



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 7R0W / pdb_00007r0w
EMDB ID : EMD-14224
Title : 2.8 Angstrom cryo-EM structure of the dimeric cytochrome b6f-PetP complex from *Synechocystis* sp. PCC 6803 with natively bound lipids and plastoquinone molecules
Authors : Farmer, D.F.; Proctor, M.S.; Malone, L.A.; Swainsbury, D.P.K.; Hawkings, F.R.; Hitchcock, A.; Johnson, M.P.
Deposited on : 2022-02-02
Resolution : 2.80 Å(reported)
Based on initial model : 7PPW

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

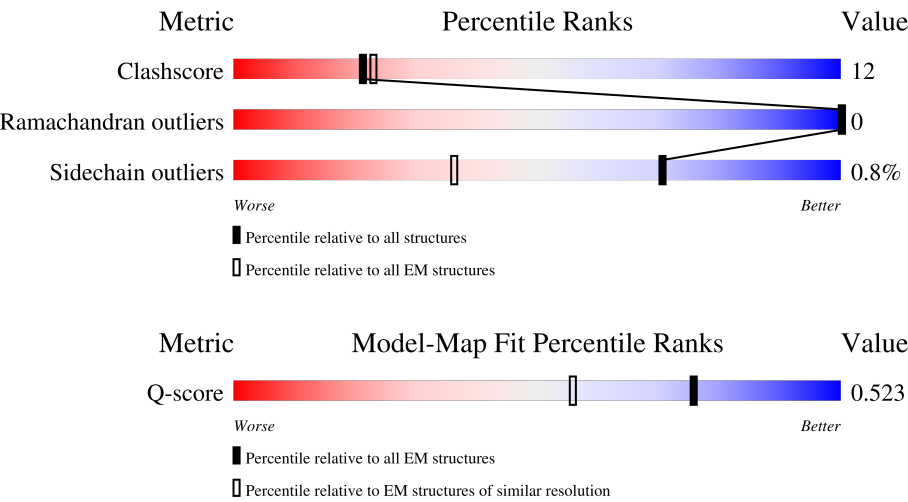
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	V	65	6% 52% 46% .
1	X	65	. 49% 49% .
2	A	222	82% 18%

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Mol	Chain	Length	Quality of chain
2	I	222	
3	B	160	
3	J	160	
4	C	328	
4	K	328	
5	E	32	
5	M	32	
6	F	36	
6	N	36	
7	G	38	
7	O	38	
8	H	29	
8	P	29	
9	D	192	
9	L	192	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	302	X	-	-	-
14	CLA	J	202	X	-	-	-
16	LMG	N	101	X	-	-	-
17	6PL	H	101	X	-	-	-
17	6PL	P	101	X	-	-	-
19	FES	D	201	-	-	X	-
19	FES	L	202	-	-	X	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 16830 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 Uncharacterized protein Cp097, conserved in cyanobacteria.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	64	Total	C	N	O	S	0	0
			500	320	85	94	1		
1	V	64	Total	C	N	O	S	0	0
			500	320	85	94	1		

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	222	Total	C	N	O	S	0	0
			1769	1175	283	299	12		
2	A	222	Total	C	N	O	S	0	0
			1769	1175	283	299	12		

- Molecule 3 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		
3	B	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		

- Molecule 4 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	279	Total	C	N	O	S	0	0
			2115	1356	352	402	5		
4	C	279	Total	C	N	O	S	0	0
			2115	1356	352	402	5		

- Molecule 5 is a protein called Cytochrome B6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	32	Total	C	N	O	S	0	0
			238	165	36	36	1		
5	E	32	Total	C	N	O	S	0	0
			238	165	36	36	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	34	Total	C	N	O	S	0	0
			248	165	38	42	3		
6	F	34	Total	C	N	O	S	0	0
			248	165	38	42	3		

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	32	Total	C	N	O	S	0	0
			242	166	37	38	1		
7	G	32	Total	C	N	O	S	0	0
			242	166	37	38	1		

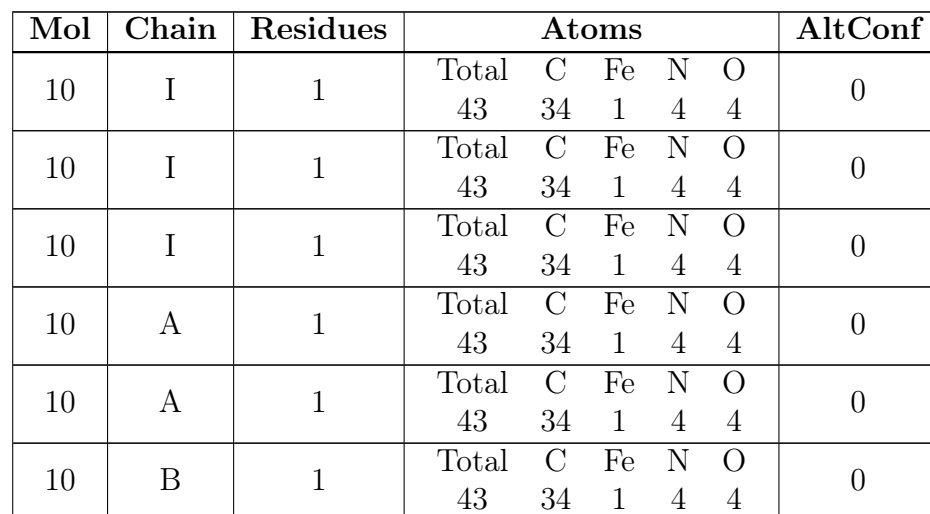
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	29	Total	C	N	O	S	0	0
			234	159	36	37	2		
8	H	29	Total	C	N	O	S	0	0
			234	159	36	37	2		

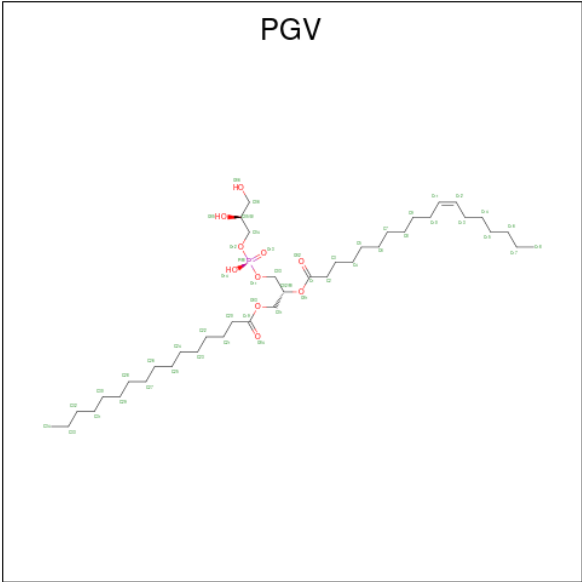
- Molecule 9 is a protein called Rieske domain, PetC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	169	Total	C	N	O	S	0	0
			1256	795	215	240	6		
9	L	169	Total	C	N	O	S	0	0
			1256	795	215	240	6		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

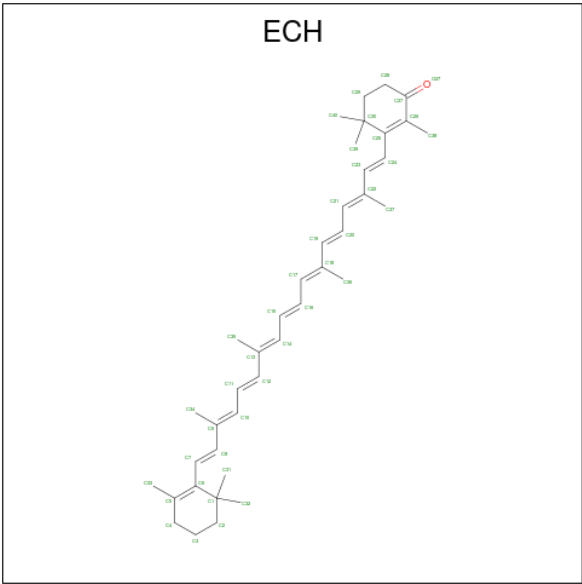


- Molecule 11 is (1R)-2-[[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



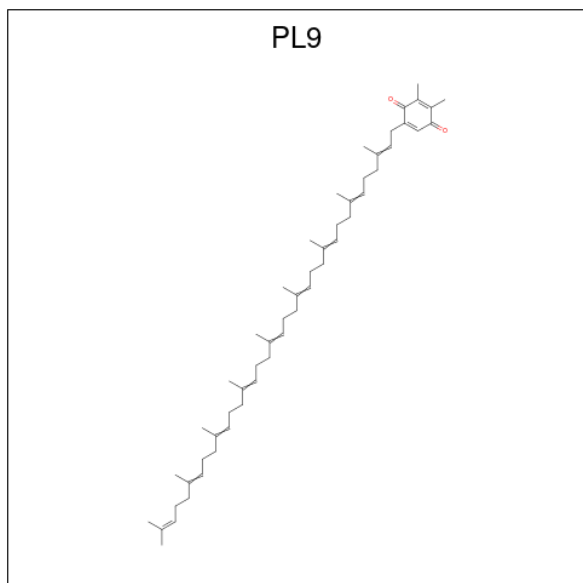
Mol	Chain	Residues	Atoms				AltConf
11	I	1	Total	C	O	P	0
			39	28	10	1	
11	J	1	Total	C	O	P	0
			41	30	10	1	
11	B	1	Total	C	O	P	0
			51	40	10	1	
11	C	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 12 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



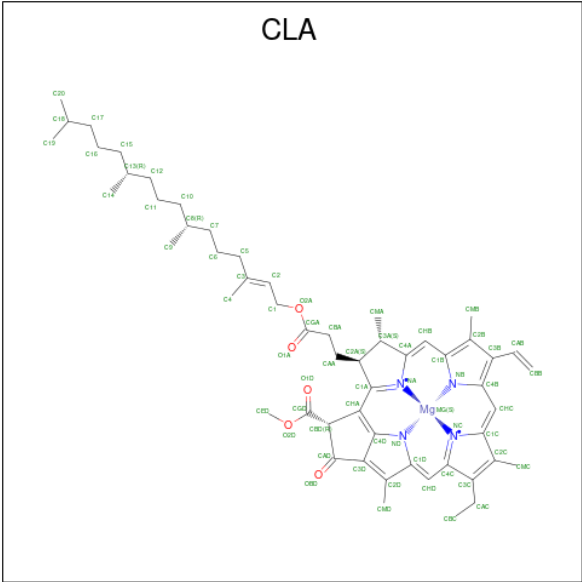
Mol	Chain	Residues	Atoms			AltConf
12	I	1	Total	C	O	0
			41	40	1	
12	A	1	Total	C	O	0
			41	40	1	

- Molecule 13 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



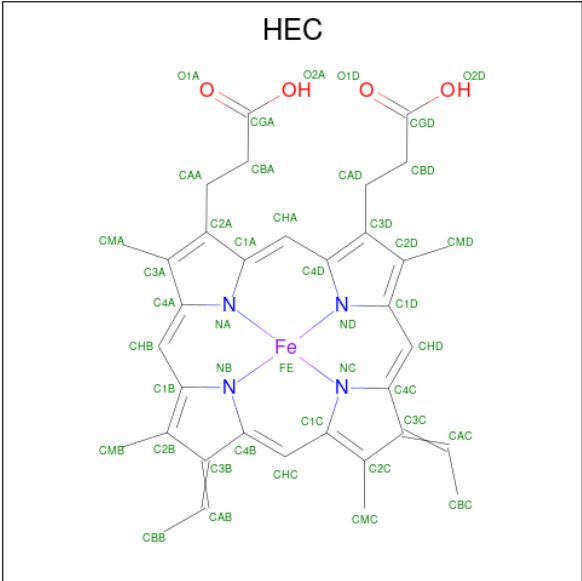
Mol	Chain	Residues	Atoms			AltConf
13	J	1	Total	C	O	0
			55	53	2	
13	A	1	Total	C	O	0
			55	53	2	

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



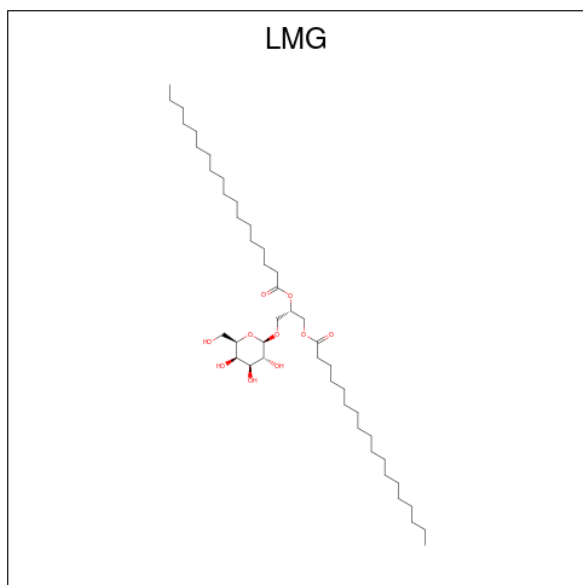
Mol	Chain	Residues	Atoms					AltConf
15	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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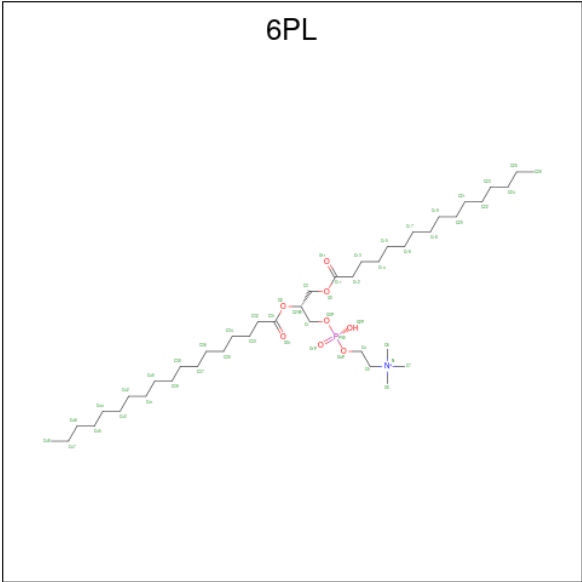
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
15	C	1	43	34	1	4	4	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



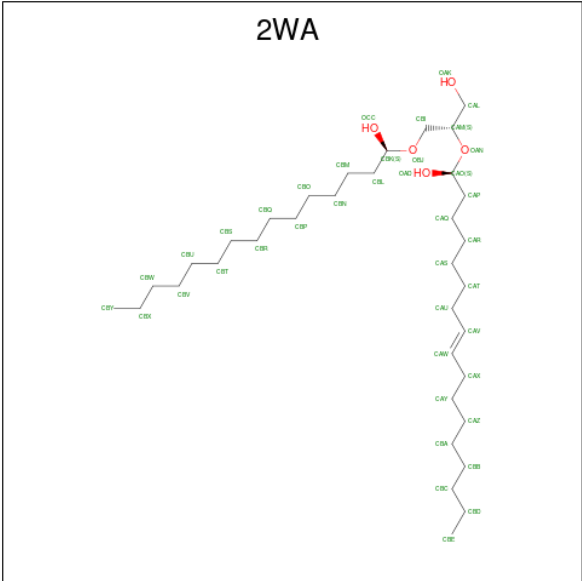
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	N	1	55	45	10	0

- Molecule 17 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: $C_{42}H_{85}NO_8P$).



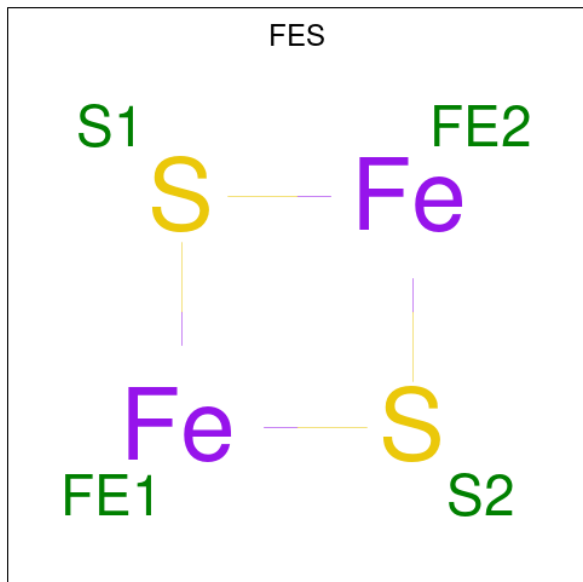
Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			51	41	1	8	1	
17	H	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 18 is (1S,8E)-1-{[(2S)-1-hydroxy-3-{[(1S)-1-hydroxypentadecyl]oxy}propan-2-yl]oxy}heptadec-8-en-1-ol (CCD ID: 2WA) (formula: C₃₅H₇₀O₅).



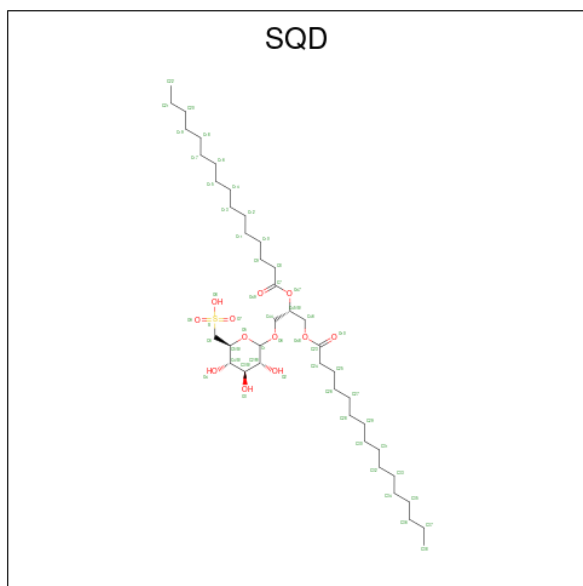
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			40	35	5	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



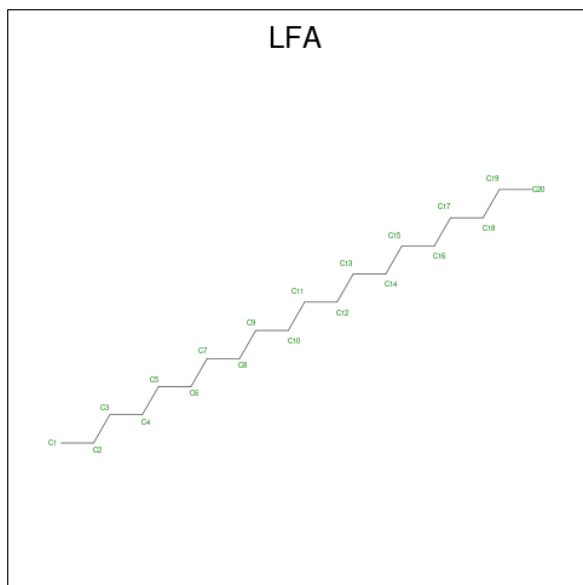
Mol	Chain	Residues	Atoms			AltConf
19	D	1	Total	Fe	S	0
			4	2	2	
19	L	1	Total	Fe	S	0
			4	2	2	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	O	S	0
			54	41	12	1	
20	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
21	E	1	Total	C	0
			20	20	

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	I	1	Total	O	0
			1	1	
22	B	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

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.

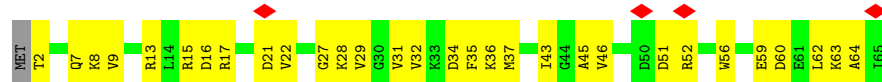
- Molecule 1: Uncharacterized protein Cp097, conserved in cyanobacteria

Chain X: 



- Molecule 1: Uncharacterized protein Cp097, conserved in cyanobacteria

Chain V: 



- Molecule 2: Cytochrome b6

Chain I: 



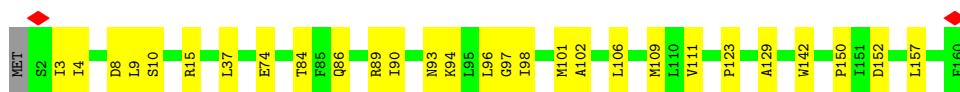
- Molecule 2: Cytochrome b6

Chain A: 

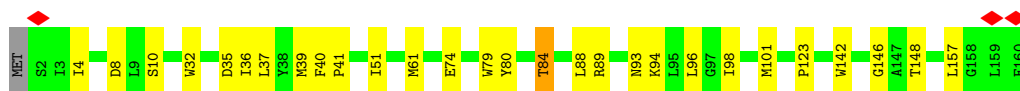
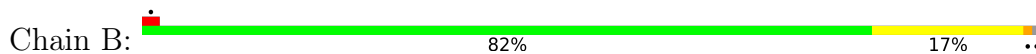


- Molecule 3: Cytochrome b6-f complex subunit 4

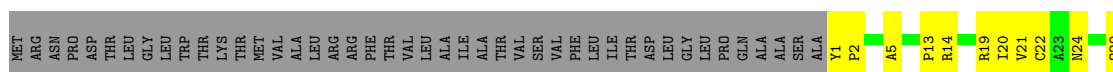
Chain J: 



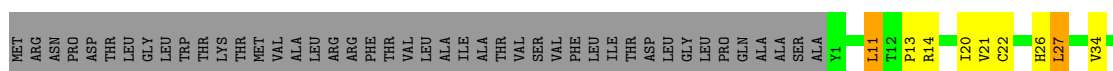
- Molecule 3: Cytochrome b6-f complex subunit 4



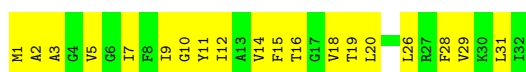
- Molecule 4: Cytochrome f



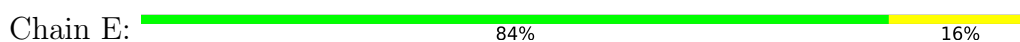
- Molecule 4: Cytochrome f



- Molecule 5: Cytochrome B6



- Molecule 5: Cytochrome B6





- Molecule 6: Cytochrome b6-f complex subunit 7

Chain N: 69% 25% 6%



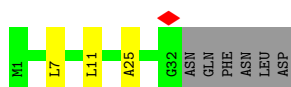
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F: 75% 17% 6%



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain O: 76% 8% 16%



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G: 61% 24% 16%



- Molecule 8: Cytochrome b6-f complex subunit 8

Chain P: 72% 28%



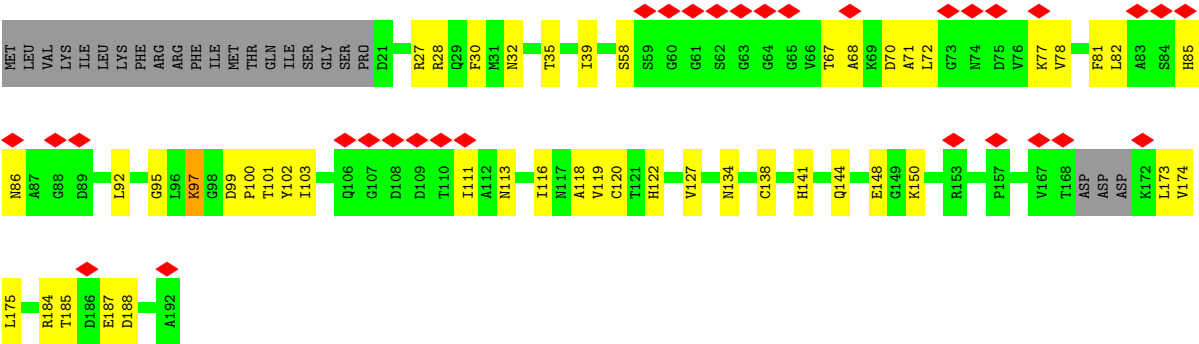
- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H: 66% 31% 3%

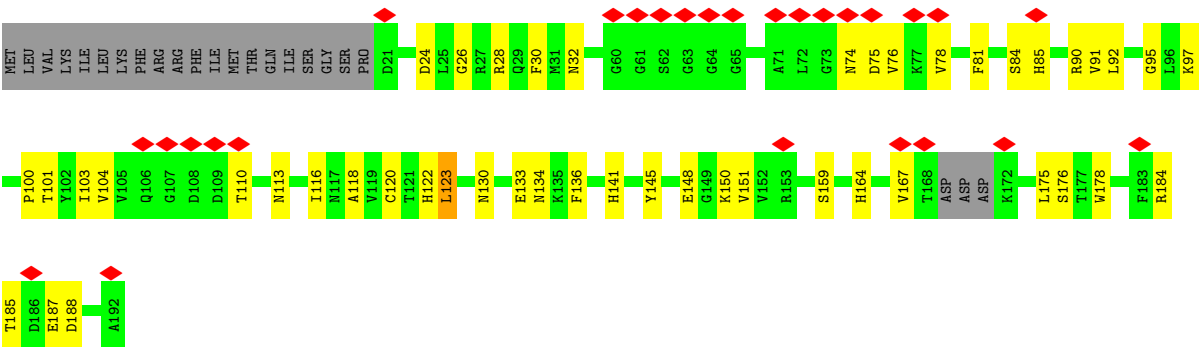


- Molecule 9: Rieske domain, PetC

Chain D: 16% 64% 24% 12%



• Molecule 9: Rieske domain, PetC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	152860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.986	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	211.99998, 211.99998, 211.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, 6PL, SQD, HEM, LFA, ECH, 2WA, PGV, CLA, FES, LMG, HEC

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	V	0.22	0/507	0.54	0/679
1	X	0.27	0/507	0.62	0/679
2	A	0.20	0/1821	0.43	0/2480
2	I	0.22	0/1821	0.43	0/2480
3	B	0.18	0/1261	0.40	0/1721
3	J	0.18	0/1261	0.44	0/1721
4	C	0.14	0/2158	0.38	0/2935
4	K	0.15	0/2158	0.39	0/2935
5	E	0.26	0/242	0.48	0/326
5	M	0.27	0/242	0.56	0/326
6	F	0.27	0/251	0.50	0/337
6	N	0.35	0/251	0.67	0/337
7	G	0.23	0/246	0.44	0/334
7	O	0.21	0/246	0.44	0/334
8	H	0.23	0/241	0.42	0/329
8	P	0.27	0/241	0.46	0/329
9	D	0.18	0/1286	0.45	1/1757 (0.1%)
9	L	0.16	0/1286	0.42	0/1757
All	All	0.19	0/16026	0.44	1/21796 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	97	LYS	CA-CB-CG	5.62	125.34	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	500	0	513	30	0
1	X	500	0	513	28	0
2	A	1769	0	1799	35	0
2	I	1769	0	1799	27	0
3	B	1223	0	1268	22	0
3	J	1223	0	1268	24	0
4	C	2115	0	2133	40	0
4	K	2115	0	2133	50	0
5	E	238	0	264	6	0
5	M	238	0	264	13	0
6	F	248	0	268	6	0
6	N	248	0	268	9	0
7	G	242	0	274	9	0
7	O	242	0	274	2	0
8	H	234	0	240	7	0
8	P	234	0	240	9	0
9	D	1256	0	1220	49	0
9	L	1256	0	1219	41	0
10	A	86	0	60	7	0
10	B	43	0	30	2	0
10	I	129	0	90	12	0
11	B	51	0	76	0	0
11	C	47	0	65	0	0
11	I	39	0	47	0	0
11	J	41	0	50	2	0
12	A	41	0	54	5	0
12	I	41	0	54	2	0
13	A	55	0	80	0	0
13	J	55	0	80	4	0
14	B	65	0	71	4	0
14	J	65	0	71	2	0
15	C	43	0	32	5	0
15	K	43	0	31	5	0
16	N	55	0	85	0	0
17	H	52	0	83	1	0
17	P	51	0	78	1	0
18	B	40	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	4	0	0	2	0
19	L	4	0	0	2	0
20	D	54	0	78	4	0
20	L	54	0	78	2	0
21	E	20	0	42	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
All	All	16830	0	17362	402	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 12.

All (402) 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)
2:I:42:CYS:SG	10:I:302:HEM:HAB	1.91	1.11
2:I:42:CYS:SG	10:I:302:HEM:CAB	2.40	1.09
2:I:42:CYS:HG	10:I:302:HEM:CAB	1.65	1.09
2:A:42:CYS:SG	10:B:301:HEM:HAB	2.02	1.00
1:V:52:ARG:O	1:V:52:ARG:NH1	2.05	0.90
2:A:42:CYS:SG	10:B:301:HEM:CAB	2.61	0.88
4:C:34:VAL:HG22	4:C:151:LEU:HD22	1.63	0.78
2:A:180:GLU:N	2:A:180:GLU:OE1	2.17	0.78
4:K:34:VAL:HG22	4:K:151:LEU:HD22	1.66	0.77
2:A:136:VAL:HG21	14:B:302:CLA:H43	1.67	0.76
2:A:7:THR:O	2:A:8:GLU:HG2	1.86	0.76
9:D:70:ASP:OD1	9:D:71:ALA:N	2.20	0.75
1:V:21:ASP:OD1	1:V:22:VAL:N	2.19	0.75
3:J:4:ILE:HD12	3:J:4:ILE:O	1.87	0.74
7:G:30:LYS:HE2	7:G:30:LYS:HA	1.71	0.73
5:E:30:LYS:HE3	5:E:30:LYS:HA	1.72	0.71
3:B:94:LYS:O	3:B:98:ILE:HD13	1.90	0.71
6:F:30:LYS:HD2	6:F:30:LYS:O	1.91	0.70
2:I:39:ILE:HD11	12:I:305:ECH:H32A	1.74	0.70
9:D:97:LYS:O	9:D:97:LYS:HD3	1.91	0.69
9:D:134:ASN:O	9:D:134:ASN:ND2	2.26	0.69
4:K:5:ALA:HB2	15:K:301:HEC:HBB3	1.75	0.68
4:K:123:GLN:OE1	4:K:123:GLN:N	2.26	0.68
4:C:271:LYS:HB2	9:D:35:THR:HG21	1.75	0.67
2:A:39:ILE:HD11	12:A:304:ECH:H32A	1.76	0.67
2:A:104:MET:O	2:A:108:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:27:ASN:ND2	8:H:27:ASN:O	2.25	0.66
9:L:150:LYS:HA	9:L:150:LYS:HE2	1.75	0.66
1:X:52:ARG:O	1:X:52:ARG:CZ	2.44	0.66
5:M:12:ILE:O	5:M:16:THR:HG23	1.95	0.65
2:I:104:MET:O	2:I:108:VAL:HG23	1.96	0.65
10:I:301:HEM:HBB2	10:I:301:HEM:HMB2	1.77	0.65
4:K:5:ALA:CB	15:K:301:HEC:HBB3	2.27	0.65
2:I:209:HIS:CD2	2:I:213:ILE:HD11	2.32	0.64
4:K:215:VAL:HG11	4:K:227:LEU:HD13	1.80	0.63
4:K:96:GLU:OE1	4:K:97:LYS:N	2.31	0.63
2:I:42:CYS:SG	10:I:302:HEM:C3B	2.83	0.62
15:K:301:HEC:HBC2	15:K:301:HEC:HHD	1.80	0.62
5:M:10:GLY:O	5:M:14:VAL:HG13	2.00	0.62
12:A:304:ECH:H40B	12:A:304:ECH:H23	1.82	0.62
4:C:34:VAL:CG2	4:C:151:LEU:HD22	2.30	0.62
6:N:30:LYS:HD2	6:N:30:LYS:O	1.99	0.61
12:I:305:ECH:H36A	6:N:19:LEU:HD21	1.82	0.61
9:L:134:ASN:OD1	9:L:134:ASN:O	2.18	0.61
4:K:88:ASP:OD1	4:K:89:ARG:N	2.32	0.61
4:C:246:GLN:HG2	4:C:251:ILE:HD11	1.82	0.61
1:X:52:ARG:O	1:X:52:ARG:NE	2.34	0.60
3:J:9:LEU:O	3:J:15:ARG:NH1	2.34	0.60
2:A:206:LEU:HD21	10:A:301:HEM:HMB3	1.83	0.60
4:K:246:GLN:HG2	4:K:251:ILE:HD11	1.83	0.60
4:K:278:VAL:HG21	9:L:28:ARG:HD3	1.83	0.59
5:M:14:VAL:O	5:M:18:VAL:HG13	2.02	0.59
4:C:13:PRO:O	4:C:21:VAL:HG13	2.02	0.59
1:V:8:LYS:HE2	1:V:8:LYS:H	1.68	0.59
1:V:15:ARG:NH2	1:V:60:ASP:OD1	2.36	0.59
2:I:110:ARG:NH2	10:I:303:HEM:O1A	2.34	0.59
1:X:13:ARG:HG3	1:X:13:ARG:HH11	1.68	0.59
5:E:1:MET:HE3	5:E:1:MET:HA	1.84	0.59
2:I:5:GLU:N	2:I:5:GLU:OE1	2.36	0.59
9:D:150:LYS:HZ3	9:D:184:ARG:HB3	1.68	0.58
5:M:20:LEU:HD13	6:N:31:LEU:HD22	1.86	0.58
9:L:164:HIS:CG	9:L:176:SER:HG	2.20	0.58
10:I:303:HEM:HBB2	10:I:303:HEM:HMB2	1.86	0.58
6:N:25:GLY:HA3	8:P:23:VAL:HG13	1.86	0.58
9:L:150:LYS:HZ2	9:L:185:THR:HG23	1.69	0.58
3:J:152:ASP:OD1	3:J:152:ASP:N	2.37	0.57
2:I:168:VAL:HG12	2:I:172:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:202:CLA:HHC	14:J:202:CLA:HBB1	1.86	0.57
6:F:6:MET:HA	6:F:9:ASN:OD1	2.04	0.57
9:L:85:HIS:CD2	9:L:91:VAL:HG21	2.40	0.57
6:N:30:LYS:HD2	6:N:30:LYS:C	2.31	0.56
14:B:302:CLA:HHC	14:B:302:CLA:HBB1	1.86	0.56
9:L:122:HIS:NE2	19:L:202:FES:S2	2.76	0.56
1:X:8:LYS:HZ3	1:X:29:VAL:HG13	1.71	0.56
8:P:19:ILE:O	8:P:23:VAL:HG12	2.04	0.56
7:O:7:LEU:O	7:O:11:LEU:HD23	2.06	0.56
9:L:92:LEU:HD22	9:L:100:PRO:HB2	1.86	0.56
9:L:110:THR:HG22	9:L:167:VAL:HG11	1.87	0.56
3:J:150:PRO:HB2	3:J:152:ASP:OD1	2.06	0.56
4:K:215:VAL:HG11	4:K:227:LEU:CD1	2.36	0.56
1:X:12:TYR:CD2	1:X:63:LYS:HE3	2.41	0.56
4:C:193:LEU:HD11	4:C:213:LEU:HD21	1.88	0.55
9:D:120:CYS:SG	19:D:201:FES:S2	3.04	0.55
5:M:1:MET:HE2	5:M:1:MET:HA	1.87	0.55
1:V:13:ARG:HB3	1:V:13:ARG:NH1	2.21	0.55
4:C:206:ASP:OD2	4:C:207:ILE:N	2.40	0.55
4:C:27:LEU:CD2	4:C:159:GLN:HB2	2.38	0.54
4:K:13:PRO:O	4:K:21:VAL:HG13	2.07	0.54
15:C:302:HEC:CBC	15:C:302:HEC:HHD	2.38	0.54
9:D:97:LYS:O	9:D:97:LYS:CD	2.54	0.54
2:I:3:SER:O	2:I:7:THR:HG23	2.06	0.54
1:V:46:VAL:HA	1:V:56:TRP:HA	1.90	0.54
1:V:21:ASP:OD1	1:V:22:VAL:HG23	2.08	0.54
1:V:34:ASP:OD1	1:V:35:PHE:N	2.41	0.54
4:K:84:ILE:HG12	4:K:114:VAL:HG21	1.90	0.54
9:D:116:ILE:HD12	9:D:116:ILE:H	1.73	0.54
3:B:89:ARG:NH2	3:B:146:GLY:O	2.41	0.53
9:L:113:ASN:OD1	9:L:113:ASN:C	2.51	0.53
4:K:35:GLU:HA	4:K:35:GLU:OE2	2.09	0.53
9:L:24:ASP:OD1	9:L:26:GLY:N	2.41	0.53
8:P:1:MET:SD	8:P:1:MET:O	2.68	0.52
1:X:40:GLY:O	1:X:41:SER:OG	2.24	0.52
1:X:52:ARG:O	1:X:52:ARG:CD	2.56	0.52
4:C:269:VAL:HG11	8:H:24:TRP:CE3	2.45	0.52
9:D:58:SER:O	9:D:58:SER:OG	2.25	0.52
9:D:188:ASP:O	9:D:188:ASP:OD2	2.27	0.52
9:D:82:LEU:HD21	9:D:111:ILE:HG23	1.92	0.52
4:K:255:VAL:HG21	8:P:6:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:55:ASP:OD2	4:C:55:ASP:C	2.53	0.52
1:X:12:TYR:CD1	1:X:12:TYR:C	2.88	0.52
4:C:155:ARG:NE	4:C:235:GLY:O	2.42	0.52
1:V:60:ASP:OD2	1:V:60:ASP:C	2.53	0.51
1:X:12:TYR:CE2	1:X:63:LYS:HE3	2.45	0.51
4:K:213:LEU:HD23	4:K:228:THR:HG22	1.93	0.51
5:M:3:ALA:O	5:M:7:ILE:HG13	2.10	0.51
9:D:102:TYR:CD2	9:D:118:ALA:HB2	2.46	0.51
18:B:303:2WA:H47	7:G:7:LEU:HD13	1.93	0.51
3:B:123:PRO:HD2	7:G:25:ALA:HB1	1.92	0.50
3:J:93:ASN:HB3	3:J:96:LEU:HD23	1.93	0.50
4:K:116:VAL:HG22	4:K:119:LEU:HD11	1.94	0.50
9:D:92:LEU:HD22	9:D:100:PRO:HB2	1.92	0.50
6:F:5:SER:O	6:F:9:ASN:OD1	2.30	0.50
1:X:12:TYR:CE1	1:X:13:ARG:HD2	2.47	0.50
4:K:284:ASN:OD1	4:K:284:ASN:C	2.54	0.50
5:M:16:THR:HA	5:M:19:THR:HG22	1.93	0.50
4:C:123:GLN:CD	4:C:123:GLN:O	2.54	0.50
1:X:4:GLU:OE1	1:X:4:GLU:N	2.45	0.50
10:I:303:HEM:HHA	10:I:303:HEM:HBA1	1.93	0.50
4:C:116:VAL:HG22	4:C:119:LEU:HD11	1.94	0.50
4:C:84:ILE:HG12	4:C:114:VAL:HG21	1.94	0.50
2:A:157:ILE:HG23	9:L:123:LEU:HD22	1.93	0.50
9:D:148:GLU:OE1	9:D:148:GLU:HA	2.10	0.50
1:V:15:ARG:HG3	1:V:15:ARG:HH11	1.76	0.50
4:K:269:VAL:HG11	8:P:24:TRP:CE3	2.47	0.49
10:A:302:HEM:HBB2	10:A:302:HEM:HMB2	1.93	0.49
9:D:150:LYS:HZ3	9:D:184:ARG:CB	2.26	0.49
9:L:123:LEU:HD12	9:L:141:HIS:CE1	2.47	0.49
3:J:129:ALA:HB2	11:J:203:PGV:H032	1.93	0.49
2:A:6:VAL:HG21	20:D:202:SQD:C7	2.42	0.49
3:B:8:ASP:OD1	3:B:10:SER:OG	2.30	0.49
3:B:74:GLU:O	3:B:74:GLU:HG3	2.13	0.49
3:B:93:ASN:ND2	3:B:96:LEU:HD23	2.27	0.49
4:K:20:ILE:HG22	4:K:22:CYS:H	1.76	0.49
9:L:151:VAL:HG23	9:L:159:SER:HA	1.95	0.49
8:P:15:PHE:CZ	8:P:19:ILE:HD11	2.47	0.49
5:M:2:ALA:O	5:M:5:VAL:HG22	2.12	0.48
4:C:88:ASP:OD1	4:C:89:ARG:N	2.46	0.48
15:C:302:HEC:CBB	15:C:302:HEC:HHC	2.43	0.48
9:L:74:ASN:OD1	9:L:74:ASN:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:161:VAL:HG22	2:I:162:PRO:HD3	1.95	0.48
4:K:212:GLU:H	4:K:212:GLU:CD	2.21	0.48
9:L:75:ASP:OD1	9:L:76:VAL:N	2.46	0.48
2:I:168:VAL:HG12	2:I:172:LEU:HD21	1.94	0.48
2:A:111:VAL:CG1	10:A:301:HEM:HMD3	2.44	0.48
15:C:302:HEC:HHD	15:C:302:HEC:HBC2	1.95	0.48
9:D:99:ASP:HB3	9:D:119:VAL:HG21	1.95	0.48
1:V:8:LYS:HB3	1:V:29:VAL:CG1	2.44	0.48
1:X:8:LYS:HD2	1:X:9:VAL:N	2.28	0.48
4:C:79:PRO:HD3	4:C:149:VAL:HG22	1.94	0.48
4:K:282:GLU:C	4:K:282:GLU:OE1	2.57	0.48
12:A:304:ECH:H31	12:A:304:ECH:C8	2.43	0.48
9:L:136:PHE:N	9:L:145:TYR:O	2.47	0.48
3:J:93:ASN:ND2	3:J:96:LEU:HD22	2.29	0.47
4:K:206:ASP:OD2	4:K:207:ILE:N	2.47	0.47
2:A:111:VAL:HG11	10:A:301:HEM:HMD3	1.96	0.47
2:I:27:ASP:OD2	2:I:214:ARG:NH2	2.47	0.47
2:I:161:VAL:N	2:I:162:PRO:CD	2.77	0.47
2:A:4:LYS:HE3	2:A:4:LYS:HA	1.96	0.47
9:D:27:ARG:HG3	9:D:27:ARG:HH11	1.79	0.47
1:V:37:MET:HE1	1:V:43:ILE:CD1	2.45	0.47
13:J:201:PL9:H222	13:J:201:PL9:H201	1.79	0.47
4:C:26:HIS:NE2	15:C:302:HEC:NC	2.62	0.47
8:H:15:PHE:CZ	8:H:19:ILE:HD11	2.48	0.47
1:V:52:ARG:O	1:V:52:ARG:HD2	2.14	0.47
9:D:85:HIS:O	9:D:86:ASN:CG	2.57	0.47
4:K:180:ILE:HG23	4:K:218:GLY:HA2	1.97	0.47
5:M:5:VAL:O	5:M:9:ILE:HD13	2.15	0.47
2:A:104:MET:SD	10:A:301:HEM:HAB	2.54	0.47
2:I:221:PRO:HG2	1:V:37:MET:HB2	1.97	0.47
9:L:78:VAL:HG21	9:L:167:VAL:HA	1.97	0.47
9:L:150:LYS:HA	9:L:150:LYS:CE	2.42	0.47
5:E:9:ILE:CD1	17:H:101:6PL:H422	2.44	0.47
4:C:190:GLY:C	4:C:191:TYR:HD1	2.22	0.46
4:K:108:GLU:OE2	4:K:108:GLU:HA	2.13	0.46
4:C:206:ASP:OD2	4:C:206:ASP:C	2.58	0.46
4:K:109:ASP:CG	4:K:109:ASP:O	2.58	0.46
9:L:116:ILE:HD12	9:L:116:ILE:H	1.80	0.46
1:V:43:ILE:N	1:V:59:GLU:OE2	2.48	0.46
4:K:284:ASN:OD1	4:K:284:ASN:O	2.33	0.46
1:V:60:ASP:O	1:V:63:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:113:ASN:C	9:D:113:ASN:OD1	2.59	0.46
9:D:116:ILE:HD12	9:D:116:ILE:N	2.30	0.46
3:J:102:ALA:O	3:J:106:LEU:HD22	2.15	0.46
3:J:102:ALA:O	3:J:106:LEU:CD2	2.64	0.46
4:K:1:TYR:HB3	4:K:2:PRO:CD	2.46	0.46
3:B:148:THR:HB	7:G:2:ILE:HD11	1.97	0.46
9:L:123:LEU:HB2	19:L:202:FES:S2	2.56	0.46
9:D:85:HIS:O	9:D:86:ASN:ND2	2.49	0.46
9:D:92:LEU:HD21	9:D:118:ALA:HB3	1.98	0.46
9:L:84:SER:C	9:L:85:HIS:CG	2.94	0.46
9:L:95:GLY:HA2	9:L:175:LEU:HD12	1.97	0.46
2:I:154:ALA:O	2:I:158:VAL:HG22	2.16	0.45
4:K:165:LEU:HD12	4:K:166:LEU:N	2.31	0.45
4:C:11:LEU:O	4:C:107:ARG:NH1	2.49	0.45
9:D:141:HIS:HB2	19:D:201:FES:S1	2.56	0.45
3:J:123:PRO:HD2	7:O:25:ALA:HB1	1.98	0.45
2:A:96:SER:OG	3:B:51:ILE:HG21	2.17	0.45
4:K:134:PRO:HG2	4:K:142:ILE:HG21	1.99	0.45
9:D:97:LYS:HD2	9:D:99:ASP:CG	2.41	0.45
8:H:17:TRP:CZ2	8:H:21:MET:HE3	2.51	0.45
2:A:133:VAL:HG21	14:B:302:CLA:H202	1.98	0.45
7:G:30:LYS:HD3	7:G:31:ARG:H	1.82	0.45
4:K:213:LEU:HD22	4:K:215:VAL:HG12	1.99	0.45
9:D:27:ARG:HH11	9:D:27:ARG:CG	2.29	0.45
1:X:18:VAL:HB	1:X:22:VAL:HB	1.98	0.45
9:L:92:LEU:HD21	9:L:118:ALA:HB3	1.99	0.45
4:K:275:ILE:HD12	4:K:275:ILE:HA	1.91	0.45
4:C:159:GLN:HG3	4:C:169:ASN:O	2.17	0.45
9:L:75:ASP:OD1	9:L:75:ASP:C	2.60	0.45
9:L:97:LYS:O	9:L:97:LYS:CG	2.64	0.45
1:X:19:SER:O	1:X:23:VAL:HG23	2.16	0.45
6:N:29:ILE:O	6:N:32:GLN:HG2	2.16	0.45
3:B:4:ILE:HG13	3:B:4:ILE:O	2.17	0.45
1:V:8:LYS:H	1:V:8:LYS:CE	2.29	0.45
9:D:111:ILE:C	9:D:111:ILE:HD12	2.42	0.44
6:F:30:LYS:HD2	6:F:30:LYS:C	2.41	0.44
1:V:51:ASP:O	1:V:52:ARG:HB3	2.17	0.44
2:I:130:MET:HG3	3:J:109:MET:HE2	1.99	0.44
5:M:26:LEU:HA	5:M:29:VAL:HG22	1.98	0.44
1:X:33:LYS:HE2	1:X:48:SER:HB3	1.99	0.44
2:I:191:TYR:CE1	2:I:195:THR:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:29:GLN:OE1	4:K:236:PHE:O	2.35	0.44
4:K:55:ASP:OD2	4:K:57:ASP:N	2.50	0.44
2:A:101:VAL:HG11	3:B:80:TYR:HB3	2.00	0.44
14:B:302:CLA:H142	14:B:302:CLA:H111	1.87	0.44
1:V:9:VAL:HG12	1:V:64:ALA:HA	1.98	0.44
2:A:10:LYS:C	2:A:10:LYS:HD2	2.42	0.44
9:D:77:LYS:HD3	9:D:78:VAL:N	2.33	0.44
7:G:30:LYS:HD3	7:G:31:ARG:N	2.32	0.44
1:X:46:VAL:HG12	1:X:54:ALA:HB1	1.99	0.44
4:K:92:GLU:CD	4:K:93:GLY:N	2.75	0.44
4:K:108:GLU:O	4:K:109:ASP:HB3	2.17	0.44
4:K:155:ARG:HD2	4:K:235:GLY:O	2.18	0.44
12:A:304:ECH:H8	12:A:304:ECH:H32	1.99	0.44
9:D:68:ALA:H	9:D:173:LEU:HD12	1.83	0.44
9:D:103:ILE:N	9:D:103:ILE:HD12	2.32	0.44
1:X:52:ARG:O	1:X:52:ARG:HD2	2.17	0.44
4:K:75:VAL:HG13	4:K:75:VAL:O	2.18	0.44
2:A:110:ARG:HD2	2:A:110:ARG:C	2.43	0.44
2:A:206:LEU:CD2	10:A:301:HEM:HMB3	2.48	0.44
9:D:92:LEU:HD21	9:D:118:ALA:CB	2.47	0.44
20:D:202:SQD:H321	20:D:202:SQD:H292	1.86	0.44
4:K:160:ILE:O	15:K:301:HEC:HMD3	2.18	0.44
4:C:91:SER:O	4:C:95:LYS:N	2.46	0.44
9:D:30:PHE:HD2	5:E:31:LEU:HD21	1.82	0.44
1:V:28:LYS:N	1:V:28:LYS:HD2	2.33	0.44
10:I:301:HEM:HBB2	10:I:301:HEM:CMB	2.47	0.43
3:J:3:ILE:HD12	3:J:3:ILE:HA	1.91	0.43
2:A:137:THR:HG22	2:A:198:LEU:HD11	2.00	0.43
2:A:191:TYR:CE1	2:A:195:THR:HG21	2.53	0.43
3:B:32:TRP:CD1	20:D:202:SQD:HO3	2.35	0.43
2:I:54:GLN:NE2	2:I:97:ALA:HB2	2.32	0.43
8:P:12:LEU:HD21	17:P:101:6PL:H352	1.99	0.43
2:A:24:ILE:N	2:A:24:ILE:HD12	2.33	0.43
18:B:303:2WA:H48	7:G:11:LEU:HD11	2.00	0.43
9:D:173:LEU:HD13	9:D:174:VAL:N	2.33	0.43
1:V:52:ARG:O	1:V:52:ARG:CD	2.66	0.43
4:K:92:GLU:OE1	4:K:93:GLY:N	2.51	0.43
4:K:215:VAL:O	4:K:215:VAL:HG13	2.18	0.43
4:C:20:ILE:HG22	4:C:22:CYS:H	1.83	0.43
20:L:201:SQD:H172	20:L:201:SQD:H142	1.84	0.43
1:X:43:ILE:N	1:X:59:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:127:VAL:HG12	9:D:138:CYS:SG	2.58	0.43
3:J:86:GLN:O	3:J:90:ILE:HG12	2.18	0.43
2:A:168:VAL:O	2:A:172:LEU:HD23	2.18	0.43
9:D:144:GLN:N	9:D:144:GLN:CD	2.77	0.43
9:L:122:HIS:CE1	9:L:141:HIS:ND1	2.87	0.43
1:V:36:LYS:HD2	1:V:56:TRP:CB	2.49	0.43
4:K:37:PRO:HA	6:N:1:MET:SD	2.58	0.43
4:C:165:LEU:HD12	4:C:166:LEU:N	2.34	0.43
2:I:5:GLU:N	2:I:5:GLU:CD	2.77	0.43
15:C:302:HEC:HHC	15:C:302:HEC:HBB2	2.01	0.43
2:I:130:MET:HE3	2:I:205:LEU:HD21	2.01	0.43
3:J:84:THR:HG22	3:J:101:MET:SD	2.59	0.43
3:J:97:GLY:O	3:J:101:MET:HG3	2.19	0.43
2:A:209:HIS:CD2	2:A:213:ILE:HD11	2.54	0.43
4:C:13:PRO:HD3	4:C:106:TYR:CD1	2.53	0.43
2:I:110:ARG:HD2	2:I:110:ARG:C	2.44	0.43
3:J:94:LYS:HD2	3:J:94:LYS:N	2.33	0.43
13:J:201:PL9:H421	13:J:201:PL9:H401	1.82	0.43
4:C:139:ASP:OD1	4:C:141:SER:OG	2.26	0.43
9:L:90:ARG:HD2	9:L:104:VAL:HG22	2.00	0.43
13:J:201:PL9:H471	13:J:201:PL9:H451	1.88	0.42
12:A:304:ECH:H36A	6:F:19:LEU:HD21	2.01	0.42
9:D:70:ASP:CG	9:D:71:ALA:N	2.76	0.42
1:V:27:GLY:C	1:V:28:LYS:HD2	2.43	0.42
1:X:36:LYS:HZ1	1:X:56:TRP:CG	2.38	0.42
2:I:55:PHE:CD2	10:I:301:HEM:HBB1	2.55	0.42
3:J:142:TRP:CD1	3:J:157:LEU:HD21	2.53	0.42
2:A:5:GLU:HA	2:A:5:GLU:OE2	2.18	0.42
4:C:13:PRO:HG2	4:C:77:MET:SD	2.59	0.42
9:L:97:LYS:O	9:L:97:LYS:HG3	2.17	0.42
1:X:12:TYR:CE2	1:X:63:LYS:CE	3.02	0.42
2:I:180:GLU:OE1	2:I:181:SER:OG	2.35	0.42
4:C:154:ASN:ND2	4:C:156:GLY:O	2.47	0.42
9:D:67:THR:HA	9:D:173:LEU:O	2.20	0.42
9:D:81:PHE:C	9:D:81:PHE:CD2	2.96	0.42
9:D:101:THR:O	9:D:103:ILE:HD12	2.18	0.42
13:J:201:PL9:H301	13:J:201:PL9:H322	1.87	0.42
9:D:81:PHE:HD2	9:D:81:PHE:O	2.03	0.42
3:B:84:THR:HG22	3:B:101:MET:HG2	2.02	0.42
4:C:257:PHE:CZ	4:C:261:ILE:HD11	2.54	0.42
9:L:148:GLU:OE2	9:L:148:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:36:LYS:HZ1	1:X:56:TRP:CD1	2.37	0.42
1:X:51:ASP:O	1:X:52:ARG:HB3	2.19	0.42
3:J:111:VAL:HG22	11:J:203:PGV:H231	2.01	0.42
14:J:202:CLA:C2	14:J:202:CLA:H93	2.49	0.42
2:A:117:PHE:HB3	2:A:125:TRP:CE3	2.55	0.42
4:C:160:ILE:HG22	4:C:166:LEU:HD22	2.00	0.42
9:L:187:GLU:OE1	9:L:188:ASP:O	2.37	0.42
1:V:15:ARG:HG2	1:V:16:ASP:OD1	2.20	0.42
3:J:74:GLU:O	3:J:74:GLU:CD	2.62	0.42
4:K:180:ILE:HG22	4:K:219:GLN:O	2.20	0.42
5:M:31:LEU:HD11	9:L:30:PHE:CD2	2.54	0.42
2:A:68:THR:HG22	2:A:70:THR:H	1.85	0.42
9:L:150:LYS:HE3	9:L:184:ARG:HB2	2.02	0.42
1:X:7:GLN:NE2	1:X:64:ALA:CB	2.83	0.42
3:J:94:LYS:O	3:J:98:ILE:HG12	2.20	0.42
9:D:81:PHE:C	9:D:81:PHE:HD2	2.28	0.42
9:L:123:LEU:HD12	9:L:141:HIS:HE1	1.85	0.42
9:L:130:ASN:OD1	9:L:130:ASN:C	2.63	0.42
4:K:14:ARG:HB2	4:K:77:MET:HE1	2.02	0.41
4:K:212:GLU:OE1	4:K:212:GLU:N	2.46	0.41
3:B:36:ILE:O	3:B:40:PHE:HB2	2.20	0.41
1:V:8:LYS:HD3	1:V:31:VAL:HG23	2.02	0.41
1:V:36:LYS:HD2	1:V:56:TRP:HB2	2.02	0.41
4:K:180:ILE:HD11	4:K:182:GLU:O	2.20	0.41
3:B:39:MET:HE3	4:C:272:LYS:CD	2.51	0.41
9:D:185:THR:HB	9:D:187:GLU:OE1	2.20	0.41
9:L:133:GLU:O	9:L:134:ASN:HB3	2.20	0.41
5:M:28:PHE:CD1	5:M:28:PHE:C	2.99	0.41
9:D:68:ALA:CB	9:D:173:LEU:HD12	2.50	0.41
9:L:164:HIS:CE1	9:L:178:TRP:HA	2.55	0.41
2:I:6:VAL:HG21	20:L:201:SQD:C7	2.50	0.41
4:C:75:VAL:HG13	4:C:75:VAL:O	2.19	0.41
4:C:268:LEU:HG	9:D:39:ILE:HD11	2.01	0.41
3:J:37:LEU:O	3:J:37:LEU:HD12	2.21	0.41
3:J:94:LYS:HE3	9:D:122:HIS:O	2.21	0.41
4:K:109:ASP:O	4:K:109:ASP:OD1	2.39	0.41
15:K:301:HEC:HHD	15:K:301:HEC:CBC	2.47	0.41
4:C:56:LEU:HD11	4:C:122:GLU:HA	2.02	0.41
3:J:86:GLN:O	3:J:89:ARG:HG2	2.21	0.41
4:K:19:ARG:NH2	4:K:24:ASN:OD1	2.51	0.41
9:D:97:LYS:HD2	9:D:99:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:81:PHE:CD2	9:L:85:HIS:CE1	3.08	0.41
1:X:47:VAL:O	1:X:54:ALA:HA	2.20	0.41
2:I:40:PHE:CE2	8:P:29:PHE:CE2	3.08	0.41
4:C:267:LEU:HB3	9:D:35:THR:HG22	2.02	0.41
1:V:13:ARG:HB3	1:V:13:ARG:CZ	2.51	0.41
1:X:7:GLN:O	1:X:32:VAL:HG23	2.21	0.41
10:I:303:HEM:HBC2	10:I:303:HEM:HMC1	2.02	0.41
3:B:39:MET:CE	8:H:25:GLY:HA3	2.51	0.41
4:C:14:ARG:HB2	4:C:77:MET:SD	2.60	0.41
4:C:70:LEU:HD23	4:C:155:ARG:O	2.20	0.41
20:D:202:SQD:H101	20:D:202:SQD:H131	1.87	0.41
5:E:7:ILE:HG22	8:H:9:VAL:HG11	2.02	0.41
6:F:27:VAL:O	6:F:31:LEU:HG	2.21	0.41
9:L:101:THR:O	9:L:103:ILE:HD13	2.21	0.41
1:X:2:THR:C	1:X:3:ILE:HD13	2.46	0.41
3:J:8:ASP:OD2	3:J:10:SER:OG	2.39	0.41
6:N:17:LEU:HD12	8:P:12:LEU:HD22	2.03	0.41
2:A:101:VAL:HG11	3:B:80:TYR:CB	2.51	0.41
2:A:114:THR:HA	2:A:222:LEU:HD21	2.03	0.41
2:A:154:ALA:O	2:A:158:VAL:HG12	2.21	0.41
2:A:155:VAL:HA	2:A:158:VAL:HG12	2.03	0.41
2:A:157:ILE:HD12	9:L:123:LEU:HD13	2.01	0.41
3:B:35:ASP:OD2	8:H:26:ARG:NH1	2.54	0.41
5:E:30:LYS:HA	5:E:30:LYS:CE	2.43	0.41
9:L:81:PHE:CZ	9:L:103:ILE:HB	2.56	0.41
10:I:303:HEM:HBC2	10:I:303:HEM:CMC	2.51	0.41
4:K:172:PHE:CZ	4:K:208:PRO:HD2	2.56	0.41
2:A:156:LYS:HA	2:A:182:VAL:HG21	2.02	0.41
3:B:79:TRP:CD1	7:G:6:LEU:HD21	2.55	0.41
4:C:203:GLU:CD	4:C:203:GLU:H	2.29	0.41
9:D:111:ILE:HD12	9:D:111:ILE:O	2.21	0.40
1:X:25:LYS:O	1:X:28:LYS:HB2	2.21	0.40
3:B:88:LEU:HD21	3:B:101:MET:SD	2.62	0.40
3:B:142:TRP:CD1	3:B:157:LEU:HD21	2.56	0.40
9:D:95:GLY:HA2	9:D:175:LEU:CD1	2.51	0.40
7:G:13:LEU:HA	7:G:16:VAL:HG12	2.04	0.40
1:X:17:ARG:HG2	1:X:18:VAL:N	2.36	0.40
2:A:108:VAL:HG22	10:A:301:HEM:HMC1	2.02	0.40
4:C:215:VAL:O	4:C:215:VAL:HG13	2.21	0.40
4:K:184:ASN:OD1	4:K:192:GLN:OE1	2.40	0.40
4:K:262:MET:HE2	5:M:15:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:4:GLU:C	6:N:4:GLU:OE1	2.65	0.40
3:B:37:LEU:O	3:B:41:PRO:CG	2.70	0.40
1:V:45:ALA:HB3	1:V:62:LEU:HD21	2.03	0.40
3:B:61:MET:HE1	4:C:242:GLU:HG2	2.03	0.40
9:D:28:ARG:O	9:D:32:ASN:ND2	2.54	0.40
1:V:7:GLN:H	1:V:32:VAL:HG22	1.87	0.40
1:V:17:ARG:HD3	1:V:17:ARG:N	2.36	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	V	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
1	X	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
2	A	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
2	I	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
3	B	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
3	J	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
4	C	275/328 (84%)	266 (97%)	9 (3%)	0	100	100
4	K	275/328 (84%)	258 (94%)	17 (6%)	0	100	100
5	E	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
5	M	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
6	F	32/36 (89%)	32 (100%)	0	0	100	100
6	N	32/36 (89%)	32 (100%)	0	0	100	100
7	G	30/38 (79%)	30 (100%)	0	0	100	100
7	O	30/38 (79%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
9	D	165/192 (86%)	160 (97%)	5 (3%)	0	100	100
9	L	165/192 (86%)	159 (96%)	6 (4%)	0	100	100
All	All	1996/2204 (91%)	1932 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	54/55 (98%)	53 (98%)	1 (2%)	50	81
1	X	54/55 (98%)	54 (100%)	0	100	100
2	A	192/192 (100%)	192 (100%)	0	100	100
2	I	192/192 (100%)	192 (100%)	0	100	100
3	B	127/128 (99%)	126 (99%)	1 (1%)	73	90
3	J	127/128 (99%)	127 (100%)	0	100	100
4	C	226/266 (85%)	223 (99%)	3 (1%)	61	86
4	K	226/266 (85%)	225 (100%)	1 (0%)	84	94
5	E	23/23 (100%)	23 (100%)	0	100	100
5	M	23/23 (100%)	22 (96%)	1 (4%)	26	60
6	F	25/27 (93%)	24 (96%)	1 (4%)	28	63
6	N	25/27 (93%)	25 (100%)	0	100	100
7	G	25/31 (81%)	25 (100%)	0	100	100
7	O	25/31 (81%)	25 (100%)	0	100	100
8	H	26/26 (100%)	24 (92%)	2 (8%)	12	36
8	P	26/26 (100%)	26 (100%)	0	100	100
9	D	132/154 (86%)	131 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	L	132/154 (86%)	129 (98%)	3 (2%)	44 78
All	All	1660/1804 (92%)	1646 (99%)	14 (1%)	70 90

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

Mol	Chain	Res	Type
4	K	96	GLU
5	M	11	TYR
3	B	84	THR
4	C	11	LEU
4	C	27	LEU
4	C	155	ARG
9	D	72	LEU
6	F	30	LYS
8	H	27	ASN
8	H	29	PHE
9	L	32	ASN
9	L	120	CYS
9	L	123	LEU
1	V	2	THR

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

Mol	Chain	Res	Type
4	K	229	ASN
4	K	246	GLN
2	A	16	ASN
2	A	22	GLN
2	A	81	ASN
4	C	125	GLN
4	C	176	ASN
4	C	246	GLN
9	D	74	ASN
9	D	86	ASN
9	D	164	HIS
9	L	29	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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$
20	SQD	D	202	-	52,54,54	1.62	8 (15%)	62,65,65	1.20	6 (9%)
16	LMG	N	101	-	55,55,55	0.90	1 (1%)	63,63,63	1.58	11 (17%)
17	6PL	H	101	-	51,51,51	0.49	0	57,59,59	1.25	6 (10%)
10	HEM	I	301	2	50,50,50	1.38	7 (14%)	67,82,82	1.07	2 (2%)
15	HEC	C	302	4	46,50,50	1.85	6 (13%)	58,82,82	1.56	5 (8%)
11	PGV	I	304	-	38,38,50	0.57	0	41,44,56	0.52	0
10	HEM	B	301	22	50,50,50	1.36	6 (12%)	67,82,82	1.12	3 (4%)
10	HEM	I	302	22	50,50,50	1.40	6 (12%)	67,82,82	1.10	3 (4%)
11	PGV	B	304	-	50,50,50	0.49	0	53,56,56	0.64	1 (1%)
10	HEM	A	302	2	50,50,50	1.34	9 (18%)	67,82,82	1.07	3 (4%)
21	LFA	E	101	-	19,19,19	0.33	0	18,18,18	0.59	0
19	FES	D	201	9	0,4,4	-	-	-	-	-
13	PL9	A	303	-	55,55,55	0.95	4 (7%)	68,69,69	1.46	9 (13%)
10	HEM	I	303	2	50,50,50	1.40	6 (12%)	67,82,82	1.06	4 (5%)
12	ECH	A	304	-	42,42,42	0.31	0	55,58,58	0.73	0
11	PGV	C	301	-	46,46,50	0.52	0	49,52,56	0.55	0
10	HEM	A	301	2	50,50,50	1.38	7 (14%)	67,82,82	1.04	3 (4%)
19	FES	L	202	9	0,4,4	-	-	-	-	-
15	HEC	K	301	4	46,50,50	1.85	6 (13%)	58,82,82	1.54	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	6PL	P	101	-	50,50,51	0.49	0	56,58,59	1.23	4 (7%)
14	CLA	B	302	-	69,73,73	1.18	6 (8%)	82,113,113	1.39	11 (13%)
14	CLA	J	202	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	13 (15%)
13	PL9	J	201	-	55,55,55	0.93	4 (7%)	68,69,69	1.46	10 (14%)
18	2WA	B	303	-	39,39,39	0.55	1 (2%)	37,41,41	0.74	1 (2%)
12	ECH	I	305	-	42,42,42	0.34	0	55,58,58	0.78	2 (3%)
20	SQD	L	201	-	52,54,54	1.59	7 (13%)	62,65,65	1.79	10 (16%)
11	PGV	J	203	-	40,40,50	0.56	0	43,46,56	0.80	2 (4%)

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
20	SQD	D	202	-	-	35/49/69/69	0/1/1/1
16	LMG	N	101	-	1/1/8/8	19/50/70/70	0/1/1/1
17	6PL	H	101	-	1/1/5/5	26/55/55/55	-
10	HEM	I	301	2	-	4/14/54/54	-
15	HEC	C	302	4	-	3/14/54/54	-
11	PGV	I	304	-	-	21/43/43/55	-
10	HEM	B	301	22	-	9/14/54/54	-
10	HEM	I	302	22	-	7/14/54/54	-
11	PGV	B	304	-	-	29/55/55/55	-
10	HEM	A	302	2	-	5/14/54/54	-
21	LFA	E	101	-	-	8/17/17/17	-
19	FES	D	201	9	-	-	0/1/1/1
13	PL9	A	303	-	-	18/53/73/73	0/1/1/1
10	HEM	I	303	2	-	4/14/54/54	-
12	ECH	A	304	-	-	10/29/66/66	0/2/2/2
11	PGV	C	301	-	-	29/51/51/55	-
10	HEM	A	301	2	-	3/14/54/54	-
19	FES	L	202	9	-	-	0/1/1/1
15	HEC	K	301	4	-	4/14/54/54	-
17	6PL	P	101	-	1/1/5/5	30/54/54/55	-
14	CLA	B	302	-	2/2/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	J	202	-	2/2/15/20	16/39/115/115	-
13	PL9	J	201	-	-	29/53/73/73	0/1/1/1
18	2WA	B	303	-	-	20/41/41/41	-
12	ECH	I	305	-	-	15/29/66/66	0/2/2/2
20	SQD	L	201	-	-	25/49/69/69	0/1/1/1
11	PGV	J	203	-	-	32/45/45/55	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	HEC	CAB-C3B	6.44	1.55	1.35
15	C	302	HEC	CAB-C3B	6.39	1.55	1.35
15	K	301	HEC	CAC-C3C	6.34	1.55	1.35
15	C	302	HEC	CAC-C3C	6.15	1.55	1.35
15	C	302	HEC	C3D-C2D	5.55	1.53	1.38
15	K	301	HEC	C3D-C2D	5.40	1.53	1.38
20	L	201	SQD	O48-C23	4.71	1.47	1.33
20	D	202	SQD	O48-C23	4.69	1.47	1.33
16	N	101	LMG	O6-C5	-3.97	1.34	1.44
20	D	202	SQD	O47-C45	-3.73	1.37	1.46
20	L	201	SQD	O47-C45	-3.69	1.37	1.46
10	A	301	HEM	FE-ND	3.62	2.06	1.94
20	L	201	SQD	O5-C1	3.53	1.50	1.41
14	B	302	CLA	C4B-NB	3.50	1.42	1.37
10	I	302	HEM	FE-NB	3.49	2.05	1.94
10	I	303	HEM	FE-ND	3.48	2.05	1.94
14	B	302	CLA	C1D-ND	3.45	1.42	1.37
10	B	301	HEM	FE-NB	3.43	2.05	1.94
14	J	202	CLA	C4B-NB	3.40	1.42	1.37
20	D	202	SQD	O5-C1	3.39	1.50	1.41
10	I	302	HEM	FE-ND	3.39	2.05	1.94
14	J	202	CLA	C1D-ND	3.35	1.42	1.37
10	I	303	HEM	FE-NA	3.22	2.05	1.95
20	L	201	SQD	O47-C7	3.22	1.43	1.34
10	I	301	HEM	FE-ND	3.21	2.04	1.94
20	D	202	SQD	O47-C7	3.17	1.43	1.34
10	I	303	HEM	FE-NC	3.08	2.05	1.95
10	A	301	HEM	FE-NA	3.06	2.05	1.95
20	L	201	SQD	C24-C23	3.04	1.59	1.50
20	D	202	SQD	C24-C23	3.00	1.59	1.50
10	A	302	HEM	FE-NC	3.00	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	301	HEM	FE-NA	2.98	2.05	1.95
10	I	301	HEM	FE-NB	2.98	2.04	1.94
10	I	301	HEM	FE-NC	2.97	2.05	1.95
10	B	301	HEM	FE-ND	2.96	2.04	1.94
10	A	302	HEM	CAB-C3B	2.95	1.55	1.47
10	I	302	HEM	FE-NC	2.94	2.04	1.95
13	J	201	PL9	C3-C4	-2.91	1.45	1.49
10	I	303	HEM	CAB-C3B	2.89	1.55	1.47
10	I	303	HEM	CAC-C3C	2.88	1.55	1.47
10	I	302	HEM	FE-NA	2.88	2.04	1.95
10	I	301	HEM	CAB-C3B	2.86	1.55	1.47
10	A	301	HEM	CAB-C3B	2.83	1.54	1.47
14	J	202	CLA	C3B-C4B	2.79	1.50	1.42
10	A	301	HEM	CAC-C3C	2.79	1.54	1.47
14	B	302	CLA	C3B-C4B	2.78	1.50	1.42
10	A	302	HEM	CAC-C3C	2.78	1.54	1.47
13	A	303	PL9	C7-C3	-2.77	1.47	1.51
10	A	302	HEM	FE-NB	2.76	2.03	1.94
10	I	301	HEM	CAC-C3C	2.75	1.54	1.47
10	I	302	HEM	CAB-C3B	2.74	1.54	1.47
10	B	301	HEM	FE-NA	2.73	2.04	1.95
10	B	301	HEM	FE-NC	2.72	2.04	1.95
10	B	301	HEM	CAC-C3C	2.71	1.54	1.47
13	A	303	PL9	C3-C4	-2.67	1.45	1.49
10	A	301	HEM	FE-NC	2.66	2.03	1.95
10	I	302	HEM	CAC-C3C	2.64	1.54	1.47
14	B	302	CLA	C1B-C2B	2.64	1.49	1.43
10	B	301	HEM	CAB-C3B	2.63	1.54	1.47
10	I	303	HEM	FE-NB	2.63	2.03	1.94
13	A	303	PL9	C53-C6	-2.53	1.45	1.50
10	A	302	HEM	FE-NA	2.51	2.03	1.95
10	A	302	HEM	FE-ND	2.49	2.02	1.94
13	J	201	PL9	C7-C3	-2.42	1.48	1.51
10	A	301	HEM	FE-NB	2.36	2.02	1.94
15	C	302	HEC	C3C-C2C	-2.31	1.33	1.41
14	J	202	CLA	C1B-C2B	2.30	1.48	1.43
14	B	302	CLA	CHC-C1C	2.26	1.43	1.38
15	K	301	HEC	C3C-C2C	-2.24	1.33	1.41
18	B	303	2WA	OAN-CAM	-2.24	1.41	1.44
14	B	302	CLA	CMD-C2D	-2.23	1.46	1.50
14	J	202	CLA	CHC-C1C	2.23	1.43	1.38
15	K	301	HEC	C3B-C2B	-2.22	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	302	HEC	C3B-C2B	-2.22	1.33	1.41
20	L	201	SQD	O9-S	2.22	1.51	1.45
20	D	202	SQD	O9-S	2.17	1.51	1.45
14	J	202	CLA	CMD-C2D	-2.17	1.46	1.50
20	L	201	SQD	O7-S	2.16	1.51	1.45
13	A	303	PL9	C6-C1	-2.15	1.45	1.48
20	D	202	SQD	O7-S	2.14	1.51	1.45
13	J	201	PL9	C6-C1	-2.12	1.45	1.48
10	A	302	HEM	CMC-C2C	2.06	1.55	1.50
13	J	201	PL9	C53-C6	-2.05	1.46	1.50
10	I	301	HEM	C2A-C3A	-2.04	1.33	1.38
15	K	301	HEC	CMC-C2C	2.03	1.54	1.50
20	D	202	SQD	C44-C45	2.03	1.57	1.50
10	A	301	HEM	C2A-C3A	-2.02	1.33	1.38
10	A	302	HEM	CMB-C2B	2.02	1.54	1.50
10	A	302	HEM	C2A-C3A	-2.02	1.33	1.38
14	J	202	CLA	CMB-C2B	-2.01	1.46	1.50
15	C	302	HEC	CMC-C2C	2.00	1.54	1.50

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	201	SQD	O6-C1-C2	7.78	120.09	108.27
17	P	101	6PL	C1-C2-C3	6.84	127.74	111.78
15	K	301	HEC	CBC-CAC-C3C	-6.43	114.58	127.43
16	N	101	LMG	O6-C5-C4	6.21	120.88	109.70
15	C	302	HEC	CBC-CAC-C3C	-6.00	115.44	127.43
13	A	303	PL9	C7-C3-C4	5.59	121.52	116.91
14	J	202	CLA	C4A-NA-C1A	5.41	109.15	106.68
14	B	302	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	J	201	PL9	C7-C3-C4	5.28	121.26	116.91
17	H	101	6PL	C2-O2-C31	5.16	130.14	117.80
15	C	302	HEC	CBB-CAB-C3B	-4.90	117.65	127.43
20	L	201	SQD	O5-C1-C2	4.44	119.49	110.37
13	A	303	PL9	C7-C3-C2	-4.35	118.26	123.39
16	N	101	LMG	O6-C5-C6	4.17	116.76	106.44
14	B	302	CLA	C9-C8-C10	4.05	125.73	111.27
20	L	201	SQD	O5-C1-O6	4.05	119.62	110.04
13	J	201	PL9	C7-C3-C2	-4.04	118.63	123.39
17	H	101	6PL	C1-C2-C3	4.00	121.11	111.78
20	L	201	SQD	O47-C7-C8	3.92	119.97	111.48
20	L	201	SQD	O9-S-O7	-3.92	101.08	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	101	6PL	O2-C2-C1	3.87	122.24	108.34
20	D	202	SQD	O9-S-O7	-3.84	101.33	113.82
15	K	301	HEC	CBB-CAB-C3B	-3.83	119.77	127.43
13	J	201	PL9	C40-C39-C41	3.82	121.86	115.23
20	D	202	SQD	O47-C7-C8	3.64	119.36	111.48
13	A	303	PL9	C40-C39-C41	3.64	121.55	115.23
14	B	302	CLA	C3B-C4B-NB	-3.33	107.55	110.53
14	J	202	CLA	CAA-C2A-C1A	-3.30	101.16	111.97
15	K	301	HEC	C4D-ND-C1D	3.27	111.16	105.82
20	L	201	SQD	O7-S-C6	3.18	111.50	106.76
20	D	202	SQD	O9-S-C6	3.18	111.50	106.76
15	C	302	HEC	C4D-ND-C1D	3.17	110.99	105.82
14	B	302	CLA	CAA-C2A-C1A	-3.17	101.59	111.97
14	J	202	CLA	C3B-C4B-NB	-3.14	107.73	110.53
20	D	202	SQD	O7-S-C6	3.09	111.38	106.76
14	J	202	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
11	J	203	PGV	C02-O01-C1	3.07	125.14	117.80
14	B	302	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	J	202	CLA	C6-C5-C3	3.04	120.87	113.47
14	J	202	CLA	C9-C8-C7	2.94	121.77	111.27
16	N	101	LMG	C1-O6-C5	-2.90	108.06	113.72
17	P	101	6PL	O2-C2-C1	2.89	118.70	108.34
14	J	202	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
16	N	101	LMG	C6-C5-C4	2.83	119.98	113.02
20	L	201	SQD	O5-C5-C4	2.80	114.74	109.70
14	J	202	CLA	C9-C8-C10	2.78	121.18	111.27
14	B	302	CLA	C6-C5-C3	2.72	120.09	113.47
13	J	201	PL9	C22-C23-C24	-2.64	121.58	127.62
14	J	202	CLA	C1-C2-C3	-2.64	121.88	126.20
17	P	101	6PL	O3-C3-C2	2.62	115.94	108.40
20	L	201	SQD	O9-S-C6	2.61	110.65	106.76
13	A	303	PL9	O2-C1-C6	2.56	124.56	120.48
17	H	101	6PL	O2-C31-C32	2.55	117.00	111.48
17	P	101	6PL	C2-O2-C31	2.53	123.85	117.80
15	C	302	HEC	C2A-C1A-NA	-2.47	107.94	110.32
14	B	302	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
13	J	201	PL9	O2-C1-C6	2.46	124.40	120.48
13	A	303	PL9	C22-C23-C24	-2.46	122.00	127.62
14	J	202	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
16	N	101	LMG	O1-C1-C2	-2.40	104.62	108.27
15	K	301	HEC	CHC-C4B-C3B	2.39	129.24	125.21
16	N	101	LMG	O2-C2-C1	-2.39	104.39	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	201	SQD	O8-S-C6	2.36	110.52	105.97
13	J	201	PL9	C37-C38-C39	-2.32	122.31	127.62
17	H	101	6PL	O2-C2-C3	2.30	116.60	108.34
10	A	302	HEM	C4D-ND-C1D	2.28	107.91	105.21
14	J	202	CLA	CHB-C1B-NB	2.28	127.47	124.05
20	L	201	SQD	O48-C23-C24	2.28	118.78	111.83
16	N	101	LMG	O6-C1-O1	-2.26	104.69	110.04
15	K	301	HEC	CMD-C2D-C1D	2.24	128.84	125.42
16	N	101	LMG	O3-C3-C2	-2.24	105.09	110.38
10	I	302	HEM	C3B-C2B-C1B	2.23	108.09	106.41
10	A	301	HEM	C1B-NB-C4B	2.23	107.85	105.21
10	B	301	HEM	C4D-ND-C1D	2.22	107.84	105.21
10	I	303	HEM	C1B-NB-C4B	2.20	107.81	105.21
13	J	201	PL9	O1-C4-C3	-2.19	118.42	120.73
13	A	303	PL9	O2-C1-C2	-2.19	116.84	121.83
11	B	304	PGV	C01-O03-C19	2.19	125.11	117.12
10	I	302	HEM	C4D-ND-C1D	2.18	107.79	105.21
13	J	201	PL9	O2-C1-C2	-2.18	116.87	121.83
13	J	201	PL9	C32-C33-C34	-2.17	122.66	127.62
16	N	101	LMG	C40-C39-C38	-2.16	103.46	114.37
10	I	303	HEM	C3B-C2B-C1B	2.16	108.03	106.41
10	A	301	HEM	C3B-C2B-C1B	2.16	108.03	106.41
10	I	301	HEM	C1B-NB-C4B	2.15	107.76	105.21
10	I	302	HEM	C1B-NB-C4B	2.15	107.76	105.21
10	B	301	HEM	C3B-C4B-NB	-2.15	107.93	109.47
10	I	301	HEM	C4D-ND-C1D	2.14	107.74	105.21
14	B	302	CLA	C9-C8-C7	2.13	118.88	111.27
11	J	203	PGV	O01-C1-C2	2.12	116.08	111.48
13	J	201	PL9	C20-C19-C21	2.12	118.91	115.23
10	I	303	HEM	C4D-ND-C1D	2.11	107.70	105.21
14	B	302	CLA	CHB-C4A-NA	2.09	127.42	124.40
10	B	301	HEM	C1B-NB-C4B	2.09	107.68	105.21
12	I	305	ECH	C11-C10-C9	2.08	130.20	127.28
15	C	302	HEC	CHC-C1C-NC	2.08	127.64	123.86
14	B	302	CLA	O2D-CGD-CBD	2.08	114.86	111.23
12	I	305	ECH	C20-C21-C22	-2.07	124.38	127.28
10	A	302	HEM	C3D-C4D-ND	-2.07	107.91	110.17
16	N	101	LMG	C38-C37-C36	-2.06	103.96	114.37
14	B	302	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
18	B	303	2WA	CBI-OBJ-CBK	2.06	118.25	113.86
15	K	301	HEC	CHC-C1C-NC	2.05	127.59	123.86
20	D	202	SQD	O8-S-C6	2.04	109.92	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	301	HEM	C4D-ND-C1D	2.03	107.61	105.21
13	A	303	PL9	O1-C4-C3	-2.03	118.59	120.73
20	D	202	SQD	O48-C23-C24	2.03	118.02	111.83
14	J	202	CLA	CMB-C2B-C3B	2.02	131.31	126.55
16	N	101	LMG	O7-C10-O9	-2.02	118.98	123.70
13	A	303	PL9	C20-C19-C21	2.02	118.73	115.23
14	J	202	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
10	I	303	HEM	C3D-C4D-ND	-2.01	107.97	110.17
13	A	303	PL9	C32-C33-C34	-2.01	123.03	127.62
10	A	302	HEM	C2A-C1A-NA	-2.00	107.93	110.15
17	H	101	6PL	O2P-P-O1P	2.00	121.75	112.44

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	J	202	CLA	C8
14	J	202	CLA	ND
14	B	302	CLA	C8
14	B	302	CLA	ND
16	N	101	LMG	C5
17	P	101	6PL	C2
17	H	101	6PL	C2

All (415) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	I	302	HEM	C2B-C3B-CAB-CBB
10	I	302	HEM	C2C-C3C-CAC-CBC
10	B	301	HEM	C2B-C3B-CAB-CBB
10	B	301	HEM	C2C-C3C-CAC-CBC
10	B	301	HEM	C4C-C3C-CAC-CBC
11	I	304	PGV	C03-O11-P-O12
11	I	304	PGV	C03-O11-P-O14
11	I	304	PGV	C04-C05-C06-O06
11	J	203	PGV	C03-O11-P-O12
11	J	203	PGV	C03-O11-P-O13
11	J	203	PGV	C03-O11-P-O14
11	J	203	PGV	O01-C02-C03-O11
11	J	203	PGV	O02-C1-O01-C02
11	J	203	PGV	C2-C1-O01-C02
11	B	304	PGV	C03-O11-P-O12
11	B	304	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
11	B	304	PGV	C04-O12-P-O11
11	B	304	PGV	C04-O12-P-O13
11	B	304	PGV	C04-O12-P-O14
11	B	304	PGV	O04-C19-O03-C01
11	B	304	PGV	C20-C19-O03-C01
11	C	301	PGV	C03-O11-P-O12
11	C	301	PGV	C03-O11-P-O13
11	C	301	PGV	C03-O11-P-O14
11	C	301	PGV	C04-O12-P-O11
11	C	301	PGV	C04-C05-C06-O06
12	I	305	ECH	C1-C6-C7-C8
12	I	305	ECH	C5-C6-C7-C8
12	I	305	ECH	C7-C8-C9-C10
12	I	305	ECH	C7-C8-C9-C34
12	I	305	ECH	C11-C12-C13-C14
12	I	305	ECH	C11-C12-C13-C35
12	I	305	ECH	C21-C22-C23-C24
12	I	305	ECH	C37-C22-C23-C24
12	A	304	ECH	C5-C6-C7-C8
12	A	304	ECH	C23-C24-C25-C30
13	J	201	PL9	C12-C13-C14-C15
13	J	201	PL9	C12-C13-C14-C16
13	J	201	PL9	C22-C23-C24-C25
13	J	201	PL9	C37-C38-C39-C40
13	J	201	PL9	C37-C38-C39-C41
13	J	201	PL9	C47-C48-C49-C51
13	A	303	PL9	C27-C28-C29-C31
13	A	303	PL9	C37-C38-C39-C41
13	A	303	PL9	C44-C46-C47-C48
15	K	301	HEC	C4C-C3C-CAC-CBC
16	N	101	LMG	O9-C10-O7-C8
17	P	101	6PL	C4-O4P-P-O3P
17	P	101	6PL	C4-O4P-P-O2P
17	P	101	6PL	O4P-C4-C5-N
17	H	101	6PL	C2-C1-O3P-P
17	H	101	6PL	C1-O3P-P-O2P
17	H	101	6PL	C1-O3P-P-O4P
17	H	101	6PL	O4P-C4-C5-N
17	H	101	6PL	O31-C31-O2-C2
17	H	101	6PL	C32-C31-O2-C2
18	B	303	2WA	OCC-CBK-CBL-CBM
20	L	201	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
20	L	201	SQD	C5-C6-S-O7
20	L	201	SQD	C5-C6-S-O8
20	L	201	SQD	C5-C6-S-O9
11	C	301	PGV	O04-C19-O03-C01
16	N	101	LMG	O10-C28-O8-C9
13	J	201	PL9	C47-C48-C49-C50
17	P	101	6PL	C12-C11-O3-C3
17	P	101	6PL	O11-C11-O3-C3
16	N	101	LMG	C29-C28-O8-C9
16	N	101	LMG	C11-C10-O7-C8
13	A	303	PL9	C15-C14-C16-C17
13	A	303	PL9	C40-C39-C41-C42
13	J	201	PL9	C18-C19-C21-C22
13	J	201	PL9	C38-C39-C41-C42
13	A	303	PL9	C38-C39-C41-C42
11	C	301	PGV	C20-C19-O03-C01
13	A	303	PL9	C22-C23-C24-C25
13	A	303	PL9	C37-C38-C39-C40
13	J	201	PL9	C22-C23-C24-C26
13	A	303	PL9	C22-C23-C24-C26
20	D	202	SQD	C29-C30-C31-C32
16	N	101	LMG	C4-C5-C6-O5
13	J	201	PL9	C20-C19-C21-C22
13	J	201	PL9	C24-C26-C27-C28
13	J	201	PL9	C34-C36-C37-C38
13	A	303	PL9	C14-C16-C17-C18
13	A	303	PL9	C29-C31-C32-C33
13	A	303	PL9	C34-C36-C37-C38
11	J	203	PGV	C20-C19-O03-C01
20	D	202	SQD	C10-C11-C12-C13
11	J	203	PGV	O04-C19-O03-C01
20	L	201	SQD	C14-C15-C16-C17
18	B	303	2WA	CAY-CAZ-CBA-CBB
11	I	304	PGV	C20-C19-O03-C01
11	B	304	PGV	C2-C3-C4-C5
11	C	301	PGV	C24-C25-C26-C27
21	E	101	LFA	C4-C5-C6-C7
11	C	301	PGV	C2-C3-C4-C5
13	A	303	PL9	C13-C14-C16-C17
14	J	202	CLA	C11-C10-C8-C9
14	J	202	CLA	C11-C12-C13-C14
14	B	302	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
12	I	305	ECH	C36-C18-C19-C20
12	A	304	ECH	C37-C22-C23-C24
12	I	305	ECH	C17-C18-C19-C20
20	L	201	SQD	O6-C44-C45-O47
11	C	301	PGV	C19-C20-C21-C22
20	D	202	SQD	C17-C18-C19-C20
13	J	201	PL9	C14-C16-C17-C18
13	A	303	PL9	C24-C26-C27-C28
11	J	203	PGV	C6-C7-C8-C9
10	A	301	HEM	C2A-CAA-CBA-CGA
14	B	302	CLA	C5-C6-C7-C8
11	C	301	PGV	O12-C04-C05-O05
11	I	304	PGV	O04-C19-O03-C01
13	J	201	PL9	C27-C28-C29-C30
11	I	304	PGV	C2-C1-O01-C02
12	I	305	ECH	C19-C20-C21-C22
11	I	304	PGV	O02-C1-O01-C02
11	C	301	PGV	O12-C04-C05-C06
14	J	202	CLA	C5-C6-C7-C8
11	B	304	PGV	C15-C16-C17-C18
17	H	101	6PL	C11-C12-C13-C14
18	B	303	2WA	OBJ-CBK-CBL-CBM
20	D	202	SQD	C2-C1-O6-C44
11	J	203	PGV	O12-C04-C05-O05
10	I	303	HEM	C1A-C2A-CAA-CBA
12	A	304	ECH	C21-C22-C23-C24
11	B	304	PGV	C04-C05-C06-O06
11	J	203	PGV	C11-C10-C9-C8
20	D	202	SQD	O5-C1-O6-C44
20	D	202	SQD	C33-C34-C35-C36
13	J	201	PL9	C7-C8-C9-C10
17	H	101	6PL	C41-C42-C43-C44
20	D	202	SQD	C9-C10-C11-C12
17	H	101	6PL	O11-C11-O3-C3
17	H	101	6PL	C12-C11-O3-C3
11	C	301	PGV	C30-C31-C32-C33
17	H	101	6PL	C43-C44-C45-C46
18	B	303	2WA	CBP-CBQ-CBR-CBS
11	B	304	PGV	O05-C05-C06-O06
17	P	101	6PL	C31-C32-C33-C34
13	J	201	PL9	C7-C8-C9-C11
20	D	202	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
16	N	101	LMG	C10-C11-C12-C13
17	H	101	6PL	C35-C36-C37-C38
11	B	304	PGV	C20-C21-C22-C23
17	P	101	6PL	C20-C21-C22-C23
18	B	303	2WA	CBL-CBM-CBN-CBO
20	D	202	SQD	C11-C12-C13-C14
21	E	101	LFA	C2-C3-C4-C5
11	J	203	PGV	C2-C3-C4-C5
11	C	301	PGV	C7-C8-C9-C10
11	B	304	PGV	C3-C4-C5-C6
16	N	101	LMG	C19-C20-C21-C22
13	A	303	PL9	C32-C33-C34-C35
11	I	304	PGV	C1-C2-C3-C4
12	A	304	ECH	C1-C6-C7-C8
12	A	304	ECH	C23-C24-C25-C26
17	H	101	6PL	C18-C19-C20-C21
20	D	202	SQD	C8-C7-O47-C45
11	C	301	PGV	C11-C10-C9-C8
10	I	301	HEM	C2A-CAA-CBA-CGA
10	A	302	HEM	C2A-CAA-CBA-CGA
17	P	101	6PL	C33-C34-C35-C36
20	L	201	SQD	C34-C35-C36-C37
13	J	201	PL9	C40-C39-C41-C42
11	J	203	PGV	C4-C5-C6-C7
20	D	202	SQD	C24-C25-C26-C27
17	H	101	6PL	C16-C17-C18-C19
20	L	201	SQD	C13-C14-C15-C16
11	B	304	PGV	C31-C32-C33-C34
18	B	303	2WA	CBQ-CBR-CBS-CBT
11	J	203	PGV	C11-C12-C13-C14
20	L	201	SQD	C33-C34-C35-C36
21	E	101	LFA	C10-C11-C12-C13
14	B	302	CLA	C16-C17-C18-C19
17	P	101	6PL	C32-C31-O2-C2
20	L	201	SQD	C8-C7-O47-C45
14	J	202	CLA	CBD-CGD-O2D-CED
20	D	202	SQD	C13-C14-C15-C16
11	I	304	PGV	C24-C25-C26-C27
16	N	101	LMG	C17-C18-C19-C20
14	B	302	CLA	C16-C17-C18-C20
20	D	202	SQD	C28-C29-C30-C31
10	I	302	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	B	301	HEM	C4B-C3B-CAB-CBB
20	D	202	SQD	C15-C16-C17-C18
20	L	201	SQD	C15-C16-C17-C18
20	L	201	SQD	C32-C33-C34-C35
11	I	304	PGV	C6-C7-C8-C9
16	N	101	LMG	O6-C5-C6-O5
20	L	201	SQD	O47-C45-C46-O48
17	P	101	6PL	C37-C38-C39-C40
11	J	203	PGV	C23-C24-C25-C26
20	L	201	SQD	C16-C17-C18-C19
20	L	201	SQD	C26-C27-C28-C29
10	I	302	HEM	C3D-CAD-CBD-CGD
11	J	203	PGV	O12-C04-C05-C06
20	D	202	SQD	C27-C28-C29-C30
11	I	304	PGV	C5-C6-C7-C8
18	B	303	2WA	CBU-CBV-CBW-CBX
18	B	303	2WA	CAR-CAS-CAT-CAU
11	C	301	PGV	C27-C28-C29-C30
17	P	101	6PL	O31-C31-O2-C2
20	D	202	SQD	O49-C7-O47-C45
20	L	201	SQD	O49-C7-O47-C45
11	B	304	PGV	C14-C15-C16-C17
11	J	203	PGV	C1-C2-C3-C4
20	D	202	SQD	C23-C24-C25-C26
18	B	303	2WA	OAN-CAO-CAP-CAQ
20	D	202	SQD	C12-C13-C14-C15
21	E	101	LFA	C15-C16-C17-C18
11	B	304	PGV	C28-C29-C30-C31
11	I	304	PGV	O03-C01-C02-C03
20	D	202	SQD	O6-C44-C45-C46
20	L	201	SQD	O6-C44-C45-C46
18	B	303	2WA	CAX-CAY-CAZ-CBA
17	H	101	6PL	C38-C39-C40-C41
20	D	202	SQD	C34-C35-C36-C37
16	N	101	LMG	C31-C32-C33-C34
14	J	202	CLA	C3-C5-C6-C7
11	I	304	PGV	C2-C3-C4-C5
11	B	304	PGV	C21-C22-C23-C24
11	B	304	PGV	C11-C10-C9-C8
18	B	303	2WA	CAW-CAX-CAY-CAZ
17	H	101	6PL	C42-C43-C44-C45
21	E	101	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	J	202	CLA	C16-C17-C18-C20
21	E	101	LFA	C14-C15-C16-C17
14	B	302	CLA	C10-C11-C12-C13
11	J	203	PGV	C7-C8-C9-C10
20	D	202	SQD	C16-C17-C18-C19
20	D	202	SQD	C19-C20-C21-C22
20	L	201	SQD	C18-C19-C20-C21
18	B	303	2WA	OAN-CAM-CBI-OBJ
16	N	101	LMG	C13-C14-C15-C16
20	L	201	SQD	C19-C20-C21-C22
20	L	201	SQD	C30-C31-C32-C33
17	H	101	6PL	C17-C18-C19-C20
14	J	202	CLA	C16-C17-C18-C19
11	C	301	PGV	C3-C4-C5-C6
11	C	301	PGV	O05-C05-C06-O06
14	B	302	CLA	C6-C7-C8-C9
11	J	203	PGV	C5-C6-C7-C8
20	D	202	SQD	C35-C36-C37-C38
17	P	101	6PL	C44-C45-C46-C47
11	J	203	PGV	C01-C02-C03-O11
17	H	101	6PL	O3P-C1-C2-C3
11	I	304	PGV	C4-C5-C6-C7
17	H	101	6PL	C20-C21-C22-C23
11	J	203	PGV	C20-C21-C22-C23
16	N	101	LMG	C7-C8-C9-O8
17	H	101	6PL	C1-C2-C3-O3
18	B	303	2WA	CAL-CAM-CBI-OBJ
20	L	201	SQD	C44-C45-C46-O48
11	J	203	PGV	C21-C22-C23-C24
11	I	304	PGV	O03-C01-C02-O01
20	D	202	SQD	O6-C44-C45-O47
20	D	202	SQD	O47-C45-C46-O48
11	I	304	PGV	C20-C21-C22-C23
11	B	304	PGV	C19-C20-C21-C22
11	I	304	PGV	C21-C22-C23-C24
16	N	101	LMG	C38-C39-C40-C41
11	J	203	PGV	C3-C4-C5-C6
11	C	301	PGV	C11-C12-C13-C14
17	P	101	6PL	C41-C42-C43-C44
17	H	101	6PL	C14-C15-C16-C17
11	I	304	PGV	C11-C10-C9-C8
12	A	304	ECH	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
11	J	203	PGV	C19-C20-C21-C22
10	B	301	HEM	C3D-CAD-CBD-CGD
15	C	302	HEC	C2A-CAA-CBA-CGA
14	J	202	CLA	O1D-CGD-O2D-CED
20	L	201	SQD	C28-C29-C30-C31
13	J	201	PL9	C35-C34-C36-C37
17	P	101	6PL	C3-C2-O2-C31
11	J	203	PGV	O03-C01-C02-C03
11	C	301	PGV	O03-C01-C02-C03
10	I	302	HEM	C4C-C3C-CAC-CBC
14	B	302	CLA	C4-C3-C5-C6
17	H	101	6PL	C5-C4-O4P-P
16	N	101	LMG	O7-C8-C9-O8
20	D	202	SQD	C30-C31-C32-C33
11	C	301	PGV	C26-C27-C28-C29
11	B	304	PGV	C4-C5-C6-C7
11	I	304	PGV	O05-C05-C06-O06
18	B	303	2WA	CBL-CBK-OBJ-CBI
14	B	302	CLA	C2-C3-C5-C6
11	J	203	PGV	C24-C25-C26-C27
17	P	101	6PL	O3P-C1-C2-C3
14	J	202	CLA	C11-C12-C13-C15
11	B	304	PGV	O12-C04-C05-O05
20	D	202	SQD	C7-C8-C9-C10
17	P	101	6PL	C2-C1-O3P-P
11	B	304	PGV	C24-C25-C26-C27
11	B	304	PGV	C27-C28-C29-C30
17	P	101	6PL	C36-C37-C38-C39
20	D	202	SQD	C44-C45-C46-O48
11	B	304	PGV	C26-C27-C28-C29
17	P	101	6PL	C38-C39-C40-C41
11	C	301	PGV	C9-C10-C11-C12
20	L	201	SQD	C27-C28-C29-C30
11	C	301	PGV	C04-O12-P-O13
12	I	305	ECH	C9-C10-C11-C12
18	B	303	2WA	CAL-CAM-OAN-CAO
14	B	302	CLA	C3-C5-C6-C7
13	J	201	PL9	C25-C24-C26-C27
13	J	201	PL9	C33-C34-C36-C37
16	N	101	LMG	C9-C8-O7-C10
17	H	101	6PL	C33-C34-C35-C36
15	K	301	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	H	101	6PL	C32-C33-C34-C35
14	B	302	CLA	C15-C16-C17-C18
11	B	304	PGV	C12-C13-C14-C15
17	P	101	6PL	C18-C19-C20-C21
11	J	203	PGV	O03-C01-C02-O01
11	C	301	PGV	O03-C01-C02-O01
17	P	101	6PL	O2-C2-C3-O3
18	B	303	2WA	CBA-CBB-CBC-CBD
18	B	303	2WA	CBK-CBL-CBM-CBN
13	J	201	PL9	C29-C31-C32-C33
17	P	101	6PL	C32-C33-C34-C35
15	K	301	HEC	C3A-C2A-CAA-CBA
10	I	303	HEM	C3A-C2A-CAA-CBA
20	D	202	SQD	C26-C27-C28-C29
16	N	101	LMG	C32-C33-C34-C35
17	P	101	6PL	C40-C41-C42-C43
11	C	301	PGV	C31-C32-C33-C34
18	B	303	2WA	CAV-CAW-CAX-CAY
20	D	202	SQD	C32-C33-C34-C35
12	I	305	ECH	C11-C10-C9-C34
12	A	304	ECH	C11-C10-C9-C34
11	C	301	PGV	C23-C24-C25-C26
16	N	101	LMG	C18-C19-C20-C21
17	P	101	6PL	C35-C36-C37-C38
15	K	301	HEC	C3D-CAD-CBD-CGD
14	J	202	CLA	C15-C16-C17-C18
11	I	304	PGV	O12-C04-C05-O05
15	C	302	HEC	CAD-CBD-CGD-O1D
17	P	101	6PL	C12-C13-C14-C15
15	C	302	HEC	CAD-CBD-CGD-O2D
12	I	305	ECH	C11-C10-C9-C8
12	A	304	ECH	C11-C10-C9-C8
17	H	101	6PL	C37-C38-C39-C40
11	B	304	PGV	C23-C24-C25-C26
14	J	202	CLA	C4-C3-C5-C6
13	J	201	PL9	C23-C24-C26-C27
13	J	201	PL9	C28-C29-C31-C32
11	C	301	PGV	C25-C26-C27-C28
11	C	301	PGV	C28-C29-C30-C31
10	I	301	HEM	CAD-CBD-CGD-O1D
10	I	301	HEM	CAD-CBD-CGD-O2D
16	N	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	P	101	6PL	C39-C40-C41-C42
13	J	201	PL9	C30-C29-C31-C32
17	P	101	6PL	C23-C24-C25-C26
21	E	101	LFA	C17-C18-C19-C20
16	N	101	LMG	C12-C13-C14-C15
10	I	302	HEM	CAA-CBA-CGA-O2A
13	A	303	PL9	C12-C11-C9-C10
11	B	304	PGV	C02-C03-O11-P
10	A	301	HEM	CAA-CBA-CGA-O2A
13	J	201	PL9	C17-C18-C19-C21
17	P	101	6PL	C1-C2-C3-O3
13	A	303	PL9	C35-C34-C36-C37
10	A	302	HEM	CAD-CBD-CGD-O2D
10	A	302	HEM	CAD-CBD-CGD-O1D
21	E	101	LFA	C11-C10-C9-C8
11	J	203	PGV	C9-C10-C11-C12
11	I	304	PGV	C02-C03-O11-P
11	J	203	PGV	C02-C03-O11-P
10	I	302	HEM	CAA-CBA-CGA-O1A
20	L	201	SQD	C9-C10-C11-C12
10	B	301	HEM	CAA-CBA-CGA-O2A
20	D	202	SQD	C45-C44-O6-C1
14	B	302	CLA	C2-C1-O2A-CGA
10	A	301	HEM	CAA-CBA-CGA-O1A
10	B	301	HEM	CAA-CBA-CGA-O1A
11	B	304	PGV	O03-C01-C02-C03
12	A	304	ECH	C11-C12-C13-C14
14	J	202	CLA	C13-C15-C16-C17
12	I	305	ECH	C23-C24-C25-C30
13	J	201	PL9	C19-C21-C22-C23
14	J	202	CLA	CAA-CBA-CGA-O2A
13	J	201	PL9	C15-C14-C16-C17
14	J	202	CLA	C2-C3-C5-C6
18	B	303	2WA	OAD-CAO-CAP-CAQ
10	I	303	HEM	CAA-CBA-CGA-O1A
20	D	202	SQD	O48-C23-C24-C25
11	C	301	PGV	C5-C6-C7-C8
14	B	302	CLA	C4B-C3B-CAB-CBB
10	B	301	HEM	CAD-CBD-CGD-O2D
14	B	302	CLA	C8-C10-C11-C12
11	J	203	PGV	O03-C19-C20-C21
11	B	304	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
11	J	203	PGV	O01-C1-C2-C3
10	I	303	HEM	CAA-CBA-CGA-O2A
14	B	302	CLA	O2A-C1-C2-C3
13	A	303	PL9	C9-C11-C12-C13
13	J	201	PL9	C12-C11-C9-C10
18	B	303	2WA	CAO-CAP-CAQ-CAR
17	P	101	6PL	C42-C43-C44-C45
10	A	302	HEM	CAA-CBA-CGA-O2A
20	D	202	SQD	C25-C26-C27-C28
11	J	203	PGV	O04-C19-C20-C21
14	J	202	CLA	CAA-CBA-CGA-O1A
20	D	202	SQD	O10-C23-C24-C25
14	J	202	CLA	C10-C11-C12-C13
10	B	301	HEM	CAD-CBD-CGD-O1D
17	H	101	6PL	C15-C16-C17-C18
20	D	202	SQD	O47-C7-C8-C9
20	L	201	SQD	O48-C23-C24-C25
10	A	302	HEM	CAA-CBA-CGA-O1A
17	P	101	6PL	C13-C14-C15-C16
10	I	301	HEM	CAA-CBA-CGA-O1A
17	P	101	6PL	C15-C16-C17-C18

There are no ring outliers.

21 monomers are involved in 64 short contacts:

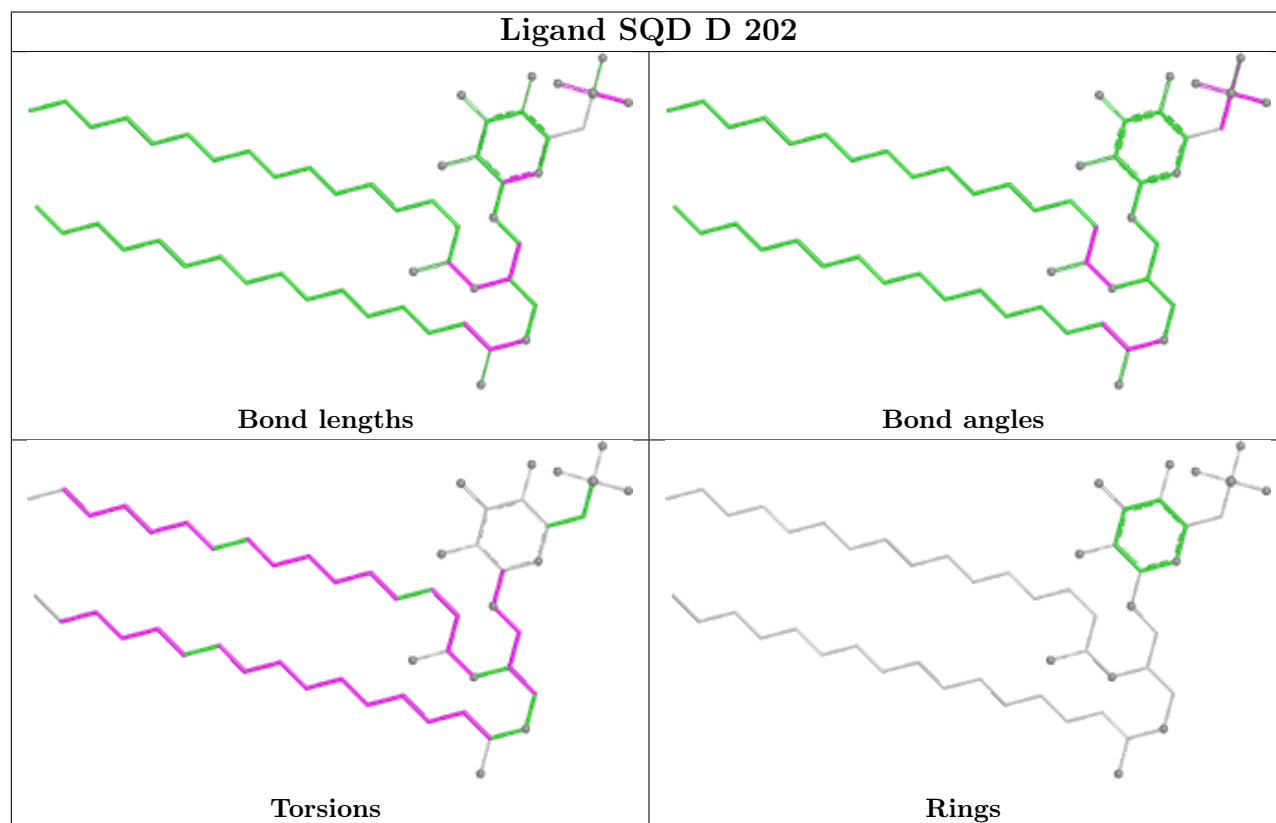
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	202	SQD	4	0
17	H	101	6PL	1	0
10	I	301	HEM	3	0
15	C	302	HEC	5	0
10	B	301	HEM	2	0
10	I	302	HEM	4	0
10	A	302	HEM	1	0
19	D	201	FES	2	0
10	I	303	HEM	5	0
12	A	304	ECH	5	0
10	A	301	HEM	6	0
19	L	202	FES	2	0
15	K	301	HEC	5	0
17	P	101	6PL	1	0
14	B	302	CLA	4	0
14	J	202	CLA	2	0

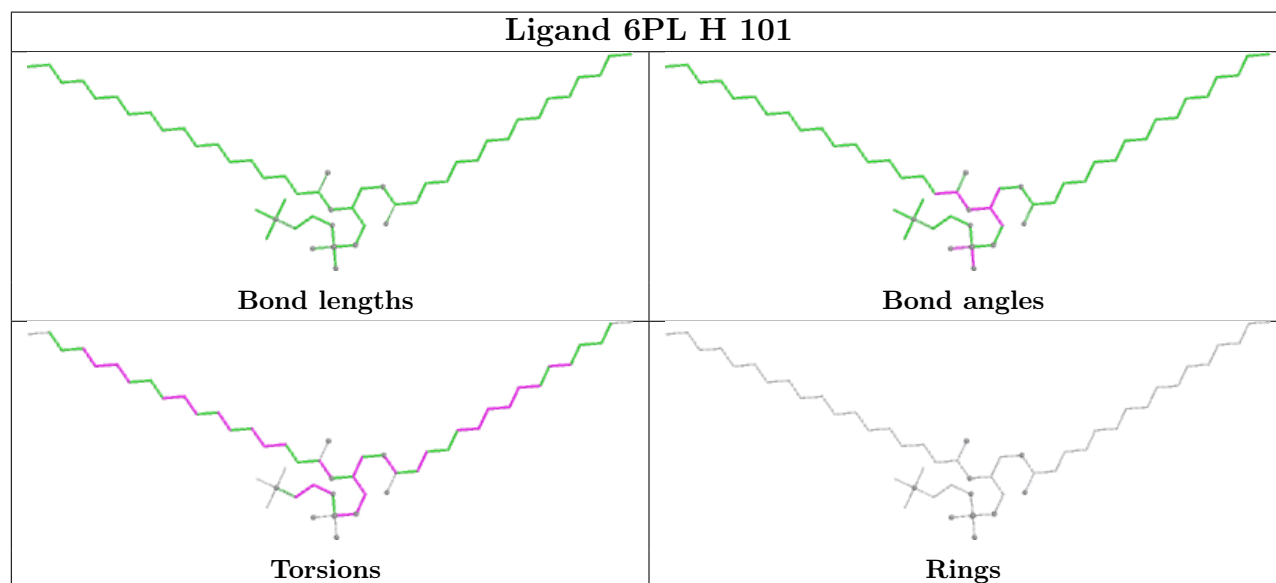
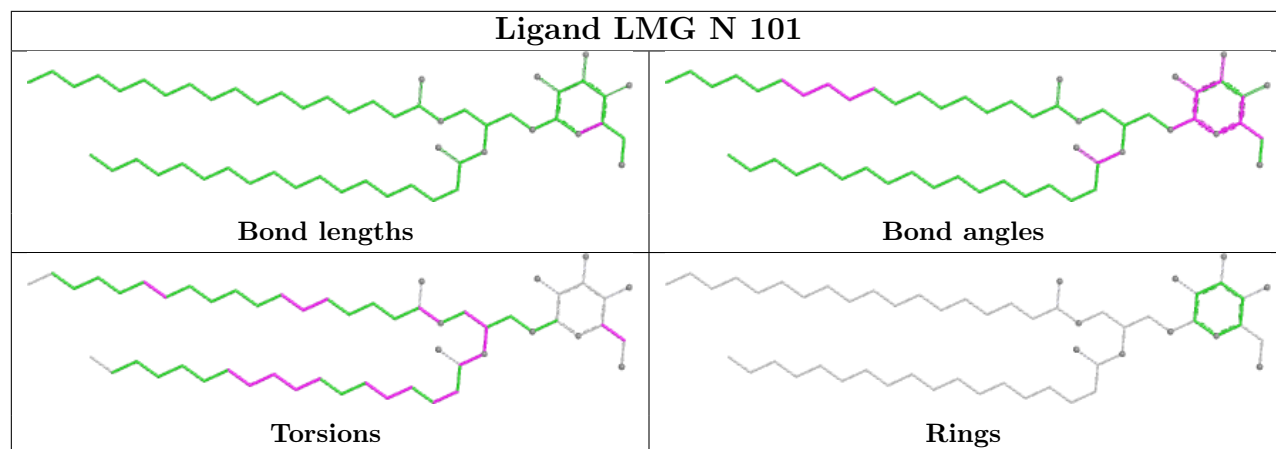
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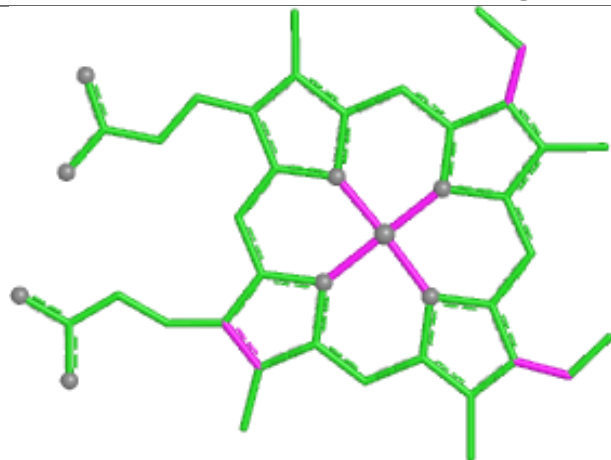
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	J	201	PL9	4	0
18	B	303	2WA	2	0
12	I	305	ECH	2	0
20	L	201	SQD	2	0
11	J	203	PGV	2	0

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.

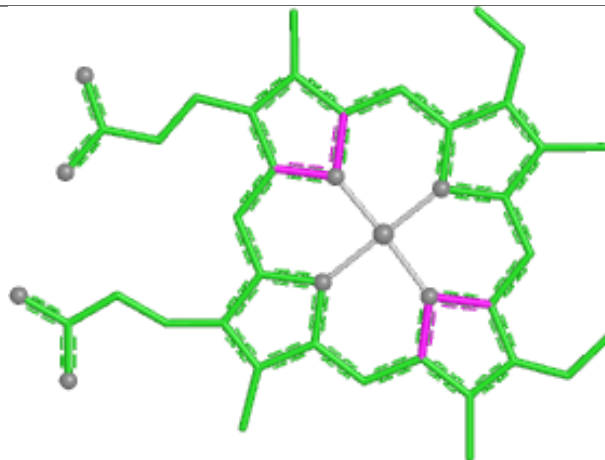




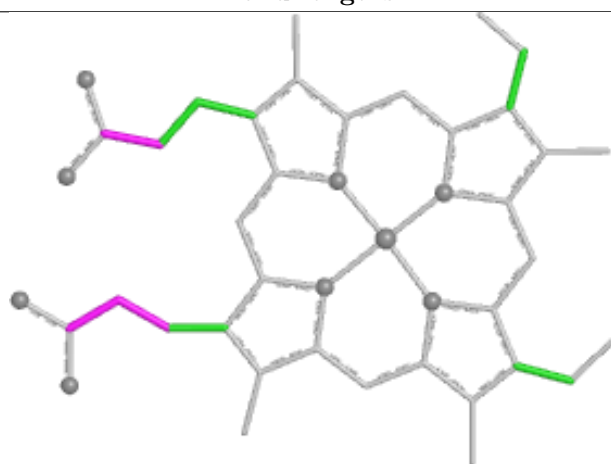
Ligand HEM I 301



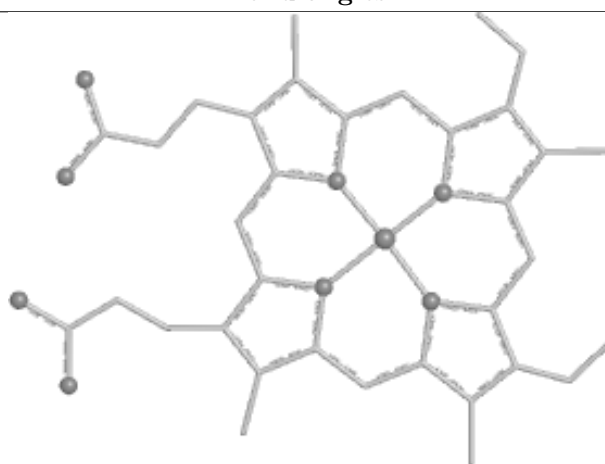
Bond lengths



Bond angles

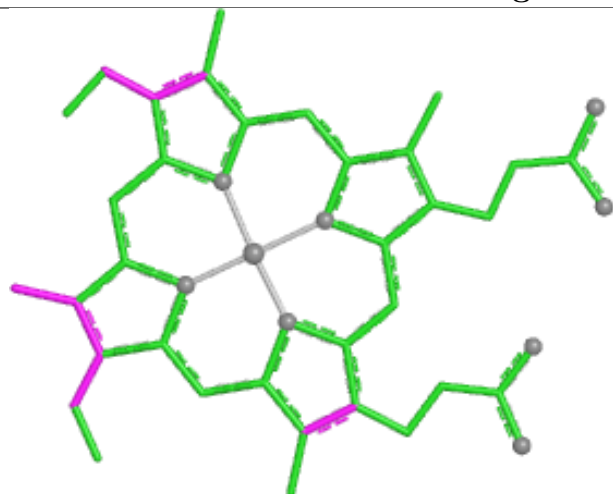


Torsions

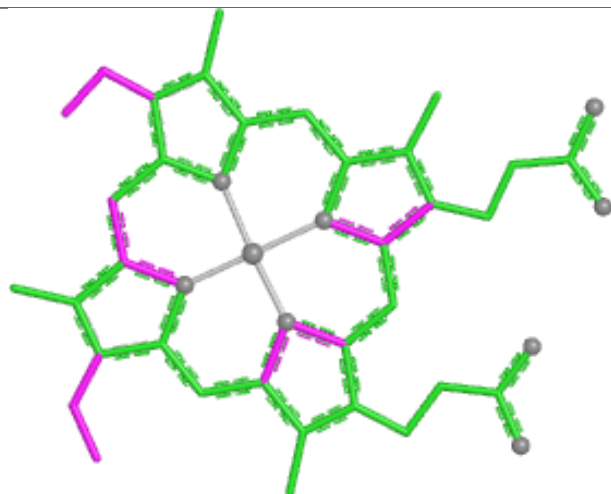


Rings

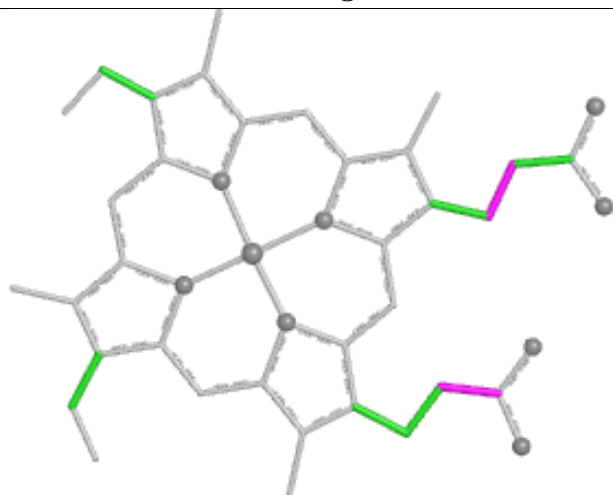
Ligand HEC C 302



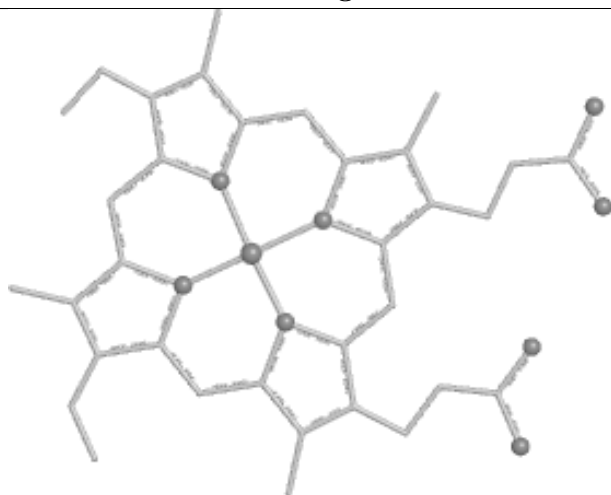
Bond lengths



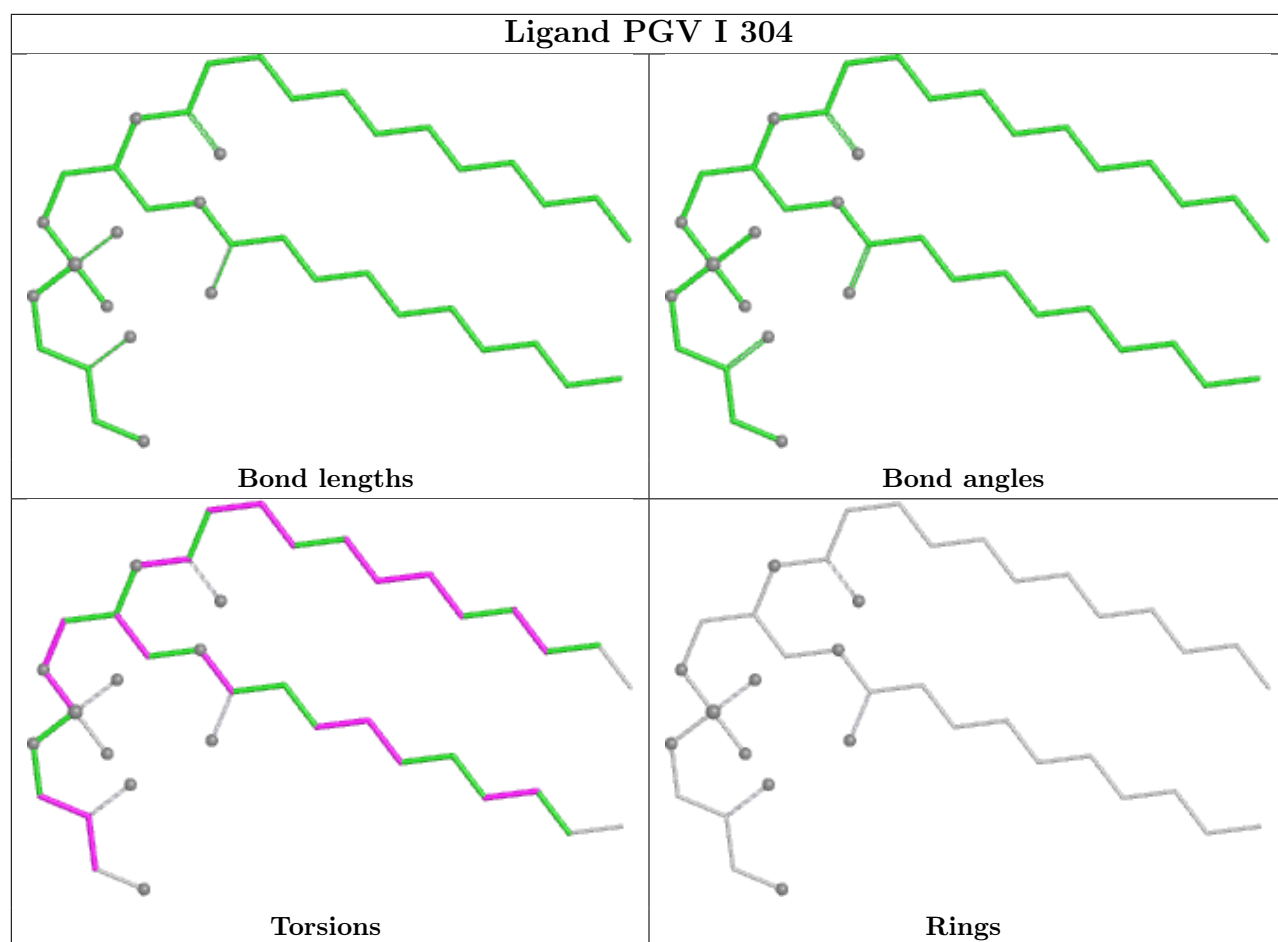
Bond angles

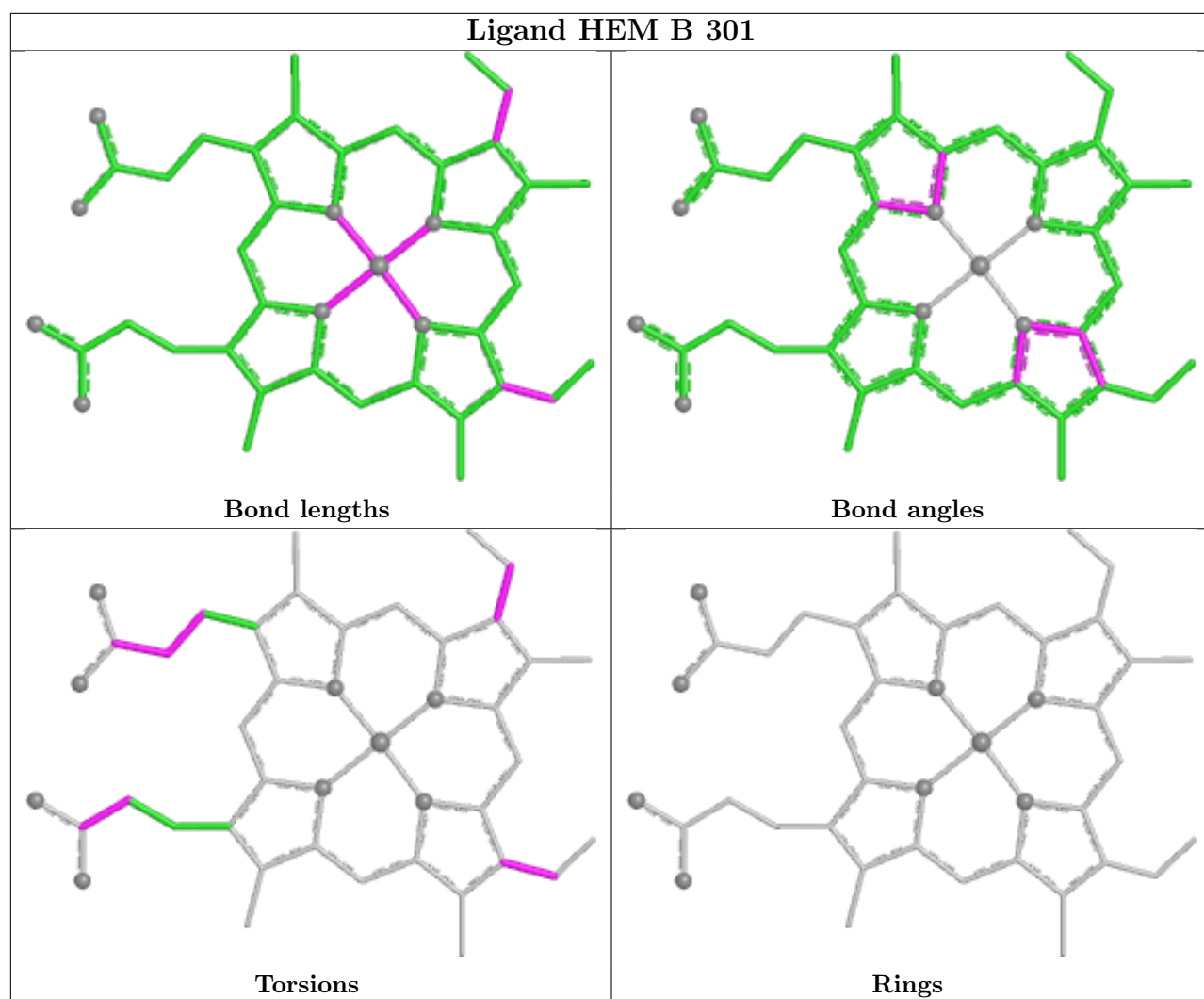


Torsions

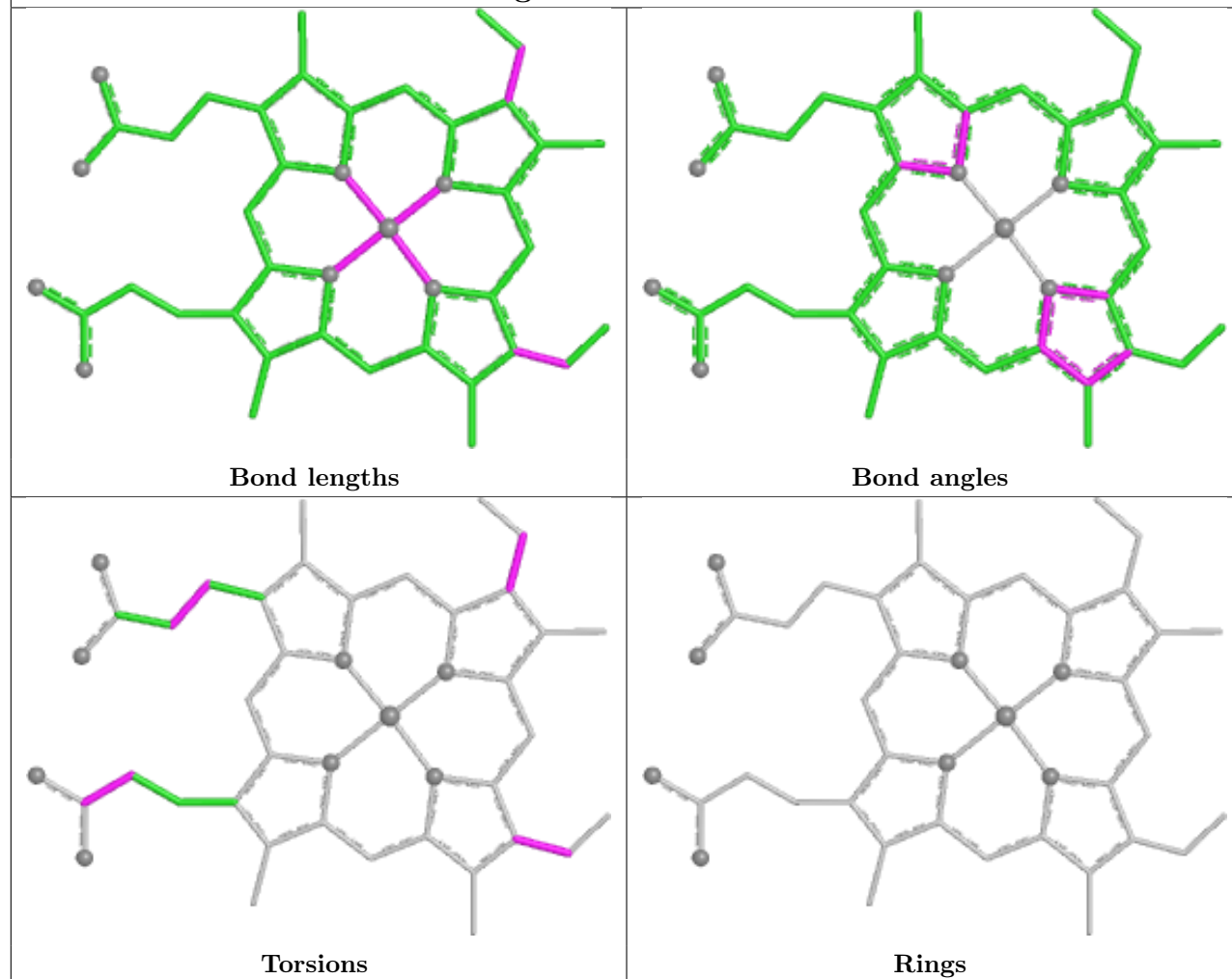


Rings

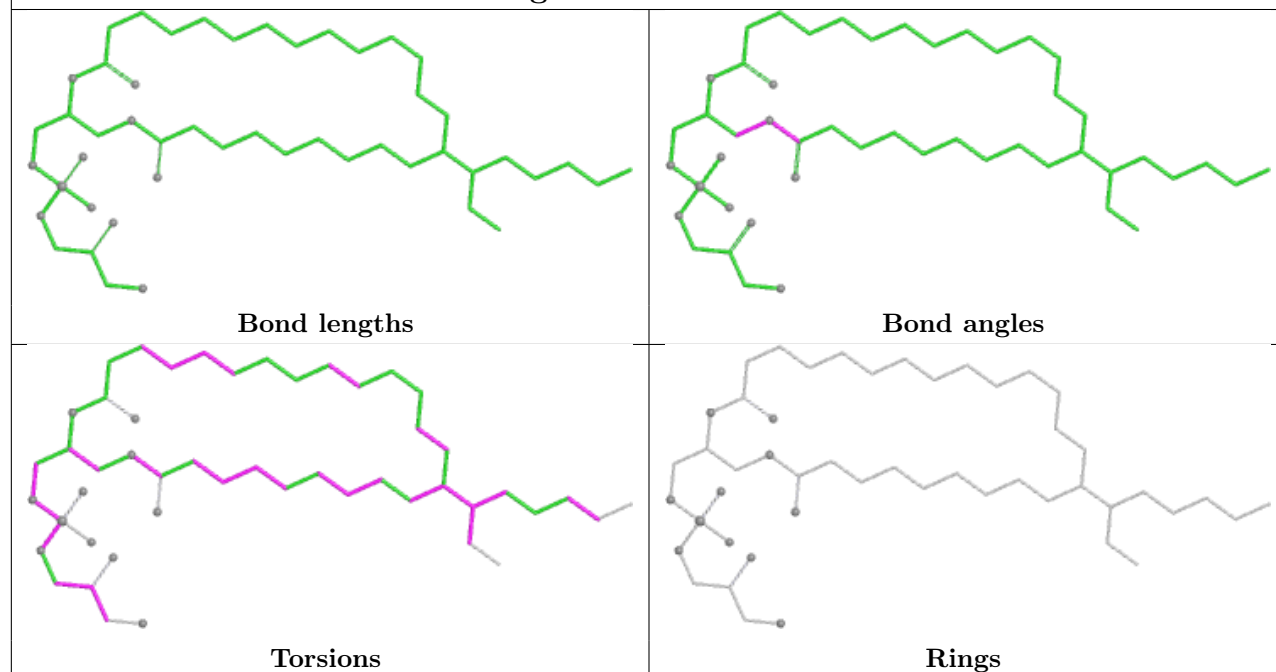


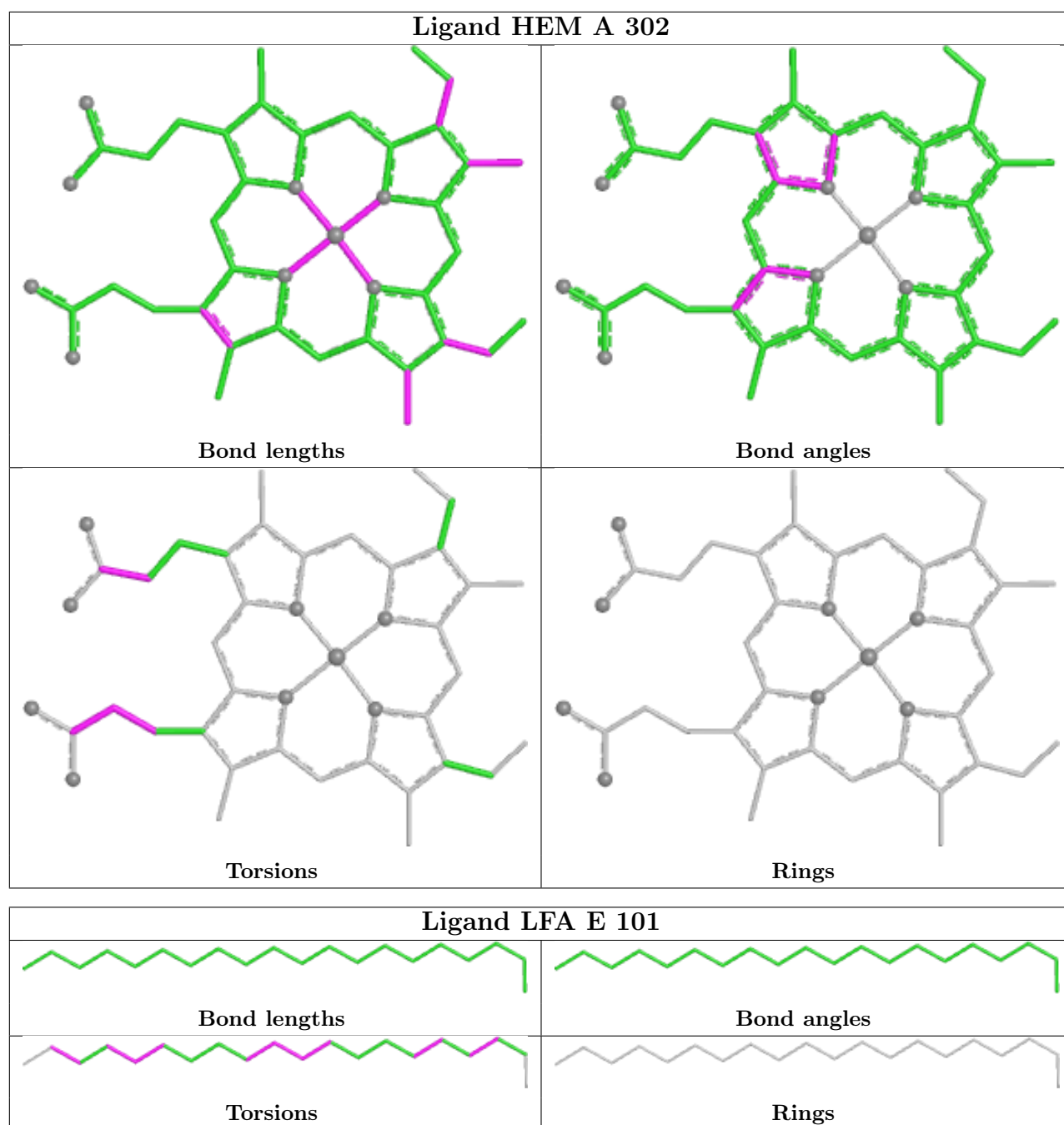


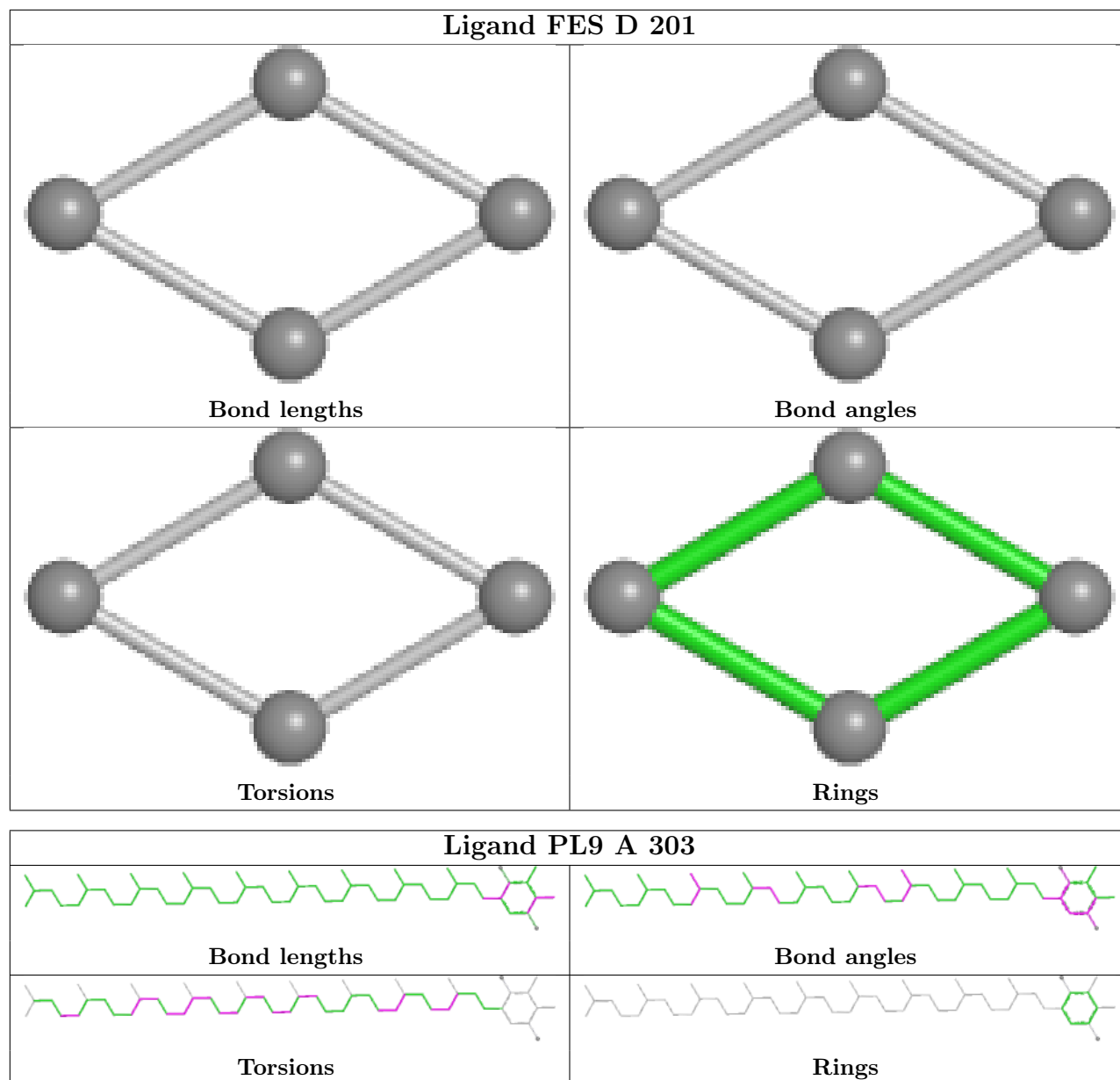
Ligand HEM I 302



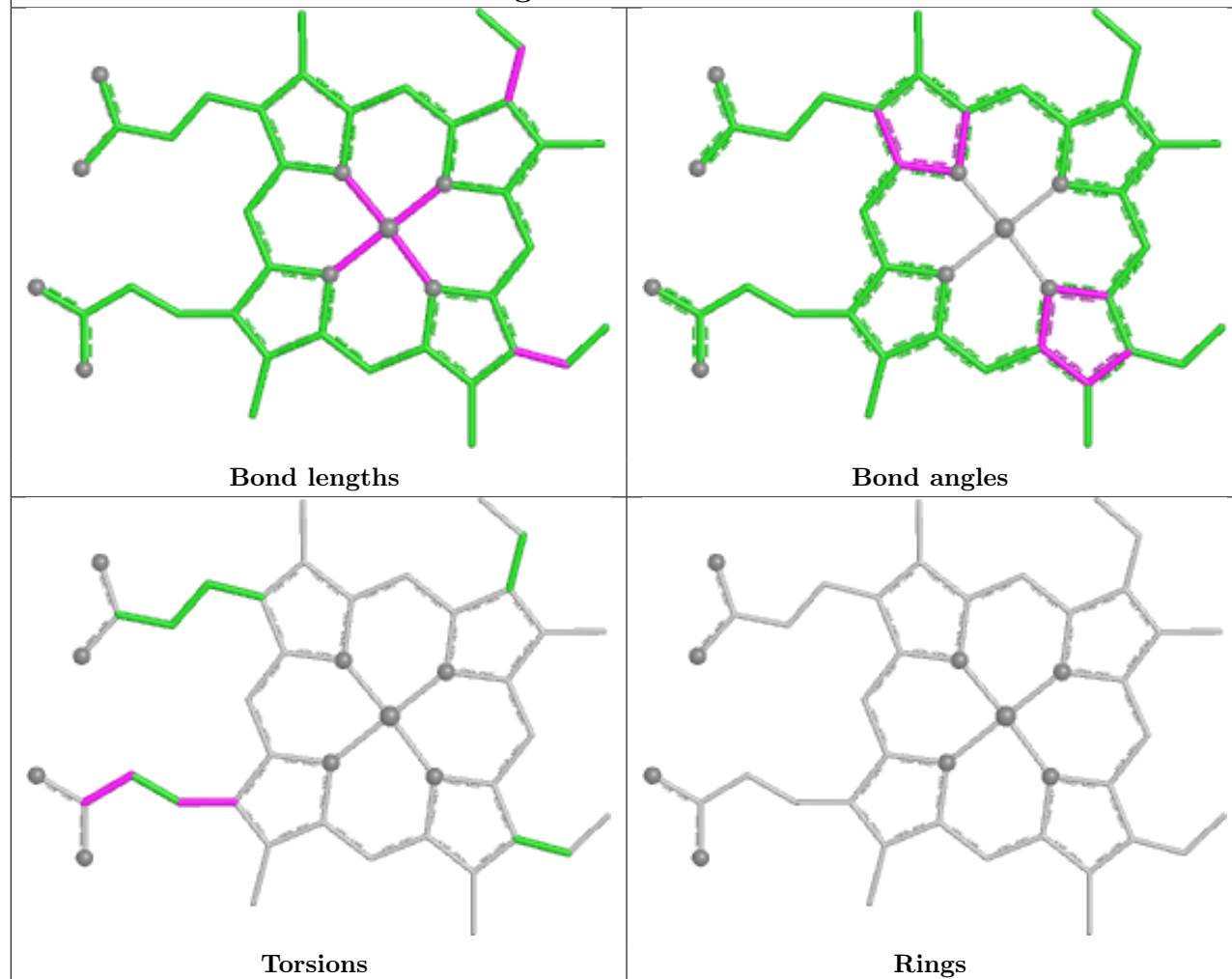
Ligand PGV B 304



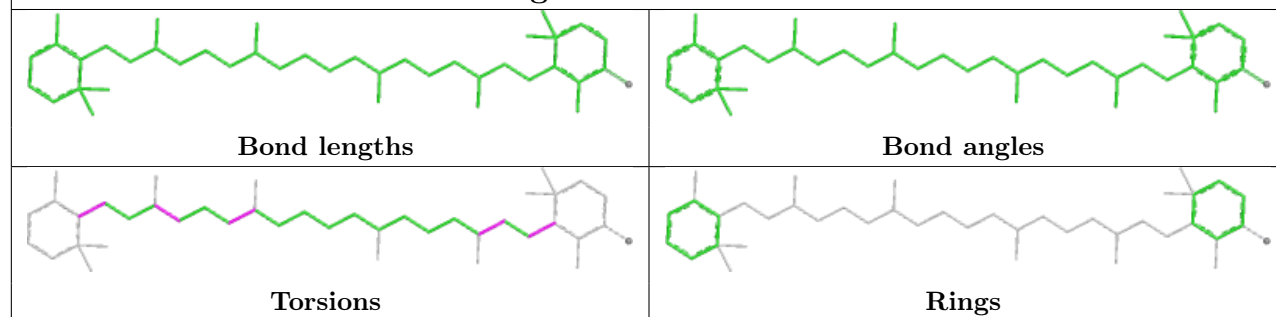


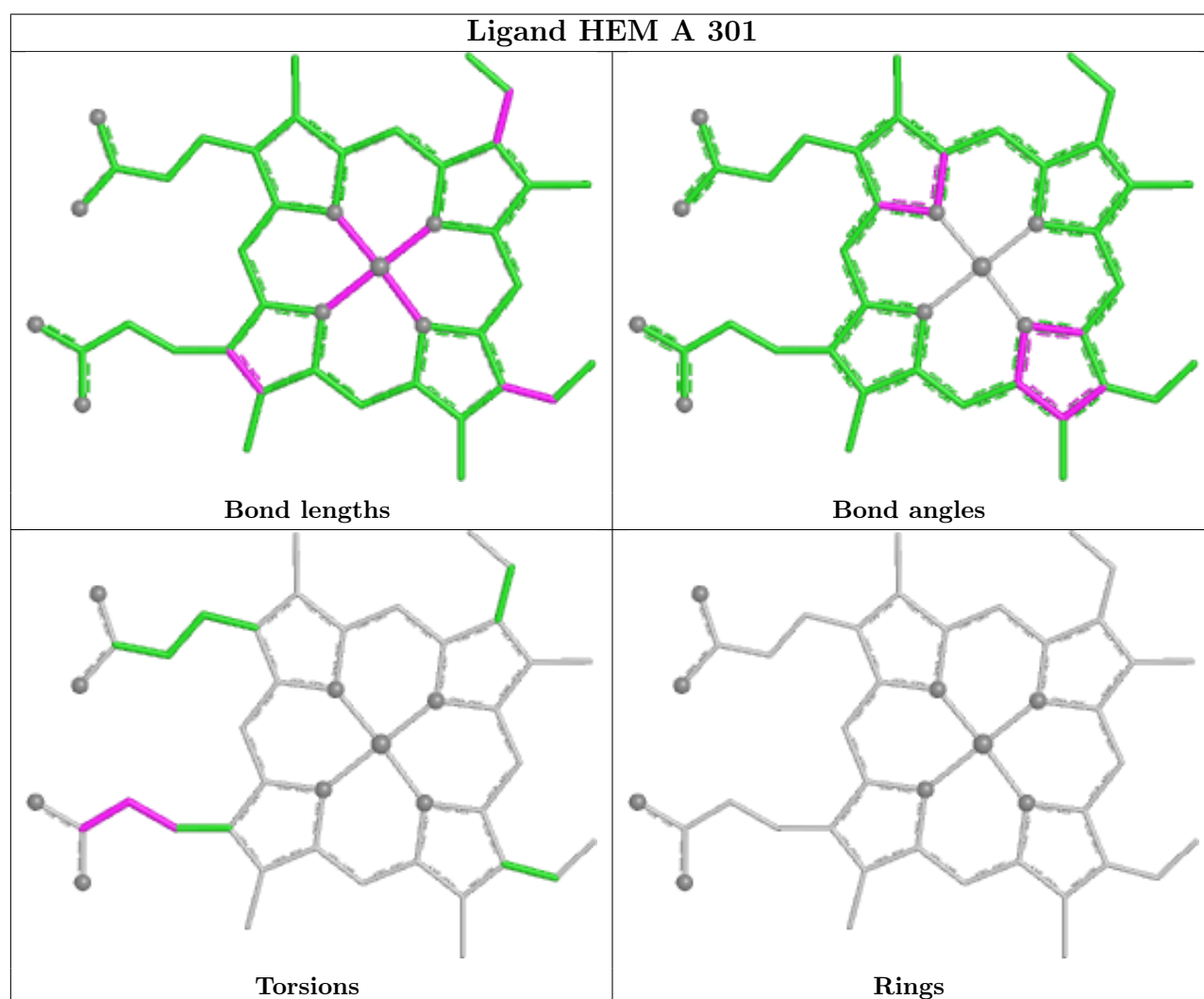
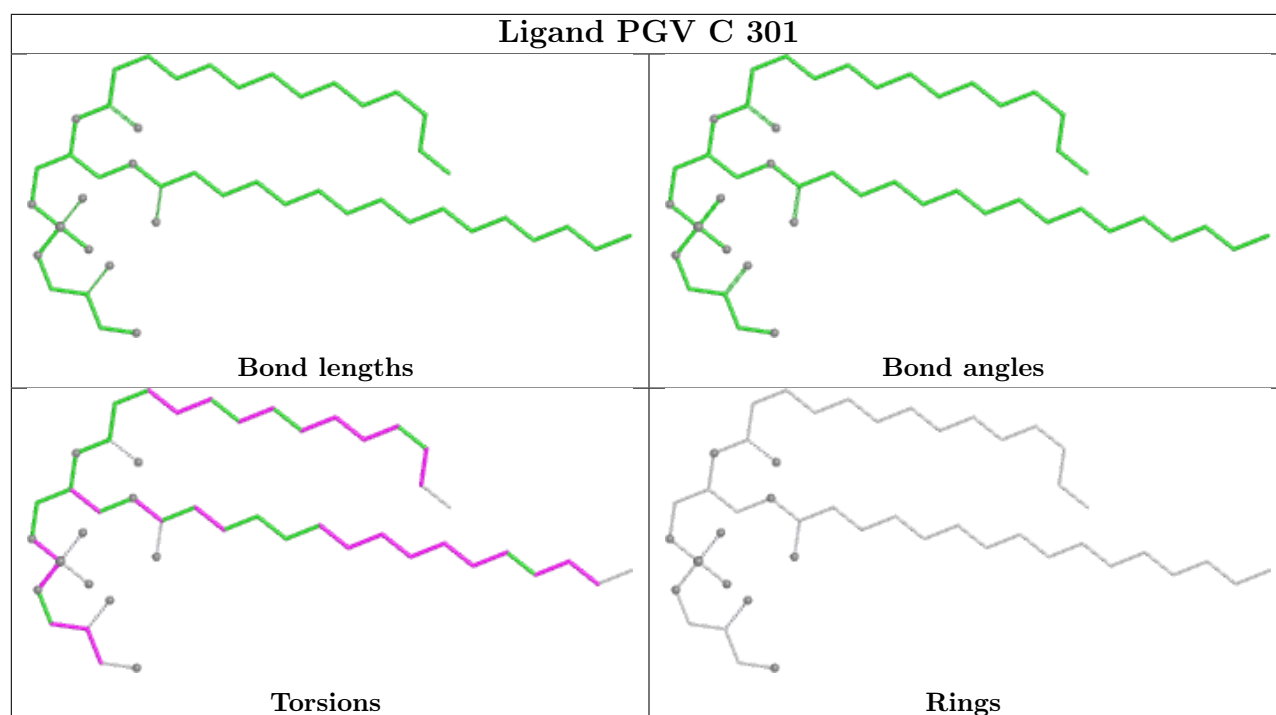


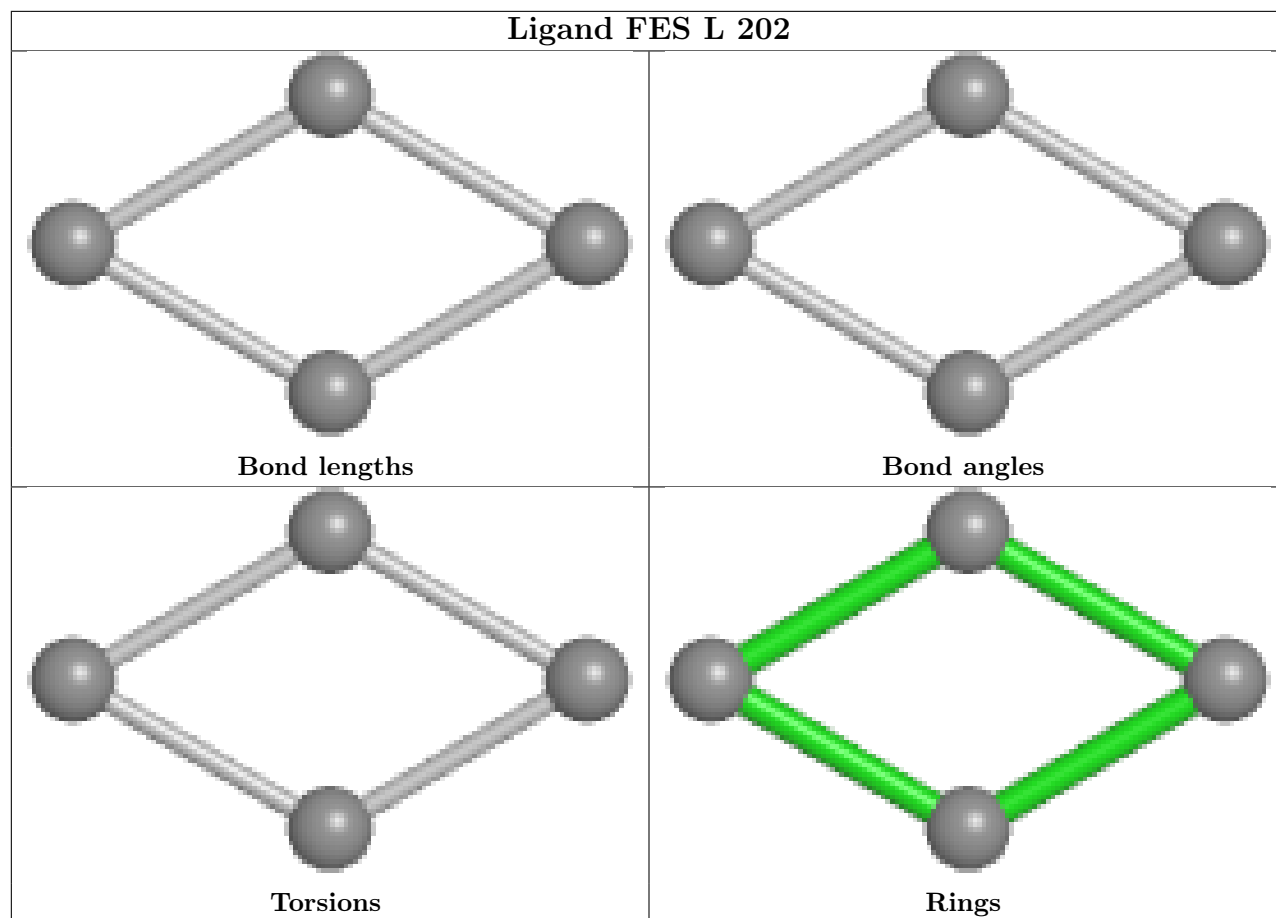
Ligand HEM I 303

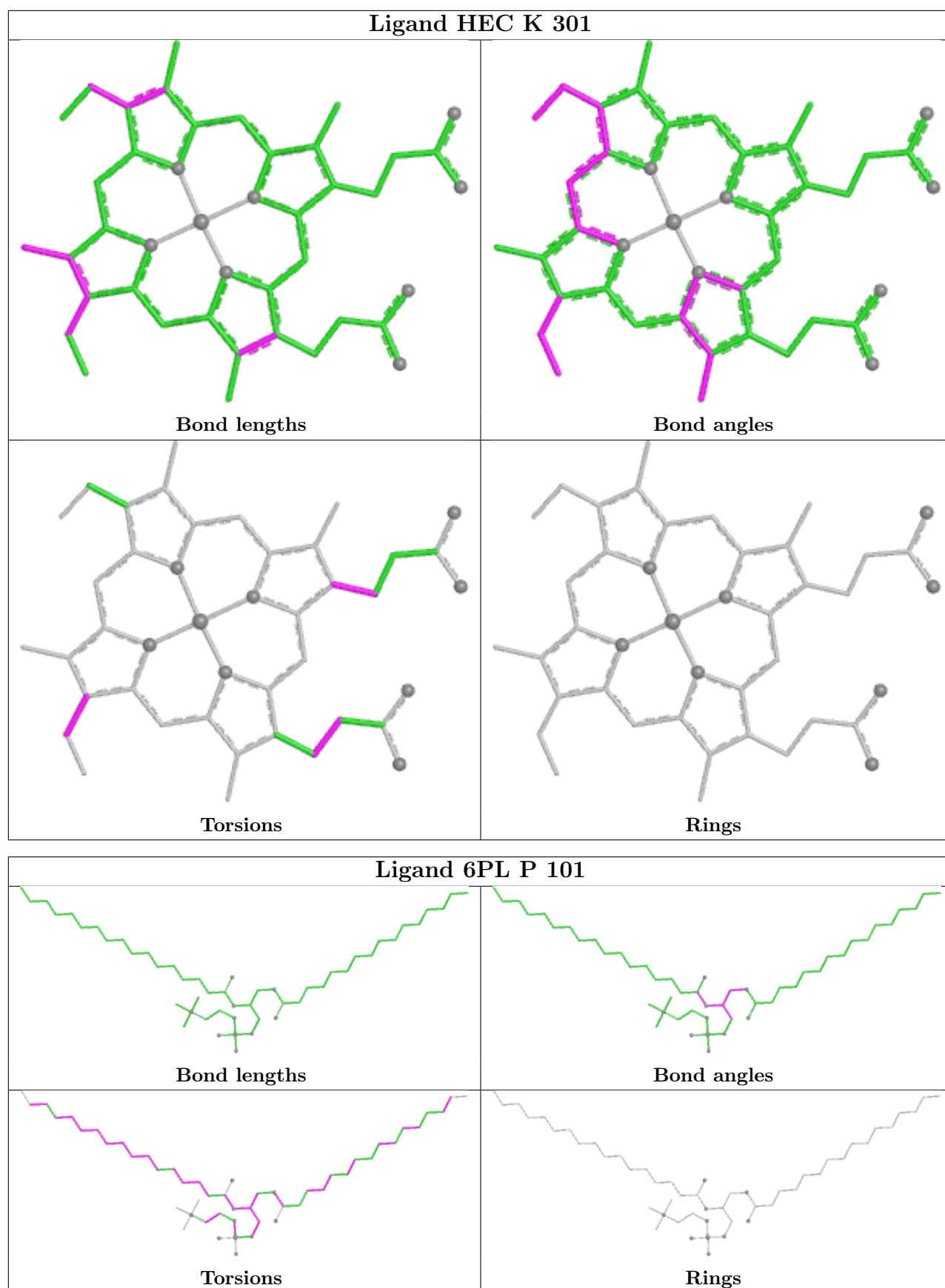


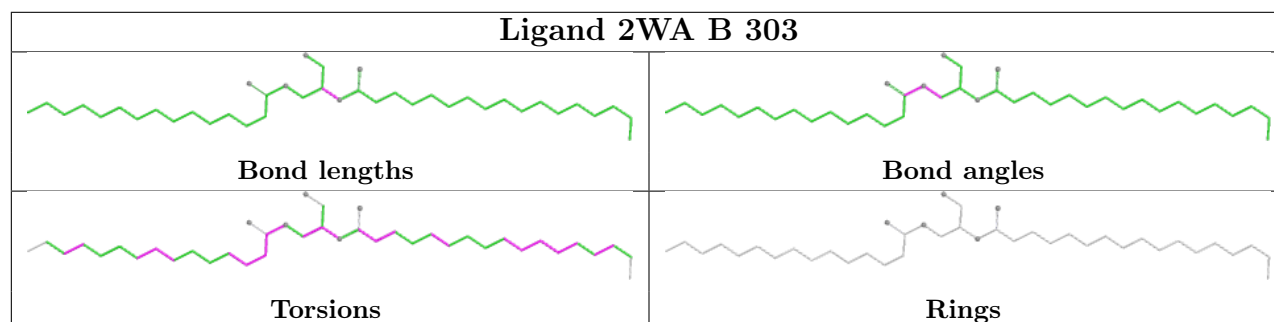
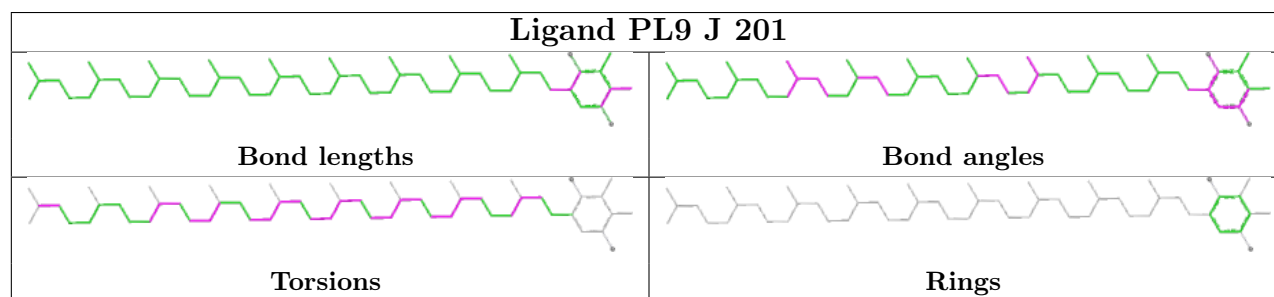
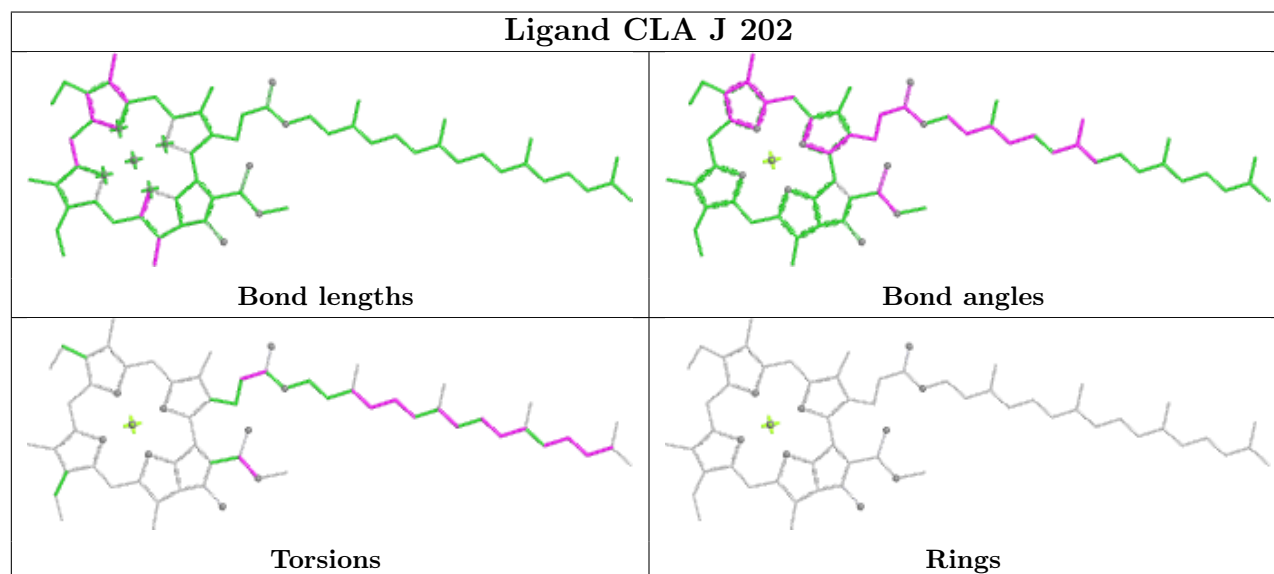
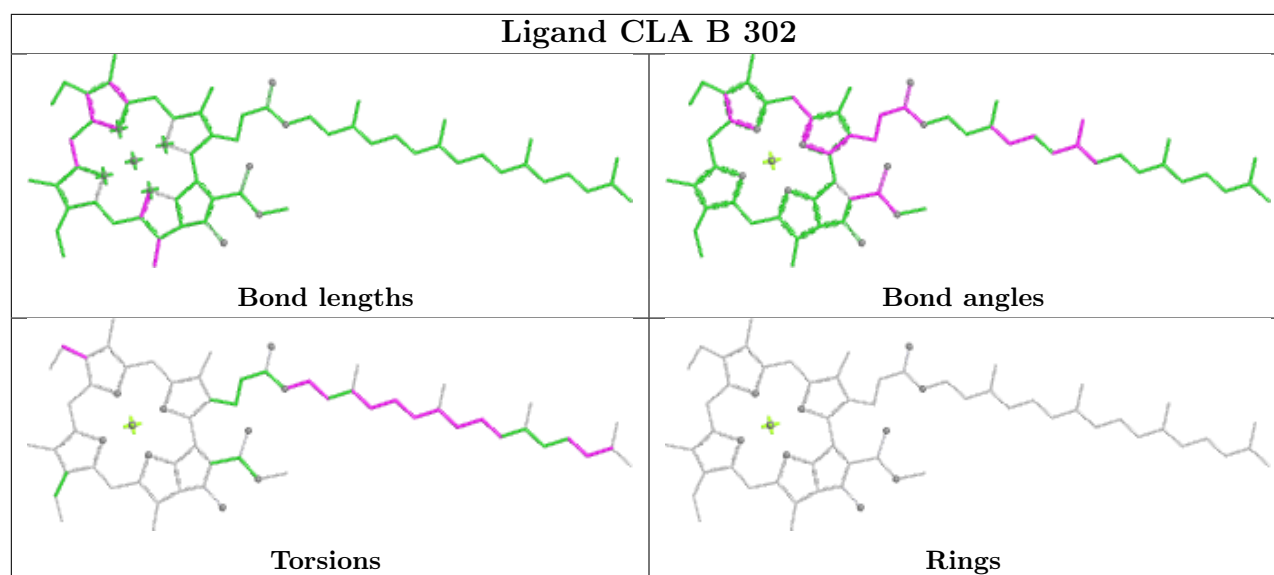
Ligand ECH A 304

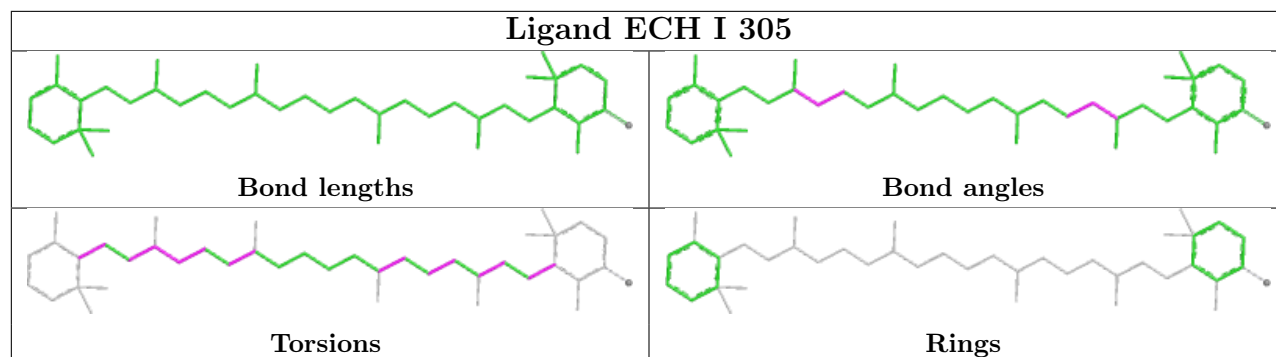
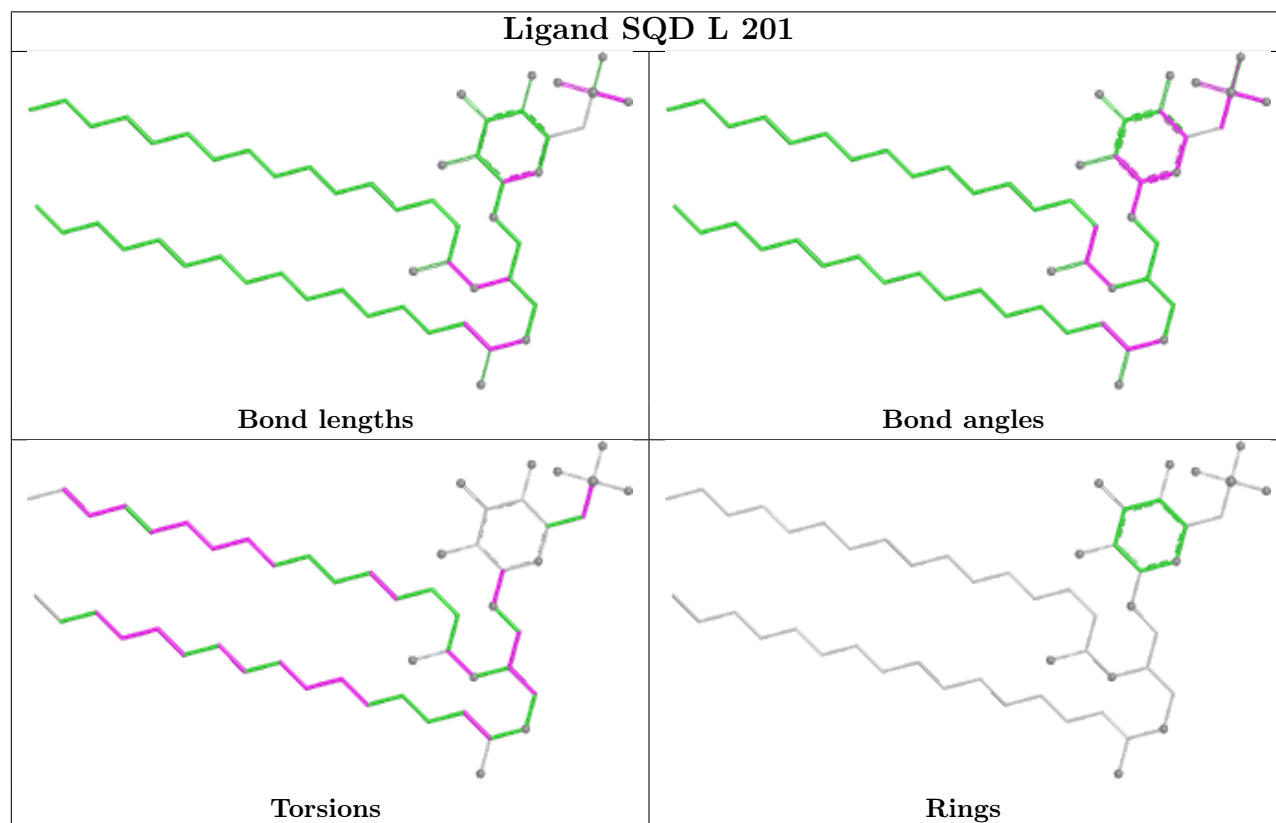


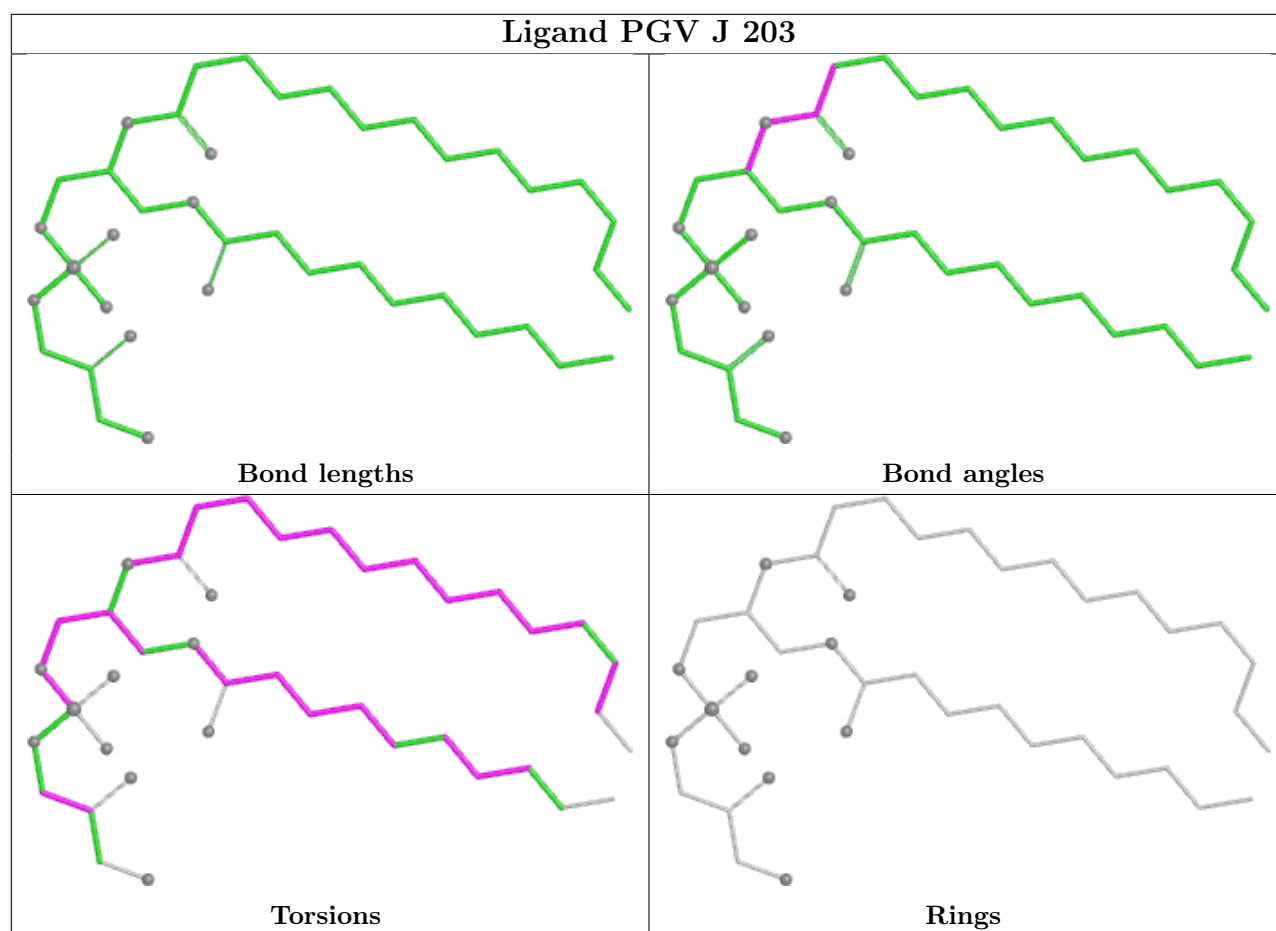








Ligand ECH I 305**Ligand SQD L 201**



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.

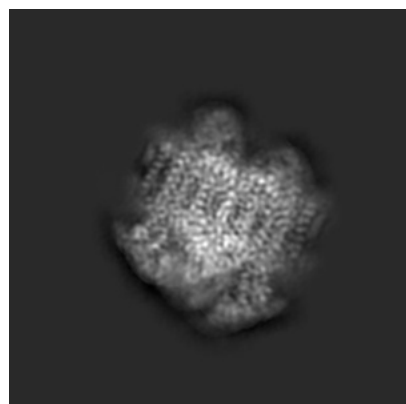
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14224. These allow visual inspection of the internal detail of the map and identification of artifacts.

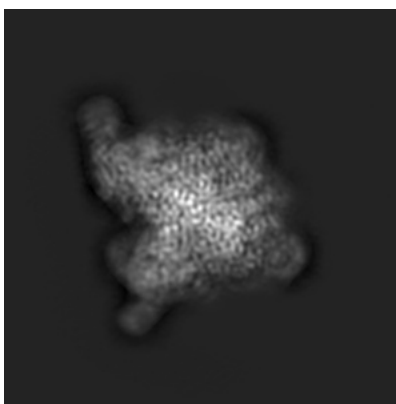
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

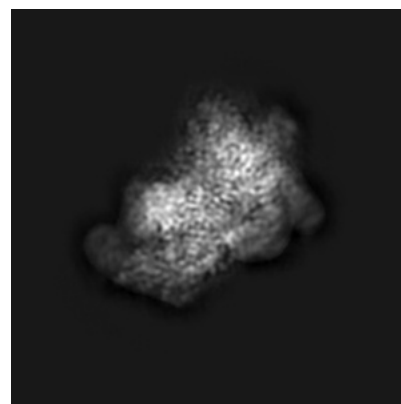
6.1.1 Primary map



X

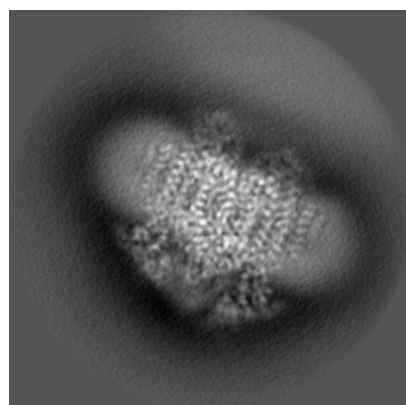


Y

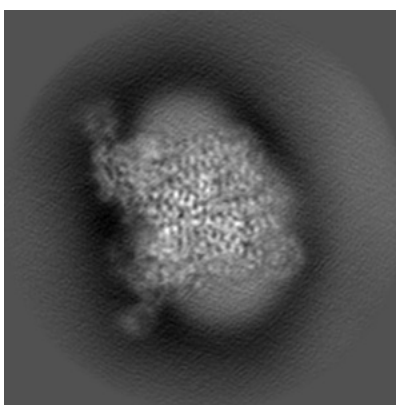


Z

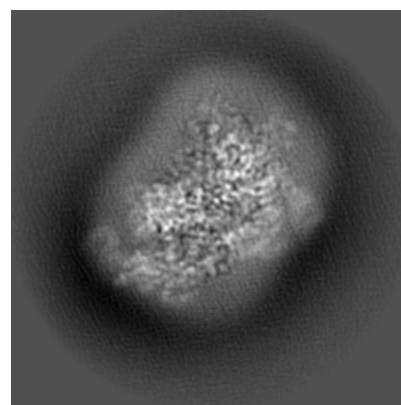
6.1.2 Raw map



X



Y

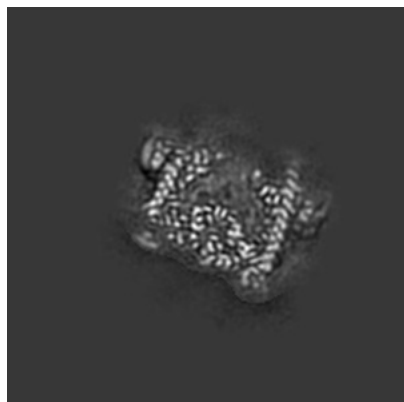


Z

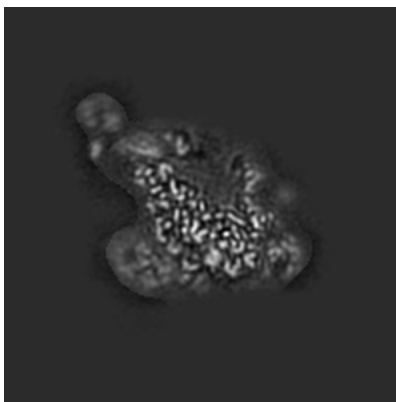
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

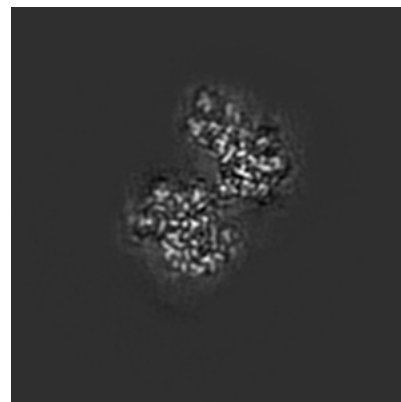
6.2.1 Primary map



X Index: 100

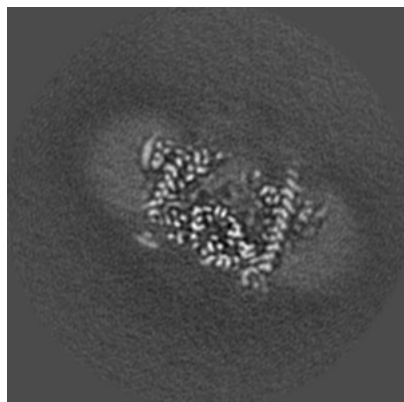


Y Index: 100

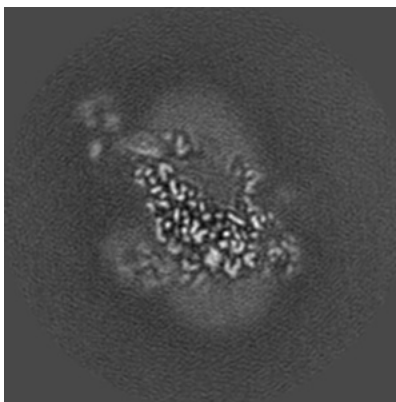


Z Index: 100

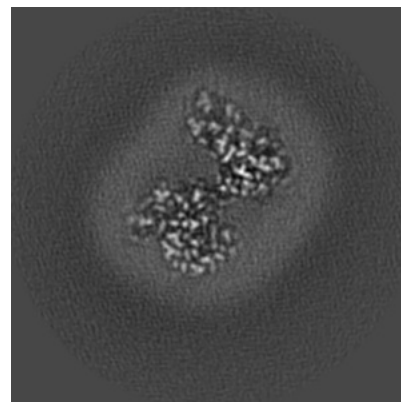
6.2.2 Raw map



X Index: 100



Y Index: 100

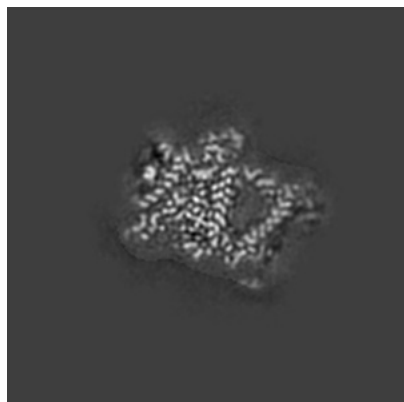


Z Index: 100

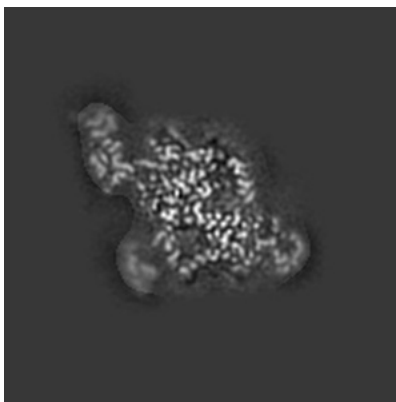
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

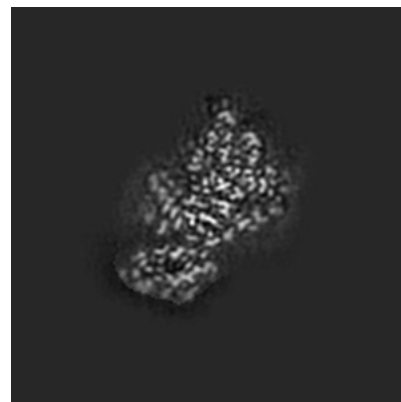
6.3.1 Primary map



X Index: 93

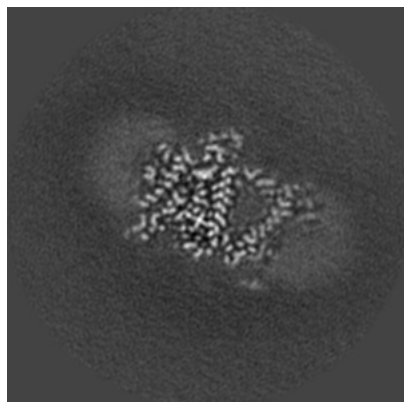


Y Index: 108

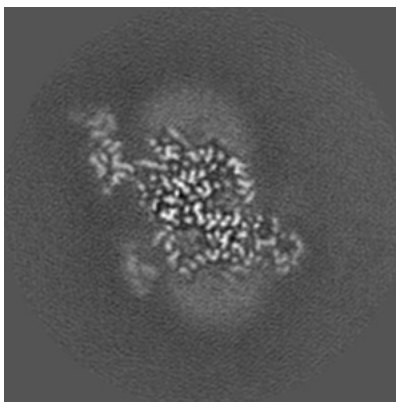


Z Index: 85

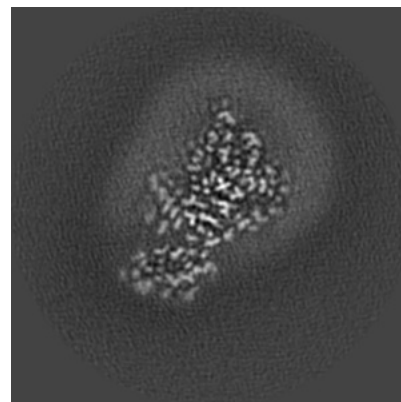
6.3.2 Raw map



X Index: 93



Y Index: 108

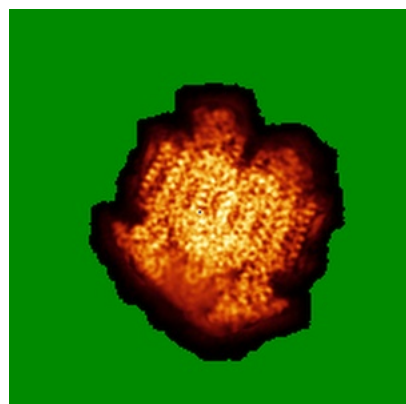


Z Index: 85

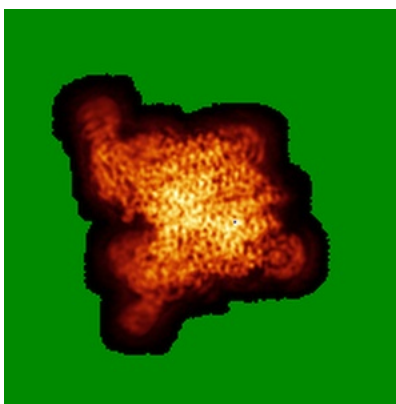
The images above show the largest variance slices of the map in three orthogonal directions.

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

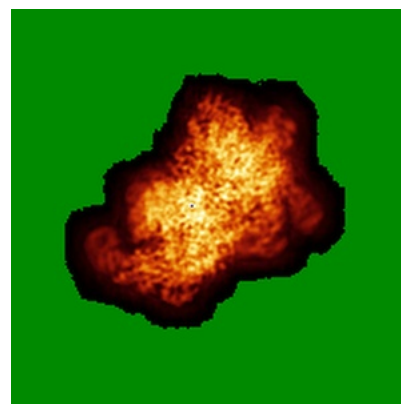
6.4.1 Primary map



X

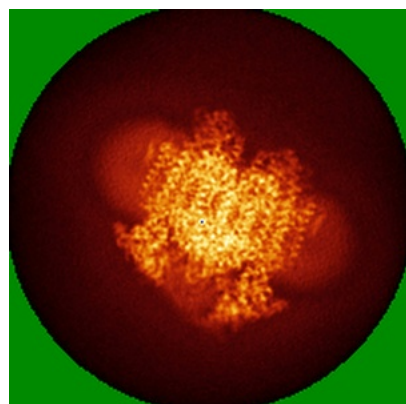


Y

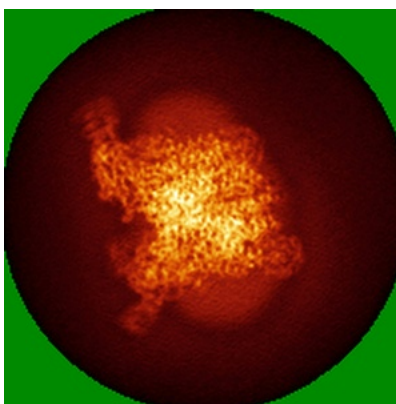


Z

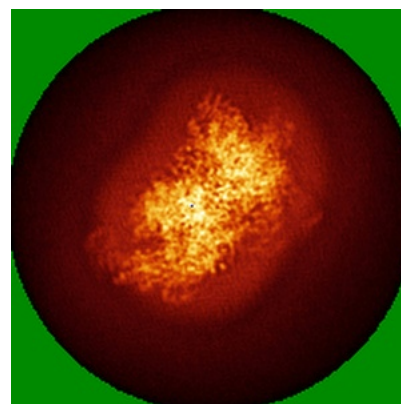
6.4.2 Raw map



X



Y

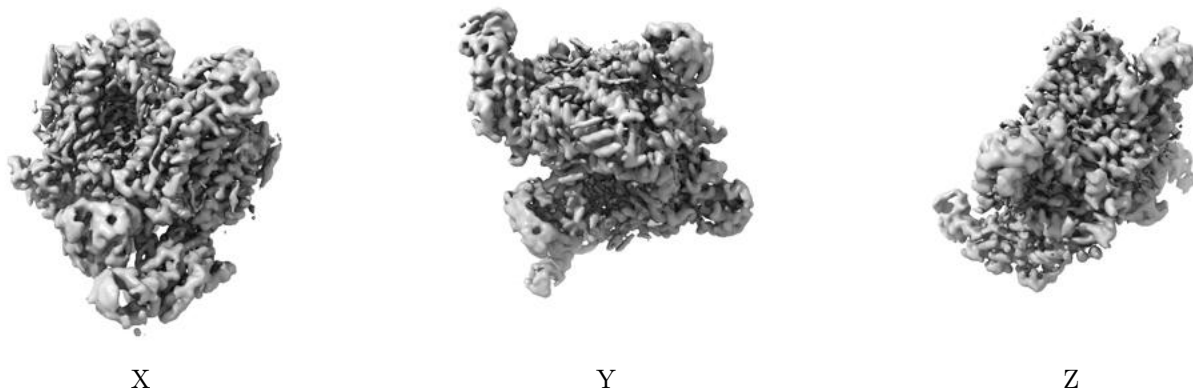


Z

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

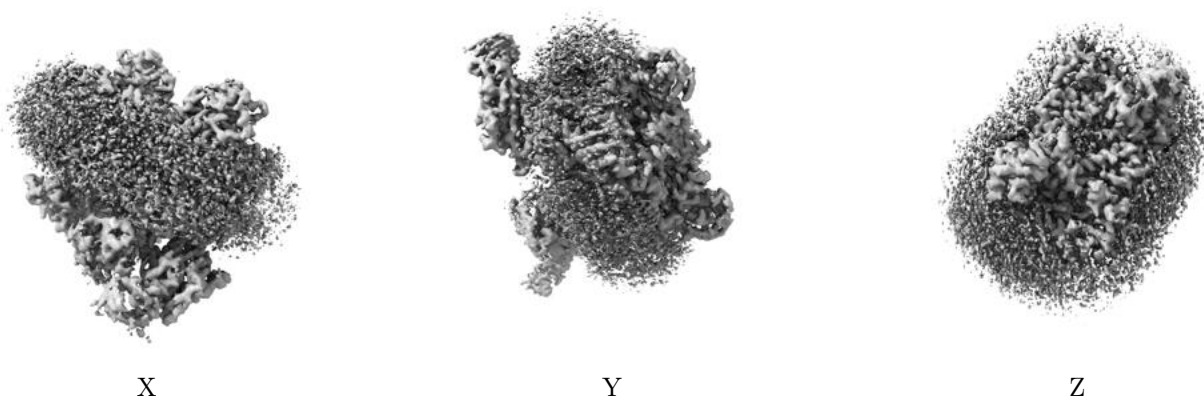
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

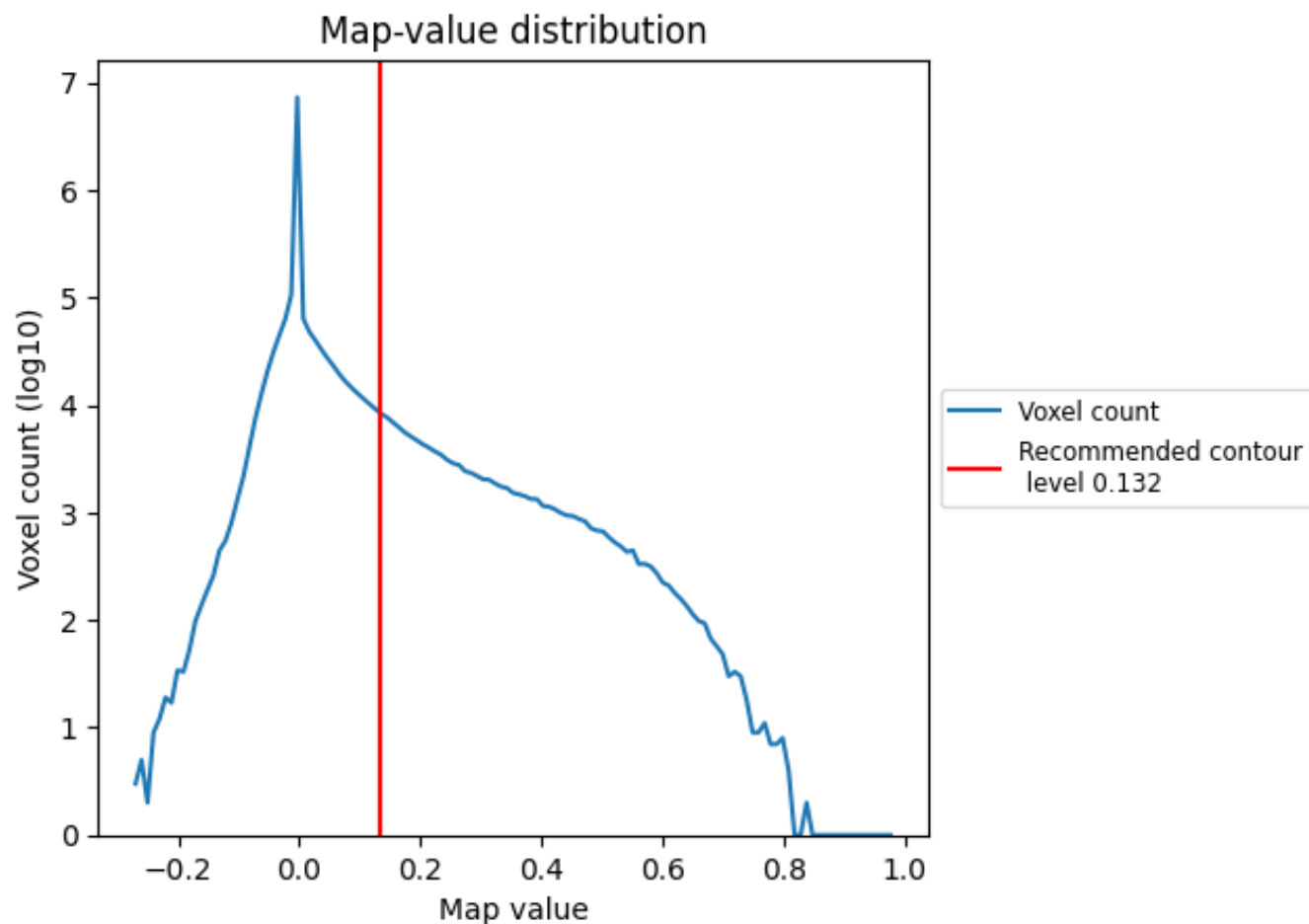
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

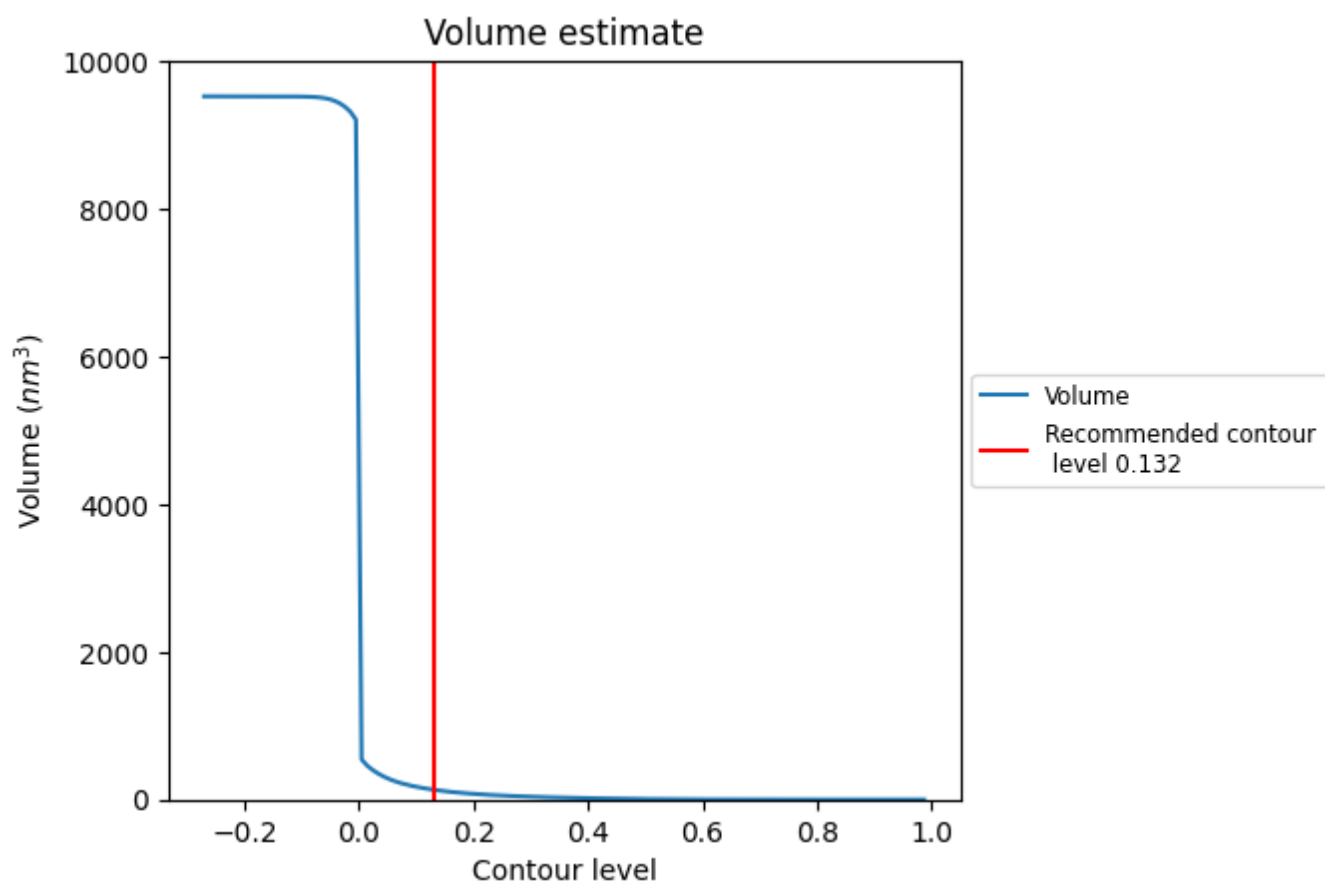
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

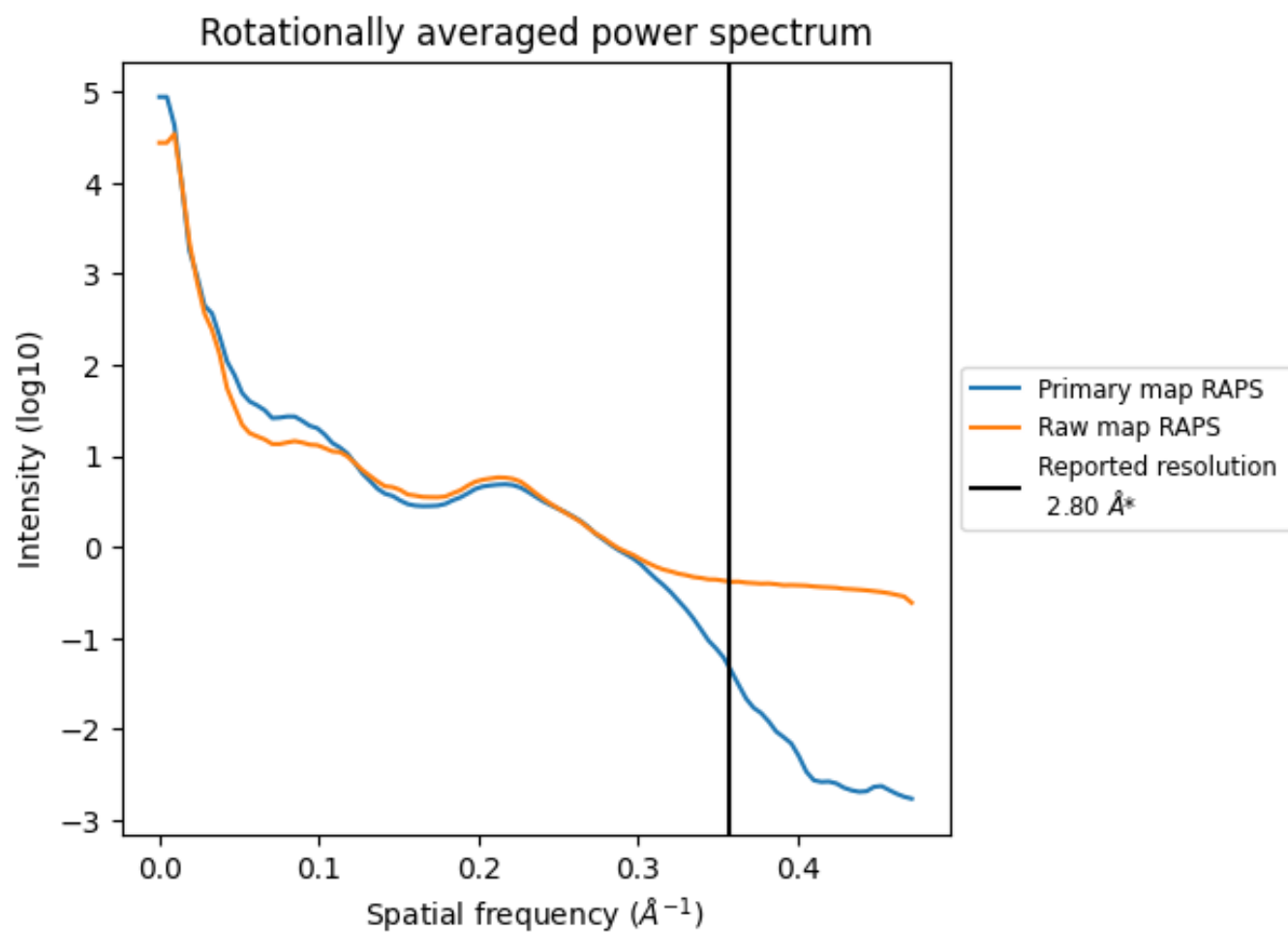
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm^3 ; this corresponds to an approximate mass of 118 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 ⓘ

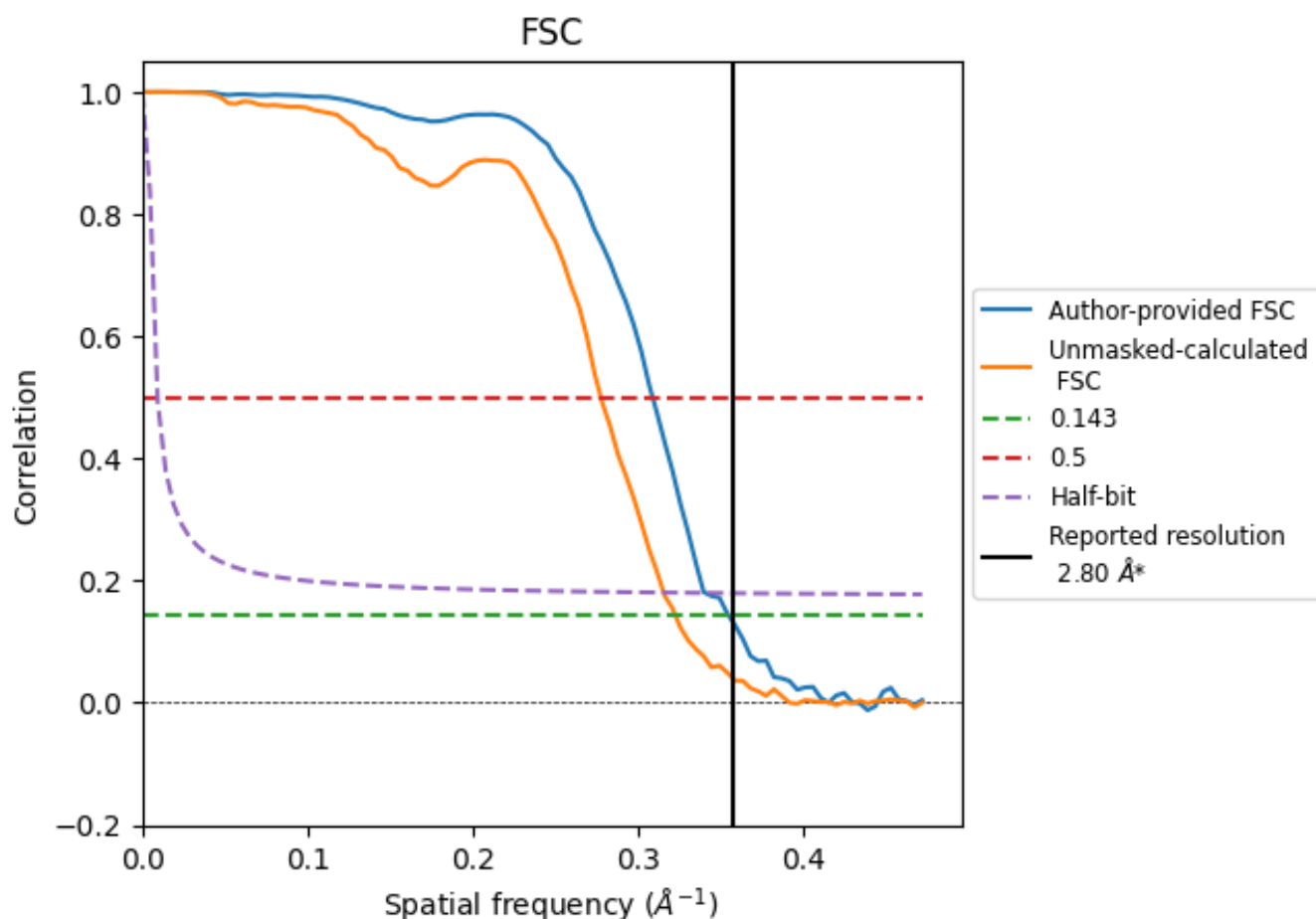


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

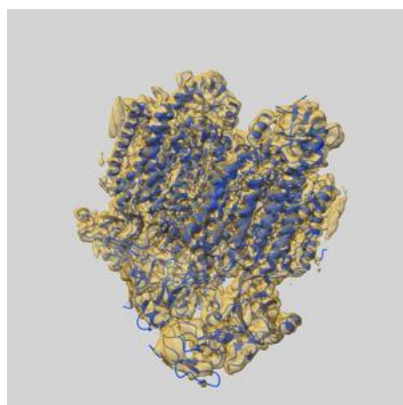
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.24	2.94
Unmasked-calculated*	3.10	3.60	3.17

*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 2.8 by more than 10 %

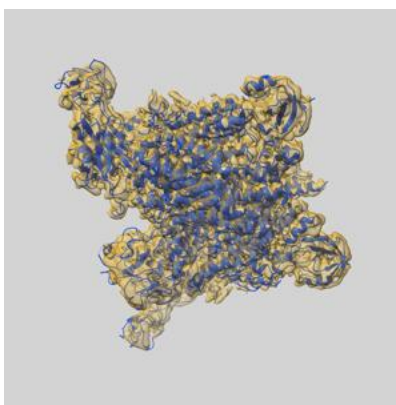
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14224 and PDB model 7R0W. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

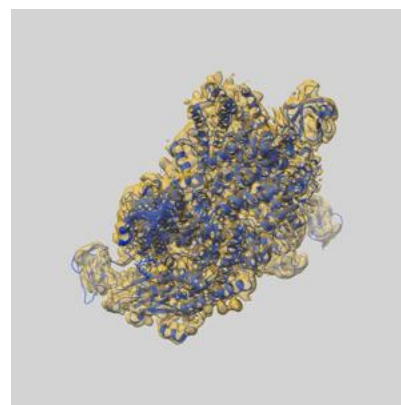
9.1 Map-model overlay [i](#)



X



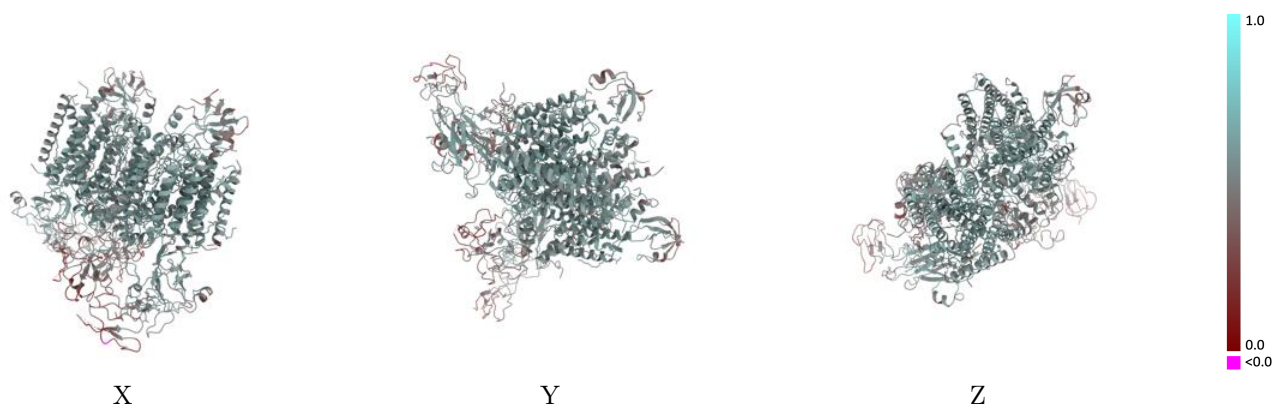
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

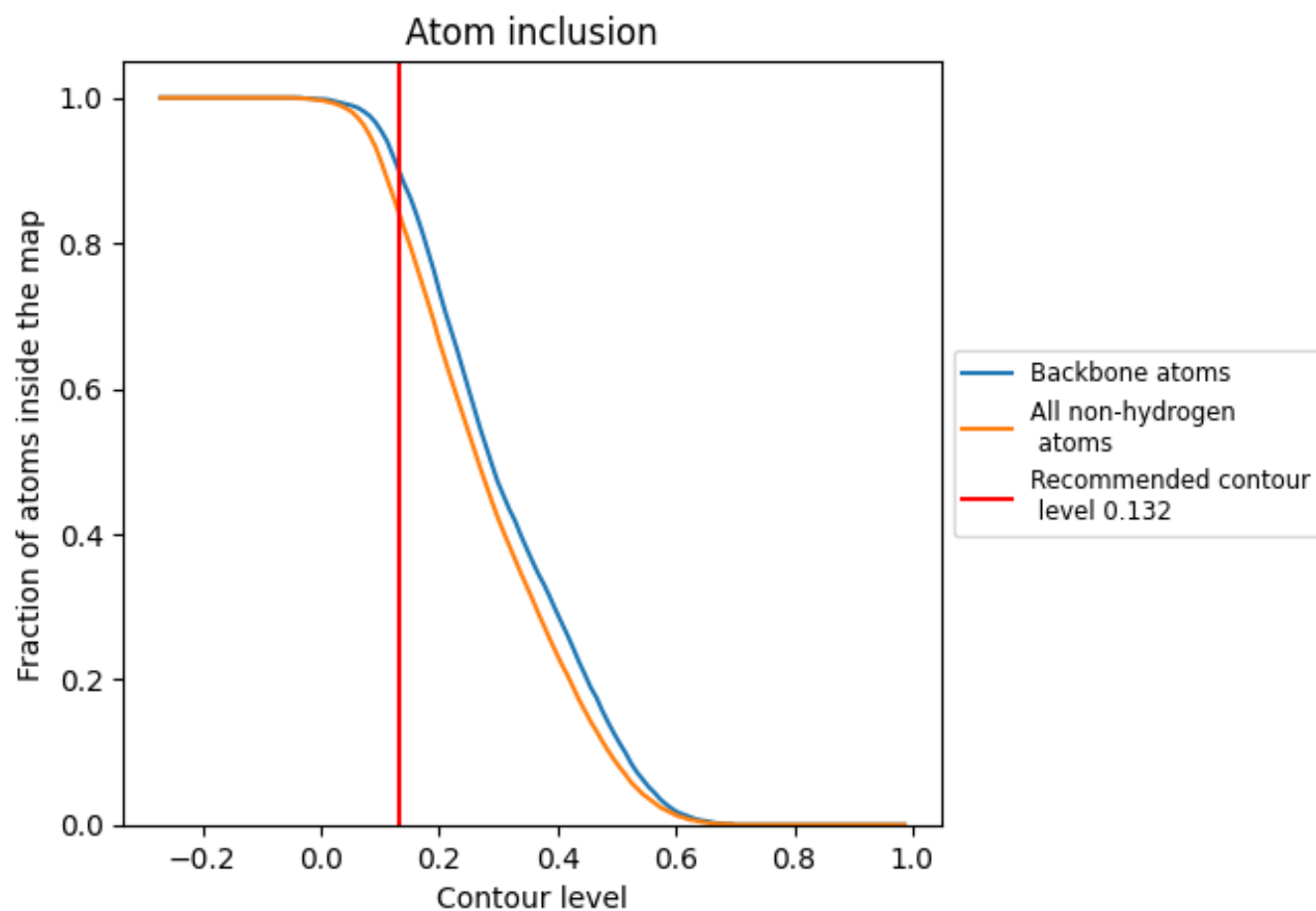


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5230
A	 0.9520	 0.5910
B	 0.8870	 0.5630
C	 0.8050	 0.5040
D	 0.6940	 0.4050
E	 0.8390	 0.5420
F	 0.9070	 0.5350
G	 0.9580	 0.5720
H	 0.9070	 0.5670
I	 0.9600	 0.5890
J	 0.8990	 0.5670
K	 0.8080	 0.5060
L	 0.7060	 0.4120
M	 0.8550	 0.5130
N	 0.8050	 0.5080
O	 0.9500	 0.5880
P	 0.9070	 0.5640
V	 0.7350	 0.4680
X	 0.7450	 0.4690

