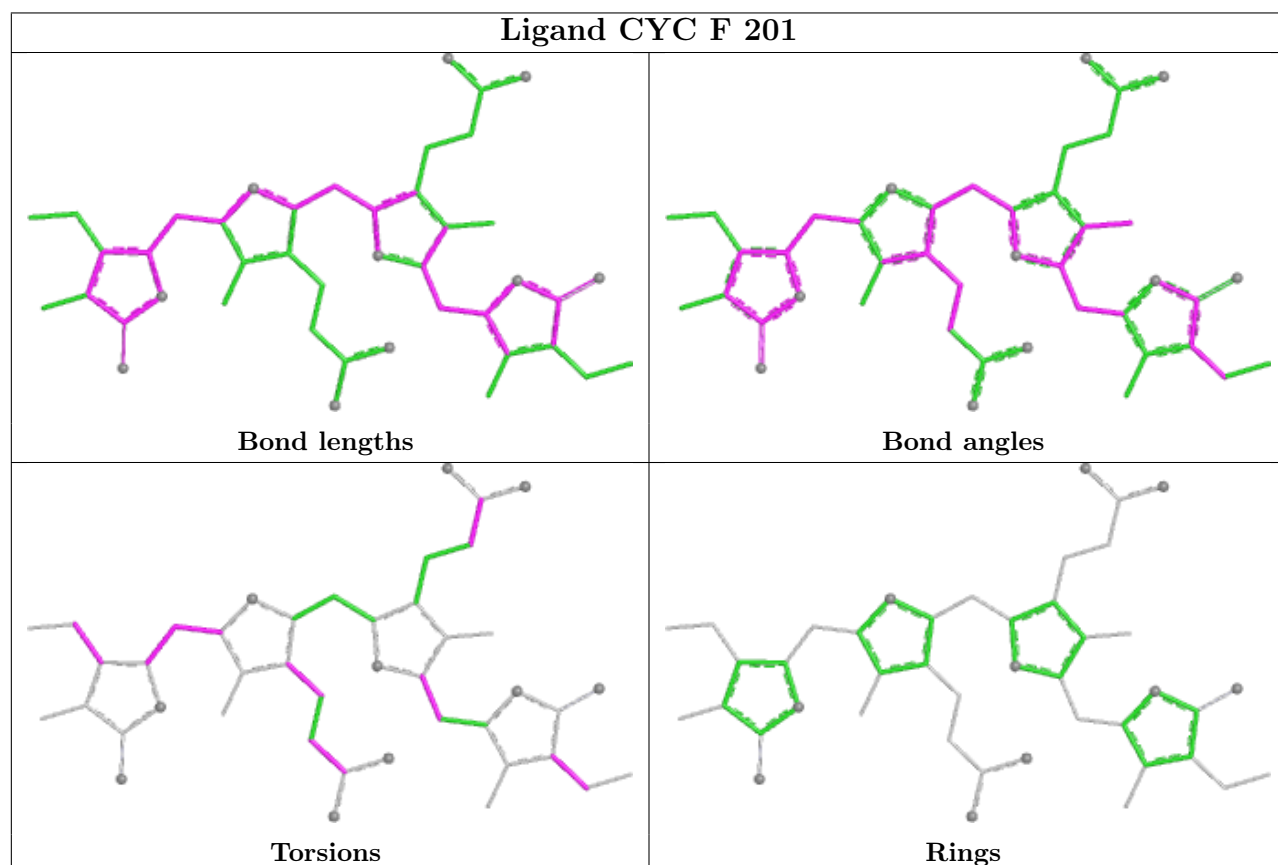
Ligand CYC Q 202

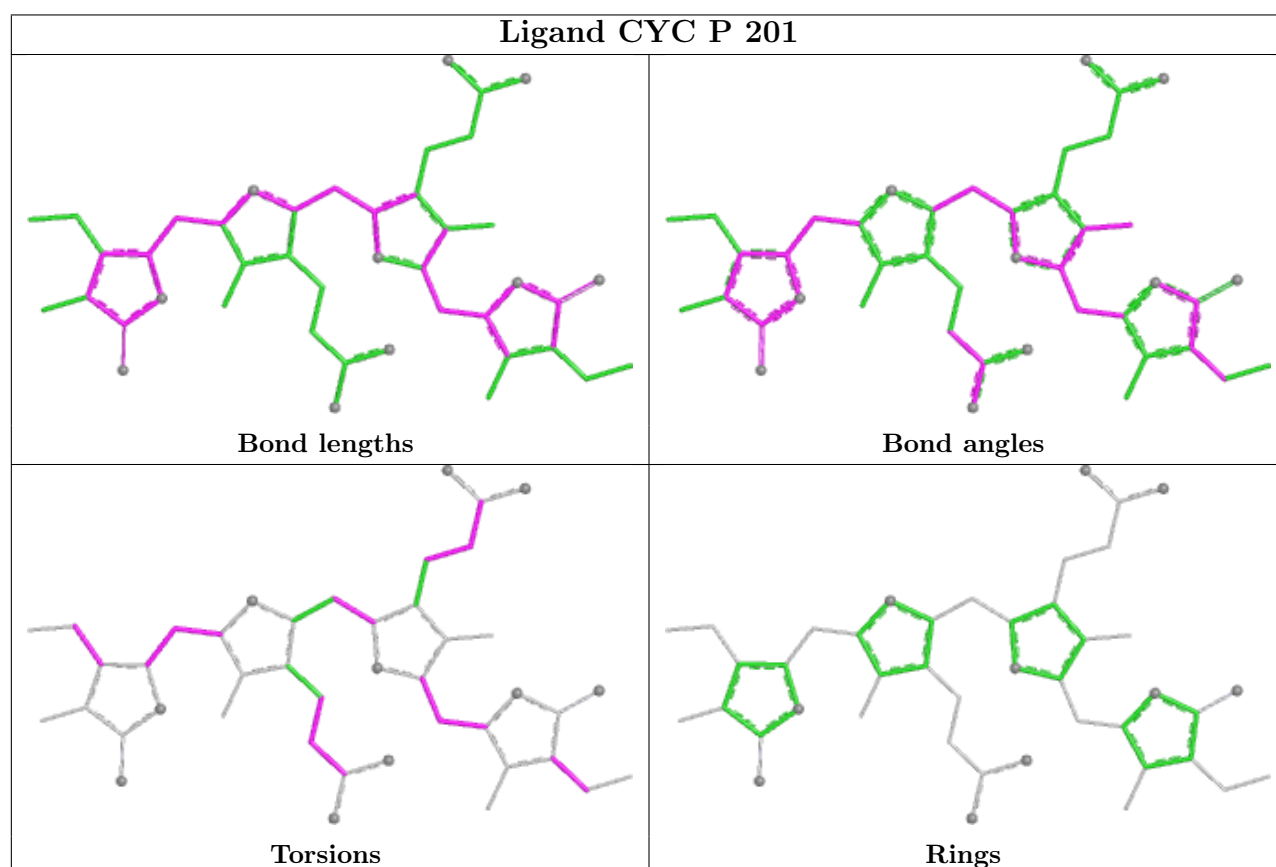
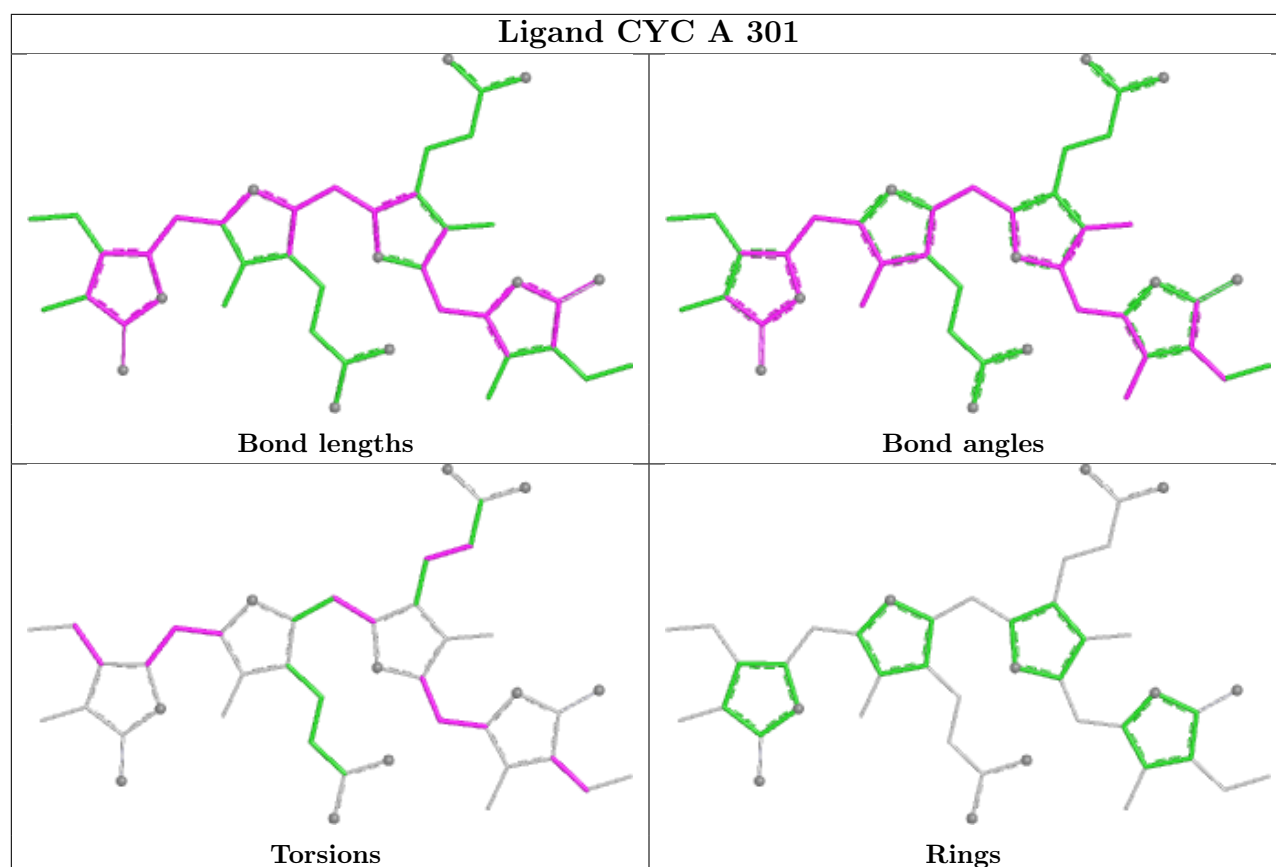


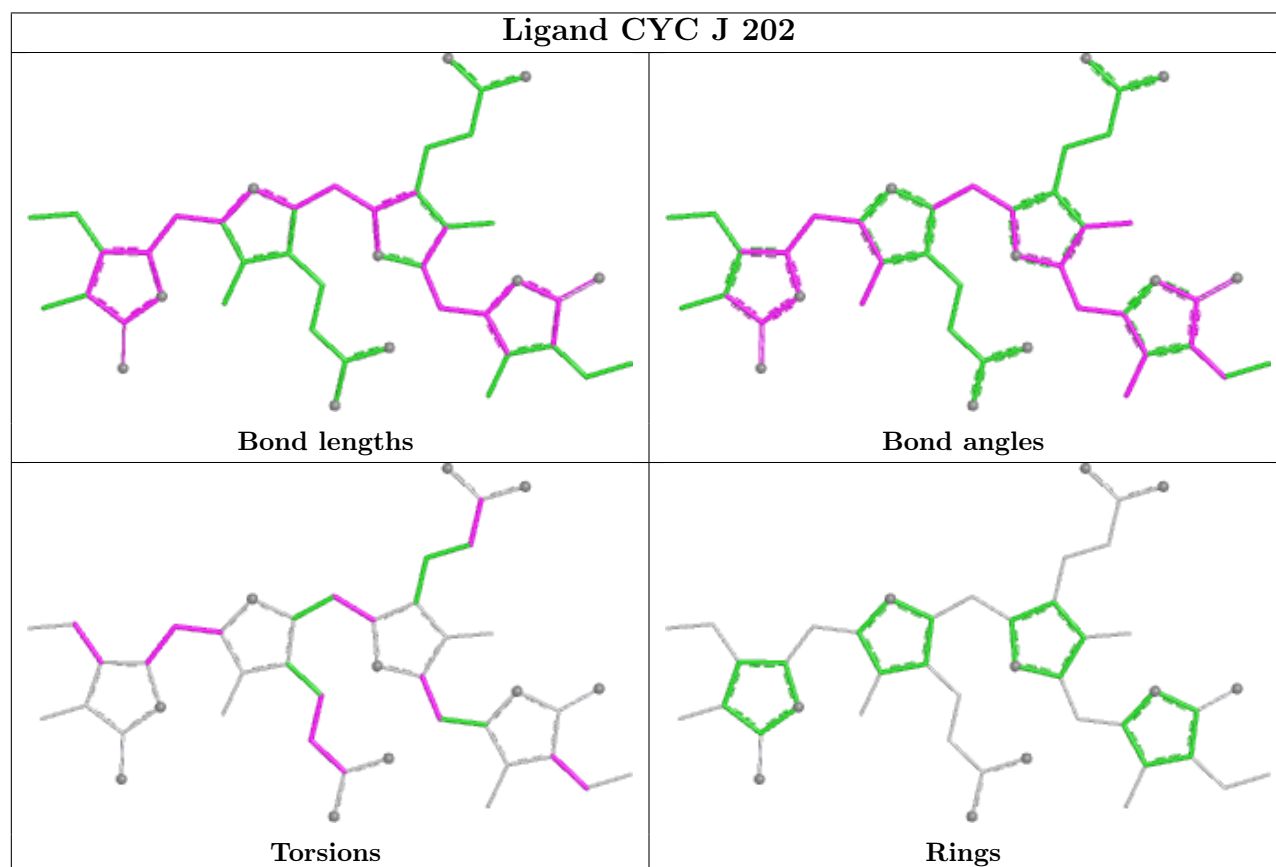
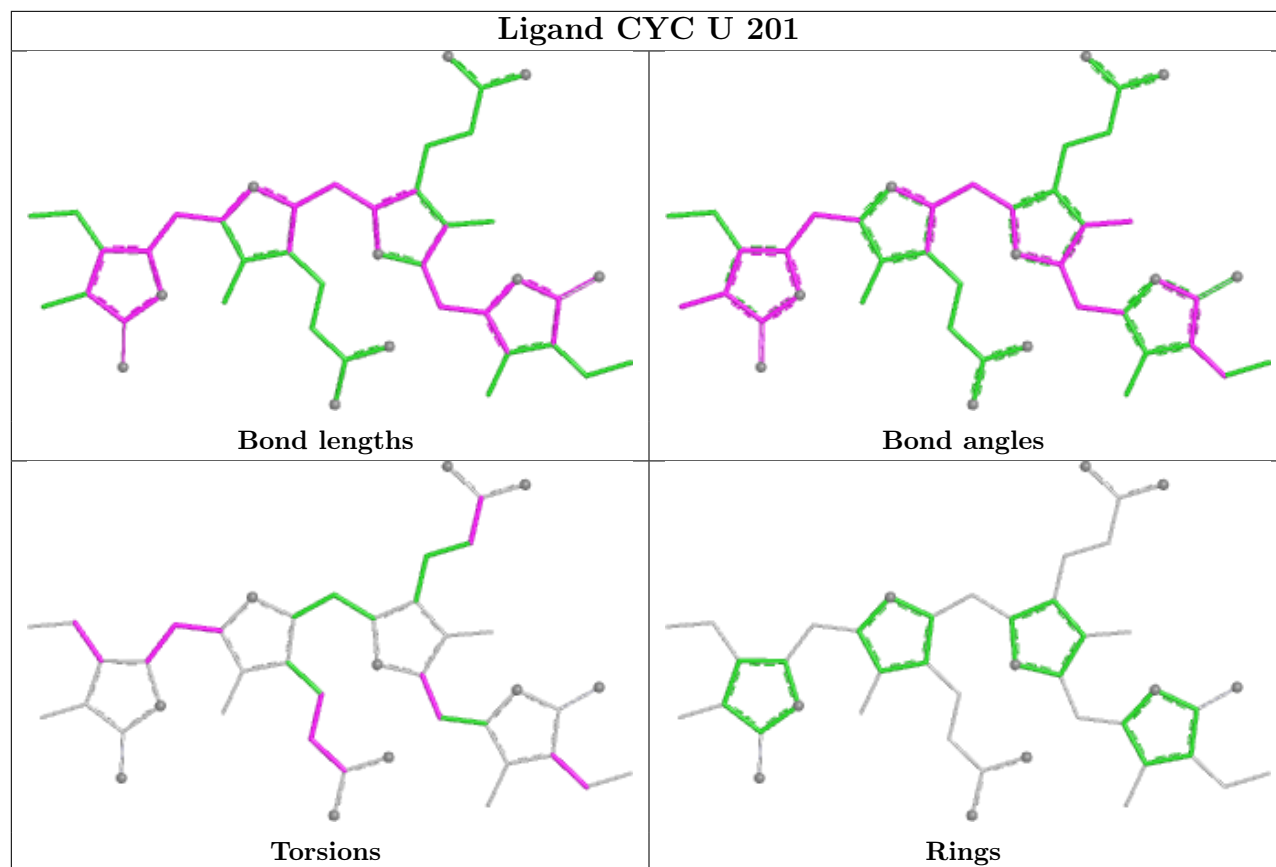
Ligand CYC a 201

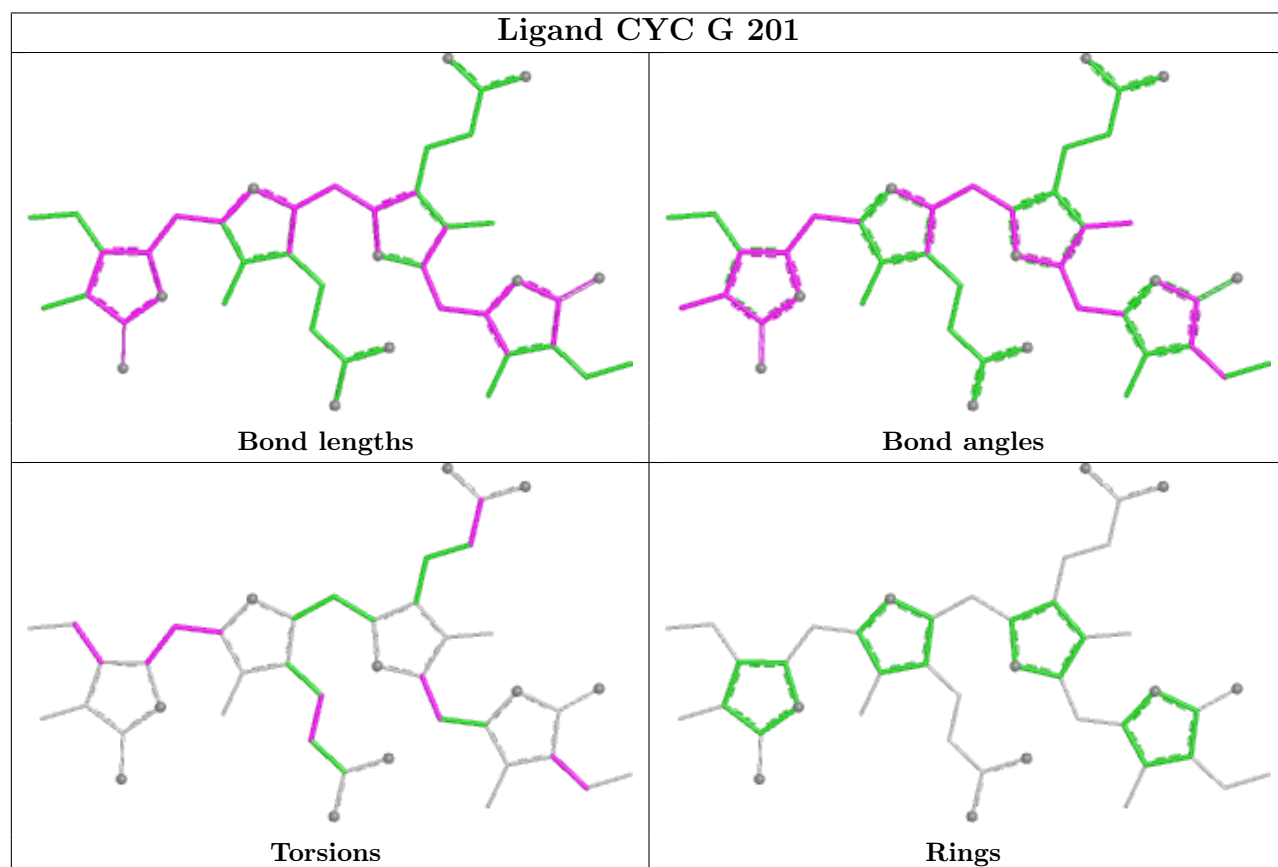
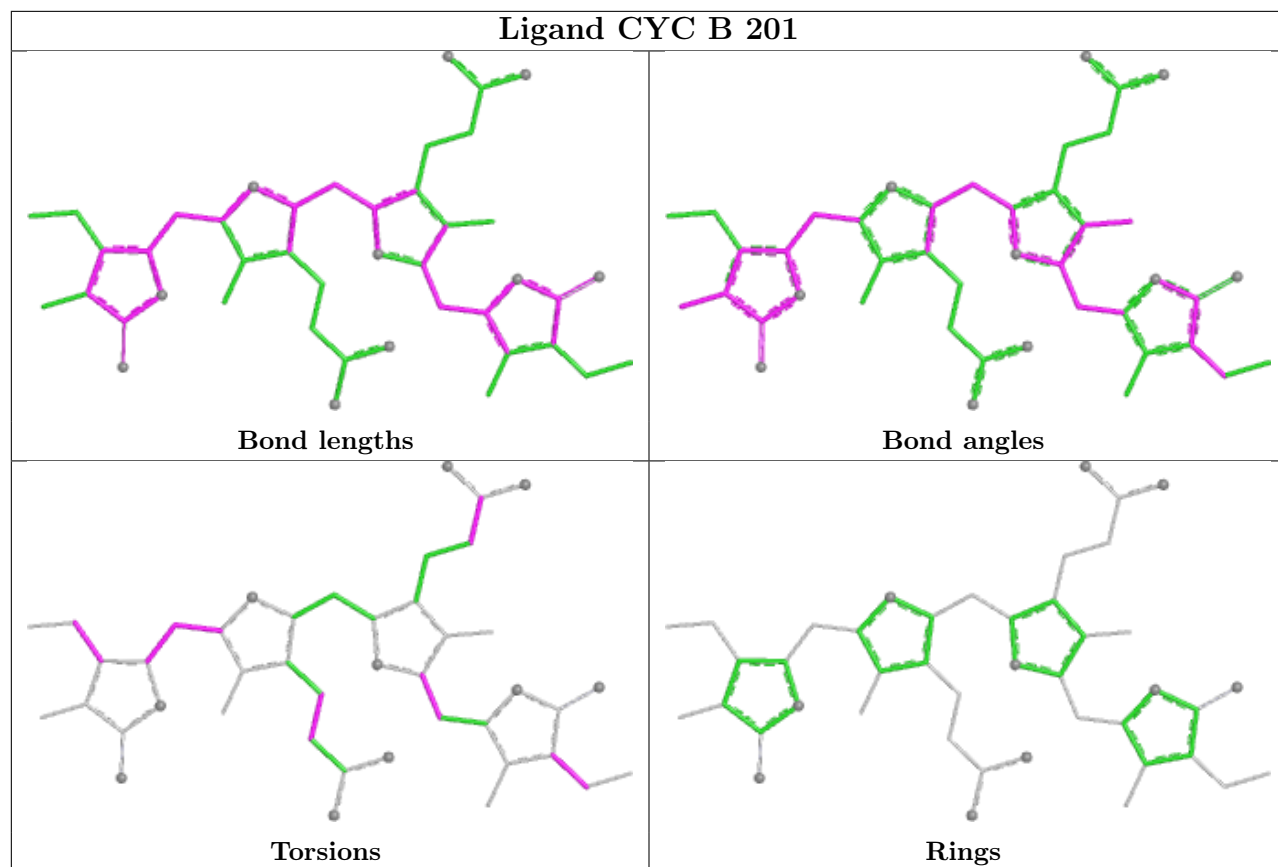


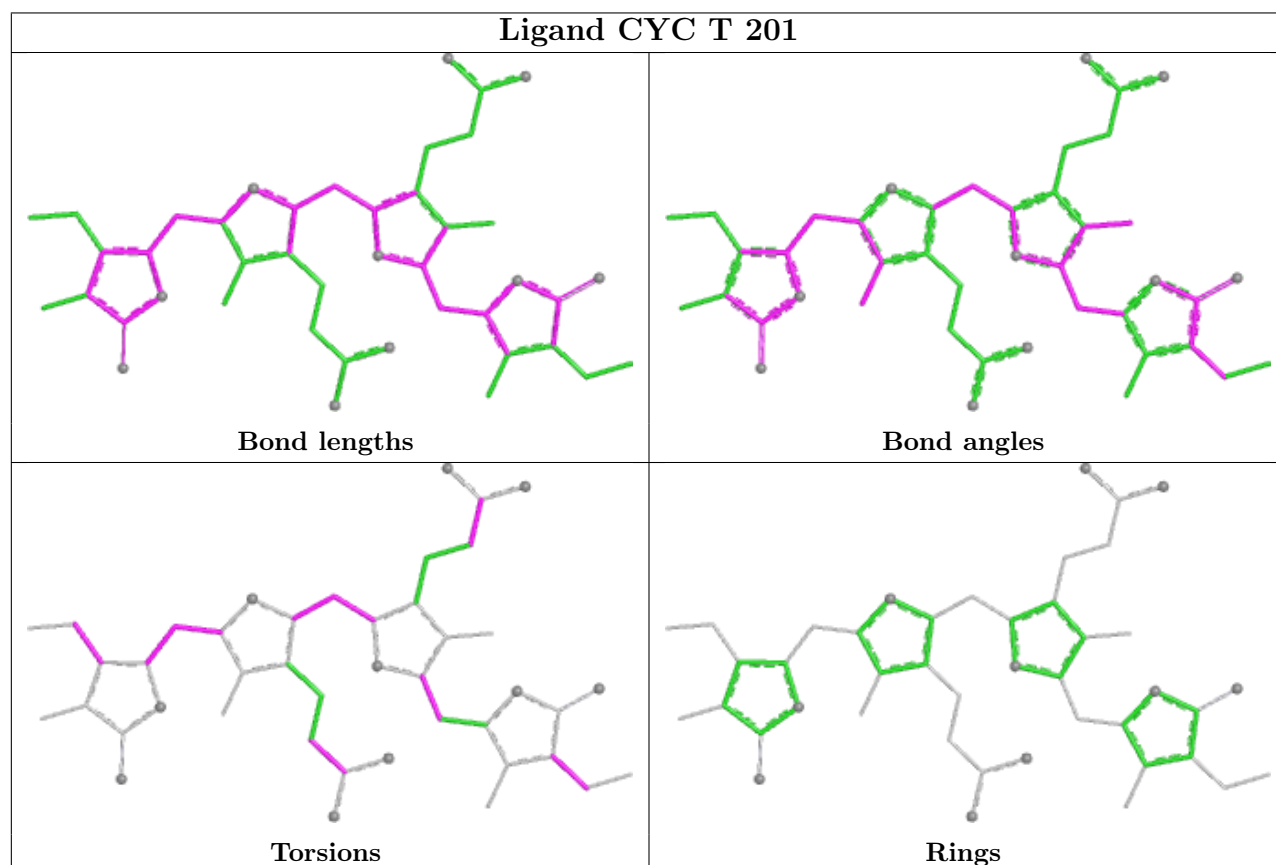
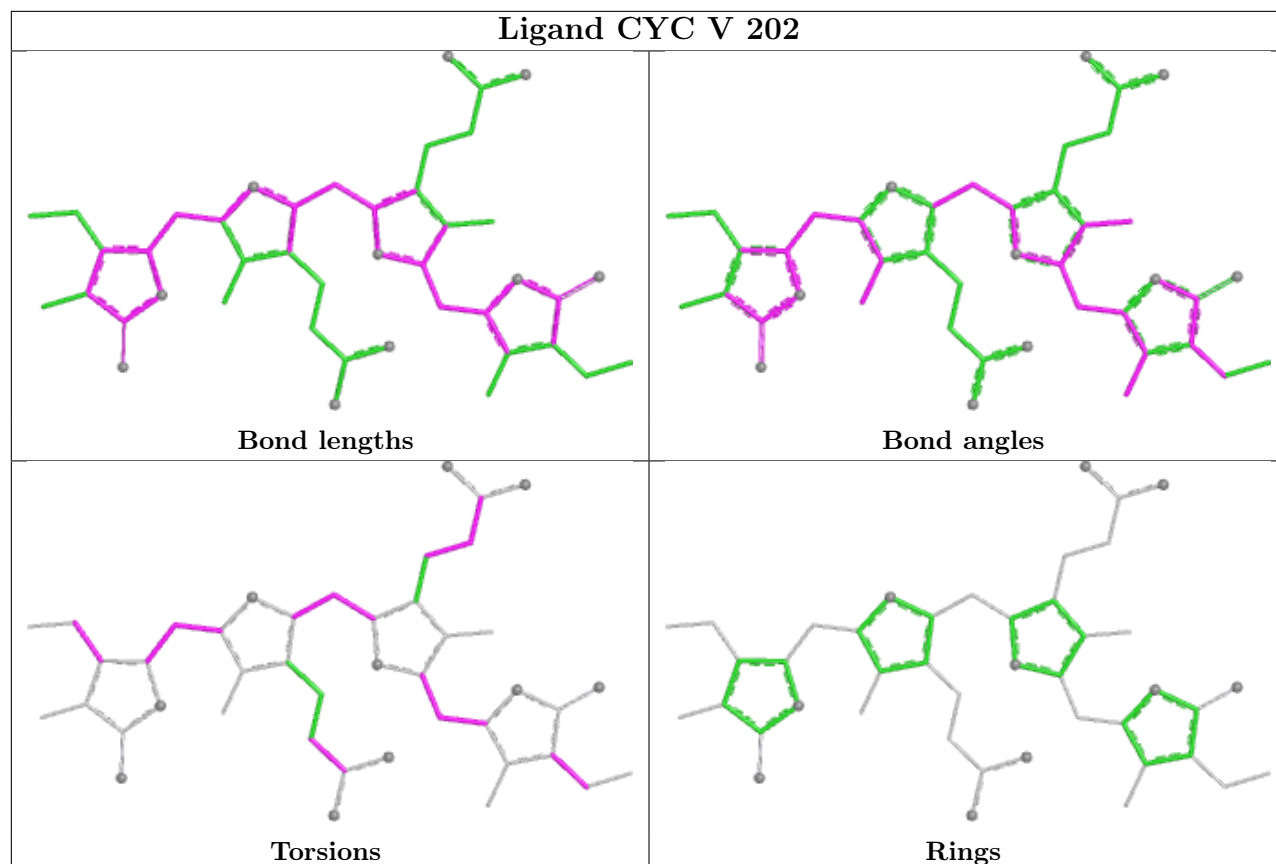
Ligand CYC F 201

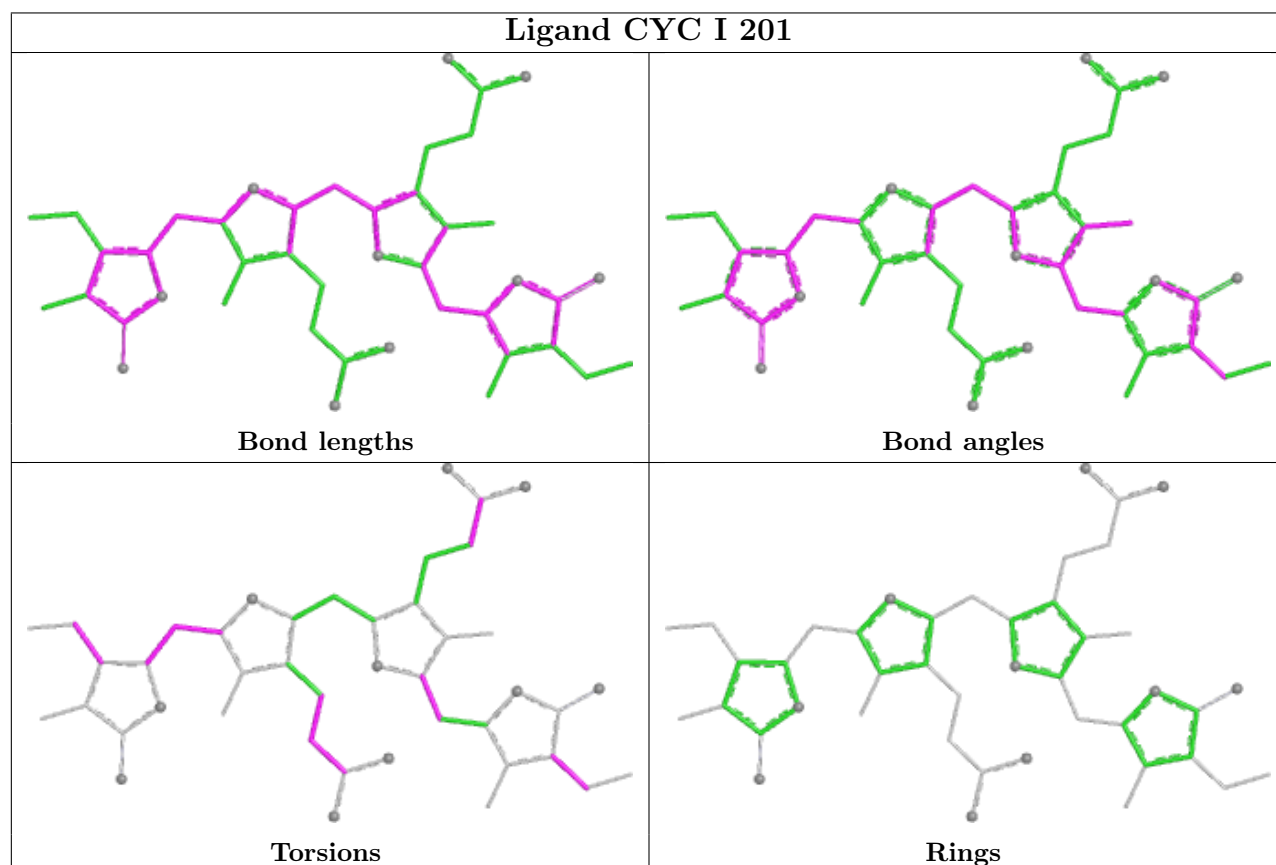
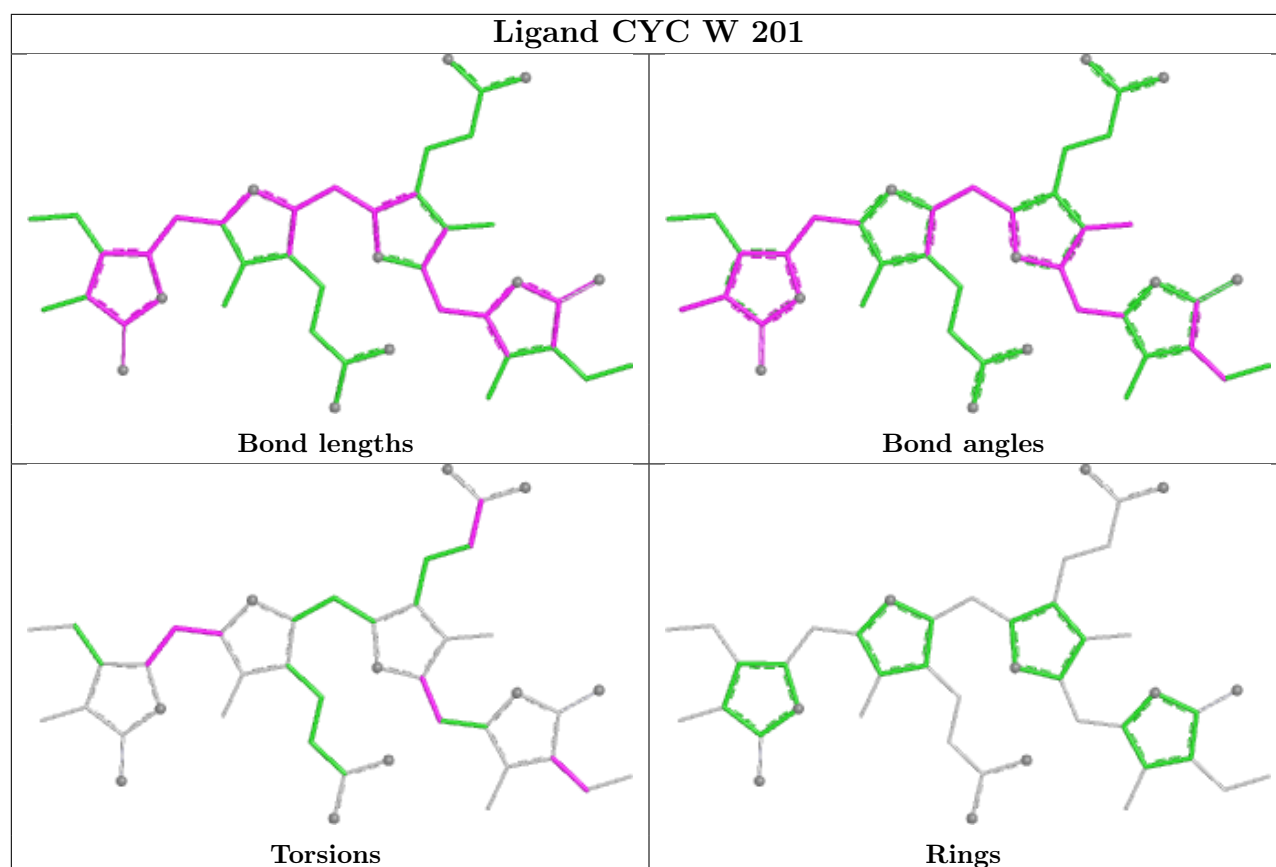


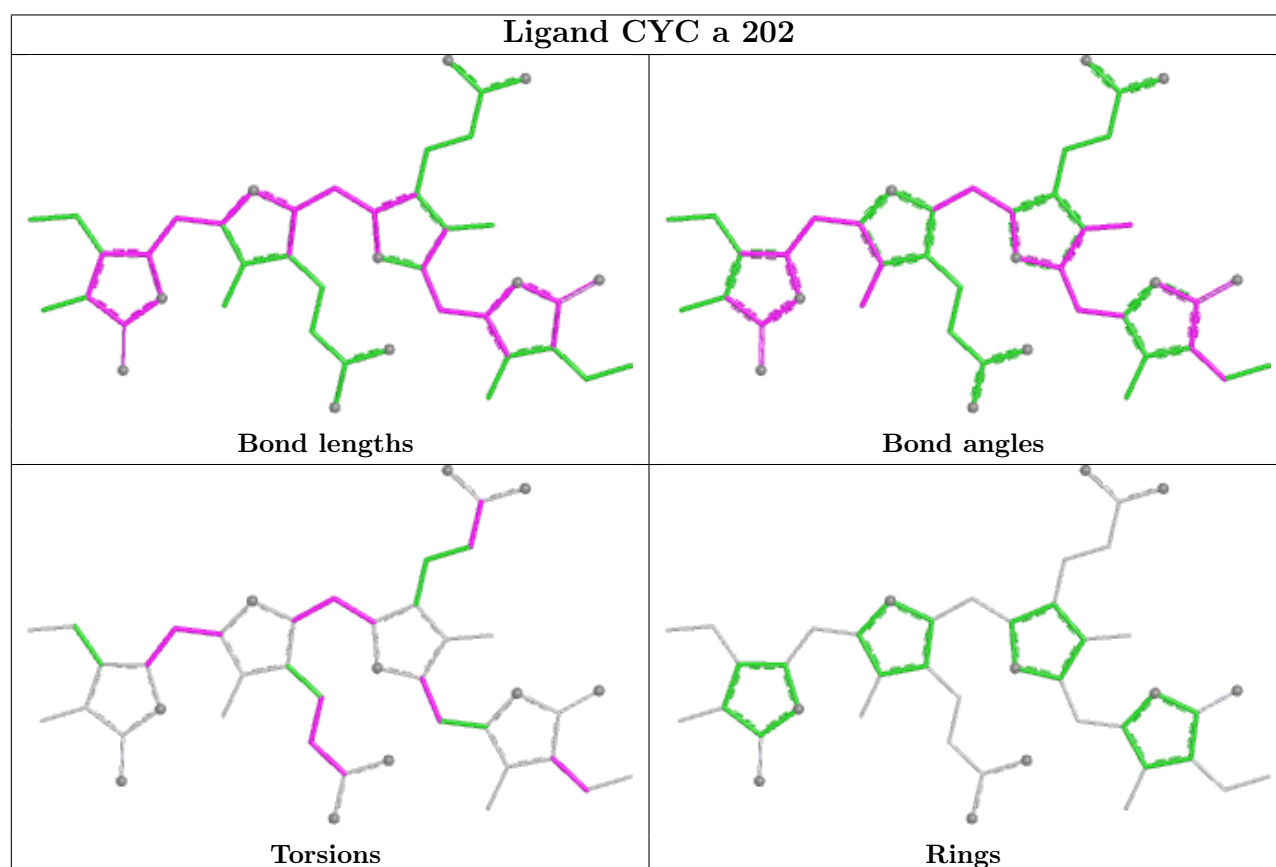
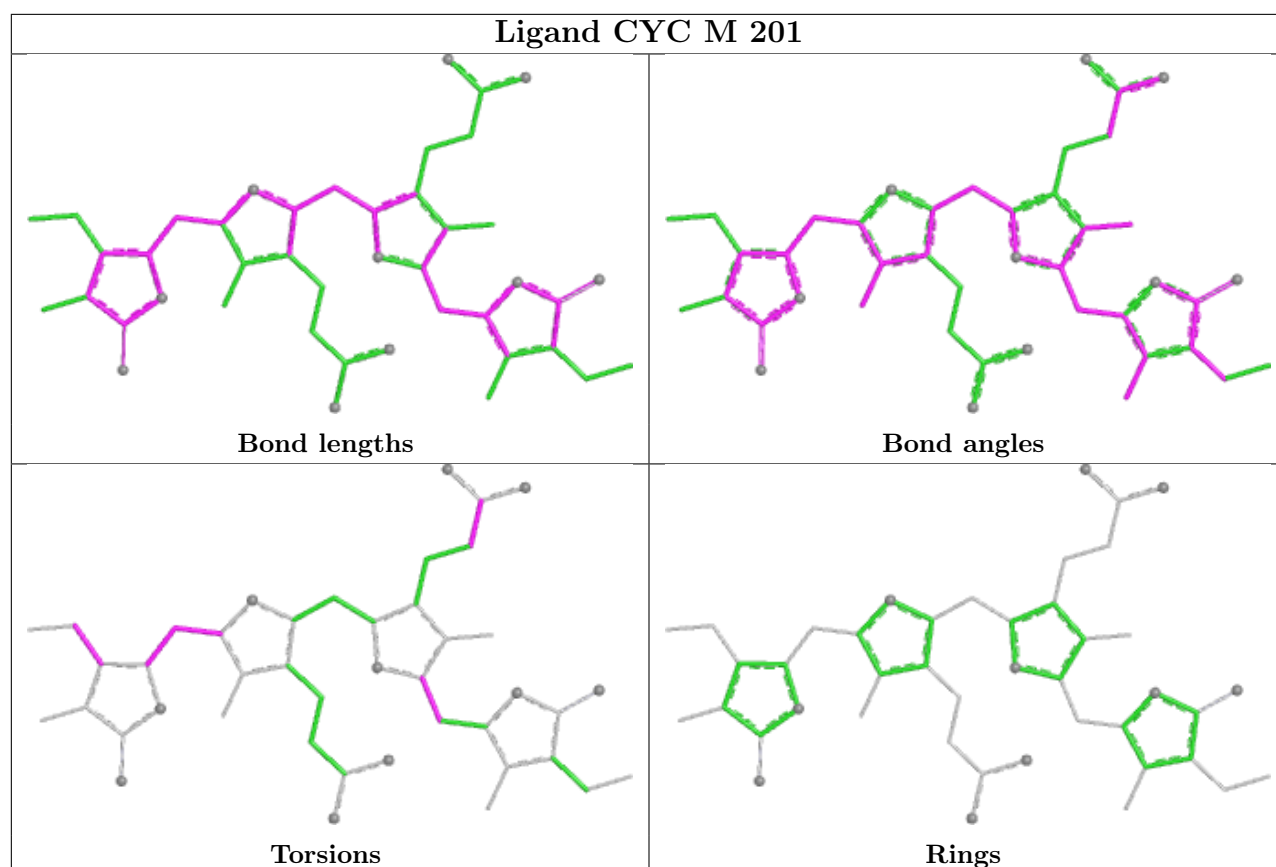


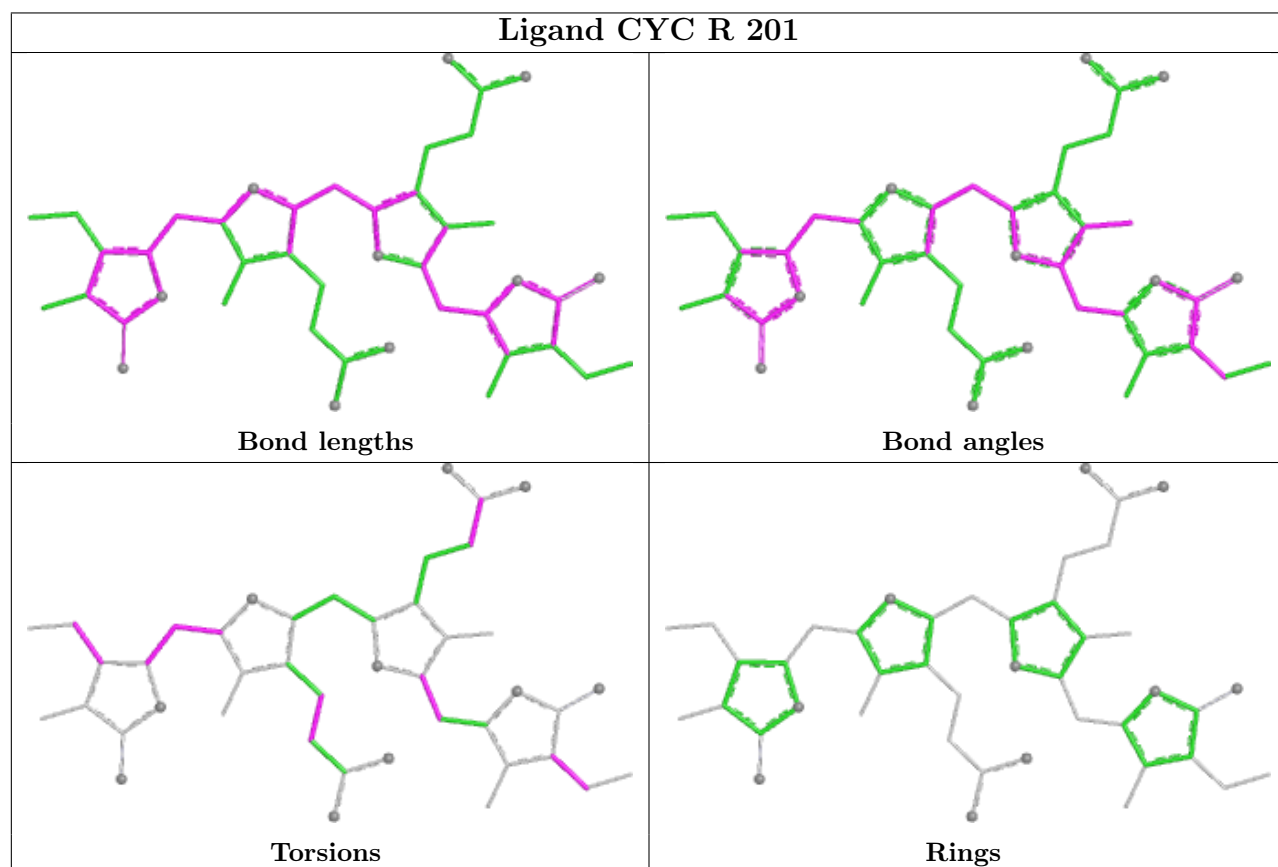
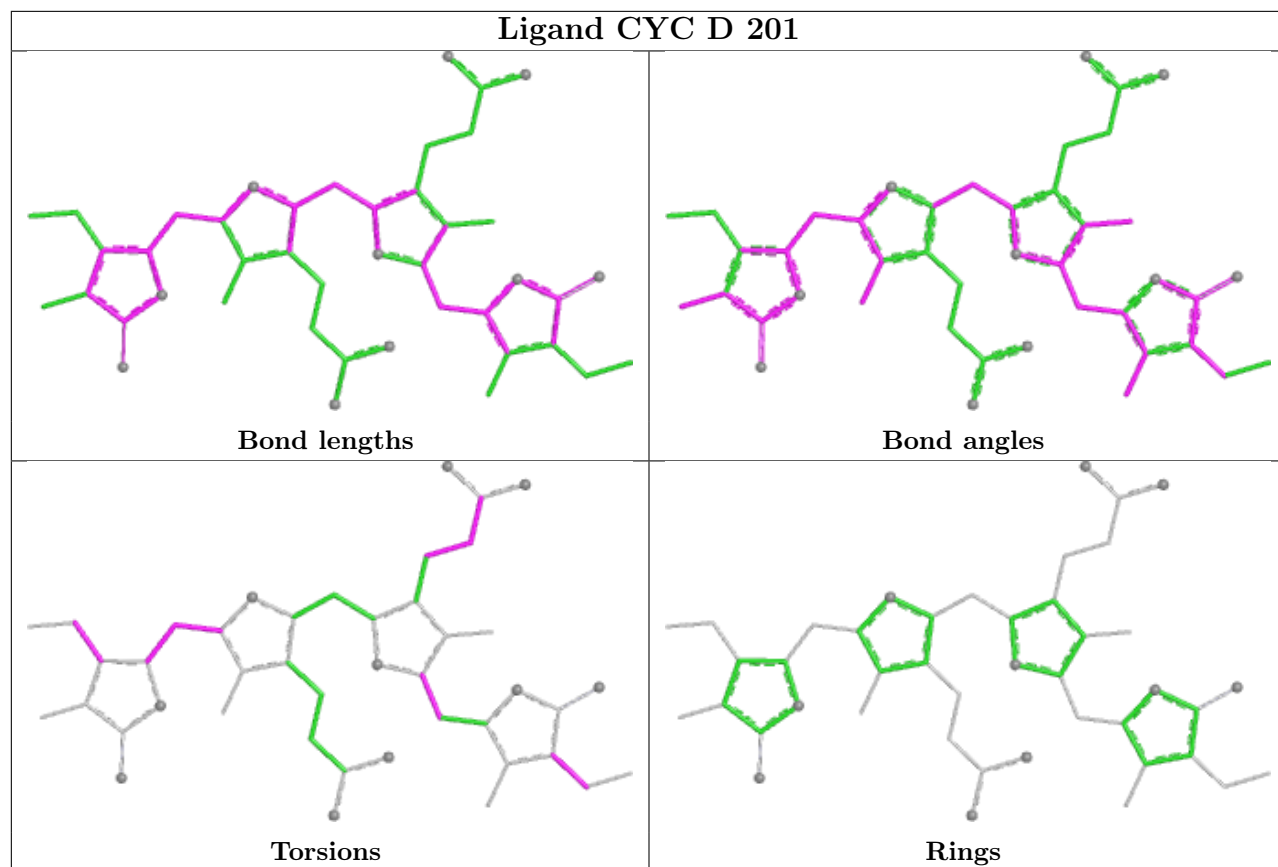


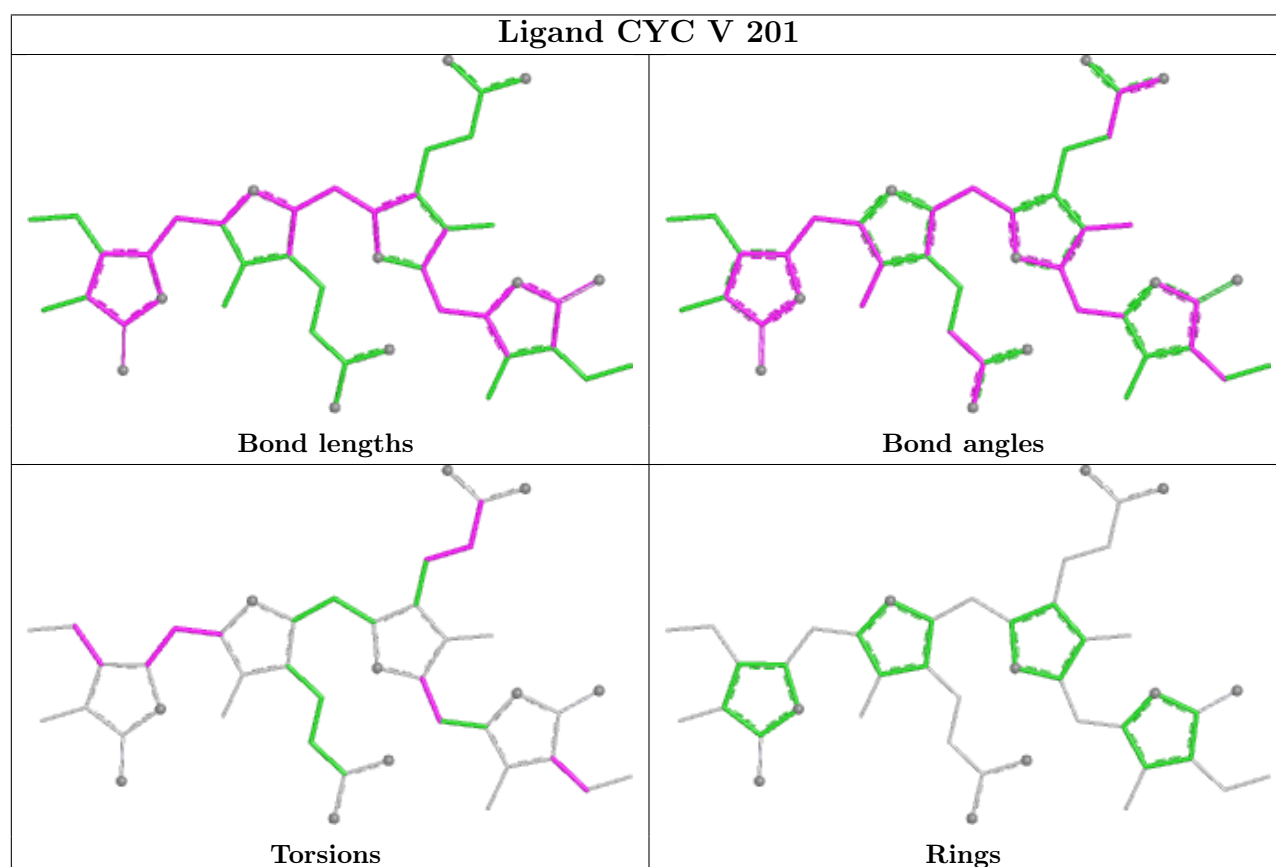
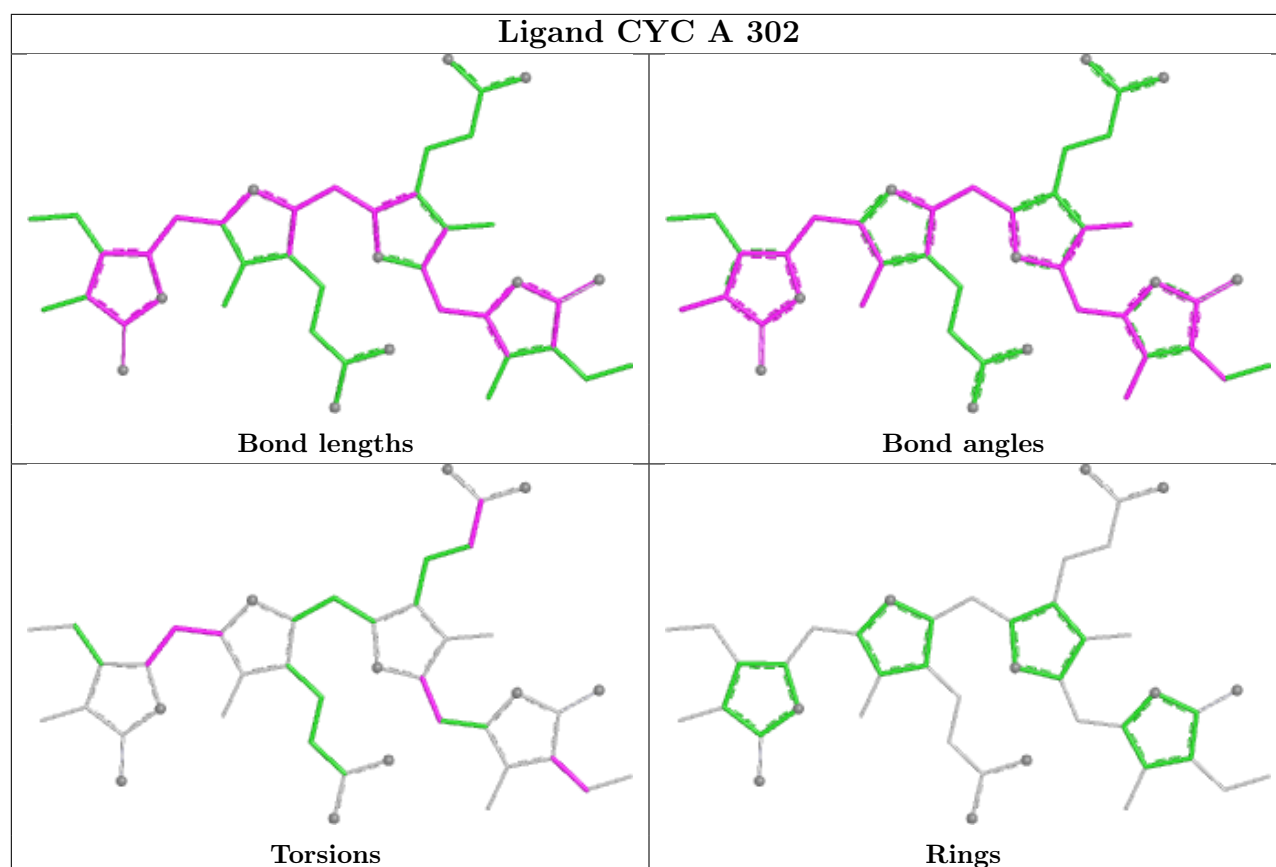


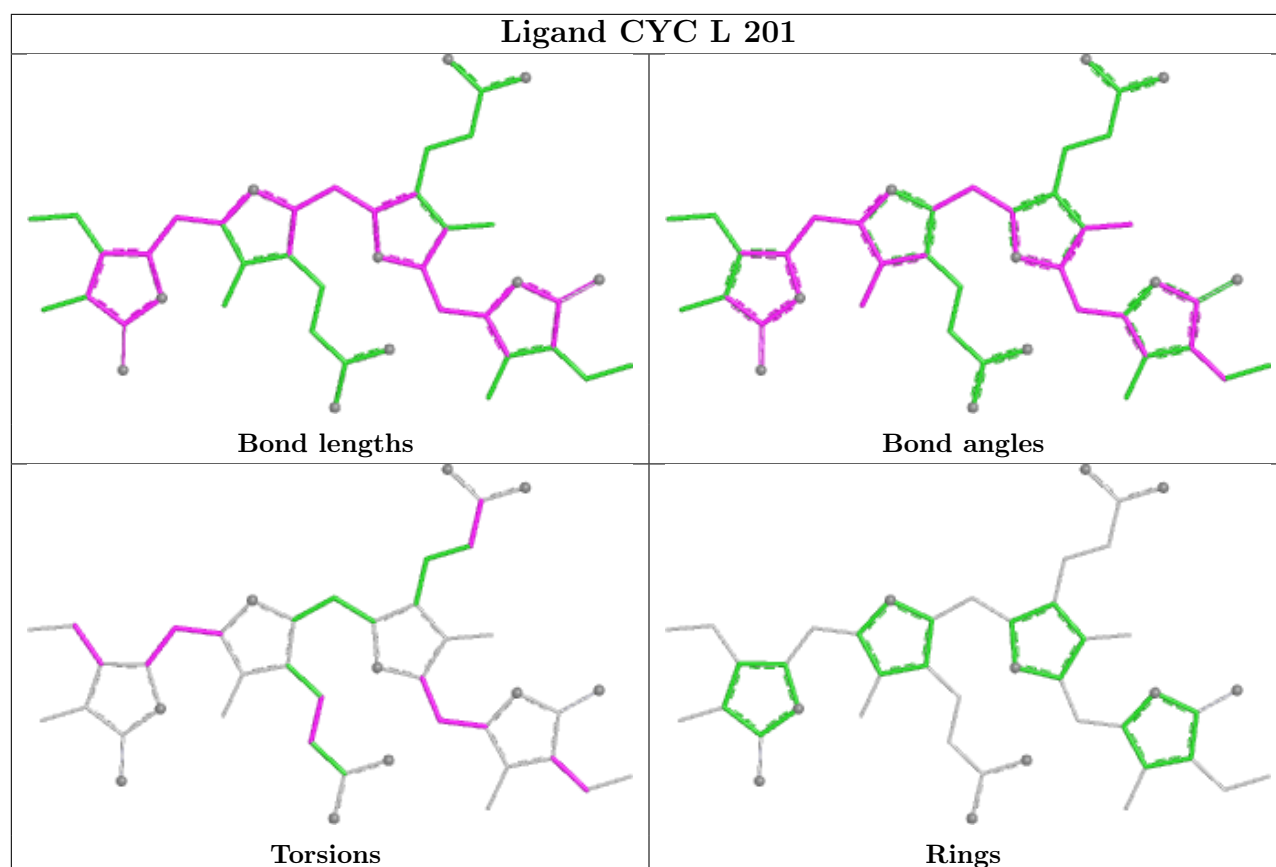












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

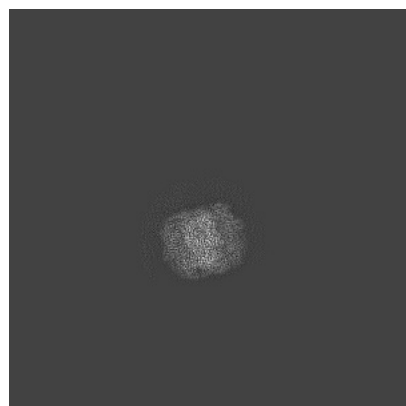
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66300. These allow visual inspection of the internal detail of the map and identification of artifacts.

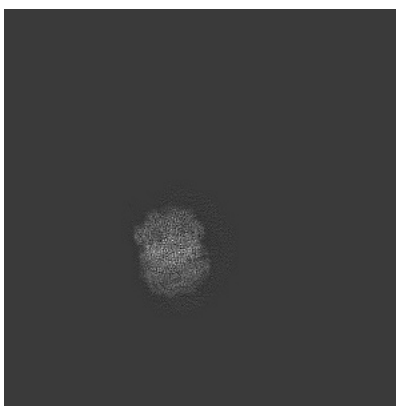
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

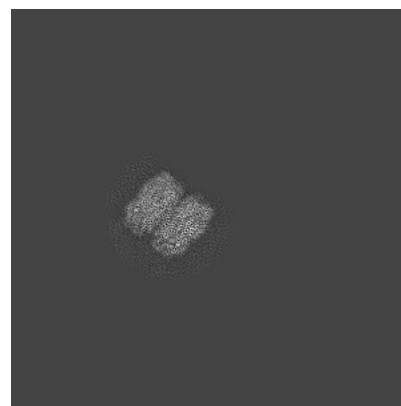
6.1.1 Primary map



X

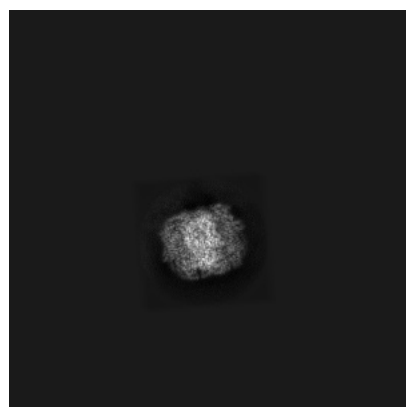


Y

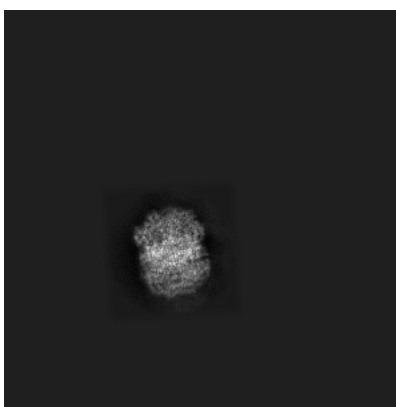


Z

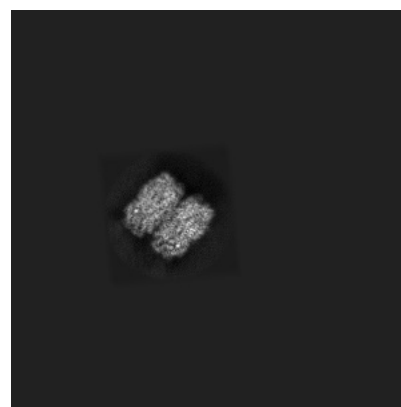
6.1.2 Raw map



X



Y

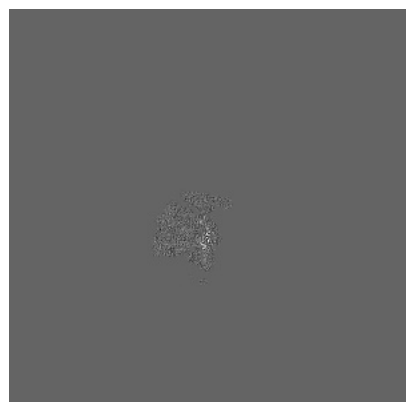


Z

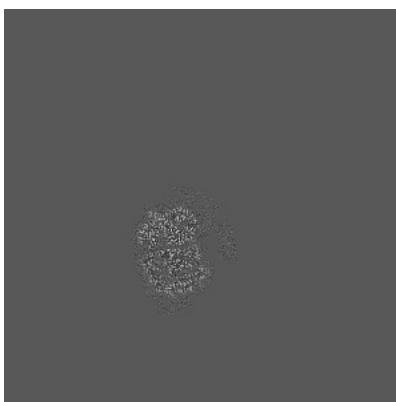
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

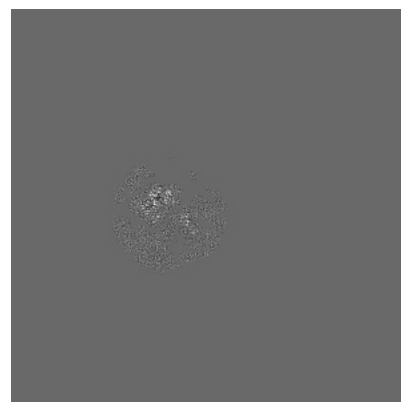
6.2.1 Primary map



X Index: 280

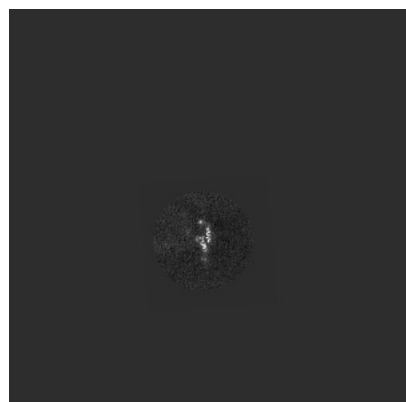


Y Index: 280



Z Index: 280

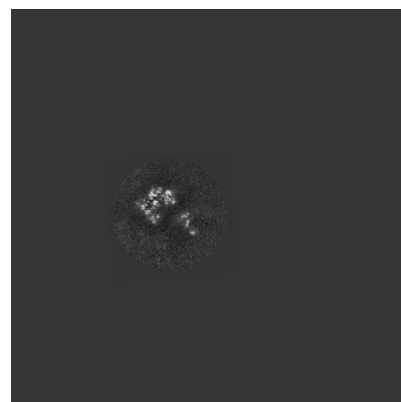
6.2.2 Raw map



X Index: 280



Y Index: 280

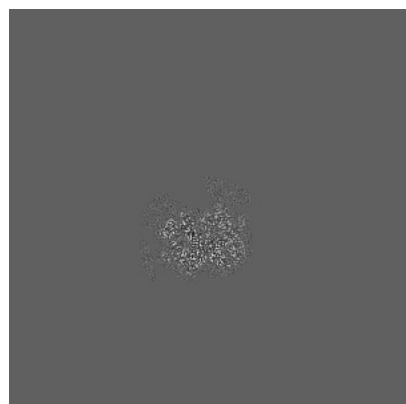


Z Index: 280

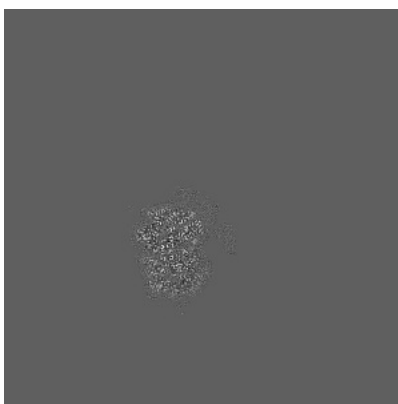
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

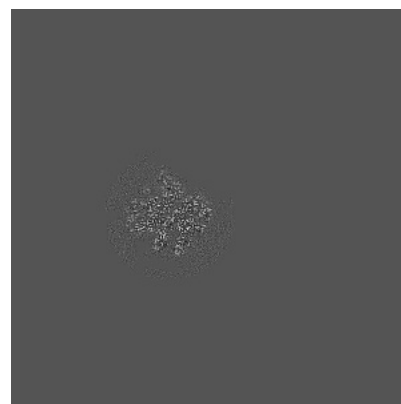
6.3.1 Primary map



X Index: 220

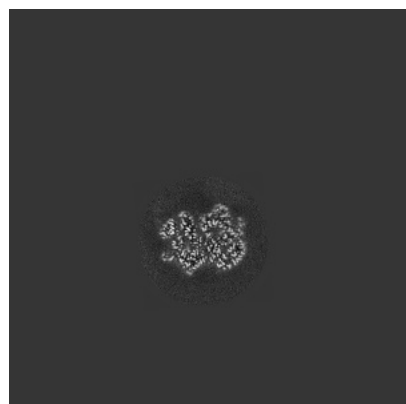


Y Index: 275

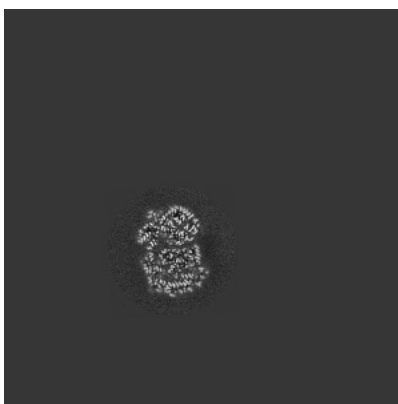


Z Index: 235

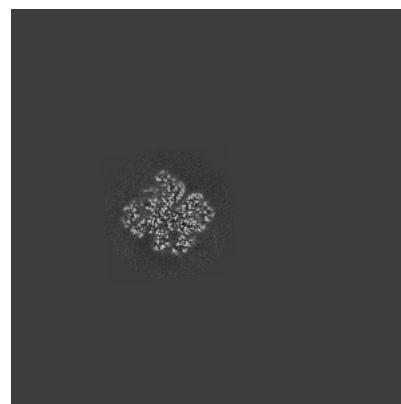
6.3.2 Raw map



X Index: 219



Y Index: 279



Z Index: 233

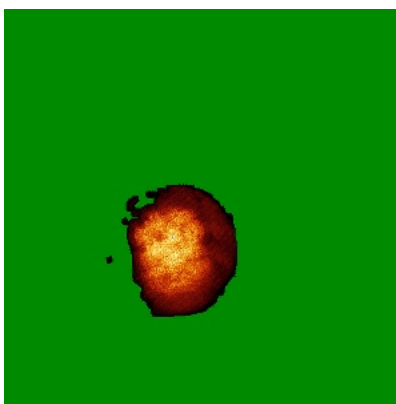
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

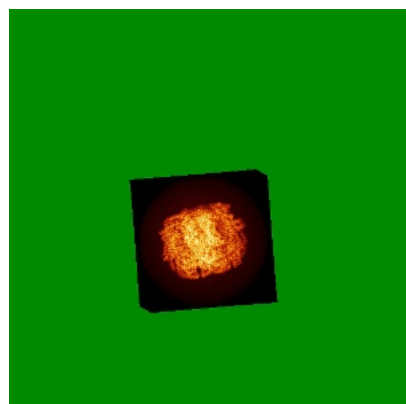


Y

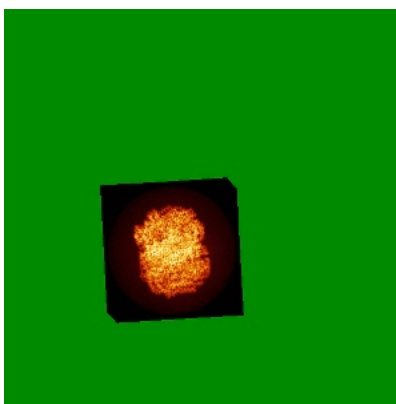


Z

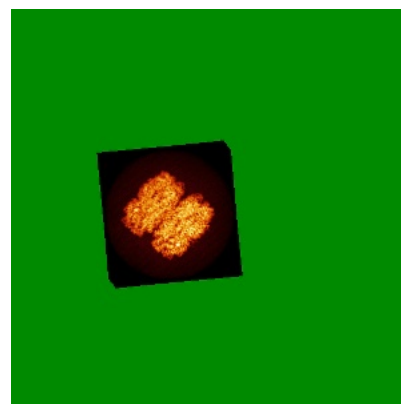
6.4.2 Raw map



X



Y

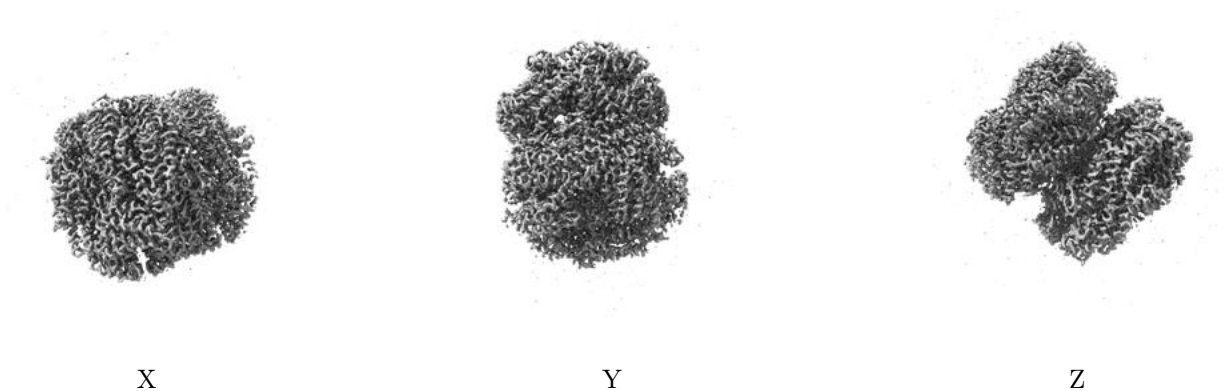


Z

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.

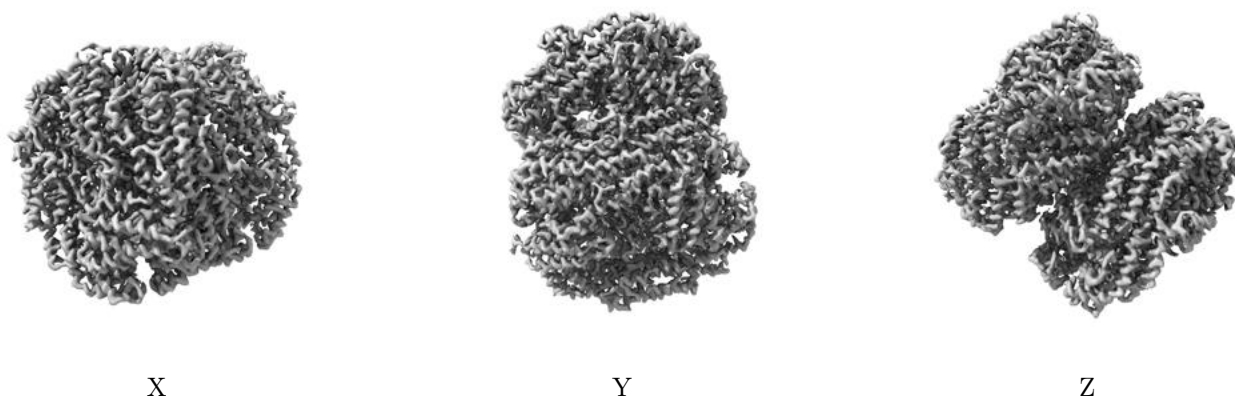
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

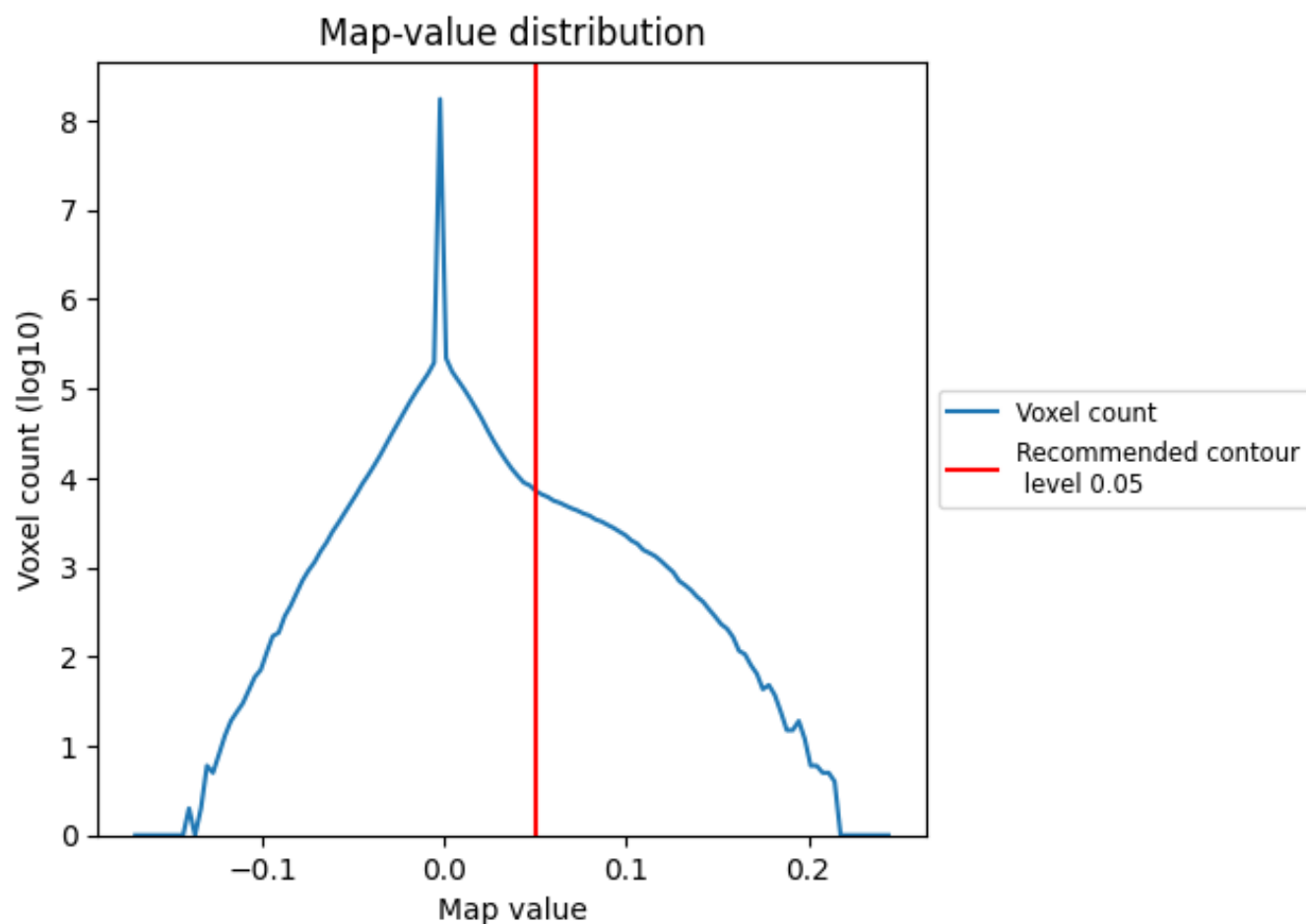
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

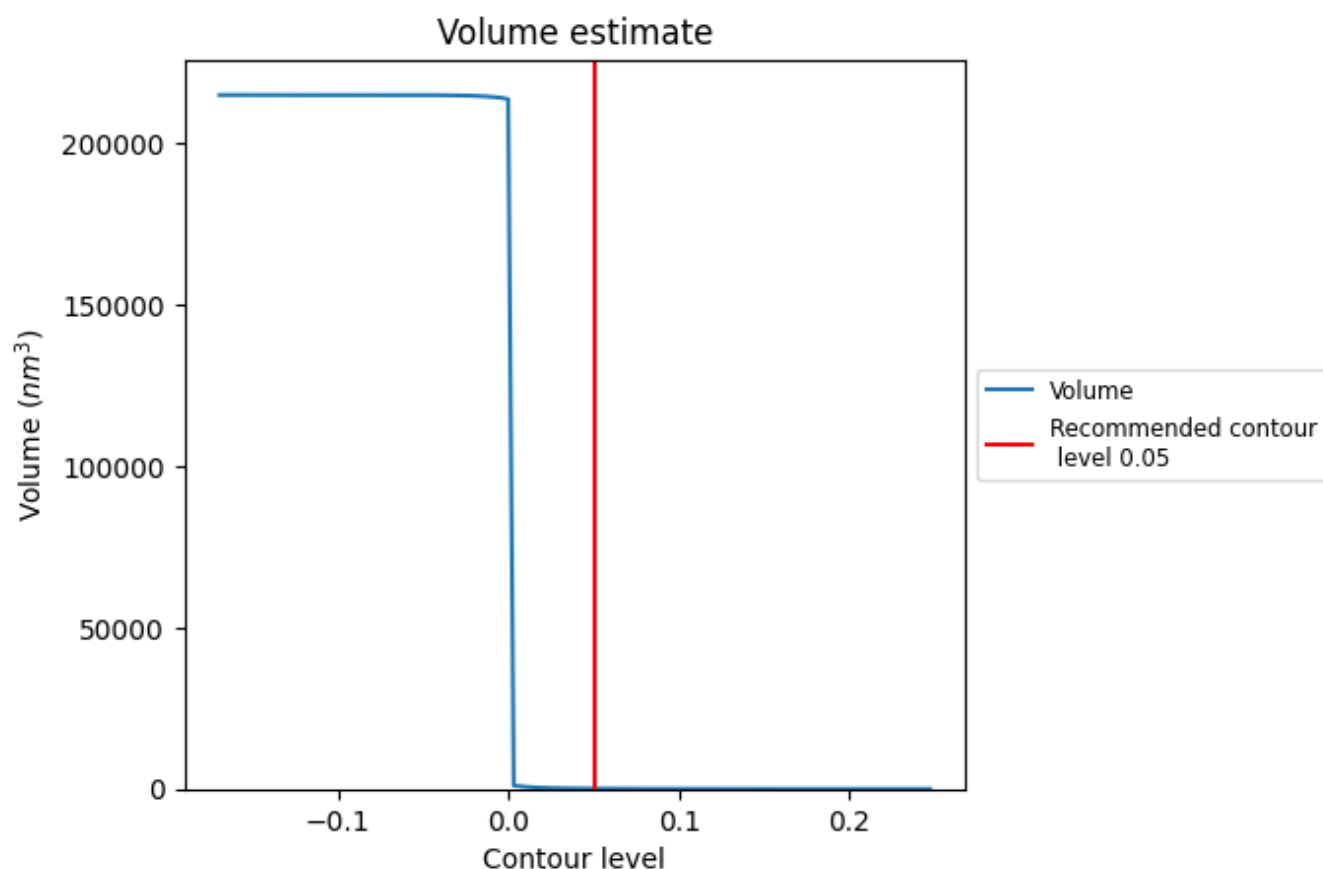
This section contains the results of statistical analysis of the map.

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.

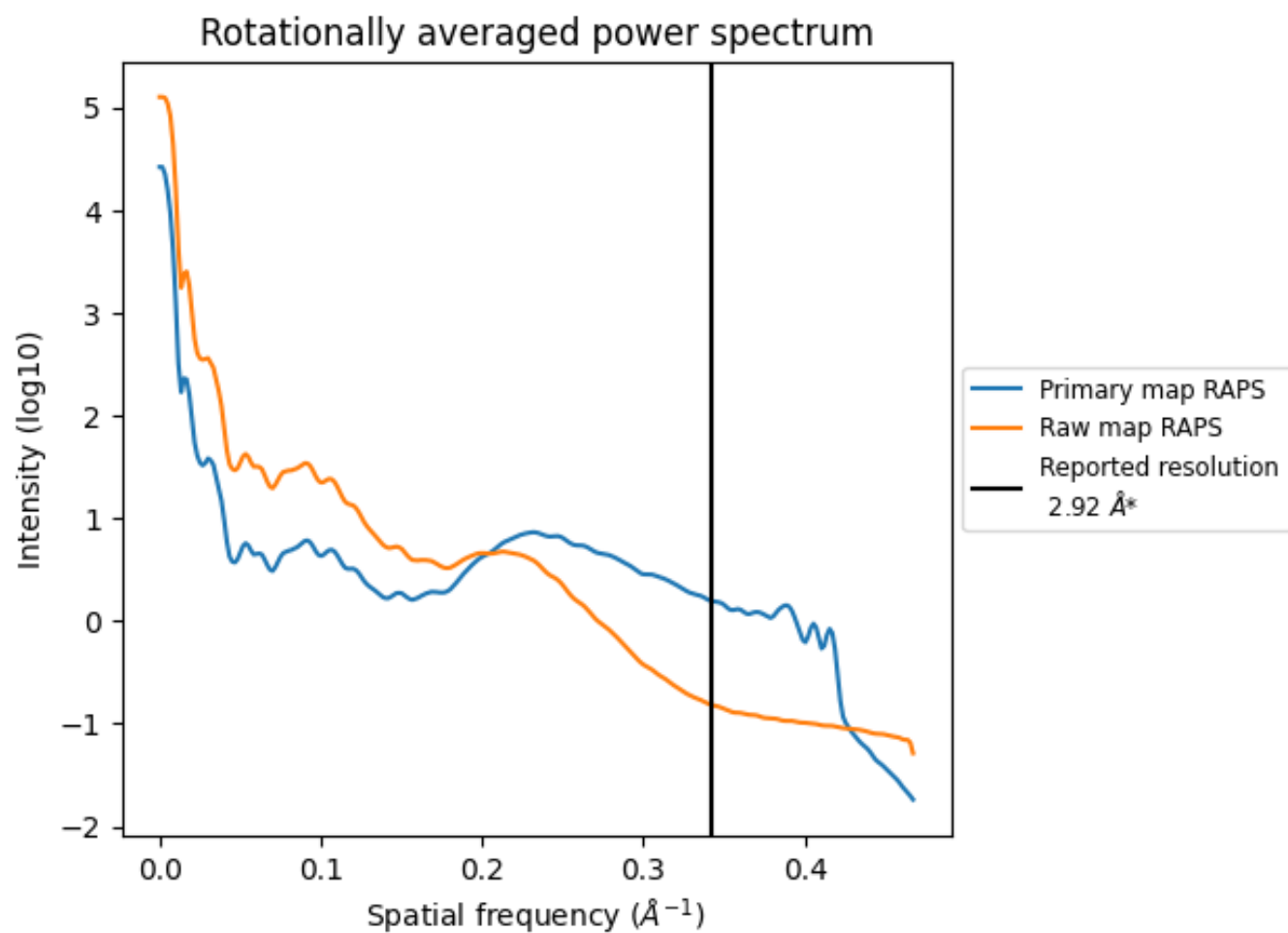
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ

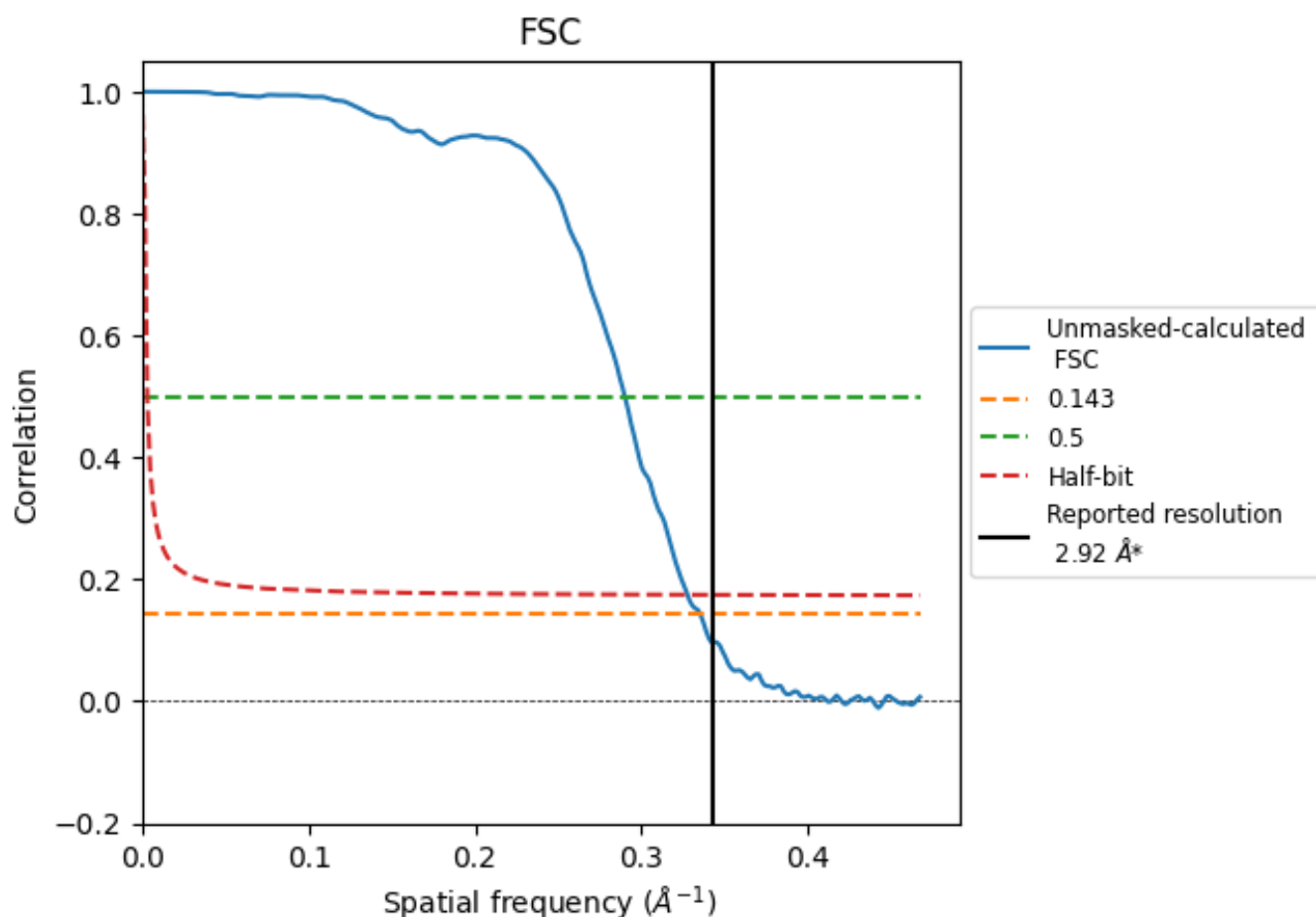


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.342 \AA^{-1}

8.2 Resolution estimates [i](#)

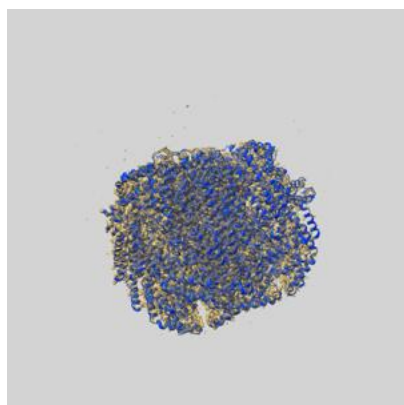
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.98	3.45	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

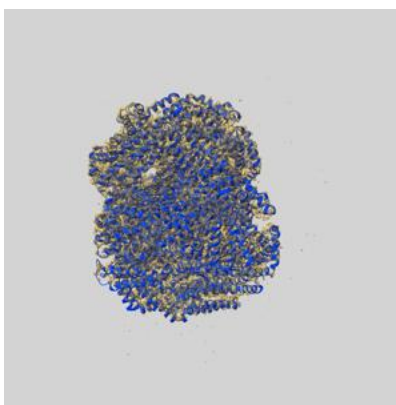
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66300 and PDB model 9X6D. Per-residue inclusion information can be found in section [3](#) on page [8](#).

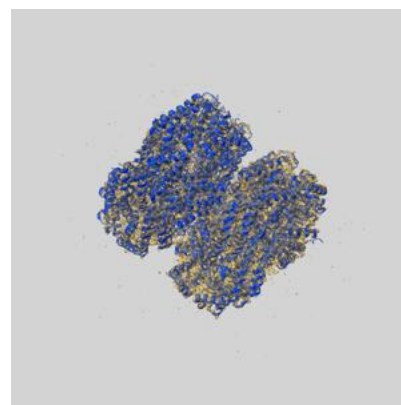
9.1 Map-model overlay [i](#)



X



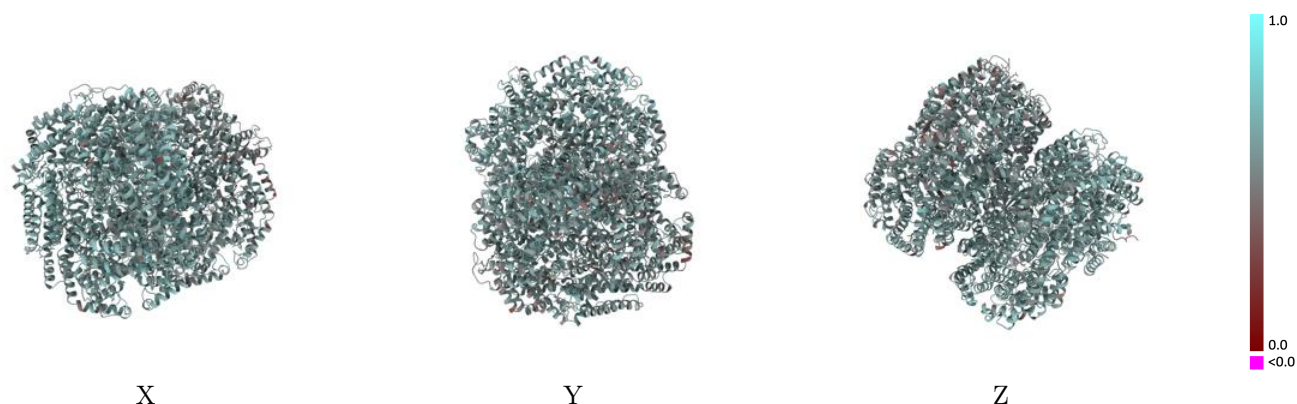
Y



Z

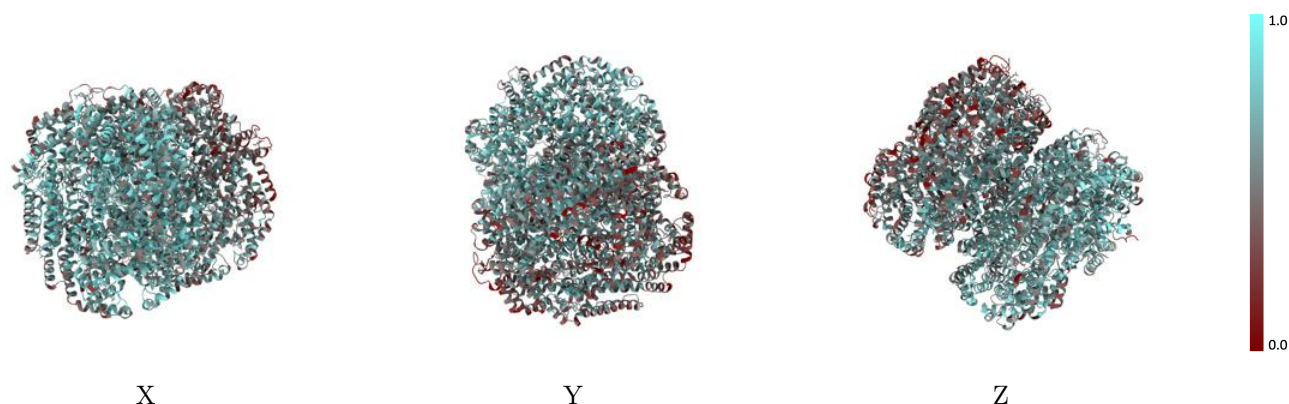
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



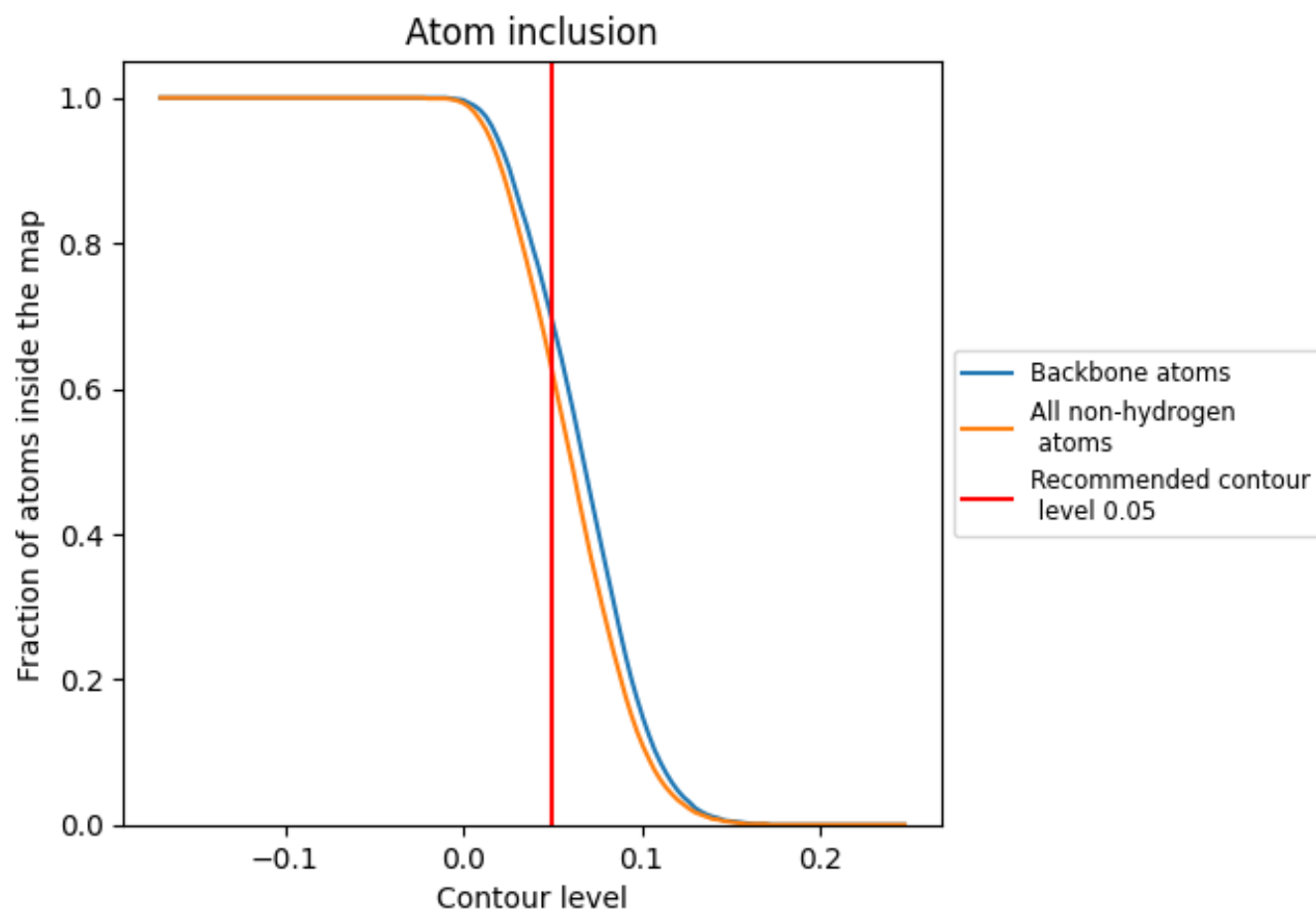
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.5900
A	 0.7420	 0.6120
B	 0.7110	 0.6160
C	 0.7100	 0.6070
D	 0.6680	 0.6020
E	 0.6620	 0.6050
F	 0.6830	 0.6060
G	 0.7090	 0.6160
H	 0.6740	 0.6050
I	 0.6850	 0.6110
J	 0.6920	 0.6100
K	 0.6710	 0.6070
L	 0.6980	 0.6100
M	 0.4840	 0.5610
N	 0.6130	 0.5820
O	 0.6310	 0.5900
P	 0.4600	 0.5440
Q	 0.4410	 0.5390
R	 0.4690	 0.5470
S	 0.4980	 0.5640
T	 0.5460	 0.5730
U	 0.5280	 0.5780
V	 0.6370	 0.5930
W	 0.6360	 0.5930
X	 0.5550	 0.5700
Y	 0.1900	 0.4670
Z	 0.7310	 0.6160
a	 0.6800	 0.6070

