



Full wwPDB EM Validation Report ⓘ

Apr 18, 2026 – 08:42 am BST

PDB ID : 9SMG / pdb_00009smg
EMDB ID : EMD-55031
Title : Reduced bovine complex I in lipid nanodisc, NADH-active-altQ10
Authors : Chung, I.; Hirst, J.
Deposited on : 2025-09-08
Resolution : 2.42 Å(reported)
Based on initial model : 7QSK

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:

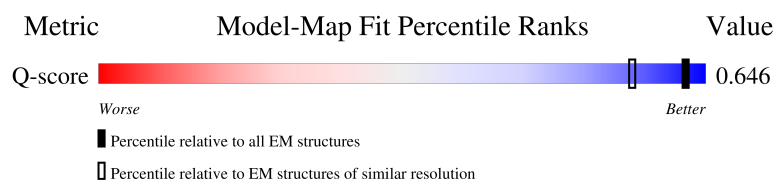
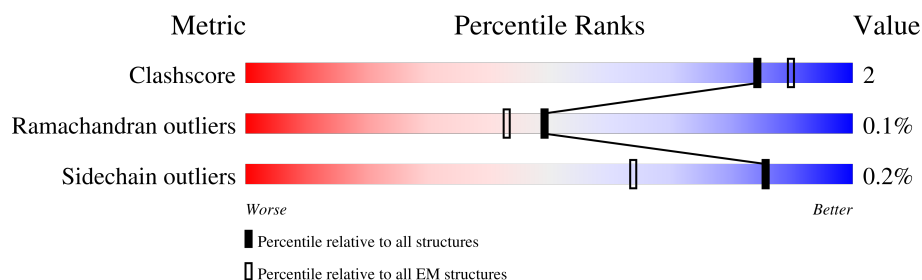
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 2.42 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.





















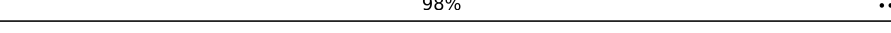

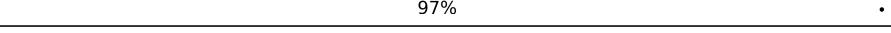
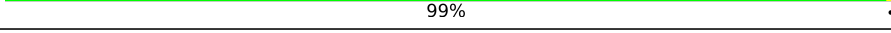
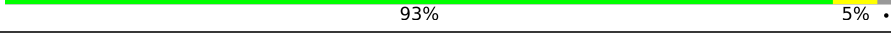

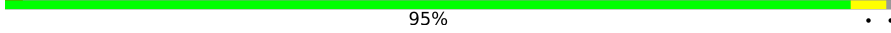
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5729 (1.92 - 2.92)

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

Mol	Chain	Length	Quality of chain
1	A	115	 86% 14%
2	B	216	 66% 6% 27%
3	C	266	 77% 21%
4	D	463	 89% 7%



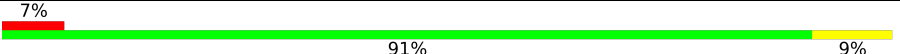
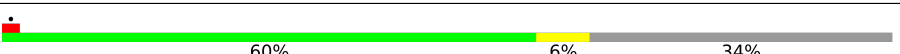
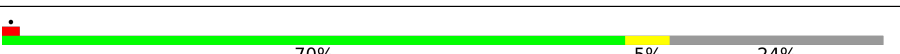
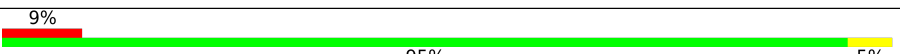
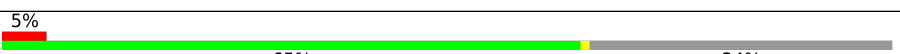
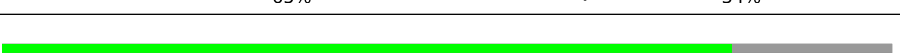

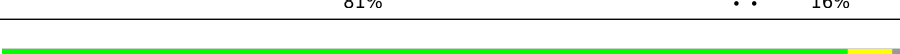
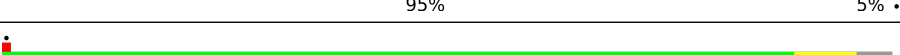

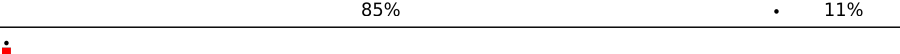
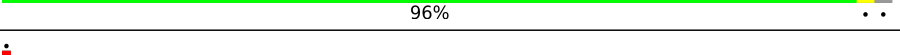
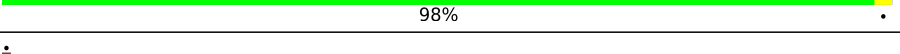

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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	121	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 70726 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1261	803	227	217	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1668	1064	280	314	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	433	Total	C	N	O	S	0	0
			3331	2099	595	617	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	690	Total	C	N	O	S	0	0
			5288	3312	922	1015	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			707	454	104	144	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	ACE	-	acetylation	UNP Q8HXG6

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	121	Total	C	N	O	S	0	0
			999	650	172	172	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	ACE	-	acetylation	UNP Q02827

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	100	Total	C	N	O	S	0	0
			838	528	160	144	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			854	548	141	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	143	Total	C	N	O	S	0	0
			1186	776	203	205	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	ACE	-	acetylation	UNP Q02367

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1067	684	188	195			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1453	910	268	267	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	97	Total	C	N	O	S	0	0
			785	496	146	140	3		

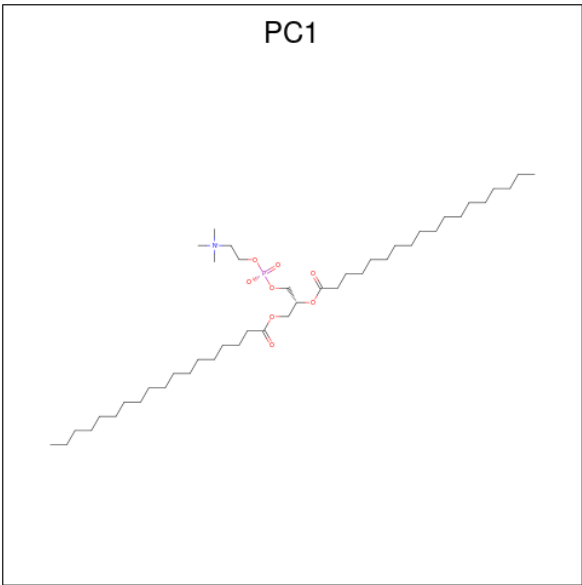
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Chain	Residue	Modelled	Actual	Comment	Reference
r	1	ACE	-	acetylation	UNP Q05752

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	I	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	P	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	h	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



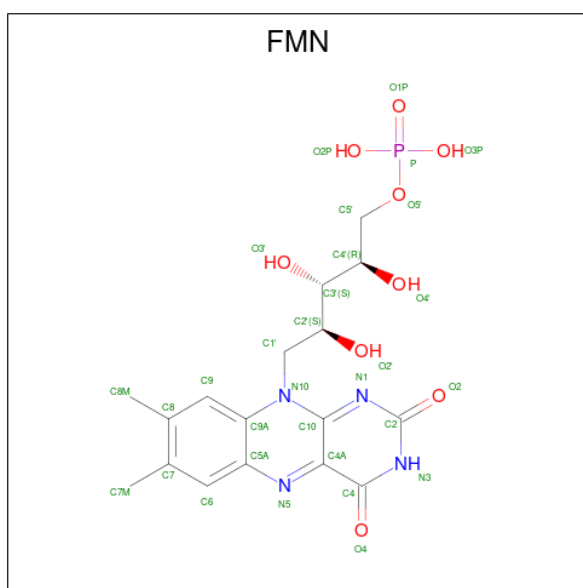
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

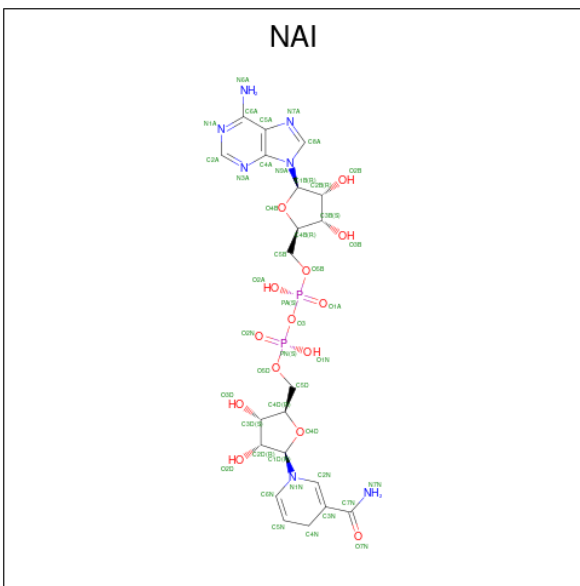
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
48	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID:

NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

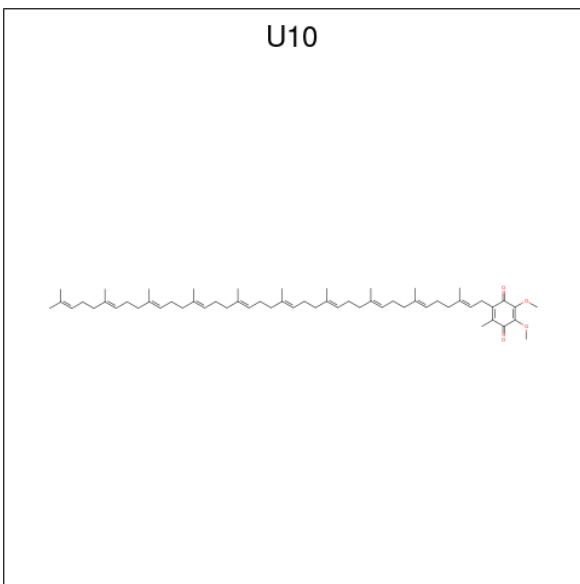


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total 44	C 21	N 7	O 14	P 2	0

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

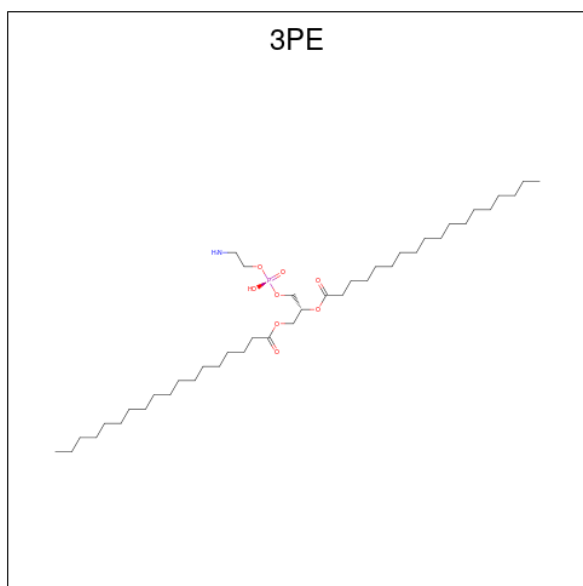
Mol	Chain	Residues	Atoms	AltConf
50	G	1	Total K 1 1	0

- Molecule 51 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			63	59	4	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



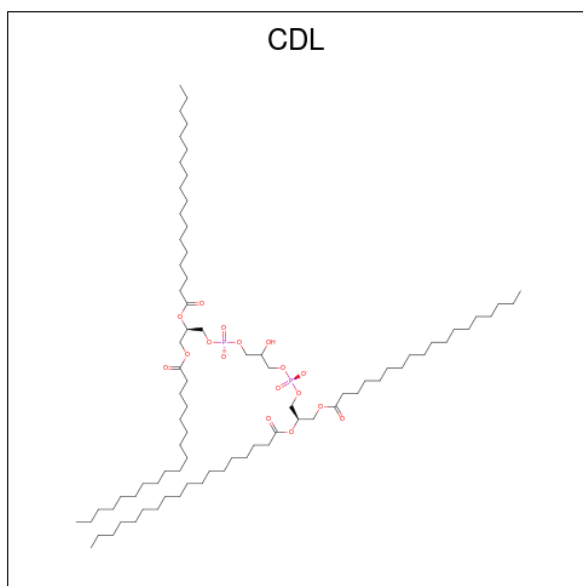
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
52	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	K	1	Total	C	N	O	P	0
			42	32	1	8	1	
52	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
52	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
52	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	N	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
52	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	Y	1	Total	C	N	O	P	0
			34	24	1	8	1	
52	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
52	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
52	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
52	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



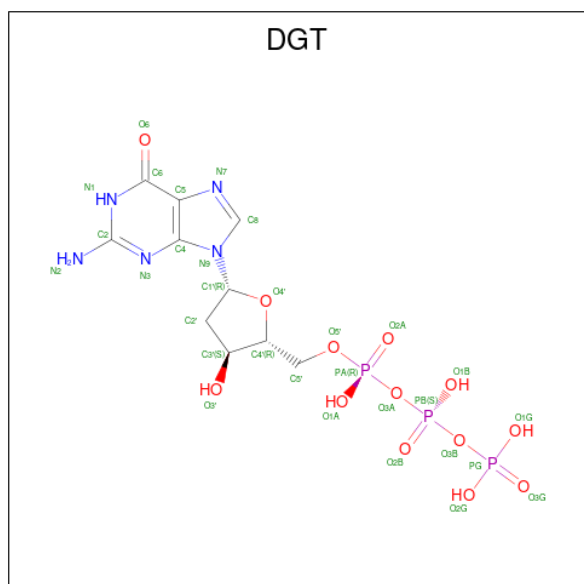
Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			69	50	17	2	
53	M	1	Total	C	O	P	0
			81	62	17	2	
53	P	1	Total	C	O	P	0
			69	50	17	2	

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Mol	Chain	Residues	Atoms				AltConf
53	X	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			78	59	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

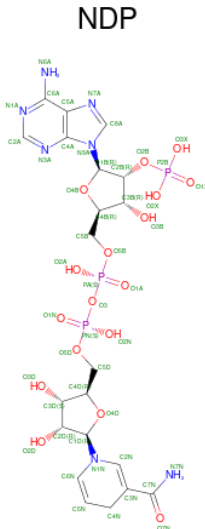


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

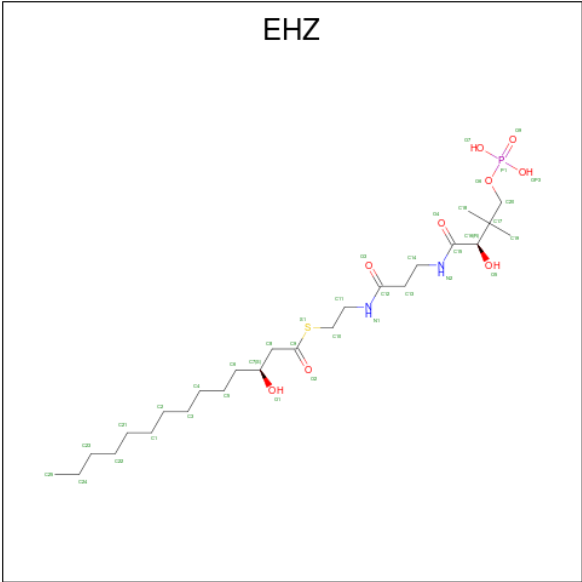


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

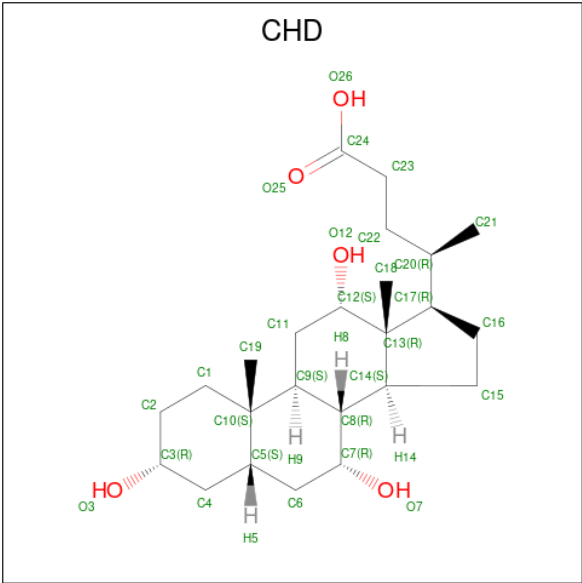
Mol	Chain	Residues	Atoms	AltConf
57	R	1	Total Zn 1 1	0

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



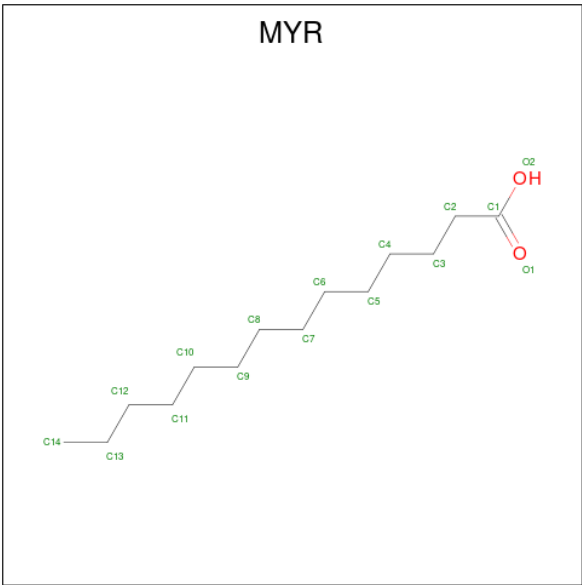
Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
58	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	32	Total	O	0
			32	32	
61	B	76	Total	O	0
			76	76	
61	C	111	Total	O	0
			111	111	
61	D	200	Total	O	0
			200	200	
61	E	31	Total	O	0
			31	31	
61	F	81	Total	O	0
			81	81	
61	G	223	Total	O	0
			223	223	
61	H	107	Total	O	0
			107	107	
61	I	100	Total	O	0
			100	100	
61	J	41	Total	O	0
			41	41	
61	K	24	Total	O	0
			24	24	

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Mol	Chain	Residues	Atoms		AltConf
61	L	61	Total 61	O 61	0
61	M	131	Total 131	O 131	0
61	N	77	Total 77	O 77	0
61	O	25	Total 25	O 25	0
61	P	87	Total 87	O 87	0
61	Q	101	Total 101	O 101	0
61	R	35	Total 35	O 35	0
61	S	1	Total 1	O 1	0
61	T	1	Total 1	O 1	0
61	V	14	Total 14	O 14	0
61	W	24	Total 24	O 24	0
61	X	33	Total 33	O 33	0
61	Y	2	Total 2	O 2	0
61	Z	52	Total 52	O 52	0
61	a	32	Total 32	O 32	0
61	b	6	Total 6	O 6	0
61	d	23	Total 23	O 23	0
61	e	31	Total 31	O 31	0
61	f	3	Total 3	O 3	0
61	g	14	Total 14	O 14	0
61	h	33	Total 33	O 33	0

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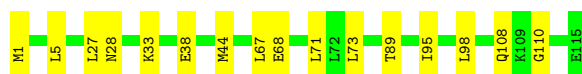
Mol	Chain	Residues	Atoms		AltConf
61	i	2	Total 2	O 2	0
61	l	22	Total 22	O 22	0
61	m	14	Total 14	O 14	0
61	n	13	Total 13	O 13	0
61	o	1	Total 1	O 1	0
61	p	36	Total 36	O 36	0
61	q	35	Total 35	O 35	0
61	r	25	Total 25	O 25	0
61	s	11	Total 11	O 11	0

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.

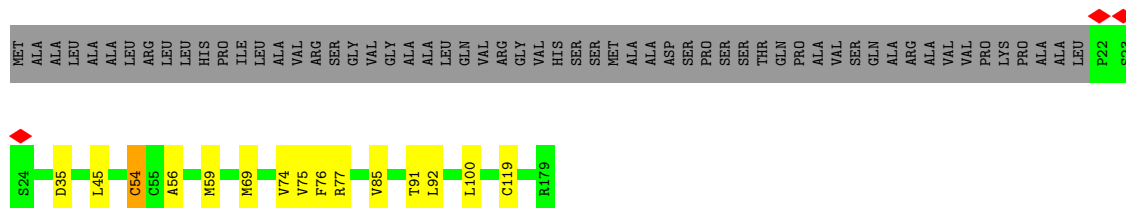
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 




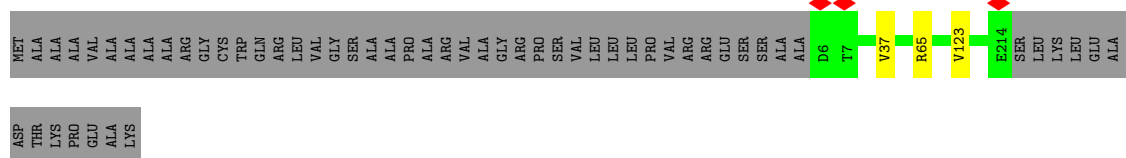
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



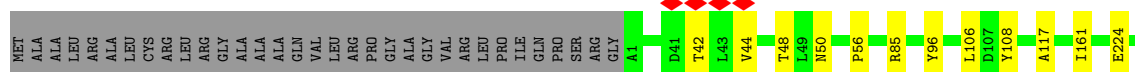
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 

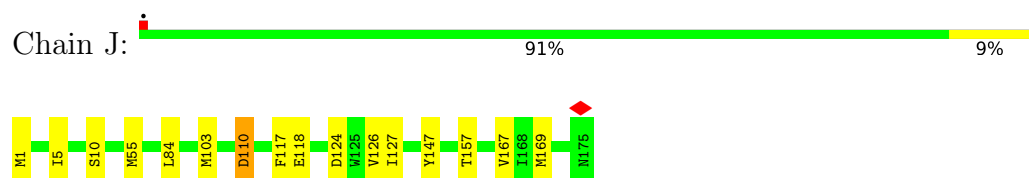


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

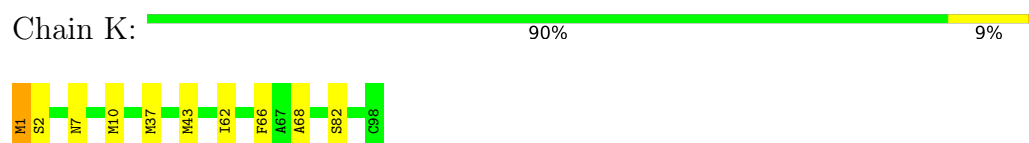
Chain D: 



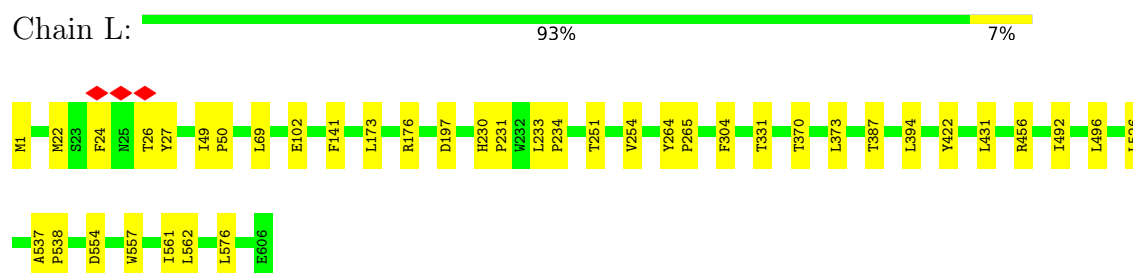
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



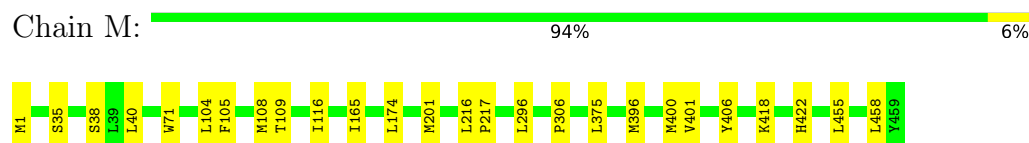
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



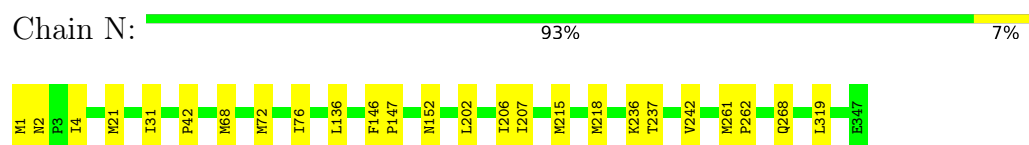
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



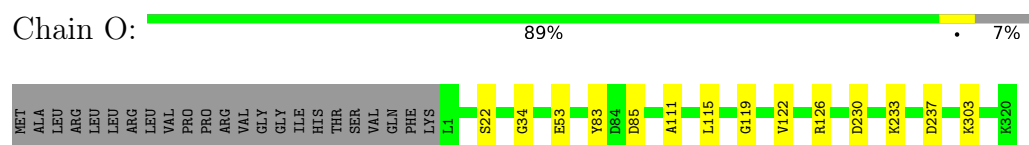
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

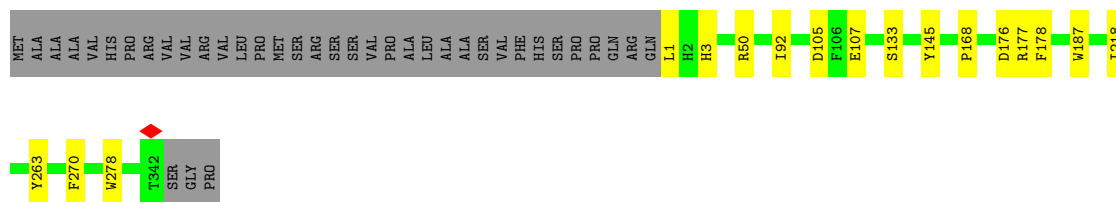


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



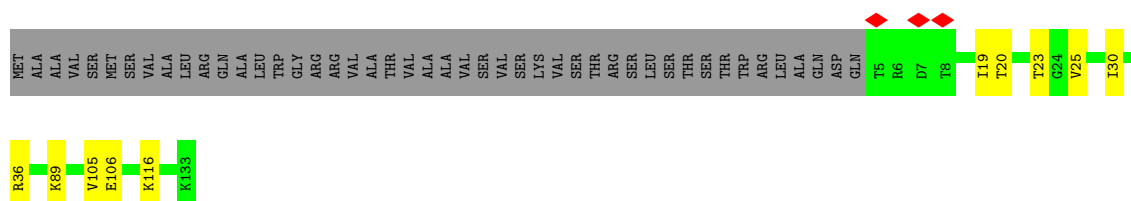
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  86% 10%



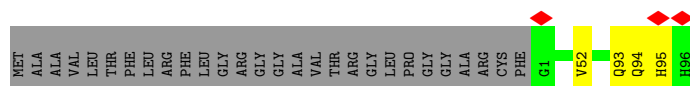
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  68% 6% 26%




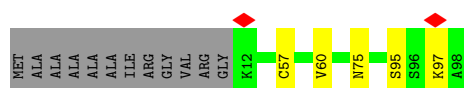
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  74% 23%



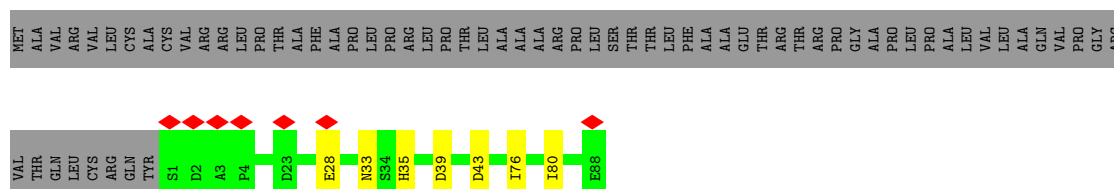
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:  83% 5% 12%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  52% 44%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  52% 44%

MET ALA VAL ARG VAL LEU CYS CYS VAL ARG LEU PRO THR ALA PHE ALA PRO LEU PRO ARG LEU PRO THR LEU ALA ALA ARG PRO LEU SER THR THR LEU PHE ALA ALA GLU THR ARG THR ARG PRO GLY ALA PRO LEU PRO ALA VAL VAL ALA GLN VAL PRO GLY ARG


VAL THR GLN LEU CYS ARG GLN TYR S1 D2 E28 N33 D46 E55 D56 G69 E88

- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:  98%

MET A1 G2 L3 I115

- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  88%

MET ALA ALA SER GLY LEU ARG GLN ALA VAL VAL ALA ALA S13 R63 N69 V95 P127

- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  97%

MET F1 L44 E79 P80 V130 V153 M171

- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  99%


ACE1 E13 K125 V140

- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  93%

MET ALA ALA S3 R27 H50 R67 R81 E92 Y124 V132 T143

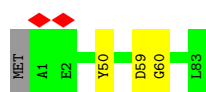
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  91%

M1 R25 R28 R53 T69 D70

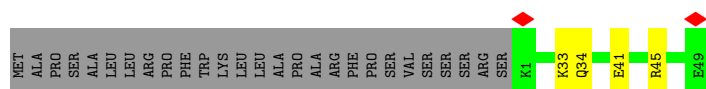
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  95%




- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  59% 5% 36%




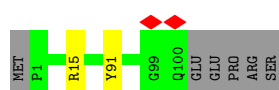
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  88% 12%




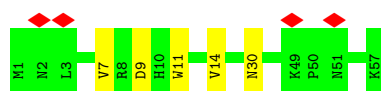
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  92% 6%



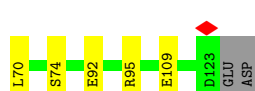
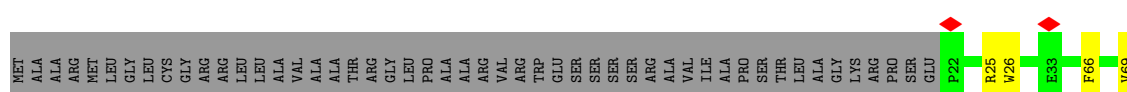
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  7% 91% 9%

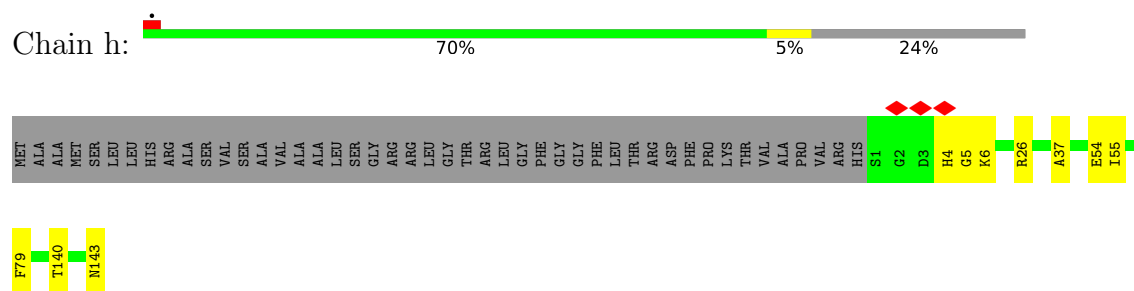


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

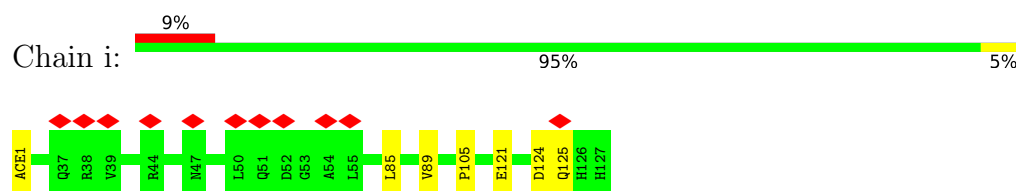
Chain g:  60% 6% 34%



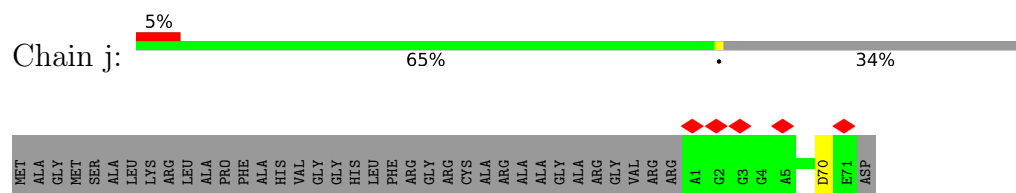
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



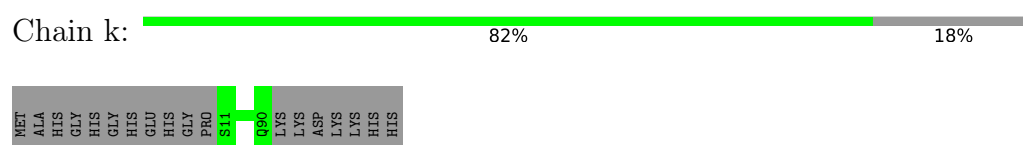
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



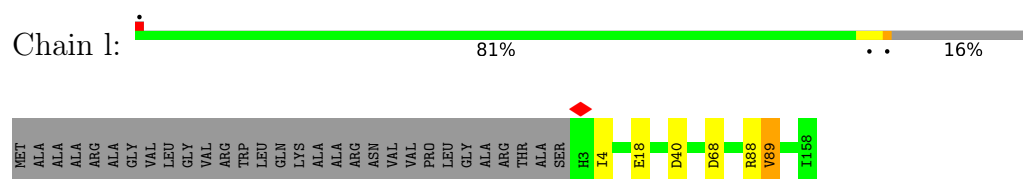
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



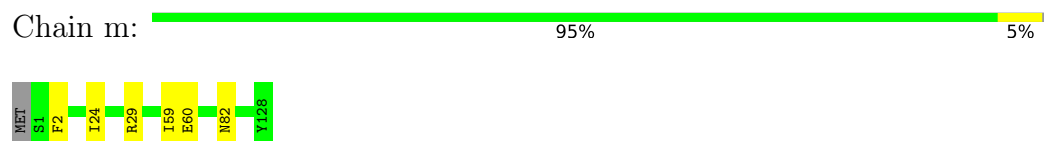
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3




- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

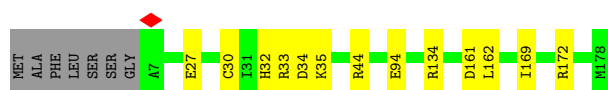


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4




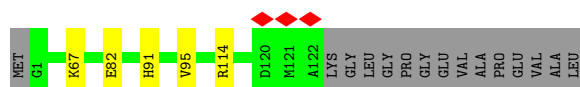
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  89% 7%



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  85% 11%



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  96%




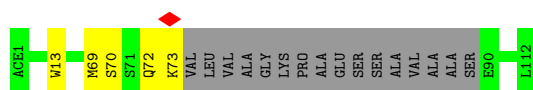
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  98%



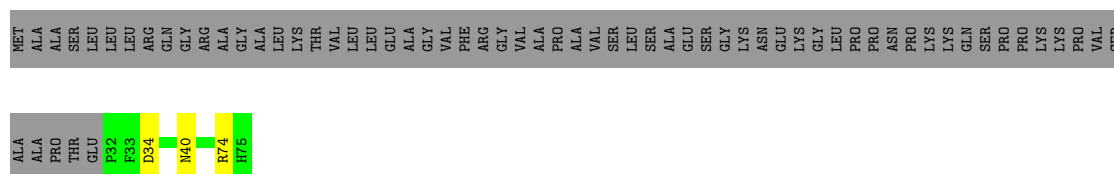
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  81% 14%



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  38% 60%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.29	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	33.956	Depositor
Minimum map value	-14.378	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.906	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75375, 0.75375, 0.75375	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, DGT, NAI, CHD, NDP, SF4, CDL, MG, K, PC1, FES, FMN, 3PE, U10, ZN, EHZ, ACE, FME, 2MR, WYK

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	0.10	0/936	0.24	0/1281
2	B	0.12	0/1280	0.29	0/1730
3	C	0.10	0/1789	0.26	0/2436
4	D	0.12	0/3537	0.26	0/4794
5	E	0.10	0/1708	0.27	0/2324
6	F	0.11	0/3406	0.25	0/4602
7	G	0.09	0/5376	0.25	0/7286
8	H	0.11	0/2571	0.30	0/3513
9	I	0.10	0/1445	0.26	0/1956
10	J	0.09	0/1370	0.23	0/1859
11	K	0.10	0/745	0.25	0/1008
12	L	0.09	0/4920	0.25	0/6694
13	M	0.09	0/3738	0.24	0/5097
14	N	0.10	0/2792	0.26	0/3800
15	O	0.09	0/2651	0.22	0/3587
16	P	0.17	0/2831	0.31	0/3841
17	Q	0.10	0/1072	0.28	0/1449
18	R	0.13	0/753	0.24	0/1014
19	S	0.08	0/711	0.22	0/956
20	T	0.11	0/719	0.30	0/971
20	U	0.10	0/719	0.19	0/971
21	V	0.10	0/948	0.20	0/1284
22	W	0.10	0/1000	0.26	0/1344
23	X	0.10	0/1439	0.25	0/1942
24	Y	0.18	0/1048	0.21	0/1423
25	Z	0.09	0/1181	0.22	0/1592
26	a	0.15	0/584	0.34	0/786
27	b	0.12	0/672	0.23	0/923
28	c	0.11	0/427	0.18	0/579
29	d	0.19	0/1027	0.26	0/1387
30	e	0.10	0/859	0.24	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.11	0/505	0.25	0/681
32	g	0.10	0/881	0.27	0/1197
33	h	0.09	0/1221	0.23	0/1651
34	i	0.18	1/1134 (0.1%)	0.24	0/1544
35	j	0.11	0/624	0.20	0/855
36	k	0.07	0/663	0.17	0/895
37	l	0.09	0/1369	0.23	0/1873
38	m	0.10	0/1094	0.21	0/1480
39	n	0.08	0/1545	0.21	0/2092
40	o	0.08	0/1073	0.22	0/1437
41	p	0.09	0/1486	0.24	0/2004
42	q	0.10	0/1250	0.22	0/1698
43	r	0.21	0/804	0.26	0/1088
44	s	0.09	0/383	0.24	0/518
All	All	0.11	1/68286 (0.0%)	0.25	0/92590

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	a	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1	ACE	C-N	5.04	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	a	25	ARG	Sidechain
26	a	28	ARG	Sidechain

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	921	0	952	16	0
2	B	1261	0	1256	13	0
3	C	1738	0	1685	2	0
4	D	3459	0	3404	15	0
5	E	1668	0	1672	8	0
6	F	3331	0	3287	17	0
7	G	5288	0	5309	21	0
8	H	2509	0	2621	20	0
9	I	1414	0	1370	8	0
10	J	1345	0	1352	15	0
11	K	745	0	785	12	0
12	L	4802	0	4960	25	0
13	M	3654	0	3852	19	0
14	N	2733	0	2912	20	0
15	O	2589	0	2565	10	0
16	P	2754	0	2773	14	0
17	Q	1049	0	1045	7	0
18	R	740	0	714	2	0
19	S	700	0	719	3	0
20	T	707	0	700	5	0
20	U	707	0	700	6	0
21	V	928	0	972	1	0
22	W	976	0	991	2	0
23	X	1402	0	1379	3	0
24	Y	1030	0	1039	1	0
25	Z	1152	0	1151	6	0
26	a	569	0	568	3	0
27	b	651	0	662	2	0
28	c	414	0	415	2	0
29	d	999	0	988	12	0
30	e	838	0	837	2	0
31	f	492	0	501	4	0
32	g	854	0	802	7	0
33	h	1186	0	1193	7	0
34	i	1097	0	1108	4	0
35	j	597	0	536	1	0
36	k	644	0	626	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1314	0	1210	5	0
38	m	1067	0	1067	5	0
39	n	1492	0	1438	8	0
40	o	1048	0	1016	4	0
41	p	1453	0	1425	4	0
42	q	1209	0	1182	2	0
43	r	785	0	795	4	0
44	s	371	0	344	3	0
45	A	70	0	88	5	0
45	B	90	0	128	2	0
45	I	40	0	54	1	0
45	M	42	0	61	1	0
45	N	39	0	52	5	0
45	P	33	0	40	2	0
45	Z	44	0	62	2	0
45	h	44	0	62	0	0
45	q	49	0	75	1	0
46	B	8	0	0	0	0
46	F	8	0	0	1	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	F	44	0	25	3	0
50	G	1	0	0	0	0
51	H	63	0	90	15	0
52	H	79	0	109	3	0
52	K	42	0	58	0	0
52	L	138	0	207	2	0
52	M	43	0	60	1	0
52	N	121	0	167	2	0
52	P	35	0	44	5	0
52	Y	173	0	219	2	0
52	b	47	0	71	2	0
52	m	41	0	59	1	0
53	L	69	0	82	0	0
53	M	81	0	112	2	0
53	P	69	0	85	1	0
53	X	86	0	125	1	0
53	d	65	0	77	2	0
53	h	78	0	100	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	q	61	0	66	2	0
54	O	31	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	0	0
57	R	1	0	0	0	0
58	T	37	0	0	3	0
58	U	37	0	0	1	0
59	i	29	0	38	1	0
60	o	15	0	27	0	0
61	A	32	0	0	0	0
61	B	76	0	0	0	0
61	C	111	0	0	0	0
61	D	200	0	0	0	0
61	E	31	0	0	1	0
61	F	81	0	0	0	0
61	G	223	0	0	1	0
61	H	107	0	0	2	0
61	I	100	0	0	0	0
61	J	41	0	0	0	0
61	K	24	0	0	0	0
61	L	61	0	0	1	0
61	M	131	0	0	0	0
61	N	77	0	0	0	0
61	O	25	0	0	0	0
61	P	87	0	0	0	0
61	Q	101	0	0	0	0
61	R	35	0	0	0	0
61	S	1	0	0	0	0
61	T	1	0	0	0	0
61	V	14	0	0	0	0
61	W	24	0	0	0	0
61	X	33	0	0	0	0
61	Y	2	0	0	0	0
61	Z	52	0	0	1	0
61	a	32	0	0	1	0
61	b	6	0	0	0	0
61	d	23	0	0	0	0
61	e	31	0	0	1	0
61	f	3	0	0	0	0
61	g	14	0	0	0	0
61	h	33	0	0	0	0
61	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	l	22	0	0	0	0
61	m	14	0	0	0	0
61	n	13	0	0	0	0
61	o	1	0	0	0	0
61	p	36	0	0	0	0
61	q	35	0	0	0	0
61	r	25	0	0	0	0
61	s	11	0	0	1	0
All	All	70726	0	69378	321	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 2.

All (321) 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)
25:Z:92:GLU:OE1	30:e:91:TYR:OH	2.02	0.78
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.67	0.75
7:G:675:ASP:OD1	7:G:678:SER:OG	2.03	0.75
51:H:701:U10:H38	51:H:701:U10:H351	1.69	0.75
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.20	0.74
12:L:197:ASP:OD1	61:L:801:HOH:O	2.07	0.73
33:h:140:THR:O	33:h:143:ASN:ND2	2.22	0.72
15:O:22:SER:OG	15:O:119:GLY:O	2.04	0.72
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.71	0.71
7:G:366:THR:O	7:G:367:THR:OG1	2.07	0.70
10:J:103:MET:HE2	11:K:10:MET:HE2	1.74	0.70
15:O:83:TYR:OH	54:O:401:DGT:O3'	2.00	0.69
7:G:293:HIS:ND1	16:P:1:LEU:HD13	2.07	0.68
8:H:227:GLU:OE2	61:H:801:HOH:O	2.13	0.66
17:Q:19:ILE:O	17:Q:23:THR:HG23	1.97	0.65
45:P:401:PC1:O22	45:P:401:PC1:H32	1.97	0.64
6:F:98:ASP:O	6:F:99:GLU:C	2.41	0.63
7:G:644:GLN:N	7:G:644:GLN:OE1	2.31	0.63
16:P:176:ASP:OD1	16:P:177:ARG:N	2.31	0.63
2:B:45:LEU:HD22	2:B:85:VAL:CG2	2.30	0.62
34:i:105:PRO:O	40:o:67:LYS:NZ	2.32	0.62
5:E:105:THR:HG22	5:E:106:THR:H	1.65	0.61
12:L:251:THR:O	12:L:254:VAL:HG22	2.00	0.61
1:A:89:THR:HG21	45:A:202:PC1:H321	1.83	0.61
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:224:GLU:OE1	9:I:40:TYR:OH	2.10	0.61
37:l:18:GLU:N	37:l:18:GLU:OE1	2.33	0.60
7:G:689:LYS:NZ	7:G:693:GLU:OE2	2.26	0.60
51:H:701:U10:H351	51:H:701:U10:C38	2.30	0.60
29:d:5:ARG:NH1	29:d:89:ASP:OD1	2.36	0.59
7:G:109:ASP:OD2	61:G:901:HOH:O	2.16	0.59
16:P:278:TRP:CH2	52:P:404:3PE:H232	2.36	0.59
29:d:9:ALA:HB1	29:d:12:GLN:NE2	2.18	0.59
31:f:30:ASN:ND2	31:f:30:ASN:O	2.36	0.58
12:L:173:LEU:HD23	52:L:701:3PE:H322	1.84	0.58
35:j:70:ASP:OD2	40:o:114:ARG:NH2	2.36	0.58
52:Y:802:3PE:H2I2	52:Y:803:3PE:H332	1.86	0.58
14:N:136:LEU:HD22	45:N:404:PC1:H3B2	1.87	0.57
12:L:26:THR:HG22	12:L:27:TYR:H	1.70	0.57
10:J:10:SER:OG	11:K:7:ASN:ND2	2.36	0.56
51:H:701:U10:H301	51:H:701:U10:C36	2.35	0.56
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.34	0.56
10:J:110:ASP:OD1	10:J:110:ASP:N	2.38	0.56
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.87	0.56
45:M:503:PC1:O13	45:M:503:PC1:H132	2.05	0.56
33:h:54:GLU:OE2	33:h:55:ILE:N	2.39	0.56
43:r:69:MET:SD	43:r:70:SER:N	2.79	0.56
5:E:91:ASN:ND2	61:E:403:HOH:O	2.39	0.55
10:J:126:VAL:HG23	10:J:127:ILE:HG23	1.88	0.55
20:U:88:GLU:OE2	33:h:6:LYS:NZ	2.39	0.55
8:H:243:LEU:CD1	52:H:702:3PE:H2C2	2.36	0.55
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.89	0.55
38:m:24:ILE:HD13	38:m:29:ARG:NE	2.21	0.55
59:i:201:CHD:H212	59:i:201:CHD:H12	1.88	0.54
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.41	0.54
15:O:230:ASP:OD1	15:O:233:LYS:N	2.39	0.54
5:E:111:ARG:NH1	6:F:260:GLY:O	2.40	0.54
10:J:157:THR:HG22	11:K:66:PHE:HE2	1.73	0.53
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.90	0.53
14:N:152:ASN:HB3	52:N:402:3PE:H222	1.90	0.53
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.74	0.53
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.43	0.53
2:B:59:MET:HE2	51:H:701:U10:H102	1.92	0.52
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.41	0.52
9:I:54:LYS:NZ	9:I:138:GLU:OE2	2.43	0.52
7:G:226:GLU:OE1	17:Q:36:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD21	8:H:3:MET:SD	2.50	0.52
4:D:42:THR:O	4:D:42:THR:HG23	2.09	0.52
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.92	0.52
39:n:134:ARG:NH1	39:n:161:ASP:OD1	2.43	0.52
52:L:701:3PE:H2D2	13:M:401:VAL:HG11	1.91	0.51
15:O:85:ASP:OD1	15:O:85:ASP:N	2.43	0.51
14:N:21:MET:HE1	45:N:404:PC1:H3B1	1.92	0.51
14:N:206:ILE:HD11	45:N:404:PC1:H382	1.92	0.51
16:P:105:ASP:OD1	16:P:107:GLU:N	2.44	0.51
25:Z:67:ARG:NH2	27:b:50:TYR:O	2.44	0.51
6:F:118:LEU:HD13	6:F:225:VAL:HG13	1.93	0.51
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.93	0.51
16:P:187:TRP:CE3	52:P:404:3PE:H252	2.46	0.51
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.39	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.10	0.50
20:T:28:GLU:N	20:T:28:GLU:OE1	2.42	0.50
53:M:502:CDL:H731	14:N:242:VAL:HG11	1.94	0.50
6:F:184:TYR:OH	49:F:503:NAI:H5N	2.11	0.50
18:R:52:VAL:O	18:R:94:GLN:N	2.44	0.50
12:L:176:ARG:NH1	13:M:400:MET:O	2.45	0.50
34:i:124:ASP:OD1	34:i:125:GLN:N	2.45	0.50
6:F:82:MET:O	6:F:91:LYS:NZ	2.31	0.50
51:H:701:U10:H301	51:H:701:U10:C33	2.40	0.50
51:H:701:U10:H301	51:H:701:U10:C34	2.42	0.50
16:P:278:TRP:CZ3	52:P:404:3PE:H232	2.47	0.50
20:T:35:HIS:N	20:T:39:ASP:OD2	2.44	0.50
12:L:264:TYR:N	12:L:265:PRO:CD	2.75	0.49
7:G:484:THR:HG22	7:G:485:GLY:H	1.76	0.49
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.94	0.49
13:M:306:PRO:HA	13:M:458:LEU:HD22	1.94	0.49
45:Z:200:PC1:O13	45:Z:200:PC1:H133	2.12	0.49
29:d:9:ALA:HB3	29:d:15:PRO:HG3	1.94	0.49
32:g:25:ARG:O	32:g:26:TRP:CG	2.65	0.49
1:A:44:MET:CE	4:D:48:THR:HG22	2.43	0.49
7:G:46:LEU:O	17:Q:116:LYS:NZ	2.45	0.49
25:Z:81:ARG:NH1	61:Z:304:HOH:O	2.46	0.49
21:V:3:LEU:HD23	21:V:3:LEU:H	1.77	0.49
39:n:34:ASP:OD1	39:n:35:LYS:N	2.46	0.49
8:H:207:LEU:O	8:H:209:SER:N	2.46	0.49
9:I:79:ALA:HB2	9:I:106:THR:HG23	1.94	0.49
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.95	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.96	0.48
37:l:4:ILE:HD11	38:m:60:GLU:OE2	2.13	0.48
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.42	0.48
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.44	0.48
20:U:28:GLU:N	20:U:28:GLU:OE1	2.44	0.48
4:D:117:ALA:HB2	4:D:367:ILE:HG12	1.95	0.48
5:E:148:CYS:SG	6:F:103:GLY:N	2.86	0.48
29:d:112:VAL:O	41:p:159:LYS:NZ	2.46	0.48
4:D:96:TYR:CE2	4:D:358:VAL:HG21	2.49	0.48
45:Z:200:PC1:H133	45:Z:200:PC1:P	2.54	0.48
37:l:40:ASP:O	38:m:82:ASN:ND2	2.46	0.48
8:H:243:LEU:HD11	52:H:702:3PE:H2C2	1.96	0.48
12:L:22:MET:SD	12:L:27:TYR:OH	2.55	0.48
3:C:65:ARG:NH1	3:C:123:VAL:O	2.45	0.47
9:I:75:GLU:O	9:I:105:ARG:NH1	2.47	0.47
13:M:201:MET:HG3	52:M:501:3PE:H2G2	1.96	0.47
7:G:356:THR:HG21	7:G:503:LEU:HD22	1.96	0.47
1:A:27:LEU:HD12	45:A:201:PC1:H131	1.97	0.47
11:K:37:MET:SD	14:N:68:MET:HE1	2.54	0.47
4:D:56:PRO:O	51:H:701:U10:H1M3	2.15	0.47
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.96	0.47
53:M:502:CDL:C73	14:N:242:VAL:HG11	2.44	0.47
52:Y:802:3PE:H2B2	52:Y:803:3PE:C37	2.44	0.47
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.47	0.47
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.96	0.47
13:M:35:SER:O	13:M:38:SER:OG	2.27	0.47
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.95	0.47
32:g:109:GLU:O	41:p:141:ARG:NE	2.48	0.47
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.97	0.47
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.50	0.47
19:S:95:SER:O	19:S:97:LYS:NZ	2.37	0.47
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.32	0.47
34:i:121:GLU:N	34:i:121:GLU:OE1	2.48	0.47
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.96	0.47
37:l:88:ARG:O	37:l:89:VAL:C	2.57	0.47
45:B:202:PC1:H142	45:B:202:PC1:O13	2.16	0.46
58:T:101:EHZ:N1	22:W:69:ASN:O	2.49	0.46
1:A:110:GLY:HA3	10:J:169:MET:HE3	1.98	0.46
8:H:179:TRP:N	8:H:180:PRO:CD	2.79	0.46
16:P:176:ASP:CG	16:P:178:PHE:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:4:HIS:HB3	33:h:5:GLY:H	1.54	0.46
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.46
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.49	0.46
29:d:67:SER:HB2	53:d:201:CDL:H762	1.96	0.46
7:G:297:GLU:OE1	7:G:297:GLU:N	2.43	0.46
14:N:215:MET:HE2	14:N:218:MET:CE	2.46	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.97	0.46
53:q:202:CDL:C34	53:q:202:CDL:H712	2.45	0.46
8:H:200:LEU:HD21	8:H:280:PHE:O	2.15	0.46
26:a:1:MET:HE3	26:a:1:MET:HA	1.98	0.46
2:B:56:ALA:HB1	51:H:701:U10:H103	1.97	0.46
4:D:358:VAL:O	4:D:359:PRO:C	2.58	0.46
7:G:140:LYS:O	7:G:148:THR:OG1	2.20	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.46
17:Q:20:THR:OG1	17:Q:30:ILE:HD13	2.16	0.46
7:G:190:MET:HE3	7:G:695:ALA:HB2	1.96	0.46
8:H:18:ALA:HB2	51:H:701:U10:H472	1.97	0.46
10:J:124:ASP:OD2	11:K:2:SER:OG	2.32	0.46
12:L:557:TRP:HB3	52:m:201:3PE:H2C1	1.97	0.46
25:Z:27:ARG:NH2	43:r:13:TRP:O	2.48	0.45
2:B:69:MET:HE1	2:B:76:PHE:CE2	2.51	0.45
20:U:56:ASP:OD1	20:U:56:ASP:N	2.50	0.45
29:d:9:ALA:HB1	29:d:12:GLN:CD	2.40	0.45
12:L:331:THR:HB	12:L:387:THR:HG22	1.99	0.45
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.49	0.45
19:S:57:CYS:O	19:S:60:VAL:HG22	2.17	0.45
40:o:82:GLU:N	40:o:82:GLU:OE1	2.49	0.45
3:C:37:VAL:HG12	43:r:69:MET:CE	2.45	0.45
8:H:23:VAL:HG11	8:H:268:MET:HE1	1.99	0.45
13:M:40:LEU:HD22	33:h:79:PHE:HB3	1.98	0.45
2:B:91:THR:HA	2:B:119:CYS:HB3	1.98	0.45
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.99	0.45
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.97	0.45
53:q:202:CDL:H742	53:q:202:CDL:H541	1.98	0.45
34:i:85:LEU:HD23	34:i:89:VAL:HG21	1.99	0.45
4:D:106:LEU:O	4:D:427:GLU:N	2.50	0.45
31:f:7:VAL:HG12	31:f:7:VAL:O	2.17	0.45
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.48	0.45
40:o:91:HIS:O	40:o:95:VAL:HG23	2.16	0.45
14:N:261:MET:HE1	52:N:403:3PE:H2I1	2.00	0.44
58:T:101:EHZ:O2	58:T:101:EHZ:O1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:HD13	8:H:236:ILE:HG21	1.98	0.44
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.99	0.44
20:U:33:ASN:OD1	20:U:33:ASN:N	2.50	0.44
1:A:71:LEU:O	10:J:147:TYR:OH	2.32	0.44
32:g:92:GLU:OE2	32:g:95:ARG:NH2	2.47	0.44
45:A:202:PC1:H332	45:A:202:PC1:H2	1.98	0.44
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.99	0.44
6:F:268:VAL:HG22	6:F:269:GLU:N	2.33	0.44
51:H:701:U10:H4M2	51:H:701:U10:O3	2.18	0.44
52:H:703:3PE:H252	9:I:30:LEU:HD13	1.99	0.44
12:L:69:LEU:HD21	13:M:455:LEU:HD11	1.99	0.44
25:Z:50:MET:N	25:Z:50:MET:HE2	2.32	0.44
13:M:406:TYR:CD1	13:M:406:TYR:C	2.96	0.44
24:Y:13:GLU:OE2	24:Y:125:LYS:NZ	2.42	0.44
38:m:24:ILE:HD13	38:m:29:ARG:CZ	2.47	0.44
15:O:111:ALA:HB1	15:O:122:VAL:HG21	2.00	0.44
19:S:75:ASN:OD1	19:S:75:ASN:N	2.50	0.44
2:B:45:LEU:O	2:B:74:VAL:HA	2.18	0.44
13:M:216:LEU:HD23	13:M:216:LEU:C	2.43	0.44
2:B:45:LEU:HD22	2:B:85:VAL:HG21	1.98	0.44
10:J:117:PHE:HB3	11:K:1:FME:HE3	2.00	0.44
5:E:105:THR:HG22	5:E:106:THR:N	2.31	0.43
20:T:76:ILE:O	20:T:80:ILE:HG12	2.17	0.43
6:F:192:LEU:C	6:F:192:LEU:HD23	2.42	0.43
44:s:40:ASN:O	44:s:40:ASN:CG	2.61	0.43
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.00	0.43
52:b:201:3PE:H12	52:b:201:3PE:H121	2.00	0.43
2:B:59:MET:CE	51:H:701:U10:H102	2.47	0.43
7:G:143:GLY:HA2	7:G:190:MET:HE2	1.99	0.43
10:J:118:GLU:N	10:J:118:GLU:OE1	2.51	0.43
16:P:133:SER:O	16:P:168:PRO:HD2	2.19	0.43
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.46	0.43
30:e:15:ARG:NH2	61:e:204:HOH:O	2.51	0.43
6:F:403:THR:HB	46:F:502:SF4:S4	2.58	0.43
16:P:50:ARG:HD2	16:P:50:ARG:C	2.43	0.43
45:A:201:PC1:C21	45:A:201:PC1:O31	2.65	0.43
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.01	0.43
5:E:192:SER:OG	5:E:194:GLU:OE1	2.23	0.43
6:F:306:LEU:C	6:F:306:LEU:HD12	2.44	0.43
20:U:55:GLU:O	20:U:59:GLY:N	2.51	0.43
1:A:95:ILE:HG21	8:H:302:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.48	0.43
32:g:26:TRP:CD1	32:g:26:TRP:C	2.96	0.43
43:r:72:GLN:O	43:r:73:LYS:HB2	2.19	0.43
15:O:237:ASP:N	15:O:237:ASP:OD1	2.52	0.43
16:P:270:PHE:CD1	45:P:401:PC1:H351	2.54	0.43
6:F:69:GLY:O	49:F:503:NAI:H2N	2.19	0.42
12:L:24:PHE:O	33:h:26:ARG:HD3	2.18	0.42
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.01	0.42
52:P:404:3PE:H262	52:P:404:3PE:H231	1.69	0.42
26:a:69:ILE:O	26:a:70:ASP:C	2.62	0.42
7:G:366:THR:HB	7:G:450:MET:HE3	2.01	0.42
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	2.01	0.42
20:T:43:ASP:OD1	22:W:63:ARG:NH2	2.53	0.42
39:n:169:ILE:O	39:n:172:ARG:NH1	2.52	0.42
7:G:254:MET:HA	7:G:260:GLU:O	2.20	0.42
8:H:142:TYR:CD1	8:H:142:TYR:C	2.96	0.42
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.54	0.42
13:M:116:ILE:HG12	13:M:174:LEU:HD13	2.02	0.42
13:M:104:LEU:HG	13:M:108:MET:HE2	2.00	0.42
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.50	0.42
16:P:145:TYR:CD1	16:P:145:TYR:C	2.98	0.42
45:N:404:PC1:H371	45:N:404:PC1:H3A1	1.65	0.42
31:f:11:TRP:O	31:f:14:VAL:HG22	2.20	0.42
37:l:68:ASP:OD1	37:l:68:ASP:N	2.52	0.42
1:A:44:MET:HE3	4:D:48:THR:HG22	2.01	0.42
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.01	0.42
2:B:75:VAL:HG11	51:H:701:U10:C31	2.49	0.42
8:H:143:GLU:OE1	61:H:802:HOH:O	2.22	0.42
14:N:72:MET:HE3	14:N:76:ILE:HD11	2.01	0.42
1:A:67:LEU:CD1	11:K:68:ALA:HB3	2.44	0.42
4:D:161:ILE:HG22	4:D:161:ILE:O	2.18	0.42
1:A:28:ASN:O	1:A:33:LYS:NZ	2.47	0.41
2:B:54:CYS:HB3	4:D:108:TYR:HB2	2.00	0.41
6:F:434:ALA:O	6:F:438:GLN:HG2	2.20	0.41
16:P:187:TRP:CE3	52:P:404:3PE:H242	2.55	0.41
20:T:33:ASN:OD1	20:T:33:ASN:N	2.53	0.41
13:M:418:LYS:NZ	39:n:94:GLU:OE2	2.45	0.41
14:N:202:LEU:HD22	45:N:404:PC1:H381	2.02	0.41
32:g:66:PHE:HD1	32:g:70:LEU:HD12	1.84	0.41
14:N:207:ILE:HD13	14:N:262:PRO:HD3	2.02	0.41
45:A:201:PC1:O13	45:A:201:PC1:H133	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:153:VAL:HG23	29:d:6:GLN:HB2	2.02	0.41
32:g:70:LEU:O	32:g:74:SER:OG	2.31	0.41
33:h:37:ALA:HA	53:h:201:CDL:H752	2.02	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.35	0.41
14:N:2:ASN:OD1	14:N:4:ILE:N	2.48	0.41
15:O:34:GLY:N	54:O:401:DGT:O1G	2.53	0.41
8:H:225:MET:HG2	51:H:701:U10:H453	2.01	0.41
12:L:422:TYR:CD1	12:L:422:TYR:C	2.99	0.41
13:M:105:PHE:O	13:M:109:THR:OG1	2.20	0.41
39:n:162:LEU:HD12	39:n:162:LEU:N	2.36	0.41
1:A:38:GLU:HG2	4:D:50:ASN:HB2	2.03	0.41
7:G:477:ILE:HD11	7:G:489:VAL:HG11	2.01	0.41
4:D:44:VAL:O	4:D:44:VAL:HG13	2.21	0.41
5:E:96:GLY:H	5:E:138:THR:HG1	1.69	0.41
6:F:95:VAL:HG11	6:F:118:LEU:HD11	2.03	0.41
13:M:296:LEU:HD21	13:M:396:MET:SD	2.61	0.41
15:O:303:LYS:O	29:d:50:ARG:NH2	2.53	0.41
16:P:176:ASP:O	16:P:177:ARG:HB2	2.21	0.41
18:R:93:GLN:O	18:R:95:HIS:N	2.48	0.41
26:a:53:ARG:NH2	61:a:105:HOH:O	2.54	0.41
52:b:201:3PE:H2I3	52:b:201:3PE:H2F2	1.89	0.41
29:d:109:TYR:CZ	41:p:152:ARG:HD3	2.56	0.41
39:n:30:CYS:O	39:n:32:HIS:N	2.53	0.41
42:q:55:PHE:CD1	42:q:55:PHE:C	2.98	0.41
44:s:34:ASP:OD1	44:s:34:ASP:N	2.54	0.41
44:s:74:ARG:NH1	61:s:102:HOH:O	2.53	0.41
2:B:92:LEU:HD13	2:B:100:LEU:HD13	2.02	0.41
12:L:492:ILE:O	12:L:496:LEU:HD23	2.20	0.41
53:X:201:CDL:C52	29:d:29:PRO:HB3	2.50	0.41
10:J:84:LEU:HG	53:P:402:CDL:C52	2.52	0.40
11:K:43:MET:SD	14:N:72:MET:HE1	2.61	0.40
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.51	0.40
28:c:33:LYS:HG3	28:c:34:GLN:N	2.36	0.40
29:d:71:VAL:HG23	53:d:201:CDL:H771	2.03	0.40
2:B:35:ASP:HB3	45:B:203:PC1:H241	2.04	0.40
2:B:76:PHE:CD2	51:H:701:U10:H13	2.56	0.40
14:N:146:PHE:N	14:N:147:PRO:CD	2.85	0.40
14:N:237:THR:HG21	14:N:319:LEU:HD11	2.03	0.40
58:T:101:EHZ:O3	58:T:101:EHZ:N2	2.54	0.40
27:b:59:ASP:OD1	27:b:60:GLY:N	2.54	0.40
45:I:203:PC1:O13	45:I:203:PC1:H152	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:561:ILE:HG13	12:L:562:LEU:N	2.37	0.40
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.52	0.40
45:q:201:PC1:O13	45:q:201:PC1:H152	2.22	0.40
6:F:101:GLU:HB2	49:F:503:NAI:H42N	2.04	0.40
51:H:701:U10:C55	51:H:701:U10:C51	3.00	0.40
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.44	0.40
11:K:66:PHE:CZ	14:N:31:ILE:HG23	2.56	0.40
12:L:394:LEU:N	12:L:394:LEU:HD12	2.36	0.40
31:f:9:ASP:OD1	31:f:9:ASP:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	155/216 (72%)	150 (97%)	5 (3%)	0	100	100
3	C	207/266 (78%)	203 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	417 (98%)	9 (2%)	1 (0%)	43	57
5	E	214/249 (86%)	207 (97%)	7 (3%)	0	100	100
6	F	431/464 (93%)	425 (99%)	5 (1%)	1 (0%)	43	57
7	G	688/727 (95%)	674 (98%)	14 (2%)	0	100	100
8	H	316/318 (99%)	311 (98%)	4 (1%)	1 (0%)	36	49
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	585 (97%)	19 (3%)	0	100	100
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	340/380 (90%)	335 (98%)	4 (1%)	1 (0%)	36	49
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	85/99 (86%)	83 (98%)	2 (2%)	0	100	100
20	T	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	110 (97%)	2 (2%)	1 (1%)	14	20
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
25	Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	119/121 (98%)	119 (100%)	0	0	100	100
30	e	98/106 (92%)	98 (100%)	0	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	100/154 (65%)	94 (94%)	6 (6%)	0	100	100
33	h	141/189 (75%)	137 (97%)	4 (3%)	0	100	100
34	i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	78/98 (80%)	76 (97%)	2 (3%)	0	100	100
37	l	154/186 (83%)	150 (97%)	3 (2%)	1 (1%)	21	30
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	o	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
41	p	171/176 (97%)	171 (100%)	0	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	93/113 (82%)	90 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8210/9214 (89%)	8056 (98%)	148 (2%)	6 (0%)	49	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	99	GLU
16	P	3	HIS
4	D	359	PRO
8	H	208	VAL
37	l	89	VAL
22	W	95	VAL

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	100/100 (100%)	100 (100%)	0	100	100
2	B	133/174 (76%)	132 (99%)	1 (1%)	73	85
3	C	190/228 (83%)	190 (100%)	0	100	100
4	D	370/392 (94%)	369 (100%)	1 (0%)	86	93
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	346/368 (94%)	345 (100%)	1 (0%)	86	93
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	273 (100%)	1 (0%)	84	92
9	I	151/175 (86%)	150 (99%)	1 (1%)	76	87
10	J	141/141 (100%)	139 (99%)	2 (1%)	59	77
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	79
12	L	533/533 (100%)	531 (100%)	2 (0%)	84	92
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	296/327 (90%)	295 (100%)	1 (0%)	86	93
17	Q	116/153 (76%)	116 (100%)	0	100	100
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	77/82 (94%)	77 (100%)	0	100	100
20	T	81/135 (60%)	81 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/101 (100%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	58 (98%)	1 (2%)	53	73
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	106/106 (100%)	106 (100%)	0	100	100
30	e	90/96 (94%)	90 (100%)	0	100	100
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	93/131 (71%)	93 (100%)	0	100	100
33	h	124/158 (78%)	124 (100%)	0	100	100
34	i	121/121 (100%)	121 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	140/159 (88%)	140 (100%)	0	100	100
38	m	114/115 (99%)	113 (99%)	1 (1%)	70	84
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	131/131 (100%)	130 (99%)	1 (1%)	73	85
43	r	86/96 (90%)	86 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	7228/7891 (92%)	7214 (100%)	14 (0%)	85	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
4	D	420	THR
6	F	105	CYS
8	H	205	SER
9	I	58	SER
10	J	5	ILE
10	J	110	ASP
11	K	82	SER
12	L	554	ASP
12	L	576	LEU
16	P	263	TYR
26	a	69	ILE
38	m	2	PHE
42	q	95	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	71	GLN
3	C	160	HIS
4	D	54	GLN
4	D	55	HIS
4	D	201	GLN
4	D	280	GLN
5	E	42	HIS
5	E	214	GLN
6	F	421	HIS
7	G	141	ASN
7	G	182	GLN
7	G	237	ASN
7	G	401	HIS
7	G	581	GLN
8	H	230	ASN
11	K	50	ASN
11	K	52	HIS
12	L	25	ASN

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Mol	Chain	Res	Type
12	L	59	GLN
12	L	354	GLN
12	L	518	ASN
13	M	139	GLN
13	M	187	HIS
13	M	251	ASN
13	M	293	HIS
13	M	304	GLN
14	N	48	HIS
14	N	134	GLN
14	N	172	GLN
15	O	190	HIS
15	O	251	GLN
15	O	287	HIS
15	O	288	GLN
16	P	8	HIS
16	P	93	ASN
16	P	131	HIS
17	Q	29	HIS
19	S	72	GLN
21	V	82	GLN
22	W	69	ASN
22	W	125	HIS
25	Z	60	GLN
25	Z	111	HIS
29	d	61	GLN
33	h	124	HIS
34	i	25	GLN
35	j	6	HIS
36	k	47	ASN
37	l	104	HIS
39	n	11	HIS
39	n	77	GLN
40	o	49	GLN
40	o	116	GLN
41	p	133	GLN
41	p	143	HIS
42	q	5	GLN
42	q	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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
12	FME	L	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.61	1 (14%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	7,9,11	1.62	2 (28%)
2	WYK	B	77	2	9,11,12	2.53	2 (22%)	7,13,15	0.58	0
13	FME	M	1	13	8,9,10	1.53	1 (12%)	7,9,11	1.79	1 (14%)
14	FME	N	1	14	8,9,10	1.52	1 (12%)	7,9,11	1.73	2 (28%)
11	FME	K	1	11	8,9,10	1.52	1 (12%)	7,9,11	1.70	2 (28%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	7,9,11	1.77	1 (14%)
4	2MR	D	85	4	10,12,13	2.45	2 (20%)	5,13,15	1.26	1 (20%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.71	2 (28%)

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
12	FME	L	1	12	-	4/7/9/11	-
10	FME	J	1	10	-	5/7/9/11	-
2	WYK	B	77	2	-	1/10/11/13	-
13	FME	M	1	13	-	2/7/9/11	-
14	FME	N	1	14	-	1/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	0/10/13/15	-
1	FME	A	1	1	-	3/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	WYK	CZ-NE	6.69	1.46	1.33
4	D	85	2MR	CZ-NH2	5.37	1.45	1.33
4	D	85	2MR	CZ-NE	5.22	1.45	1.34
13	M	1	FME	CN-N	3.73	1.45	1.33
14	N	1	FME	CN-N	3.71	1.45	1.33
11	K	1	FME	CN-N	3.70	1.45	1.33
8	H	1	FME	CN-N	3.69	1.45	1.33
10	J	1	FME	CN-N	3.69	1.45	1.33
1	A	1	FME	CN-N	3.65	1.45	1.33
12	L	1	FME	CN-N	3.64	1.45	1.33
2	B	77	WYK	CZ-NH2	-2.19	1.25	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	CE-SD-CG	3.46	112.27	100.40
14	N	1	FME	CE-SD-CG	3.15	111.23	100.40
8	H	1	FME	CE-SD-CG	2.94	110.51	100.40
11	K	1	FME	CE-SD-CG	2.94	110.51	100.40
1	A	1	FME	CE-SD-CG	2.73	109.78	100.40
12	L	1	FME	CE-SD-CG	2.56	109.18	100.40
10	J	1	FME	CE-SD-CG	2.44	108.80	100.40
11	K	1	FME	O1-CN-N	-2.09	119.76	125.27
14	N	1	FME	O1-CN-N	-2.09	119.77	125.27
4	D	85	2MR	CD-NE-CZ	-2.07	119.53	123.41
1	A	1	FME	O1-CN-N	-2.06	119.85	125.27
10	J	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	CA-CB-CG-SD

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Mol	Chain	Res	Type	Atoms
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
2	B	77	WYK	CA-CB-CG-OH
11	K	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
10	J	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
13	M	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 for Mogul analysis.

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
52	3PE	M	501	-	42,42,50	0.94	4 (9%)	45,47,55	1.07	2 (4%)
47	FES	G	803	7	0,4,4	-	-	-	-	-
52	3PE	Y	804	-	26,26,50	1.20	4 (15%)	29,31,55	1.23	2 (6%)
45	PC1	P	401	-	32,32,53	1.58	6 (18%)	38,40,61	0.94	2 (5%)
46	SF4	G	801	7	0,12,12	-	-	-	-	-
52	3PE	Y	805	-	40,40,50	0.96	3 (7%)	43,45,55	1.11	2 (4%)
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.51	5 (14%)
53	CDL	h	201	-	77,77,99	1.02	7 (9%)	83,89,111	1.14	5 (6%)
52	3PE	K	101	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)
52	3PE	N	402	-	30,30,50	1.10	4 (13%)	33,35,55	1.06	2 (6%)
52	3PE	b	201	-	46,46,50	0.97	4 (8%)	49,51,55	1.12	2 (4%)
53	CDL	P	402	-	68,68,99	1.07	7 (10%)	74,80,111	1.05	3 (4%)
46	SF4	I	202	9	0,12,12	-	-	-	-	-
52	3PE	Y	801	-	30,30,50	1.07	4 (13%)	33,35,55	1.15	3 (9%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
45	PC1	A	201	-	34,34,53	1.51	6 (17%)	40,42,61	1.00	2 (5%)
45	PC1	Z	200	-	43,43,53	1.44	6 (13%)	49,51,61	0.97	2 (4%)
46	SF4	I	201	9	0,12,12	-	-	-	-	-
52	3PE	H	703	-	44,44,50	0.91	4 (9%)	47,49,55	1.13	3 (6%)
45	PC1	B	203	-	43,43,53	1.40	6 (13%)	49,51,61	0.95	2 (4%)
52	3PE	H	702	-	33,33,50	1.09	4 (12%)	36,38,55	1.37	3 (8%)
45	PC1	B	202	-	45,45,53	1.41	6 (13%)	51,53,61	0.94	2 (3%)
54	DGT	O	401	55	29,33,33	3.19	14 (48%)	44,52,52	2.10	12 (27%)
52	3PE	L	701	-	43,43,50	0.94	4 (9%)	46,48,55	1.02	2 (4%)
52	3PE	m	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.12	2 (4%)
58	EHZ	T	101	20	29,36,37	1.71	5 (17%)	35,44,47	1.26	2 (5%)
53	CDL	X	201	-	85,85,99	0.99	7 (8%)	91,97,111	1.08	6 (6%)
52	3PE	L	704	-	48,48,50	0.90	4 (8%)	51,53,55	1.01	2 (3%)
49	NAI	F	503	-	45,48,48	3.75	19 (42%)	60,73,73	1.85	15 (25%)
47	FES	E	301	5	0,4,4	-	-	-	-	-
53	CDL	d	201	-	64,64,99	1.10	6 (9%)	70,76,111	1.09	4 (5%)
52	3PE	Y	802	-	39,39,50	0.96	4 (10%)	42,44,55	1.14	2 (4%)
52	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.08	2 (4%)
52	3PE	N	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.15	2 (4%)
52	3PE	Y	803	-	33,33,50	1.09	4 (12%)	36,38,55	1.09	2 (5%)
45	PC1	I	203	-	39,39,53	1.46	6 (15%)	45,47,61	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PC1	h	202	-	43,43,53	1.41	6 (13%)	49,51,61	1.02	2 (4%)
48	FMN	F	501	-	33,33,33	2.81	10 (30%)	48,50,50	1.70	12 (25%)
59	CHD	i	201	-	32,32,32	3.28	10 (31%)	51,51,51	1.85	13 (25%)
60	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.86	0
45	PC1	A	202	-	34,34,53	1.53	6 (17%)	40,42,61	1.13	3 (7%)
53	CDL	L	702	-	68,68,99	1.08	7 (10%)	74,80,111	0.99	4 (5%)
53	CDL	q	202	-	60,60,99	1.14	7 (11%)	66,72,111	1.15	5 (7%)
53	CDL	M	502	-	80,80,99	1.02	7 (8%)	86,92,111	1.20	5 (5%)
45	PC1	M	503	-	41,41,53	1.41	6 (14%)	47,49,61	1.18	2 (4%)
51	U10	H	701	-	63,63,63	0.62	2 (3%)	76,79,79	0.60	0
52	3PE	N	403	-	48,48,50	0.89	4 (8%)	51,53,55	1.01	2 (3%)
45	PC1	q	201	-	48,48,53	1.35	6 (12%)	54,56,61	1.06	2 (3%)
52	3PE	P	404	-	34,34,50	1.04	4 (11%)	37,39,55	1.21	2 (5%)
46	SF4	B	201	2	0,12,12	-	-	-	-	-
56	NDP	P	403	-	49,52,52	3.97	24 (48%)	66,80,80	2.08	14 (21%)
45	PC1	N	404	-	38,38,53	1.45	6 (15%)	44,46,61	1.04	2 (4%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-

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
52	3PE	M	501	-	-	17/46/46/54	-
47	FES	G	803	7	-	-	0/1/1/1
52	3PE	Y	804	-	-	17/30/30/54	-
45	PC1	P	401	-	-	10/36/36/57	-
52	3PE	Y	805	-	-	13/44/44/54	-
58	EHZ	U	101	20	-	9/42/44/45	-
46	SF4	G	801	7	-	-	0/6/5/5
53	CDL	h	201	-	-	34/88/88/110	-
52	3PE	K	101	-	-	18/45/45/54	-
52	3PE	N	402	-	-	15/34/34/54	-
52	3PE	b	201	-	-	18/50/50/54	-
53	CDL	P	402	-	-	33/79/79/110	-
52	3PE	Y	801	-	-	23/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SF4	I	202	9	-	-	0/6/5/5
46	SF4	F	502	6	-	-	0/6/5/5
45	PC1	A	201	-	-	9/38/38/57	-
45	PC1	Z	200	-	-	21/47/47/57	-
52	3PE	H	703	-	-	13/48/48/54	-
46	SF4	I	201	9	-	-	0/6/5/5
45	PC1	B	203	-	-	13/47/47/57	-
52	3PE	H	702	-	-	17/37/37/54	-
45	PC1	B	202	-	-	14/49/49/57	-
54	DGT	O	401	55	-	3/22/34/34	0/3/3/3
52	3PE	L	701	-	-	21/47/47/54	-
52	3PE	m	201	-	-	18/44/44/54	-
58	EHZ	T	101	20	-	17/42/44/45	-
53	CDL	X	201	-	-	38/96/96/110	-
52	3PE	L	704	-	-	19/52/52/54	-
46	SF4	B	201	2	-	-	0/6/5/5
49	NAI	F	503	-	-	6/29/72/72	0/5/5/5
47	FES	E	301	5	-	-	0/1/1/1
53	CDL	d	201	-	-	33/75/75/110	-
52	3PE	Y	802	-	-	18/43/43/54	-
52	3PE	N	401	-	-	19/44/44/54	-
52	3PE	Y	803	-	-	12/37/37/54	-
45	PC1	I	203	-	-	11/43/43/57	-
45	PC1	h	202	-	-	14/47/47/57	-
48	FMN	F	501	-	-	1/18/18/18	0/3/3/3
59	CHD	i	201	-	-	0/9/74/74	0/4/4/4
60	MYR	o	201	40	-	2/11/12/13	-
45	PC1	A	202	-	-	11/38/38/57	-
53	CDL	L	702	-	-	24/79/79/110	-
53	CDL	q	202	-	-	28/71/71/110	-
53	CDL	M	502	-	-	39/91/91/110	-
45	PC1	M	503	-	-	6/45/45/57	-
51	U10	H	701	-	-	24/63/87/87	0/1/1/1
52	3PE	N	403	-	-	18/52/52/54	-
45	PC1	q	201	-	-	18/52/52/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	P	404	-	-	15/38/38/54	-
52	3PE	L	703	-	-	19/48/48/54	-
56	NDP	P	403	-	-	3/34/77/77	0/5/5/5
45	PC1	N	404	-	-	11/42/42/57	-
46	SF4	G	802	7	-	-	0/6/5/5

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	403	NDP	C6N-C5N	12.12	1.55	1.33
49	F	503	NAI	C6N-C5N	11.32	1.53	1.33
59	i	201	CHD	C11-C12	9.01	1.68	1.53
49	F	503	NAI	O4B-C1B	8.64	1.62	1.42
49	F	503	NAI	O4D-C1D	8.56	1.62	1.42
56	P	403	NDP	C2B-C1B	-8.49	1.31	1.53
56	P	403	NDP	O4B-C1B	8.42	1.61	1.42
56	P	403	NDP	O4D-C1D	8.37	1.61	1.42
56	P	403	NDP	C7N-N7N	8.28	1.55	1.33
54	O	401	DGT	C2'-C3'	-7.60	1.32	1.52
48	F	501	FMN	C4A-N5	7.27	1.44	1.30
59	i	201	CHD	C16-C15	7.19	1.73	1.54
49	F	503	NAI	C2B-C1B	-7.07	1.30	1.53
56	P	403	NDP	C2D-C1D	-7.07	1.30	1.53
49	F	503	NAI	C2D-C1D	-6.85	1.31	1.53
48	F	501	FMN	C10-N1	6.53	1.46	1.33
54	O	401	DGT	C4-N3	6.49	1.49	1.34
49	F	503	NAI	O4D-C4D	-6.40	1.30	1.45
49	F	503	NAI	C2N-C3N	6.34	1.52	1.34
56	P	403	NDP	O4D-C4D	-6.32	1.30	1.45
49	F	503	NAI	O4B-C4B	-6.23	1.31	1.45
59	i	201	CHD	C13-C17	6.14	1.66	1.55
56	P	403	NDP	C6A-N6A	5.68	1.48	1.34
58	T	101	EHZ	C12-N1	5.63	1.46	1.33
54	O	401	DGT	C2-N3	5.51	1.46	1.33
48	F	501	FMN	C5A-N5	5.44	1.50	1.39
59	i	201	CHD	C8-C9	5.44	1.64	1.53
56	P	403	NDP	P2B-O2B	5.42	1.69	1.59
54	O	401	DGT	O4'-C4'	5.38	1.57	1.45
58	U	101	EHZ	C15-N2	5.38	1.45	1.33
58	U	101	EHZ	C12-N1	5.33	1.45	1.33
59	i	201	CHD	C20-C17	-5.27	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	T	101	EHZ	C15-N2	5.22	1.45	1.33
59	i	201	CHD	O12-C12	-5.20	1.35	1.43
56	P	403	NDP	O4B-C4B	-5.20	1.33	1.45
54	O	401	DGT	O4'-C1'	-5.15	1.30	1.42
48	F	501	FMN	C9A-N10	4.99	1.49	1.41
56	P	403	NDP	C2N-C3N	4.84	1.48	1.34
59	i	201	CHD	C6-C5	4.79	1.61	1.53
54	O	401	DGT	C2-N2	4.77	1.45	1.34
48	F	501	FMN	C2-N1	4.76	1.48	1.36
49	F	503	NAI	C6A-N6A	4.60	1.45	1.34
49	F	503	NAI	C7N-N7N	4.54	1.45	1.33
48	F	501	FMN	C2-N3	4.32	1.49	1.39
59	i	201	CHD	C6-C7	4.10	1.59	1.52
59	i	201	CHD	C15-C14	4.06	1.62	1.54
56	P	403	NDP	O2D-C2D	3.95	1.52	1.43
48	F	501	FMN	C4-N3	3.95	1.46	1.38
45	B	202	PC1	O31-C31	3.94	1.44	1.33
56	P	403	NDP	O7N-C7N	-3.91	1.15	1.24
54	O	401	DGT	C2'-C1'	3.89	1.63	1.52
54	O	401	DGT	C5'-C4'	-3.89	1.39	1.51
45	Z	200	PC1	O31-C31	3.88	1.44	1.33
45	h	202	PC1	O31-C31	3.88	1.44	1.33
45	I	203	PC1	O31-C31	3.87	1.44	1.33
45	P	401	PC1	O31-C31	3.86	1.44	1.33
45	q	201	PC1	O31-C31	3.85	1.44	1.33
45	M	503	PC1	O31-C31	3.83	1.44	1.33
45	A	202	PC1	O31-C31	3.76	1.44	1.33
56	P	403	NDP	C5A-C4A	-3.74	1.32	1.39
45	B	203	PC1	O31-C31	3.74	1.44	1.33
48	F	501	FMN	C10-N10	3.73	1.45	1.37
45	P	401	PC1	O21-C21	3.72	1.44	1.34
45	N	404	PC1	O31-C31	3.68	1.44	1.33
45	A	202	PC1	O21-C21	3.68	1.44	1.34
45	Z	200	PC1	O21-C21	3.66	1.44	1.34
45	h	202	PC1	O21-C21	3.64	1.44	1.34
45	A	201	PC1	O31-C31	3.60	1.43	1.33
45	q	201	PC1	O21-C21	3.60	1.44	1.34
45	A	201	PC1	O21-C21	3.59	1.44	1.34
45	B	203	PC1	O21-C21	3.58	1.44	1.34
45	M	503	PC1	O21-C21	3.57	1.44	1.34
45	N	404	PC1	O21-C21	3.51	1.44	1.34
49	F	503	NAI	C6N-N1N	3.51	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	I	203	PC1	O21-C21	3.50	1.44	1.34
56	P	403	NDP	C8A-N9A	-3.47	1.31	1.37
45	B	202	PC1	O21-C21	3.44	1.44	1.34
56	P	403	NDP	C4N-C3N	3.40	1.56	1.49
54	O	401	DGT	C5-N7	-3.10	1.33	1.39
48	F	501	FMN	O2-C2	-3.10	1.18	1.24
49	F	503	NAI	O3D-C3D	-2.94	1.36	1.43
49	F	503	NAI	O2B-C2B	2.92	1.49	1.43
49	F	503	NAI	O2D-C2D	2.90	1.49	1.43
49	F	503	NAI	O3B-C3B	-2.84	1.36	1.43
53	M	502	CDL	OB8-CB7	2.82	1.41	1.33
48	F	501	FMN	O4-C4	-2.74	1.18	1.23
53	h	201	CDL	OB8-CB7	2.71	1.41	1.33
56	P	403	NDP	C4N-C5N	2.71	1.56	1.48
45	B	202	PC1	O21-C2	-2.68	1.39	1.46
53	q	202	CDL	OA6-CA4	-2.67	1.39	1.46
53	X	201	CDL	OB8-CB7	2.67	1.41	1.33
54	O	401	DGT	C2-N1	2.67	1.44	1.37
53	L	702	CDL	OA6-CA4	-2.66	1.39	1.46
45	N	404	PC1	O21-C2	-2.64	1.40	1.46
53	q	202	CDL	OB8-CB7	2.63	1.41	1.33
49	F	503	NAI	C5A-C4A	-2.63	1.34	1.39
53	d	201	CDL	OB8-CB7	2.63	1.41	1.33
52	Y	805	3PE	O21-C2	-2.62	1.40	1.46
53	M	502	CDL	OA6-CA4	-2.62	1.40	1.46
45	I	203	PC1	O21-C2	-2.61	1.40	1.46
52	b	201	3PE	O21-C2	-2.61	1.40	1.46
53	M	502	CDL	OB6-CB5	2.60	1.41	1.34
52	Y	803	3PE	O21-C2	-2.59	1.40	1.46
52	L	703	3PE	O31-C31	2.59	1.40	1.33
52	b	201	3PE	O31-C31	2.59	1.40	1.33
51	H	701	U10	C3-C2	-2.58	1.41	1.48
45	B	203	PC1	O21-C2	-2.58	1.40	1.46
53	P	402	CDL	OB8-CB7	2.58	1.40	1.33
54	O	401	DGT	O3'-C3'	2.58	1.48	1.43
52	Y	805	3PE	O31-C31	2.57	1.40	1.33
53	h	201	CDL	OA6-CA4	-2.56	1.40	1.46
53	X	201	CDL	OB6-CB5	2.56	1.41	1.34
53	h	201	CDL	OA8-CA7	2.56	1.40	1.33
53	L	702	CDL	OB8-CB7	2.56	1.40	1.33
53	q	202	CDL	OB6-CB5	2.55	1.41	1.34
52	L	704	3PE	O31-C31	2.55	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	701	3PE	O21-C2	-2.55	1.40	1.46
54	O	401	DGT	C5-C6	2.54	1.53	1.44
52	N	402	3PE	O21-C2	-2.54	1.40	1.46
53	d	201	CDL	OA8-CA7	2.54	1.40	1.33
53	L	702	CDL	OA8-CA7	2.53	1.40	1.33
53	L	702	CDL	OB6-CB5	2.53	1.41	1.34
53	h	201	CDL	OB6-CB5	2.53	1.41	1.34
53	X	201	CDL	OA6-CA4	-2.51	1.40	1.46
52	N	403	3PE	O21-C2	-2.51	1.40	1.46
52	Y	804	3PE	O31-C31	2.51	1.40	1.33
45	h	202	PC1	O21-C2	-2.50	1.40	1.46
56	P	403	NDP	O3B-C3B	-2.49	1.37	1.43
52	H	702	3PE	O21-C2	-2.49	1.40	1.46
52	P	404	3PE	O31-C31	2.49	1.40	1.33
52	m	201	3PE	O21-C2	-2.49	1.40	1.46
53	X	201	CDL	OA8-CA7	2.49	1.40	1.33
52	K	101	3PE	O21-C2	-2.49	1.40	1.46
45	A	202	PC1	O21-C2	-2.48	1.40	1.46
53	P	402	CDL	OB6-CB4	-2.47	1.40	1.46
45	P	401	PC1	P-O11	2.47	1.69	1.59
53	P	402	CDL	OB6-CB5	2.47	1.41	1.34
53	d	201	CDL	OB6-CB5	2.46	1.41	1.34
53	d	201	CDL	OA6-CA4	-2.45	1.40	1.46
56	P	403	NDP	O3D-C3D	-2.45	1.37	1.43
52	M	501	3PE	O21-C2	-2.44	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.44	1.40	1.46
49	F	503	NAI	C5A-N7A	-2.44	1.34	1.39
54	O	401	DGT	C6-N1	2.43	1.43	1.38
53	M	502	CDL	OA8-CA7	2.43	1.40	1.33
54	O	401	DGT	O6-C6	-2.43	1.19	1.23
52	N	403	3PE	O31-C31	2.43	1.40	1.33
45	B	202	PC1	P-O11	2.42	1.69	1.59
52	Y	803	3PE	O31-C31	2.42	1.40	1.33
53	P	402	CDL	OA8-CA7	2.42	1.40	1.33
52	K	101	3PE	O31-C31	2.42	1.40	1.33
45	M	503	PC1	O21-C2	-2.42	1.40	1.46
52	L	703	3PE	O21-C2	-2.42	1.40	1.46
45	q	201	PC1	O21-C2	-2.41	1.40	1.46
52	N	401	3PE	O31-C31	2.40	1.40	1.33
52	Y	804	3PE	O21-C21	2.40	1.41	1.34
52	M	501	3PE	O31-C31	2.40	1.40	1.33
45	A	201	PC1	P-O11	2.40	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Z	200	PC1	O21-C2	-2.39	1.40	1.46
45	q	201	PC1	P-O11	2.38	1.69	1.59
52	H	703	3PE	O31-C3	-2.38	1.39	1.45
52	N	402	3PE	O31-C31	2.38	1.40	1.33
45	A	201	PC1	O21-C2	-2.38	1.40	1.46
58	U	101	EHZ	C9-S1	2.38	1.81	1.76
53	h	201	CDL	OB6-CB4	-2.37	1.40	1.46
56	P	403	NDP	C7N-C3N	2.37	1.53	1.48
52	L	704	3PE	O21-C21	2.37	1.41	1.34
53	q	202	CDL	OA8-CA7	2.36	1.40	1.33
52	H	703	3PE	O21-C2	-2.36	1.40	1.46
53	L	702	CDL	OB6-CB4	-2.36	1.40	1.46
52	N	401	3PE	O21-C2	-2.36	1.40	1.46
45	M	503	PC1	C22-C21	2.36	1.57	1.50
45	N	404	PC1	P-O11	2.35	1.68	1.59
53	X	201	CDL	OA6-CA5	2.35	1.40	1.34
51	H	701	U10	C4-C5	-2.35	1.42	1.48
52	L	701	3PE	O31-C31	2.34	1.40	1.33
56	P	403	NDP	C6N-N1N	2.34	1.43	1.37
53	q	202	CDL	OB6-CB4	-2.34	1.40	1.46
56	P	403	NDP	C5A-N7A	-2.34	1.34	1.39
52	Y	802	3PE	O21-C2	-2.34	1.40	1.46
45	B	203	PC1	P-O11	2.34	1.68	1.59
52	Y	802	3PE	O21-C21	2.33	1.40	1.34
45	Z	200	PC1	P-O11	2.33	1.68	1.59
45	P	401	PC1	O21-C2	-2.32	1.40	1.46
45	Z	200	PC1	C22-C21	2.32	1.57	1.50
45	h	202	PC1	P-O11	2.32	1.68	1.59
58	T	101	EHZ	O4-C15	-2.31	1.18	1.23
45	I	203	PC1	P-O11	2.31	1.68	1.59
52	P	404	3PE	O21-C21	2.31	1.40	1.34
52	Y	802	3PE	O31-C31	2.31	1.40	1.33
52	H	702	3PE	O31-C31	2.31	1.40	1.33
45	I	203	PC1	C22-C21	2.30	1.57	1.50
45	A	202	PC1	P-O11	2.30	1.68	1.59
52	m	201	3PE	O31-C31	2.30	1.40	1.33
52	H	703	3PE	O21-C21	2.29	1.40	1.34
52	H	702	3PE	O31-C3	-2.29	1.39	1.45
45	q	201	PC1	C22-C21	2.29	1.57	1.50
45	P	401	PC1	C22-C21	2.29	1.57	1.50
58	T	101	EHZ	C9-S1	2.28	1.81	1.76
52	Y	801	3PE	O21-C2	-2.28	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	404	3PE	O21-C2	-2.28	1.40	1.46
49	F	503	NAI	O7N-C7N	-2.28	1.19	1.24
52	K	101	3PE	O21-C21	2.27	1.40	1.34
52	L	701	3PE	O31-C3	-2.26	1.40	1.45
53	X	201	CDL	OB6-CB4	-2.26	1.40	1.46
52	N	401	3PE	O21-C21	2.26	1.40	1.34
52	N	403	3PE	O31-C3	-2.26	1.40	1.45
58	U	101	EHZ	O3-C12	-2.26	1.18	1.23
56	P	403	NDP	PA-O5B	2.25	1.68	1.59
52	N	402	3PE	O31-C3	-2.25	1.40	1.45
45	A	201	PC1	C22-C21	2.24	1.57	1.50
45	M	503	PC1	P-O11	2.24	1.68	1.59
45	A	202	PC1	C22-C21	2.23	1.57	1.50
53	d	201	CDL	OA6-CA5	2.23	1.40	1.34
45	B	203	PC1	C22-C21	2.22	1.57	1.50
56	P	403	NDP	P2B-O1X	2.22	1.57	1.50
58	U	101	EHZ	O4-C15	-2.22	1.19	1.23
52	m	201	3PE	O31-C3	-2.22	1.40	1.45
52	Y	801	3PE	O21-C21	2.21	1.40	1.34
52	H	702	3PE	O21-C21	2.21	1.40	1.34
58	T	101	EHZ	O3-C12	-2.21	1.18	1.23
52	H	703	3PE	O31-C31	2.21	1.39	1.33
45	h	202	PC1	C22-C21	2.20	1.57	1.50
52	M	501	3PE	O21-C21	2.20	1.40	1.34
53	q	202	CDL	OA8-CA6	-2.20	1.40	1.45
52	Y	801	3PE	O31-C31	2.20	1.39	1.33
53	M	502	CDL	OB6-CB4	-2.20	1.41	1.46
45	I	203	PC1	P-O13	2.20	1.68	1.59
52	L	701	3PE	O21-C21	2.20	1.40	1.34
52	N	402	3PE	O21-C21	2.20	1.40	1.34
52	M	501	3PE	O31-C3	-2.19	1.40	1.45
45	P	401	PC1	P-O13	2.19	1.68	1.59
53	P	402	CDL	OA8-CA6	-2.18	1.40	1.45
53	P	402	CDL	OA6-CA4	-2.18	1.41	1.46
45	A	201	PC1	P-O13	2.17	1.68	1.59
52	m	201	3PE	O21-C21	2.16	1.40	1.34
52	L	703	3PE	O21-C21	2.16	1.40	1.34
52	b	201	3PE	O21-C21	2.16	1.40	1.34
53	L	702	CDL	OA6-CA5	2.16	1.40	1.34
53	P	402	CDL	OA6-CA5	2.15	1.40	1.34
52	L	704	3PE	O21-C2	-2.15	1.41	1.46
52	N	401	3PE	O31-C3	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	h	201	CDL	OA6-CA5	2.14	1.40	1.34
52	Y	805	3PE	O21-C21	2.14	1.40	1.34
52	L	704	3PE	O31-C3	-2.13	1.40	1.45
52	P	404	3PE	O31-C3	-2.13	1.40	1.45
45	h	202	PC1	P-O13	2.13	1.67	1.59
53	M	502	CDL	OA6-CA5	2.13	1.40	1.34
45	A	202	PC1	P-O13	2.12	1.67	1.59
59	i	201	CHD	C13-C12	-2.12	1.51	1.54
53	M	502	CDL	OA8-CA6	-2.11	1.40	1.45
52	Y	803	3PE	O21-C21	2.11	1.40	1.34
52	Y	803	3PE	O31-C3	-2.11	1.40	1.45
45	B	202	PC1	C22-C21	2.10	1.56	1.50
45	N	404	PC1	P-O13	2.10	1.67	1.59
52	Y	804	3PE	O21-C2	-2.10	1.41	1.46
52	N	403	3PE	O21-C21	2.10	1.40	1.34
45	q	201	PC1	P-O13	2.10	1.67	1.59
45	Z	200	PC1	P-O13	2.10	1.67	1.59
45	N	404	PC1	C22-C21	2.09	1.56	1.50
52	K	101	3PE	O31-C3	-2.09	1.40	1.45
52	Y	802	3PE	O31-C3	-2.08	1.40	1.45
49	F	503	NAI	C7N-C3N	2.08	1.53	1.48
45	B	202	PC1	P-O13	2.06	1.67	1.59
53	q	202	CDL	OA6-CA5	2.06	1.40	1.34
53	L	702	CDL	OA8-CA6	-2.05	1.40	1.45
52	b	201	3PE	O31-C3	-2.05	1.40	1.45
53	X	201	CDL	OA8-CA6	-2.04	1.40	1.45
52	Y	801	3PE	O31-C3	-2.04	1.40	1.45
45	B	203	PC1	P-O13	2.03	1.67	1.59
45	M	503	PC1	P-O13	2.01	1.67	1.59
53	h	201	CDL	OA8-CA6	-2.01	1.40	1.45
52	Y	804	3PE	O31-C3	-2.00	1.40	1.45

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	403	NDP	N6A-C6A-N1A	-6.40	104.33	118.35
54	O	401	DGT	C5-C4-N3	-5.55	119.46	128.46
56	P	403	NDP	C5A-C6A-N6A	5.45	135.30	123.43
56	P	403	NDP	C5A-C4A-N3A	-5.42	119.68	126.75
54	O	401	DGT	C1'-N9-C8	5.38	139.91	127.85
58	U	101	EHZ	C8-C9-S1	5.35	120.25	113.63
56	P	403	NDP	N3A-C2A-N1A	-5.29	120.33	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	F	503	NAI	C5A-C4A-N3A	-5.26	119.89	126.75
49	F	503	NAI	N3A-C2A-N1A	-5.21	120.45	128.60
56	P	403	NDP	C4A-N9A-C1B	-5.13	114.37	126.59
54	O	401	DGT	C1'-N9-C4	-4.86	112.00	125.48
53	M	502	CDL	OB6-CB5-C51	4.68	121.59	111.50
56	P	403	NDP	C1B-N9A-C8A	4.68	137.70	127.14
52	N	401	3PE	O21-C21-C22	4.63	121.48	111.50
54	O	401	DGT	C2-N3-C4	4.63	120.55	112.30
59	i	201	CHD	C14-C13-C12	4.58	111.67	107.40
49	F	503	NAI	N6A-C6A-N1A	-4.55	108.40	118.35
59	i	201	CHD	C17-C13-C12	4.53	121.81	117.67
45	M	503	PC1	O21-C21-C22	4.48	121.16	111.50
53	X	201	CDL	OB6-CB5-C51	4.42	121.03	111.50
52	H	703	3PE	O21-C21-C22	4.34	120.86	111.50
52	P	404	3PE	O21-C21-C22	4.26	120.68	111.50
53	M	502	CDL	OA6-CA5-C11	4.24	120.63	111.50
48	F	501	FMN	C7M-C7-C6	4.19	127.23	119.49
52	Y	802	3PE	O21-C21-C22	4.16	120.46	111.50
52	m	201	3PE	O21-C21-C22	4.15	120.45	111.50
52	H	702	3PE	O21-C21-C22	4.15	120.44	111.50
59	i	201	CHD	C17-C13-C14	4.14	104.27	100.09
56	P	403	NDP	N9A-C8A-N7A	-4.14	108.25	113.91
48	F	501	FMN	C9-C8-C7	4.12	125.58	119.67
45	q	201	PC1	O21-C21-C22	4.09	120.32	111.50
53	h	201	CDL	OA6-CA5-C11	4.05	120.24	111.50
53	h	201	CDL	OB6-CB5-C51	4.02	120.16	111.50
52	L	704	3PE	O21-C21-C22	3.99	120.11	111.50
52	K	101	3PE	O21-C21-C22	3.99	120.11	111.50
52	b	201	3PE	O21-C21-C22	3.96	120.03	111.50
52	Y	805	3PE	O21-C21-C22	3.95	120.02	111.50
49	F	503	NAI	N9A-C8A-N7A	-3.95	108.52	113.91
45	A	202	PC1	O21-C21-C22	3.91	119.92	111.50
53	q	202	CDL	OA6-CA5-C11	3.87	119.85	111.50
53	d	201	CDL	OA6-CA5-C11	3.87	119.84	111.50
52	Y	804	3PE	O21-C21-C22	3.87	119.84	111.50
49	F	503	NAI	C5A-C6A-N6A	3.85	131.81	123.43
58	T	101	EHZ	C10-S1-C9	3.84	113.83	101.87
45	Z	200	PC1	O21-C21-C22	3.84	119.77	111.50
52	L	703	3PE	O21-C21-C22	3.80	119.69	111.50
52	M	501	3PE	O21-C21-C22	3.79	119.67	111.50
53	q	202	CDL	OB6-CB5-C51	3.77	119.63	111.50
45	h	202	PC1	O21-C21-C22	3.77	119.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	403	NDP	C2A-N3A-C4A	3.66	120.40	111.75
45	B	203	PC1	O21-C21-C22	3.66	119.39	111.50
45	N	404	PC1	O21-C21-C22	3.66	119.38	111.50
45	B	202	PC1	O21-C21-C22	3.64	119.35	111.50
45	A	201	PC1	O21-C21-C22	3.64	119.34	111.50
52	Y	803	3PE	O21-C21-C22	3.59	119.24	111.50
58	T	101	EHZ	C8-C9-S1	3.54	118.00	113.63
59	i	201	CHD	C18-C13-C12	-3.53	105.47	109.07
49	F	503	NAI	C2A-N3A-C4A	3.49	120.00	111.75
52	P	404	3PE	O31-C31-C32	3.48	122.83	111.91
54	O	401	DGT	N9-C4-N3	3.47	132.90	125.94
52	L	701	3PE	O21-C21-C22	3.45	118.94	111.50
48	F	501	FMN	C4-N3-C2	-3.45	119.27	125.64
52	H	702	3PE	O31-C31-C32	3.42	120.34	111.38
53	L	702	CDL	OB6-CB5-C51	3.41	118.85	111.50
45	P	401	PC1	O21-C21-C22	3.37	118.77	111.50
53	P	402	CDL	OB6-CB5-C51	3.36	118.74	111.50
53	X	201	CDL	OA6-CA5-C11	3.34	118.70	111.50
53	L	702	CDL	OA6-CA5-C11	3.33	118.68	111.50
52	Y	804	3PE	O31-C31-C32	3.32	122.34	111.91
52	N	403	3PE	O21-C21-C22	3.31	118.63	111.50
52	Y	801	3PE	O21-C21-C22	3.27	118.54	111.50
59	i	201	CHD	C18-C13-C17	-3.21	106.18	111.21
53	M	502	CDL	OB8-CB7-C71	3.20	121.95	111.91
45	I	203	PC1	O31-C31-C32	3.20	121.94	111.91
56	P	403	NDP	C5A-N7A-C8A	3.15	107.98	103.51
56	P	403	NDP	N3A-C4A-N9A	3.13	132.24	127.08
48	F	501	FMN	C8M-C8-C7	-3.11	114.37	120.74
54	O	401	DGT	C2-N1-C6	-3.10	119.45	125.10
53	P	402	CDL	OA6-CA5-C11	3.09	118.17	111.50
59	i	201	CHD	C13-C17-C20	-3.09	115.81	119.50
49	F	503	NAI	C5A-N7A-C8A	3.06	107.86	103.51
53	q	202	CDL	CA4-OA6-CA5	-3.04	110.30	117.79
59	i	201	CHD	C18-C13-C14	-3.02	106.48	111.21
45	M	503	PC1	O31-C31-C32	3.00	121.34	111.91
52	N	402	3PE	O21-C21-C22	2.94	117.85	111.50
53	P	402	CDL	OA8-CA7-C31	2.93	121.09	111.91
59	i	201	CHD	C11-C12-C13	2.90	114.22	111.24
53	d	201	CDL	OB6-CB5-C51	2.90	118.88	110.80
53	X	201	CDL	OB8-CB7-C71	2.89	120.98	111.91
45	Z	200	PC1	O31-C31-C32	2.87	120.92	111.91
54	O	401	DGT	N9-C8-N7	-2.86	108.00	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	I	203	PC1	O21-C21-C22	2.85	117.65	111.50
54	O	401	DGT	PA-O3A-PB	-2.82	123.14	132.83
49	F	503	NAI	C1D-N1N-C2N	-2.81	116.44	121.11
52	L	703	3PE	O31-C31-C32	2.79	120.65	111.91
48	F	501	FMN	C4A-C10-N10	2.78	120.55	116.48
49	F	503	NAI	PN-O3-PA	-2.77	123.33	132.83
53	q	202	CDL	OA8-CA7-C31	2.75	120.55	111.91
45	h	202	PC1	O31-C31-C32	2.74	120.50	111.91
53	h	201	CDL	OA8-CA7-C31	2.73	120.46	111.91
54	O	401	DGT	C5-C6-N1	2.71	120.08	113.19
56	P	403	NDP	PN-O3-PA	-2.71	123.53	132.83
45	q	201	PC1	O31-C31-C32	2.69	120.35	111.91
52	L	704	3PE	O31-C31-C32	2.69	120.34	111.91
52	N	403	3PE	O31-C31-C32	2.68	120.32	111.91
49	F	503	NAI	N3A-C4A-N9A	2.67	131.48	127.08
52	N	402	3PE	O31-C31-C32	2.67	120.28	111.91
48	F	501	FMN	C4A-C4-N3	2.65	119.93	113.19
53	d	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
56	P	403	NDP	C2B-C1B-N9A	-2.64	109.09	113.53
53	d	201	CDL	OA8-CA7-C31	2.62	120.14	111.91
53	h	201	CDL	CA4-OA6-CA5	-2.62	111.34	117.79
54	O	401	DGT	PB-O3B-PG	-2.62	123.85	132.83
45	A	201	PC1	O31-C31-C32	2.60	120.08	111.91
52	M	501	3PE	O31-C31-C32	2.60	120.07	111.91
45	B	202	PC1	O31-C31-C32	2.60	120.06	111.91
48	F	501	FMN	C10-C4A-N5	-2.58	119.37	124.86
52	Y	803	3PE	O31-C31-C32	2.57	119.98	111.91
53	h	201	CDL	OB8-CB7-C71	2.57	119.97	111.91
53	M	502	CDL	OA8-CA7-C31	2.56	119.93	111.91
53	M	502	CDL	CA4-OA6-CA5	-2.54	111.53	117.79
45	P	401	PC1	O31-C31-C32	2.54	119.88	111.91
48	F	501	FMN	C6-C7-C8	-2.54	116.03	119.67
48	F	501	FMN	O4-C4-C4A	-2.51	119.95	126.60
54	O	401	DGT	O6-C6-C5	-2.51	119.95	126.60
48	F	501	FMN	C9A-C5A-N5	-2.50	119.71	122.43
53	X	201	CDL	OA8-CA7-C31	2.49	119.72	111.91
45	A	202	PC1	O31-C31-C32	2.48	119.67	111.91
52	Y	801	3PE	O13-C11-C12	2.47	118.35	109.10
49	F	503	NAI	C4A-C5A-N7A	-2.47	107.61	110.62
49	F	503	NAI	C5A-C4A-N9A	2.45	108.63	105.78
52	b	201	3PE	O31-C31-C32	2.44	119.56	111.91
52	K	101	3PE	O31-C31-C32	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	L	702	CDL	OA8-CA7-C31	2.35	119.29	111.91
59	i	201	CHD	C6-C5-C4	-2.35	108.48	111.19
52	L	701	3PE	O31-C31-C32	2.34	119.26	111.91
52	Y	802	3PE	O31-C31-C32	2.34	119.25	111.91
56	P	403	NDP	C4A-C5A-N7A	-2.34	107.77	110.62
53	L	702	CDL	OB8-CB7-C71	2.33	119.21	111.91
52	Y	805	3PE	O31-C31-C32	2.32	119.18	111.91
58	U	101	EHZ	C13-C12-N1	2.31	120.31	116.42
45	A	202	PC1	C2-O21-C21	-2.29	112.15	117.79
59	i	201	CHD	C16-C17-C20	-2.28	108.61	112.15
52	N	401	3PE	O31-C31-C32	2.27	119.02	111.91
59	i	201	CHD	C6-C7-C8	2.26	113.89	111.48
52	Y	801	3PE	O31-C31-C32	2.25	118.97	111.91
58	U	101	EHZ	C7-C8-C9	-2.22	108.82	113.89
54	O	401	DGT	C8-N7-C5	2.22	108.26	104.24
53	q	202	CDL	OB8-CB7-C71	2.21	118.85	111.91
52	m	201	3PE	O31-C31-C32	2.19	118.78	111.91
45	N	404	PC1	O31-C31-C32	2.18	118.74	111.91
49	F	503	NAI	C2D-C3D-C4D	2.12	106.77	102.64
49	F	503	NAI	C3D-C2D-C1D	2.12	105.46	101.43
58	U	101	EHZ	C10-S1-C9	2.10	108.42	101.87
53	X	201	CDL	OB6-CB5-OB7	-2.09	118.65	123.70
59	i	201	CHD	C15-C14-C8	2.09	121.25	118.33
53	X	201	CDL	C12-C11-CA5	-2.08	106.04	113.62
52	H	703	3PE	C3-C2-C1	-2.08	106.88	111.79
45	B	203	PC1	O31-C31-C32	2.07	118.41	111.91
59	i	201	CHD	C21-C20-C22	-2.06	107.13	110.36
48	F	501	FMN	C4A-C10-N1	-2.06	119.95	124.73
49	F	503	NAI	C6A-C5A-C4A	2.06	119.95	117.18
58	U	101	EHZ	O2-C9-S1	-2.05	119.95	122.61
52	H	703	3PE	O31-C31-C32	2.03	118.28	111.91
52	H	702	3PE	P-O13-C11	-2.03	111.60	121.59
56	P	403	NDP	C4A-N9A-C8A	2.02	107.92	105.73
48	F	501	FMN	C4-C4A-C10	2.01	120.17	116.79

There are no chirality outliers.

All (742) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PC1	O13-C11-C12-N
45	A	201	PC1	C22-C21-O21-C2
45	B	203	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	I	203	PC1	C1-O11-P-O12
45	I	203	PC1	C1-O11-P-O14
45	P	401	PC1	C2-C1-O11-P
45	Z	200	PC1	C1-O11-P-O14
45	Z	200	PC1	O13-C11-C12-N
45	Z	200	PC1	O11-C1-C2-O21
45	h	202	PC1	C11-O13-P-O14
45	h	202	PC1	C1-O11-P-O14
45	h	202	PC1	C2-C1-O11-P
45	q	201	PC1	O13-C11-C12-N
45	q	201	PC1	O22-C21-O21-C2
51	H	701	U10	C7-C8-C9-C10
51	H	701	U10	C7-C8-C9-C11
51	H	701	U10	C37-C38-C39-C40
51	H	701	U10	C37-C38-C39-C41
51	H	701	U10	C42-C43-C44-C45
51	H	701	U10	C42-C43-C44-C46
51	H	701	U10	C51-C52-C53-C54
52	H	702	3PE	C22-C21-O21-C2
52	H	703	3PE	C11-O13-P-O12
52	H	703	3PE	C11-O13-P-O14
52	H	703	3PE	O13-C11-C12-N
52	H	703	3PE	C22-C21-O21-C2
52	L	701	3PE	C1-O11-P-O14
52	L	701	3PE	O13-C11-C12-N
52	L	703	3PE	C11-O13-P-O14
52	L	704	3PE	C1-O11-P-O12
52	L	704	3PE	O22-C21-O21-C2
52	L	704	3PE	C22-C21-O21-C2
52	N	401	3PE	O13-C11-C12-N
52	N	401	3PE	C22-C21-O21-C2
52	P	404	3PE	C1-O11-P-O12
52	P	404	3PE	C1-O11-P-O14
52	P	404	3PE	C2-C1-O11-P
52	P	404	3PE	C3-C2-O21-C21
52	P	404	3PE	C22-C21-O21-C2
52	Y	801	3PE	C12-C11-O13-P
52	Y	801	3PE	O13-C11-C12-N
52	Y	801	3PE	O22-C21-O21-C2
52	Y	801	3PE	C22-C21-O21-C2
52	Y	802	3PE	C11-O13-P-O11
52	Y	803	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
52	Y	804	3PE	C1-O11-P-O12
52	Y	804	3PE	C1-O11-P-O14
52	Y	804	3PE	C2-C1-O11-P
52	Y	804	3PE	O13-C11-C12-N
52	Y	805	3PE	C1-O11-P-O14
52	b	201	3PE	C12-C11-O13-P
52	m	201	3PE	C1-O11-P-O14
52	m	201	3PE	C11-O13-P-O14
52	m	201	3PE	C12-C11-O13-P
52	m	201	3PE	O22-C21-O21-C2
53	L	702	CDL	CB3-OB5-PB2-OB4
53	M	502	CDL	C1-CA2-OA2-PA1
53	M	502	CDL	C11-CA5-OA6-CA4
53	M	502	CDL	CB2-OB2-PB2-OB3
53	M	502	CDL	CB2-OB2-PB2-OB4
53	P	402	CDL	CA3-OA5-PA1-OA3
53	P	402	CDL	C11-CA5-OA6-CA4
53	P	402	CDL	CB2-OB2-PB2-OB3
53	P	402	CDL	CB2-OB2-PB2-OB4
53	P	402	CDL	CB2-OB2-PB2-OB5
53	P	402	CDL	C51-CB5-OB6-CB4
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CA2-OA2-PA1-OA4
53	X	201	CDL	CA2-OA2-PA1-OA5
53	X	201	CDL	CA3-OA5-PA1-OA4
53	X	201	CDL	CB4-CB3-OB5-PB2
53	X	201	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	CA3-OA5-PA1-OA3
53	d	201	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	C11-CA5-OA6-CA4
53	q	202	CDL	CA3-OA5-PA1-OA3
53	q	202	CDL	C11-CA5-OA6-CA4
53	q	202	CDL	CB3-OB5-PB2-OB3
54	O	401	DGT	C5'-O5'-PA-O3A
56	P	403	NDP	C2B-O2B-P2B-O3X
58	T	101	EHZ	C5-C6-C7-C8
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	S1-C10-C11-N1
58	T	101	EHZ	C10-C11-N1-C12

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Mol	Chain	Res	Type	Atoms
58	T	101	EHZ	C12-C13-C14-N2
58	T	101	EHZ	C15-C16-C17-C19
58	T	101	EHZ	C15-C16-C17-C20
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
52	L	701	3PE	O32-C31-O31-C3
52	L	704	3PE	O32-C31-O31-C3
45	N	404	PC1	O32-C31-O31-C3
45	h	202	PC1	O32-C31-O31-C3
45	q	201	PC1	O32-C31-O31-C3
52	K	101	3PE	O32-C31-O31-C3
52	P	404	3PE	O32-C31-O31-C3
52	Y	801	3PE	O32-C31-O31-C3
52	Y	802	3PE	O32-C31-O31-C3
53	L	702	CDL	OB9-CB7-OB8-CB6
53	M	502	CDL	OB9-CB7-OB8-CB6
45	A	201	PC1	O22-C21-O21-C2
45	A	202	PC1	O22-C21-O21-C2
45	B	203	PC1	O22-C21-O21-C2
52	H	702	3PE	O22-C21-O21-C2
52	H	703	3PE	O22-C21-O21-C2
52	N	401	3PE	O22-C21-O21-C2
52	P	404	3PE	O22-C21-O21-C2
53	M	502	CDL	OA7-CA5-OA6-CA4
53	P	402	CDL	OA7-CA5-OA6-CA4
53	P	402	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	OA7-CA5-OA6-CA4
53	q	202	CDL	OA7-CA5-OA6-CA4
45	B	203	PC1	C32-C31-O31-C3
45	M	503	PC1	C32-C31-O31-C3
45	N	404	PC1	C32-C31-O31-C3
45	q	201	PC1	C32-C31-O31-C3
52	K	101	3PE	C32-C31-O31-C3
52	L	701	3PE	C32-C31-O31-C3
52	L	704	3PE	C32-C31-O31-C3
52	P	404	3PE	C32-C31-O31-C3
52	Y	801	3PE	C32-C31-O31-C3
52	Y	802	3PE	C32-C31-O31-C3
53	L	702	CDL	C71-CB7-OB8-CB6
45	A	202	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	q	201	PC1	C22-C21-O21-C2
52	m	201	3PE	C22-C21-O21-C2
53	X	201	CDL	OB9-CB7-OB8-CB6
52	N	403	3PE	O32-C31-O31-C3
45	A	202	PC1	C32-C31-O31-C3
45	h	202	PC1	C32-C31-O31-C3
52	Y	804	3PE	C32-C31-O31-C3
53	M	502	CDL	C71-CB7-OB8-CB6
51	H	701	U10	C22-C23-C24-C25
51	H	701	U10	C22-C23-C24-C26
45	B	203	PC1	O32-C31-O31-C3
52	Y	804	3PE	O32-C31-O31-C3
53	L	702	CDL	O1-C1-CB2-OB2
53	M	502	CDL	O1-C1-CA2-OA2
53	d	201	CDL	O1-C1-CA2-OA2
53	X	201	CDL	C71-CB7-OB8-CB6
45	M	503	PC1	O32-C31-O31-C3
52	L	701	3PE	C22-C21-O21-C2
52	Y	802	3PE	C22-C21-O21-C2
53	h	201	CDL	C51-CB5-OB6-CB4
52	M	501	3PE	C26-C27-C28-C29
52	N	403	3PE	C32-C31-O31-C3
52	N	402	3PE	C2-C1-O11-P
45	A	202	PC1	O32-C31-O31-C3
51	H	701	U10	C30-C29-C31-C32
51	H	701	U10	C28-C29-C31-C32
51	H	701	U10	C24-C26-C27-C28
51	H	701	U10	C44-C46-C47-C48
45	P	401	PC1	C32-C31-O31-C3
52	m	201	3PE	C32-C31-O31-C3
53	L	702	CDL	CA2-C1-CB2-OB2
53	M	502	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	OB7-CB5-OB6-CB4
45	P	401	PC1	O32-C31-O31-C3
52	m	201	3PE	O32-C31-O31-C3
45	I	203	PC1	C32-C31-O31-C3
52	N	401	3PE	C32-C31-O31-C3
52	N	402	3PE	C32-C31-O31-C3
45	N	404	PC1	C34-C35-C36-C37
45	A	201	PC1	O11-C1-C2-O21
52	M	501	3PE	O21-C2-C3-O31
45	I	203	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
52	L	701	3PE	O22-C21-O21-C2
52	Y	802	3PE	O22-C21-O21-C2
52	N	402	3PE	O32-C31-O31-C3
45	Z	200	PC1	C26-C27-C28-C29
58	T	101	EHZ	C5-C6-C7-O1
53	P	402	CDL	C31-CA7-OA8-CA6
52	Y	802	3PE	C2-C1-O11-P
52	Y	803	3PE	C31-C32-C33-C34
52	P	404	3PE	C21-C22-C23-C24
52	N	401	3PE	O32-C31-O31-C3
51	H	701	U10	C49-C51-C52-C53
52	P	404	3PE	C23-C24-C25-C26
53	P	402	CDL	OA9-CA7-OA8-CA6
52	L	704	3PE	C33-C34-C35-C36
45	B	203	PC1	C11-O13-P-O11
45	I	203	PC1	C1-O11-P-O13
45	Z	200	PC1	C1-O11-P-O13
45	h	202	PC1	C11-O13-P-O11
45	h	202	PC1	C1-O11-P-O13
45	q	201	PC1	C1-O11-P-O13
52	H	703	3PE	C11-O13-P-O11
52	K	101	3PE	C1-O11-P-O13
52	L	703	3PE	C11-O13-P-O11
52	L	704	3PE	C1-O11-P-O13
52	N	403	3PE	C1-O11-P-O13
52	P	404	3PE	C1-O11-P-O13
52	Y	801	3PE	C1-O11-P-O13
52	Y	801	3PE	C11-O13-P-O11
52	Y	803	3PE	C11-O13-P-O11
52	Y	804	3PE	C1-O11-P-O13
52	Y	805	3PE	C1-O11-P-O13
52	m	201	3PE	C1-O11-P-O13
53	L	702	CDL	CB3-OB5-PB2-OB2
53	M	502	CDL	CA2-OA2-PA1-OA5
53	M	502	CDL	CB2-OB2-PB2-OB5
53	P	402	CDL	CA3-OA5-PA1-OA2
53	P	402	CDL	CB3-OB5-PB2-OB2
53	X	201	CDL	CA3-OA5-PA1-OA2
53	d	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA2-OA2-PA1-OA5
53	q	202	CDL	CB2-OB2-PB2-OB5
53	M	502	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	q	202	CDL	C71-CB7-OB8-CB6
52	m	201	3PE	C21-C22-C23-C24
53	d	201	CDL	CB2-C1-CA2-OA2
45	A	201	PC1	C32-C31-O31-C3
52	L	703	3PE	C26-C27-C28-C29
53	q	202	CDL	C71-C72-C73-C74
52	N	403	3PE	C27-C28-C29-C2A
52	L	701	3PE	C23-C24-C25-C26
52	L	703	3PE	C39-C3A-C3B-C3C
53	d	201	CDL	O1-C1-CB2-OB2
52	H	702	3PE	C25-C26-C27-C28
52	N	403	3PE	C35-C36-C37-C38
52	Y	801	3PE	C32-C33-C34-C35
53	X	201	CDL	C34-C35-C36-C37
53	X	201	CDL	C59-C60-C61-C62
58	U	101	EHZ	C1-C21-C22-C23
53	q	202	CDL	OB9-CB7-OB8-CB6
45	h	202	PC1	C2A-C2B-C2C-C2D
52	Y	805	3PE	C25-C26-C27-C28
53	M	502	CDL	C35-C36-C37-C38
53	d	201	CDL	C76-C77-C78-C79
53	h	201	CDL	C39-C40-C41-C42
52	L	703	3PE	C33-C34-C35-C36
53	h	201	CDL	C37-C38-C39-C40
45	N	404	PC1	C31-C32-C33-C34
45	B	202	PC1	C25-C26-C27-C28
52	Y	805	3PE	C24-C25-C26-C27
52	b	201	3PE	C28-C29-C2A-C2B
45	q	201	PC1	C2B-C2C-C2D-C2E
52	M	501	3PE	C23-C24-C25-C26
52	m	201	3PE	C32-C33-C34-C35
53	M	502	CDL	C61-C62-C63-C64
53	M	502	CDL	C71-C72-C73-C74
53	P	402	CDL	C31-C32-C33-C34
52	b	201	3PE	C34-C35-C36-C37
45	B	203	PC1	C22-C23-C24-C25
52	N	401	3PE	C29-C2A-C2B-C2C
45	I	203	PC1	C22-C23-C24-C25
52	N	403	3PE	C38-C39-C3A-C3B
52	b	201	3PE	C23-C24-C25-C26
52	m	201	3PE	C24-C25-C26-C27
45	I	203	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
52	H	702	3PE	C26-C27-C28-C29
52	L	704	3PE	C23-C24-C25-C26
45	h	202	PC1	C27-C28-C29-C2A
45	A	201	PC1	O32-C31-O31-C3
53	M	502	CDL	OA9-CA7-OA8-CA6
53	L	702	CDL	CB5-C51-C52-C53
53	P	402	CDL	CA2-C1-CB2-OB2
53	q	202	CDL	C12-C13-C14-C15
53	P	402	CDL	C62-C63-C64-C65
45	Z	200	PC1	C23-C24-C25-C26
52	M	501	3PE	C32-C31-O31-C3
52	b	201	3PE	C32-C31-O31-C3
52	H	702	3PE	C2A-C2B-C2C-C2D
58	U	101	EHZ	C3-C4-C5-C6
53	X	201	CDL	C41-C42-C43-C44
52	M	501	3PE	O32-C31-O31-C3
52	b	201	3PE	O32-C31-O31-C3
45	Z	200	PC1	C2A-C2B-C2C-C2D
53	d	201	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	OB7-CB5-OB6-CB4
52	N	401	3PE	C31-C32-C33-C34
53	M	502	CDL	CA5-C11-C12-C13
53	d	201	CDL	C31-CA7-OA8-CA6
53	d	201	CDL	C42-C43-C44-C45
45	Z	200	PC1	C36-C37-C38-C39
53	h	201	CDL	C11-C12-C13-C14
58	U	101	EHZ	C21-C1-C2-C3
45	q	201	PC1	C2-C3-O31-C31
52	H	703	3PE	C23-C24-C25-C26
45	Z	200	PC1	C32-C31-O31-C3
60	o	201	MYR	C7-C8-C9-C10
53	d	201	CDL	C11-CA5-OA6-CA4
53	d	201	CDL	C51-CB5-OB6-CB4
52	N	402	3PE	O11-C1-C2-O21
53	L	702	CDL	C32-C33-C34-C35
52	H	703	3PE	C2C-C2D-C2E-C2F
53	X	201	CDL	C23-C24-C25-C26
45	h	202	PC1	C23-C24-C25-C26
52	m	201	3PE	C2C-C2D-C2E-C2F
52	Y	804	3PE	C2-C3-O31-C31
45	A	201	PC1	C32-C33-C34-C35
53	X	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	CA5-C11-C12-C13
52	Y	803	3PE	C34-C35-C36-C37
52	M	501	3PE	C22-C21-O21-C2
45	q	201	PC1	C11-O13-P-O11
52	b	201	3PE	C11-O13-P-O11
53	L	702	CDL	CB2-OB2-PB2-OB5
53	q	202	CDL	CA3-OA5-PA1-OA2
45	M	503	PC1	C21-C22-C23-C24
51	H	701	U10	C6-C7-C8-C9
45	Z	200	PC1	O11-C1-C2-C3
52	Y	801	3PE	O11-C1-C2-C3
52	Y	804	3PE	O11-C1-C2-C3
52	Y	805	3PE	O11-C1-C2-C3
53	P	402	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OB5-CB3-CB4-CB6
45	q	201	PC1	C34-C35-C36-C37
53	P	402	CDL	C51-C52-C53-C54
45	N	404	PC1	C37-C38-C39-C3A
45	M	503	PC1	C22-C23-C24-C25
52	L	701	3PE	C2D-C2E-C2F-C2G
53	q	202	CDL	C51-CB5-OB6-CB4
52	K	101	3PE	C27-C28-C29-C2A
53	M	502	CDL	C81-C82-C83-C84
53	X	201	CDL	C57-C58-C59-C60
52	H	702	3PE	C1-C2-C3-O31
52	M	501	3PE	C1-C2-C3-O31
52	N	403	3PE	C1-C2-C3-O31
52	Y	804	3PE	C1-C2-C3-O31
53	X	201	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	CB3-CB4-CB6-OB8
52	Y	801	3PE	C34-C35-C36-C37
58	U	101	EHZ	C2-C1-C21-C22
52	b	201	3PE	C29-C2A-C2B-C2C
53	L	702	CDL	C12-C13-C14-C15
53	M	502	CDL	C77-C78-C79-C80
45	P	401	PC1	O21-C21-C22-C23
53	d	201	CDL	OA9-CA7-OA8-CA6
45	Z	200	PC1	C35-C36-C37-C38
52	Y	804	3PE	O31-C31-C32-C33
52	L	701	3PE	C26-C27-C28-C29
53	d	201	CDL	C43-C44-C45-C46
53	h	201	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
52	Y	801	3PE	C31-C32-C33-C34
52	Y	805	3PE	C31-C32-C33-C34
49	F	503	NAI	C2D-C1D-N1N-C2N
45	I	203	PC1	O11-C1-C2-O21
52	P	404	3PE	O31-C31-C32-C33
52	M	501	3PE	C37-C38-C39-C3A
53	P	402	CDL	O1-C1-CB2-OB2
52	b	201	3PE	C31-C32-C33-C34
58	T	101	EHZ	O5-C16-C17-C18
58	T	101	EHZ	O5-C16-C17-C19
45	B	203	PC1	C36-C37-C38-C39
52	K	101	3PE	O21-C21-C22-C23
45	P	401	PC1	C23-C24-C25-C26
45	Z	200	PC1	O32-C31-O31-C3
52	Y	802	3PE	C23-C24-C25-C26
52	M	501	3PE	O22-C21-O21-C2
52	K	101	3PE	C22-C21-O21-C2
52	N	402	3PE	C22-C21-O21-C2
45	I	203	PC1	C26-C27-C28-C29
53	P	402	CDL	C71-CB7-OB8-CB6
52	N	403	3PE	C2A-C2B-C2C-C2D
45	I	203	PC1	O11-C1-C2-C3
52	N	402	3PE	O11-C1-C2-C3
52	Y	803	3PE	C22-C23-C24-C25
52	Y	802	3PE	C31-C32-C33-C34
52	L	703	3PE	O13-C11-C12-N
52	H	702	3PE	C27-C28-C29-C2A
52	N	403	3PE	C34-C35-C36-C37
53	h	201	CDL	C52-C53-C54-C55
45	A	202	PC1	O31-C31-C32-C33
53	P	402	CDL	C1-CB2-OB2-PB2
60	o	201	MYR	C2-C3-C4-C5
52	M	501	3PE	C2E-C2F-C2G-C2H
52	Y	802	3PE	C28-C29-C2A-C2B
45	B	202	PC1	C33-C34-C35-C36
52	L	703	3PE	C38-C39-C3A-C3B
45	N	404	PC1	C1-C2-C3-O31
52	N	401	3PE	C1-C2-C3-O31
52	m	201	3PE	C1-C2-C3-O31
53	h	201	CDL	CA3-CA4-CA6-OA8
53	q	202	CDL	OB7-CB5-OB6-CB4
52	K	101	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
52	L	703	3PE	C35-C36-C37-C38
45	q	201	PC1	C21-C22-C23-C24
45	I	203	PC1	C21-C22-C23-C24
45	B	202	PC1	C35-C36-C37-C38
52	L	701	3PE	O11-C1-C2-O21
52	L	704	3PE	O11-C1-C2-O21
52	Y	803	3PE	O11-C1-C2-O21
52	Y	804	3PE	O11-C1-C2-O21
53	M	502	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	OA5-CA3-CA4-OA6
53	h	201	CDL	OB5-CB3-CB4-OB6
53	q	202	CDL	OB5-CB3-CB4-OB6
45	B	202	PC1	C21-C22-C23-C24
53	M	502	CDL	CB5-C51-C52-C53
52	Y	801	3PE	O21-C21-C22-C23
53	h	201	CDL	O1-C1-CB2-OB2
52	K	101	3PE	C36-C37-C38-C39
52	N	401	3PE	O21-C2-C3-O31
52	N	403	3PE	O21-C2-C3-O31
52	m	201	3PE	O21-C2-C3-O31
53	h	201	CDL	C71-CB7-OB8-CB6
53	h	201	CDL	C75-C76-C77-C78
53	M	502	CDL	C37-C38-C39-C40
52	K	101	3PE	O22-C21-O21-C2
52	N	402	3PE	O22-C21-O21-C2
52	Y	803	3PE	C2-C1-O11-P
45	N	404	PC1	C35-C36-C37-C38
52	N	401	3PE	C22-C23-C24-C25
53	h	201	CDL	C38-C39-C40-C41
52	L	704	3PE	C36-C37-C38-C39
52	b	201	3PE	C2B-C2C-C2D-C2E
45	q	201	PC1	C38-C39-C3A-C3B
45	A	201	PC1	O11-C1-C2-C3
45	M	503	PC1	O11-C1-C2-C3
52	L	701	3PE	O11-C1-C2-C3
52	L	704	3PE	O11-C1-C2-C3
52	N	401	3PE	O11-C1-C2-C3
52	Y	803	3PE	O11-C1-C2-C3
52	N	401	3PE	C25-C26-C27-C28
45	N	404	PC1	C2-C3-O31-C31
45	P	401	PC1	C3-C2-O21-C21
52	L	704	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
53	P	402	CDL	CA6-CA4-OA6-CA5
53	d	201	CDL	CB6-CB4-OB6-CB5
52	Y	802	3PE	C27-C28-C29-C2A
45	B	202	PC1	C1-C2-C3-O31
48	F	501	FMN	C4'-C5'-O5'-P
52	Y	801	3PE	C2-C1-O11-P
53	L	702	CDL	CB3-CB4-CB6-OB8
53	q	202	CDL	CA3-CA4-CA6-OA8
52	Y	805	3PE	O11-C1-C2-O21
53	X	201	CDL	OA5-CA3-CA4-OA6
52	M	501	3PE	O21-C21-C22-C23
45	q	201	PC1	C23-C24-C25-C26
52	L	701	3PE	C25-C26-C27-C28
58	T	101	EHZ	O1-C7-C8-C9
58	U	101	EHZ	O1-C7-C8-C9
49	F	503	NAI	O4D-C1D-N1N-C2N
53	P	402	CDL	OB9-CB7-OB8-CB6
52	Y	805	3PE	C35-C36-C37-C38
45	N	404	PC1	O21-C2-C3-O31
52	L	701	3PE	O21-C2-C3-O31
52	Y	801	3PE	O21-C2-C3-O31
53	L	702	CDL	OB6-CB4-CB6-OB8
53	P	402	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OB9-CB7-OB8-CB6
53	X	201	CDL	C12-C11-CA5-OA6
52	M	501	3PE	C2B-C2C-C2D-C2E
49	F	503	NAI	C5D-O5D-PN-O3
52	N	403	3PE	C29-C2A-C2B-C2C
51	H	701	U10	C16-C17-C18-C19
52	b	201	3PE	C26-C27-C28-C29
53	L	702	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	C35-C36-C37-C38
52	M	501	3PE	C24-C25-C26-C27
52	N	403	3PE	O31-C31-C32-C33
45	B	203	PC1	C27-C28-C29-C2A
45	h	202	PC1	C33-C34-C35-C36
52	L	703	3PE	O22-C21-O21-C2
45	A	202	PC1	C11-O13-P-O11
52	N	403	3PE	C11-O13-P-O11
52	m	201	3PE	C11-O13-P-O11
45	B	203	PC1	C2-C1-O11-P
45	B	203	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	q	201	PC1	C11-O13-P-O12
45	q	201	PC1	C1-O11-P-O12
52	K	101	3PE	C1-O11-P-O14
52	N	403	3PE	C1-O11-P-O12
52	Y	801	3PE	C1-O11-P-O12
52	Y	801	3PE	C1-O11-P-O14
52	Y	801	3PE	C11-O13-P-O12
52	Y	803	3PE	C11-O13-P-O12
52	b	201	3PE	C1-O11-P-O14
52	b	201	3PE	C11-O13-P-O12
53	L	702	CDL	CB2-OB2-PB2-OB4
53	L	702	CDL	CB3-OB5-PB2-OB3
53	M	502	CDL	CA2-OA2-PA1-OA3
53	M	502	CDL	CA2-OA2-PA1-OA4
53	M	502	CDL	CA3-OA5-PA1-OA4
53	P	402	CDL	CA3-OA5-PA1-OA4
53	P	402	CDL	CB3-OB5-PB2-OB3
53	X	201	CDL	CA3-OA5-PA1-OA3
53	d	201	CDL	CA2-OA2-PA1-OA4
53	q	202	CDL	CA2-OA2-PA1-OA3
53	q	202	CDL	CB2-OB2-PB2-OB4
54	O	401	DGT	C5'-O5'-PA-O1A
52	L	704	3PE	C31-C32-C33-C34
53	q	202	CDL	C17-C18-C19-C20
53	M	502	CDL	OB5-CB3-CB4-CB6
45	q	201	PC1	C24-C25-C26-C27
52	L	704	3PE	C2D-C2E-C2F-C2G
52	H	703	3PE	C37-C38-C39-C3A
53	M	502	CDL	C55-C56-C57-C58
53	L	702	CDL	C51-CB5-OB6-CB4
45	A	202	PC1	C12-C11-O13-P
52	H	702	3PE	C12-C11-O13-P
52	M	501	3PE	C12-C11-O13-P
52	N	402	3PE	C12-C11-O13-P
52	Y	805	3PE	C12-C11-O13-P
52	K	101	3PE	C21-C22-C23-C24
45	M	503	PC1	O11-C1-C2-O21
52	Y	801	3PE	O11-C1-C2-O21
53	P	402	CDL	OB5-CB3-CB4-OB6
53	X	201	CDL	OB5-CB3-CB4-OB6
52	L	701	3PE	C36-C37-C38-C39
52	L	703	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	A	202	PC1	C21-C22-C23-C24
49	F	503	NAI	C2D-C1D-N1N-C6N
45	A	202	PC1	O13-C11-C12-N
45	h	202	PC1	O13-C11-C12-N
52	K	101	3PE	C22-C23-C24-C25
52	M	501	3PE	C28-C29-C2A-C2B
52	Y	802	3PE	C1-C2-C3-O31
53	P	402	CDL	CA3-CA4-CA6-OA8
58	T	101	EHZ	O5-C16-C17-C20
52	H	702	3PE	O21-C2-C3-O31
52	N	402	3PE	O21-C2-C3-O31
52	Y	802	3PE	O21-C2-C3-O31
53	X	201	CDL	OB6-CB4-CB6-OB8
53	d	201	CDL	OB6-CB4-CB6-OB8
53	q	202	CDL	OA6-CA4-CA6-OA8
52	H	703	3PE	C2-C1-O11-P
45	Z	200	PC1	C33-C34-C35-C36
53	M	502	CDL	C74-C75-C76-C77
52	H	702	3PE	C21-C22-C23-C24
45	B	202	PC1	O32-C31-O31-C3
53	h	201	CDL	OA9-CA7-OA8-CA6
52	Y	802	3PE	O21-C21-C22-C23
49	F	503	NAI	O4D-C1D-N1N-C6N
52	L	703	3PE	C36-C37-C38-C39
52	L	704	3PE	C38-C39-C3A-C3B
52	Y	804	3PE	C22-C21-O21-C2
53	q	202	CDL	C19-C20-C21-C22
53	M	502	CDL	C72-C73-C74-C75
45	A	201	PC1	C3-C2-O21-C21
45	q	201	PC1	C3-C2-O21-C21
52	N	402	3PE	C3-C2-O21-C21
52	Y	801	3PE	C3-C2-O21-C21
53	M	502	CDL	CA2-C1-CB2-OB2
45	B	202	PC1	C32-C31-O31-C3
52	N	401	3PE	C2A-C2B-C2C-C2D
45	B	202	PC1	C3B-C3C-C3D-C3E
52	N	403	3PE	C24-C25-C26-C27
53	X	201	CDL	C55-C56-C57-C58
53	d	201	CDL	CA4-CA3-OA5-PA1
53	q	202	CDL	C1-CA2-OA2-PA1
52	N	401	3PE	O11-C1-C2-O21
52	Y	804	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
53	M	502	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	OA7-CA5-OA6-CA4
52	L	701	3PE	C27-C28-C29-C2A
52	Y	804	3PE	O21-C2-C3-O31
53	h	201	CDL	OB6-CB4-CB6-OB8
52	N	402	3PE	C1-O11-P-O13
52	N	402	3PE	C11-O13-P-O11
53	X	201	CDL	CB2-OB2-PB2-OB5
53	d	201	CDL	CA3-OA5-PA1-OA2
53	d	201	CDL	CB2-OB2-PB2-OB5
52	K	101	3PE	C39-C3A-C3B-C3C
53	P	402	CDL	C54-C55-C56-C57
53	X	201	CDL	C20-C21-C22-C23
52	H	702	3PE	O31-C31-C32-C33
52	M	501	3PE	C2C-C2D-C2E-C2F
56	P	403	NDP	O4D-C1D-N1N-C6N
52	P	404	3PE	O32-C31-C32-C33
53	h	201	CDL	C36-C37-C38-C39
58	U	101	EHZ	C5-C6-C7-C8
45	q	201	PC1	C29-C2A-C2B-C2C
45	B	202	PC1	O21-C21-C22-C23
52	H	702	3PE	C29-C2A-C2B-C2C
45	Z	200	PC1	C21-C22-C23-C24
53	h	201	CDL	C31-CA7-OA8-CA6
52	Y	801	3PE	C22-C23-C24-C25
52	Y	802	3PE	C24-C25-C26-C27
53	h	201	CDL	C13-C14-C15-C16
52	L	703	3PE	C34-C35-C36-C37
53	M	502	CDL	C64-C65-C66-C67
53	X	201	CDL	OA5-CA3-CA4-CA6
45	B	202	PC1	C34-C35-C36-C37
53	X	201	CDL	C11-C12-C13-C14
52	L	701	3PE	C29-C2A-C2B-C2C
51	H	701	U10	C45-C44-C46-C47
52	Y	802	3PE	C2D-C2E-C2F-C2G
52	H	702	3PE	O32-C31-C32-C33
45	P	401	PC1	O22-C21-C22-C23
58	U	101	EHZ	S1-C10-C11-N1
52	K	101	3PE	C35-C36-C37-C38
53	X	201	CDL	C14-C15-C16-C17
45	B	202	PC1	C22-C23-C24-C25
56	P	403	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	C15-C16-C17-C18
52	Y	801	3PE	C1-C2-C3-O31
52	b	201	3PE	O21-C21-C22-C23
53	M	502	CDL	C58-C59-C60-C61
52	Y	804	3PE	O32-C31-C32-C33
45	P	401	PC1	C32-C33-C34-C35
53	M	502	CDL	C60-C61-C62-C63
53	P	402	CDL	C58-C59-C60-C61
53	P	402	CDL	CB5-C51-C52-C53
52	L	701	3PE	C3-C2-O21-C21
52	Y	804	3PE	C3-C2-O21-C21
53	X	201	CDL	CB3-CB4-OB6-CB5
53	X	201	CDL	CB6-CB4-OB6-CB5
51	H	701	U10	C20-C19-C21-C22
53	q	202	CDL	CA2-OA2-PA1-OA5
52	N	403	3PE	C25-C26-C27-C28
45	Z	200	PC1	C24-C25-C26-C27
53	X	201	CDL	OB5-CB3-CB4-CB6
52	N	401	3PE	C37-C38-C39-C3A
45	B	202	PC1	O21-C2-C3-O31
53	h	201	CDL	OA6-CA4-CA6-OA8
45	N	404	PC1	C39-C3A-C3B-C3C
53	L	702	CDL	C35-C36-C37-C38
53	q	202	CDL	C15-C16-C17-C18
45	Z	200	PC1	C37-C38-C39-C3A
51	H	701	U10	C39-C41-C42-C43
53	q	202	CDL	C1-CB2-OB2-PB2
45	Z	200	PC1	C28-C29-C2A-C2B
52	K	101	3PE	O22-C21-C22-C23
51	H	701	U10	C43-C44-C46-C47
52	N	401	3PE	C35-C36-C37-C38
53	M	502	CDL	C51-CB5-OB6-CB4
45	B	203	PC1	C34-C35-C36-C37
52	M	501	3PE	O11-C1-C2-O21
52	b	201	3PE	C2E-C2F-C2G-C2H
51	H	701	U10	C5-C4-O4-C4M
53	X	201	CDL	C51-C52-C53-C54
52	b	201	3PE	O11-C1-C2-C3
53	h	201	CDL	OA5-CA3-CA4-CA6
53	h	201	CDL	OB5-CB3-CB4-CB6
53	X	201	CDL	C19-C20-C21-C22
53	d	201	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	C52-C51-CB5-OB6
45	A	202	PC1	O32-C31-C32-C33
53	q	202	CDL	C52-C51-CB5-OB6
53	L	702	CDL	CB4-CB3-OB5-PB2
52	L	703	3PE	C22-C23-C24-C25
53	L	702	CDL	C36-C37-C38-C39
52	H	702	3PE	C24-C25-C26-C27
49	F	503	NAI	C3D-C4D-C5D-O5D
53	q	202	CDL	CB3-OB5-PB2-OB2
52	H	702	3PE	C1-C2-O21-C21
52	L	701	3PE	C1-C2-O21-C21
45	h	202	PC1	C21-C22-C23-C24
52	Y	803	3PE	O22-C21-O21-C2
52	N	401	3PE	C26-C27-C28-C29
53	P	402	CDL	C16-C17-C18-C19
51	H	701	U10	C18-C19-C21-C22
52	L	703	3PE	O21-C21-C22-C23
52	L	704	3PE	C22-C23-C24-C25
52	N	402	3PE	C1-C2-C3-O31
53	d	201	CDL	CB3-CB4-CB6-OB8
51	H	701	U10	C11-C12-C13-C14
53	L	702	CDL	C53-C54-C55-C56
52	Y	801	3PE	O22-C21-C22-C23
58	T	101	EHZ	C15-C16-C17-C18
53	h	201	CDL	C72-C71-CB7-OB8
53	d	201	CDL	C71-C72-C73-C74
53	q	202	CDL	OB5-CB3-CB4-CB6
53	M	502	CDL	C32-C31-CA7-OA8
53	d	201	CDL	C52-C51-CB5-OB7
52	Y	802	3PE	C29-C2A-C2B-C2C
45	B	203	PC1	O21-C21-C22-C23
53	X	201	CDL	C11-CA5-OA6-CA4
53	L	702	CDL	C54-C55-C56-C57
54	O	401	DGT	PB-O3A-PA-O1A
51	H	701	U10	C41-C42-C43-C44
45	B	202	PC1	C38-C39-C3A-C3B
53	q	202	CDL	C52-C51-CB5-OB7
52	Y	803	3PE	C36-C37-C38-C39
53	h	201	CDL	C72-C71-CB7-OB9
52	L	701	3PE	C1-C2-C3-O31
52	L	703	3PE	O31-C31-C32-C33
52	b	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
52	P	404	3PE	C36-C37-C38-C39
52	L	703	3PE	C23-C24-C25-C26
53	d	201	CDL	C72-C71-CB7-OB8
52	b	201	3PE	C2-C1-O11-P
53	d	201	CDL	CB4-CB3-OB5-PB2
53	M	502	CDL	C32-C31-CA7-OA9
52	L	703	3PE	C3A-C3B-C3C-C3D
45	A	202	PC1	C11-O13-P-O14
45	B	202	PC1	C11-O13-P-O14
45	P	401	PC1	C11-O13-P-O14
45	Z	200	PC1	C11-C12-N-C13
45	Z	200	PC1	C11-C12-N-C15
52	H	702	3PE	C11-O13-P-O14
52	K	101	3PE	C1-O11-P-O12
52	N	402	3PE	C1-O11-P-O14
52	N	402	3PE	C11-O13-P-O14
52	N	403	3PE	C1-O11-P-O14
53	L	702	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	C73-C74-C75-C76
58	T	101	EHZ	C3-C4-C5-C6
52	L	703	3PE	O22-C21-C22-C23
52	H	702	3PE	C3-C2-O21-C21
52	H	703	3PE	C1-C2-O21-C21
52	N	403	3PE	C12-C11-O13-P
52	Y	803	3PE	C12-C11-O13-P
53	d	201	CDL	CA3-CA4-OA6-CA5
53	d	201	CDL	CA6-CA4-OA6-CA5
52	Y	805	3PE	C28-C29-C2A-C2B
58	T	101	EHZ	C2-C1-C21-C22
45	B	203	PC1	O22-C21-C22-C23
52	L	704	3PE	C29-C2A-C2B-C2C
53	q	202	CDL	C11-C12-C13-C14
45	Z	200	PC1	C11-C12-N-C14
45	Z	200	PC1	O21-C21-C22-C23
52	H	703	3PE	O21-C21-C22-C23
52	L	701	3PE	O21-C21-C22-C23
52	L	704	3PE	O31-C31-C32-C33
52	P	404	3PE	O21-C21-C22-C23
53	P	402	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C71-C72-C73-C74
45	N	404	PC1	O21-C21-C22-C23
52	Y	802	3PE	O31-C31-C32-C33
52	Y	805	3PE	O21-C21-C22-C23
53	M	502	CDL	CA7-C31-C32-C33
53	d	201	CDL	C72-C71-CB7-OB9
53	M	502	CDL	C84-C85-C86-C87
52	N	401	3PE	O32-C31-C32-C33
52	m	201	3PE	O32-C31-C32-C33
52	K	101	3PE	O31-C31-C32-C33
52	N	401	3PE	O31-C31-C32-C33
52	Y	805	3PE	O31-C31-C32-C33
52	m	201	3PE	O31-C31-C32-C33
45	h	202	PC1	C2B-C2C-C2D-C2E
52	K	101	3PE	O32-C31-C32-C33
52	L	701	3PE	O22-C21-C22-C23
52	Y	802	3PE	O32-C31-C32-C33
53	X	201	CDL	C15-C16-C17-C18
52	L	703	3PE	O32-C31-C32-C33
52	L	704	3PE	O32-C31-C32-C33
53	P	402	CDL	C52-C51-CB5-OB7
52	m	201	3PE	C2A-C2B-C2C-C2D
52	H	703	3PE	O22-C21-C22-C23
52	Y	805	3PE	O32-C31-C32-C33
45	P	401	PC1	O31-C31-C32-C33

There are no ring outliers.

34 monomers are involved in 72 short contacts:

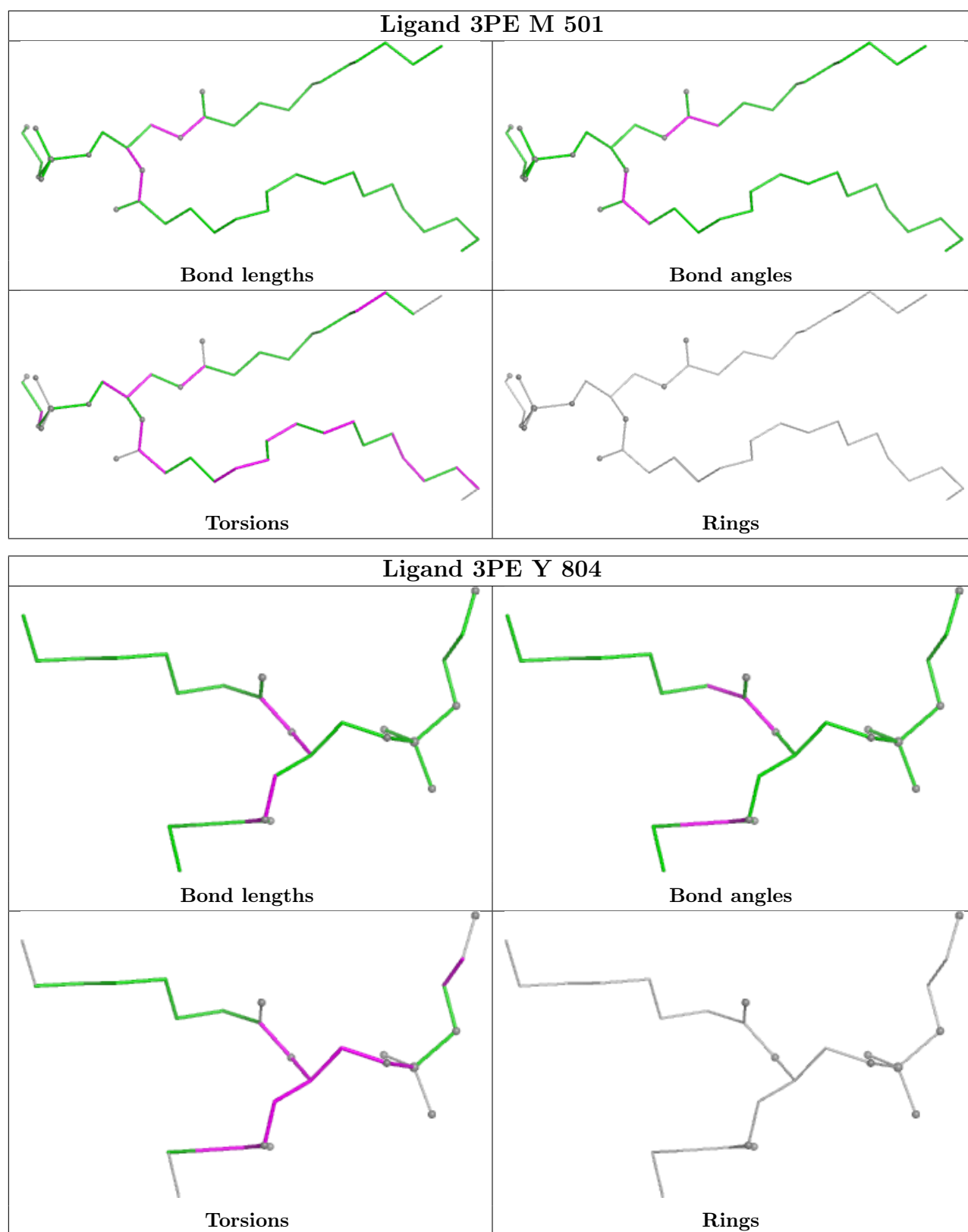
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	M	501	3PE	1	0
45	P	401	PC1	2	0
58	U	101	EHZ	1	0
53	h	201	CDL	1	0
52	N	402	3PE	1	0
52	b	201	3PE	2	0
53	P	402	CDL	1	0
46	F	502	SF4	1	0
45	A	201	PC1	3	0
45	Z	200	PC1	2	0
52	H	703	3PE	1	0
45	B	203	PC1	1	0

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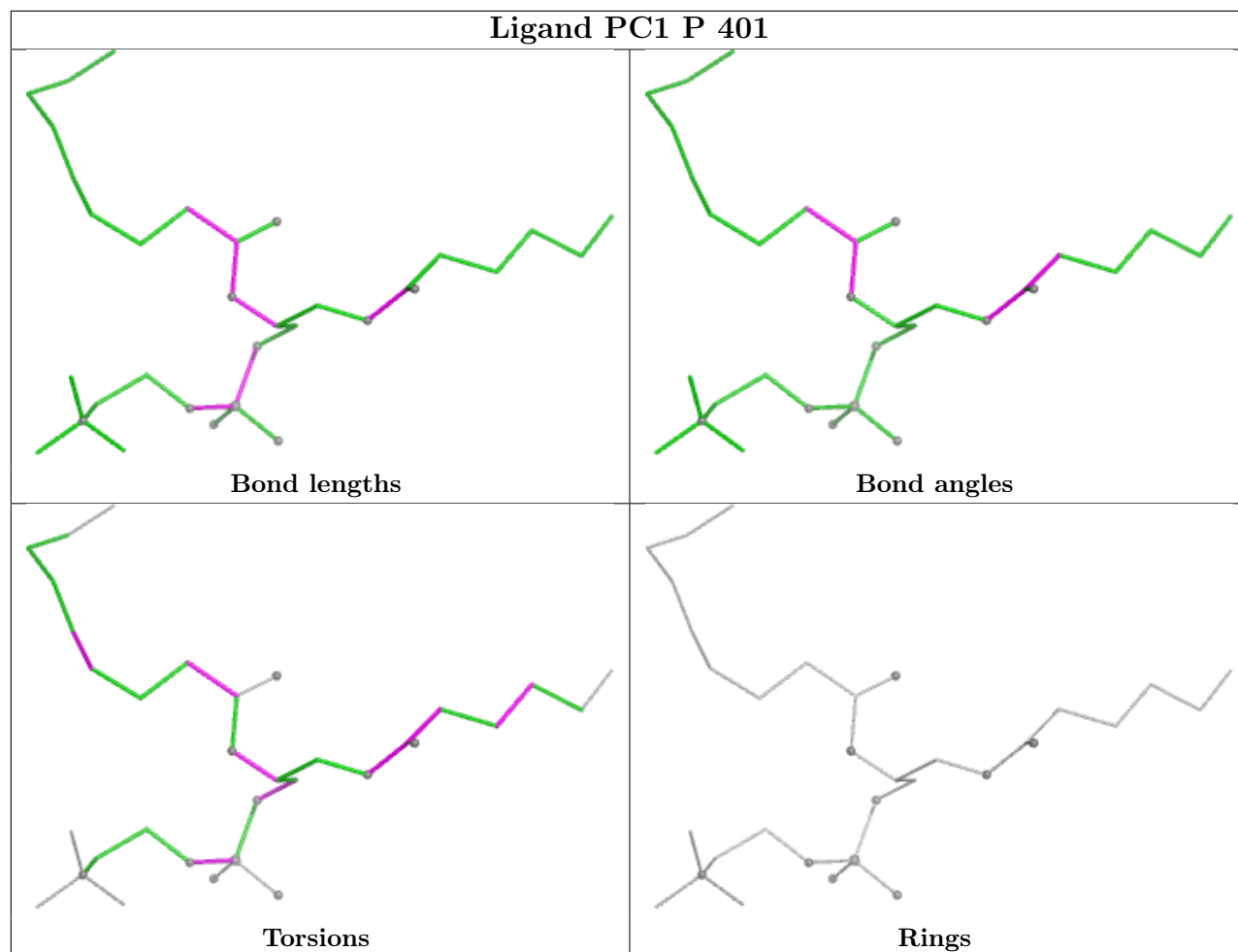
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	H	702	3PE	2	0
45	B	202	PC1	1	0
54	O	401	DGT	2	0
52	L	701	3PE	2	0
52	m	201	3PE	1	0
58	T	101	EHZ	3	0
53	X	201	CDL	1	0
49	F	503	NAI	3	0
53	d	201	CDL	2	0
52	Y	802	3PE	2	0
52	Y	803	3PE	2	0
45	I	203	PC1	1	0
59	i	201	CHD	1	0
45	A	202	PC1	2	0
53	q	202	CDL	2	0
53	M	502	CDL	2	0
45	M	503	PC1	1	0
51	H	701	U10	15	0
52	N	403	3PE	1	0
45	q	201	PC1	1	0
52	P	404	3PE	5	0
45	N	404	PC1	5	0

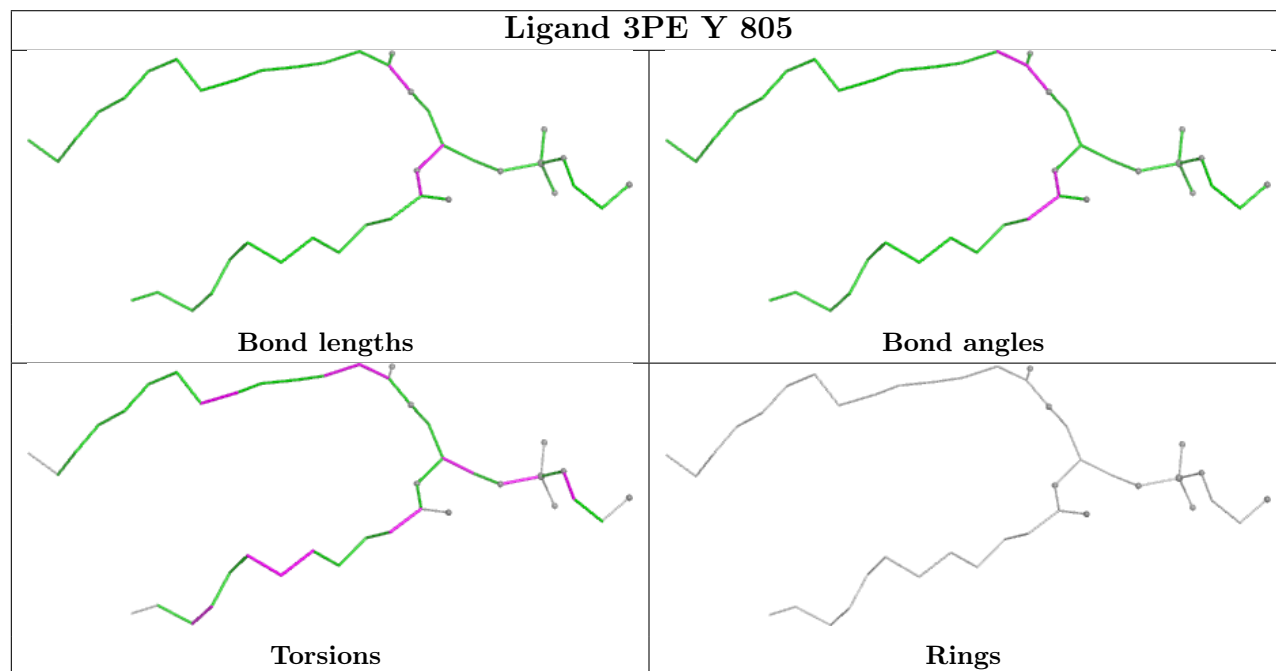
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

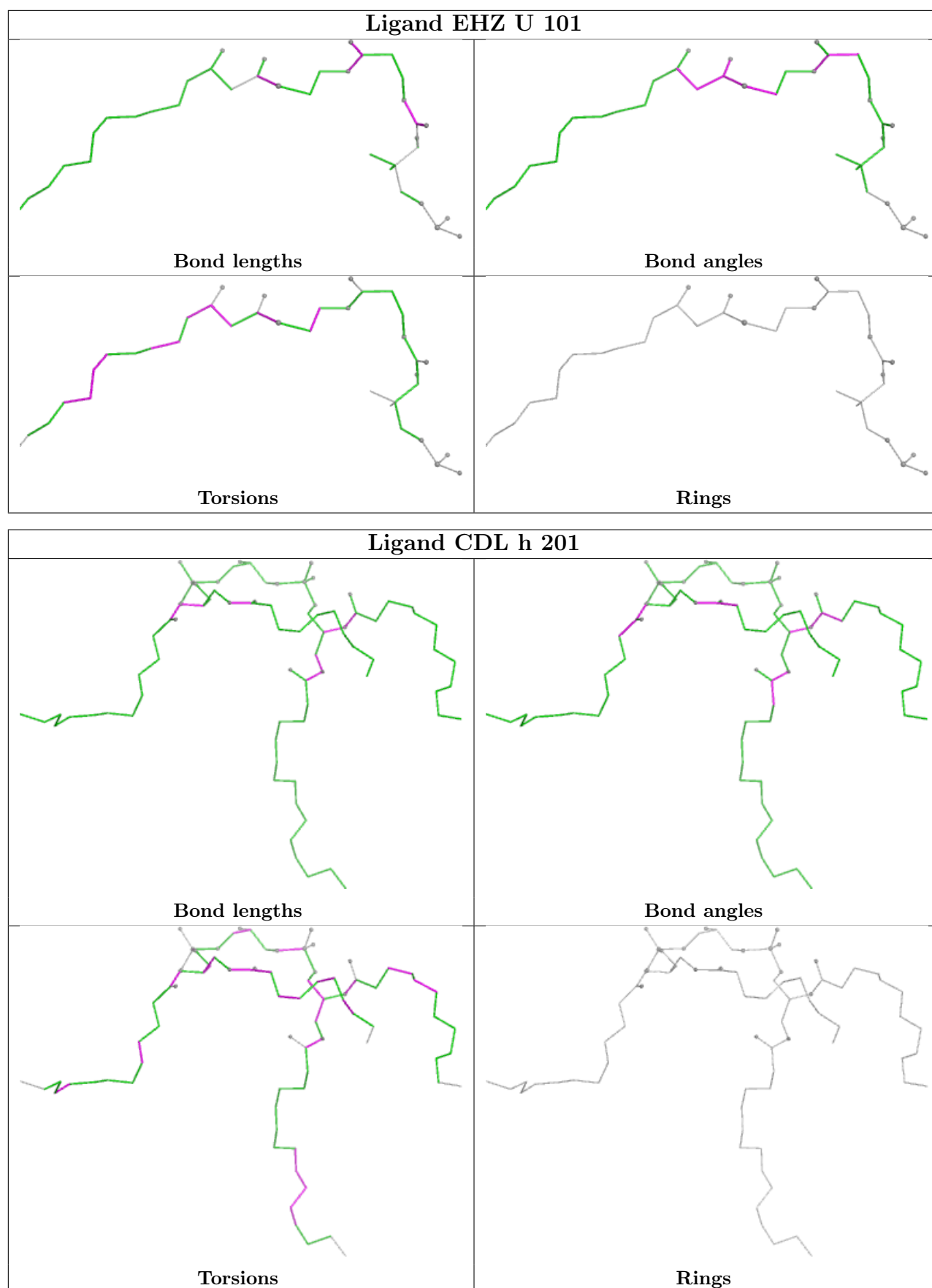


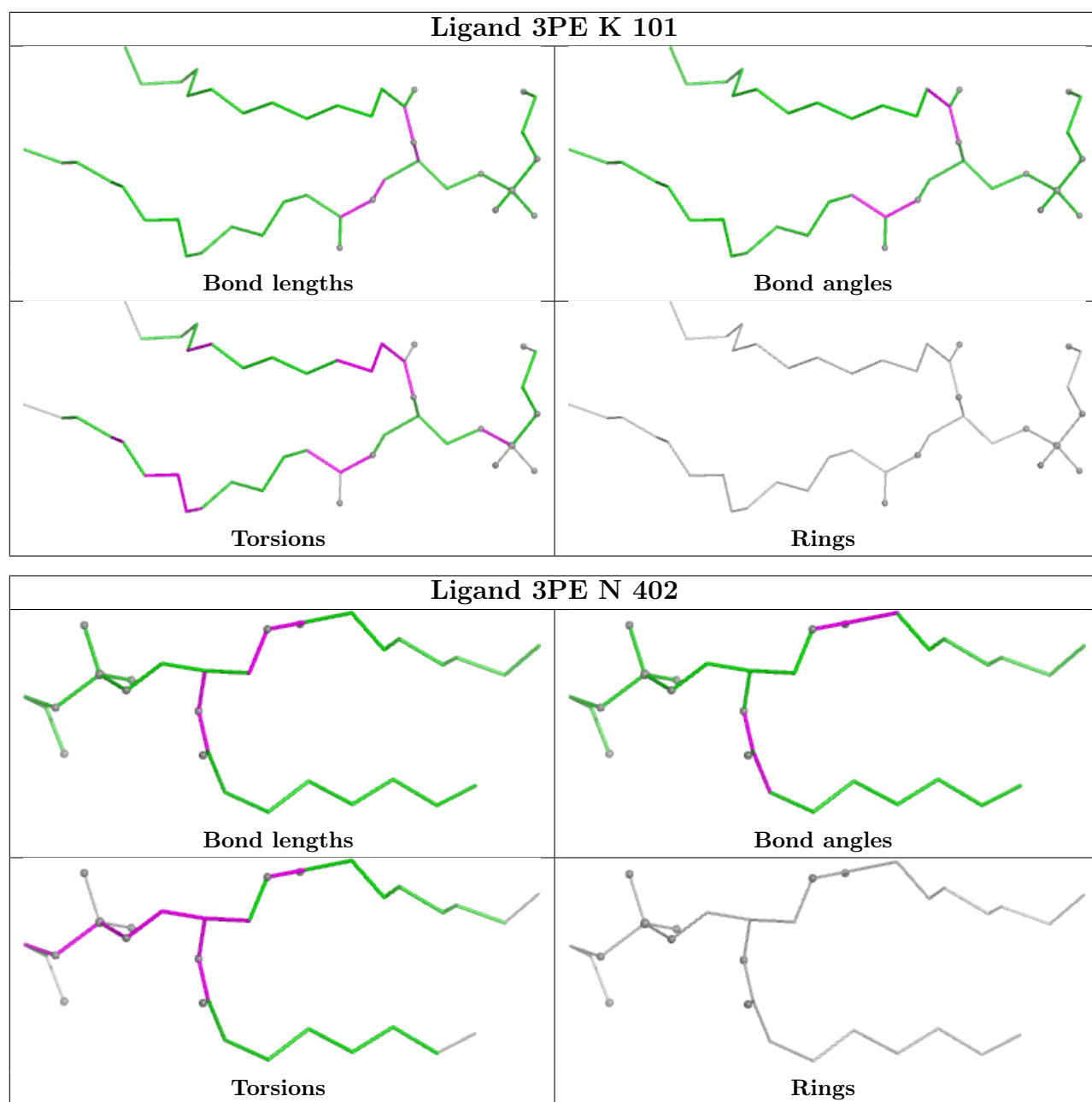
Ligand PC1 P 401

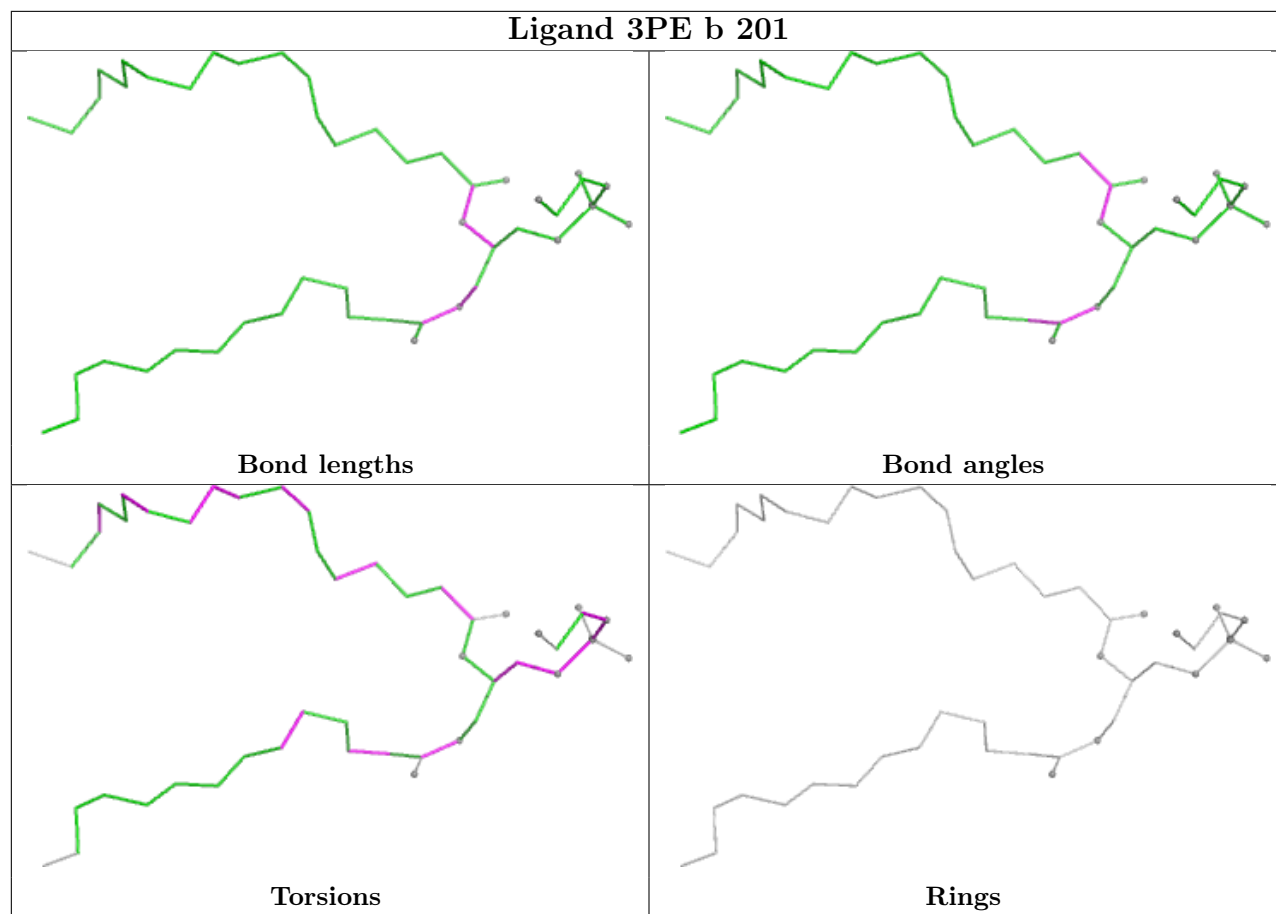


Ligand 3PE Y 805

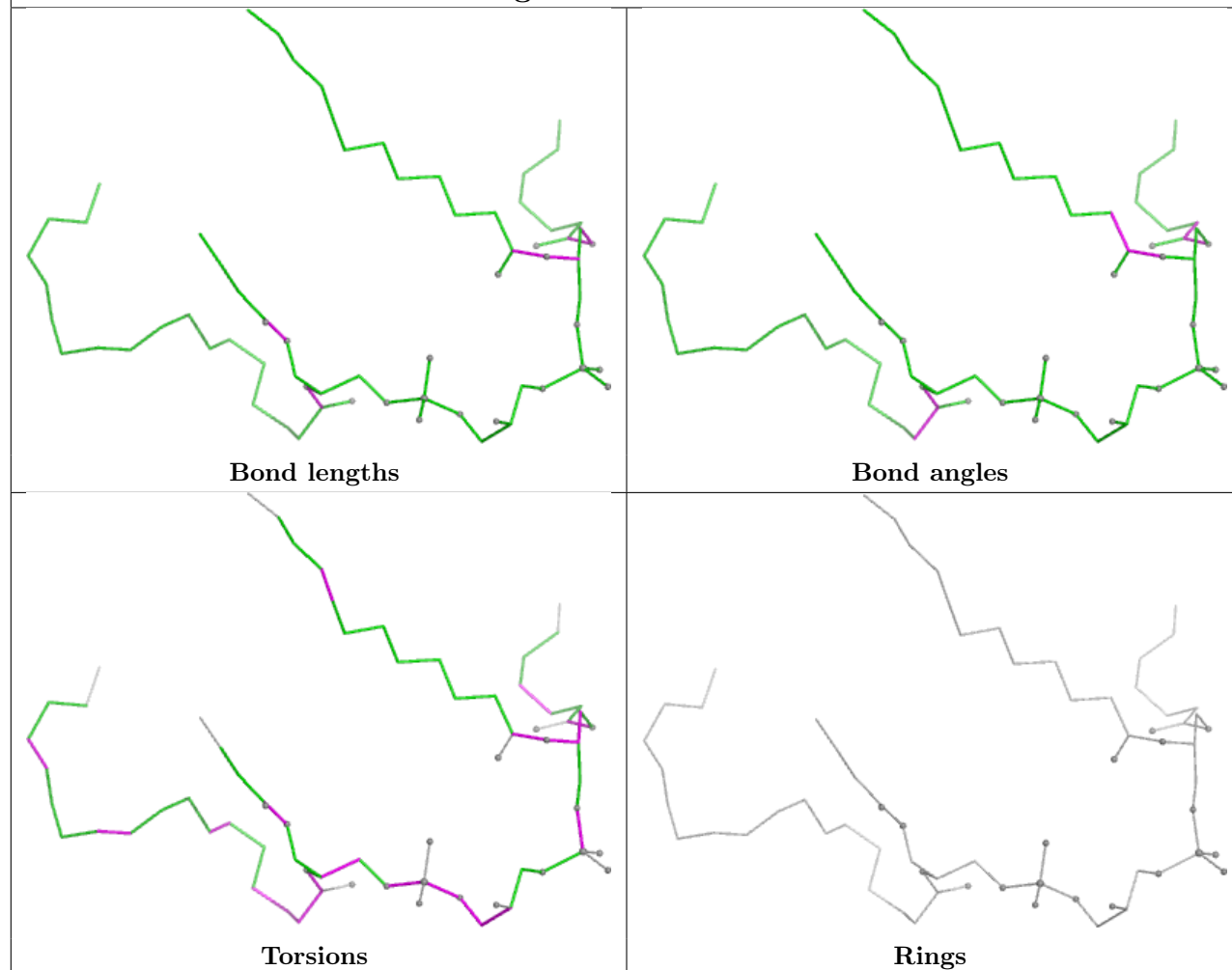




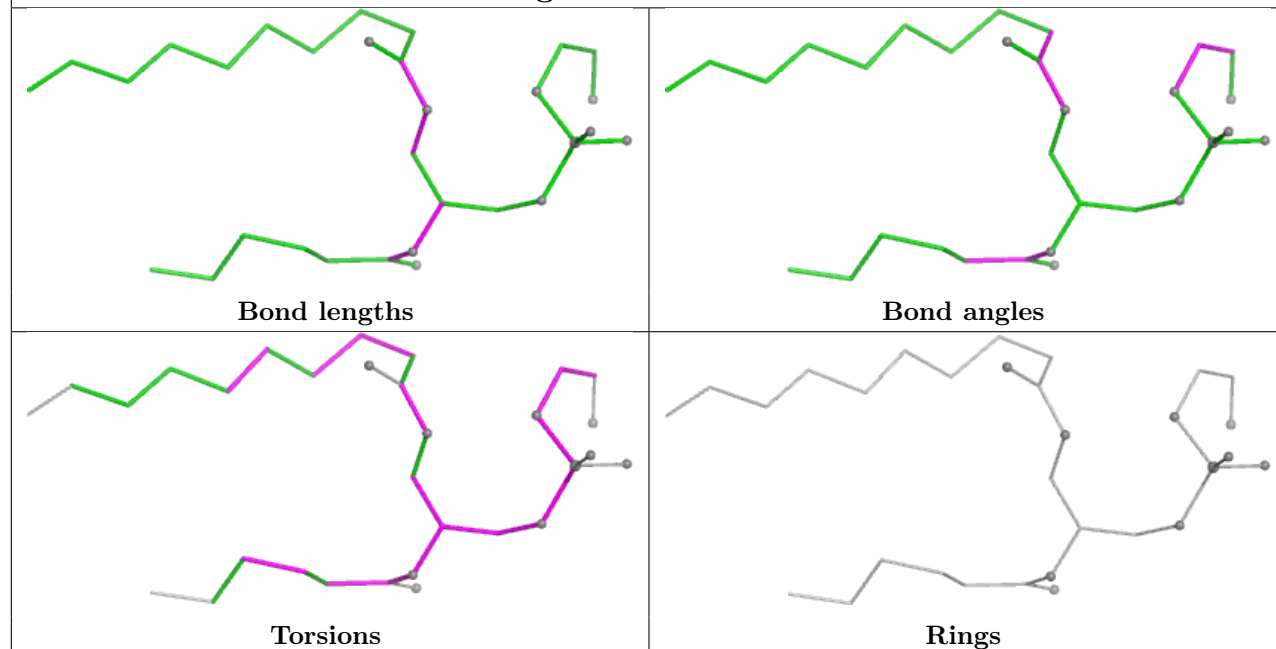


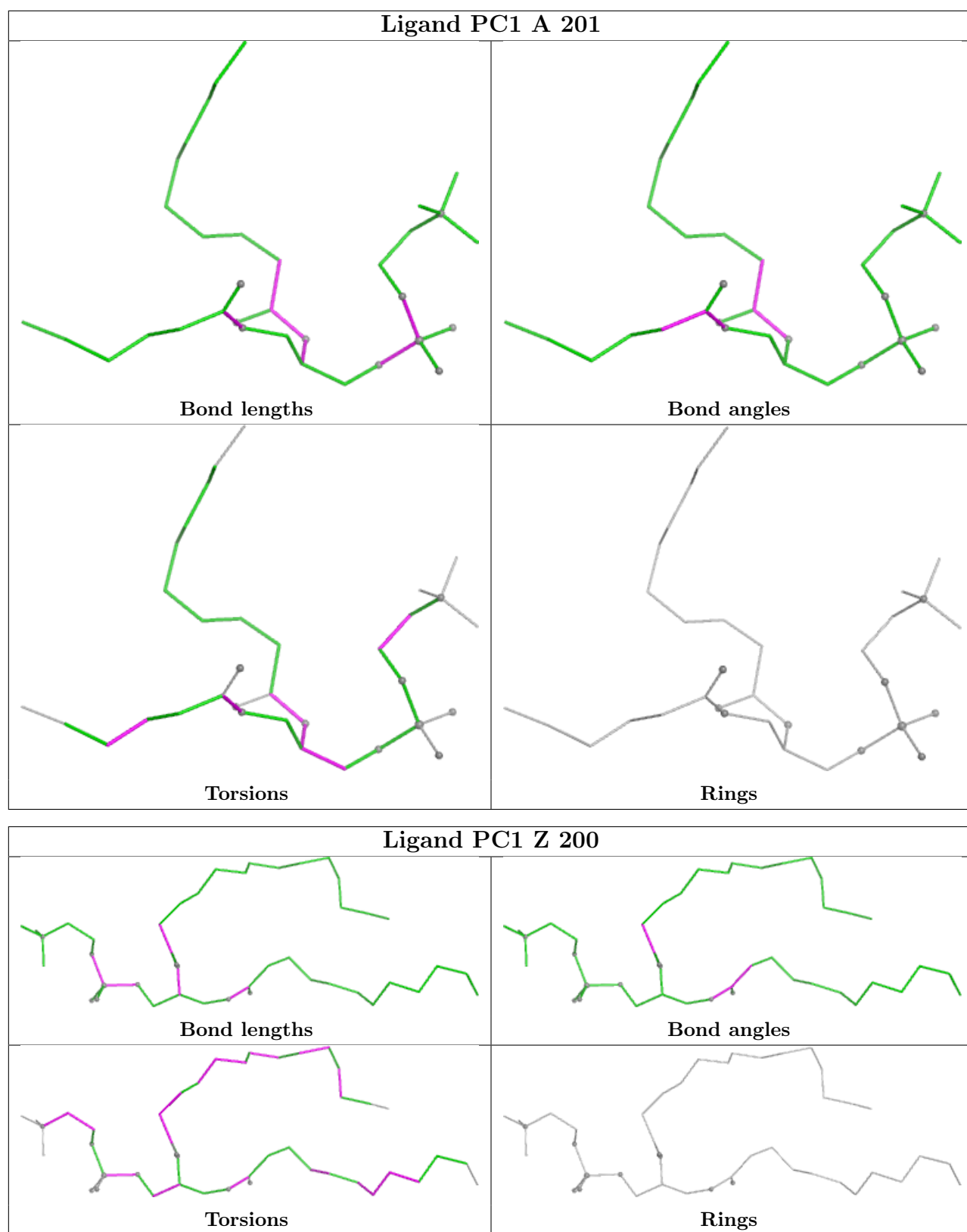


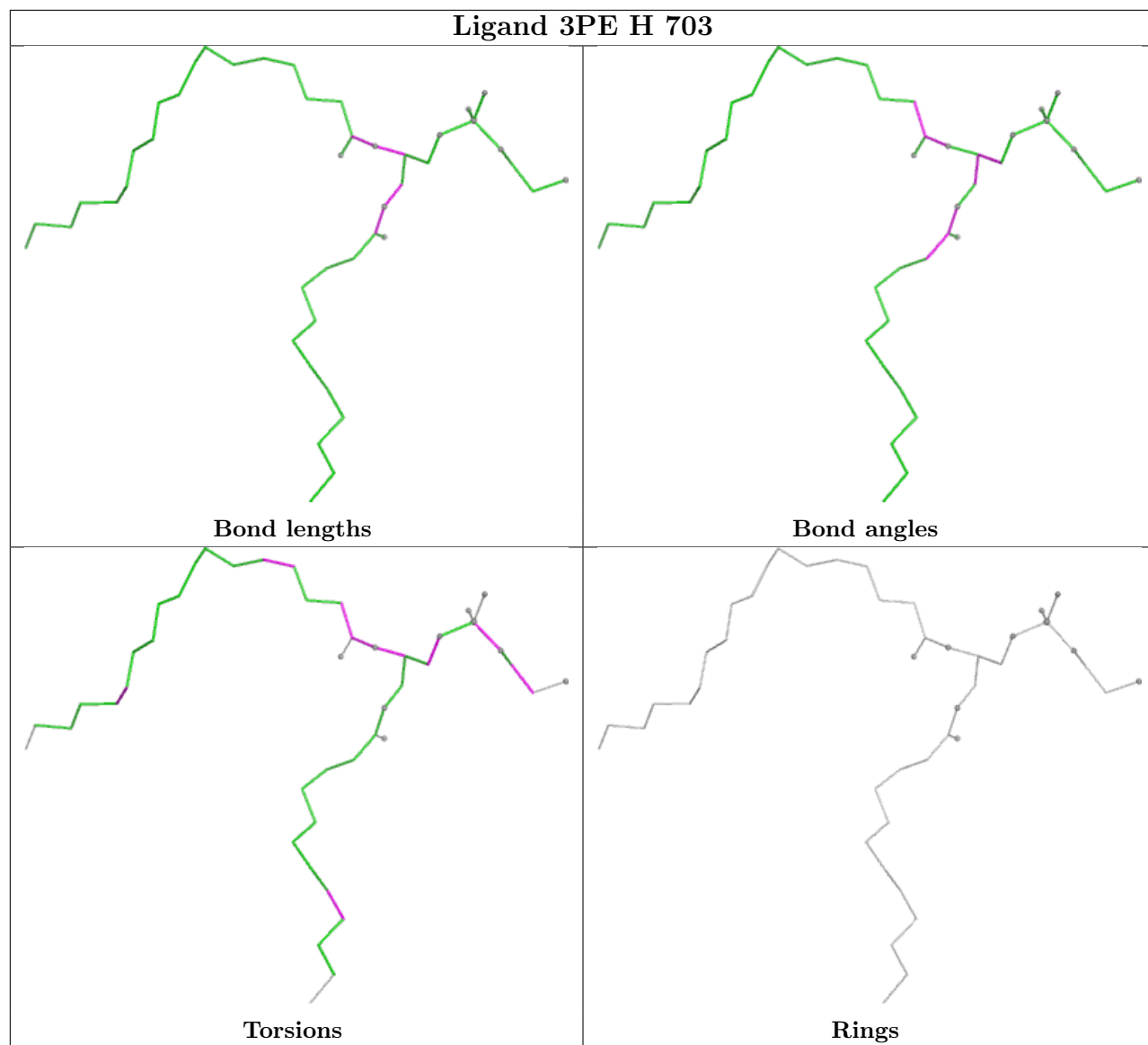
Ligand CDL P 402

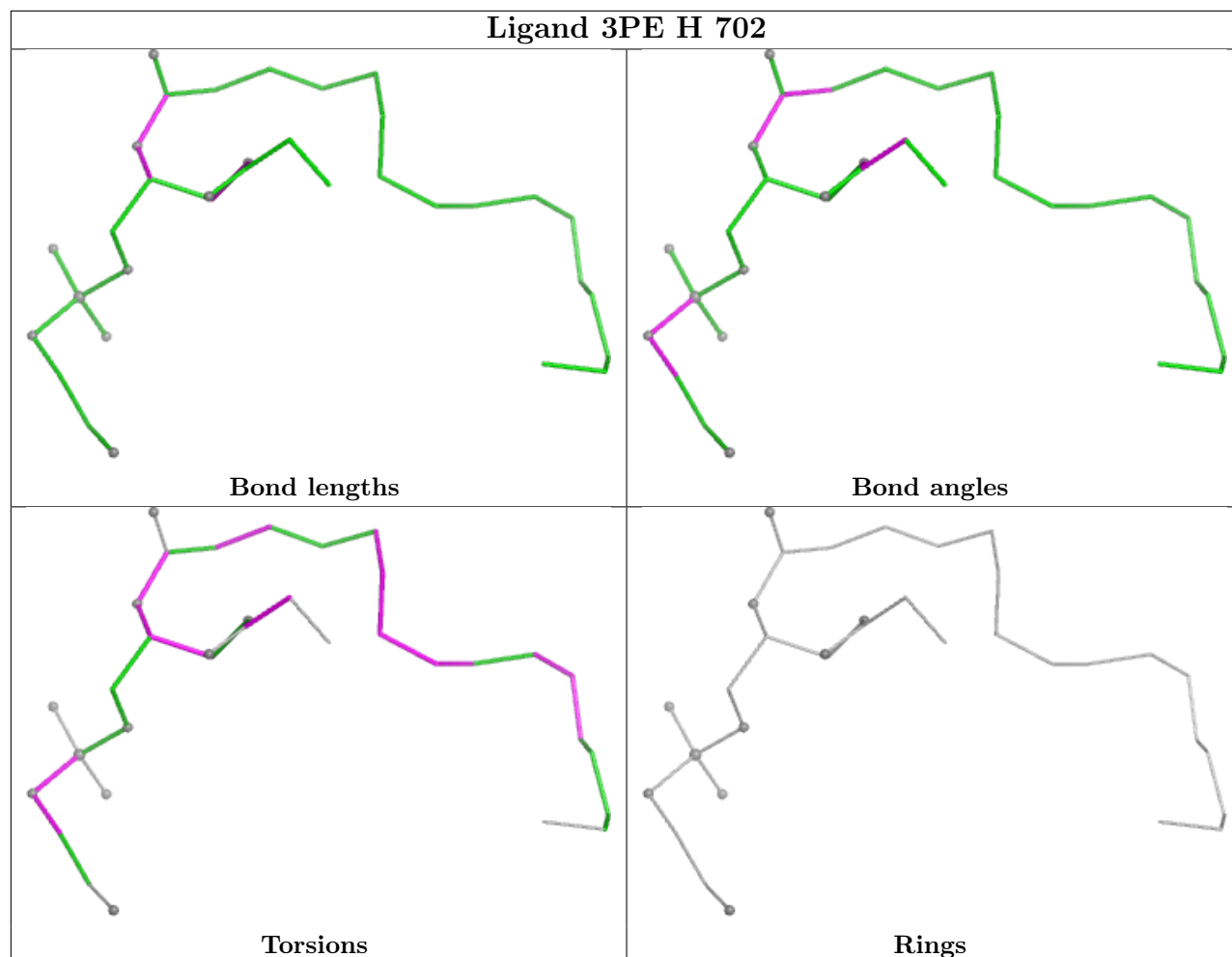
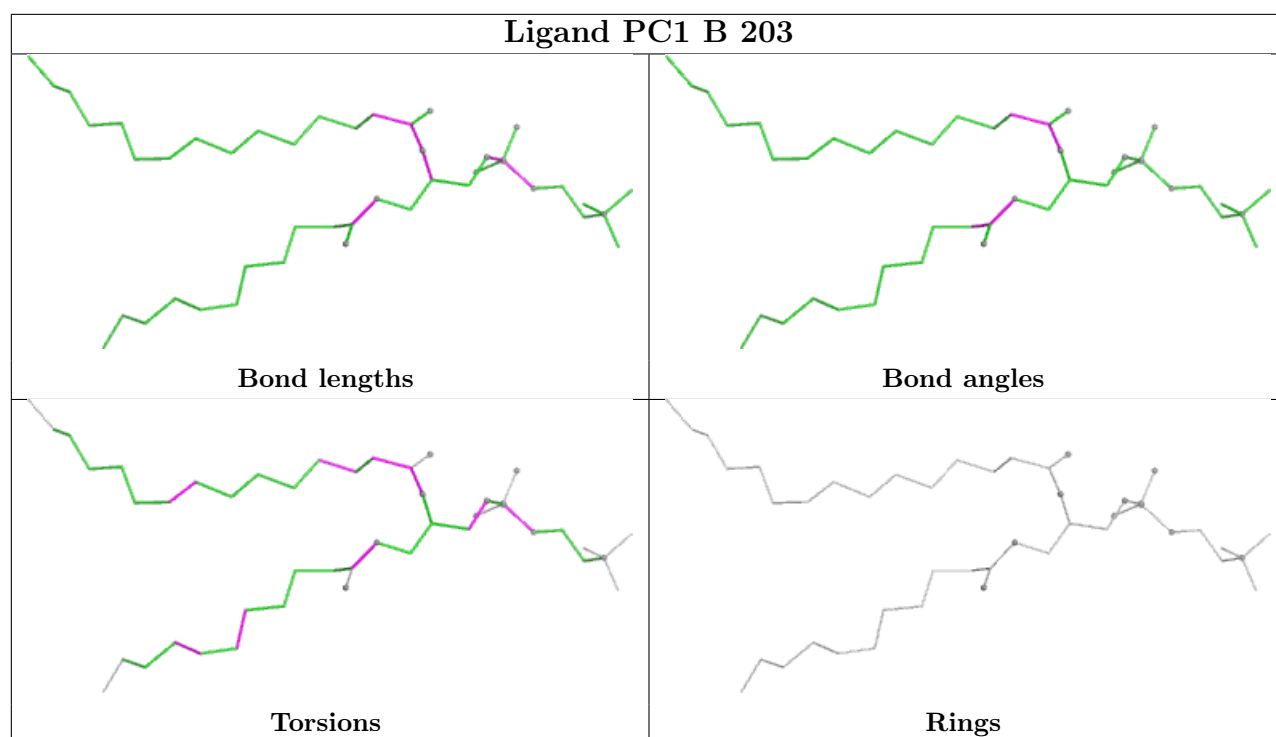


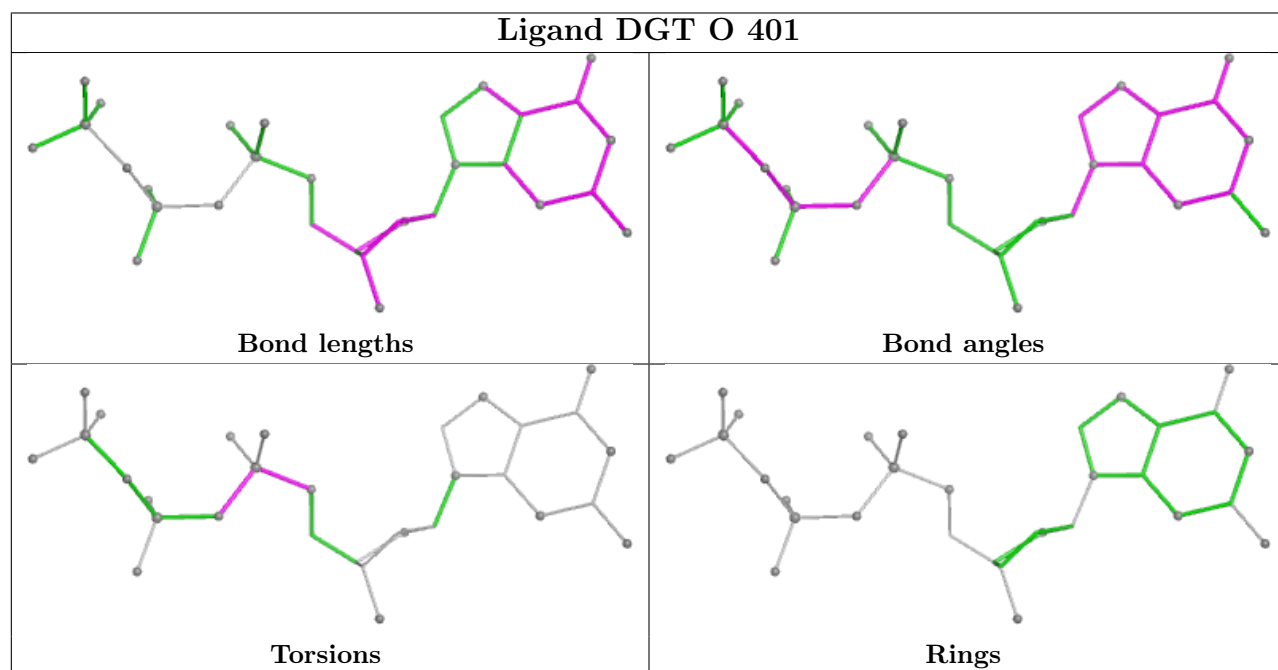
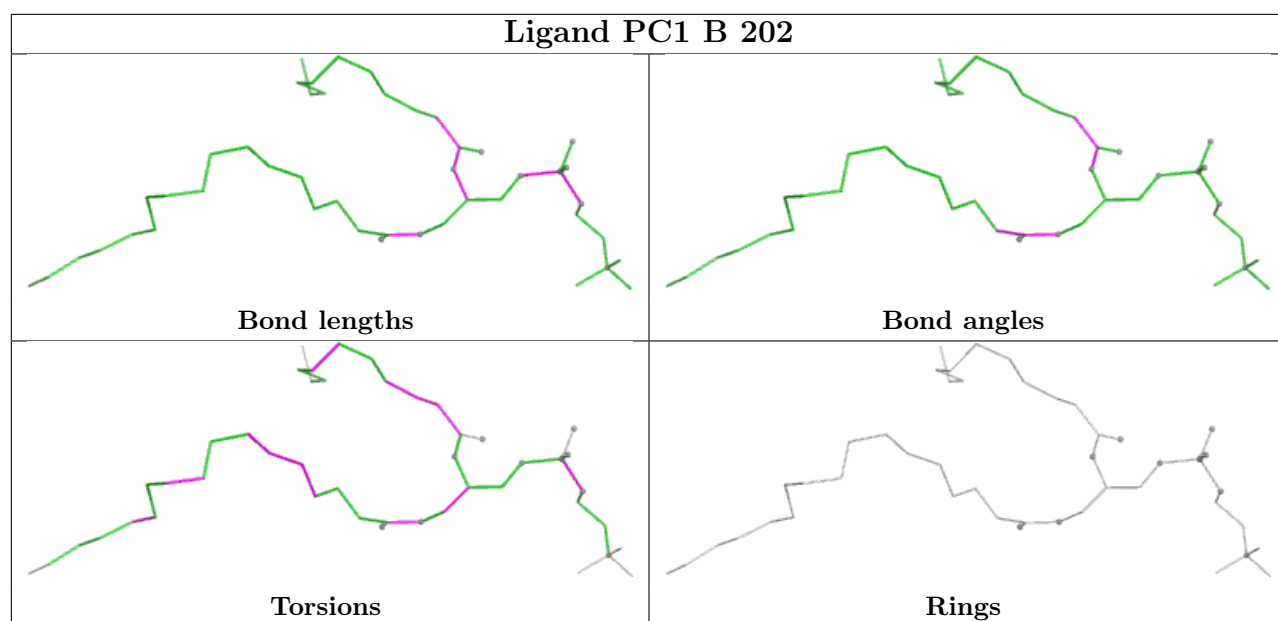
Ligand 3PE Y 801

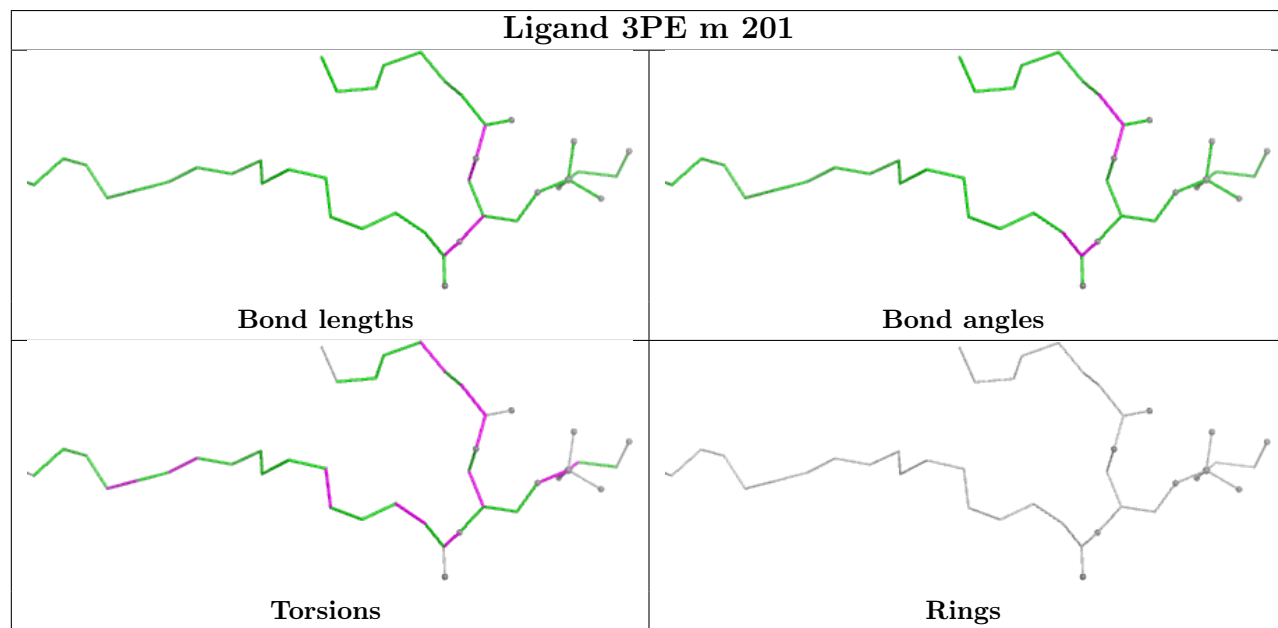
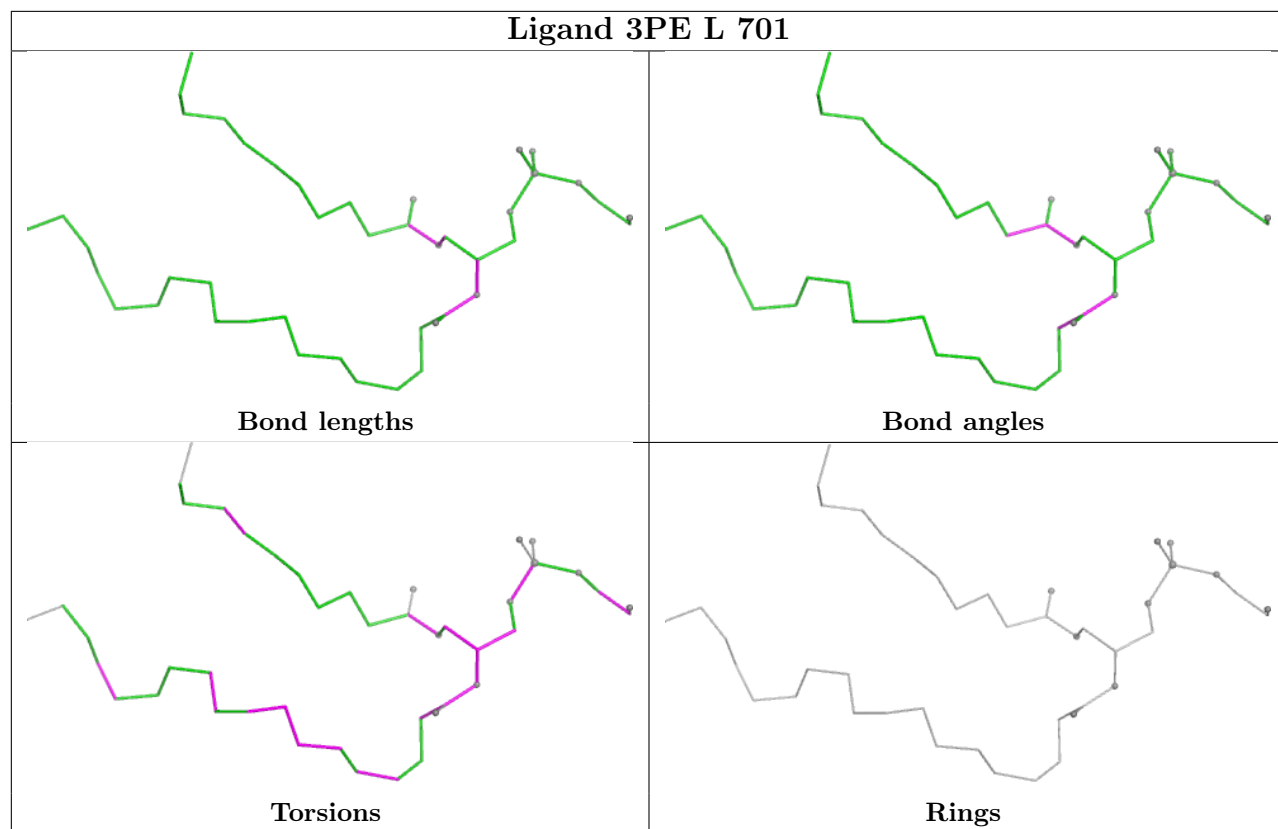


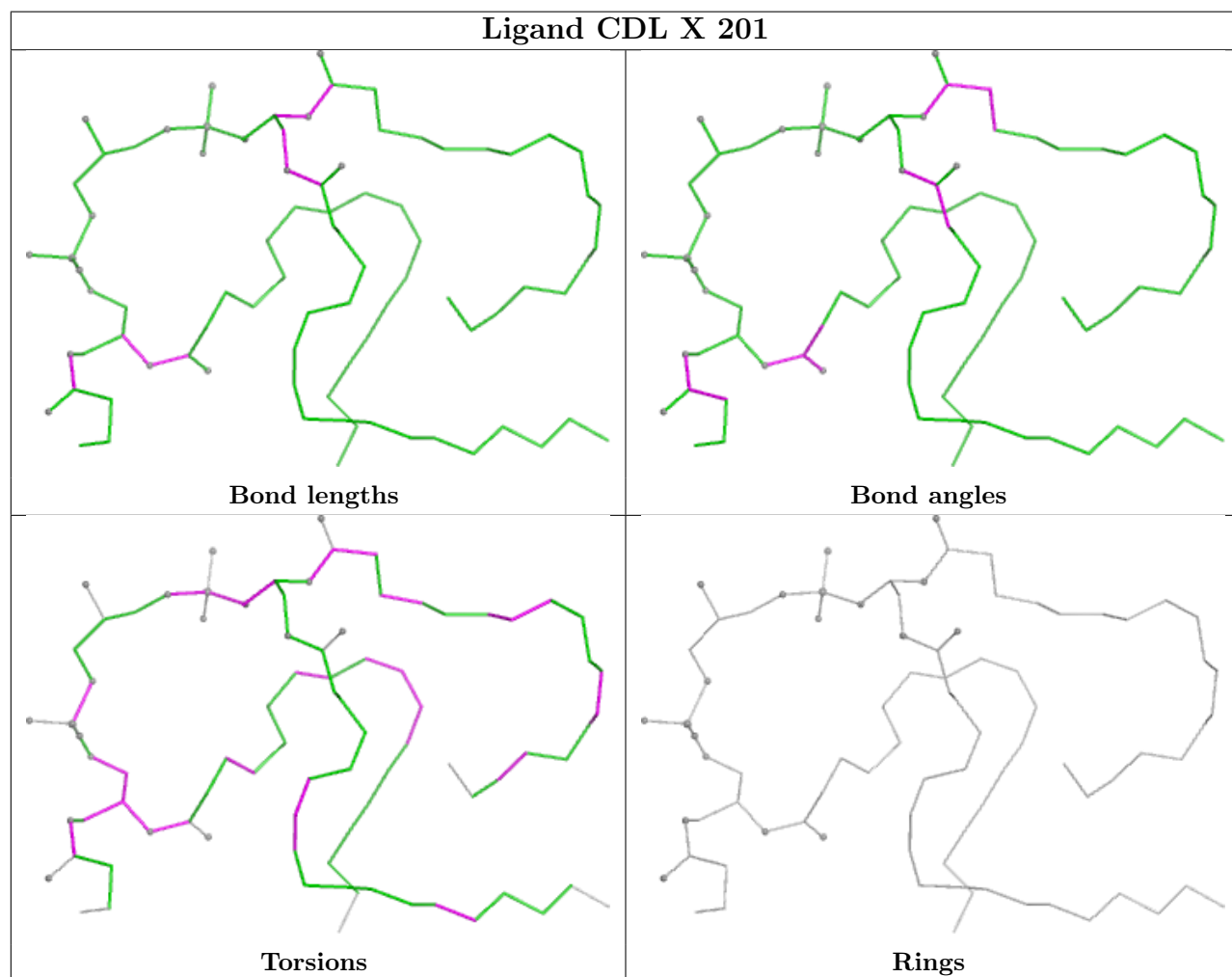
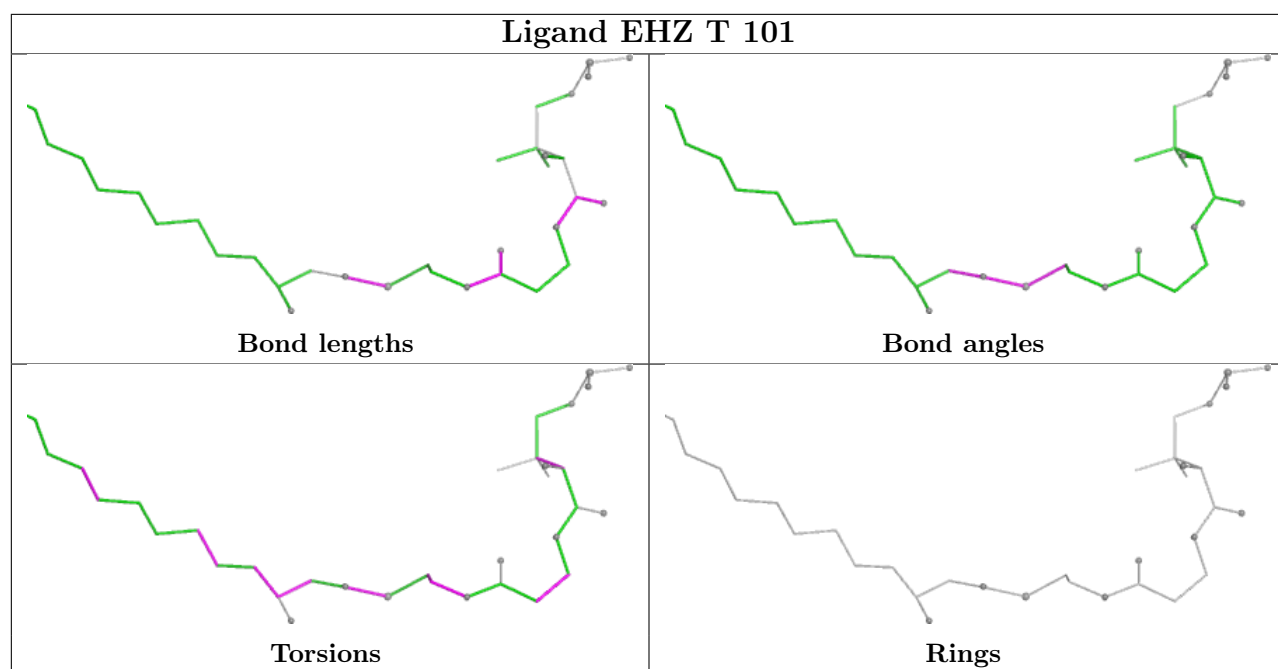


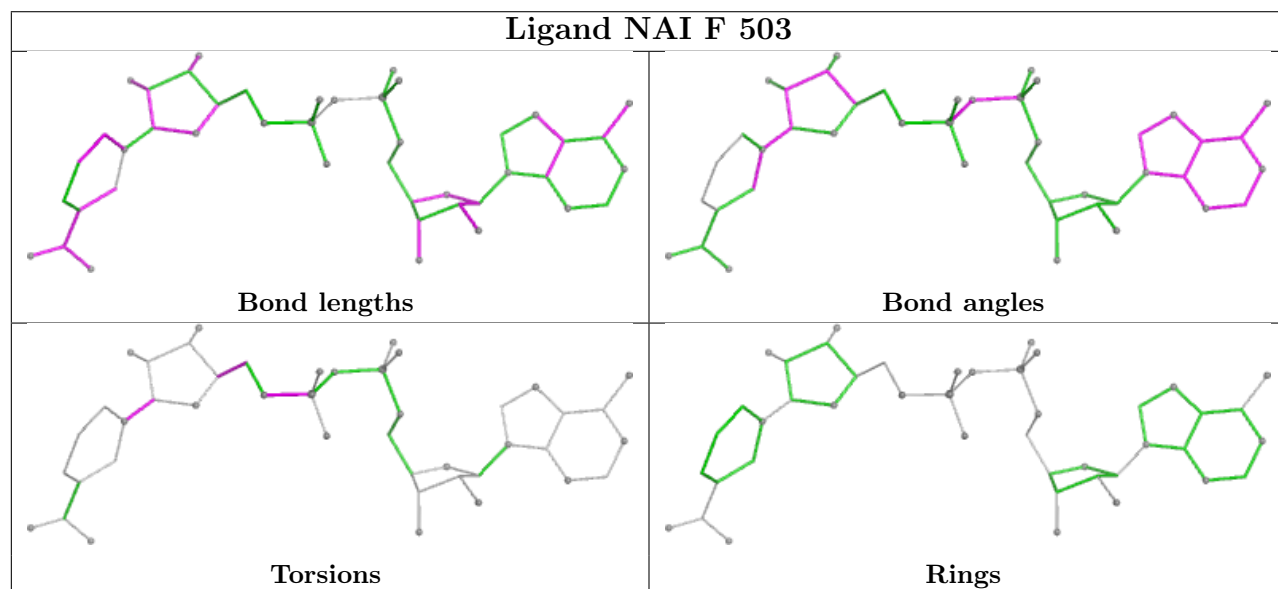
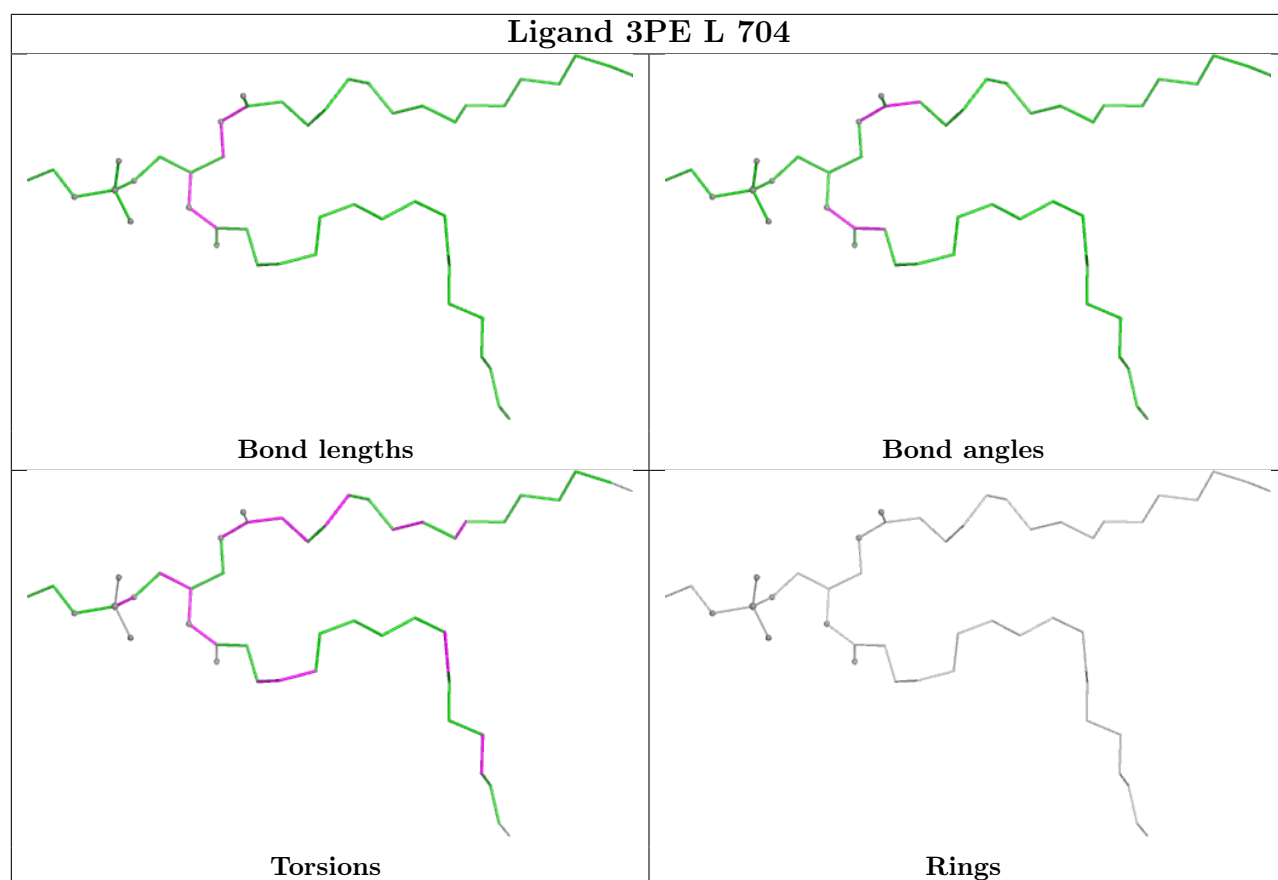


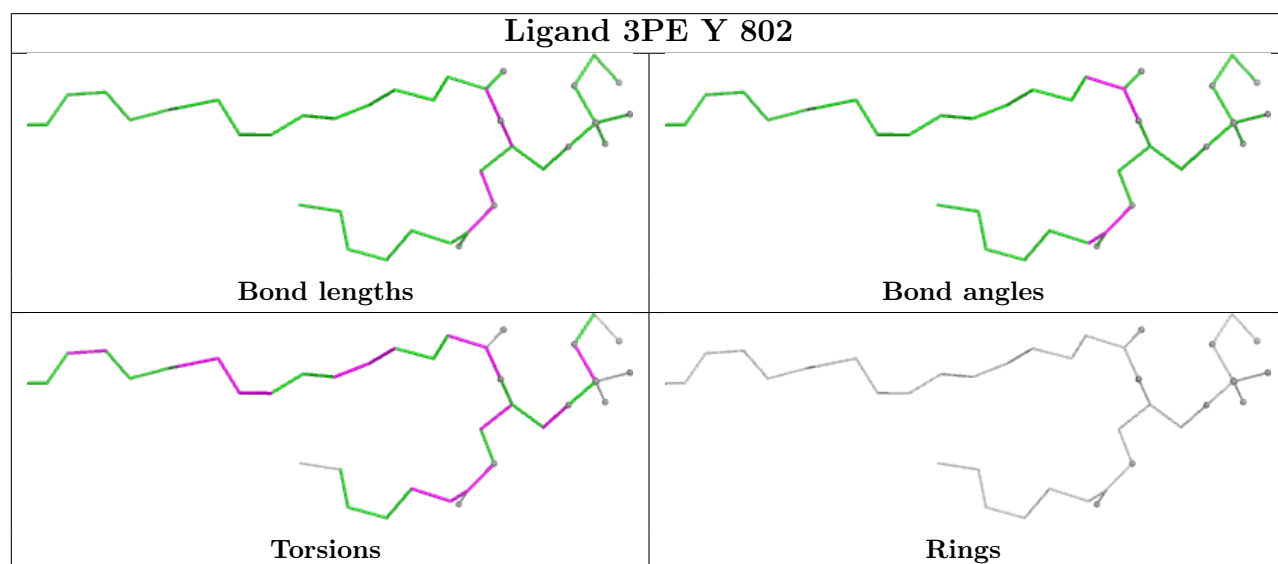
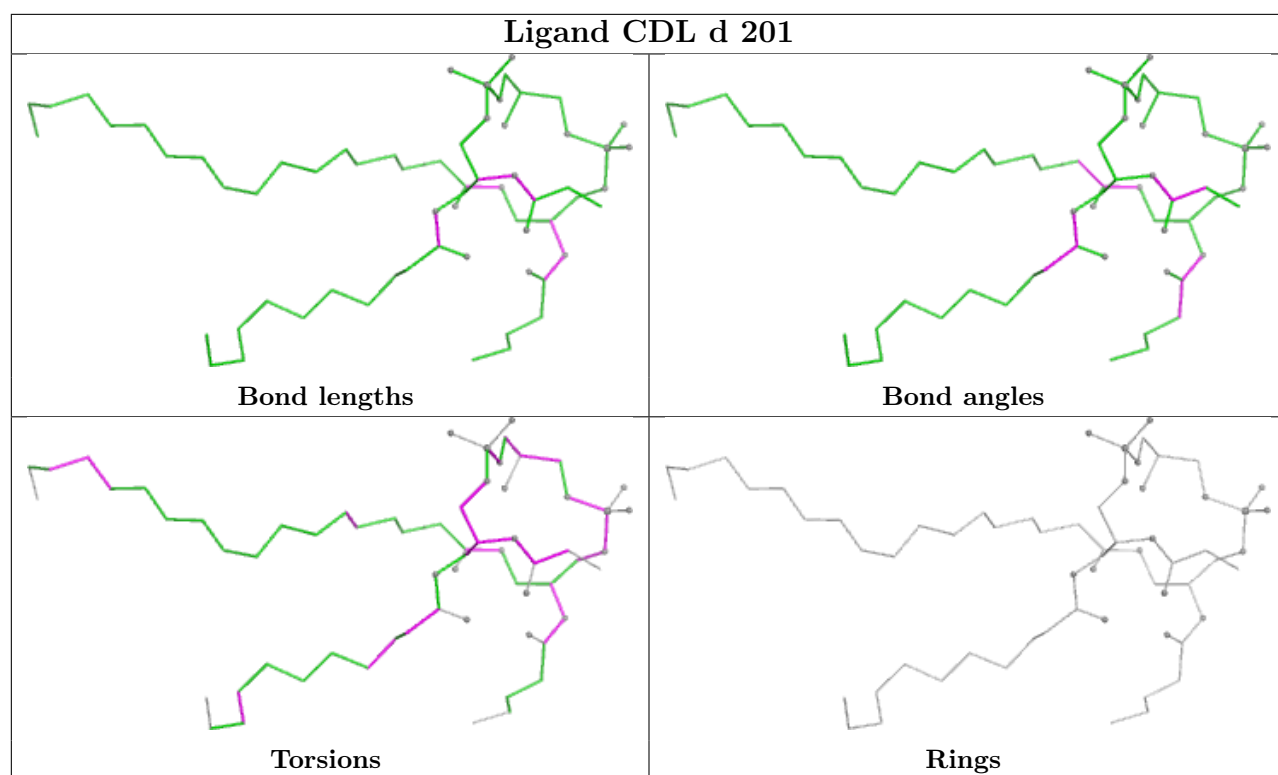


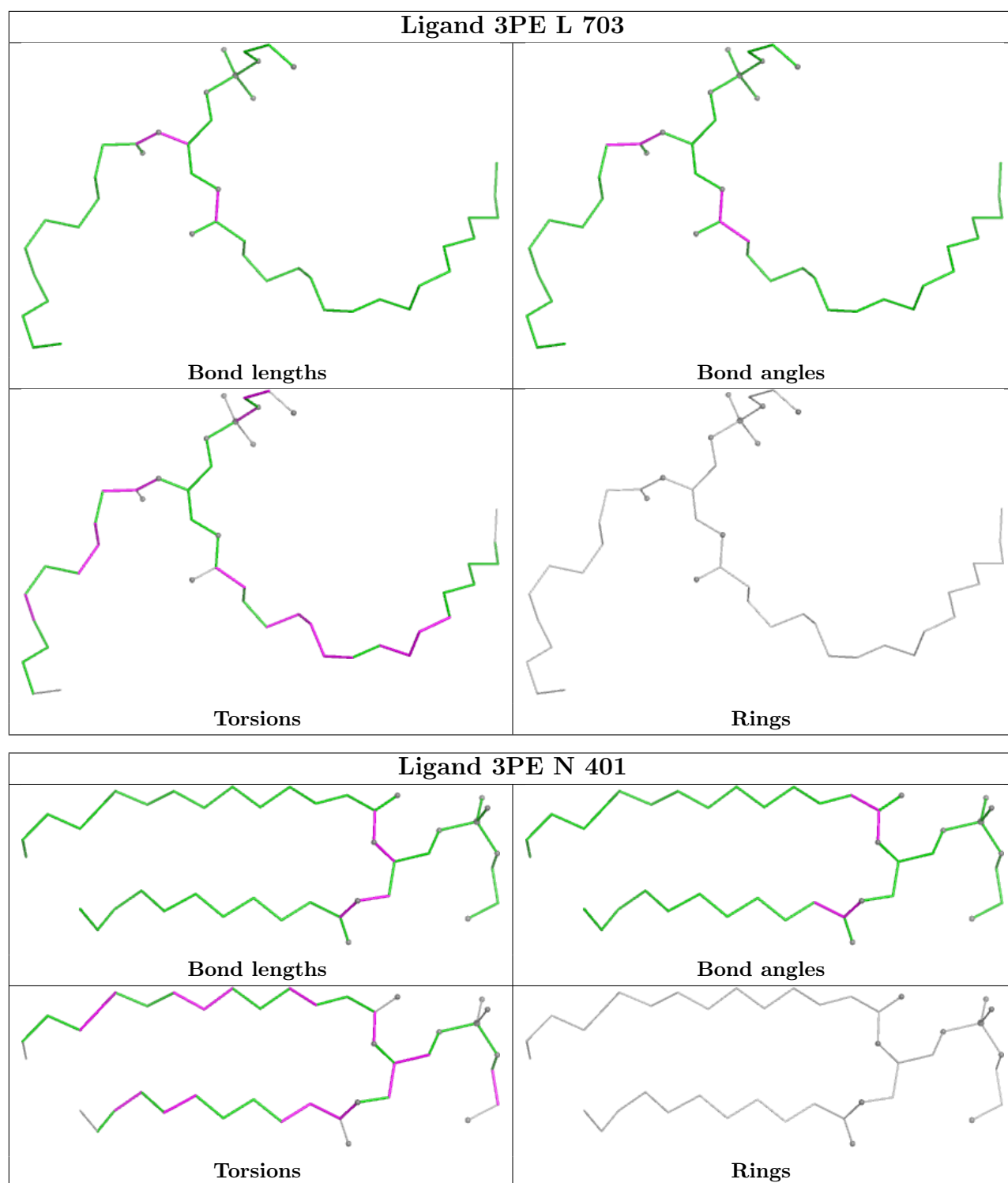


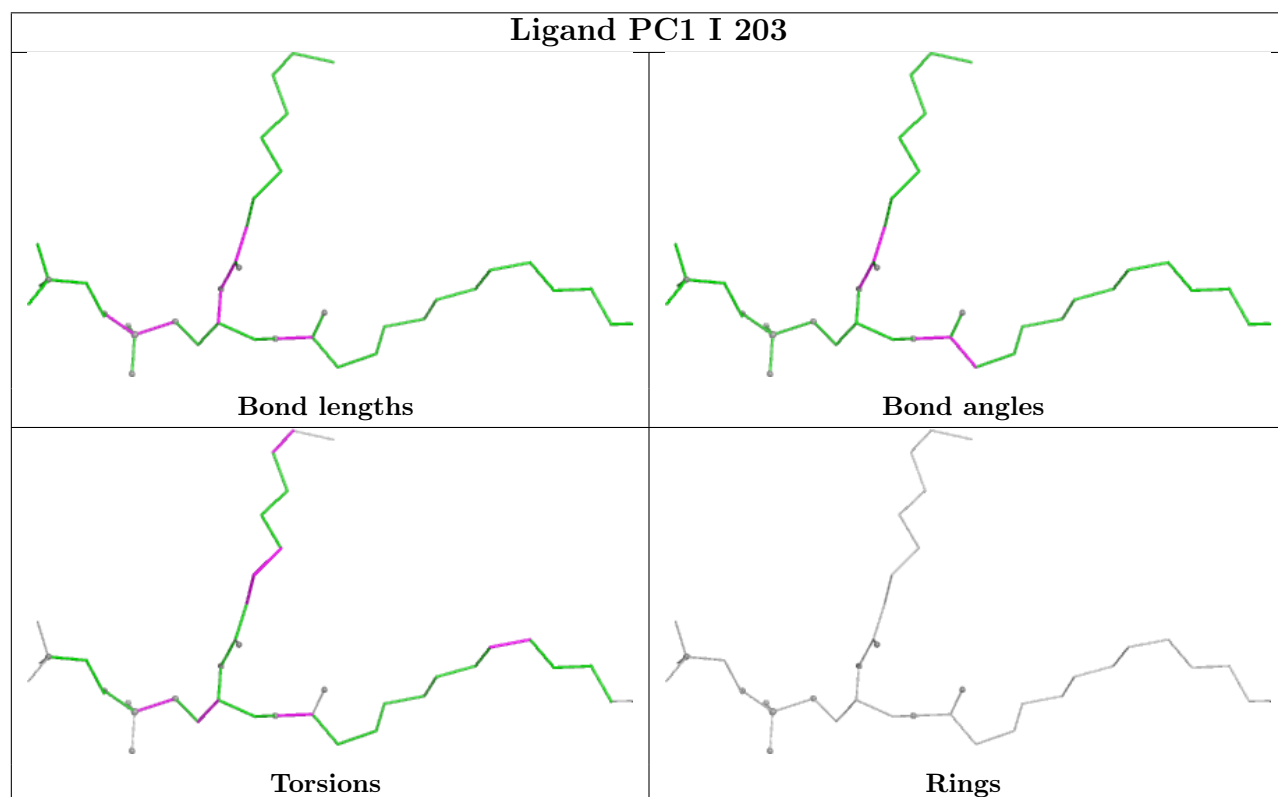
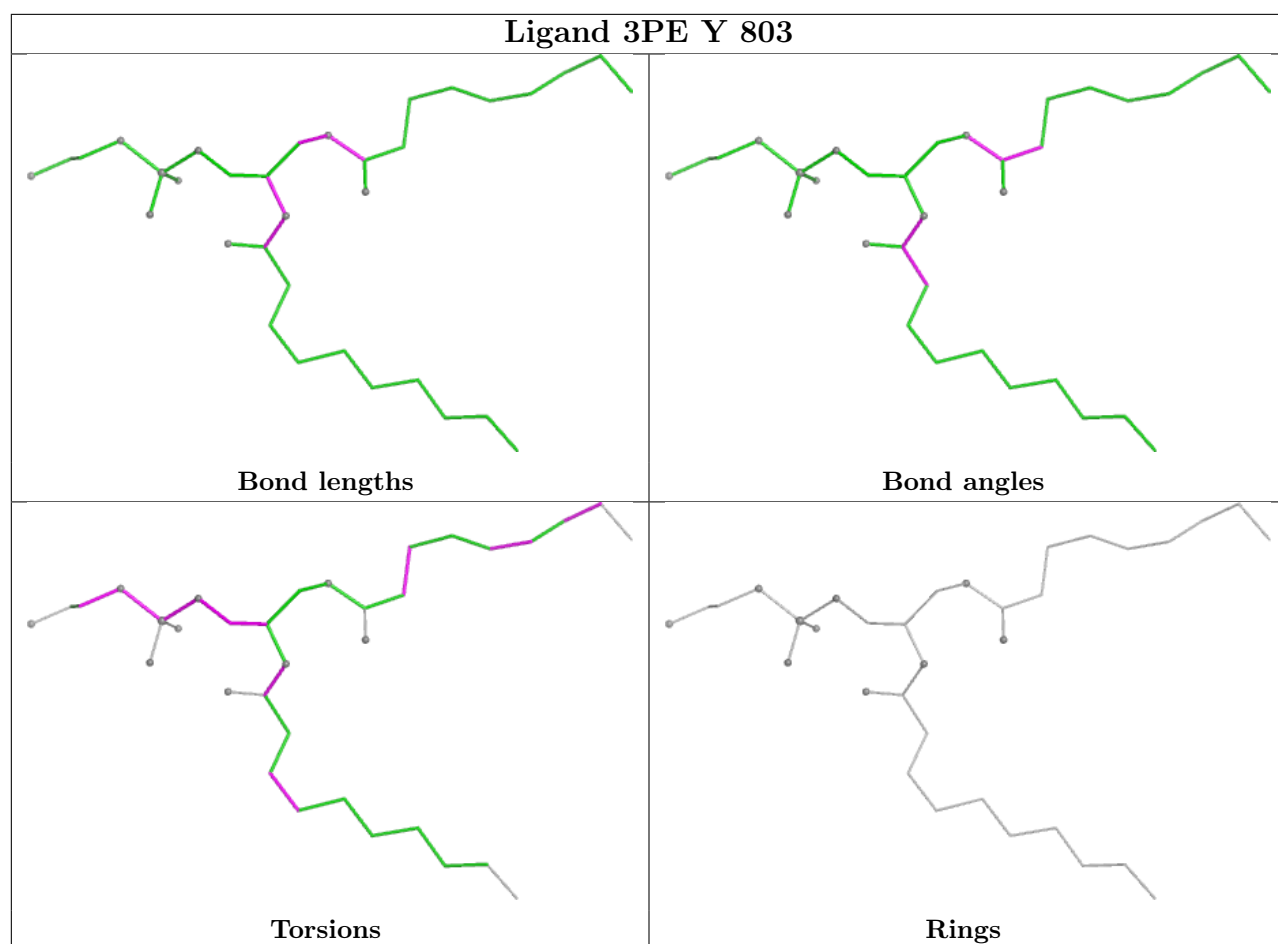


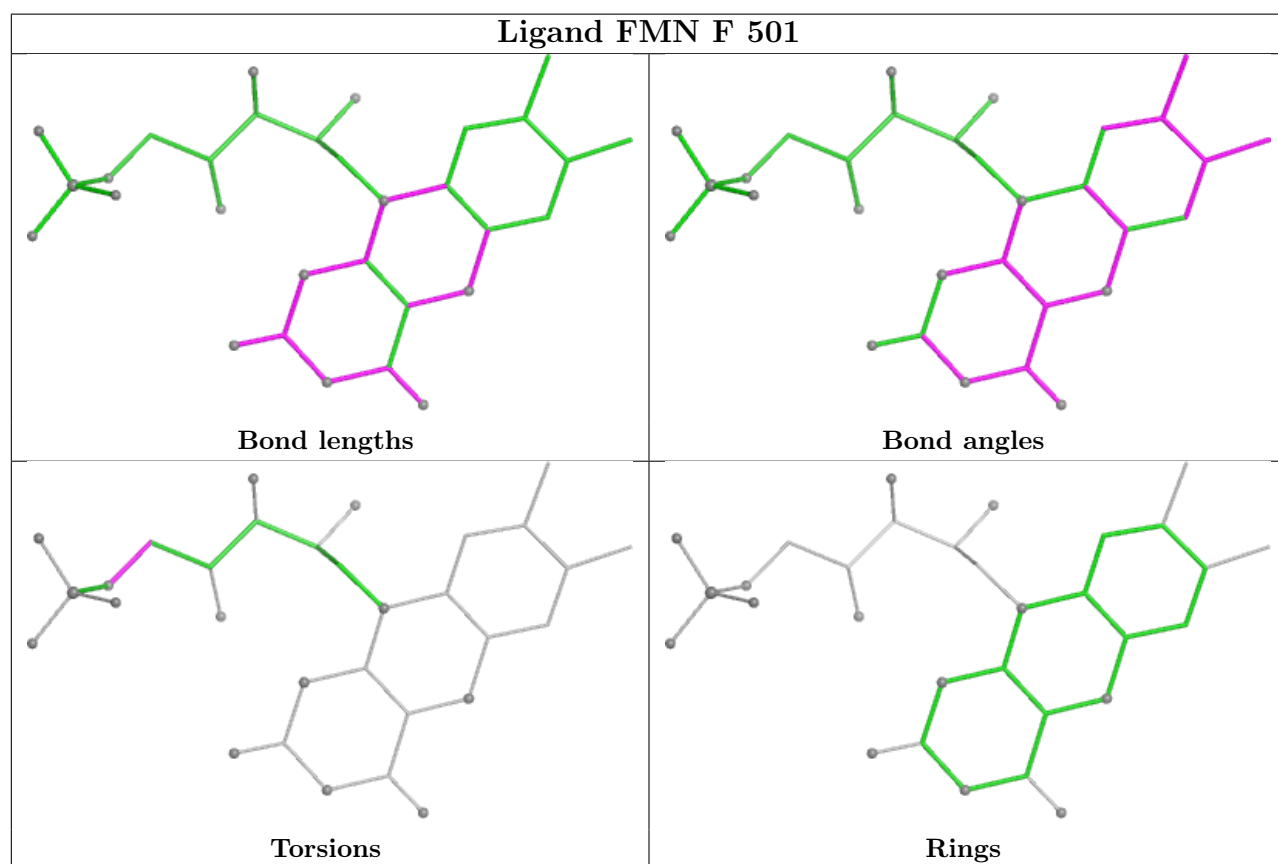
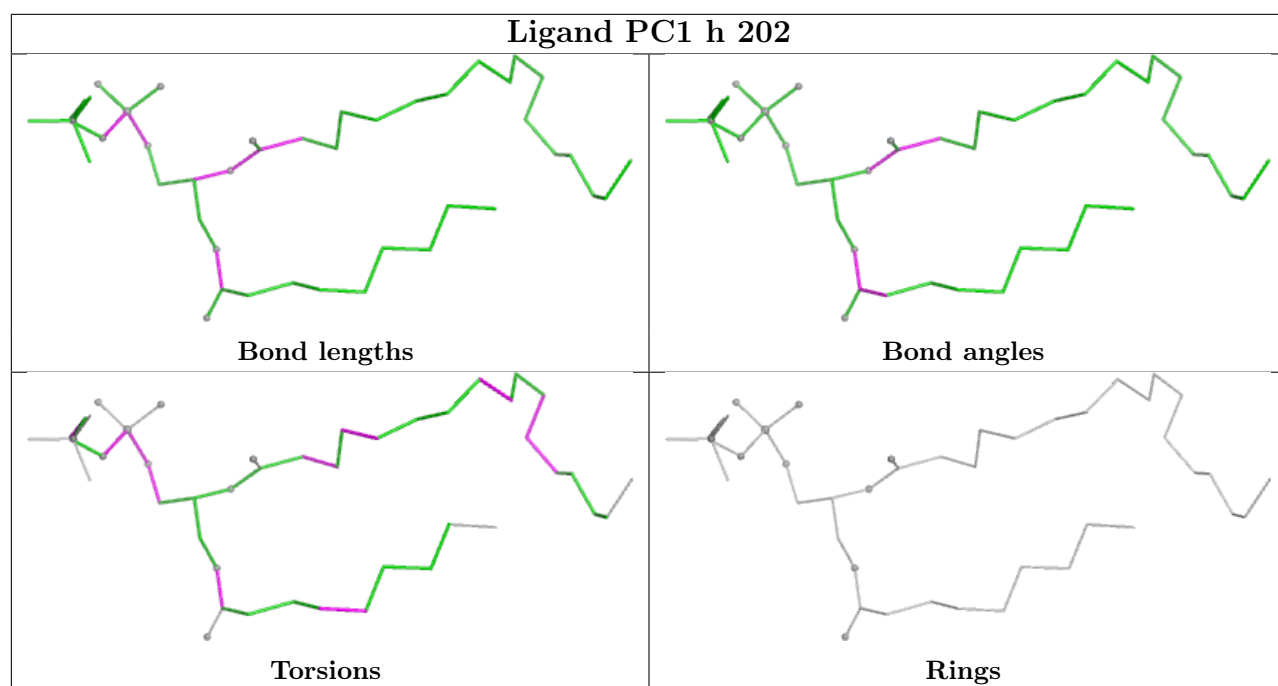




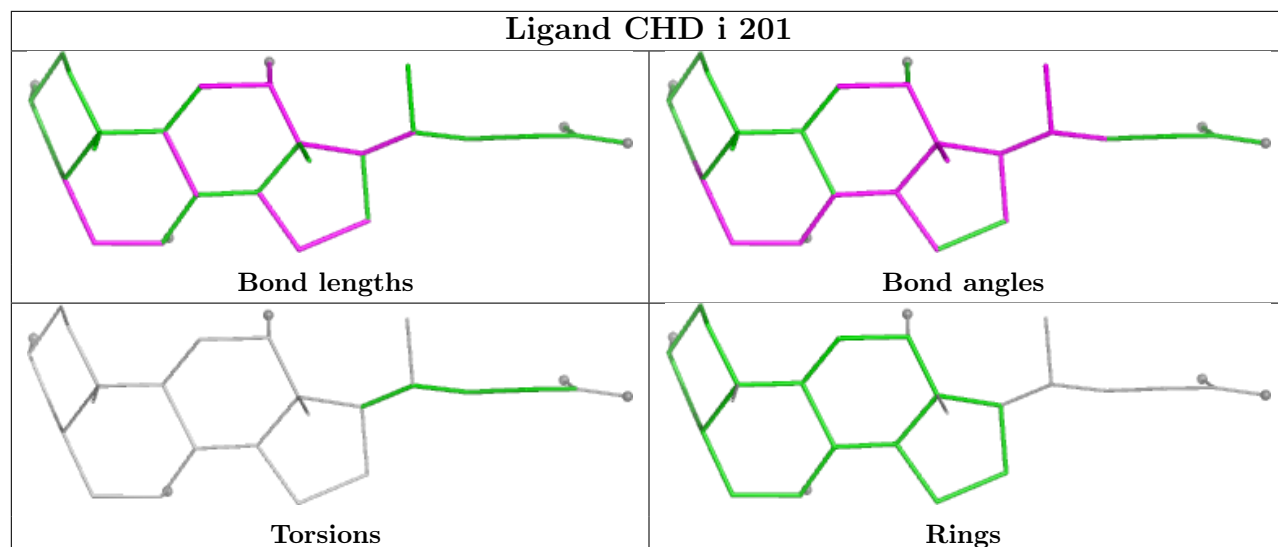




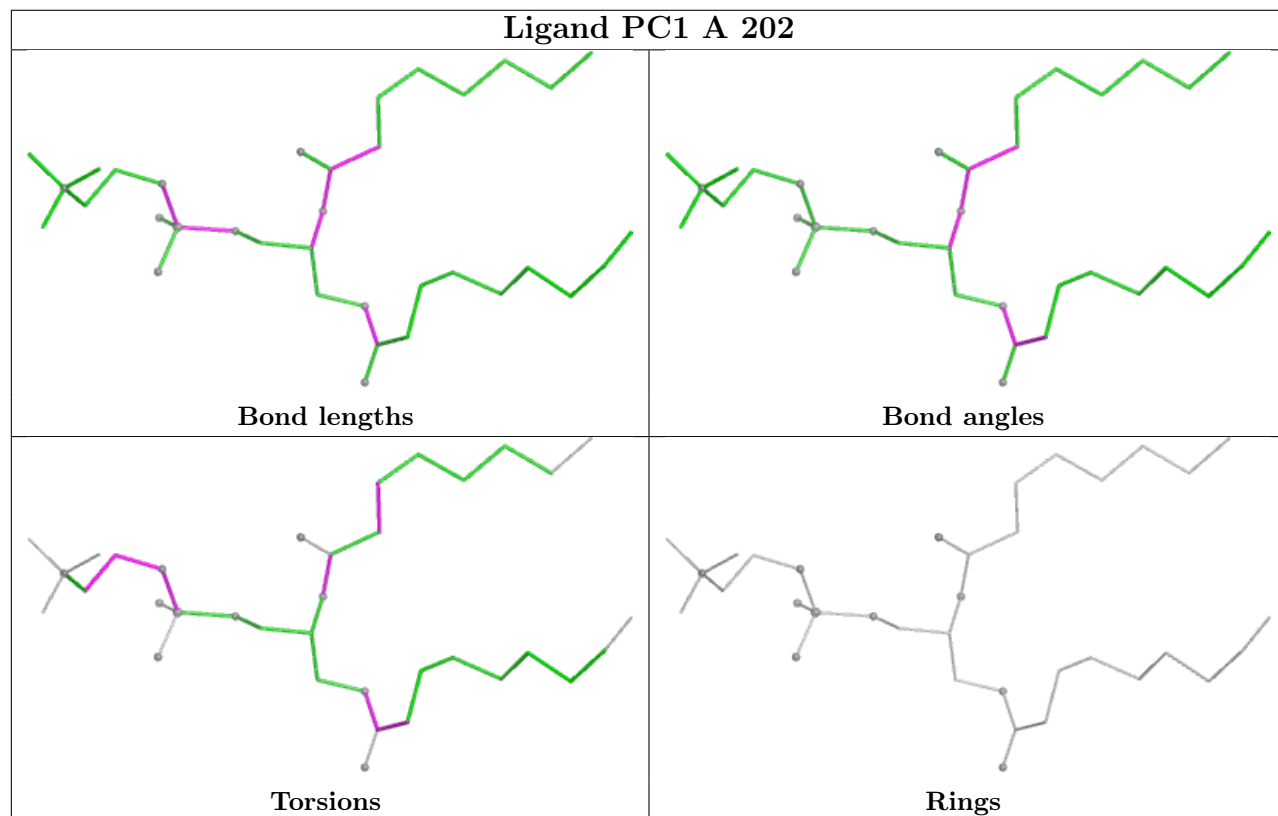


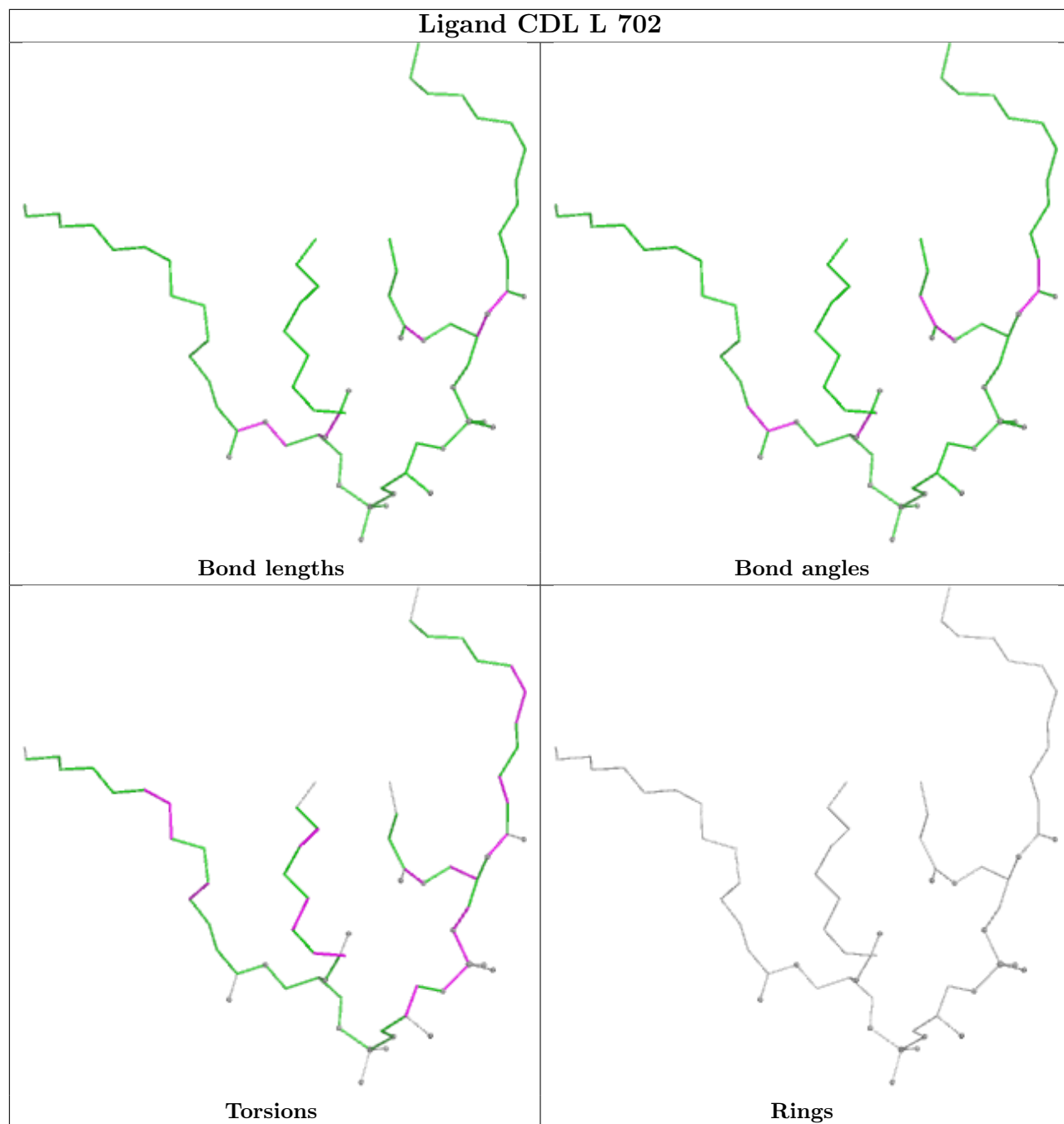


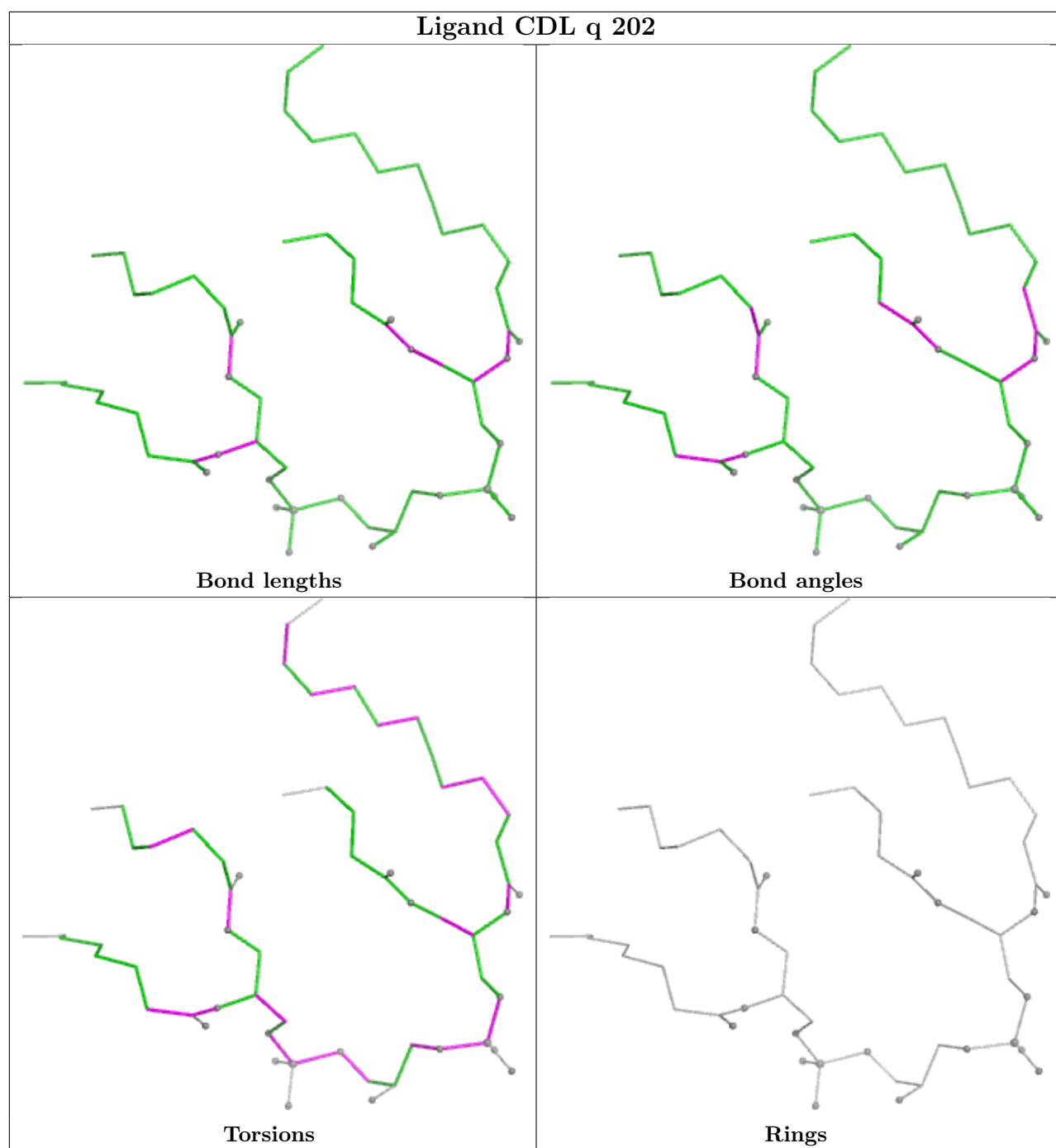
Ligand CHD i 201

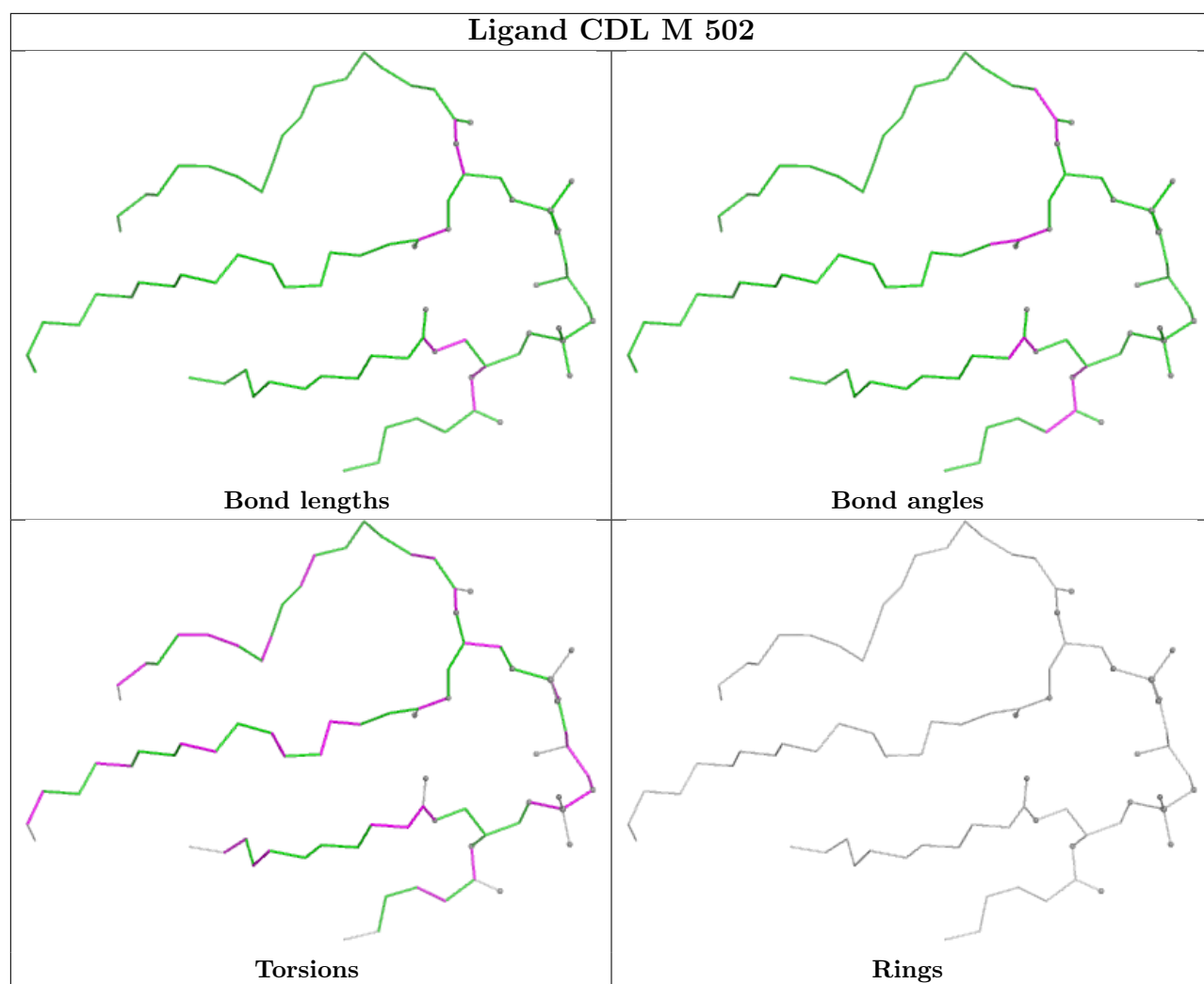


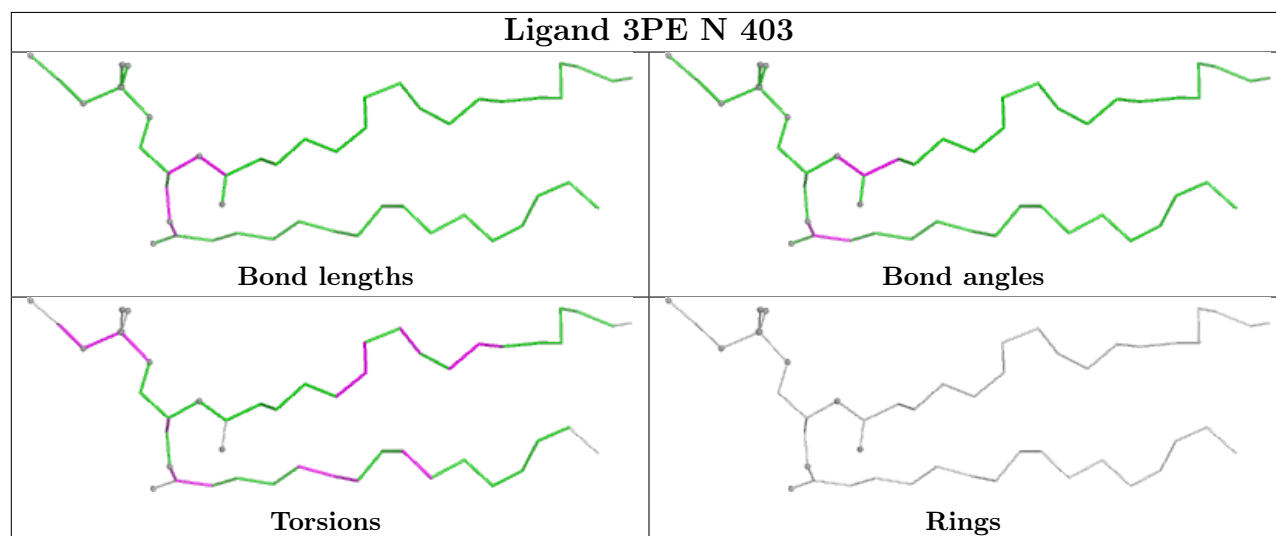
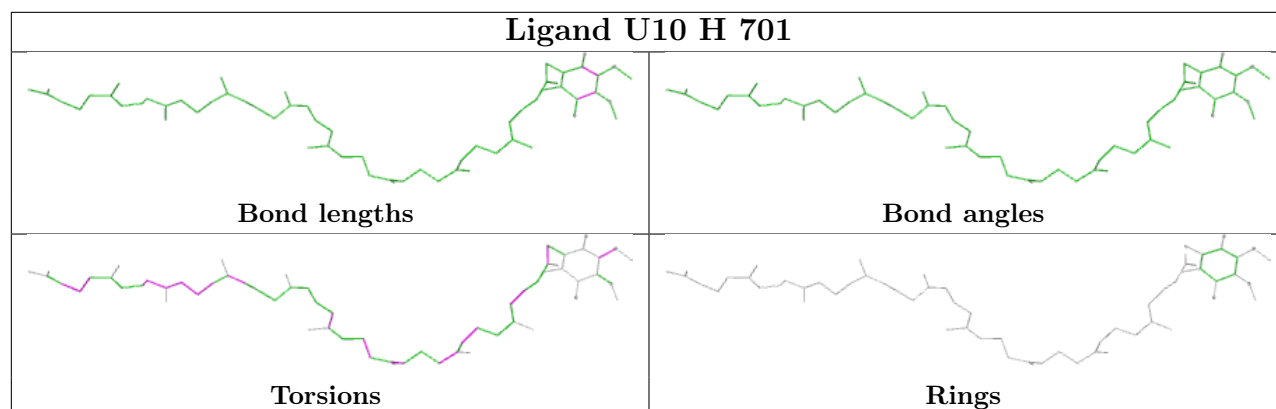
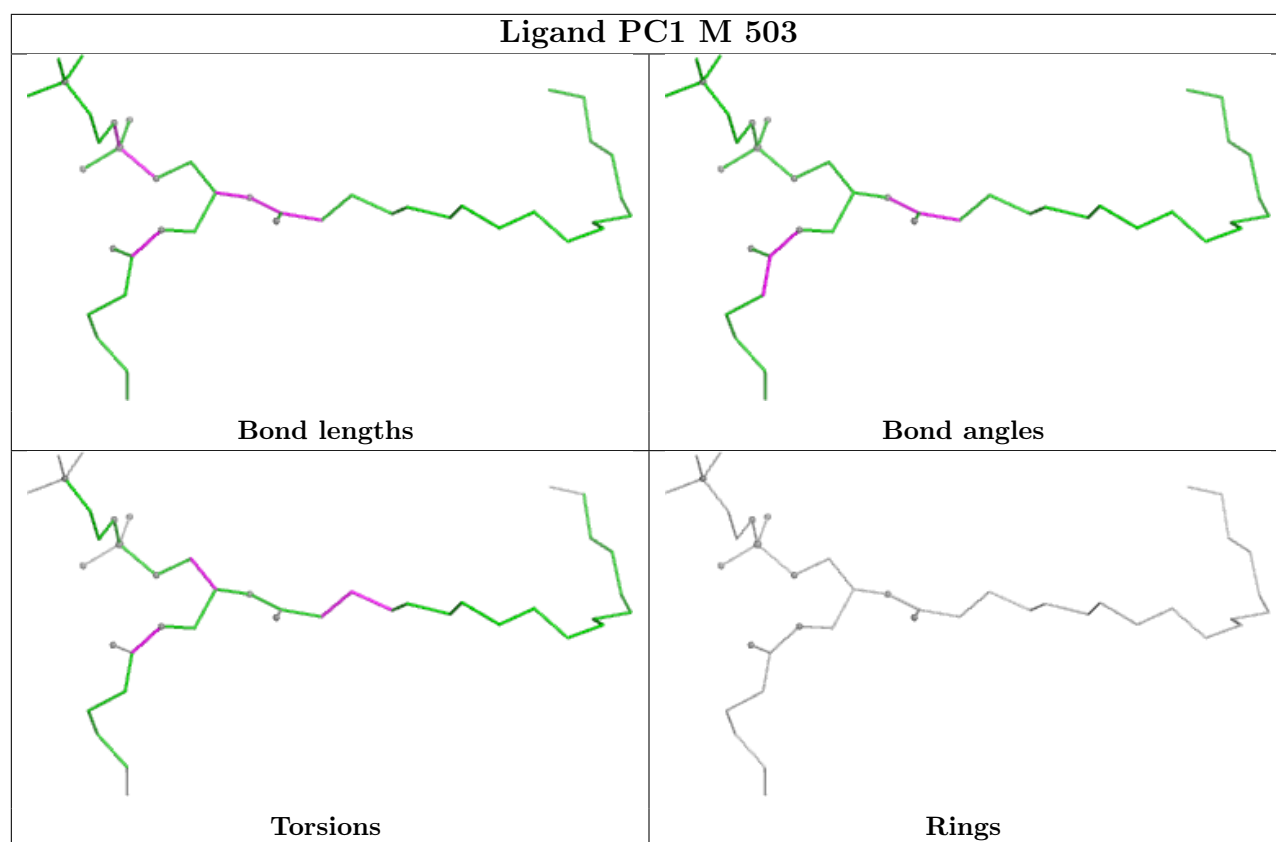
Ligand PC1 A 202

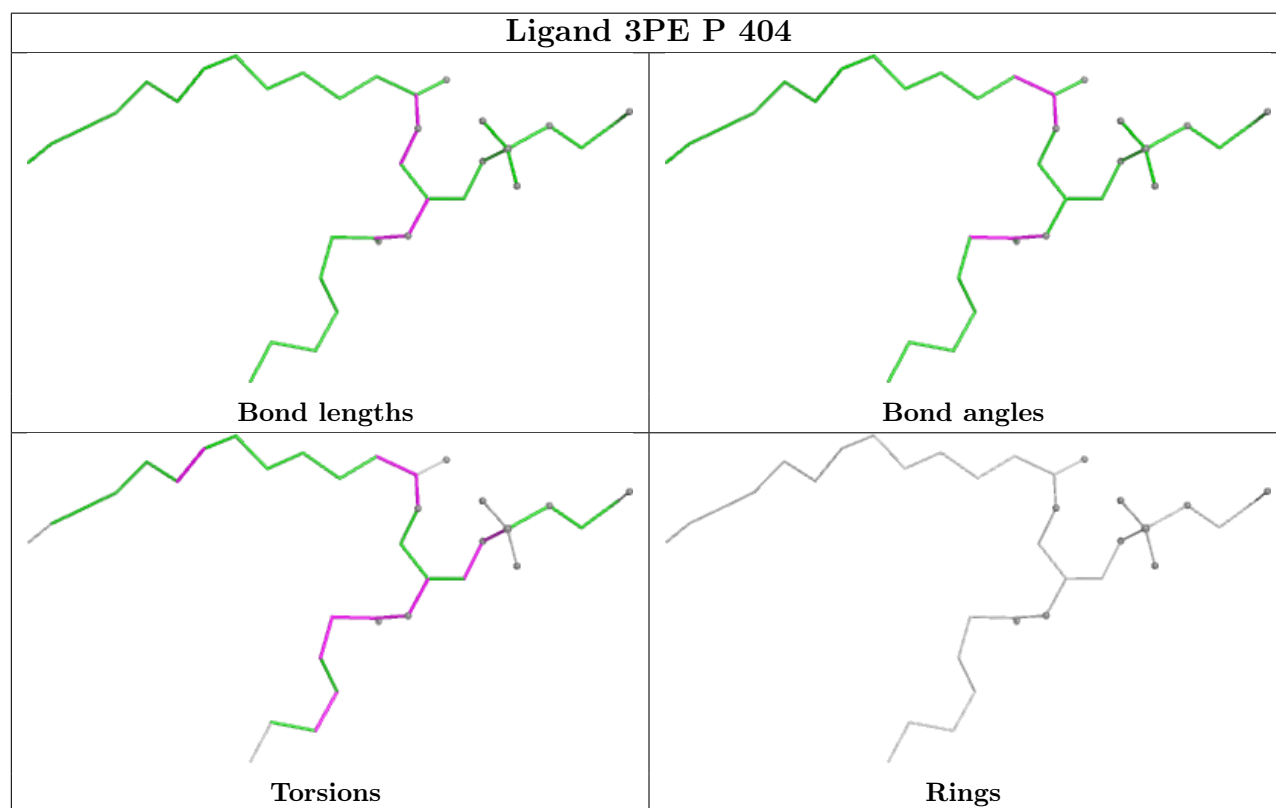
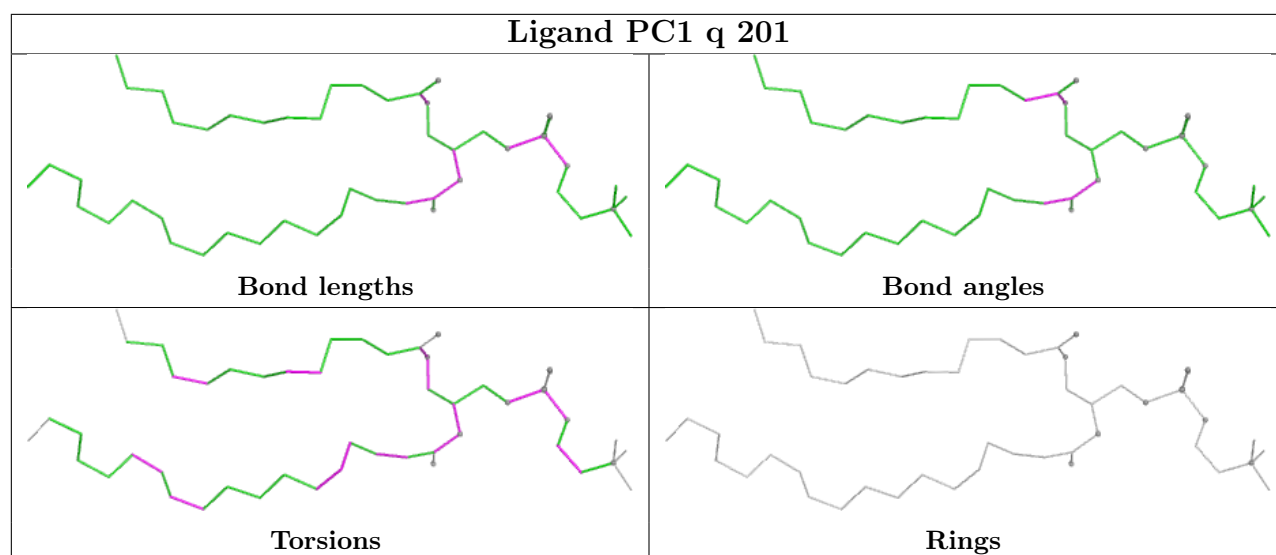


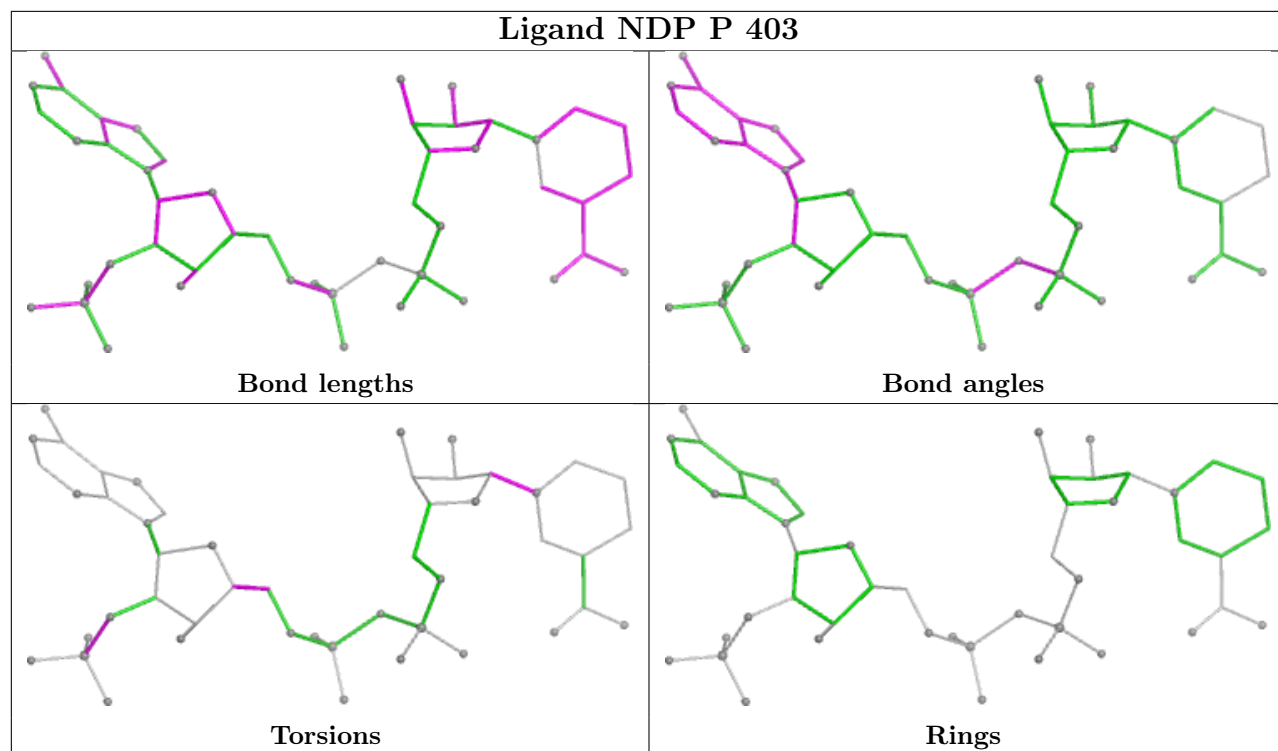


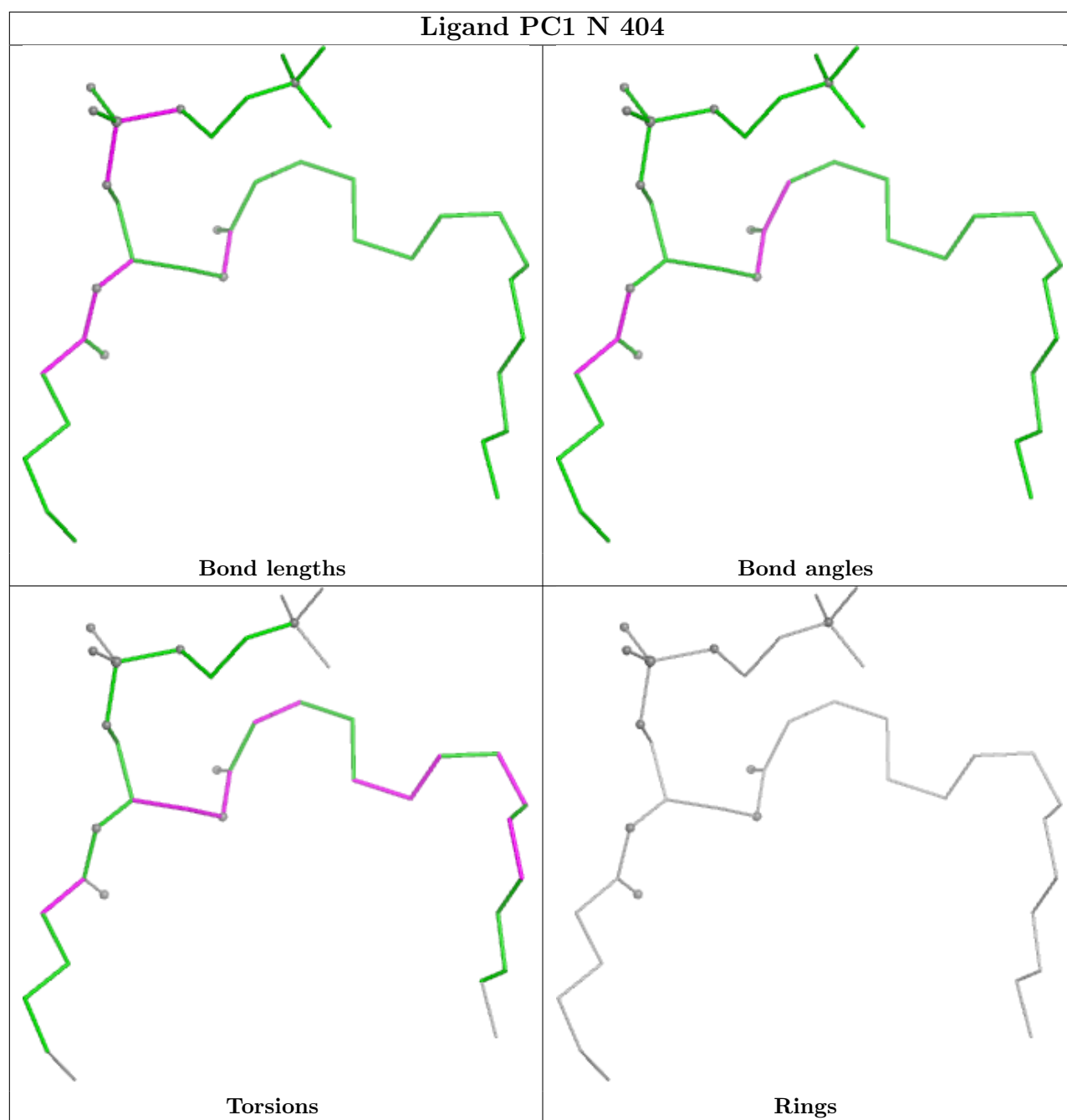












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

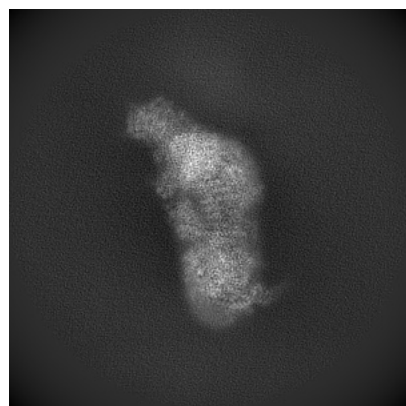
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55031. These allow visual inspection of the internal detail of the map and identification of artifacts.

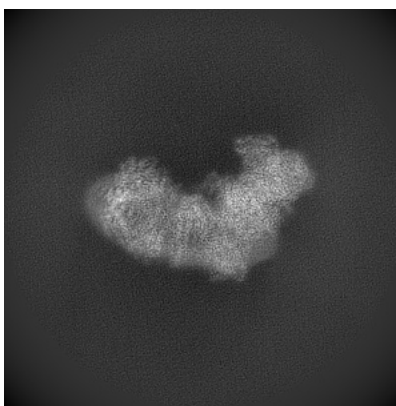
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

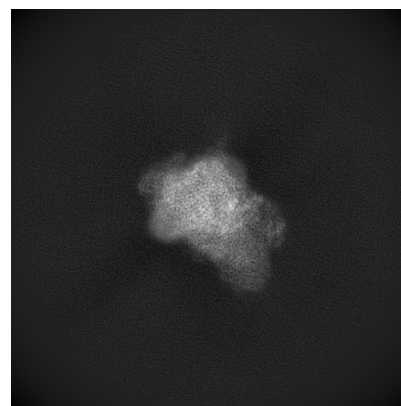
6.1.1 Primary map



X

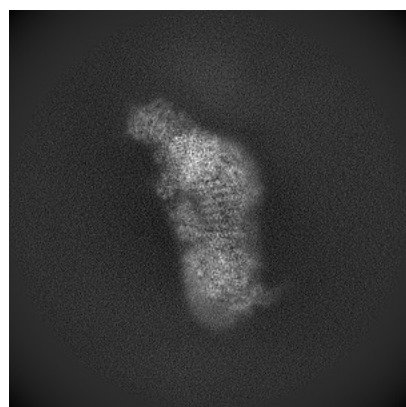


Y

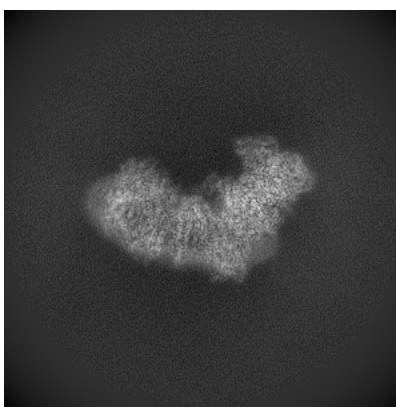


Z

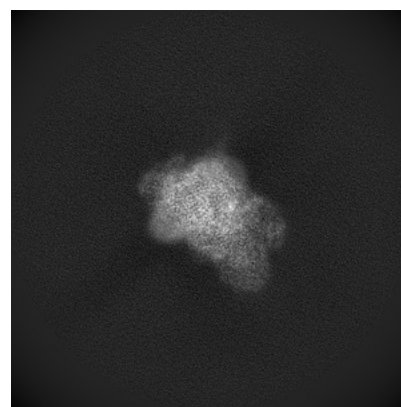
6.1.2 Raw map



X



Y

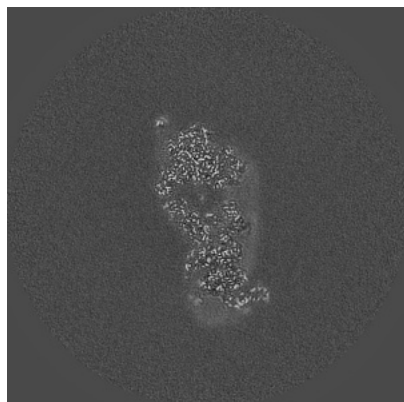


Z

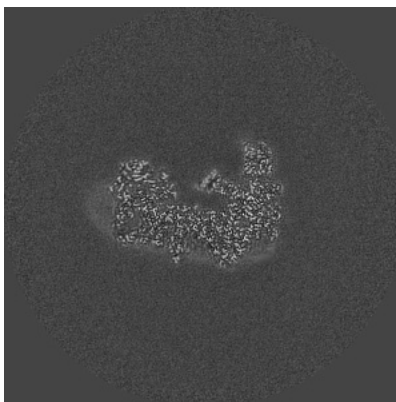
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

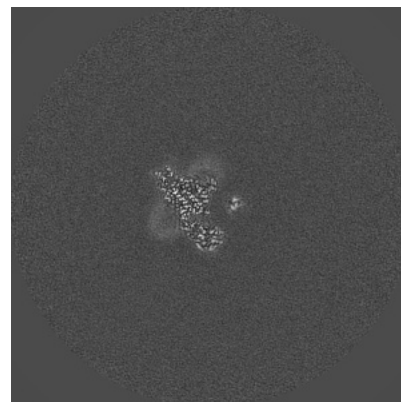
6.2.1 Primary map



X Index: 320

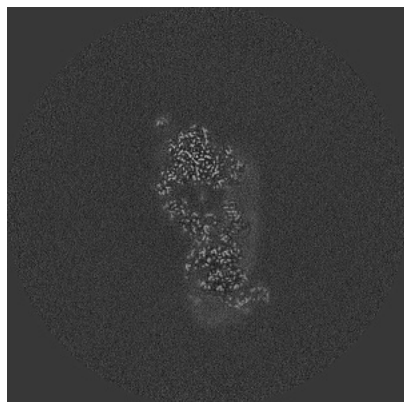


Y Index: 320

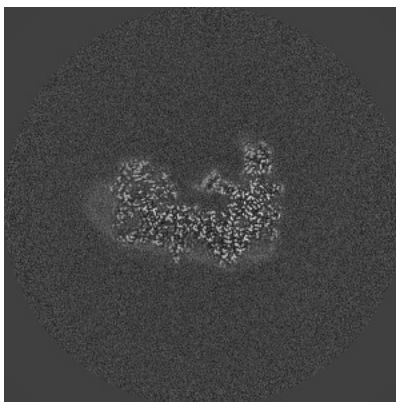


Z Index: 320

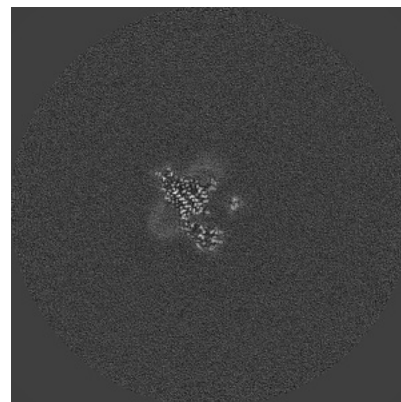
6.2.2 Raw map



X Index: 320



Y Index: 320

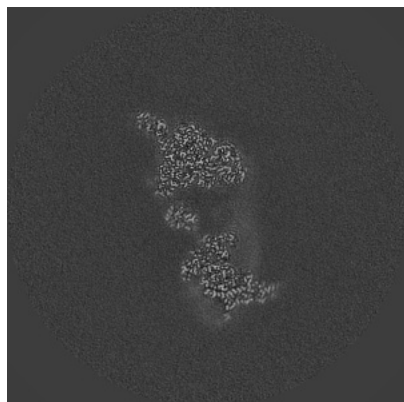


Z Index: 320

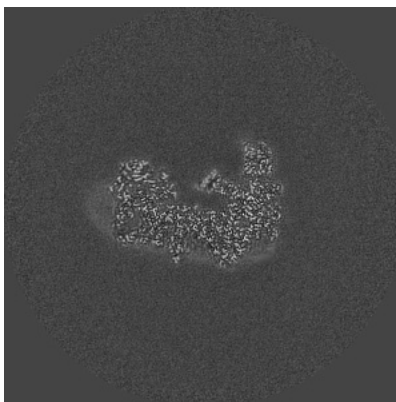
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

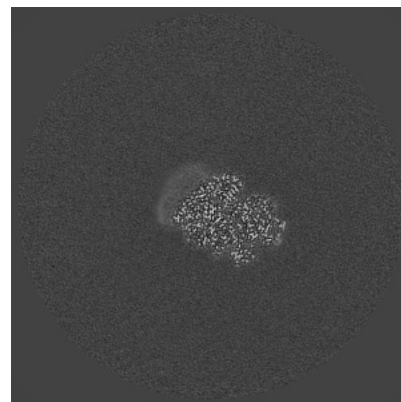
6.3.1 Primary map



X Index: 336

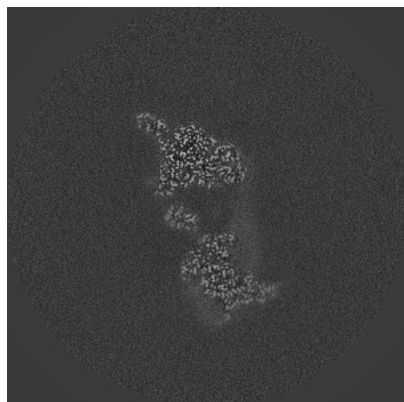


Y Index: 320

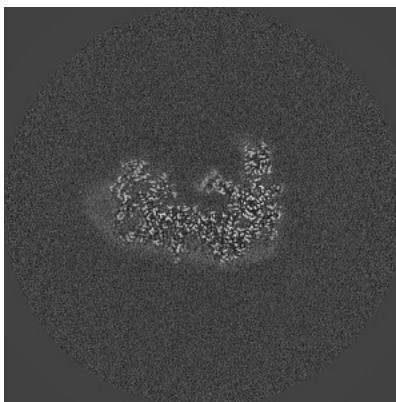


Z Index: 408

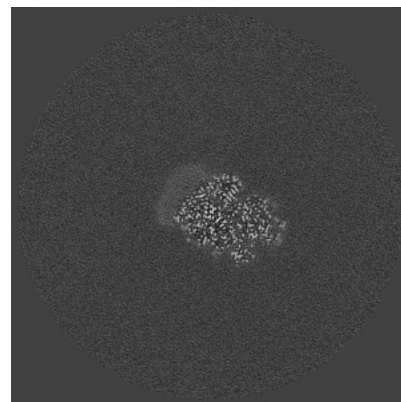
6.3.2 Raw map



X Index: 336



Y Index: 319

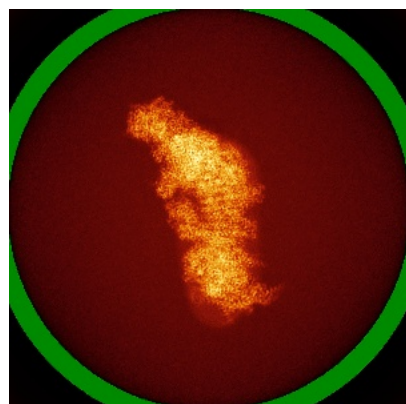


Z Index: 408

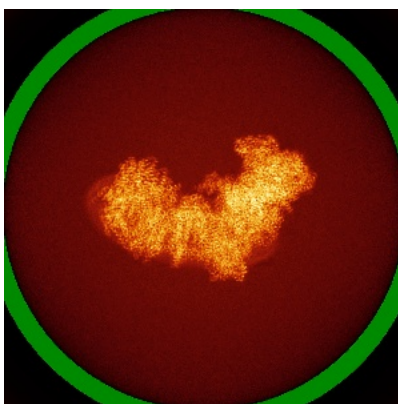
The images above show the largest variance slices of the map in three orthogonal directions.

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

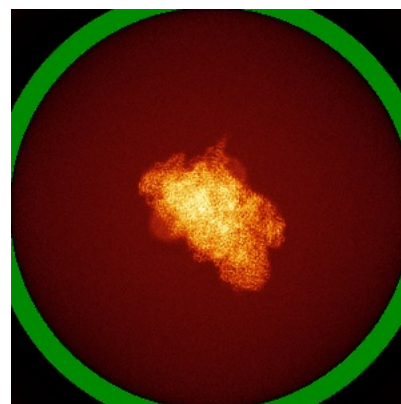
6.4.1 Primary map



X

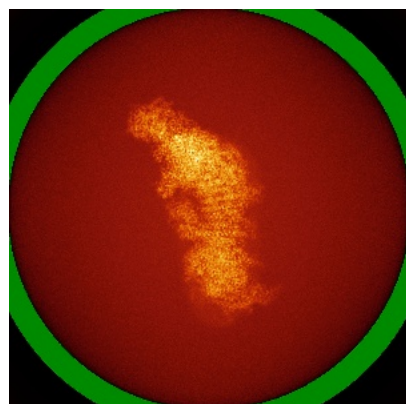


Y

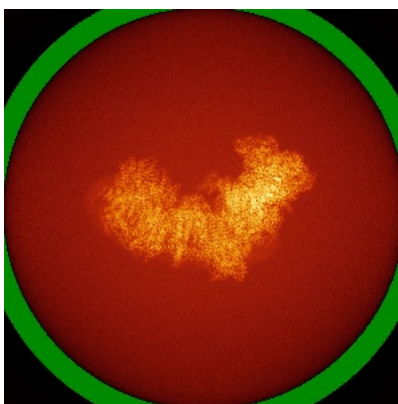


Z

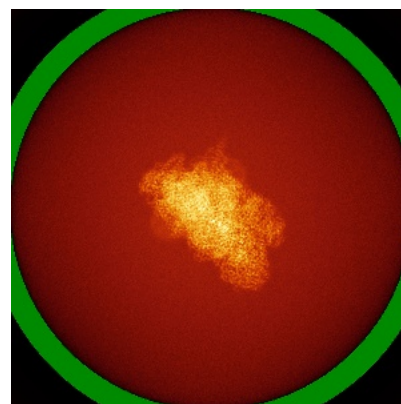
6.4.2 Raw map



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



X



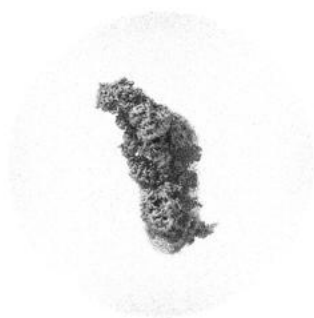
Y



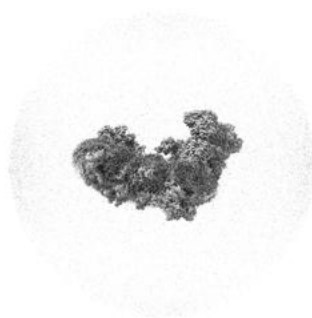
Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

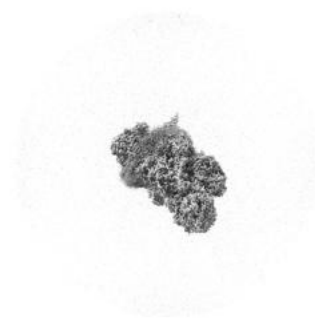
6.5.2 Raw map



X



Y



Z

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.

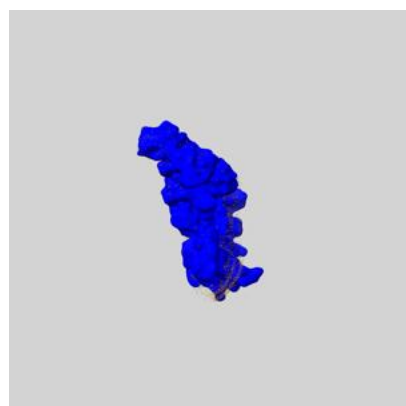
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

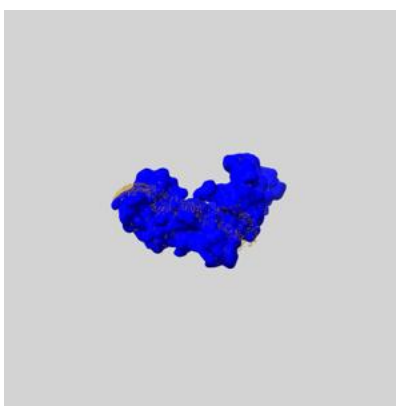
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

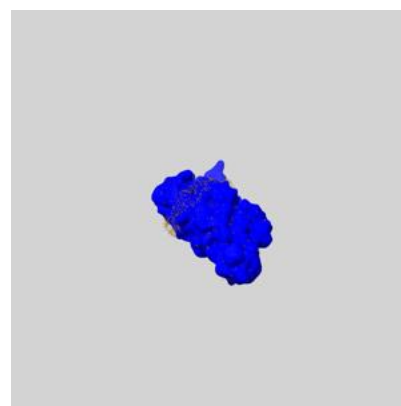
6.6.1 emd_55031_msk_1.map [i](#)



X



Y

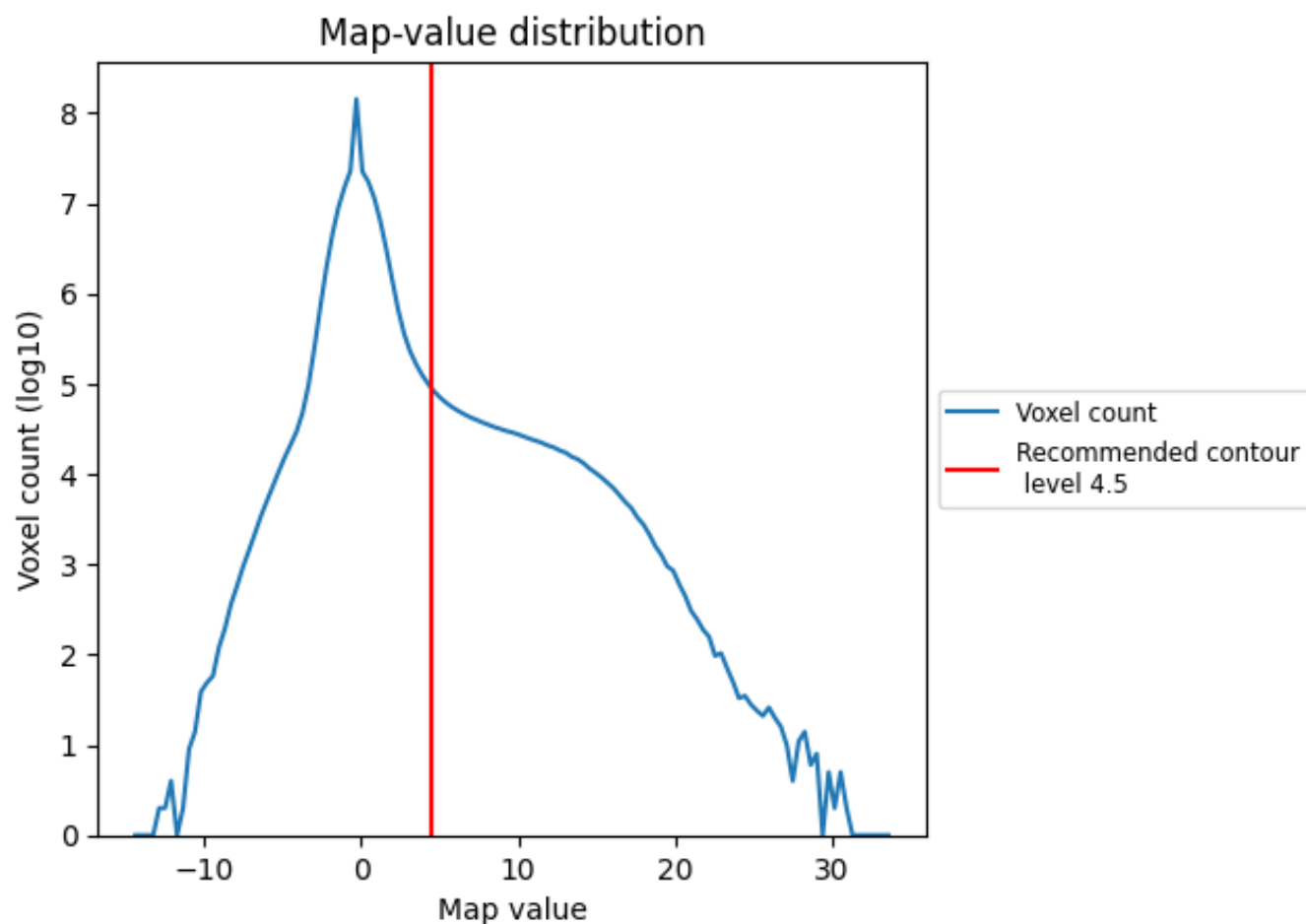


Z

7 Map analysis [i](#)

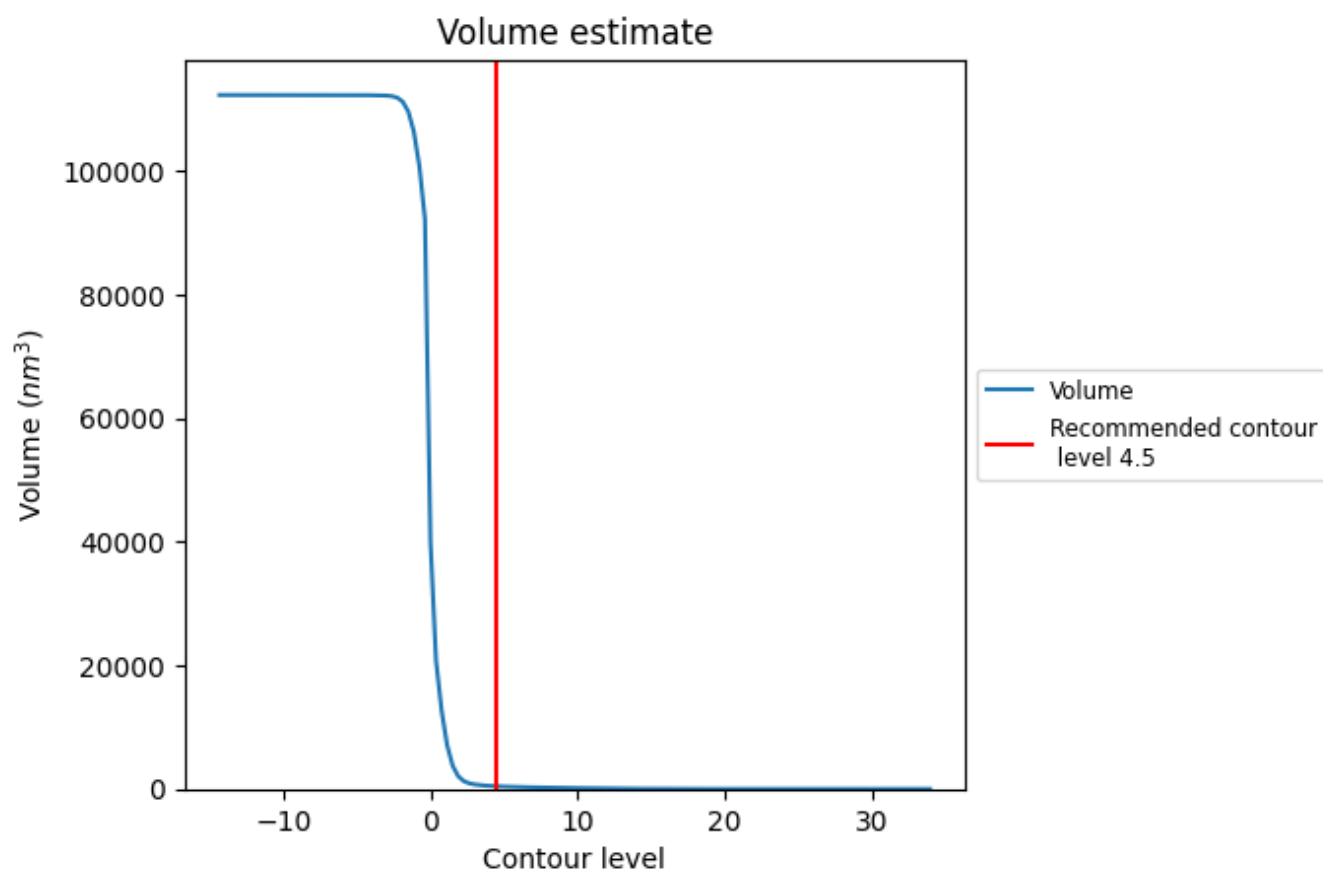
This section contains the results of statistical analysis of the map.

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.

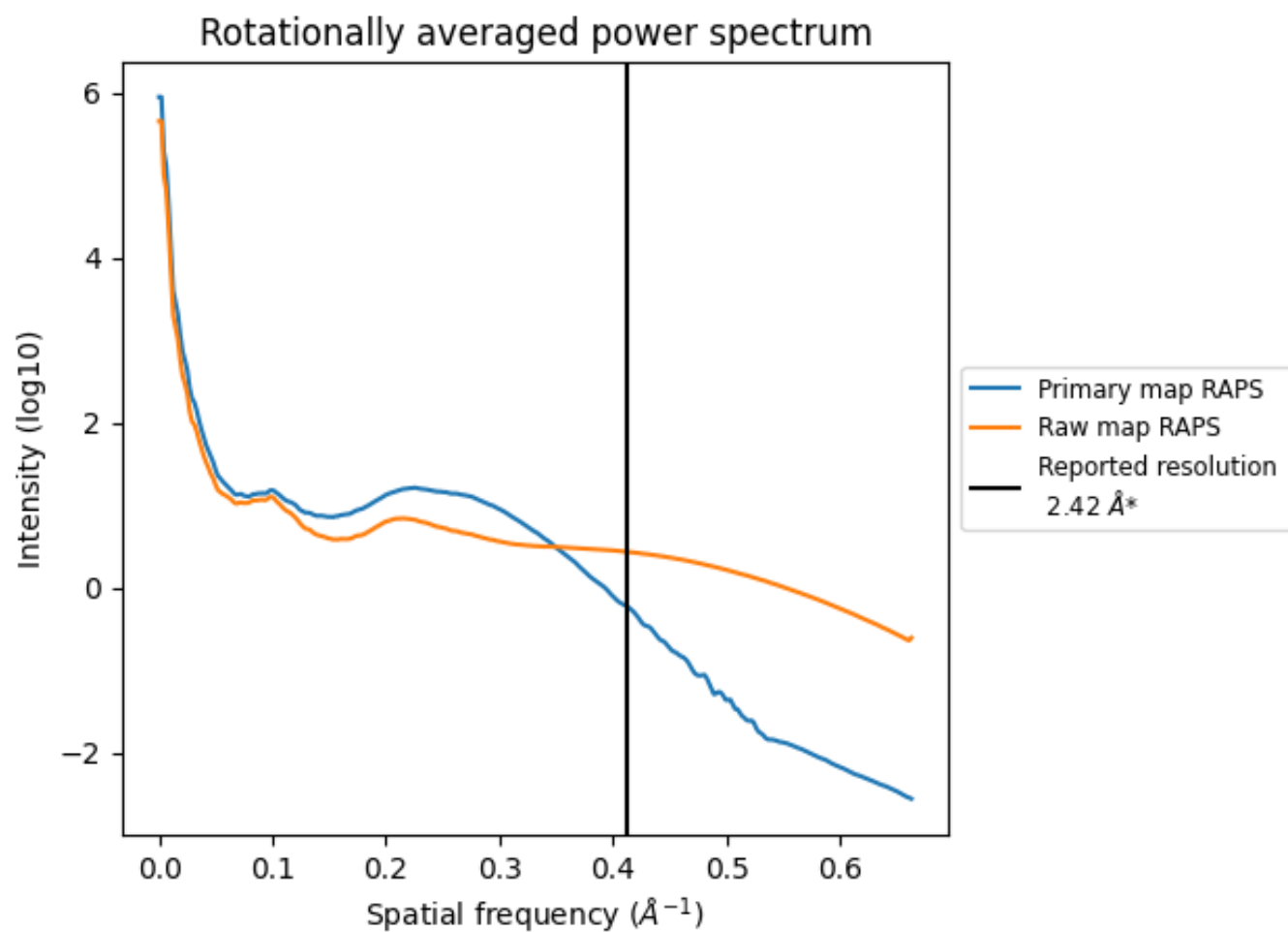
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm^3 ; this corresponds to an approximate mass of 389 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 ⓘ

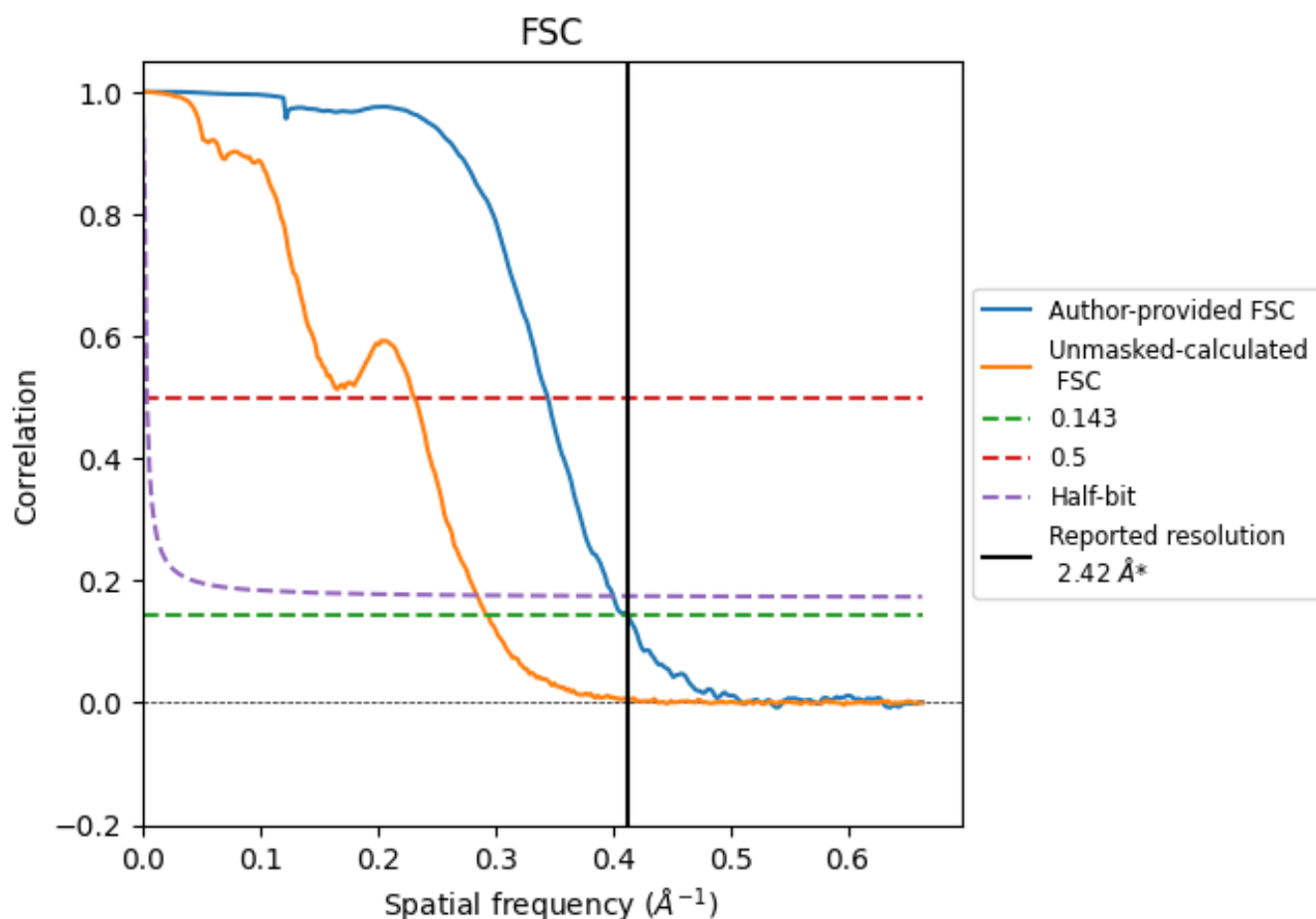


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 \AA^{-1}

8.2 Resolution estimates [i](#)

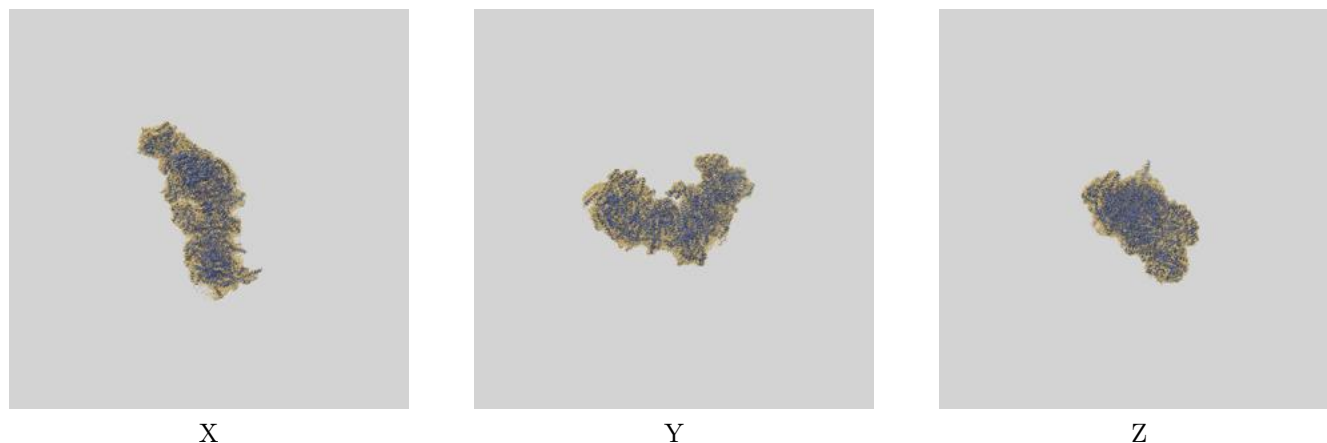
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.90	2.50
Unmasked-calculated*	3.42	4.32	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

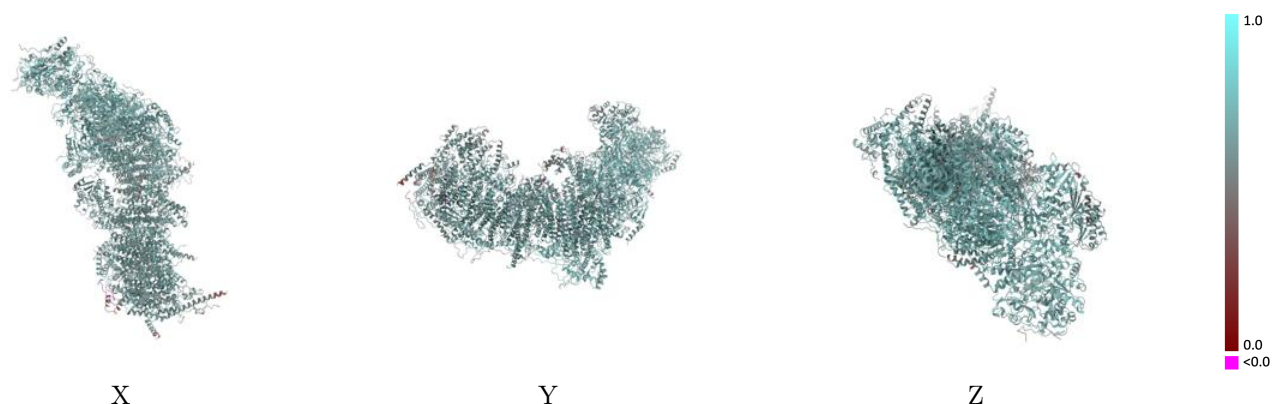
This section contains information regarding the fit between EMDB map EMD-55031 and PDB model 9SMG. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



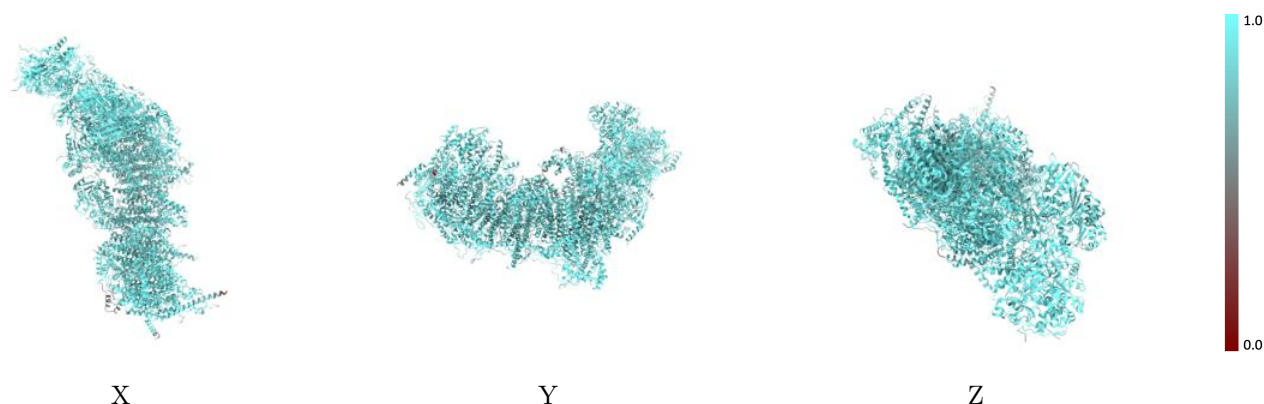
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



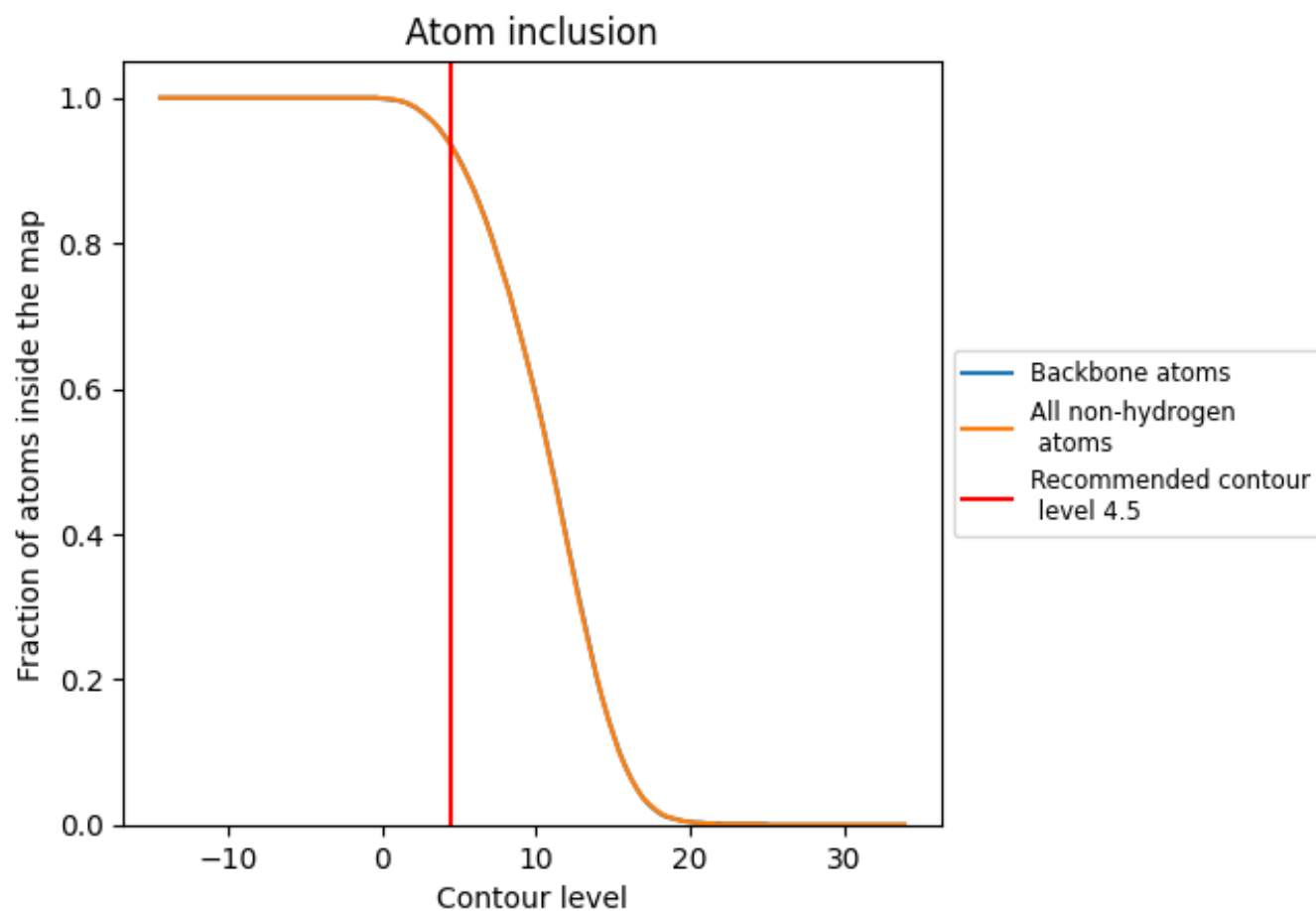
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6460
A	 0.9520	 0.6810
B	 0.9680	 0.6940
C	 0.9650	 0.6990
D	 0.9710	 0.7020
E	 0.9400	 0.6300
F	 0.9590	 0.6510
G	 0.9510	 0.6640
H	 0.9690	 0.6930
I	 0.9820	 0.7060
J	 0.9590	 0.6720
K	 0.9760	 0.6930
L	 0.9490	 0.6370
M	 0.9800	 0.6890
N	 0.9750	 0.6930
O	 0.9250	 0.6190
P	 0.9340	 0.6540
Q	 0.9270	 0.6750
R	 0.9250	 0.6630
S	 0.8910	 0.5650
T	 0.7600	 0.5040
U	 0.8750	 0.5630
V	 0.9100	 0.6440
W	 0.9220	 0.6530
X	 0.9160	 0.6290
Y	 0.8900	 0.6030
Z	 0.9370	 0.6540
a	 0.9730	 0.6710
b	 0.8920	 0.6210
c	 0.8910	 0.5950
d	 0.9230	 0.6400
e	 0.9140	 0.6370
f	 0.8100	 0.5640
g	 0.8890	 0.6120
h	 0.9190	 0.6330



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Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8220	 0.5230
j	 0.8640	 0.5360
k	 0.8540	 0.5410
l	 0.9260	 0.6080
m	 0.9110	 0.6080
n	 0.9160	 0.5970
o	 0.8660	 0.5460
p	 0.9190	 0.6180
q	 0.9200	 0.6560
r	 0.9340	 0.6540
s	 0.9360	 0.6200