Full wwPDB EM Validation Report

Aug 26, 2026 – 05:04 pm BST

PDB ID	:	8ASJ / pdb_00008asj
EMDB ID	:	EMD-15617
Title	:	Four subunit cytochrome b-c1 complex from Rhodobacter sphaeroides in native nanodiscs - focussed refinement in the b-c conformation
Authors	:	Swainsbury, D.J.K.; Hawkings, F.R.; Martin, E.C.; Musial, S.; Salisbury, J.H.; Jackson, P.J.; Farmer, D.A.; Johnson, M.P.; Siebert, C.A.; Hitchcock, A.; Hunter, C.N.
Deposited on	:	2022-08-19
Resolution	:	3.75 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:

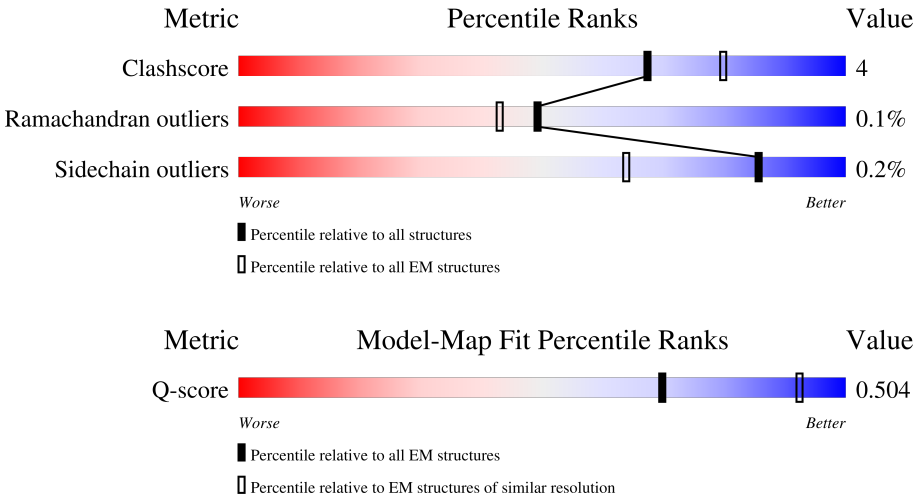
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.75 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	10301 (3.25 - 4.25)

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 <=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	187	14% 90% 6%
1	E	187	71% 75% 21%
2	B	445	91% 7%

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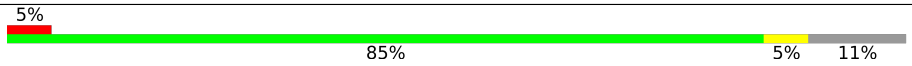
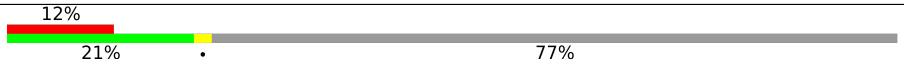
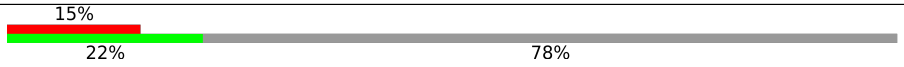
Mol	Chain	Length	Quality of chain
2	F	445	
3	C	285	
3	G	285	
4	D	124	
4	H	124	

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
5	FES	E	201	-	-	X	-
8	HEC	C	301	X	-	-	-
8	HEC	G	301	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14720 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	179	Total	C	N	O	S	0	0
			1342	845	237	254	6		
1	E	181	Total	C	N	O	S	0	0
			1357	854	241	256	6		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	433	Total	C	N	O	S	0	0
			3477	2345	552	564	16		
2	F	432	Total	C	N	O	S	0	0
			3471	2342	551	562	16		

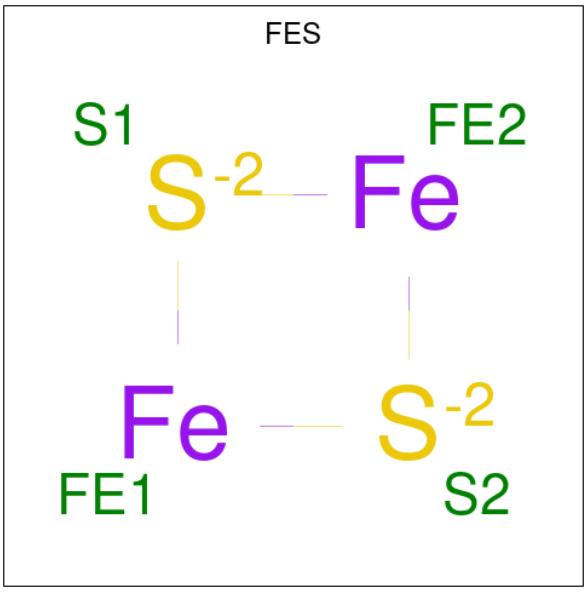
- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	254	Total	C	N	O	S	0	0
			1944	1235	324	372	13		
3	G	254	Total	C	N	O	S	0	0
			1944	1235	324	372	13		

- Molecule 4 is a protein called Cytochrome b-c1 subunit IV.

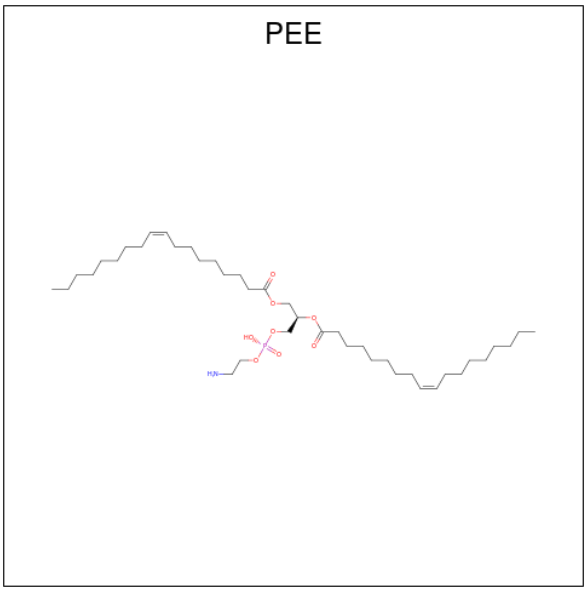
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	29	Total	C	N	O	0	0
			222	149	38	35		
4	H	27	Total	C	N	O	0	0
			203	136	35	32		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			4	2	2	
5	E	1	Total	Fe	S	0
			4	2	2	

- Molecule 6 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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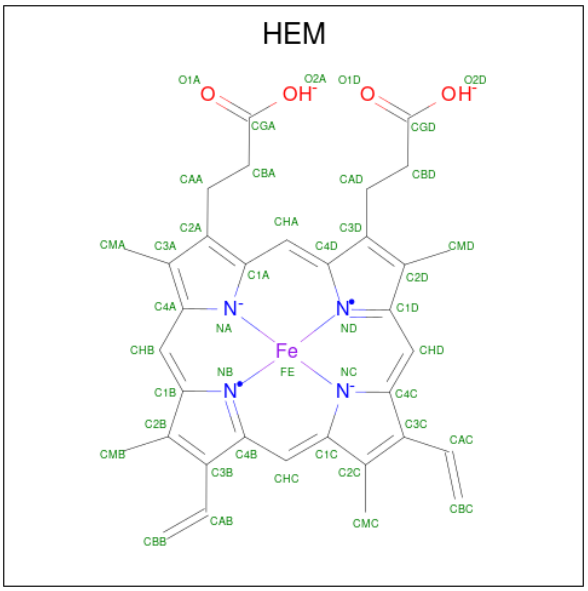
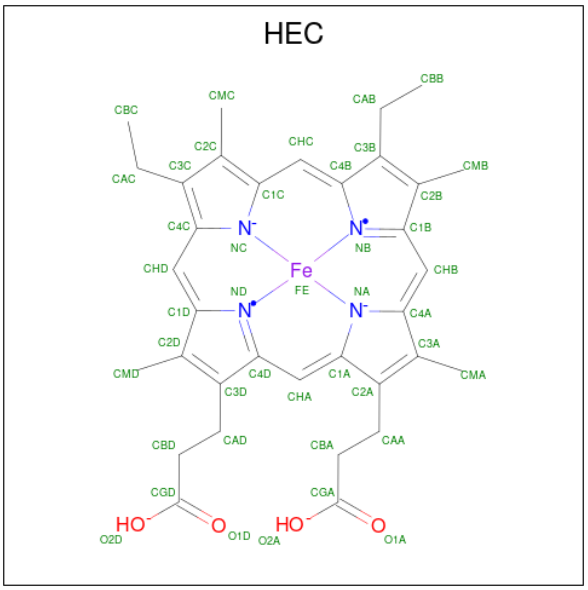
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
6	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
6	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
6	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
6	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
6	F	1	Total	C	N	O	P	0
			31	21	1	8	1	
6	F	1	Total	C	N	O	P	0
			30	20	1	8	1	
6	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	F	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



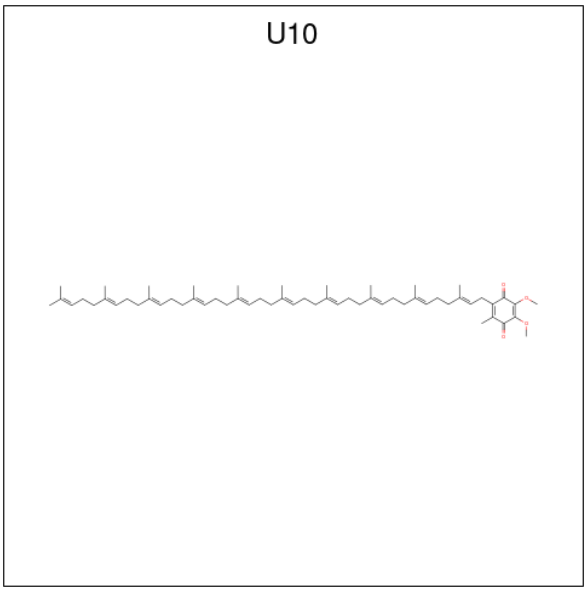
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

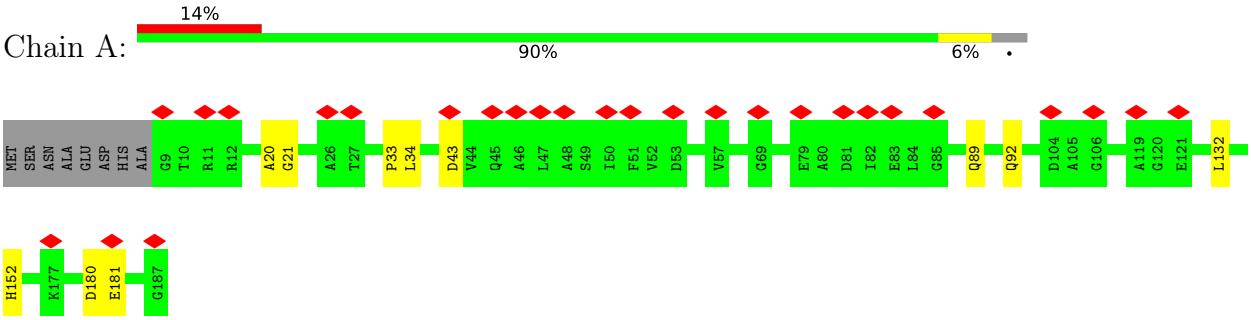


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	F	1	42	38	4	0

3 Residue-property plots (i)

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

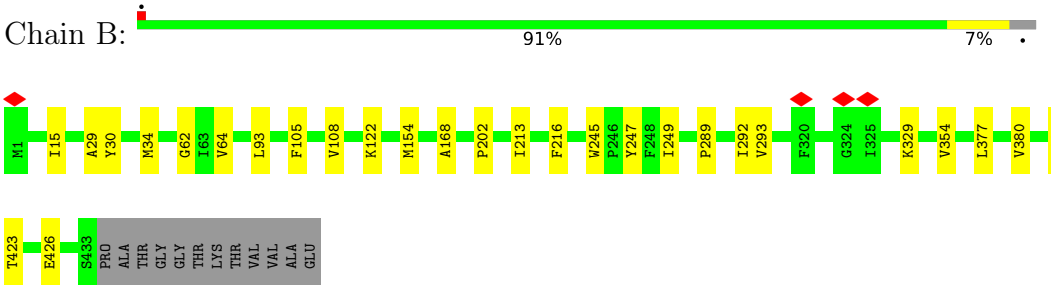
• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

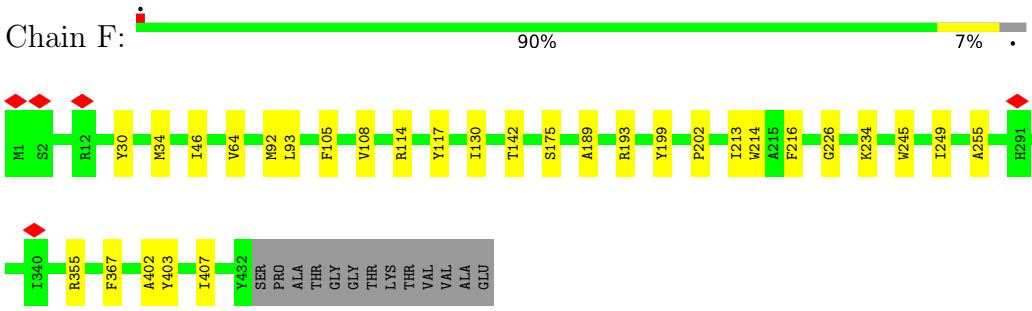


• Molecule 2: Cytochrome b



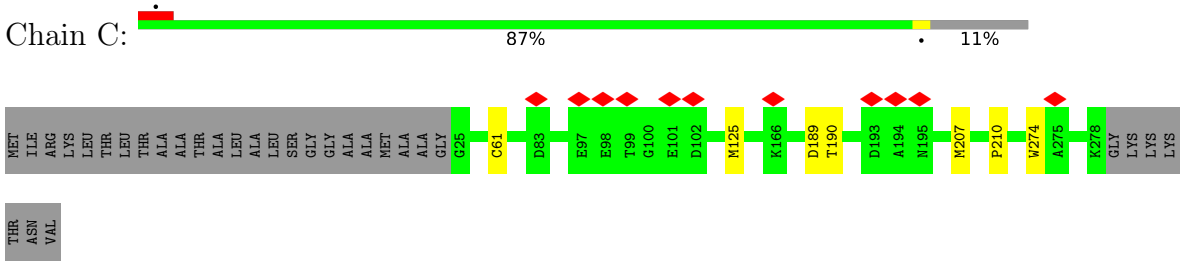
• Molecule 2: Cytochrome b

Chain F:



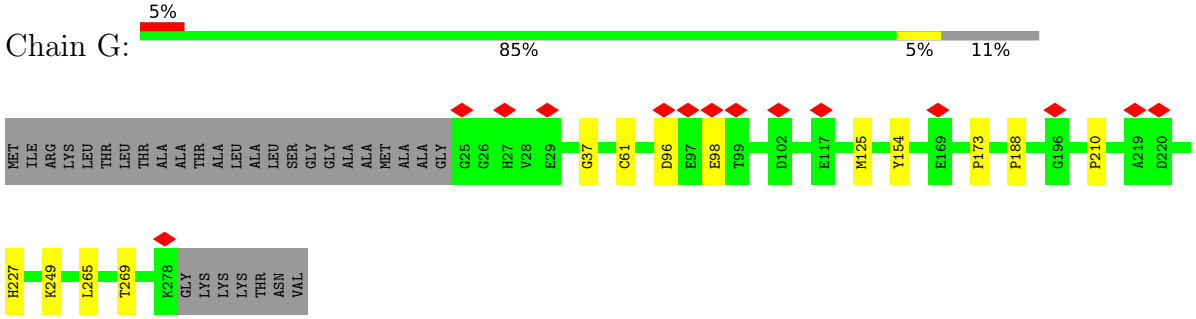
• Molecule 3: Cytochrome c1

Chain C:



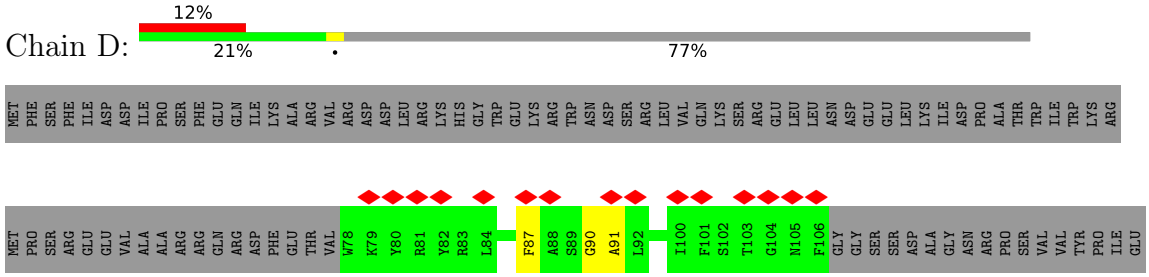
• Molecule 3: Cytochrome c1

Chain G:



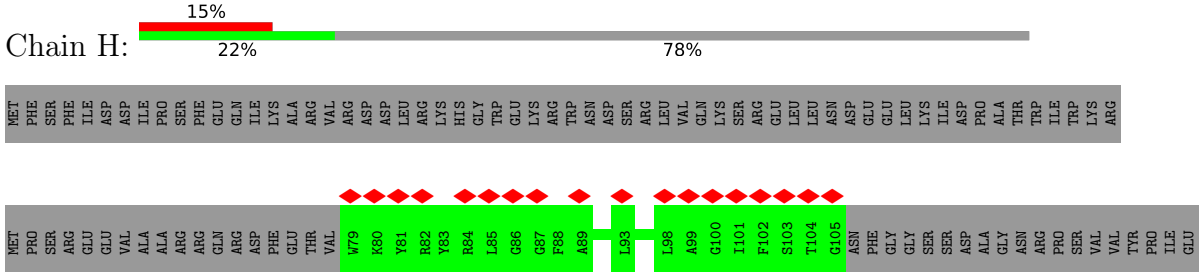
• Molecule 4: Cytochrome b-c1 subunit IV

Chain D:



• Molecule 4: Cytochrome b-c1 subunit IV

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72118	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	257.796, 257.796, 257.796	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1717999, 1.1717999, 1.1717999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, HEC, FES, HEM, PEE

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	0/1372	0.39	0/1868
1	E	0.15	0/1388	0.51	0/1890
2	B	0.14	0/3609	0.41	0/4950
2	F	0.13	0/3603	0.37	0/4942
3	C	0.10	0/2001	0.30	0/2721
3	G	0.10	0/2001	0.31	0/2721
4	D	0.13	0/228	0.50	0/306
4	H	0.10	0/208	0.33	0/279
All	All	0.13	0/14410	0.38	0/19677

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

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	1342	0	1307	10	0
1	E	1357	0	1319	29	0
2	B	3477	0	3458	19	0
2	F	3471	0	3453	24	0
3	C	1944	0	1840	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1944	0	1840	11	0
4	D	222	0	222	3	0
4	H	203	0	207	0	0
5	A	4	0	0	0	0
5	E	4	0	0	3	0
6	A	51	0	82	11	0
6	B	230	0	311	9	0
6	E	34	0	42	1	0
6	F	137	0	173	5	0
7	B	86	0	60	2	0
7	F	86	0	60	5	0
8	C	43	0	31	4	0
8	G	43	0	31	8	0
9	F	42	0	55	1	0
All	All	14720	0	14491	111	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 4.

All (111) 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:61:CYS:SG	8:C:301:HEC:CAC	2.54	0.96
3:C:61:CYS:SG	8:C:301:HEC:HAC	2.11	0.90
1:E:131:HIS:HE1	5:E:201:FES:S2	1.92	0.89
1:A:21:GLY:HA2	6:A:202:PEE:H38	1.53	0.88
3:G:210:PRO:HB2	8:G:301:HEC:HBB3	1.65	0.78
1:E:19:THR:HG22	3:G:265:LEU:HB3	1.69	0.74
3:G:61:CYS:SG	8:G:301:HEC:CAC	2.76	0.73
1:A:20:ALA:HA	6:A:202:PEE:H62	1.70	0.73
6:B:507:PEE:H37	2:F:130:ILE:HD12	1.74	0.70
1:E:131:HIS:CE1	5:E:201:FES:S2	2.83	0.69
2:B:29:ALA:HB1	6:B:508:PEE:H23	1.77	0.66
8:G:301:HEC:HBB2	8:G:301:HEC:HHC	1.81	0.63
2:F:202:PRO:HG2	7:F:502:HEM:HMC1	1.81	0.63
1:A:33:PRO:HG2	6:B:504:PEE:H48	1.80	0.62
3:G:61:CYS:SG	8:G:301:HEC:C3C	2.89	0.61
1:E:15:LEU:O	1:E:19:THR:HG23	2.01	0.60
1:A:21:GLY:HA3	6:A:202:PEE:H43	1.84	0.58
2:F:105:PHE:HA	2:F:108:VAL:HG22	1.85	0.58
6:B:504:PEE:H49	6:B:504:PEE:H18	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:MET:HE2	3:C:210:PRO:HG3	1.86	0.58
1:E:126:TRP:CE2	1:E:174:PRO:HB3	2.39	0.58
3:G:125:MET:HG2	8:G:301:HEC:HMA3	1.84	0.58
2:F:214:TRP:CD1	6:F:503:PEE:H16	2.39	0.57
8:G:301:HEC:HHC	8:G:301:HEC:CBB	2.35	0.56
1:A:21:GLY:CA	6:A:202:PEE:H43	2.35	0.56
2:B:168:ALA:HB2	2:B:329:LYS:HE2	1.88	0.55
2:B:245:TRP:HE3	2:B:249:ILE:HD12	1.73	0.54
3:G:61:CYS:SG	8:G:301:HEC:C2C	2.96	0.53
2:B:122:LYS:NZ	2:B:354:VAL:O	2.36	0.53
8:C:301:HEC:HMC1	8:C:301:HEC:HBC3	1.91	0.53
1:E:77:ARG:HA	1:E:81:ASP:HB3	1.91	0.53
1:E:75:ARG:HH12	1:E:146:GLY:HA2	1.74	0.53
2:F:213:ILE:HA	2:F:216:PHE:CE2	2.44	0.52
2:B:154:MET:HE1	2:B:293:VAL:H	1.75	0.52
2:F:226:GLY:O	2:F:355:ARG:NH1	2.40	0.52
1:E:100:ASN:ND2	1:E:102:ASN:OD1	2.42	0.52
3:G:37:GLY:O	3:G:249:LYS:NZ	2.34	0.52
3:G:173:PRO:HD3	3:G:188:PRO:HG3	1.91	0.52
2:B:105:PHE:HA	2:B:108:VAL:HG22	1.92	0.51
2:B:213:ILE:HA	2:B:216:PHE:CD2	2.46	0.51
3:C:125:MET:HG2	8:C:301:HEC:HMA2	1.93	0.50
1:E:97:ASN:O	1:E:114:ARG:NH2	2.42	0.50
1:E:125:MET:HE2	1:E:160:GLY:HA3	1.93	0.50
2:F:245:TRP:HE3	2:F:249:ILE:HD12	1.77	0.49
1:A:180:ASP:OD1	1:A:181:GLU:N	2.44	0.49
6:A:202:PEE:H36	4:D:87:PHE:CE2	2.48	0.49
2:F:302:TYR:CZ	2:F:306:ARG:HD3	2.48	0.48
1:E:139:GLY:O	1:E:140:VAL:HG22	2.13	0.48
2:F:402:ALA:HB2	6:F:506:PEE:H39	1.96	0.47
2:F:403:TYR:HA	2:F:407:ILE:HD12	1.95	0.47
6:B:508:PEE:H72	6:B:508:PEE:H37	1.94	0.47
2:F:175:SER:HB3	6:F:505:PEE:H1	1.96	0.47
3:G:96:ASP:OD1	3:G:98:GLU:N	2.44	0.47
1:E:125:MET:HG3	1:E:171:LEU:HD23	1.96	0.46
2:F:213:ILE:HA	2:F:216:PHE:CD2	2.49	0.46
1:E:156:TYR:OH	5:E:201:FES:S2	2.63	0.46
1:E:117:ASP:OD1	1:E:117:ASP:N	2.48	0.46
1:A:34:LEU:HD22	2:B:64:VAL:HG21	1.98	0.46
2:F:46:ILE:HD12	2:F:255:ALA:HB1	1.98	0.46
2:F:114:ARG:NH1	7:F:501:HEM:O2A	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:503:PEE:O4	6:B:503:PEE:H3	2.15	0.46
2:F:30:TYR:CZ	2:F:34:MET:HG3	2.51	0.46
1:E:77:ARG:HE	1:E:81:ASP:CG	2.23	0.45
2:B:15:ILE:HA	6:B:507:PEE:H11	1.99	0.45
2:B:423:THR:HG23	2:B:426:GLU:H	1.81	0.45
1:E:157:ASP:OD1	1:E:158:SER:N	2.49	0.45
6:A:202:PEE:H26	6:A:202:PEE:H31	1.55	0.45
3:C:189:ASP:OD1	3:C:190:THR:N	2.50	0.45
2:B:390:ASP:OD1	2:B:391:TRP:N	2.50	0.45
1:E:11:ARG:HB3	1:E:13:ASP:OD1	2.17	0.45
2:F:117:TYR:HB2	2:F:367:PHE:CZ	2.52	0.45
2:B:62:GLY:HA3	7:B:502:HEM:C3C	2.52	0.44
6:A:202:PEE:H74	6:B:508:PEE:C37	2.47	0.44
1:E:74:ILE:HD12	1:E:184:ILE:HG23	1.99	0.44
3:G:154:TYR:OH	3:G:227:HIS:ND1	2.45	0.44
1:E:112:GLN:C	1:E:114:ARG:H	2.25	0.44
6:F:503:PEE:H14	6:F:503:PEE:C30	2.47	0.44
2:B:213:ILE:HA	2:B:216:PHE:CE2	2.53	0.44
1:E:64:THR:HG23	1:E:73:PHE:CZ	2.53	0.44
1:A:132:LEU:HD12	1:A:152:HIS:CE1	2.53	0.44
6:F:506:PEE:H27	6:F:506:PEE:H22	1.81	0.43
2:F:199:TYR:CE2	7:F:502:HEM:HBC1	2.53	0.43
2:F:64:VAL:HG11	2:F:93:LEU:HD13	2.00	0.43
1:E:146:GLY:HA2	1:E:158:SER:HA	2.00	0.43
2:F:189:ALA:HB1	2:F:193:ARG:HH21	1.84	0.43
2:B:30:TYR:CZ	2:B:34:MET:HG3	2.54	0.43
1:E:74:ILE:HG12	1:E:124:VAL:HG22	2.01	0.43
1:E:93:LEU:HD22	1:E:161:ARG:NH1	2.33	0.43
2:B:64:VAL:HG11	2:B:93:LEU:HD13	2.01	0.43
2:F:294:PRO:HG3	9:F:507:U10:C2	2.49	0.43
8:G:301:HEC:HBC2	8:G:301:HEC:HHD	2.01	0.43
1:A:89:GLN:N	1:A:92:GLN:OE1	2.46	0.42
6:A:202:PEE:H45	4:D:90:GLY:C	2.44	0.42
2:B:247:TYR:HB3	3:C:274:TRP:CZ2	2.54	0.42
2:B:202:PRO:HG2	7:B:502:HEM:HMC3	2.01	0.42
1:E:49:SER:HB3	1:E:51:PHE:CE1	2.55	0.42
2:F:199:TYR:CZ	7:F:502:HEM:HBC1	2.55	0.42
6:E:202:PEE:H14	2:F:92:MET:HG2	2.02	0.41
6:A:202:PEE:H46	4:D:91:ALA:HA	2.01	0.41
1:E:131:HIS:CD2	1:E:132:LEU:HG	2.55	0.41
2:F:234:LYS:HE2	2:F:234:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:THR:HG21	7:F:502:HEM:HBB2	2.03	0.41
1:A:43:ASP:N	1:A:43:ASP:OD1	2.53	0.41
6:A:202:PEE:H74	6:B:508:PEE:H61	2.03	0.40
6:A:202:PEE:H66	6:A:202:PEE:H61	1.31	0.40
1:E:126:TRP:CZ2	1:E:174:PRO:HB3	2.56	0.40
2:B:289:PRO:HD2	2:B:292:ILE:HD11	2.03	0.40
2:B:377:LEU:HA	2:B:380:VAL:HG12	2.03	0.40
1:E:19:THR:HG21	3:G:269:THR:OG1	2.21	0.40
1:E:127:GLY:O	1:E:136:PRO:HD2	2.22	0.40
1:E:129:CYS:HB2	1:E:136:PRO:HD3	2.04	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	177/187 (95%)	169 (96%)	8 (4%)	0	100	100
1	E	179/187 (96%)	155 (87%)	22 (12%)	2 (1%)	11	40
2	B	431/445 (97%)	424 (98%)	7 (2%)	0	100	100
2	F	430/445 (97%)	421 (98%)	9 (2%)	0	100	100
3	C	252/285 (88%)	246 (98%)	6 (2%)	0	100	100
3	G	252/285 (88%)	245 (97%)	7 (3%)	0	100	100
4	D	27/124 (22%)	27 (100%)	0	0	100	100
4	H	25/124 (20%)	24 (96%)	1 (4%)	0	100	100
All	All	1773/2082 (85%)	1711 (96%)	60 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	57	VAL
1	E	140	VAL

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	138/144 (96%)	138 (100%)	0	100 100
1	E	139/144 (96%)	137 (99%)	2 (1%)	59 70
2	B	358/366 (98%)	357 (100%)	1 (0%)	86 84
2	F	357/366 (98%)	357 (100%)	0	100 100
3	C	203/222 (91%)	203 (100%)	0	100 100
3	G	203/222 (91%)	203 (100%)	0	100 100
4	D	19/105 (18%)	19 (100%)	0	100 100
4	H	17/105 (16%)	17 (100%)	0	100 100
All	All	1434/1674 (86%)	1431 (100%)	3 (0%)	85 87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	385	THR
1	E	123	LEU
1	E	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	HIS
2	B	384	GLN
1	E	131	HIS
2	F	8	HIS
2	F	174	HIS
2	F	276	HIS

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Mol	Chain	Res	Type
3	G	118	ASN
3	G	133	HIS
3	G	270	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)

21 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	$\#\|Z\| > 2$
6	PEE	B	503	-	37,37,50	1.23	2 (5%)	40,42,55	1.45	6 (15%)
8	HEC	G	301	3	50,50,50	1.80	8 (16%)	68,82,82	1.73	16 (23%)
6	PEE	B	508	-	50,50,50	1.12	2 (4%)	53,55,55	1.41	6 (11%)
7	HEM	B	502	2	50,50,50	1.38	6 (12%)	66,82,82	1.26	7 (10%)
7	HEM	B	501	2	50,50,50	1.35	6 (12%)	66,82,82	1.22	8 (12%)
6	PEE	A	202	-	50,50,50	1.12	3 (6%)	53,55,55	1.24	4 (7%)
6	PEE	B	505	-	30,30,50	1.28	2 (6%)	33,35,55	1.26	3 (9%)
6	PEE	B	506	-	31,31,50	1.26	2 (6%)	34,36,55	1.12	2 (5%)
6	PEE	F	506	-	43,43,50	1.19	2 (4%)	46,48,55	1.11	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	U10	F	507	-	42,42,63	2.61	13 (30%)	50,53,79	1.66	11 (22%)
6	PEE	F	504	-	29,29,50	1.24	2 (6%)	32,34,55	1.13	2 (6%)
5	FES	E	201	1	0,4,4	-	-	-		
6	PEE	F	503	-	30,30,50	1.25	2 (6%)	33,35,55	1.11	2 (6%)
6	PEE	B	507	-	46,46,50	1.14	2 (4%)	49,51,55	1.23	3 (6%)
8	HEC	C	301	3	50,50,50	1.82	9 (18%)	68,82,82	1.72	12 (17%)
6	PEE	E	202	-	33,33,50	1.24	2 (6%)	36,38,55	1.13	3 (8%)
5	FES	A	201	1	0,4,4	-	-	-		
6	PEE	B	504	-	30,30,50	1.24	2 (6%)	33,35,55	1.12	2 (6%)
6	PEE	F	505	-	31,31,50	1.22	2 (6%)	34,36,55	1.00	2 (5%)
7	HEM	F	502	2	50,50,50	1.38	6 (12%)	66,82,82	1.23	7 (10%)
7	HEM	F	501	2	50,50,50	1.36	7 (14%)	66,82,82	1.22	7 (10%)

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
6	PEE	B	503	-	-	26/41/41/54	-
8	HEC	G	301	3	1/1/3/7	12/14/54/54	-
6	PEE	B	508	-	-	25/54/54/54	-
7	HEM	B	502	2	-	7/14/54/54	-
7	HEM	B	501	2	-	6/14/54/54	-
6	PEE	A	202	-	-	9/54/54/54	-
6	PEE	B	505	-	-	16/34/34/54	-
6	PEE	B	506	-	-	10/35/35/54	-
6	PEE	F	506	-	-	20/47/47/54	-
9	U10	F	507	-	-	14/38/62/87	0/1/1/1
6	PEE	F	504	-	-	16/33/33/54	-
5	FES	E	201	1	-	-	0/1/1/1
6	PEE	F	503	-	-	11/34/34/54	-
6	PEE	B	507	-	-	22/50/50/54	-
8	HEC	C	301	3	1/1/3/7	12/14/54/54	-
6	PEE	E	202	-	-	22/37/37/54	-
5	FES	A	201	1	-	-	0/1/1/1
6	PEE	B	504	-	-	24/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEE	F	505	-	-	11/35/35/54	-
7	HEM	F	502	2	-	8/14/54/54	-
7	HEM	F	501	2	-	4/14/54/54	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	301	HEC	C3D-C2D	7.96	1.53	1.36
8	G	301	HEC	C3D-C2D	7.94	1.53	1.36
9	F	507	U10	C8-C9	6.16	1.47	1.33
9	F	507	U10	C18-C19	6.04	1.47	1.33
9	F	507	U10	C23-C24	6.02	1.47	1.33
9	F	507	U10	C13-C14	6.01	1.47	1.33
9	F	507	U10	C28-C29	5.98	1.47	1.33
9	F	507	U10	O3-C3	-5.12	1.24	1.36
9	F	507	U10	O4-C4	-5.02	1.24	1.36
8	C	301	HEC	FE-NB	4.51	2.08	1.94
8	C	301	HEC	FE-ND	4.33	2.08	1.94
8	G	301	HEC	FE-NB	4.16	2.07	1.94
8	G	301	HEC	FE-ND	3.94	2.07	1.94
7	B	502	HEM	FE-ND	3.38	2.05	1.94
7	F	502	HEM	FE-NB	3.34	2.05	1.94
7	B	501	HEM	FE-NB	3.31	2.05	1.94
7	F	501	HEM	FE-NB	3.31	2.05	1.94
7	F	502	HEM	FE-ND	3.30	2.05	1.94
9	F	507	U10	C4-C5	-3.24	1.39	1.48
7	B	502	HEM	FE-NB	3.23	2.04	1.94
9	F	507	U10	C3-C2	-3.12	1.39	1.48
7	B	501	HEM	FE-NA	2.99	2.05	1.95
6	B	503	PEE	O3-C30	2.98	1.42	1.33
7	F	502	HEM	FE-NC	2.93	2.05	1.95
6	E	202	PEE	O3-C30	2.91	1.41	1.33
7	F	501	HEM	FE-NA	2.90	2.04	1.95
6	A	202	PEE	O3-C30	2.90	1.41	1.33
7	B	502	HEM	FE-NC	2.88	2.04	1.95
6	B	505	PEE	O3-C30	2.88	1.41	1.33
6	B	508	PEE	O3-C30	2.87	1.41	1.33
8	C	301	HEC	FE-NC	2.87	2.04	1.95
7	F	501	HEM	CAB-C3B	2.87	1.55	1.47
7	F	502	HEM	FE-NA	2.86	2.04	1.95
7	F	501	HEM	FE-ND	2.85	2.03	1.94
6	B	503	PEE	O2-C10	2.84	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	PEE	O3-C30	2.84	1.41	1.33
7	B	502	HEM	CAB-C3B	2.84	1.55	1.47
7	F	502	HEM	CAB-C3B	2.82	1.55	1.47
6	B	507	PEE	O3-C30	2.82	1.41	1.33
7	B	501	HEM	CAB-C3B	2.82	1.55	1.47
7	F	501	HEM	CAC-C3C	2.81	1.55	1.47
6	F	506	PEE	O3-C30	2.81	1.41	1.33
7	B	501	HEM	CAC-C3C	2.80	1.55	1.47
6	B	506	PEE	O3-C30	2.80	1.41	1.33
7	B	502	HEM	FE-NA	2.79	2.04	1.95
6	F	505	PEE	O3-C30	2.79	1.41	1.33
6	F	504	PEE	O3-C30	2.79	1.41	1.33
6	F	503	PEE	O3-C30	2.78	1.41	1.33
7	B	501	HEM	FE-ND	2.77	2.03	1.94
8	C	301	HEC	FE-NA	2.76	2.04	1.95
7	F	502	HEM	CAC-C3C	2.76	1.55	1.47
8	G	301	HEC	FE-NC	2.75	2.04	1.95
7	B	501	HEM	FE-NC	2.74	2.04	1.95
7	F	501	HEM	FE-NC	2.71	2.04	1.95
6	B	506	PEE	O2-C10	2.71	1.42	1.34
9	F	507	U10	C6-C5	-2.69	1.39	1.46
7	B	502	HEM	CAC-C3C	2.67	1.54	1.47
6	F	506	PEE	O2-C10	2.62	1.41	1.34
6	F	503	PEE	O2-C10	2.62	1.41	1.34
6	B	504	PEE	O2-C10	2.62	1.41	1.34
6	E	202	PEE	O2-C10	2.62	1.41	1.34
6	B	508	PEE	O2-C10	2.59	1.41	1.34
8	G	301	HEC	FE-NA	2.56	2.03	1.95
6	F	505	PEE	O2-C10	2.55	1.41	1.34
9	F	507	U10	C6-C1	2.44	1.39	1.35
8	G	301	HEC	CAB-C3B	2.42	1.57	1.51
6	F	504	PEE	O2-C10	2.42	1.41	1.34
6	B	505	PEE	O2-C10	2.42	1.41	1.34
6	B	507	PEE	O2-C10	2.41	1.41	1.34
9	F	507	U10	C33-C34	2.40	1.47	1.29
6	A	202	PEE	O2-C10	2.30	1.40	1.34
9	F	507	U10	C1-C2	-2.23	1.39	1.47
8	C	301	HEC	CAB-C3B	2.17	1.56	1.51
8	C	301	HEC	CMB-C2B	2.15	1.55	1.50
8	C	301	HEC	CMC-C2C	2.15	1.55	1.50
6	A	202	PEE	O2-C2	-2.04	1.41	1.46
8	G	301	HEC	CMB-C2B	2.02	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	301	HEC	CAC-C3C	2.01	1.56	1.51
8	C	301	HEC	CAC-C3C	2.01	1.56	1.51
7	F	501	HEM	CMB-C2B	2.00	1.55	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	301	HEC	C1D-ND-C4D	6.44	111.72	105.07
8	G	301	HEC	C1D-ND-C4D	6.25	111.53	105.07
8	C	301	HEC	CMC-C2C-C1C	-5.29	117.32	125.37
6	B	503	PEE	C40-C39-C38	-5.06	85.91	124.73
6	B	507	PEE	C40-C39-C38	-5.04	86.07	124.73
6	B	508	PEE	O2-C10-C11	4.35	120.87	111.50
6	B	508	PEE	C40-C39-C38	-4.34	91.41	124.73
6	B	505	PEE	O2-C10-C11	4.29	120.75	111.50
6	B	504	PEE	O2-C10-C11	4.06	120.24	111.50
6	A	202	PEE	O2-C10-C11	4.04	120.20	111.50
6	F	503	PEE	O2-C10-C11	3.94	119.99	111.50
6	F	504	PEE	O2-C10-C11	3.89	119.89	111.50
8	G	301	HEC	CAB-C3B-C4B	3.82	129.77	124.81
6	B	507	PEE	O2-C10-C11	3.72	119.51	111.50
6	F	506	PEE	O2-C10-C11	3.71	119.50	111.50
6	E	202	PEE	O2-C10-C11	3.70	119.47	111.50
8	G	301	HEC	CAC-C3C-C4C	3.64	129.96	124.92
9	F	507	U10	C17-C18-C19	-3.48	119.28	127.66
8	C	301	HEC	CAC-C3C-C4C	-3.44	120.14	124.92
6	B	503	PEE	O2-C10-C11	3.28	118.56	111.50
6	F	505	PEE	O2-C10-C11	3.26	118.53	111.50
6	A	202	PEE	C40-C39-C38	-3.20	100.16	124.73
6	B	506	PEE	O2-C10-C11	3.19	118.38	111.50
9	F	507	U10	C4M-O4-C4	3.17	127.71	116.47
9	F	507	U10	C25-C24-C26	3.17	120.60	115.27
7	F	501	HEM	C4D-ND-C1D	3.15	108.33	105.07
6	F	506	PEE	C40-C39-C38	-3.13	100.56	126.37
7	B	501	HEM	C4D-ND-C1D	3.12	108.29	105.07
8	G	301	HEC	CMC-C2C-C1C	-3.07	120.69	125.37
6	A	202	PEE	O3-C30-C31	3.03	121.42	111.91
8	C	301	HEC	CMB-C2B-C1B	-3.03	120.43	125.04
7	B	502	HEM	C4C-NC-C1C	2.99	108.28	105.35
7	F	501	HEM	C1B-NB-C4B	2.98	108.15	105.07
6	B	508	PEE	O3-C30-C31	2.97	121.22	111.91
7	F	502	HEM	C1B-NB-C4B	2.97	108.14	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	501	HEM	C1B-NB-C4B	2.95	108.12	105.07
8	G	301	HEC	C4B-NB-C1B	2.95	108.12	105.07
7	B	502	HEM	C1B-NB-C4B	2.94	108.11	105.07
7	B	501	HEM	C4C-NC-C1C	2.93	108.22	105.35
7	F	502	HEM	C4A-NA-C1A	2.92	108.21	105.35
8	G	301	HEC	CAC-C3C-C2C	-2.90	122.22	126.86
9	F	507	U10	C30-C29-C31	2.89	120.13	115.27
7	B	501	HEM	C4A-NA-C1A	2.88	108.17	105.35
7	F	501	HEM	C4A-NA-C1A	2.88	108.17	105.35
6	B	503	PEE	O3-C30-C31	2.85	120.86	111.91
7	F	501	HEM	C4C-NC-C1C	2.83	108.11	105.35
7	B	502	HEM	C4D-ND-C1D	2.81	107.98	105.07
7	F	502	HEM	C4D-ND-C1D	2.81	107.98	105.07
9	F	507	U10	C12-C13-C14	-2.75	121.05	127.66
6	B	505	PEE	O3-C30-C31	2.74	120.52	111.91
7	B	502	HEM	C4A-NA-C1A	2.74	108.03	105.35
9	F	507	U10	C20-C19-C21	2.72	119.85	115.27
7	F	502	HEM	C4C-NC-C1C	2.68	107.97	105.35
8	C	301	HEC	CAC-C3C-C2C	2.67	131.15	126.86
9	F	507	U10	C27-C28-C29	-2.66	121.25	127.66
9	F	507	U10	C10-C9-C11	2.65	119.73	115.27
6	F	506	PEE	O3-C30-C31	2.64	120.19	111.91
6	B	503	PEE	C2-O2-C10	2.64	124.28	117.79
6	E	202	PEE	O3-C30-C31	2.62	120.12	111.91
8	G	301	HEC	CHC-C4B-C3B	2.61	130.23	125.33
6	F	503	PEE	O3-C30-C31	2.59	120.04	111.91
9	F	507	U10	C15-C14-C16	2.59	119.63	115.27
6	B	506	PEE	O3-C30-C31	2.59	120.02	111.91
8	C	301	HEC	C4B-NB-C1B	2.58	107.74	105.07
6	B	507	PEE	O3-C30-C31	2.54	119.89	111.91
6	B	508	PEE	C17-C18-C19	2.54	144.22	124.73
8	G	301	HEC	C4A-NA-C1A	2.48	107.77	105.35
6	B	504	PEE	O3-C30-C31	2.46	119.62	111.91
6	F	504	PEE	O3-C30-C31	2.43	119.55	111.91
8	G	301	HEC	CHC-C4B-NB	-2.42	121.39	124.37
8	G	301	HEC	CAA-CBA-CGA	-2.38	108.49	113.60
9	F	507	U10	C22-C23-C24	-2.38	121.94	127.66
9	F	507	U10	C1-C6-C5	-2.36	117.36	119.58
6	B	508	PEE	C37-C38-C39	-2.32	106.93	124.73
7	F	501	HEM	C3D-C4D-ND	-2.28	107.63	110.17
8	G	301	HEC	C1B-C2B-C3B	2.23	109.30	106.96
6	B	508	PEE	C22-C21-C20	-2.23	104.08	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	503	PEE	O3-C3-C2	2.23	114.91	108.43
8	C	301	HEC	C4A-NA-C1A	2.20	107.50	105.35
7	B	501	HEM	C3D-C4D-ND	-2.19	107.73	110.17
8	C	301	HEC	CAB-C3B-C4B	-2.15	122.02	124.81
6	F	505	PEE	O3-C30-C31	2.14	118.64	111.91
6	B	505	PEE	C2-O2-C10	-2.14	112.53	117.79
6	E	202	PEE	C37-C38-C39	-2.14	112.30	126.84
7	F	502	HEM	C2A-C1A-NA	-2.13	107.76	110.15
7	F	501	HEM	CAD-CBD-CGD	-2.12	109.04	113.60
7	F	502	HEM	C3B-C2B-C1B	2.12	108.06	106.49
7	B	501	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
8	C	301	HEC	CBB-CAB-C3B	2.11	118.25	112.43
6	B	503	PEE	O2-C2-C1	2.11	116.04	108.40
8	C	301	HEC	CAB-C3B-C2B	2.11	131.14	127.53
7	B	502	HEM	C3B-C2B-C1B	2.08	108.03	106.49
8	C	301	HEC	CAA-CBA-CGA	-2.08	109.12	113.60
8	G	301	HEC	CAD-C3D-C4D	2.08	128.30	124.66
6	A	202	PEE	C23-C24-C25	-2.08	103.87	114.42
7	F	502	HEM	CAD-CBD-CGD	-2.07	109.15	113.60
8	G	301	HEC	CAB-C3B-C2B	-2.07	124.00	127.53
7	F	501	HEM	C2A-C1A-NA	-2.05	107.85	110.15
8	C	301	HEC	CAD-C3D-C4D	2.05	128.24	124.66
7	B	502	HEM	CAD-CBD-CGD	-2.04	109.21	113.60
7	B	501	HEM	C2A-C1A-NA	-2.04	107.87	110.15
7	B	502	HEM	C2A-C1A-NA	-2.02	107.89	110.15
8	G	301	HEC	C3C-C4C-NC	-2.02	107.89	110.15
7	B	501	HEM	C3B-C2B-C1B	2.01	107.98	106.49
8	G	301	HEC	C4C-NC-C1C	2.00	107.31	105.35
8	G	301	HEC	C2A-C1A-NA	-2.00	108.38	110.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	301	HEC	NA
8	G	301	HEC	NA

All (275) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	202	PEE	C11-C10-O2-C2
6	A	202	PEE	O4-C10-O2-C2
6	B	503	PEE	C1-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
6	B	503	PEE	C4-O4P-P-O2P
6	B	503	PEE	C4-O4P-P-O1P
6	B	503	PEE	C5-C4-O4P-P
6	B	503	PEE	O4P-C4-C5-N
6	B	504	PEE	C11-C10-O2-C2
6	B	504	PEE	C1-O3P-P-O2P
6	B	504	PEE	C4-O4P-P-O1P
6	B	504	PEE	C5-C4-O4P-P
6	B	505	PEE	O3P-C1-C2-O2
6	B	505	PEE	O2-C2-C3-O3
6	B	505	PEE	C1-O3P-P-O2P
6	B	505	PEE	C1-O3P-P-O1P
6	B	505	PEE	C1-O3P-P-O4P
6	B	505	PEE	C4-O4P-P-O2P
6	B	505	PEE	O5-C30-O3-C3
6	B	505	PEE	C31-C30-O3-C3
6	B	506	PEE	O3P-C1-C2-O2
6	B	506	PEE	C4-O4P-P-O2P
6	B	506	PEE	C4-O4P-P-O1P
6	B	507	PEE	O4P-C4-C5-N
6	B	508	PEE	O4-C10-O2-C2
6	B	508	PEE	C5-C4-O4P-P
6	E	202	PEE	C11-C10-O2-C2
6	E	202	PEE	C5-C4-O4P-P
6	F	503	PEE	C11-C10-O2-C2
6	F	503	PEE	C4-O4P-P-O1P
6	F	503	PEE	C5-C4-O4P-P
6	F	505	PEE	C4-O4P-P-O2P
6	F	505	PEE	C4-O4P-P-O1P
8	C	301	HEC	C1A-C2A-CAA-CBA
8	C	301	HEC	C3A-C2A-CAA-CBA
8	G	301	HEC	C2A-CAA-CBA-CGA
8	G	301	HEC	C2B-C3B-CAB-CBB
8	G	301	HEC	C4B-C3B-CAB-CBB
9	F	507	U10	C9-C11-C12-C13
9	F	507	U10	C14-C16-C17-C18
8	G	301	HEC	C4C-C3C-CAC-CBC
8	C	301	HEC	C4B-C3B-CAB-CBB
8	C	301	HEC	C2B-C3B-CAB-CBB
8	C	301	HEC	C2C-C3C-CAC-CBC
8	G	301	HEC	C2C-C3C-CAC-CBC
8	C	301	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	B	504	PEE	O5-C30-O3-C3
6	B	507	PEE	O5-C30-O3-C3
6	B	508	PEE	O5-C30-O3-C3
6	E	202	PEE	O5-C30-O3-C3
6	B	504	PEE	O4-C10-O2-C2
6	E	202	PEE	O4-C10-O2-C2
6	F	503	PEE	O4-C10-O2-C2
6	B	508	PEE	C31-C30-O3-C3
6	E	202	PEE	C31-C30-O3-C3
6	B	508	PEE	C11-C10-O2-C2
6	B	504	PEE	C31-C30-O3-C3
6	B	507	PEE	C31-C30-O3-C3
9	F	507	U10	C7-C8-C9-C10
9	F	507	U10	C22-C23-C24-C25
6	F	504	PEE	O4-C10-O2-C2
9	F	507	U10	C7-C8-C9-C11
9	F	507	U10	C22-C23-C24-C26
6	A	202	PEE	O5-C30-O3-C3
6	F	506	PEE	C31-C30-O3-C3
6	F	504	PEE	C11-C10-O2-C2
6	A	202	PEE	C31-C30-O3-C3
8	C	301	HEC	C2A-CAA-CBA-CGA
8	C	301	HEC	C3D-CAD-CBD-CGD
8	G	301	HEC	C3D-CAD-CBD-CGD
9	F	507	U10	C29-C31-C32-C33
6	F	506	PEE	O5-C30-O3-C3
9	F	507	U10	C20-C19-C21-C22
6	F	504	PEE	C30-C31-C32-C33
6	B	504	PEE	C10-C11-C12-C13
6	B	503	PEE	C16-C17-C18-C19
6	B	505	PEE	C16-C17-C18-C19
6	B	506	PEE	C16-C17-C18-C19
6	B	508	PEE	C2-C3-O3-C30
6	B	503	PEE	C1-O3P-P-O4P
6	B	503	PEE	C4-O4P-P-O3P
6	B	504	PEE	C1-O3P-P-O4P
6	B	504	PEE	C4-O4P-P-O3P
6	B	506	PEE	C4-O4P-P-O3P
6	B	507	PEE	C1-O3P-P-O4P
6	B	508	PEE	C4-O4P-P-O3P
6	E	202	PEE	C1-O3P-P-O4P
6	F	503	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
6	F	505	PEE	C1-O3P-P-O4P
6	F	505	PEE	C4-O4P-P-O3P
6	F	506	PEE	C1-O3P-P-O4P
6	B	504	PEE	C30-C31-C32-C33
6	B	503	PEE	O4-C10-O2-C2
6	F	505	PEE	O4-C10-O2-C2
6	B	504	PEE	C13-C14-C15-C16
6	B	503	PEE	C11-C10-O2-C2
6	F	505	PEE	C11-C10-O2-C2
6	B	504	PEE	C32-C33-C34-C35
6	B	507	PEE	C32-C33-C34-C35
6	A	202	PEE	C23-C24-C25-C26
6	B	503	PEE	C34-C35-C36-C37
6	B	508	PEE	C20-C21-C22-C23
6	B	508	PEE	C21-C22-C23-C24
6	F	504	PEE	C11-C12-C13-C14
6	B	504	PEE	O4P-C4-C5-N
6	F	504	PEE	O4P-C4-C5-N
6	B	507	PEE	C23-C24-C25-C26
6	B	503	PEE	C39-C40-C41-C42
6	B	507	PEE	C11-C12-C13-C14
6	F	506	PEE	C11-C10-O2-C2
6	B	508	PEE	C35-C36-C37-C38
6	B	508	PEE	C43-C44-C45-C46
6	E	202	PEE	C34-C35-C36-C37
6	B	508	PEE	C13-C14-C15-C16
6	F	506	PEE	O4-C10-O2-C2
9	F	507	U10	C18-C19-C21-C22
8	G	301	HEC	C1A-C2A-CAA-CBA
6	A	202	PEE	C19-C20-C21-C22
6	B	503	PEE	C35-C36-C37-C38
6	F	504	PEE	C32-C33-C34-C35
6	B	503	PEE	O2-C2-C3-O3
6	E	202	PEE	C12-C13-C14-C15
6	F	503	PEE	C31-C32-C33-C34
6	F	504	PEE	C4-O4P-P-O3P
6	E	202	PEE	C31-C32-C33-C34
6	B	505	PEE	O3P-C1-C2-C3
6	B	507	PEE	C34-C35-C36-C37
6	B	504	PEE	C1-C2-C3-O3
6	F	505	PEE	C3-C2-O2-C10
6	F	506	PEE	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
6	B	508	PEE	C44-C45-C46-C47
6	E	202	PEE	C15-C16-C17-C18
6	B	503	PEE	O3P-C1-C2-C3
6	B	504	PEE	O3P-C1-C2-C3
6	B	506	PEE	O3P-C1-C2-C3
6	B	503	PEE	C30-C31-C32-C33
6	B	503	PEE	O2-C10-C11-C12
6	B	504	PEE	C2-C1-O3P-P
6	E	202	PEE	C2-C1-O3P-P
6	B	503	PEE	C1-C2-C3-O3
6	E	202	PEE	C1-C2-C3-O3
6	F	506	PEE	C1-C2-C3-O3
6	B	508	PEE	C17-C18-C19-C20
8	G	301	HEC	C3A-C2A-CAA-CBA
6	B	505	PEE	C4-O4P-P-O3P
6	B	504	PEE	O3P-C1-C2-O2
6	F	503	PEE	O3-C30-C31-C32
6	F	506	PEE	C2-C1-O3P-P
6	F	504	PEE	C13-C14-C15-C16
9	F	507	U10	C32-C33-C34-C35
6	B	503	PEE	C14-C15-C16-C17
6	A	202	PEE	C11-C12-C13-C14
6	B	503	PEE	C13-C14-C15-C16
6	F	506	PEE	C18-C19-C20-C21
6	E	202	PEE	C3-C2-O2-C10
6	F	503	PEE	C3-C2-O2-C10
7	B	501	HEM	C2B-C3B-CAB-CBB
7	B	501	HEM	C2C-C3C-CAC-CBC
7	F	501	HEM	C2C-C3C-CAC-CBC
7	F	502	HEM	C2B-C3B-CAB-CBB
6	B	505	PEE	C1-C2-C3-O3
6	F	505	PEE	C2-C1-O3P-P
6	B	503	PEE	O3P-C1-C2-O2
6	E	202	PEE	C36-C37-C38-C39
6	B	508	PEE	O2-C2-C3-O3
6	E	202	PEE	O2-C2-C3-O3
6	F	504	PEE	O2-C2-C3-O3
6	A	202	PEE	C12-C13-C14-C15
6	B	504	PEE	C34-C35-C36-C37
6	B	504	PEE	C12-C13-C14-C15
6	B	507	PEE	C14-C15-C16-C17
6	B	503	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
6	B	503	PEE	C1-O3P-P-O1P
6	B	504	PEE	C1-O3P-P-O1P
6	B	505	PEE	C4-O4P-P-O1P
6	B	506	PEE	C1-O3P-P-O2P
6	B	507	PEE	C1-O3P-P-O2P
6	B	508	PEE	C4-O4P-P-O2P
6	E	202	PEE	C1-O3P-P-O1P
6	E	202	PEE	C4-O4P-P-O2P
6	F	504	PEE	C4-O4P-P-O1P
6	F	505	PEE	C1-O3P-P-O2P
6	F	506	PEE	C1-O3P-P-O1P
6	B	505	PEE	C11-C10-O2-C2
6	F	504	PEE	C5-C4-O4P-P
6	B	508	PEE	C31-C32-C33-C34
6	B	507	PEE	C18-C19-C20-C21
6	F	506	PEE	O2-C2-C3-O3
6	B	503	PEE	C31-C32-C33-C34
6	B	507	PEE	C40-C41-C42-C43
6	B	508	PEE	C23-C24-C25-C26
6	B	506	PEE	C3-C2-O2-C10
6	B	505	PEE	O4-C10-O2-C2
6	B	507	PEE	C2-C1-O3P-P
6	A	202	PEE	C1-O3P-P-O4P
6	F	504	PEE	C1-O3P-P-O4P
6	F	506	PEE	C4-O4P-P-O3P
6	B	508	PEE	C1-C2-C3-O3
6	B	503	PEE	O4-C10-C11-C12
6	F	506	PEE	C11-C12-C13-C14
7	B	502	HEM	C2B-C3B-CAB-CBB
7	B	502	HEM	C2C-C3C-CAC-CBC
7	F	502	HEM	C2C-C3C-CAC-CBC
6	E	202	PEE	O4P-C4-C5-N
8	G	301	HEC	CAA-CBA-CGA-O2A
6	B	507	PEE	C22-C23-C24-C25
7	B	501	HEM	C4B-C3B-CAB-CBB
7	B	501	HEM	C4C-C3C-CAC-CBC
7	B	502	HEM	C4B-C3B-CAB-CBB
7	F	502	HEM	C4C-C3C-CAC-CBC
7	B	501	HEM	CAA-CBA-CGA-O1A
7	F	501	HEM	CAA-CBA-CGA-O1A
8	C	301	HEC	CAA-CBA-CGA-O2A
6	B	506	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	503	PEE	C38-C39-C40-C41
7	F	502	HEM	CAA-CBA-CGA-O2A
7	F	502	HEM	CAA-CBA-CGA-O1A
6	B	508	PEE	C36-C37-C38-C39
6	B	504	PEE	C3-C2-O2-C10
7	F	502	HEM	CAD-CBD-CGD-O2D
6	E	202	PEE	C14-C15-C16-C17
6	B	507	PEE	C21-C22-C23-C24
6	F	504	PEE	C31-C30-O3-C3
7	B	502	HEM	CAA-CBA-CGA-O2A
6	E	202	PEE	C10-C11-C12-C13
7	F	501	HEM	CAA-CBA-CGA-O2A
8	G	301	HEC	CAA-CBA-CGA-O1A
6	F	504	PEE	O5-C30-O3-C3
7	B	501	HEM	CAA-CBA-CGA-O2A
8	C	301	HEC	CAA-CBA-CGA-O1A
7	B	502	HEM	CAA-CBA-CGA-O1A
7	F	502	HEM	CAD-CBD-CGD-O1D
6	B	506	PEE	C13-C14-C15-C16
6	F	505	PEE	O3P-C1-C2-C3
7	B	502	HEM	CAD-CBD-CGD-O2D
6	F	506	PEE	C20-C21-C22-C23
7	B	502	HEM	CAD-CBD-CGD-O1D
6	B	507	PEE	O2-C10-C11-C12
9	F	507	U10	C30-C29-C31-C32
6	F	506	PEE	C16-C17-C18-C19
6	B	507	PEE	O4-C10-O2-C2
6	F	503	PEE	C13-C14-C15-C16
6	B	507	PEE	O3-C30-C31-C32
9	F	507	U10	C28-C29-C31-C32
8	G	301	HEC	CAD-CBD-CGD-O1D
7	F	501	HEM	C4C-C3C-CAC-CBC
7	F	502	HEM	C4B-C3B-CAB-CBB
6	F	503	PEE	O5-C30-C31-C32
8	C	301	HEC	CAD-CBD-CGD-O1D
6	B	508	PEE	C38-C39-C40-C41
6	B	505	PEE	C32-C33-C34-C35
6	F	505	PEE	O2-C2-C3-O3
8	G	301	HEC	CAD-CBD-CGD-O2D
6	F	506	PEE	C36-C37-C38-C39
6	B	508	PEE	O2-C10-C11-C12
6	B	508	PEE	C19-C20-C21-C22

Continued on next page...

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Mol	Chain	Res	Type	Atoms
8	C	301	HEC	CAD-CBD-CGD-O2D
6	F	503	PEE	C15-C16-C17-C18
6	B	507	PEE	O4-C10-C11-C12
6	B	507	PEE	O5-C30-C31-C32
6	F	506	PEE	C33-C34-C35-C36
6	F	504	PEE	C1-C2-C3-O3
6	E	202	PEE	O3-C30-C31-C32
6	B	508	PEE	C32-C33-C34-C35
6	F	504	PEE	C4-O4P-P-O2P
6	F	506	PEE	C1-O3P-P-O2P
6	F	506	PEE	C4-O4P-P-O1P
6	B	504	PEE	O2-C2-C3-O3
9	F	507	U10	C15-C14-C16-C17
9	F	507	U10	C11-C12-C13-C14
6	B	508	PEE	C1-C2-O2-C10
6	F	506	PEE	C5-C4-O4P-P
6	B	504	PEE	C11-C12-C13-C14
6	E	202	PEE	O5-C30-C31-C32
6	B	507	PEE	C10-C11-C12-C13
6	B	507	PEE	C11-C10-O2-C2

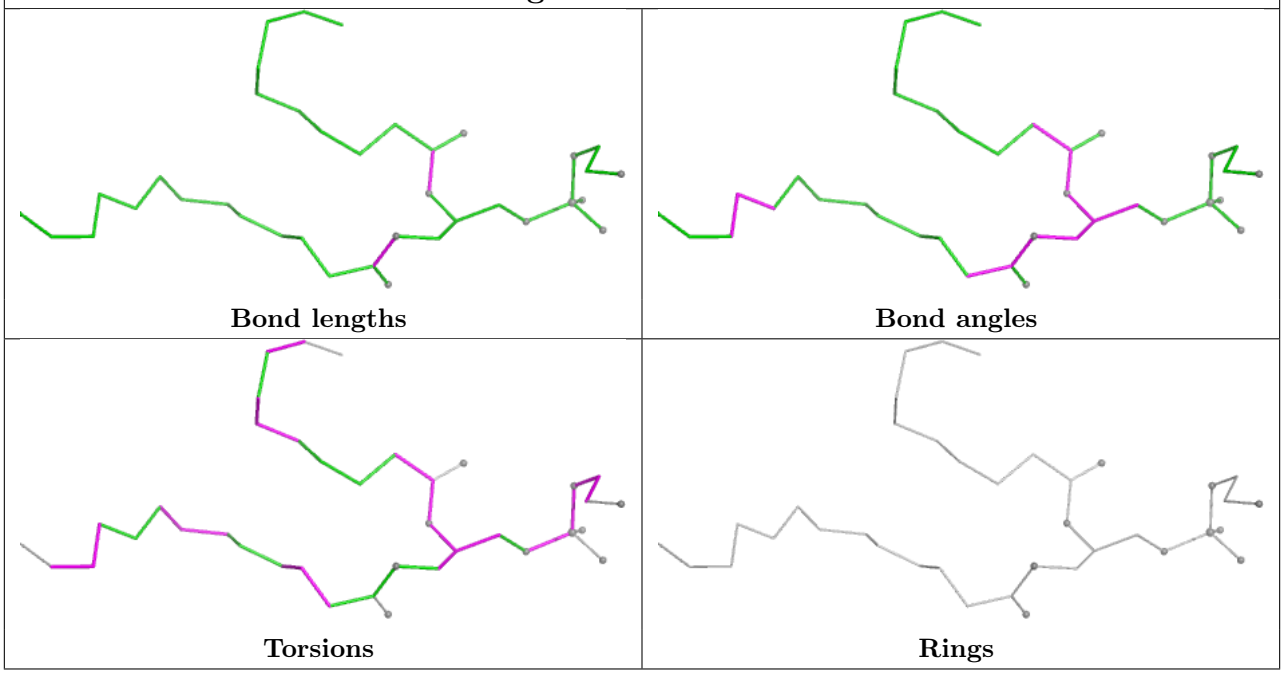
There are no ring outliers.

16 monomers are involved in 47 short contacts:

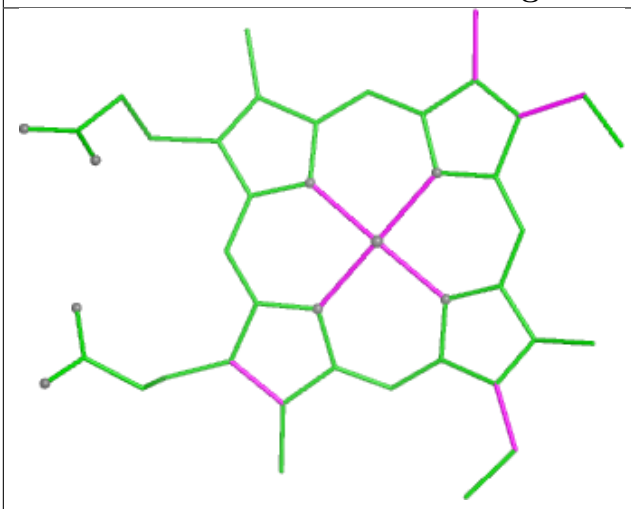
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	503	PEE	1	0
8	G	301	HEC	8	0
6	B	508	PEE	4	0
7	B	502	HEM	2	0
6	A	202	PEE	11	0
6	F	506	PEE	2	0
9	F	507	U10	1	0
5	E	201	FES	3	0
6	F	503	PEE	2	0
6	B	507	PEE	2	0
8	C	301	HEC	4	0
6	E	202	PEE	1	0
6	B	504	PEE	2	0
6	F	505	PEE	1	0
7	F	502	HEM	4	0
7	F	501	HEM	1	0

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 then 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.

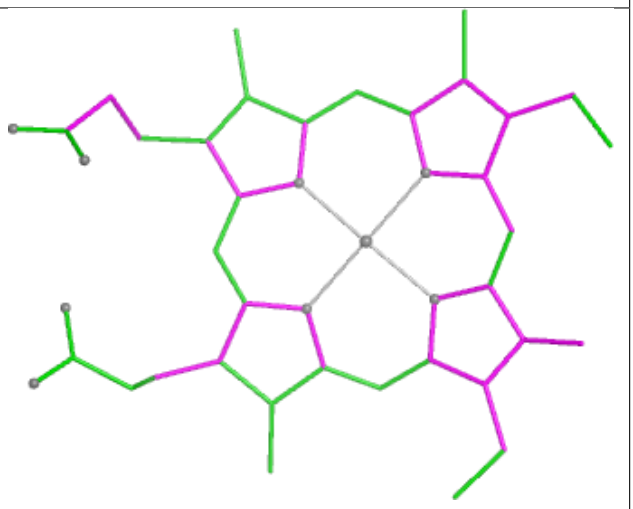
Ligand PEE B 503



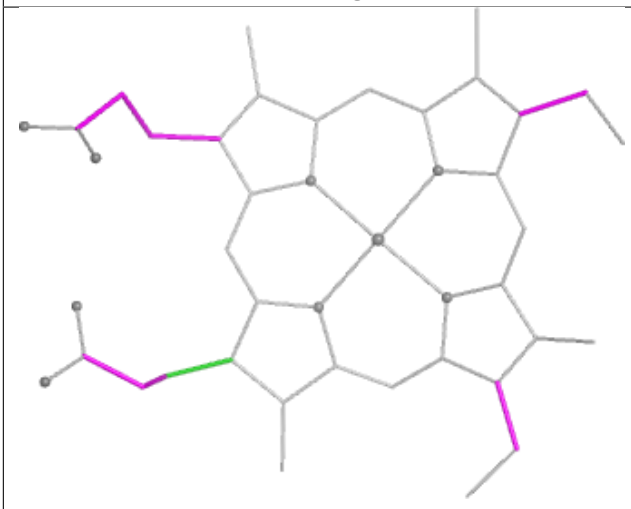
Ligand HEC G 301



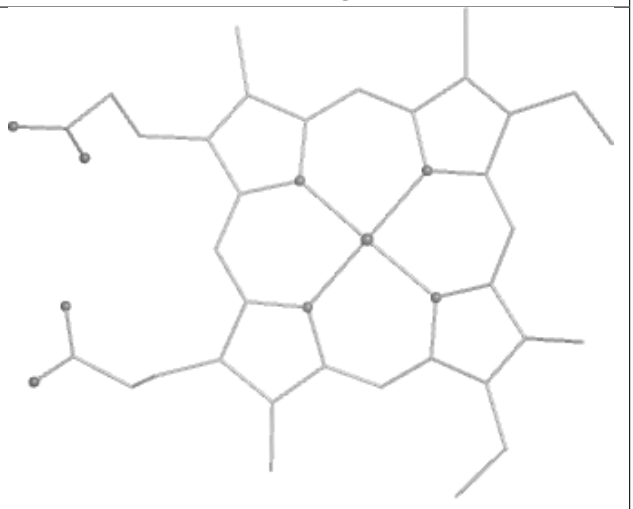
Bond lengths



Bond angles

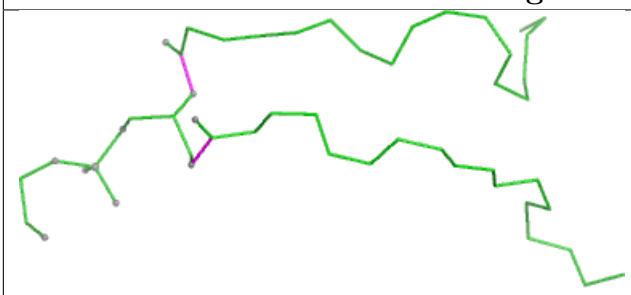


Torsions



Rings

Ligand PEE B 508



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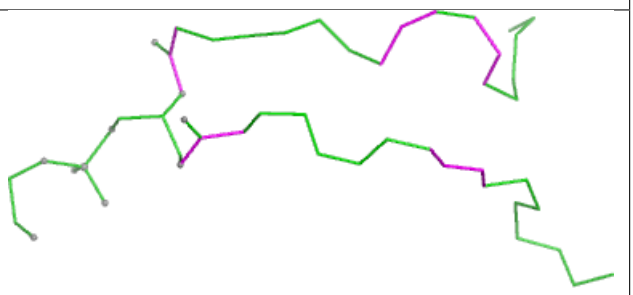
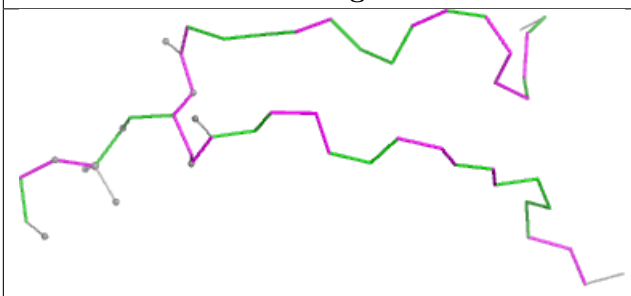


Bond angles

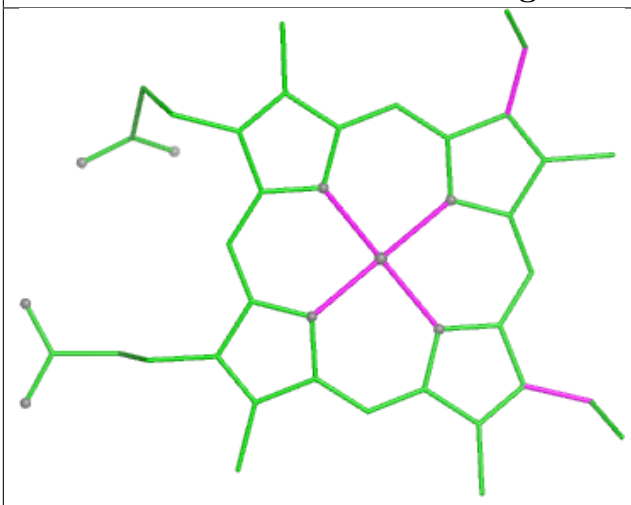


Torsions



Rings

Ligand HEM B 502



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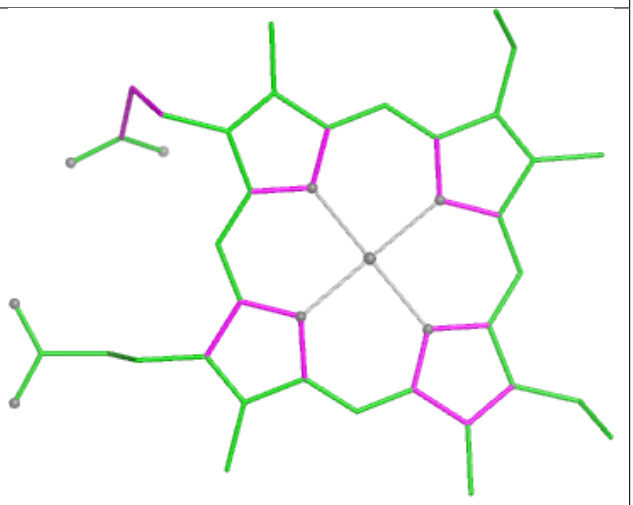

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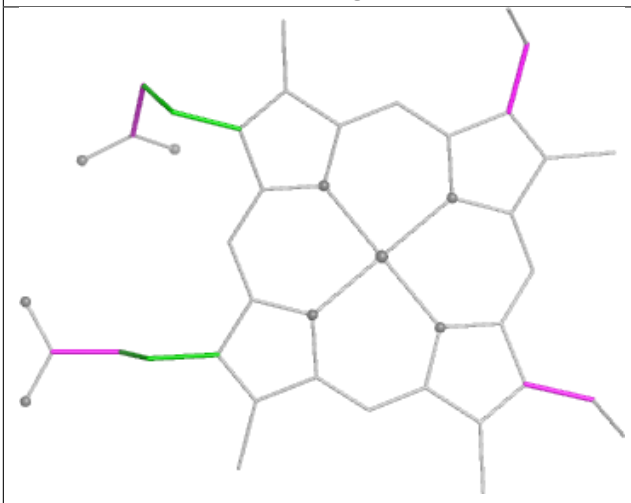

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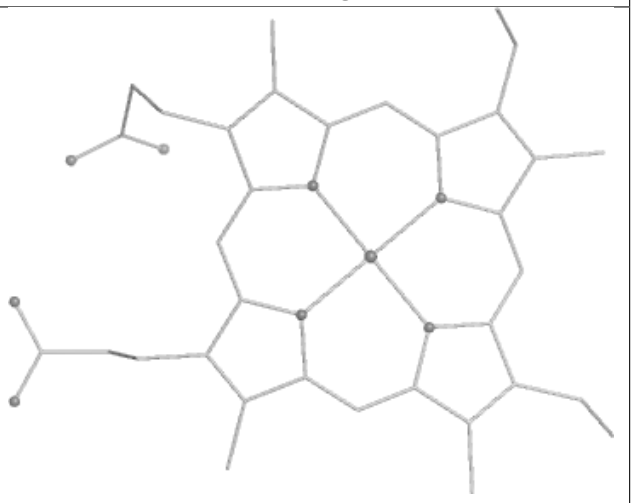

Rings

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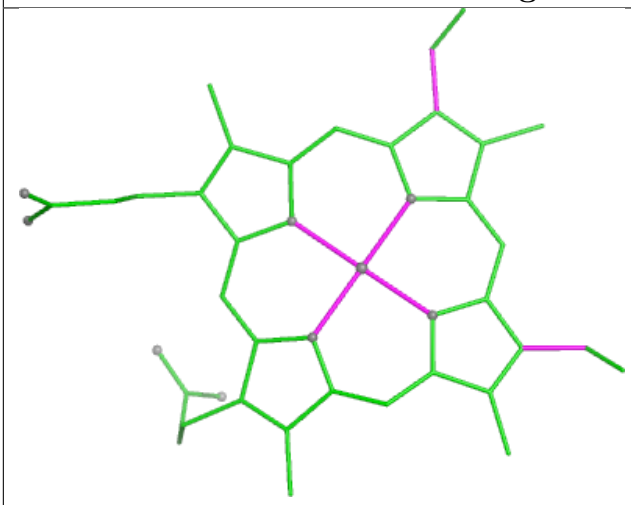

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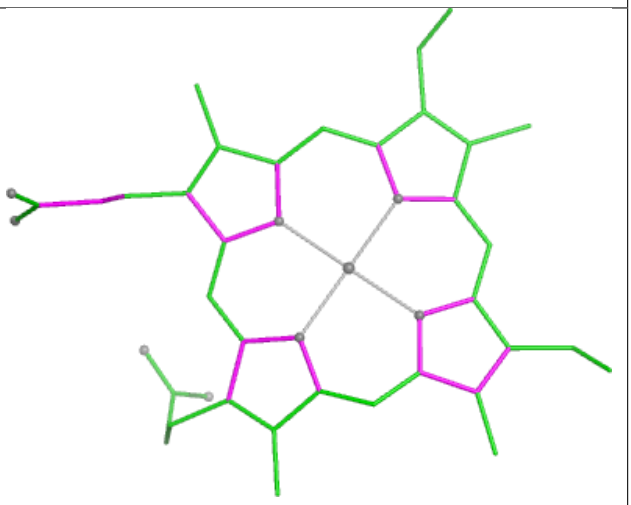

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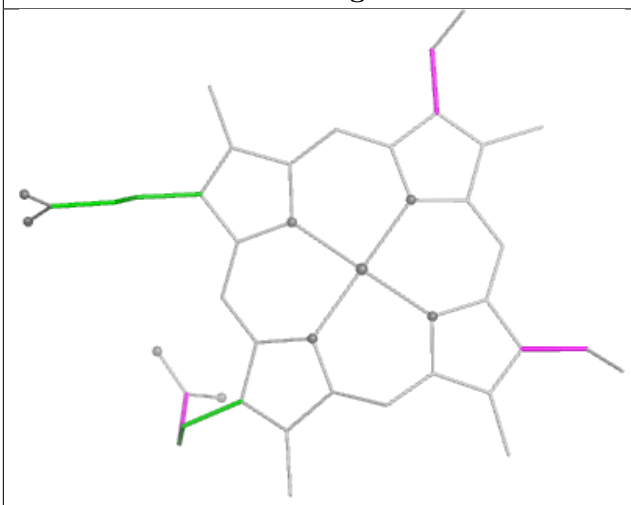

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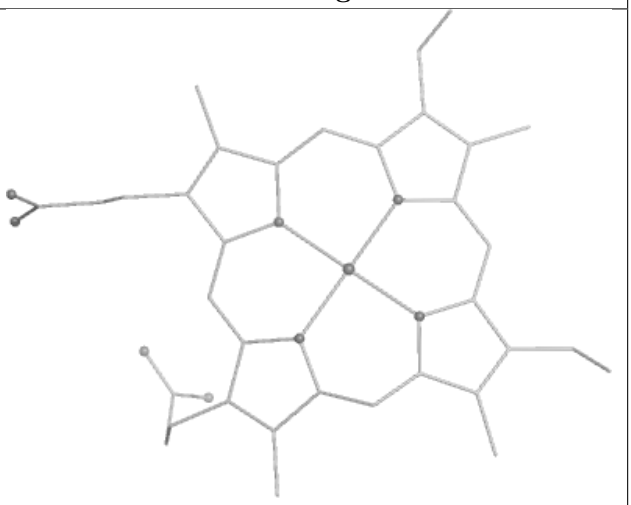
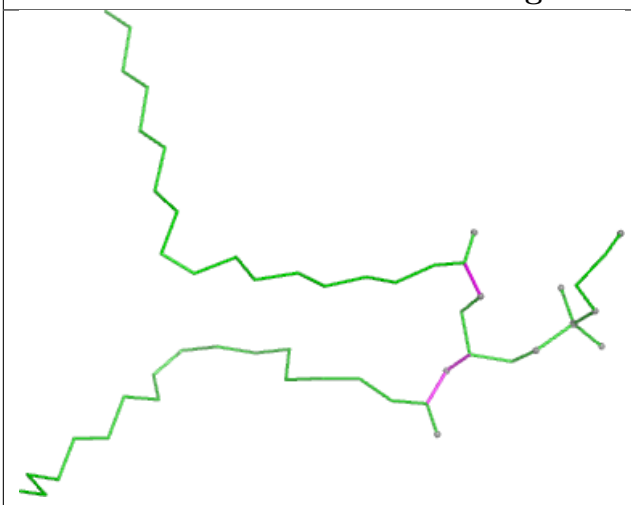


Rings

Ligand PEE A 202



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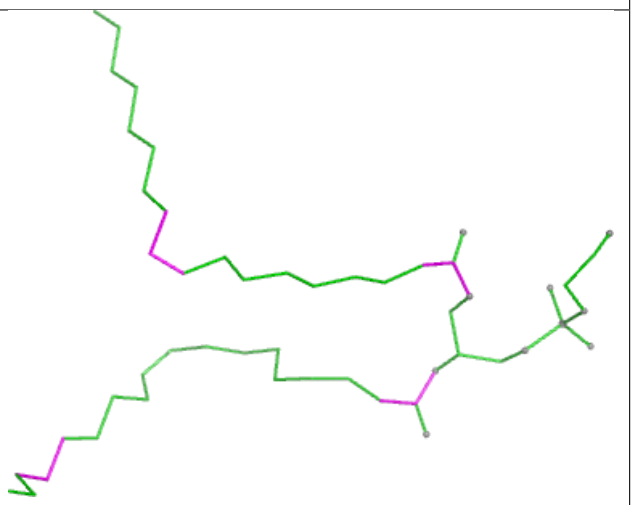

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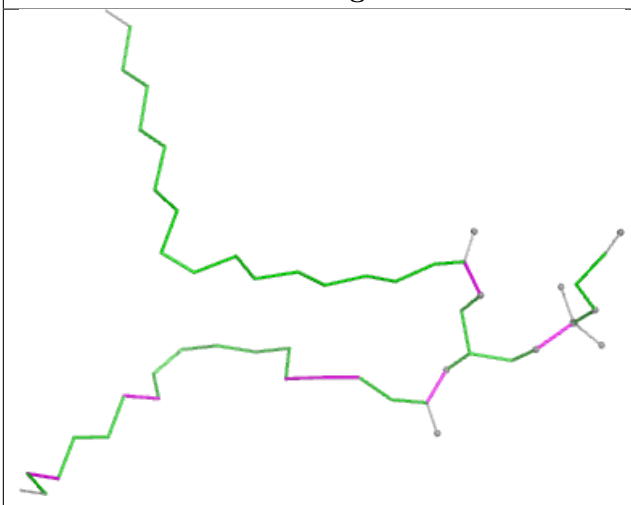

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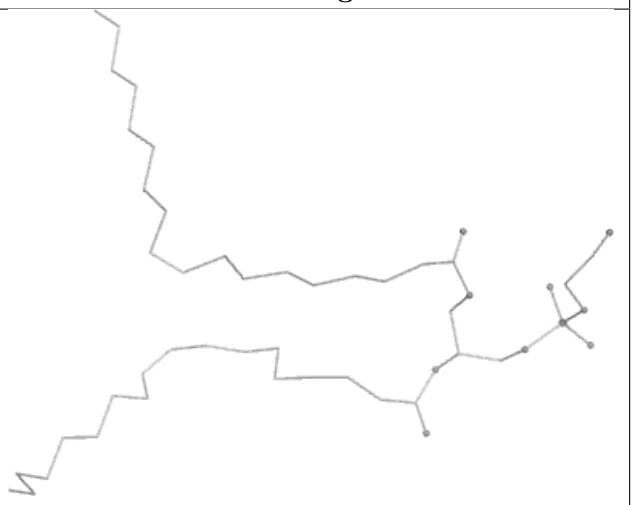
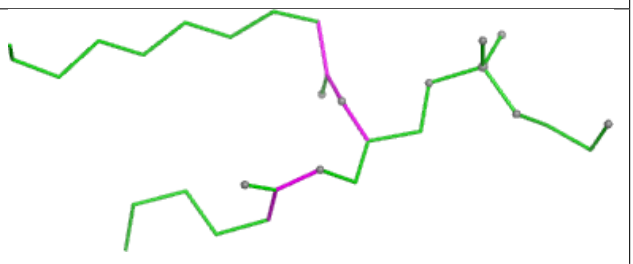


Rings

Ligand PEE B 505



Bond lengths



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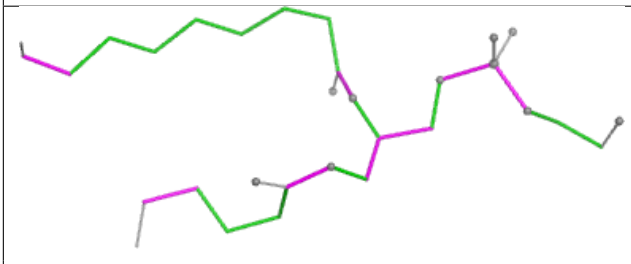

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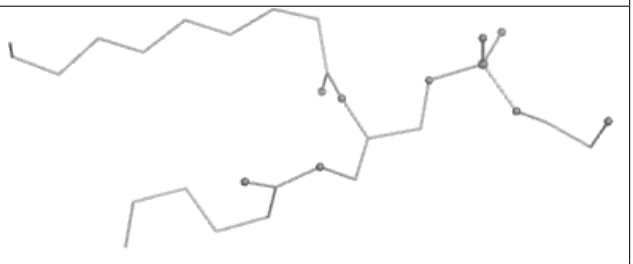

Rings

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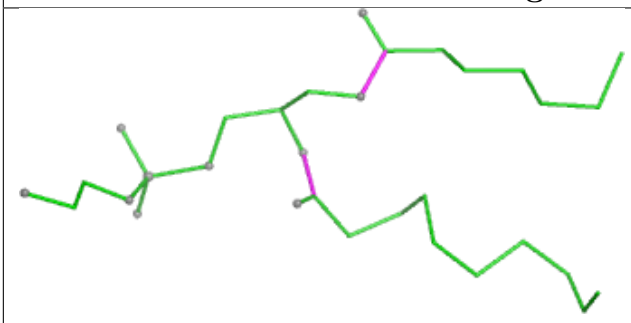

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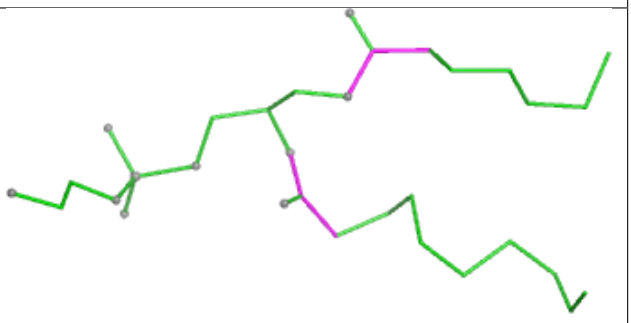

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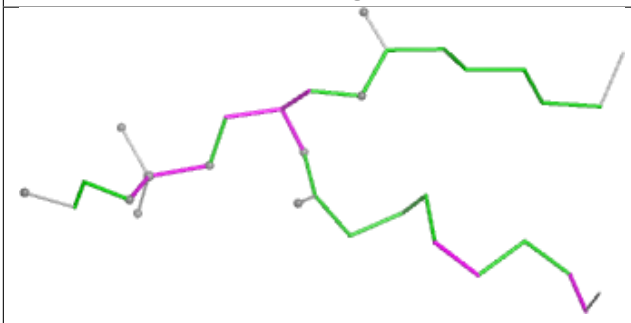

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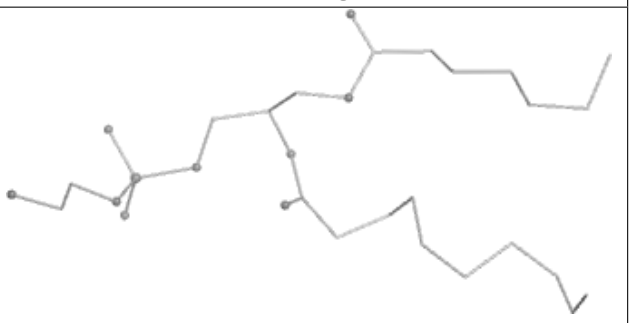

Rings

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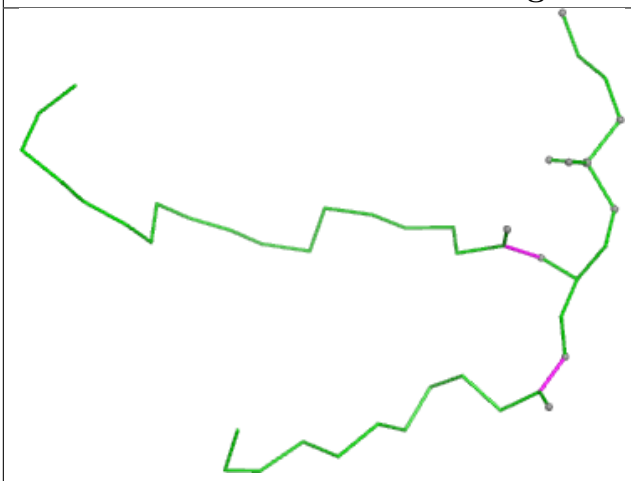

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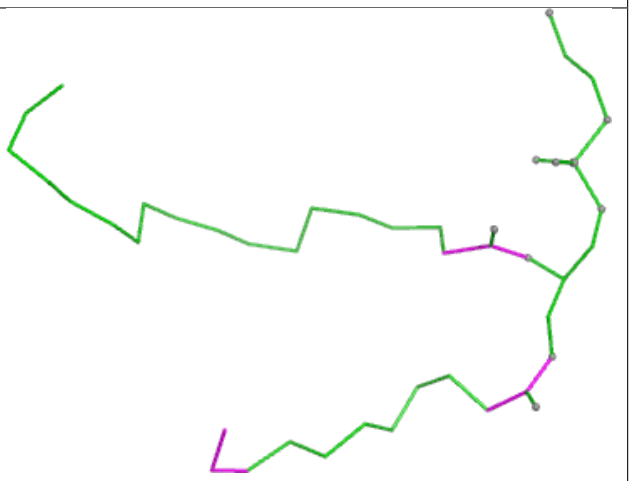

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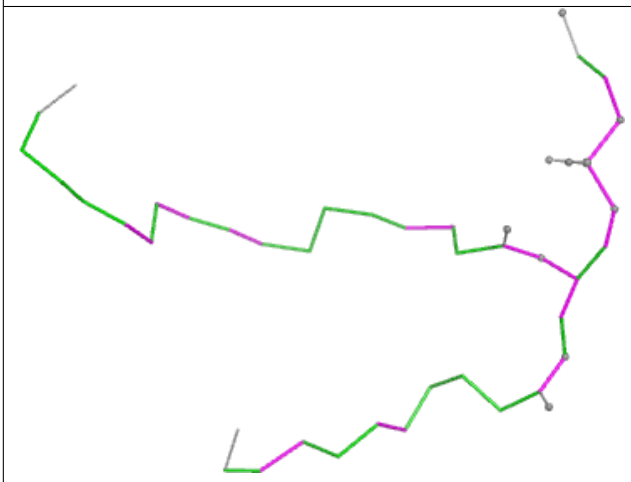
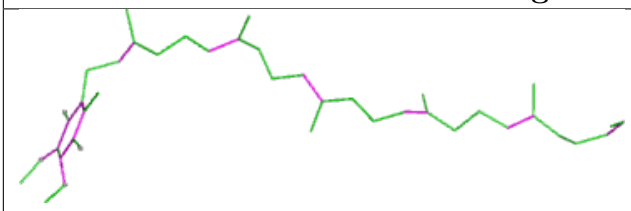


Torsions



Rings

Ligand U10 F 507



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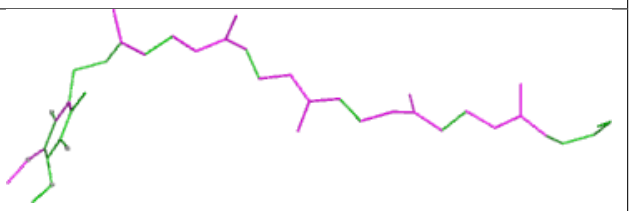
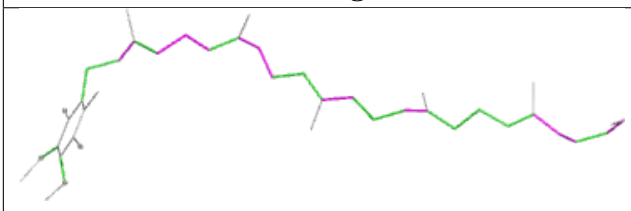


Bond angles



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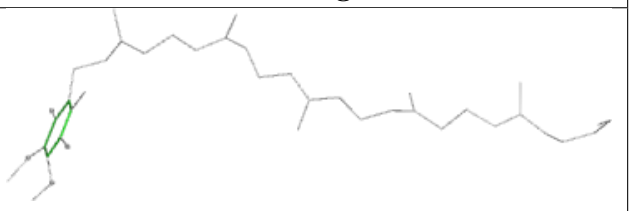

Rings

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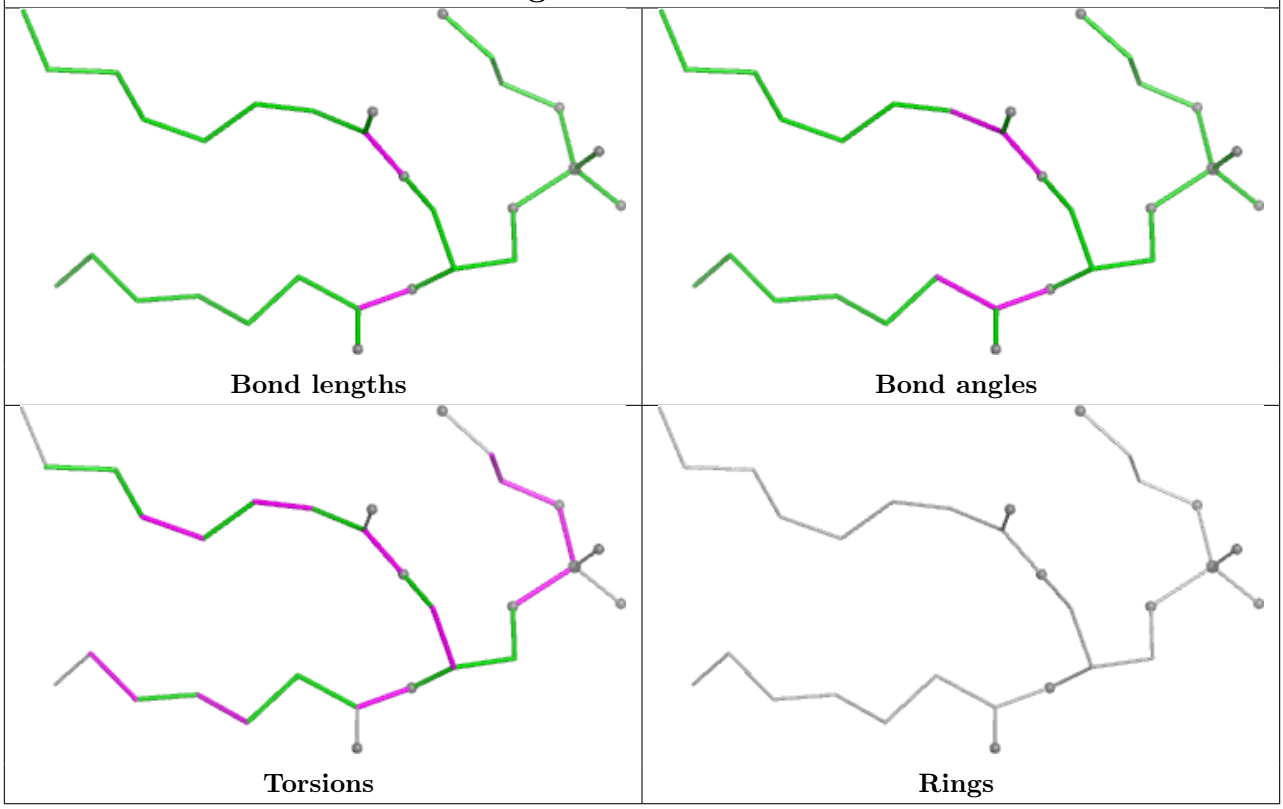
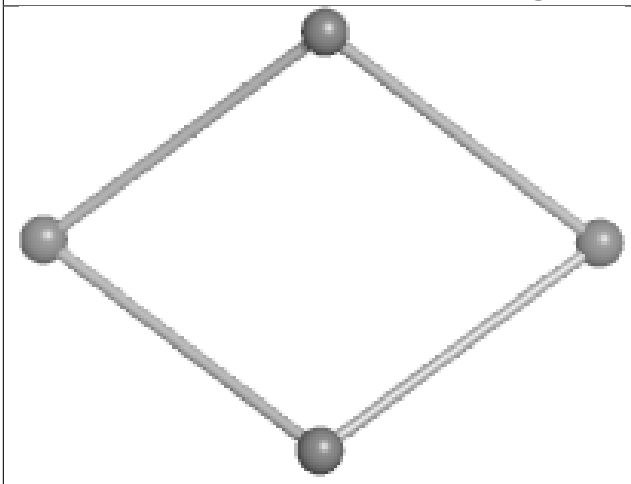


Ligand FES E 201



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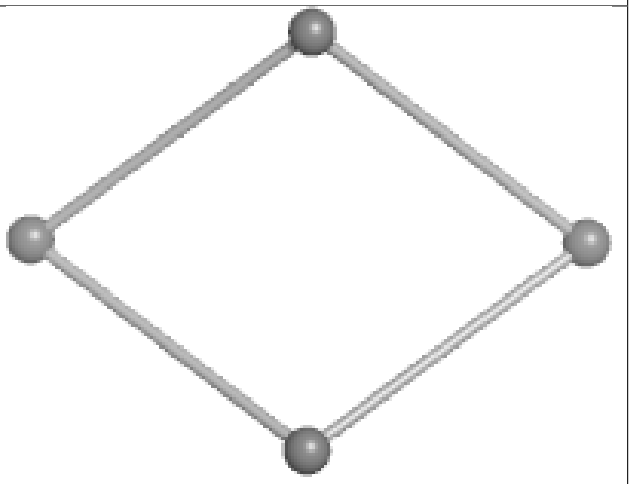

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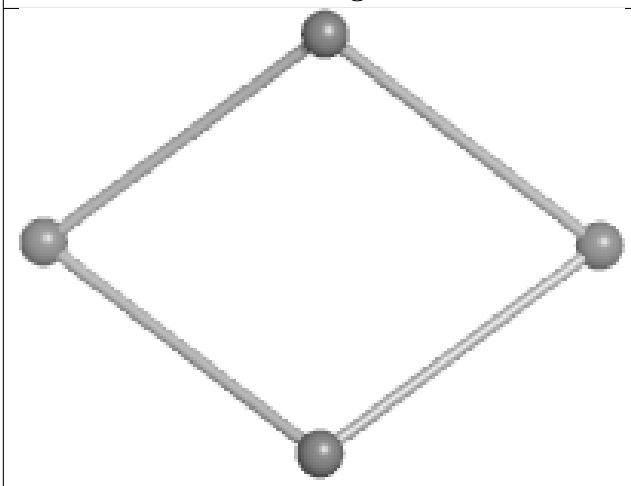

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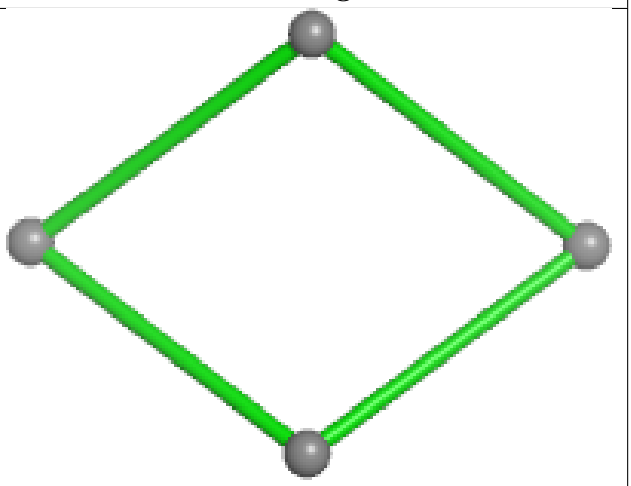

Rings

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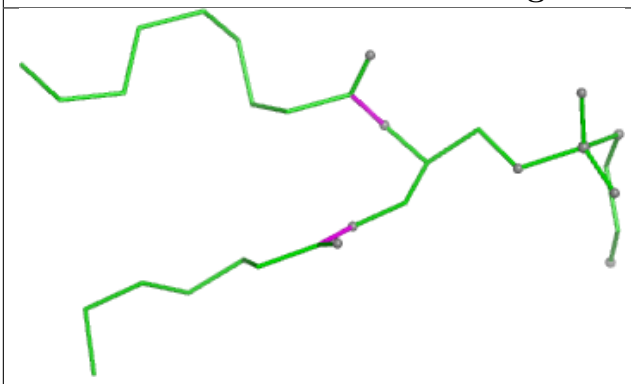

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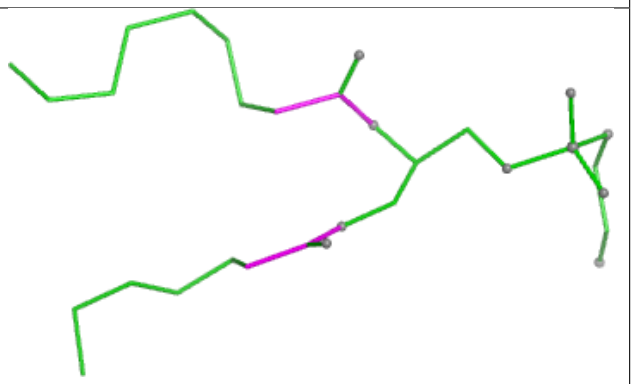

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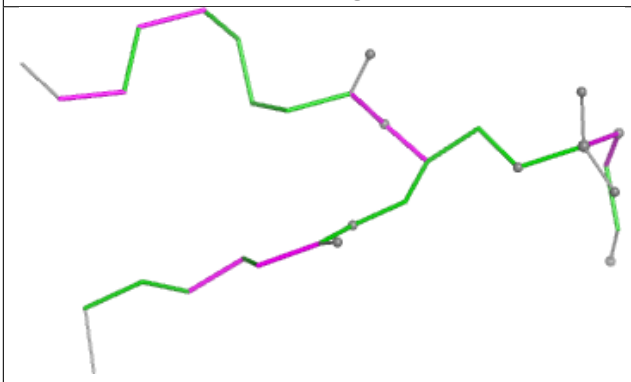

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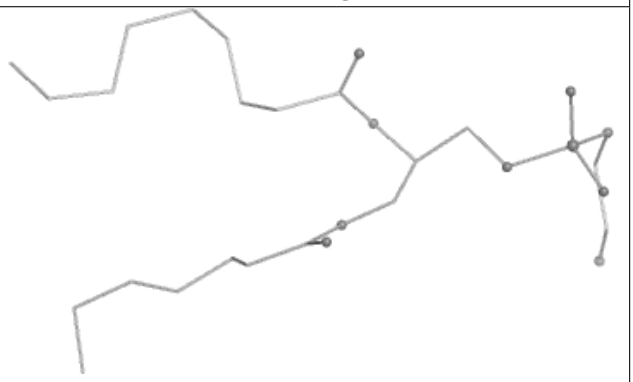

Rings

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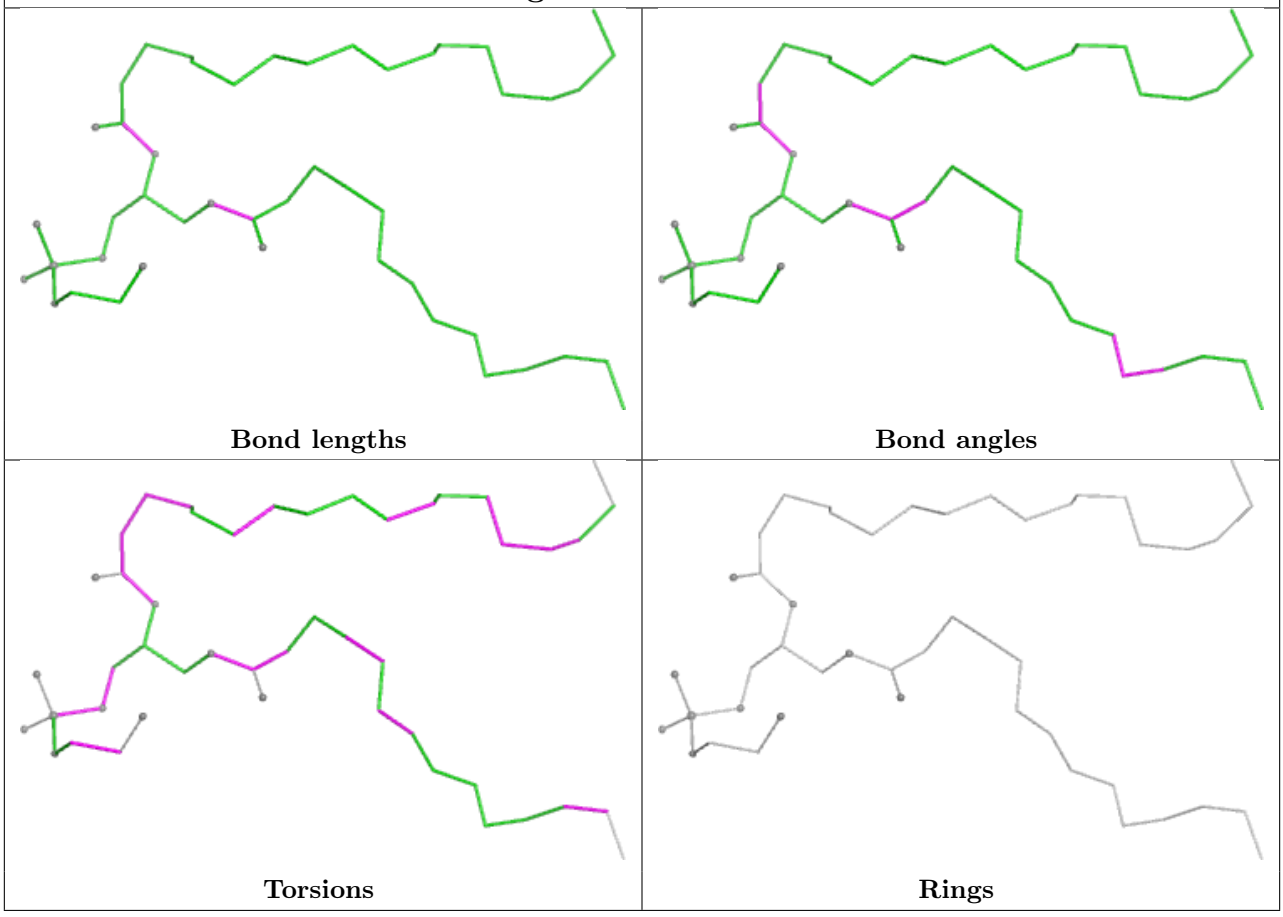
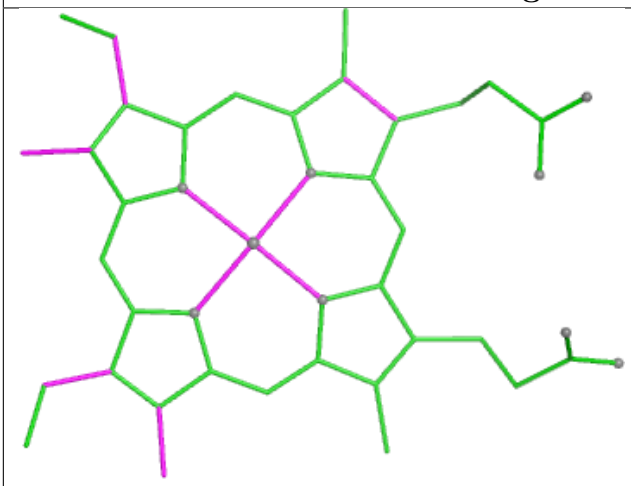


Ligand HEC C 301



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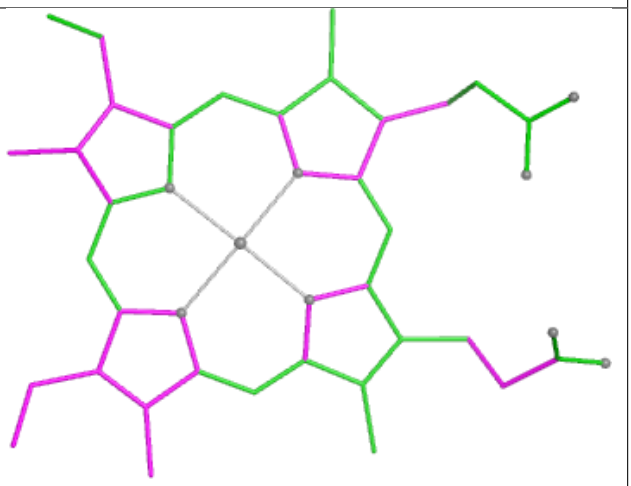
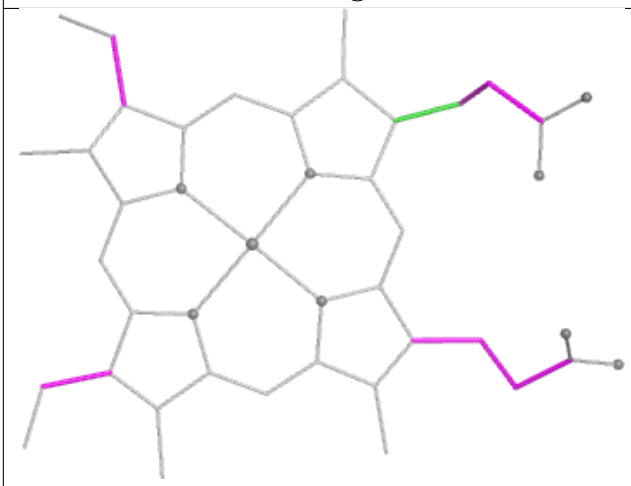


Bond angles



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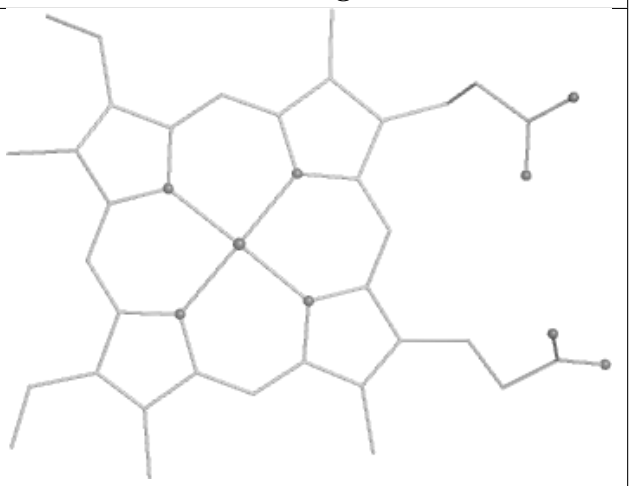

Rings

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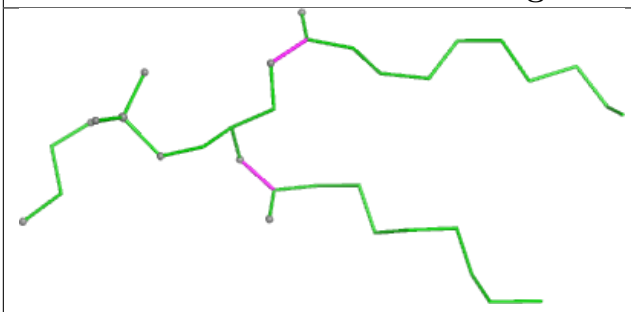
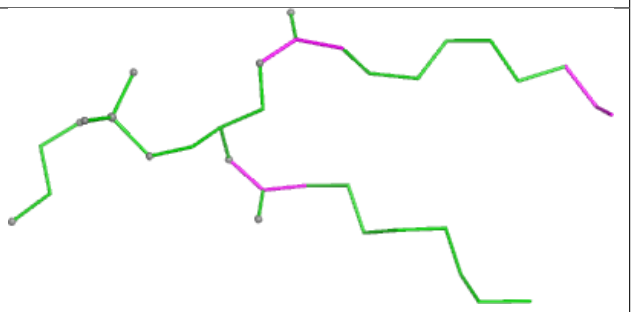
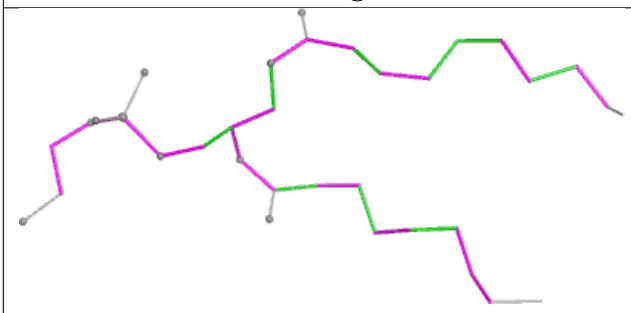


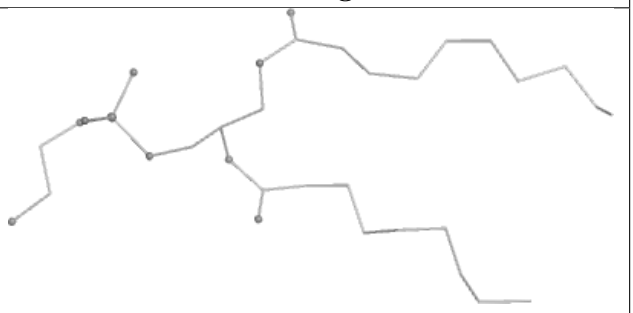
Bond lengths



Bond angles

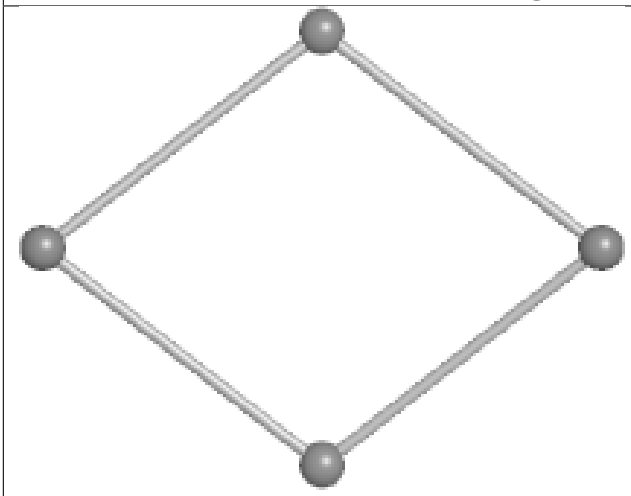


Torsions

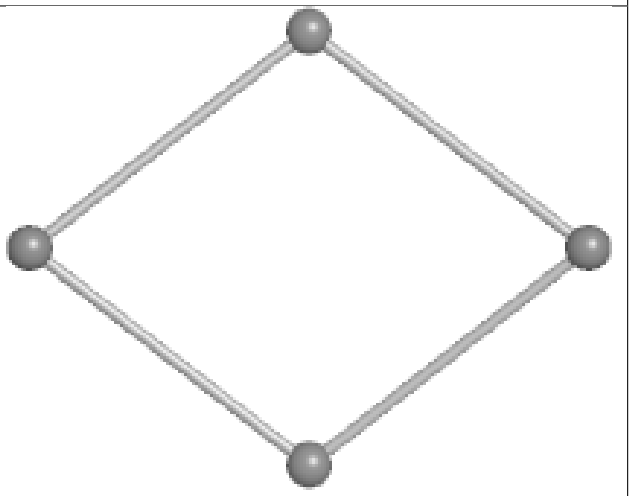


Rings

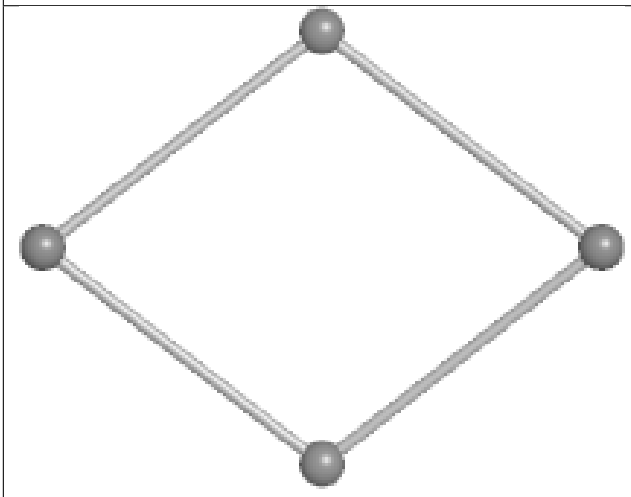
Ligand FES A 201



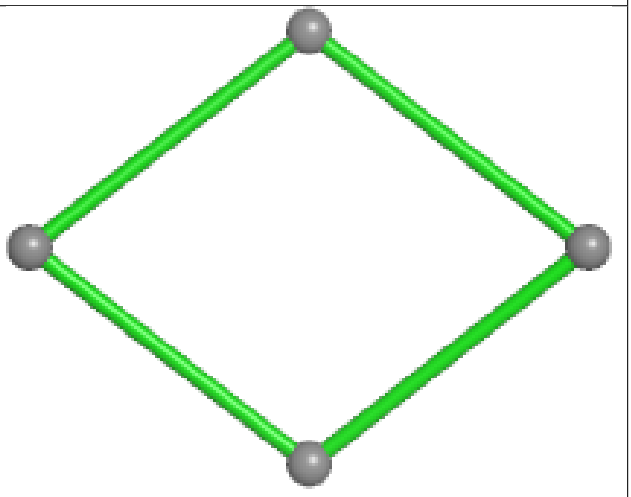
Bond lengths



Bond angles

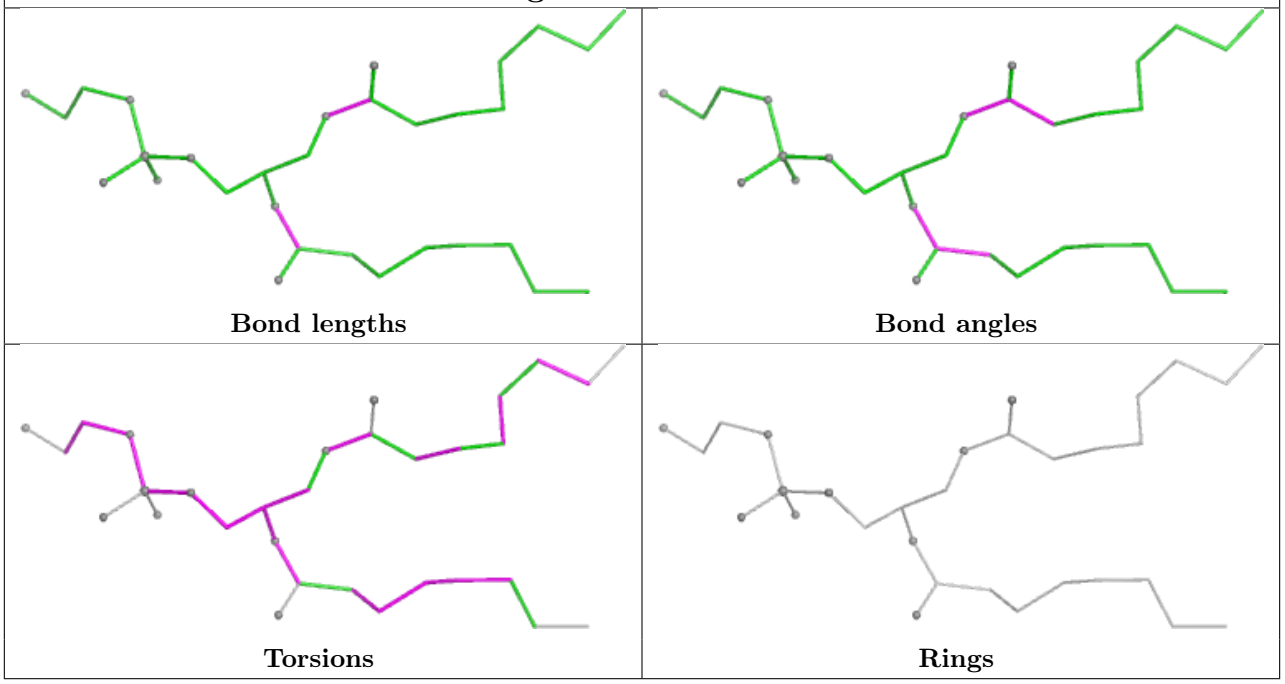


Torsions

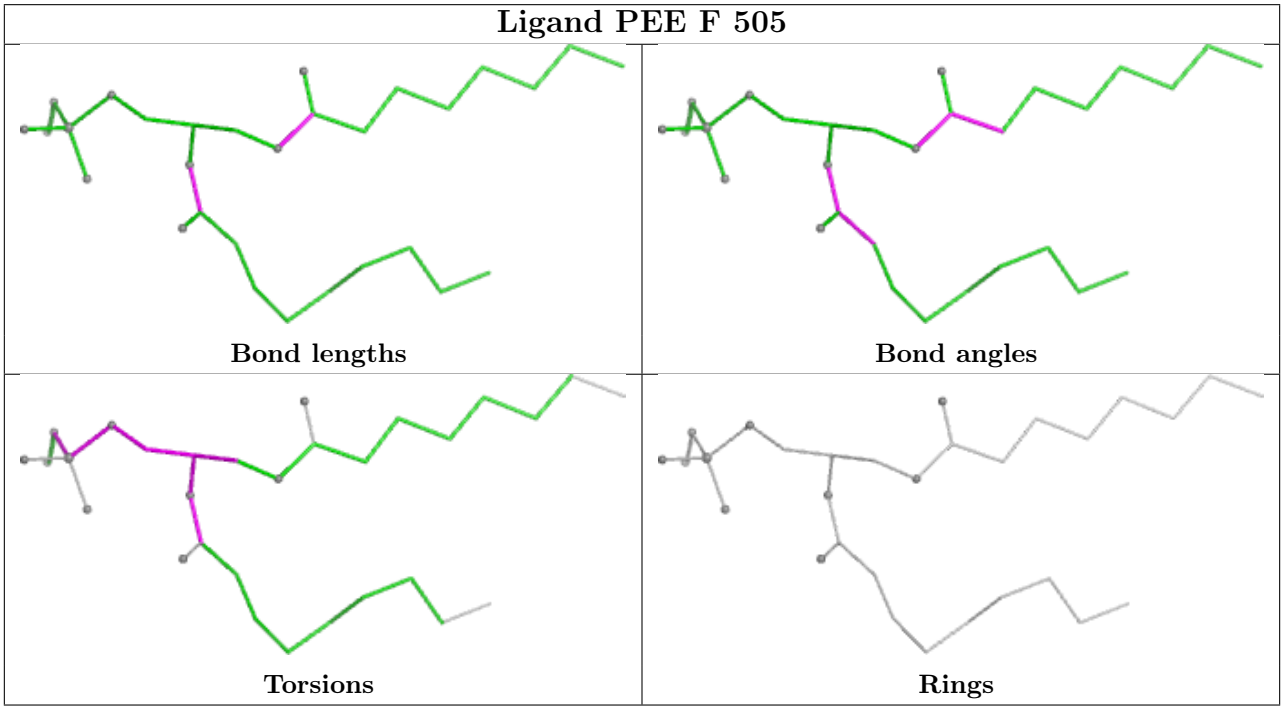


Rings

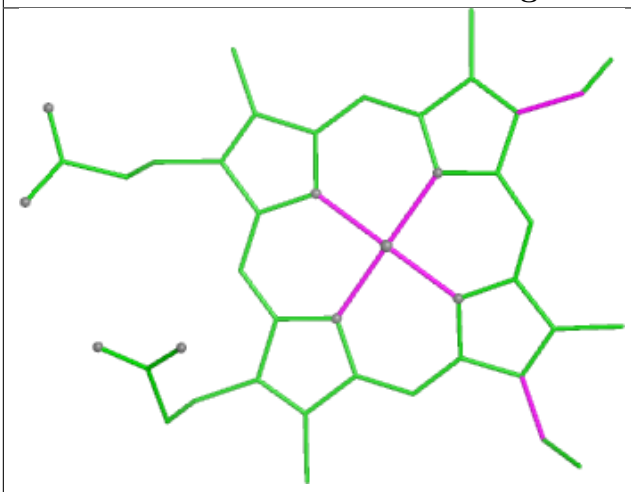
Ligand PEE B 504



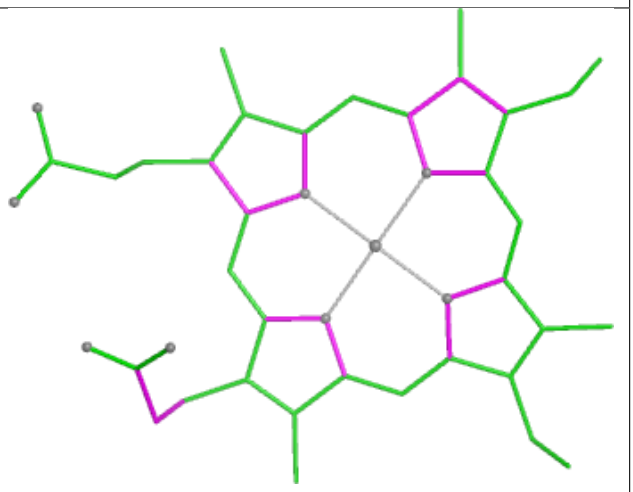
Ligand PEE F 505



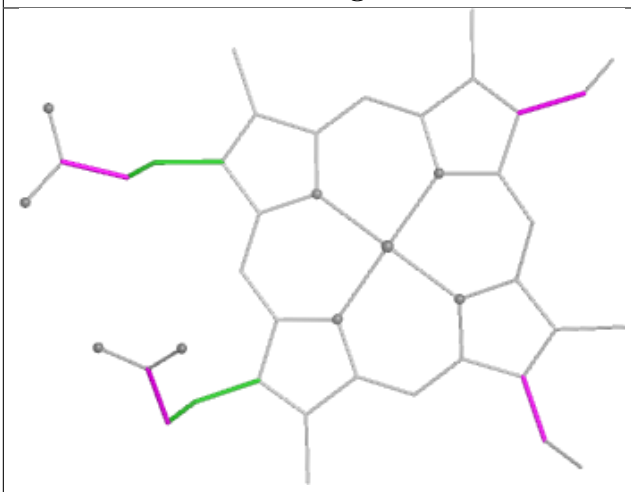
Ligand HEM F 502



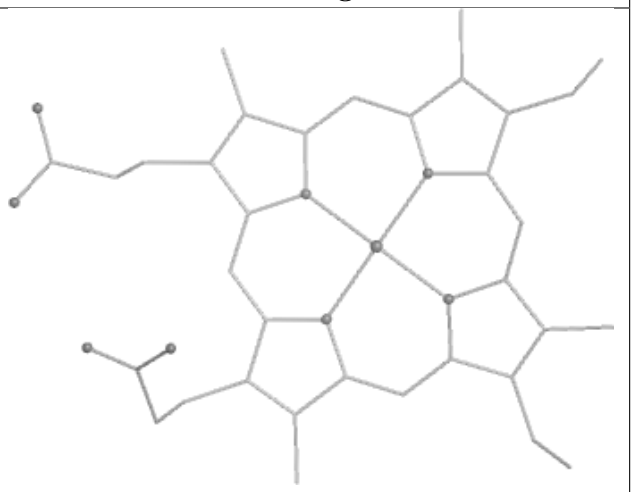
Bond lengths



Bond angles

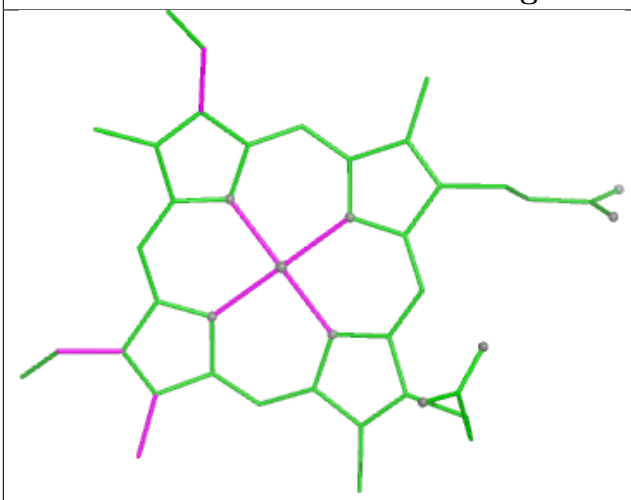


Torsions

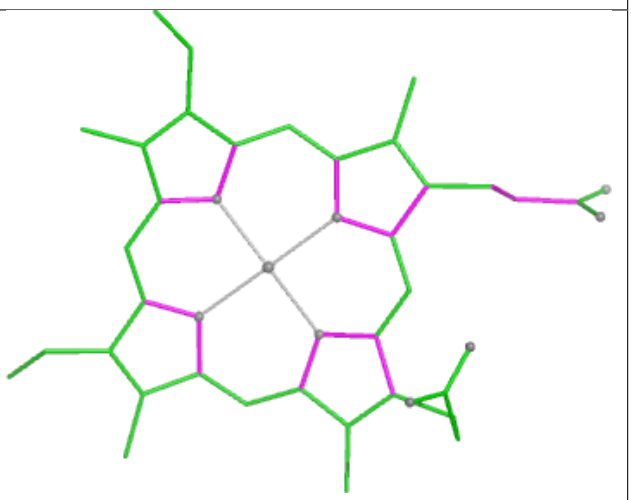


Rings

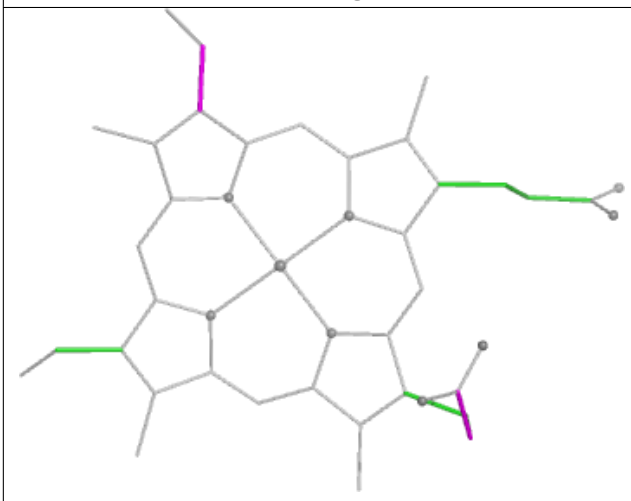
Ligand HEM F 501



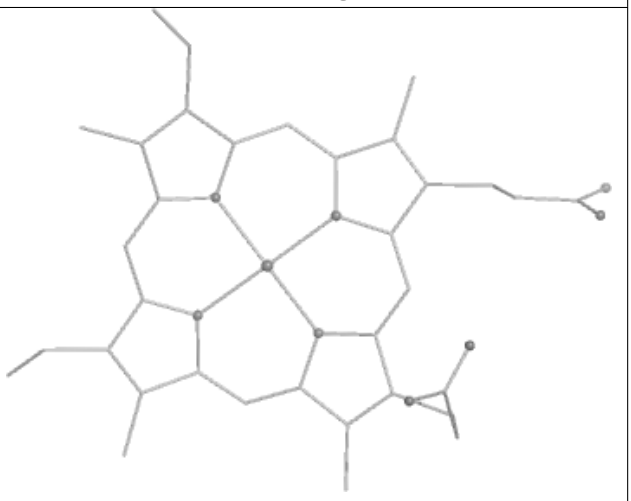
Bond lengths



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.

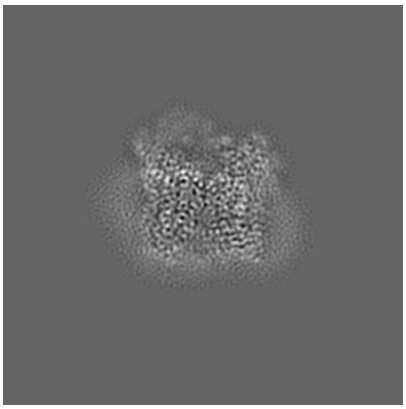
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15617. These allow visual inspection of the internal detail of the map and identification of artifacts.

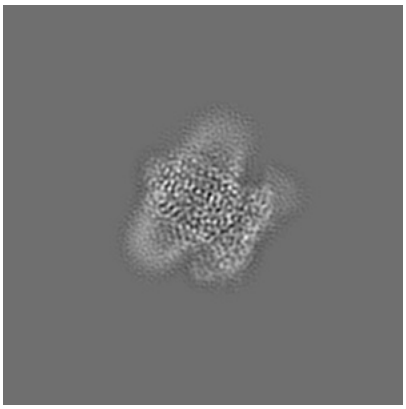
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

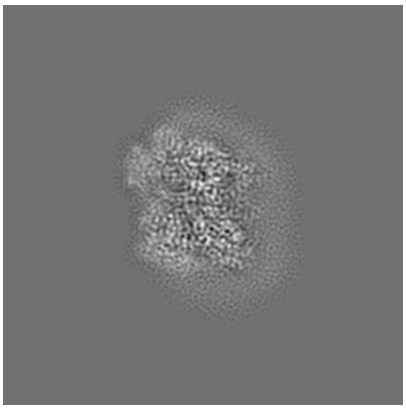
6.1.1 Primary map



X

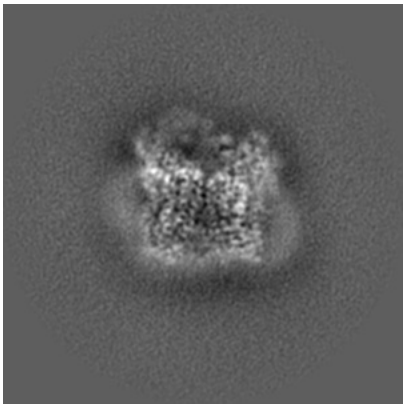


Y

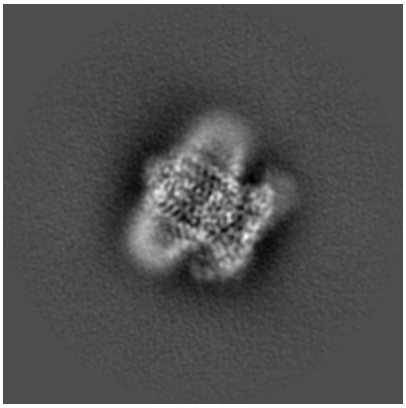


Z

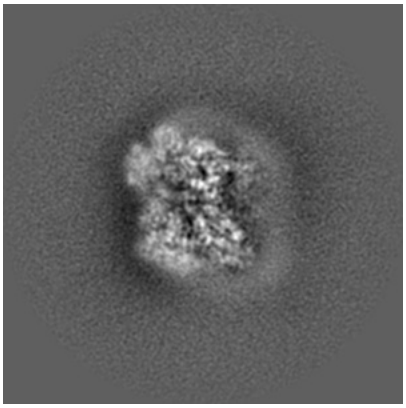
6.1.2 Raw map



X



Y

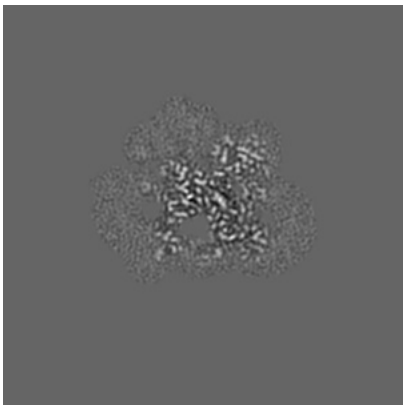


Z

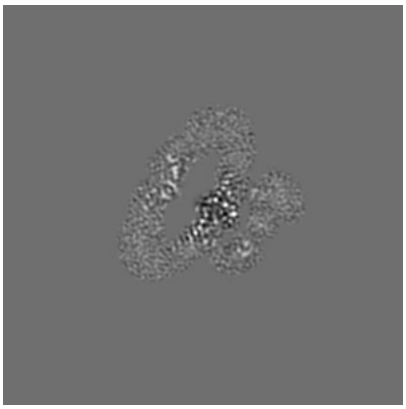
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

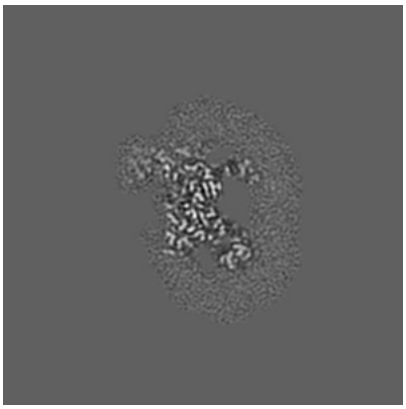
6.2.1 Primary map



X Index: 110

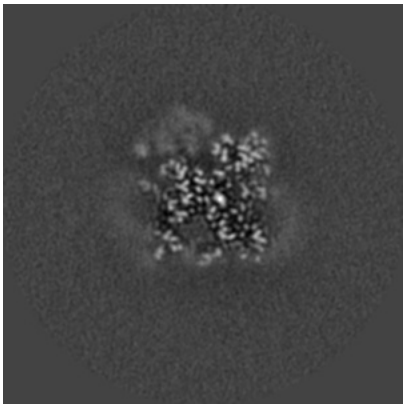


Y Index: 110

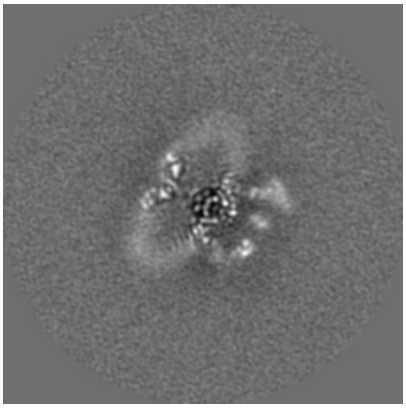


Z Index: 110

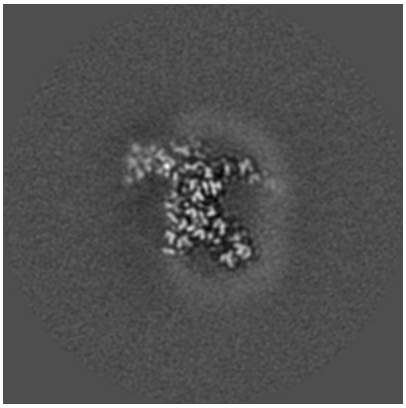
6.2.2 Raw map



X Index: 110



Y Index: 110

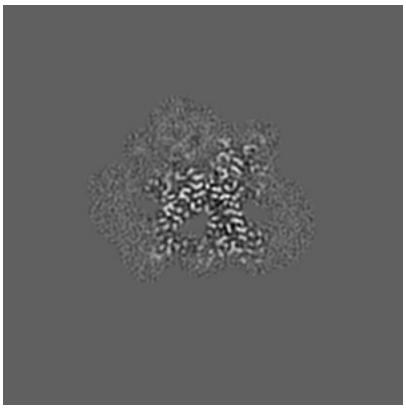


Z Index: 110

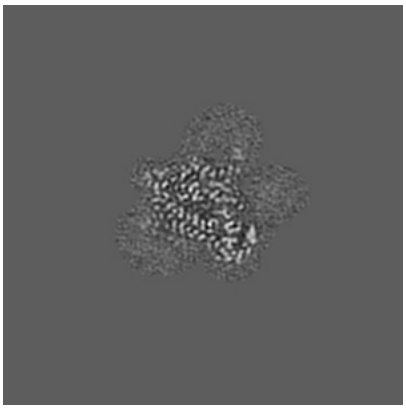
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

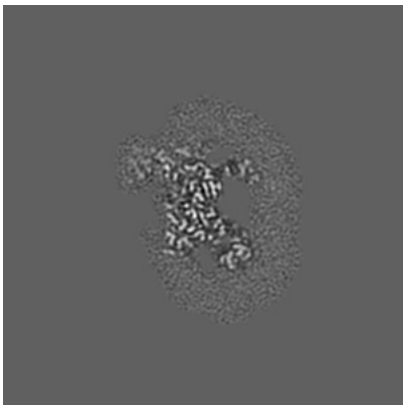
6.3.1 Primary map



X Index: 113

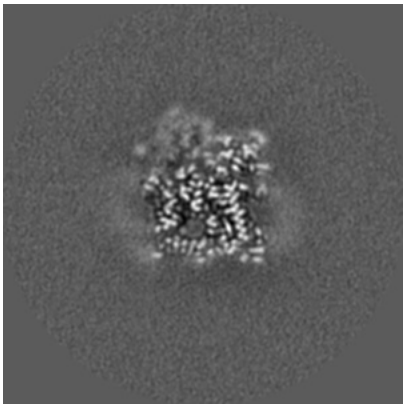


Y Index: 90

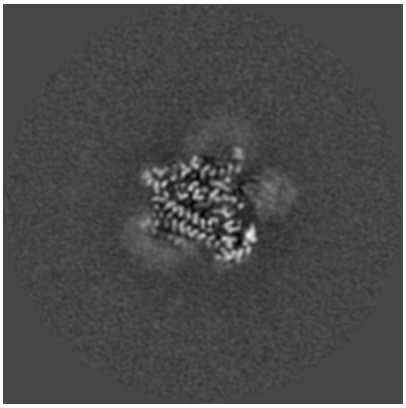


Z Index: 110

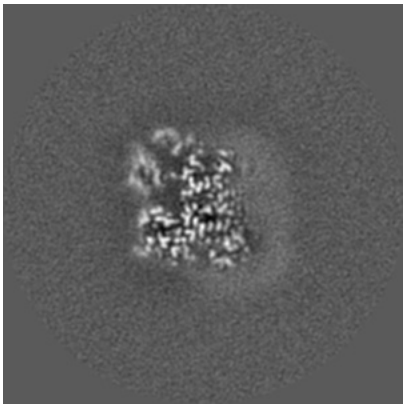
6.3.2 Raw map



X Index: 114



Y Index: 90

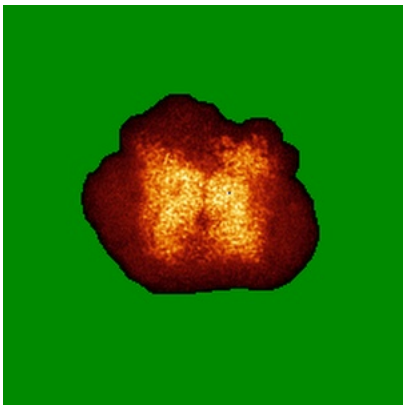


Z Index: 124

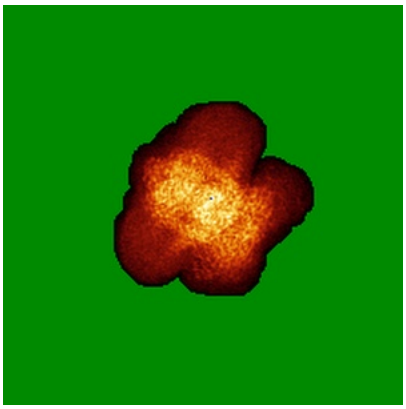
The images above show the largest variance slices of the map in three orthogonal directions.

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

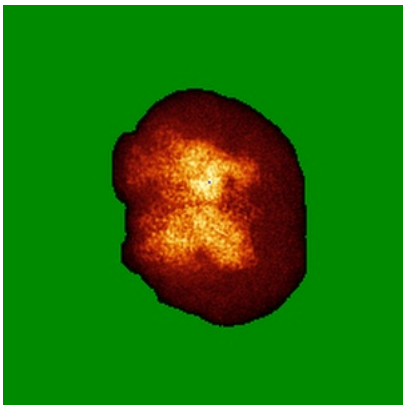
6.4.1 Primary map



X

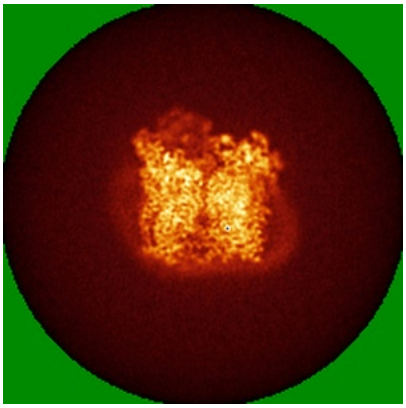


Y

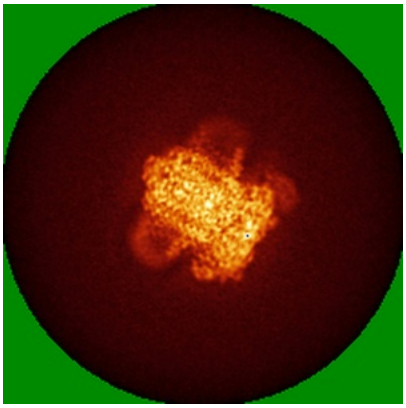


Z

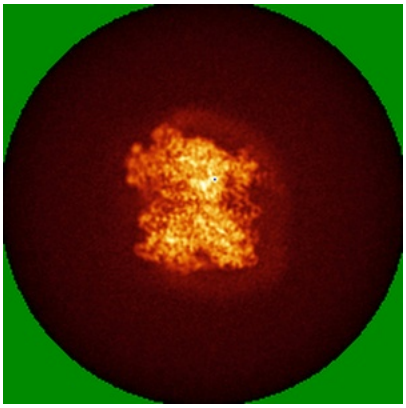
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

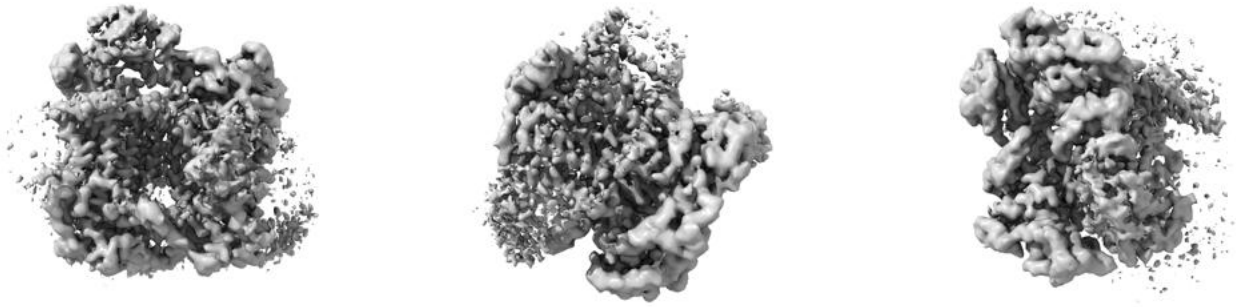
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

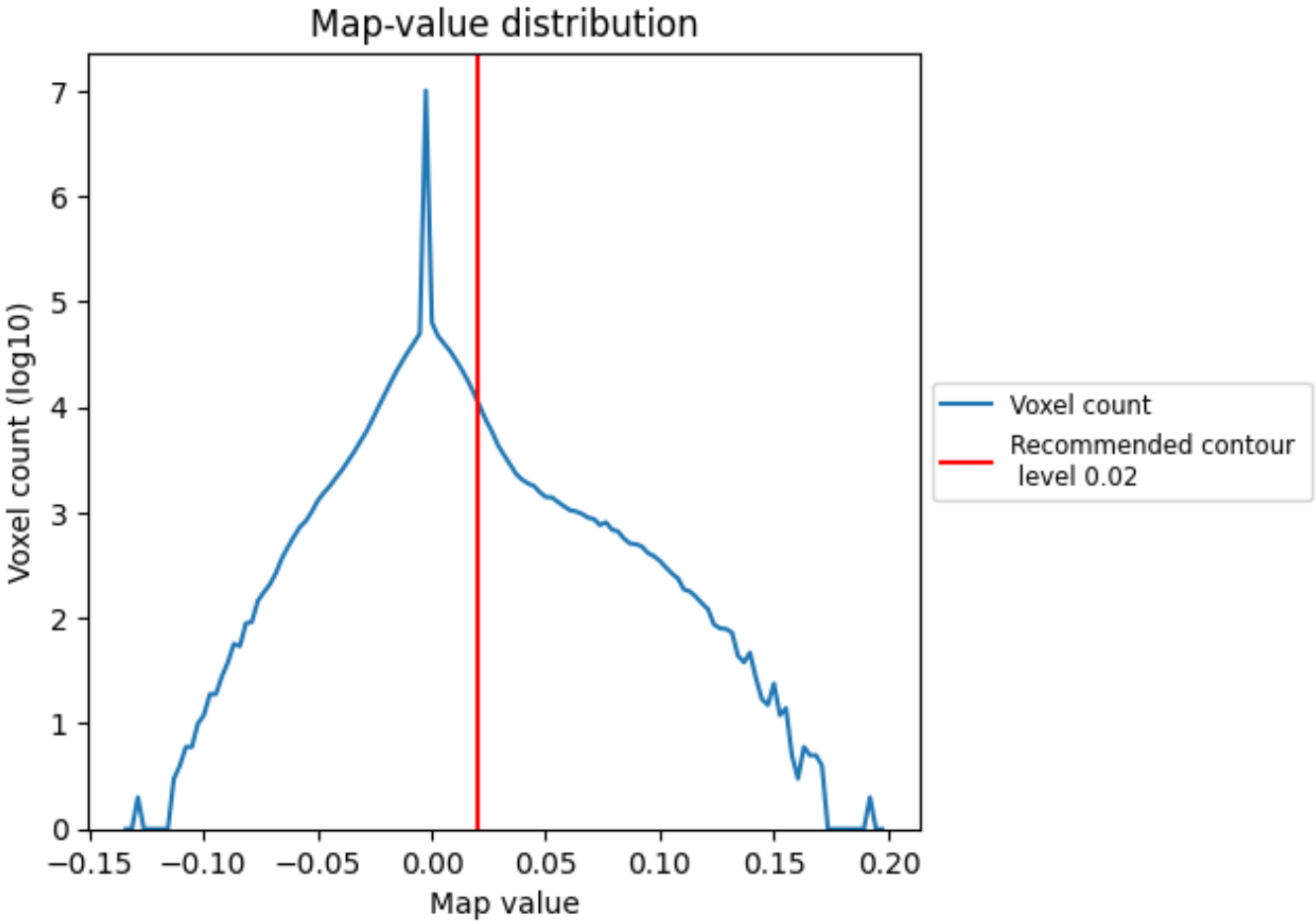
6.6 Mask visualisation (i)

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

7 Map analysis

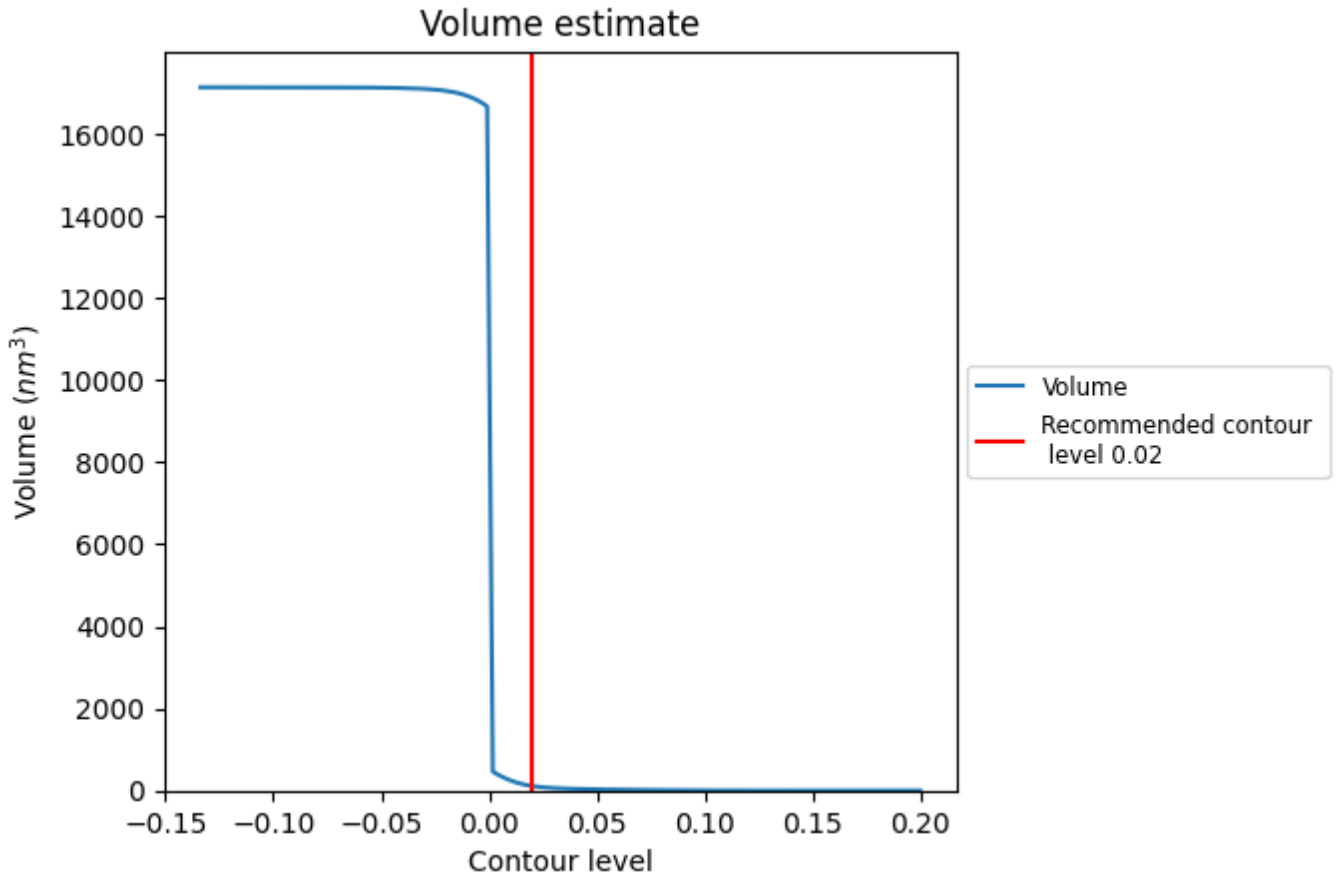
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

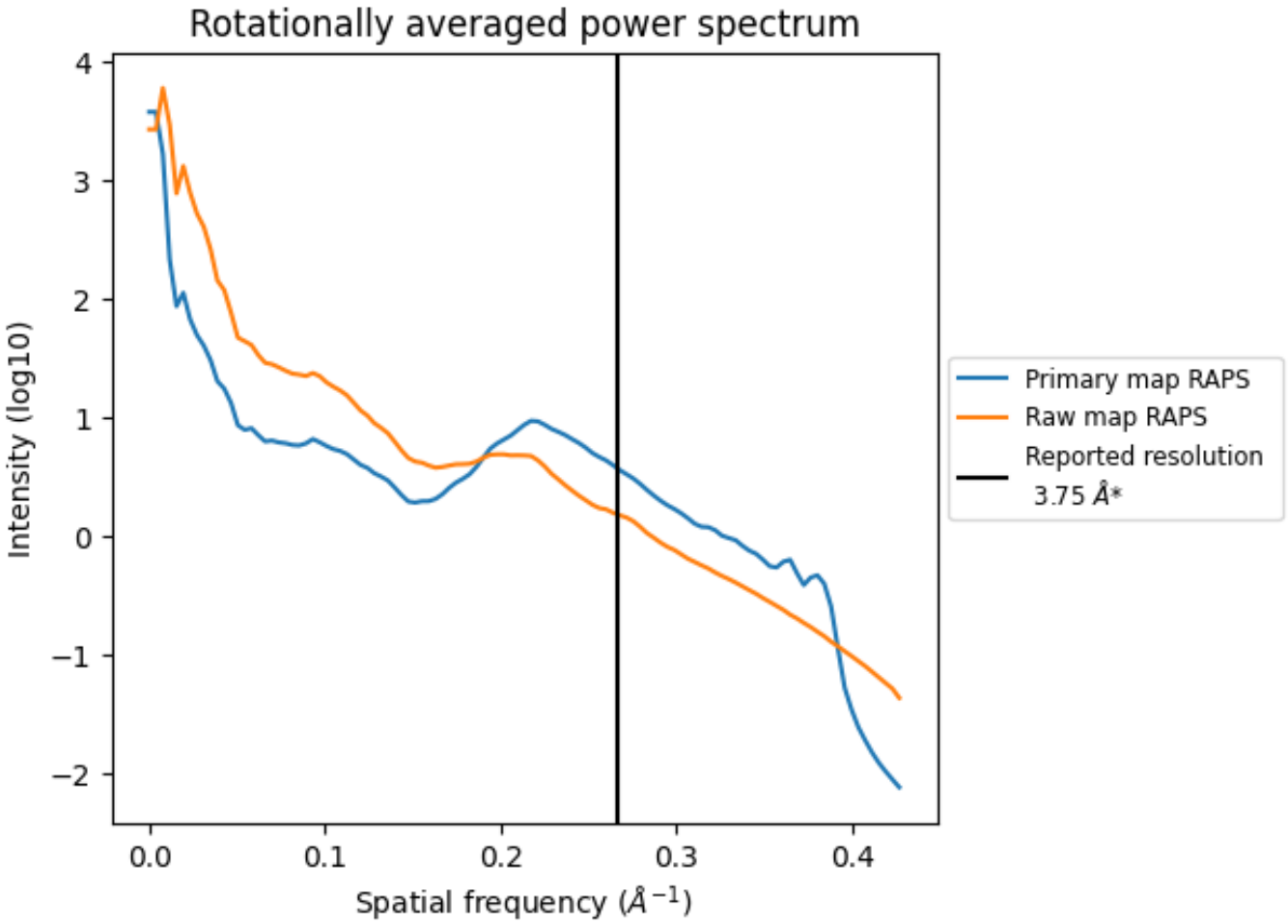
7.2 Volume estimate



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 99 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)

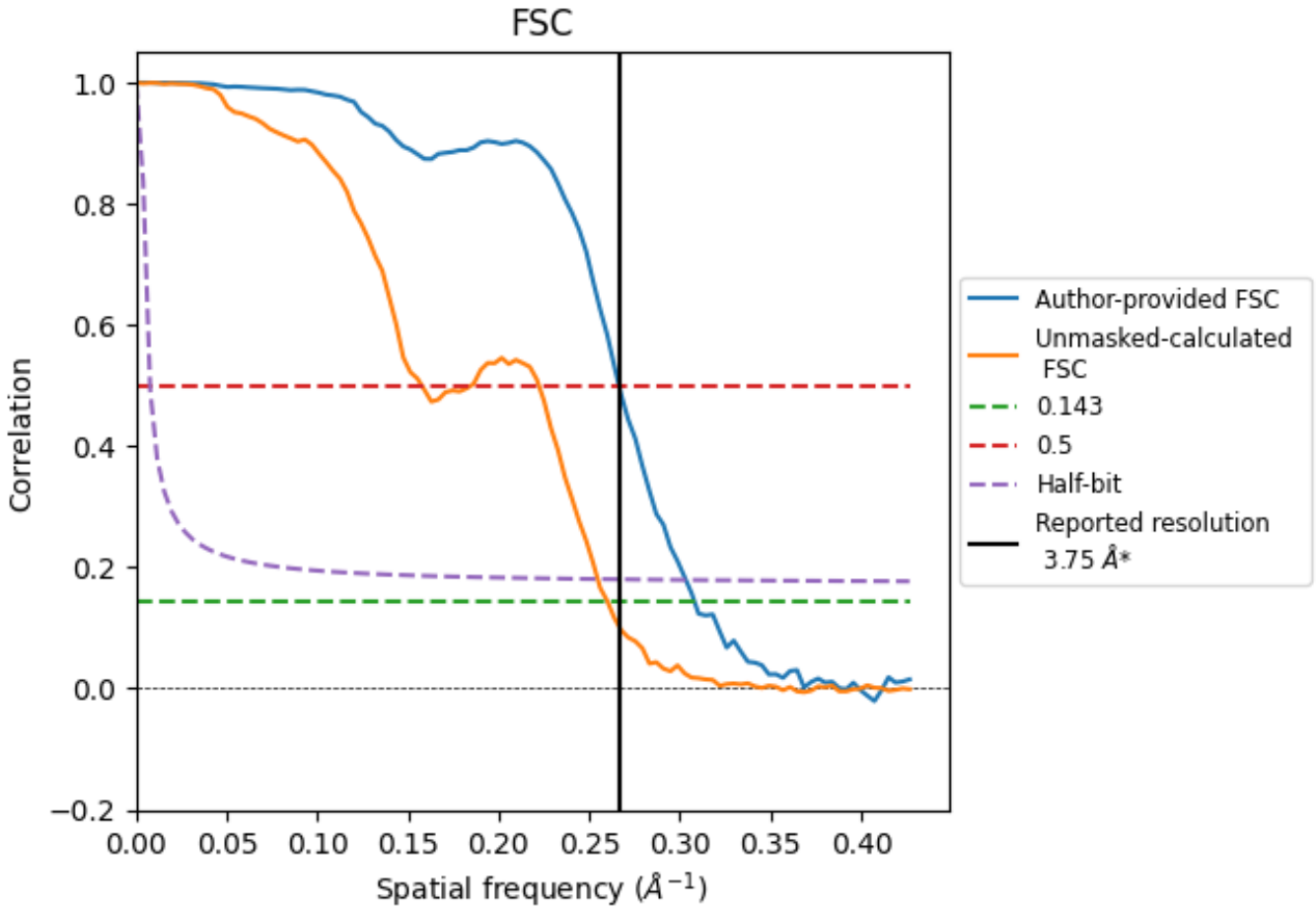


*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

8.2 Resolution estimates (i)

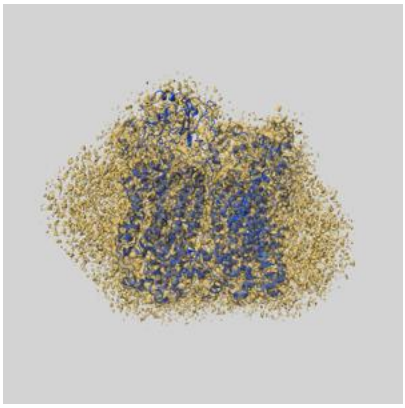
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.75	-
Author-provided FSC curve	3.25	3.76	3.30
Unmasked-calculated*	3.84	6.35	3.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 6.35 differs from the reported value 3.75 by more than 10 %

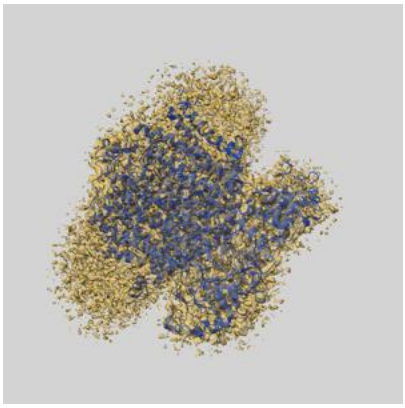
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15617 and PDB model 8ASJ. Per-residue inclusion information can be found in section 3 on page 9.

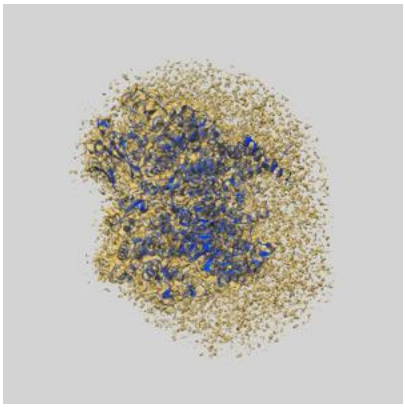
9.1 Map-model overlay



X



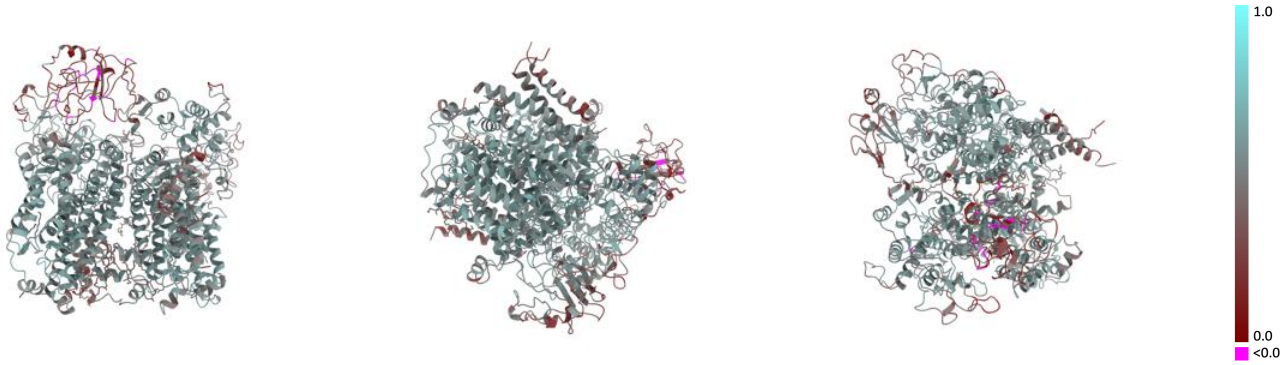
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

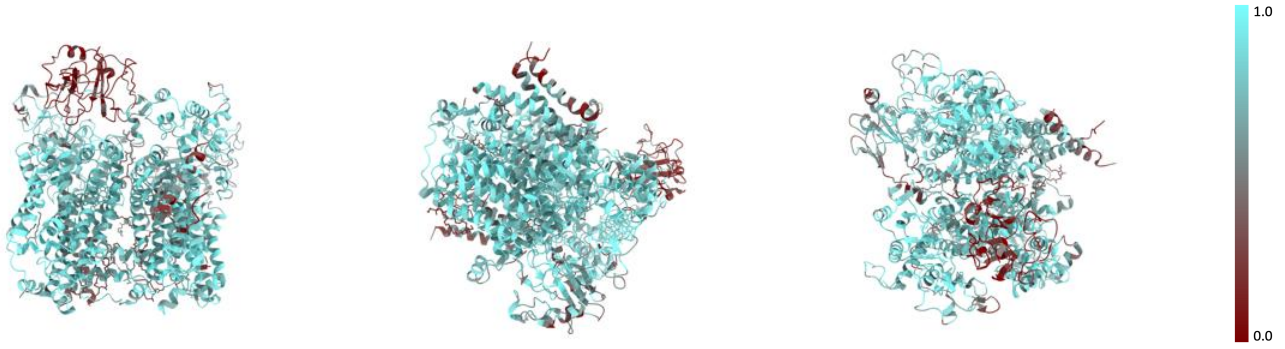
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

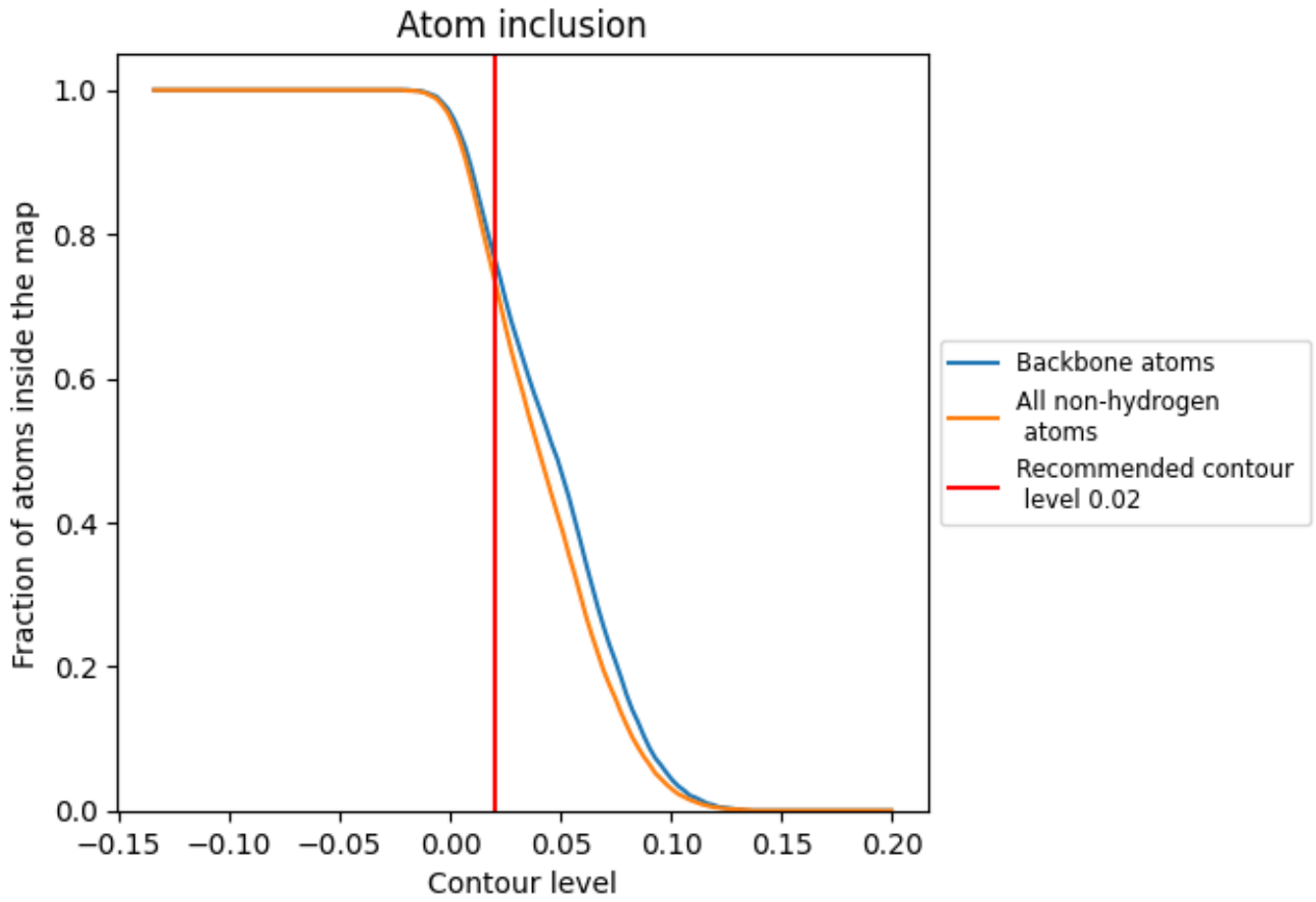
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 74% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.5040
A	0.6760	0.4450
B	0.8300	0.5610
C	0.7910	0.5180
D	0.3950	0.2660
E	0.2760	0.2740
F	0.8290	0.5640
G	0.7860	0.5130
H	0.3720	0.3650

