Full wwPDB EM Validation Report

Oct 26, 2026 – 02:57 PM EDT

PDB ID	:	9OCX / pdb_00009ocx
EMDB ID	:	EMD-70334
Title	:	Cryo-EM structure of the CIII2 featuring FES in b-position from Bacillus subtilis
Authors	:	Gu, M.; Zheng, W.; Zong, Y.; Zhang, K.; Zhu, J.
Deposited on	:	2025-04-25
Resolution	:	3.40 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:

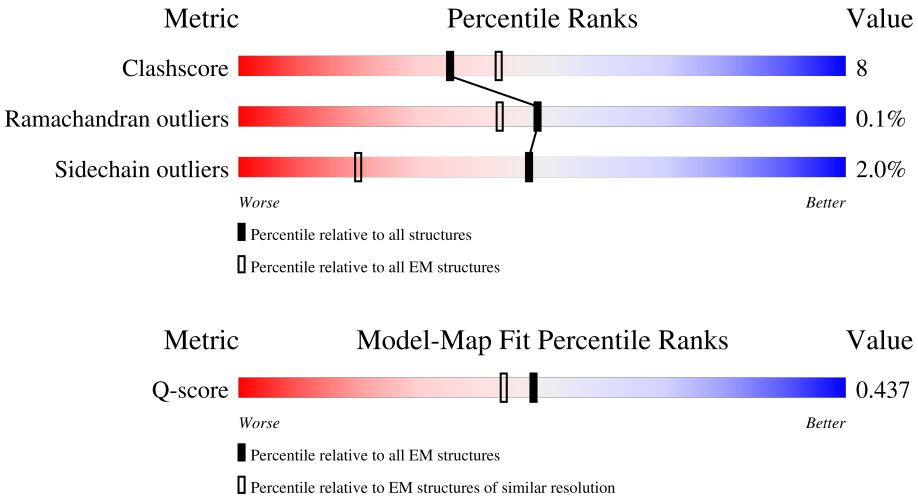
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



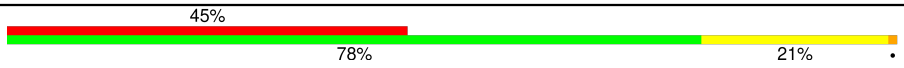
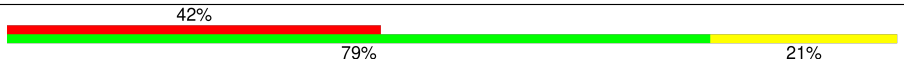
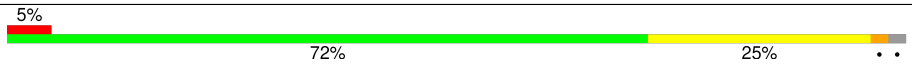
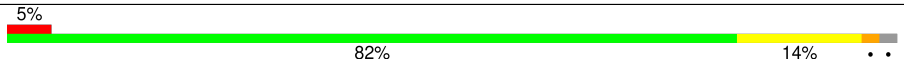
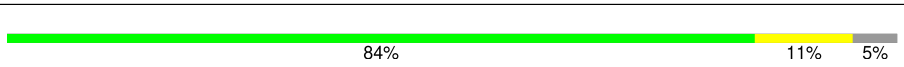
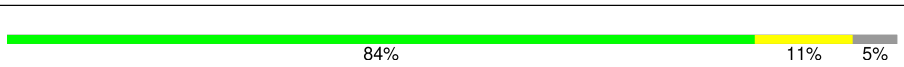
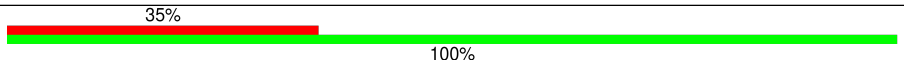
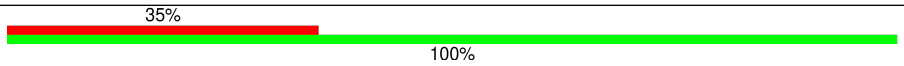
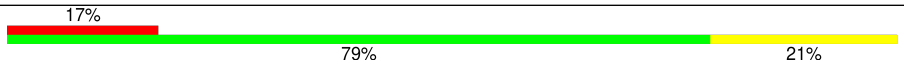
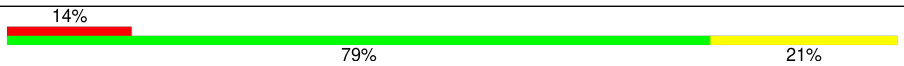
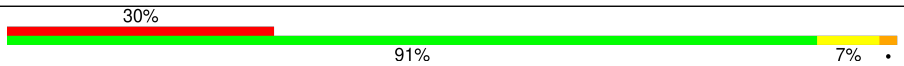
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	167	60% 74% 23%
1	a	167	22% 73% 20% 5%
2	B	224	83% 16%
2	b	224	88% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	255	
3	c	255	
4	D	57	
4	d	57	
5	E	81	
5	e	81	
6	F	23	
6	f	23	
7	G	29	
7	g	29	
8	H	44	
8	h	44	

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
10	HEC	B	301	X	-	-	-
10	HEC	C	302	X	-	-	-
10	HEC	b	305	X	-	-	-
10	HEC	c	302	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14444 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 Menaquinol:cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	163	Total	C	N	O	S	0	0
			1290	825	216	239	10		
1	a	158	Total	C	N	O	S	0	0
			1255	804	208	234	9		

- Molecule 2 is a protein called Menaquinol:cytochrome c reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1804	1207	292	293	12		
2	b	224	Total	C	N	O	S	0	0
			1804	1207	292	293	12		

- Molecule 3 is a protein called Menaquinol:cytochrome c reductase cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			1986	1293	325	357	11		
3	c	255	Total	C	N	O	S	0	0
			1986	1293	325	357	11		

- Molecule 4 is a protein called YqgW.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	56	Total	C	N	O	S	0	0
			433	297	68	66	2		
4	d	56	Total	C	N	O	S	0	0
			433	297	68	66	2		

- Molecule 5 is a protein called YqgY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	77	Total	C	N	O	S	0	0
			645	447	91	101	6		
5	e	77	Total	C	N	O	S	0	0
			645	447	91	101	6		

- Molecule 6 is a protein called QcrF.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	23	Total	C	N	O	0	0
			114	69	23	22		
6	f	23	Total	C	N	O	0	0
			114	69	23	22		

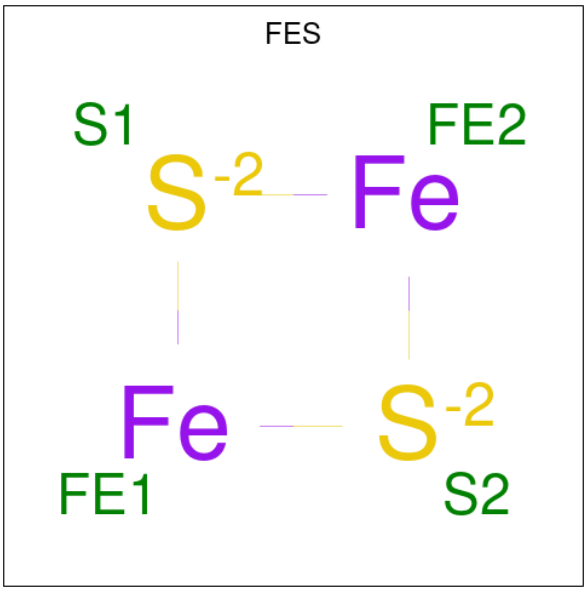
- Molecule 7 is a protein called QcrG.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	29	Total	C	N	O	S	0	0
			221	147	32	39	3		
7	g	29	Total	C	N	O	S	0	0
			221	147	32	39	3		

- Molecule 8 is a protein called YqzM.

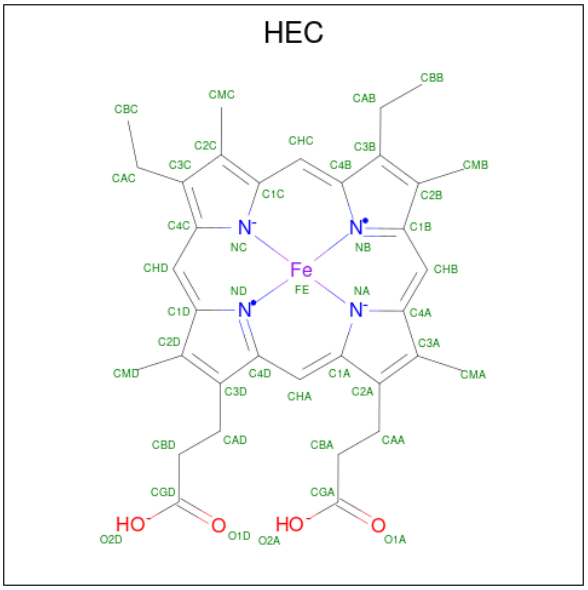
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	44	Total	C	N	O	S	0	0
			342	223	55	62	2		
8	h	44	Total	C	N	O	S	0	0
			342	223	55	62	2		

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	Fe	S	0
			4	2	2	
9	a	1	Total	Fe	S	0
			4	2	2	

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



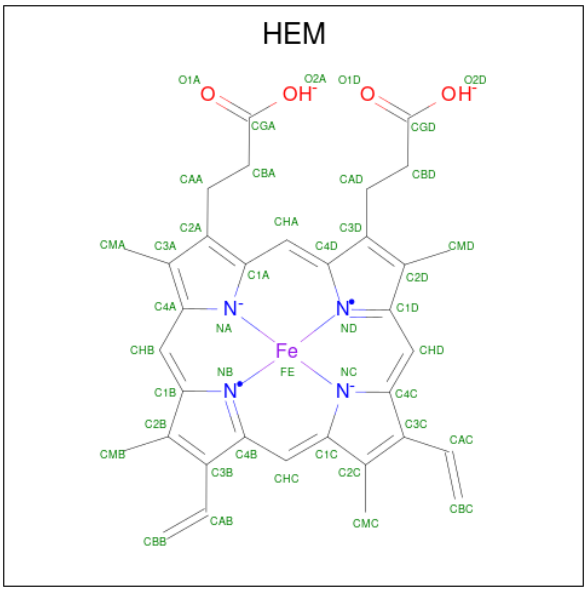
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

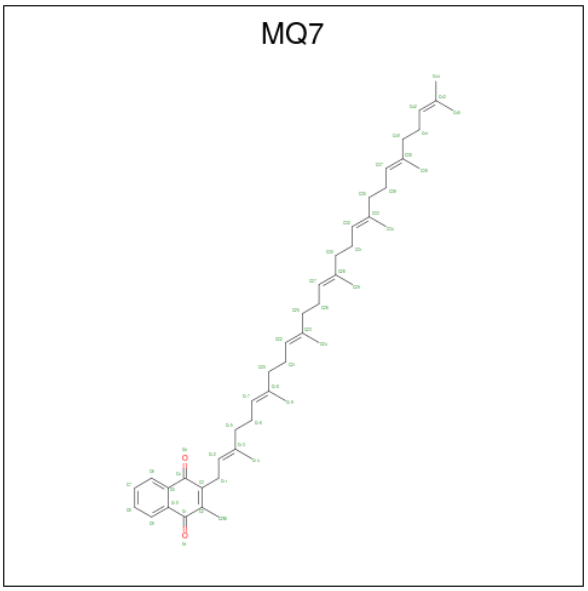
Mol	Chain	Residues	Atoms					AltConf
10	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



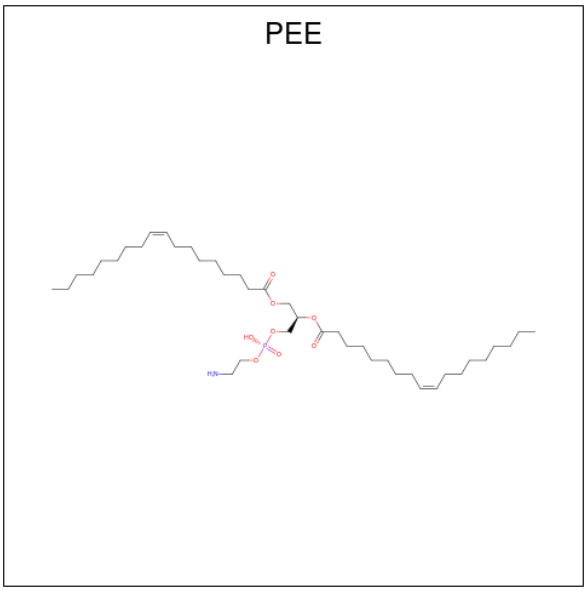
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



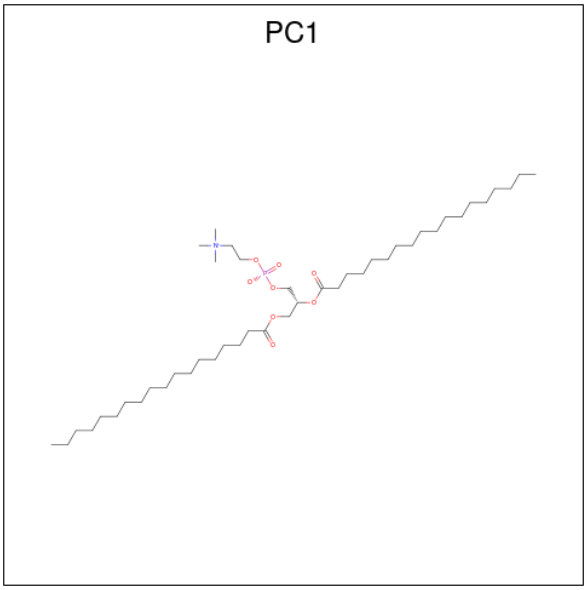
Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C O 48 46 2	0
12	C	1	Total C O 48 46 2	0
12	b	1	Total C O 48 46 2	0
12	c	1	Total C O 48 46 2	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



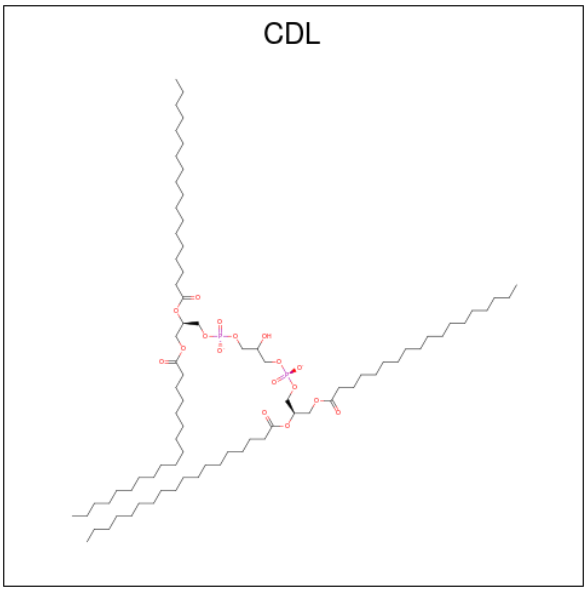
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
13	c	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	e	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	E	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	b	1	Total	C	O	P	0
			98	79	17	2	

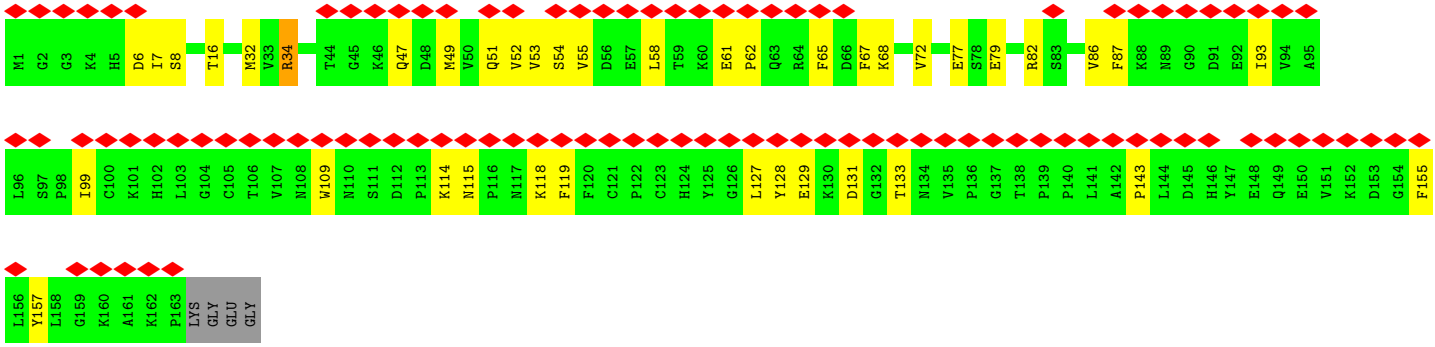
3 Residue-property plots (i)

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: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain A:

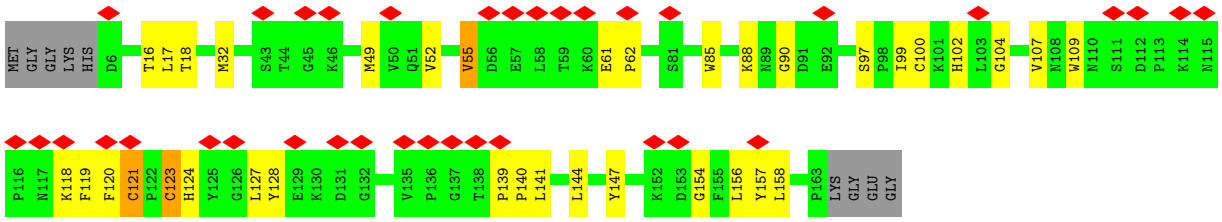




• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

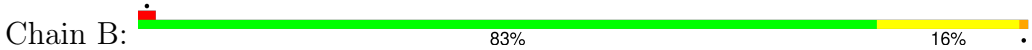
Chain a:

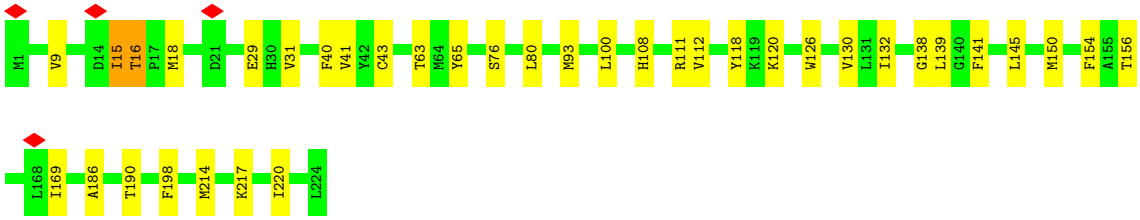




• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain B:

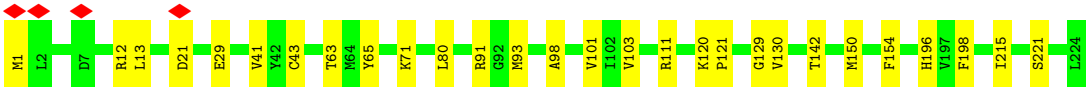




• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain b:





• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain C:

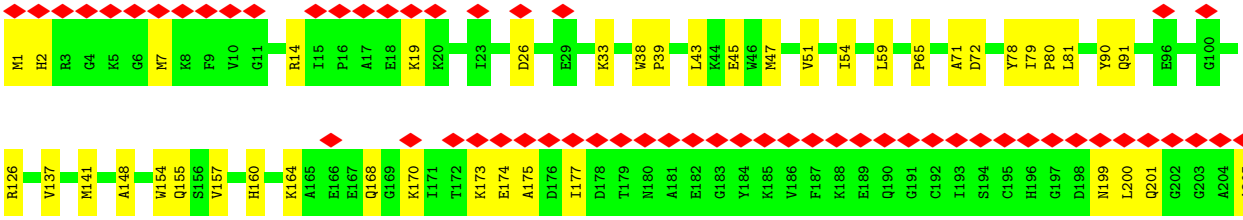




• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain c:

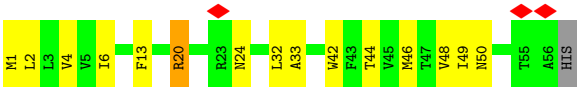




• Molecule 4: YqgW

Chain D:

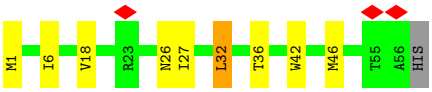




• Molecule 4: YqgW

Chain d:





• Molecule 5: YqgY

Chain E:

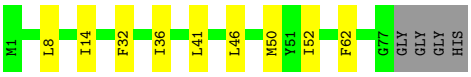




• Molecule 5: YqgY

Chain e:

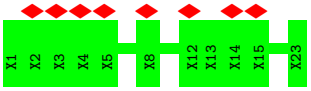




• Molecule 6: QcrF

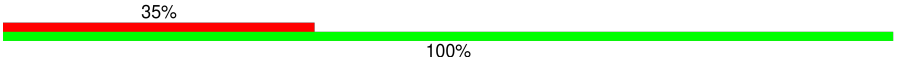
Chain F:

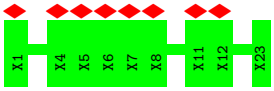




• Molecule 6: QcrF

Chain f:





• Molecule 7: QcrG

Chain G:

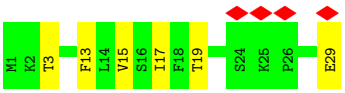




• Molecule 7: QcrG

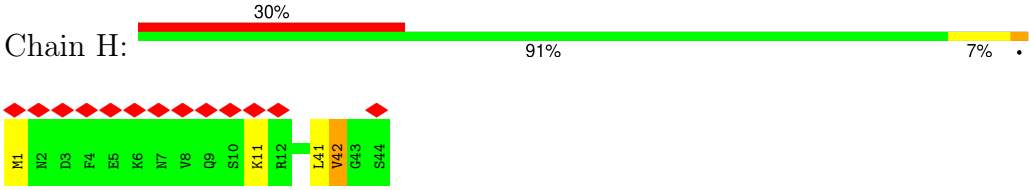
Chain g:





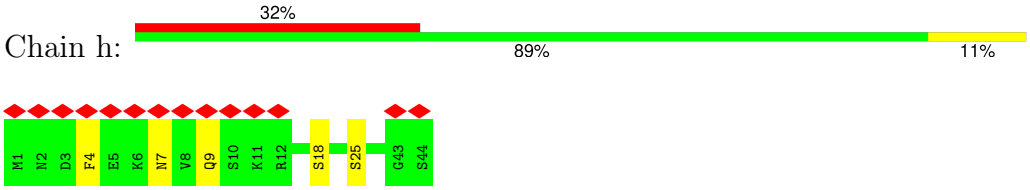
• Molecule 8: YqzM

Chain H:



• Molecule 8: YqzM

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39080	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.579	Depositor
Minimum map value	-1.190	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	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: PC1, FES, HEC, MQ7, CDL, PEE, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.15	0/1326	0.41	0/1796
1	a	0.14	0/1290	0.34	0/1750
2	B	0.31	0/1863	0.53	0/2533
2	b	0.14	0/1863	0.31	0/2533
3	C	0.31	0/2040	0.47	0/2759
3	c	0.11	0/2040	0.32	0/2759
4	D	0.37	0/444	0.69	0/605
4	d	0.16	0/444	0.45	0/605
5	E	0.12	0/667	0.27	0/900
5	e	0.13	0/667	0.26	0/900
7	G	0.12	0/224	0.32	0/299
7	g	0.17	0/224	0.33	0/299
8	H	0.13	0/349	0.36	0/468
8	h	0.11	0/349	0.22	0/468
All	All	0.21	0/13790	0.40	0/18674

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	20	ARG	Sidechain

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	1290	0	1256	32	0
1	a	1255	0	1217	25	0
2	B	1804	0	1813	44	0
2	b	1804	0	1813	22	0
3	C	1986	0	1999	54	0
3	c	1986	0	1997	42	0
4	D	433	0	463	11	0
4	d	433	0	463	7	0
5	E	645	0	642	9	0
5	e	645	0	642	8	0
6	F	114	0	25	0	0
6	f	114	0	25	0	0
7	G	221	0	241	3	0
7	g	221	0	241	6	0
8	H	342	0	334	4	0
8	h	342	0	334	3	0
9	A	4	0	0	0	0
9	a	4	0	0	1	0
10	B	43	0	31	3	0
10	C	43	0	32	1	0
10	b	43	0	32	2	0
10	c	43	0	30	3	0
11	B	86	0	60	2	0
11	b	86	0	60	2	0
12	B	48	0	64	3	0
12	C	48	0	64	2	0
12	b	48	0	64	2	0
12	c	48	0	64	4	0
13	C	46	0	65	3	0
13	c	51	0	76	4	0
13	e	34	0	42	2	0
14	E	36	0	46	0	0
15	b	98	0	149	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14444	0	14384	231	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 8.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HG11	3:C:119:LEU:CD1	1.22	1.57
2:B:130:VAL:CG1	3:C:119:LEU:HD11	1.45	1.44
2:B:130:VAL:CG1	3:C:119:LEU:CD1	1.95	1.44
2:B:130:VAL:HG11	3:C:119:LEU:HD12	1.19	1.10
2:B:130:VAL:CB	3:C:119:LEU:HD11	1.86	1.04
2:B:130:VAL:HG11	3:C:119:LEU:HD13	1.40	1.02
3:c:164:LYS:O	3:c:168:GLN:HB2	1.62	0.97
2:B:130:VAL:CB	3:C:119:LEU:CD1	2.46	0.90
2:B:130:VAL:HG12	3:C:119:LEU:HD11	1.54	0.86
1:A:16:THR:HG21	5:E:52:ILE:HD12	1.55	0.85
2:B:18:MET:HE3	2:B:18:MET:H	1.41	0.84
1:a:52:VAL:HG11	1:a:158:LEU:HD23	1.58	0.84
2:B:130:VAL:HB	3:C:119:LEU:HD11	1.61	0.82
4:D:46:MET:HA	4:D:49:ILE:HG22	1.68	0.76
1:a:119:PHE:HB2	1:a:128:TYR:HB2	1.69	0.75
2:B:130:VAL:HG21	3:C:119:LEU:HD12	1.72	0.70
3:c:207:PRO:HG3	10:c:302:HEC:HBA2	1.76	0.67
2:B:214:MET:HG2	2:b:13:LEU:HD21	1.74	0.67
3:C:174:GLU:HA	3:C:201:GLN:HE21	1.61	0.64
4:d:42:TRP:CE2	4:d:46:MET:HE1	2.33	0.64
4:D:42:TRP:CE2	4:D:46:MET:HE1	2.33	0.64
1:A:129:GLU:HG2	1:A:131:ASP:H	1.63	0.63
13:c:303:PEE:H64	13:c:303:PEE:H24	1.79	0.63
2:B:9:VAL:HG12	2:B:15:ILE:HG21	1.79	0.63
3:c:79:ILE:H	3:c:168:GLN:HE21	1.44	0.63
1:a:99:ILE:HG23	1:a:104:GLY:HA2	1.81	0.63
1:a:16:THR:HG21	5:e:52:ILE:HD12	1.81	0.62
3:c:1:MET:HB3	3:c:14:ARG:HD3	1.81	0.62
1:a:62:PRO:HB3	1:a:85:TRP:HB3	1.82	0.62
2:b:65:TYR:HB2	2:b:80:LEU:HD12	1.84	0.60
2:B:130:VAL:HB	3:C:119:LEU:CD1	2.26	0.60
2:B:169:ILE:HD12	2:B:169:ILE:O	2.01	0.60
3:c:43:LEU:O	3:c:47:MET:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:CG1	3:C:119:LEU:HD12	1.95	0.58
2:B:130:VAL:CG2	3:C:119:LEU:HD12	2.33	0.58
2:B:154:PHE:HB3	3:C:80:PRO:HB3	1.84	0.58
2:B:31:VAL:HG21	10:B:301:HEC:HBB1	1.85	0.58
2:B:150:MET:HE1	3:C:69:ARG:CZ	2.33	0.58
3:c:59:LEU:HD22	13:e:101:PEE:H25	1.85	0.58
1:a:62:PRO:HD2	1:a:109:TRP:CE2	2.39	0.57
3:C:121:ALA:N	3:C:122:PRO:HD2	2.20	0.57
4:D:44:THR:O	4:D:48:VAL:HG12	2.04	0.56
10:B:301:HEC:HHC	3:C:41:PHE:HE2	1.70	0.56
7:g:13:PHE:O	7:g:17:ILE:HG22	2.05	0.55
12:B:304:MQ7:H412	12:C:301:MQ7:H452	1.88	0.55
2:B:15:ILE:O	2:B:15:ILE:HG13	2.06	0.55
2:b:103:VAL:HG21	13:e:101:PEE:H58	1.88	0.55
3:C:97:TYR:HE2	4:D:50:ASN:HD22	1.54	0.55
1:A:62:PRO:HD2	1:A:109:TRP:CE2	2.42	0.54
5:e:46:LEU:HD23	5:e:50:MET:HG2	1.89	0.54
2:B:100:LEU:HD12	3:C:52:PHE:HZ	1.73	0.54
1:a:107:VAL:HG12	1:a:121:CYS:HB2	1.89	0.54
1:a:118:LYS:HD3	1:a:127:LEU:HD11	1.89	0.54
3:c:220:LYS:HG2	3:c:242:LEU:HG	1.90	0.54
3:C:78:TYR:CD1	3:C:168:GLN:HG2	2.43	0.53
2:b:154:PHE:HB3	3:c:80:PRO:HB3	1.89	0.53
1:A:49:MET:SD	1:A:157:TYR:HB3	2.48	0.53
3:c:90:TYR:CD1	12:c:301:MQ7:H8	2.44	0.53
7:G:19:THR:HG22	7:G:22:TYR:H	1.73	0.53
4:d:32:LEU:O	4:d:36:THR:HG22	2.09	0.53
3:C:140:GLY:HA3	4:D:13:PHE:HE2	1.74	0.53
1:A:133:THR:HA	1:A:143:PRO:HB3	1.91	0.53
1:a:97:SER:HB3	1:a:147:TYR:HE1	1.74	0.53
3:C:174:GLU:HA	3:C:201:GLN:NE2	2.23	0.52
2:b:150:MET:HB3	3:c:78:TYR:CE1	2.43	0.52
3:C:25:LYS:HA	8:H:11:LYS:NZ	2.25	0.52
1:A:55:VAL:HG23	1:A:58:LEU:HD12	1.92	0.52
3:C:163:ALA:O	3:C:167:GLU:HG3	2.09	0.52
3:C:222:ILE:HG12	3:C:227:LYS:HD3	1.91	0.51
1:a:49:MET:SD	1:a:157:TYR:HB3	2.50	0.51
2:B:198:PHE:HE2	2:b:63:THR:HG21	1.75	0.51
8:H:11:LYS:HA	8:H:11:LYS:HE2	1.92	0.51
1:A:32:MET:HE2	2:B:93:MET:HE1	1.93	0.51
1:A:7:ILE:HG22	1:A:8:SER:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:ILE:HG12	5:E:62:PHE:CE2	2.46	0.51
3:C:125:ASP:HB3	13:C:303:PEE:H10	1.93	0.51
3:C:148:ALA:HB2	4:D:6:ILE:HG21	1.91	0.51
2:b:129:GLY:C	11:b:302:HEM:HBC2	2.36	0.51
1:a:61:GLU:HB3	1:a:109:TRP:CZ2	2.46	0.50
2:B:41:VAL:HG12	2:B:111:ARG:HG3	1.92	0.50
2:B:65:TYR:HB2	2:B:80:LEU:HD12	1.93	0.50
2:B:16:THR:H	2:B:18:MET:HE1	1.77	0.50
2:B:145:LEU:HD22	2:B:156:THR:HG21	1.94	0.50
3:c:177:ILE:HB	3:c:199:ASN:HB3	1.94	0.50
1:A:62:PRO:HA	1:A:86:VAL:O	2.11	0.50
2:B:18:MET:H	2:B:18:MET:CE	2.18	0.49
15:b:304:CDL:HB62	15:b:304:CDL:H742	1.94	0.49
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.77	0.49
2:B:108:HIS:O	2:B:112:VAL:HG23	2.12	0.49
3:C:91:GLN:NE2	3:C:155:GLN:HG2	2.28	0.49
2:b:150:MET:HG2	3:c:71:ALA:HA	1.94	0.49
3:c:1:MET:HG2	3:c:2:HIS:HD2	1.78	0.49
1:A:49:MET:HA	1:A:49:MET:HE2	1.95	0.48
3:C:136:PRO:HD2	4:D:20:ARG:HH22	1.77	0.48
1:a:16:THR:HG21	5:e:52:ILE:CD1	2.43	0.48
1:a:123:CYS:HB2	9:a:201:FES:S2	2.53	0.48
1:A:67:PHE:CE2	1:A:82:ARG:HB2	2.47	0.48
3:c:54:ILE:HG12	5:e:62:PHE:CE2	2.47	0.48
3:c:205:ALA:O	10:c:302:HEC:HHB	2.12	0.48
13:c:303:PEE:H49	13:c:303:PEE:H8	1.53	0.48
2:B:130:VAL:CB	3:C:119:LEU:HD12	2.29	0.48
1:a:128:TYR:CE2	1:a:144:LEU:HG	2.49	0.48
1:A:51:GLN:HG2	1:A:157:TYR:HE1	1.78	0.48
1:A:6:ASP:C	1:A:7:ILE:HD13	2.39	0.47
5:e:32:PHE:O	5:e:36:ILE:HG22	2.14	0.47
3:C:210:VAL:HA	3:C:252:THR:HG22	1.97	0.47
3:C:220:LYS:HG2	3:C:242:LEU:HG	1.95	0.47
3:C:25:LYS:HA	8:H:11:LYS:HZ3	1.78	0.47
2:B:40:PHE:O	2:B:43:CYS:HB3	2.15	0.47
2:b:41:VAL:C	2:b:43:CYS:H	2.22	0.47
11:B:303:HEM:HBC2	11:B:303:HEM:HHD	1.96	0.47
3:C:112:GLY:C	3:C:114:ALA:H	2.23	0.46
2:B:138:GLY:O	2:B:139:LEU:C	2.58	0.46
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.78	0.46
2:b:111:ARG:HA	7:g:17:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:HG2	1:A:157:TYR:CE1	2.52	0.45
1:A:68:LYS:HD2	1:A:79:GLU:OE1	2.15	0.45
3:C:110:MET:HB2	3:C:111:PRO:HD3	1.98	0.45
3:c:215:LYS:HB2	3:c:218:GLU:HG3	1.99	0.45
1:a:139:PRO:N	1:a:140:PRO:HD2	2.32	0.45
2:B:43:CYS:HB2	10:B:301:HEC:HBC2	1.51	0.45
8:H:41:LEU:O	8:H:42:VAL:HG22	2.17	0.45
1:a:18:THR:HG21	8:h:18:SER:O	2.16	0.45
12:b:303:MQ7:H262	12:b:303:MQ7:H241	1.73	0.45
1:A:54:SER:HA	1:A:155:PHE:HA	1.98	0.45
3:C:82:PRO:HG2	3:C:87:LEU:HD23	1.99	0.45
3:c:51:VAL:HG21	5:e:8:LEU:HD22	1.98	0.45
1:A:47:GLN:HE22	1:A:49:MET:HE2	1.81	0.45
1:A:49:MET:HG3	1:A:157:TYR:CD1	2.51	0.45
1:a:102:HIS:HE1	1:a:124:HIS:CG	2.34	0.45
12:b:303:MQ7:H312	12:b:303:MQ7:H291	1.84	0.45
10:b:305:HEC:HMC2	3:c:45:GLU:HA	1.99	0.45
3:c:148:ALA:HB2	4:d:6:ILE:HG21	1.99	0.44
4:d:1:MET:HA	4:d:1:MET:HE2	1.99	0.44
3:C:200:LEU:HB3	3:C:209:LEU:HB2	1.98	0.44
1:A:115:ASN:ND2	1:A:118:LYS:HB2	2.33	0.44
2:B:217:LYS:HE2	12:B:304:MQ7:O4	2.18	0.44
3:c:7:MET:HE3	3:c:7:MET:HB3	1.93	0.44
12:C:301:MQ7:H362	12:C:301:MQ7:H341	1.46	0.44
1:a:55:VAL:HB	1:a:154:GLY:C	2.43	0.44
2:B:63:THR:HG21	2:b:198:PHE:HE2	1.82	0.44
1:A:47:GLN:HE22	1:A:49:MET:CE	2.30	0.44
8:h:4:PHE:HA	8:h:7:ASN:HD21	1.82	0.44
3:c:26:ASP:HA	8:h:9:GLN:HG3	1.99	0.44
3:c:174:GLU:HA	3:c:201:GLN:NE2	2.33	0.44
12:c:301:MQ7:H311	12:c:301:MQ7:H291	1.78	0.44
3:C:131:ARG:HD2	3:C:133:TRP:CZ2	2.53	0.43
3:C:57:LEU:HD23	3:C:57:LEU:HA	1.88	0.43
1:a:120:PHE:CD1	1:a:120:PHE:C	2.96	0.43
3:c:173:LYS:HE3	3:c:175:ALA:H	1.83	0.43
3:c:91:GLN:NE2	3:c:155:GLN:HG2	2.34	0.43
3:c:126:ARG:HH21	4:d:26:ASN:ND2	2.16	0.43
2:b:21:ASP:OD1	2:b:21:ASP:C	2.62	0.43
3:C:116:GLY:C	3:C:118:LEU:H	2.26	0.43
1:a:32:MET:HE3	2:b:93:MET:HE1	2.01	0.43
2:b:111:ARG:HA	7:g:17:ILE:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:216:PRO:HA	3:c:219:ILE:HD12	2.00	0.43
7:g:15:VAL:O	7:g:19:THR:HG22	2.19	0.43
3:C:173:LYS:HA	3:C:173:LYS:HD2	1.84	0.43
3:C:195:CYS:SG	10:C:302:HEC:HHC	2.59	0.43
1:a:62:PRO:HD2	1:a:109:TRP:CZ2	2.54	0.43
2:b:142:THR:HG22	2:b:196:HIS:HB2	1.99	0.43
5:E:44:LEU:HD12	5:E:44:LEU:HA	1.81	0.43
2:b:29:GLU:HB2	3:c:33:LYS:HB2	2.00	0.43
1:A:61:GLU:HA	1:A:62:PRO:HD3	1.92	0.42
2:B:120:LYS:NZ	2:b:12:ARG:HH12	2.17	0.42
7:G:21:GLY:HA2	7:G:26:PRO:HA	2.00	0.42
2:B:220:ILE:HD12	2:B:220:ILE:HA	1.93	0.42
3:c:170:LYS:HA	3:c:170:LYS:HD2	1.82	0.42
1:A:52:VAL:HG12	1:A:53:VAL:HG13	2.00	0.42
13:C:303:PEE:H69	13:C:303:PEE:H63	1.92	0.42
2:b:91:ARG:NH1	3:c:65:PRO:HB2	2.35	0.42
2:b:130:VAL:N	11:b:302:HEM:HBC2	2.34	0.42
3:C:9:PHE:HD1	3:C:10:VAL:HG13	1.85	0.42
3:C:42:LEU:HD12	3:C:42:LEU:HA	1.89	0.42
1:A:72:VAL:HG23	1:A:77:GLU:HG3	2.02	0.42
2:B:118:TYR:HB3	2:B:126:TRP:CE3	2.54	0.42
3:c:137:VAL:HB	13:c:303:PEE:O1P	2.19	0.42
5:E:29:LEU:HD23	5:E:29:LEU:HA	1.84	0.42
3:c:230:MET:HE1	10:c:302:HEC:C4B	2.50	0.42
12:c:301:MQ7:H412	12:c:301:MQ7:H391	1.84	0.42
1:a:52:VAL:HG13	1:a:156:LEU:HB3	2.02	0.42
1:a:88:LYS:HG2	1:a:90:GLY:H	1.83	0.42
3:C:200:LEU:O	3:C:210:VAL:HG13	2.20	0.42
4:D:50:ASN:CG	4:D:50:ASN:O	2.63	0.42
5:E:18:MET:HE2	5:E:18:MET:HB2	1.87	0.42
2:b:98:ALA:O	2:b:101:VAL:HG12	2.20	0.42
2:B:217:LYS:NZ	12:B:304:MQ7:H201	2.35	0.42
3:C:51:VAL:HG21	5:E:8:LEU:HD22	2.02	0.42
3:C:182:GLU:HA	3:C:185:LYS:HD2	2.02	0.42
3:C:222:ILE:HG23	3:C:227:LYS:HB2	2.02	0.42
3:c:81:LEU:HD13	3:c:160:HIS:CE1	2.55	0.41
5:e:41:LEU:HD23	5:e:41:LEU:HA	1.86	0.41
3:C:170:LYS:O	3:C:171:ILE:HG13	2.20	0.41
7:g:29:GLU:N	7:g:29:GLU:OE1	2.53	0.41
1:A:114:LYS:HB3	1:A:114:LYS:HE2	1.87	0.41
2:B:186:ALA:O	2:B:190:THR:HG23	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:59:LEU:HD23	5:E:59:LEU:HA	1.89	0.41
3:c:154:TRP:HE1	7:g:3:THR:HG21	1.86	0.41
4:d:46:MET:HB2	4:d:46:MET:HE3	1.70	0.41
2:B:100:LEU:HD12	3:C:52:PHE:CZ	2.55	0.41
4:D:32:LEU:O	4:D:33:ALA:C	2.63	0.41
3:c:19:LYS:HD2	3:c:19:LYS:HA	1.83	0.41
3:c:200:LEU:HD23	3:c:209:LEU:HD13	2.02	0.41
2:B:132:ILE:HG21	11:B:303:HEM:HBA2	2.03	0.41
3:c:177:ILE:HD12	3:c:177:ILE:HA	1.98	0.41
5:e:14:ILE:HD13	5:e:14:ILE:HA	1.92	0.41
2:B:138:GLY:O	2:B:141:PHE:N	2.54	0.41
3:C:114:ALA:HB1	13:C:303:PEE:H62	2.02	0.41
3:c:38:TRP:HB3	3:c:39:PRO:HD3	2.02	0.41
13:c:303:PEE:H57	4:d:36:THR:HG21	2.01	0.41
1:A:53:VAL:HG11	1:A:65:PHE:CG	2.56	0.41
5:E:21:LEU:HD23	5:E:21:LEU:HA	1.79	0.41
2:b:150:MET:HE2	3:c:72:ASP:HB3	2.02	0.41
3:c:79:ILE:H	3:c:168:GLN:NE2	2.16	0.41
1:A:62:PRO:CA	1:A:87:PHE:HB3	2.52	0.40
5:E:50:MET:HE3	5:E:50:MET:HB3	1.91	0.40
1:A:119:PHE:HB2	1:A:128:TYR:HB2	2.03	0.40
3:C:120:LEU:HD13	3:C:120:LEU:HA	1.86	0.40
1:a:128:TYR:HE2	1:a:144:LEU:HG	1.86	0.40
2:b:120:LYS:HA	2:b:121:PRO:HA	1.92	0.40
1:A:86:VAL:HG12	1:A:93:ILE:HD11	2.02	0.40
4:D:1:MET:O	4:D:4:VAL:HG22	2.22	0.40
10:b:305:HEC:HMC2	3:c:45:GLU:O	2.21	0.40
3:c:90:TYR:HD1	12:c:301:MQ7:H8	1.84	0.40
3:c:244:GLU:HA	3:c:247:LYS:HG2	2.02	0.40
1:A:61:GLU:OE1	1:A:61:GLU:C	2.65	0.40
1:a:49:MET:HE2	1:a:49:MET:HA	2.02	0.40
1:A:34:ARG:HA	1:A:34:ARG:HD2	1.88	0.40
4:D:24:ASN:OD1	4:D:24:ASN:O	2.40	0.40
7:G:3:THR:O	7:G:7:MET:HG2	2.22	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	161/167 (96%)	147 (91%)	14 (9%)	0	100	100
1	a	156/167 (93%)	149 (96%)	7 (4%)	0	100	100
2	B	222/224 (99%)	213 (96%)	7 (3%)	2 (1%)	14	42
2	b	222/224 (99%)	215 (97%)	7 (3%)	0	100	100
3	C	253/255 (99%)	228 (90%)	25 (10%)	0	100	100
3	c	253/255 (99%)	237 (94%)	16 (6%)	0	100	100
4	D	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
4	d	54/57 (95%)	54 (100%)	0	0	100	100
5	E	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
5	e	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
7	G	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
7	g	27/29 (93%)	27 (100%)	0	0	100	100
8	H	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
8	h	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
All	All	1663/1714 (97%)	1572 (94%)	89 (5%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	THR
2	B	15	ILE

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	142/144 (99%)	140 (99%)	2 (1%)	59	70
1	a	139/144 (96%)	133 (96%)	6 (4%)	26	51
2	B	188/188 (100%)	186 (99%)	2 (1%)	65	74
2	b	188/188 (100%)	184 (98%)	4 (2%)	47	64
3	C	205/205 (100%)	200 (98%)	5 (2%)	43	62
3	c	205/205 (100%)	203 (99%)	2 (1%)	68	75
4	D	45/46 (98%)	44 (98%)	1 (2%)	45	63
4	d	45/46 (98%)	42 (93%)	3 (7%)	15	41
5	E	66/67 (98%)	66 (100%)	0	100	100
5	e	66/67 (98%)	66 (100%)	0	100	100
7	G	25/25 (100%)	25 (100%)	0	100	100
7	g	25/25 (100%)	25 (100%)	0	100	100
8	H	37/37 (100%)	35 (95%)	2 (5%)	20	47
8	h	37/37 (100%)	36 (97%)	1 (3%)	39	60
All	All	1413/1424 (99%)	1385 (98%)	28 (2%)	48	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	99	ILE
2	B	29	GLU
2	B	76	SER
3	C	60	THR
3	C	83	ASP
3	C	118	LEU
3	C	120	LEU
3	C	135	ARG
4	D	2	LEU
8	H	1	MET
8	H	42	VAL
1	a	17	LEU
1	a	55	VAL
1	a	100	CYS
1	a	121	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	123	CYS
1	a	141	LEU
2	b	1	MET
2	b	71	LYS
2	b	215	ILE
2	b	221	SER
3	c	141	MET
3	c	157	VAL
4	d	18	VAL
4	d	27	ILE
4	d	32	LEU
8	h	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	89	ASN
2	B	108	HIS
2	B	115	GLN
3	C	91	GLN
3	C	190	GLN
4	D	24	ASN
4	D	26	ASN
4	D	50	ASN
1	a	108	ASN
3	c	190	GLN
3	c	199	ASN
5	e	34	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	$\#\|Z\|>2$
11	HEM	B	302	2	50,50,50	1.57	9 (18%)	67,82,82	1.66	13 (19%)
10	HEC	B	301	2	50,50,50	3.01	29 (58%)	68,82,82	2.35	27 (39%)
13	PEE	e	101	-	33,33,50	0.34	0	36,38,55	0.45	0
12	MQ7	b	303	-	49,49,49	0.39	0	61,63,63	0.63	1 (1%)
10	HEC	b	305	2	50,50,50	2.87	26 (52%)	68,82,82	2.54	26 (38%)
13	PEE	C	303	-	45,45,50	0.32	0	48,50,55	0.38	0
11	HEM	b	302	2	50,50,50	1.57	9 (18%)	67,82,82	1.58	12 (17%)
12	MQ7	B	304	-	49,49,49	0.41	1 (2%)	61,63,63	0.51	1 (1%)
11	HEM	B	303	2	50,50,50	1.84	14 (28%)	67,82,82	1.24	6 (8%)
10	HEC	c	302	3	50,50,50	3.84	33 (66%)	68,82,82	9.14	32 (47%)
10	HEC	C	302	-	50,50,50	3.05	29 (58%)	68,82,82	2.27	28 (41%)
13	PEE	c	303	-	50,50,50	0.30	0	53,55,55	0.33	0
12	MQ7	c	301	-	49,49,49	0.38	0	61,63,63	0.52	1 (1%)
9	FES	A	201	1	0,4,4	-	-	-		
9	FES	a	201	1	0,4,4	-	-	-		
12	MQ7	C	301	-	49,49,49	0.37	0	61,63,63	0.53	1 (1%)
14	PC1	E	101	-	35,35,53	0.60	0	41,43,61	0.53	1 (2%)
15	CDL	b	304	-	97,97,99	0.26	0	103,109,111	0.45	1 (0%)
11	HEM	b	301	2	50,50,50	1.56	8 (16%)	67,82,82	1.65	12 (17%)

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
11	HEM	B	302	2	-	7/14/54/54	-
10	HEC	B	301	2	1/1/3/7	11/14/54/54	-
13	PEE	e	101	-	-	5/37/37/54	-
12	MQ7	b	303	-	-	12/41/61/61	0/2/2/2
10	HEC	b	305	2	1/1/3/7	9/14/54/54	-
13	PEE	C	303	-	-	17/49/49/54	-
11	HEM	b	302	2	-	4/14/54/54	-
12	MQ7	B	304	-	-	5/41/61/61	0/2/2/2
11	HEM	B	303	2	-	7/14/54/54	-
10	HEC	c	302	3	1/1/3/7	7/14/54/54	-
10	HEC	C	302	-	1/1/3/7	7/14/54/54	-
13	PEE	c	303	-	-	12/54/54/54	-
12	MQ7	c	301	-	-	11/41/61/61	0/2/2/2
9	FES	A	201	1	-	-	0/1/1/1
12	MQ7	C	301	-	-	16/41/61/61	0/2/2/2
9	FES	a	201	1	-	-	0/1/1/1
14	PC1	E	101	-	-	13/39/39/57	-
15	CDL	b	304	-	-	8/108/108/110	-
11	HEM	b	301	2	-	9/14/54/54	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	302	HEC	CAC-C3C	9.97	1.76	1.51
10	c	302	HEC	CMC-C2C	9.55	1.70	1.50
10	c	302	HEC	C3B-C2B	5.68	1.49	1.36
10	C	302	HEC	C3B-C2B	5.60	1.48	1.36
10	c	302	HEC	C3D-C2D	5.55	1.48	1.36
10	B	301	HEC	C2A-C3A	5.51	1.48	1.36
10	c	302	HEC	C2A-C3A	5.48	1.48	1.36
10	c	302	HEC	CHB-C4A	5.45	1.49	1.38
10	C	302	HEC	C2A-C3A	5.43	1.48	1.36
10	B	301	HEC	C3B-C2B	5.42	1.48	1.36
10	c	302	HEC	CHD-C1D	5.42	1.49	1.38
10	c	302	HEC	CHA-C1A	5.41	1.49	1.38
10	C	302	HEC	C3D-C2D	5.40	1.48	1.36
10	C	302	HEC	CHB-C4A	5.37	1.48	1.38
10	c	302	HEC	CHC-C4B	5.31	1.49	1.38
10	C	302	HEC	CHA-C1A	5.30	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	302	HEM	FE-NB	5.29	2.11	1.94
11	b	301	HEM	FE-NB	5.28	2.11	1.94
11	b	302	HEM	FE-NB	5.25	2.11	1.94
10	B	301	HEC	C3D-C2D	5.22	1.48	1.36
10	B	301	HEC	CHB-C4A	5.16	1.48	1.38
10	b	305	HEC	FE-NB	5.15	2.10	1.94
10	C	302	HEC	CHD-C1D	5.15	1.48	1.38
10	C	302	HEC	CHC-C4B	5.13	1.48	1.38
10	B	301	HEC	CHA-C1A	5.13	1.48	1.38
10	b	305	HEC	FE-ND	5.08	2.10	1.94
10	b	305	HEC	C3B-C2B	5.07	1.47	1.36
10	c	302	HEC	C4C-C3C	5.03	1.54	1.44
10	B	301	HEC	CHC-C4B	5.02	1.48	1.38
10	b	305	HEC	C2A-C3A	4.99	1.47	1.36
10	b	305	HEC	C3D-C2D	4.98	1.47	1.36
10	c	302	HEC	C3C-C2C	-4.90	1.26	1.38
10	c	302	HEC	CHD-C4C	4.86	1.50	1.39
10	B	301	HEC	FE-ND	4.82	2.09	1.94
10	B	301	HEC	CHD-C1D	4.81	1.48	1.38
10	B	301	HEC	FE-NB	4.80	2.09	1.94
10	b	305	HEC	CHB-C4A	4.79	1.47	1.38
10	b	305	HEC	CHA-C1A	4.79	1.47	1.38
10	b	305	HEC	CHD-C1D	4.72	1.47	1.38
10	b	305	HEC	FE-NA	4.69	2.10	1.95
10	C	302	HEC	FE-NB	4.67	2.09	1.94
10	C	302	HEC	FE-ND	4.67	2.09	1.94
10	b	305	HEC	FE-NC	4.66	2.10	1.95
10	c	302	HEC	FE-NB	4.51	2.08	1.94
10	c	302	HEC	C1C-NC	-4.49	1.31	1.39
10	c	302	HEC	FE-ND	4.47	2.08	1.94
10	B	301	HEC	FE-NA	4.46	2.09	1.95
10	c	302	HEC	CHC-C1C	4.45	1.49	1.39
10	B	301	HEC	FE-NC	4.45	2.09	1.95
11	B	303	HEM	C1D-C2D	-4.37	1.35	1.44
10	c	302	HEC	CHA-C4D	4.37	1.49	1.39
10	C	302	HEC	FE-NC	4.31	2.09	1.95
10	c	302	HEC	CHB-C1B	4.31	1.49	1.39
10	C	302	HEC	CHA-C4D	4.27	1.48	1.39
10	C	302	HEC	FE-NA	4.26	2.09	1.95
11	b	302	HEM	FE-NC	4.24	2.09	1.95
10	C	302	HEC	CHB-C1B	4.20	1.48	1.39
10	c	302	HEC	FE-NA	4.20	2.09	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	301	HEM	FE-NC	4.19	2.09	1.95
10	C	302	HEC	CHD-C4C	4.17	1.48	1.39
10	b	305	HEC	CHC-C4B	4.15	1.46	1.38
11	B	302	HEM	FE-NC	4.15	2.08	1.95
10	c	302	HEC	FE-NC	4.11	2.08	1.95
10	C	302	HEC	CHC-C1C	4.11	1.48	1.39
11	B	303	HEM	C4D-C3D	-4.10	1.38	1.45
10	B	301	HEC	CHA-C4D	4.07	1.48	1.39
10	B	301	HEC	CHB-C1B	4.04	1.48	1.39
10	B	301	HEC	CHD-C4C	4.03	1.48	1.39
10	B	301	HEC	CHC-C1C	4.02	1.48	1.39
11	B	303	HEM	C3C-C4C	-3.99	1.39	1.46
10	b	305	HEC	CHD-C4C	3.95	1.48	1.39
10	c	302	HEC	C4C-NC	-3.92	1.32	1.39
10	C	302	HEC	C3C-C2C	3.81	1.48	1.38
10	b	305	HEC	CHA-C4D	3.79	1.47	1.39
10	b	305	HEC	CHB-C1B	3.75	1.47	1.39
10	B	301	HEC	C3C-C2C	3.75	1.48	1.38
11	B	303	HEM	C1A-C2A	-3.74	1.37	1.44
11	B	303	HEM	C1C-C2C	-3.62	1.38	1.45
10	b	305	HEC	CHC-C1C	3.49	1.47	1.39
10	c	302	HEC	C1C-C2C	3.44	1.51	1.43
11	b	301	HEM	C1B-NB	-3.31	1.34	1.40
11	b	302	HEM	C1B-NB	-3.30	1.34	1.40
11	B	303	HEM	C1B-C2B	-3.26	1.37	1.44
10	b	305	HEC	C3C-C2C	3.25	1.47	1.38
11	B	302	HEM	C1B-NB	-3.23	1.34	1.40
11	B	302	HEM	C4D-ND	-3.19	1.34	1.40
11	b	302	HEM	C4D-ND	-3.19	1.34	1.40
10	c	302	HEC	C1D-ND	-3.18	1.34	1.40
11	b	301	HEM	C4D-ND	-3.17	1.34	1.40
10	C	302	HEC	C4B-NB	-3.14	1.34	1.40
11	B	303	HEM	C4A-C3A	-3.12	1.35	1.43
10	b	305	HEC	C4B-NB	-3.11	1.34	1.40
10	c	302	HEC	C4B-NB	-3.10	1.34	1.40
10	B	301	HEC	C4B-NB	-3.06	1.34	1.40
11	B	303	HEM	C3B-C4B	-3.05	1.39	1.44
10	B	301	HEC	C1D-ND	-3.04	1.35	1.40
10	C	302	HEC	C1D-ND	-3.02	1.35	1.40
11	B	303	HEM	C1B-NB	-2.89	1.35	1.40
10	b	305	HEC	C1D-ND	-2.86	1.35	1.40
10	C	302	HEC	C1C-C2C	2.73	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	HEC	C1C-C2C	2.71	1.49	1.43
10	b	305	HEC	C4C-C3C	2.64	1.49	1.44
11	B	303	HEM	C4D-ND	-2.62	1.35	1.40
10	c	302	HEC	C4A-NA	-2.56	1.34	1.39
10	c	302	HEC	C4D-C3D	2.55	1.49	1.45
10	C	302	HEC	C4D-C3D	2.54	1.49	1.45
10	b	305	HEC	C1B-C2B	2.52	1.49	1.44
10	C	302	HEC	C4C-NC	-2.51	1.34	1.39
10	c	302	HEC	C1B-C2B	2.50	1.49	1.44
10	B	301	HEC	C1A-NA	-2.50	1.34	1.39
10	C	302	HEC	C4A-NA	-2.49	1.34	1.39
10	C	302	HEC	C1B-C2B	2.48	1.49	1.44
11	b	302	HEM	FE-ND	-2.46	1.87	1.94
10	c	302	HEC	C1A-NA	-2.46	1.35	1.39
10	B	301	HEC	C4D-C3D	2.45	1.49	1.45
10	C	302	HEC	C1A-NA	-2.45	1.35	1.39
11	B	302	HEM	FE-ND	-2.44	1.87	1.94
10	B	301	HEC	C4A-NA	-2.43	1.35	1.39
10	B	301	HEC	C4C-NC	-2.41	1.35	1.39
11	b	301	HEM	FE-ND	-2.40	1.87	1.94
11	B	303	HEM	C1A-NA	-2.38	1.35	1.39
11	b	302	HEM	C1C-C2C	-2.36	1.40	1.45
10	B	301	HEC	C1B-C2B	2.36	1.49	1.44
11	b	301	HEM	C1C-C2C	-2.36	1.40	1.45
10	c	302	HEC	C1D-C2D	2.34	1.49	1.44
10	c	302	HEC	C1A-C2A	2.33	1.49	1.45
11	B	302	HEM	C1C-C2C	-2.33	1.40	1.45
10	C	302	HEC	C1D-C2D	2.29	1.49	1.44
10	C	302	HEC	C1A-C2A	2.28	1.49	1.45
10	b	305	HEC	C4D-C3D	2.27	1.48	1.45
10	c	302	HEC	C4B-C3B	2.25	1.48	1.45
10	b	305	HEC	C4A-NA	-2.22	1.35	1.39
10	b	305	HEC	C1D-C2D	2.22	1.49	1.44
10	C	302	HEC	C1C-NC	-2.21	1.35	1.39
10	b	305	HEC	C1A-NA	-2.20	1.35	1.39
10	B	301	HEC	C1C-NC	-2.20	1.35	1.39
11	b	302	HEM	C1D-ND	-2.20	1.34	1.38
10	B	301	HEC	C4B-C3B	2.20	1.48	1.45
11	B	303	HEM	FE-NC	2.19	2.02	1.95
10	b	305	HEC	C1C-NC	-2.19	1.35	1.39
10	C	302	HEC	C4B-C3B	2.19	1.48	1.45
11	B	303	HEM	FE-NB	2.17	2.01	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	HEC	C1D-C2D	2.17	1.48	1.44
11	B	303	HEM	C1C-NC	-2.16	1.35	1.39
10	B	301	HEC	C1A-C2A	2.16	1.49	1.45
10	b	305	HEC	C1A-C2A	2.15	1.49	1.45
10	B	301	HEC	C4C-C3C	2.12	1.48	1.44
11	B	302	HEM	C1D-ND	-2.08	1.34	1.38
11	b	301	HEM	C1D-ND	-2.07	1.34	1.38
10	C	302	HEC	C4C-C3C	2.07	1.48	1.44
11	b	301	HEM	C3C-C4C	-2.06	1.42	1.46
11	B	302	HEM	C3C-C4C	-2.06	1.42	1.46
12	B	304	MQ7	C3-C2	2.05	1.38	1.35
10	c	302	HEC	C4A-C3A	2.05	1.49	1.45
11	b	302	HEM	C4B-NB	-2.03	1.34	1.38
11	B	302	HEM	C3B-C4B	2.02	1.48	1.44
10	c	302	HEC	C4D-ND	-2.02	1.34	1.38
11	b	302	HEM	C3C-C4C	-2.02	1.42	1.46

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	c	302	HEC	CAC-C3C-C2C	-52.62	43.63	126.89
10	c	302	HEC	CMC-C2C-C3C	-46.71	26.56	125.62
10	c	302	HEC	CAC-C3C-C4C	13.67	143.72	124.91
10	c	302	HEC	CBC-CAC-C3C	12.34	145.86	112.42
10	c	302	HEC	CMC-C2C-C1C	6.50	135.32	125.42
10	c	302	HEC	C3C-C4C-NC	6.20	117.03	110.15
10	b	305	HEC	C1B-C2B-C3B	-5.95	100.72	106.98
10	B	301	HEC	C1B-C2B-C3B	-5.77	100.91	106.98
10	C	302	HEC	C1B-C2B-C3B	-5.63	101.06	106.98
10	c	302	HEC	C1B-C2B-C3B	-5.54	101.15	106.98
10	b	305	HEC	C2B-C1B-NB	5.45	116.20	109.90
10	b	305	HEC	C2A-C1A-NA	5.34	115.48	110.32
10	b	305	HEC	C3D-C4D-ND	5.24	115.42	110.35
11	b	301	HEM	CHC-C4B-NB	5.22	130.04	124.42
10	C	302	HEC	C1C-C2C-C3C	-5.07	101.01	106.82
10	B	301	HEC	C1C-C2C-C3C	-4.93	101.17	106.82
10	B	301	HEC	C2A-C1A-NA	4.90	115.05	110.32
10	B	301	HEC	C2B-C1B-NB	4.86	115.52	109.90
11	b	302	HEM	CHC-C4B-NB	4.82	129.62	124.42
11	B	302	HEM	CHC-C4B-NB	4.80	129.59	124.42
10	b	305	HEC	CBC-CAC-C3C	4.75	125.30	112.42
10	b	305	HEC	C1C-C2C-C3C	-4.70	101.44	106.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	305	HEC	C2D-C1D-ND	4.66	115.20	109.84
10	B	301	HEC	CBC-CAC-C3C	4.58	124.83	112.42
10	c	302	HEC	CBB-CAB-C3B	4.55	124.77	112.42
10	b	305	HEC	CAC-C3C-C4C	4.54	131.16	124.91
10	C	302	HEC	CBB-CAB-C3B	4.54	124.73	112.42
10	C	302	HEC	CBC-CAC-C3C	4.52	124.68	112.42
11	B	302	HEM	CHD-C1D-ND	4.47	129.23	124.42
10	B	301	HEC	CBB-CAB-C3B	4.44	124.46	112.42
11	b	301	HEM	CHD-C1D-ND	4.43	129.19	124.42
10	C	302	HEC	C2B-C1B-NB	4.38	114.97	109.90
10	c	302	HEC	C4C-C3C-C2C	-4.38	100.09	106.87
10	b	305	HEC	CBB-CAB-C3B	4.37	124.28	112.42
10	B	301	HEC	C2D-C1D-ND	4.37	114.86	109.84
10	B	301	HEC	C3D-C4D-ND	4.33	114.53	110.35
10	b	305	HEC	C3B-C4B-NB	4.22	114.80	110.17
10	c	302	HEC	C2B-C1B-NB	4.11	114.65	109.90
10	B	301	HEC	C1D-C2D-C3D	-4.07	102.69	106.98
10	C	302	HEC	C2A-C1A-NA	4.00	114.18	110.32
10	b	305	HEC	C2C-C1C-NC	3.98	116.53	110.14
11	b	302	HEM	CHD-C1D-ND	3.98	128.70	124.42
10	b	305	HEC	C1D-C2D-C3D	-3.93	102.85	106.98
10	C	302	HEC	C3D-C4D-ND	3.89	114.11	110.35
10	c	302	HEC	C2A-C1A-NA	3.78	113.97	110.32
10	C	302	HEC	C1D-C2D-C3D	-3.78	103.00	106.98
11	b	301	HEM	CHA-C4D-ND	3.72	128.97	124.37
10	C	302	HEC	C2D-C1D-ND	3.72	114.12	109.84
11	B	302	HEM	CHA-C4D-ND	3.69	128.93	124.37
10	c	302	HEC	C1D-C2D-C3D	-3.69	103.10	106.98
11	B	302	HEM	CHB-C1B-NB	3.59	128.80	124.37
11	b	302	HEM	CHA-C4D-ND	3.57	128.79	124.37
10	c	302	HEC	CHD-C4C-NC	-3.54	117.44	123.86
10	c	302	HEC	CHB-C1B-NB	-3.52	120.64	124.42
11	B	303	HEM	CHD-C4C-NC	-3.51	120.63	124.45
10	B	301	HEC	C1A-C2A-C3A	-3.51	102.49	107.11
11	b	301	HEM	CHB-C1B-NB	3.45	128.64	124.37
10	c	302	HEC	C4C-NC-C1C	-3.45	100.20	105.82
10	c	302	HEC	C3D-C4D-ND	3.44	113.68	110.35
10	b	305	HEC	C1A-C2A-C3A	-3.39	102.64	107.11
10	c	302	HEC	C2D-C1D-ND	3.33	113.67	109.84
10	C	302	HEC	CHB-C1B-NB	-3.31	120.86	124.42
11	B	302	HEM	C1B-NB-C4B	3.28	109.09	105.21
10	B	301	HEC	C2C-C1C-NC	3.27	115.38	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	302	HEM	CHB-C1B-NB	3.26	128.40	124.37
11	b	302	HEM	C1B-NB-C4B	3.25	109.05	105.21
10	C	302	HEC	C1A-C2A-C3A	-3.24	102.85	107.11
10	b	305	HEC	C3A-C4A-NA	3.17	115.50	109.64
10	c	302	HEC	CHB-C4A-NA	-3.17	121.00	124.45
10	c	302	HEC	C1A-C2A-C3A	-3.15	102.95	107.11
12	b	303	MQ7	C11-C3-C2	-3.11	119.55	124.89
11	b	301	HEM	C1B-NB-C4B	3.09	108.87	105.21
10	C	302	HEC	CHA-C4D-ND	-3.09	121.10	124.42
10	C	302	HEC	C2C-C1C-NC	3.08	115.07	110.14
10	C	302	HEC	CHA-C1A-NA	-3.06	121.12	124.45
10	B	301	HEC	C3C-C4C-NC	3.01	113.49	110.15
10	C	302	HEC	CHB-C4A-NA	-2.97	121.22	124.45
10	b	305	HEC	C4D-C3D-C2D	-2.95	102.60	106.89
10	C	302	HEC	CMC-C2C-C3C	2.94	131.85	125.62
10	c	302	HEC	CHA-C4D-ND	-2.89	121.31	124.42
10	c	302	HEC	CHA-C1A-NA	-2.87	121.33	124.45
10	b	305	HEC	C4A-C3A-C2A	-2.86	102.72	106.97
10	B	301	HEC	CMC-C2C-C3C	2.83	131.62	125.62
10	b	305	HEC	CMC-C2C-C3C	2.82	131.60	125.62
10	b	305	HEC	CHC-C1C-C2C	-2.79	119.31	127.43
10	B	301	HEC	C4A-C3A-C2A	-2.79	102.83	106.97
10	B	301	HEC	C3B-C4B-NB	2.76	113.20	110.17
10	C	302	HEC	C4D-C3D-C2D	-2.74	102.90	106.89
11	B	302	HEM	CHD-C1D-C2D	-2.74	120.71	125.03
11	B	302	HEM	C3B-C4B-NB	-2.73	107.51	109.47
10	B	301	HEC	C3A-C4A-NA	2.73	114.69	109.64
10	B	301	HEC	C4D-C3D-C2D	-2.73	102.92	106.89
11	B	302	HEM	CHD-C4C-NC	2.72	127.41	124.45
11	b	301	HEM	CHD-C1D-C2D	-2.71	120.75	125.03
10	c	302	HEC	C4D-C3D-C2D	-2.70	102.96	106.89
10	c	302	HEC	C4A-C3A-C2A	-2.70	102.97	106.97
10	c	302	HEC	CHD-C1D-ND	-2.67	121.06	124.37
10	B	301	HEC	CHB-C4A-NA	-2.65	121.57	124.45
11	B	303	HEM	CHD-C4C-C3C	2.65	129.68	125.21
10	B	301	HEC	CHB-C1B-NB	-2.65	121.57	124.42
10	C	302	HEC	C4A-C3A-C2A	-2.65	103.05	106.97
10	b	305	HEC	C3C-C4C-NC	2.64	113.08	110.15
11	b	301	HEM	CHD-C4C-NC	2.64	127.33	124.45
12	C	301	MQ7	C11-C3-C2	-2.62	120.40	124.89
11	b	302	HEM	C3B-C4B-NB	-2.58	107.61	109.47
10	B	301	HEC	CHA-C4D-ND	-2.51	121.72	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	302	HEC	C3C-C4C-NC	2.51	112.94	110.15
10	C	302	HEC	C3B-C4B-NB	2.50	112.91	110.17
11	b	302	HEM	C4C-CHD-C1D	-2.49	120.73	126.02
10	C	302	HEC	CAC-C3C-C2C	2.44	130.74	126.89
10	B	301	HEC	CAC-C3C-C2C	2.43	130.74	126.89
11	B	303	HEM	CAD-C3D-C4D	2.42	128.91	124.70
10	C	302	HEC	CHD-C1D-ND	-2.41	121.38	124.37
12	c	301	MQ7	C11-C3-C2	-2.41	120.77	124.89
11	b	301	HEM	C3B-C4B-NB	-2.38	107.76	109.47
10	C	302	HEC	CAD-C3D-C4D	2.37	128.83	124.70
10	C	302	HEC	C3A-C4A-NA	2.37	114.02	109.64
12	B	304	MQ7	C11-C3-C2	-2.37	120.83	124.89
10	c	302	HEC	C2C-C1C-NC	2.35	113.92	110.14
11	b	301	HEM	CHA-C4D-C3D	-2.35	120.89	125.23
10	B	301	HEC	CAA-CBA-CGA	-2.35	107.43	113.67
10	c	302	HEC	C3A-C4A-NA	2.35	113.97	109.64
10	B	301	HEC	CHA-C1A-NA	-2.33	121.91	124.45
14	E	101	PC1	O12-P-O14	2.33	123.29	112.44
11	b	302	HEM	CHD-C1D-C2D	-2.33	121.35	125.03
10	B	301	HEC	CAD-C3D-C4D	2.33	128.75	124.70
10	c	302	HEC	CAD-C3D-C4D	2.33	128.75	124.70
10	b	305	HEC	CHB-C1B-C2B	-2.32	121.36	125.03
15	b	304	CDL	OB6-CB5-C51	2.31	116.49	111.48
10	b	305	HEC	CMD-C2D-C1D	2.30	128.63	125.03
11	B	302	HEM	CHA-C4D-C3D	-2.30	120.99	125.23
11	b	302	HEM	CHD-C4C-NC	2.27	126.93	124.45
11	B	303	HEM	CHA-C4D-C3D	2.26	129.39	125.23
11	b	301	HEM	C1A-CHA-C4D	-2.26	120.94	126.25
10	B	301	HEC	CMD-C2D-C1D	2.25	128.55	125.03
10	C	302	HEC	CHC-C4B-NB	-2.24	121.59	124.37
11	B	303	HEM	C4A-CHB-C1B	-2.24	120.98	126.25
11	B	303	HEM	CHA-C4D-ND	-2.23	121.61	124.37
10	B	301	HEC	CHD-C1D-ND	-2.23	121.61	124.37
10	C	302	HEC	CMD-C2D-C1D	2.23	128.51	125.03
11	B	302	HEM	C1A-CHA-C4D	-2.22	121.02	126.25
10	b	305	HEC	CAD-C3D-C4D	2.20	128.53	124.70
10	b	305	HEC	CAB-C3B-C2B	2.19	131.59	127.56
10	C	302	HEC	CMA-C3A-C4A	2.18	128.57	124.73
10	b	305	HEC	CHA-C4D-C3D	-2.18	121.60	124.77
10	c	302	HEC	CHC-C1C-NC	-2.18	119.91	123.86
11	b	302	HEM	C4A-CHB-C1B	-2.17	121.14	126.25
10	B	301	HEC	CMB-C2B-C3B	2.16	131.98	126.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	302	HEM	C1A-CHA-C4D	-2.15	121.19	126.25
10	c	302	HEC	CMD-C2D-C1D	2.14	128.38	125.03
11	b	302	HEM	CHA-C4D-C3D	-2.14	121.29	125.23
10	C	302	HEC	CMB-C2B-C3B	2.11	131.85	126.15
11	b	301	HEM	CHA-C1A-NA	2.11	127.68	123.86
10	c	302	HEC	C3B-C4B-NB	2.10	112.47	110.17
11	b	301	HEM	CHB-C1B-C2B	-2.09	121.00	126.95
10	b	305	HEC	CMA-C3A-C4A	2.09	128.41	124.73
10	c	302	HEC	CMA-C3A-C4A	2.08	128.40	124.73
11	B	302	HEM	CHB-C1B-C2B	-2.06	121.08	126.95
11	B	302	HEM	CHA-C1A-NA	2.05	127.58	123.86
10	b	305	HEC	CHB-C4A-C3A	-2.04	121.24	125.49
10	c	302	HEC	CMB-C2B-C3B	2.03	131.65	126.15
11	B	302	HEM	C4C-CHD-C1D	-2.01	121.74	126.02

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	301	HEC	NA
10	C	302	HEC	NA
10	b	305	HEC	NA
10	c	302	HEC	NA

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	301	HEC	C1A-C2A-CAA-CBA
11	B	302	HEM	C2C-C3C-CAC-CBC
11	B	303	HEM	C2A-CAA-CBA-CGA
11	b	301	HEM	C2C-C3C-CAC-CBC
11	b	302	HEM	C2B-C3B-CAB-CBB
11	b	302	HEM	C2C-C3C-CAC-CBC
12	C	301	MQ7	C12-C11-C3-C2
12	C	301	MQ7	C12-C11-C3-C4
13	C	303	PEE	C11-C10-O2-C2
13	C	303	PEE	C4-O4P-P-O3P
13	C	303	PEE	C5-C4-O4P-P
13	c	303	PEE	C2-C1-O3P-P
13	c	303	PEE	C1-O3P-P-O1P
13	c	303	PEE	C1-O3P-P-O4P
13	c	303	PEE	O5-C30-O3-C3
13	c	303	PEE	C31-C30-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	101	PEE	C4-O4P-P-O1P
14	E	101	PC1	O13-C11-C12-N
15	b	304	CDL	C1-CA2-OA2-PA1
15	b	304	CDL	OB7-CB5-OB6-CB4
15	b	304	CDL	C51-CB5-OB6-CB4
15	b	304	CDL	OB9-CB7-OB8-CB6
15	b	304	CDL	C71-CB7-OB8-CB6
10	b	305	HEC	C2C-C3C-CAC-CBC
10	B	301	HEC	C4B-C3B-CAB-CBB
10	C	302	HEC	C4B-C3B-CAB-CBB
10	B	301	HEC	C4C-C3C-CAC-CBC
10	C	302	HEC	C4C-C3C-CAC-CBC
10	b	305	HEC	C4C-C3C-CAC-CBC
10	c	302	HEC	C4C-C3C-CAC-CBC
10	b	305	HEC	C4B-C3B-CAB-CBB
10	c	302	HEC	C4B-C3B-CAB-CBB
10	B	301	HEC	C2B-C3B-CAB-CBB
10	C	302	HEC	C2B-C3B-CAB-CBB
10	b	305	HEC	C2B-C3B-CAB-CBB
10	c	302	HEC	C2B-C3B-CAB-CBB
13	C	303	PEE	O4-C10-O2-C2
10	B	301	HEC	C2C-C3C-CAC-CBC
10	C	302	HEC	C2C-C3C-CAC-CBC
10	c	302	HEC	C2C-C3C-CAC-CBC
12	b	303	MQ7	C24-C23-C25-C26
12	b	303	MQ7	C34-C33-C35-C36
10	B	301	HEC	C3A-C2A-CAA-CBA
11	B	303	HEM	C4D-C3D-CAD-CBD
12	C	301	MQ7	C34-C33-C35-C36
12	b	303	MQ7	C29-C28-C30-C31
12	b	303	MQ7	C39-C38-C40-C41
12	c	301	MQ7	C29-C28-C30-C31
12	c	301	MQ7	C39-C38-C40-C41
12	C	301	MQ7	C32-C33-C35-C36
12	b	303	MQ7	C22-C23-C25-C26
12	b	303	MQ7	C27-C28-C30-C31
12	b	303	MQ7	C37-C38-C40-C41
12	c	301	MQ7	C27-C28-C30-C31
12	c	301	MQ7	C37-C38-C40-C41
12	C	301	MQ7	C33-C35-C36-C37
11	B	302	HEM	C2A-CAA-CBA-CGA
11	b	301	HEM	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	C	301	MQ7	C11-C12-C13-C14
12	C	301	MQ7	C11-C12-C13-C15
12	C	301	MQ7	C16-C17-C18-C20
12	b	303	MQ7	C32-C33-C35-C36
11	B	303	HEM	C2D-C3D-CAD-CBD
11	B	303	HEM	C3D-CAD-CBD-CGD
12	C	301	MQ7	C16-C17-C18-C19
14	E	101	PC1	C31-C32-C33-C34
13	C	303	PEE	C37-C38-C39-C40
14	E	101	PC1	C22-C21-O21-C2
11	b	301	HEM	C2B-C3B-CAB-CBB
11	B	302	HEM	C4C-C3C-CAC-CBC
11	b	301	HEM	C4C-C3C-CAC-CBC
11	b	302	HEM	C4B-C3B-CAB-CBB
11	b	302	HEM	C4C-C3C-CAC-CBC
13	C	303	PEE	C2-C1-O3P-P
10	B	301	HEC	C3D-CAD-CBD-CGD
14	E	101	PC1	O22-C21-O21-C2
14	E	101	PC1	C21-C22-C23-C24
10	c	302	HEC	C3D-CAD-CBD-CGD
13	C	303	PEE	O3P-C1-C2-C3
14	E	101	PC1	C23-C24-C25-C26
12	C	301	MQ7	C41-C42-C43-C44
14	E	101	PC1	O21-C2-C3-O31
12	b	303	MQ7	C12-C11-C3-C2
11	B	303	HEM	C4C-C3C-CAC-CBC
11	b	301	HEM	C4B-C3B-CAB-CBB
12	b	303	MQ7	C12-C11-C3-C4
13	c	303	PEE	C5-C4-O4P-P
13	e	101	PEE	C5-C4-O4P-P
13	e	101	PEE	O2-C2-C3-O3
13	c	303	PEE	C18-C19-C20-C21
13	e	101	PEE	C36-C37-C38-C39
13	C	303	PEE	O2-C2-C3-O3
13	C	303	PEE	C1-C2-C3-O3
13	c	303	PEE	C36-C37-C38-C39
13	c	303	PEE	C38-C39-C40-C41
13	C	303	PEE	C4-O4P-P-O1P
15	b	304	CDL	CB2-OB2-PB2-OB3
12	B	304	MQ7	C34-C33-C35-C36
12	C	301	MQ7	C41-C42-C43-C45
13	C	303	PEE	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	303	PEE	C1-C2-O2-C10
12	c	301	MQ7	C13-C15-C16-C17
13	C	303	PEE	C18-C19-C20-C21
12	c	301	MQ7	C24-C23-C25-C26
13	C	303	PEE	C36-C37-C38-C39
12	C	301	MQ7	C24-C23-C25-C26
12	B	304	MQ7	C32-C33-C35-C36
12	C	301	MQ7	C14-C13-C15-C16
10	b	305	HEC	C3D-CAD-CBD-CGD
14	E	101	PC1	C32-C33-C34-C35
12	c	301	MQ7	C22-C23-C25-C26
11	b	301	HEM	CAA-CBA-CGA-O1A
12	c	301	MQ7	C14-C13-C15-C16
12	C	301	MQ7	C22-C23-C25-C26
11	B	302	HEM	CAD-CBD-CGD-O2D
11	B	303	HEM	CAD-CBD-CGD-O1D
11	B	303	HEM	CAD-CBD-CGD-O2D
13	c	303	PEE	C14-C15-C16-C17
12	C	301	MQ7	C12-C13-C15-C16
11	B	302	HEM	CAD-CBD-CGD-O1D
11	b	301	HEM	CAD-CBD-CGD-O1D
12	B	304	MQ7	C20-C21-C22-C23
12	b	303	MQ7	C14-C13-C15-C16
11	b	301	HEM	CAD-CBD-CGD-O2D
11	b	301	HEM	CAA-CBA-CGA-O2A
14	E	101	PC1	C1-C2-C3-O31
13	C	303	PEE	O3P-C1-C2-O2
12	c	301	MQ7	C19-C18-C20-C21
12	B	304	MQ7	C3-C11-C12-C13
13	c	303	PEE	C16-C17-C18-C19
11	B	302	HEM	CAA-CBA-CGA-O2A
14	E	101	PC1	O11-C1-C2-C3
10	B	301	HEC	CAA-CBA-CGA-O2A
10	C	302	HEC	CAA-CBA-CGA-O2A
11	B	302	HEM	CAA-CBA-CGA-O1A
10	C	302	HEC	CAA-CBA-CGA-O1A
12	C	301	MQ7	C26-C27-C28-C29
10	B	301	HEC	CAA-CBA-CGA-O1A
10	b	305	HEC	CAA-CBA-CGA-O2A
10	c	302	HEC	CAD-CBD-CGD-O1D
10	b	305	HEC	CAA-CBA-CGA-O1A
10	c	302	HEC	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	c	301	MQ7	C12-C13-C15-C16
12	c	301	MQ7	C17-C18-C20-C21
10	B	301	HEC	CAD-CBD-CGD-O2D
14	E	101	PC1	O21-C21-C22-C23
10	b	305	HEC	CAD-CBD-CGD-O2D
13	e	101	PEE	C1-C2-O2-C10
12	b	303	MQ7	C40-C41-C42-C43
12	B	304	MQ7	C33-C35-C36-C37
13	C	303	PEE	C34-C35-C36-C37
10	B	301	HEC	CAD-CBD-CGD-O1D
15	b	304	CDL	C55-C56-C57-C58
14	E	101	PC1	O22-C21-C22-C23
13	C	303	PEE	C38-C39-C40-C41
10	b	305	HEC	CAD-CBD-CGD-O1D
14	E	101	PC1	C34-C35-C36-C37
15	b	304	CDL	C31-C32-C33-C34
10	C	302	HEC	CAD-CBD-CGD-O2D
13	c	303	PEE	C31-C32-C33-C34

There are no ring outliers.

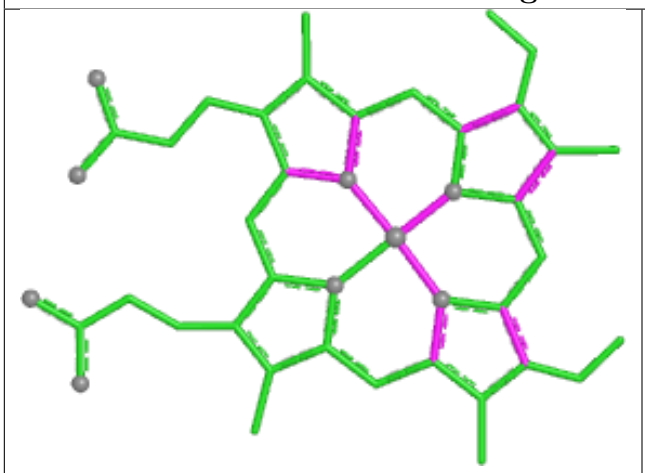
15 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	301	HEC	3	0
13	e	101	PEE	2	0
12	b	303	MQ7	2	0
10	b	305	HEC	2	0
13	C	303	PEE	3	0
11	b	302	HEM	2	0
12	B	304	MQ7	3	0
11	B	303	HEM	2	0
10	c	302	HEC	3	0
10	C	302	HEC	1	0
13	c	303	PEE	4	0
12	c	301	MQ7	4	0
9	a	201	FES	1	0
12	C	301	MQ7	2	0
15	b	304	CDL	1	0

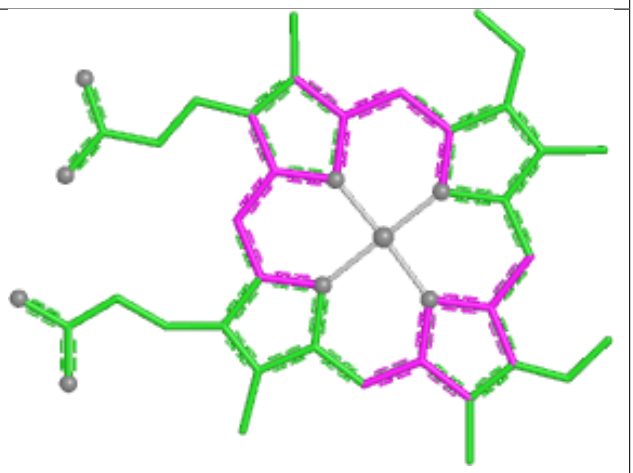
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

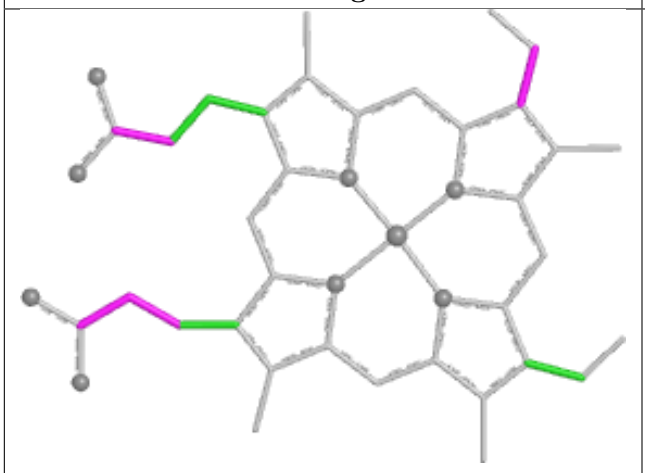
Ligand HEM B 302



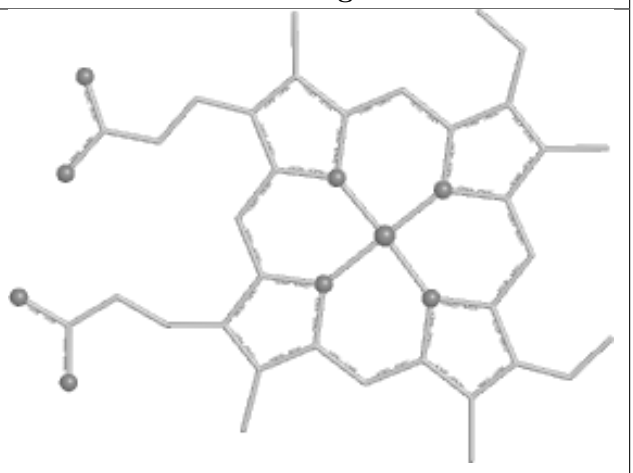
Bond lengths



Bond angles

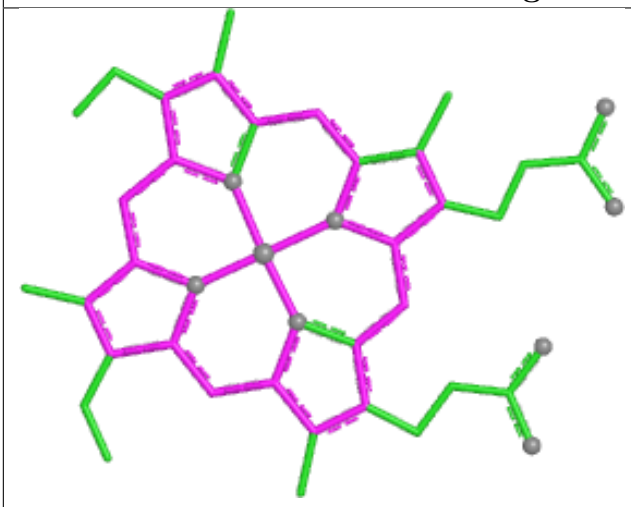


Torsions

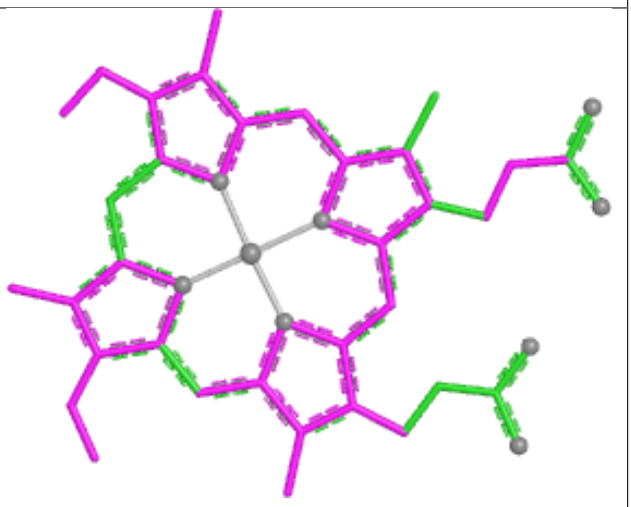


Rings

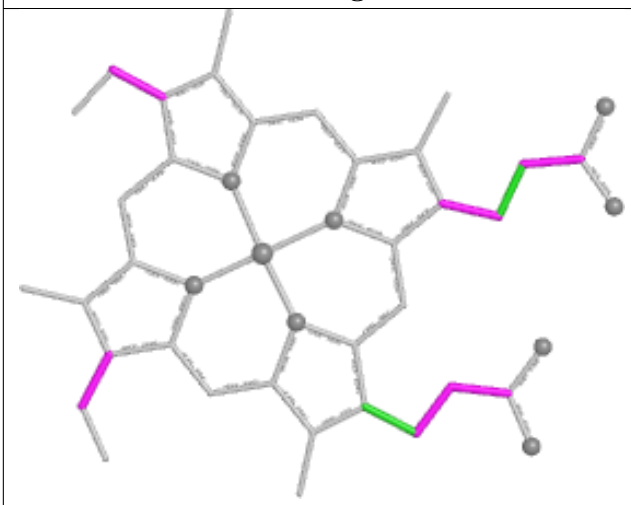
Ligand HEC B 301



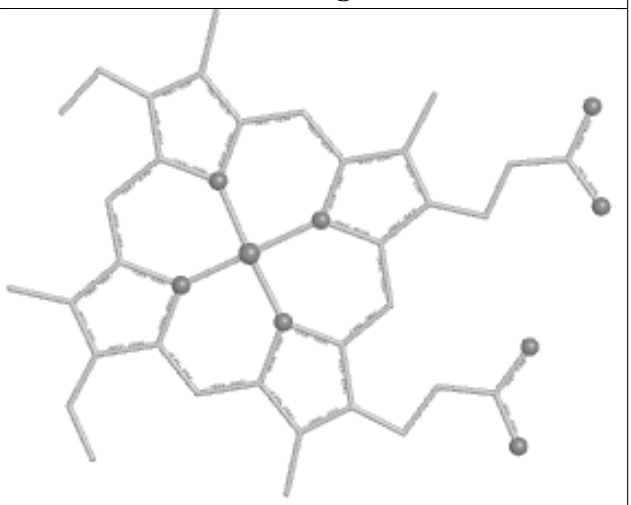
Bond lengths



Bond angles

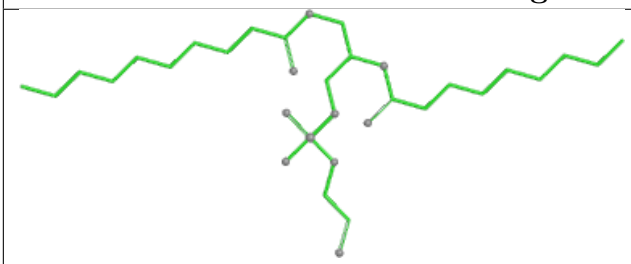


Torsions

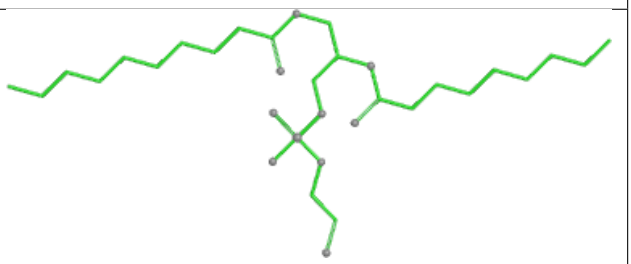


Rings

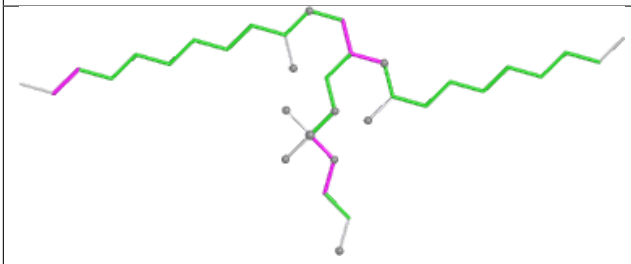
Ligand PEE e 101



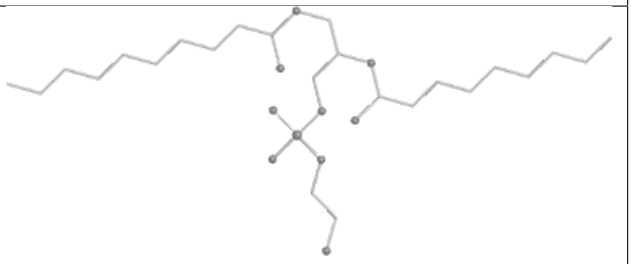
Bond lengths



Bond angles



Torsions



Rings

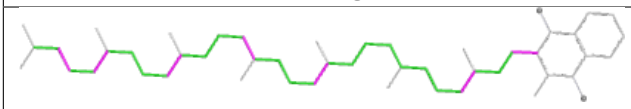
Ligand MQ7 b 303



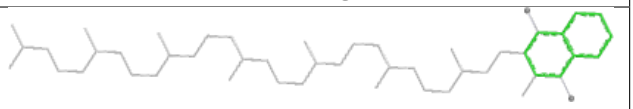
Bond lengths



Bond angles

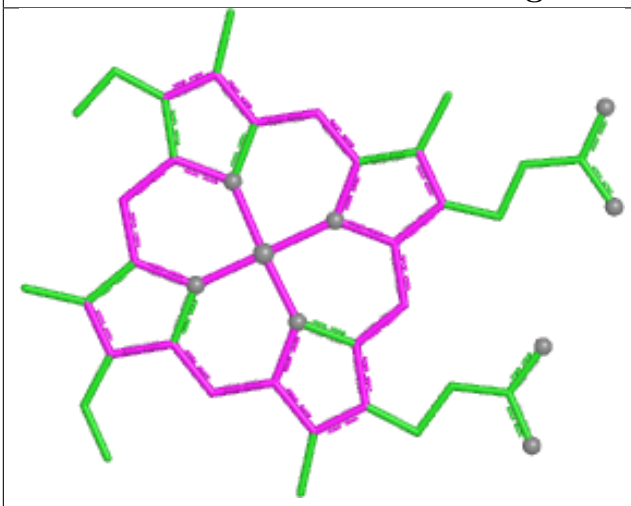


Torsions

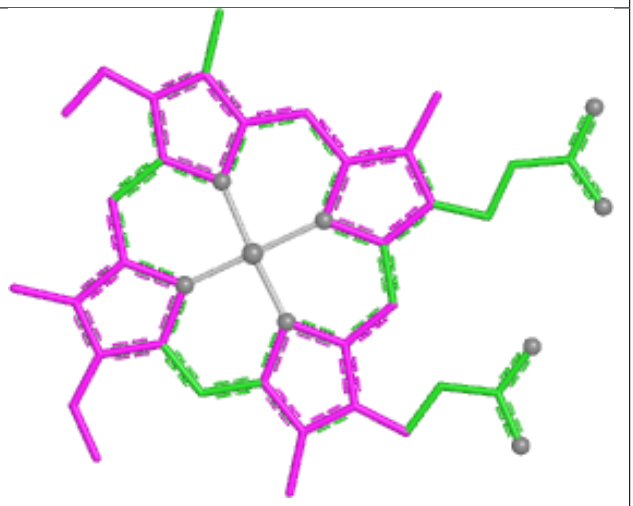


Rings

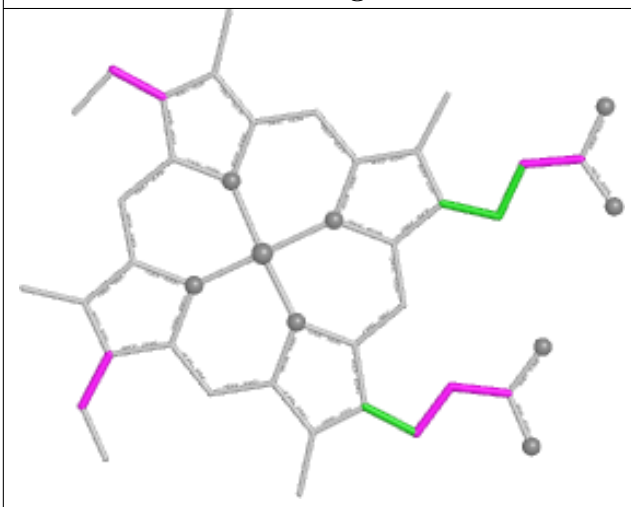
Ligand HEC b 305



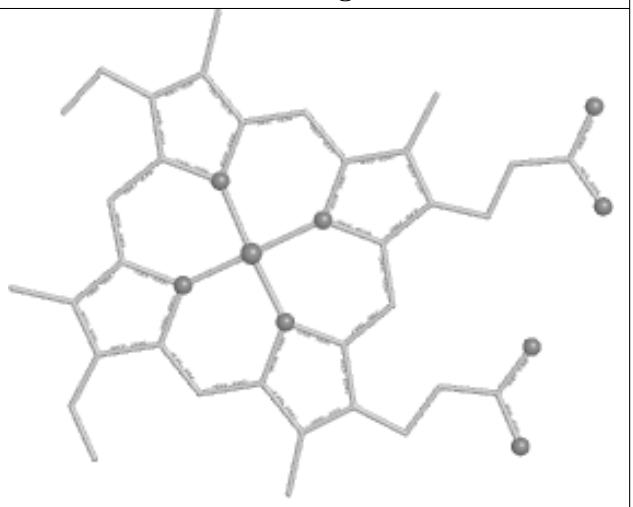
Bond lengths



Bond angles

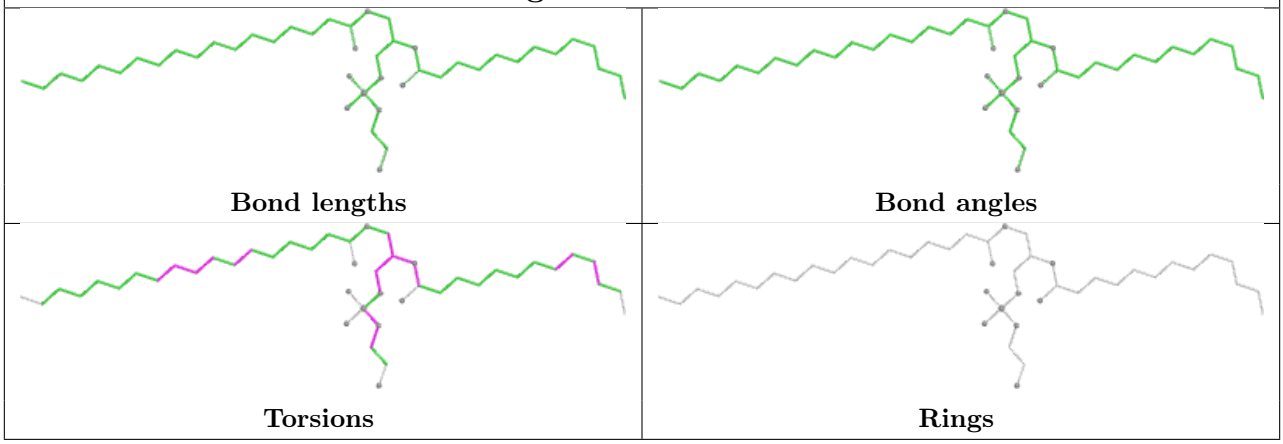


Torsions

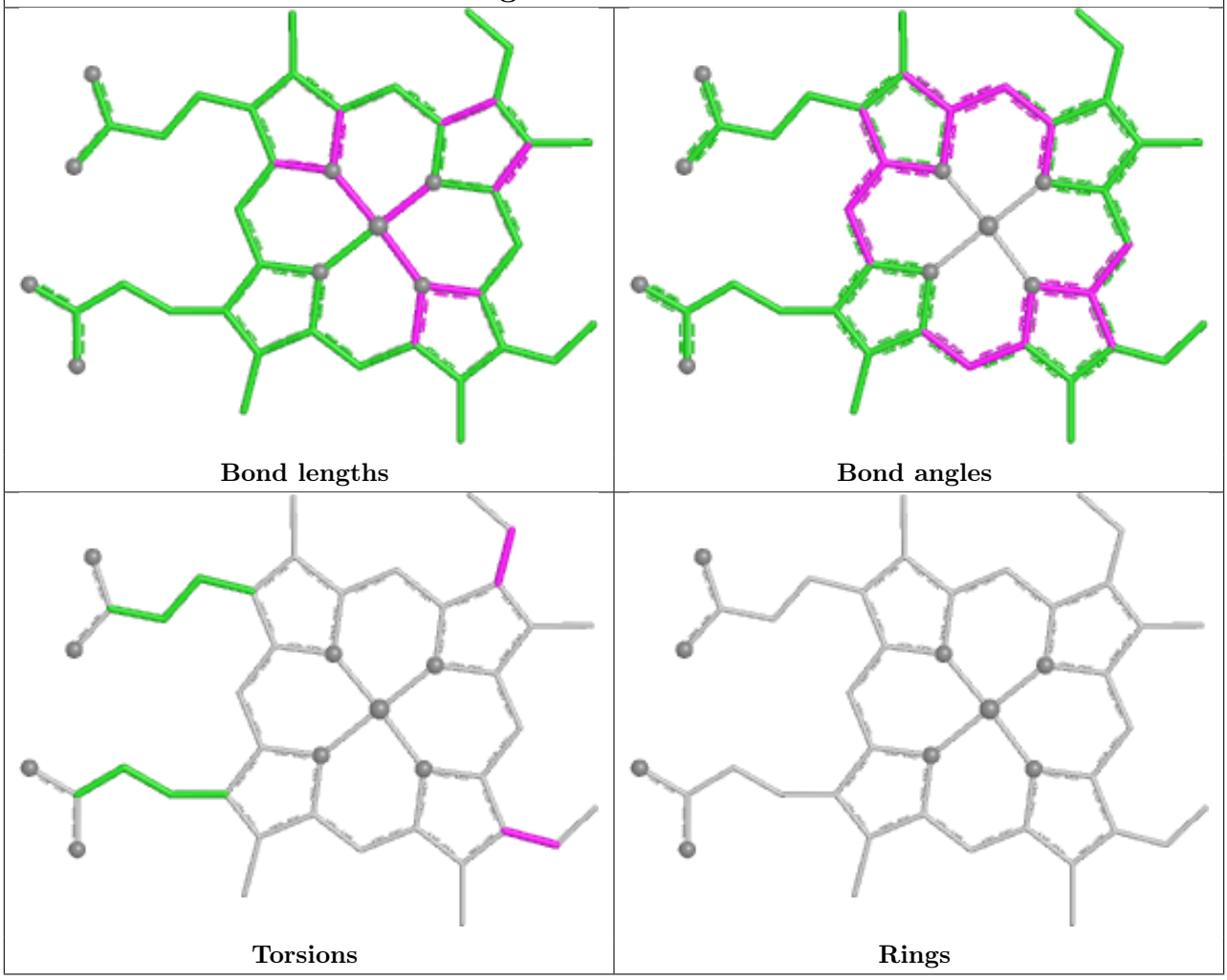


Rings

Ligand PEE C 303



Ligand HEM b 302



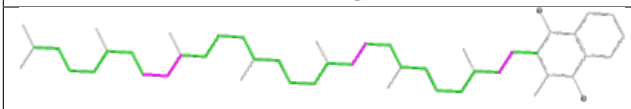
Ligand MQ7 B 304



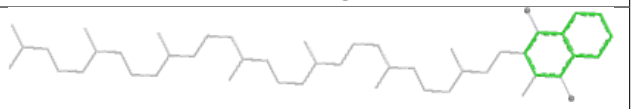
Bond lengths



Bond angles

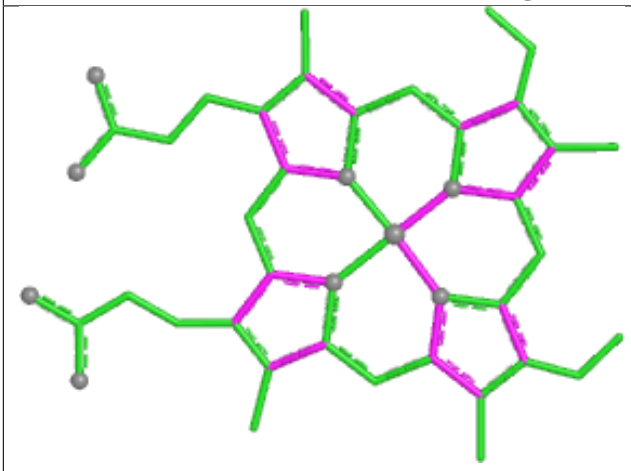


Torsions

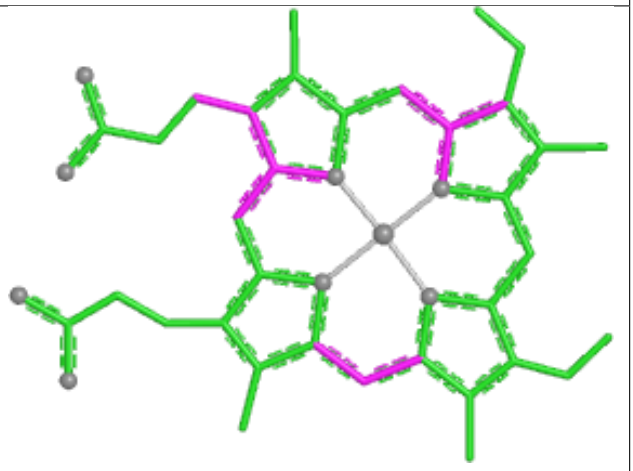


Rings

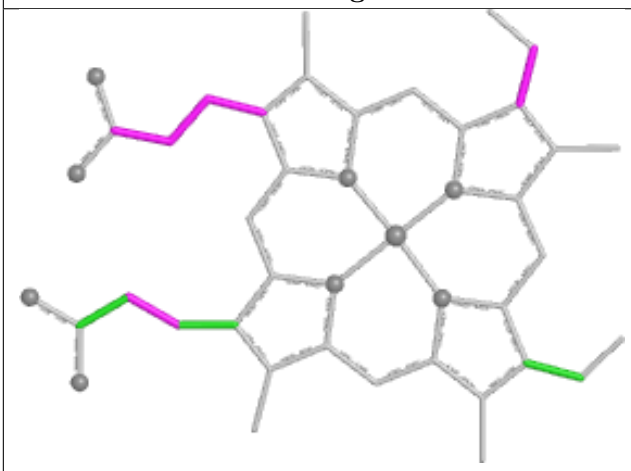
Ligand HEM B 303



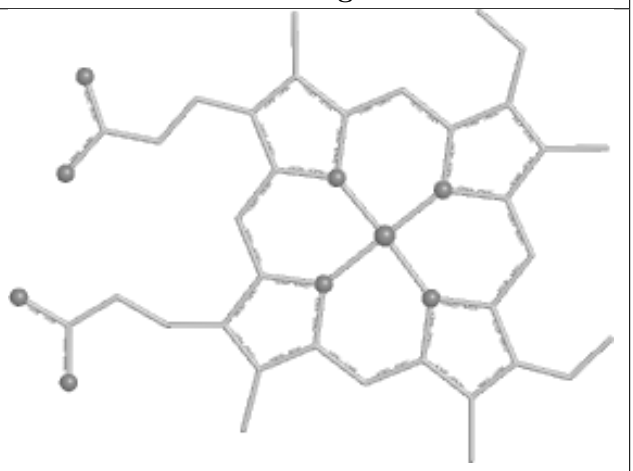
Bond lengths



Bond angles

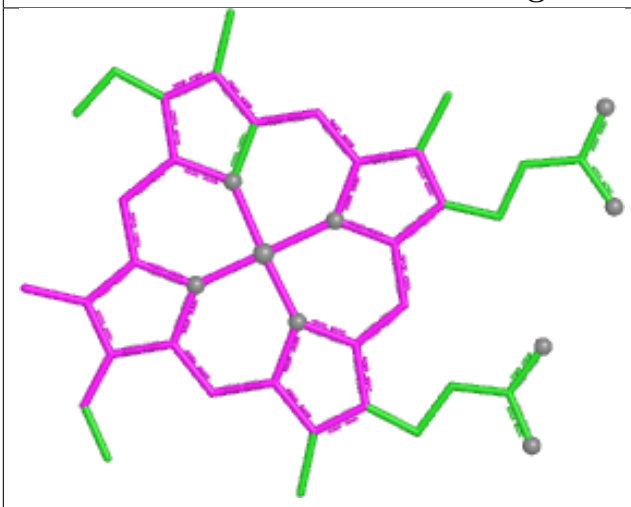


Torsions

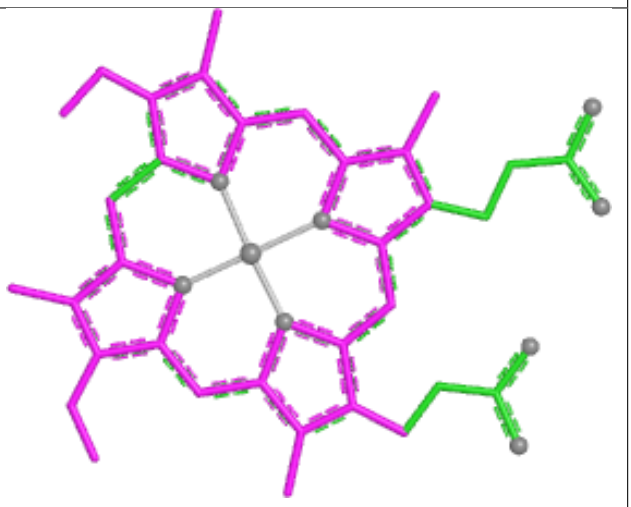


Rings

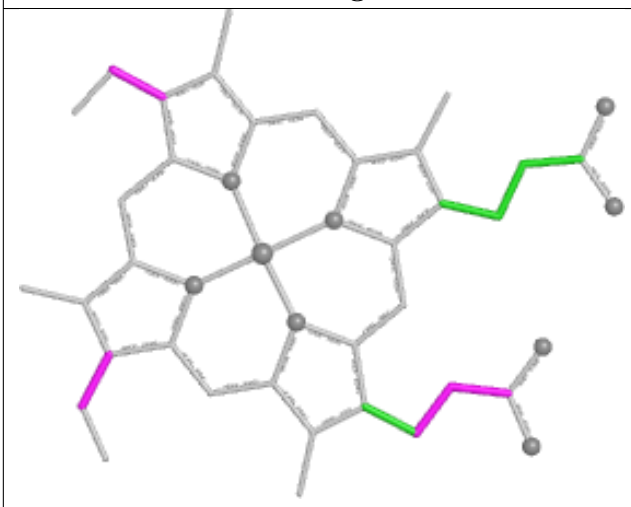
Ligand HEC c 302



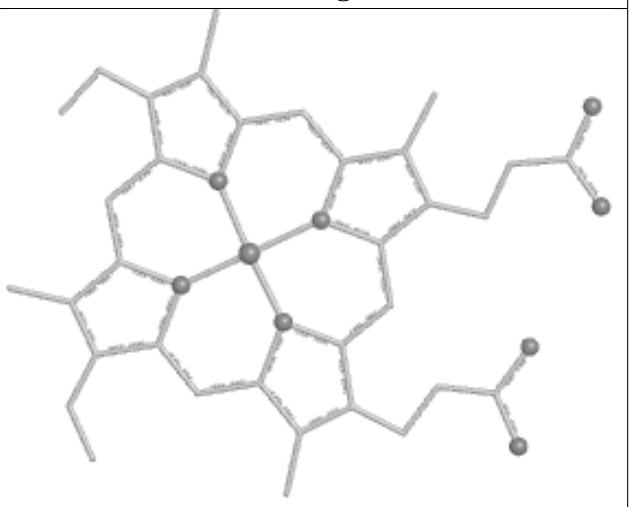
Bond lengths



Bond angles

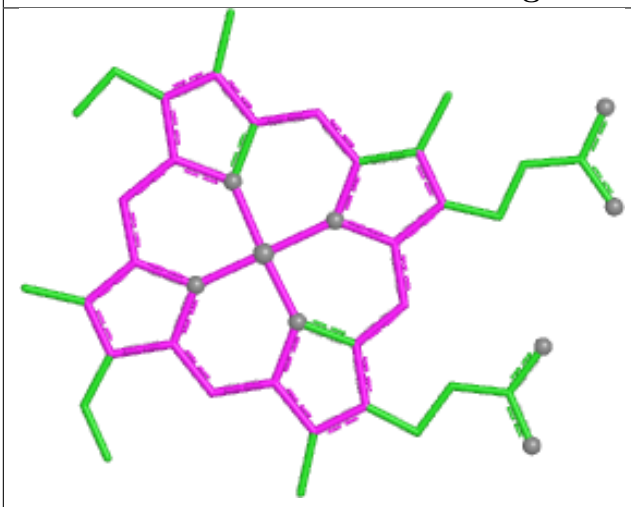


Torsions

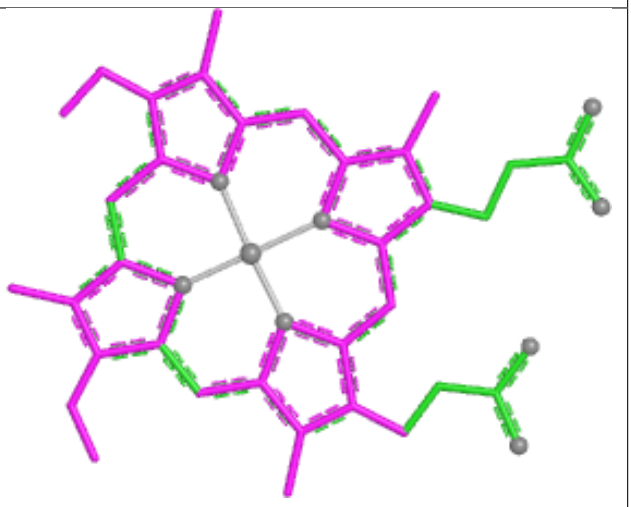


Rings

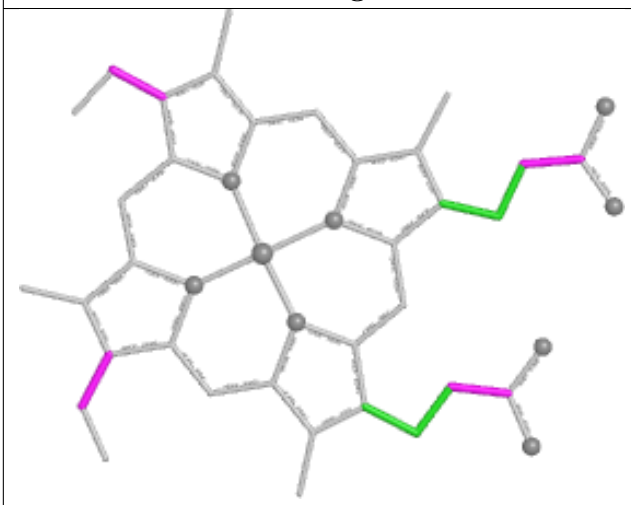
Ligand HEC C 302



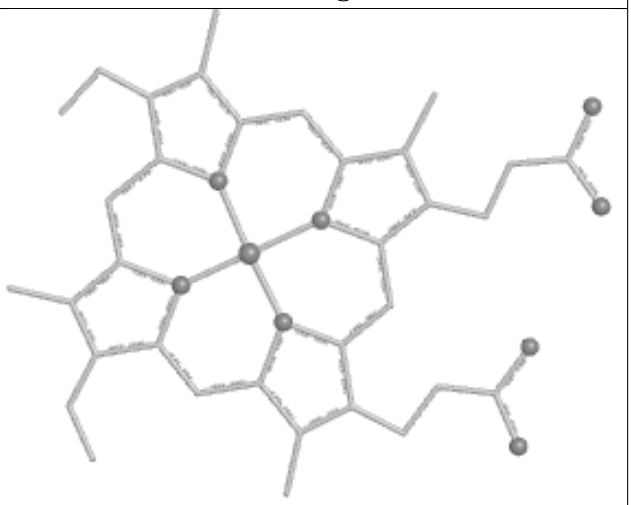
Bond lengths



Bond angles

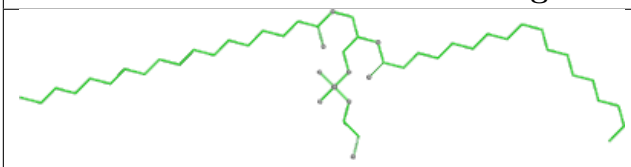


Torsions

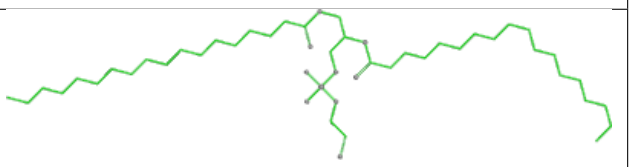


Rings

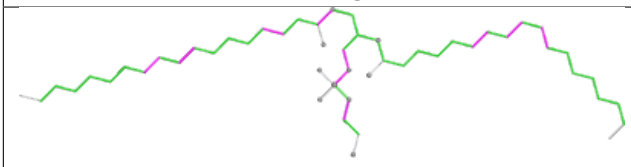
Ligand PEE c 303



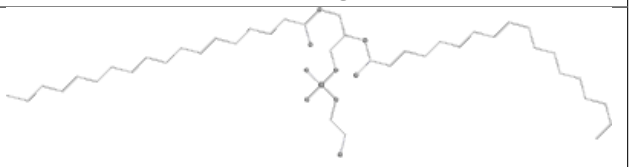
Bond lengths



Bond angles

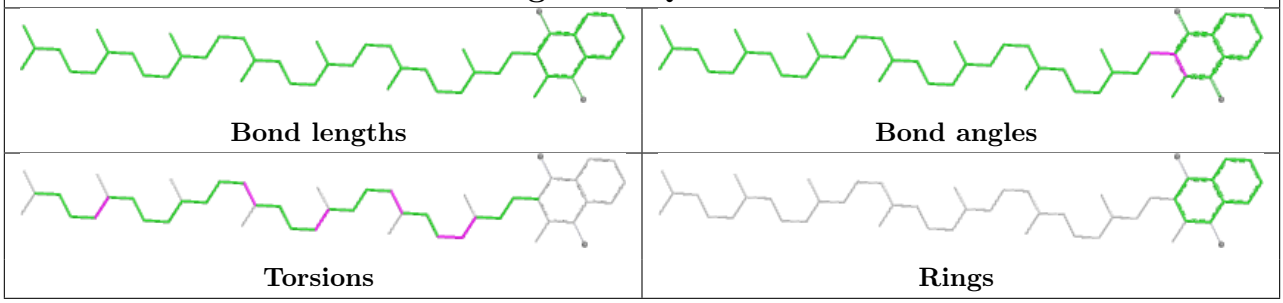


Torsions

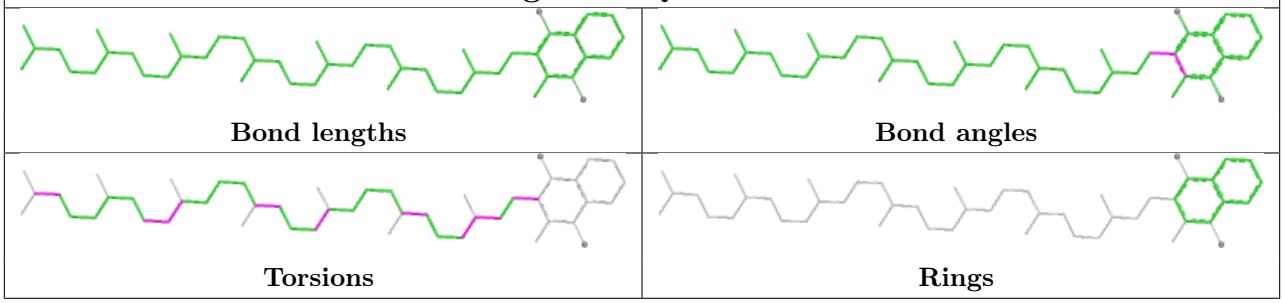


Rings

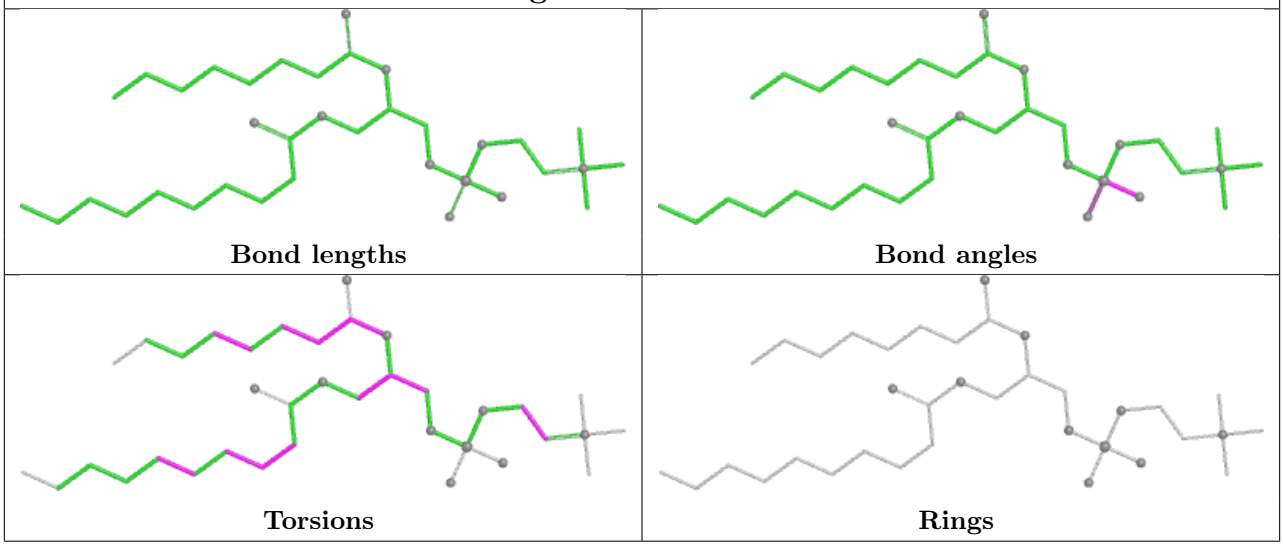
Ligand MQ7 c 301



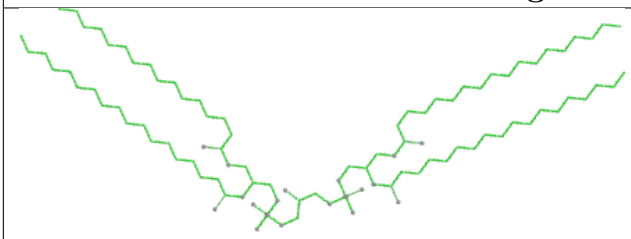
Ligand MQ7 C 301



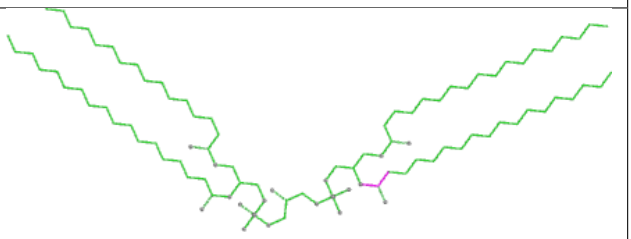
Ligand PC1 E 101



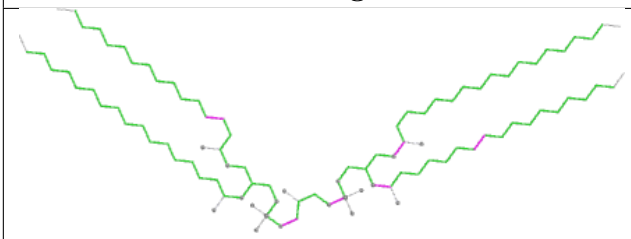
Ligand CDL b 304



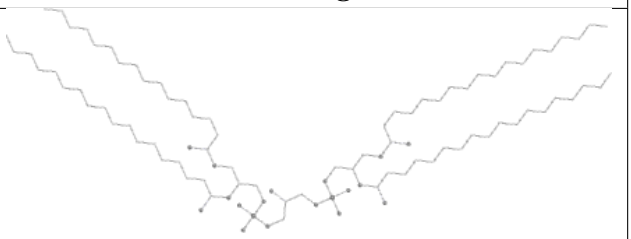
Bond lengths



Bond angles

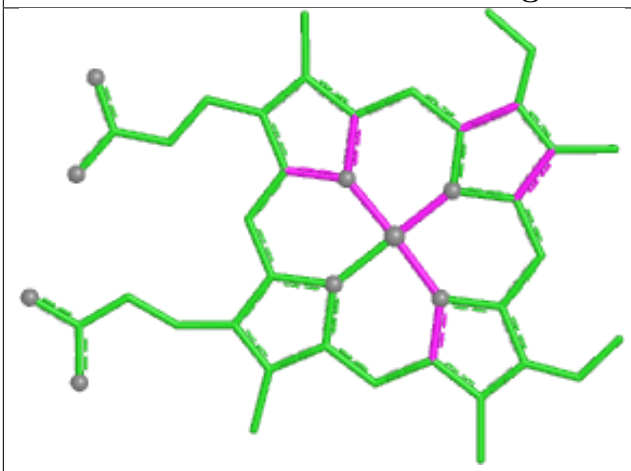


Torsions

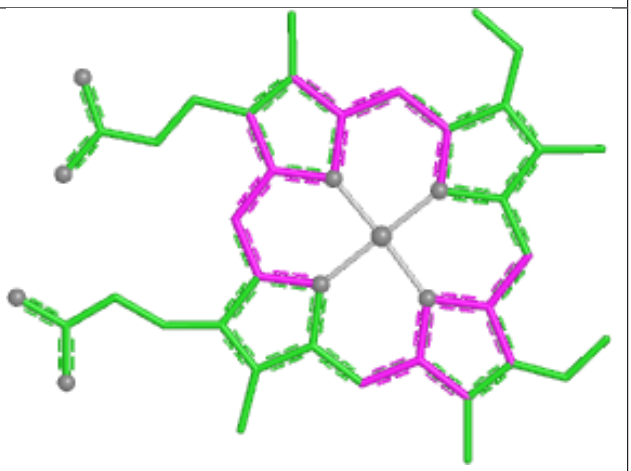


Rings

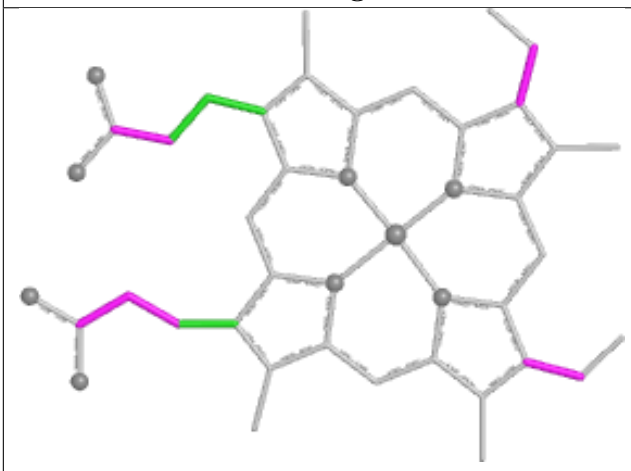
Ligand HEM b 301



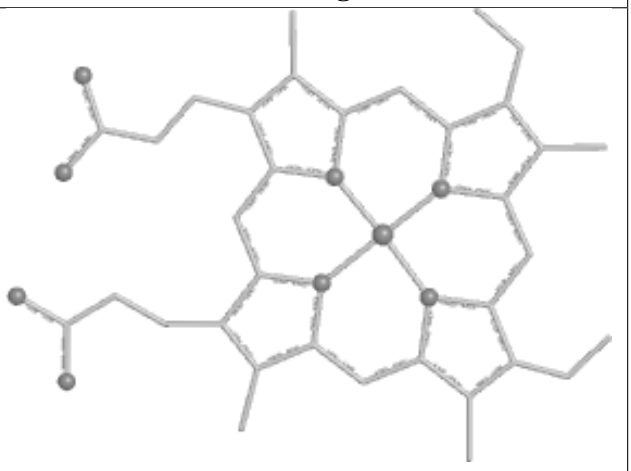
Bond lengths



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.

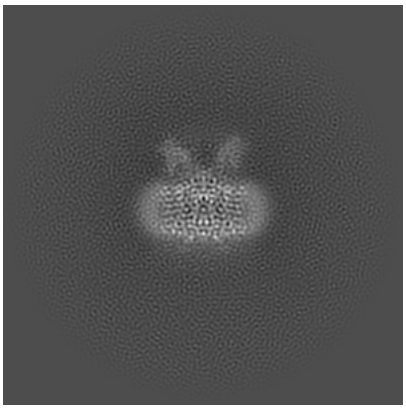
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70334. These allow visual inspection of the internal detail of the map and identification of artifacts.

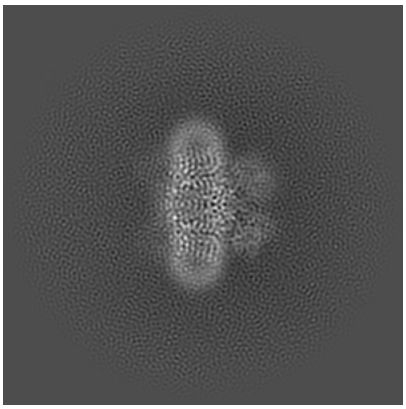
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

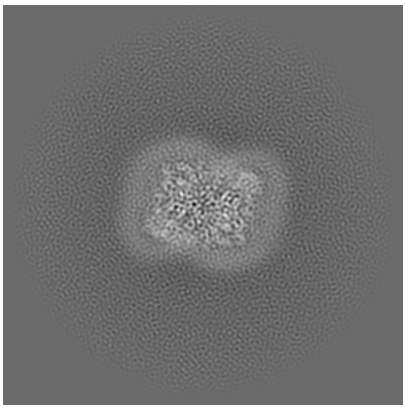
6.1.1 Primary map



X

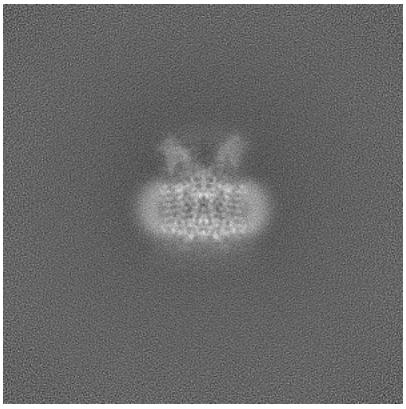


Y

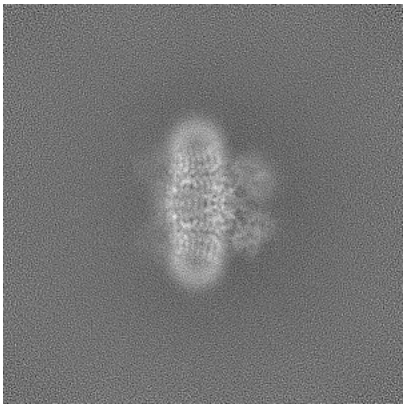


Z

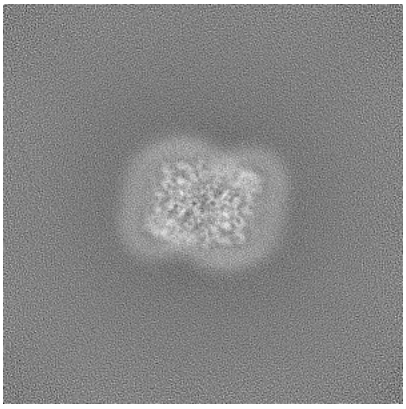
6.1.2 Raw map



X



Y

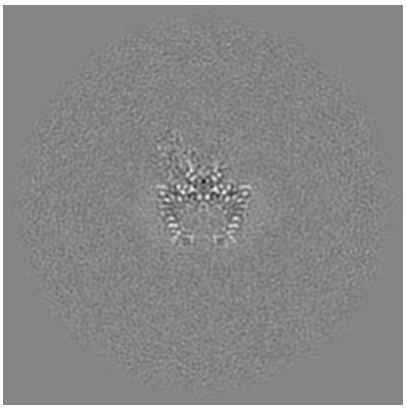


Z

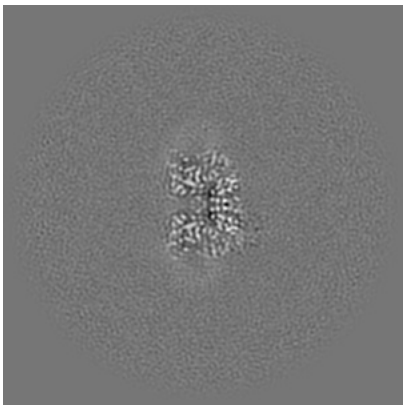
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

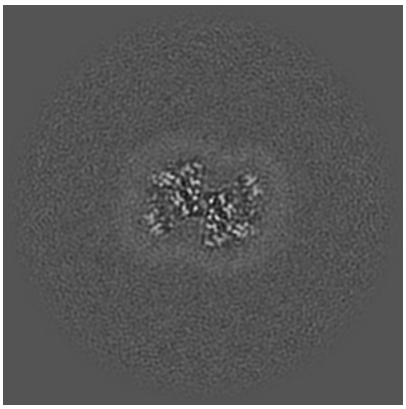
6.2.1 Primary map



X Index: 180

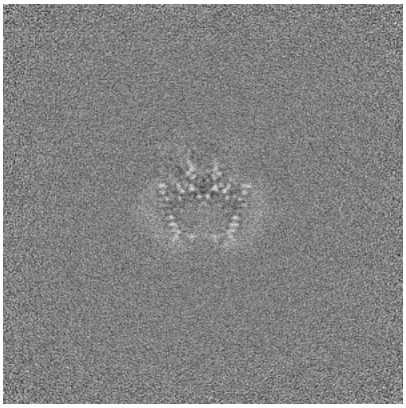


Y Index: 180

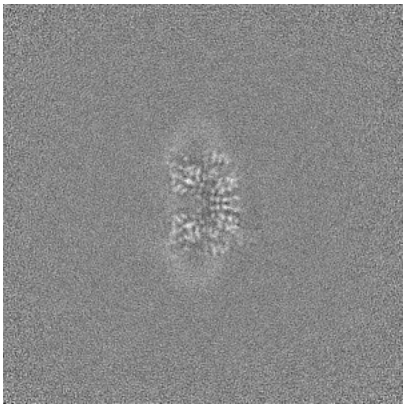


Z Index: 180

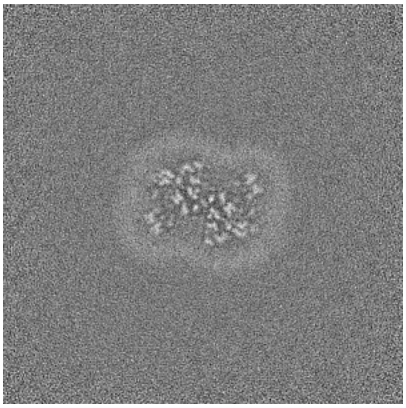
6.2.2 Raw map



X Index: 180



Y Index: 180

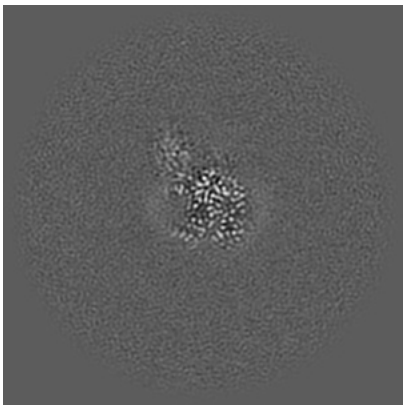


Z Index: 180

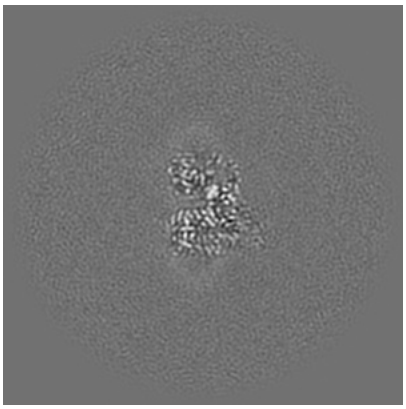
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

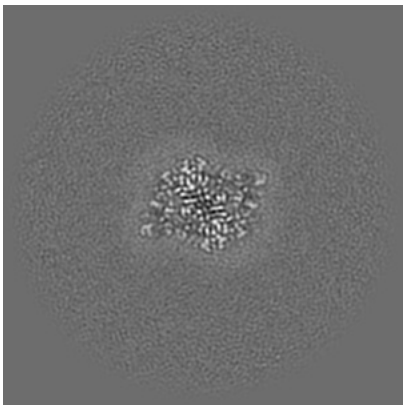
6.3.1 Primary map



X Index: 166

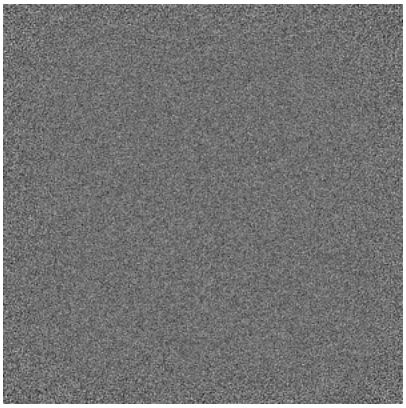


Y Index: 177

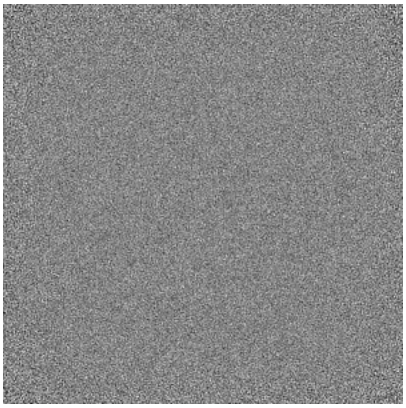


Z Index: 190

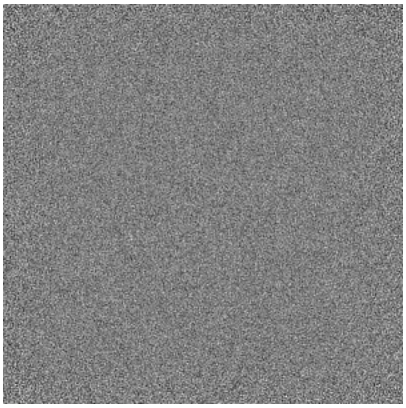
6.3.2 Raw map



X Index: 0



Y Index: 0

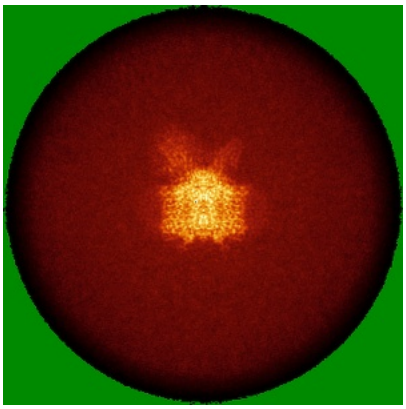


Z Index: 0

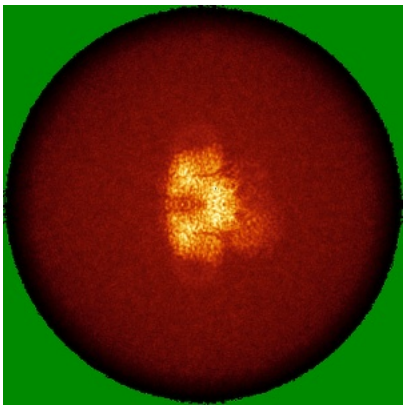
The images above show the largest variance slices of the map in three orthogonal directions.

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

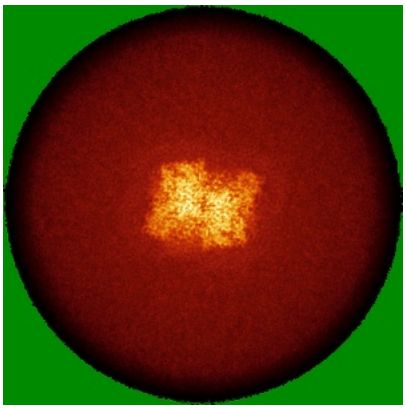
6.4.1 Primary map



X

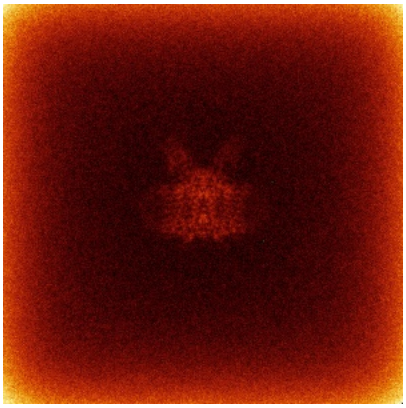


Y

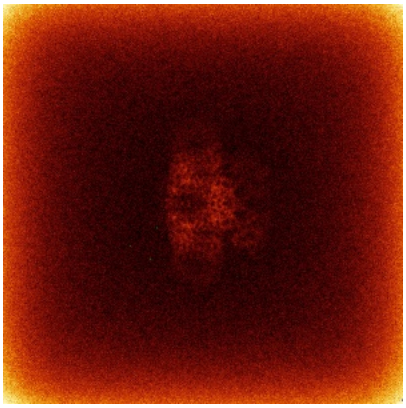


Z

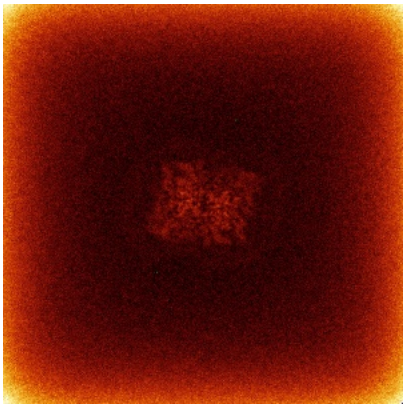
6.4.2 Raw map



X



Y

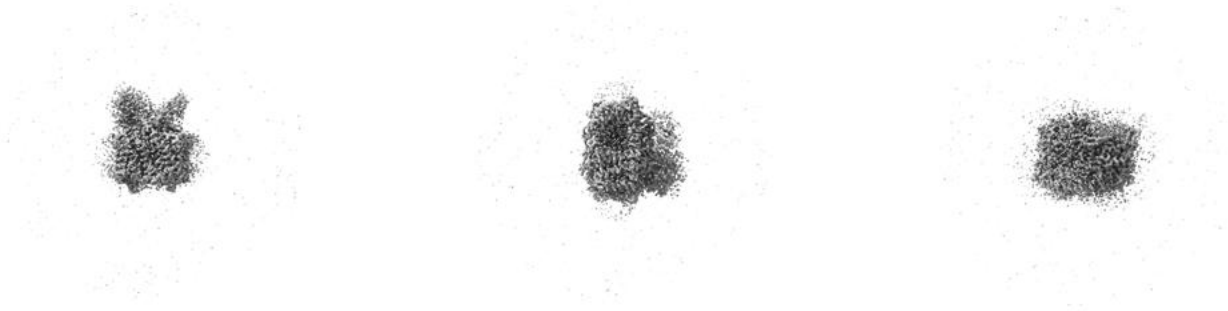


Z

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)

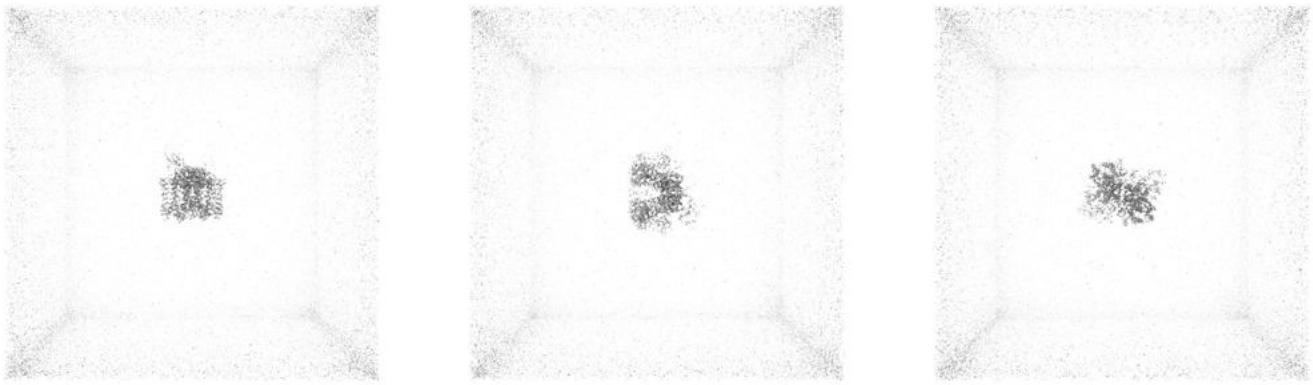
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

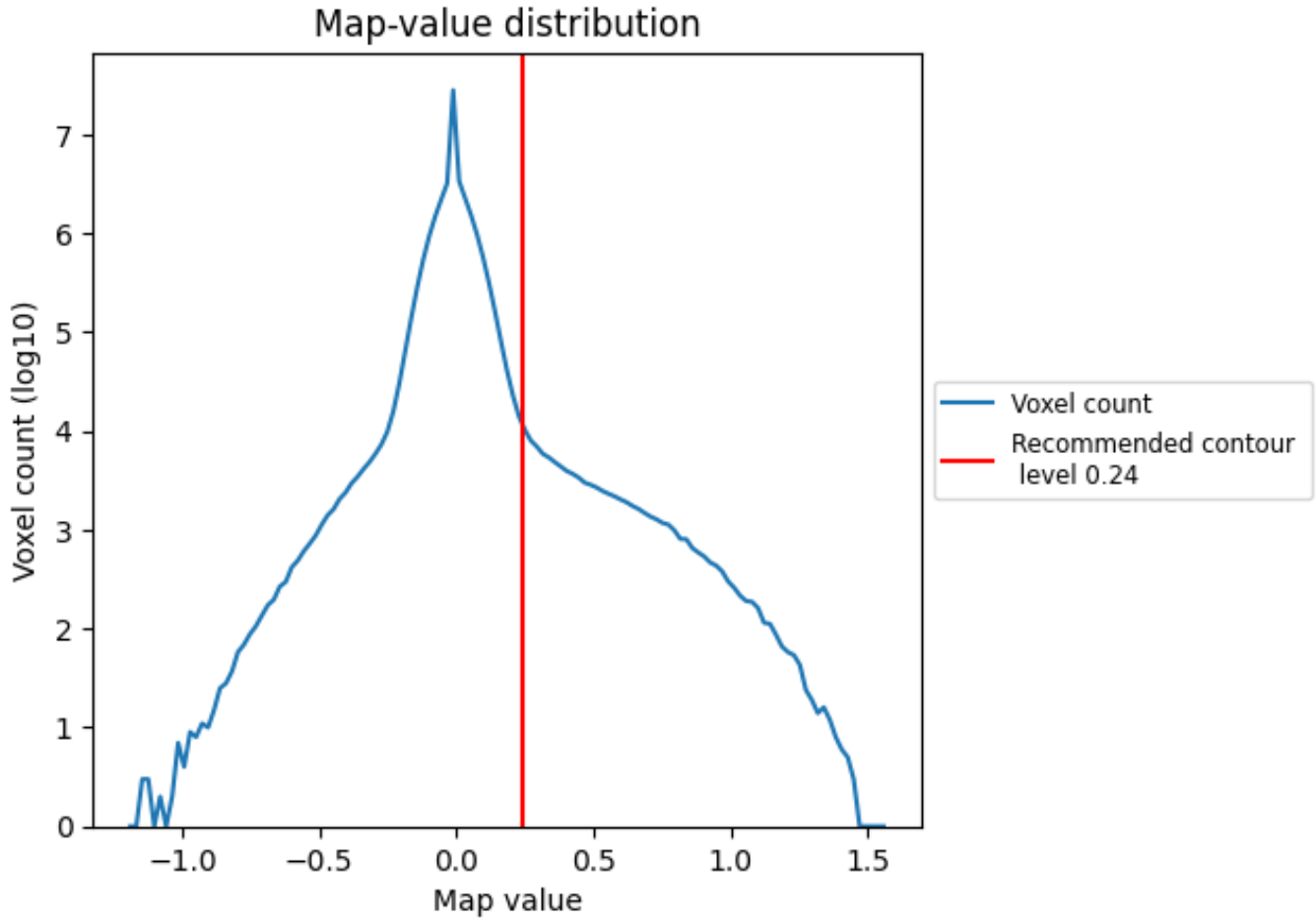
6.6 Mask visualisation (i)

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

7 Map analysis

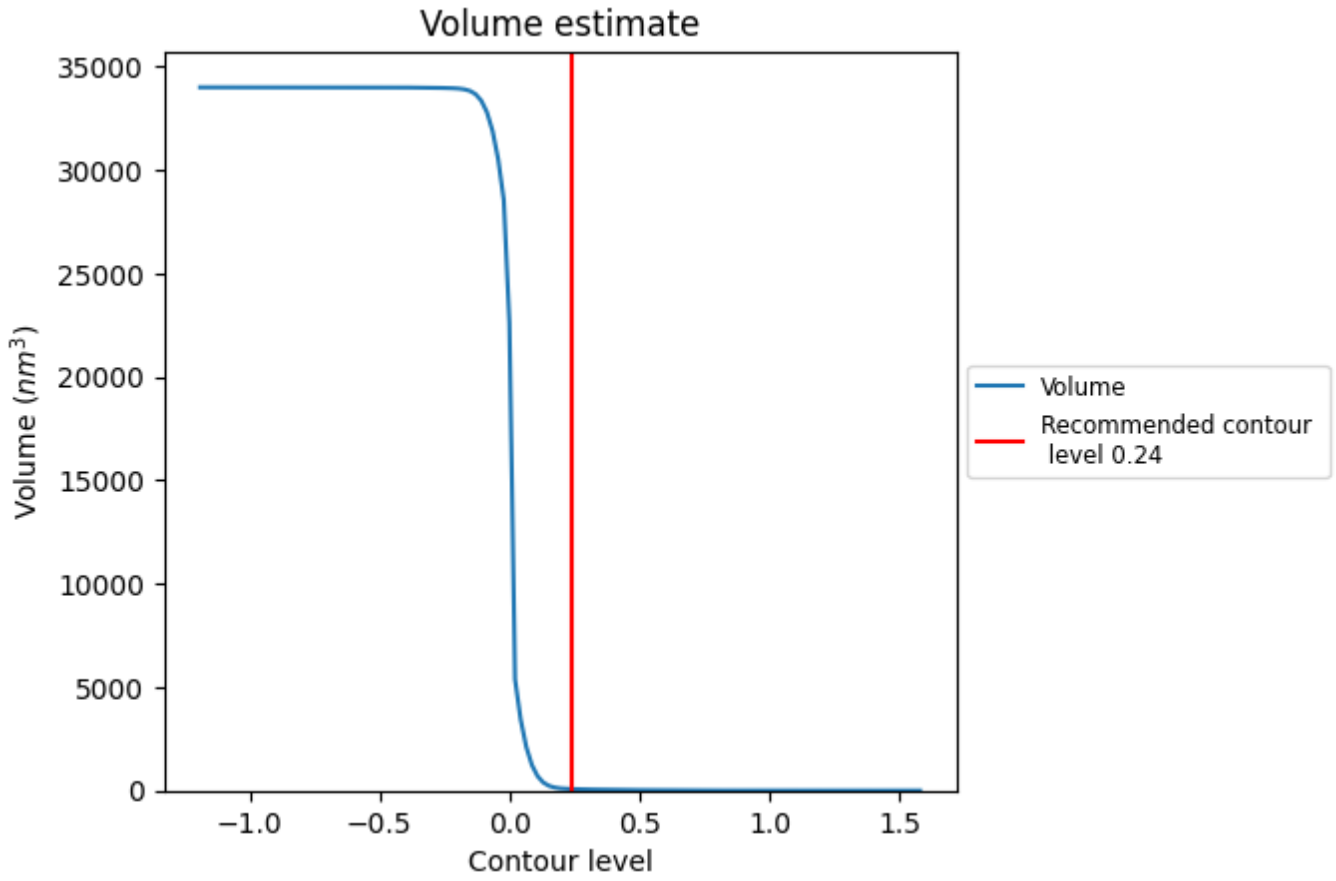
This section contains the results of statistical analysis of the map.

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.

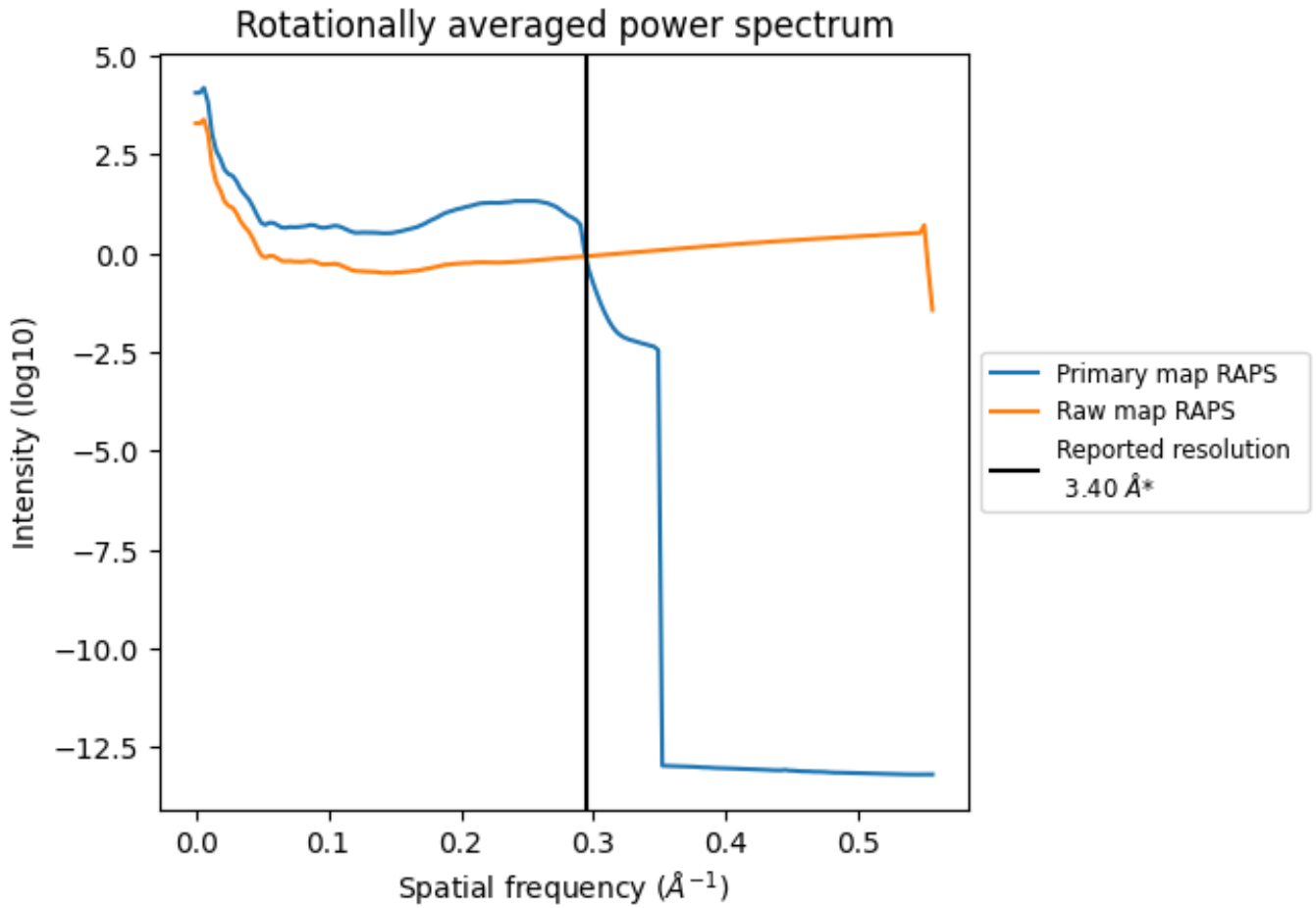
7.2 Volume estimate



The volume at the recommended contour level is 72 nm^3; this corresponds to an approximate mass of 65 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)

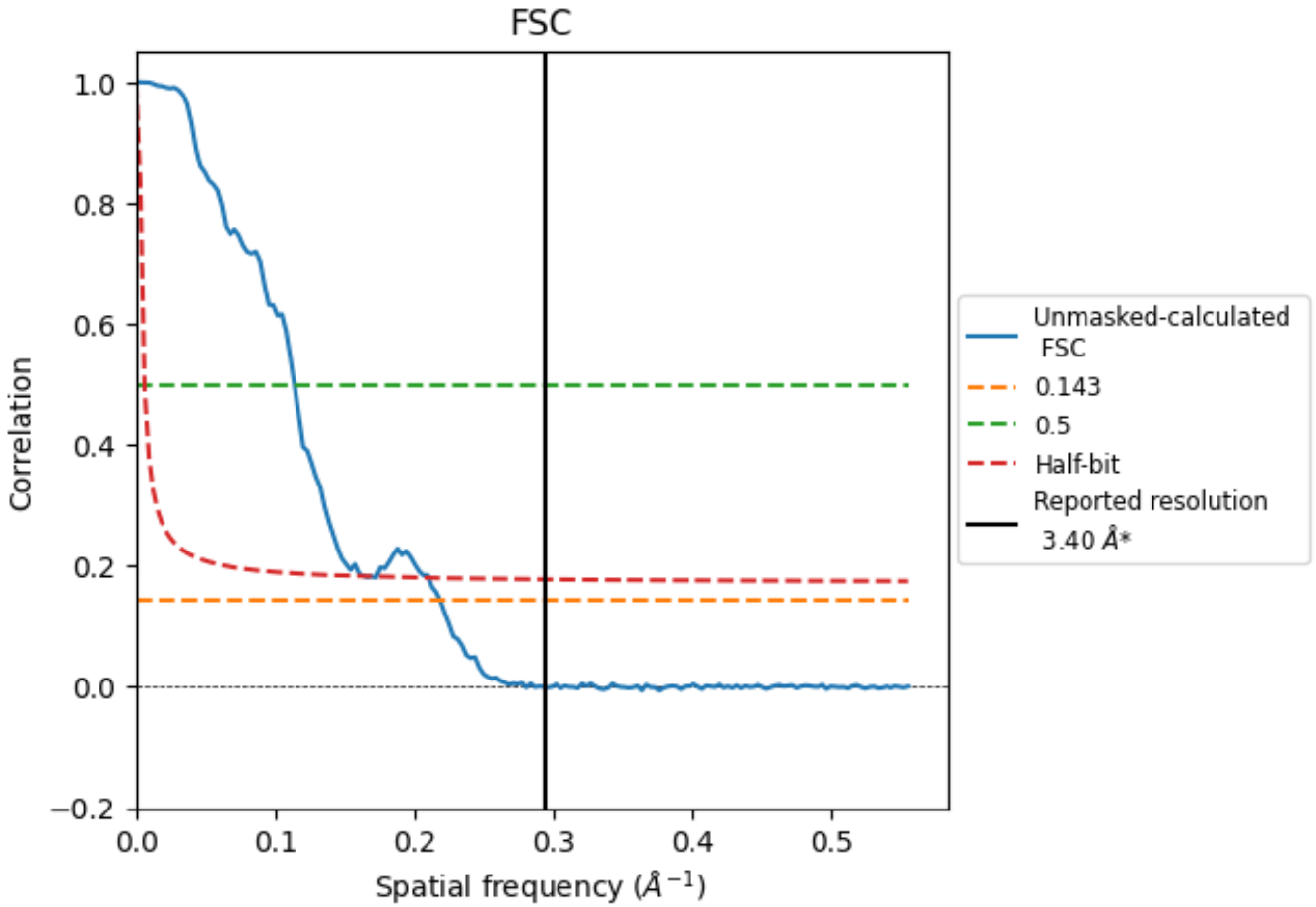


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

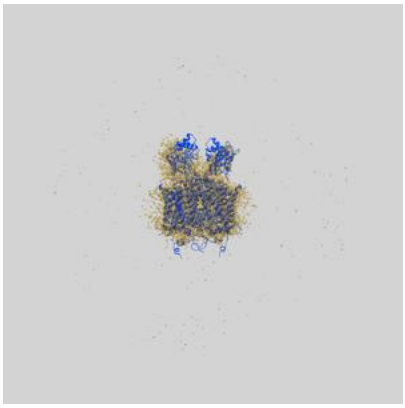
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.57	8.76	6.05

*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 4.57 differs from the reported value 3.4 by more than 10 %

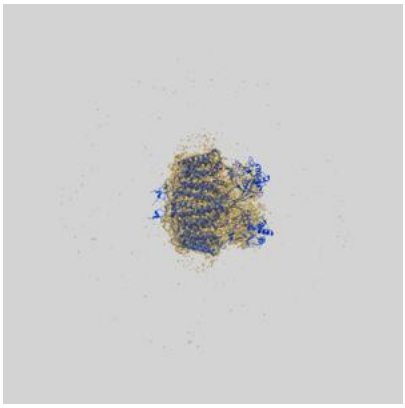
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70334 and PDB model 9OCX. Per-residue inclusion information can be found in section 3 on page 11.

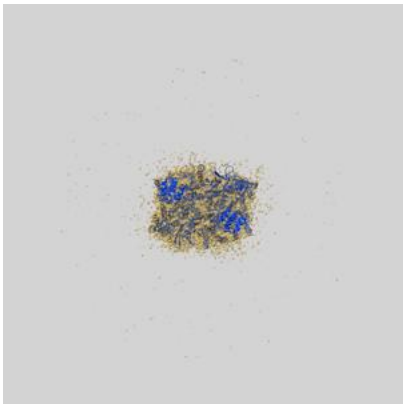
9.1 Map-model overlay



X



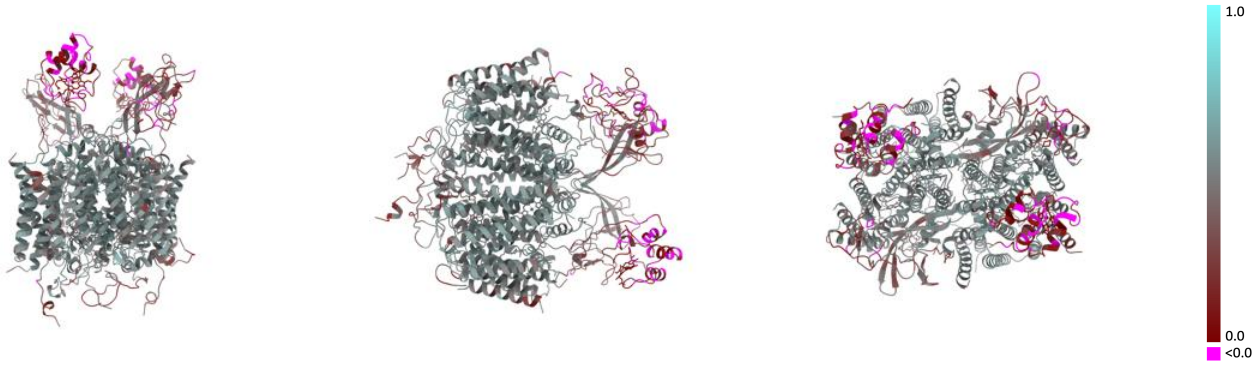
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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.

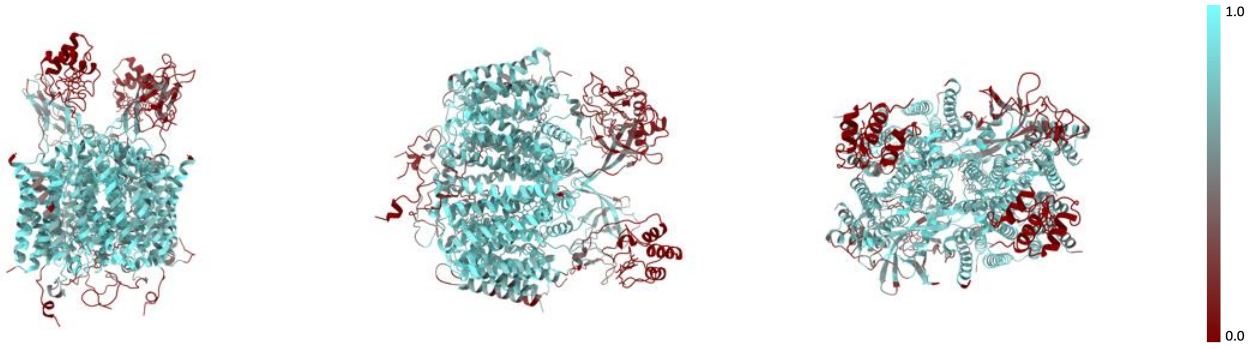
9.2 Q-score mapped to coordinate model (i)



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.

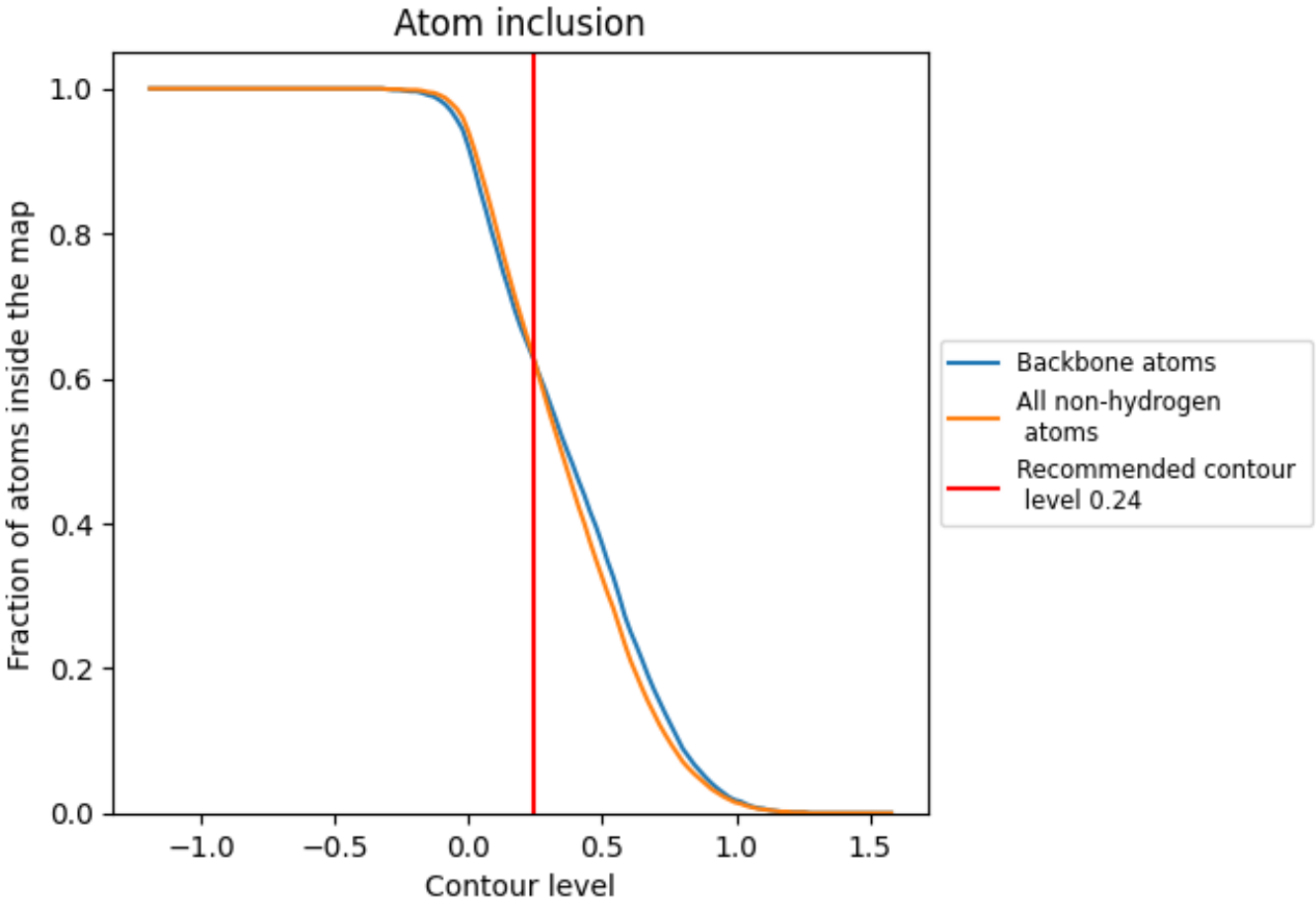
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.24).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.4370
A	0.3640	0.3440
B	0.8270	0.5260
C	0.4600	0.3480
D	0.7210	0.4870
E	0.8430	0.5210
F	0.5260	0.4100
G	0.6270	0.4310
H	0.5680	0.4460
a	0.6110	0.3890
b	0.8080	0.5260
c	0.4890	0.3620
d	0.7070	0.4820
e	0.8410	0.5220
f	0.5350	0.4280
g	0.6910	0.4870
h	0.5620	0.4430

