



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 01:39 pm BST

PDB ID : 8AC4
EMDB ID : EMD-15333
Title : Complex III₂ from *Yarrowia lipolytica*, apo, c-position
Authors : Wieferig, J.P.; Kuhlbrandt, W.
Deposited on : 2022-07-05
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

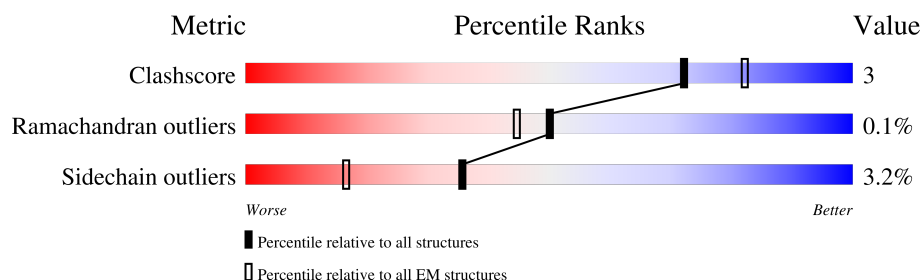
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	385	
1	N	385	
2	E	225	
2	P	225	
3	G	128	
3	R	128	
4	F	137	
4	Q	137	

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Mol	Chain	Length	Quality of chain
5	A	474	 86%6%8%
5	L	474	 87%5%8%
6	B	417	 87%9%.
6	M	417	 87%9%.
7	D	330	 68%5%26%
7	O	330	 69%5%26%
8	H	93	 86%. . 9%
8	S	93	 86%. . 9%
9	I	69	 72%6%22%
9	T	69	 74%. 22%
10	J	82	 83%7%. 9%
10	U	82	 83%9%9%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32540 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		
1	N	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	186	Total	C	N	O	S	0	0
			1445	920	248	268	9		
2	E	61	Total	C	N	O	S	0	0
			465	297	76	89	3		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	124	Total	C	N	O	S	0	0
			994	640	162	190	2		
3	R	124	Total	C	N	O	S	0	0
			994	640	162	190	2		

- Molecule 4 is a protein called YALI0F24673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	71	Total	C	N	O	S	0	0
			579	361	99	115	4		
4	Q	71	Total	C	N	O	S	0	0
			579	361	99	115	4		

- Molecule 5 is a protein called YALI0A14806p.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		
5	L	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		
6	M	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		

- Molecule 7 is a protein called YALI0A17468p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		
7	O	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			690	459	118	111	2		
8	S	85	Total	C	N	O	S	0	0
			690	459	118	111	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			452	297	76	78	1		
9	T	54	Total	C	N	O	S	0	0
			452	297	76	78	1		

- Molecule 10 is a protein called YALI0C12210p.

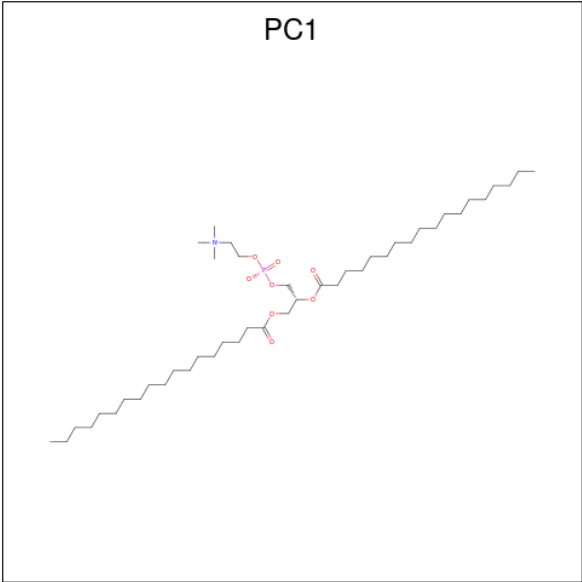
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	75	Total	C	N	O	0	0
			598	403	99	96		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	75	Total	C	N	O	0	0
			598	403	99	96		

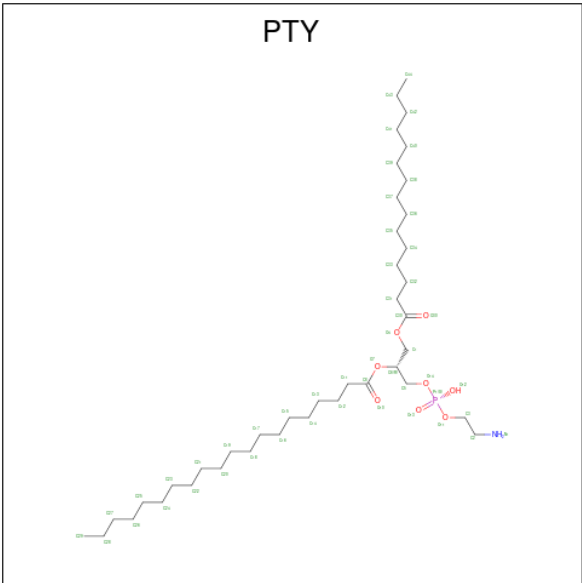
- # HEM

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



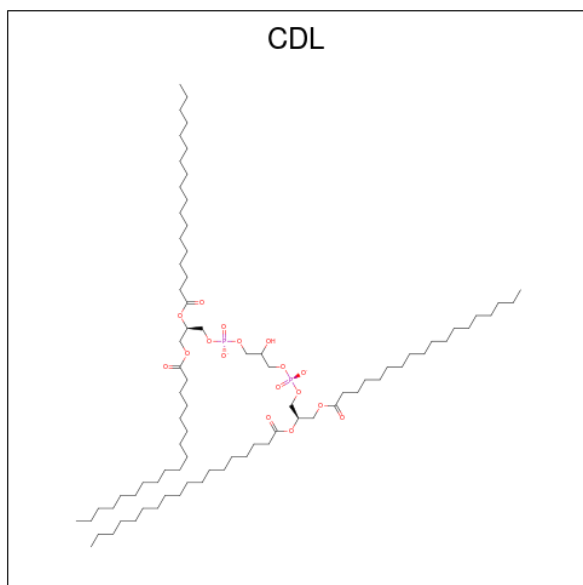
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	T	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	E	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



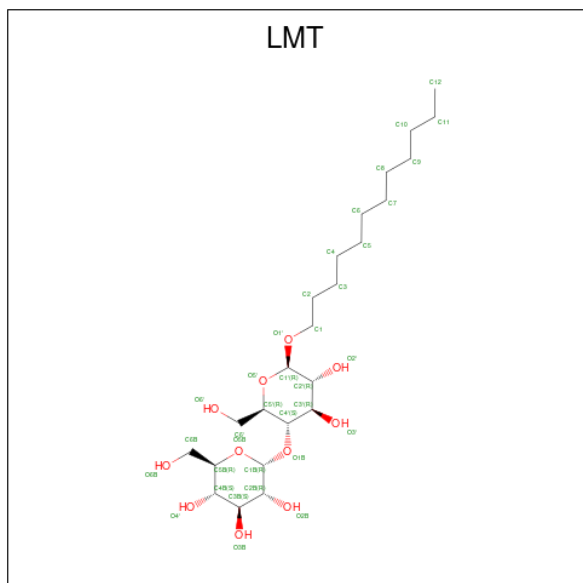
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	A	1	Total	C	O	P	0
			42	25	15	2	
14	A	1	Total	C	O	P	0
			47	30	15	2	
14	H	1	Total	C	O	P	0
			50	31	17	2	
14	H	1	Total	C	O	P	0
			39	20	17	2	
14	N	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			48	29	17	2	
14	L	1	Total	C	O	P	0
			42	25	15	2	

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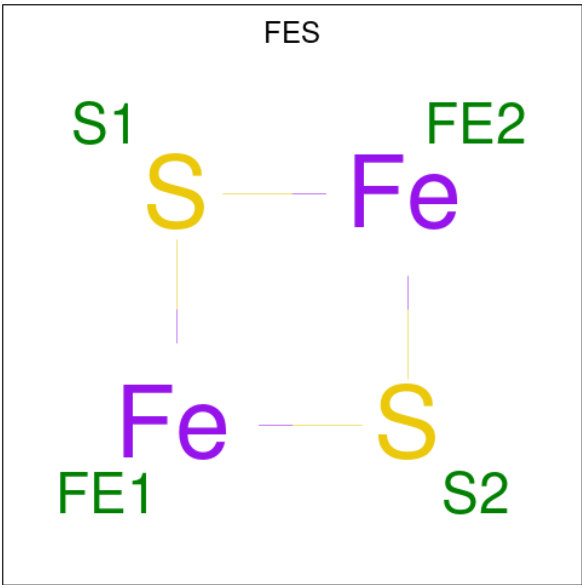
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			47	30	15	2	
14	S	1	Total	C	O	P	0
			39	20	17	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



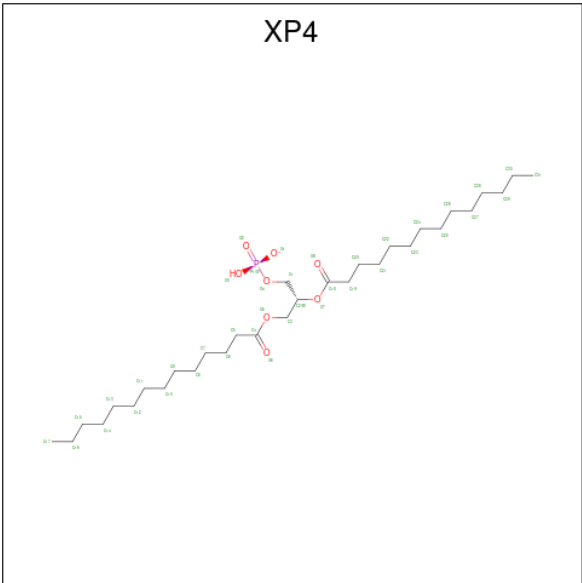
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			35	24	11	
15	P	1	Total	C	O	0
			35	24	11	
15	J	1	Total	C	O	0
			35	24	11	
15	N	1	Total	C	O	0
			35	24	11	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



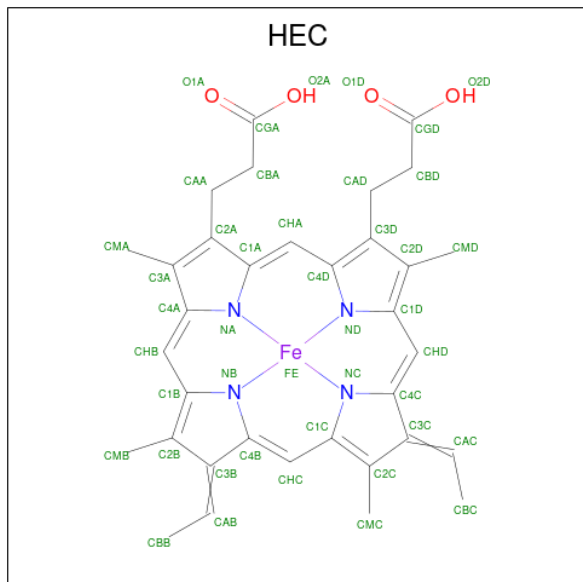
Mol	Chain	Residues	Atoms			AltConf
16	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: C₃₁H₆₀O₈P).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			24	15	8	1	
17	U	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).




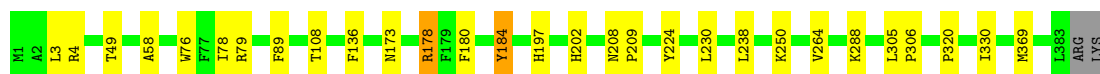
Mol	Chain	Residues	Atoms					AltConf
18	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
18	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

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.

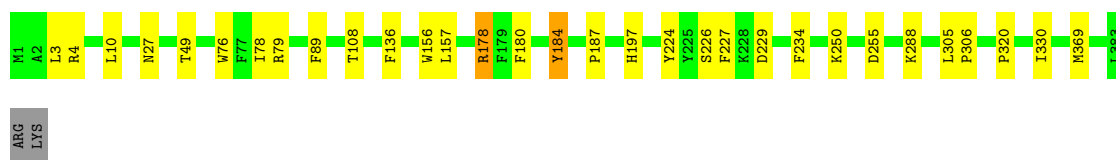
- Molecule 1: Cytochrome b

Chain C:  92% 7% ..



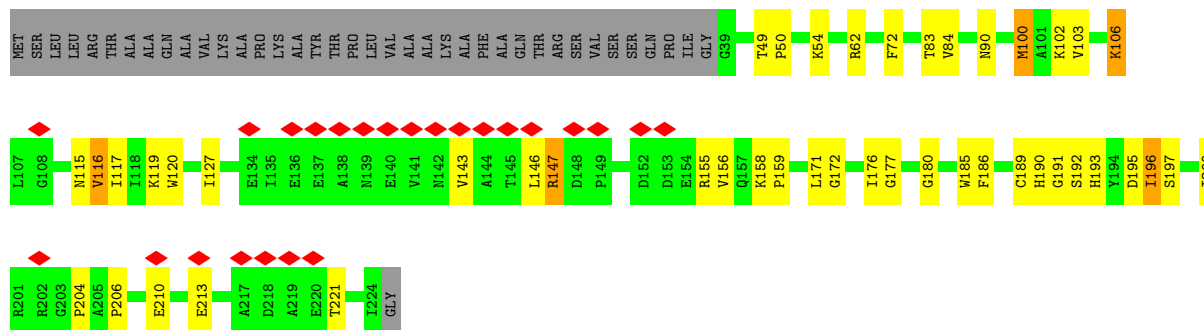
- Molecule 1: Cytochrome b

Chain N:  91% 8% ..



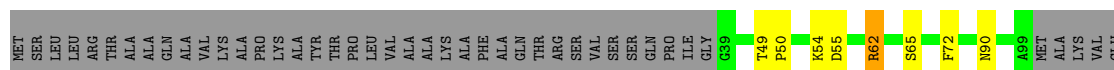
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

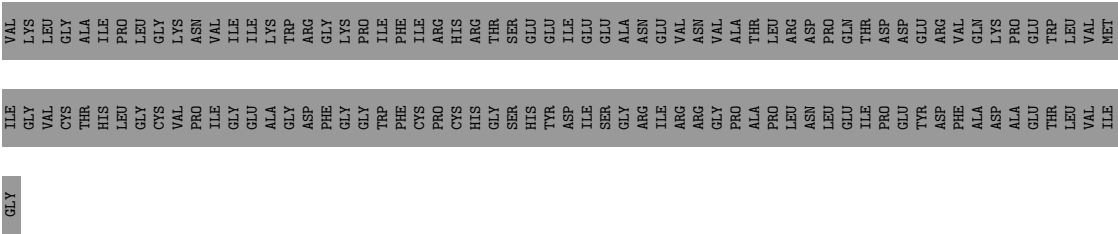
Chain P:  11% 62% 18% . 17%



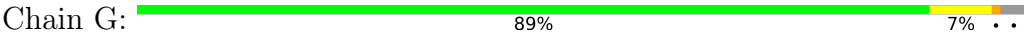
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:  24% . 73%

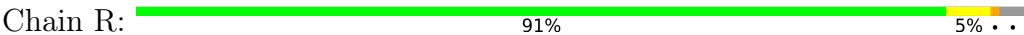




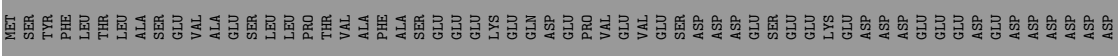
• Molecule 3: Cytochrome b-c1 complex subunit 7



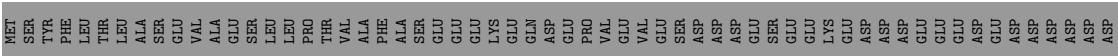
• Molecule 3: Cytochrome b-c1 complex subunit 7



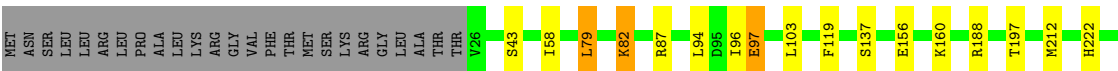
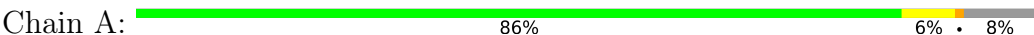
• Molecule 4: YALI0F24673p

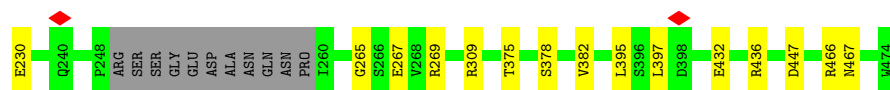


• Molecule 4: YALI0F24673p



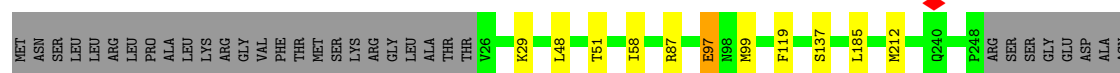
• Molecule 5: YALI0A14806p





• Molecule 5: YALI0A14806p

Chain L: 87% 5% 8%



• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 87% 9% 4%



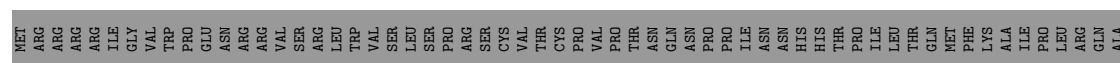
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 87% 9% 4%

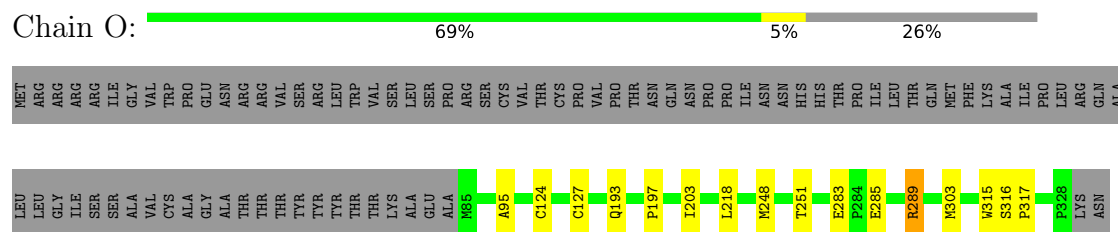


• Molecule 7: YALI0A17468p

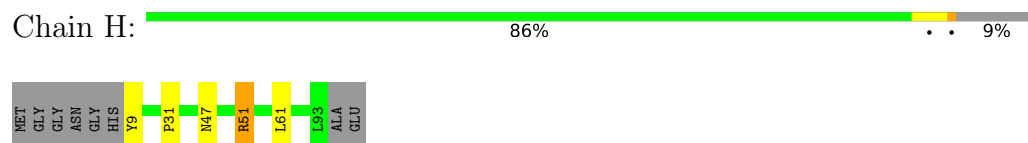
Chain D: 68% 5% 26%



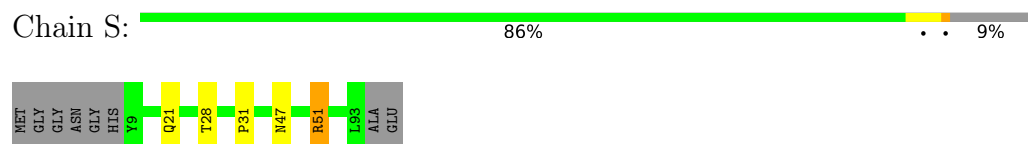
• Molecule 7: YALI0A17468p



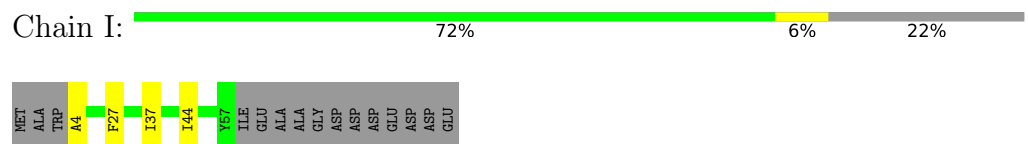
- Molecule 8: Cytochrome b-c1 complex subunit 8



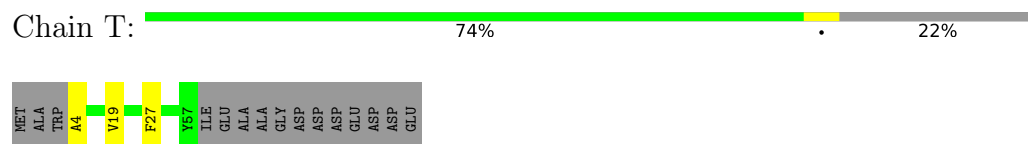
- Molecule 8: Cytochrome b-c1 complex subunit 8



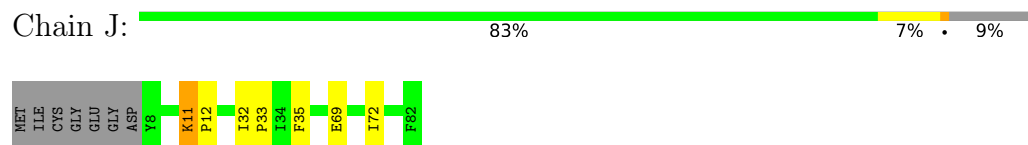
- Molecule 9: Complex III subunit 9



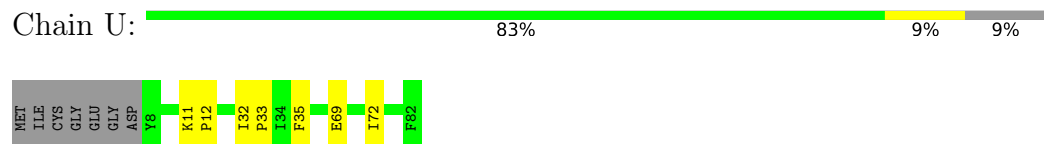
- Molecule 9: Complex III subunit 9



- Molecule 10: YALI0C12210p



- Molecule 10: YALI0C12210p



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192544	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	301.32, 301.32, 301.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, HEM, CDL, LMT, HEC, XP4, FES, PC1

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	C	0.45	0/3153	0.78	1/4305 (0.0%)
1	N	0.44	0/3153	0.77	1/4305 (0.0%)
2	E	0.45	0/474	0.75	1/637 (0.2%)
2	P	0.38	0/1479	0.80	1/2003 (0.0%)
3	G	0.41	0/1012	0.73	0/1373
3	R	0.42	1/1012 (0.1%)	0.74	0/1373
4	F	0.29	0/595	0.66	0/805
4	Q	0.30	0/595	0.67	0/805
5	A	0.38	0/3510	0.76	2/4768 (0.0%)
5	L	0.38	0/3510	0.78	4/4768 (0.1%)
6	B	0.35	0/3069	0.76	3/4178 (0.1%)
6	M	0.35	0/3069	0.76	3/4178 (0.1%)
7	D	0.39	0/1950	0.78	3/2656 (0.1%)
7	O	0.40	0/1950	0.77	2/2656 (0.1%)
8	H	0.40	1/717 (0.1%)	0.71	0/975
8	S	0.40	0/717	0.72	0/975
9	I	0.46	1/465 (0.2%)	0.65	0/629
9	T	0.45	1/465 (0.2%)	0.65	0/629
10	J	0.37	0/620	0.66	0/846
10	U	0.37	0/620	0.66	0/846
All	All	0.39	4/32135 (0.0%)	0.76	21/43710 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	4	ALA	N-CA	5.65	1.57	1.46
9	I	4	ALA	N-CA	5.60	1.57	1.46
3	R	2	ALA	N-CA	5.22	1.56	1.46
8	H	9	TYR	N-CA	5.11	1.56	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	90	ARG	CG-CD-NE	-7.67	95.69	111.80
6	M	90	ARG	CG-CD-NE	-7.65	95.74	111.80
5	L	269	ARG	NE-CZ-NH2	-7.61	116.49	120.30
6	B	215	GLN	CB-CA-C	-7.46	95.49	110.40
6	M	215	GLN	CB-CA-C	-7.38	95.64	110.40
5	A	269	ARG	CG-CD-NE	-6.93	97.25	111.80
7	O	283	GLU	CB-CA-C	-6.42	97.55	110.40
5	A	309	ARG	CG-CD-NE	-6.37	98.43	111.80
2	P	100	MET	C-N-CA	-6.34	105.84	121.70
5	L	269	ARG	NE-CZ-NH1	6.34	123.47	120.30
5	L	309	ARG	CG-CD-NE	-6.29	98.58	111.80
7	D	283	GLU	CB-CA-C	-5.66	99.09	110.40
6	B	158	ARG	CG-CD-NE	-5.61	100.02	111.80
2	E	62	ARG	CB-CG-CD	-5.49	97.33	111.60
7	D	283	GLU	CB-CG-CD	-5.49	99.39	114.20
6	M	158	ARG	CG-CD-NE	-5.46	100.33	111.80
5	L	269	ARG	CG-CD-NE	-5.41	100.45	111.80
1	N	4	ARG	CG-CD-NE	-5.18	100.93	111.80
1	C	4	ARG	CG-CD-NE	-5.13	101.03	111.80
7	O	289	ARG	CG-CD-NE	-5.04	101.21	111.80
7	D	289	ARG	CG-CD-NE	-5.03	101.23	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3052	0	3113	20	0
1	N	3052	0	3113	19	0
2	E	465	0	459	2	0
2	P	1445	0	1426	30	0
3	G	994	0	1022	3	0
3	R	994	0	1022	3	0
4	F	579	0	511	1	0
4	Q	579	0	511	1	0
5	A	3446	0	3369	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	3446	0	3369	9	0
6	B	3008	0	2991	21	0
6	M	3008	0	2991	20	0
7	D	1893	0	1834	24	0
7	O	1893	0	1834	20	0
8	H	690	0	673	4	0
8	S	690	0	673	5	0
9	I	452	0	435	2	0
9	T	452	0	435	1	0
10	J	598	0	615	4	0
10	U	598	0	615	4	0
11	C	86	0	60	8	0
11	N	86	0	60	8	0
12	C	38	0	50	1	0
12	I	32	0	38	0	0
12	N	38	0	50	1	0
12	T	32	0	38	2	0
13	C	41	0	58	3	0
13	E	41	0	58	1	0
13	N	41	0	58	9	0
13	P	41	0	58	10	0
14	A	89	0	85	3	0
14	C	48	0	40	2	0
14	H	89	0	66	3	0
14	L	89	0	85	1	0
14	N	98	0	84	5	0
14	S	39	0	22	2	0
15	C	35	0	46	1	0
15	J	35	0	46	1	0
15	N	35	0	46	0	0
15	P	35	0	46	0	0
16	P	4	0	0	0	0
17	A	24	0	22	1	0
17	U	24	0	22	1	0
18	D	43	0	32	12	0
18	O	43	0	32	13	0
All	All	32540	0	32213	209	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 3.

All (209) 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)
7:O:124:CYS:SG	18:O:401:HEC:HBB3	1.62	1.39
7:D:124:CYS:SG	18:D:401:HEC:HBB3	1.62	1.38
2:P:189:CYS:O	7:D:235:MET:CE	1.68	1.38
2:P:84:VAL:CG2	13:P:303:PTY:H441	1.54	1.35
2:P:189:CYS:O	7:D:235:MET:HE1	1.11	1.23
2:P:84:VAL:HG23	13:P:303:PTY:C44	1.66	1.23
7:O:124:CYS:SG	18:O:401:HEC:CBB	2.34	1.15
7:D:124:CYS:SG	18:D:401:HEC:CBB	2.33	1.15
7:D:127:CYS:SG	18:D:401:HEC:CAC	2.37	1.12
7:O:127:CYS:SG	18:O:401:HEC:CAC	2.39	1.09
7:O:127:CYS:SG	18:O:401:HEC:HBC3	1.95	1.06
7:D:127:CYS:SG	18:D:401:HEC:HBC3	1.96	1.05
7:D:127:CYS:SG	18:D:401:HEC:CBC	2.48	1.01
7:O:127:CYS:SG	18:O:401:HEC:CBC	2.48	1.01
7:D:124:CYS:SG	18:D:401:HEC:CAB	2.51	0.98
7:O:124:CYS:SG	18:O:401:HEC:CAB	2.52	0.97
2:P:189:CYS:O	7:D:235:MET:HE3	1.66	0.94
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.51	0.93
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.51	0.91
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.09	0.84
5:A:395:LEU:HD23	6:B:34:ILE:HD12	1.61	0.81
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.64	0.79
1:C:264:VAL:HA	2:P:171:LEU:O	1.83	0.78
1:C:58:ALA:H	1:C:173:ASN:HD22	1.28	0.77
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.20	0.71
11:C:502:HEM:HBC2	11:C:502:HEM:HMC2	1.72	0.71
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.21	0.71
5:A:395:LEU:HD22	6:B:98:GLN:HG2	1.72	0.70
7:O:251:THR:HG21	18:O:401:HEC:HMC2	1.74	0.69
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.75	0.68
13:C:504:PTY:H112	13:C:504:PTY:HC12	1.77	0.67
6:B:236:ARG:HD3	6:M:170:TYR:CE1	2.29	0.67
2:P:84:VAL:HG23	13:P:303:PTY:H441	0.74	0.67
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	1.92	0.67
7:D:127:CYS:SG	18:D:401:HEC:C3C	2.84	0.66
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.77	0.65
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.77	0.64
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.80	0.64
7:O:127:CYS:SG	18:O:401:HEC:C3C	2.86	0.64
6:M:91:GLU:HG2	6:M:364:MET:HE2	1.80	0.63
5:A:395:LEU:CD2	6:B:34:ILE:HD12	2.27	0.63
8:S:47:ASN:O	8:S:51:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:251:THR:HG21	18:D:401:HEC:HMC2	1.80	0.62
7:O:124:CYS:SG	18:O:401:HEC:C3B	2.88	0.62
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.82	0.61
2:P:84:VAL:CG2	13:P:303:PTY:C44	2.45	0.61
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.83	0.61
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.83	0.61
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.83	0.60
8:H:47:ASN:O	8:H:51:ARG:HG2	2.01	0.60
6:M:318:ALA:O	6:M:322:VAL:HG23	2.01	0.60
7:D:124:CYS:SG	18:D:401:HEC:C3B	2.88	0.60
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.82	0.60
11:N:501:HEM:HBB2	11:N:501:HEM:CMB	2.30	0.59
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.82	0.59
5:A:395:LEU:HD23	6:B:34:ILE:CD1	2.32	0.59
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.83	0.59
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.84	0.59
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.39	0.58
1:C:58:ALA:H	1:C:173:ASN:ND2	2.01	0.57
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.34	0.57
5:A:43:SER:CB	5:A:222:HIS:HD2	2.18	0.57
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.70	0.56
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.04	0.56
8:H:51:ARG:HH21	14:H:701:CDL:HA22	1.70	0.56
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.35	0.56
7:O:203:ILE:HG12	18:O:401:HEC:HMA3	1.86	0.56
11:N:501:HEM:HBB2	11:N:501:HEM:HMB1	1.88	0.56
7:D:203:ILE:HG12	18:D:401:HEC:HMA3	1.88	0.55
5:A:378:SER:HA	5:A:432:GLU:OE1	2.06	0.55
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.41	0.55
2:P:155:ARG:NH1	2:P:197:SER:O	2.39	0.54
11:C:501:HEM:CMB	11:C:501:HEM:HBB2	2.38	0.54
1:C:320:PRO:HD2	3:G:31:TYR:CE1	2.43	0.54
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.91	0.53
6:M:91:GLU:HG2	6:M:364:MET:CE	2.40	0.52
7:D:317:PRO:HG3	8:H:31:PRO:HD3	1.91	0.52
2:P:191:GLY:HA3	7:D:232:ALA:HB1	1.91	0.52
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.92	0.52
1:C:3:LEU:HD11	14:N:506:CDL:HB32	1.91	0.52
2:E:49:THR:N	2:E:50:PRO:HD2	2.25	0.51
5:L:395:LEU:HD12	6:M:34:ILE:CG2	2.39	0.51
2:P:103:VAL:HG22	2:P:120:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:229:ASP:HB2	13:N:505:PTY:H382	1.92	0.51
1:N:320:PRO:HD2	3:R:31:TYR:CE1	2.45	0.51
6:M:59:LYS:HB3	6:M:129:VAL:HG13	1.91	0.51
11:N:502:HEM:CMB	11:N:502:HEM:HBB2	2.41	0.51
2:P:186:PHE:CE1	2:P:191:GLY:HA2	2.45	0.50
7:O:317:PRO:HG3	8:S:31:PRO:HD3	1.94	0.50
7:D:218:LEU:HD11	18:D:401:HEC:HMB2	1.94	0.50
7:O:218:LEU:HD11	18:O:401:HEC:HMB2	1.93	0.50
2:P:83:THR:HA	13:P:303:PTY:H121	1.94	0.49
1:N:49:THR:HG21	1:N:78:ILE:HD13	1.94	0.49
11:C:501:HEM:HBB2	11:C:501:HEM:HMB1	1.94	0.49
14:N:504:CDL:HA21	8:S:51:ARG:HH21	1.77	0.49
2:P:84:VAL:HG23	13:P:303:PTY:C43	2.40	0.49
14:A:3002:CDL:H132	14:A:3002:CDL:H522	1.94	0.48
14:H:701:CDL:OB3	14:H:702:CDL:O1	2.30	0.48
13:P:303:PTY:H141	13:P:303:PTY:H311	1.94	0.48
14:C:505:CDL:HB32	1:N:3:LEU:HD11	1.96	0.48
14:N:504:CDL:OB3	14:S:101:CDL:O1	2.31	0.48
2:P:49:THR:N	2:P:50:PRO:HD2	2.29	0.48
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.50	0.47
10:U:35:PHE:HE1	17:U:101:XP4:H8	1.80	0.47
13:C:504:PTY:H132	2:E:72:PHE:CD2	2.49	0.47
5:A:82:LYS:HA	5:A:82:LYS:HD3	1.64	0.47
1:C:49:THR:HG21	1:C:78:ILE:HD13	1.95	0.47
17:A:3003:XP4:H8	10:J:35:PHE:HE1	1.80	0.47
5:L:267:GLU:HG3	8:S:28:THR:HG22	1.97	0.47
1:N:156:TRP:CE3	1:N:157:LEU:HG	2.50	0.46
13:P:303:PTY:H331	13:P:303:PTY:H361	1.72	0.46
7:D:248:MET:HB2	18:D:401:HEC:C1D	2.45	0.46
11:C:502:HEM:HBC2	11:C:502:HEM:CMC	2.43	0.46
2:P:180:GLY:HA2	2:P:186:PHE:HB2	1.97	0.46
2:P:103:VAL:HG22	2:P:120:TRP:HD1	1.81	0.46
6:M:47:TYR:HB3	6:M:220:VAL:CG1	2.45	0.46
13:N:505:PTY:H372	13:N:505:PTY:H402	1.70	0.46
13:N:505:PTY:H112	13:N:505:PTY:HC12	1.98	0.45
13:N:505:PTY:H331	13:N:505:PTY:H362	1.51	0.45
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.65	0.45
15:J:101:LMT:H71	15:J:101:LMT:H41	1.75	0.45
1:C:202:HIS:HD2	15:C:506:LMT:O3'	2.00	0.45
1:N:226:SER:HB3	13:N:505:PTY:H321	2.00	0.44
13:N:505:PTY:H111	12:T:201:PC1:O31	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:171:LEU:HD12	2:P:190:HIS:CE1	2.52	0.44
14:H:702:CDL:HA62	14:H:702:CDL:H311	1.58	0.44
6:M:249:ILE:HD11	6:M:393:LEU:HD21	2.00	0.44
7:O:248:MET:HB2	18:O:401:HEC:C1D	2.48	0.44
2:P:193:HIS:O	2:P:200:ILE:HD12	2.18	0.44
6:B:47:TYR:HB3	6:B:220:VAL:CG1	2.47	0.44
5:L:375:THR:C	5:L:436:ARG:HH12	2.22	0.43
1:C:305:LEU:N	1:C:306:PRO:CD	2.81	0.43
13:C:504:PTY:HC31	5:A:467:ASN:CG	2.38	0.43
1:N:305:LEU:N	1:N:306:PRO:CD	2.82	0.43
5:A:375:THR:C	5:A:436:ARG:HH12	2.22	0.43
1:N:27:ASN:HB2	14:N:504:CDL:OB4	2.18	0.43
1:N:108:THR:HA	14:N:506:CDL:OA4	2.18	0.43
10:J:69:GLU:HA	10:J:72:ILE:HD12	2.00	0.43
10:U:32:ILE:HB	10:U:33:PRO:HD3	2.01	0.43
10:U:69:GLU:HA	10:U:72:ILE:HD12	2.00	0.43
2:P:106:LYS:HA	2:P:221:THR:HG22	2.01	0.43
6:B:48:ALA:HB1	6:B:53:VAL:HG12	2.01	0.43
2:P:147:ARG:HE	2:P:147:ARG:HB2	1.29	0.43
5:A:119:PHE:HE1	6:B:349:ALA:HB2	1.84	0.43
6:B:34:ILE:HD13	6:B:100:LEU:HD23	2.01	0.42
6:B:236:ARG:HD3	6:M:170:TYR:CD1	2.54	0.42
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.54	0.42
1:C:320:PRO:HD2	3:G:31:TYR:CZ	2.55	0.42
2:P:196:ILE:H	2:P:196:ILE:HG12	1.55	0.42
2:P:210:GLU:H	2:P:210:GLU:HG2	1.69	0.42
7:O:316:SER:N	7:O:317:PRO:CD	2.83	0.42
13:P:303:PTY:H161	13:P:303:PTY:H132	1.81	0.42
6:B:249:ILE:HD11	6:B:302:PHE:HB2	2.02	0.42
10:J:11:LYS:HD2	10:J:12:PRO:HD2	2.01	0.42
6:M:53:VAL:HG12	6:M:173:VAL:HG13	2.02	0.42
2:P:84:VAL:HG22	13:P:303:PTY:H441	1.78	0.42
7:D:316:SER:N	7:D:317:PRO:CD	2.82	0.42
1:N:227:PHE:HZ	13:N:505:PTY:HC6	1.85	0.42
11:C:501:HEM:HHD	11:C:501:HEM:CBC	2.49	0.42
5:L:395:LEU:HD12	6:M:34:ILE:HG22	2.01	0.42
5:A:79:LEU:HD12	5:A:79:LEU:HA	1.89	0.42
6:M:175:LEU:HA	6:M:178:VAL:HG12	2.01	0.42
6:M:249:ILE:CD1	6:M:393:LEU:HD21	2.50	0.42
14:S:101:CDL:HA62	14:S:101:CDL:H311	1.65	0.42
1:N:76:TRP:CG	7:O:285:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TRP:CG	7:D:285:GLU:HG3	2.54	0.42
1:C:108:THR:HA	14:C:505:CDL:OA4	2.19	0.42
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.54	0.42
2:P:192:SER:HB3	2:P:204:PRO:HD2	2.02	0.42
7:D:105:LEU:HB3	9:I:44:ILE:HD12	2.02	0.42
2:P:177:GLY:HA2	2:P:185:TRP:CD1	2.54	0.42
6:B:247:LEU:HD13	6:B:393:LEU:HB3	2.01	0.41
9:T:19:VAL:HG22	12:T:201:PC1:H332	2.02	0.41
3:R:71:VAL:HG11	8:S:21:GLN:HG2	2.02	0.41
5:L:97:GLU:HB3	6:M:339:ARG:HD3	2.02	0.41
14:L:3001:CDL:H1	14:L:3002:CDL:HA4	2.02	0.41
6:B:29:ASP:HB2	6:B:200:PRO:HD3	2.02	0.41
5:L:119:PHE:HE1	6:M:349:ALA:HB2	1.85	0.41
5:A:265:GLY:HA3	5:A:447:ASP:HB3	2.01	0.41
6:B:175:LEU:HA	6:B:178:VAL:HG12	2.01	0.41
10:J:32:ILE:HB	10:J:33:PRO:HD3	2.02	0.41
1:N:224:TYR:HB3	7:O:315:TRP:CZ2	2.56	0.41
1:N:234:PHE:CZ	7:O:303:MET:HE2	2.56	0.41
2:P:156:VAL:HG21	2:P:159:PRO:HA	2.03	0.41
5:A:58:ILE:HG12	5:A:212:MET:HG2	2.02	0.41
5:A:97:GLU:HG3	6:B:343:LYS:HE2	2.01	0.41
5:A:97:GLU:HB3	6:B:339:ARG:HD2	2.03	0.41
8:H:61:LEU:HD23	8:H:61:LEU:HA	1.95	0.41
13:E:401:PTY:H141	13:E:401:PTY:H311	2.02	0.41
6:M:29:ASP:HB2	6:M:200:PRO:HD3	2.03	0.41
5:A:96:ILE:HG12	5:A:103:LEU:HD13	2.02	0.41
11:N:502:HEM:HBB2	11:N:502:HEM:HMB1	2.03	0.41
13:N:505:PTY:H311	13:N:505:PTY:H342	1.30	0.41
1:C:238:LEU:HD13	7:D:300:ILE:HG22	2.02	0.41
5:A:160:LYS:HD2	5:A:160:LYS:HA	1.91	0.41
5:L:58:ILE:HG12	5:L:212:MET:HG2	2.03	0.41
1:N:178:ARG:HE	1:N:178:ARG:HB3	1.50	0.40
2:P:116:VAL:HG23	2:P:127:ILE:O	2.21	0.40
2:P:147:ARG:HD2	2:P:206:PRO:HA	2.03	0.40
9:I:37:ILE:HD13	9:I:37:ILE:HA	1.97	0.40
1:N:10:LEU:HD23	1:N:10:LEU:HA	1.89	0.40
1:C:208:ASN:HB2	1:C:209:PRO:HD2	2.03	0.40
2:P:72:PHE:HE2	13:N:505:PTY:H152	1.86	0.40
6:B:241:ASN:HB3	6:B:314:ILE:HD12	2.03	0.40
6:M:332:VAL:HG23	6:M:383:PRO:HB3	2.03	0.40
1:C:224:TYR:HB3	7:D:315:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:265:GLY:HA3	5:L:447:ASP:HB3	2.03	0.40
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.89	0.40
7:O:197:PRO:HG3	18:O:401:HEC:HMD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
1	N	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
2	E	59/225 (26%)	58 (98%)	1 (2%)	0	100	100
2	P	184/225 (82%)	171 (93%)	12 (6%)	1 (0%)	25	49
3	G	122/128 (95%)	122 (100%)	0	0	100	100
3	R	122/128 (95%)	122 (100%)	0	0	100	100
4	F	69/137 (50%)	66 (96%)	3 (4%)	0	100	100
4	Q	69/137 (50%)	66 (96%)	3 (4%)	0	100	100
5	A	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
5	L	434/474 (92%)	422 (97%)	12 (3%)	0	100	100
6	B	400/417 (96%)	383 (96%)	16 (4%)	1 (0%)	37	61
6	M	400/417 (96%)	386 (96%)	14 (4%)	0	100	100
7	D	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
7	O	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
9	I	52/69 (75%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
10	J	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
10	U	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
All	All	3955/4680 (84%)	3851 (97%)	102 (3%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	368	SER
2	P	172	GLY

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	C	331/333 (99%)	322 (97%)	9 (3%)	40	69
1	N	331/333 (99%)	320 (97%)	11 (3%)	33	62
2	E	49/182 (27%)	44 (90%)	5 (10%)	6	15
2	P	154/182 (85%)	136 (88%)	18 (12%)	4	11
3	G	113/117 (97%)	105 (93%)	8 (7%)	12	30
3	R	113/117 (97%)	110 (97%)	3 (3%)	40	69
4	F	61/123 (50%)	58 (95%)	3 (5%)	21	47
4	Q	61/123 (50%)	60 (98%)	1 (2%)	58	82
5	A	377/407 (93%)	366 (97%)	11 (3%)	37	67
5	L	377/407 (93%)	366 (97%)	11 (3%)	37	67
6	B	311/322 (97%)	301 (97%)	10 (3%)	34	63
6	M	311/322 (97%)	302 (97%)	9 (3%)	37	67
7	D	192/268 (72%)	191 (100%)	1 (0%)	86	95
7	O	192/268 (72%)	191 (100%)	1 (0%)	86	95
8	H	67/71 (94%)	66 (98%)	1 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	67/71 (94%)	66 (98%)	1 (2%)	60	83
9	I	46/57 (81%)	45 (98%)	1 (2%)	47	76
9	T	46/57 (81%)	45 (98%)	1 (2%)	47	76
10	J	63/68 (93%)	62 (98%)	1 (2%)	58	82
10	U	63/68 (93%)	63 (100%)	0	100	100
All	All	3325/3896 (85%)	3219 (97%)	106 (3%)	36	63

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ARG
1	C	89	PHE
1	C	136	PHE
1	C	178	ARG
1	C	184	TYR
1	C	197	HIS
1	C	250	LYS
1	C	288	LYS
1	C	369	MET
2	P	54	LYS
2	P	62	ARG
2	P	90	ASN
2	P	100	MET
2	P	102	LYS
2	P	106	LYS
2	P	115	ASN
2	P	116	VAL
2	P	117	ILE
2	P	119	LYS
2	P	143	VAL
2	P	146	LEU
2	P	147	ARG
2	P	158	LYS
2	P	176	ILE
2	P	195	ASP
2	P	196	ILE
2	P	213	GLU
3	G	3	SER
3	G	6	SER
3	G	17	SER

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Mol	Chain	Res	Type
3	G	22	LYS
3	G	23	ILE
3	G	40	LEU
3	G	50	GLU
3	G	123	GLU
4	F	83	HIS
4	F	96	HIS
4	F	100	GLU
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	137	SER
5	A	197	THR
5	A	230	GLU
5	A	267	GLU
5	A	397	LEU
5	A	466	ARG
6	B	45	SER
6	B	60	PHE
6	B	79	LEU
6	B	102	GLN
6	B	119	LYS
6	B	247	LEU
6	B	249	ILE
6	B	261	SER
6	B	345	LYS
6	B	376	GLU
7	D	193	GLN
8	H	51	ARG
9	I	27	PHE
10	J	11	LYS
1	N	79	ARG
1	N	89	PHE
1	N	136	PHE
1	N	178	ARG
1	N	184	TYR
1	N	187	PRO
1	N	197	HIS
1	N	250	LYS
1	N	255	ASP

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Mol	Chain	Res	Type
1	N	288	LYS
1	N	369	MET
2	E	54	LYS
2	E	55	ASP
2	E	62	ARG
2	E	65	SER
2	E	90	ASN
3	R	17	SER
3	R	22	LYS
3	R	23	ILE
4	Q	83	HIS
5	L	29	LYS
5	L	48	LEU
5	L	51	THR
5	L	87	ARG
5	L	97	GLU
5	L	99	MET
5	L	137	SER
5	L	185	LEU
5	L	378	SER
5	L	441	LYS
5	L	466	ARG
6	M	19	GLU
6	M	32	SER
6	M	60	PHE
6	M	101	LYS
6	M	119	LYS
6	M	272	SER
6	M	273	VAL
6	M	331	GLU
6	M	376	GLU
7	O	193	GLN
8	S	51	ARG
9	T	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	11	ASN
1	C	14	ASN
1	C	173	ASN
1	C	202	HIS

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Mol	Chain	Res	Type
1	C	332	ASN
2	P	90	ASN
3	G	54	ASN
4	F	132	HIS
5	A	74	HIS
5	A	222	HIS
6	B	87	HIS
6	B	215	GLN
10	J	70	HIS
1	N	14	ASN
1	N	202	HIS
1	N	332	ASN
2	E	90	ASN
4	Q	132	HIS
6	M	87	HIS
6	M	92	HIS
6	M	184	GLN
6	M	215	GLN
10	U	70	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CDL	H	701	-	49,49,99	0.38	0	55,61,111	0.72	0
18	HEC	O	401	7	32,50,50	1.82	10 (31%)	24,82,82	2.90	8 (33%)
14	CDL	N	506	-	47,47,99	0.51	0	53,59,111	0.91	3 (5%)
12	PC1	T	201	-	31,31,53	0.40	0	37,39,61	0.61	0
11	HEM	C	502	1	41,50,50	1.39	6 (14%)	45,82,82	2.45	22 (48%)
18	HEC	D	401	7	32,50,50	1.77	9 (28%)	24,82,82	3.00	6 (25%)
15	LMT	P	302	-	36,36,36	0.53	0	47,47,47	1.02	5 (10%)
13	PTY	C	504	-	40,40,49	0.37	0	43,45,54	0.58	0
14	CDL	A	3001	-	41,41,99	0.56	0	45,51,111	0.69	1 (2%)
14	CDL	L	3002	-	46,46,99	0.39	0	51,56,111	0.87	3 (5%)
15	LMT	J	101	-	36,36,36	0.55	0	47,47,47	1.20	5 (10%)
12	PC1	N	503	-	37,37,53	0.72	0	43,45,61	0.85	1 (2%)
13	PTY	N	505	-	40,40,49	0.39	0	43,45,54	0.75	2 (4%)
14	CDL	L	3001	-	41,41,99	0.43	0	45,51,111	0.75	1 (2%)
13	PTY	E	401	-	40,40,49	0.44	0	43,45,54	0.49	0
16	FES	P	301	2	0,4,4	-	-	-	-	-
11	HEM	N	502	1	41,50,50	1.38	6 (14%)	45,82,82	2.33	21 (46%)
12	PC1	C	503	-	37,37,53	0.79	1 (2%)	43,45,61	1.01	3 (6%)
14	CDL	C	505	-	47,47,99	0.49	0	53,59,111	0.92	3 (5%)
14	CDL	A	3002	-	46,46,99	0.40	0	51,56,111	0.83	2 (3%)
14	CDL	N	504	-	49,49,99	0.48	1 (2%)	55,61,111	0.58	0
15	LMT	C	506	-	36,36,36	0.56	0	47,47,47	1.42	10 (21%)
13	PTY	P	303	-	40,40,49	0.50	0	43,45,54	0.63	0
14	CDL	S	101	-	38,38,99	0.49	0	44,50,111	1.25	5 (11%)
12	PC1	I	201	-	31,31,53	0.41	0	37,39,61	0.67	0
17	XP4	A	3003	-	23,23,39	1.50	2 (8%)	27,28,44	2.60	9 (33%)
15	LMT	N	507	-	36,36,36	0.51	0	47,47,47	1.14	4 (8%)
17	XP4	U	101	-	23,23,39	1.47	2 (8%)	27,28,44	2.41	7 (25%)
11	HEM	C	501	1	41,50,50	1.48	6 (14%)	45,82,82	2.39	15 (33%)
14	CDL	H	702	-	38,38,99	0.45	0	44,50,111	1.20	4 (9%)
11	HEM	N	501	1	41,50,50	1.52	7 (17%)	45,82,82	2.28	15 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	H	701	-	-	34/59/59/110	-
18	HEC	O	401	7	-	2/10/54/54	-
14	CDL	N	506	-	-	28/57/57/110	-
12	PC1	T	201	-	-	13/35/35/57	-
11	HEM	C	502	1	-	4/12/54/54	-
18	HEC	D	401	7	-	2/10/54/54	-
15	LMT	P	302	-	-	6/21/61/61	0/2/2/2
13	PTY	C	504	-	-	29/44/44/53	-
14	CDL	A	3001	-	-	15/48/48/110	-
14	CDL	L	3002	-	-	27/54/54/110	-
15	LMT	J	101	-	-	14/21/61/61	0/2/2/2
12	PC1	N	503	-	-	13/41/41/57	-
13	PTY	N	505	-	-	30/44/44/53	-
14	CDL	L	3001	-	-	20/48/48/110	-
13	PTY	E	401	-	-	26/44/44/53	-
16	FES	P	301	2	-	-	0/1/1/1
11	HEM	N	502	1	-	4/12/54/54	-
12	PC1	C	503	-	-	13/41/41/57	-
14	CDL	C	505	-	-	30/57/57/110	-
14	CDL	A	3002	-	-	30/54/54/110	-
14	CDL	N	504	-	-	35/59/59/110	-
15	LMT	C	506	-	-	15/21/61/61	0/2/2/2
13	PTY	P	303	-	-	25/44/44/53	-
14	CDL	S	101	-	-	29/48/48/110	-
12	PC1	I	201	-	-	15/35/35/57	-
17	XP4	A	3003	-	-	1/24/24/41	-
15	LMT	N	507	-	-	13/21/61/61	0/2/2/2
17	XP4	U	101	-	-	3/24/24/41	-
11	HEM	C	501	1	-	5/12/54/54	-
14	CDL	H	702	-	-	29/48/48/110	-
11	HEM	N	501	1	-	5/12/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	101	XP4	O7-C18	5.28	1.47	1.35
17	A	3003	XP4	O7-C18	5.22	1.47	1.35
18	D	401	HEC	C2B-C3B	4.48	1.45	1.40
18	O	401	HEC	C3C-C2C	4.12	1.45	1.40
11	N	501	HEM	C3C-C2C	-4.09	1.34	1.40
11	N	502	HEM	C1B-NB	-3.91	1.33	1.40
17	A	3003	XP4	O5-C4	3.91	1.44	1.33
11	C	501	HEM	C3C-C2C	-3.85	1.35	1.40
11	C	502	HEM	C1B-NB	-3.84	1.33	1.40
18	O	401	HEC	C2B-C3B	3.83	1.44	1.40
18	D	401	HEC	C3C-C2C	3.71	1.44	1.40
11	N	501	HEM	C4B-NB	-3.58	1.31	1.38
17	U	101	XP4	O5-C4	3.54	1.43	1.33
11	N	501	HEM	C1B-NB	-3.41	1.34	1.40
11	C	501	HEM	C4B-NB	-3.35	1.31	1.38
11	C	501	HEM	C4D-ND	-3.30	1.34	1.40
11	C	501	HEM	C1B-NB	-3.28	1.34	1.40
11	N	501	HEM	C4D-ND	-3.07	1.35	1.40
11	N	502	HEM	C4B-NB	-3.02	1.32	1.38
11	C	502	HEM	C1D-ND	-2.78	1.33	1.38
18	O	401	HEC	C3D-C2D	2.71	1.45	1.37
18	O	401	HEC	C2A-C3A	2.70	1.45	1.37
11	C	502	HEM	FE-NB	2.66	2.10	1.96
11	N	501	HEM	FE-NB	2.58	2.09	1.96
12	C	503	PC1	C22-C21	2.52	1.58	1.50
18	D	401	HEC	C3D-C2D	2.52	1.45	1.37
18	O	401	HEC	CAA-C2A	-2.47	1.47	1.52
18	D	401	HEC	C2A-C3A	2.46	1.45	1.37
11	C	501	HEM	FE-NB	2.44	2.08	1.96
18	O	401	HEC	CAD-C3D	-2.42	1.48	1.52
18	D	401	HEC	C1B-NB	-2.40	1.31	1.36
11	C	502	HEM	C4B-NB	-2.33	1.34	1.38
18	D	401	HEC	C2A-C1A	2.33	1.47	1.42
11	N	502	HEM	C1D-ND	-2.31	1.34	1.38
11	C	502	HEM	CAA-C2A	-2.30	1.48	1.52
18	O	401	HEC	C4D-ND	-2.29	1.31	1.36
11	N	501	HEM	CHB-C1B	2.27	1.40	1.35
11	C	502	HEM	CHA-C4D	2.27	1.40	1.35
11	N	502	HEM	C4D-ND	-2.26	1.36	1.40
18	D	401	HEC	C4D-ND	-2.25	1.31	1.36
18	D	401	HEC	C1C-NC	-2.21	1.31	1.36
11	N	501	HEM	O2D-CGD	-2.16	1.23	1.30
18	O	401	HEC	C4D-CHA	2.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	501	HEM	O2D-CGD	-2.13	1.23	1.30
18	D	401	HEC	CAD-C3D	-2.10	1.49	1.52
14	N	504	CDL	C15-C14	2.09	1.67	1.49
11	N	502	HEM	FE-NB	2.08	2.07	1.96
18	O	401	HEC	C1B-NB	-2.06	1.31	1.36
11	N	502	HEM	CAA-C2A	-2.02	1.49	1.52
18	O	401	HEC	C3A-C4A	2.02	1.47	1.42

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	3003	XP4	O7-C18-C19	8.28	126.32	111.09
18	D	401	HEC	CMB-C2B-C3B	8.01	135.23	125.82
17	U	101	XP4	O7-C18-C19	7.97	125.75	111.09
18	D	401	HEC	C1D-C2D-C3D	-7.59	101.72	107.00
18	O	401	HEC	C1D-C2D-C3D	-7.32	101.91	107.00
11	N	502	HEM	CHC-C4B-NB	7.29	132.35	124.43
18	O	401	HEC	CMB-C2B-C3B	7.14	134.21	125.82
11	C	502	HEM	CHC-C4B-NB	6.48	131.47	124.43
11	C	501	HEM	CHC-C4B-NB	6.46	131.44	124.43
11	N	501	HEM	CBA-CAA-C2A	-6.22	102.01	112.62
11	C	501	HEM	CBA-CAA-C2A	-6.05	102.30	112.62
11	N	501	HEM	CHA-C4D-ND	5.90	131.67	124.38
17	A	3003	XP4	O7-C18-O8	-5.71	111.61	122.96
17	U	101	XP4	O7-C18-O8	-5.67	111.70	122.96
11	C	501	HEM	CHA-C4D-ND	5.32	130.95	124.38
11	N	501	HEM	CHC-C4B-NB	5.24	130.13	124.43
18	D	401	HEC	CAA-CBA-CGA	-5.10	99.46	113.76
11	N	501	HEM	CHD-C1D-ND	4.88	129.73	124.43
18	O	401	HEC	CMC-C2C-C3C	4.79	131.45	125.82
18	O	401	HEC	CAA-CBA-CGA	-4.64	100.76	113.76
11	C	501	HEM	CHD-C1D-ND	4.57	129.40	124.43
18	D	401	HEC	CMC-C2C-C3C	4.56	131.19	125.82
18	O	401	HEC	CBD-CAD-C3D	-4.52	104.91	112.62
11	C	502	HEM	C1B-NB-C4B	4.51	109.73	105.07
15	C	506	LMT	C1'-O5'-C5'	4.43	122.39	113.69
11	C	501	HEM	C1B-NB-C4B	4.33	109.55	105.07
11	N	502	HEM	C1B-NB-C4B	4.23	109.44	105.07
11	C	502	HEM	C4C-CHD-C1D	-4.17	117.06	122.56
11	C	502	HEM	CHA-C4D-ND	4.14	129.49	124.38
11	C	501	HEM	CAD-CBD-CGD	-4.12	104.74	113.60
18	D	401	HEC	CBD-CAD-C3D	-4.11	105.60	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	502	HEM	C4B-CHC-C1C	-3.91	117.39	122.56
17	A	3003	XP4	P1-O4-C1	3.90	129.05	118.30
11	C	502	HEM	CMA-C3A-C4A	-3.85	122.54	128.46
15	J	101	LMT	C1-O1'-C1'	-3.75	107.62	113.84
11	N	501	HEM	CHA-C4D-C3D	-3.70	118.39	125.33
11	N	501	HEM	C1B-NB-C4B	3.66	108.86	105.07
11	C	502	HEM	CHD-C1D-ND	3.66	128.41	124.43
14	S	101	CDL	CB4-OB6-CB5	3.63	124.67	117.90
11	N	502	HEM	CHB-C1B-NB	3.60	128.82	124.38
17	A	3003	XP4	O4-P1-O2	-3.58	96.43	106.47
11	C	502	HEM	CHA-C4D-C3D	-3.54	118.68	125.33
14	H	702	CDL	CB4-OB6-CB5	3.54	124.49	117.90
17	U	101	XP4	O5-C4-O6	-3.49	114.78	123.59
11	C	501	HEM	CHA-C4D-C3D	-3.48	118.80	125.33
14	L	3001	CDL	OB6-CB4-CB3	-3.42	97.57	109.56
11	N	502	HEM	C4C-CHD-C1D	-3.38	118.09	122.56
11	C	502	HEM	CHD-C1D-C2D	-3.31	119.80	124.98
11	N	502	HEM	CHD-C1D-C2D	-3.28	119.85	124.98
11	N	501	HEM	CAD-CBD-CGD	-3.27	106.57	113.60
11	N	502	HEM	CHC-C4B-C3B	-3.26	119.57	124.57
11	C	501	HEM	CHD-C1D-C2D	-3.24	119.92	124.98
14	C	505	CDL	OB6-CB4-CB3	3.24	120.12	108.40
17	A	3003	XP4	O5-C4-O6	-3.21	115.50	123.59
17	U	101	XP4	P1-O4-C1	3.18	127.06	118.30
15	J	101	LMT	O5'-C1'-O1'	-3.18	102.44	109.97
11	C	502	HEM	CHB-C1B-NB	3.16	128.29	124.38
11	C	502	HEM	C2C-C3C-C4C	3.09	109.05	106.90
11	N	502	HEM	CHD-C1D-ND	3.08	127.78	124.43
11	C	501	HEM	CMA-C3A-C4A	-3.08	123.73	128.46
11	C	502	HEM	C3C-C4C-NC	-3.07	105.15	110.94
17	A	3003	XP4	O5-C4-C5	3.06	121.52	111.91
17	U	101	XP4	O5-C4-C5	3.04	121.44	111.91
12	C	503	PC1	O22-C21-C22	3.02	135.53	123.73
17	A	3003	XP4	O1-P1-O4	2.93	114.54	106.73
11	N	502	HEM	CBA-CAA-C2A	-2.90	107.68	112.62
14	N	506	CDL	OB6-CB4-CB3	2.89	118.88	108.40
14	H	702	CDL	OB6-CB4-CB6	2.87	118.79	108.40
14	H	702	CDL	OA5-PA1-OA3	-2.87	97.86	109.07
11	N	501	HEM	CHD-C1D-C2D	-2.86	120.51	124.98
11	C	502	HEM	CBA-CAA-C2A	-2.84	107.77	112.62
14	A	3002	CDL	OA6-CA4-CA6	2.84	118.68	108.40
11	C	502	HEM	CHC-C4B-C3B	-2.81	120.26	124.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S	101	CDL	OB6-CB5-C51	2.77	116.19	111.09
12	C	503	PC1	O21-C21-C22	-2.77	105.52	111.50
11	C	501	HEM	C4A-C3A-C2A	2.76	108.92	107.00
11	N	501	HEM	C4A-C3A-C2A	2.73	108.90	107.00
18	O	401	HEC	CMD-C2D-C3D	2.73	130.09	124.94
14	S	101	CDL	OB6-CB4-CB6	2.71	118.23	108.40
15	P	302	LMT	C4-C3-C2	-2.71	100.67	114.42
11	N	502	HEM	O2D-CGD-CBD	2.71	122.73	114.03
15	N	507	LMT	C3B-C4B-C5B	2.70	115.06	110.24
14	C	505	CDL	CB4-OB6-CB5	2.69	124.42	117.79
15	C	506	LMT	O5'-C5'-C4'	2.69	115.42	109.75
11	N	502	HEM	C3C-C4C-NC	-2.67	105.91	110.94
11	N	502	HEM	CAD-C3D-C4D	2.67	129.32	124.66
11	C	502	HEM	C4B-CHC-C1C	-2.66	119.05	122.56
11	N	502	HEM	CHA-C4D-ND	2.64	127.64	124.38
11	C	501	HEM	CHC-C4B-C3B	-2.63	120.55	124.57
15	N	507	LMT	C1B-O5B-C5B	2.60	118.80	113.69
11	C	502	HEM	O2D-CGD-CBD	2.60	122.39	114.03
14	L	3002	CDL	OA6-CA4-CA6	2.59	117.80	108.40
15	C	506	LMT	C1B-O5B-C5B	2.58	118.75	113.69
15	C	506	LMT	O5'-C1'-C2'	2.55	115.75	110.35
15	N	507	LMT	O5B-C5B-C4B	2.51	114.25	109.69
11	C	502	HEM	CBD-CAD-C3D	-2.51	105.65	112.63
14	S	101	CDL	OA5-PA1-OA3	-2.50	99.30	109.07
14	N	506	CDL	CB4-OB6-CB5	2.50	123.93	117.79
14	L	3002	CDL	OA2-PA1-OA3	2.48	118.77	109.07
11	C	502	HEM	CAD-C3D-C4D	2.47	128.97	124.66
14	A	3001	CDL	OB8-CB6-CB4	2.46	117.65	105.77
15	C	506	LMT	C3B-C4B-C5B	2.40	114.53	110.24
13	N	505	PTY	O7-C8-C11	2.40	116.67	111.50
14	A	3002	CDL	OA2-PA1-OA3	2.39	118.39	109.07
14	L	3002	CDL	OA5-PA1-OA3	-2.38	99.75	109.07
15	J	101	LMT	C1'-O5'-C5'	-2.38	109.01	113.69
15	N	507	LMT	C1'-O5'-C5'	2.35	118.31	113.69
15	C	506	LMT	O1'-C1'-C2'	-2.35	104.63	108.30
11	N	501	HEM	CHC-C4B-C3B	-2.35	120.98	124.57
15	C	506	LMT	O5B-C5B-C4B	2.34	113.95	109.69
17	U	101	XP4	O3-P1-O4	-2.32	100.57	106.73
11	N	502	HEM	CBD-CAD-C3D	-2.30	106.22	112.63
11	N	502	HEM	CMA-C3A-C4A	-2.30	124.94	128.46
11	C	501	HEM	CHB-C1B-NB	2.30	127.22	124.38
11	C	501	HEM	CMD-C2D-C1D	2.29	128.53	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	502	HEM	CHA-C4D-C3D	-2.28	121.06	125.33
17	A	3003	XP4	O5-C3-C2	-2.27	101.84	108.43
14	S	101	CDL	OB6-CB4-CB3	2.26	116.58	108.40
12	C	503	PC1	C23-C22-C21	2.25	121.81	113.62
11	N	501	HEM	CHB-C1B-NB	2.23	127.13	124.38
11	C	502	HEM	C4A-C3A-C2A	2.22	108.54	107.00
11	C	502	HEM	O2A-CGA-O1A	-2.21	117.79	123.30
15	P	302	LMT	C2'-C3'-C4'	2.20	114.72	109.68
11	N	502	HEM	CHB-C1B-C2B	-2.19	120.67	126.72
14	C	505	CDL	OA6-CA5-C11	2.19	116.22	111.50
11	N	502	HEM	CMD-C2D-C1D	2.19	128.37	125.04
11	C	502	HEM	O2A-CGA-CBA	2.19	121.05	114.03
11	C	501	HEM	C3B-C2B-C1B	-2.19	104.86	106.49
11	N	501	HEM	CMC-C2C-C3C	-2.18	120.60	124.68
15	P	302	LMT	O5'-C1'-O1'	-2.17	104.84	109.97
14	N	506	CDL	OB6-CB4-CB6	2.16	116.22	108.40
18	O	401	HEC	O1D-CGD-CBD	-2.14	116.20	123.08
18	O	401	HEC	O2A-CGA-CBA	2.13	120.89	114.03
12	N	503	PC1	O22-C21-C22	2.13	132.05	123.73
15	P	302	LMT	O1'-C1'-C2'	2.12	111.62	108.30
13	N	505	PTY	O7-C6-C5	2.12	116.09	108.40
15	C	506	LMT	C6-C5-C4	-2.12	103.66	114.42
14	H	702	CDL	OB6-CB5-C51	2.12	114.99	111.09
15	J	101	LMT	O1'-C1'-C2'	2.11	111.59	108.30
11	C	502	HEM	CMA-C3A-C2A	2.10	128.90	124.94
17	U	101	XP4	O5-C3-C2	-2.09	102.34	108.43
11	C	501	HEM	CBB-CAB-C3B	-2.08	117.28	127.62
18	D	401	HEC	CMA-C3A-C2A	2.08	128.86	124.94
11	N	501	HEM	CBB-CAB-C3B	-2.07	117.32	127.62
15	C	506	LMT	O2'-C2'-C1'	-2.07	105.02	110.05
11	N	502	HEM	O1D-CGD-CBD	-2.06	116.45	123.08
11	N	502	HEM	C2D-C1D-ND	2.05	112.34	109.88
11	N	502	HEM	O2A-CGA-O1A	-2.04	118.21	123.30
17	A	3003	XP4	O3-P1-O4	-2.04	101.30	106.73
11	N	501	HEM	C4D-ND-C1D	2.03	107.17	105.07
15	P	302	LMT	C1-O1'-C1'	-2.02	110.49	113.84
11	C	502	HEM	CBB-CAB-C3B	-2.02	117.56	127.62
15	J	101	LMT	C3-C2-C1	-2.02	104.53	113.49
15	C	506	LMT	C7-C6-C5	-2.01	104.24	114.42
11	N	501	HEM	CMD-C2D-C1D	2.00	128.09	125.04

There are no chirality outliers.

All (515) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	I	201	PC1	C11-O13-P-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	O21-C2-C3-O31
13	C	504	PTY	N1-C2-C3-O11
13	C	504	PTY	C11-C8-O7-C6
13	C	504	PTY	C3-O11-P1-O13
13	P	303	PTY	C5-O14-P1-O11
13	P	303	PTY	C5-O14-P1-O12
13	N	505	PTY	C11-C8-O7-C6
13	N	505	PTY	C3-O11-P1-O12
13	N	505	PTY	C3-O11-P1-O13
13	N	505	PTY	C5-O14-P1-O13
13	E	401	PTY	N1-C2-C3-O11
13	E	401	PTY	C3-O11-P1-O13
13	E	401	PTY	C5-O14-P1-O12
14	C	505	CDL	O1-C1-CA2-OA2
14	C	505	CDL	CA3-OA5-PA1-OA3
14	C	505	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	CB2-OB2-PB2-OB3
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB2-OB2-PB2-OB5
14	C	505	CDL	CB3-OB5-PB2-OB3
14	C	505	CDL	CB3-OB5-PB2-OB4
14	A	3001	CDL	OA5-CA3-CA4-OA6
14	A	3001	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	CA2-OA2-PA1-OA3
14	A	3002	CDL	CA2-OA2-PA1-OA4
14	A	3002	CDL	CA2-OA2-PA1-OA5
14	A	3002	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	CA2-OA2-PA1-OA4
14	H	702	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CB3-OB5-PB2-OB4
14	N	504	CDL	CA2-OA2-PA1-OA3
14	N	504	CDL	CA2-OA2-PA1-OA4
14	N	506	CDL	CB2-C1-CA2-OA2
14	N	506	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
14	N	506	CDL	C11-CA5-OA6-CA4
14	N	506	CDL	CB2-OB2-PB2-OB3
14	N	506	CDL	CB2-OB2-PB2-OB4
14	N	506	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	CB3-OB5-PB2-OB4
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	L	3001	CDL	CB3-CB4-CB6-OB8
14	L	3002	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	CA2-OA2-PA1-OA3
14	L	3002	CDL	CA2-OA2-PA1-OA4
14	L	3002	CDL	CA2-OA2-PA1-OA5
14	L	3002	CDL	OB5-CB3-CB4-OB6
14	S	101	CDL	CA2-OA2-PA1-OA4
14	S	101	CDL	OA9-CA7-OA8-CA6
14	S	101	CDL	C31-CA7-OA8-CA6
14	S	101	CDL	CB3-OB5-PB2-OB2
14	S	101	CDL	CB3-OB5-PB2-OB4
14	S	101	CDL	C51-CB5-OB6-CB4
15	J	101	LMT	C2-C1-O1'-C1'
17	U	101	XP4	C1-O4-P1-O3
14	H	702	CDL	C51-CB5-OB6-CB4
14	H	702	CDL	OB9-CB7-OB8-CB6
14	S	101	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	CB4-CB6-OB8-CB7
12	T	201	PC1	C32-C31-O31-C3
14	H	702	CDL	C71-CB7-OB8-CB6
14	S	101	CDL	C71-CB7-OB8-CB6
14	H	702	CDL	OB7-CB5-OB6-CB4
12	T	201	PC1	O32-C31-O31-C3
14	A	3001	CDL	OA9-CA7-OA8-CA6
14	H	701	CDL	OB9-CB7-OB8-CB6
14	N	504	CDL	OB9-CB7-OB8-CB6
14	S	101	CDL	OB7-CB5-OB6-CB4
13	C	504	PTY	O10-C8-O7-C6
13	N	505	PTY	O10-C8-O7-C6
14	N	506	CDL	OA7-CA5-OA6-CA4
14	H	701	CDL	C71-CB7-OB8-CB6
14	N	504	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	OA9-CA7-OA8-CA6
15	J	101	LMT	O5'-C5'-C6'-O6'
14	A	3001	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	C31-CA7-OA8-CA6
14	L	3001	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	C31-CA7-OA8-CA6
14	C	505	CDL	OA7-CA5-OA6-CA4
14	L	3001	CDL	OA9-CA7-OA8-CA6
14	L	3001	CDL	OB9-CB7-OB8-CB6
15	J	101	LMT	C4-C5-C6-C7
13	N	505	PTY	C31-C32-C33-C34
14	A	3002	CDL	O1-C1-CB2-OB2
14	N	504	CDL	O1-C1-CA2-OA2
14	N	506	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3002	CDL	O1-C1-CB2-OB2
13	E	401	PTY	C35-C36-C37-C38
14	A	3001	CDL	OB6-CB4-CB6-OB8
14	A	3002	CDL	C11-CA5-OA6-CA4
14	L	3002	CDL	C11-CA5-OA6-CA4
13	C	504	PTY	C31-C32-C33-C34
13	C	504	PTY	C35-C36-C37-C38
13	P	303	PTY	C37-C38-C39-C40
13	N	505	PTY	C33-C34-C35-C36
15	N	507	LMT	O5'-C5'-C6'-O6'
14	N	504	CDL	OA9-CA7-OA8-CA6
15	C	506	LMT	O5'-C5'-C6'-O6'
15	N	507	LMT	O5B-C5B-C6B-O6B
15	J	101	LMT	C4'-C5'-C6'-O6'
15	P	302	LMT	C11-C10-C9-C8
15	C	506	LMT	O5B-C5B-C6B-O6B
13	N	505	PTY	C37-C38-C39-C40
13	P	303	PTY	C35-C36-C37-C38
15	J	101	LMT	C2-C3-C4-C5
14	C	505	CDL	CA2-C1-CB2-OB2
14	H	702	CDL	CB2-C1-CA2-OA2
14	N	504	CDL	CB2-C1-CA2-OA2
14	N	504	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	OA7-CA5-OA6-CA4
14	L	3002	CDL	OA7-CA5-OA6-CA4
15	N	507	LMT	C4'-C5'-C6'-O6'
12	C	503	PC1	C32-C31-O31-C3
12	I	201	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
13	P	303	PTY	C31-C30-O4-C1
14	L	3002	CDL	CA7-C31-C32-C33
14	N	504	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	OB5-CB3-CB4-OB6
14	S	101	CDL	O1-C1-CA2-OA2
15	C	506	LMT	C4'-C5'-C6'-O6'
14	L	3001	CDL	OB6-CB4-CB6-OB8
14	N	504	CDL	C51-CB5-OB6-CB4
13	N	505	PTY	C8-C11-C12-C13
12	I	201	PC1	C31-C32-C33-C34
14	H	701	CDL	CB7-C71-C72-C73
13	E	401	PTY	C40-C41-C42-C43
14	C	505	CDL	CA7-C31-C32-C33
14	A	3001	CDL	CB7-C71-C72-C73
14	A	3002	CDL	CA7-C31-C32-C33
14	H	701	CDL	CA5-C11-C12-C13
14	N	504	CDL	CA5-C11-C12-C13
14	N	504	CDL	CB7-C71-C72-C73
15	J	101	LMT	O5B-C5B-C6B-O6B
12	I	201	PC1	C21-C22-C23-C24
12	T	201	PC1	C21-C22-C23-C24
14	N	506	CDL	CA7-C31-C32-C33
12	C	503	PC1	O32-C31-O31-C3
13	P	303	PTY	C33-C34-C35-C36
15	C	506	LMT	O1'-C1-C2-C3
12	T	201	PC1	C31-C32-C33-C34
14	H	702	CDL	O1-C1-CB2-OB2
14	N	504	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	S	101	CDL	O1-C1-CB2-OB2
14	N	504	CDL	OB7-CB5-OB6-CB4
12	I	201	PC1	O32-C31-O31-C3
13	P	303	PTY	O30-C30-O4-C1
13	E	401	PTY	C8-C11-C12-C13
15	C	506	LMT	C4B-C5B-C6B-O6B
12	T	201	PC1	C11-O13-P-O11
13	N	505	PTY	C3-O11-P1-O14
13	N	505	PTY	C5-O14-P1-O11
13	E	401	PTY	C5-O14-P1-O11
14	C	505	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	CA2-OA2-PA1-OA5
14	N	506	CDL	CB2-OB2-PB2-OB5
14	S	101	CDL	CA2-OA2-PA1-OA5
12	N	503	PC1	C32-C31-O31-C3
14	A	3002	CDL	C51-CB5-OB6-CB4
15	N	507	LMT	C4B-C5B-C6B-O6B
13	P	303	PTY	C30-C31-C32-C33
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	CA2-C1-CB2-OB2
14	S	101	CDL	CB2-C1-CA2-OA2
14	L	3001	CDL	CB7-C71-C72-C73
13	E	401	PTY	C30-C31-C32-C33
13	C	504	PTY	C16-C17-C18-C19
15	N	507	LMT	C7-C8-C9-C10
13	P	303	PTY	C16-C17-C18-C19
13	N	505	PTY	C32-C33-C34-C35
14	A	3001	CDL	C71-C72-C73-C74
14	N	504	CDL	C74-C75-C76-C77
15	C	506	LMT	C4-C5-C6-C7
13	E	401	PTY	C13-C14-C15-C16
14	C	505	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	O1-C1-CA2-OA2
14	L	3002	CDL	O1-C1-CA2-OA2
13	E	401	PTY	C16-C17-C18-C19
13	E	401	PTY	C38-C39-C40-C41
14	H	701	CDL	C71-C72-C73-C74
13	P	303	PTY	C34-C35-C36-C37
14	H	701	CDL	C73-C74-C75-C76
15	C	506	LMT	C3-C4-C5-C6
15	P	302	LMT	C4-C5-C6-C7
12	N	503	PC1	O32-C31-O31-C3
15	C	506	LMT	C5-C6-C7-C8
14	N	506	CDL	OB7-CB5-OB6-CB4
15	C	506	LMT	C6-C7-C8-C9
13	C	504	PTY	C8-C11-C12-C13
14	A	3002	CDL	C33-C34-C35-C36
12	C	503	PC1	C28-C29-C2A-C2B
14	N	504	CDL	C71-C72-C73-C74
14	L	3002	CDL	C12-C13-C14-C15
14	L	3002	CDL	C33-C34-C35-C36
13	E	401	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	C31-C32-C33-C34
14	H	701	CDL	CB5-C51-C52-C53
14	H	701	CDL	C74-C75-C76-C77
15	P	302	LMT	C7-C8-C9-C10
13	P	303	PTY	C31-C32-C33-C34
13	N	505	PTY	C16-C17-C18-C19
14	H	701	CDL	C11-C12-C13-C14
15	C	506	LMT	C2-C3-C4-C5
14	A	3002	CDL	OB7-CB5-OB6-CB4
13	C	504	PTY	C38-C39-C40-C41
12	T	201	PC1	C33-C34-C35-C36
13	C	504	PTY	C37-C38-C39-C40
13	E	401	PTY	C32-C33-C34-C35
14	A	3001	CDL	C73-C74-C75-C76
13	E	401	PTY	C31-C30-O4-C1
14	N	506	CDL	C51-CB5-OB6-CB4
13	P	303	PTY	C11-C12-C13-C14
14	N	504	CDL	C73-C74-C75-C76
14	L	3001	CDL	CA7-C31-C32-C33
14	N	506	CDL	CA2-C1-CB2-OB2
12	N	503	PC1	C28-C29-C2A-C2B
14	C	505	CDL	OB7-CB5-OB6-CB4
15	J	101	LMT	C1-C2-C3-C4
13	N	505	PTY	C34-C35-C36-C37
15	N	507	LMT	C2-C3-C4-C5
14	A	3002	CDL	C12-C13-C14-C15
13	P	303	PTY	C13-C14-C15-C16
13	P	303	PTY	C40-C41-C42-C43
15	N	507	LMT	C1-C2-C3-C4
13	P	303	PTY	C8-C11-C12-C13
14	L	3002	CDL	CA5-C11-C12-C13
14	C	505	CDL	C51-CB5-OB6-CB4
14	H	701	CDL	C51-CB5-OB6-CB4
13	E	401	PTY	O14-C5-C6-O7
14	N	504	CDL	C11-C12-C13-C14
15	J	101	LMT	C6-C7-C8-C9
14	H	701	CDL	OB7-CB5-OB6-CB4
12	C	503	PC1	O21-C2-C3-O31
12	N	503	PC1	O21-C2-C3-O31
12	C	503	PC1	C22-C23-C24-C25
13	N	505	PTY	C12-C13-C14-C15
14	L	3001	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
12	N	503	PC1	C22-C23-C24-C25
13	E	401	PTY	O30-C30-O4-C1
13	C	504	PTY	C5-O14-P1-O11
14	H	701	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	CA3-OA5-PA1-OA2
14	N	506	CDL	C31-C32-C33-C34
13	N	505	PTY	O14-C5-C6-C1
14	A	3002	CDL	OA5-CA3-CA4-CA6
14	L	3002	CDL	OA5-CA3-CA4-CA6
13	P	303	PTY	C41-C42-C43-C44
13	N	505	PTY	C30-C31-C32-C33
13	N	505	PTY	C36-C37-C38-C39
13	E	401	PTY	C14-C15-C16-C17
14	L	3002	CDL	C31-C32-C33-C34
12	C	503	PC1	C27-C28-C29-C2A
15	N	507	LMT	C3-C4-C5-C6
14	C	505	CDL	CB2-C1-CA2-OA2
14	A	3002	CDL	CB2-C1-CA2-OA2
13	P	303	PTY	C14-C15-C16-C17
13	N	505	PTY	C15-C16-C17-C18
15	J	101	LMT	C7-C8-C9-C10
13	N	505	PTY	O4-C1-C6-C5
14	H	701	CDL	CB3-CB4-CB6-OB8
14	N	504	CDL	C75-C76-C77-C78
13	E	401	PTY	C41-C42-C43-C44
14	A	3001	CDL	C31-C32-C33-C34
15	N	507	LMT	C9-C10-C11-C12
13	E	401	PTY	C11-C12-C13-C14
13	N	505	PTY	C41-C42-C43-C44
12	N	503	PC1	C26-C27-C28-C29
14	L	3002	CDL	C11-C12-C13-C14
15	J	101	LMT	C9-C10-C11-C12
12	N	503	PC1	C27-C28-C29-C2A
14	A	3002	CDL	CA6-CA4-OA6-CA5
13	C	504	PTY	C41-C42-C43-C44
14	H	701	CDL	C75-C76-C77-C78
14	N	504	CDL	OA5-CA3-CA4-OA6
14	N	504	CDL	OB5-CB3-CB4-OB6
13	N	505	PTY	C14-C15-C16-C17
13	E	401	PTY	C12-C13-C14-C15
15	C	506	LMT	C11-C10-C9-C8
14	L	3001	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	CB2-C1-CA2-OA2
14	L	3002	CDL	CB2-C1-CA2-OA2
13	C	504	PTY	C40-C41-C42-C43
12	I	201	PC1	C34-C35-C36-C37
13	E	401	PTY	O14-C5-C6-C1
14	H	701	CDL	OB5-CB3-CB4-CB6
15	C	506	LMT	C9-C10-C11-C12
15	N	507	LMT	C5-C6-C7-C8
14	N	504	CDL	CB5-C51-C52-C53
13	C	504	PTY	C17-C18-C19-C20
13	N	505	PTY	C38-C39-C40-C41
13	E	401	PTY	C33-C34-C35-C36
15	C	506	LMT	C2-C1-O1'-C1'
11	C	501	HEM	C3D-CAD-CBD-CGD
14	C	505	CDL	C31-C32-C33-C34
12	C	503	PC1	C1-C2-C3-O31
15	P	302	LMT	C3-C4-C5-C6
13	C	504	PTY	C39-C40-C41-C42
14	C	505	CDL	C13-C14-C15-C16
12	C	503	PC1	C26-C27-C28-C29
14	A	3001	CDL	CB3-OB5-PB2-OB2
14	H	701	CDL	OA5-CA3-CA4-OA6
14	H	701	CDL	OB5-CB3-CB4-OB6
14	N	506	CDL	O1-C1-CB2-OB2
13	C	504	PTY	C32-C33-C34-C35
14	A	3002	CDL	C34-C35-C36-C37
14	A	3002	CDL	CB5-C51-C52-C53
13	N	505	PTY	O4-C1-C6-O7
14	S	101	CDL	OB6-CB4-CB6-OB8
13	P	303	PTY	C38-C39-C40-C41
14	H	701	CDL	C72-C73-C74-C75
14	L	3002	CDL	C51-CB5-OB6-CB4
14	N	504	CDL	C51-C52-C53-C54
14	C	505	CDL	CA4-CA3-OA5-PA1
15	N	507	LMT	C11-C10-C9-C8
11	N	501	HEM	C3D-CAD-CBD-CGD
14	N	504	CDL	OA7-CA5-OA6-CA4
12	I	201	PC1	C22-C21-O21-C2
14	H	702	CDL	OB5-CB3-CB4-CB6
14	N	504	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	C72-C73-C74-C75
12	I	201	PC1	C22-C23-C24-C25
14	H	702	CDL	CB6-CB4-OB6-CB5
14	L	3002	CDL	CA6-CA4-OA6-CA5
14	S	101	CDL	CB6-CB4-OB6-CB5
13	C	504	PTY	C31-C30-O4-C1
14	A	3002	CDL	C31-CA7-OA8-CA6
15	P	302	LMT	O5'-C1'-O1'-C1
12	N	503	PC1	C1-C2-C3-O31
12	T	201	PC1	C1-C2-C3-O31
13	C	504	PTY	O4-C1-C6-C5
14	N	504	CDL	CA3-CA4-CA6-OA8
14	N	506	CDL	CA4-CA3-OA5-PA1
13	P	303	PTY	O14-C5-C6-O7
14	S	101	CDL	OB5-CB3-CB4-OB6
12	N	503	PC1	C33-C34-C35-C36
14	L	3002	CDL	C52-C53-C54-C55
12	N	503	PC1	O22-C21-O21-C2
14	H	701	CDL	OA6-CA4-CA6-OA8
14	H	701	CDL	OB6-CB4-CB6-OB8
14	N	504	CDL	OA6-CA4-CA6-OA8
15	C	506	LMT	C7-C8-C9-C10
13	C	504	PTY	O30-C30-O4-C1
14	H	701	CDL	OA7-CA5-OA6-CA4
14	A	3002	CDL	CA5-C11-C12-C13
14	L	3002	CDL	C34-C35-C36-C37
13	E	401	PTY	C3-O11-P1-O14
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	L	3001	CDL	O1-C1-CA2-OA2
12	I	201	PC1	C11-O13-P-O14
12	T	201	PC1	C11-C12-N-C14
13	C	504	PTY	C5-O14-P1-O12
13	C	504	PTY	C5-O14-P1-O13
13	P	303	PTY	C5-O14-P1-O13
13	N	505	PTY	C5-O14-P1-O12
14	C	505	CDL	CA3-OA5-PA1-OA4
14	H	701	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB3-OB5-PB2-OB3
14	S	101	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	C31-CA7-OA8-CA6
14	H	701	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	OB5-CB3-CB4-CB6
14	A	3001	CDL	C72-C73-C74-C75
14	C	505	CDL	C32-C33-C34-C35
14	H	701	CDL	C51-C52-C53-C54
13	C	504	PTY	O14-C5-C6-O7
14	C	505	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OB5-CB3-CB4-OB6
14	N	506	CDL	OA5-CA3-CA4-OA6
14	A	3002	CDL	OA9-CA7-OA8-CA6
13	E	401	PTY	C36-C37-C38-C39
14	H	701	CDL	CA3-CA4-CA6-OA8
14	A	3002	CDL	OA6-CA4-CA6-OA8
14	A	3002	CDL	C13-C14-C15-C16
14	N	506	CDL	C32-C33-C34-C35
14	N	504	CDL	C11-CA5-OA6-CA4
14	L	3002	CDL	OB7-CB5-OB6-CB4
15	P	302	LMT	C5-C6-C7-C8
12	T	201	PC1	C11-C12-N-C15
17	A	3003	XP4	C5-C6-C7-C8
13	N	505	PTY	O30-C30-O4-C1
14	N	506	CDL	OA9-CA7-OA8-CA6
17	U	101	XP4	C1-O4-P1-O2
13	N	505	PTY	O14-C5-C6-O7
13	C	504	PTY	C13-C14-C15-C16
13	C	504	PTY	O4-C1-C6-O7
14	H	702	CDL	OB6-CB4-CB6-OB8
13	C	504	PTY	C3-O11-P1-O14
13	P	303	PTY	C3-O11-P1-O14
14	A	3002	CDL	CB2-OB2-PB2-OB5
14	A	3002	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CB2-OB2-PB2-OB5
14	L	3002	CDL	CB2-OB2-PB2-OB5
14	S	101	CDL	CB2-OB2-PB2-OB5
14	A	3001	CDL	C72-C71-CB7-OB8
15	J	101	LMT	O1'-C1-C2-C3
14	H	702	CDL	CB3-CB4-CB6-OB8
14	N	504	CDL	CB3-CB4-CB6-OB8
14	S	101	CDL	CB3-CB4-CB6-OB8
13	N	505	PTY	C31-C30-O4-C1
14	H	702	CDL	CB4-CB3-OB5-PB2
14	A	3001	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	C31-CA7-OA8-CA6
15	J	101	LMT	C3-C4-C5-C6
13	C	504	PTY	C30-C31-C32-C33
11	N	502	HEM	CAD-CBD-CGD-O2D
15	N	507	LMT	C6-C7-C8-C9
11	C	502	HEM	CAA-CBA-CGA-O1A
12	I	201	PC1	C32-C33-C34-C35
14	L	3002	CDL	CB5-C51-C52-C53
11	C	501	HEM	CAA-CBA-CGA-O2A
14	C	505	CDL	OB6-CB4-CB6-OB8
13	C	504	PTY	C6-C5-O14-P1
14	S	101	CDL	CB4-CB3-OB5-PB2
11	C	501	HEM	CAA-CBA-CGA-O1A
11	C	502	HEM	CAD-CBD-CGD-O2D
11	N	501	HEM	CAA-CBA-CGA-O2A
18	D	401	HEC	CAA-CBA-CGA-O1A
14	H	702	CDL	CA3-CA4-CA6-OA8
14	S	101	CDL	CA3-CA4-CA6-OA8
11	C	502	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAA-CBA-CGA-O1A
12	T	201	PC1	C11-C12-N-C13
14	C	505	CDL	CA3-OA5-PA1-OA2
11	C	502	HEM	CAA-CBA-CGA-O2A
13	C	504	PTY	C12-C13-C14-C15
12	I	201	PC1	O22-C21-O21-C2
14	C	505	CDL	C11-C12-C13-C14
14	A	3002	CDL	C51-C52-C53-C54
11	N	502	HEM	CAD-CBD-CGD-O1D
14	A	3002	CDL	C31-C32-C33-C34
18	D	401	HEC	CAA-CBA-CGA-O2A
15	J	101	LMT	C11-C10-C9-C8
13	P	303	PTY	C12-C13-C14-C15
12	T	201	PC1	C32-C33-C34-C35
14	S	101	CDL	OA5-CA3-CA4-OA6
11	N	502	HEM	CAA-CBA-CGA-O2A
18	O	401	HEC	CAA-CBA-CGA-O2A
13	C	504	PTY	O14-C5-C6-C1
14	C	505	CDL	OA5-CA3-CA4-CA6
14	N	506	CDL	OA5-CA3-CA4-CA6
14	C	505	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
14	S	101	CDL	C32-C31-CA7-OA8
15	C	506	LMT	C1-C2-C3-C4
14	H	701	CDL	C12-C13-C14-C15
12	I	201	PC1	C33-C34-C35-C36
13	N	505	PTY	C13-C14-C15-C16
17	U	101	XP4	C1-O4-P1-O1
13	N	505	PTY	C1-C6-O7-C8
11	C	501	HEM	CAD-CBD-CGD-O2D
14	H	701	CDL	C72-C71-CB7-OB8
14	N	506	CDL	C32-C31-CA7-OA8
18	O	401	HEC	CAA-CBA-CGA-O1A
14	C	505	CDL	C32-C31-CA7-OA8
14	N	504	CDL	C72-C71-CB7-OB8
12	I	201	PC1	O21-C21-C22-C23
12	N	503	PC1	O31-C31-C32-C33
13	P	303	PTY	O4-C30-C31-C32
14	H	702	CDL	C32-C31-CA7-OA9
14	L	3002	CDL	OA6-CA4-CA6-OA8
14	S	101	CDL	C32-C31-CA7-OA9
11	N	501	HEM	CAD-CBD-CGD-O2D
12	C	503	PC1	O31-C31-C32-C33
12	C	503	PC1	C11-C12-N-C15
14	H	701	CDL	C11-CA5-OA6-CA4
14	H	702	CDL	C72-C71-CB7-OB8
14	S	101	CDL	C72-C71-CB7-OB8
14	L	3002	CDL	C51-C52-C53-C54
12	N	503	PC1	C22-C21-O21-C2
14	H	701	CDL	C72-C71-CB7-OB9
14	H	701	CDL	CA2-C1-CB2-OB2
14	C	505	CDL	C32-C31-CA7-OA9
14	N	506	CDL	C32-C31-CA7-OA9
14	A	3002	CDL	CB2-OB2-PB2-OB3
14	H	702	CDL	CB2-OB2-PB2-OB3
14	N	506	CDL	CA3-OA5-PA1-OA4
14	L	3002	CDL	CB2-OB2-PB2-OB3
14	S	101	CDL	CB2-OB2-PB2-OB3
14	N	504	CDL	C72-C71-CB7-OB9
13	P	303	PTY	O30-C30-C31-C32
15	J	101	LMT	C5-C6-C7-C8
11	C	501	HEM	CAD-CBD-CGD-O1D
14	H	701	CDL	CA3-CA4-OA6-CA5
14	N	504	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
14	N	506	CDL	CB6-CB4-OB6-CB5
12	C	503	PC1	C33-C34-C35-C36
13	P	303	PTY	C15-C16-C17-C18
12	C	503	PC1	C11-C12-N-C13
11	N	501	HEM	CAD-CBD-CGD-O1D
12	N	503	PC1	O32-C31-C32-C33
15	N	507	LMT	C4-C5-C6-C7
13	E	401	PTY	O4-C30-C31-C32
12	I	201	PC1	O22-C21-C22-C23
12	C	503	PC1	O32-C31-C32-C33
13	E	401	PTY	O30-C30-C31-C32

There are no ring outliers.

27 monomers are involved in 86 short contacts:

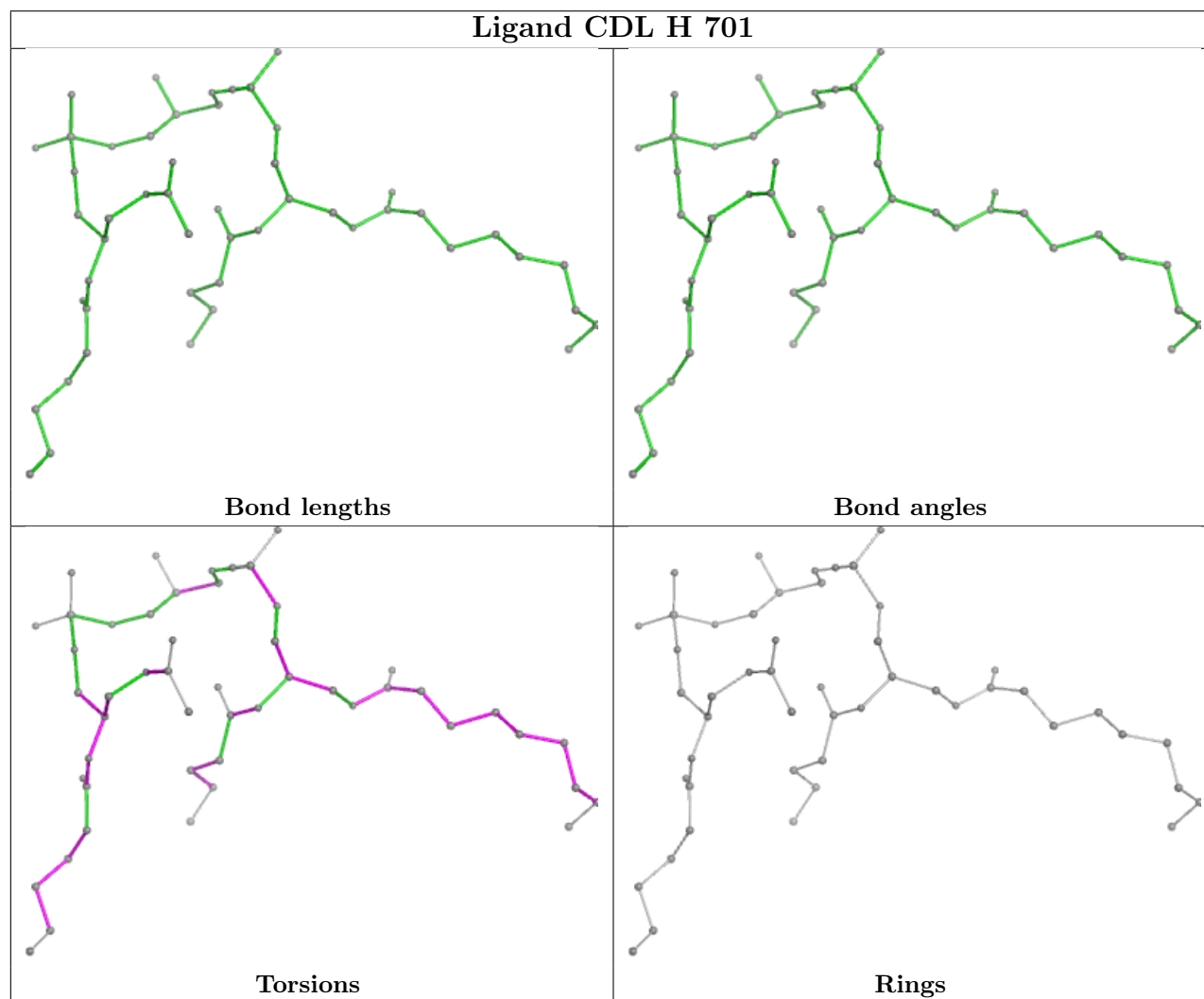
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14	H	701	CDL	2	0
18	O	401	HEC	13	0
14	N	506	CDL	2	0
12	T	201	PC1	2	0
11	C	502	HEM	2	0
18	D	401	HEC	12	0
13	C	504	PTY	3	0
14	A	3001	CDL	2	0
14	L	3002	CDL	1	0
15	J	101	LMT	1	0
12	N	503	PC1	1	0
13	N	505	PTY	9	0
14	L	3001	CDL	1	0
13	E	401	PTY	1	0
11	N	502	HEM	3	0
12	C	503	PC1	1	0
14	C	505	CDL	2	0
14	A	3002	CDL	2	0
14	N	504	CDL	3	0
15	C	506	LMT	1	0
13	P	303	PTY	10	0
14	S	101	CDL	2	0
17	A	3003	XP4	1	0
17	U	101	XP4	1	0
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14	H	702	CDL	2	0

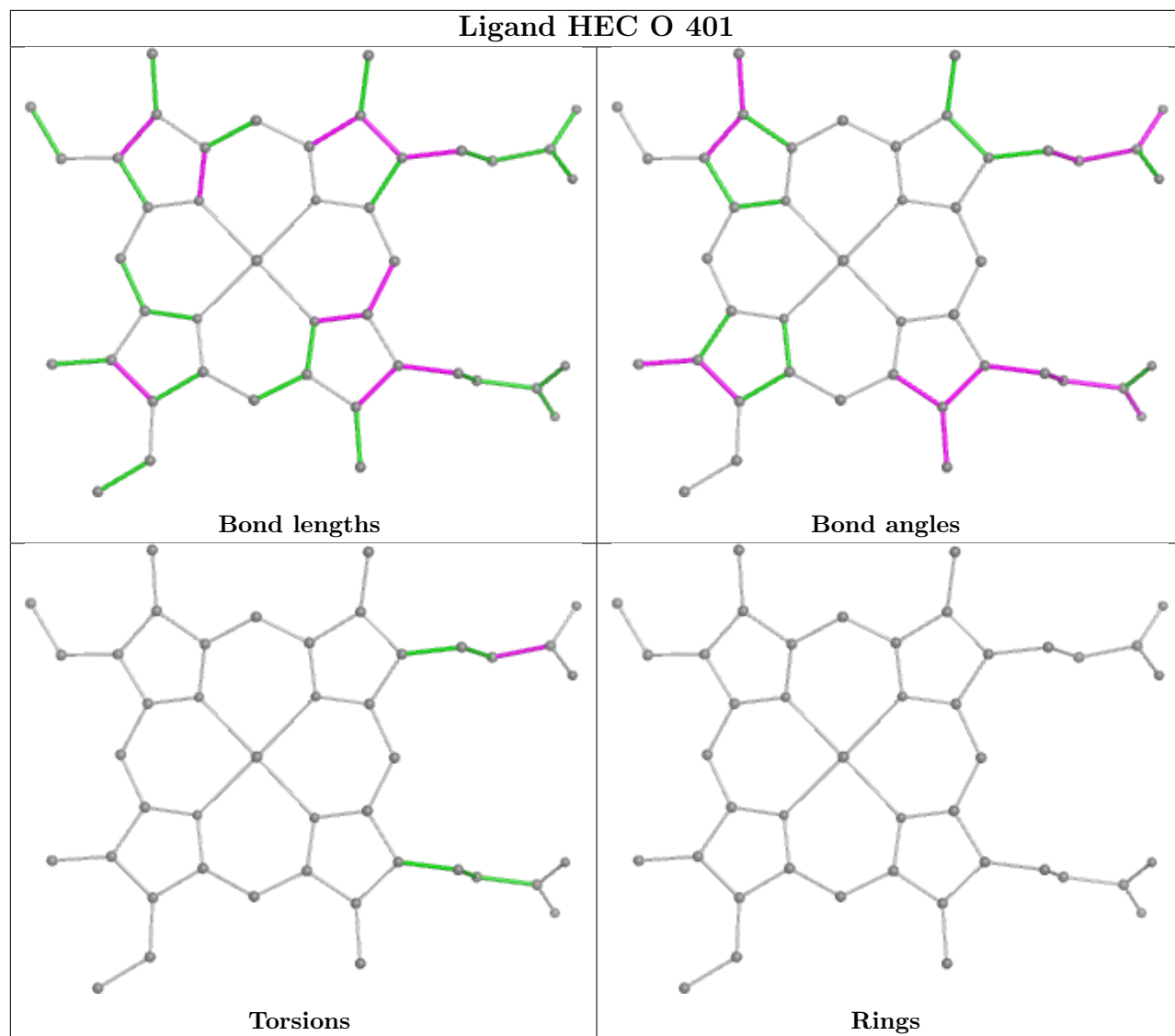
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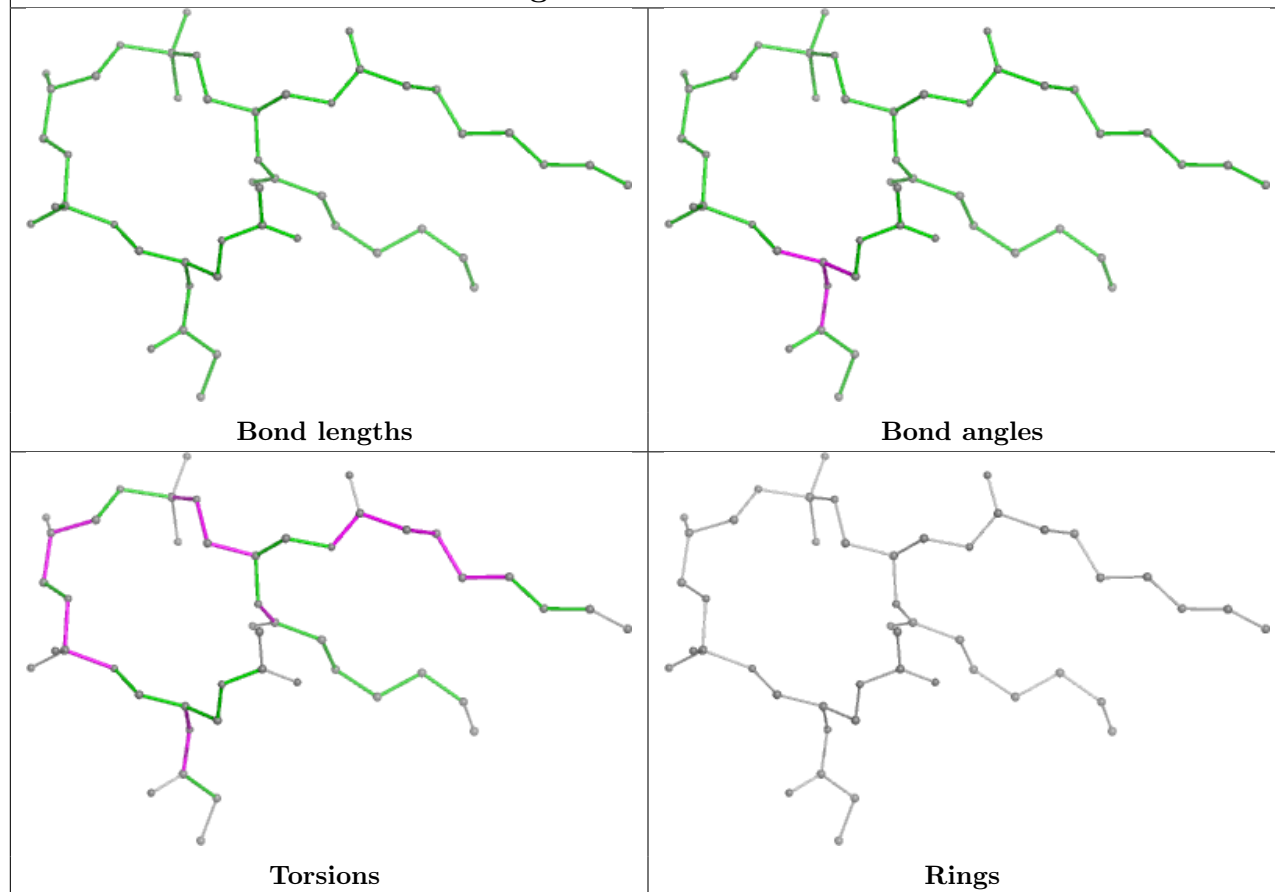
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	501	HEM	5	0

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.

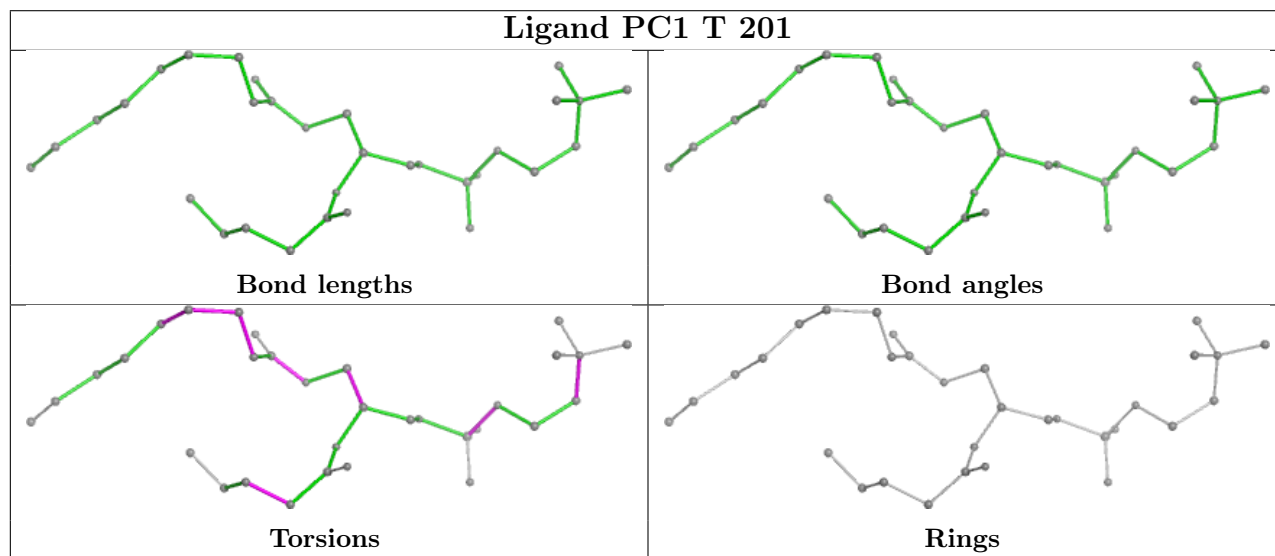


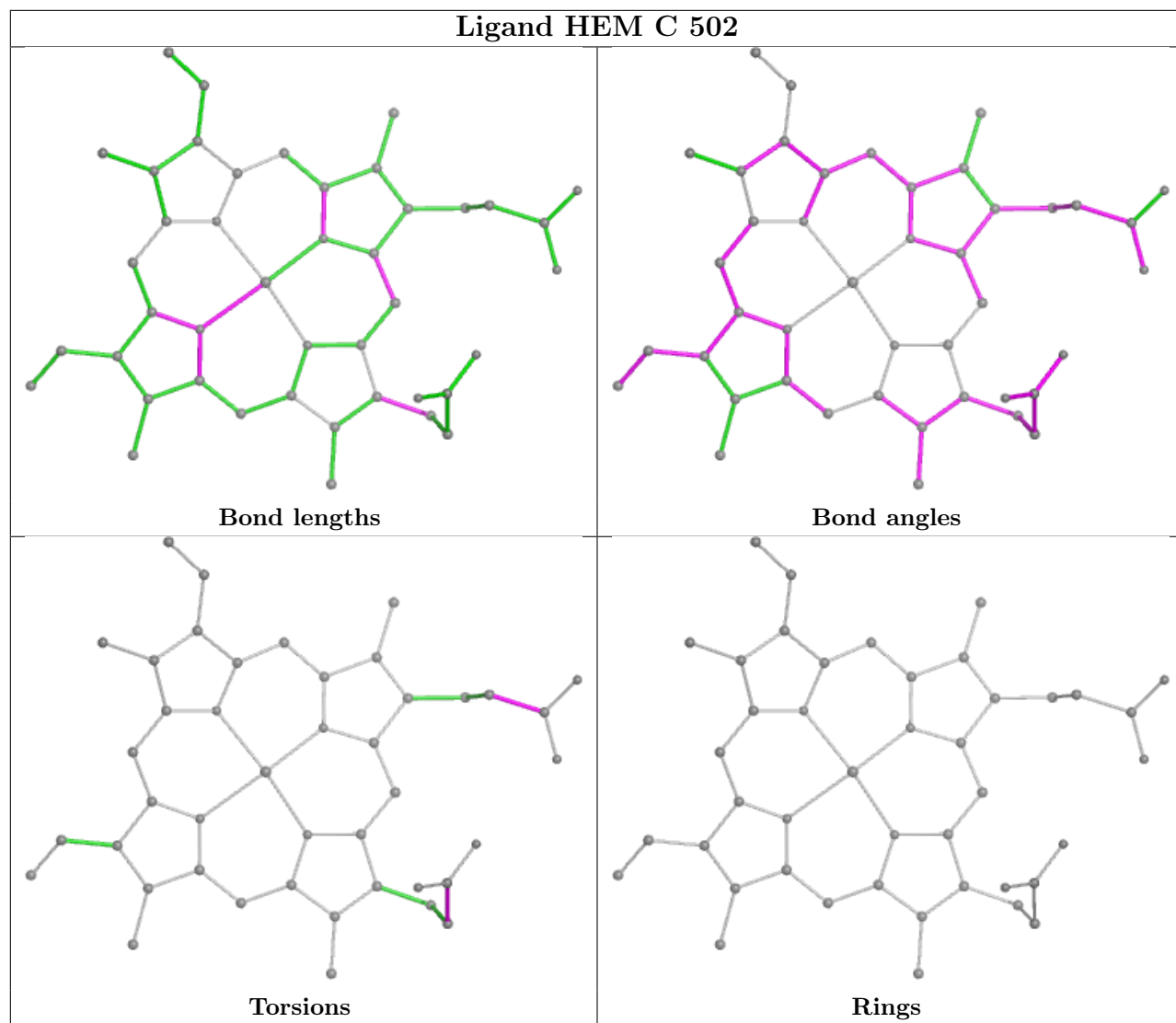


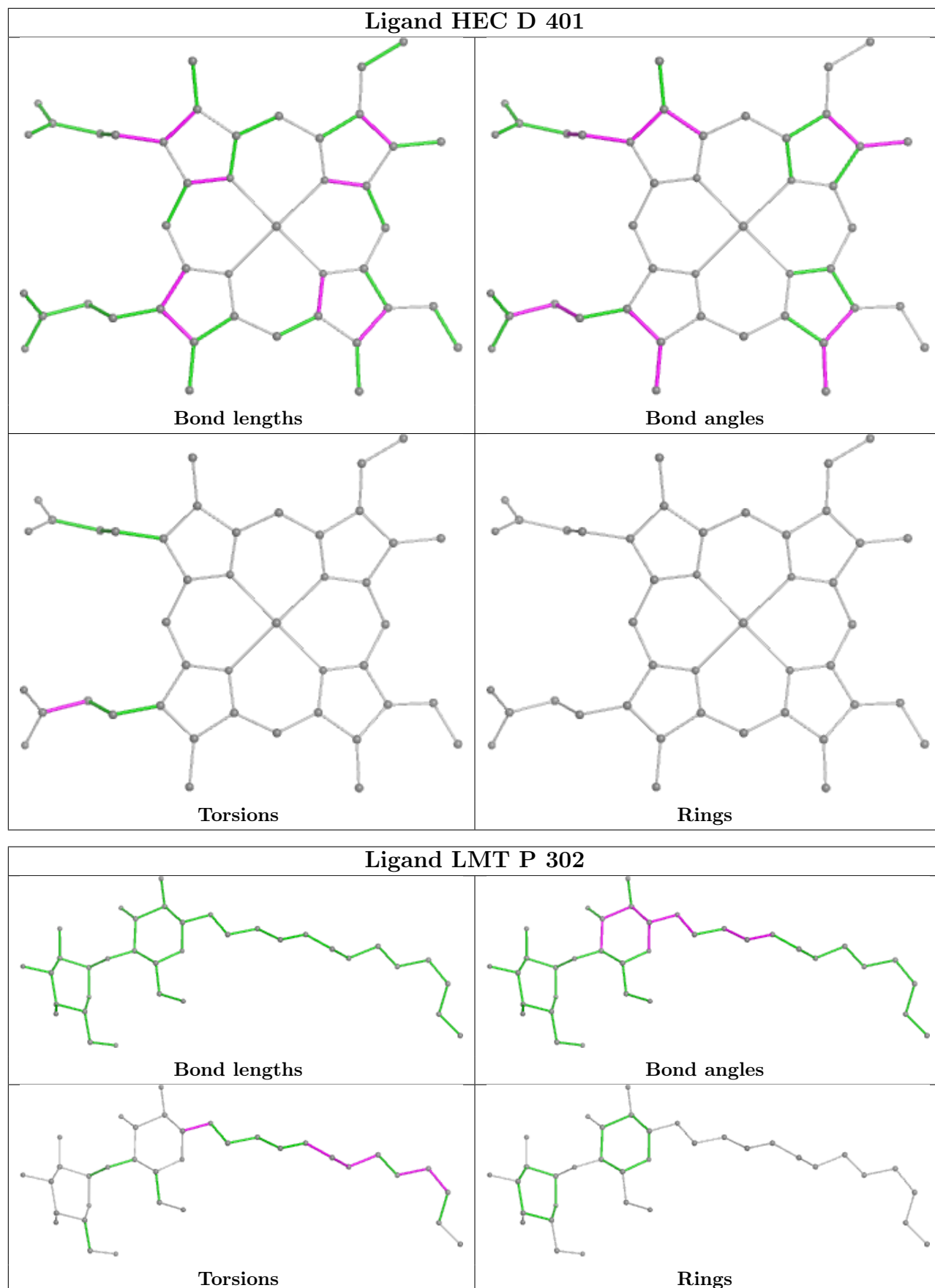
Ligand CDL N 506

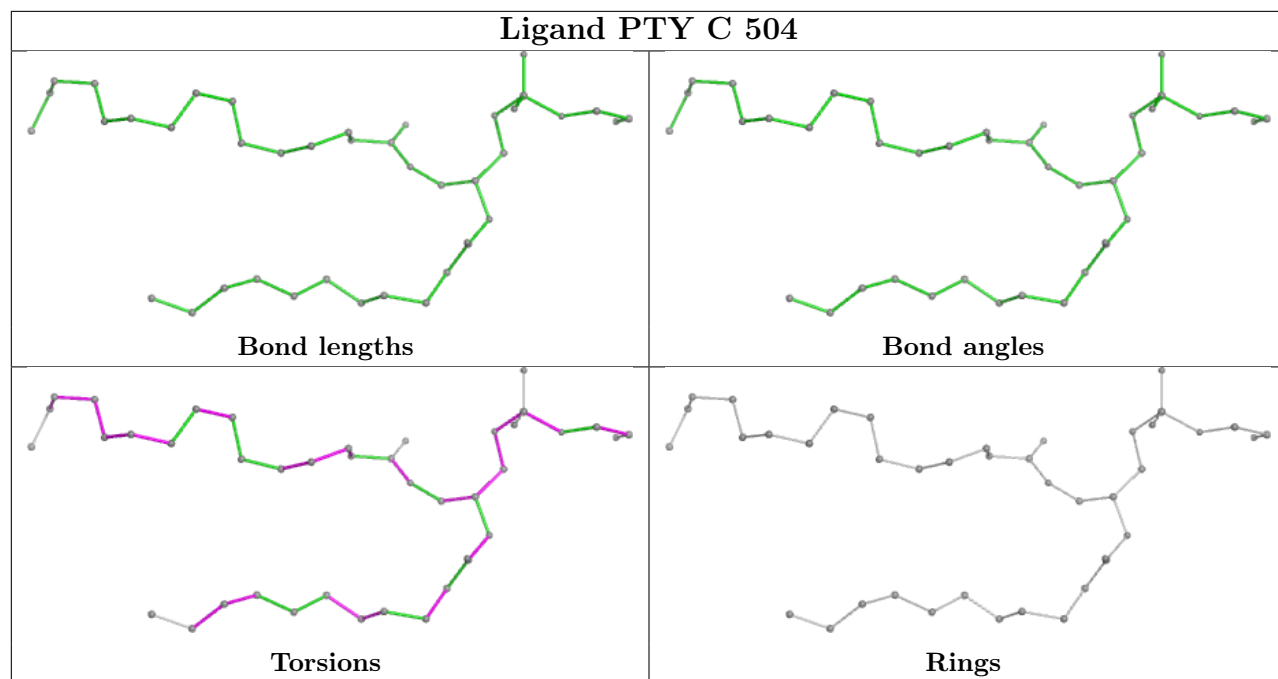


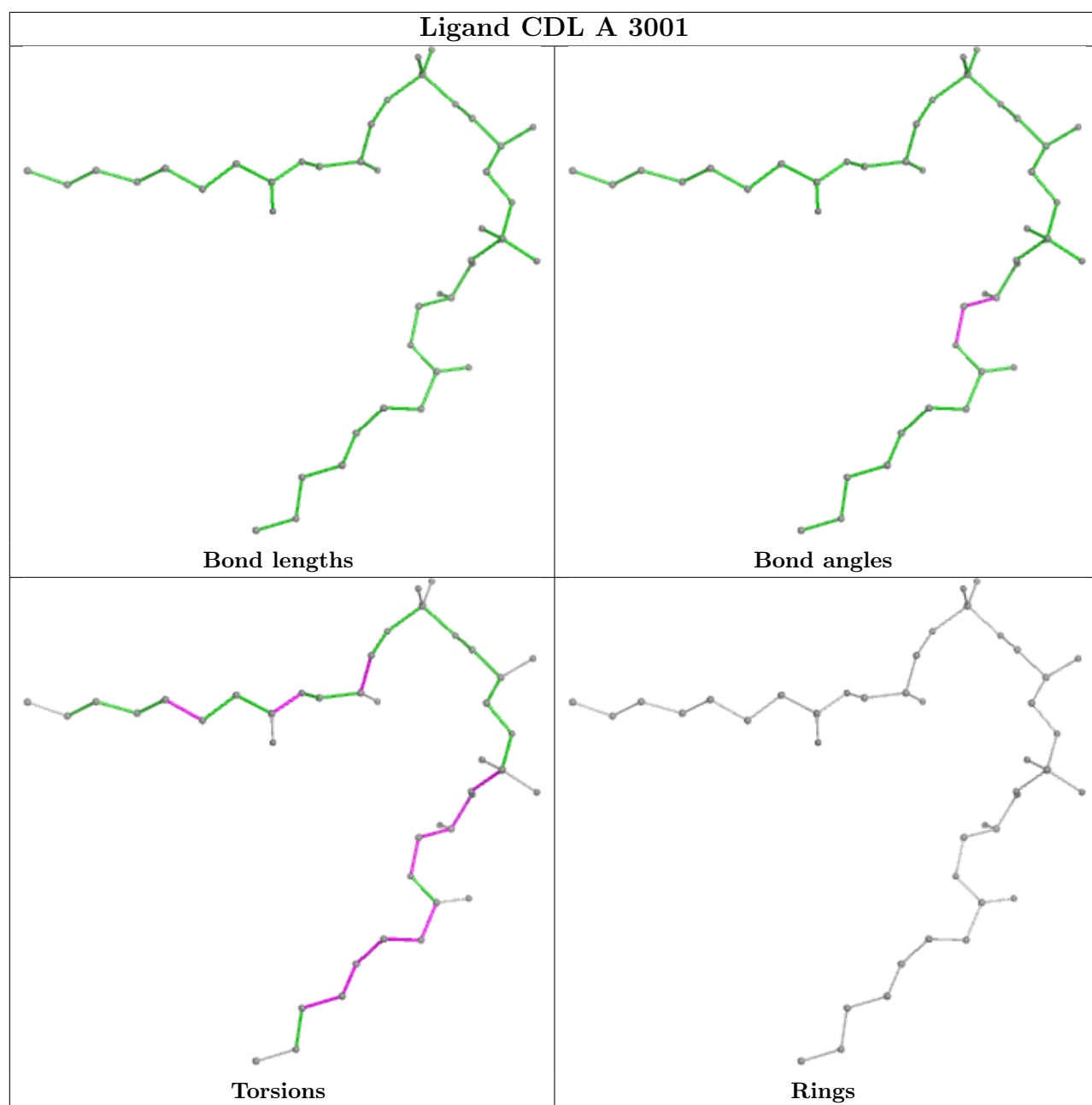
Ligand PC1 T 201

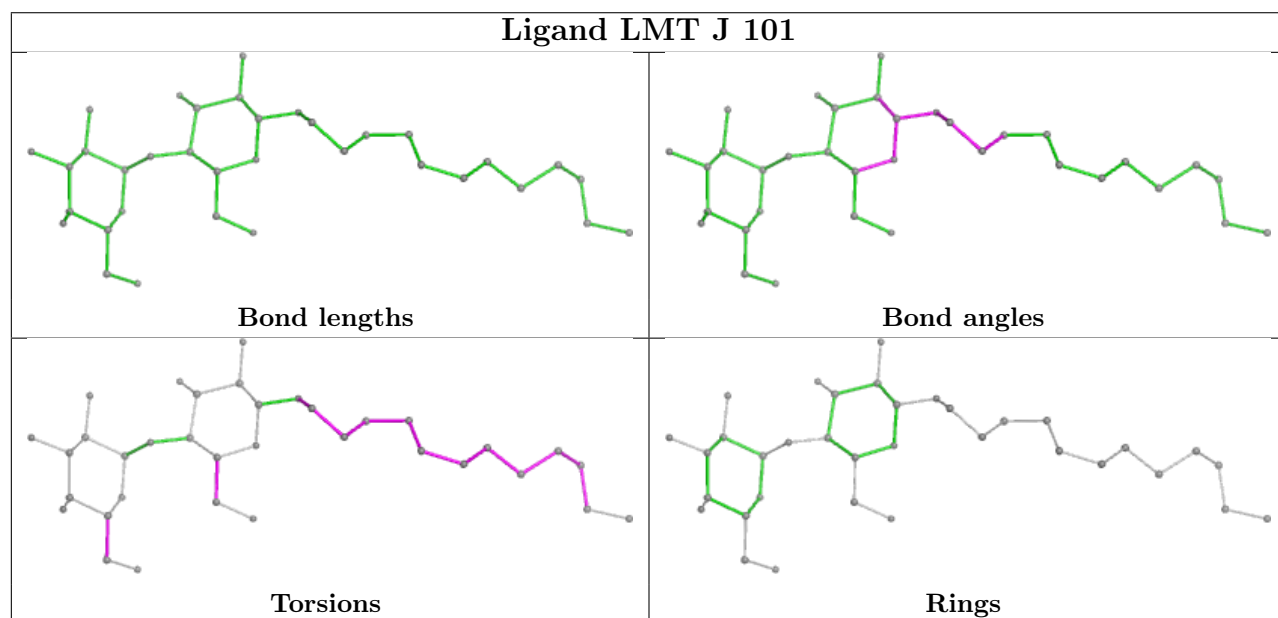
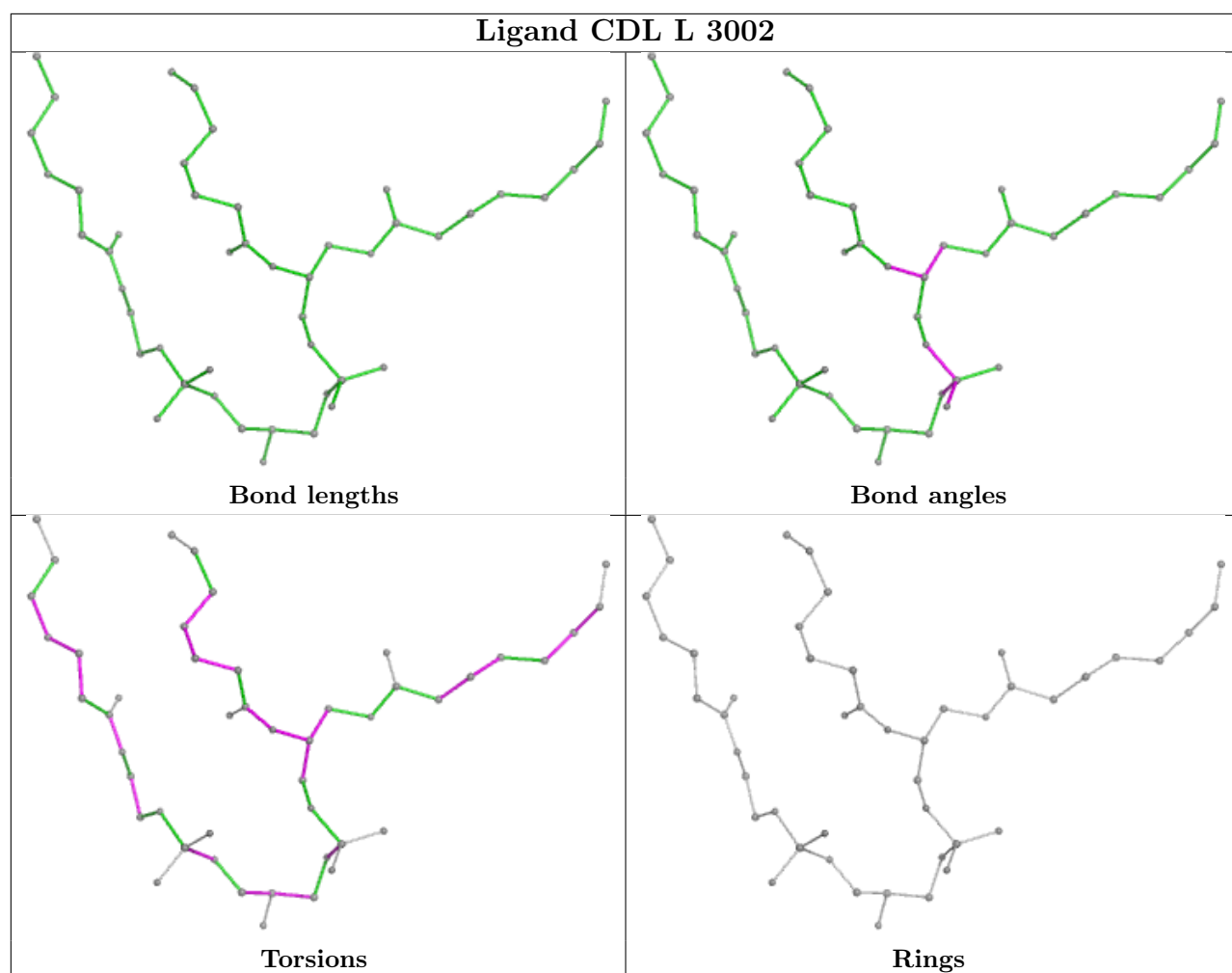


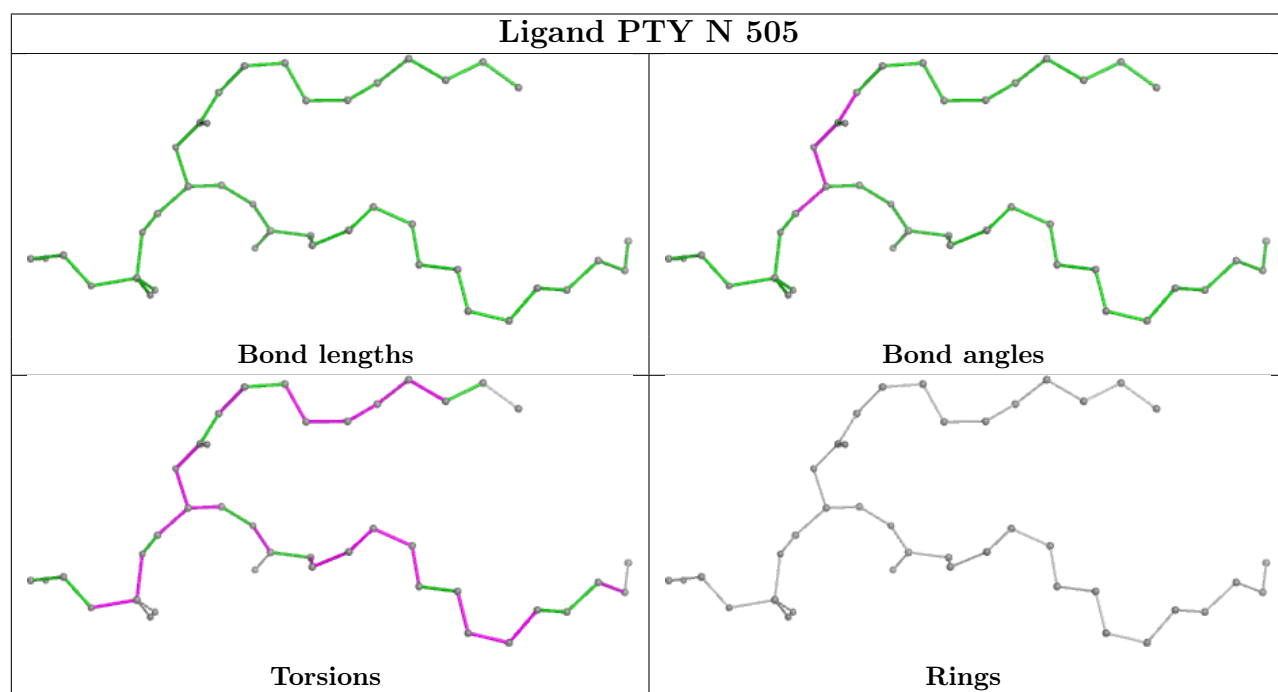
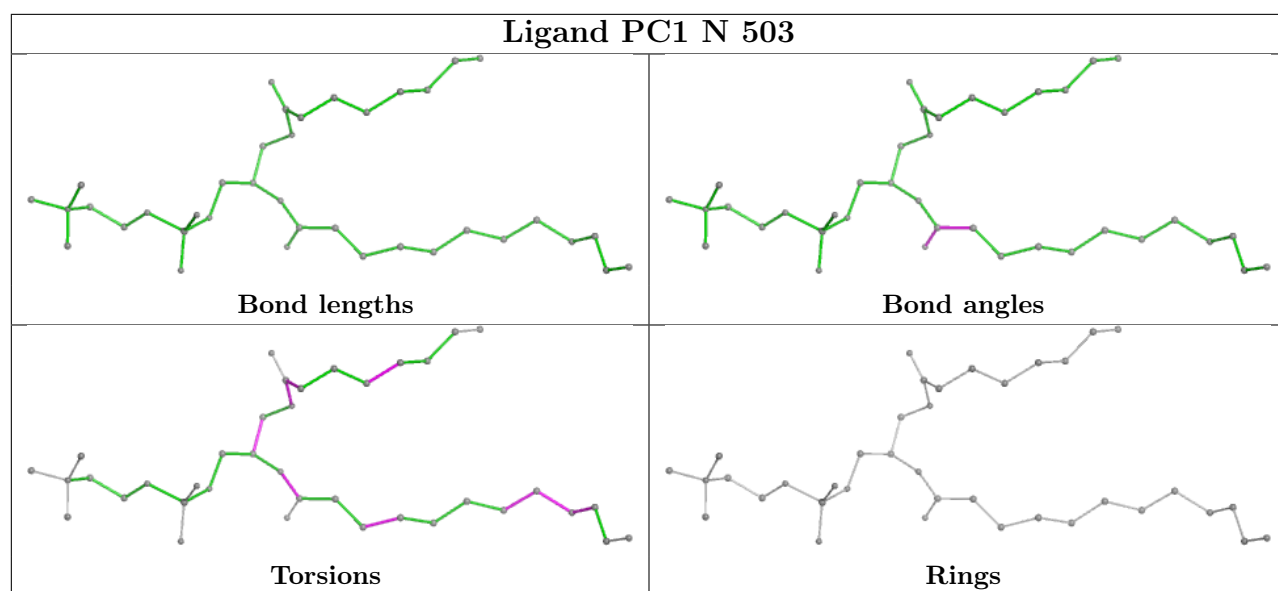


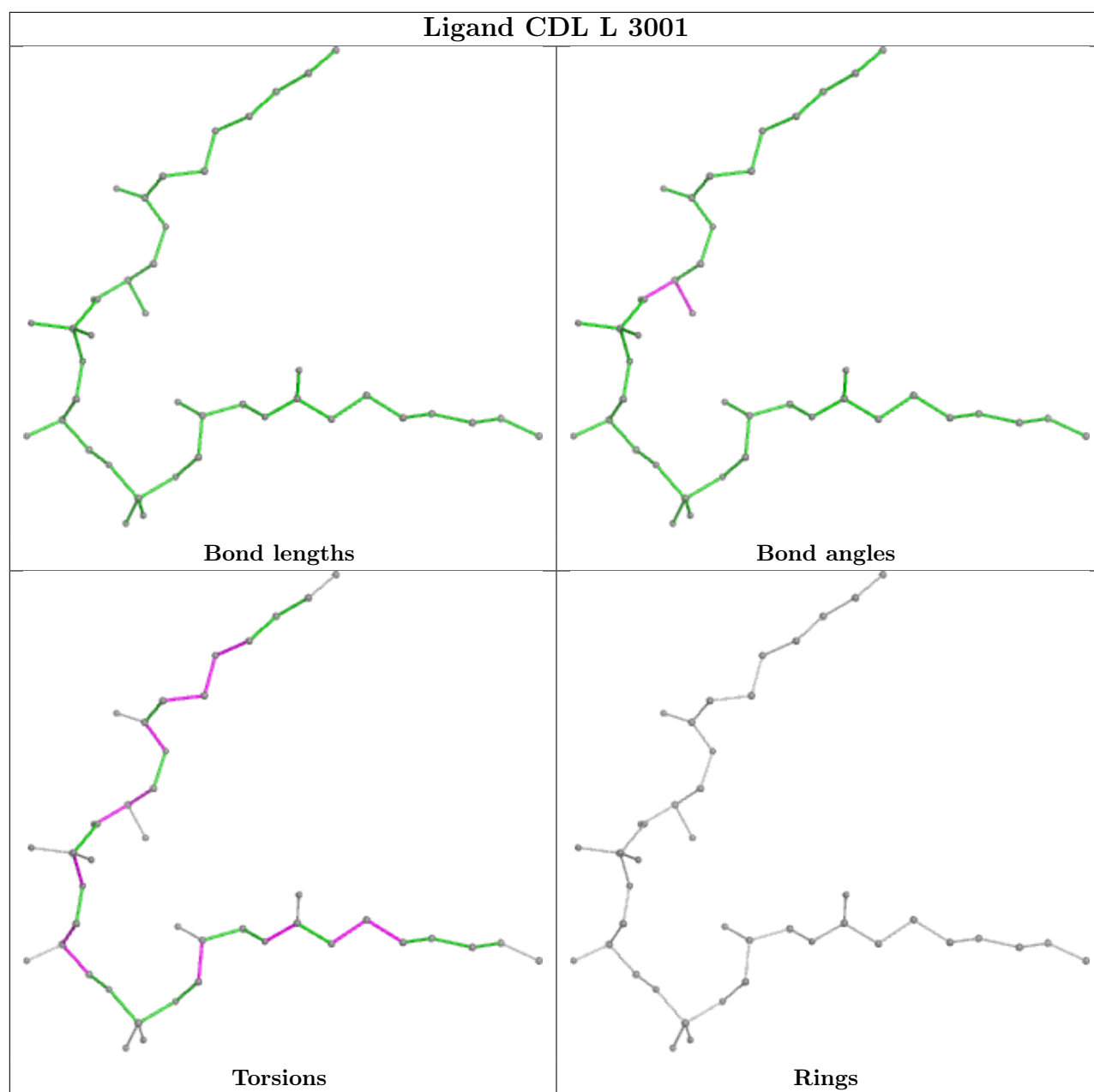


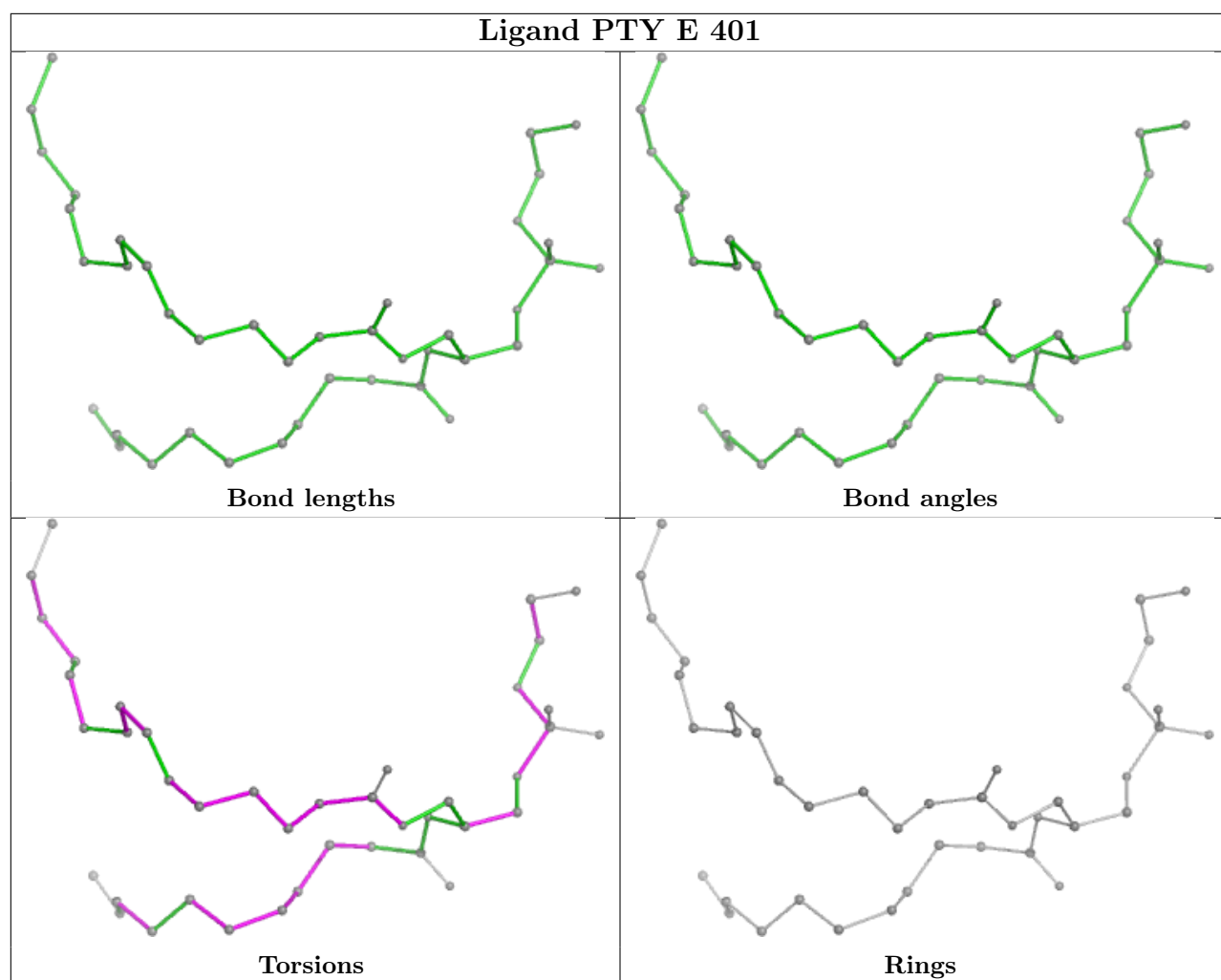


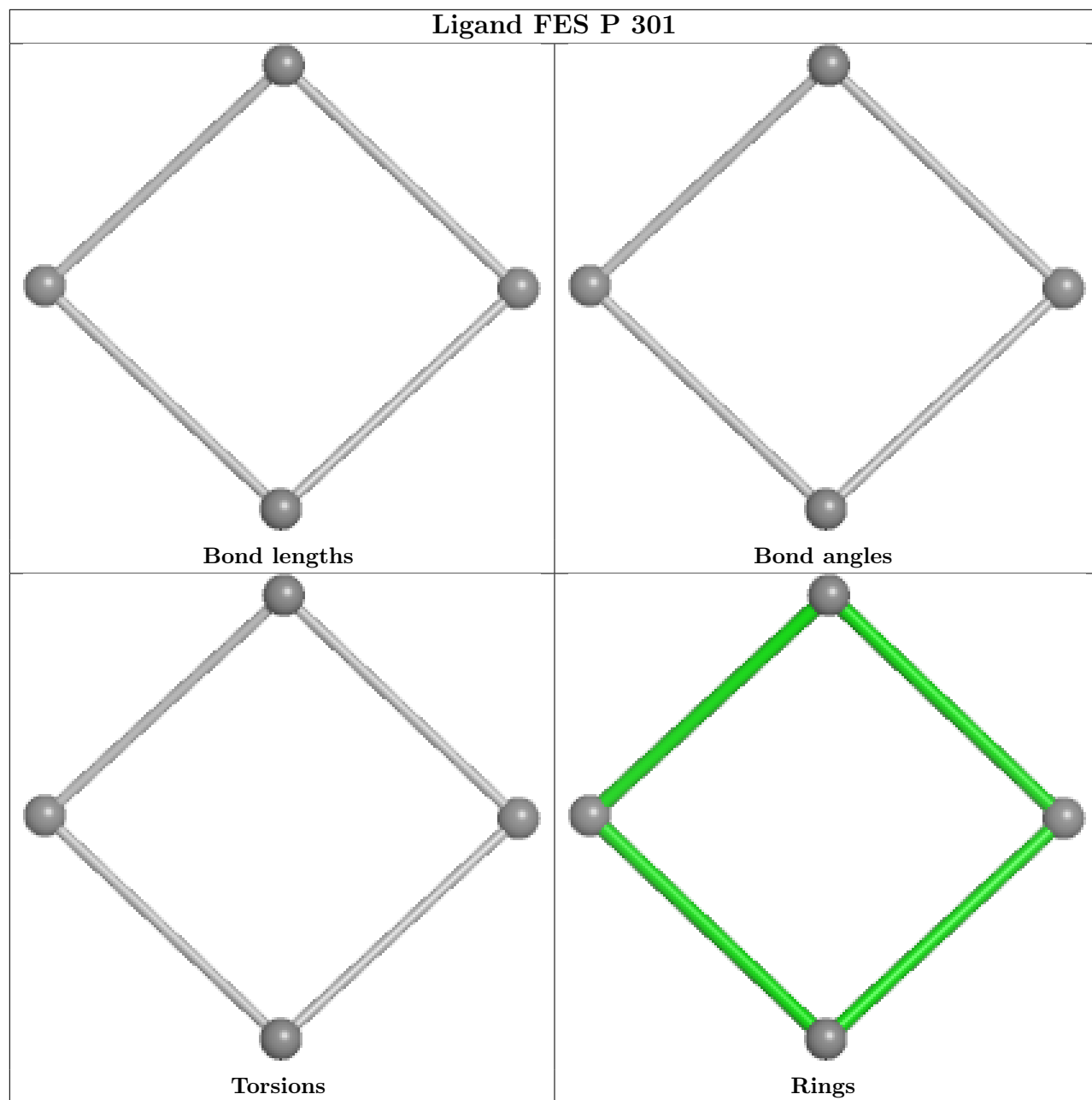


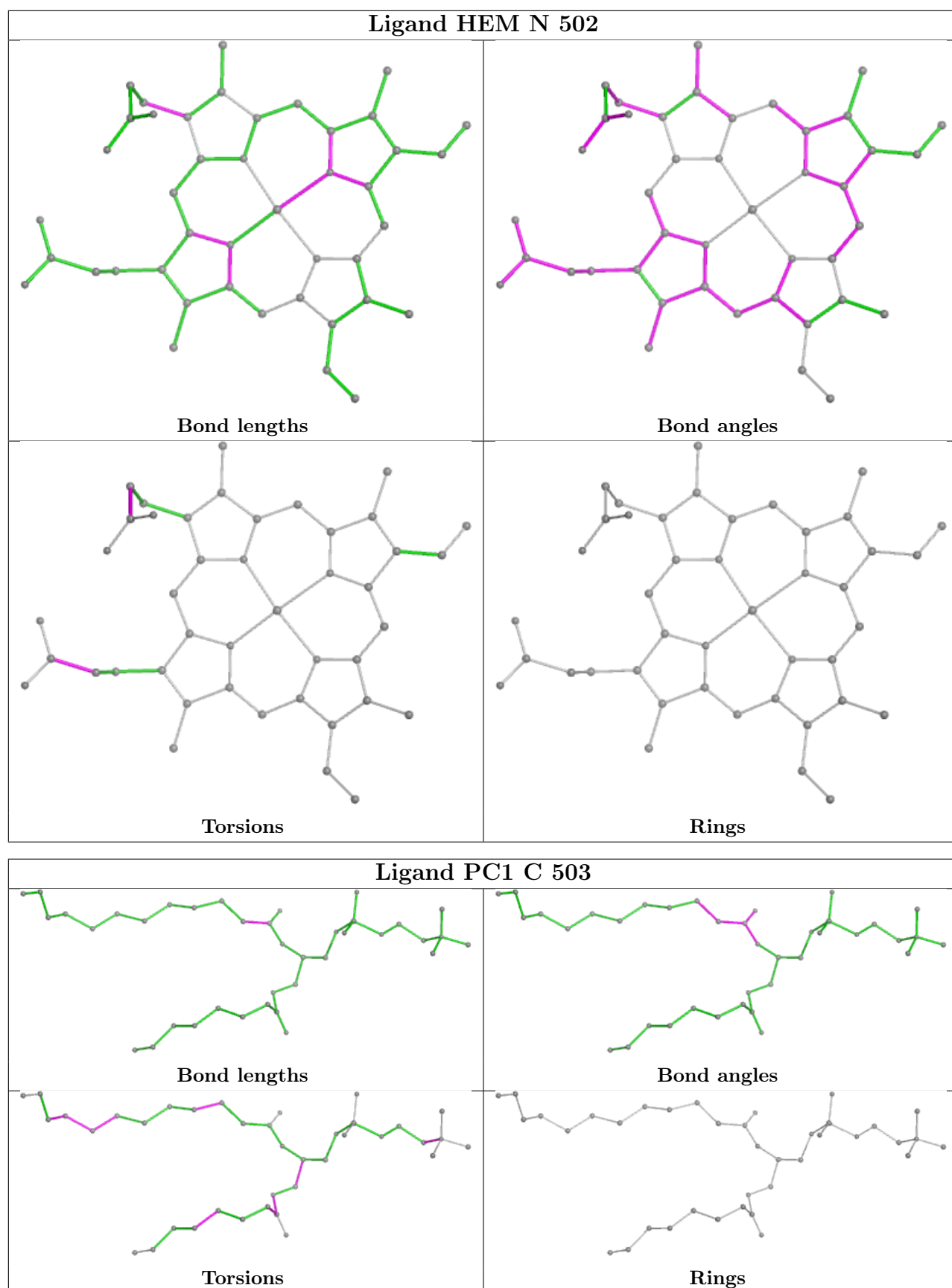


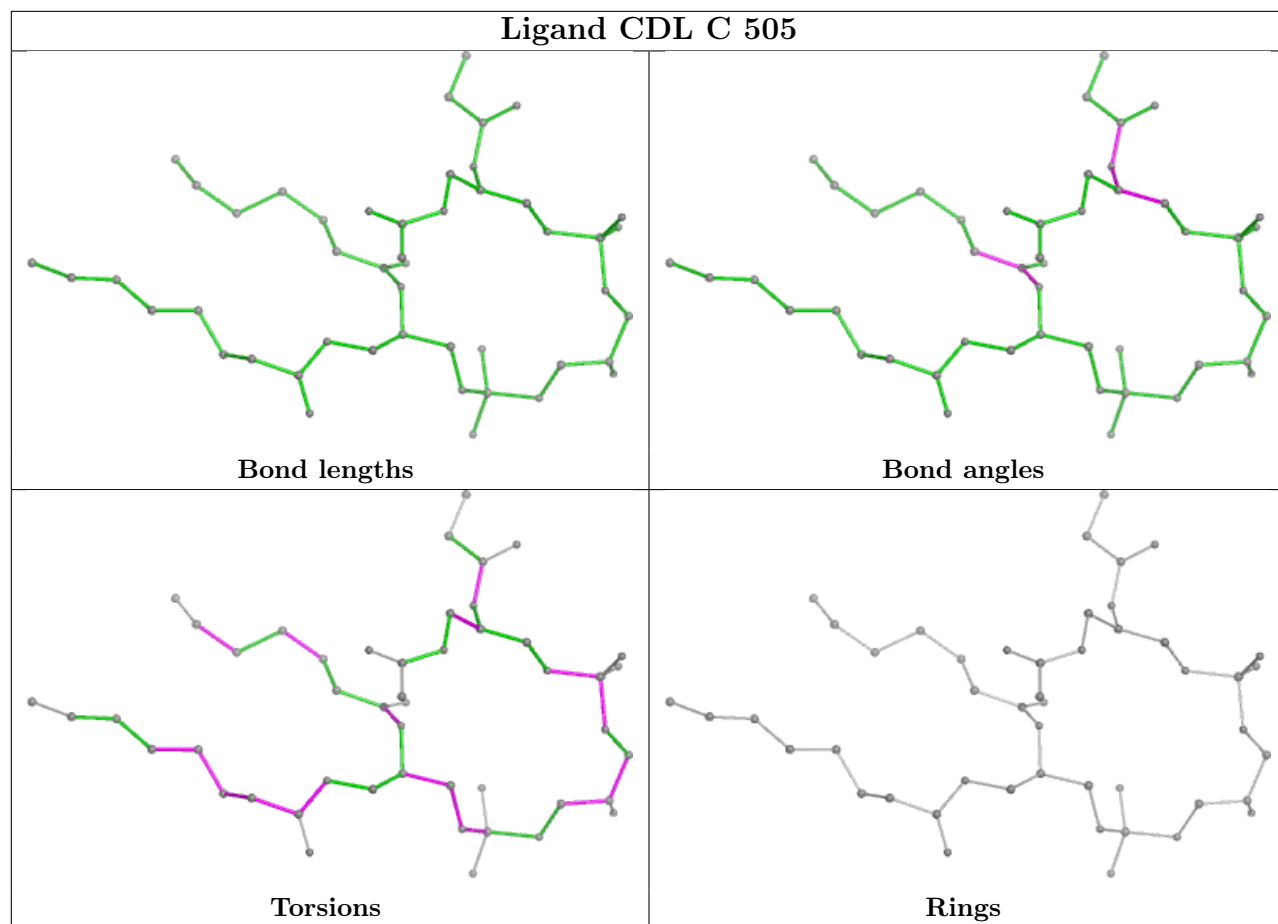


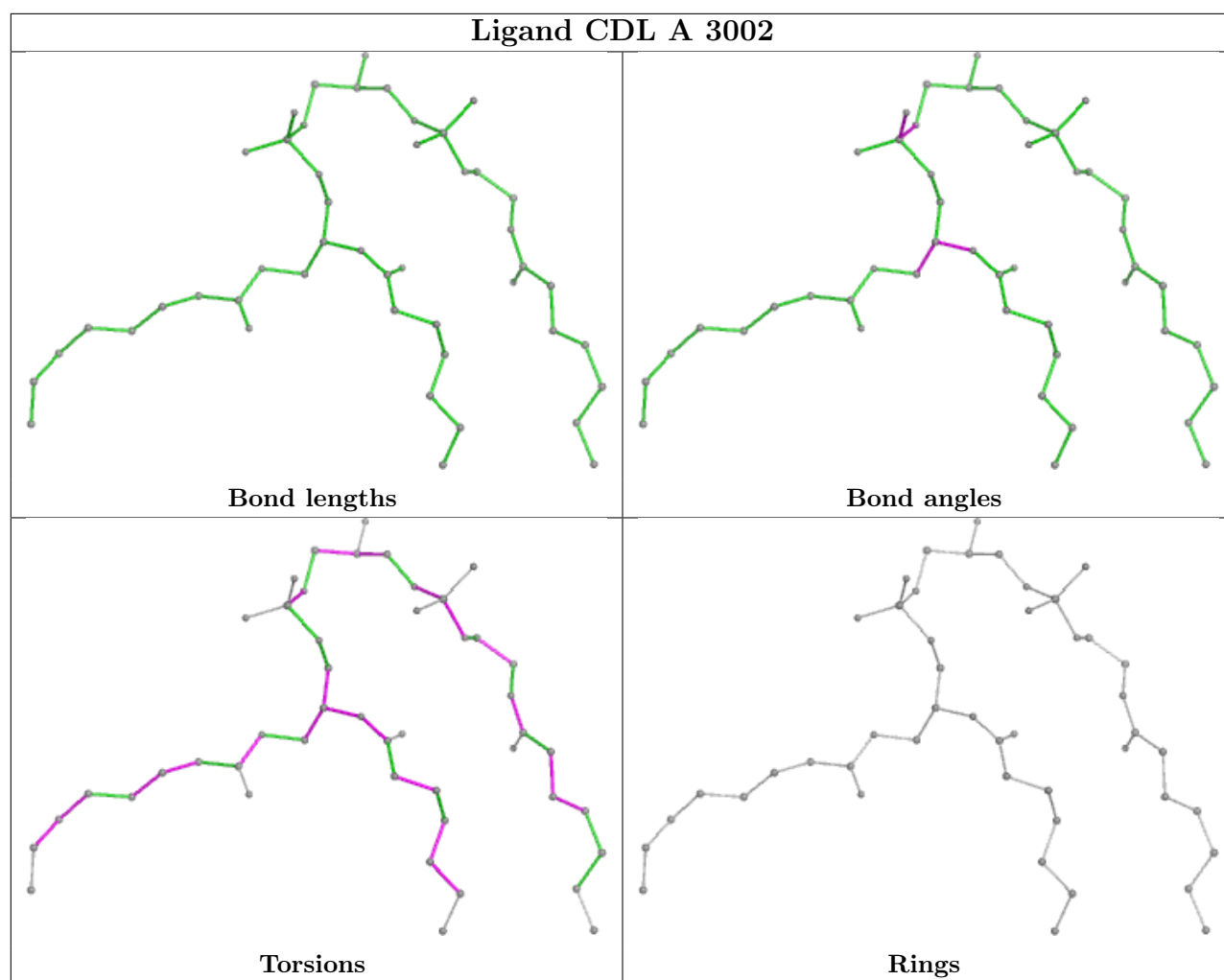


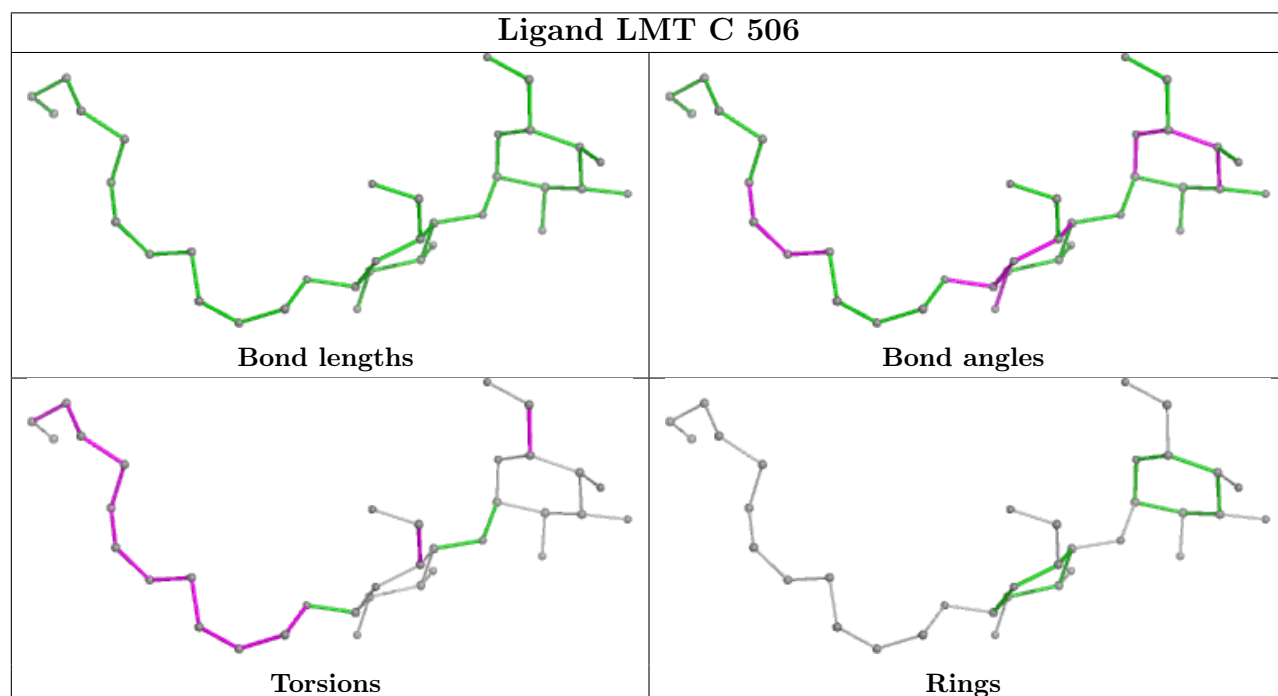
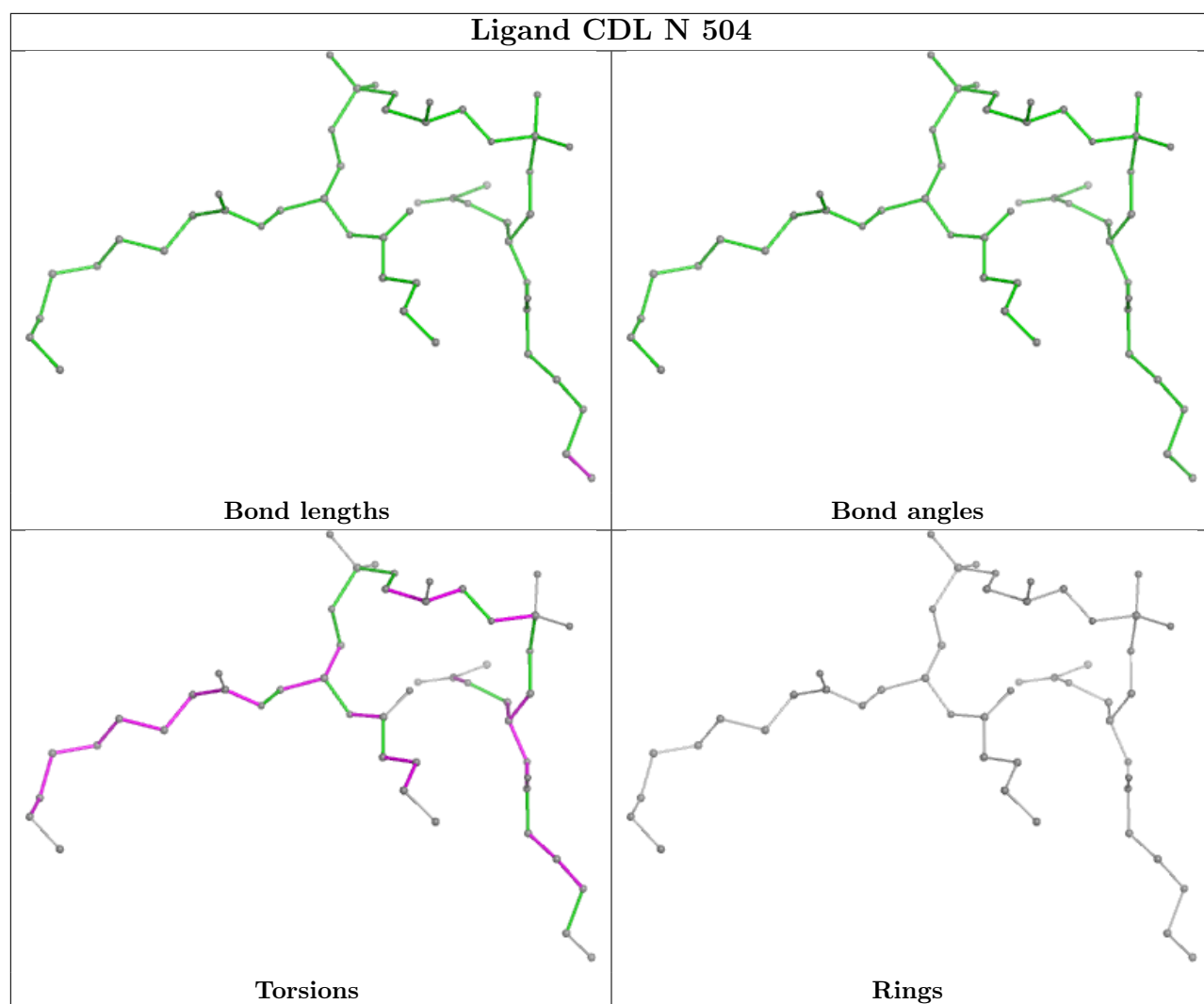


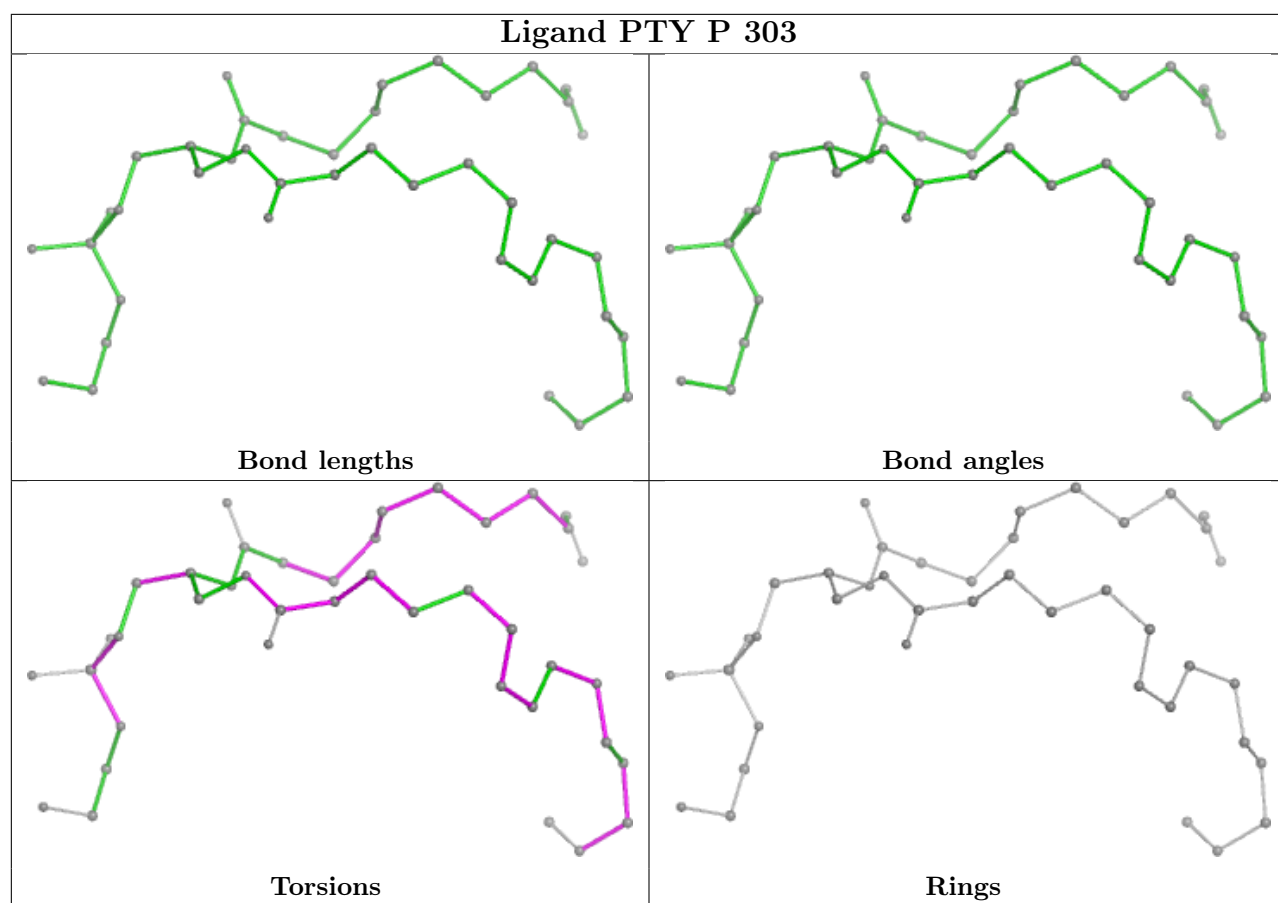




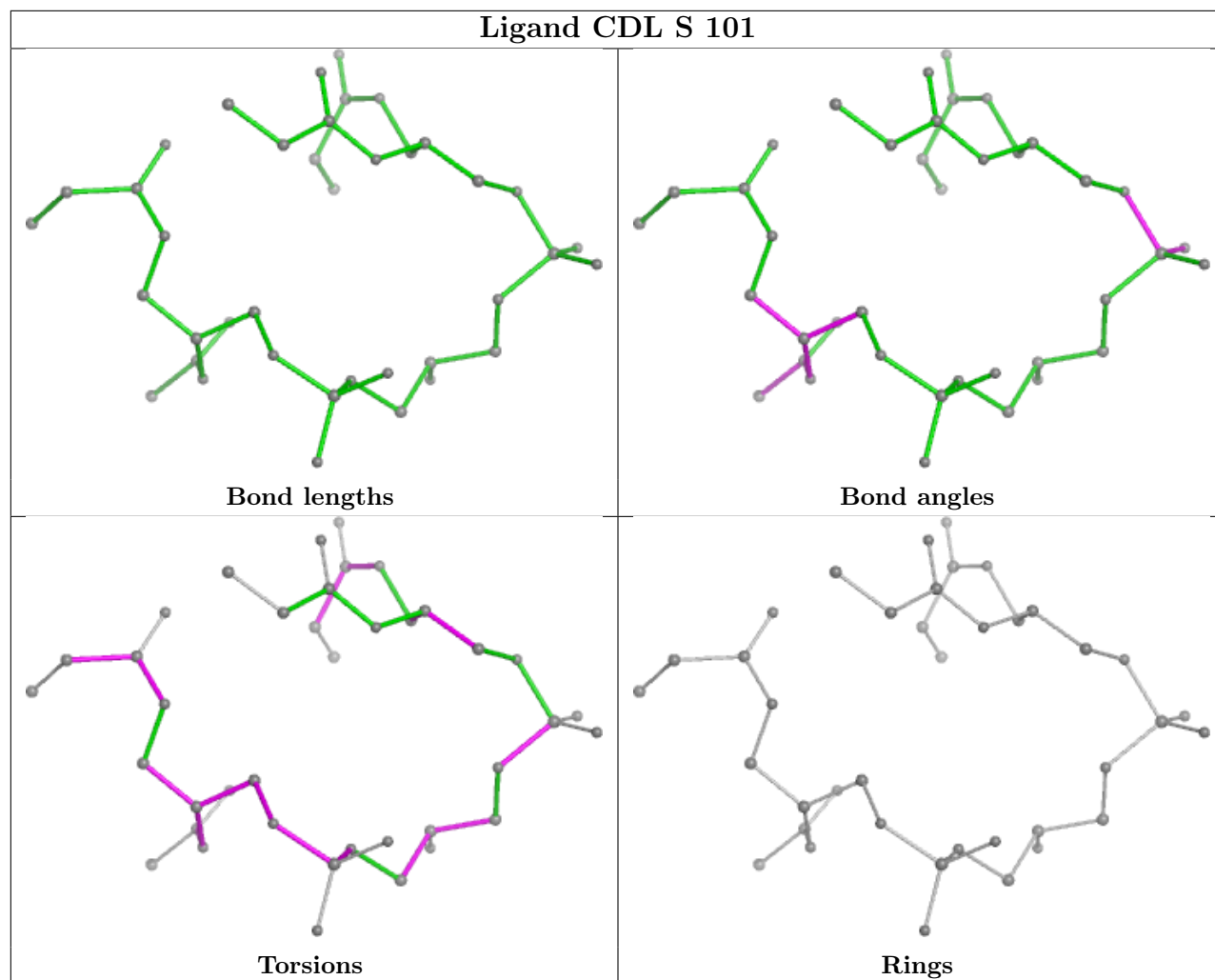




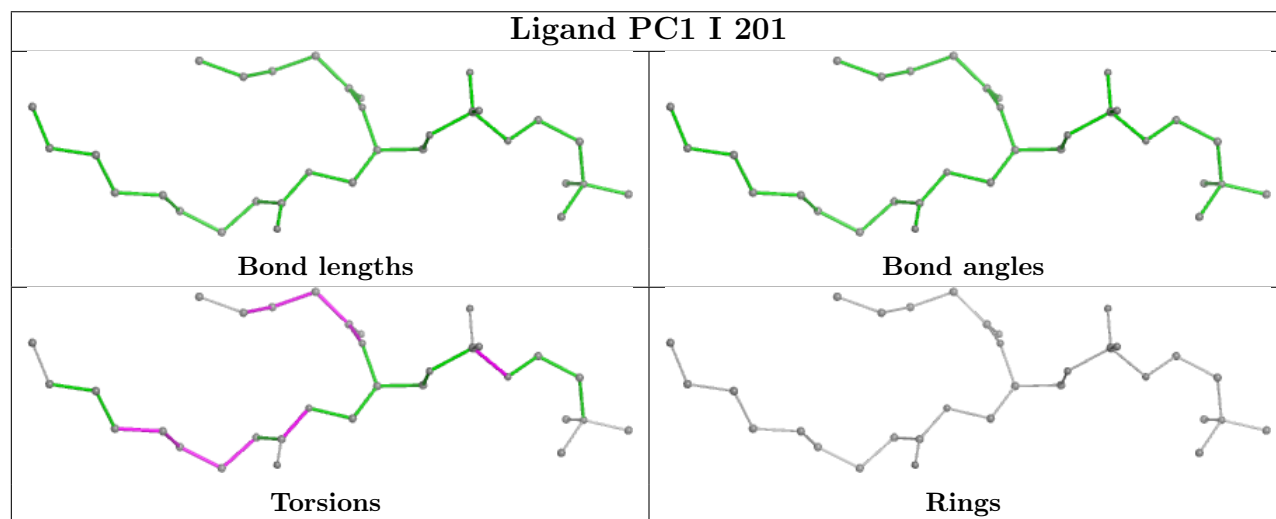


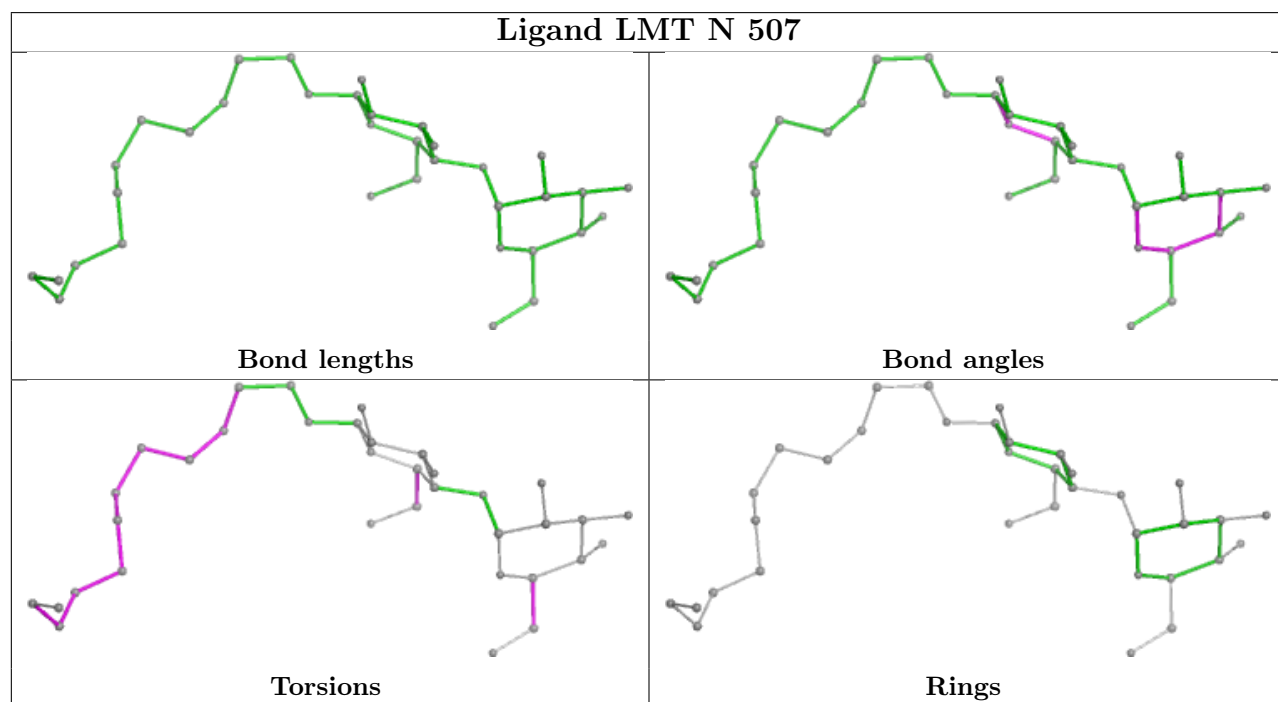
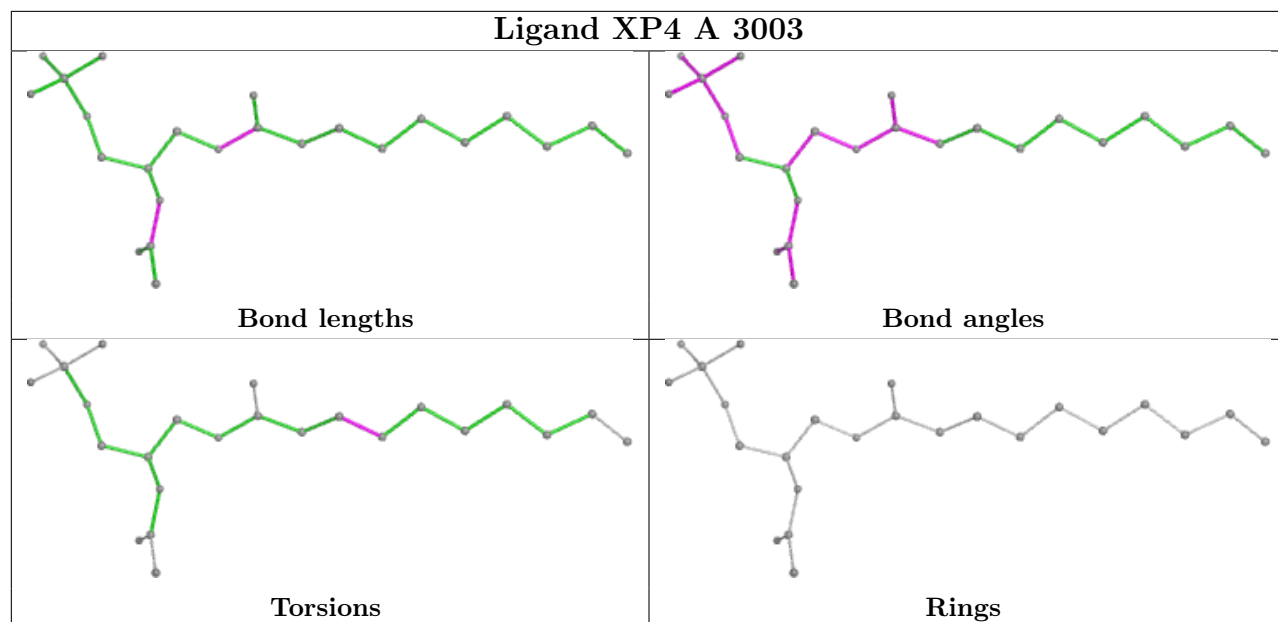


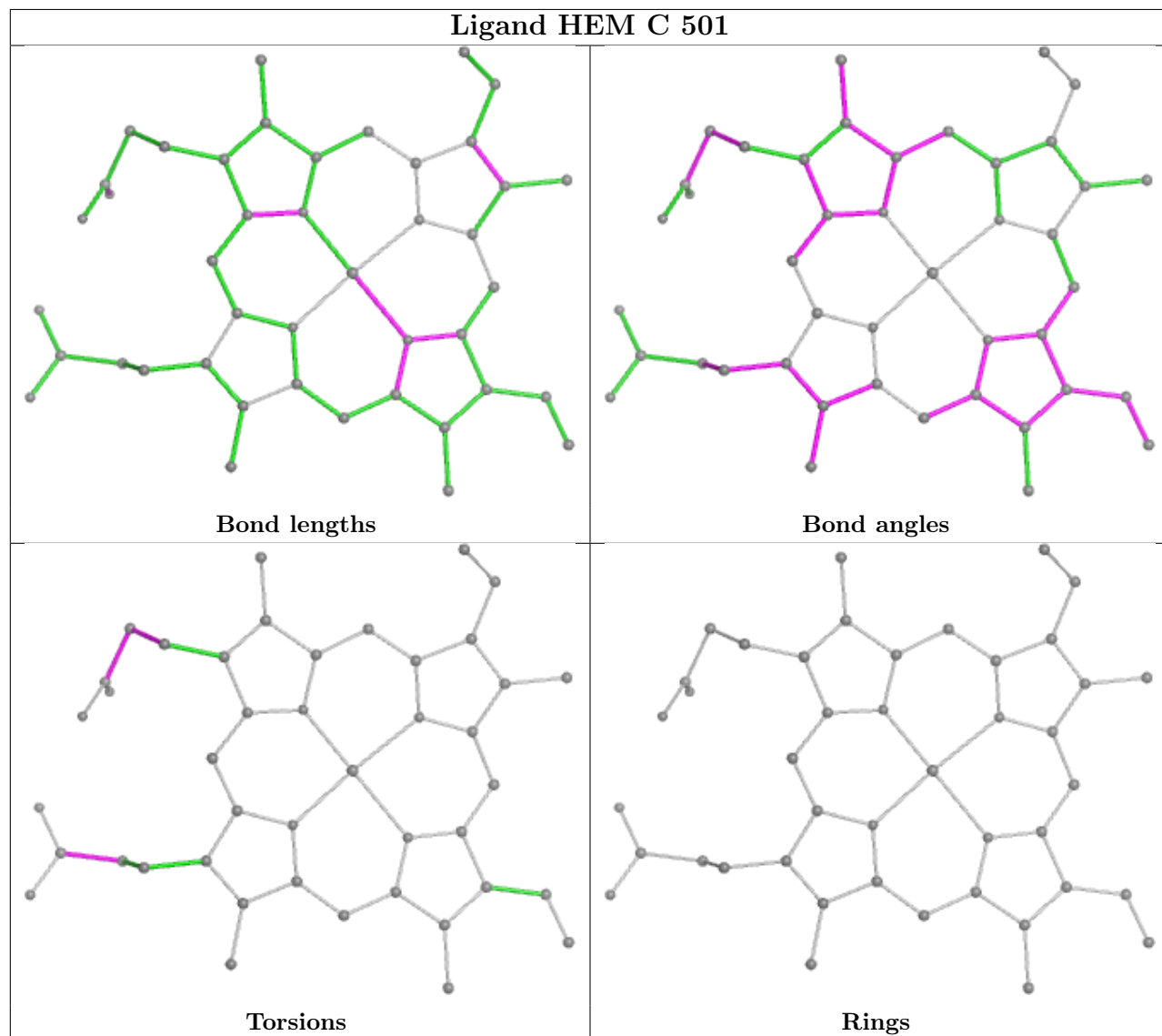
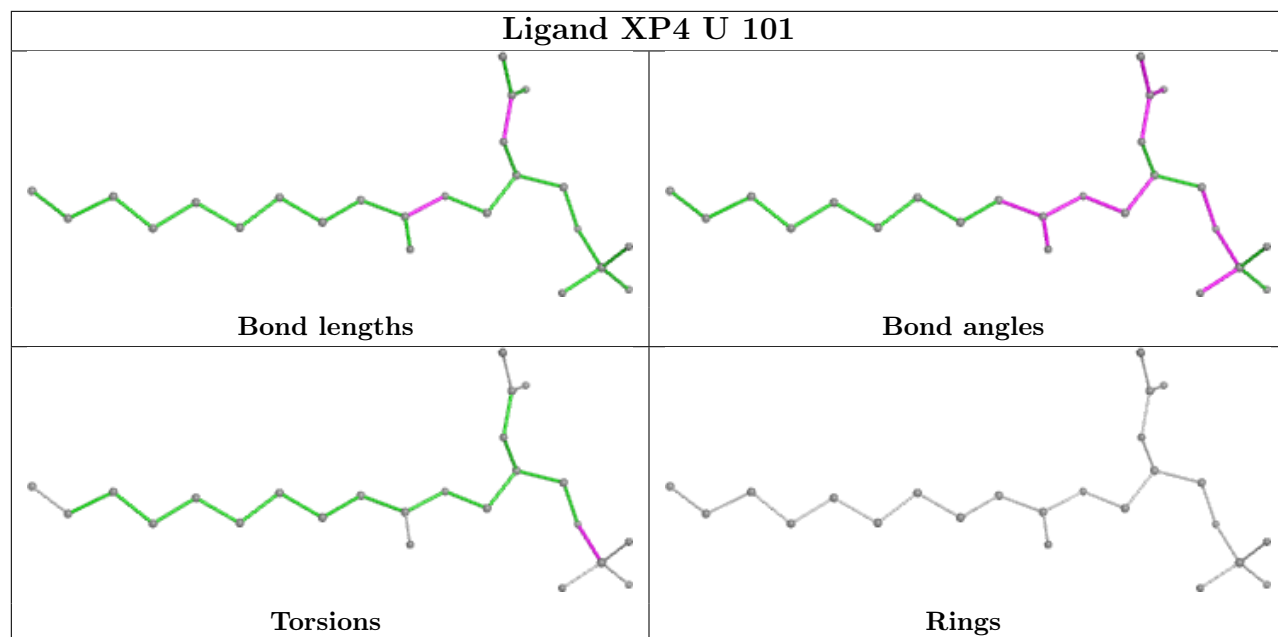
Ligand CDL S 101

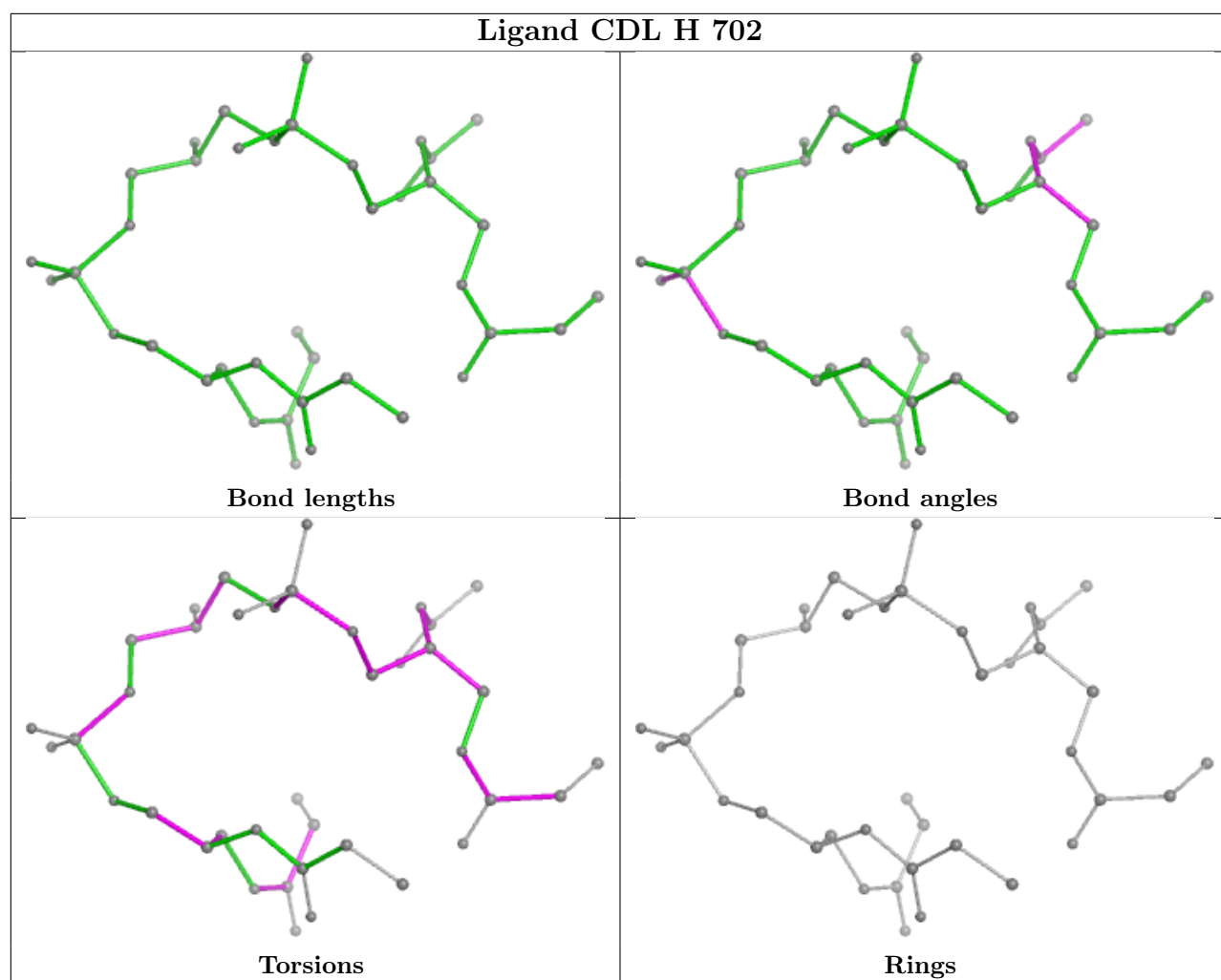


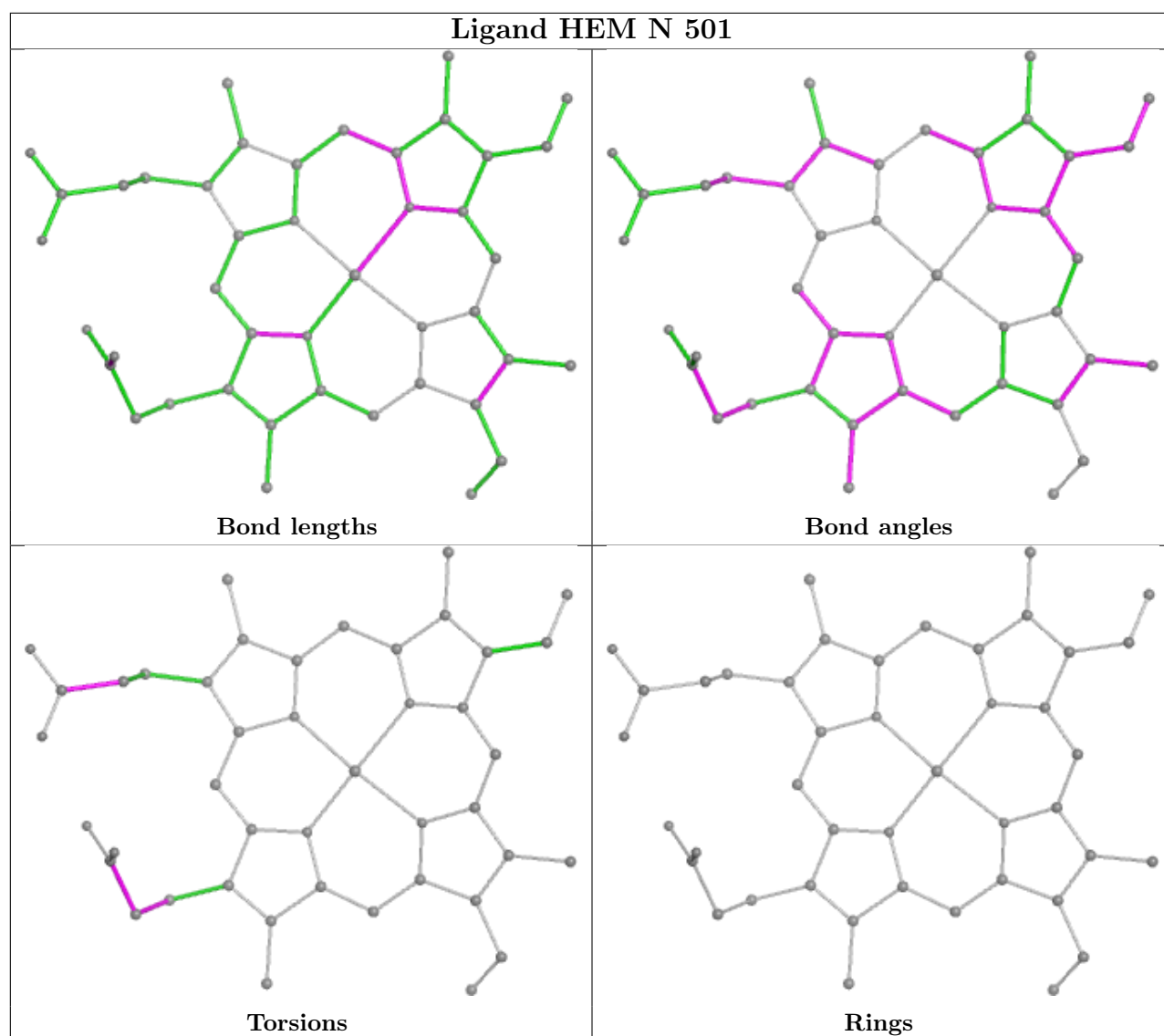
Ligand PC1 I 201











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

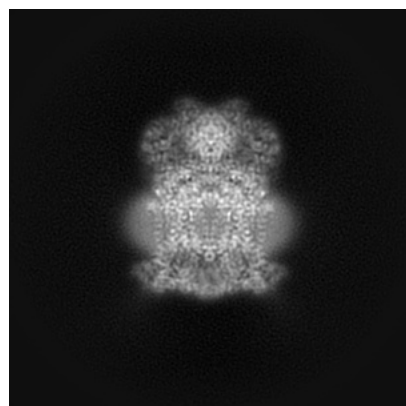
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15333. These allow visual inspection of the internal detail of the map and identification of artifacts.

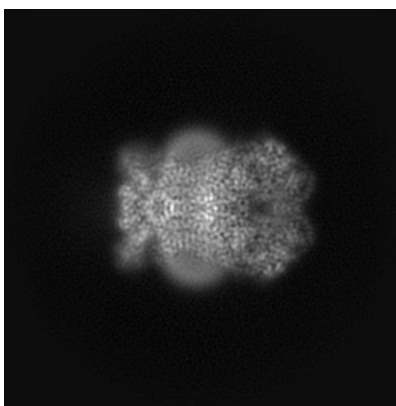
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

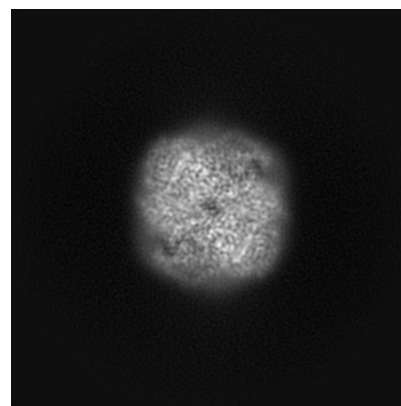
6.1.1 Primary map



X

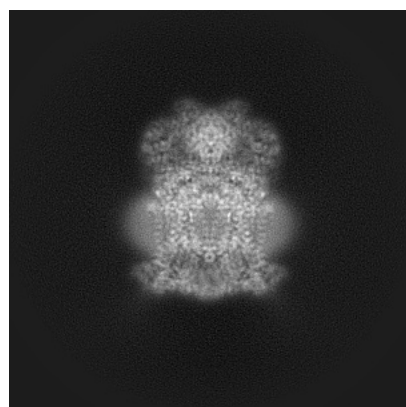


Y

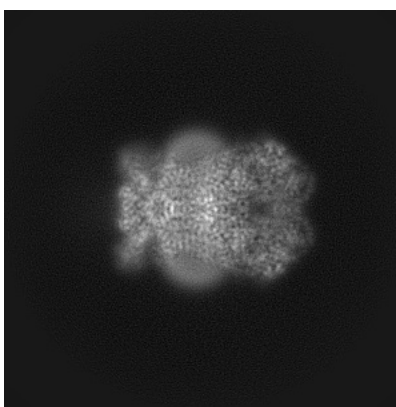


Z

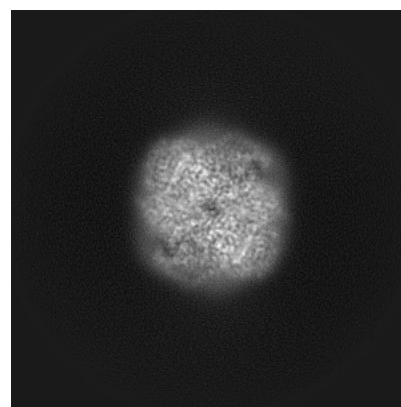
6.1.2 Raw map



X



Y

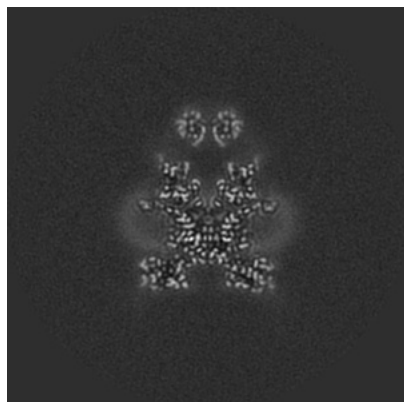


Z

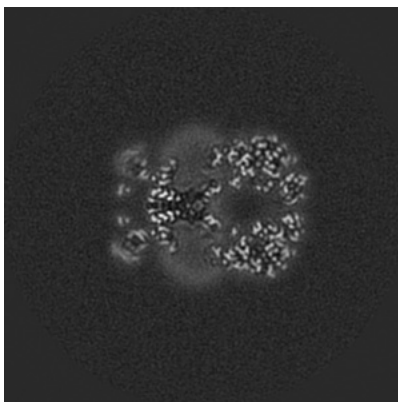
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

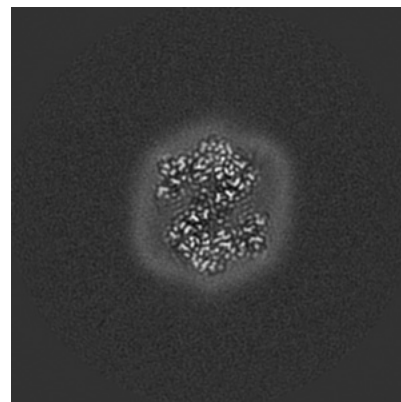
6.2.1 Primary map



X Index: 180

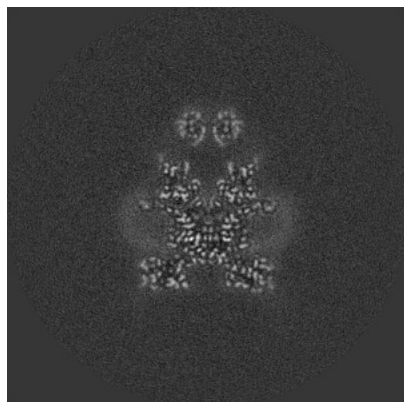


Y Index: 180

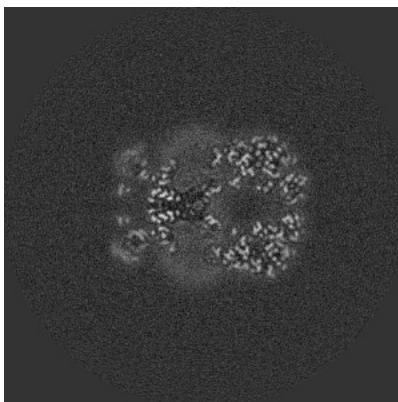


Z Index: 180

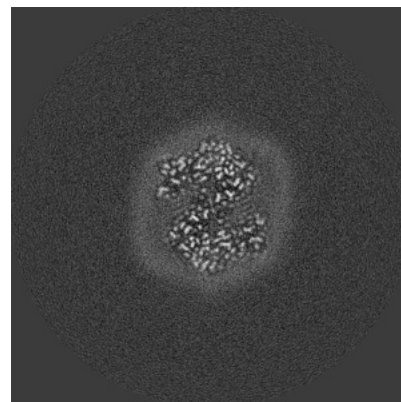
6.2.2 Raw map



X Index: 180



Y Index: 180

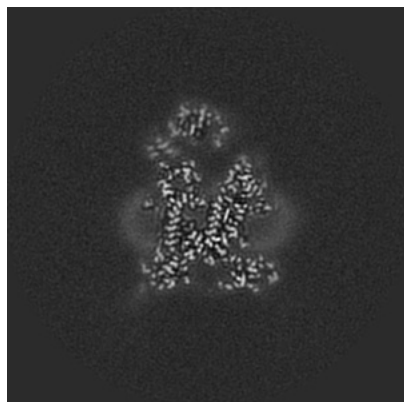


Z Index: 180

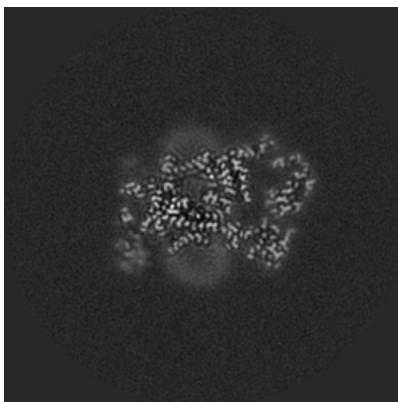
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

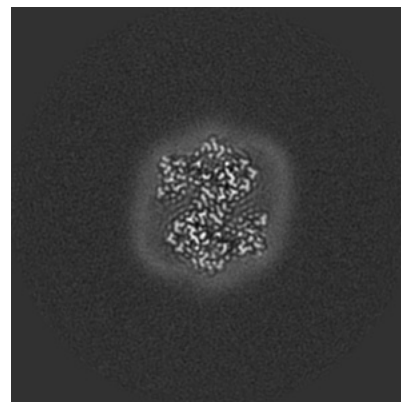
6.3.1 Primary map



X Index: 187

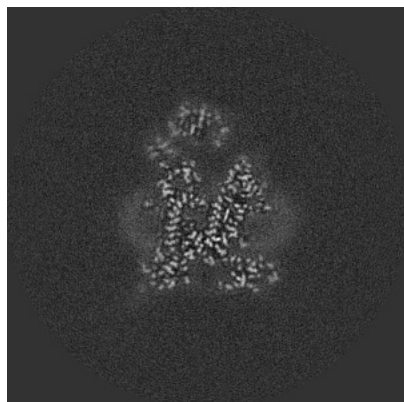


Y Index: 166

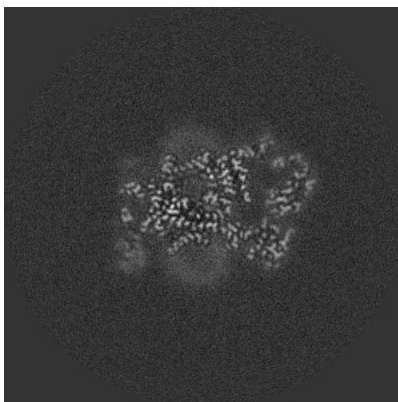


Z Index: 182

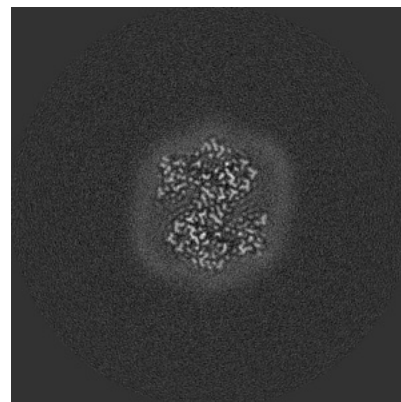
6.3.2 Raw map



X Index: 187



Y Index: 166

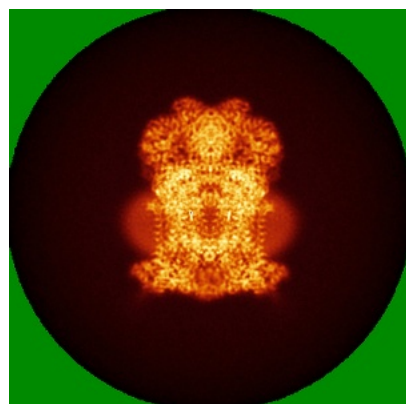


Z Index: 182

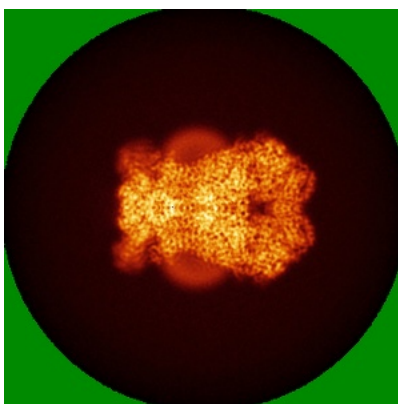
The images above show the largest variance slices of the map in three orthogonal directions.

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

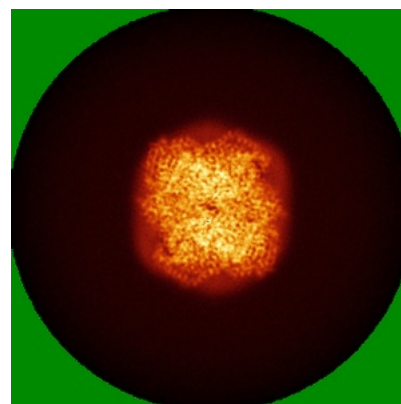
6.4.1 Primary map



X

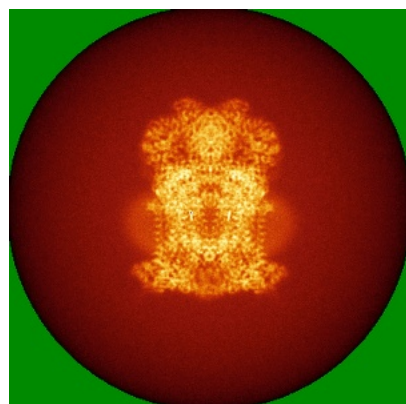


Y

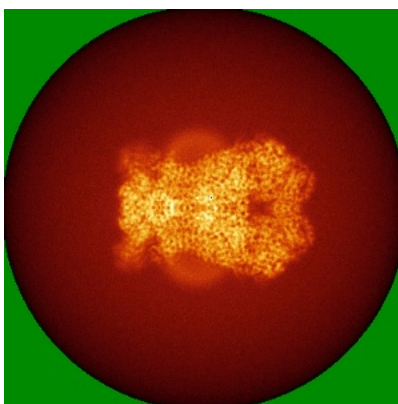


Z

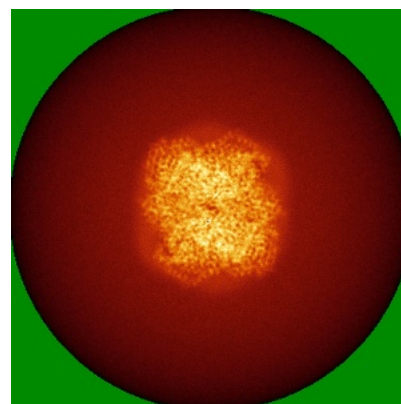
6.4.2 Raw map



X



Y

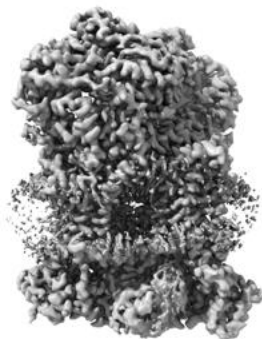


Z

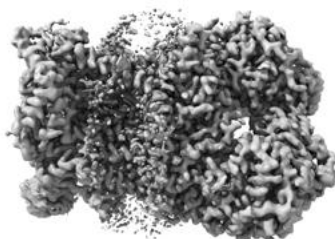
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

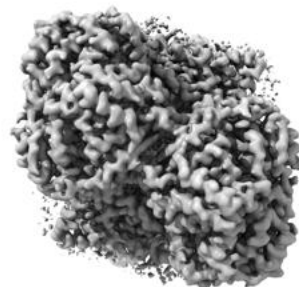
6.5.1 Primary map



X



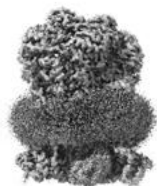
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

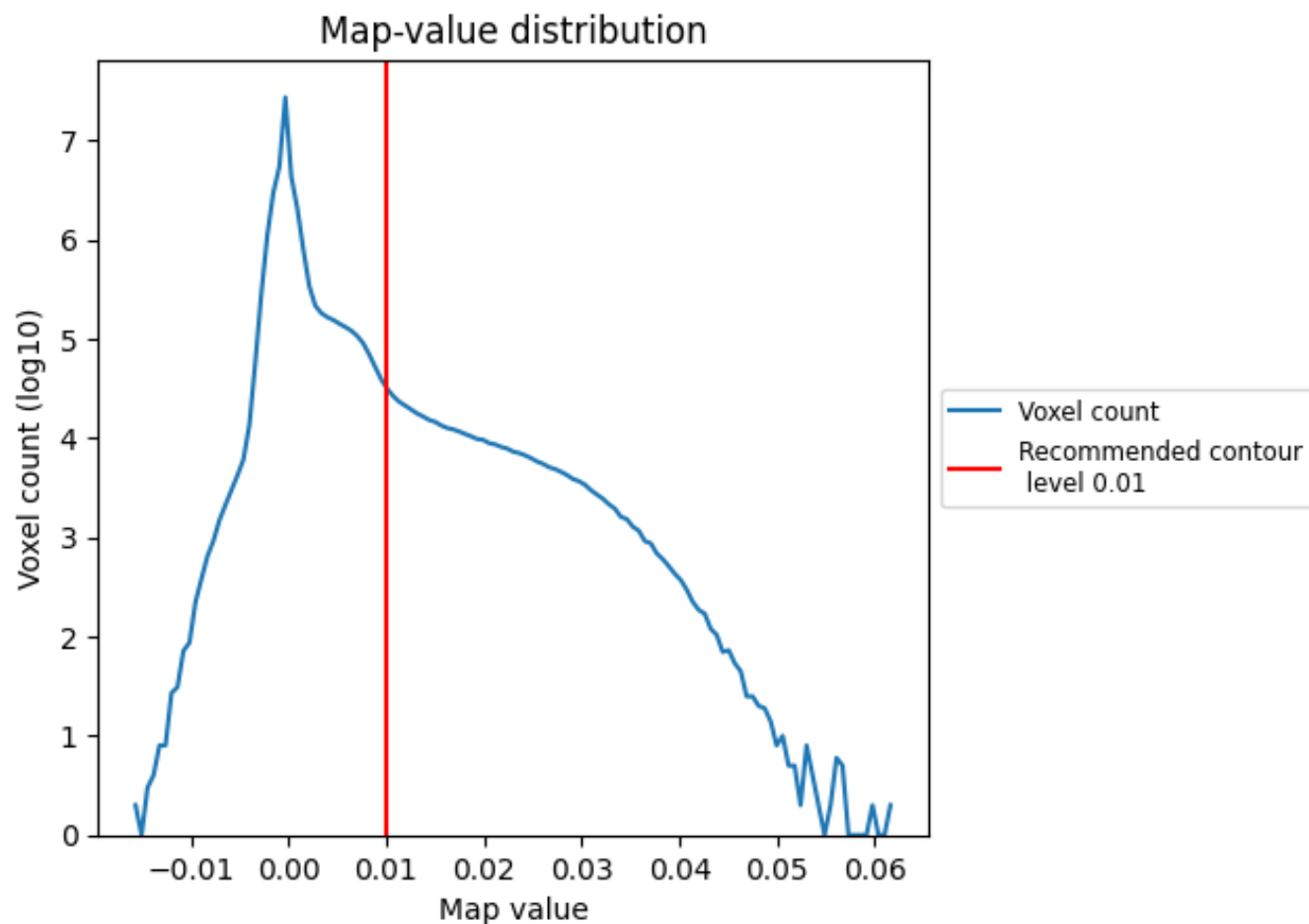
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

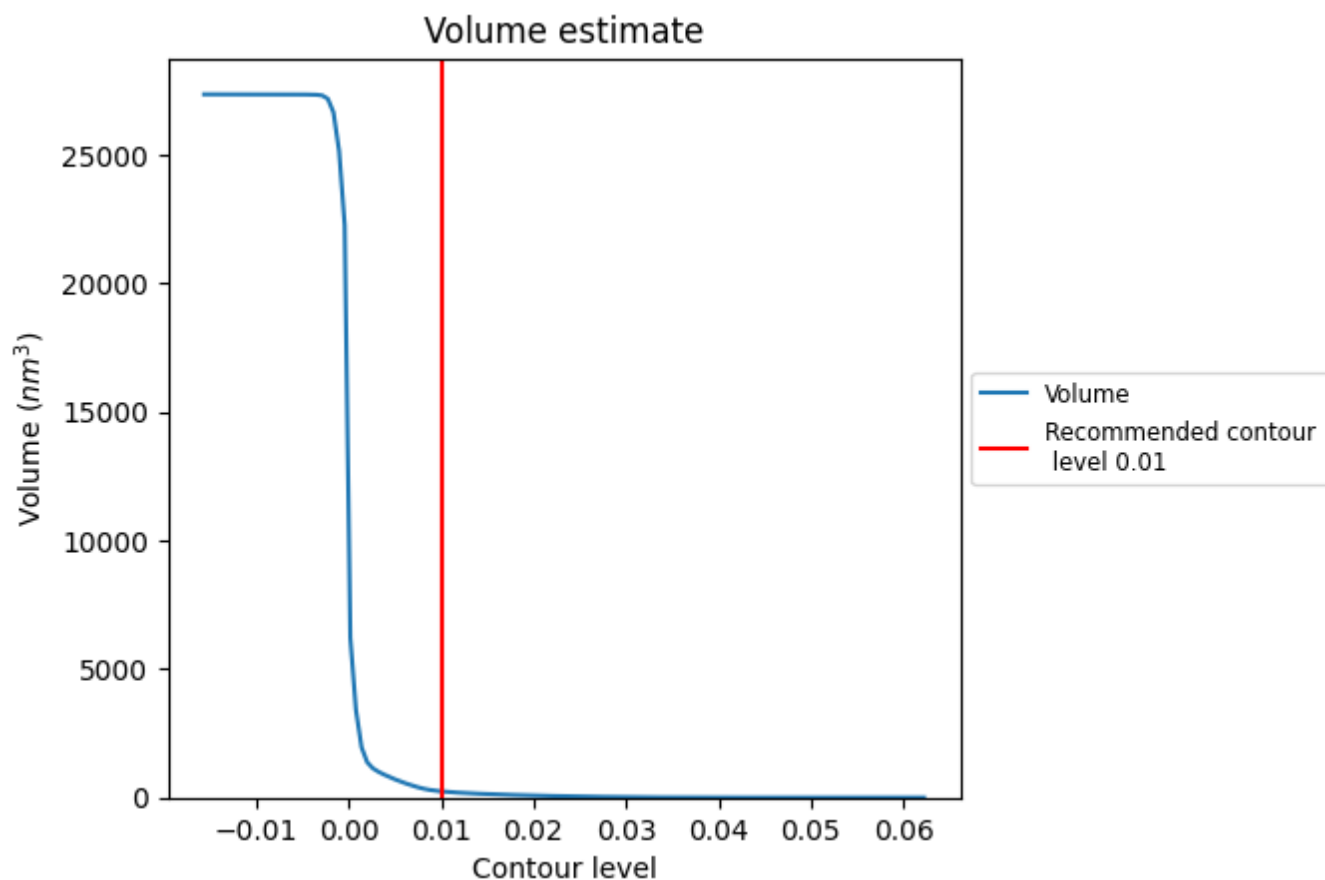
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

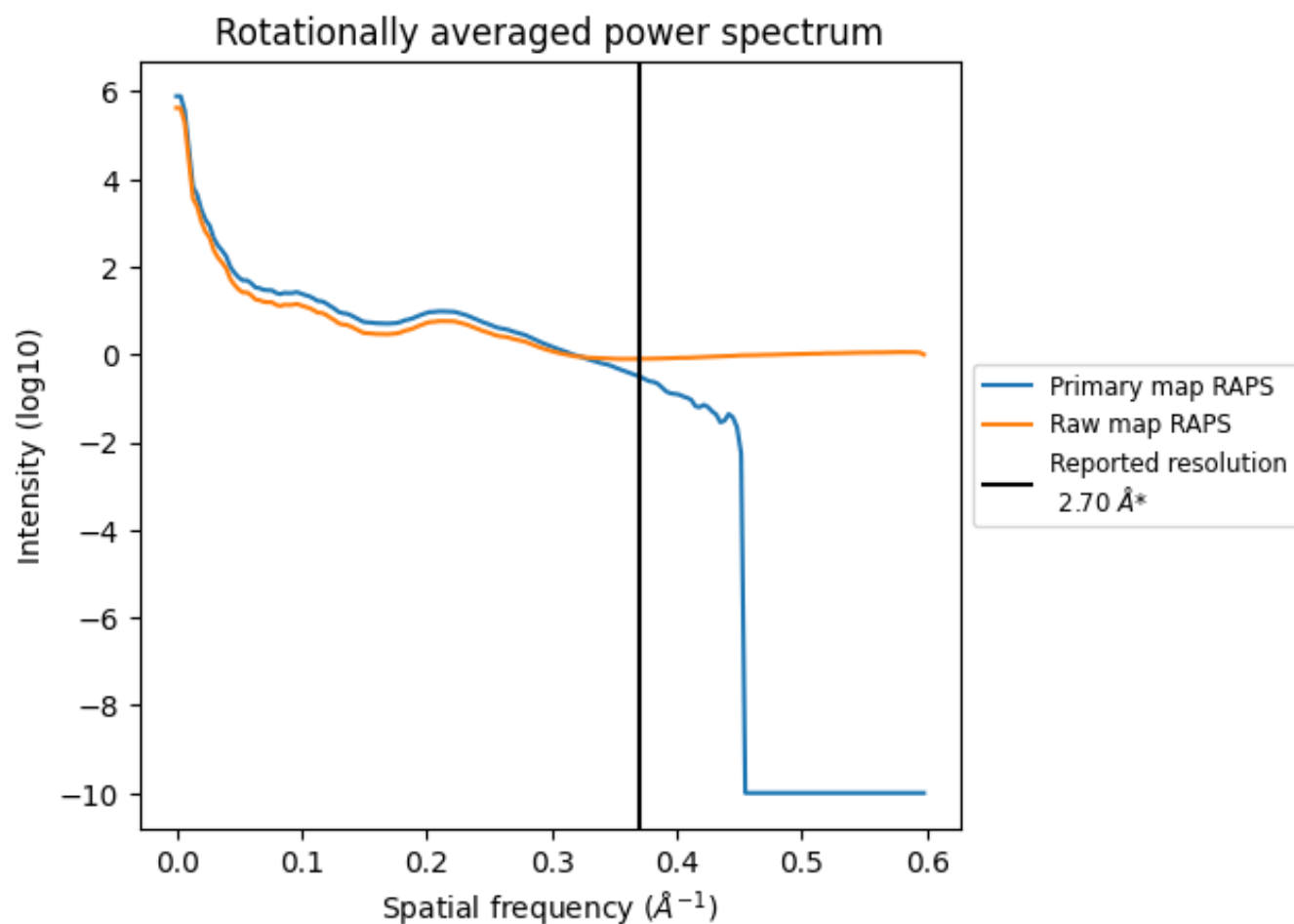
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm^3 ; this corresponds to an approximate mass of 217 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 ⓘ

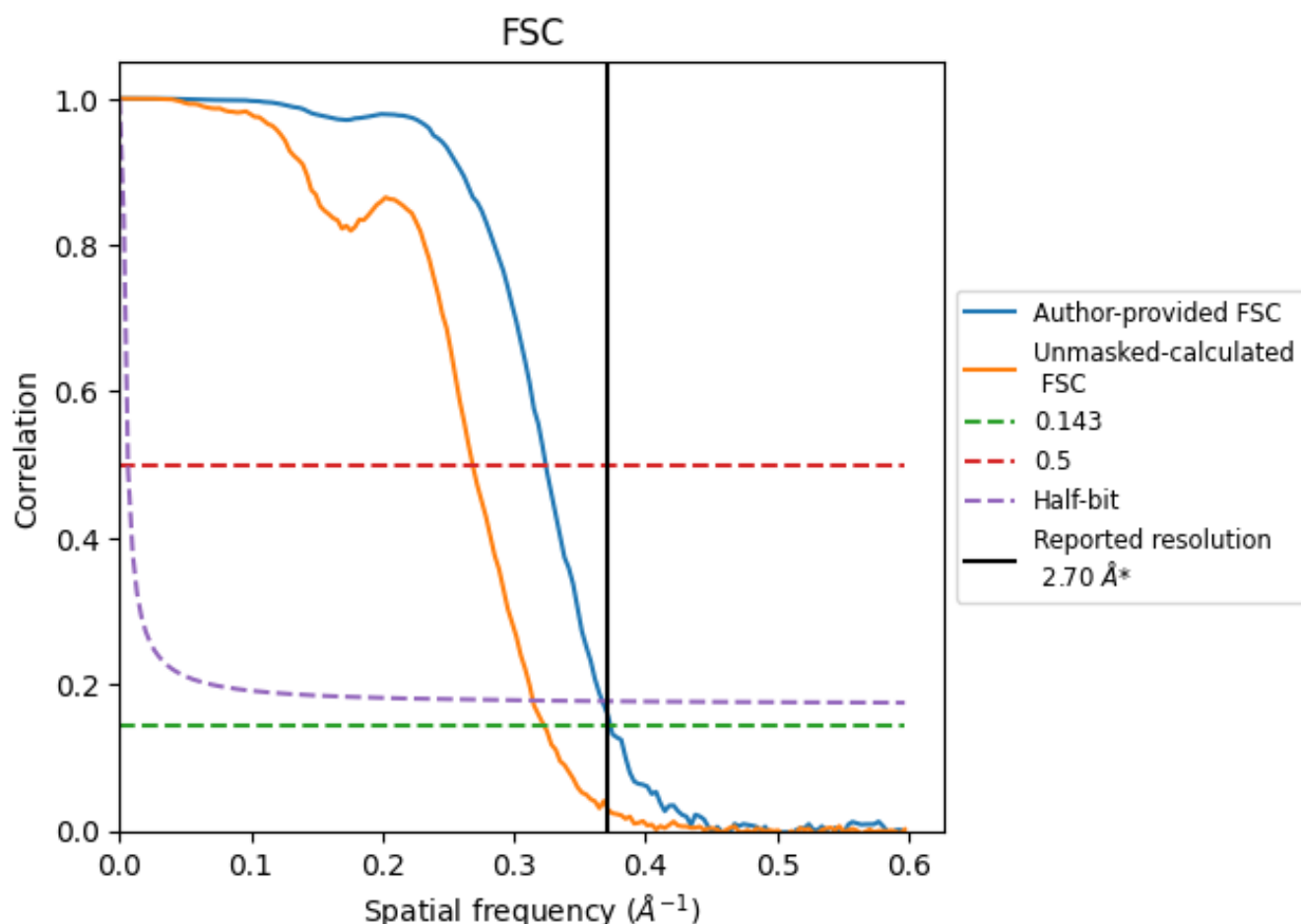


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

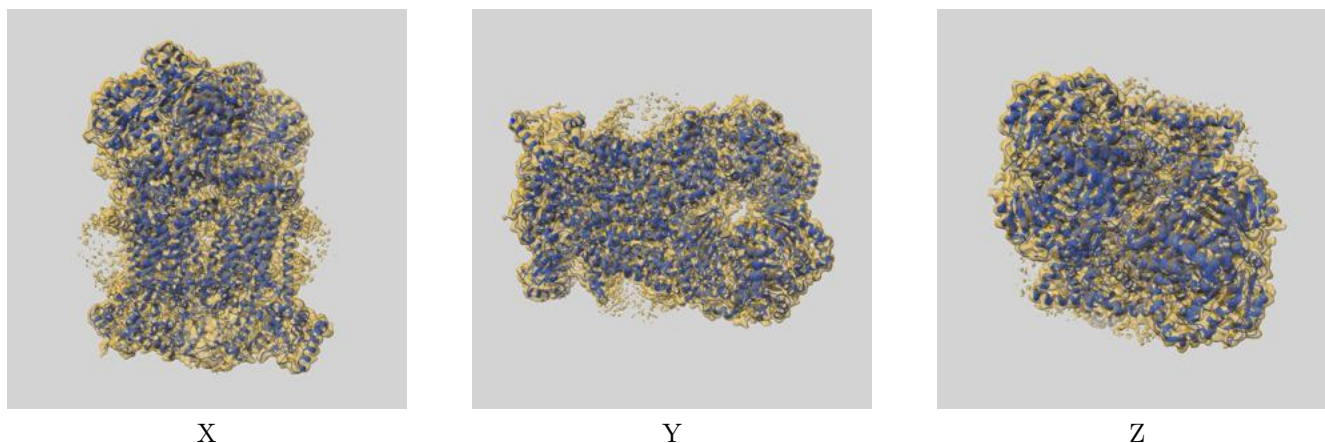
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.08	2.72
Unmasked-calculated*	3.10	3.72	3.18

*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 3.10 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

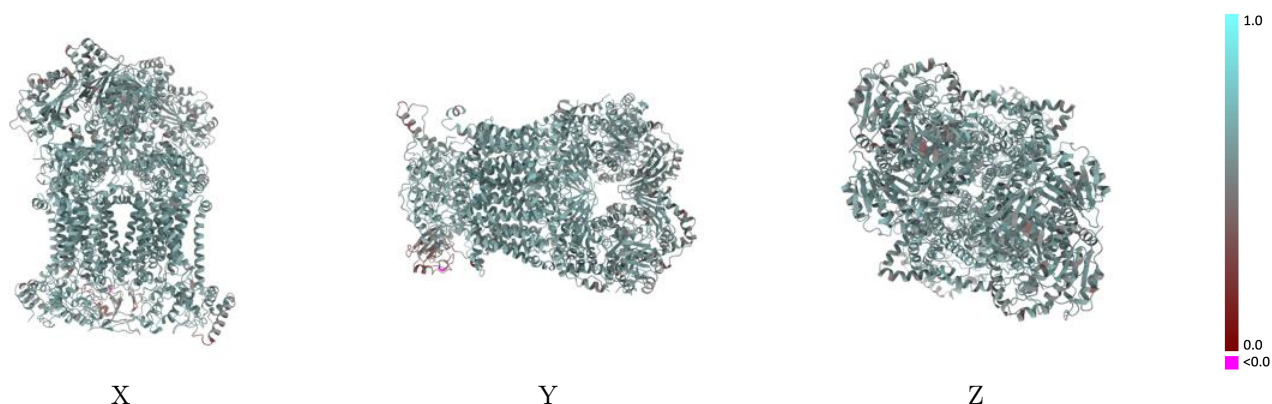
This section contains information regarding the fit between EMDB map EMD-15333 and PDB model 8AC4. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



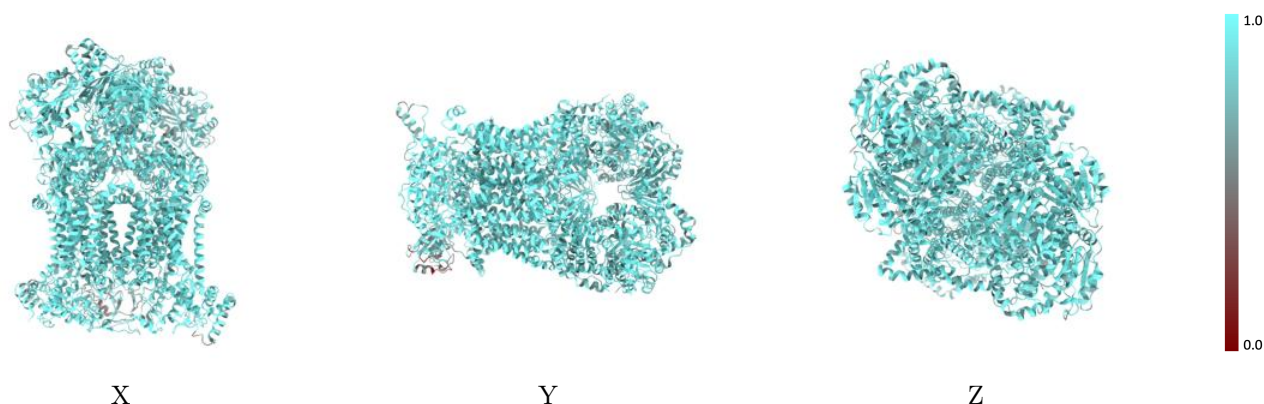
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



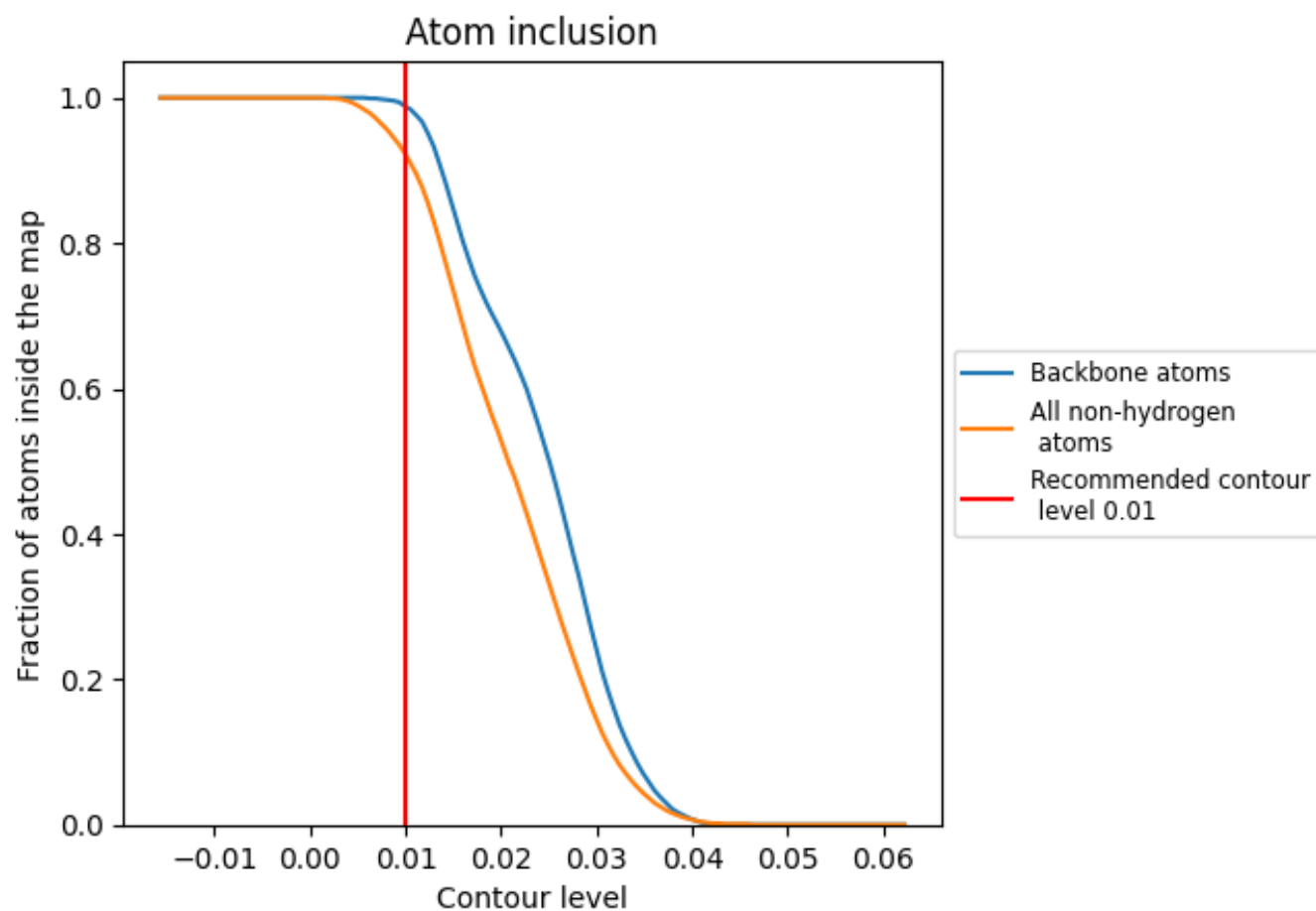
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9220	 0.5890
A	 0.9110	 0.5860
B	 0.9080	 0.5760
C	 0.9680	 0.6230
D	 0.9500	 0.6110
E	 0.9420	 0.6150
F	 0.8260	 0.5060
G	 0.9280	 0.6030
H	 0.9590	 0.6050
I	 0.9600	 0.6130
J	 0.8950	 0.5750
L	 0.9130	 0.5850
M	 0.9130	 0.5770
N	 0.9680	 0.6230
O	 0.9480	 0.6100
P	 0.7560	 0.4710
Q	 0.8340	 0.5100
R	 0.9230	 0.6020
S	 0.9590	 0.6040
T	 0.9560	 0.6060
U	 0.9130	 0.5850

