



Full wwPDB EM Validation Report ⓘ

Nov 2, 2025 – 12:29 PM JST

PDB ID : 9LB1 / pdb_00009lb1
EMDB ID : EMD-62935
Title : Cryo-EM structure of the MK4-bound succinate dehydrogenase from *Chloroflexus aurantiacus*
Authors : Zhang, X.; Wu, J.Y.; Xu, X.L.
Deposited on : 2025-01-02
Resolution : 2.90 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

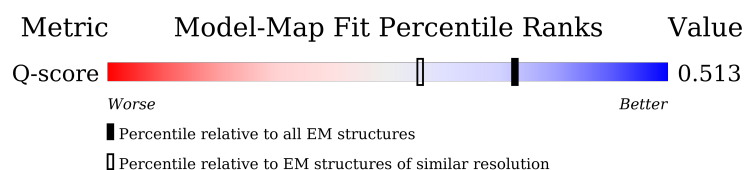
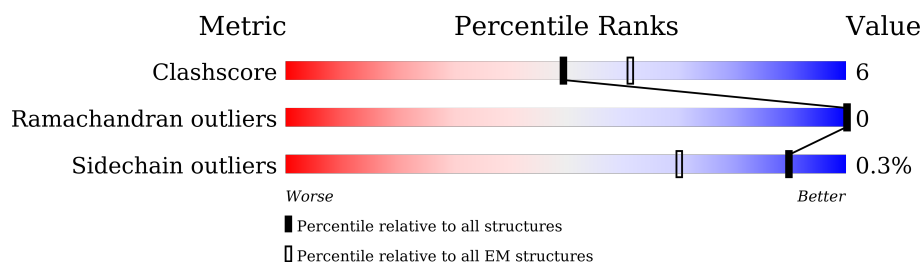
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	657	
1	D	657	
1	G	657	
2	B	260	

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Mol	Chain	Length	Quality of chain
2	E	260	 84% 15%
2	H	260	 89% 10%
3	C	239	 88% 12%
3	F	239	 85% 15%
3	I	239	 89% 11%

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
7	F3S	B	303	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27122 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 Succinate dehydrogenase or fumarate reductase, flavoprotein subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	631	Total	C	N	O	S	0	0
			4948	3115	896	915	22		
1	D	631	Total	C	N	O	S	0	0
			4948	3115	896	915	22		
1	G	631	Total	C	N	O	S	0	0
			4948	3115	896	915	22		

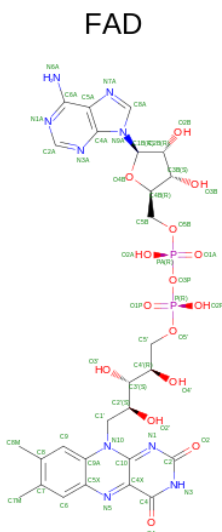
- Molecule 2 is a protein called 4Fe-4S ferredoxin iron-sulfur binding domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	257	Total	C	N	O	S	0	0
			1929	1202	338	366	23		
2	E	257	Total	C	N	O	S	0	0
			1929	1202	338	366	23		
2	H	257	Total	C	N	O	S	0	0
			1929	1202	338	366	23		

- Molecule 3 is a protein called Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family.

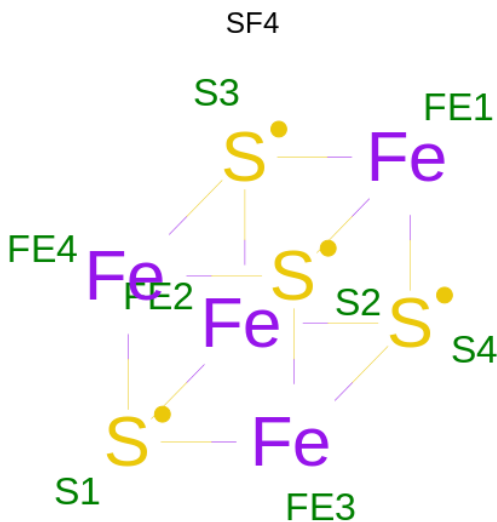
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		
3	F	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		
3	I	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



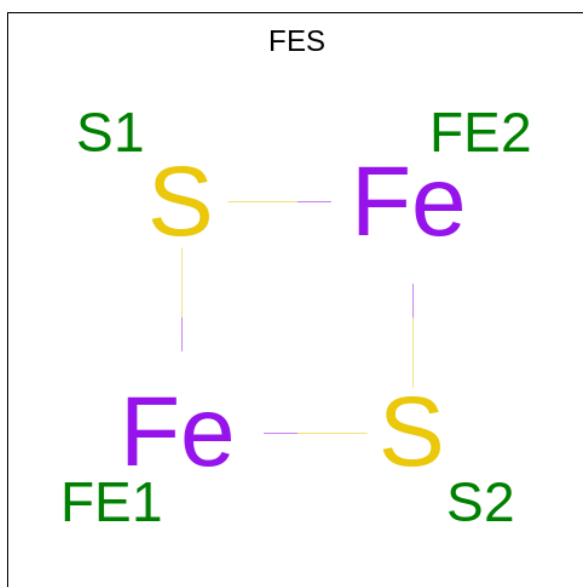
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



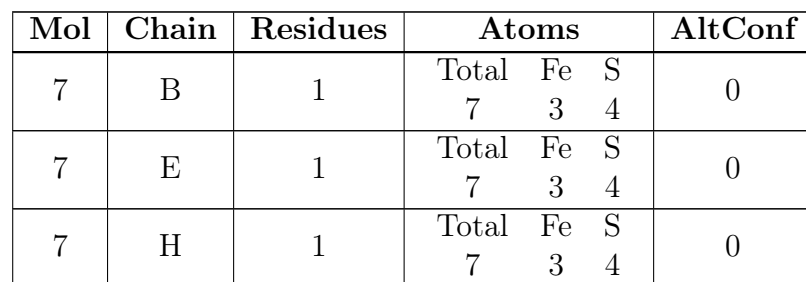
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	Fe	S	0
			8	4	4	
5	E	1	Total	Fe	S	0
			8	4	4	
5	H	1	Total	Fe	S	0
			8	4	4	

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	Fe	S	0
			4	2	2	
6	E	1	Total	Fe	S	0
			4	2	2	
6	H	1	Total	Fe	S	0
			4	2	2	

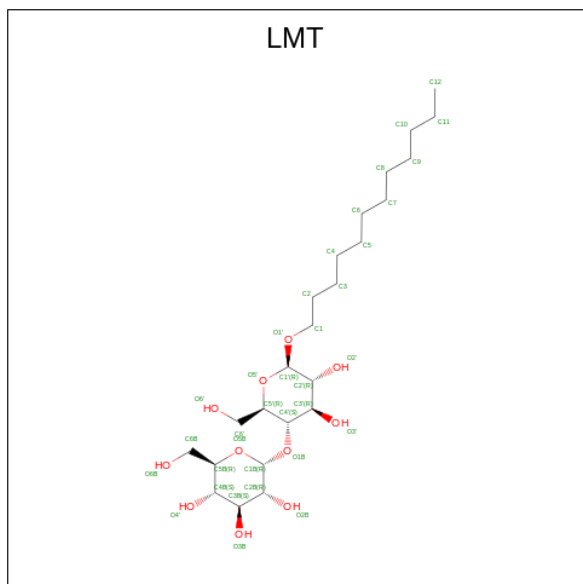
- Molecule 7 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



- [illegible]

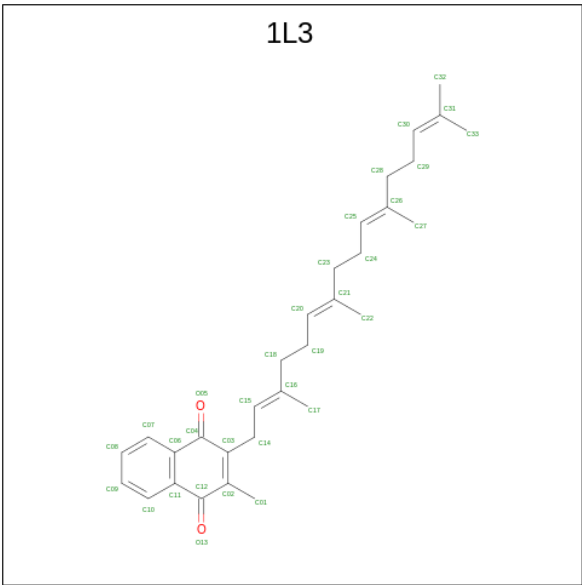
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 9 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			34	23	11	
9	F	1	Total	C	O	0
			35	24	11	
9	I	1	Total	C	O	0
			35	24	11	

- Molecule 10 is Menaquinone-4 (CCD ID: 1L3) (formula: $C_{31}H_{40}O_2$) (labeled as "Ligand of Interest" by depositor).

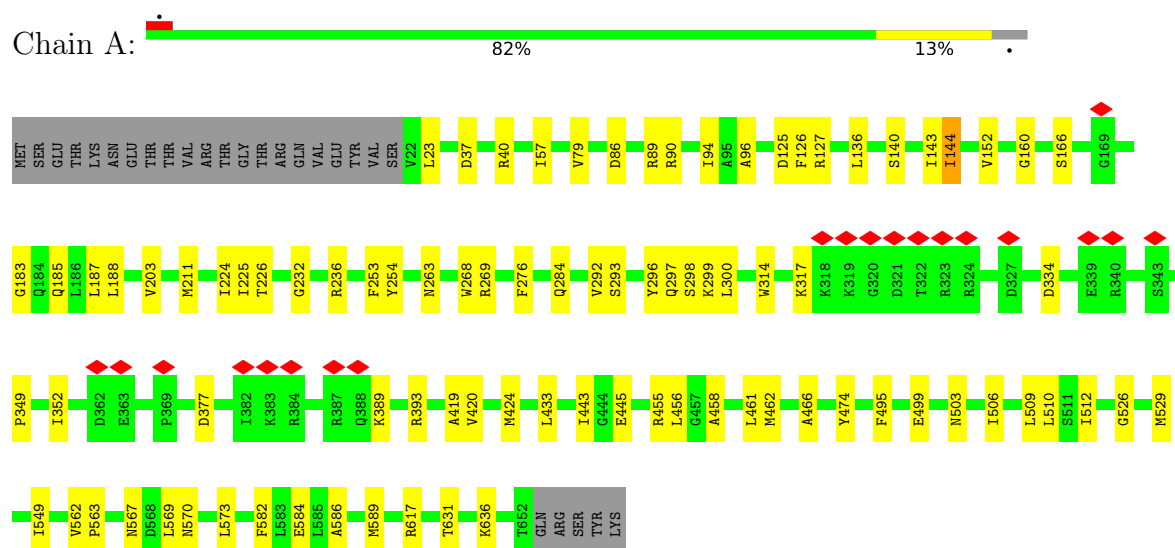


Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			22	20	2	
10	C	1	Total	C	O	0
			22	20	2	
10	F	1	Total	C	O	0
			22	20	2	
10	F	1	Total	C	O	0
			22	20	2	
10	I	1	Total	C	O	0
			22	20	2	
10	I	1	Total	C	O	0
			22	20	2	

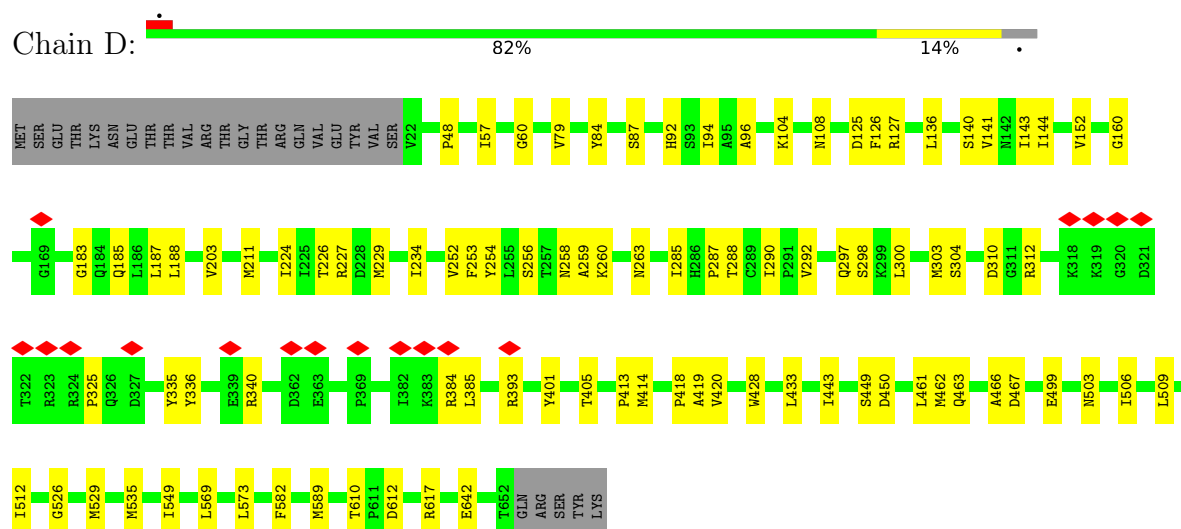
3 Residue-property plots

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.

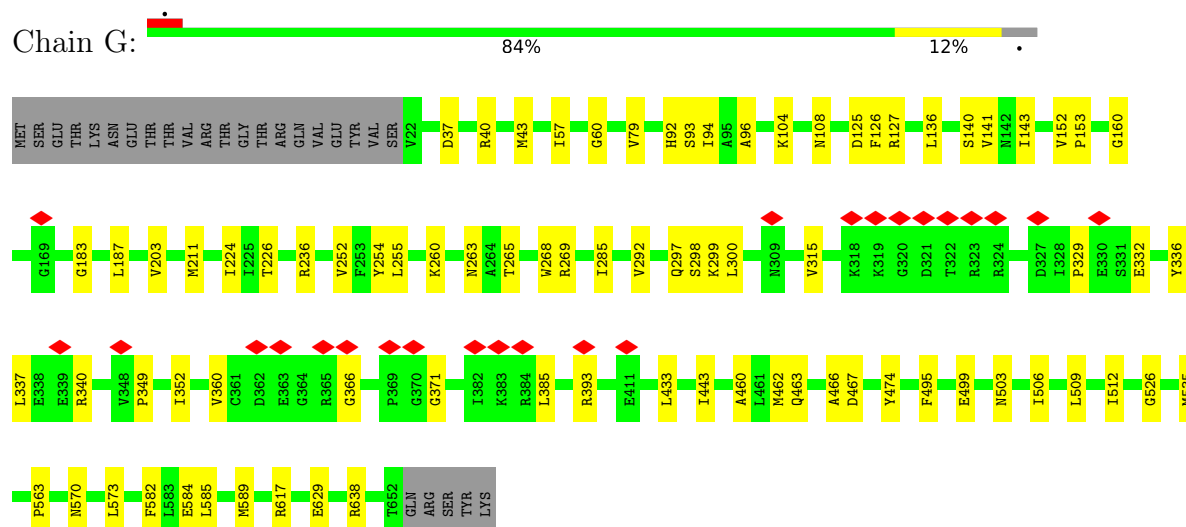
- Molecule 1: Succinate dehydrogenase or fumarate reductase, flavoprotein subunit



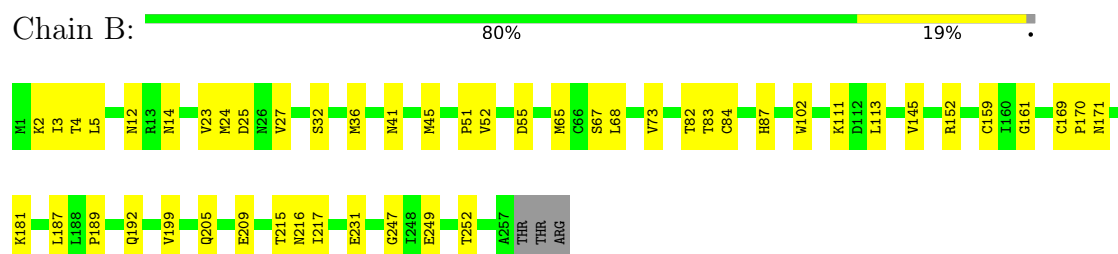
- Molecule 1: Succinate dehydrogenase or fumarate reductase, flavoprotein subunit



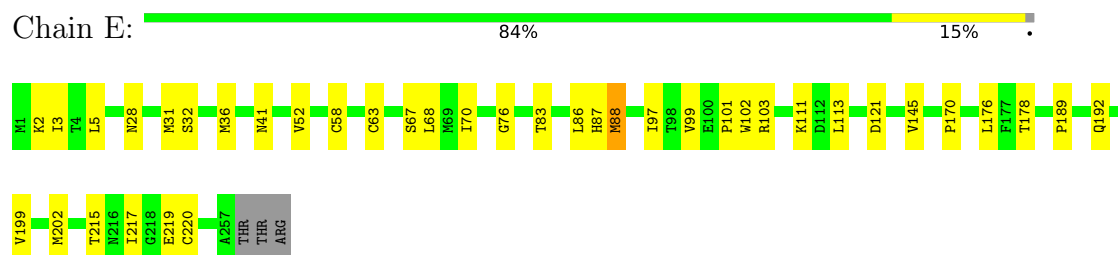
- Molecule 1: Succinate dehydrogenase or fumarate reductase, flavoprotein subunit



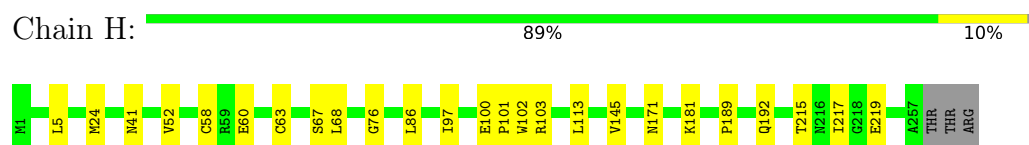
- Molecule 2: 4Fe-4S ferredoxin iron-sulfur binding domain protein



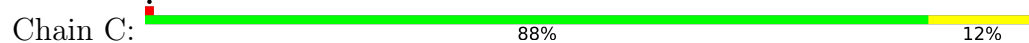
- Molecule 2: 4Fe-4S ferredoxin iron-sulfur binding domain protein



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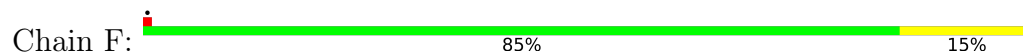


- Molecule 3: Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family

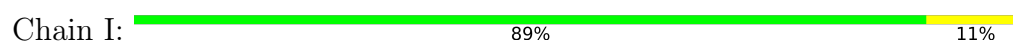




- Molecule 3: Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family



- Molecule 3: Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44018	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.319	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	192.0, 192.0, 192.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.64, 0.64, 0.64	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FAD, 1L3, LMT, FES, F3S, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.10	0/5055	0.24	0/6835
1	D	0.10	0/5055	0.24	0/6835
1	G	0.11	0/5055	0.25	0/6835
2	B	0.11	0/1963	0.24	0/2663
2	E	0.13	0/1963	0.29	0/2663
2	H	0.11	0/1963	0.24	0/2663
3	C	0.11	0/1988	0.24	0/2702
3	F	0.15	0/1988	0.26	0/2702
3	I	0.16	0/1988	0.28	0/2702
All	All	0.12	0/27018	0.25	0/36600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	4948	0	4857	56	0
1	D	4948	0	4857	55	0
1	G	4948	0	4857	48	0
2	B	1929	0	1911	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1929	0	1911	28	0
2	H	1929	0	1911	18	0
3	C	1927	0	1929	22	0
3	F	1927	0	1929	26	0
3	I	1927	0	1929	19	0
4	A	53	0	31	3	0
4	D	53	0	31	2	0
4	G	53	0	31	3	0
5	B	8	0	0	0	0
5	E	8	0	0	0	0
5	H	8	0	0	0	0
6	B	4	0	0	0	0
6	E	4	0	0	0	0
6	H	4	0	0	0	0
7	B	7	0	0	4	0
7	E	7	0	0	1	0
7	H	7	0	0	1	0
8	C	86	0	60	6	0
8	F	86	0	60	11	0
8	I	86	0	60	6	0
9	C	34	0	40	1	0
9	F	35	0	45	1	0
9	I	35	0	45	2	0
10	C	44	0	0	0	0
10	F	44	0	0	1	0
10	I	44	0	0	0	0
All	All	27122	0	26494	297	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 6.

All (297) 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)
8:F:302:HEM:HBB2	8:F:302:HEM:HHC	1.64	0.78
3:I:107:TYR:HB2	3:I:110:HIS:HB2	1.66	0.76
8:I:302:HEM:HHC	8:I:302:HEM:HBB2	1.69	0.74
1:G:255:LEU:HB3	1:G:300:LEU:HD11	1.70	0.73
3:F:82:ILE:HD11	8:F:301:HEM:HMC1	1.73	0.68
1:D:211:MET:HA	1:D:226:THR:HG22	1.76	0.67
1:D:252:VAL:HG11	1:D:589:MET:HE1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:TYR:HB2	3:C:110:HIS:HB2	1.77	0.66
1:D:104:LYS:HG2	1:D:141:VAL:HG12	1.76	0.66
1:G:211:MET:HA	1:G:226:THR:HG22	1.78	0.66
3:F:96:LEU:HD13	3:F:106:ARG:HD2	1.78	0.65
2:B:170:PRO:HG2	2:B:217:ILE:HD13	1.76	0.65
1:A:297:GLN:NE2	1:A:299:LYS:O	2.30	0.65
3:F:21:THR:HG21	3:F:81:HIS:HB2	1.78	0.65
1:G:104:LYS:HG2	1:G:141:VAL:HG12	1.80	0.64
1:A:136:LEU:HD11	1:A:462:MET:HG2	1.79	0.64
2:B:247:GLY:O	3:C:1:MET:N	2.31	0.64
2:H:101:PRO:HG3	2:H:113:LEU:HA	1.79	0.63
2:H:171:ASN:ND2	2:H:215:THR:OG1	2.26	0.63
1:A:143:ILE:HD11	1:A:466:ALA:HB2	1.81	0.63
1:D:143:ILE:HD11	1:D:466:ALA:HB2	1.79	0.63
1:A:140:SER:HA	1:A:143:ILE:HD12	1.82	0.62
1:A:314:TRP:HE1	1:A:377:ASP:HB2	1.64	0.62
3:C:21:THR:HG21	3:C:81:HIS:HB2	1.81	0.62
1:G:136:LEU:HD11	1:G:462:MET:HG2	1.81	0.62
2:E:178:THR:HG23	2:E:202:MET:HE2	1.80	0.62
2:B:231:GLU:N	2:B:231:GLU:OE1	2.31	0.62
3:I:21:THR:HG21	3:I:81:HIS:HB2	1.81	0.62
2:E:103:ARG:HH12	3:F:101:ILE:HB	1.65	0.61
1:G:252:VAL:HG11	1:G:589:MET:HE1	1.82	0.61
2:B:216:ASN:N	7:B:303:F3S:S2	2.74	0.61
8:F:301:HEM:HBB1	8:F:302:HEM:HBC1	1.83	0.61
3:F:131:PHE:CG	3:F:181:THR:HG21	2.36	0.60
2:E:28:ASN:H	2:E:31:MET:HE3	1.67	0.60
1:G:140:SER:HA	1:G:143:ILE:HD12	1.83	0.60
1:A:211:MET:HA	1:A:226:THR:HG22	1.84	0.60
1:D:140:SER:HA	1:D:143:ILE:HD12	1.83	0.60
1:G:366:GLY:HA2	1:G:371:GLY:HA2	1.84	0.60
2:E:101:PRO:HG3	2:E:113:LEU:HA	1.83	0.60
2:B:169:CYS:CB	7:B:303:F3S:S1	2.89	0.59
3:C:14:LYS:HZ1	9:C:303:LMT:H4'	1.67	0.59
2:B:171:ASN:OD1	2:B:215:THR:OG1	2.21	0.59
1:D:499:GLU:OE2	1:D:503:ASN:ND2	2.36	0.59
3:I:131:PHE:CG	3:I:181:THR:HG21	2.38	0.59
1:A:96:ALA:HB3	1:A:183:GLY:HA3	1.84	0.58
1:A:349:PRO:HD2	1:A:352:ILE:HD12	1.85	0.58
1:D:94:ILE:HB	1:D:187:LEU:HD23	1.84	0.58
1:G:143:ILE:HD11	1:G:466:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:302:HEM:HMC2	8:F:302:HEM:HBC2	1.85	0.58
3:F:57:GLY:O	3:F:61:PHE:N	2.35	0.58
1:G:349:PRO:HD2	1:G:352:ILE:HD12	1.86	0.58
3:C:131:PHE:CG	3:C:181:THR:HG21	2.39	0.57
1:A:90:ARG:NH2	2:B:161:GLY:O	2.36	0.57
1:G:260:LYS:HE3	1:G:298:SER:HB2	1.86	0.57
1:G:499:GLU:OE2	1:G:503:ASN:ND2	2.38	0.57
2:H:219:GLU:N	7:H:303:F3S:S2	2.78	0.57
3:I:14:LYS:NZ	3:I:87:SER:OG	2.38	0.56
1:G:254:TYR:H	1:G:526:GLY:HA3	1.70	0.56
2:B:169:CYS:HB2	7:B:303:F3S:S1	2.46	0.56
1:D:310:ASP:OD2	1:D:393:ARG:NH1	2.39	0.56
1:G:329:PRO:HG2	1:G:332:GLU:HB2	1.87	0.56
3:F:161:THR:HA	3:F:164:ASN:HD22	1.71	0.56
1:D:256:SER:OG	1:D:258:ASN:OD1	2.20	0.55
1:A:254:TYR:H	1:A:526:GLY:HA3	1.72	0.55
1:D:260:LYS:HE3	1:D:298:SER:HB2	1.87	0.55
1:A:236:ARG:HD2	1:A:495:PHE:HB3	1.88	0.55
3:F:25:LEU:HB3	8:F:301:HEM:HMB1	1.89	0.55
1:G:236:ARG:HD2	1:G:495:PHE:HB3	1.89	0.55
3:I:171:ASN:HB3	3:I:174:ILE:HG12	1.89	0.55
1:A:268:TRP:NE1	1:A:584:GLU:OE1	2.35	0.55
1:G:385:LEU:HD22	1:G:393:ARG:HH22	1.72	0.55
2:H:189:PRO:HA	2:H:192:GLN:HG2	1.89	0.55
3:I:135:HIS:CE1	3:I:139:LEU:HD12	2.42	0.55
3:C:25:LEU:HB3	8:C:301:HEM:HMB1	1.89	0.54
9:F:303:LMT:H5B	9:F:303:LMT:H6D	1.90	0.54
1:D:125:ASP:OD1	1:D:617:ARG:NH1	2.41	0.54
3:C:14:LYS:NZ	3:C:87:SER:OG	2.35	0.54
3:C:125:GLY:O	8:C:301:HEM:HBC2	2.08	0.54
2:B:45:MET:HG3	2:B:51:PRO:HG3	1.90	0.53
1:A:499:GLU:OE2	1:A:503:ASN:ND2	2.41	0.53
3:C:57:GLY:O	3:C:61:PHE:N	2.41	0.53
2:E:41:ASN:OD1	2:E:52:VAL:N	2.40	0.53
1:G:463:GLN:NE2	1:G:467:ASP:OD2	2.42	0.53
1:G:96:ALA:HB3	1:G:183:GLY:HA3	1.90	0.53
1:G:292:VAL:HB	1:G:297:GLN:HB3	1.91	0.52
1:D:288:THR:OG1	1:D:304:SER:O	2.24	0.52
1:D:463:GLN:NE2	1:D:467:ASP:OD2	2.41	0.52
1:D:325:PRO:HB2	1:D:413:PRO:HG2	1.91	0.52
1:G:125:ASP:OD1	1:G:617:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASP:HB3	2:B:65:MET:HG3	1.92	0.52
1:D:300:LEU:HD22	1:D:419:ALA:HB2	1.91	0.52
3:I:25:LEU:HB3	8:I:301:HEM:HMB1	1.92	0.52
3:C:18:MET:SD	8:C:301:HEM:HBD1	2.50	0.51
2:H:100:GLU:OE2	2:H:103:ARG:NH2	2.43	0.51
1:D:433:LEU:HD13	1:D:443:ILE:HG22	1.92	0.51
3:F:78:VAL:O	3:F:82:ILE:HG12	2.10	0.51
2:H:171:ASN:HD21	2:H:215:THR:HG1	1.56	0.51
3:I:125:GLY:O	8:I:301:HEM:HBC2	2.10	0.51
3:F:147:GLU:HB3	3:F:150:GLN:HG3	1.93	0.51
3:F:54:ARG:NH1	8:F:302:HEM:O2A	2.41	0.51
2:H:5:LEU:HD23	2:H:97:ILE:HG13	1.91	0.51
2:E:170:PRO:HG2	2:E:217:ILE:HD13	1.91	0.51
1:G:585:LEU:HG	1:G:589:MET:HE2	1.92	0.51
3:F:6:THR:HA	3:F:9:ARG:HD3	1.93	0.50
2:E:176:LEU:HD22	2:E:220:CYS:HB3	1.92	0.50
2:E:219:GLU:N	7:E:303:F3S:S1	2.83	0.50
1:G:299:LYS:NZ	2:H:60:GLU:OE2	2.44	0.50
2:B:2:LYS:HG3	2:B:25:ASP:HA	1.93	0.50
1:G:40:ARG:HA	1:G:43:MET:HE2	1.93	0.50
1:A:79:VAL:HB	1:A:203:VAL:HG22	1.93	0.50
2:E:189:PRO:HA	2:E:192:GLN:HG2	1.93	0.50
1:G:79:VAL:HB	1:G:203:VAL:HG22	1.93	0.50
1:G:268:TRP:NE1	1:G:584:GLU:OE1	2.32	0.50
3:C:78:VAL:O	3:C:82:ILE:HG12	2.12	0.50
2:B:189:PRO:HA	2:B:192:GLN:HG2	1.92	0.50
1:A:300:LEU:HD22	1:A:419:ALA:HB2	1.94	0.50
1:D:401:TYR:O	1:D:405:THR:OG1	2.30	0.49
2:B:32:SER:HA	2:B:87:HIS:HA	1.93	0.49
2:B:4:THR:HG23	2:B:23:VAL:HG22	1.93	0.49
1:G:337:LEU:H	1:G:340:ARG:HG2	1.77	0.49
1:A:253:PHE:CE1	1:A:529:MET:HB3	2.48	0.49
2:B:3:ILE:HG21	2:B:36:MET:HE1	1.94	0.49
2:E:70:ILE:HG12	2:E:99:VAL:HG12	1.95	0.49
2:H:217:ILE:HG12	3:I:117:ALA:HB3	1.95	0.49
2:B:68:LEU:HB2	2:B:83:THR:HG21	1.95	0.48
3:C:135:HIS:ND1	3:C:178:TYR:OH	2.44	0.48
1:D:136:LEU:HD11	1:D:462:MET:HG3	1.96	0.48
1:G:629:GLU:HB3	1:G:638:ARG:HB3	1.96	0.48
1:A:389:LYS:HB3	1:A:393:ARG:HH21	1.78	0.48
1:D:79:VAL:HB	1:D:203:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ALA:HB1	8:C:301:HEM:HMD3	1.95	0.48
3:I:135:HIS:ND1	3:I:178:TYR:OH	2.37	0.48
1:A:89:ARG:NH2	2:B:159:CYS:O	2.46	0.48
1:A:509:LEU:HA	1:A:512:ILE:HD12	1.95	0.48
3:C:112:ARG:NH1	3:C:118:ASP:OD1	2.42	0.48
1:G:509:LEU:HA	1:G:512:ILE:HD12	1.96	0.48
1:D:292:VAL:HB	1:D:297:GLN:HB3	1.95	0.48
2:B:67:SER:HB2	2:B:102:TRP:NE1	2.29	0.47
2:B:215:THR:N	7:B:303:F3S:S2	2.87	0.47
2:B:249:GLU:OE2	3:C:9:ARG:NH1	2.47	0.47
2:H:58:CYS:HB3	2:H:63:CYS:HB3	1.97	0.47
8:C:302:HEM:HHC	8:C:302:HEM:HBB2	1.94	0.47
1:G:94:ILE:HD12	1:G:187:LEU:HB3	1.95	0.47
1:D:126:PHE:O	1:D:127:ARG:NH1	2.46	0.47
1:G:315:VAL:HG21	1:G:360:VAL:HG11	1.96	0.47
3:F:82:ILE:CD1	8:F:301:HEM:HMC1	2.44	0.47
1:G:160:GLY:HA2	2:H:145:VAL:O	2.15	0.47
1:A:126:PHE:O	1:A:127:ARG:NH1	2.45	0.47
8:I:301:HEM:HBB1	8:I:302:HEM:HBC1	1.95	0.47
3:I:182:MET:HE1	3:I:185:LEU:HD23	1.95	0.47
1:D:96:ALA:HB3	1:D:183:GLY:HA3	1.97	0.46
1:G:433:LEU:HD13	1:G:443:ILE:HG22	1.97	0.46
2:H:76:GLY:HA3	2:H:86:LEU:HD22	1.97	0.46
2:E:68:LEU:HB2	2:E:83:THR:HG21	1.96	0.46
1:A:57:ILE:HD13	1:A:224:ILE:HG12	1.97	0.46
2:E:170:PRO:HB3	3:F:112:ARG:NH2	2.30	0.46
1:G:92:HIS:CE1	4:G:701:FAD:HM81	2.50	0.46
1:D:108:ASN:OD1	1:G:474:TYR:OH	2.22	0.46
3:F:56:LEU:HB3	3:F:66:LEU:HD12	1.97	0.46
3:C:65:HIS:ND1	3:I:34:TYR:OH	2.40	0.46
1:D:506:ILE:HG23	1:D:573:LEU:HD21	1.96	0.46
2:E:58:CYS:HB3	2:E:63:CYS:HB3	1.96	0.46
1:G:563:PRO:O	1:G:570:ASN:ND2	2.38	0.46
1:A:506:ILE:HG23	1:A:573:LEU:HD21	1.97	0.46
1:A:458:ALA:HA	4:A:701:FAD:HN3	1.81	0.46
2:B:41:ASN:OD1	2:B:52:VAL:N	2.39	0.46
2:E:67:SER:HB2	2:E:102:TRP:CE2	2.50	0.46
1:A:125:ASP:OD1	1:A:617:ARG:NH1	2.47	0.45
1:A:529:MET:HE3	1:A:549:ILE:HD11	1.98	0.45
2:B:24:MET:HE2	2:B:27:VAL:HG22	1.98	0.45
1:A:474:TYR:OH	1:G:108:ASN:OD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:O	1:A:570:ASN:ND2	2.36	0.45
1:D:84:TYR:HB2	1:D:229:MET:HE1	1.98	0.45
2:E:76:GLY:HA3	2:E:86:LEU:HD22	1.98	0.45
1:A:461:LEU:HG	4:A:701:FAD:C2	2.47	0.45
1:D:290:ILE:HG12	1:D:303:MET:HE2	1.98	0.45
3:F:104:VAL:O	10:F:305:1L3:O13	2.34	0.45
3:C:21:THR:HG23	3:C:77:SER:HB3	1.98	0.45
3:C:131:PHE:CD2	3:C:181:THR:HG21	2.52	0.45
1:G:57:ILE:HD13	1:G:224:ILE:HG12	1.98	0.45
1:G:126:PHE:O	1:G:127:ARG:NH1	2.47	0.45
9:I:303:LMT:H5B	9:I:303:LMT:H6D	1.98	0.45
1:D:610:THR:HG23	1:D:612:ASP:H	1.82	0.45
1:D:92:HIS:HD1	1:D:259:ALA:HB2	1.82	0.45
1:D:336:TYR:HB2	1:D:340:ARG:HH21	1.82	0.45
3:I:131:PHE:CD2	3:I:181:THR:HG21	2.52	0.45
1:D:253:PHE:CE1	1:D:529:MET:HB3	2.53	0.44
3:F:160:GLU:O	3:F:164:ASN:ND2	2.50	0.44
3:F:192:GLY:HA2	3:F:195:SER:HB2	2.00	0.44
2:H:181:LYS:HA	2:H:181:LYS:HD3	1.78	0.44
1:A:225:ILE:HD12	1:A:236:ARG:HG2	1.98	0.44
1:A:445:GLU:HB2	4:A:701:FAD:H5'2	1.99	0.44
2:B:82:THR:OG1	2:B:84:CYS:SG	2.75	0.44
1:D:254:TYR:H	1:D:526:GLY:HA3	1.82	0.44
2:E:67:SER:HB2	2:E:102:TRP:NE1	2.32	0.44
3:I:188:HIS:NE2	8:I:301:HEM:NA	2.65	0.44
2:B:205:GLN:NE2	2:B:209:GLU:OE2	2.51	0.44
1:A:569:LEU:HD23	2:B:111:LYS:HB2	1.99	0.44
1:A:94:ILE:HD12	1:A:187:LEU:HB3	1.99	0.44
1:A:166:SER:HB2	1:D:48:PRO:HG2	1.99	0.44
2:B:12:ASN:ND2	2:B:14:ASN:OD1	2.50	0.44
8:F:302:HEM:HBC2	8:F:302:HEM:CMC	2.47	0.44
2:H:67:SER:HB2	2:H:102:TRP:CE2	2.53	0.44
1:A:284:GLN:HB2	1:A:424:MET:SD	2.58	0.43
3:C:82:ILE:HD11	8:C:301:HEM:HMC3	1.99	0.43
1:D:287:PRO:HA	1:D:418:PRO:HB3	2.00	0.43
1:G:506:ILE:HG23	1:G:573:LEU:HD21	1.99	0.43
1:A:160:GLY:HA2	2:B:145:VAL:O	2.18	0.43
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.88	0.43
1:D:509:LEU:HA	1:D:512:ILE:HD12	2.00	0.43
2:E:2:LYS:C	2:E:3:ILE:HD12	2.43	0.43
1:A:631:THR:OG1	1:A:636:LYS:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ARG:HB2	1:D:335:TYR:HE2	1.83	0.43
2:B:5:LEU:HD11	2:B:36:MET:HE2	2.00	0.43
1:D:535:MET:H	1:D:535:MET:HG2	1.60	0.43
1:A:433:LEU:HD13	1:A:443:ILE:HG22	1.99	0.43
3:I:186:ALA:HB2	3:I:223:PHE:HB2	2.01	0.43
1:A:253:PHE:CE2	1:A:420:VAL:HG21	2.54	0.43
1:D:285:ILE:HG22	1:D:420:VAL:HA	2.01	0.43
1:D:384:ARG:HG2	1:D:385:LEU:HD12	2.01	0.43
3:I:54:ARG:HB3	3:I:64:GLU:HG2	2.00	0.43
3:F:125:GLY:O	8:F:301:HEM:HBC2	2.19	0.43
1:A:232:GLY:HA3	1:A:567:ASN:HA	2.00	0.42
1:D:227:ARG:HB2	1:D:234:ILE:HD13	2.01	0.42
3:C:112:ARG:HH12	3:C:118:ASP:CG	2.25	0.42
1:D:461:LEU:HG	4:D:701:FAD:C2	2.49	0.42
3:F:131:PHE:CD2	3:F:181:THR:HG21	2.54	0.42
1:G:93:SER:HB2	1:G:187:LEU:HD22	2.01	0.42
1:G:265:THR:O	1:G:269:ARG:HG2	2.19	0.42
1:A:23:LEU:HD21	1:A:276:PHE:HD2	1.85	0.42
1:A:254:TYR:CZ	1:A:298:SER:HB3	2.53	0.42
1:G:285:ILE:HD13	1:G:535:MET:HE2	2.01	0.42
2:H:215:THR:HB	2:H:217:ILE:HG13	2.00	0.42
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.77	0.42
1:D:152:VAL:HG13	1:D:185:GLN:HB3	2.01	0.42
1:G:336:TYR:O	1:G:337:LEU:HB2	2.19	0.42
1:A:144:ILE:HD13	1:A:144:ILE:HA	1.92	0.42
1:D:263:ASN:HA	1:D:582:PHE:HZ	1.84	0.42
1:D:263:ASN:HA	1:D:582:PHE:CZ	2.55	0.42
1:D:449:SER:OG	1:D:450:ASP:N	2.53	0.42
8:I:302:HEM:HHC	8:I:302:HEM:CBB	2.45	0.42
2:B:215:THR:HB	2:B:217:ILE:HG13	2.02	0.42
1:A:510:LEU:HD12	1:A:562:VAL:HG23	2.02	0.42
1:D:92:HIS:ND1	1:D:259:ALA:HB2	2.35	0.42
1:D:428:TRP:NE1	1:D:642:GLU:OE1	2.35	0.42
1:D:60:GLY:HA2	4:D:701:FAD:H1B	2.02	0.41
1:D:87:SER:OG	2:E:121:ASP:OD2	2.29	0.41
3:I:139:LEU:HA	3:I:139:LEU:HD23	1.83	0.41
1:A:152:VAL:HG13	1:A:185:GLN:HB3	2.02	0.41
1:A:317:LYS:HG2	1:A:334:ASP:HB2	2.02	0.41
1:A:549:ILE:HD13	1:A:549:ILE:HA	1.97	0.41
2:E:88:MET:HE2	2:E:88:MET:HB3	1.99	0.41
2:H:24:MET:HE2	2:H:24:MET:HB3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:82:ILE:HG22	9:I:303:LMT:H101	2.03	0.41
2:B:68:LEU:HD21	2:B:113:LEU:HD13	2.03	0.41
3:C:47:ASN:ND2	3:C:159:TYR:O	2.53	0.41
1:D:160:GLY:HA2	2:E:145:VAL:O	2.21	0.41
1:G:263:ASN:HA	1:G:582:PHE:HZ	1.85	0.41
1:G:263:ASN:HA	1:G:582:PHE:CZ	2.55	0.41
2:B:181:LYS:HA	2:B:181:LYS:HD3	1.78	0.41
1:D:401:TYR:CZ	1:D:414:MET:HG3	2.56	0.41
1:D:549:ILE:HD13	1:D:549:ILE:HA	1.91	0.41
2:E:28:ASN:O	2:E:31:MET:HG2	2.21	0.41
3:F:146:TYR:OH	3:F:164:ASN:O	2.39	0.41
3:F:229:PHE:HB2	3:F:230:PRO:HD3	2.02	0.41
1:G:37:ASP:OD1	1:G:40:ARG:NH2	2.40	0.41
2:E:68:LEU:HD21	2:E:113:LEU:HD13	2.03	0.41
3:F:85:ALA:HB1	8:F:301:HEM:HMD3	2.02	0.41
3:F:188:HIS:NE2	8:F:301:HEM:NA	2.69	0.41
1:A:86:ASP:H	2:B:65:MET:HE1	1.85	0.41
1:A:94:ILE:HB	1:A:187:LEU:HD23	2.02	0.41
1:A:263:ASN:HA	1:A:582:PHE:CZ	2.55	0.41
2:B:152:ARG:HB3	2:B:187:LEU:HD13	2.03	0.41
1:D:57:ILE:HD13	1:D:224:ILE:HG12	2.03	0.41
2:E:70:ILE:HB	2:E:76:GLY:HA2	2.02	0.41
2:E:215:THR:HG22	2:E:215:THR:O	2.21	0.41
3:F:186:ALA:HB2	3:F:223:PHE:HB2	2.02	0.41
1:G:152:VAL:HA	1:G:153:PRO:HD3	1.91	0.41
1:A:37:ASP:OD1	1:A:40:ARG:NH2	2.45	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.91	0.41
1:A:263:ASN:HA	1:A:582:PHE:HZ	1.86	0.41
3:C:186:ALA:HB2	3:C:223:PHE:HB2	2.03	0.40
2:E:5:LEU:HD23	2:E:97:ILE:HB	2.02	0.40
1:G:460:ALA:HB3	4:G:701:FAD:N1	2.35	0.40
2:H:68:LEU:HD21	2:H:113:LEU:HD13	2.03	0.40
3:I:172:PRO:HA	3:I:175:VAL:HG22	2.03	0.40
1:A:293:SER:O	1:A:296:TYR:OH	2.38	0.40
2:E:32:SER:HA	2:E:87:HIS:HA	2.04	0.40
1:A:455:ARG:HD2	1:A:456:LEU:O	2.20	0.40
2:B:12:ASN:HD22	2:B:14:ASN:H	1.69	0.40
1:D:443:ILE:HB	1:D:467:ASP:HB3	2.04	0.40
3:F:182:MET:HE2	3:F:226:ASN:HB3	2.02	0.40
2:H:41:ASN:OD1	2:H:52:VAL:N	2.42	0.40
1:A:586:ALA:O	1:A:589:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:LEU:HD23	2:E:111:LYS:HB2	2.02	0.40
2:E:36:MET:HE2	2:E:36:MET:HB3	1.93	0.40
1:G:60:GLY:HA2	4:G:701:FAD:H1B	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	629/657 (96%)	610 (97%)	19 (3%)	0	100	100
1	D	629/657 (96%)	611 (97%)	18 (3%)	0	100	100
1	G	629/657 (96%)	611 (97%)	18 (3%)	0	100	100
2	B	255/260 (98%)	251 (98%)	4 (2%)	0	100	100
2	E	255/260 (98%)	252 (99%)	3 (1%)	0	100	100
2	H	255/260 (98%)	251 (98%)	4 (2%)	0	100	100
3	C	237/239 (99%)	235 (99%)	2 (1%)	0	100	100
3	F	237/239 (99%)	233 (98%)	4 (2%)	0	100	100
3	I	237/239 (99%)	234 (99%)	3 (1%)	0	100	100
All	All	3363/3468 (97%)	3288 (98%)	75 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/529 (95%)	502 (100%)	2 (0%)	89	97
1	D	504/529 (95%)	503 (100%)	1 (0%)	92	98
1	G	504/529 (95%)	504 (100%)	0	100	100
2	B	209/212 (99%)	206 (99%)	3 (1%)	62	86
2	E	209/212 (99%)	207 (99%)	2 (1%)	73	91
2	H	209/212 (99%)	209 (100%)	0	100	100
3	C	198/198 (100%)	198 (100%)	0	100	100
3	F	198/198 (100%)	197 (100%)	1 (0%)	86	96
3	I	198/198 (100%)	198 (100%)	0	100	100
All	All	2733/2817 (97%)	2724 (100%)	9 (0%)	90	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ILE
1	A	292	VAL
2	B	73	VAL
2	B	199	VAL
2	B	252	THR
1	D	144	ILE
2	E	88	MET
2	E	199	VAL
3	F	56	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	142	ASN
1	A	171	GLN
1	A	258	ASN
1	A	478	ASN
2	B	125	GLN
2	B	197	GLN
3	C	47	ASN
3	C	63	HIS
1	D	47	ASN

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Mol	Chain	Res	Type
1	D	50	ASN
1	D	197	GLN
1	D	503	ASN
1	D	603	HIS
2	E	125	GLN
3	F	47	ASN
3	F	109	GLN
3	F	164	ASN
1	G	92	HIS
1	G	192	GLN
1	G	197	GLN
1	G	258	ASN
1	G	309	ASN
1	G	403	GLN
1	G	478	ASN
1	G	603	HIS
2	H	125	GLN
3	I	150	GLN
3	I	163	ASN
3	I	170	GLN

5.3.3 RNA [i](#)

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	$\# Z > 2$
10	1L3	F	305	-	23,23,34	3.72	15 (65%)	28,31,45	2.52	8 (28%)
6	FES	H	302	2	0,4,4	-	-	-	-	-
8	HEM	C	301	3	41,50,50	1.32	4 (9%)	45,82,82	1.82	11 (24%)
4	FAD	A	701	-	53,58,58	0.49	0	68,89,89	0.52	2 (2%)
4	FAD	D	701	-	53,58,58	0.48	0	68,89,89	0.52	2 (2%)
6	FES	E	302	2	0,4,4	-	-	-	-	-
10	1L3	C	305	-	23,23,34	3.72	14 (60%)	28,31,45	2.53	8 (28%)
10	1L3	F	304	-	23,23,34	3.74	15 (65%)	28,31,45	2.54	8 (28%)
8	HEM	F	301	3	41,50,50	1.33	5 (12%)	45,82,82	1.86	12 (26%)
10	1L3	I	305	-	23,23,34	3.72	14 (60%)	28,31,45	2.51	8 (28%)
9	LMT	I	303	-	36,36,36	1.16	6 (16%)	47,47,47	1.01	2 (4%)
10	1L3	I	304	-	23,23,34	3.74	14 (60%)	28,31,45	2.49	8 (28%)
8	HEM	C	302	3	41,50,50	1.32	5 (12%)	45,82,82	1.80	8 (17%)
8	HEM	I	301	3	41,50,50	1.40	6 (14%)	45,82,82	1.87	12 (26%)
5	SF4	E	301	2	0,12,12	-	-	-	-	-
9	LMT	C	303	-	35,35,36	1.14	5 (14%)	46,46,47	0.98	3 (6%)
10	1L3	C	304	-	23,23,34	3.74	14 (60%)	28,31,45	2.49	8 (28%)
9	LMT	F	303	-	36,36,36	1.17	6 (16%)	47,47,47	1.03	2 (4%)
5	SF4	B	301	2	0,12,12	-	-	-	-	-
8	HEM	F	302	3	41,50,50	1.31	5 (12%)	45,82,82	1.79	9 (20%)
7	F3S	E	303	2	0,9,9	-	-	-	-	-
5	SF4	H	301	2	0,12,12	-	-	-	-	-
7	F3S	B	303	2	0,9,9	-	-	-	-	-
8	HEM	I	302	3	41,50,50	1.34	5 (12%)	45,82,82	1.88	11 (24%)
7	F3S	H	303	2	0,9,9	-	-	-	-	-
6	FES	B	302	2	0,4,4	-	-	-	-	-
4	FAD	G	701	-	53,58,58	0.48	0	68,89,89	0.51	2 (2%)

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
10	1L3	F	305	-	-	2/10/30/43	0/2/2/2
6	FES	H	302	2	-	-	0/1/1/1
8	HEM	C	301	3	-	6/12/54/54	-
4	FAD	A	701	-	-	9/30/50/50	0/6/6/6
4	FAD	D	701	-	-	10/30/50/50	0/6/6/6
6	FES	E	302	2	-	-	0/1/1/1
10	1L3	F	304	-	-	4/10/30/43	0/2/2/2
8	HEM	F	301	3	-	4/12/54/54	-
10	1L3	I	305	-	-	2/10/30/43	0/2/2/2
9	LMT	I	303	-	-	12/21/61/61	0/2/2/2
10	1L3	I	304	-	-	3/10/30/43	0/2/2/2
8	HEM	C	302	3	-	0/12/54/54	-
8	HEM	I	301	3	-	6/12/54/54	-
5	SF4	E	301	2	-	-	0/6/5/5
9	LMT	C	303	-	-	7/20/60/61	0/2/2/2
10	1L3	C	304	-	-	5/10/30/43	0/2/2/2
7	F3S	H	303	2	-	-	0/3/3/3
9	LMT	F	303	-	-	6/21/61/61	0/2/2/2
5	SF4	B	301	2	-	-	0/6/5/5
8	HEM	F	302	3	-	1/12/54/54	-
7	F3S	E	303	2	-	-	0/3/3/3
5	SF4	H	301	2	-	-	0/6/5/5
8	HEM	I	302	3	-	0/12/54/54	-
7	F3S	B	303	2	-	-	0/3/3/3
10	1L3	C	305	-	-	3/10/30/43	0/2/2/2
6	FES	B	302	2	-	-	0/1/1/1
4	FAD	G	701	-	-	10/30/50/50	0/6/6/6

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	304	1L3	C15-C16	8.83	1.54	1.33
10	I	304	1L3	C15-C16	8.83	1.54	1.33
10	C	304	1L3	C15-C16	8.83	1.54	1.33
10	I	305	1L3	C15-C16	8.79	1.54	1.33
10	F	305	1L3	C15-C16	8.79	1.54	1.33
10	C	305	1L3	C15-C16	8.76	1.54	1.33
10	F	304	1L3	O13-C12	8.48	1.41	1.23
10	C	304	1L3	O13-C12	8.46	1.41	1.23
10	C	305	1L3	O13-C12	8.45	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	305	1L3	O13-C12	8.45	1.41	1.23
10	I	304	1L3	O13-C12	8.45	1.41	1.23
10	F	305	1L3	O13-C12	8.41	1.41	1.23
10	F	304	1L3	O05-C04	8.36	1.40	1.23
10	C	304	1L3	O05-C04	8.36	1.40	1.23
10	C	305	1L3	O05-C04	8.36	1.40	1.23
10	I	304	1L3	O05-C04	8.35	1.40	1.23
10	I	305	1L3	O05-C04	8.35	1.40	1.23
10	F	305	1L3	O05-C04	8.35	1.40	1.23
10	I	304	1L3	C14-C15	3.71	1.56	1.50
10	C	304	1L3	C14-C15	3.71	1.56	1.50
8	I	301	HEM	C1B-NB	-3.67	1.34	1.40
10	C	305	1L3	C14-C15	3.66	1.55	1.50
10	F	304	1L3	C14-C15	3.66	1.55	1.50
10	F	305	1L3	C14-C15	3.62	1.55	1.50
10	I	305	1L3	C14-C15	3.61	1.55	1.50
10	F	304	1L3	C03-C02	3.56	1.41	1.35
10	I	304	1L3	C03-C02	3.54	1.41	1.35
8	I	301	HEM	C4D-ND	-3.52	1.34	1.40
10	C	305	1L3	C03-C02	3.49	1.41	1.35
10	I	305	1L3	C03-C02	3.49	1.41	1.35
10	F	305	1L3	C02-C12	-3.49	1.40	1.48
10	C	304	1L3	C03-C02	3.49	1.41	1.35
8	F	301	HEM	C1B-NB	-3.48	1.34	1.40
10	F	304	1L3	C02-C12	-3.48	1.40	1.48
10	C	305	1L3	C02-C12	-3.45	1.40	1.48
10	I	305	1L3	C02-C12	-3.45	1.40	1.48
10	F	305	1L3	C03-C02	3.44	1.41	1.35
10	I	304	1L3	C02-C12	-3.44	1.40	1.48
8	C	301	HEM	C4D-ND	-3.43	1.34	1.40
10	C	304	1L3	C02-C12	-3.43	1.40	1.48
8	F	301	HEM	C4D-ND	-3.41	1.34	1.40
8	C	302	HEM	C1B-NB	-3.39	1.34	1.40
8	C	301	HEM	C1B-NB	-3.36	1.34	1.40
10	I	304	1L3	C20-C21	3.33	1.54	1.29
10	C	304	1L3	C20-C21	3.33	1.54	1.29
10	F	304	1L3	C20-C21	3.32	1.54	1.29
10	I	305	1L3	C20-C21	3.32	1.54	1.29
10	C	305	1L3	C20-C21	3.32	1.54	1.29
10	F	305	1L3	C20-C21	3.31	1.54	1.29
8	C	302	HEM	C4D-ND	-3.28	1.34	1.40
8	I	302	HEM	C1B-NB	-3.28	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	302	HEM	C4D-ND	-3.28	1.34	1.40
8	F	302	HEM	C1B-NB	-3.27	1.34	1.40
8	F	302	HEM	C4D-ND	-3.18	1.34	1.40
8	F	302	HEM	FE-NB	3.04	2.11	1.96
8	I	302	HEM	FE-NB	2.90	2.11	1.96
8	F	301	HEM	FE-NB	2.88	2.11	1.96
8	C	302	HEM	FE-NB	2.87	2.11	1.96
8	C	301	HEM	FE-NB	2.85	2.11	1.96
10	F	304	1L3	C14-C03	2.74	1.55	1.51
9	C	303	LMT	O3'-C3'	-2.73	1.36	1.43
10	F	305	1L3	C14-C03	2.71	1.55	1.51
10	I	304	1L3	C14-C03	2.71	1.55	1.51
9	F	303	LMT	O3'-C3'	-2.69	1.36	1.43
10	C	304	1L3	C14-C03	2.68	1.55	1.51
8	I	301	HEM	FE-NB	2.67	2.10	1.96
10	I	305	1L3	C14-C03	2.66	1.55	1.51
10	C	305	1L3	C14-C03	2.65	1.55	1.51
9	I	303	LMT	O3'-C3'	-2.64	1.36	1.43
10	F	304	1L3	C03-C04	-2.56	1.40	1.47
10	F	305	1L3	C03-C04	-2.53	1.40	1.47
10	I	305	1L3	C03-C04	-2.53	1.40	1.47
10	I	304	1L3	C03-C04	-2.52	1.40	1.47
10	C	304	1L3	C03-C04	-2.51	1.40	1.47
10	C	305	1L3	C03-C04	-2.51	1.40	1.47
8	I	301	HEM	C1D-ND	-2.51	1.33	1.38
10	F	304	1L3	C22-C21	-2.48	1.39	1.49
10	I	304	1L3	C22-C21	-2.48	1.39	1.49
10	C	305	1L3	C22-C21	-2.47	1.39	1.49
10	C	304	1L3	C22-C21	-2.47	1.39	1.49
10	I	305	1L3	C22-C21	-2.47	1.39	1.49
10	F	305	1L3	C22-C21	-2.47	1.39	1.49
10	F	305	1L3	C10-C11	2.44	1.43	1.39
10	I	304	1L3	C07-C06	2.42	1.43	1.39
10	C	305	1L3	C07-C06	2.42	1.43	1.39
10	I	305	1L3	C07-C06	2.42	1.43	1.39
10	I	304	1L3	C10-C11	2.41	1.43	1.39
10	C	304	1L3	C10-C11	2.40	1.43	1.39
10	I	305	1L3	C10-C11	2.40	1.43	1.39
10	C	304	1L3	C07-C06	2.39	1.43	1.39
10	F	304	1L3	C10-C11	2.39	1.43	1.39
9	I	303	LMT	O3B-C3B	-2.39	1.37	1.43
9	F	303	LMT	O3B-C3B	-2.38	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	304	1L3	C07-C06	2.38	1.43	1.39
9	F	303	LMT	O2B-C2B	-2.37	1.37	1.43
10	C	305	1L3	C10-C11	2.37	1.43	1.39
9	I	303	LMT	O2B-C2B	-2.36	1.37	1.43
9	C	303	LMT	O2B-C2B	-2.35	1.37	1.43
10	F	305	1L3	C07-C06	2.34	1.43	1.39
8	I	301	HEM	C4B-NB	-2.34	1.34	1.38
9	C	303	LMT	O2'-C2'	-2.34	1.37	1.43
9	C	303	LMT	O3B-C3B	-2.33	1.37	1.43
9	F	303	LMT	O2'-C2'	-2.29	1.37	1.43
9	I	303	LMT	O2'-C2'	-2.28	1.37	1.43
8	I	302	HEM	C3B-C4B	2.16	1.49	1.44
9	C	303	LMT	O4'-C4B	-2.15	1.37	1.43
9	F	303	LMT	O4'-C4B	-2.12	1.38	1.43
10	C	304	1L3	C06-C04	-2.11	1.44	1.48
8	C	302	HEM	C3B-C4B	2.11	1.49	1.44
10	F	305	1L3	C06-C04	-2.11	1.44	1.48
10	C	305	1L3	C11-C12	-2.10	1.44	1.48
8	F	302	HEM	CHB-C1B	2.10	1.40	1.35
10	I	305	1L3	C11-C12	-2.09	1.44	1.48
10	F	305	1L3	C11-C12	-2.09	1.44	1.48
8	I	301	HEM	FE-ND	-2.09	1.86	1.96
10	I	305	1L3	C06-C04	-2.07	1.44	1.48
10	I	304	1L3	C06-C04	-2.07	1.44	1.48
9	I	303	LMT	O4'-C4B	-2.06	1.38	1.43
10	F	304	1L3	C11-C12	-2.06	1.44	1.48
9	F	303	LMT	O1'-C1'	-2.05	1.36	1.40
10	F	305	1L3	C01-C02	2.04	1.55	1.50
8	F	301	HEM	C1D-ND	-2.04	1.34	1.38
10	F	304	1L3	C06-C04	-2.04	1.44	1.48
8	C	302	HEM	CHB-C1B	2.03	1.40	1.35
10	C	304	1L3	C11-C12	-2.03	1.44	1.48
8	F	302	HEM	C3B-C4B	2.02	1.48	1.44
8	I	302	HEM	CHB-C1B	2.02	1.40	1.35
10	I	304	1L3	C11-C12	-2.01	1.44	1.48
9	I	303	LMT	O1'-C1'	-2.01	1.36	1.40
10	F	304	1L3	C01-C02	2.01	1.55	1.50
8	C	301	HEM	C1D-ND	-2.01	1.34	1.38
8	F	301	HEM	CHB-C1B	2.01	1.40	1.35
10	C	305	1L3	C06-C04	-2.00	1.44	1.48

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	304	1L3	C14-C15-C16	-8.77	112.19	126.79
10	I	304	1L3	C14-C15-C16	-8.46	112.71	126.79
10	C	304	1L3	C14-C15-C16	-8.45	112.72	126.79
10	F	305	1L3	C14-C15-C16	-8.38	112.83	126.79
10	C	305	1L3	C14-C15-C16	-8.34	112.90	126.79
10	I	305	1L3	C14-C15-C16	-8.32	112.94	126.79
10	C	305	1L3	C18-C16-C15	-6.02	108.93	121.12
10	F	305	1L3	C18-C16-C15	-5.90	109.18	121.12
10	I	305	1L3	C18-C16-C15	-5.89	109.19	121.12
10	C	304	1L3	C18-C16-C15	-5.55	109.88	121.12
10	F	304	1L3	C18-C16-C15	-5.55	109.90	121.12
10	I	304	1L3	C18-C16-C15	-5.50	110.00	121.12
10	C	305	1L3	C17-C16-C15	-5.36	109.94	123.68
10	F	304	1L3	C17-C16-C15	-5.32	110.02	123.68
10	I	304	1L3	C17-C16-C15	-5.29	110.10	123.68
10	F	305	1L3	C17-C16-C15	-5.23	110.27	123.68
10	I	305	1L3	C17-C16-C15	-5.21	110.32	123.68
10	C	304	1L3	C17-C16-C15	-5.20	110.35	123.68
8	C	301	HEM	CHC-C4B-NB	5.06	129.93	124.43
8	F	301	HEM	CHC-C4B-NB	5.05	129.92	124.43
8	I	301	HEM	CHC-C4B-NB	4.70	129.54	124.43
8	I	302	HEM	CHD-C1D-ND	4.46	129.27	124.43
8	F	302	HEM	CHD-C1D-ND	4.44	129.26	124.43
8	C	302	HEM	CHD-C1D-ND	4.31	129.12	124.43
8	C	302	HEM	CHC-C4B-NB	4.29	129.09	124.43
8	F	302	HEM	CHC-C4B-NB	4.26	129.06	124.43
8	C	301	HEM	CHD-C1D-ND	4.11	128.90	124.43
8	F	301	HEM	CHD-C1D-ND	4.08	128.86	124.43
8	I	302	HEM	CHC-C4B-NB	4.08	128.86	124.43
8	I	302	HEM	CHA-C4D-ND	3.98	129.29	124.38
8	C	302	HEM	CHA-C4D-ND	3.95	129.26	124.38
8	I	301	HEM	CHD-C1D-ND	3.92	128.69	124.43
8	C	302	HEM	C1B-NB-C4B	3.86	109.06	105.07
8	I	302	HEM	C1B-NB-C4B	3.85	109.05	105.07
8	F	302	HEM	C1B-NB-C4B	3.83	109.03	105.07
8	I	302	HEM	CHB-C1B-NB	3.82	129.10	124.38
10	C	304	1L3	C17-C16-C18	-3.79	108.90	115.27
8	I	301	HEM	CHB-C1B-NB	3.77	129.04	124.38
8	F	301	HEM	CHA-C4D-ND	3.71	128.97	124.38
10	I	304	1L3	C17-C16-C18	-3.69	109.07	115.27
8	I	301	HEM	C1B-NB-C4B	3.68	108.87	105.07
10	F	304	1L3	C17-C16-C18	-3.67	109.09	115.27
8	C	301	HEM	C1B-NB-C4B	3.66	108.85	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	301	HEM	CHA-C4D-ND	3.62	128.85	124.38
8	F	301	HEM	C1B-NB-C4B	3.57	108.76	105.07
10	I	305	1L3	C17-C16-C18	-3.57	109.27	115.27
8	F	301	HEM	CHB-C1B-NB	3.56	128.78	124.38
10	F	305	1L3	C17-C16-C18	-3.56	109.29	115.27
10	C	305	1L3	C17-C16-C18	-3.50	109.38	115.27
8	F	302	HEM	CHA-C4D-ND	3.50	128.71	124.38
8	I	302	HEM	CBA-CAA-C2A	-3.49	106.67	112.62
8	C	301	HEM	CHB-C1B-NB	3.48	128.69	124.38
8	C	302	HEM	CHB-C1B-NB	3.43	128.62	124.38
8	C	301	HEM	CHA-C4D-ND	3.38	128.55	124.38
8	F	302	HEM	CHB-C1B-NB	3.32	128.48	124.38
8	I	301	HEM	CAD-CBD-CGD	-3.30	106.50	113.60
10	F	304	1L3	C22-C21-C20	2.89	150.23	126.37
10	C	304	1L3	C22-C21-C20	2.89	150.20	126.37
8	I	301	HEM	CHD-C1D-C2D	-2.88	120.47	124.98
9	I	303	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
10	I	305	1L3	C22-C21-C20	2.86	149.95	126.37
10	I	304	1L3	C22-C21-C20	2.86	149.95	126.37
10	C	305	1L3	C22-C21-C20	2.85	149.93	126.37
10	F	305	1L3	C22-C21-C20	2.85	149.90	126.37
9	F	303	LMT	C1'-O5'-C5'	-2.83	108.13	113.69
8	C	301	HEM	CHD-C1D-C2D	-2.75	120.69	124.98
8	F	302	HEM	CHD-C1D-C2D	-2.73	120.71	124.98
8	F	301	HEM	CAD-CBD-CGD	-2.67	107.86	113.60
10	I	305	1L3	C01-C02-C03	-2.65	120.08	124.40
8	I	302	HEM	CAD-CBD-CGD	-2.65	107.91	113.60
10	F	305	1L3	C01-C02-C03	-2.60	120.16	124.40
8	I	302	HEM	CHD-C1D-C2D	-2.59	120.93	124.98
8	I	302	HEM	CHA-C4D-C3D	-2.58	120.48	125.33
4	D	701	FAD	P-O3P-PA	-2.56	124.03	132.83
8	C	302	HEM	CHD-C1D-C2D	-2.56	120.98	124.98
8	I	301	HEM	CAA-CBA-CGA	-2.56	106.59	113.76
4	A	701	FAD	P-O3P-PA	-2.55	124.08	132.83
8	C	301	HEM	CAD-CBD-CGD	-2.53	108.16	113.60
8	F	301	HEM	CHD-C1D-C2D	-2.52	121.04	124.98
8	F	301	HEM	CHA-C4D-C3D	-2.52	120.59	125.33
8	F	301	HEM	CBA-CAA-C2A	-2.51	108.33	112.62
10	C	305	1L3	C01-C02-C03	-2.51	120.31	124.40
10	F	304	1L3	C01-C02-C03	-2.50	120.32	124.40
9	F	303	LMT	C3'-C4'-C5'	-2.49	105.22	110.93
10	C	304	1L3	C01-C02-C03	-2.47	120.37	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	304	1L3	C01-C02-C03	-2.46	120.39	124.40
9	I	303	LMT	C3'-C4'-C5'	-2.45	105.30	110.93
8	F	301	HEM	CMC-C2C-C3C	2.43	129.22	124.68
4	G	701	FAD	P-O3P-PA	-2.41	124.56	132.83
8	C	302	HEM	C4D-ND-C1D	2.41	107.56	105.07
10	C	305	1L3	C19-C20-C21	-2.37	112.21	131.07
10	I	305	1L3	C19-C20-C21	-2.37	112.21	131.07
8	C	302	HEM	CHA-C4D-C3D	-2.37	120.89	125.33
10	F	305	1L3	C19-C20-C21	-2.36	112.33	131.07
10	C	304	1L3	C19-C20-C21	-2.32	112.62	131.07
8	F	302	HEM	CHA-C4D-C3D	-2.32	120.98	125.33
10	I	304	1L3	C19-C20-C21	-2.31	112.68	131.07
10	F	304	1L3	C19-C20-C21	-2.31	112.71	131.07
8	C	301	HEM	CHA-C4D-C3D	-2.29	121.02	125.33
9	C	303	LMT	O5'-C5'-C6'	2.28	112.11	106.44
4	A	701	FAD	C5A-C6A-N6A	2.27	123.81	120.35
4	G	701	FAD	C5A-C6A-N6A	2.27	123.80	120.35
8	I	301	HEM	CHA-C4D-C3D	-2.26	121.09	125.33
4	D	701	FAD	C5A-C6A-N6A	2.26	123.78	120.35
8	F	302	HEM	CMC-C2C-C3C	2.26	128.90	124.68
8	I	302	HEM	C4D-ND-C1D	2.23	107.38	105.07
10	I	305	1L3	C01-C02-C12	2.21	119.94	116.27
8	I	302	HEM	CHB-C1B-C2B	-2.20	120.65	126.72
8	I	301	HEM	CHB-C1B-C2B	-2.19	120.66	126.72
8	C	301	HEM	CMC-C2C-C3C	2.17	128.73	124.68
9	C	303	LMT	O5'-C5'-C4'	2.16	114.31	109.75
10	F	305	1L3	C01-C02-C12	2.16	119.85	116.27
8	C	301	HEM	CBA-CAA-C2A	-2.13	108.98	112.62
8	F	301	HEM	C4D-ND-C1D	2.13	107.27	105.07
8	F	301	HEM	CHB-C1B-C2B	-2.12	120.86	126.72
10	C	305	1L3	C01-C02-C12	2.10	119.76	116.27
9	C	303	LMT	O1'-C1'-C2'	2.08	111.55	108.30
8	F	302	HEM	C4B-C3B-C2B	-2.07	105.47	107.11
10	F	304	1L3	C01-C02-C12	2.05	119.67	116.27
8	C	301	HEM	CHB-C1B-C2B	-2.05	121.06	126.72
8	I	301	HEM	O2D-CGD-CBD	2.03	120.55	114.03
8	I	301	HEM	C4D-ND-C1D	2.01	107.15	105.07
10	I	304	1L3	C01-C02-C12	2.00	119.59	116.27
10	C	304	1L3	C01-C02-C12	2.00	119.59	116.27

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	FAD	O4B-C4B-C5B-O5B
4	A	701	FAD	C3B-C4B-C5B-O5B
4	A	701	FAD	C1'-C2'-C3'-C4'
4	D	701	FAD	C5B-O5B-PA-O1A
4	D	701	FAD	C2'-C3'-C4'-O4'
4	D	701	FAD	C2'-C3'-C4'-C5'
4	D	701	FAD	O3'-C3'-C4'-O4'
4	D	701	FAD	O3'-C3'-C4'-C5'
4	G	701	FAD	O4B-C4B-C5B-O5B
4	G	701	FAD	C3B-C4B-C5B-O5B
4	G	701	FAD	O3'-C3'-C4'-C5'
8	C	301	HEM	C2B-C3B-CAB-CBB
8	C	301	HEM	C4B-C3B-CAB-CBB
8	F	301	HEM	C2B-C3B-CAB-CBB
8	F	301	HEM	C4B-C3B-CAB-CBB
8	I	301	HEM	C2B-C3B-CAB-CBB
10	C	305	1L3	C14-C15-C16-C17
10	F	304	1L3	C14-C15-C16-C17
10	F	305	1L3	C14-C15-C16-C17
10	I	304	1L3	C14-C15-C16-C17
10	I	304	1L3	C16-C18-C19-C20
10	I	305	1L3	C14-C15-C16-C17
9	F	303	LMT	O5B-C5B-C6B-O6B
9	I	303	LMT	O5B-C5B-C6B-O6B
9	F	303	LMT	O5'-C5'-C6'-O6'
9	I	303	LMT	O5'-C5'-C6'-O6'
9	F	303	LMT	C4B-C5B-C6B-O6B
9	F	303	LMT	C4'-C5'-C6'-O6'
9	I	303	LMT	C4B-C5B-C6B-O6B
4	G	701	FAD	O3'-C3'-C4'-O4'
4	D	701	FAD	C3B-C4B-C5B-O5B
4	G	701	FAD	C2'-C3'-C4'-O4'
10	C	304	1L3	C15-C16-C18-C19
10	C	305	1L3	C15-C16-C18-C19
10	F	304	1L3	C15-C16-C18-C19
10	I	304	1L3	C15-C16-C18-C19
9	I	303	LMT	C4'-C5'-C6'-O6'
10	C	304	1L3	C16-C18-C19-C20
10	F	304	1L3	C16-C18-C19-C20
10	C	304	1L3	C14-C15-C16-C18
8	I	301	HEM	C4D-C3D-CAD-CBD
8	I	301	HEM	C2D-C3D-CAD-CBD
10	C	305	1L3	C16-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
4	G	701	FAD	C2'-C3'-C4'-C5'
8	C	301	HEM	C2D-C3D-CAD-CBD
8	C	301	HEM	C4D-C3D-CAD-CBD
9	C	303	LMT	O5B-C1B-O1B-C4'
9	I	303	LMT	C2-C1-O1'-C1'
9	I	303	LMT	O1'-C1-C2-C3
10	C	304	1L3	C14-C15-C16-C17
9	C	303	LMT	C1-C2-C3-C4
8	I	301	HEM	C4B-C3B-CAB-CBB
9	I	303	LMT	C5-C6-C7-C8
4	D	701	FAD	O4B-C4B-C5B-O5B
9	I	303	LMT	C11-C10-C9-C8
9	I	303	LMT	C3-C4-C5-C6
4	A	701	FAD	O2'-C2'-C3'-O3'
9	F	303	LMT	C1-C2-C3-C4
9	C	303	LMT	C3-C4-C5-C6
4	G	701	FAD	C4'-C5'-O5'-P
4	G	701	FAD	P-O3P-PA-O5B
4	A	701	FAD	O2'-C2'-C3'-C4'
8	F	302	HEM	C4B-C3B-CAB-CBB
4	D	701	FAD	C5'-O5'-P-O3P
4	A	701	FAD	PA-O3P-P-O2P
9	I	303	LMT	C1-C2-C3-C4
4	A	701	FAD	C1'-C2'-C3'-O3'
9	C	303	LMT	C5-C6-C7-C8
10	I	305	1L3	C17-C16-C18-C19
10	F	305	1L3	C17-C16-C18-C19
4	G	701	FAD	PA-O3P-P-O2P
8	F	301	HEM	CAA-CBA-CGA-O1A
8	I	301	HEM	CAA-CBA-CGA-O1A
8	C	301	HEM	CAA-CBA-CGA-O1A
9	C	303	LMT	O5'-C5'-C6'-O6'
8	I	301	HEM	CAA-CBA-CGA-O2A
8	F	301	HEM	CAA-CBA-CGA-O2A
8	C	301	HEM	CAA-CBA-CGA-O2A
10	F	304	1L3	C18-C19-C20-C21
10	C	304	1L3	C18-C19-C20-C21
9	C	303	LMT	C7-C8-C9-C10
4	A	701	FAD	PA-O3P-P-O1P
4	G	701	FAD	PA-O3P-P-O1P
9	C	303	LMT	C2-C3-C4-C5
4	A	701	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
4	D	701	FAD	C5'-O5'-P-O1P
9	I	303	LMT	O5'-C1'-O1'-C1
9	I	303	LMT	C4-C5-C6-C7
4	D	701	FAD	C4'-C5'-O5'-P
9	F	303	LMT	C5'-C4'-O1B-C1B

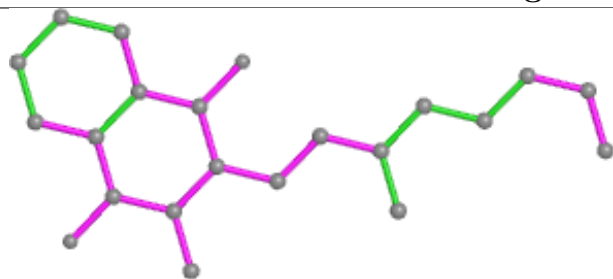
There are no ring outliers.

16 monomers are involved in 42 short contacts:

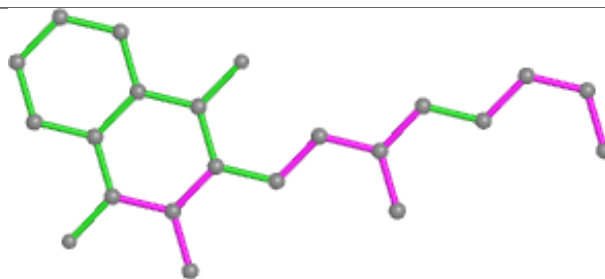
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	305	1L3	1	0
8	C	301	HEM	5	0
4	A	701	FAD	3	0
4	D	701	FAD	2	0
8	F	301	HEM	7	0
9	I	303	LMT	2	0
8	C	302	HEM	1	0
8	I	301	HEM	4	0
9	C	303	LMT	1	0
9	F	303	LMT	1	0
8	F	302	HEM	5	0
7	E	303	F3S	1	0
7	B	303	F3S	4	0
8	I	302	HEM	3	0
7	H	303	F3S	1	0
4	G	701	FAD	3	0

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.

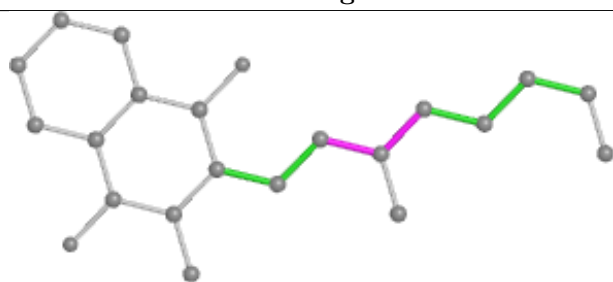
Ligand 1L3 F 305



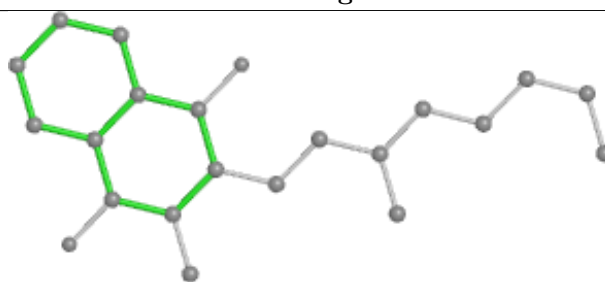
Bond lengths



Bond angles

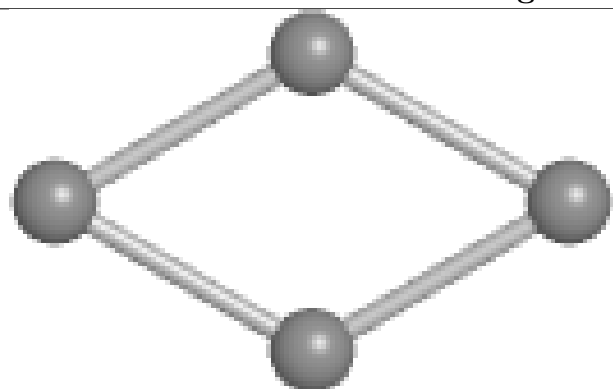


Torsions

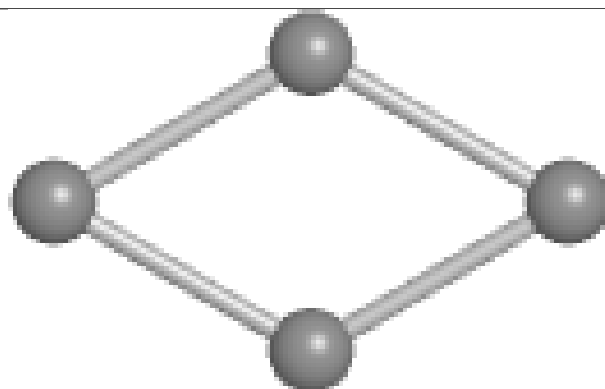


Rings

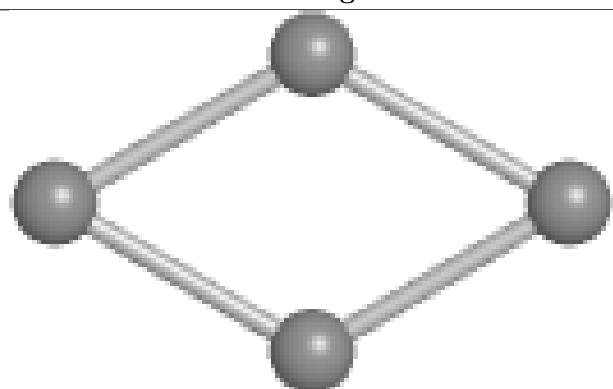
Ligand FES H 302



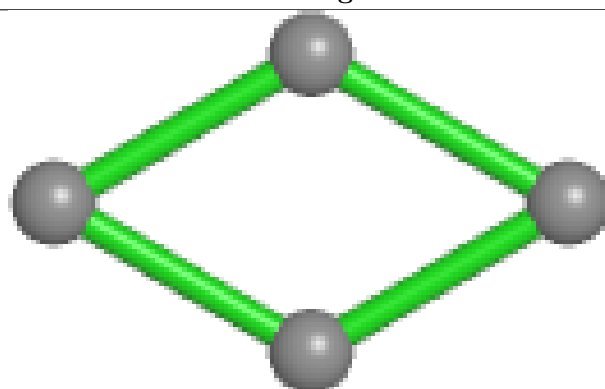
Bond lengths



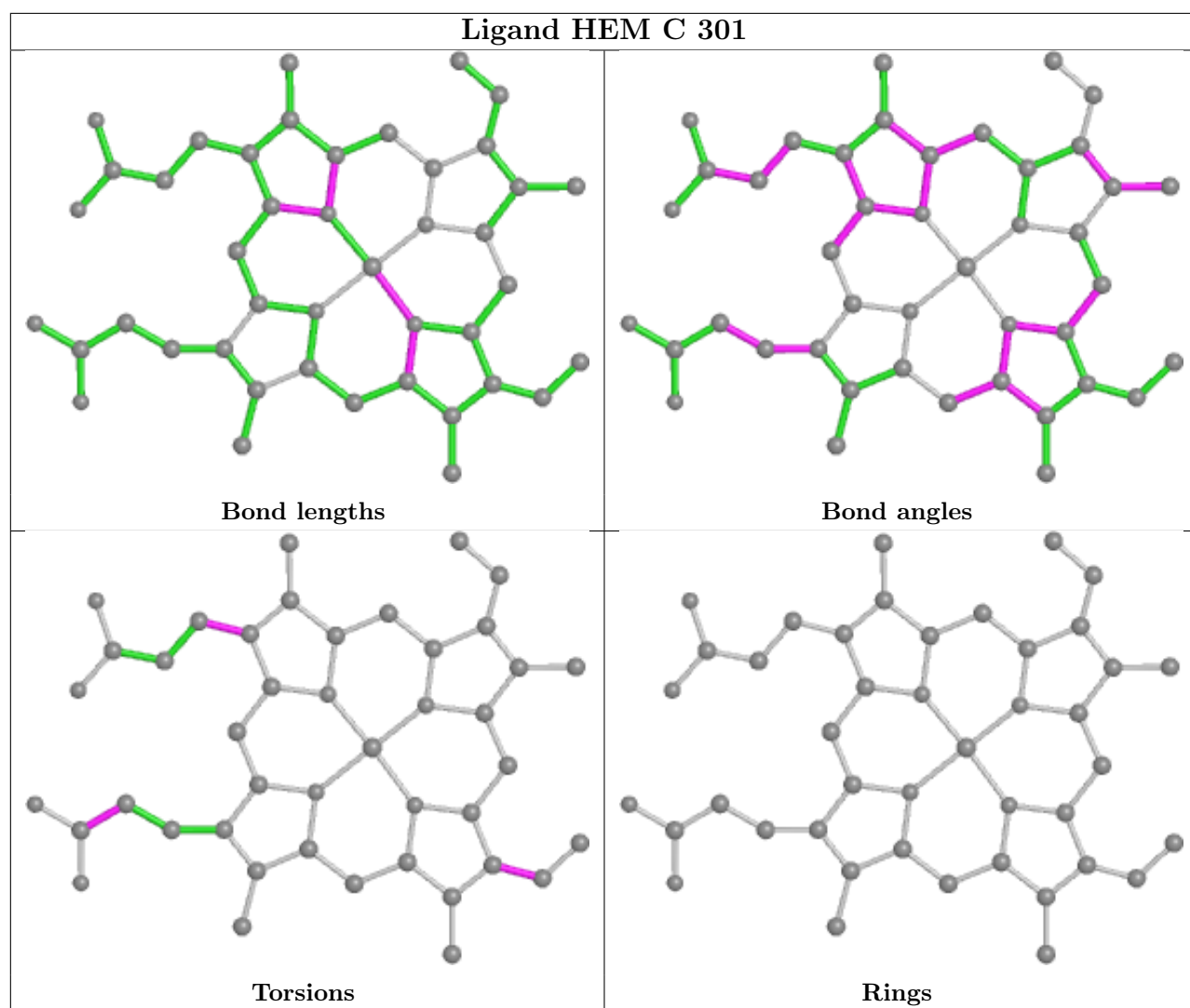
Bond angles

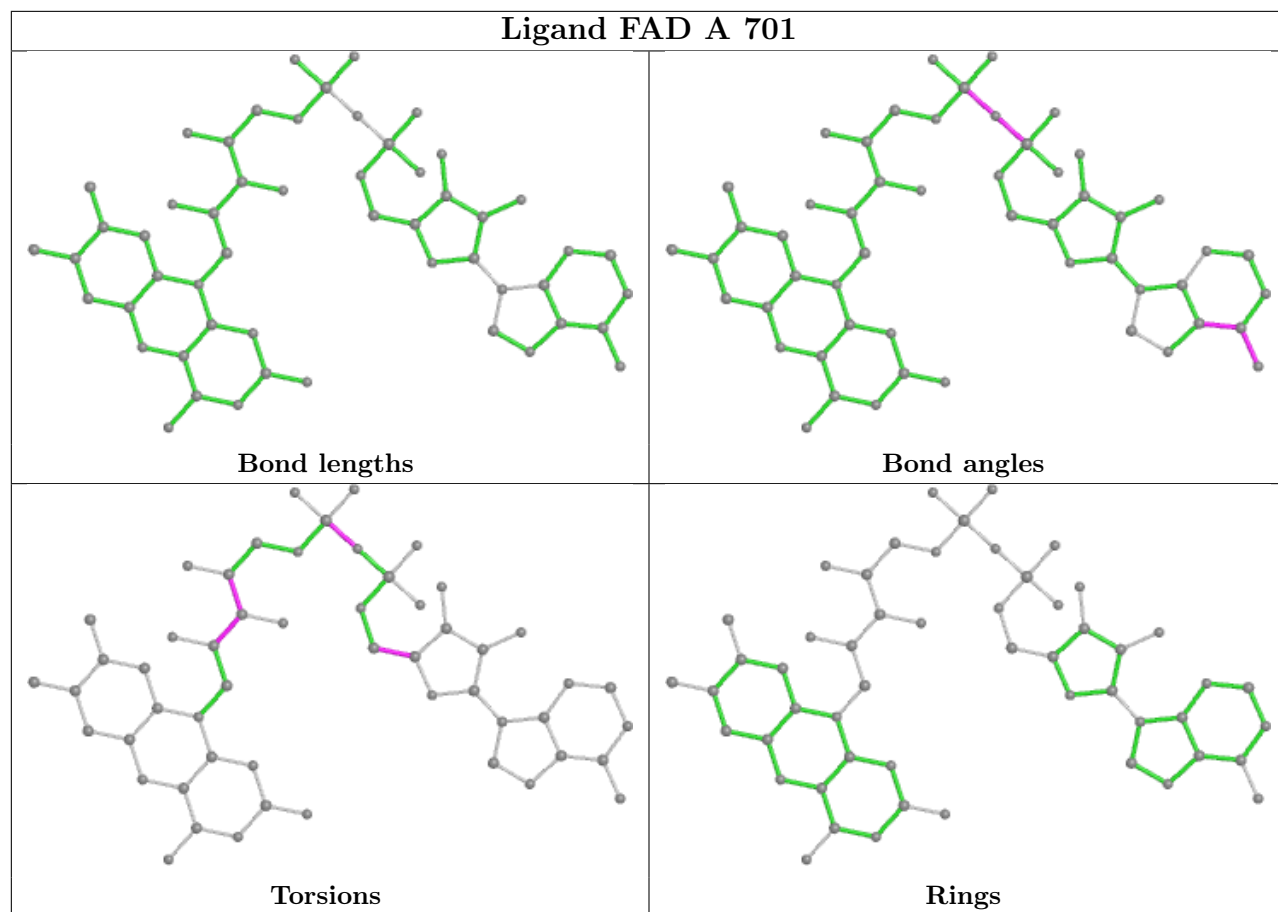


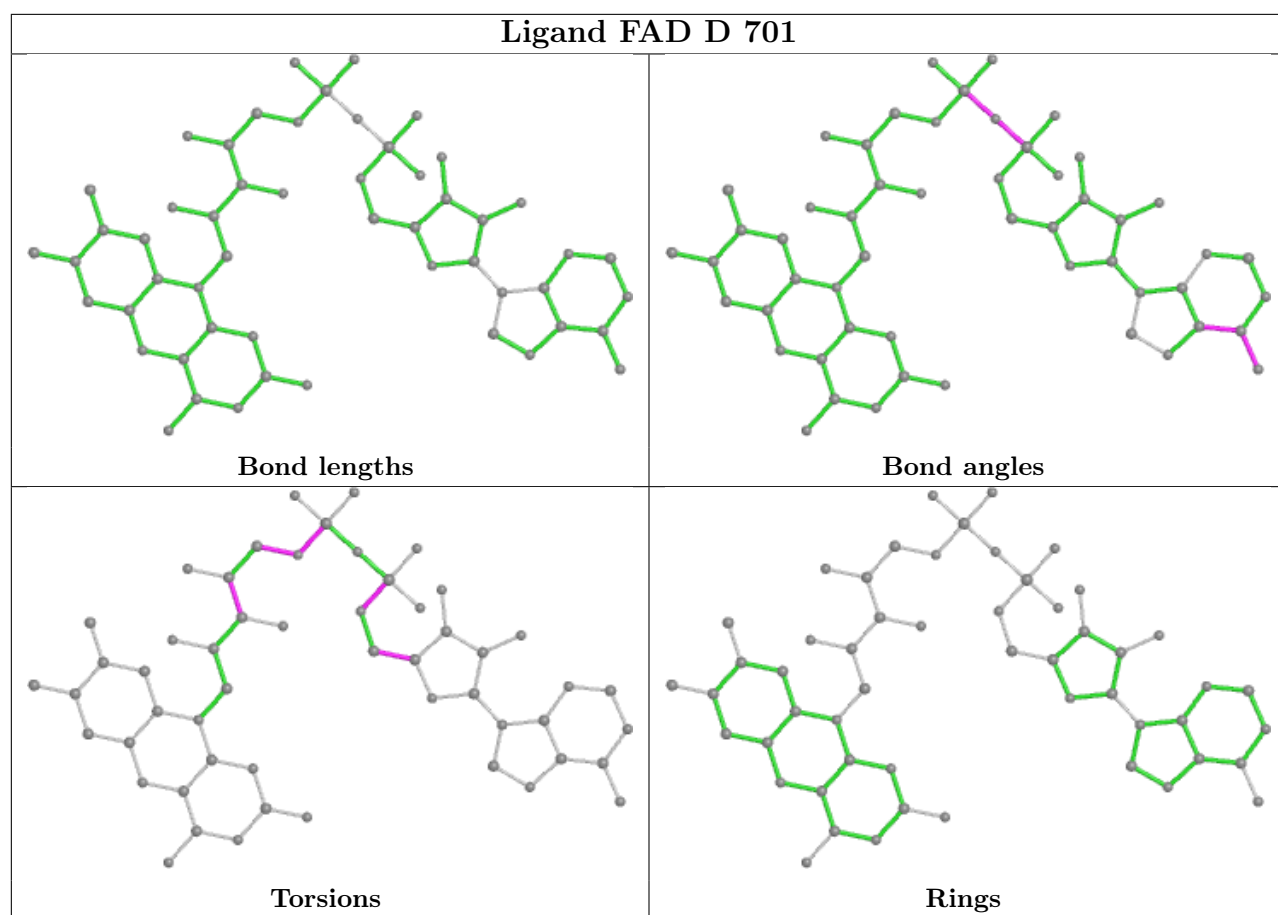
Torsions

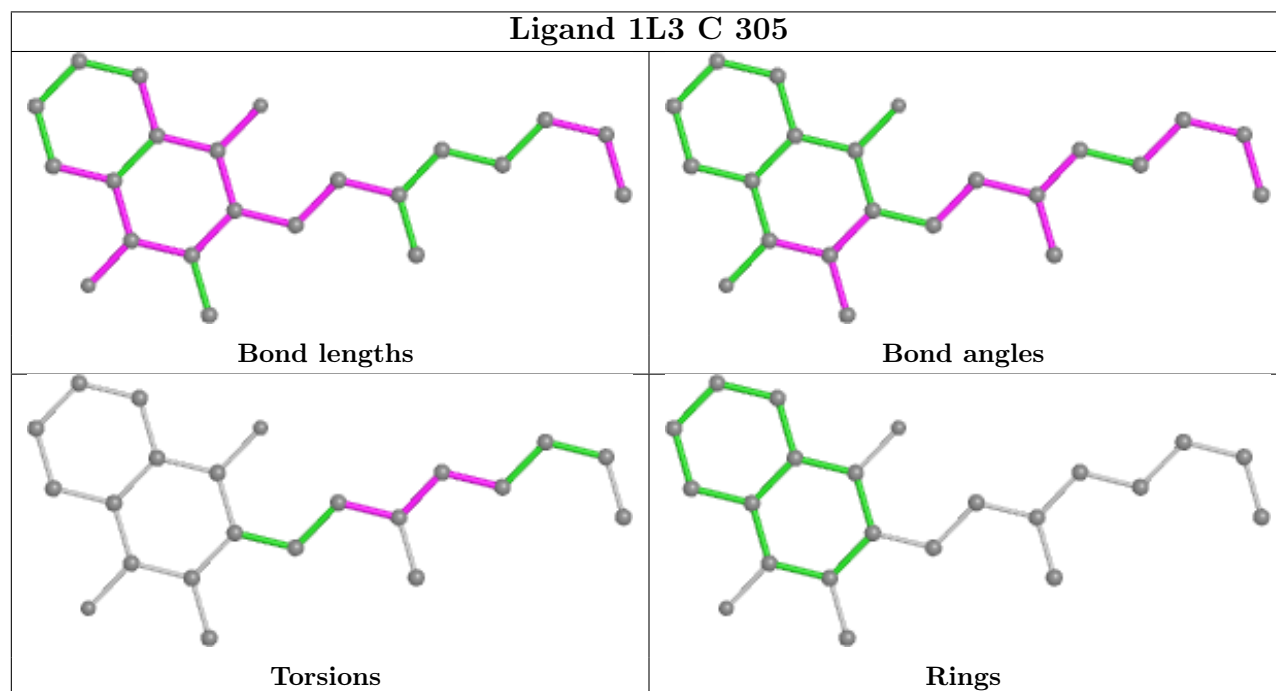
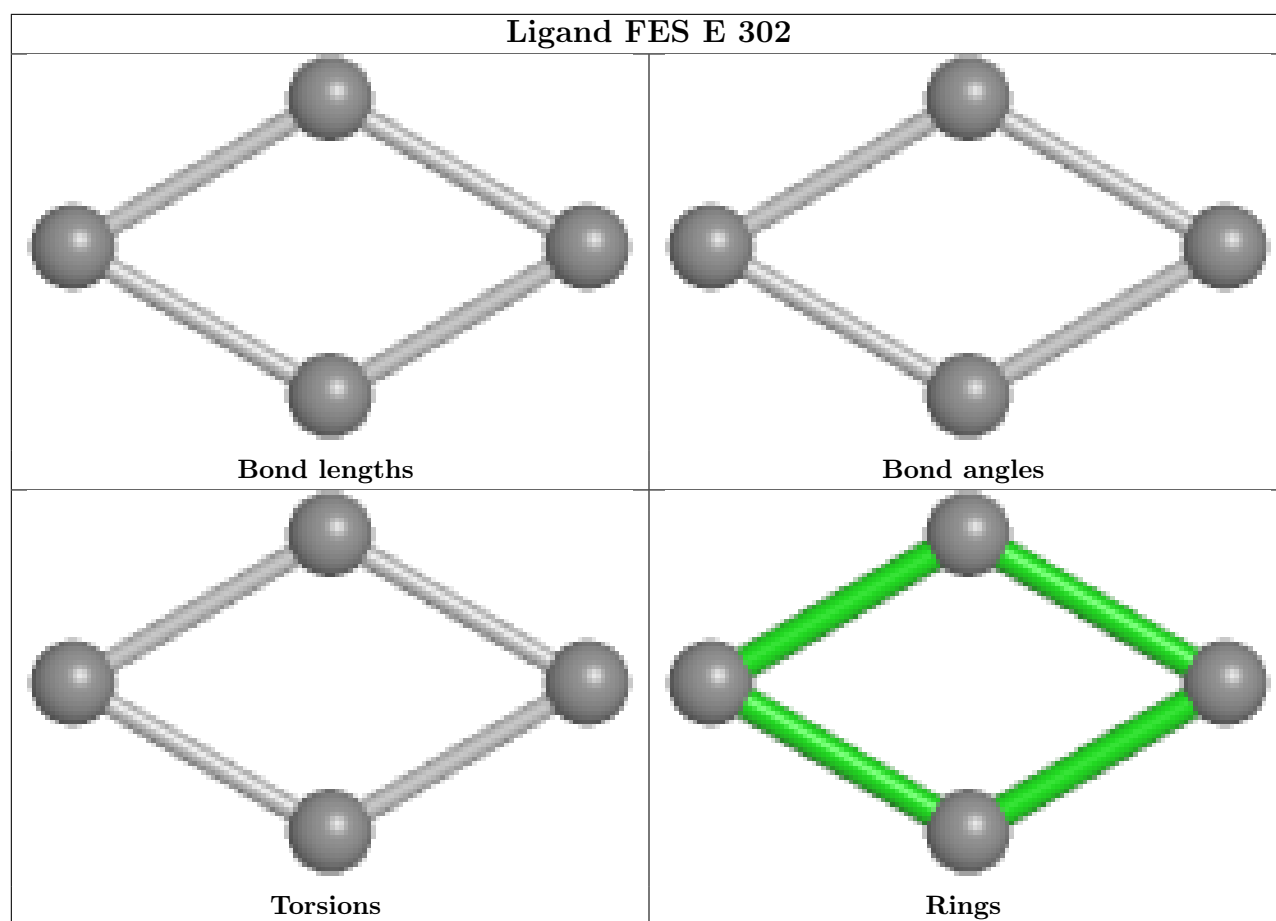


Rings

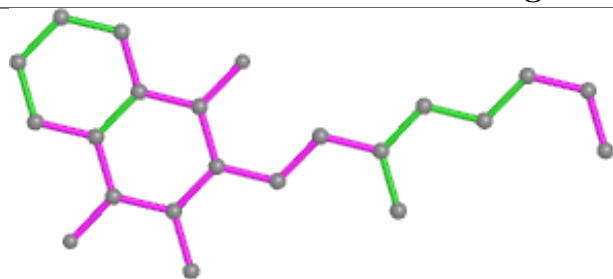




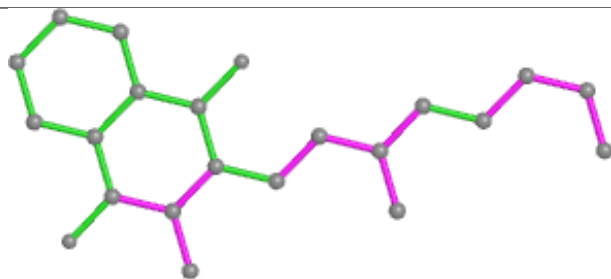




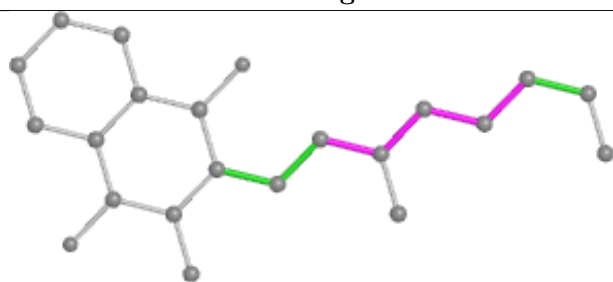
Ligand 1L3 F 304



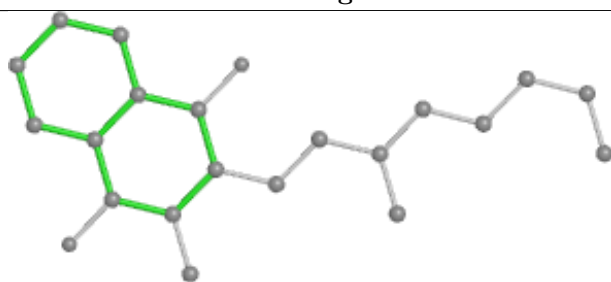
Bond lengths



Bond angles

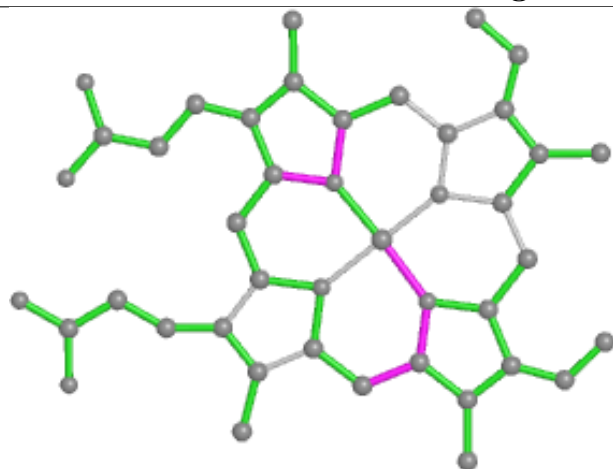


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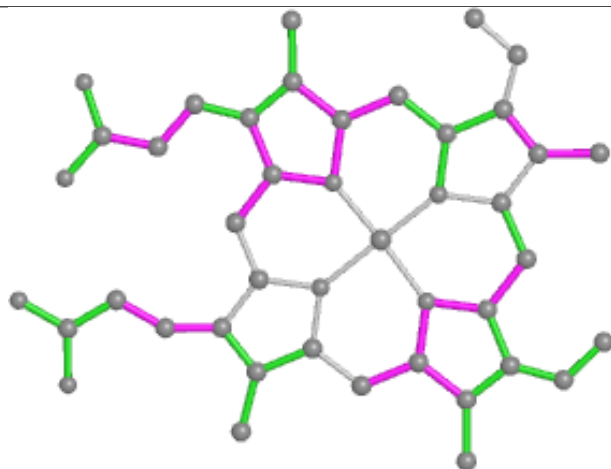


Rings

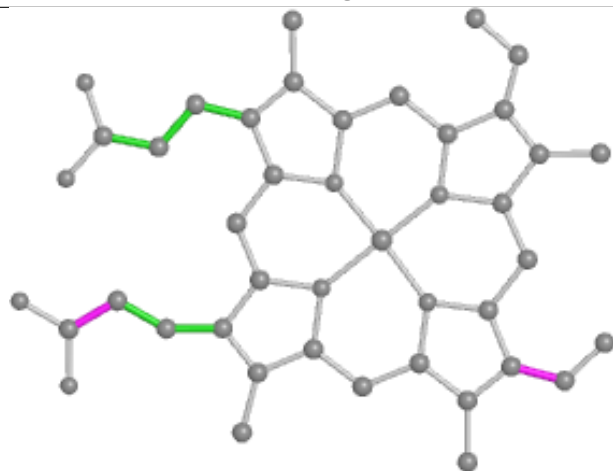
Ligand HEM F 301



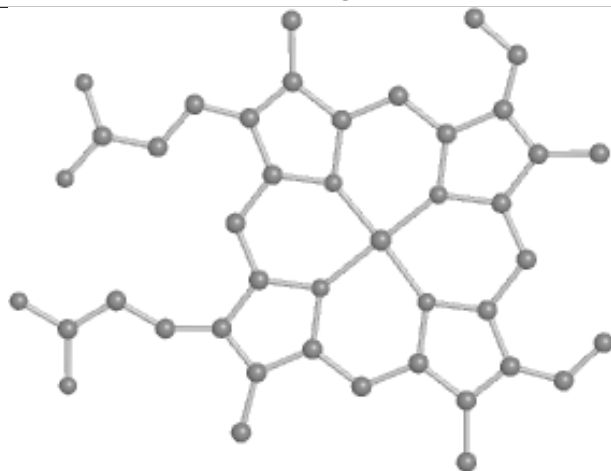
Bond lengths



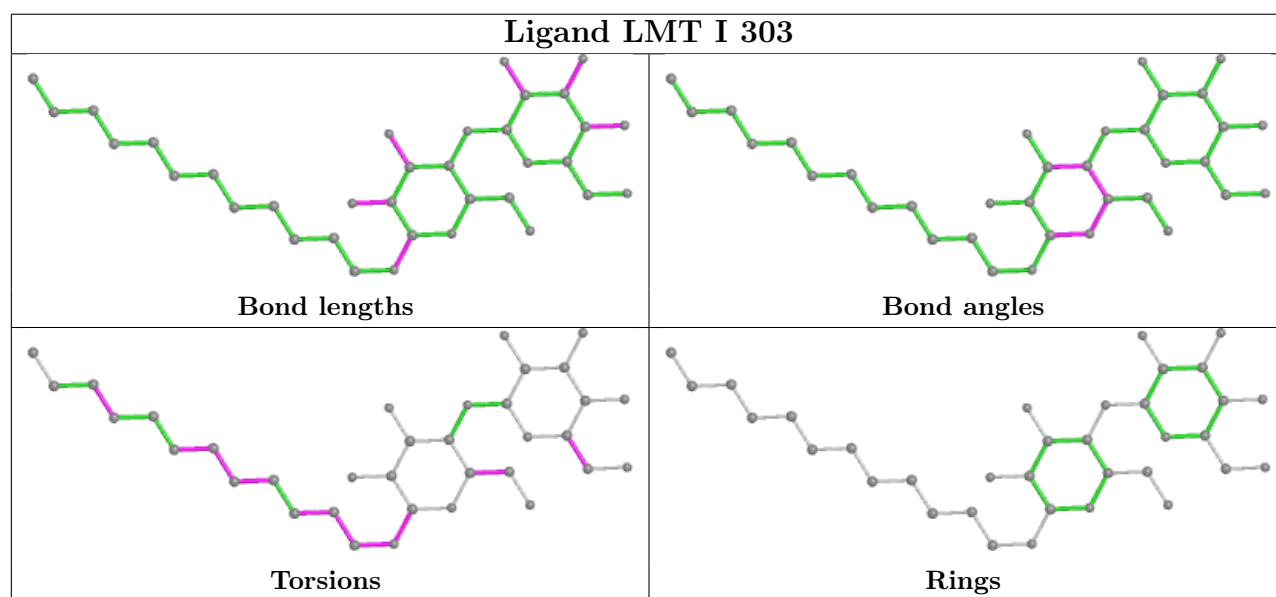
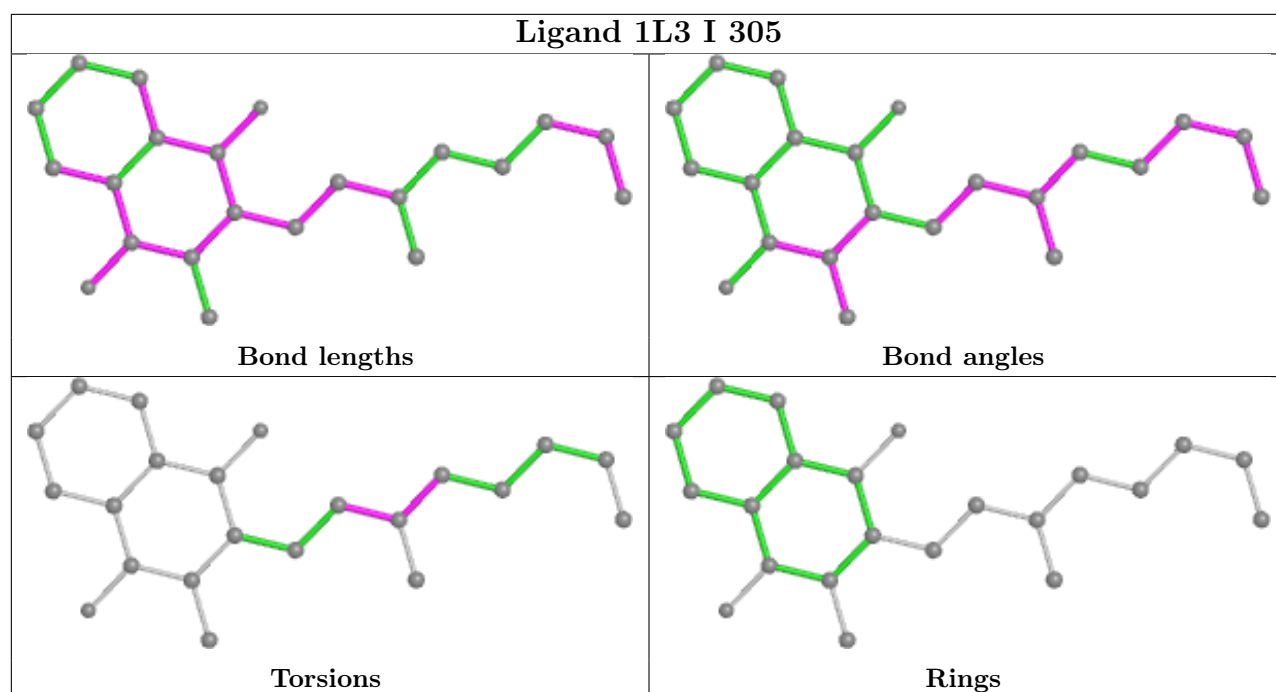
Bond angles



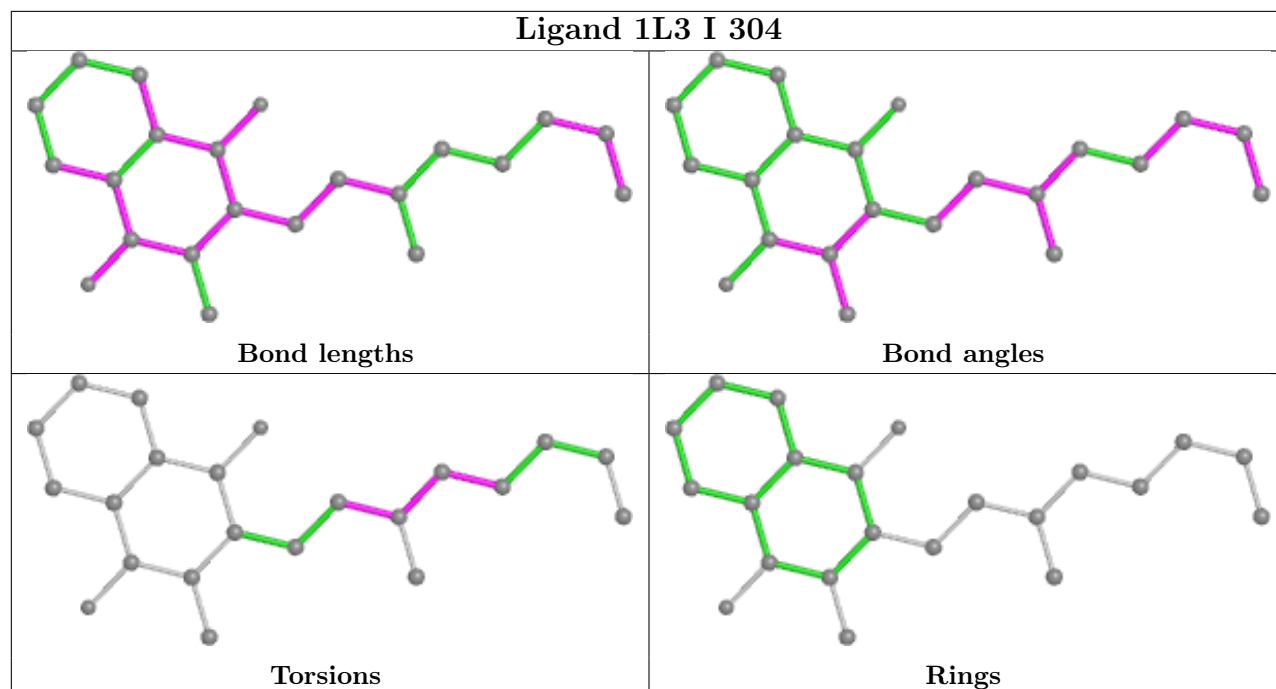
Torsions



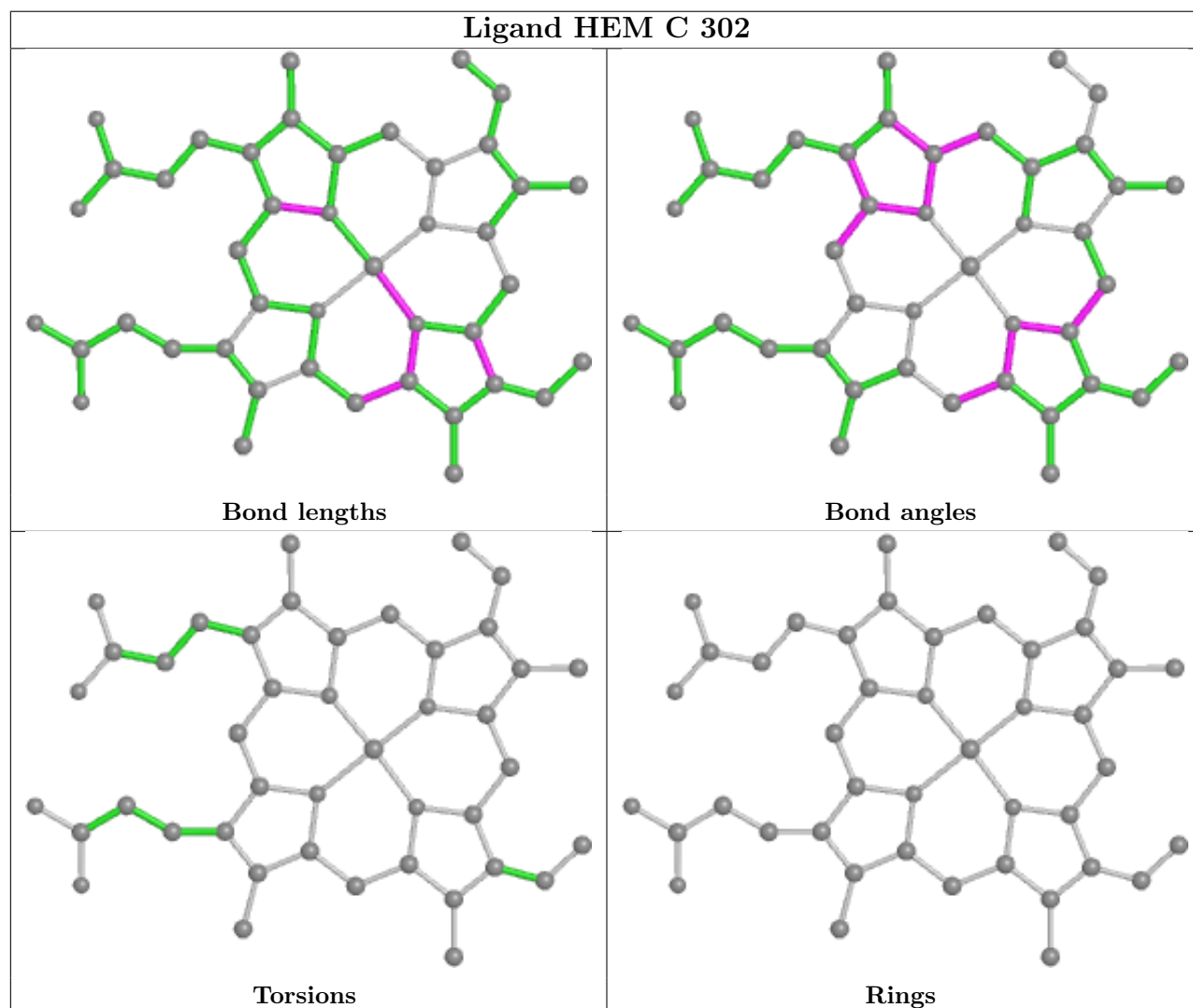
Rings

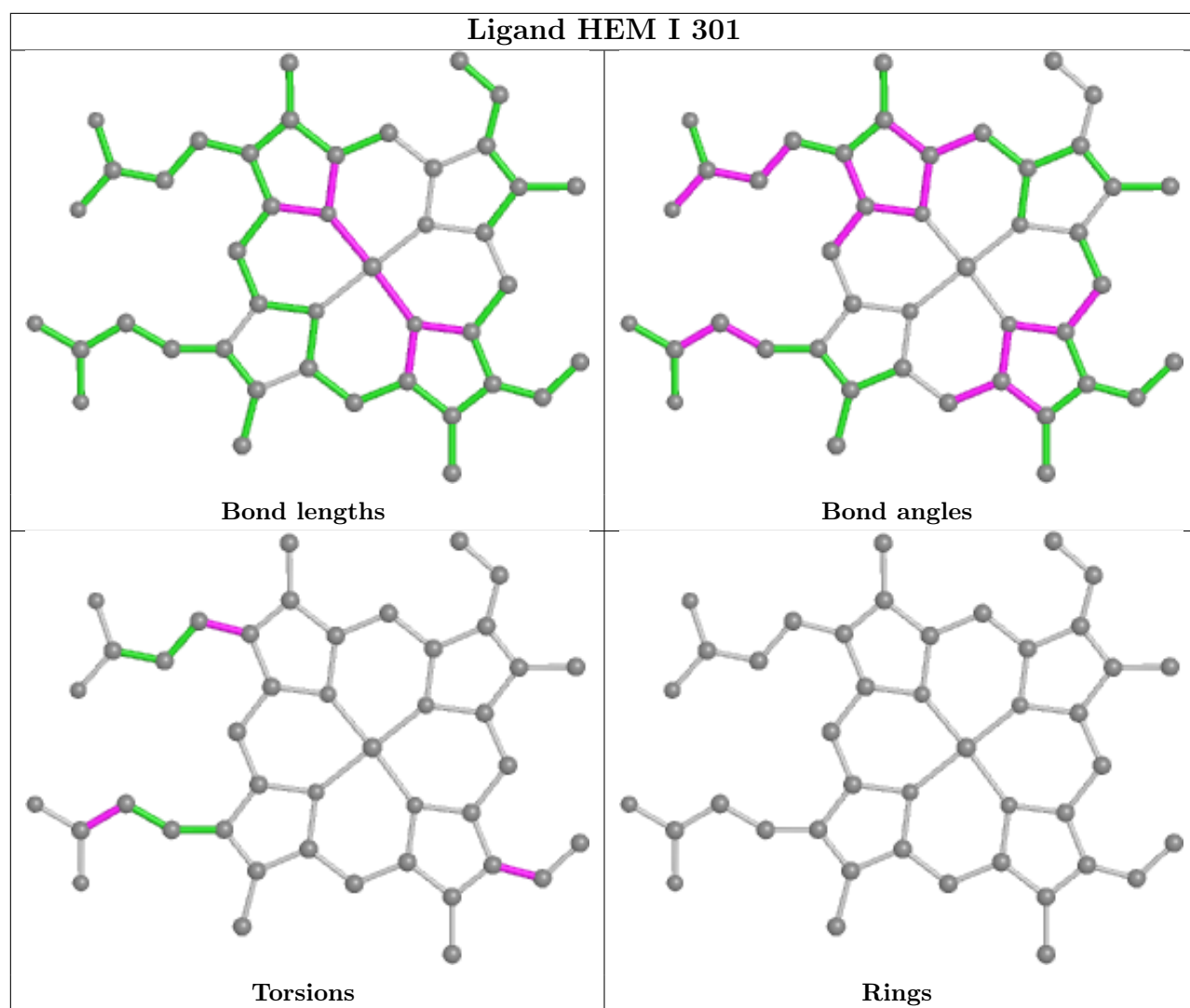


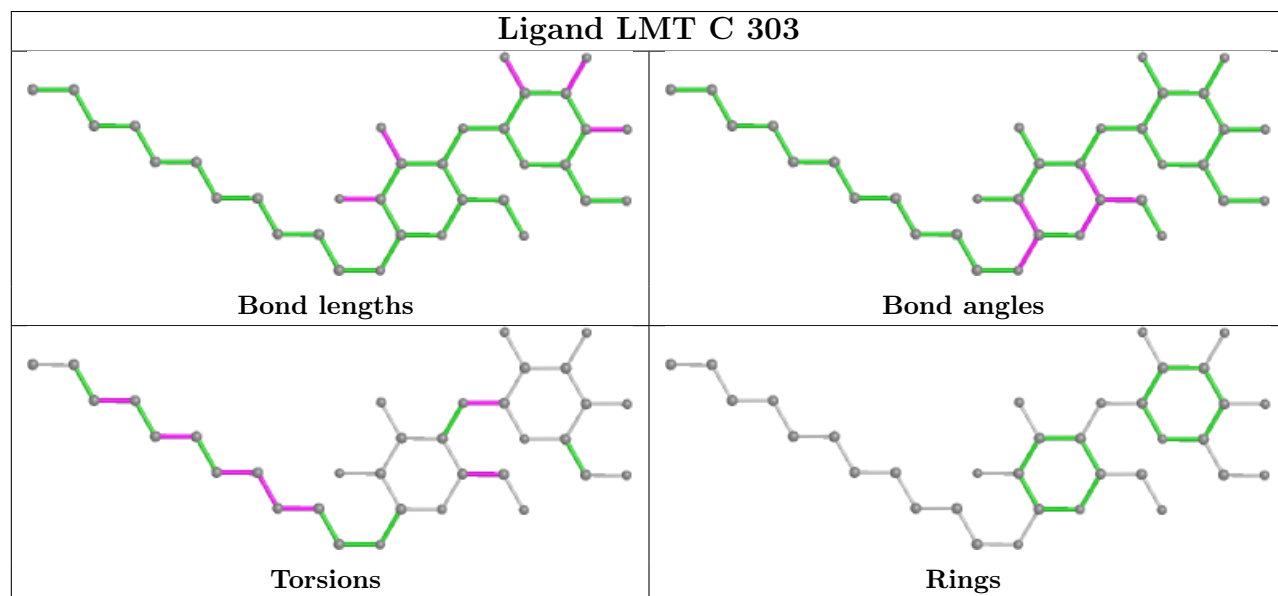
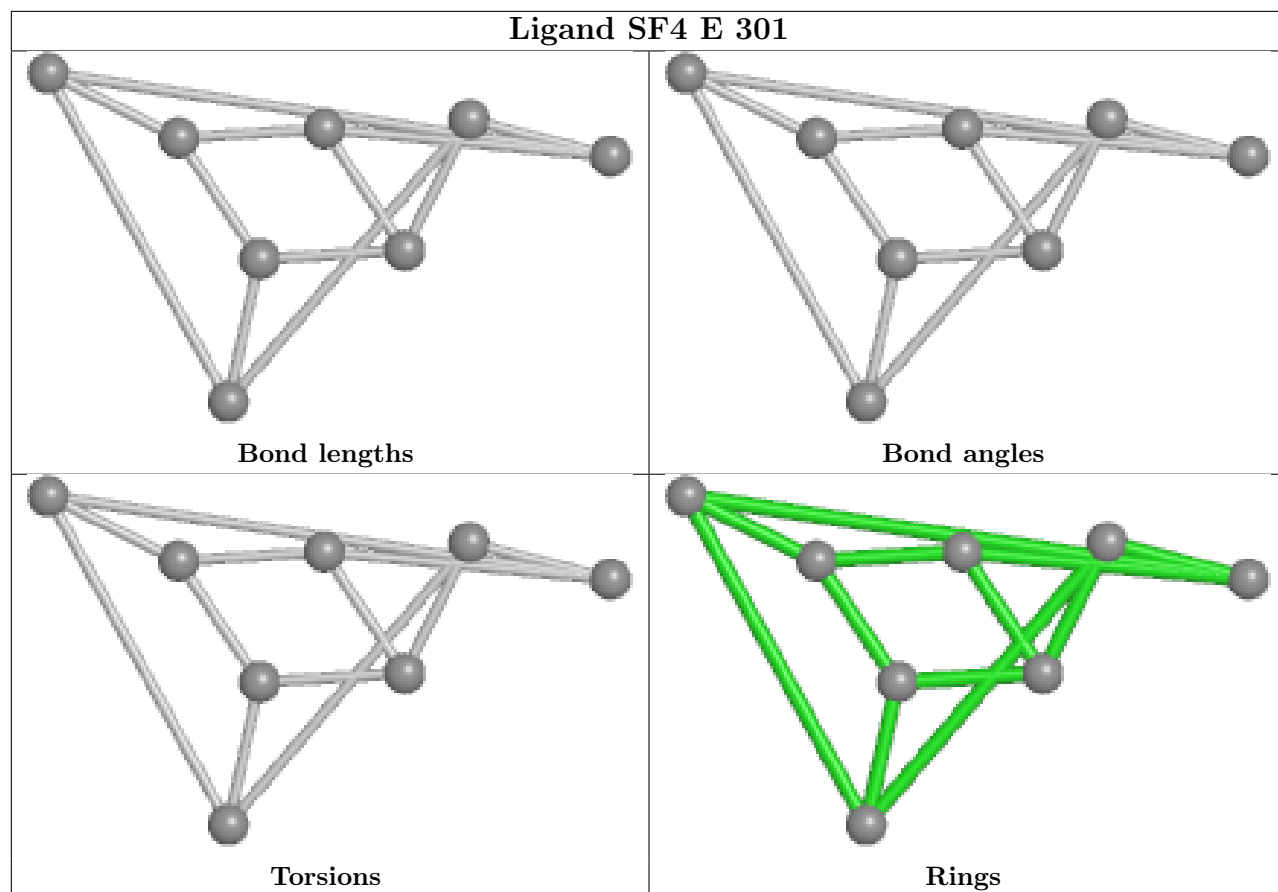
Ligand 1L3 I 304

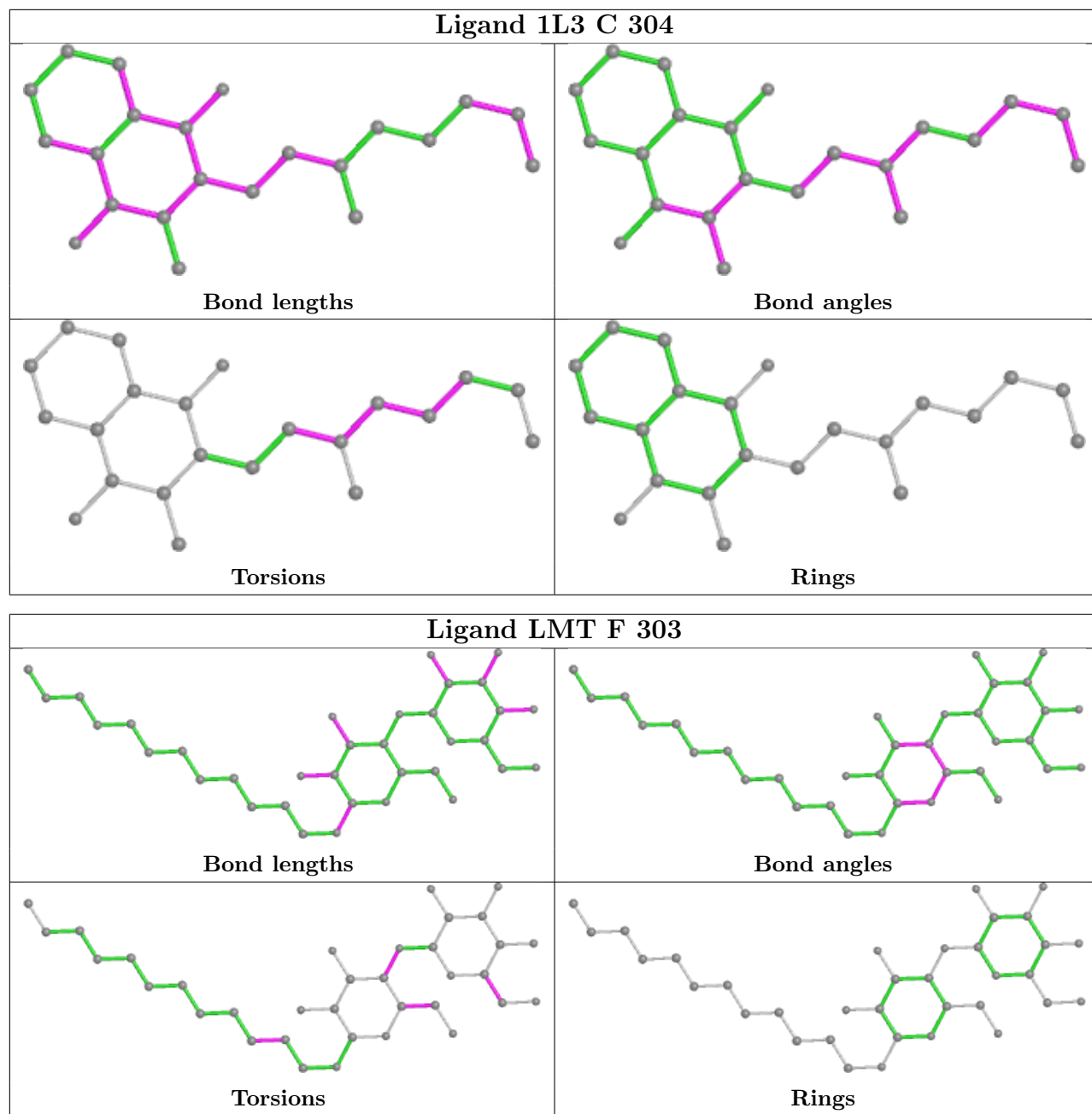


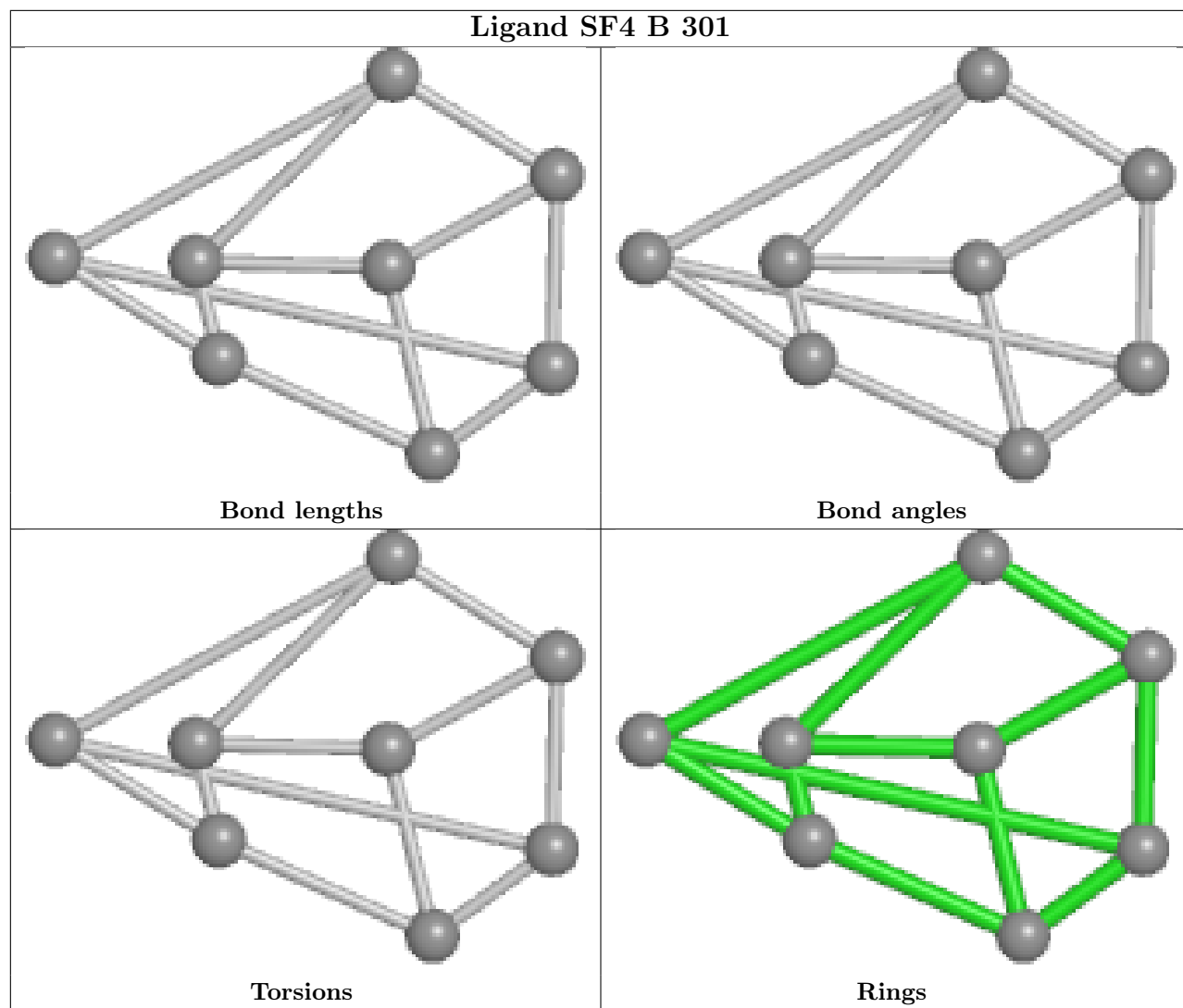
Ligand HEM C 302

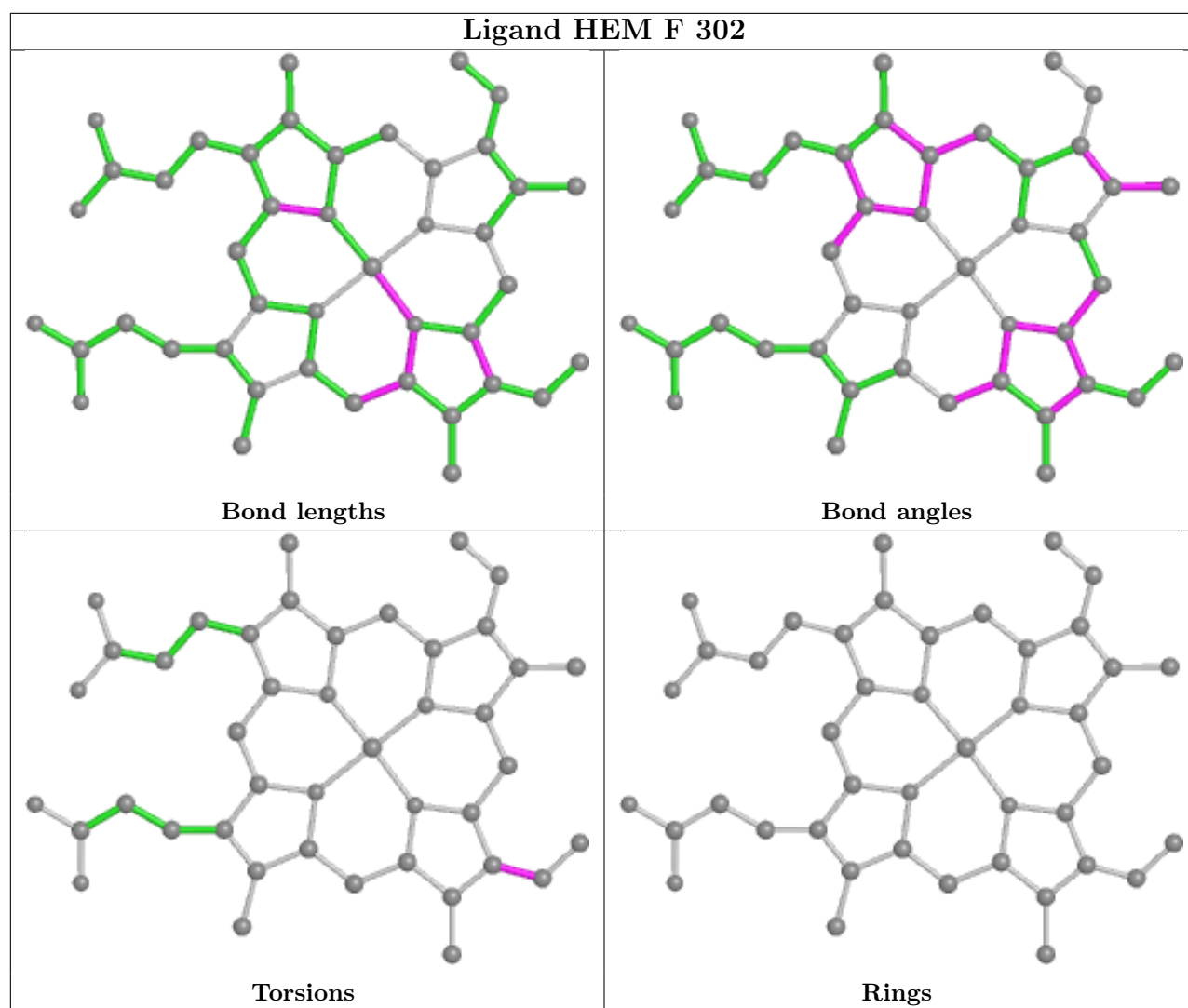


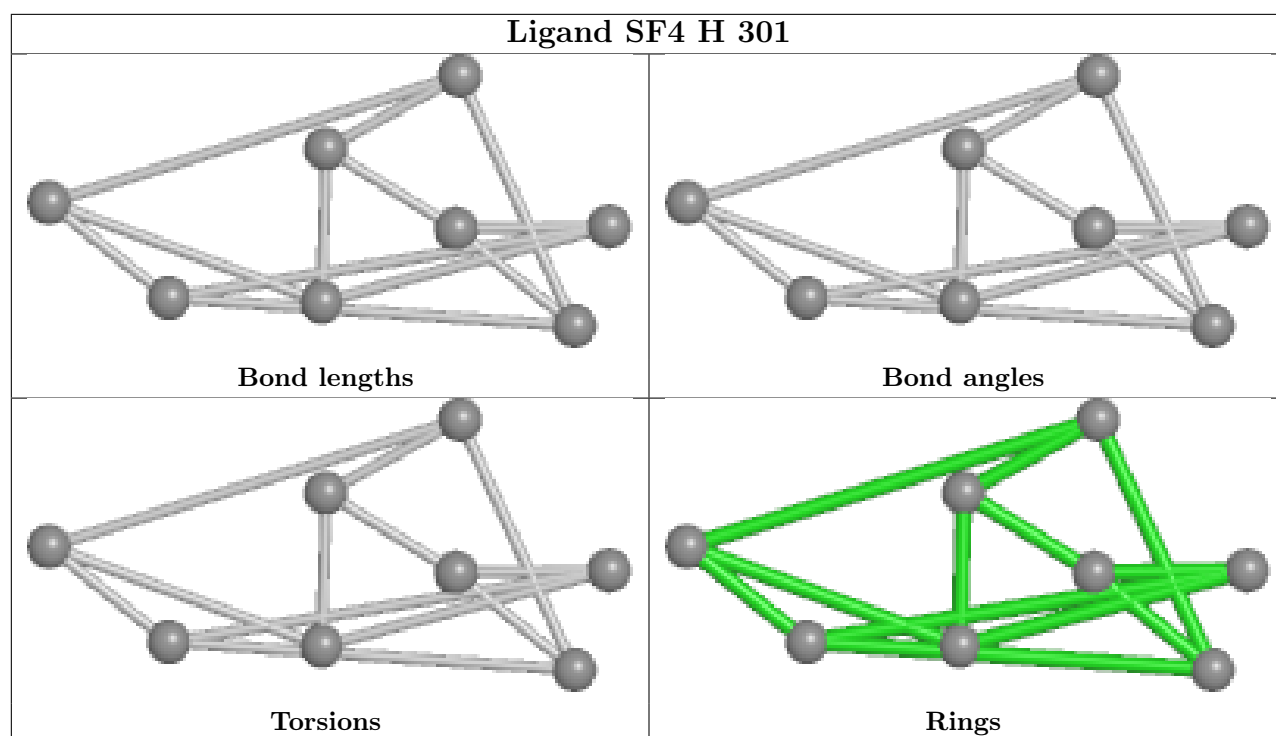
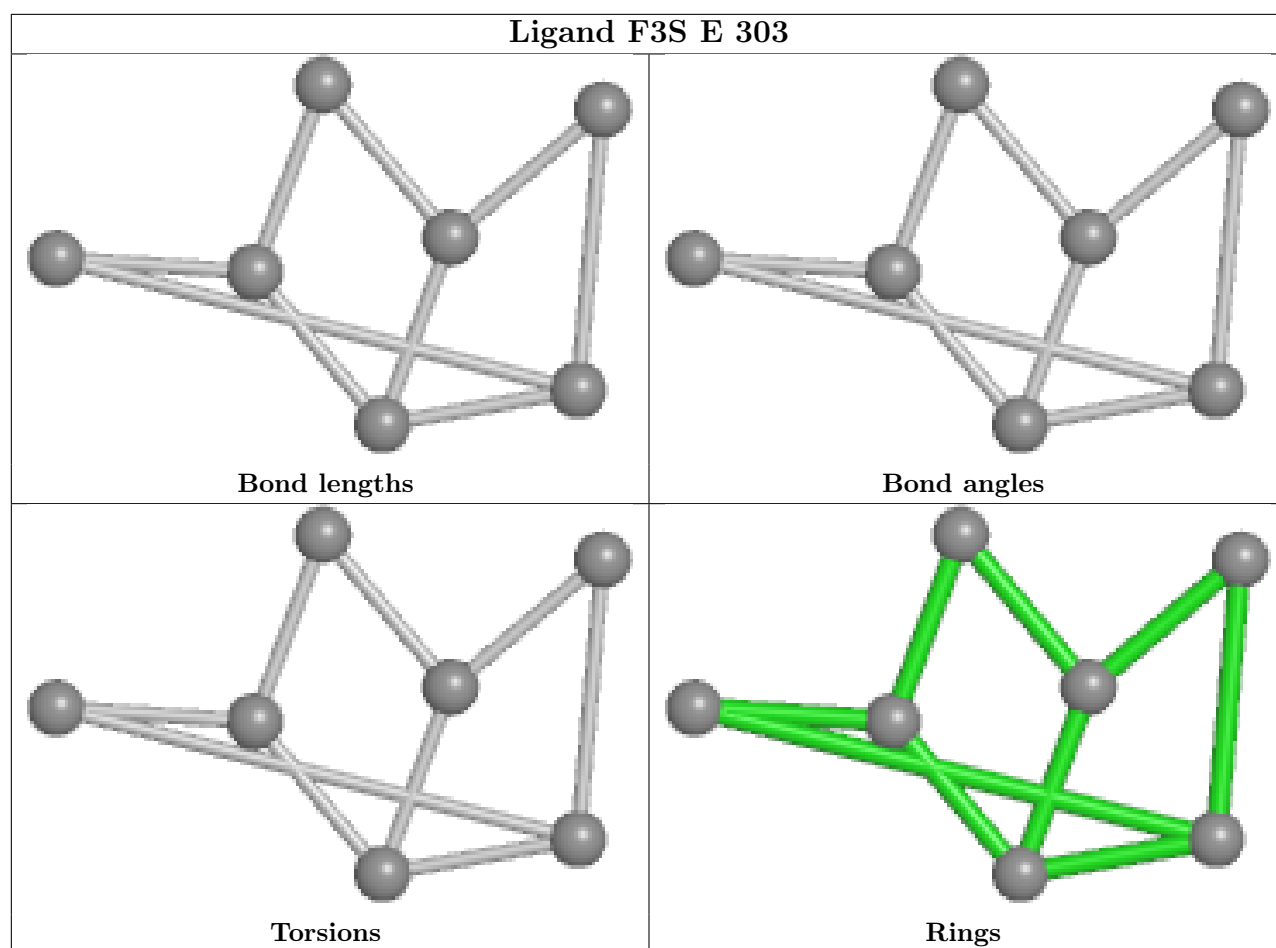


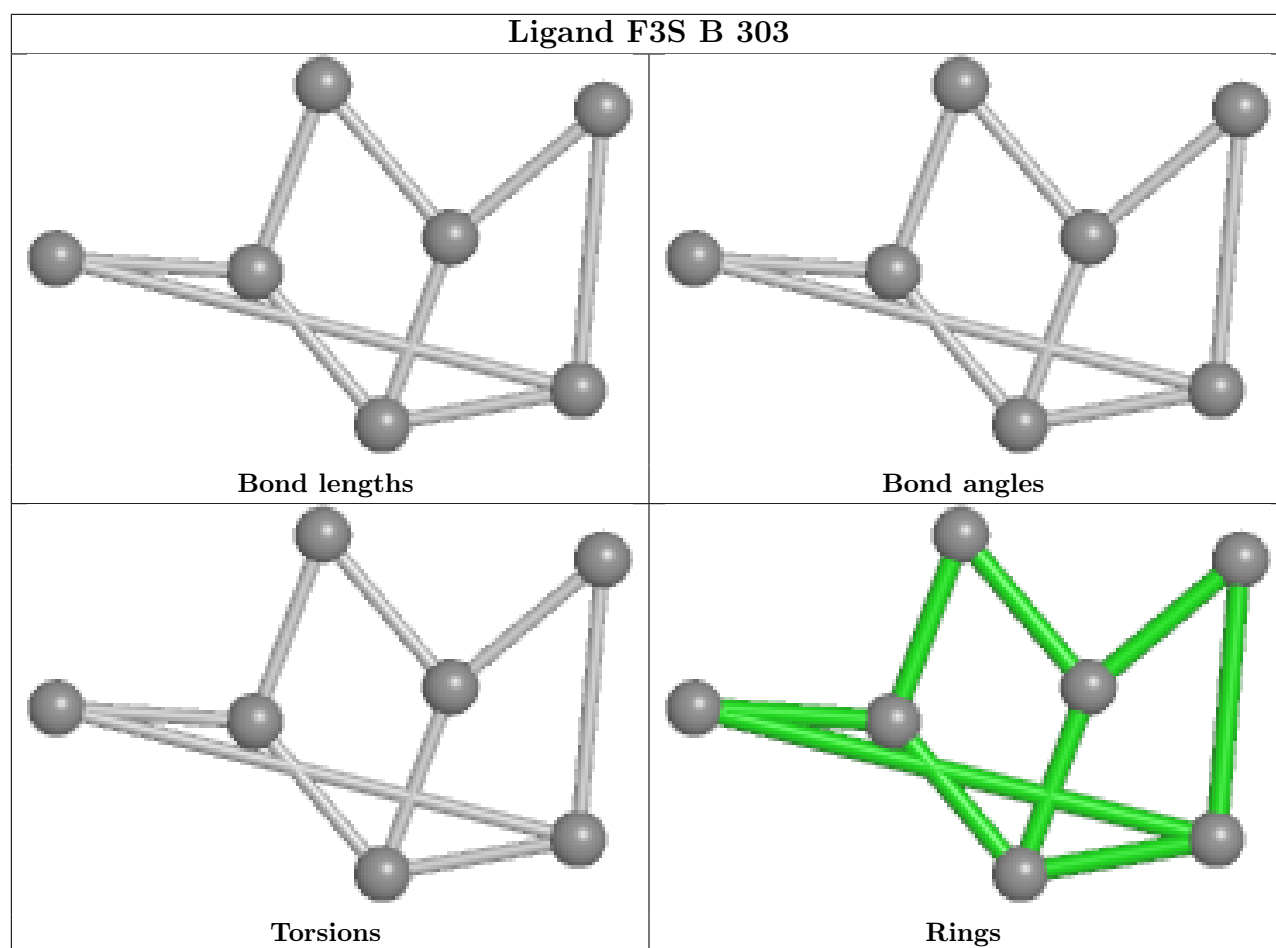


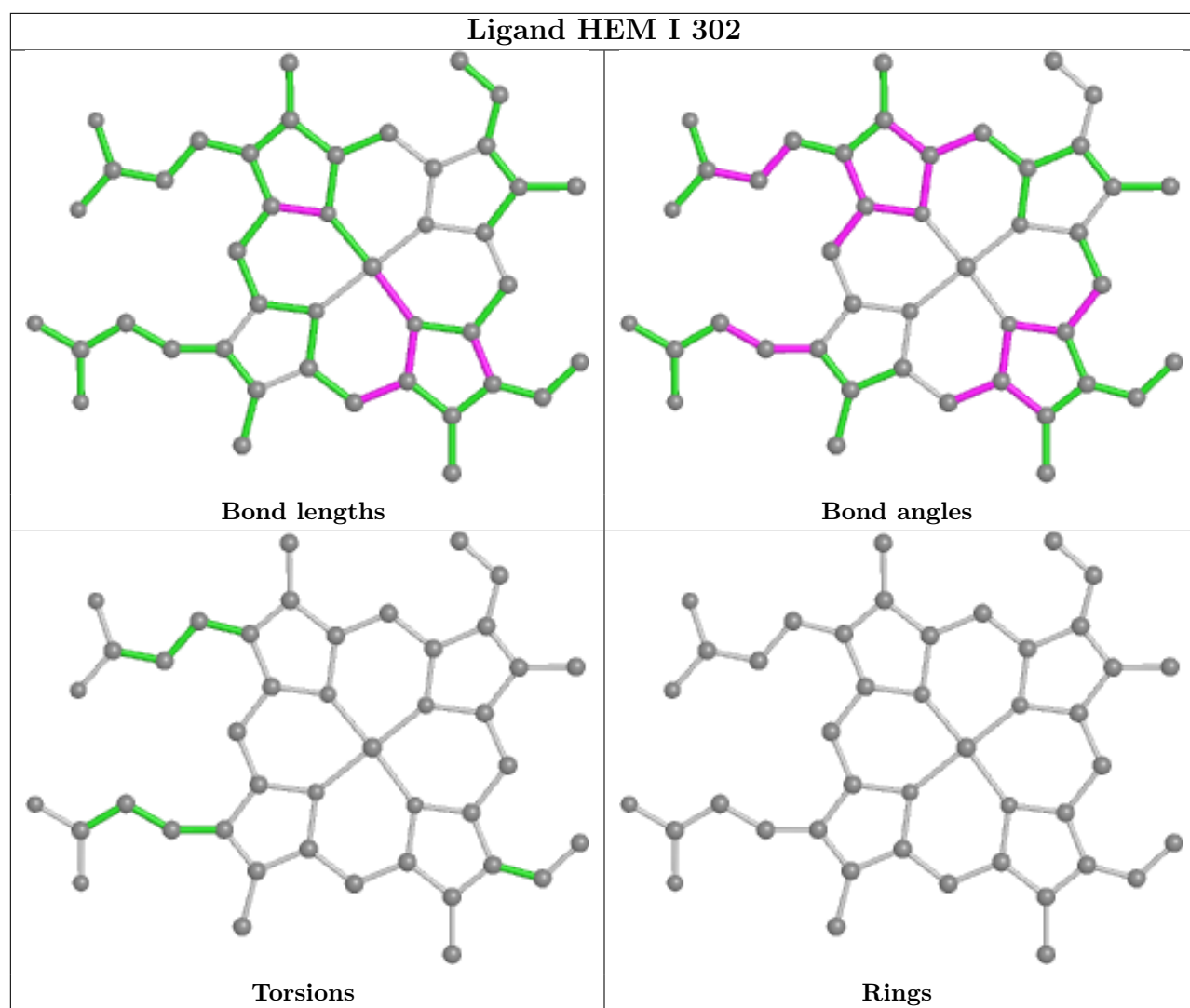


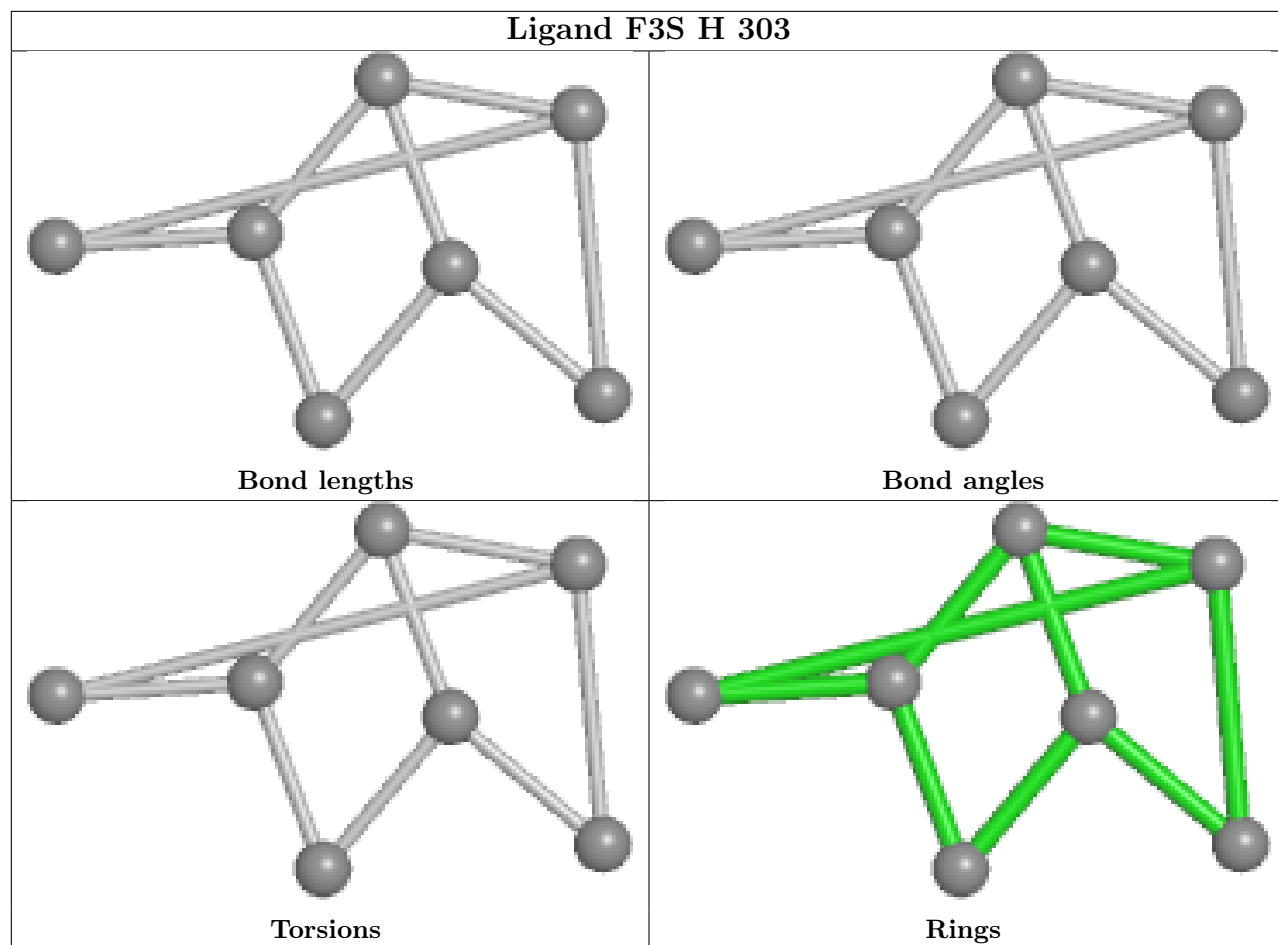


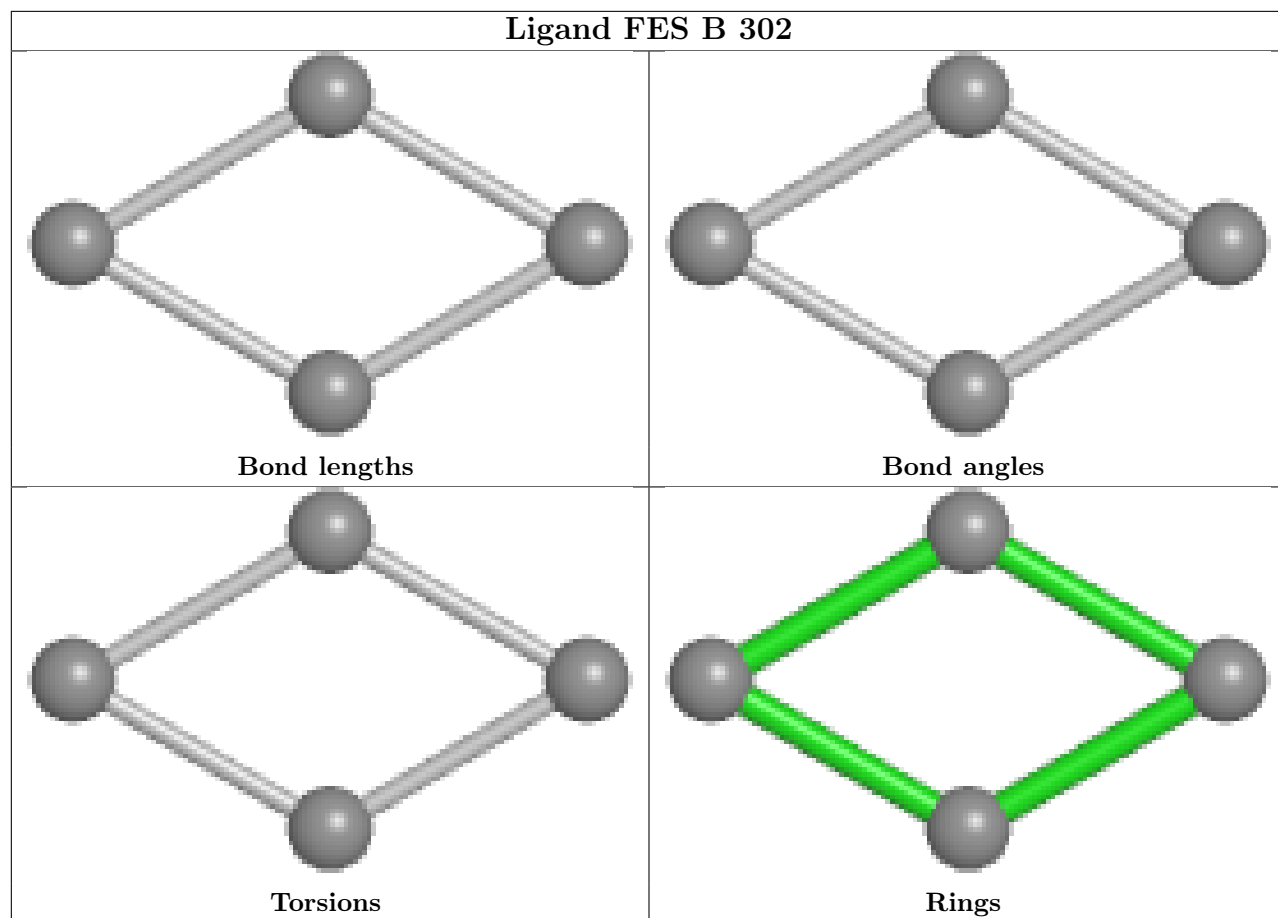


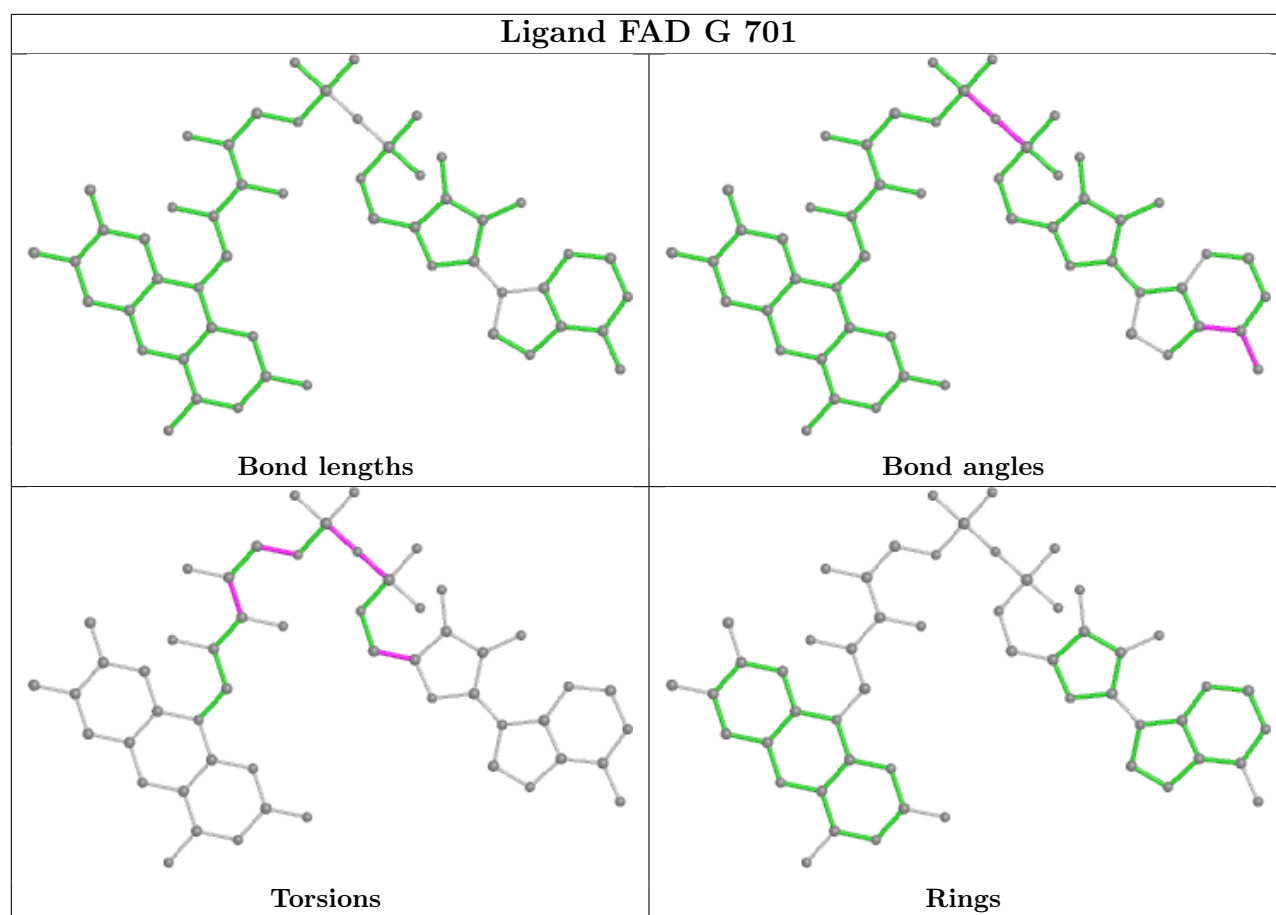












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

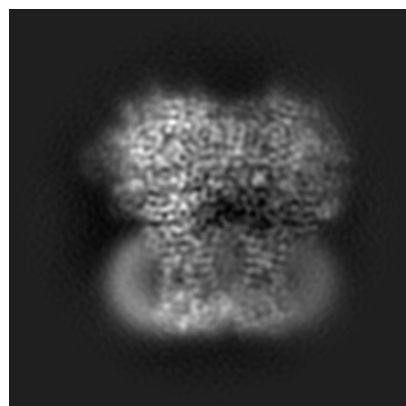
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62935. These allow visual inspection of the internal detail of the map and identification of artifacts.

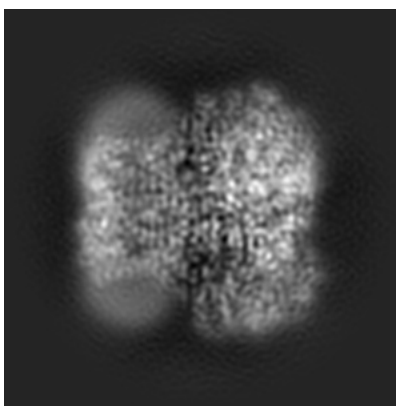
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

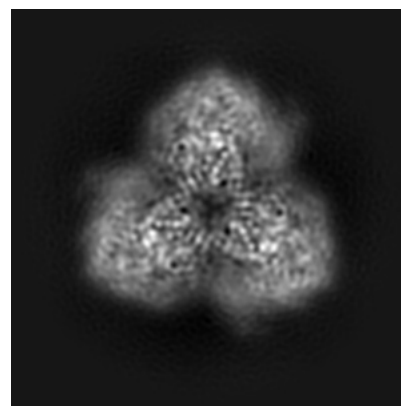
6.1.1 Primary map



X

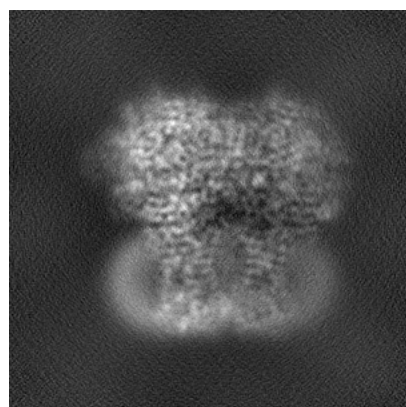


Y

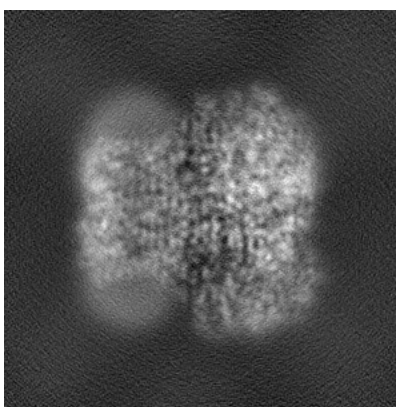


Z

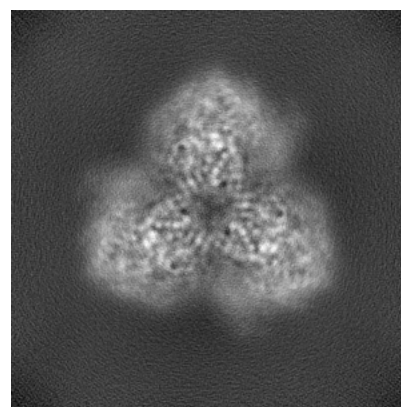
6.1.2 Raw map



X



Y

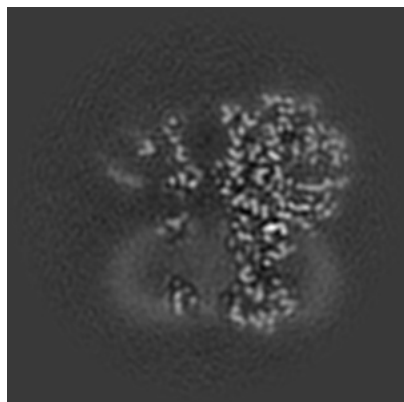


Z

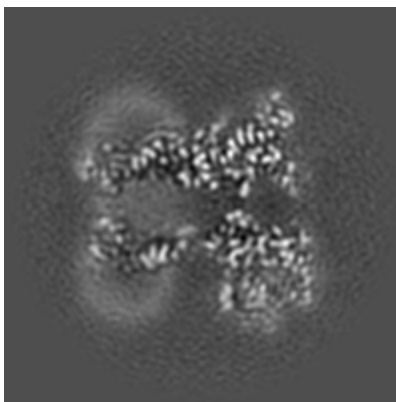
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

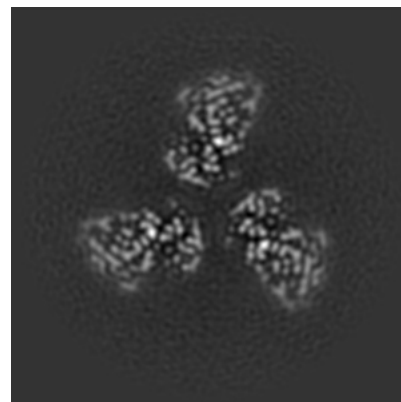
6.2.1 Primary map



X Index: 150

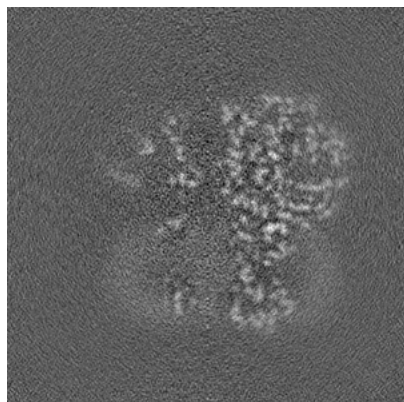


Y Index: 150

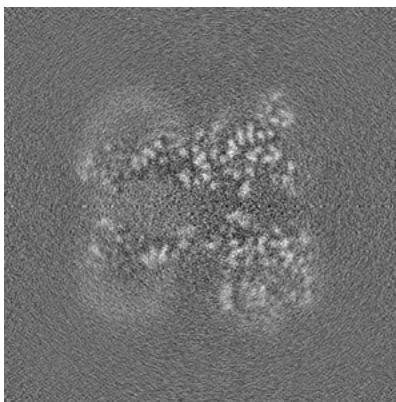


Z Index: 150

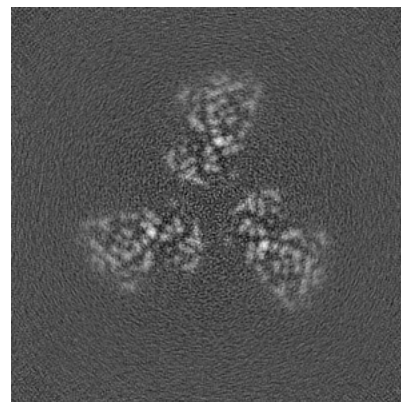
6.2.2 Raw map



X Index: 150



Y Index: 150

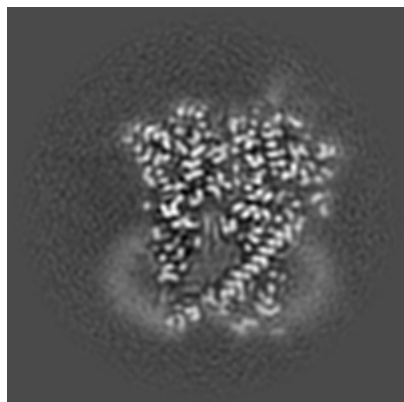


Z Index: 150

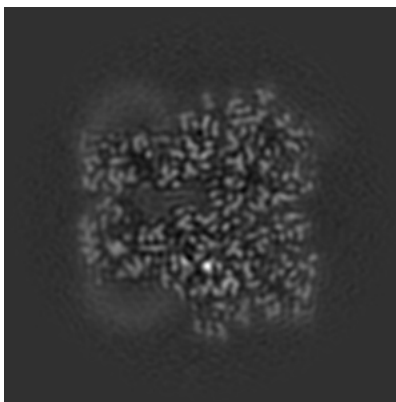
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

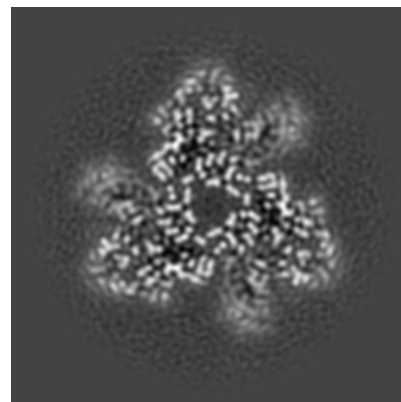
6.3.1 Primary map



X Index: 133

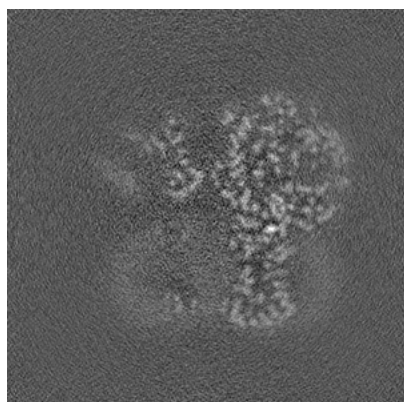


Y Index: 130

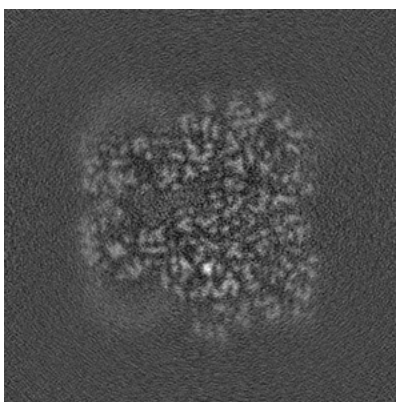


Z Index: 192

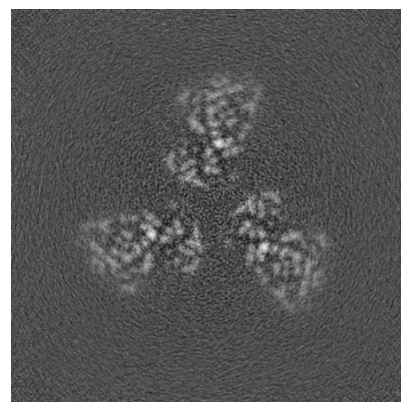
6.3.2 Raw map



X Index: 152



Y Index: 130

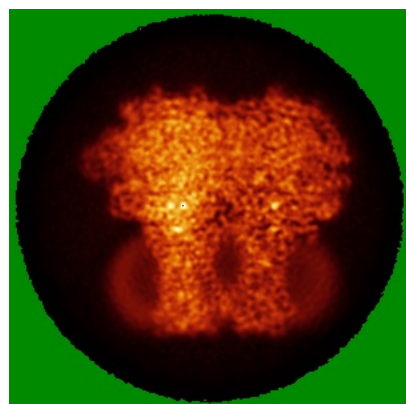


Z Index: 150

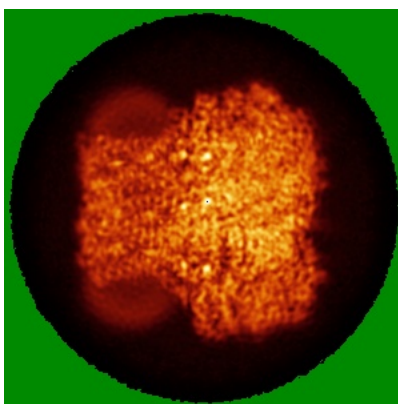
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

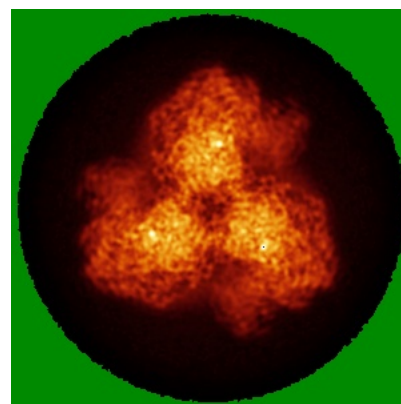
6.4.1 Primary map



X

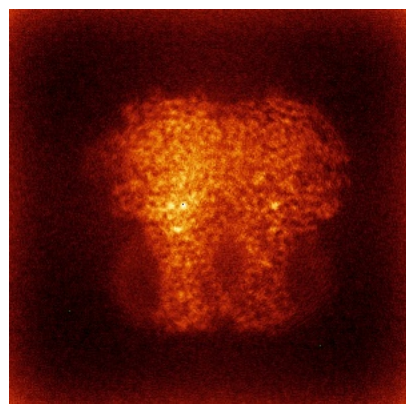


Y

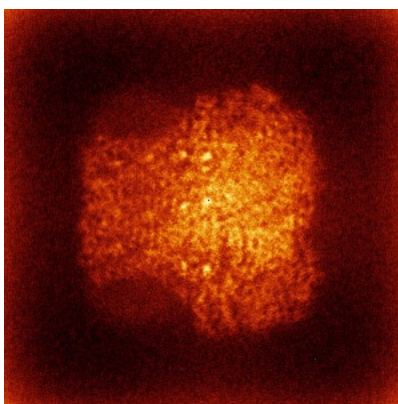


Z

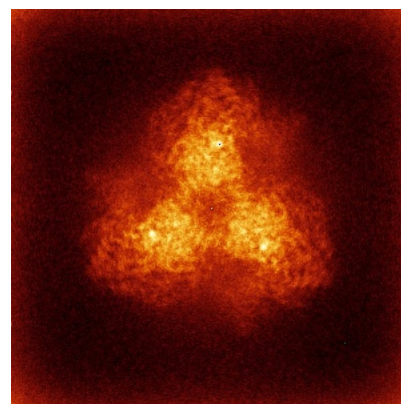
6.4.2 Raw map



X



Y

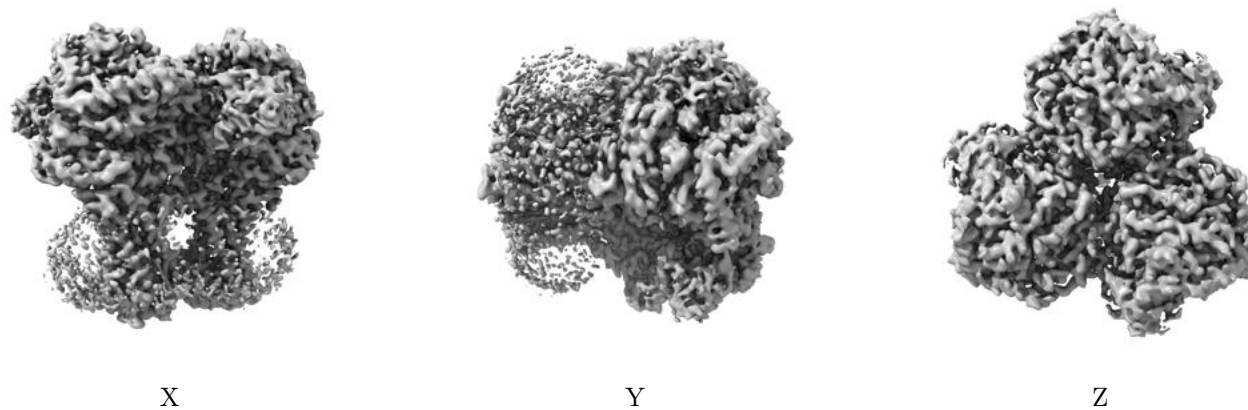


Z

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.

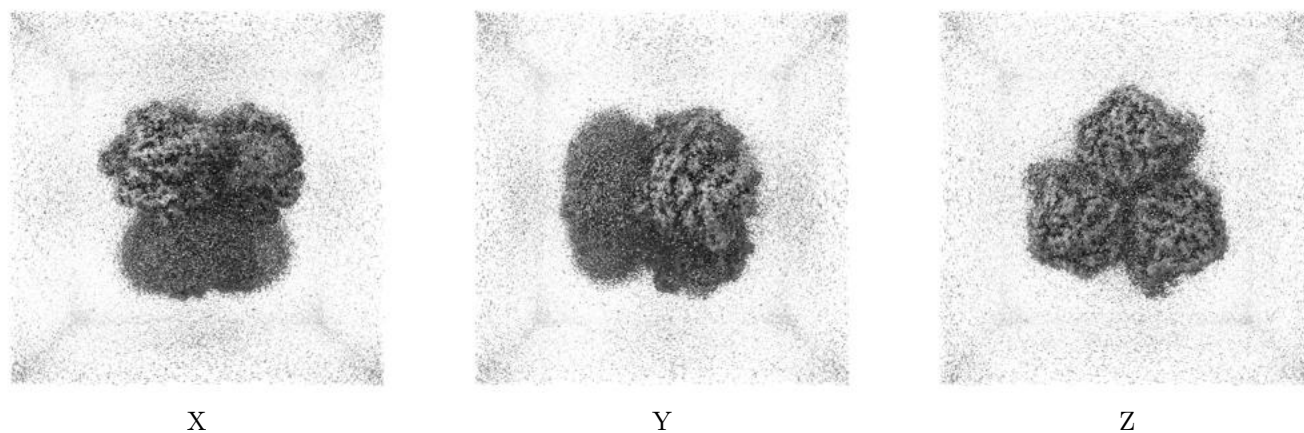
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

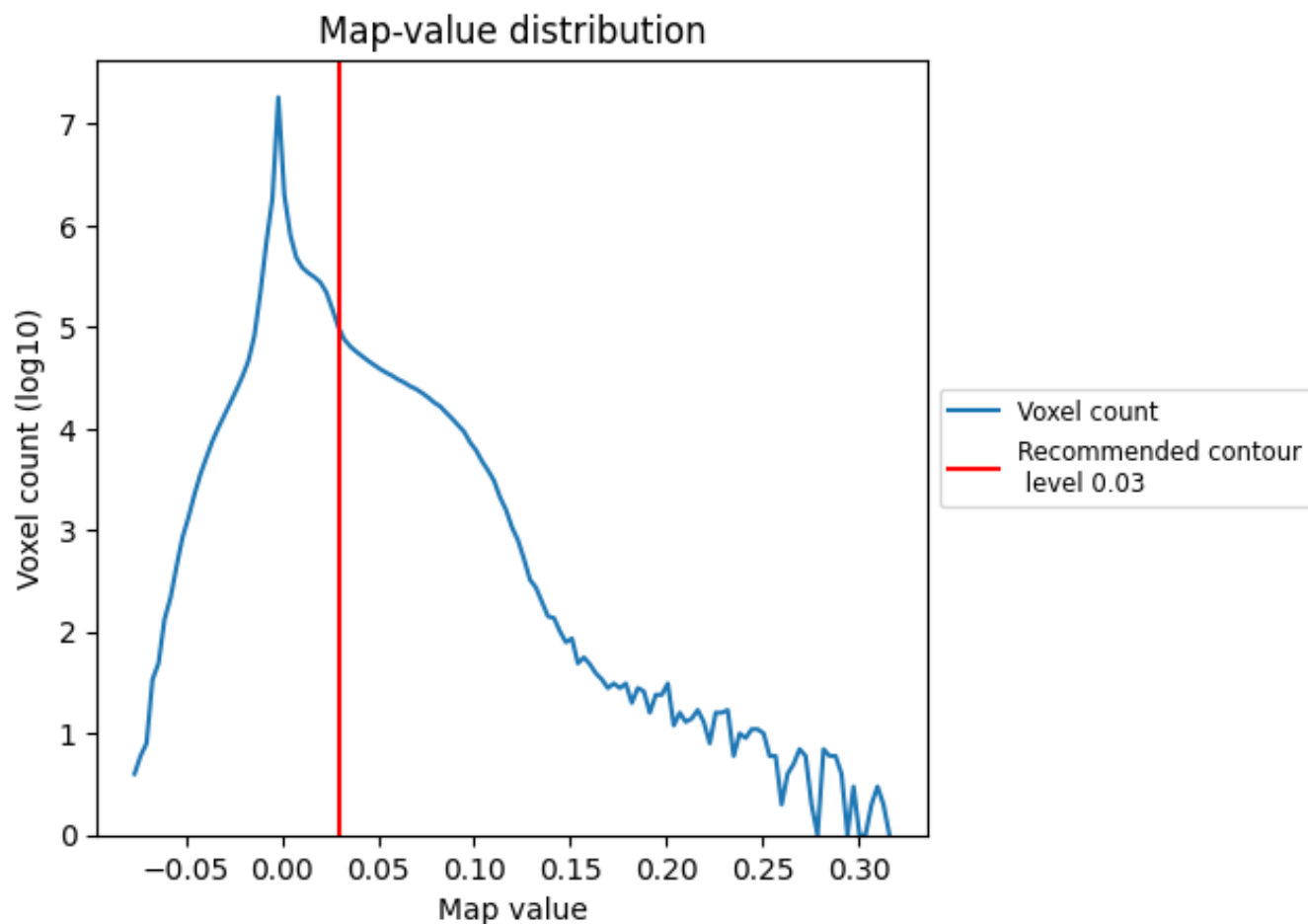
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

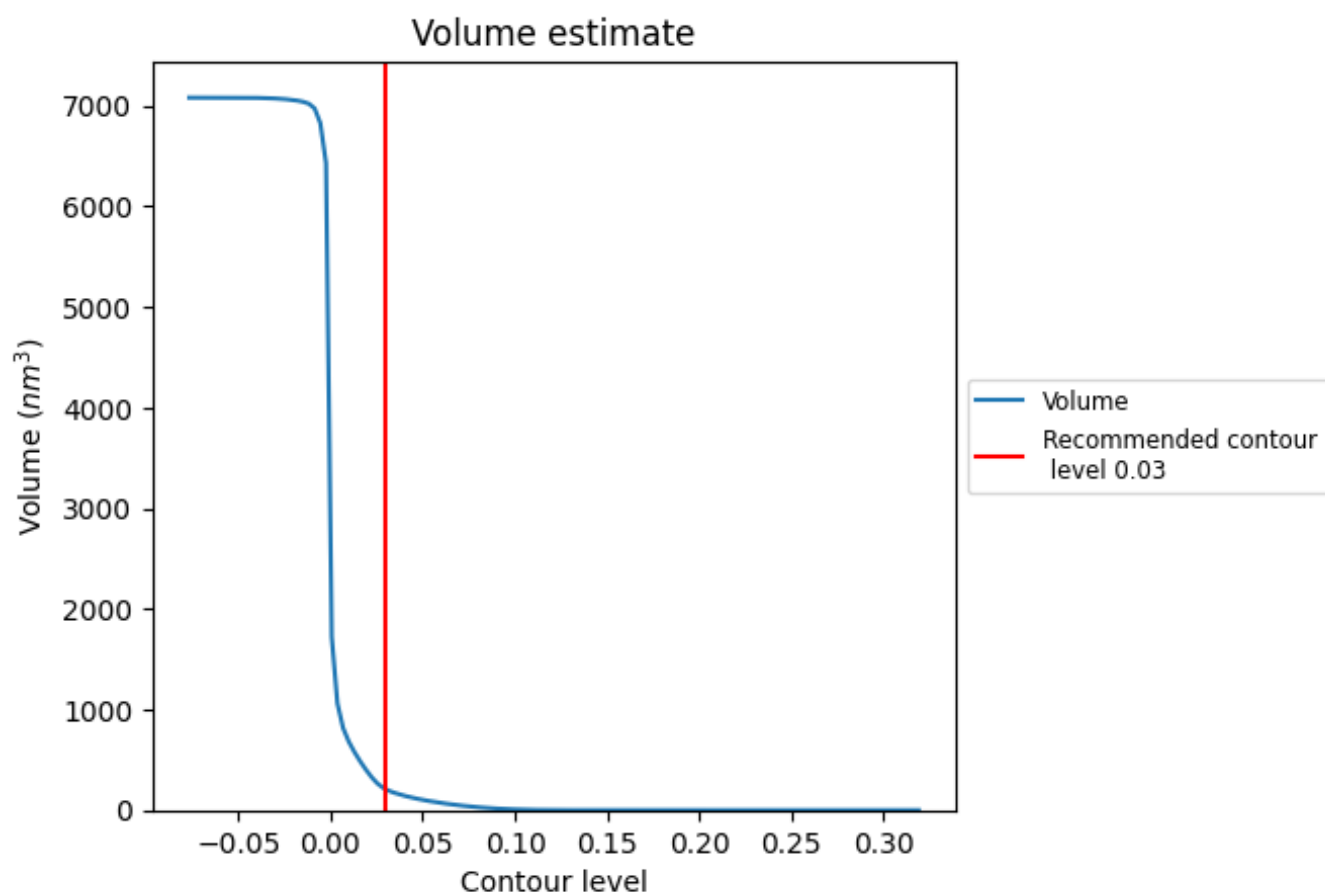
This section contains the results of statistical analysis of the map.

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.

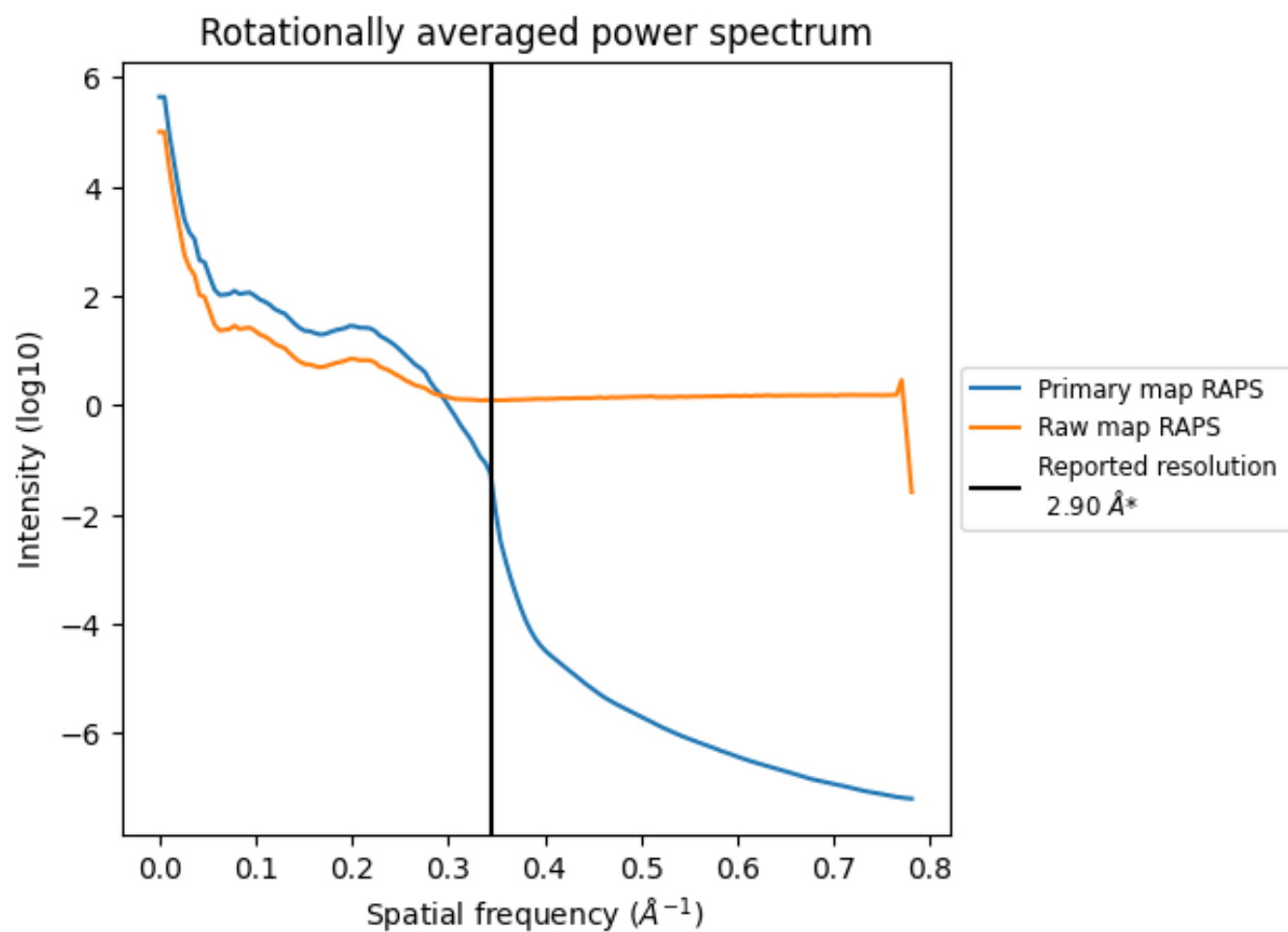
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 188 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 [i](#)

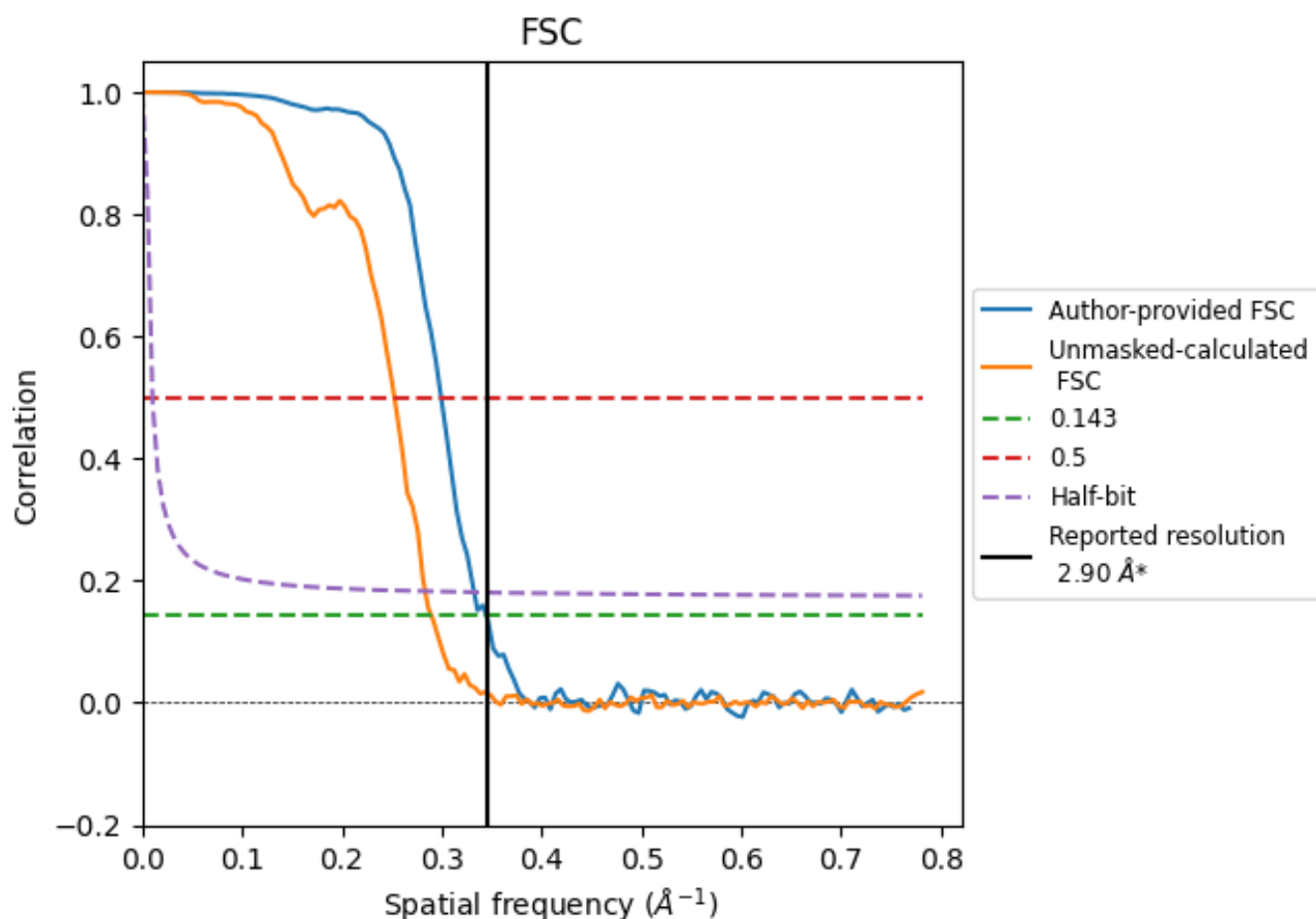


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates

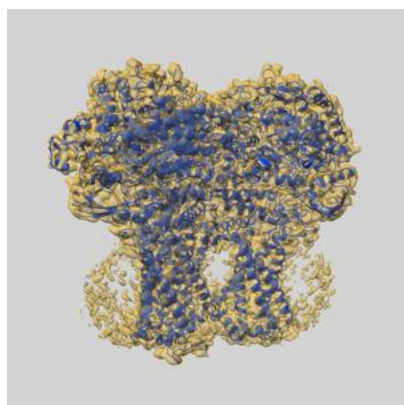
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.34	3.01
Unmasked-calculated*	3.45	3.96	3.53

*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 3.45 differs from the reported value 2.9 by more than 10 %

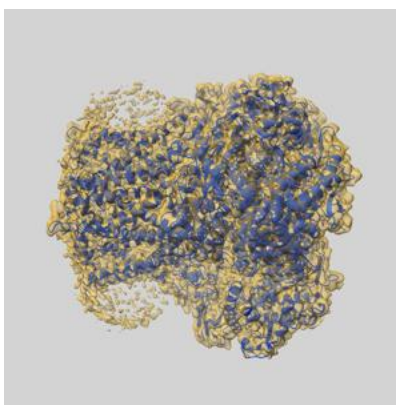
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62935 and PDB model 9LB1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

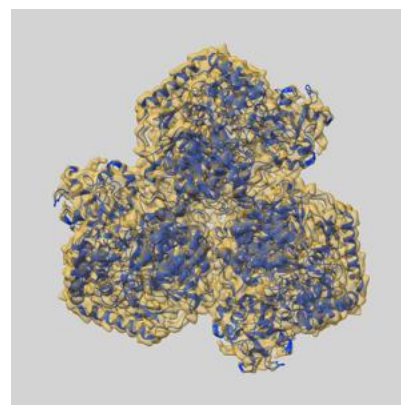
9.1 Map-model overlay [i](#)



X



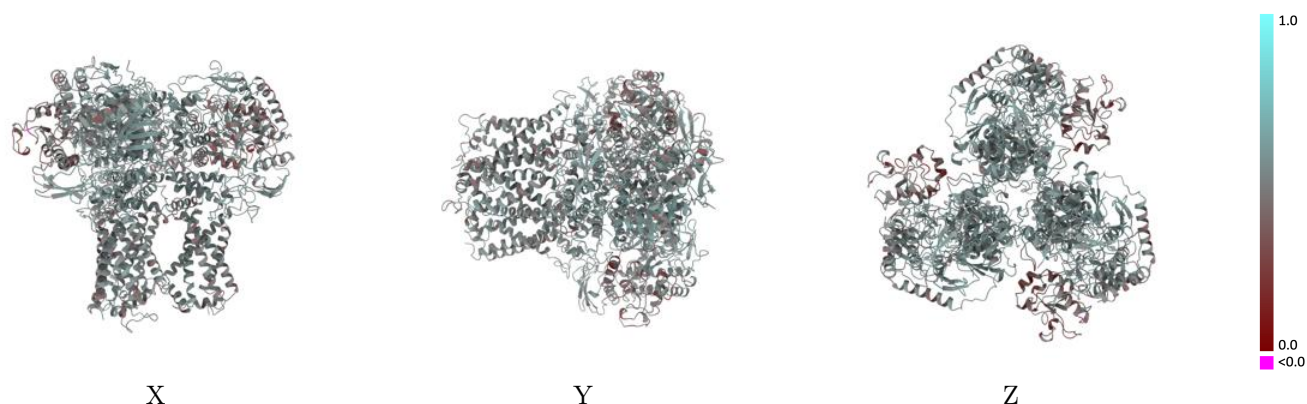
Y



Z

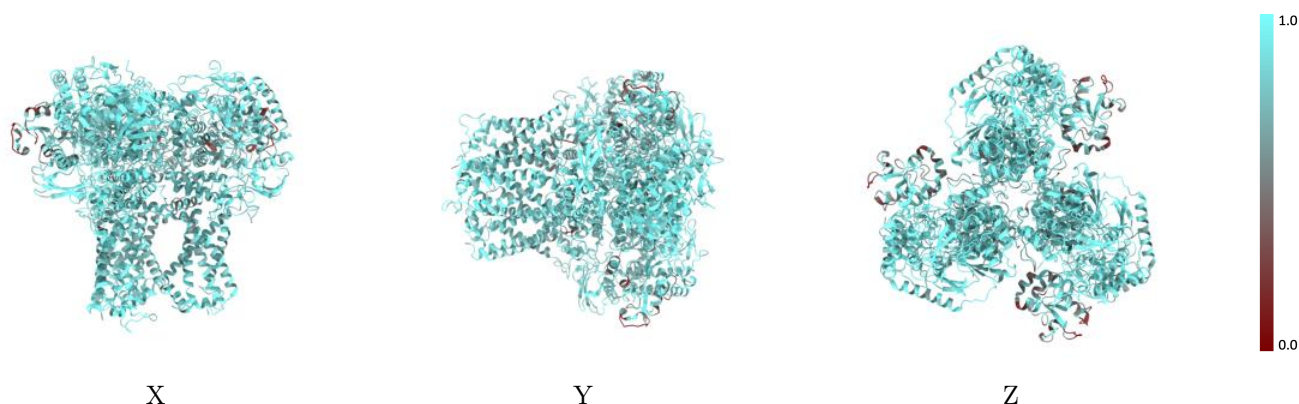
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



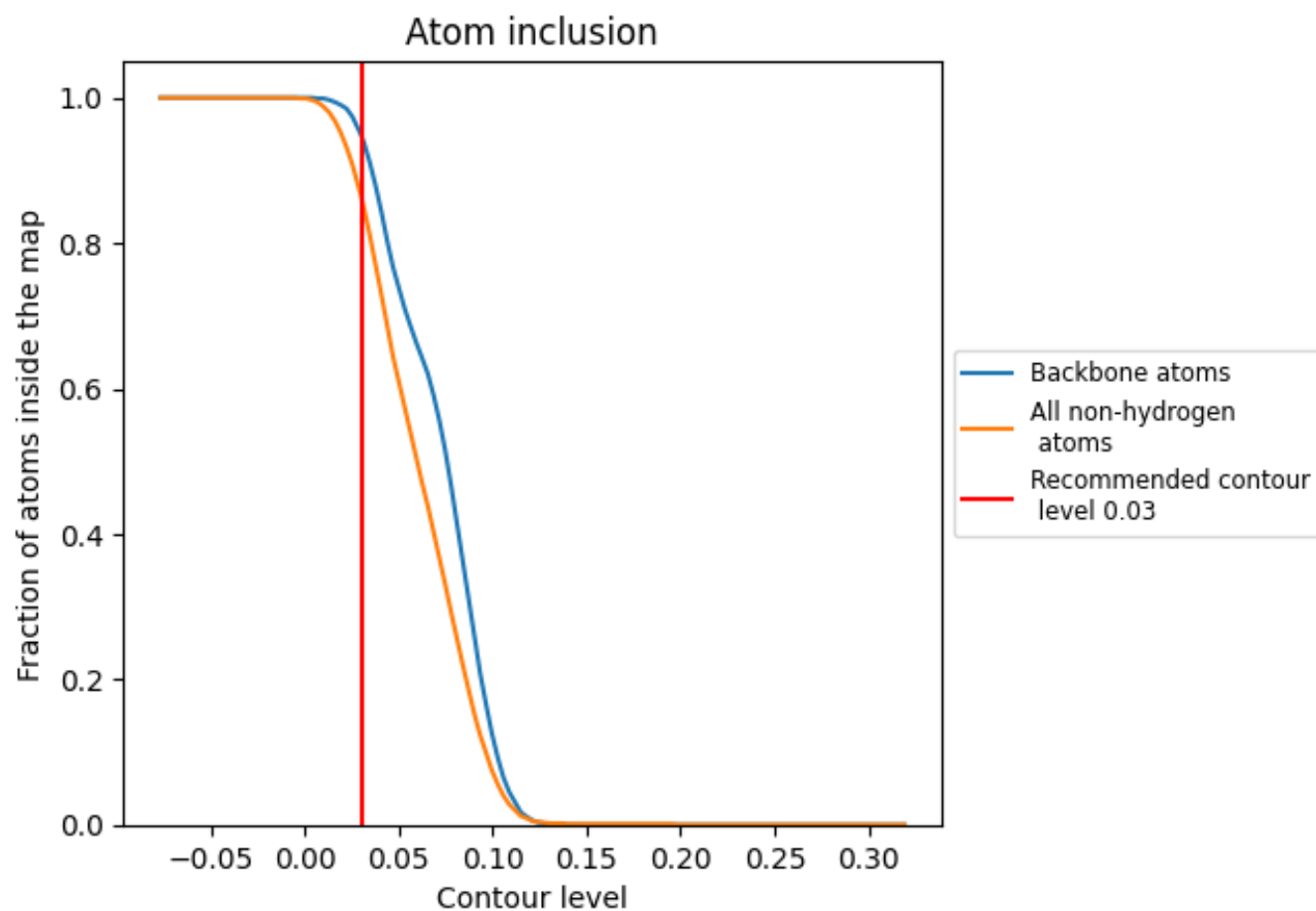
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8650	<div><div></div></div> 0.5130
A	<div><div></div></div> 0.8660	<div><div></div></div> 0.5110
B	<div><div></div></div> 0.8960	<div><div></div></div> 0.5360
C	<div><div></div></div> 0.8430	<div><div></div></div> 0.5060
D	<div><div></div></div> 0.8620	<div><div></div></div> 0.5100
E	<div><div></div></div> 0.8990	<div><div></div></div> 0.5370
F	<div><div></div></div> 0.8460	<div><div></div></div> 0.5030
G	<div><div></div></div> 0.8570	<div><div></div></div> 0.5050
H	<div><div></div></div> 0.8890	<div><div></div></div> 0.5310
I	<div><div></div></div> 0.8480	<div><div></div></div> 0.5000

1.0

0.0

<0.0