



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:04 AM JST

PDB ID : 9LAZ / pdb_00009laz
EMDB ID : EMD-62933
Title : Cryo-EM structure of the lipid-bound succinate dehydrogenase from *Chloroflexus aurantiacus*
Authors : Zhang, X.; Wu, J.Y.; Xu, X.L.
Deposited on : 2025-01-02
Resolution : 2.69 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:

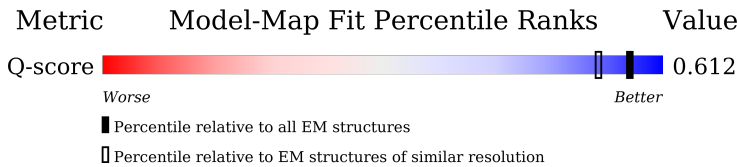
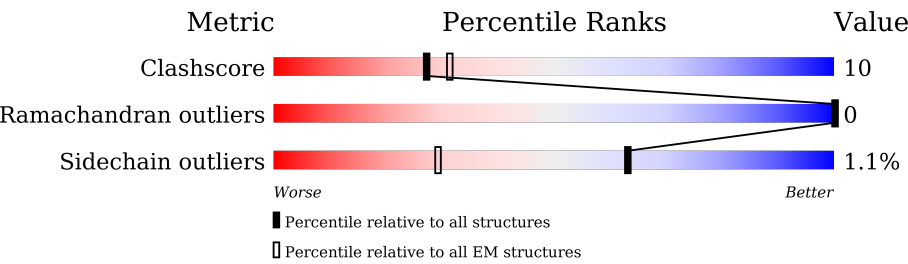
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.69 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	9309 (2.19 - 3.19)

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	74%22%.
1	D	657	74%21%.
1	G	657	77%19%.
2	B	260	77%22%.

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Mol	Chain	Length	Quality of chain
2	E	260	 70% 29%
2	H	260	 69% 29%
3	C	239	 75% 25%
3	F	239	 80% 20%
3	I	239	 74% 26%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 27469 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		

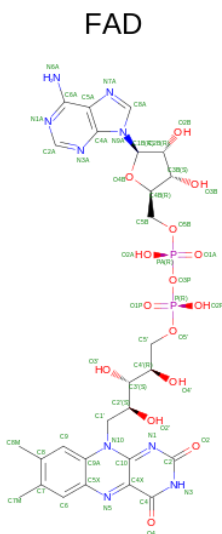
- Molecule 2 is a protein called 4Fe-4S ferredoxin iron-sulfur binding domain protein.

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.

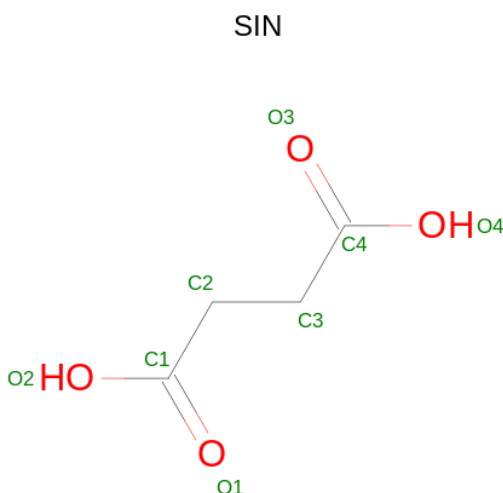
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		
3	F	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		
3	I	239	Total	C	N	O	S	0	0
			1927	1285	321	314	7		

- 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 SUCCINIC ACID (CCD ID: SIN) (formula: $\text{C}_4\text{H}_6\text{O}_4$).



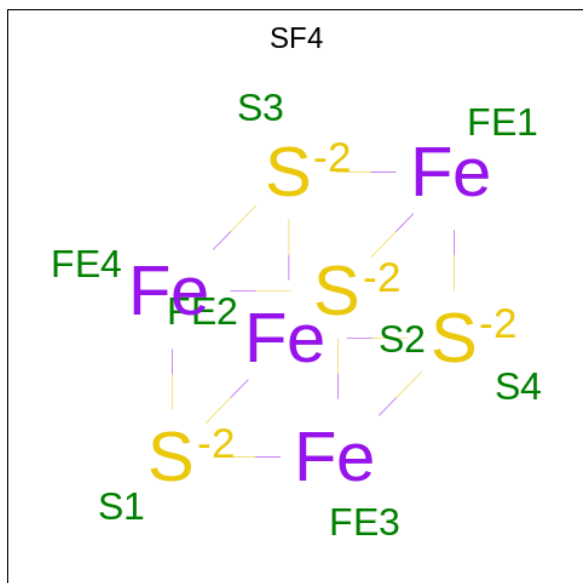
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			8	4	4	

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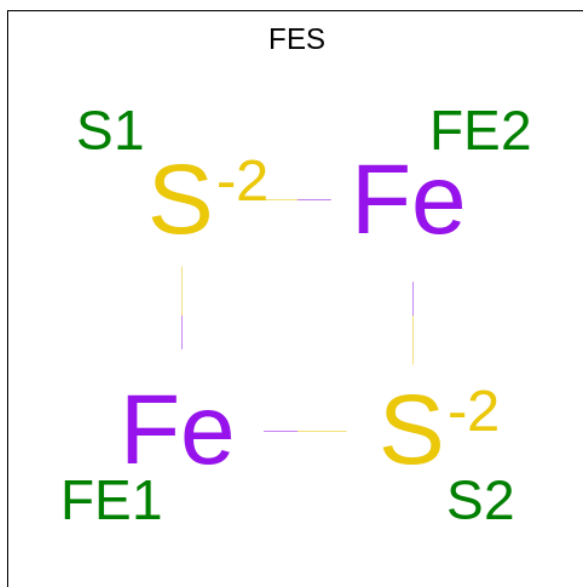
Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	C	O	0
			8	4	4	
5	G	1	Total	C	O	0
			8	4	4	

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



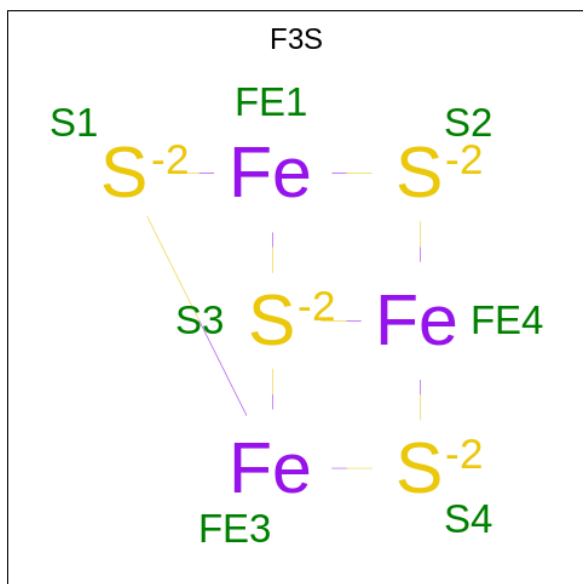
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	Fe	S	0
			8	4	4	
6	E	1	Total	Fe	S	0
			8	4	4	
6	H	1	Total	Fe	S	0
			8	4	4	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



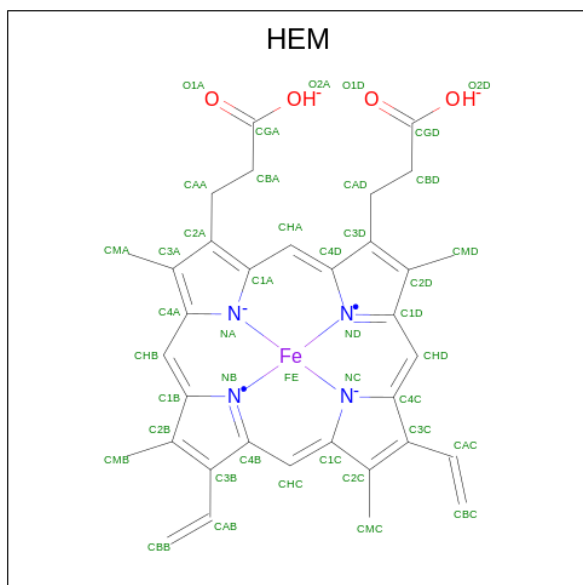
Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	Fe	S	0
			4	2	2	
7	E	1	Total	Fe	S	0
			4	2	2	
7	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



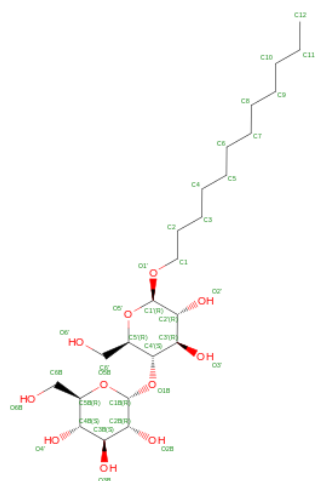
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total 7	Fe 3	S 4	0
8	E	1	Total 7	Fe 3	S 4	0
8	H	1	Total 7	Fe 3	S 4	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total 31	C 20	O 10	P 1	0
11	F	1	Total 30	C 19	O 10	P 1	0
11	I	1	Total 33	C 22	O 10	P 1	0

- Molecule 12 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).

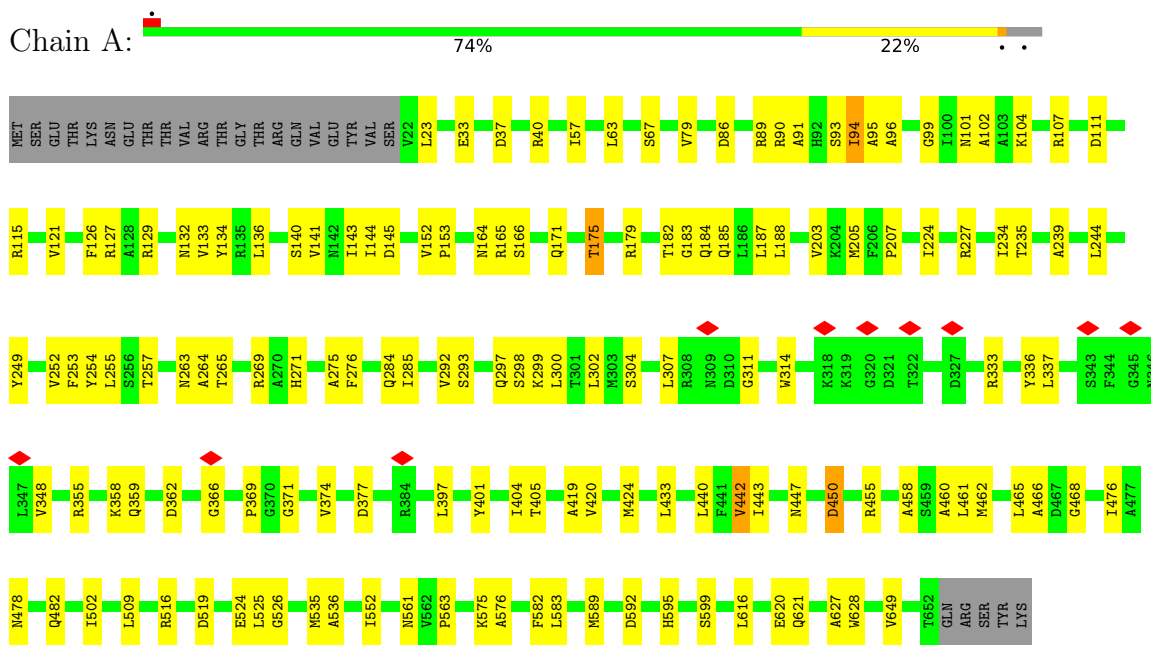


Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total 49	C 39	N 1	O 8	P 1	0
12	C	1	Total 41	C 31	N 1	O 8	P 1	0
12	F	1	Total 44	C 34	N 1	O 8	P 1	0
12	F	1	Total 49	C 39	N 1	O 8	P 1	0
12	I	1	Total 44	C 34	N 1	O 8	P 1	0
12	I	1	Total 49	C 39	N 1	O 8	P 1	0

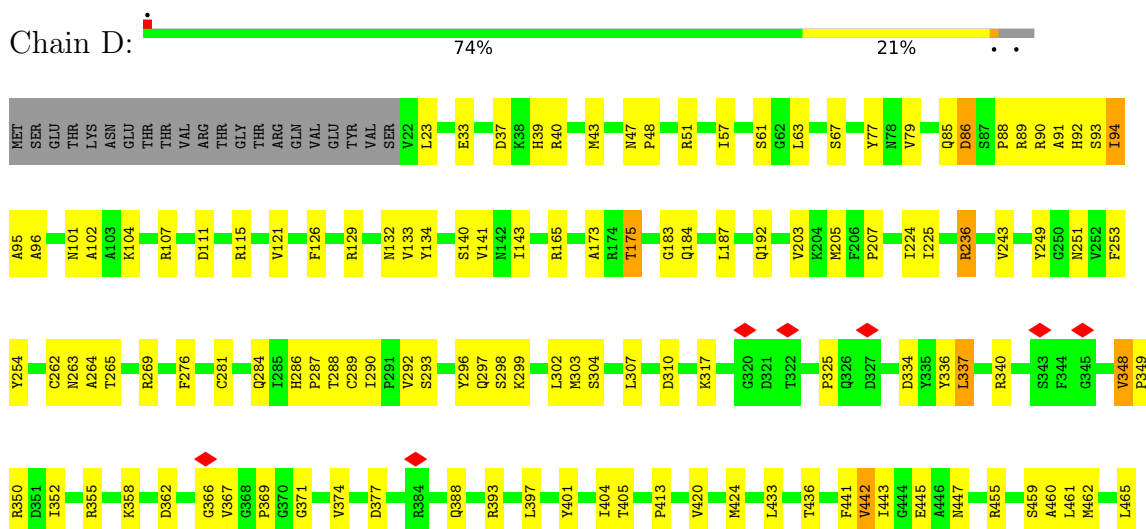
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



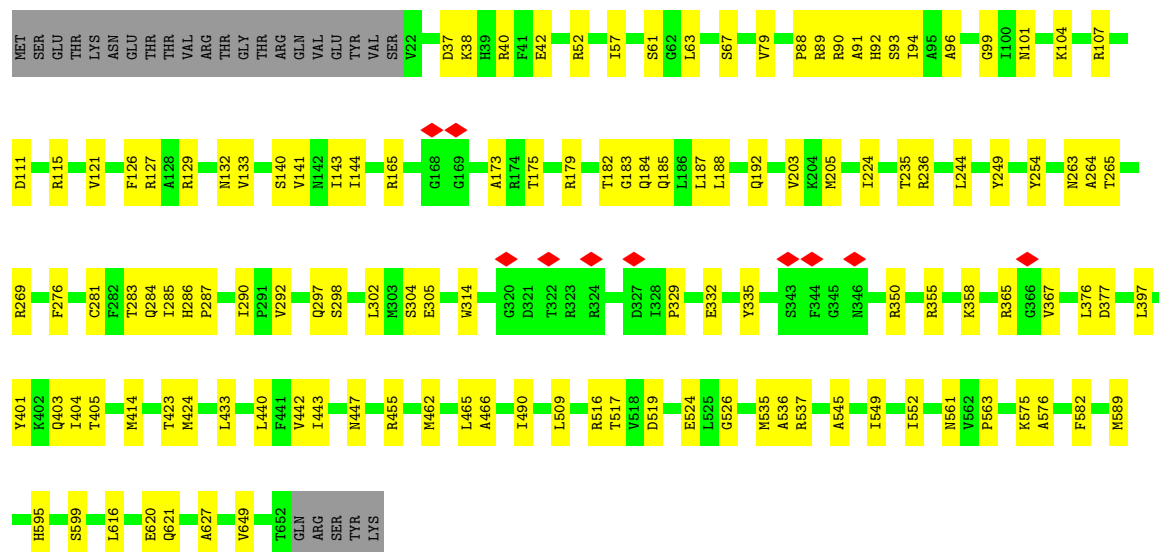
- Molecule 1: Succinate dehydrogenase or fumarate reductase, flavoprotein subunit





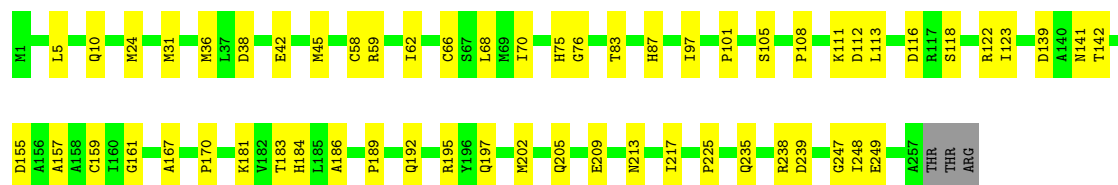
- Molecule 1: Succinate dehydrogenase or fumarate reductase, flavoprotein subunit

Chain G: 77% 19%



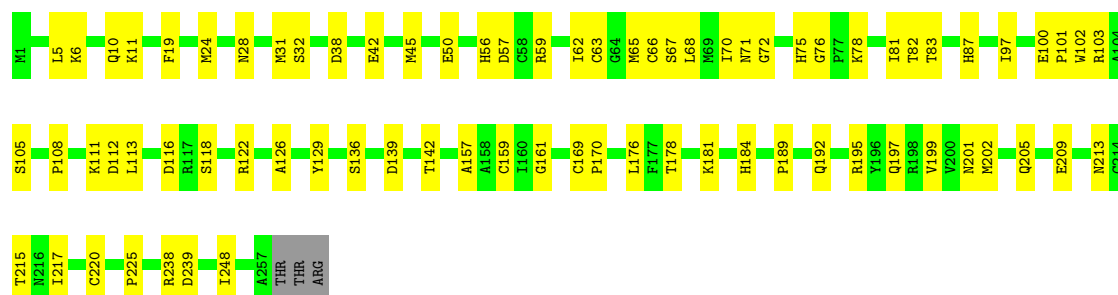
- Molecule 2: 4Fe-4S ferredoxin iron-sulfur binding domain protein

Chain B: 77% 22%



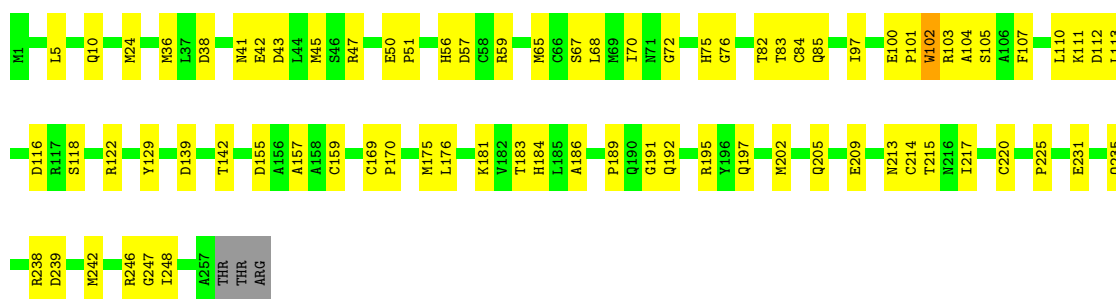
- Molecule 2: 4Fe-4S ferredoxin iron-sulfur binding domain protein

Chain E: 70% 29%



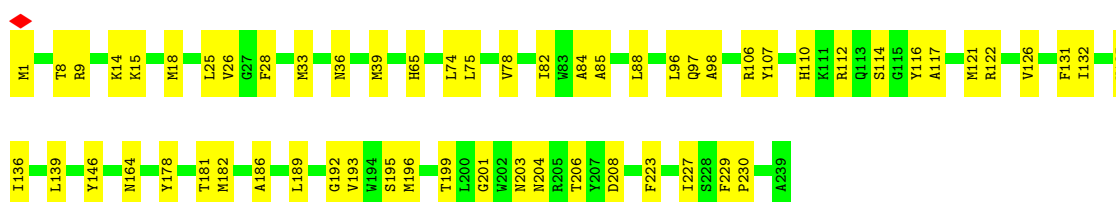
- Molecule 2: 4Fe-4S ferredoxin iron-sulfur binding domain protein

Chain H: 69% 29%



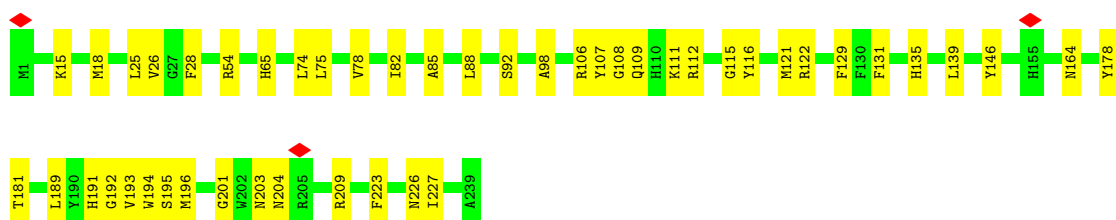
- Molecule 3: Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family

Chain C: 75% 25%



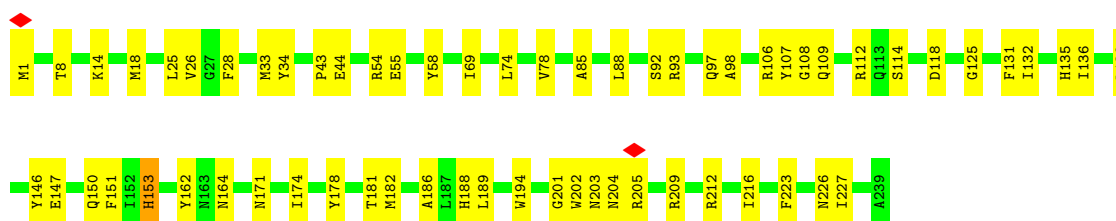
- Molecule 3: Succinate dehydrogenase (Or fumarate reductase) cytochrome b subunit, b558 family

Chain F: 80% 20%



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

Chain I: 74% 26%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69415	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	2.056	Depositor
Minimum map value	-1.367	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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, SIN, PEV, FES, PGV, FAD, F3S, HEM, LMT

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	0.12	0/5055	0.28	0/6835
1	D	0.11	0/5055	0.26	0/6835
1	G	0.11	0/5055	0.26	0/6835
2	B	0.13	0/1963	0.28	0/2663
2	E	0.13	0/1963	0.30	0/2663
2	H	0.13	0/1963	0.29	0/2663
3	C	0.14	0/1988	0.30	0/2702
3	F	0.12	0/1988	0.25	0/2702
3	I	0.15	0/1988	0.28	0/2702
All	All	0.12	0/27018	0.28	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	101	0
1	D	4948	0	4857	101	0
1	G	4948	0	4857	78	0
2	B	1929	0	1911	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1929	0	1911	58	0
2	H	1929	0	1911	58	0
3	C	1927	0	1929	47	0
3	F	1927	0	1929	40	0
3	I	1927	0	1929	50	0
4	A	53	0	31	6	0
4	D	53	0	31	6	0
4	G	53	0	31	2	0
5	A	8	0	4	1	0
5	D	8	0	4	0	0
5	G	8	0	4	1	0
6	B	8	0	0	0	0
6	E	8	0	0	0	0
6	H	8	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
7	H	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	1	0
8	H	7	0	0	1	0
9	C	86	0	60	10	0
9	F	86	0	60	14	0
9	I	86	0	60	8	0
10	C	62	0	68	2	0
10	F	63	0	73	2	0
10	I	64	0	75	1	0
11	C	31	0	32	2	0
11	F	30	0	30	1	0
11	I	33	0	36	2	0
12	C	90	0	132	2	0
12	F	93	0	138	1	0
12	I	93	0	141	2	0
All	All	27469	0	27101	533	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:ILE:HG12	9:C:301:HEM:HBC2	1.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:MET:HE1	9:C:301:HEM:HBD1	1.47	0.96
3:F:18:MET:HE1	9:F:302:HEM:HBD1	1.51	0.93
3:I:25:LEU:HB3	9:I:302:HEM:HBB2	1.56	0.88
1:D:336:TYR:HB2	1:D:340:ARG:HD2	1.63	0.80
3:C:135:HIS:HE1	3:C:139:LEU:HD12	1.47	0.77
9:F:303:HEM:HH3	9:F:303:HEM:HBB2	1.67	0.77
1:G:304:SER:HB3	1:G:397:LEU:HD11	1.68	0.76
1:D:90:ARG:NH2	2:E:161:GLY:O	2.21	0.74
1:A:254:TYR:H	1:A:526:GLY:HA3	1.53	0.73
1:D:94:ILE:HG23	1:D:187:LEU:HD23	1.68	0.73
1:G:90:ARG:HD2	2:H:65:MET:HG2	1.71	0.73
1:G:254:TYR:H	1:G:526:GLY:HA3	1.55	0.71
2:E:205:GLN:NE2	2:E:209:GLU:OE2	2.22	0.71
1:D:287:PRO:HD3	1:D:350:ARG:HD3	1.72	0.70
1:D:254:TYR:H	1:D:526:GLY:HA3	1.55	0.70
2:B:205:GLN:NE2	2:B:209:GLU:OE2	2.25	0.69
2:H:205:GLN:NE2	2:H:209:GLU:OE2	2.25	0.69
1:G:129:ARG:HH21	1:G:132:ASN:HD21	1.42	0.68
1:D:104:LYS:HG2	1:D:141:VAL:HG12	1.77	0.67
3:C:204:ASN:HD22	11:C:304:PGV:H032	1.59	0.67
1:A:94:ILE:HG22	1:A:184:GLN:HA	1.76	0.66
1:D:304:SER:HB3	1:D:397:LEU:HD11	1.77	0.66
1:A:104:LYS:HG2	1:A:141:VAL:HG12	1.77	0.66
1:A:94:ILE:HG23	1:A:187:LEU:HD23	1.77	0.65
2:B:101:PRO:HG3	2:B:113:LEU:HA	1.78	0.65
3:F:131:PHE:CG	3:F:181:THR:HG21	2.32	0.65
1:G:96:ALA:HB3	1:G:183:GLY:HA3	1.79	0.64
1:G:433:LEU:HD13	1:G:443:ILE:HG22	1.80	0.64
1:A:140:SER:HA	1:A:143:ILE:HD12	1.79	0.64
1:G:37:ASP:OD1	1:G:40:ARG:NH2	2.30	0.64
1:D:140:SER:HA	1:D:143:ILE:HD12	1.78	0.64
2:H:43:ASP:OD1	2:H:47:ARG:NH2	2.32	0.63
1:D:143:ILE:HD11	1:D:466:ALA:HB2	1.79	0.63
3:F:193:VAL:HA	3:F:196:MET:HE2	1.81	0.63
1:A:143:ILE:HD11	1:A:466:ALA:HB2	1.81	0.63
1:D:433:LEU:HD13	1:D:443:ILE:HG22	1.80	0.63
1:D:563:PRO:HG3	2:E:45:MET:HG2	1.80	0.63
3:I:85:ALA:HB1	9:I:302:HEM:HMD2	1.81	0.63
2:H:238:ARG:HG3	3:I:201:GLY:HA3	1.79	0.62
1:A:433:LEU:HD13	1:A:443:ILE:HG22	1.80	0.62
3:I:204:ASN:HD22	11:I:305:PGV:H031	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:ARG:HD2	10:C:305:LMT:H6D	1.81	0.62
1:D:96:ALA:HB3	1:D:183:GLY:HA3	1.81	0.61
3:F:85:ALA:HB1	9:F:302:HEM:HMD3	1.82	0.61
1:A:90:ARG:NH2	2:B:161:GLY:O	2.33	0.61
3:I:135:HIS:CE1	3:I:139:LEU:HD12	2.35	0.61
1:D:290:ILE:HD12	1:D:404:ILE:HD12	1.83	0.61
1:A:563:PRO:HG3	2:B:45:MET:HG2	1.82	0.61
3:C:131:PHE:CG	3:C:181:THR:HG21	2.35	0.61
2:E:189:PRO:HA	2:E:192:GLN:HG2	1.83	0.61
3:F:54:ARG:NH2	9:F:303:HEM:O2A	2.32	0.61
3:I:131:PHE:CG	3:I:181:THR:HG21	2.36	0.61
2:H:247:GLY:O	3:I:1:MET:N	2.33	0.60
1:D:304:SER:H	1:D:397:LEU:HD21	1.66	0.60
1:D:129:ARG:HH21	1:D:132:ASN:HD21	1.50	0.60
9:F:302:HEM:HBC2	9:F:302:HEM:HMC1	1.82	0.60
1:G:143:ILE:HD11	1:G:466:ALA:HB2	1.83	0.60
2:B:68:LEU:HD12	2:B:83:THR:HG21	1.83	0.60
3:I:18:MET:HE1	9:I:302:HEM:HBD1	1.83	0.60
1:A:129:ARG:HH21	1:A:132:ASN:HD21	1.47	0.60
1:D:63:LEU:HD22	1:D:465:LEU:HD21	1.84	0.59
3:I:135:HIS:HE1	3:I:139:LEU:HD12	1.68	0.59
3:F:25:LEU:HB3	9:F:302:HEM:HMB1	1.84	0.59
2:H:50:GLU:OE2	2:H:111:LYS:NZ	2.32	0.59
1:D:37:ASP:OD1	1:D:40:ARG:NH2	2.33	0.59
1:A:96:ALA:HB3	1:A:183:GLY:HA3	1.84	0.59
1:D:101:ASN:OD1	1:D:175:THR:OG1	2.20	0.59
2:E:213:ASN:OD1	3:F:92:SER:OG	2.20	0.59
2:E:170:PRO:HB3	3:F:112:ARG:HH21	1.67	0.58
2:H:100:GLU:OE2	3:I:108:GLY:N	2.35	0.58
1:G:284:GLN:NE2	1:G:455:ARG:O	2.32	0.58
2:E:139:ASP:HB3	2:E:142:THR:HG23	1.85	0.58
2:B:139:ASP:HB3	2:B:142:THR:HG23	1.85	0.58
1:A:37:ASP:OD1	1:A:40:ARG:NH2	2.34	0.58
1:D:94:ILE:HG22	1:D:184:GLN:HA	1.85	0.58
1:D:126:PHE:HE1	1:D:649:VAL:HG12	1.68	0.58
1:D:86:ASP:OD2	1:D:90:ARG:NH1	2.37	0.58
9:C:301:HEM:HBB1	9:C:302:HEM:HBC1	1.87	0.57
1:A:300:LEU:HD22	1:A:419:ALA:HB2	1.85	0.57
1:G:314:TRP:HE1	1:G:377:ASP:HB2	1.69	0.57
1:D:307:LEU:HD21	1:D:397:LEU:HD13	1.85	0.57
2:E:6:LYS:HG2	2:E:19:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ILE:HD13	1:G:224:ILE:HG12	1.86	0.57
1:A:333:ARG:NH1	1:A:377:ASP:OD2	2.37	0.57
2:B:213:ASN:ND2	9:C:301:HEM:O2D	2.36	0.57
1:G:620:GLU:HG2	1:G:621:GLN:HG3	1.86	0.57
2:H:139:ASP:HB3	2:H:142:THR:HG23	1.84	0.57
2:B:105:SER:HA	3:C:98:ALA:HB3	1.86	0.57
1:G:126:PHE:HE1	1:G:649:VAL:HG12	1.69	0.57
1:G:140:SER:HA	1:G:143:ILE:HD12	1.87	0.57
1:A:91:ALA:O	1:A:94:ILE:HG13	2.04	0.57
1:A:126:PHE:HE1	1:A:649:VAL:HG12	1.69	0.57
1:A:293:SER:HA	1:A:369:PRO:HG2	1.87	0.57
1:G:89:ARG:NH2	2:H:159:CYS:O	2.38	0.57
1:G:104:LYS:HG2	1:G:141:VAL:HG12	1.87	0.57
1:A:67:SER:OG	1:A:468:GLY:HA3	2.05	0.56
2:E:100:GLU:OE2	3:F:108:GLY:N	2.38	0.56
2:E:238:ARG:HG3	3:F:201:GLY:HA3	1.87	0.56
1:A:249:TYR:HB3	1:A:264:ALA:HB2	1.86	0.56
2:E:238:ARG:NH1	3:F:201:GLY:O	2.37	0.56
3:F:82:ILE:HG22	10:F:304:LMT:H91	1.88	0.56
1:G:101:ASN:OD1	1:G:175:THR:OG1	2.22	0.56
1:G:290:ILE:HD12	1:G:404:ILE:HD12	1.86	0.56
1:D:620:GLU:OE2	1:D:621:GLN:NE2	2.37	0.56
1:G:401:TYR:O	1:G:405:THR:OG1	2.22	0.56
9:I:302:HEM:HBD2	9:I:302:HEM:HMD1	1.88	0.56
3:I:135:HIS:ND1	3:I:178:TYR:OH	2.30	0.56
1:A:458:ALA:HA	4:A:701:FAD:HN3	1.71	0.56
1:G:249:TYR:HB3	1:G:264:ALA:HB2	1.87	0.56
2:E:57:ASP:HB2	2:E:65:MET:SD	2.46	0.56
1:D:225:ILE:HD13	1:D:236:ARG:HB3	1.88	0.55
3:C:107:TYR:HB2	3:C:110:HIS:HB2	1.88	0.55
3:I:146:TYR:OH	3:I:164:ASN:O	2.23	0.55
1:G:179:ARG:NH1	2:H:155:ASP:OD1	2.28	0.55
2:H:213:ASN:OD1	3:I:92:SER:OG	2.25	0.55
1:D:310:ASP:OD2	1:D:393:ARG:NH1	2.40	0.55
9:F:302:HEM:HBB1	9:F:303:HEM:HBC1	1.89	0.55
1:A:86:ASP:OD2	1:A:90:ARG:NH1	2.38	0.55
2:E:67:SER:HB2	2:E:102:TRP:CE2	2.42	0.55
1:G:304:SER:H	1:G:397:LEU:HD21	1.72	0.55
1:A:519:ASP:OD2	1:A:575:LYS:NZ	2.34	0.55
3:I:202:TRP:HA	11:I:305:PGV:H011	1.89	0.55
2:B:249:GLU:OE2	3:C:9:ARG:NE	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:LEU:HD22	1:G:465:LEU:HD21	1.88	0.54
1:G:63:LEU:O	1:G:67:SER:OG	2.21	0.54
1:G:88:PRO:HG3	1:G:205:MET:HE2	1.90	0.54
1:A:401:TYR:O	1:A:405:THR:OG1	2.22	0.54
1:D:57:ILE:HD13	1:D:224:ILE:HG12	1.89	0.54
2:E:32:SER:HA	2:E:87:HIS:HA	1.90	0.54
1:D:89:ARG:NH2	2:E:159:CYS:O	2.39	0.54
1:G:101:ASN:HB2	1:G:462:MET:HE2	1.90	0.54
3:I:8:THR:O	3:I:14:LYS:NZ	2.40	0.54
1:A:57:ILE:HD13	1:A:224:ILE:HG12	1.89	0.53
1:D:92:HIS:CE1	4:D:701:FAD:HM83	2.43	0.53
1:A:311:GLY:HA2	1:A:377:ASP:O	2.08	0.53
2:E:170:PRO:HG2	2:E:217:ILE:HD13	1.89	0.53
1:D:94:ILE:HD13	2:E:62:ILE:HG23	1.90	0.53
1:D:79:VAL:HB	1:D:203:VAL:HG22	1.90	0.53
2:E:38:ASP:O	2:E:42:GLU:HG2	2.08	0.53
1:A:79:VAL:HB	1:A:203:VAL:HG22	1.89	0.53
2:H:169:CYS:O	3:I:106:ARG:NH1	2.36	0.53
1:A:358:LYS:NZ	1:A:362:ASP:OD2	2.34	0.53
2:B:66:CYS:HB3	2:B:83:THR:HB	1.89	0.53
3:C:192:GLY:HA2	3:C:195:SER:HB2	1.90	0.53
2:H:57:ASP:HB2	2:H:65:MET:HG3	1.91	0.53
1:A:94:ILE:HD13	2:B:62:ILE:HG23	1.91	0.53
2:B:5:LEU:HD23	2:B:97:ILE:HB	1.91	0.53
1:G:519:ASP:OD2	1:G:575:LYS:NZ	2.40	0.53
1:A:89:ARG:NH2	2:B:159:CYS:O	2.43	0.52
1:D:284:GLN:NE2	1:D:455:ARG:O	2.40	0.52
1:D:39:HIS:HD2	1:D:43:MET:HE2	1.74	0.52
12:C:306:PEV:H322	12:C:306:PEV:H122	1.91	0.52
1:A:101:ASN:OD1	1:A:175:THR:OG1	2.25	0.52
1:A:171:GLN:NE2	1:D:47:ASN:OD1	2.41	0.52
1:D:63:LEU:O	1:D:67:SER:OG	2.20	0.52
3:I:74:LEU:HD22	12:I:307:PEV:H252	1.92	0.52
1:A:63:LEU:HD22	1:A:465:LEU:HD21	1.92	0.52
1:D:460:ALA:HB3	4:D:701:FAD:N1	2.25	0.52
1:A:284:GLN:NE2	1:A:455:ARG:O	2.34	0.52
2:B:108:PRO:HD2	2:B:116:ASP:HB3	1.91	0.52
3:C:146:TYR:OH	3:C:164:ASN:O	2.26	0.52
1:D:253:PHE:CG	1:D:420:VAL:HG21	2.45	0.52
2:B:189:PRO:HA	2:B:192:GLN:HG2	1.92	0.51
1:A:620:GLU:OE2	1:A:621:GLN:NE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HB2	1:A:535:MET:HE1	1.91	0.51
2:H:38:ASP:O	2:H:42:GLU:HG2	2.10	0.51
1:G:94:ILE:HD12	1:G:187:LEU:HB3	1.93	0.51
2:H:70:ILE:HB	2:H:76:GLY:HA2	1.93	0.51
2:H:170:PRO:HG2	2:H:217:ILE:HD13	1.92	0.51
2:H:195:ARG:NH2	2:H:239:ASP:OD1	2.43	0.51
2:E:70:ILE:HB	2:E:76:GLY:HA2	1.93	0.51
1:G:620:GLU:OE2	1:G:621:GLN:NE2	2.43	0.51
2:B:247:GLY:O	3:C:1:MET:N	2.44	0.51
3:C:117:ALA:O	3:C:121:MET:HB2	2.11	0.51
1:D:254:TYR:CZ	1:D:298:SER:HB2	2.46	0.51
1:D:445:GLU:OE1	4:D:701:FAD:O4'	2.25	0.51
2:E:213:ASN:ND2	9:F:302:HEM:O2D	2.43	0.51
3:F:112:ARG:HD2	3:F:116:TYR:CD2	2.45	0.51
1:G:287:PRO:HD3	1:G:350:ARG:HD3	1.92	0.51
1:G:376:LEU:HB3	1:G:414:MET:HG2	1.92	0.51
1:A:111:ASP:HA	1:A:115:ARG:HD2	1.91	0.51
2:E:108:PRO:HD2	2:E:116:ASP:HB3	1.91	0.51
2:B:111:LYS:HG3	2:B:112:ASP:H	1.75	0.51
1:D:107:ARG:HG3	1:D:173:ALA:HB3	1.92	0.51
1:D:293:SER:HA	1:D:369:PRO:HG2	1.93	0.51
2:E:71:ASN:O	3:F:111:LYS:HE2	2.11	0.51
2:E:176:LEU:HD22	2:E:220:CYS:HB2	1.93	0.51
2:B:75:HIS:CD2	2:B:225:PRO:HG3	2.46	0.50
2:B:116:ASP:OD1	2:B:118:SER:OG	2.27	0.50
2:B:238:ARG:HG3	3:C:201:GLY:HA3	1.92	0.50
3:I:125:GLY:O	9:I:302:HEM:HBC2	2.11	0.50
2:E:197:GLN:HA	2:E:248:ILE:HG21	1.92	0.50
1:D:377:ASP:HB3	1:D:413:PRO:HB3	1.94	0.50
2:E:103:ARG:HG2	3:F:107:TYR:CE1	2.47	0.50
1:G:276:PHE:HB3	1:G:627:ALA:HB1	1.94	0.50
2:H:72:GLY:HA2	3:I:109:GLN:O	2.12	0.50
2:H:189:PRO:HA	2:H:192:GLN:HG2	1.93	0.50
2:H:197:GLN:HA	2:H:248:ILE:HG21	1.94	0.50
3:C:97:GLN:HA	3:C:97:GLN:OE1	2.11	0.50
2:B:70:ILE:HB	2:B:76:GLY:HA2	1.94	0.50
3:F:146:TYR:OH	3:F:164:ASN:O	2.27	0.50
1:A:302:LEU:HD22	4:A:701:FAD:HM73	1.94	0.49
2:E:72:GLY:HA2	3:F:109:GLN:O	2.12	0.49
2:H:100:GLU:HG2	2:H:103:ARG:HH21	1.77	0.49
2:H:215:THR:N	8:H:303:F3S:S4	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:69:ILE:HD11	12:I:301:PEV:H382	1.94	0.49
1:A:285:ILE:HD13	1:A:535:MET:HG2	1.94	0.49
2:B:195:ARG:NH2	2:B:239:ASP:OD1	2.42	0.49
2:B:170:PRO:HG2	2:B:217:ILE:HD13	1.95	0.49
2:H:181:LYS:HB3	2:H:202:MET:HE1	1.93	0.49
1:A:179:ARG:NH1	2:B:155:ASP:OD1	2.30	0.49
1:A:104:LYS:NZ	1:A:145:ASP:OD1	2.34	0.49
1:A:136:LEU:HD11	1:A:462:MET:HG2	1.95	0.49
1:D:92:HIS:O	1:D:93:SER:OG	2.24	0.49
1:A:129:ARG:HH21	1:A:132:ASN:ND2	2.11	0.49
1:A:509:LEU:HD22	1:A:576:ALA:HB1	1.93	0.49
2:B:24:MET:HE2	2:B:36:MET:HG3	1.94	0.49
1:D:249:TYR:HB3	1:D:264:ALA:HB2	1.94	0.49
1:D:509:LEU:HD22	1:D:576:ALA:HB1	1.95	0.49
2:H:67:SER:HB2	2:H:102:TRP:CE2	2.48	0.49
2:H:217:ILE:HD11	3:I:118:ASP:HB3	1.95	0.49
2:E:101:PRO:HG3	2:E:113:LEU:HA	1.93	0.49
2:H:75:HIS:CD2	2:H:225:PRO:HG3	2.47	0.48
2:H:111:LYS:HG3	2:H:112:ASP:H	1.78	0.48
1:D:85:GLN:NE2	2:E:57:ASP:OD2	2.45	0.48
4:D:701:FAD:O3'	4:D:701:FAD:H9	2.14	0.48
2:H:186:ALA:O	2:H:192:GLN:NE2	2.40	0.48
2:B:38:ASP:O	2:B:42:GLU:HG2	2.14	0.48
2:B:181:LYS:HB3	2:B:202:MET:HE1	1.94	0.48
3:C:18:MET:HG3	3:C:84:ALA:HB3	1.95	0.48
3:F:135:HIS:CE1	3:F:139:LEU:HD12	2.49	0.48
1:D:296:TYR:CE1	2:E:31:MET:HG3	2.49	0.48
2:E:63:CYS:SG	2:E:65:MET:HG2	2.54	0.48
3:F:226:ASN:O	9:F:303:HEM:HBB1	2.14	0.48
1:G:509:LEU:HD22	1:G:576:ALA:HB1	1.95	0.48
1:A:336:TYR:O	1:A:337:LEU:HB2	2.13	0.48
1:A:620:GLU:HG2	1:A:621:GLN:HG3	1.95	0.48
1:D:94:ILE:HD12	1:D:95:ALA:N	2.29	0.48
3:F:192:GLY:HA2	3:F:195:SER:HB2	1.95	0.48
1:G:107:ARG:HG3	1:G:173:ALA:HB3	1.96	0.48
3:I:28:PHE:CD1	3:I:74:LEU:HD11	2.48	0.48
2:H:101:PRO:HG3	2:H:113:LEU:HA	1.96	0.48
2:H:238:ARG:NH1	3:I:201:GLY:O	2.42	0.48
1:A:265:THR:O	1:A:269:ARG:HG2	2.14	0.48
1:A:276:PHE:HB3	1:A:627:ALA:HB1	1.96	0.48
1:D:358:LYS:HB2	1:D:535:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:VAL:HB	1:D:447:ASN:HB3	1.95	0.48
1:D:461:LEU:HG	4:D:701:FAD:C2	2.44	0.48
2:E:195:ARG:NH2	2:E:239:ASP:OD1	2.46	0.48
3:F:18:MET:HE2	3:F:88:LEU:HD12	1.96	0.48
2:H:68:LEU:HD12	2:H:83:THR:HG21	1.96	0.48
1:D:51:ARG:HG2	1:D:77:TYR:CZ	2.49	0.47
3:F:139:LEU:HD13	9:F:303:HEM:HMA1	1.96	0.47
1:G:79:VAL:HB	1:G:203:VAL:HG22	1.95	0.47
1:A:126:PHE:O	1:A:127:ARG:NH1	2.46	0.47
3:C:195:SER:O	3:C:199:THR:OG1	2.30	0.47
1:D:288:THR:HG22	1:D:303:MET:HE3	1.96	0.47
1:A:244:LEU:HG	1:A:440:LEU:HD11	1.96	0.47
2:B:197:GLN:HA	2:B:248:ILE:HG21	1.95	0.47
3:C:186:ALA:HB2	3:C:223:PHE:HB2	1.97	0.47
1:A:254:TYR:CZ	1:A:298:SER:HB2	2.50	0.47
1:A:292:VAL:HB	1:A:297:GLN:HB3	1.97	0.47
2:B:183:THR:HG23	2:B:235:GLN:HG2	1.97	0.47
3:C:65:HIS:ND1	3:I:34:TYR:OH	2.33	0.47
3:C:203:ASN:HD21	3:C:208:ASP:HA	1.78	0.47
2:E:68:LEU:HD12	2:E:83:THR:HG21	1.97	0.47
3:F:28:PHE:CD1	3:F:74:LEU:HD11	2.49	0.47
1:A:442:VAL:HB	1:A:447:ASN:HB3	1.97	0.47
2:E:75:HIS:CD2	2:E:225:PRO:HG3	2.50	0.47
2:H:170:PRO:HB3	3:I:112:ARG:NH2	2.30	0.47
3:C:204:ASN:OD1	3:C:206:THR:OG1	2.23	0.47
2:E:111:LYS:HG3	2:E:112:ASP:H	1.80	0.47
2:H:10:GLN:H	2:H:112:ASP:HA	1.80	0.47
2:H:24:MET:HE2	2:H:36:MET:HG3	1.97	0.47
1:A:132:ASN:HB3	1:A:450:ASP:OD1	2.15	0.47
2:B:170:PRO:O	3:C:96:LEU:HD11	2.15	0.47
1:D:111:ASP:HA	1:D:115:ARG:HD2	1.95	0.47
2:E:116:ASP:OD1	2:E:118:SER:OG	2.31	0.47
1:G:535:MET:HE3	1:G:535:MET:HB2	1.73	0.47
1:G:285:ILE:HD13	1:G:535:MET:SD	2.55	0.46
1:G:38:LYS:O	1:G:42:GLU:HG3	2.16	0.46
1:G:111:ASP:HA	1:G:115:ARG:HD2	1.96	0.46
1:A:535:MET:HB2	1:A:535:MET:HE3	1.72	0.46
2:B:31:MET:HE3	2:B:36:MET:HB2	1.98	0.46
1:D:91:ALA:O	1:D:94:ILE:HG13	2.15	0.46
3:C:135:HIS:NE2	9:C:302:HEM:NB	2.64	0.46
1:D:61:SER:OG	1:D:88:PRO:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:ARG:NH2	1:G:490:ILE:O	2.48	0.46
3:C:28:PHE:CD1	3:C:74:LEU:HD11	2.50	0.46
3:C:85:ALA:HB1	9:C:301:HEM:HMD3	1.97	0.46
2:H:231:GLU:OE2	3:I:205:ARG:NE	2.45	0.46
1:D:336:TYR:CD2	1:D:337:LEU:HD13	2.51	0.46
2:E:56:HIS:CE1	2:E:59:ARG:HH21	2.33	0.46
1:A:107:ARG:HH11	1:A:164:ASN:HB2	1.80	0.46
1:D:39:HIS:CD2	1:D:43:MET:HE2	2.51	0.46
3:I:18:MET:HE1	9:I:302:HEM:CBD	2.44	0.46
1:D:336:TYR:O	1:D:337:LEU:HB2	2.16	0.46
2:E:5:LEU:HD23	2:E:97:ILE:HB	1.98	0.46
1:A:99:GLY:HA2	1:A:182:THR:HG21	1.98	0.45
3:C:25:LEU:CB	9:C:301:HEM:HMB3	2.46	0.45
1:D:39:HIS:O	1:D:43:MET:HG3	2.16	0.45
1:D:599:SER:HB2	1:D:616:LEU:H	1.81	0.45
1:A:23:LEU:HD21	1:A:276:PHE:HD2	1.81	0.45
2:B:217:ILE:O	3:C:114:SER:OG	2.31	0.45
3:F:122:ARG:HD2	10:F:306:LMT:H6D	1.98	0.45
3:I:147:GLU:HB2	3:I:150:GLN:HG3	1.98	0.45
3:I:186:ALA:HB2	3:I:223:PHE:HB2	1.98	0.45
1:D:85:GLN:HE21	2:E:57:ASP:CG	2.24	0.45
2:E:178:THR:HG23	2:E:202:MET:HE2	1.98	0.45
9:I:302:HEM:HMD1	9:I:302:HEM:CBD	2.46	0.45
1:D:506:ILE:HG23	1:D:573:LEU:HD21	1.98	0.45
1:A:599:SER:HB2	1:A:616:LEU:H	1.81	0.45
1:D:401:TYR:O	1:D:405:THR:OG1	2.27	0.45
1:G:61:SER:OG	1:G:88:PRO:HB3	2.16	0.45
1:G:93:SER:HB2	1:G:187:LEU:HD22	1.98	0.45
2:B:157:ALA:HB2	2:B:184:HIS:CD2	2.51	0.45
1:G:314:TRP:HB3	1:G:335:TYR:CD1	2.52	0.45
1:D:90:ARG:HD2	2:E:65:MET:HB3	1.99	0.45
2:E:70:ILE:HD11	2:E:83:THR:HG23	1.98	0.45
3:F:65:HIS:CD2	12:F:301:PEV:H131	2.51	0.45
1:D:317:LYS:HD2	1:D:334:ASP:HB2	1.99	0.45
1:D:336:TYR:OH	1:D:374:VAL:HG11	2.17	0.45
1:D:535:MET:HE3	1:D:535:MET:HB2	1.73	0.45
3:F:209:ARG:HA	3:F:209:ARG:HD2	1.84	0.45
1:A:424:MET:HE2	1:A:424:MET:HB2	1.80	0.45
1:D:286:HIS:HB3	1:D:289:CYS:SG	2.57	0.45
2:E:24:MET:HE2	2:E:24:MET:HB3	1.82	0.45
1:G:254:TYR:CZ	1:G:298:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:PRO:HG2	1:G:332:GLU:HG3	2.00	0.45
3:I:26:VAL:HG22	3:I:189:LEU:HD22	1.99	0.45
3:I:151:PHE:HE2	3:I:153:HIS:CD2	2.35	0.45
2:B:167:ALA:O	3:C:106:ARG:NH2	2.50	0.44
1:D:286:HIS:CD2	1:D:302:LEU:HG	2.52	0.44
1:G:403:GLN:NE2	2:H:85:GLN:O	2.47	0.44
1:A:33:GLU:HA	1:A:134:TYR:CE1	2.53	0.44
1:A:263:ASN:HA	1:A:582:PHE:CZ	2.51	0.44
1:A:461:LEU:HG	4:A:701:FAD:C2	2.46	0.44
1:A:592:ASP:OD1	1:A:628:TRP:NE1	2.47	0.44
1:G:99:GLY:HA2	1:G:182:THR:HG21	1.99	0.44
2:H:5:LEU:HD23	2:H:97:ILE:HB	2.00	0.44
2:B:238:ARG:NH1	3:C:201:GLY:O	2.41	0.44
2:E:50:GLU:OE2	2:E:111:LYS:NZ	2.40	0.44
3:I:33:MET:HE3	3:I:33:MET:HB3	1.84	0.44
3:I:178:TYR:O	3:I:182:MET:HG2	2.17	0.44
3:F:112:ARG:HD3	3:F:115:GLY:O	2.17	0.44
2:H:103:ARG:HG2	3:I:107:TYR:CE2	2.52	0.44
2:B:123:ILE:HA	2:B:205:GLN:HG2	1.99	0.44
3:C:126:VAL:HG21	10:C:305:LMT:H41	1.98	0.44
3:C:223:PHE:O	3:C:227:ILE:HG12	2.18	0.44
1:D:85:GLN:HB3	1:D:90:ARG:HB2	1.99	0.44
1:D:366:GLY:HA2	1:D:371:GLY:HA2	1.98	0.44
2:E:157:ALA:HB2	2:E:184:HIS:CD2	2.52	0.44
2:B:70:ILE:HD11	2:B:83:THR:HG23	2.00	0.44
3:C:112:ARG:HG3	3:C:116:TYR:CE2	2.53	0.44
1:G:358:LYS:HB2	1:G:535:MET:HE1	1.99	0.44
3:I:18:MET:HE2	3:I:88:LEU:HD12	1.99	0.44
3:I:93:ARG:O	3:I:97:GLN:HG2	2.18	0.44
1:A:107:ARG:HD2	1:A:164:ASN:HB2	2.00	0.44
3:C:15:LYS:NZ	9:C:301:HEM:O1D	2.51	0.44
1:D:424:MET:HE2	1:D:424:MET:HB2	1.84	0.44
2:E:66:CYS:SG	2:E:82:THR:HB	2.58	0.44
2:H:176:LEU:HD22	2:H:220:CYS:HB2	2.00	0.44
1:A:255:LEU:HD12	1:A:292:VAL:HG11	2.00	0.43
1:A:355:ARG:HD2	1:A:536:ALA:HB2	2.00	0.43
2:B:186:ALA:O	2:B:192:GLN:NE2	2.46	0.43
2:E:105:SER:HA	3:F:98:ALA:HB3	2.00	0.43
1:G:283:THR:HG22	1:G:423:THR:HG22	1.98	0.43
3:I:54:ARG:HH22	9:I:303:HEM:CGA	2.31	0.43
1:A:96:ALA:HA	4:A:701:FAD:C6	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:HB2	5:A:702:SIN:H22	1.99	0.43
1:G:192:GLN:HB3	2:H:129:TYR:HB3	2.00	0.43
1:A:359:GLN:O	1:A:359:GLN:NE2	2.41	0.43
1:D:88:PRO:HG3	1:D:205:MET:HE2	2.00	0.43
1:G:516:ARG:O	1:G:561:ASN:N	2.50	0.43
2:H:56:HIS:CE1	2:H:59:ARG:HH21	2.36	0.43
3:I:194:TRP:HE1	3:I:203:ASN:HD21	1.67	0.43
2:B:238:ARG:HD3	11:C:304:PGV:H22	2.00	0.43
1:D:269:ARG:HA	1:D:269:ARG:HD2	1.81	0.43
1:G:52:ARG:H	1:G:52:ARG:HG3	1.63	0.43
1:G:286:HIS:CD2	1:G:302:LEU:HG	2.53	0.43
3:I:55:GLU:HG2	3:I:58:TYR:HB2	2.00	0.43
1:D:281:CYS:HB2	1:D:537:ARG:HH12	1.83	0.43
2:E:10:GLN:H	2:E:112:ASP:HA	1.83	0.43
3:F:121:MET:HE3	9:F:302:HEM:CHA	2.48	0.43
1:G:281:CYS:HB2	1:G:537:ARG:HH12	1.83	0.43
3:C:33:MET:HE3	3:C:33:MET:HB3	1.78	0.43
3:C:229:PHE:HB2	3:C:230:PRO:HD3	2.01	0.43
1:D:192:GLN:HB3	2:E:129:TYR:HB3	2.00	0.43
2:E:169:CYS:O	3:F:106:ARG:NH1	2.38	0.43
3:F:194:TRP:HE1	3:F:203:ASN:HD21	1.66	0.43
2:H:110:LEU:HD21	2:H:116:ASP:HB2	2.00	0.43
3:F:129:PHE:HB2	9:F:302:HEM:HBC2	2.01	0.43
1:G:92:HIS:HD2	4:G:701:FAD:O1A	2.01	0.43
1:G:265:THR:O	1:G:269:ARG:HG2	2.19	0.43
1:G:589:MET:HE2	1:G:589:MET:HB3	1.95	0.43
3:I:212:ARG:O	3:I:216:ILE:HG13	2.19	0.43
1:A:253:PHE:CG	1:A:420:VAL:HG21	2.53	0.43
3:C:36:ASN:O	3:C:39:MET:HG2	2.19	0.43
3:C:193:VAL:HA	3:C:196:MET:HE2	2.01	0.43
1:G:244:LEU:HG	1:G:440:LEU:HD11	2.01	0.43
3:C:15:LYS:HG2	3:C:88:LEU:HD13	2.01	0.42
3:F:135:HIS:ND1	3:F:178:TYR:OH	2.46	0.42
1:A:205:MET:HG3	1:A:207:PRO:HD3	2.00	0.42
1:D:251:ASN:ND2	1:D:262:CYS:HB2	2.35	0.42
2:E:28:ASN:HB3	2:E:31:MET:HB2	1.99	0.42
3:F:15:LYS:HA	3:F:15:LYS:HD2	1.76	0.42
2:B:141:ASN:ND2	2:E:136:SER:O	2.51	0.42
1:D:325:PRO:HB2	1:D:413:PRO:HG2	2.00	0.42
3:F:26:VAL:HG22	3:F:189:LEU:HD22	2.01	0.42
2:H:45:MET:HG2	2:H:51:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:ARG:HE	2:H:209:GLU:CD	2.27	0.42
1:A:121:VAL:HG23	1:A:133:VAL:HG11	2.00	0.42
2:B:122:ARG:HE	2:B:209:GLU:CD	2.27	0.42
3:C:8:THR:O	3:C:14:LYS:NZ	2.53	0.42
3:I:44:GLU:H	3:I:44:GLU:HG2	1.64	0.42
3:I:171:ASN:HB3	3:I:174:ILE:HG12	2.02	0.42
1:D:121:VAL:HG23	1:D:133:VAL:HG11	2.01	0.42
1:D:276:PHE:CD2	1:D:436:THR:HG21	2.54	0.42
1:G:91:ALA:HB1	4:G:701:FAD:O1A	2.19	0.42
1:G:599:SER:HB2	1:G:616:LEU:H	1.84	0.42
2:H:41:ASN:O	2:H:45:MET:HG3	2.20	0.42
2:H:105:SER:HA	3:I:98:ALA:HB3	2.01	0.42
1:A:284:GLN:HB2	1:A:424:MET:SD	2.60	0.42
1:A:525:LEU:HD13	1:A:583:LEU:HD23	2.02	0.42
1:D:352:ILE:HG13	1:D:355:ARG:HH22	1.85	0.42
1:G:121:VAL:HG23	1:G:133:VAL:HG11	2.01	0.42
2:H:183:THR:HG23	2:H:235:GLN:HG2	2.00	0.42
1:A:336:TYR:OH	1:A:374:VAL:HG11	2.20	0.42
1:A:478:ASN:O	1:A:482:GLN:HG3	2.19	0.42
1:D:243:VAL:HA	1:D:441:PHE:O	2.20	0.42
1:D:292:VAL:HB	1:D:297:GLN:HB3	2.02	0.42
1:D:459:SER:HA	1:D:462:MET:HE3	2.01	0.42
3:F:223:PHE:O	3:F:227:ILE:HG12	2.19	0.42
1:G:305:GLU:HG3	5:G:702:SIN:C1	2.50	0.42
2:H:70:ILE:HD11	2:H:83:THR:HG23	2.02	0.42
2:H:217:ILE:O	3:I:114:SER:HB3	2.20	0.42
1:A:227:ARG:HB2	1:A:234:ILE:HD13	2.01	0.42
2:E:122:ARG:HE	2:E:209:GLU:CD	2.28	0.42
3:F:54:ARG:HH22	9:F:303:HEM:CGA	2.31	0.42
1:G:126:PHE:O	1:G:127:ARG:NH1	2.52	0.42
1:G:132:ASN:OD1	1:G:132:ASN:N	2.52	0.42
1:G:188:LEU:HD23	1:G:188:LEU:HA	1.90	0.42
1:A:165:ARG:O	1:A:175:THR:HB	2.20	0.42
1:G:263:ASN:HA	1:G:582:PHE:CZ	2.55	0.42
2:H:175:MET:HG2	2:H:214:CYS:HB2	2.00	0.42
1:A:299:LYS:NZ	2:B:58:CYS:O	2.45	0.42
3:F:204:ASN:HD22	11:F:305:PGV:H011	1.85	0.42
1:A:102:ALA:HA	1:A:140:SER:HB2	2.01	0.41
1:A:166:SER:HB2	1:D:48:PRO:HG2	2.02	0.41
1:A:314:TRP:HE1	1:A:377:ASP:HB2	1.85	0.41
2:E:126:ALA:O	2:E:201:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:GLN:OE1	1:G:185:GLN:NE2	2.53	0.41
1:G:292:VAL:HB	1:G:297:GLN:HB3	2.02	0.41
1:G:355:ARG:HD2	1:G:536:ALA:HB2	2.02	0.41
1:A:136:LEU:HG	1:A:462:MET:HE3	2.02	0.41
2:E:181:LYS:HA	2:E:181:LYS:HD3	1.82	0.41
2:E:199:VAL:HG11	2:E:239:ASP:HB3	2.02	0.41
9:F:302:HEM:HBC2	9:F:302:HEM:CMC	2.50	0.41
1:G:165:ARG:O	1:G:175:THR:HB	2.20	0.41
2:H:82:THR:OG1	2:H:84:CYS:SG	2.78	0.41
1:A:524:GLU:HG2	1:A:552:ILE:HD13	2.02	0.41
12:C:307:PEV:H322	12:C:307:PEV:H352	1.89	0.41
1:D:129:ARG:HE	1:D:132:ASN:HD21	1.66	0.41
1:D:276:PHE:HB3	1:D:627:ALA:HB1	2.02	0.41
1:D:460:ALA:N	4:D:701:FAD:O2	2.54	0.41
3:I:223:PHE:O	3:I:227:ILE:HG12	2.20	0.41
10:I:304:LMT:H5B	10:I:304:LMT:H6D	2.02	0.41
2:B:10:GLN:H	2:B:112:ASP:HA	1.86	0.41
2:B:24:MET:HE3	2:B:24:MET:HB3	1.91	0.41
3:C:75:LEU:HA	3:C:75:LEU:HD23	1.81	0.41
3:C:131:PHE:CD2	3:C:181:THR:HG21	2.54	0.41
1:D:33:GLU:HA	1:D:134:TYR:CE1	2.54	0.41
1:D:165:ARG:O	1:D:175:THR:HB	2.20	0.41
1:D:263:ASN:HA	1:D:582:PHE:CZ	2.54	0.41
1:D:265:THR:O	1:D:269:ARG:HG2	2.19	0.41
3:F:121:MET:HE2	3:F:191:HIS:HD2	1.84	0.41
1:G:365:ARG:HA	1:G:365:ARG:HD3	1.81	0.41
1:G:545:ALA:O	1:G:549:ILE:HG12	2.20	0.41
1:A:460:ALA:N	4:A:701:FAD:O2	2.53	0.41
2:E:215:THR:N	8:E:303:F3S:S2	2.93	0.41
1:G:524:GLU:HG2	1:G:552:ILE:HD13	2.02	0.41
2:H:242:MET:HE2	2:H:242:MET:HB2	1.88	0.41
2:H:242:MET:O	2:H:246:ARG:HG3	2.21	0.41
3:I:182:MET:SD	3:I:226:ASN:HB3	2.61	0.41
1:A:184:GLN:OE1	1:A:185:GLN:NE2	2.53	0.41
1:A:502:ILE:HD13	1:A:502:ILE:HA	1.86	0.41
3:C:192:GLY:O	3:C:196:MET:HG2	2.21	0.41
2:H:104:ALA:HB3	2:H:107:PHE:HB2	2.02	0.41
1:A:255:LEU:HD13	1:A:298:SER:HA	2.02	0.41
1:A:404:ILE:HA	2:B:87:HIS:NE2	2.35	0.41
1:D:236:ARG:HD3	1:D:495:PHE:HB3	2.02	0.41
3:F:75:LEU:HD23	3:F:75:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284:GLN:HB2	1:G:424:MET:SD	2.61	0.41
2:H:157:ALA:HB2	2:H:184:HIS:CD2	2.56	0.41
1:A:94:ILE:HD12	1:A:95:ALA:N	2.35	0.41
1:A:299:LYS:HG2	2:B:59:ARG:HB2	2.03	0.41
1:A:307:LEU:HD23	1:A:397:LEU:HD13	2.03	0.41
3:C:25:LEU:HB2	9:C:301:HEM:HMB3	2.01	0.41
3:C:139:LEU:HD13	9:C:302:HEM:HMA1	2.01	0.41
1:D:358:LYS:NZ	1:D:362:ASP:OD2	2.53	0.41
1:A:57:ILE:HG13	1:A:239:ALA:HB2	2.03	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.90	0.41
1:A:271:HIS:HA	1:A:275:ALA:O	2.21	0.41
1:D:23:LEU:HD21	1:D:276:PHE:HD2	1.85	0.41
1:D:348:VAL:HG12	1:D:349:PRO:HD2	2.03	0.41
2:E:78:LYS:HB3	2:E:81:ILE:HD11	2.03	0.41
3:I:132:ILE:O	3:I:136:ILE:HG12	2.21	0.41
1:A:144:ILE:HD13	1:A:144:ILE:HA	1.86	0.41
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.93	0.41
1:A:460:ALA:HB3	4:A:701:FAD:N1	2.35	0.41
1:G:144:ILE:HD13	1:G:144:ILE:HA	1.84	0.41
3:C:26:VAL:HG22	3:C:189:LEU:HD22	2.02	0.40
1:D:101:ASN:HB2	1:D:462:MET:HE2	2.03	0.40
2:E:11:LYS:HB2	2:E:11:LYS:HE3	1.76	0.40
1:G:424:MET:HB2	1:G:424:MET:HE2	1.78	0.40
1:A:366:GLY:HA2	1:A:371:GLY:HA2	2.03	0.40
1:A:516:ARG:O	1:A:561:ASN:N	2.50	0.40
1:D:388:GLN:CD	1:D:388:GLN:H	2.30	0.40
3:I:131:PHE:CD2	3:I:181:THR:HG21	2.56	0.40
1:A:252:VAL:HG11	1:A:589:MET:SD	2.60	0.40
2:B:181:LYS:HA	2:B:181:LYS:HD3	1.82	0.40
3:C:178:TYR:O	3:C:182:MET:HG2	2.22	0.40
1:D:102:ALA:HA	1:D:140:SER:HB2	2.03	0.40
1:D:205:MET:HG3	1:D:207:PRO:HD3	2.03	0.40
3:I:43:PRO:HB3	3:I:162:TYR:CD2	2.57	0.40
3:C:132:ILE:O	3:C:136:ILE:HG12	2.22	0.40
1:G:442:VAL:HB	1:G:447:ASN:HB3	2.03	0.40
2:H:116:ASP:OD1	2:H:118:SER:OG	2.38	0.40
1:D:524:GLU:HG2	1:D:552:ILE:HD13	2.03	0.40
1:G:563:PRO:HG3	2:H:45:MET:HG2	2.04	0.40
2:H:191:GLY:O	2:H:195:ARG:HB3	2.21	0.40
3:I:209:ARG:HA	3:I:209:ARG:HD2	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	629/657 (96%)	621 (99%)	8 (1%)	0	100	100
1	D	629/657 (96%)	616 (98%)	13 (2%)	0	100	100
1	G	629/657 (96%)	619 (98%)	10 (2%)	0	100	100
2	B	255/260 (98%)	247 (97%)	8 (3%)	0	100	100
2	E	255/260 (98%)	247 (97%)	8 (3%)	0	100	100
2	H	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
3	C	237/239 (99%)	231 (98%)	6 (2%)	0	100	100
3	F	237/239 (99%)	235 (99%)	2 (1%)	0	100	100
3	I	237/239 (99%)	234 (99%)	3 (1%)	0	100	100
All	All	3363/3468 (97%)	3298 (98%)	65 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/529 (95%)	494 (98%)	10 (2%)	48	76
1	D	504/529 (95%)	494 (98%)	10 (2%)	48	76
1	G	504/529 (95%)	500 (99%)	4 (1%)	73	88
2	B	209/212 (99%)	209 (100%)	0	100	100
2	E	209/212 (99%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	209/212 (99%)	208 (100%)	1 (0%)	81	92
3	C	198/198 (100%)	197 (100%)	1 (0%)	81	92
3	F	198/198 (100%)	197 (100%)	1 (0%)	81	92
3	I	198/198 (100%)	195 (98%)	3 (2%)	57	81
All	All	2733/2817 (97%)	2703 (99%)	30 (1%)	63	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	94	ILE
1	A	175	THR
1	A	235	THR
1	A	257	THR
1	A	348	VAL
1	A	442	VAL
1	A	450	ASP
1	A	476	ILE
1	A	595	HIS
3	C	78	VAL
1	D	86	ASP
1	D	94	ILE
1	D	175	THR
1	D	236	ARG
1	D	299	LYS
1	D	337	LEU
1	D	348	VAL
1	D	367	VAL
1	D	442	VAL
1	D	595	HIS
3	F	78	VAL
1	G	235	THR
1	G	367	VAL
1	G	517	THR
1	G	595	HIS
2	H	102	TRP
3	I	78	VAL
3	I	153	HIS
3	I	188	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	105	ASN
1	A	171	GLN
1	A	185	GLN
1	A	346	ASN
1	A	432	ASN
1	A	571	GLN
3	C	163	ASN
3	C	203	ASN
1	D	47	ASN
1	D	132	ASN
1	D	164	ASN
1	D	185	GLN
2	E	235	GLN
1	G	185	GLN
1	G	197	GLN
1	G	286	HIS
1	G	359	GLN
1	G	559	ASN
3	I	63	HIS
3	I	153	HIS
3	I	163	ASN

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](#)

36 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
9	HEM	F	302	3	50,50,50	1.59	8 (16%)	66,82,82	1.80	16 (24%)
8	F3S	E	303	2	0,9,9	-	-	-		
11	PGV	C	304	-	30,30,50	0.62	0	33,36,56	0.56	0
9	HEM	I	302	3	50,50,50	1.59	7 (14%)	66,82,82	1.62	11 (16%)
9	HEM	I	303	3	50,50,50	1.55	7 (14%)	66,82,82	1.71	15 (22%)
10	LMT	C	305	-	29,29,36	1.29	5 (17%)	40,40,47	1.11	3 (7%)
6	SF4	H	301	2	0,12,12	-	-	-		
10	LMT	F	306	-	29,29,36	1.25	5 (17%)	40,40,47	0.99	2 (5%)
9	HEM	F	303	3	50,50,50	1.60	7 (14%)	66,82,82	1.66	12 (18%)
5	SIN	D	702	-	7,7,7	1.02	0	8,8,8	1.66	1 (12%)
6	SF4	E	301	2	0,12,12	-	-	-		
5	SIN	G	702	-	7,7,7	1.02	0	8,8,8	1.66	1 (12%)
10	LMT	C	303	-	35,35,36	1.14	5 (14%)	46,46,47	0.98	3 (6%)
9	HEM	C	302	3	50,50,50	1.56	7 (14%)	66,82,82	1.73	13 (19%)
7	FES	B	302	2	0,4,4	-	-	-		
12	PEV	F	301	-	43,43,48	0.49	0	46,48,53	0.57	0
7	FES	H	302	2	0,4,4	-	-	-		
12	PEV	I	301	-	43,43,48	0.50	0	46,48,53	0.53	0
4	FAD	G	701	-	56,58,58	0.33	0	81,89,89	0.32	1 (1%)
10	LMT	I	306	-	30,30,36	1.28	5 (16%)	41,41,47	1.08	2 (4%)
4	FAD	D	701	-	56,58,58	0.35	0	81,89,89	0.36	0
12	PEV	C	306	-	48,48,48	0.48	0	51,53,53	0.50	0
12	PEV	I	307	-	48,48,48	0.48	0	51,53,53	0.49	0
4	FAD	A	701	-	56,58,58	0.34	0	81,89,89	0.29	0
12	PEV	F	307	-	48,48,48	0.47	0	51,53,53	0.50	0
5	SIN	A	702	-	7,7,7	1.01	0	8,8,8	1.66	2 (25%)
7	FES	E	302	2	0,4,4	-	-	-		
10	LMT	I	304	-	36,36,36	1.16	6 (16%)	47,47,47	1.07	2 (4%)
8	F3S	B	303	2	0,9,9	-	-	-		
9	HEM	C	301	3	50,50,50	1.58	7 (14%)	66,82,82	1.75	16 (24%)
8	F3S	H	303	2	0,9,9	-	-	-		
11	PGV	I	305	-	32,32,50	0.58	0	35,38,56	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SF4	B	301	2	0,12,12	-	-	-		
11	PGV	F	305	-	29,29,50	0.62	0	32,35,56	0.59	0
12	PEV	C	307	-	40,40,48	0.52	0	43,45,53	0.54	0
10	LMT	F	304	-	36,36,36	1.16	6 (16%)	47,47,47	1.06	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
9	HEM	F	302	3	-	2/14/54/54	-
8	F3S	E	303	2	-	-	0/3/3/3
11	PGV	C	304	-	-	17/35/35/55	-
9	HEM	I	302	3	-	7/14/54/54	-
9	HEM	I	303	3	-	6/14/54/54	-
10	LMT	C	305	-	-	11/14/54/61	0/2/2/2
6	SF4	H	301	2	-	-	0/6/5/5
10	LMT	F	306	-	-	7/14/54/61	0/2/2/2
9	HEM	F	303	3	-	1/14/54/54	-
5	SIN	D	702	-	-	4/5/5/5	-
6	SF4	E	301	2	-	-	0/6/5/5
5	SIN	G	702	-	-	5/5/5/5	-
10	LMT	C	303	-	-	8/20/60/61	0/2/2/2
9	HEM	C	302	3	-	5/14/54/54	-
7	FES	B	302	2	-	-	0/1/1/1
12	PEV	F	301	-	-	23/47/47/52	-
7	FES	H	302	2	-	-	0/1/1/1
12	PEV	I	301	-	-	20/47/47/52	-
4	FAD	G	701	-	-	3/34/50/50	0/6/6/6
10	LMT	I	306	-	-	2/15/55/61	0/2/2/2
4	FAD	D	701	-	-	18/34/50/50	0/6/6/6
12	PEV	C	306	-	-	21/52/52/52	-
12	PEV	I	307	-	-	19/52/52/52	-
4	FAD	A	701	-	-	18/34/50/50	0/6/6/6
12	PEV	F	307	-	-	13/52/52/52	-
5	SIN	A	702	-	-	3/5/5/5	-
7	FES	E	302	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	I	304	-	-	13/21/61/61	0/2/2/2
9	HEM	C	301	3	-	4/14/54/54	-
8	F3S	B	303	2	-	-	0/3/3/3
8	F3S	H	303	2	-	-	0/3/3/3
11	PGV	I	305	-	-	14/37/37/55	-
6	SF4	B	301	2	-	-	0/6/5/5
11	PGV	F	305	-	-	12/34/34/55	-
12	PEV	C	307	-	-	11/44/44/52	-
10	LMT	F	304	-	-	13/21/61/61	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	303	HEM	FE-NB	5.43	2.11	1.94
9	I	303	HEM	FE-NB	5.28	2.11	1.94
9	I	302	HEM	FE-NB	5.27	2.11	1.94
9	C	302	HEM	FE-NB	5.23	2.11	1.94
9	C	301	HEM	FE-NB	5.10	2.10	1.94
9	F	302	HEM	FE-NB	5.06	2.10	1.94
9	I	302	HEM	FE-NC	4.39	2.10	1.95
9	F	302	HEM	FE-NC	4.37	2.09	1.95
9	I	303	HEM	FE-NC	4.20	2.09	1.95
9	C	301	HEM	FE-NC	4.18	2.09	1.95
9	C	302	HEM	FE-NC	4.11	2.09	1.95
9	F	303	HEM	FE-NC	4.09	2.09	1.95
9	F	303	HEM	C1B-NB	-3.67	1.34	1.40
9	F	302	HEM	C4D-ND	-3.58	1.34	1.40
9	C	301	HEM	C4D-ND	-3.55	1.34	1.40
9	C	301	HEM	C1B-NB	-3.49	1.34	1.40
9	F	302	HEM	C1B-NB	-3.48	1.34	1.40
9	I	302	HEM	C1B-NB	-3.43	1.34	1.40
9	C	302	HEM	C4D-ND	-3.35	1.34	1.40
9	C	302	HEM	C1B-NB	-3.33	1.34	1.40
9	I	302	HEM	C4D-ND	-3.27	1.34	1.40
9	I	303	HEM	C1B-NB	-3.25	1.34	1.40
9	I	303	HEM	C4D-ND	-3.19	1.34	1.40
9	F	303	HEM	C4D-ND	-3.15	1.34	1.40
10	F	304	LMT	O3'-C3'	-2.73	1.36	1.43
10	C	305	LMT	O3'-C3'	-2.71	1.36	1.43
10	C	303	LMT	O3'-C3'	-2.67	1.36	1.43
10	I	304	LMT	O3'-C3'	-2.67	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	306	LMT	O3'-C3'	-2.65	1.36	1.43
10	F	306	LMT	O3'-C3'	-2.63	1.36	1.43
9	F	302	HEM	FE-ND	-2.58	1.86	1.94
9	F	303	HEM	FE-ND	-2.52	1.87	1.94
9	C	301	HEM	FE-ND	-2.51	1.87	1.94
9	C	302	HEM	C1C-C2C	-2.48	1.40	1.45
9	C	302	HEM	FE-ND	-2.45	1.87	1.94
9	I	302	HEM	C1C-C2C	-2.41	1.40	1.45
10	C	303	LMT	O2'-C2'	-2.39	1.37	1.43
10	I	304	LMT	O2B-C2B	-2.39	1.37	1.43
9	F	302	HEM	C1C-C2C	-2.38	1.40	1.45
10	C	303	LMT	O2B-C2B	-2.37	1.37	1.43
9	C	301	HEM	C1C-C2C	-2.37	1.40	1.45
10	F	306	LMT	O2B-C2B	-2.37	1.37	1.43
10	F	306	LMT	O2'-C2'	-2.37	1.37	1.43
10	F	304	LMT	O2B-C2B	-2.37	1.37	1.43
9	F	303	HEM	C1C-C2C	-2.36	1.40	1.45
10	F	306	LMT	O3B-C3B	-2.34	1.37	1.43
9	I	302	HEM	FE-ND	-2.33	1.87	1.94
10	F	304	LMT	O3B-C3B	-2.33	1.37	1.43
10	C	303	LMT	O3B-C3B	-2.32	1.37	1.43
10	I	306	LMT	O3B-C3B	-2.32	1.37	1.43
10	F	304	LMT	O2'-C2'	-2.31	1.37	1.43
10	I	304	LMT	O3B-C3B	-2.30	1.37	1.43
10	C	305	LMT	O3B-C3B	-2.30	1.37	1.43
10	I	304	LMT	O2'-C2'	-2.30	1.37	1.43
10	I	306	LMT	O2B-C2B	-2.28	1.37	1.43
9	F	303	HEM	C3B-C4B	2.28	1.49	1.44
10	C	305	LMT	O2'-C2'	-2.25	1.37	1.43
9	I	303	HEM	FE-ND	-2.24	1.87	1.94
9	I	302	HEM	C1D-ND	-2.23	1.34	1.38
9	I	303	HEM	C1C-C2C	-2.22	1.40	1.45
10	C	305	LMT	O4'-C4B	-2.15	1.37	1.43
10	I	306	LMT	O4'-C4B	-2.13	1.38	1.43
9	F	302	HEM	C1D-ND	-2.13	1.34	1.38
10	C	303	LMT	O4'-C4B	-2.13	1.38	1.43
10	C	305	LMT	O2B-C2B	-2.12	1.38	1.43
10	F	306	LMT	O4'-C4B	-2.10	1.38	1.43
10	F	304	LMT	O4'-C4B	-2.09	1.38	1.43
10	I	304	LMT	O4'-C4B	-2.08	1.38	1.43
10	I	306	LMT	O2'-C2'	-2.08	1.38	1.43
10	I	304	LMT	O1'-C1'	-2.06	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	303	HEM	C3B-C4B	2.04	1.48	1.44
9	C	302	HEM	C3C-C4C	-2.04	1.42	1.46
10	F	304	LMT	O1'-C1'	-2.04	1.36	1.40
9	F	302	HEM	C4B-NB	-2.03	1.34	1.38
9	C	301	HEM	C1D-ND	-2.03	1.34	1.38

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	302	HEM	CHC-C4B-NB	5.25	130.12	124.42
9	C	301	HEM	CHC-C4B-NB	5.18	130.05	124.42
9	F	302	HEM	CHC-C4B-NB	5.00	129.85	124.42
9	I	302	HEM	CHC-C4B-NB	4.91	129.76	124.42
9	I	303	HEM	CHC-C4B-NB	4.67	129.49	124.42
9	I	303	HEM	CHD-C1D-ND	4.48	129.28	124.42
9	F	303	HEM	CHC-C4B-NB	4.40	129.20	124.42
9	F	302	HEM	CAD-CBD-CGD	-4.34	104.26	113.60
9	I	302	HEM	CHD-C1D-ND	4.34	129.13	124.42
9	C	302	HEM	CHD-C1D-ND	4.31	129.10	124.42
9	F	302	HEM	CHA-C4D-ND	4.15	129.49	124.37
9	C	301	HEM	CHD-C1D-ND	4.09	128.87	124.42
9	F	302	HEM	CHD-C1D-ND	4.02	128.79	124.42
9	F	303	HEM	CHD-C1D-ND	3.97	128.74	124.42
9	F	303	HEM	CHB-C1B-NB	3.97	129.26	124.37
9	C	302	HEM	C1B-NB-C4B	3.93	109.13	105.07
9	F	303	HEM	C1B-NB-C4B	3.90	109.11	105.07
9	C	301	HEM	C1B-NB-C4B	3.86	109.06	105.07
9	C	302	HEM	CHA-C4D-ND	3.85	129.13	124.37
9	C	301	HEM	CHA-C4D-ND	3.74	128.98	124.37
9	I	303	HEM	CHA-C4D-ND	3.72	128.96	124.37
9	C	301	HEM	CAD-CBD-CGD	-3.67	105.70	113.60
9	F	302	HEM	CHB-C1B-NB	3.67	128.90	124.37
9	C	301	HEM	CHB-C1B-NB	3.64	128.86	124.37
9	F	302	HEM	C1B-NB-C4B	3.60	108.79	105.07
9	I	303	HEM	CHB-C1B-NB	3.52	128.71	124.37
9	F	303	HEM	CHA-C4D-ND	3.52	128.71	124.37
9	C	302	HEM	CHB-C1B-NB	3.43	128.61	124.37
10	C	305	LMT	C1'-O5'-C5'	-3.43	106.96	113.69
9	I	302	HEM	C1B-NB-C4B	3.41	108.60	105.07
9	I	303	HEM	C1B-NB-C4B	3.40	108.58	105.07
9	C	302	HEM	C4C-NC-C1C	3.37	108.65	105.35
9	I	302	HEM	CHB-C1B-NB	3.28	128.42	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	302	HEM	CHD-C1D-C2D	-3.23	119.94	124.98
10	I	304	LMT	C1'-O5'-C5'	-3.23	107.35	113.69
9	C	301	HEM	C4C-NC-C1C	3.22	108.50	105.35
9	I	303	HEM	C4C-NC-C1C	3.16	108.44	105.35
10	I	306	LMT	C1'-O5'-C5'	-2.99	107.81	113.69
10	F	304	LMT	C1'-O5'-C5'	-2.98	107.83	113.69
9	F	302	HEM	C4C-NC-C1C	2.96	108.25	105.35
9	I	302	HEM	CHA-C4D-ND	2.89	127.94	124.37
9	F	302	HEM	CHD-C1D-C2D	-2.87	120.50	124.98
9	C	302	HEM	CHD-C4C-NC	2.85	127.52	124.44
9	C	301	HEM	CHD-C4C-NC	2.85	127.52	124.44
9	I	303	HEM	CAA-CBA-CGA	-2.82	107.55	113.60
9	F	303	HEM	C4C-NC-C1C	2.69	107.99	105.35
9	C	301	HEM	CHD-C1D-C2D	-2.65	120.84	124.98
9	F	303	HEM	CHD-C4C-NC	2.63	127.28	124.44
9	F	303	HEM	CAA-CBA-CGA	-2.62	107.97	113.60
9	C	302	HEM	CHD-C1D-C2D	-2.61	120.90	124.98
9	F	302	HEM	CHA-C4D-C3D	-2.57	120.51	125.33
10	F	306	LMT	O5'-C5'-C6'	2.56	112.81	106.44
9	I	303	HEM	CHD-C1D-C2D	-2.53	121.02	124.98
9	I	303	HEM	C4D-ND-C1D	2.50	107.66	105.07
9	C	302	HEM	CHA-C4D-C3D	-2.48	120.66	125.33
9	F	303	HEM	CHD-C1D-C2D	-2.45	121.16	124.98
9	C	301	HEM	CHA-C4D-C3D	-2.39	120.85	125.33
10	F	304	LMT	C3'-C4'-C5'	-2.39	105.45	110.93
9	F	303	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
9	F	302	HEM	CHD-C4C-NC	2.35	126.98	124.44
9	F	303	HEM	CHB-C1B-C2B	-2.35	120.22	126.73
9	C	301	HEM	CAA-CBA-CGA	-2.34	108.58	113.60
9	I	303	HEM	CAD-CBD-CGD	-2.31	108.63	113.60
9	I	302	HEM	CAA-CBA-CGA	-2.30	108.64	113.60
9	F	302	HEM	C4B-C3B-C2B	-2.29	105.29	107.11
9	C	301	HEM	C4D-ND-C1D	2.28	107.43	105.07
10	I	304	LMT	O5B-C5B-C4B	2.28	113.84	109.69
10	C	303	LMT	O5'-C5'-C6'	2.28	112.11	106.44
11	I	305	PGV	C02-O01-C1	2.28	123.39	117.79
10	C	305	LMT	C2'-C3'-C4'	2.26	114.84	109.68
9	F	302	HEM	CAA-CBA-CGA	-2.26	108.74	113.60
9	F	302	HEM	C4D-ND-C1D	2.24	107.38	105.07
9	F	302	HEM	C1A-CHA-C4D	-2.23	121.04	126.34
9	I	302	HEM	C4C-NC-C1C	2.23	107.53	105.35
9	I	303	HEM	CHA-C4D-C3D	-2.22	121.15	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	303	HEM	CHB-C1B-C2B	-2.22	120.56	126.73
9	C	302	HEM	C4D-ND-C1D	2.21	107.36	105.07
9	F	303	HEM	C4A-NA-C1A	2.18	107.49	105.35
9	I	302	HEM	C4A-NA-C1A	2.18	107.49	105.35
9	C	302	HEM	C1A-CHA-C4D	-2.17	121.19	126.34
9	I	303	HEM	C1A-CHA-C4D	-2.17	121.19	126.34
10	C	303	LMT	O5'-C5'-C4'	2.16	114.31	109.75
9	F	302	HEM	CHB-C1B-C2B	-2.16	120.72	126.73
9	C	301	HEM	CHB-C1B-C2B	-2.15	120.75	126.73
10	I	306	LMT	C3B-C4B-C5B	-2.15	106.41	110.24
10	C	303	LMT	O1'-C1'-C2'	2.14	111.64	108.30
10	F	306	LMT	O1'-C1'-C2'	2.14	111.64	108.30
5	G	702	SIN	C2-C3-C4	-2.13	109.02	113.60
9	I	303	HEM	CHD-C4C-NC	2.13	126.74	124.44
9	C	302	HEM	C4A-NA-C1A	2.11	107.41	105.35
9	C	301	HEM	C1A-CHA-C4D	-2.10	121.35	126.34
9	I	303	HEM	C4A-NA-C1A	2.07	107.37	105.35
9	C	302	HEM	CAA-CBA-CGA	-2.07	109.16	113.60
5	A	702	SIN	O4-C4-C3	2.06	120.66	114.03
10	C	305	LMT	O5B-C5B-C4B	2.06	113.44	109.69
9	I	302	HEM	C1A-CHA-C4D	-2.05	121.47	126.34
9	C	301	HEM	C4A-CHB-C1B	-2.04	121.50	126.34
5	D	702	SIN	C2-C3-C4	-2.04	109.22	113.60
4	G	701	FAD	P-O3P-PA	-2.04	125.83	132.83
9	F	302	HEM	CAD-C3D-C2D	2.02	131.65	127.88
9	I	302	HEM	CHB-C1B-C2B	-2.02	121.13	126.73
5	A	702	SIN	O2-C1-C2	2.00	120.47	114.03
9	C	301	HEM	C4C-CHD-C1D	-2.00	121.74	126.06

There are no chirality outliers.

All (280) 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'-O3'
4	A	701	FAD	C1'-C2'-C3'-C4'
4	A	701	FAD	O2'-C2'-C3'-C4'
4	A	701	FAD	C2'-C3'-C4'-O4'
4	A	701	FAD	O3'-C3'-C4'-O4'
4	A	701	FAD	C5'-O5'-P-O1P
4	A	701	FAD	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
4	A	701	FAD	C5'-O5'-P-O3P
4	D	701	FAD	O4B-C4B-C5B-O5B
4	D	701	FAD	C3B-C4B-C5B-O5B
4	D	701	FAD	N10-C1'-C2'-O2'
4	D	701	FAD	N10-C1'-C2'-C3'
4	D	701	FAD	C1'-C2'-C3'-O3'
4	D	701	FAD	C1'-C2'-C3'-C4'
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	C3'-C4'-C5'-O5'
4	D	701	FAD	O4'-C4'-C5'-O5'
4	G	701	FAD	O4B-C4B-C5B-O5B
4	G	701	FAD	C3B-C4B-C5B-O5B
9	C	301	HEM	C2B-C3B-CAB-CBB
9	F	302	HEM	C2D-C3D-CAD-CBD
9	F	302	HEM	C4D-C3D-CAD-CBD
9	I	302	HEM	C2D-C3D-CAD-CBD
10	C	305	LMT	C2B-C1B-O1B-C4'
10	C	305	LMT	C2'-C1'-O1'-C1
10	C	305	LMT	O5'-C1'-O1'-C1
10	F	306	LMT	C2'-C1'-O1'-C1
10	F	306	LMT	O5'-C1'-O1'-C1
10	I	306	LMT	C2-C1-O1'-C1'
11	C	304	PGV	C03-O11-P-O13
11	C	304	PGV	O01-C02-C03-O11
11	C	304	PGV	O12-C04-C05-C06
11	C	304	PGV	O02-C1-O01-C02
11	F	305	PGV	O03-C01-C02-O01
11	I	305	PGV	C2-C1-O01-C02
12	C	306	PEV	C32-C31-O2-C2
12	C	306	PEV	C4-O4P-P-O2P
12	C	307	PEV	O2-C2-C3-O3
12	F	301	PEV	C1-O3P-P-O1P
12	F	301	PEV	C1-O3P-P-O2P
12	F	301	PEV	C5-C4-O4P-P
12	F	307	PEV	C1-O3P-P-O1P
12	I	301	PEV	C32-C31-O2-C2
12	I	301	PEV	O2-C2-C3-O3
12	I	301	PEV	C1-O3P-P-O2P
12	I	301	PEV	C4-O4P-P-O1P
12	I	307	PEV	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
10	C	305	LMT	O5B-C1B-O1B-C4'
11	I	305	PGV	O04-C19-O03-C01
12	C	306	PEV	O11-C11-O3-C3
12	F	301	PEV	O11-C11-O3-C3
12	C	306	PEV	O31-C31-O2-C2
12	F	307	PEV	O31-C31-O2-C2
12	I	301	PEV	O31-C31-O2-C2
11	I	305	PGV	C20-C19-O03-C01
12	C	306	PEV	C12-C11-O3-C3
12	F	301	PEV	C12-C11-O3-C3
11	C	304	PGV	C2-C1-O01-C02
12	F	307	PEV	C32-C31-O2-C2
9	I	302	HEM	C4D-C3D-CAD-CBD
11	I	305	PGV	O02-C1-O01-C02
10	I	304	LMT	O5'-C5'-C6'-O6'
11	C	304	PGV	O12-C04-C05-O05
10	C	303	LMT	C4'-C5'-C6'-O6'
10	C	305	LMT	C4'-C5'-C6'-O6'
4	A	701	FAD	O2'-C2'-C3'-O3'
4	D	701	FAD	O2'-C2'-C3'-O3'
9	C	301	HEM	C2D-C3D-CAD-CBD
10	I	304	LMT	C4'-C5'-C6'-O6'
4	D	701	FAD	O2'-C2'-C3'-C4'
12	I	307	PEV	C2-C1-O3P-P
4	A	701	FAD	O3'-C3'-C4'-C5'
4	D	701	FAD	O3'-C3'-C4'-C5'
9	C	301	HEM	C4D-C3D-CAD-CBD
4	A	701	FAD	C2'-C3'-C4'-C5'
12	F	301	PEV	C32-C31-O2-C2
10	F	306	LMT	C4'-C5'-C6'-O6'
10	F	304	LMT	C4'-C5'-C6'-O6'
10	F	304	LMT	O5'-C5'-C6'-O6'
10	C	305	LMT	O5'-C5'-C6'-O6'
12	F	301	PEV	C31-C32-C33-C34
10	C	303	LMT	O5B-C1B-O1B-C4'
11	F	305	PGV	C19-C20-C21-C22
11	I	305	PGV	C19-C20-C21-C22
5	A	702	SIN	C1-C2-C3-C4
12	F	301	PEV	O31-C31-O2-C2
9	C	302	HEM	C2A-CAA-CBA-CGA
10	C	303	LMT	O5'-C5'-C6'-O6'
10	F	304	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	G	702	SIN	C1-C2-C3-C4
11	F	305	PGV	C04-O12-P-O11
11	I	305	PGV	C03-O11-P-O12
12	C	306	PEV	C4-O4P-P-O3P
12	F	301	PEV	C1-O3P-P-O4P
12	F	301	PEV	C4-O4P-P-O3P
12	I	307	PEV	C4-O4P-P-O3P
10	F	306	LMT	O1'-C1-C2-C3
10	I	304	LMT	O1'-C1-C2-C3
11	F	305	PGV	C2-C1-O01-C02
12	C	306	PEV	C36-C37-C38-C39
11	F	305	PGV	O02-C1-O01-C02
12	C	306	PEV	C14-C15-C16-C17
12	C	306	PEV	C22-C23-C24-C25
12	F	301	PEV	C34-C35-C36-C37
12	I	307	PEV	C22-C23-C24-C25
12	C	307	PEV	C38-C39-C40-C41
11	C	304	PGV	C04-C05-C06-O06
12	C	306	PEV	C12-C13-C14-C15
12	I	301	PEV	C34-C35-C36-C37
12	F	301	PEV	C37-C38-C39-C40
12	F	301	PEV	C35-C36-C37-C38
12	I	301	PEV	C17-C18-C19-C20
10	F	304	LMT	C4-C5-C6-C7
10	C	305	LMT	C2-C1-O1'-C1'
11	I	305	PGV	C22-C23-C24-C25
12	F	301	PEV	C12-C13-C14-C15
12	F	307	PEV	C33-C34-C35-C36
12	F	301	PEV	C38-C39-C40-C41
12	I	307	PEV	C32-C31-O2-C2
12	C	306	PEV	C13-C14-C15-C16
12	C	306	PEV	C34-C35-C36-C37
10	F	304	LMT	C5-C6-C7-C8
9	C	302	HEM	C2B-C3B-CAB-CBB
9	C	302	HEM	C2C-C3C-CAC-CBC
9	I	303	HEM	C2B-C3B-CAB-CBB
10	I	304	LMT	C3-C4-C5-C6
10	I	304	LMT	C4-C5-C6-C7
9	C	301	HEM	C4B-C3B-CAB-CBB
9	C	302	HEM	C4B-C3B-CAB-CBB
9	F	303	HEM	C4B-C3B-CAB-CBB
10	F	304	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	I	307	PEV	O31-C31-O2-C2
10	I	304	LMT	O5B-C1B-O1B-C4'
10	C	303	LMT	C5-C6-C7-C8
12	F	301	PEV	C40-C41-C42-C43
4	A	701	FAD	C3'-C4'-C5'-O5'
12	C	307	PEV	C14-C15-C16-C17
12	C	307	PEV	C1-C2-C3-O3
12	F	307	PEV	C22-C23-C24-C25
12	C	306	PEV	C41-C42-C43-C44
11	C	304	PGV	O05-C05-C06-O06
10	I	304	LMT	C2-C3-C4-C5
10	C	305	LMT	O5B-C5B-C6B-O6B
12	F	307	PEV	C2-C1-O3P-P
11	C	304	PGV	C1-C2-C3-C4
4	A	701	FAD	PA-O3P-P-O1P
10	I	306	LMT	O5'-C1'-O1'-C1
12	C	307	PEV	O3P-C1-C2-C3
12	I	301	PEV	C16-C17-C18-C19
10	F	304	LMT	O5B-C1B-O1B-C4'
4	A	701	FAD	O4'-C4'-C5'-O5'
10	F	306	LMT	C2-C1-O1'-C1'
10	I	304	LMT	C2-C1-O1'-C1'
12	C	306	PEV	C1-C2-C3-O3
12	I	301	PEV	C1-C2-C3-O3
12	I	307	PEV	C33-C34-C35-C36
12	I	307	PEV	C15-C16-C17-C18
12	C	306	PEV	C1-O3P-P-O4P
12	I	301	PEV	C33-C34-C35-C36
12	F	307	PEV	C34-C35-C36-C37
12	C	307	PEV	O3P-C1-C2-O2
12	C	307	PEV	C42-C43-C44-C45
12	I	301	PEV	C22-C23-C24-C25
11	F	305	PGV	C20-C21-C22-C23
11	I	305	PGV	O12-C04-C05-C06
11	C	304	PGV	C2-C3-C4-C5
12	I	301	PEV	C21-C22-C23-C24
10	C	303	LMT	C3-C4-C5-C6
4	A	701	FAD	P-O3P-PA-O5B
10	C	305	LMT	C3'-C4'-O1B-C1B
9	I	302	HEM	C2B-C3B-CAB-CBB
9	I	303	HEM	C2C-C3C-CAC-CBC
11	I	305	PGV	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
12	F	301	PEV	C3-C2-O2-C31
10	C	303	LMT	C4-C5-C6-C7
4	D	701	FAD	C4'-C5'-O5'-P
11	F	305	PGV	O03-C01-C02-C03
9	C	302	HEM	C4C-C3C-CAC-CBC
9	I	303	HEM	C4B-C3B-CAB-CBB
11	F	305	PGV	C1-C2-C3-C4
12	C	306	PEV	O2-C2-C3-O3
12	F	301	PEV	O2-C2-C3-O3
12	I	307	PEV	C12-C11-O3-C3
4	D	701	FAD	C5B-O5B-PA-O3P
12	F	301	PEV	C32-C33-C34-C35
10	C	305	LMT	O1'-C1-C2-C3
11	C	304	PGV	C03-O11-P-O12
12	I	301	PEV	C1-O3P-P-O4P
12	I	307	PEV	C1-O3P-P-O4P
12	I	307	PEV	C42-C43-C44-C45
10	C	305	LMT	C5'-C4'-O1B-C1B
12	F	301	PEV	C2-C1-O3P-P
4	D	701	FAD	C5B-O5B-PA-O1A
4	D	701	FAD	C5B-O5B-PA-O2A
11	F	305	PGV	C04-O12-P-O13
11	I	305	PGV	C03-O11-P-O13
12	F	301	PEV	C4-O4P-P-O1P
12	I	307	PEV	C4-O4P-P-O2P
11	C	304	PGV	C01-C02-C03-O11
12	C	307	PEV	C13-C14-C15-C16
12	C	306	PEV	C5-C4-O4P-P
12	I	301	PEV	O3P-C1-C2-O2
12	F	307	PEV	C42-C43-C44-C45
12	I	307	PEV	O11-C11-O3-C3
11	F	305	PGV	O12-C04-C05-O05
10	F	304	LMT	C3-C4-C5-C6
12	F	301	PEV	C1-C2-C3-O3
11	I	305	PGV	O03-C01-C02-O01
10	I	304	LMT	C5'-C4'-O1B-C1B
10	C	303	LMT	C1-C2-C3-C4
12	I	301	PEV	C15-C16-C17-C18
12	I	307	PEV	C32-C33-C34-C35
12	F	307	PEV	C12-C13-C14-C15
10	C	303	LMT	C7-C8-C9-C10
11	F	305	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	I	301	PEV	O3P-C1-C2-C3
10	F	304	LMT	C9-C10-C11-C12
10	F	304	LMT	C5'-C4'-O1B-C1B
12	C	307	PEV	C4-O4P-P-O3P
12	F	307	PEV	C1-O3P-P-O4P
12	F	307	PEV	C4-O4P-P-O3P
11	I	305	PGV	C1-C2-C3-C4
11	I	305	PGV	O03-C01-C02-C03
12	I	307	PEV	C1-C2-C3-O3
4	G	701	FAD	PA-O3P-P-O2P
10	F	304	LMT	C7-C8-C9-C10
10	F	304	LMT	C2B-C1B-O1B-C4'
10	I	304	LMT	C2B-C1B-O1B-C4'
12	I	301	PEV	C31-C32-C33-C34
5	G	702	SIN	C2-C3-C4-O3
12	C	306	PEV	C17-C18-C19-C20
10	I	304	LMT	C5-C6-C7-C8
5	G	702	SIN	C2-C3-C4-O4
5	A	702	SIN	C2-C3-C4-O3
5	D	702	SIN	O1-C1-C2-C3
5	D	702	SIN	C2-C3-C4-O4
11	C	304	PGV	C04-O12-P-O11
5	D	702	SIN	O2-C1-C2-C3
10	I	304	LMT	C6-C7-C8-C9
5	D	702	SIN	C2-C3-C4-O3
11	C	304	PGV	C4-C5-C6-C7
12	C	306	PEV	C44-C45-C46-C47
5	A	702	SIN	C2-C3-C4-O4
4	A	701	FAD	PA-O3P-P-O2P
10	F	306	LMT	C1-C2-C3-C4
12	I	301	PEV	C32-C33-C34-C35
12	C	307	PEV	O4P-C4-C5-N6
5	G	702	SIN	O2-C1-C2-C3
9	I	302	HEM	C2C-C3C-CAC-CBC
12	F	301	PEV	C39-C40-C41-C42
11	C	304	PGV	O01-C1-C2-C3
12	F	307	PEV	C31-C32-C33-C34
10	F	306	LMT	O5'-C5'-C6'-O6'
9	I	302	HEM	C4B-C3B-CAB-CBB
9	I	302	HEM	C4C-C3C-CAC-CBC
9	I	303	HEM	C4C-C3C-CAC-CBC
9	I	303	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	I	307	PEV	C12-C13-C14-C15
12	I	301	PEV	C20-C21-C22-C23
5	G	702	SIN	O1-C1-C2-C3
12	I	307	PEV	C13-C14-C15-C16
11	I	305	PGV	C23-C24-C25-C26
11	F	305	PGV	O12-C04-C05-C06
12	I	307	PEV	C41-C42-C43-C44
11	C	304	PGV	C04-O12-P-O13
12	C	306	PEV	C1-O3P-P-O2P
12	C	307	PEV	C4-O4P-P-O1P
12	F	307	PEV	C4-O4P-P-O1P
12	I	301	PEV	C1-O3P-P-O1P
11	C	304	PGV	O02-C1-C2-C3
10	I	304	LMT	C3'-C4'-O1B-C1B
9	I	303	HEM	CAA-CBA-CGA-O2A
12	C	306	PEV	C42-C43-C44-C45
9	I	302	HEM	CAA-CBA-CGA-O2A
12	I	307	PEV	C37-C38-C39-C40
10	F	304	LMT	C4B-C5B-C6B-O6B

There are no ring outliers.

25 monomers are involved in 65 short contacts:

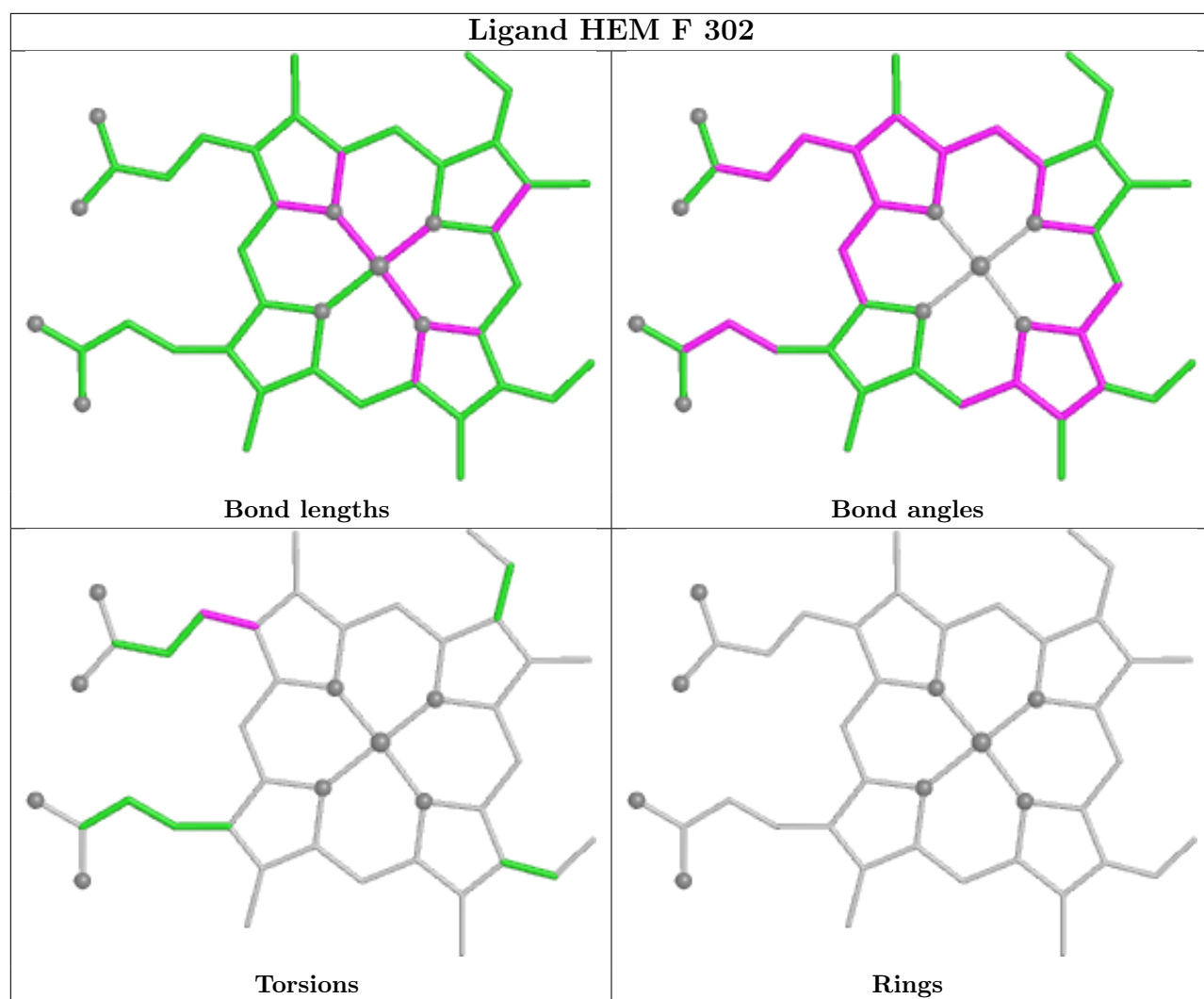
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	302	HEM	9	0
8	E	303	F3S	1	0
11	C	304	PGV	2	0
9	I	302	HEM	7	0
9	I	303	HEM	1	0
10	C	305	LMT	2	0
10	F	306	LMT	1	0
9	F	303	HEM	6	0
5	G	702	SIN	1	0
9	C	302	HEM	3	0
12	F	301	PEV	1	0
12	I	301	PEV	1	0
4	G	701	FAD	2	0
4	D	701	FAD	6	0
12	C	306	PEV	1	0
12	I	307	PEV	1	0
4	A	701	FAD	6	0
5	A	702	SIN	1	0

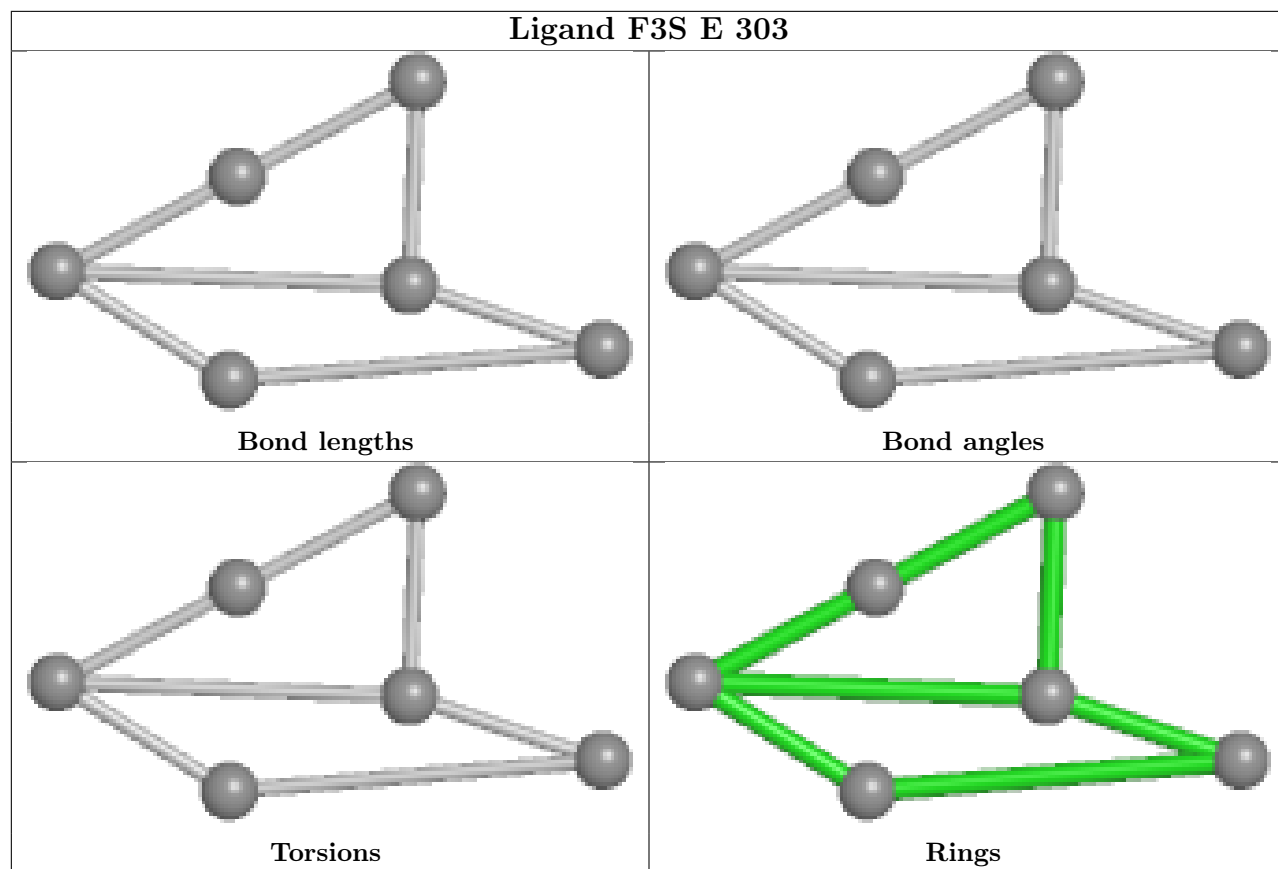
Continued on next page...

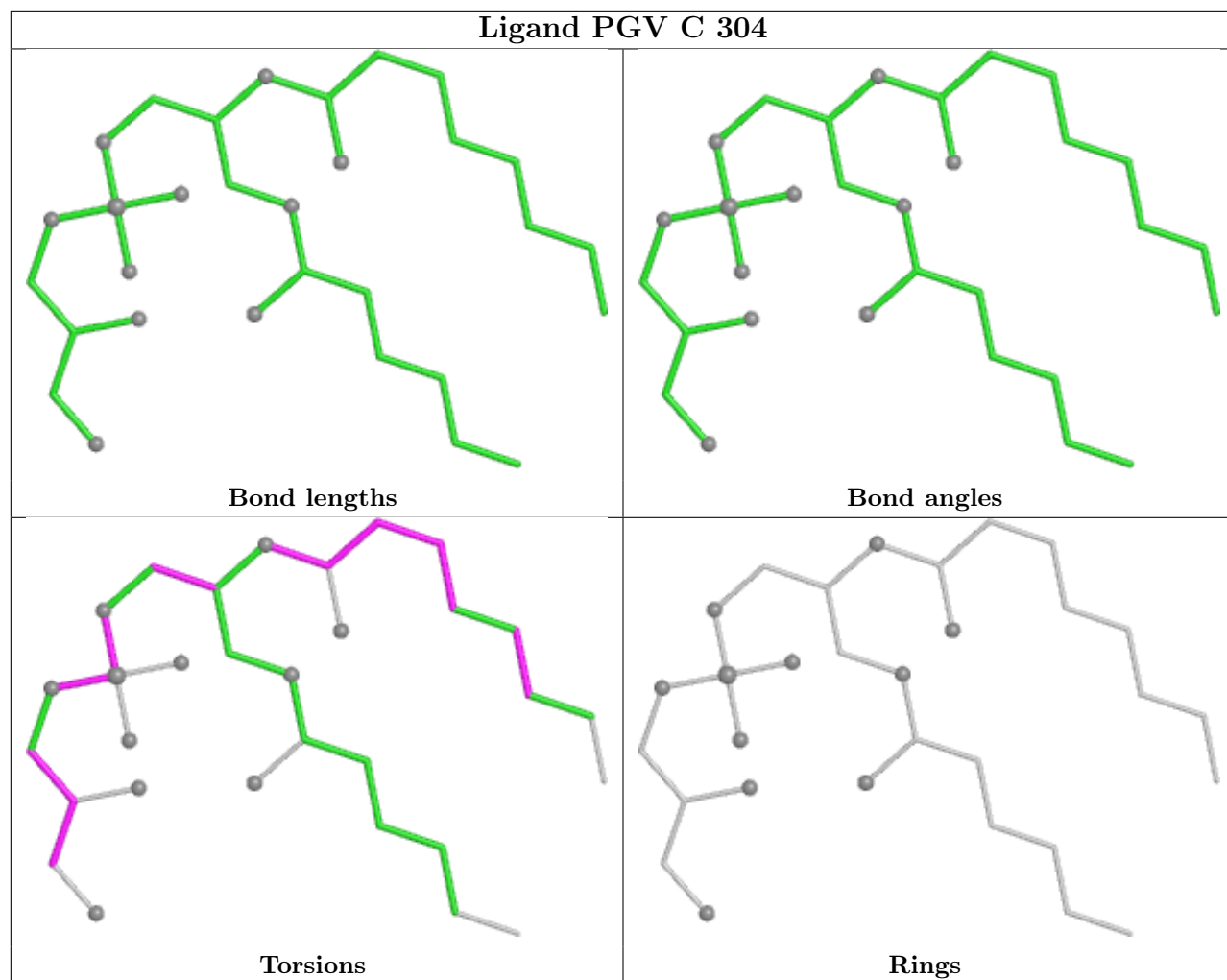
Continued from previous page...

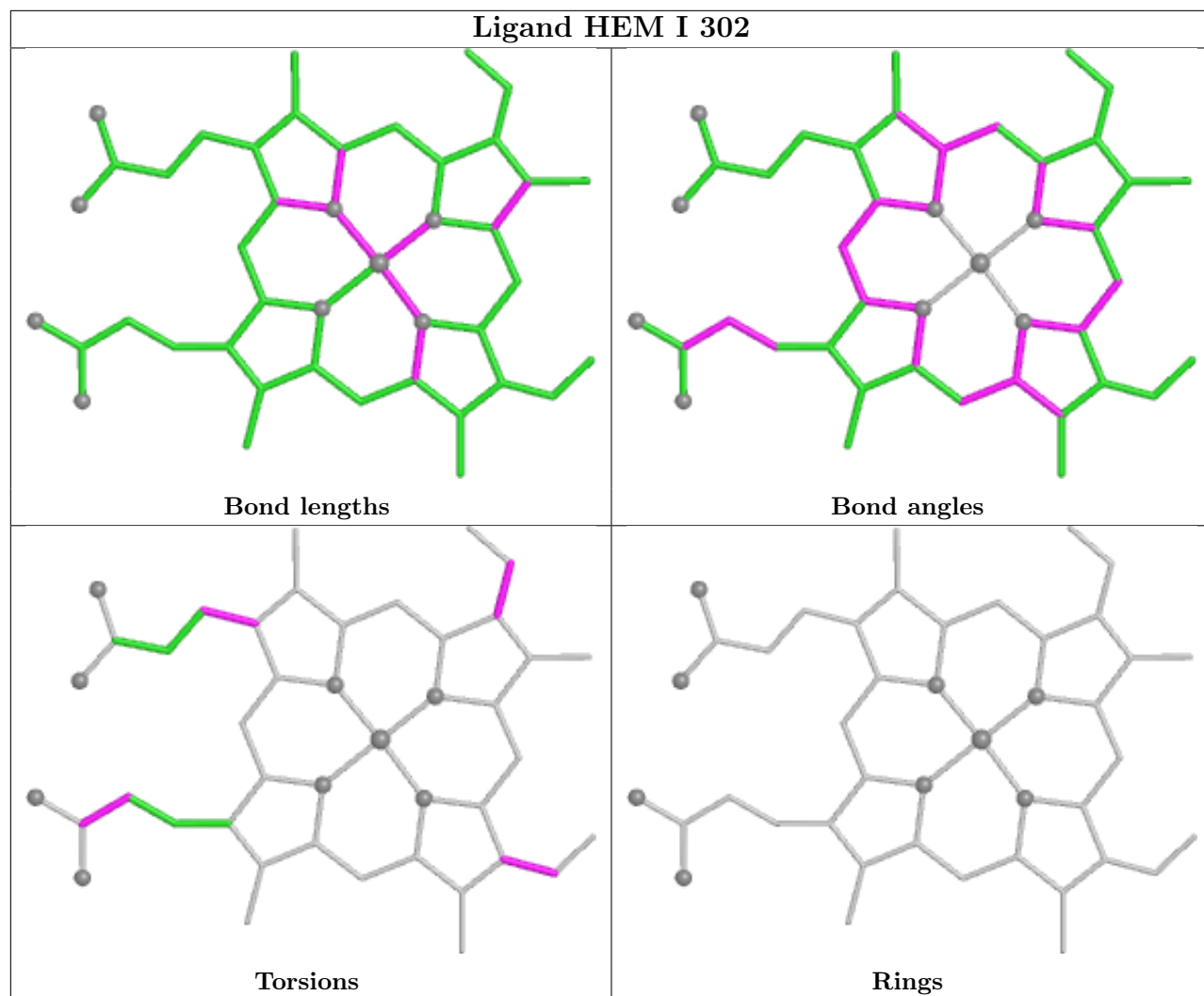
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	304	LMT	1	0
9	C	301	HEM	8	0
8	H	303	F3S	1	0
11	I	305	PGV	2	0
11	F	305	PGV	1	0
12	C	307	PEV	1	0
10	F	304	LMT	1	0

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.

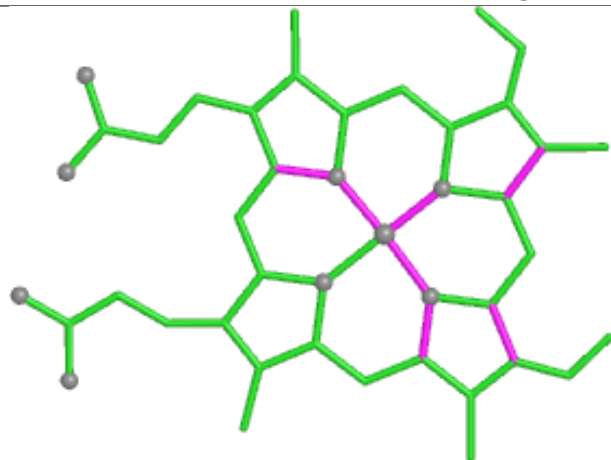




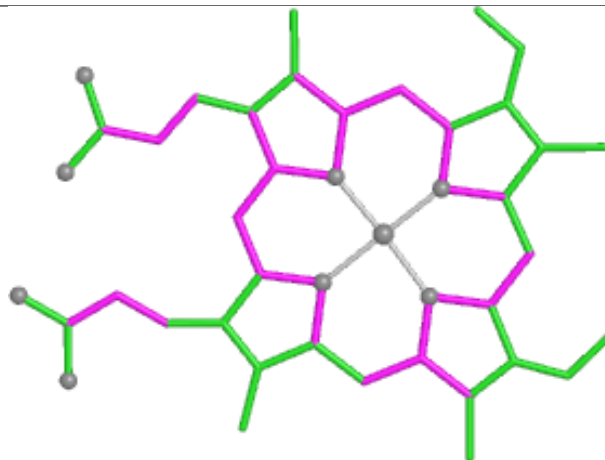




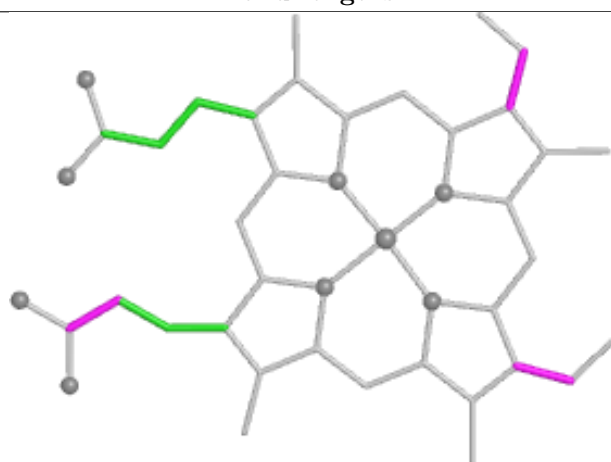
Ligand HEM I 303



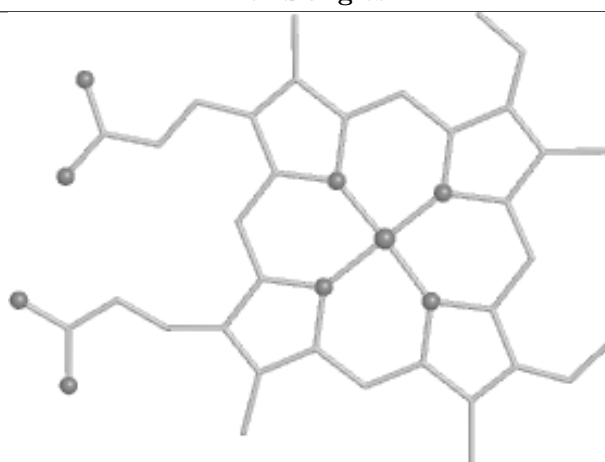
Bond lengths



Bond angles

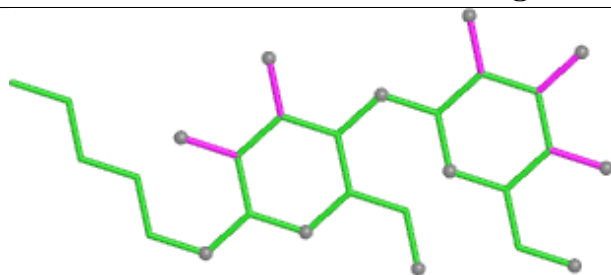


Torsions

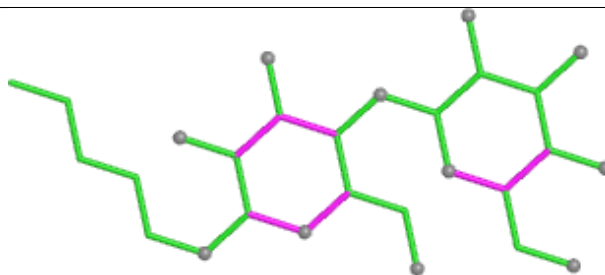


Rings

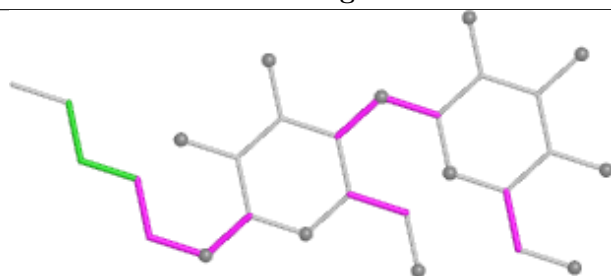
Ligand LMT C 305



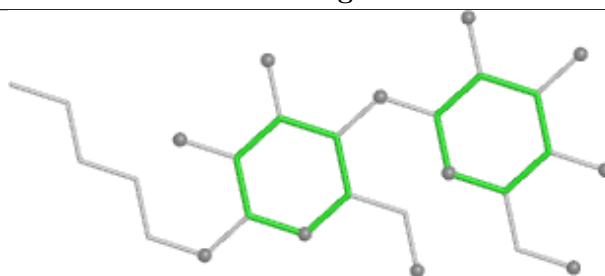
Bond lengths



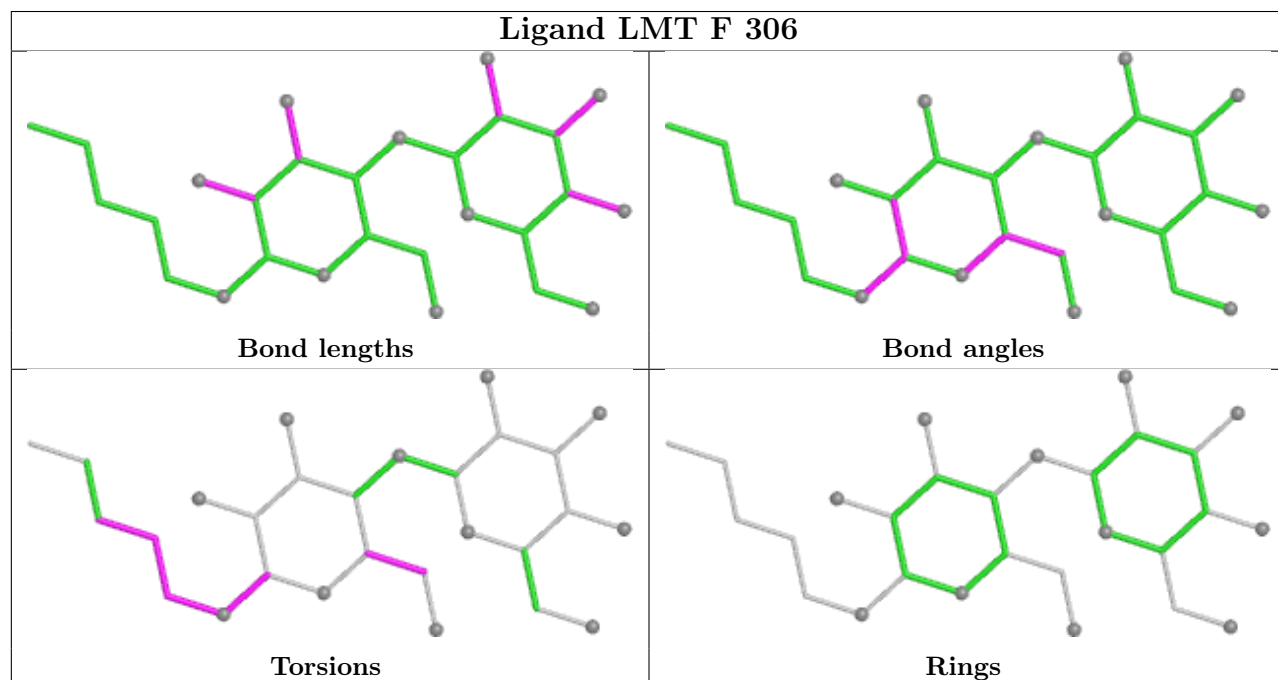
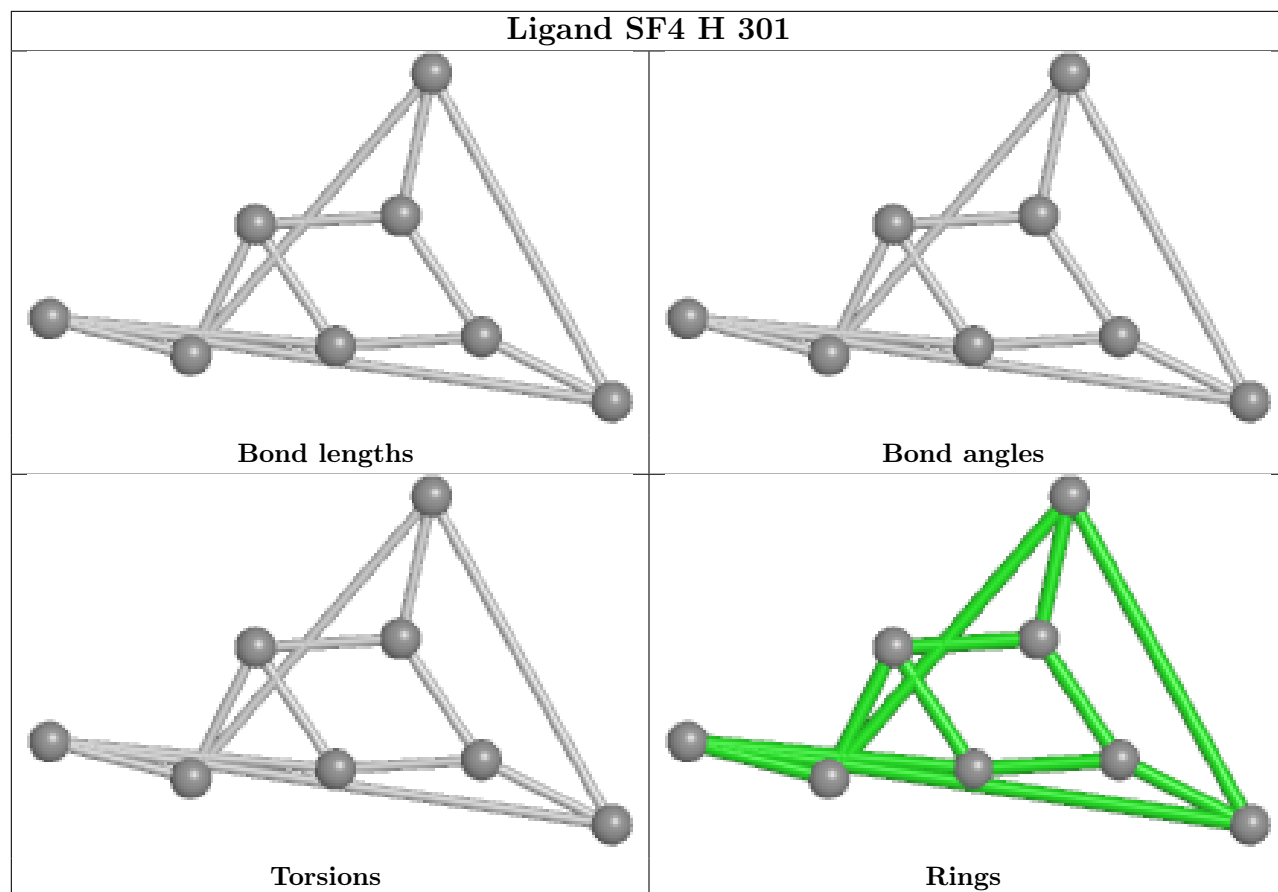
Bond angles

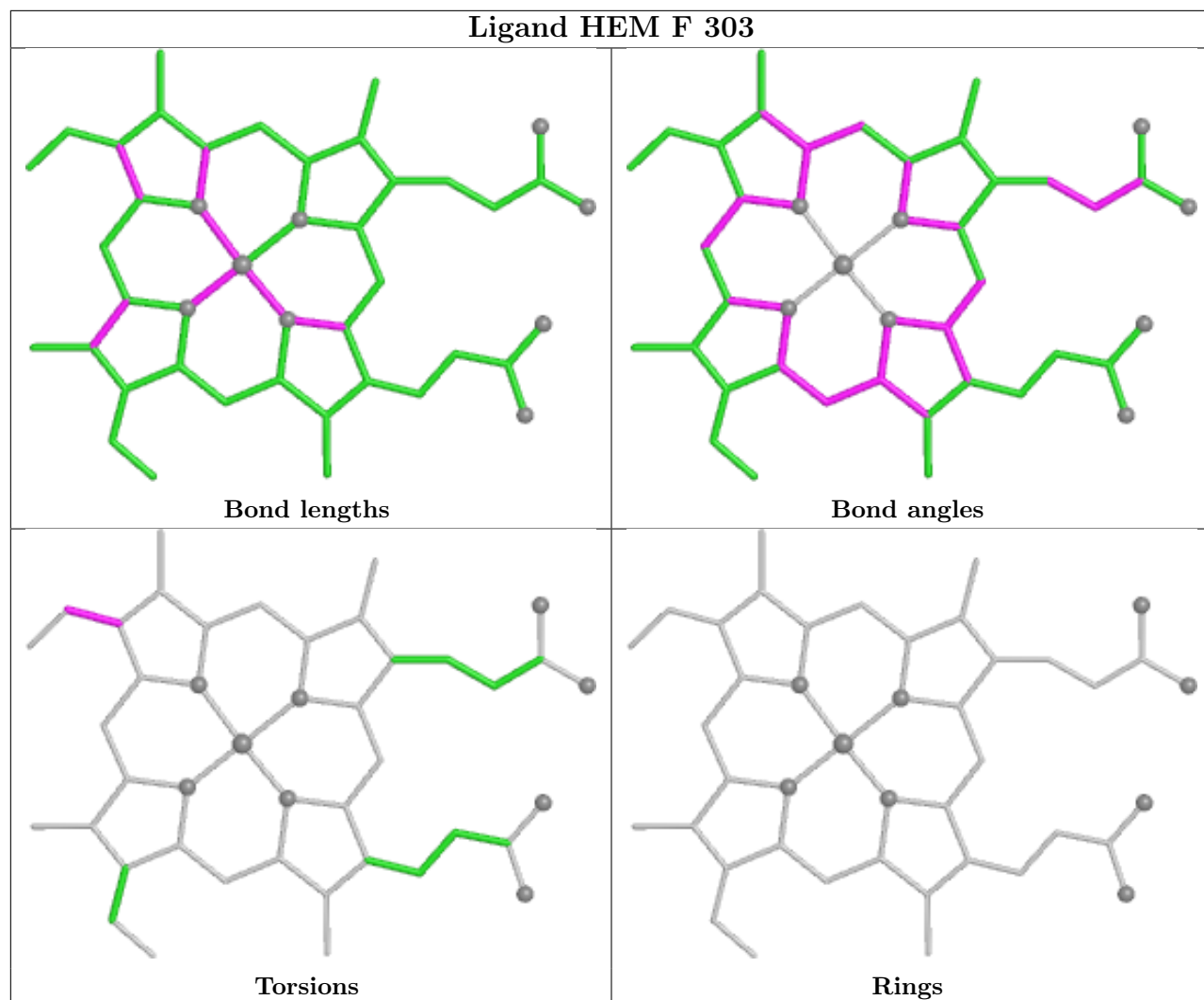


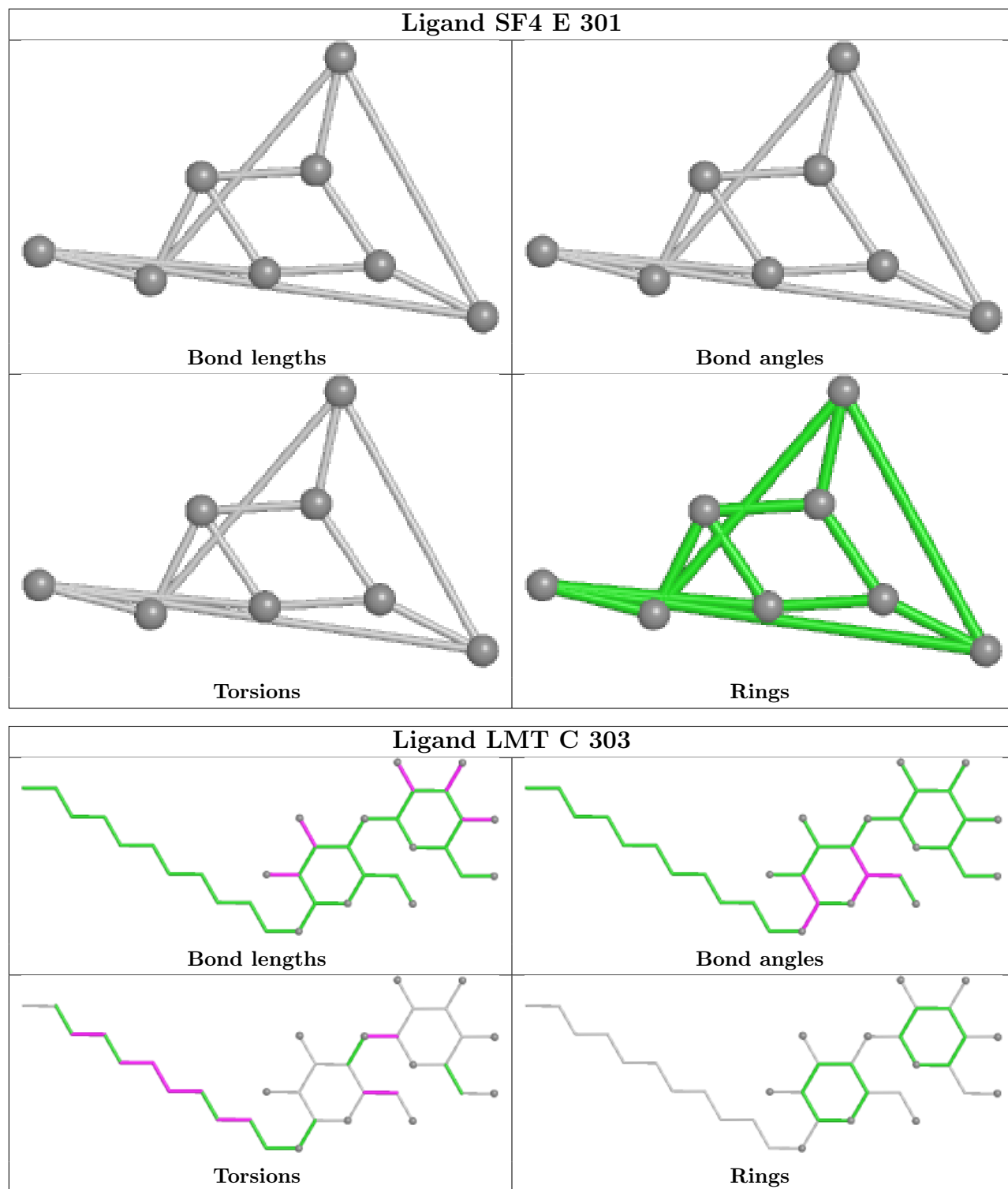
Torsions

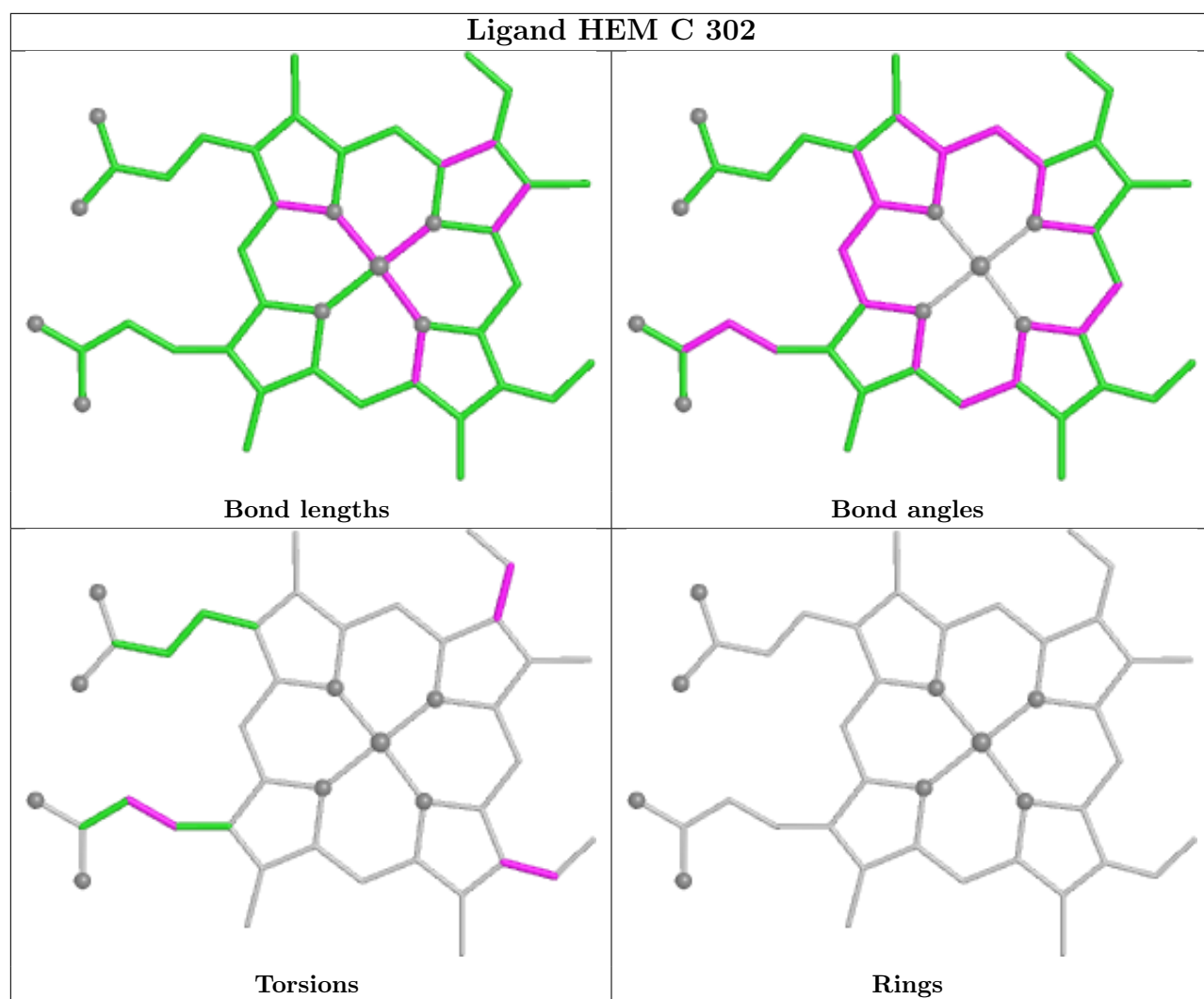


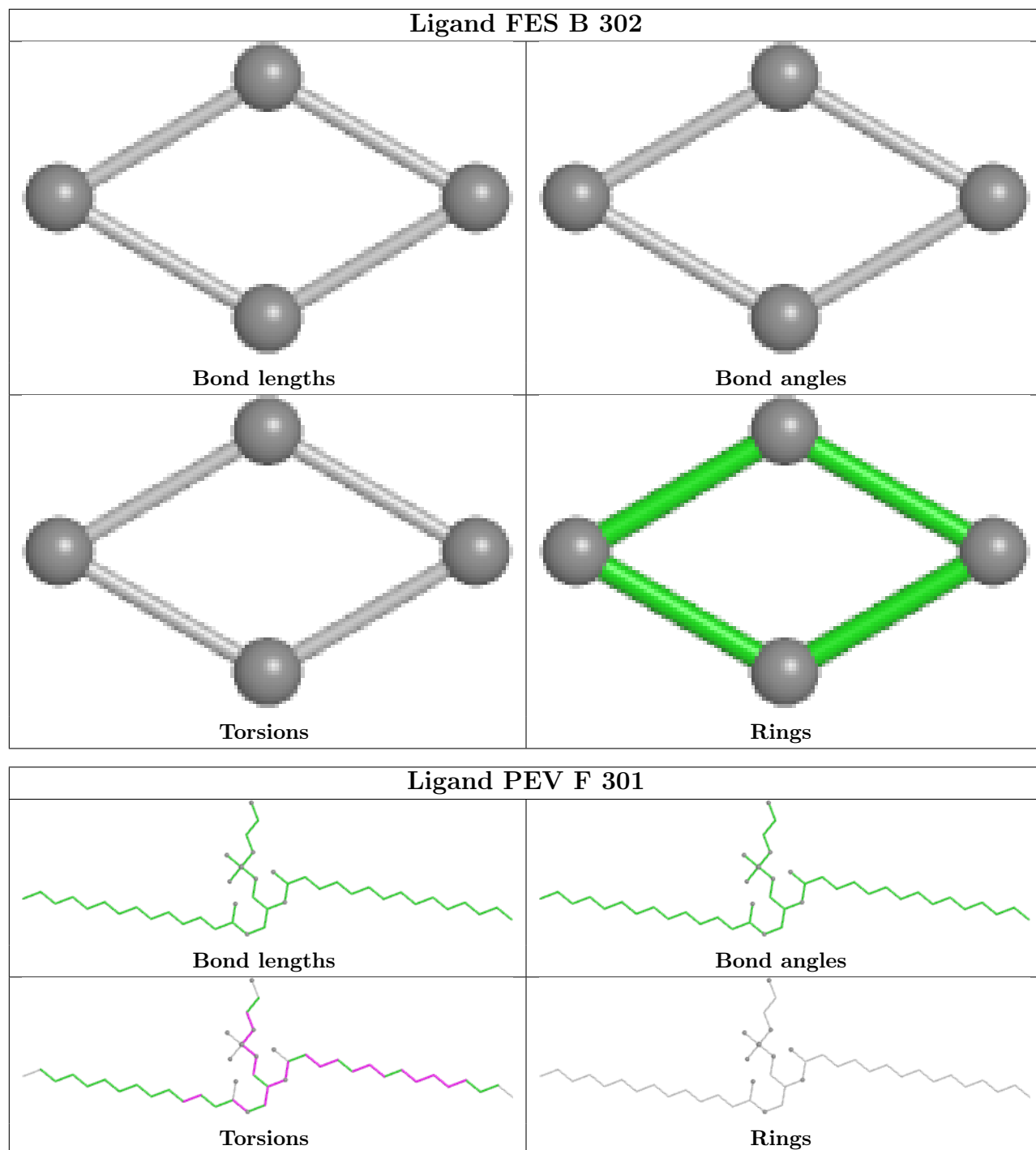
Rings

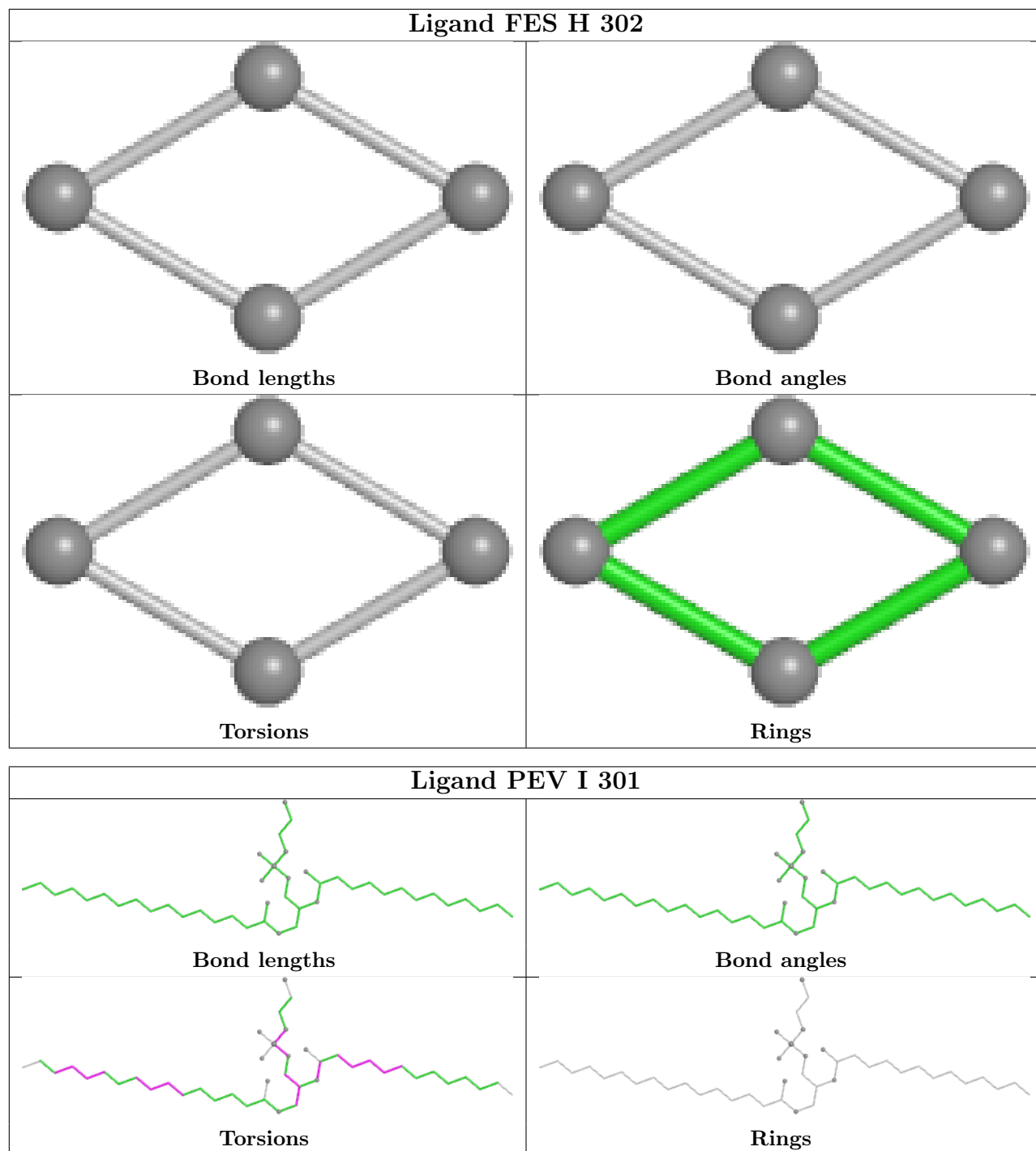


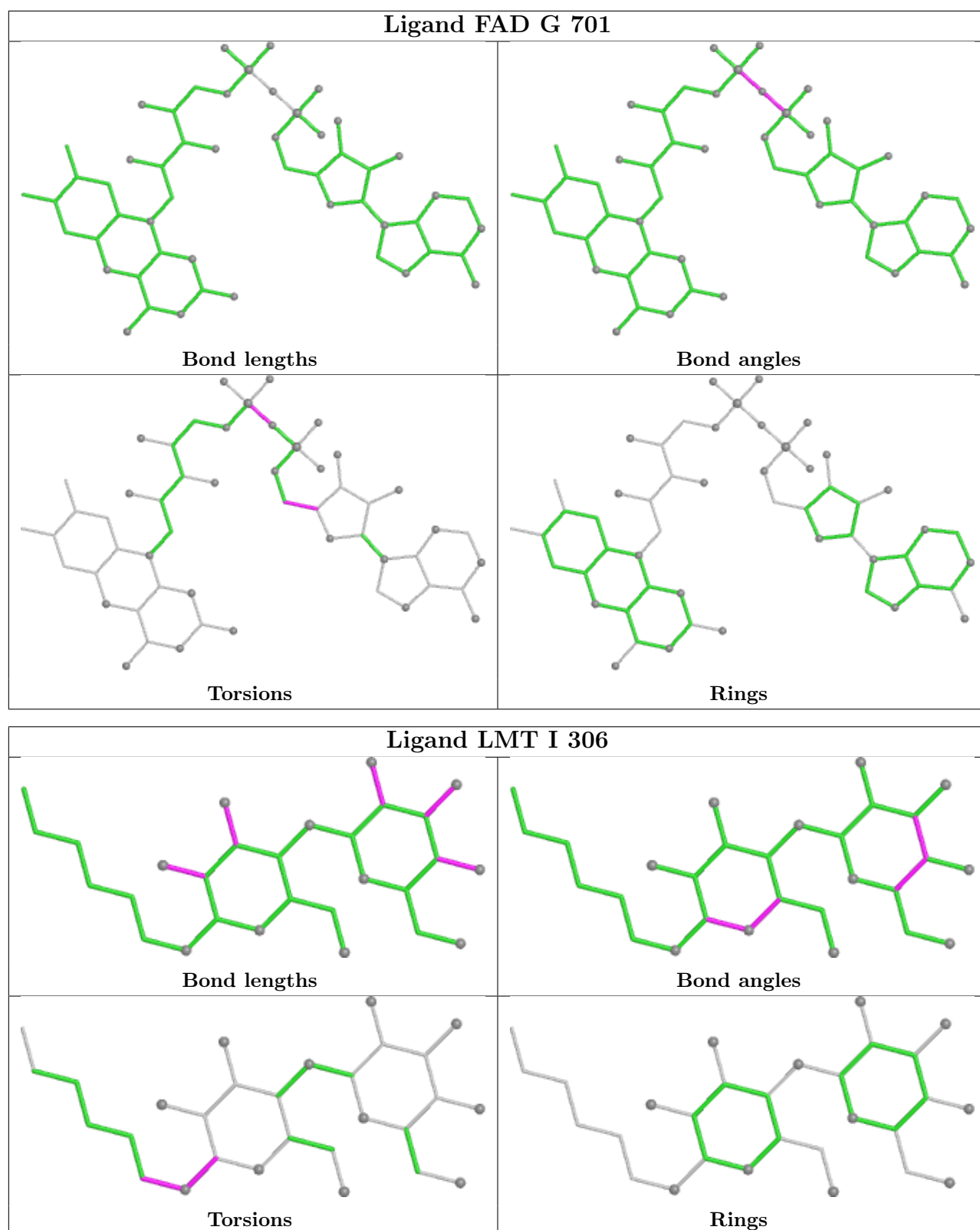


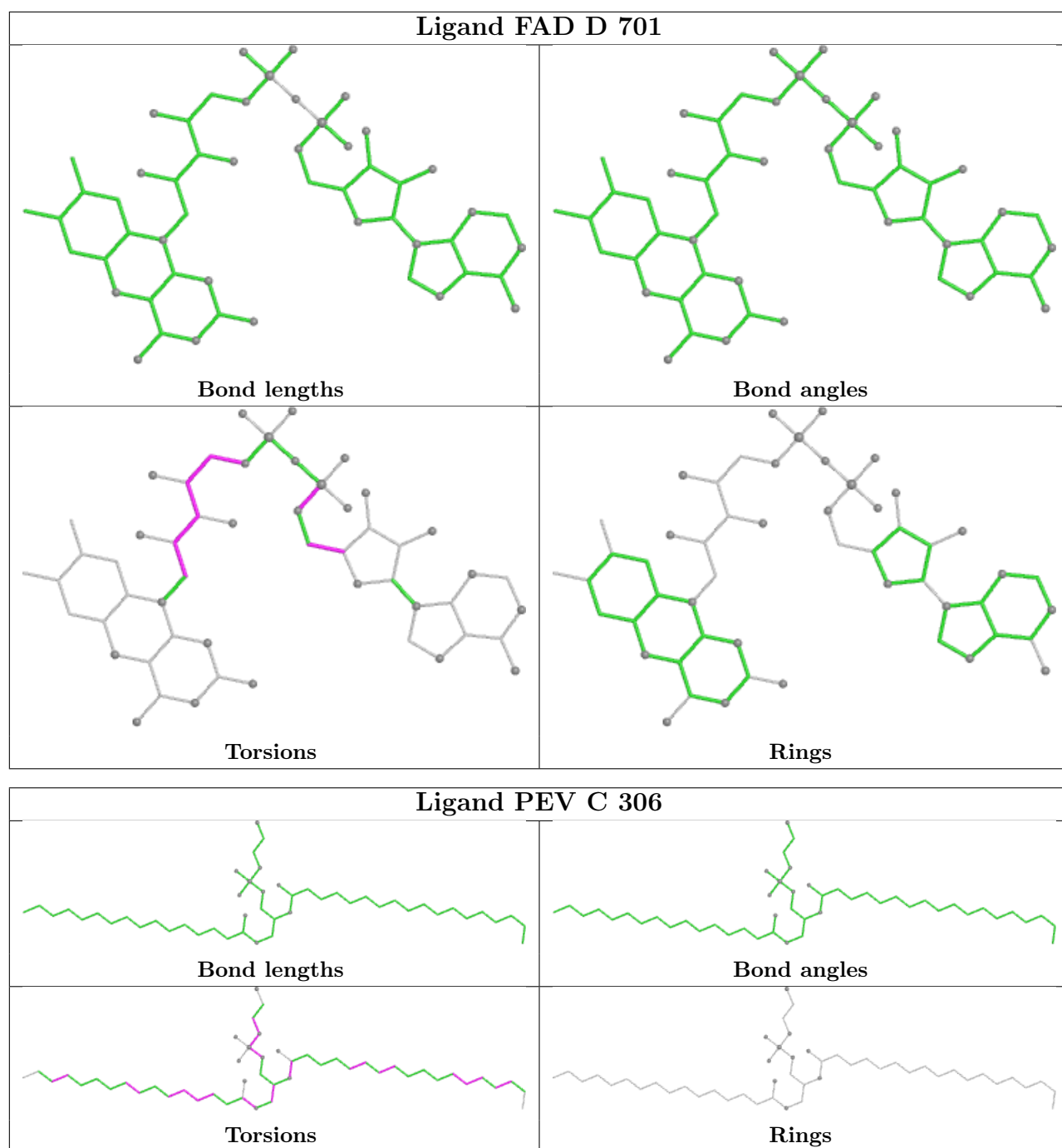


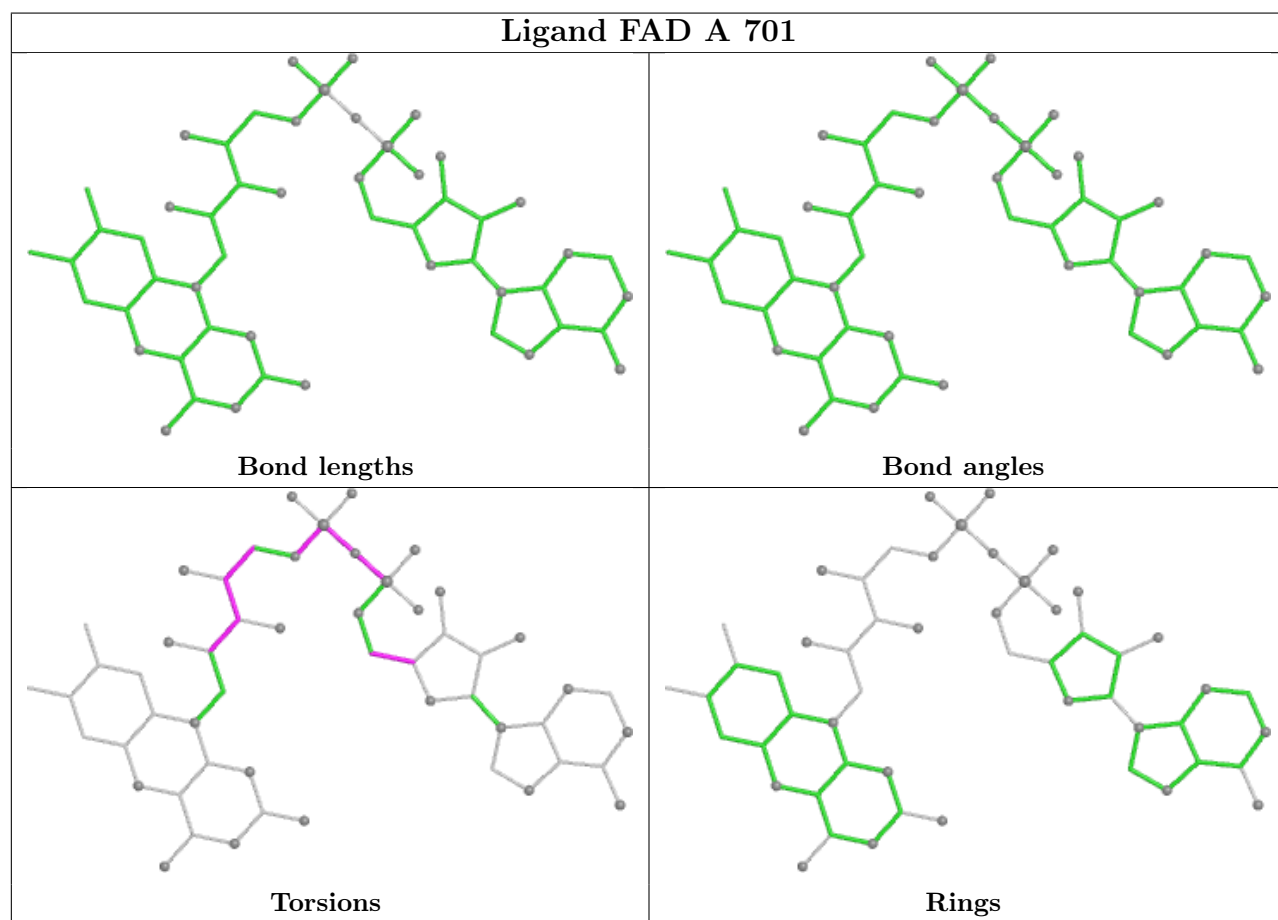
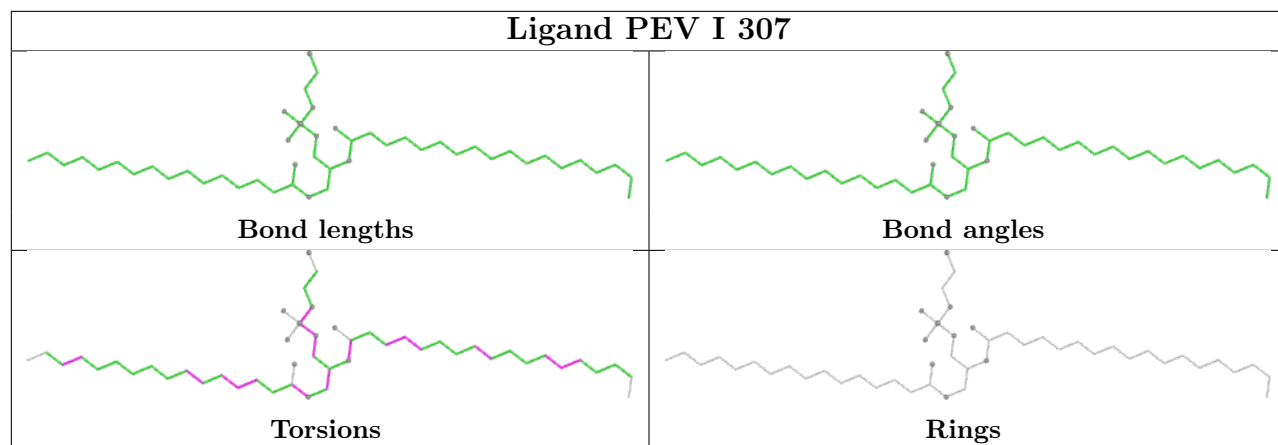


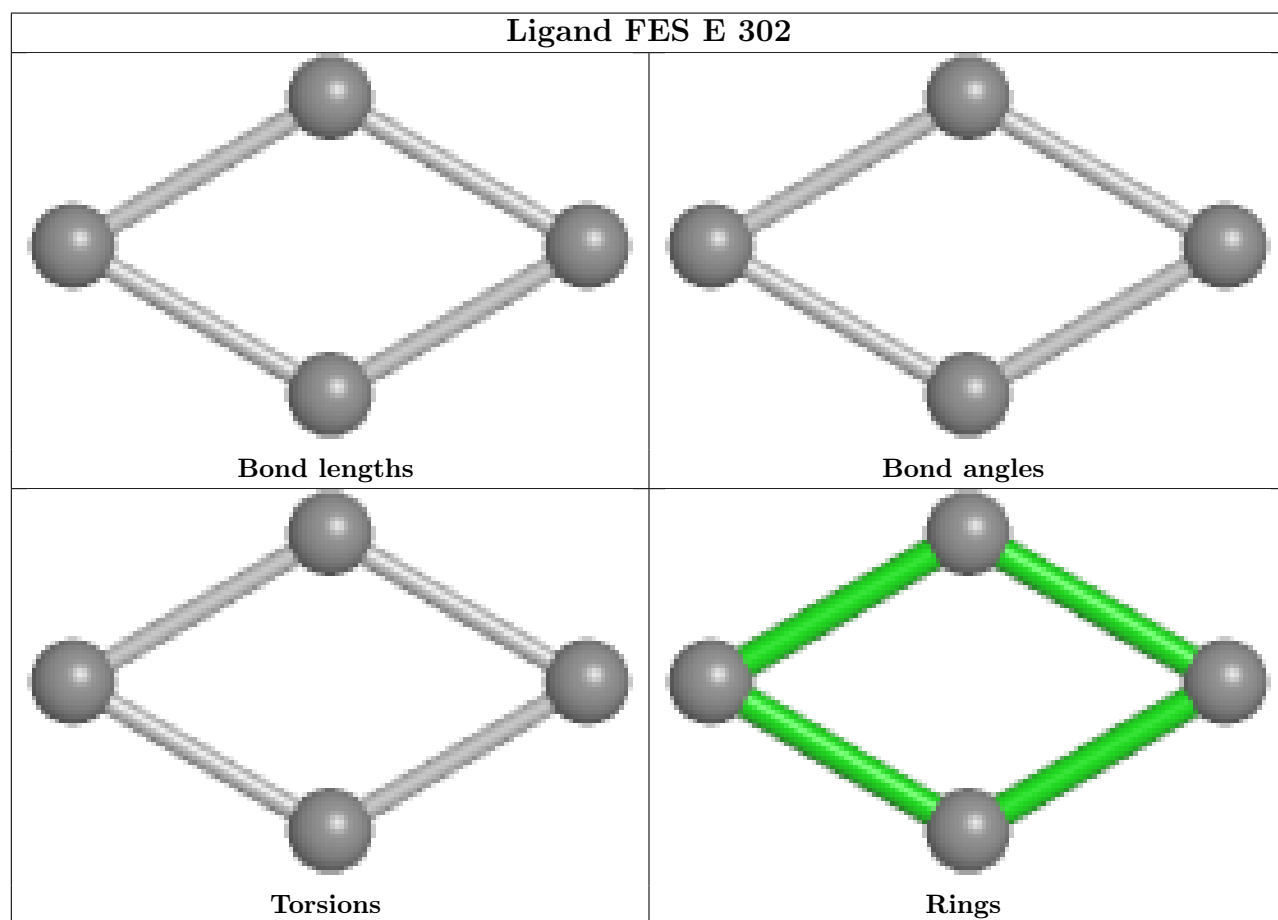
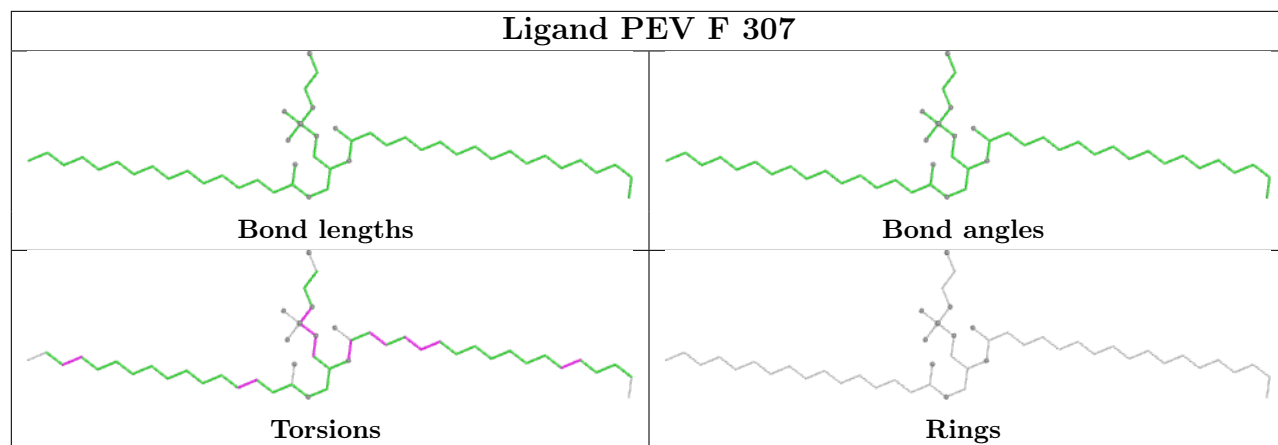


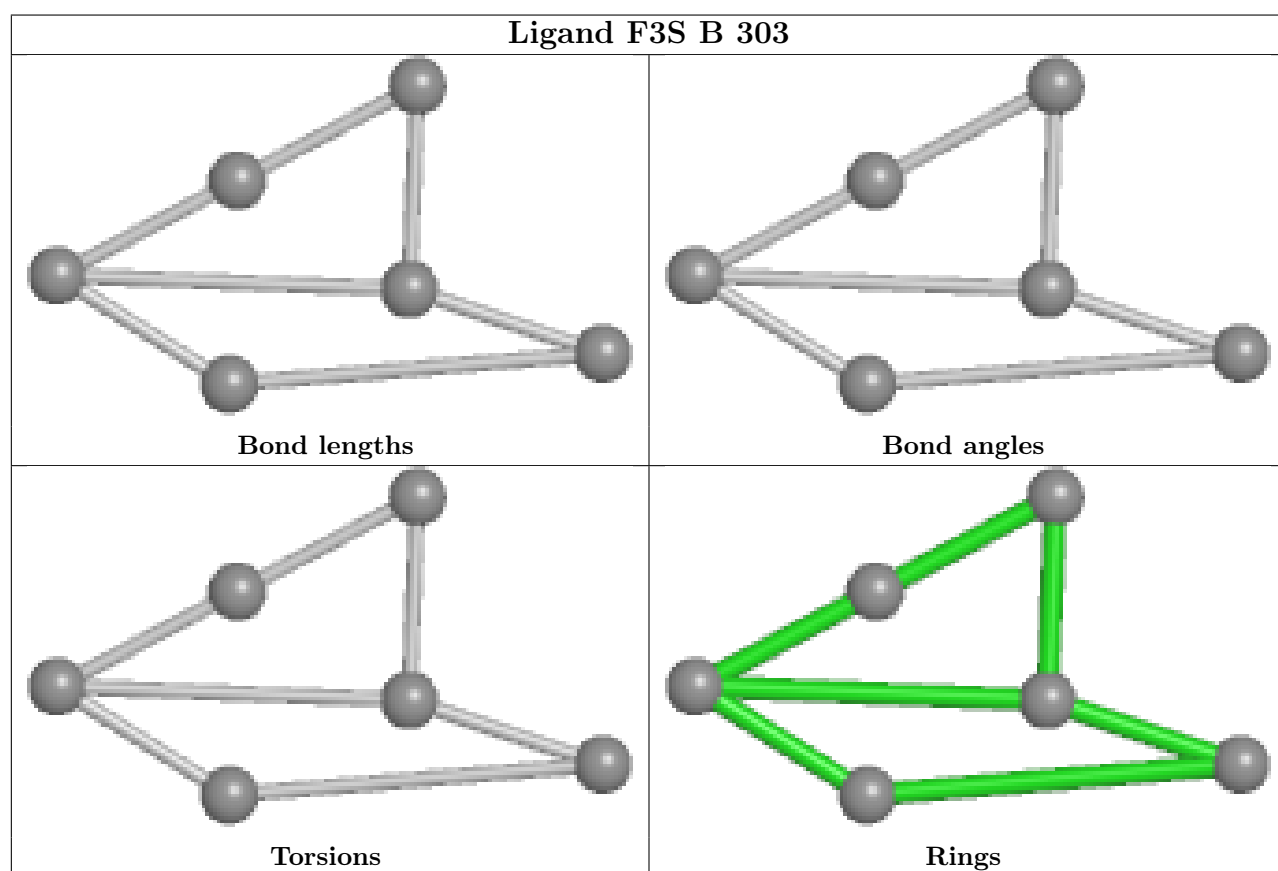
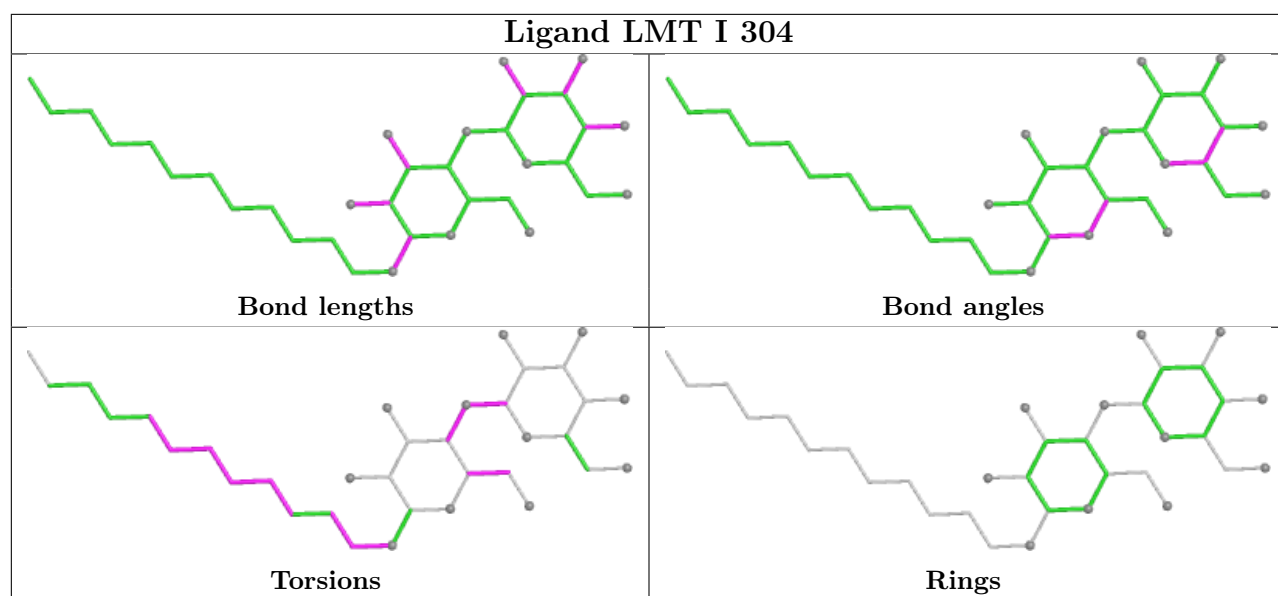


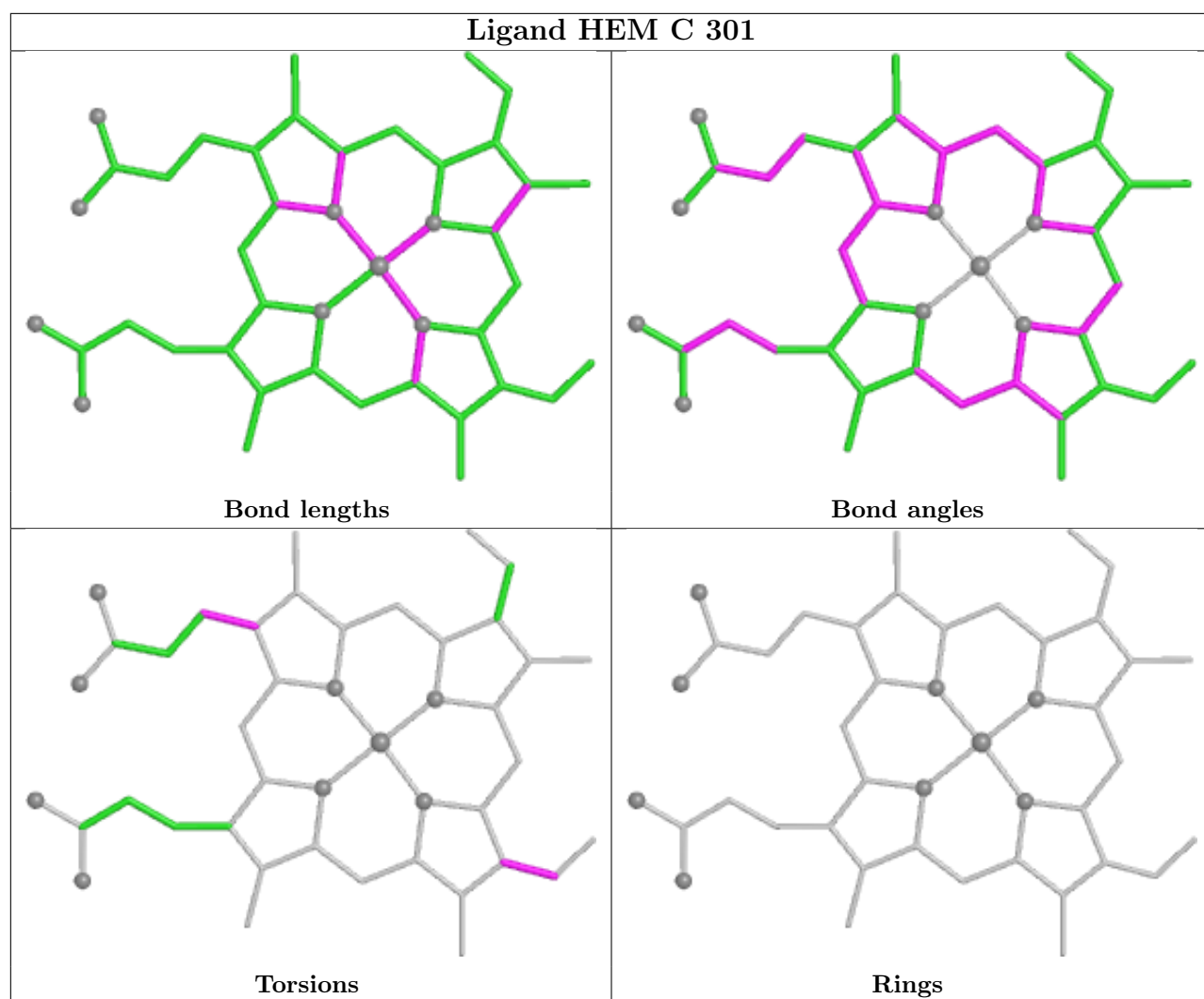


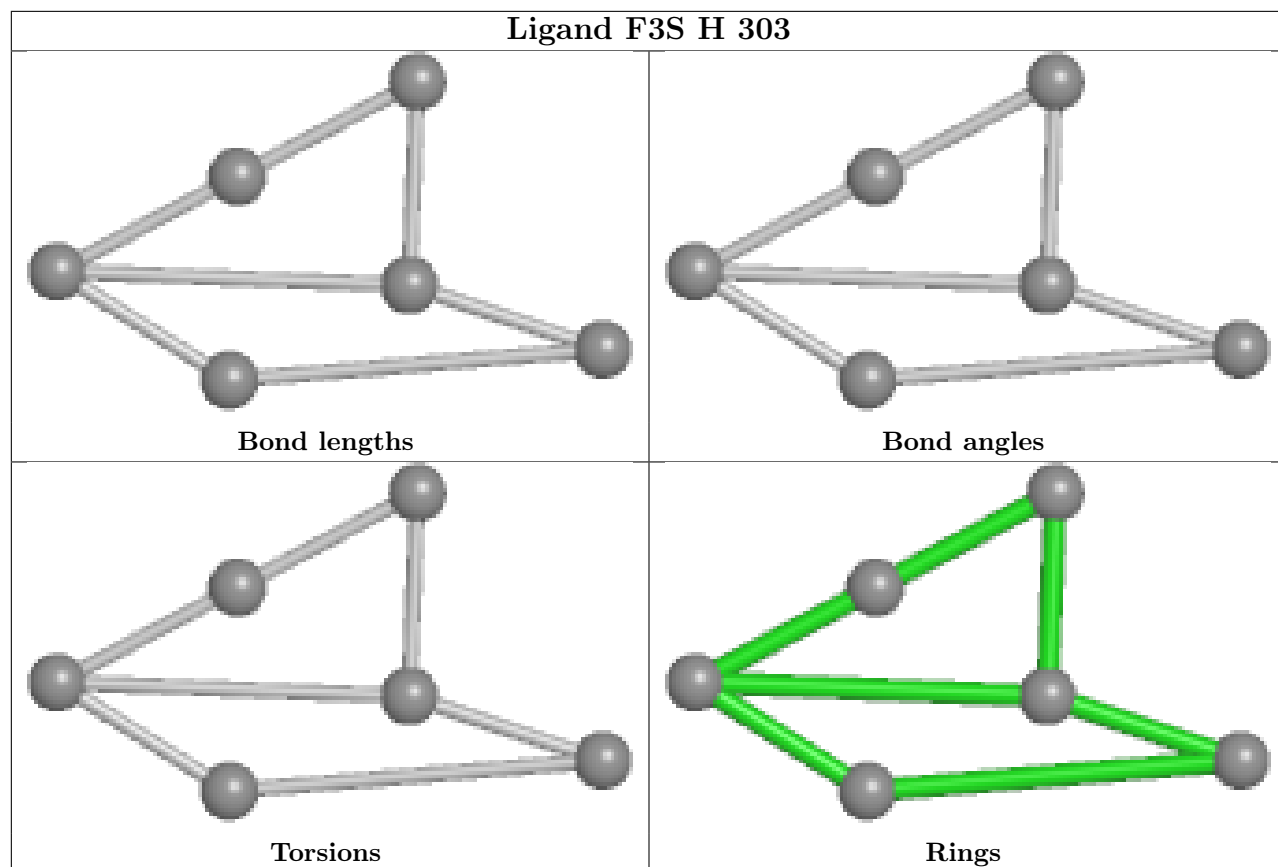


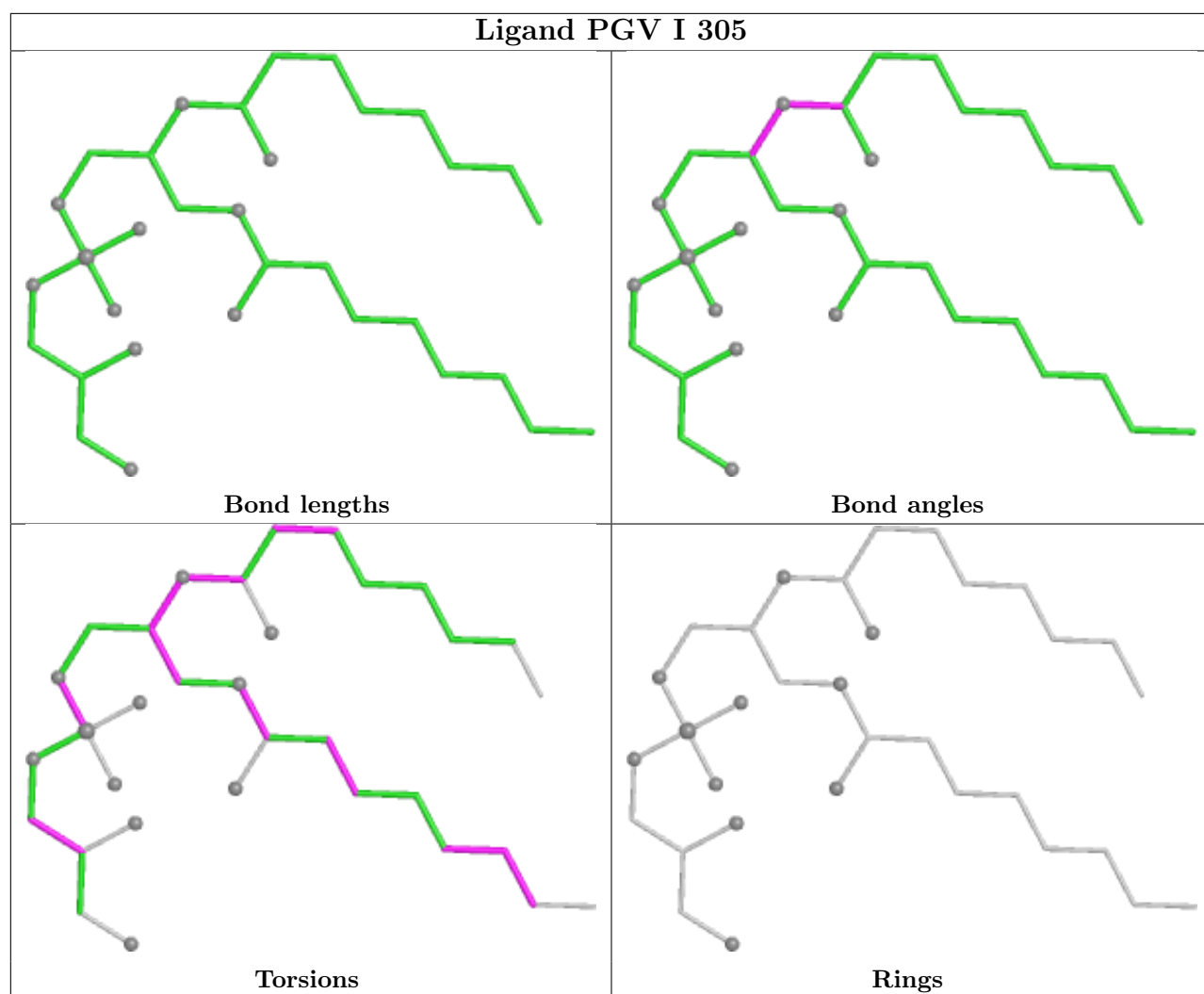


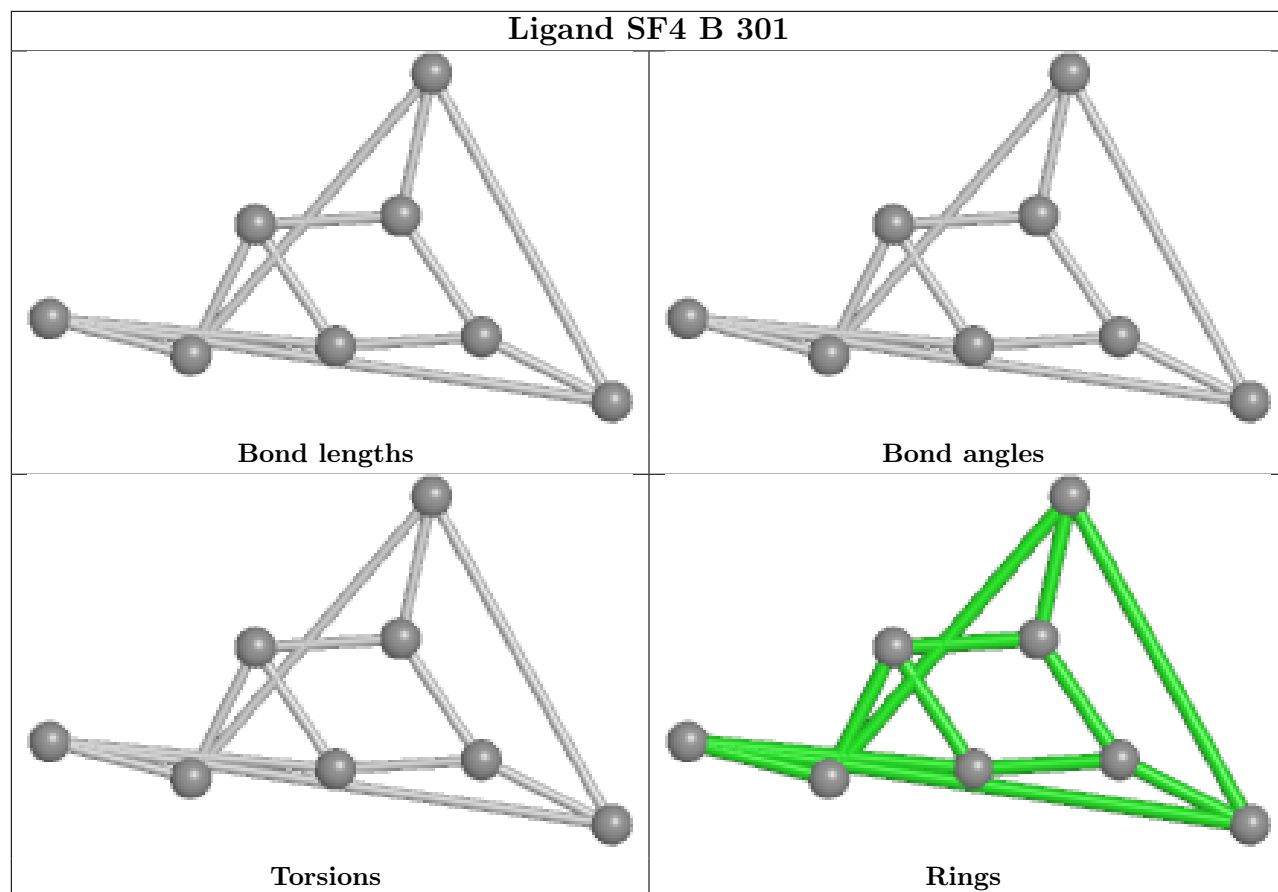


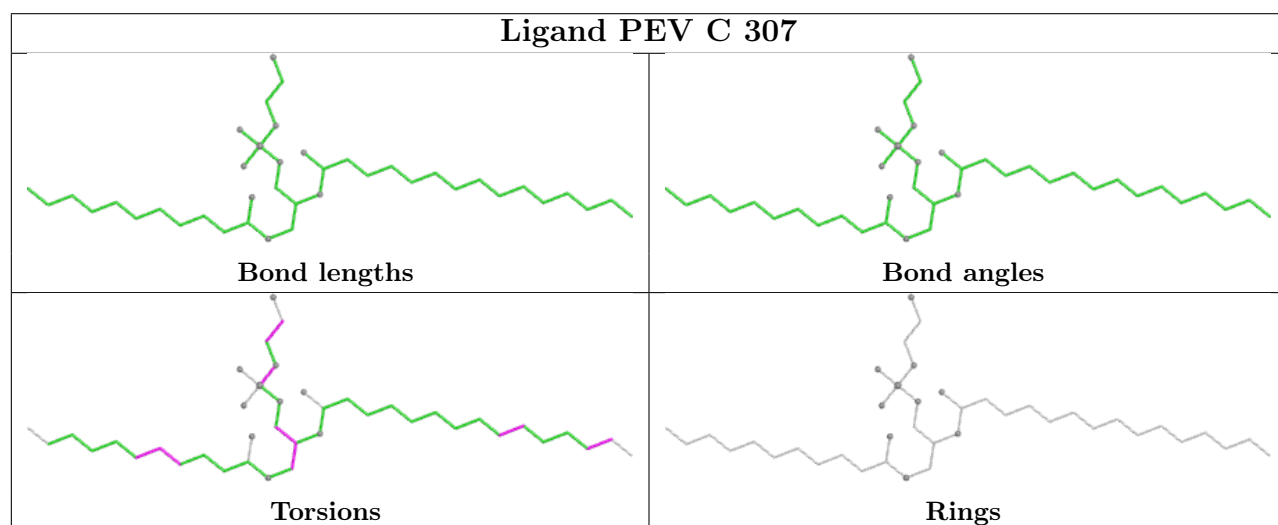
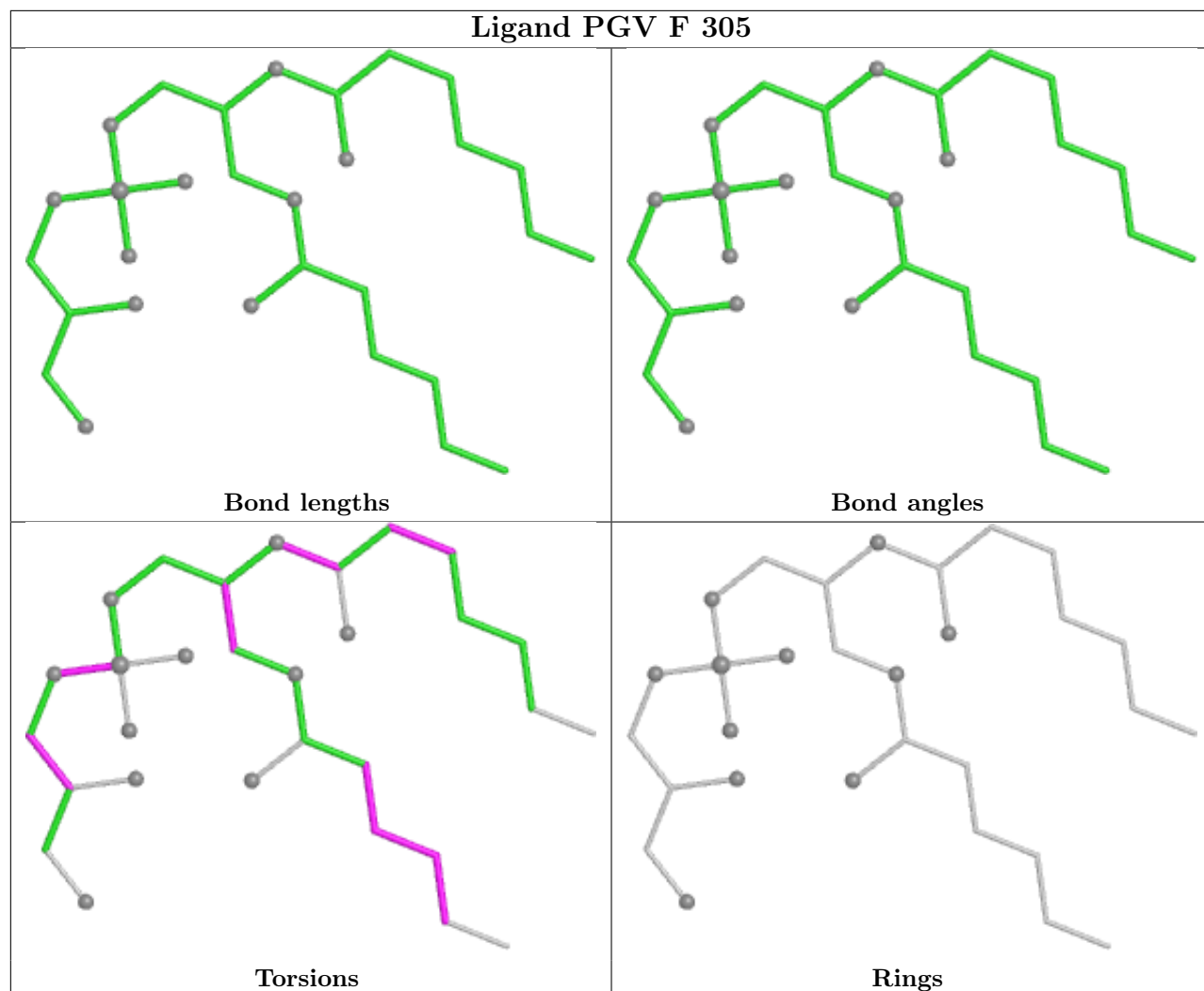


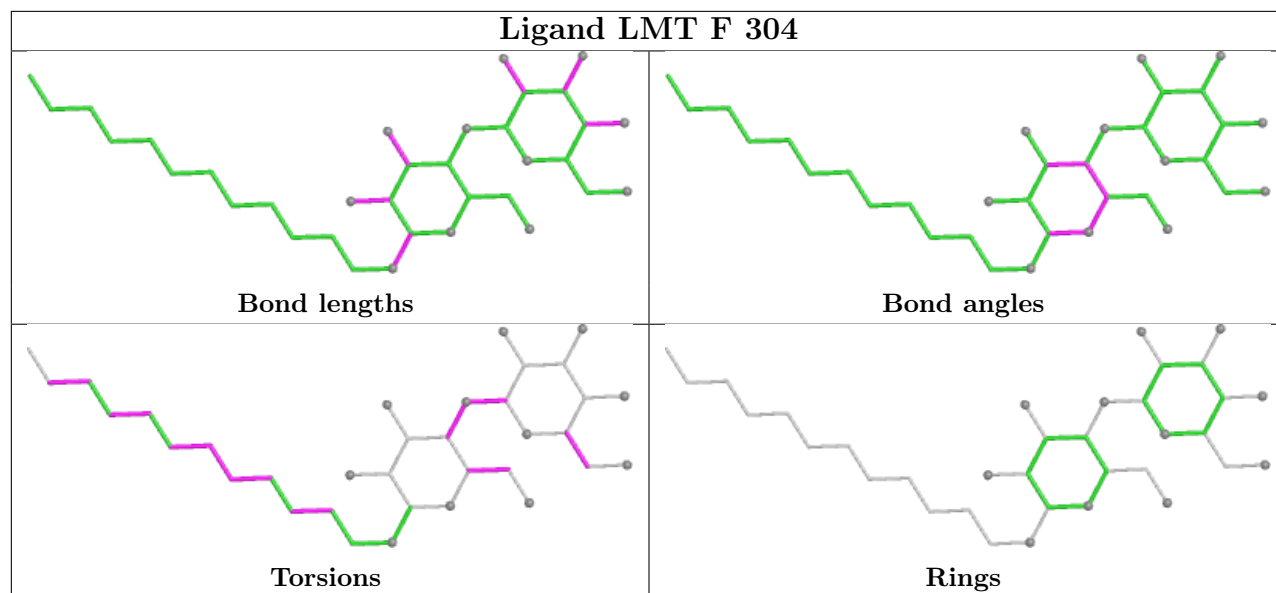












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

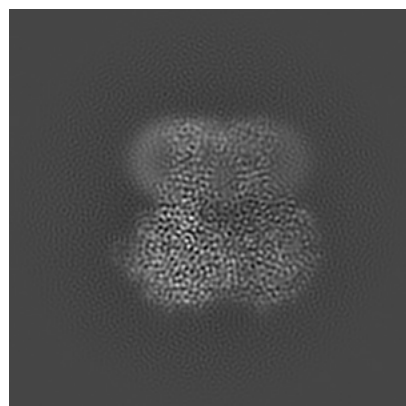
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62933. These allow visual inspection of the internal detail of the map and identification of artifacts.

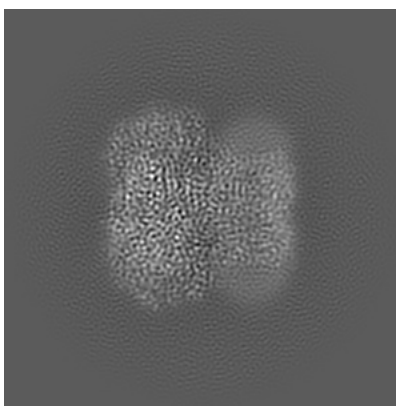
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

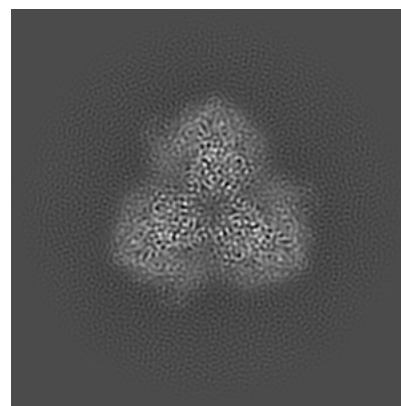
6.1.1 Primary map



X

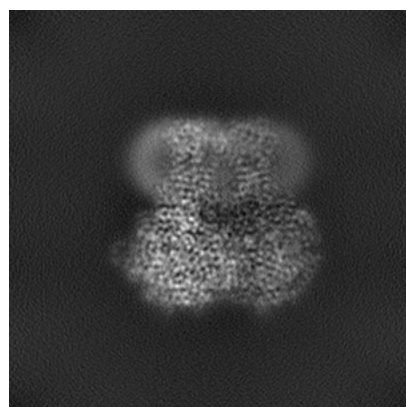


Y

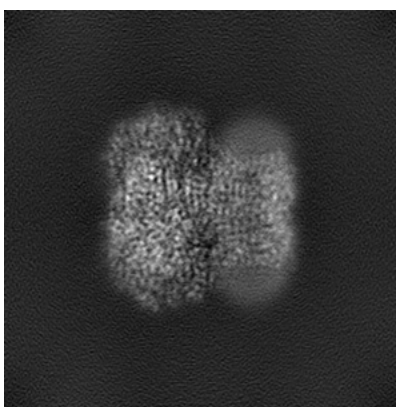


Z

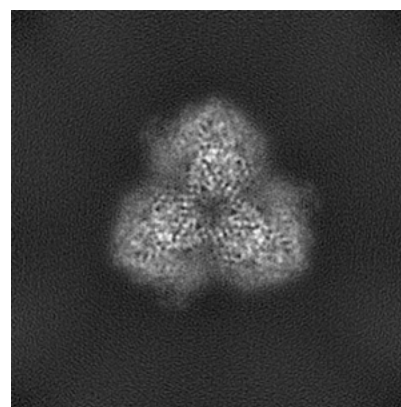
6.1.2 Raw map



X



Y

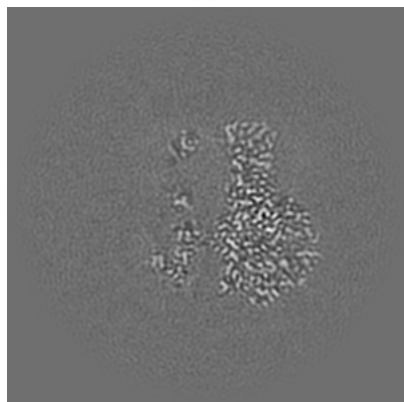


Z

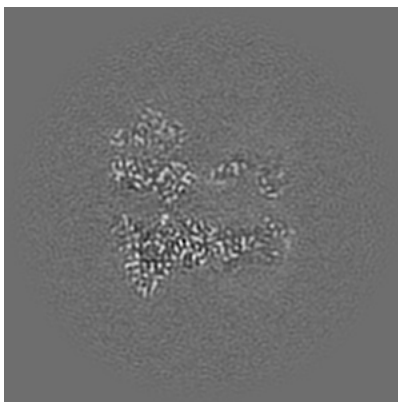
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

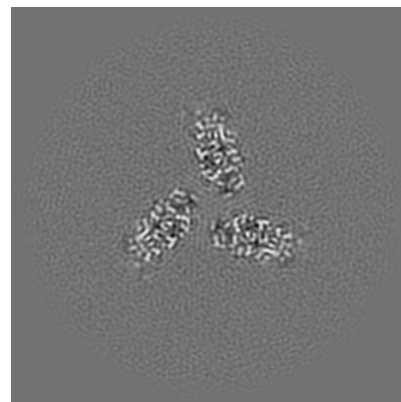
6.2.1 Primary map



X Index: 128

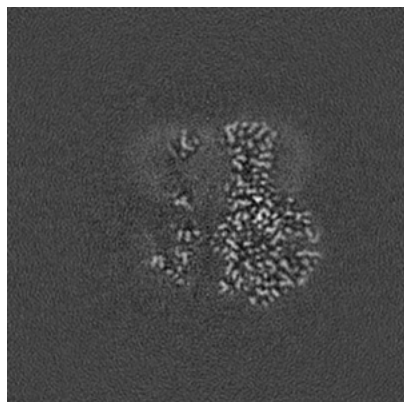


Y Index: 128

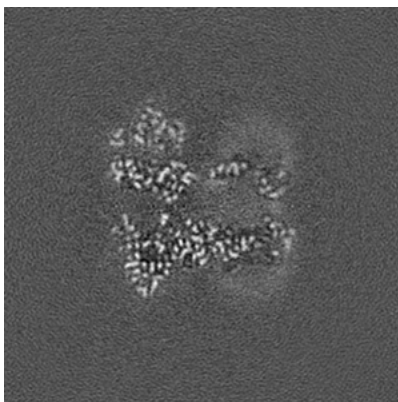


Z Index: 128

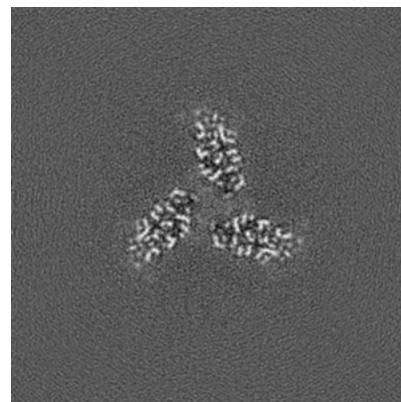
6.2.2 Raw map



X Index: 128



Y Index: 128

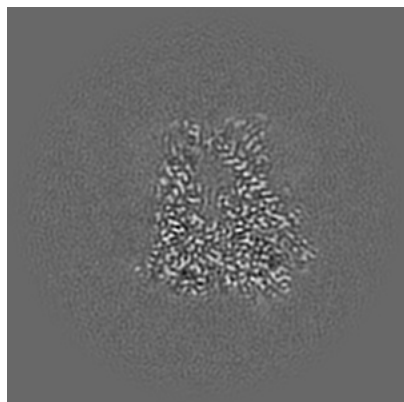


Z Index: 128

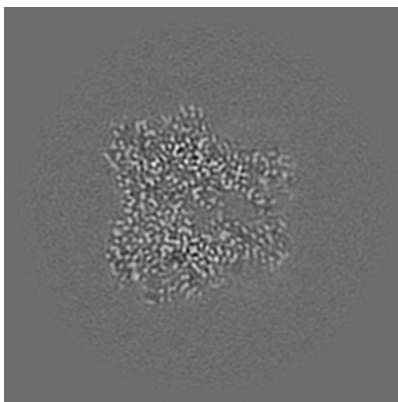
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

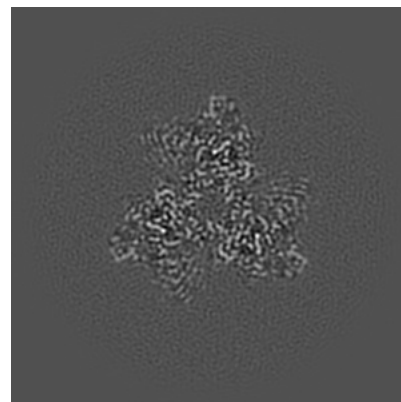
6.3.1 Primary map



X Index: 140

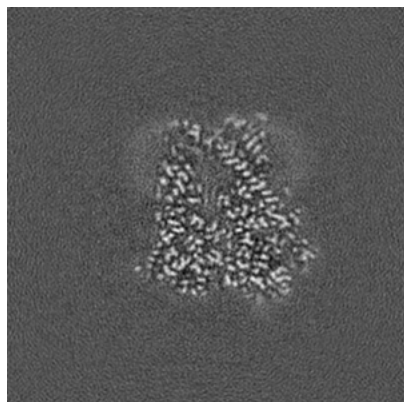


Y Index: 110

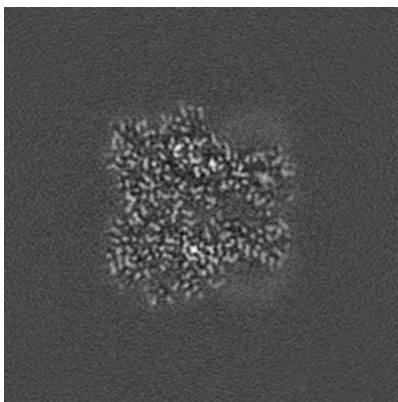


Z Index: 98

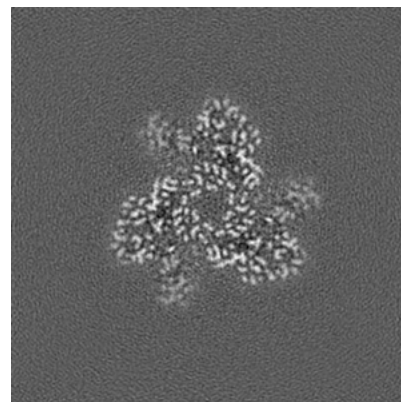
6.3.2 Raw map



X Index: 140



Y Index: 111

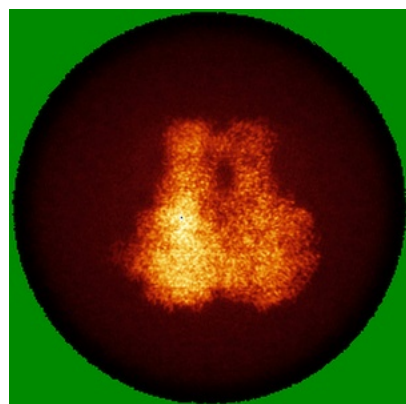


Z Index: 94

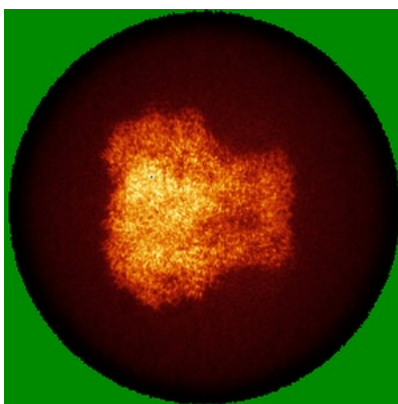
The images above show the largest variance slices of the map in three orthogonal directions.

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

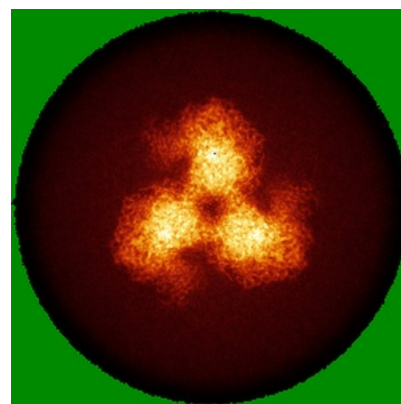
6.4.1 Primary map



X

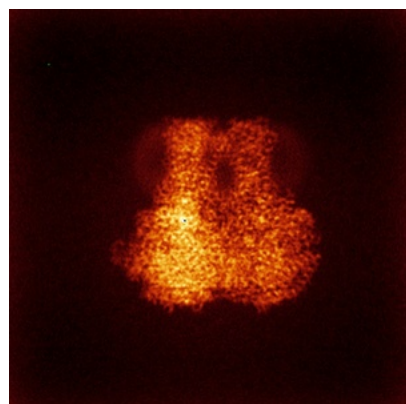


Y

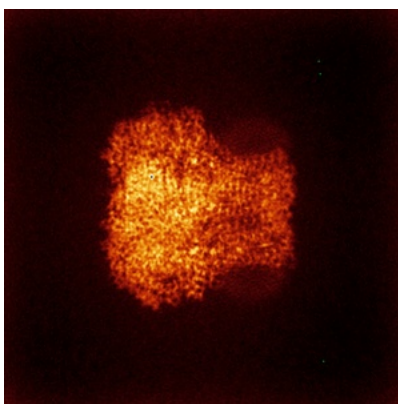


Z

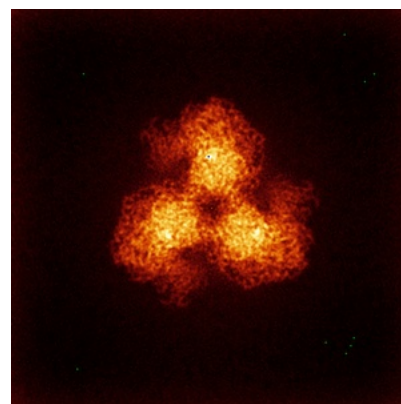
6.4.2 Raw map



X



Y

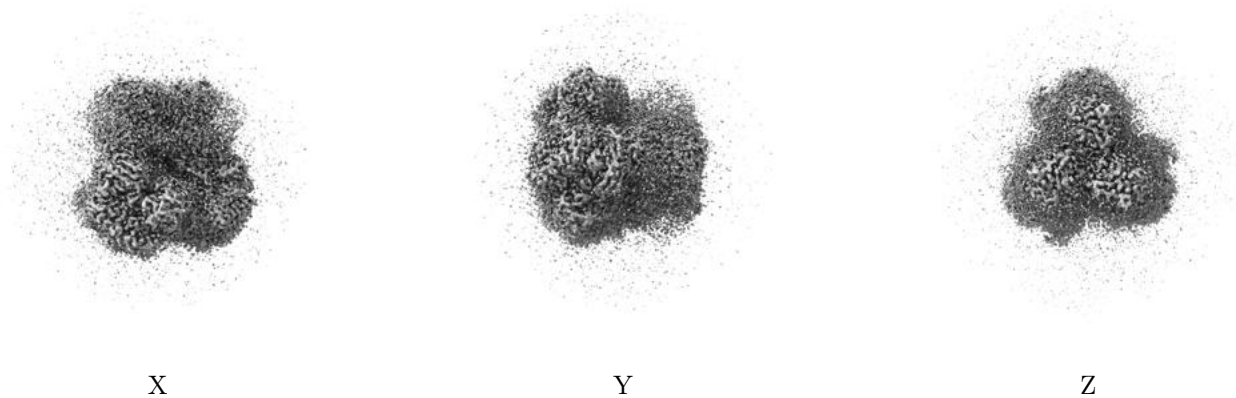


Z

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.

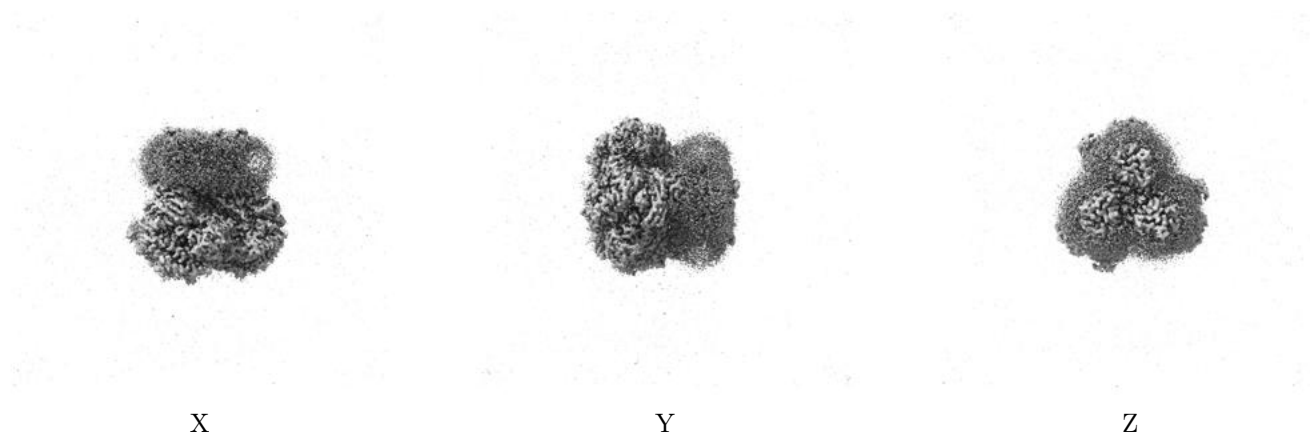
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

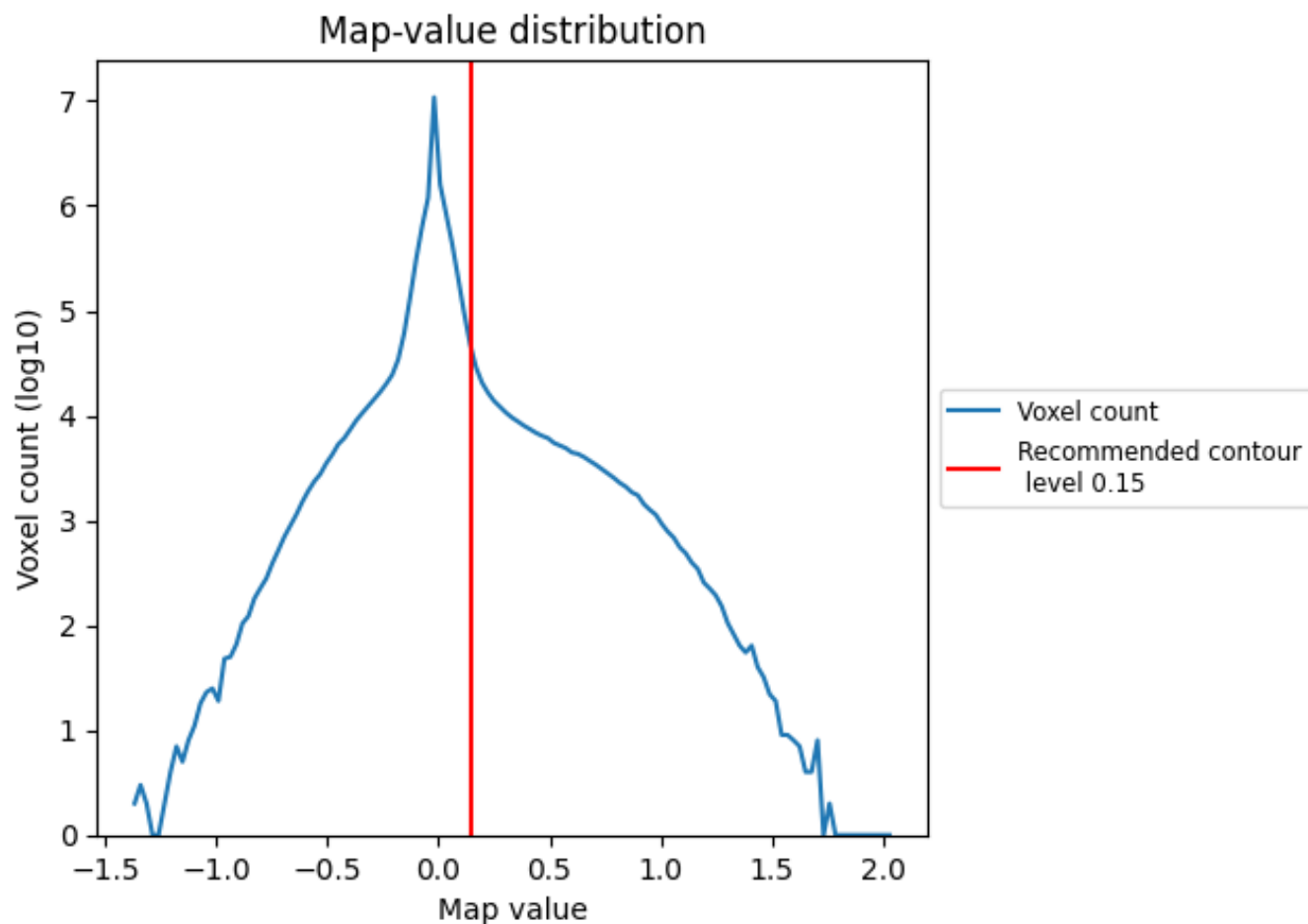
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

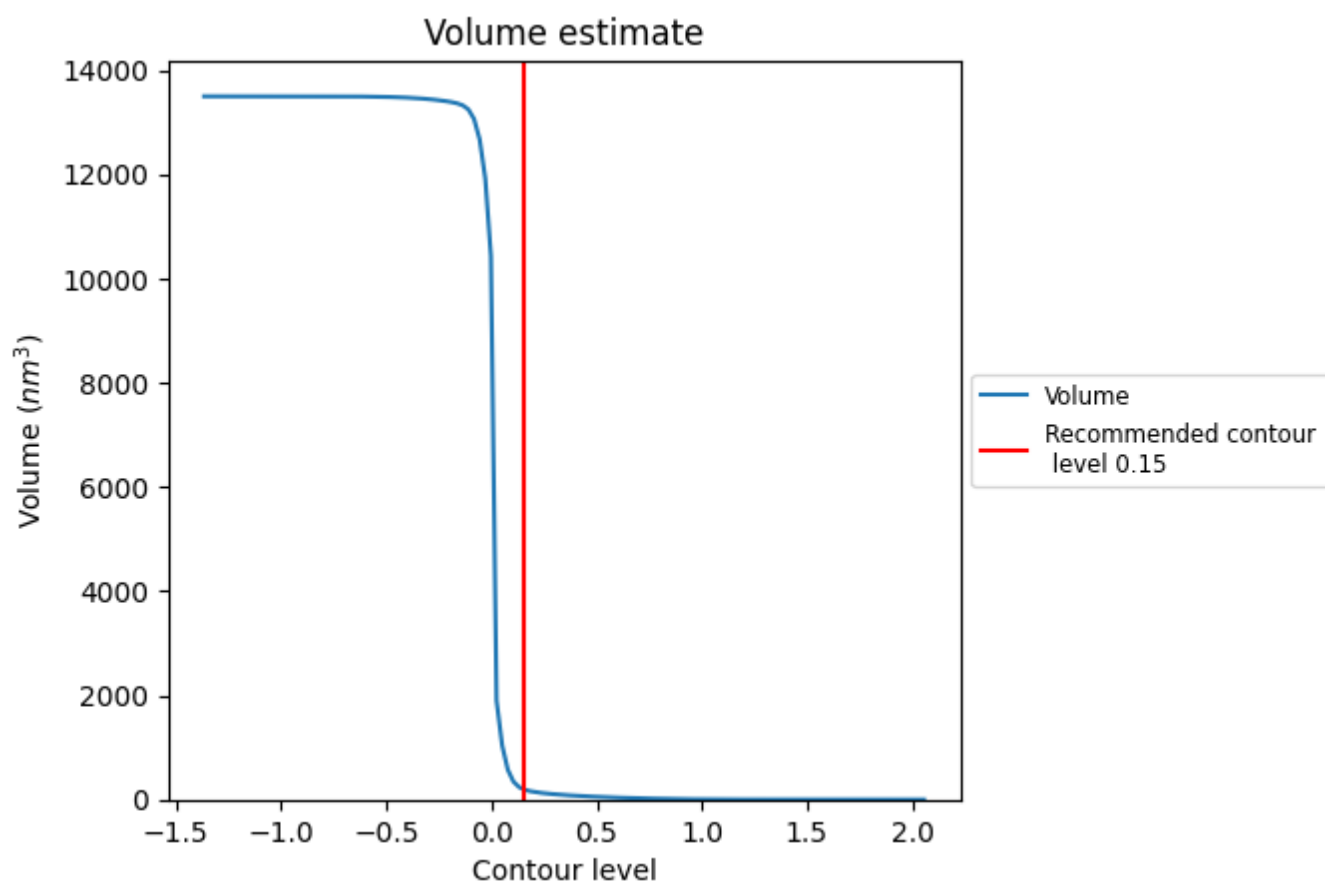
This section contains the results of statistical analysis of the map.

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.

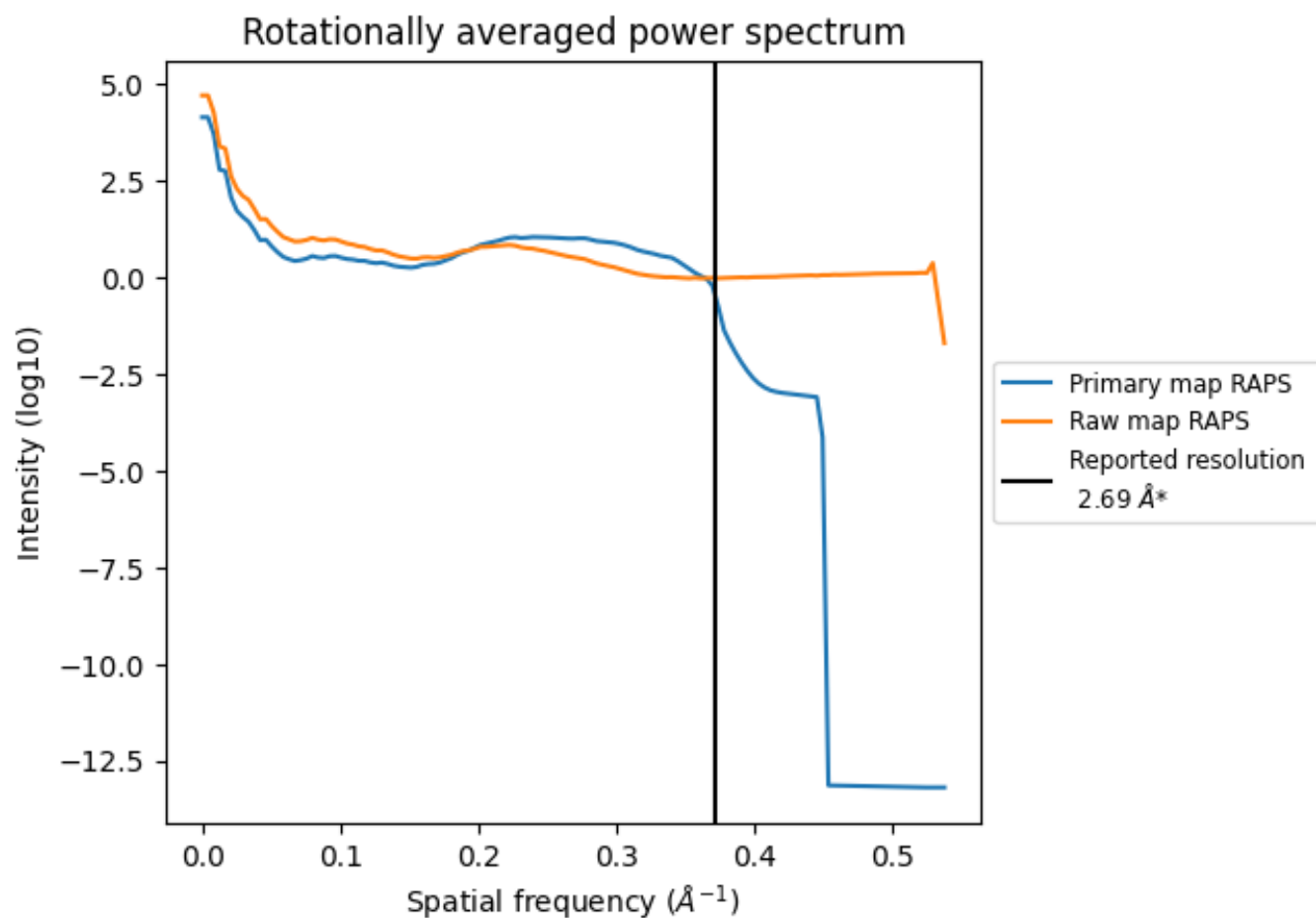
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 183 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 ⓘ

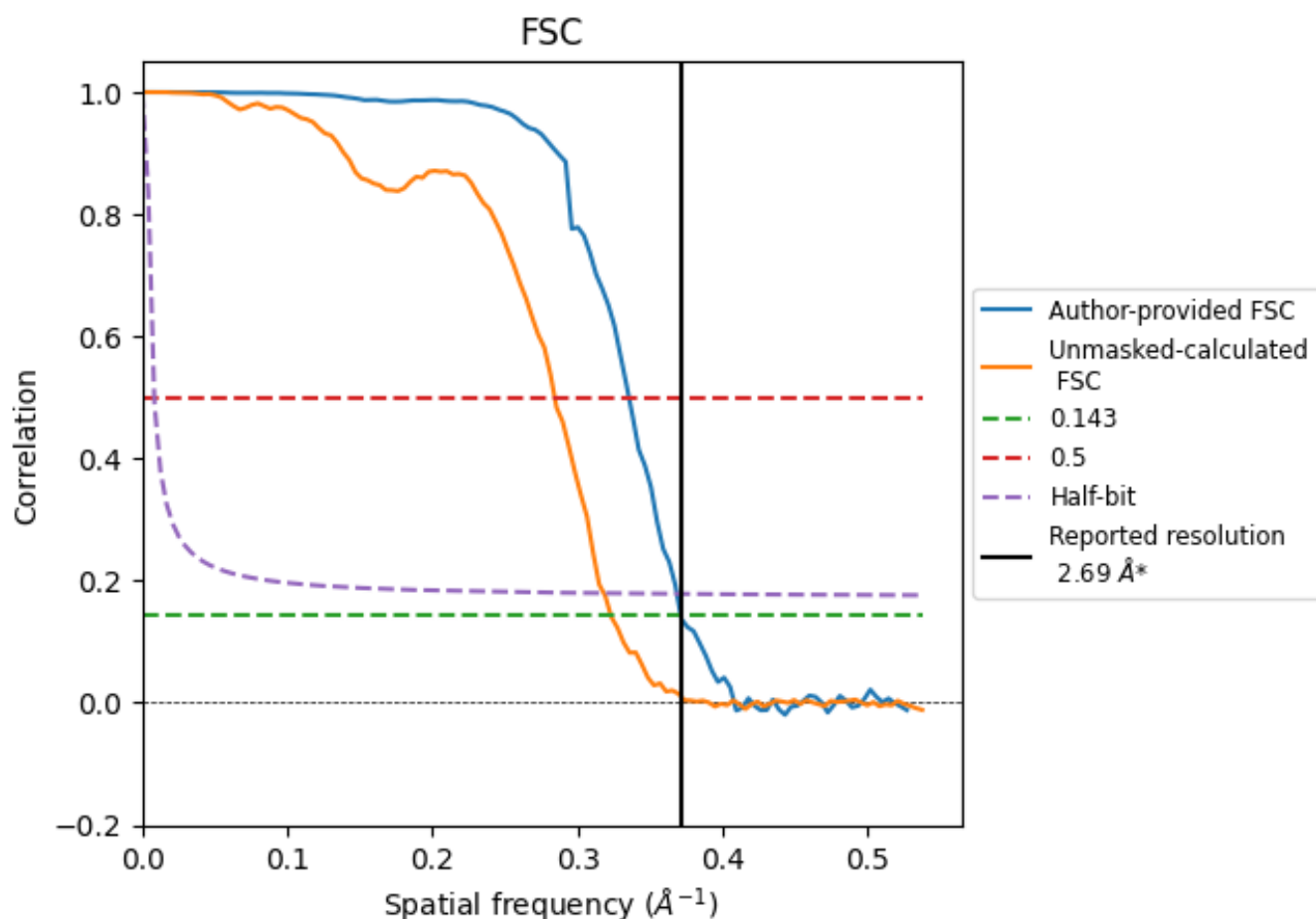


*Reported resolution corresponds to spatial frequency of 0.372 $\text{\AA}^{-1}$

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 0.372 $\text{\AA}^{-1}$

8.2 Resolution estimates

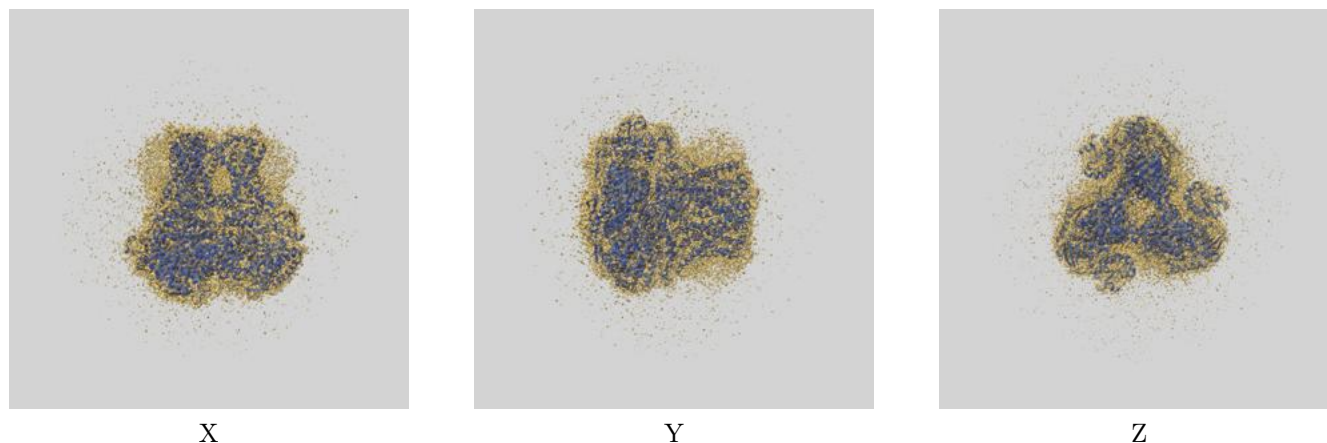
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	2.98	2.71
Unmasked-calculated*	3.10	3.52	3.14

*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 2.69 by more than 10 %

9 Map-model fit [i](#)

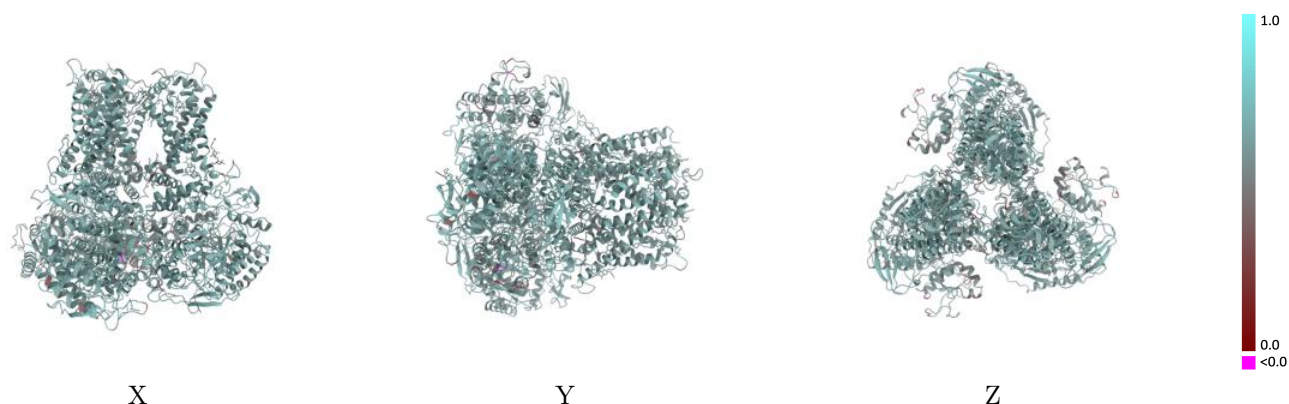
This section contains information regarding the fit between EMDB map EMD-62933 and PDB model 9LAZ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



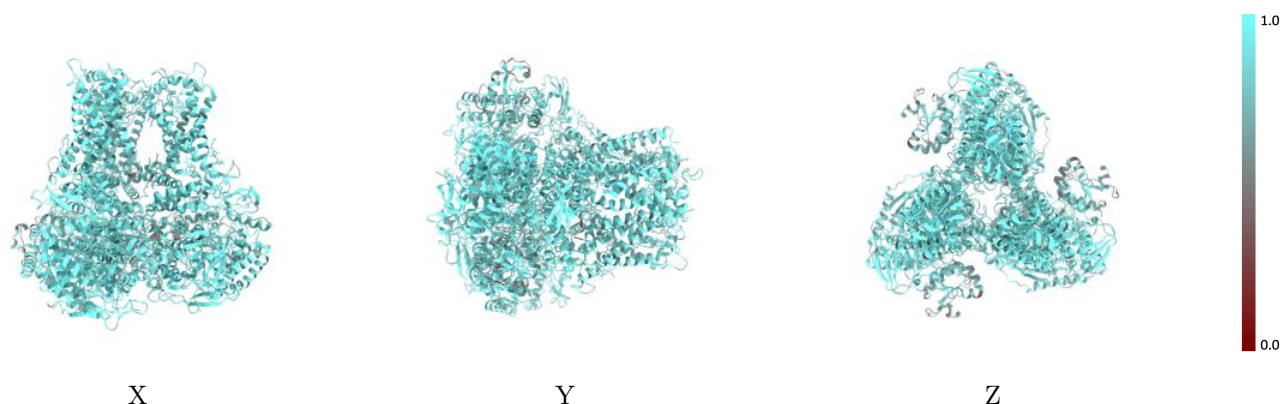
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



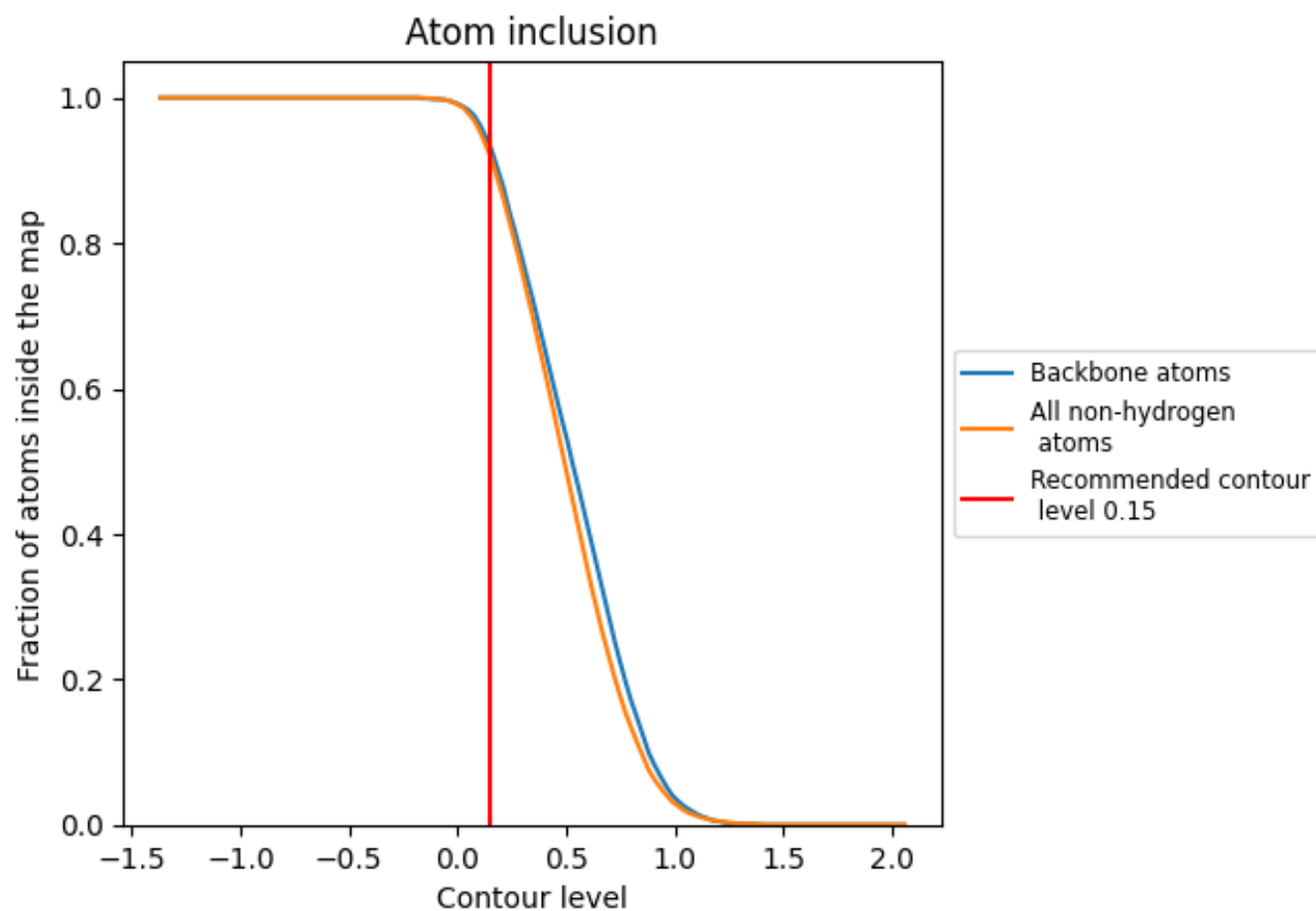
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.6120
A	0.9160	0.6120
B	0.9460	0.6300
C	0.9030	0.5970
D	0.9190	0.6120
E	0.9470	0.6310
F	0.9030	0.5980
G	0.9180	0.6110
H	0.9420	0.6290
I	0.8970	0.5970

1.0

0.0

<0.0