Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 02:31 PM EDT

PDB ID	:	9OCT / pdb_00009oct
EMDB ID	:	EMD-70331
Title	:	Cryo-EM structure of the cytochrome bc complex (CIII2) from Bacillus subtilis
Authors	:	Zong, Y.; Zheng, W.; Gu, M.; Zhang, K.; Zhu, J.
Deposited on	:	2025-04-25
Resolution	:	2.60 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:

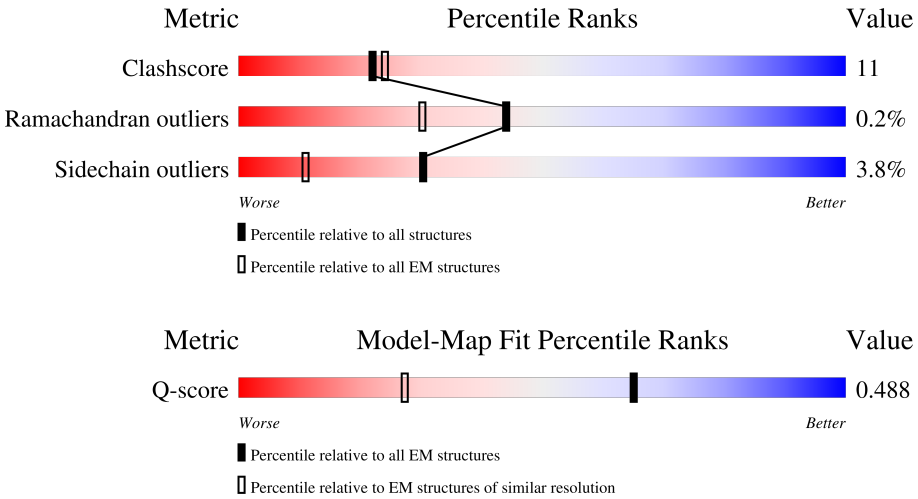
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.60 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.



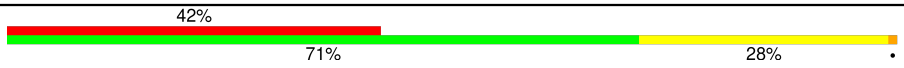
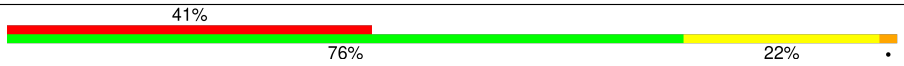
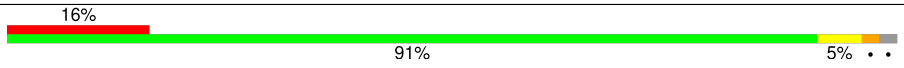
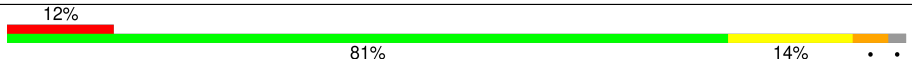
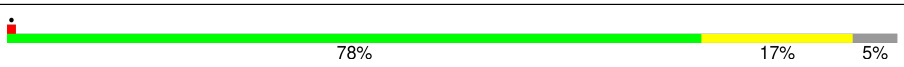
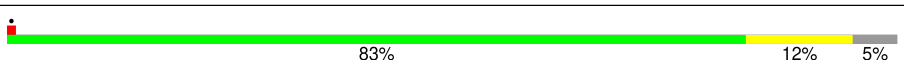
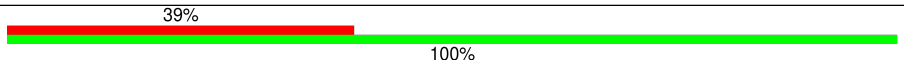
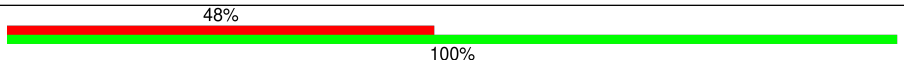
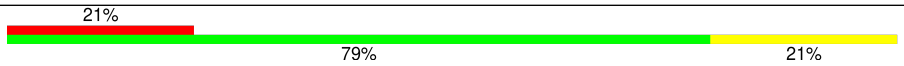
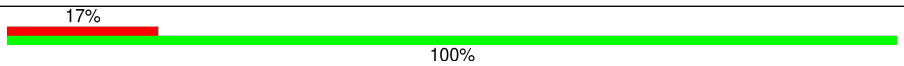
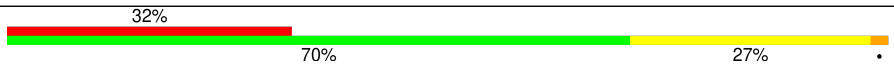
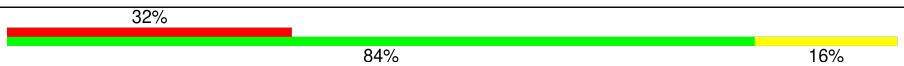
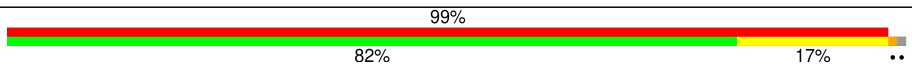
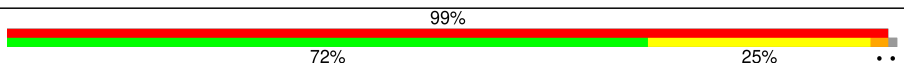
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	70%, 62%, 35%
1	a	167	67%, 63%, 29%, 5%
2	B	224	62%, 35%
2	b	224	72%, 26%

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	
9	I	120	
9	i	120	

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	FES	A	201	-	-	X	-
11	HEC	B	301	X	-	-	-
11	HEC	C	301	X	-	-	-
11	HEC	b	301	X	-	-	-
11	HEC	c	302	X	-	-	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 16361 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		

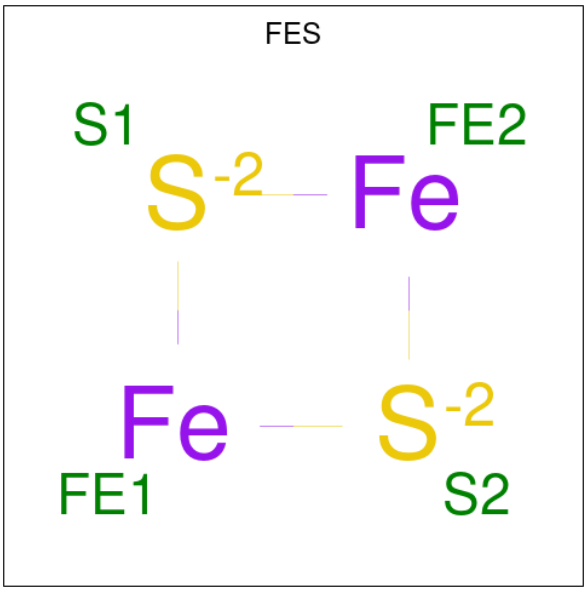
- Molecule 8 is a protein called YqzM.

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 a protein called YlbA.

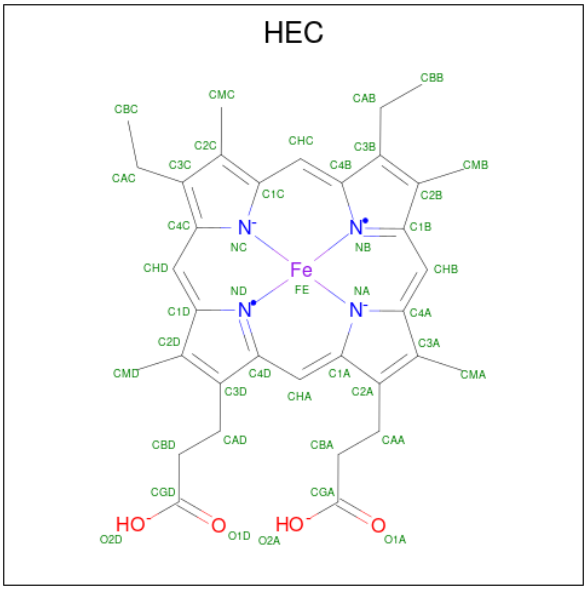
Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			941	603	153	181	4		
9	i	119	Total	C	N	O	S	0	0
			941	603	153	181	4		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



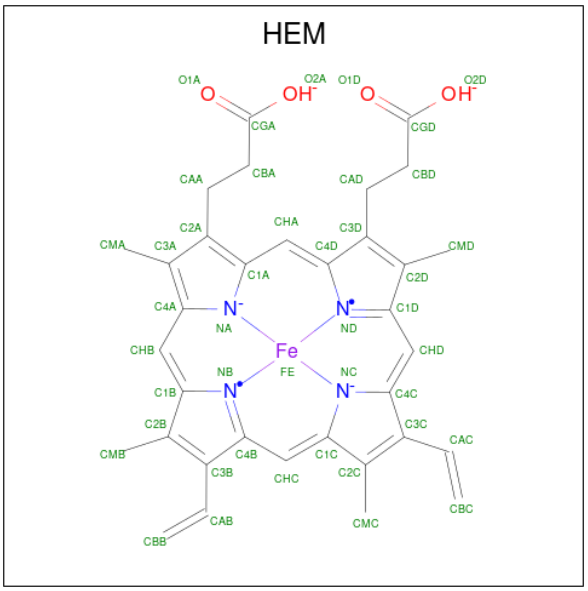
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

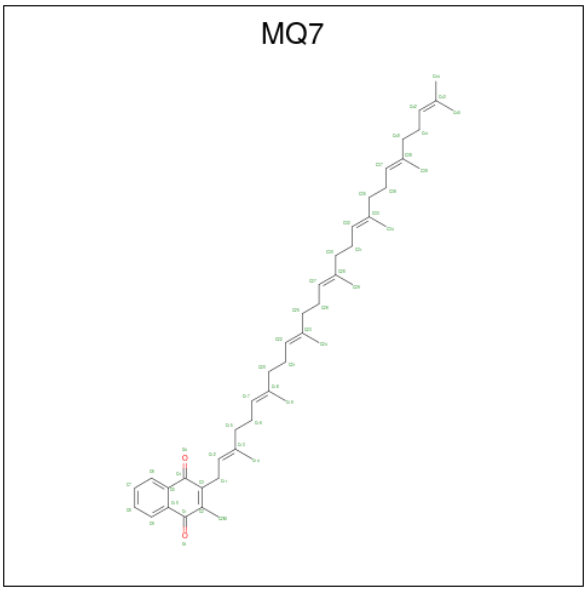
Mol	Chain	Residues	Atoms					AltConf
11	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



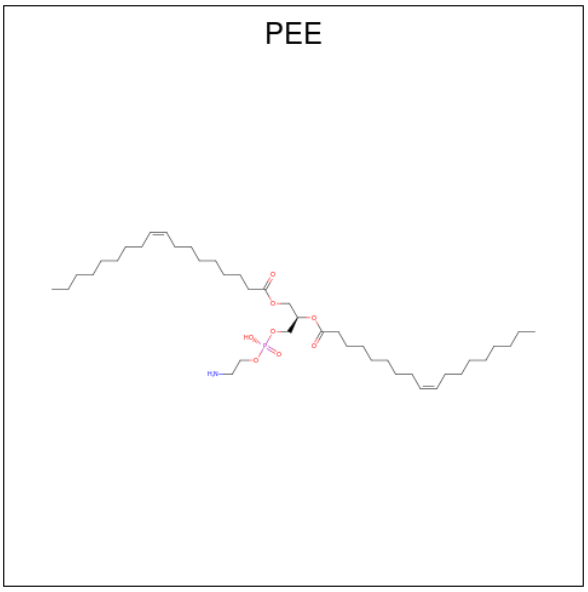
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



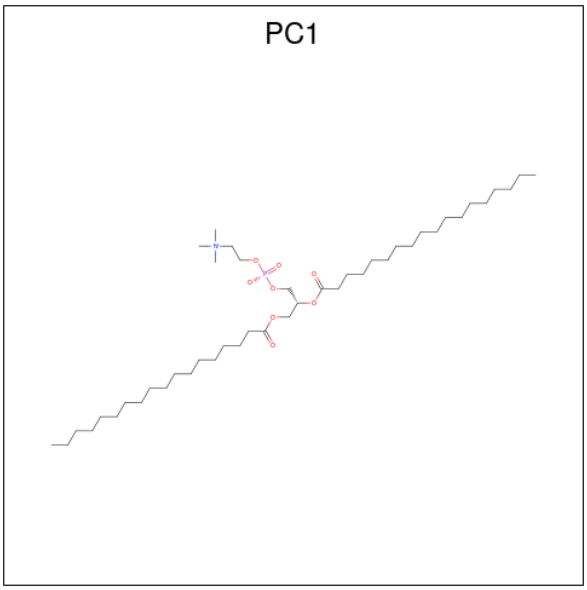
Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total C O 48 46 2	0
13	B	1	Total C O 48 46 2	0
13	b	1	Total C O 48 46 2	0
13	c	1	Total C O 48 46 2	0

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



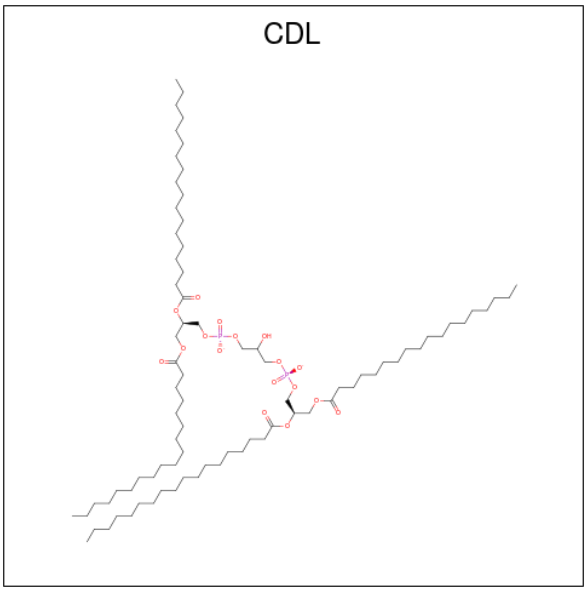
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
14	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
14	c	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	e	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 15 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
15	E	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

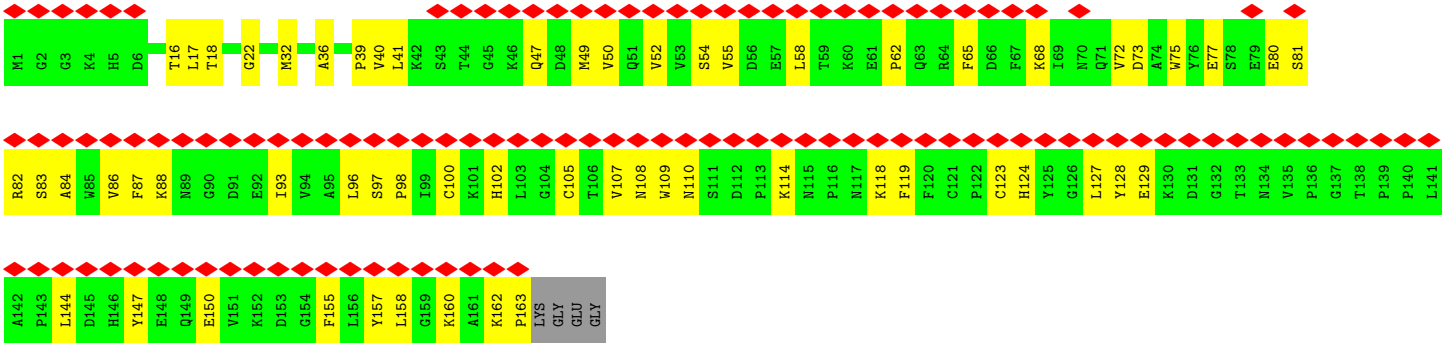
3 Residue-property plots (i)

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:

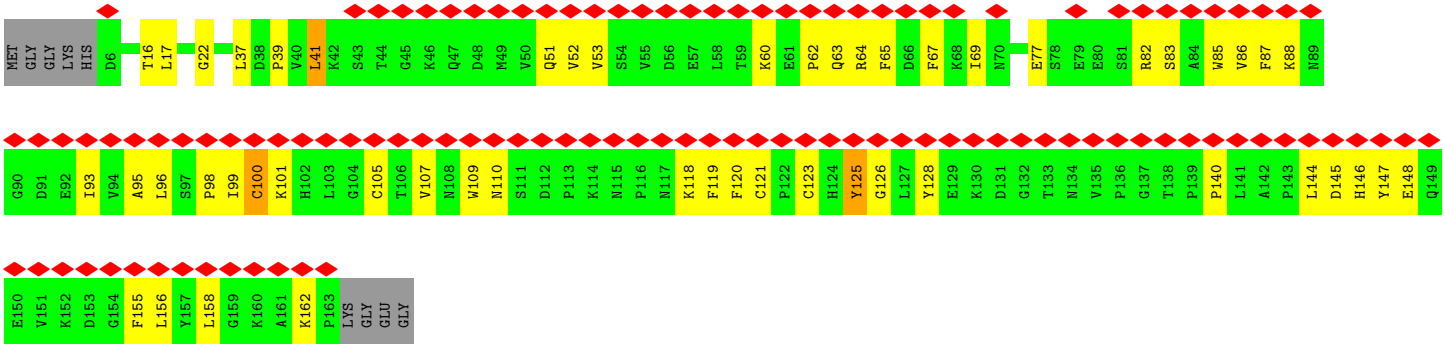




• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain a:

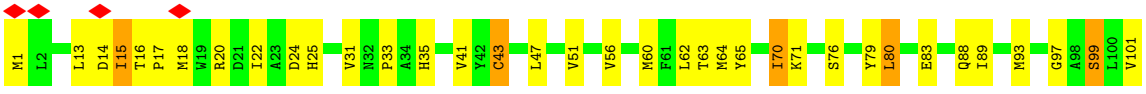




• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain B:



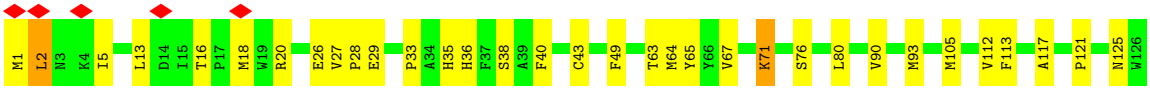


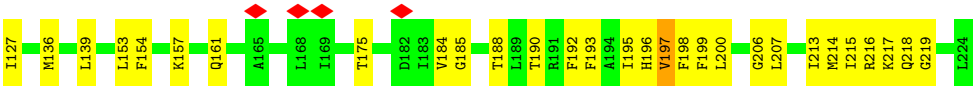


• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain b:



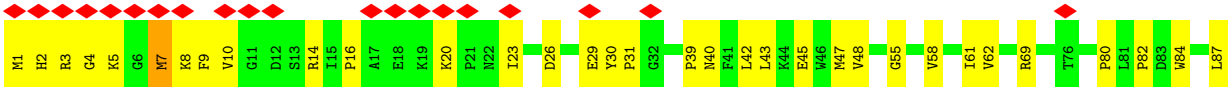


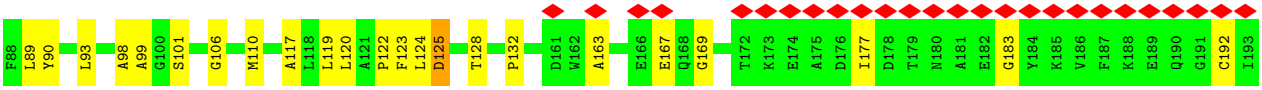


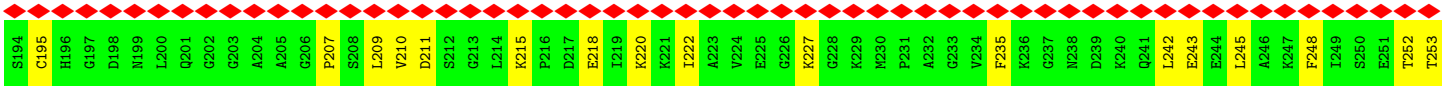
• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain C:







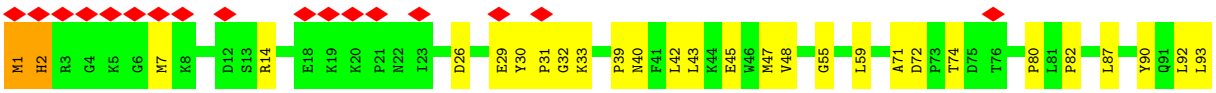


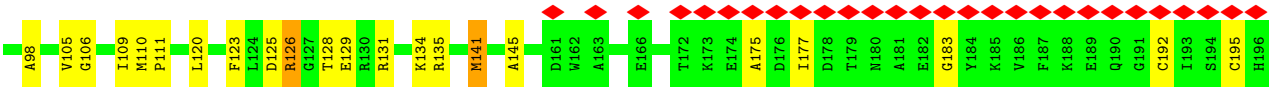


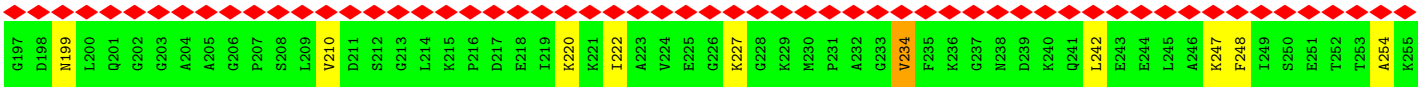
• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain c:



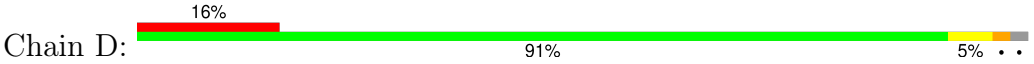


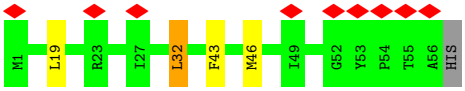




• Molecule 4: YqgW

Chain D:

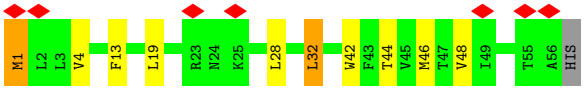




• Molecule 4: YqgW

Chain d:





• Molecule 5: YqgY

Chain E:

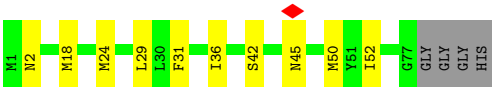




• Molecule 5: YqgY

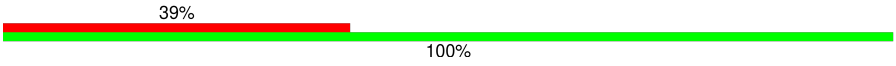
Chain e:

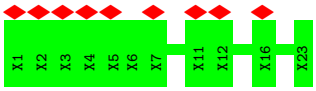




• Molecule 6: QcrF

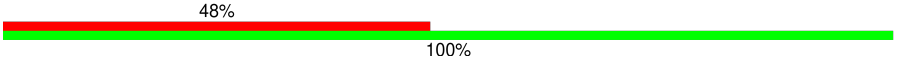
Chain F:

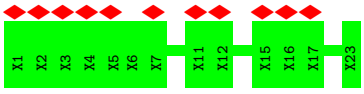




• Molecule 6: QcrF

Chain f:

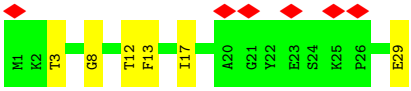




• Molecule 7: QcrG

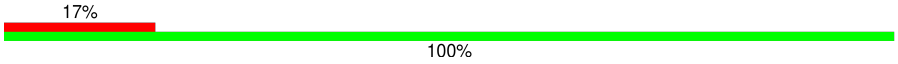
Chain G:

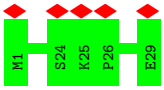




• Molecule 7: QcrG

Chain g:

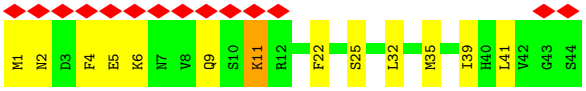




• Molecule 8: YqzM

Chain H:

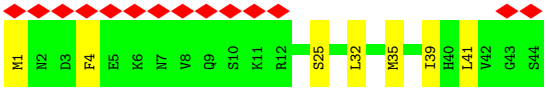




• Molecule 8: YqzM

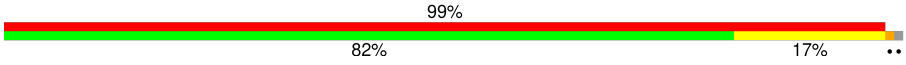
Chain h:

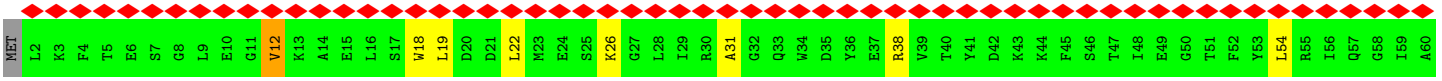


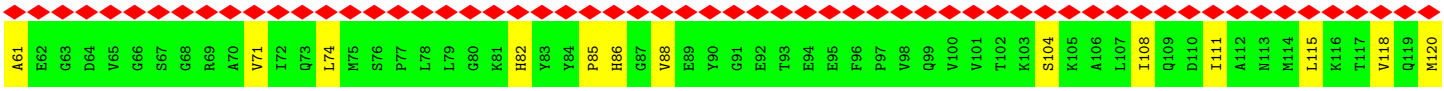


• Molecule 9: YlbA

Chain I:

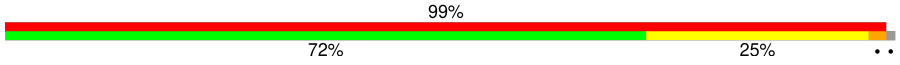


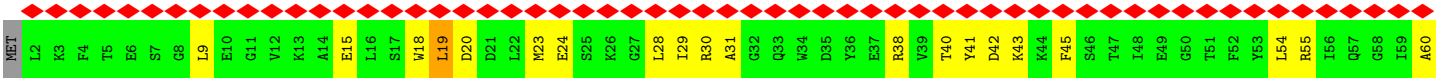


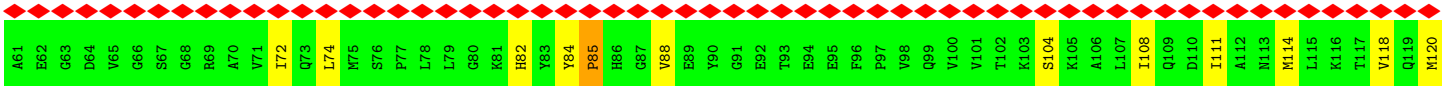


• Molecule 9: YlbA

Chain i:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195628	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	2.724	Depositor
Minimum map value	-1.514	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, HEC, HEM, FES, PC1, PEE, MQ7

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	0.24	0/1326	0.42	0/1796
1	a	0.26	0/1290	0.46	0/1750
2	B	0.44	0/1863	0.52	0/2533
2	b	0.43	0/1863	0.47	0/2533
3	C	0.33	0/2040	0.52	1/2759 (0.0%)
3	c	0.30	0/2040	0.48	1/2759 (0.0%)
4	D	0.24	0/444	0.36	0/605
4	d	0.25	0/444	0.31	0/605
5	E	0.34	0/667	0.39	0/900
5	e	0.35	0/667	0.38	0/900
7	G	0.27	0/224	0.43	0/299
7	g	0.25	0/224	0.30	0/299
8	H	0.26	0/349	0.37	0/468
8	h	0.25	0/349	0.32	0/468
9	I	0.14	0/959	0.32	0/1291
9	i	0.14	0/959	0.40	0/1291
All	All	0.32	0/15708	0.45	2/21256 (0.0%)

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
9	i	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	125	ASP	CA-CB-CG	6.65	119.25	112.60
3	c	7	MET	CB-CA-C	-6.30	109.29	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	i	84	TYR	Peptide

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	1254	47	0
1	a	1255	0	1216	40	0
2	B	1804	0	1813	74	0
2	b	1804	0	1813	50	0
3	C	1986	0	1997	60	0
3	c	1986	0	1997	57	0
4	D	433	0	463	3	0
4	d	433	0	463	7	0
5	E	645	0	642	8	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	4	0
7	g	221	0	241	0	0
8	H	342	0	334	10	0
8	h	342	0	334	5	0
9	I	941	0	938	19	0
9	i	941	0	938	23	0
10	A	4	0	0	5	0
10	a	4	0	0	0	0
11	B	43	0	31	6	0
11	C	43	0	32	2	0
11	b	43	0	31	6	0
11	c	43	0	30	1	0
12	B	86	0	60	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	b	86	0	60	3	0
13	B	96	0	128	12	0
13	b	48	0	64	7	0
13	c	48	0	64	8	0
14	C	44	0	57	3	0
14	a	40	0	48	2	0
14	c	47	0	65	7	0
14	e	34	0	42	4	0
15	E	37	0	48	0	0
16	b	98	0	149	7	0
All	All	16361	0	16285	375	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 11.

All (375) 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)
1:A:124:HIS:CE1	10:A:201:FES:S2	2.40	1.10
1:a:121:CYS:HB2	1:a:123:CYS:SG	1.96	1.06
1:a:100:CYS:SG	1:a:105:CYS:CB	2.57	0.93
1:a:121:CYS:CB	1:a:123:CYS:SG	2.64	0.81
1:a:101:LYS:HZ1	1:a:145:ASP:HB2	1.45	0.80
1:a:100:CYS:SG	1:a:105:CYS:HB3	2.18	0.79
1:A:119:PHE:HB2	1:A:128:TYR:HB2	1.65	0.77
2:B:132:ILE:HG21	12:B:303:HEM:HBA2	1.68	0.76
2:B:25:HIS:HA	9:I:86:HIS:HE1	1.51	0.76
1:A:98:PRO:HA	1:A:107:VAL:HG22	1.68	0.75
1:a:126:GLY:HA2	1:a:140:PRO:HD3	1.67	0.74
11:b:301:HEC:C1C	3:c:45:GLU:HB3	2.18	0.74
1:a:96:LEU:HD23	1:a:144:LEU:HB2	1.69	0.74
3:c:141:MET:HB3	14:c:303:PEE:H21	1.71	0.73
2:B:97:GLY:O	2:B:101:VAL:HG23	1.89	0.72
1:a:147:TYR:HB2	1:a:158:LEU:HD12	1.71	0.72
13:B:304:MQ7:H8	3:C:90:TYR:HD1	1.56	0.71
3:c:90:TYR:HD1	13:c:301:MQ7:H8	1.54	0.71
1:A:49:MET:HE2	1:A:157:TYR:HB3	1.71	0.71
9:i:9:LEU:HB3	9:i:74:LEU:HD23	1.73	0.70
2:B:130:VAL:HG11	3:C:119:LEU:HB2	1.72	0.70
2:b:207:LEU:HD11	13:c:301:MQ7:H32	1.75	0.69
1:a:62:PRO:HA	1:a:86:VAL:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:16:THR:HG21	5:e:52:ILE:HD12	1.74	0.69
1:A:72:VAL:HG13	1:A:77:GLU:HG3	1.75	0.69
1:a:107:VAL:HG12	1:a:121:CYS:HB3	1.74	0.68
12:B:303:HEM:HBD1	12:B:303:HEM:HHA	1.75	0.68
2:b:154:PHE:HB3	3:c:80:PRO:HB3	1.75	0.68
3:C:58:VAL:O	3:C:62:VAL:HG22	1.94	0.66
2:B:25:HIS:HA	9:I:86:HIS:CE1	2.30	0.66
3:C:119:LEU:O	3:C:120:LEU:HB2	1.94	0.66
1:A:102:HIS:HB3	10:A:201:FES:S2	2.36	0.65
2:b:49:PHE:HD2	11:b:301:HEC:HMB2	1.62	0.65
1:a:101:LYS:HD3	1:a:144:LEU:HA	1.78	0.65
1:A:54:SER:HA	1:A:155:PHE:HA	1.78	0.64
16:b:305:CDL:H762	16:b:305:CDL:HA61	1.80	0.64
1:A:58:LEU:HB2	1:A:88:LYS:HE3	1.80	0.64
1:a:96:LEU:HG	1:a:146:HIS:HB3	1.80	0.64
3:c:131:ARG:HH21	3:c:134:LYS:HG3	1.62	0.64
1:A:49:MET:HE3	1:A:50:VAL:H	1.61	0.64
3:C:43:LEU:O	3:C:47:MET:HG3	1.98	0.64
2:b:2:LEU:HA	2:b:5:ILE:HD12	1.80	0.63
3:C:220:LYS:HG2	3:C:242:LEU:HG	1.81	0.63
3:c:43:LEU:O	3:c:47:MET:HG3	1.98	0.63
2:B:105:MET:HG3	12:B:303:HEM:CGD	2.28	0.62
2:b:90:VAL:HA	2:b:93:MET:HE2	1.81	0.62
3:C:1:MET:HE3	3:C:14:ARG:HB3	1.82	0.62
7:G:8:GLY:O	7:G:12:THR:HG23	2.00	0.62
12:B:303:HEM:HBC2	12:B:303:HEM:HHD	1.82	0.62
2:b:26:GLU:HG3	3:c:30:TYR:HD1	1.64	0.61
3:c:1:MET:HB3	3:c:14:ARG:HD2	1.82	0.61
2:B:217:LYS:HD3	2:b:13:LEU:HD22	1.82	0.61
1:A:109:TRP:CD1	1:A:110:ASN:HD22	2.18	0.61
2:B:169:ILE:O	2:B:173:VAL:HG23	2.01	0.61
2:B:216:ARG:HD3	13:B:305:MQ7:H2M2	1.81	0.61
1:A:105:CYS:HB2	1:A:123:CYS:SG	2.42	0.60
2:B:18:MET:HE2	13:b:304:MQ7:H152	1.82	0.60
3:c:2:HIS:H	3:c:2:HIS:CD2	2.18	0.60
5:e:18:MET:HE2	14:e:101:PEE:H58	1.84	0.60
4:d:46:MET:HA	4:d:46:MET:HE2	1.84	0.59
2:b:206:GLY:HA3	13:c:301:MQ7:H401	1.84	0.59
3:C:209:LEU:HD23	11:C:301:HEC:HBA2	1.83	0.59
1:a:95:ALA:HB3	1:a:158:LEU:HD11	1.83	0.59
2:B:193:PHE:O	2:B:197:VAL:HB	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:305:CDL:HA61	16:b:305:CDL:H731	1.85	0.59
3:c:220:LYS:HG2	3:c:242:LEU:HG	1.83	0.58
8:H:35:MET:O	8:H:39:ILE:HG13	2.04	0.58
1:A:105:CYS:HB3	10:A:201:FES:S2	2.43	0.58
8:h:35:MET:O	8:h:39:ILE:HG13	2.04	0.58
2:B:31:VAL:HG21	11:B:301:HEC:HBB1	1.86	0.57
13:B:304:MQ7:H7	3:C:93:LEU:HD12	1.85	0.57
2:B:111:ARG:HA	7:G:17:ILE:HG23	1.86	0.57
9:I:26:LYS:HG3	9:I:111:ILE:HD11	1.86	0.57
3:c:177:ILE:HD11	3:c:199:ASN:O	2.05	0.57
2:b:40:PHE:O	2:b:43:CYS:HB2	2.04	0.57
2:b:35:HIS:HE1	9:i:31:ALA:HB1	1.70	0.57
9:i:60:ALA:HA	9:i:72:ILE:HD13	1.87	0.57
1:A:62:PRO:HA	1:A:87:PHE:HB3	1.88	0.56
3:C:98:ALA:HB1	3:C:106:GLY:HA3	1.87	0.56
2:B:13:LEU:HD13	13:b:304:MQ7:H242	1.86	0.56
2:B:133:PHE:HD2	12:B:303:HEM:O1D	1.89	0.56
2:B:184:VAL:HG13	2:B:188:THR:HG21	1.87	0.56
2:b:184:VAL:HG13	2:b:188:THR:HG21	1.87	0.56
2:B:13:LEU:HD21	2:b:214:MET:HG2	1.87	0.56
11:B:301:HEC:HBC1	3:C:48:VAL:HG21	1.87	0.56
2:B:161:GLN:HE22	2:B:174:LYS:HE2	1.70	0.56
3:C:235:PHE:HE1	3:C:245:LEU:HD23	1.70	0.56
2:b:157:LYS:O	2:b:161:GLN:HG2	2.05	0.56
16:b:305:CDL:H851	16:b:305:CDL:H381	1.87	0.56
3:C:31:PRO:HG3	9:I:88:VAL:HG23	1.87	0.55
13:b:304:MQ7:H291	13:b:304:MQ7:H32	1.87	0.55
3:C:163:ALA:O	3:C:167:GLU:HG3	2.05	0.55
1:a:148:GLU:HB3	1:a:162:LYS:HD2	1.88	0.55
3:c:175:ALA:HB1	3:c:254:ALA:HB1	1.87	0.55
4:D:46:MET:HA	4:D:46:MET:HE2	1.89	0.55
3:C:10:VAL:HG13	2:b:121:PRO:HG3	1.89	0.55
3:C:3:ARG:NE	3:C:4:GLY:H	2.04	0.54
2:b:16:THR:O	2:b:20:ARG:HG2	2.07	0.54
2:b:193:PHE:O	2:b:197:VAL:HB	2.06	0.54
2:b:65:TYR:O	2:b:76:SER:HB2	2.07	0.54
9:I:12:VAL:HG11	9:I:115:LEU:HD13	1.90	0.54
12:B:303:HEM:HBD1	12:B:303:HEM:CHA	2.38	0.53
3:c:125:ASP:OD1	14:c:303:PEE:H11	2.08	0.53
2:B:56:VAL:O	2:B:60:MET:HG3	2.08	0.53
2:B:47:LEU:O	2:B:51:VAL:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:63:GLN:HE22	1:a:65:PHE:HB2	1.72	0.53
1:A:105:CYS:CB	10:A:201:FES:S2	2.96	0.53
2:B:125:ASN:HD21	2:B:215:ILE:HG13	1.74	0.53
5:E:67:THR:HG23	5:E:71:ILE:HD12	1.90	0.53
3:c:31:PRO:HG2	9:i:82:HIS:CD2	2.43	0.53
2:B:217:LYS:HG2	13:B:305:MQ7:O4	2.08	0.53
1:a:101:LYS:NZ	1:a:145:ASP:HB2	2.22	0.52
14:c:303:PEE:H55	4:d:32:LEU:HB3	1.90	0.52
1:A:39:PRO:HB2	2:b:175:THR:HG22	1.91	0.52
3:C:4:GLY:HA2	9:i:85:PRO:HG2	1.91	0.52
3:C:9:PHE:CE2	9:i:85:PRO:HG3	2.45	0.52
12:B:302:HEM:HHC	12:B:302:HEM:HBB2	1.90	0.52
1:a:51:GLN:HE22	1:a:155:PHE:HB3	1.74	0.52
2:B:70:ILE:HD12	2:B:71:LYS:H	1.75	0.52
2:B:99:SER:HB3	3:C:84:TRP:HE1	1.75	0.52
14:a:202:PEE:O4P	14:a:202:PEE:H8	2.10	0.52
2:B:112:VAL:HG13	2:B:117:ALA:HB3	1.92	0.51
8:H:9:GLN:HE22	9:I:38:ARG:HD2	1.76	0.51
12:B:303:HEM:HHA	12:B:303:HEM:CBD	2.39	0.51
2:B:70:ILE:HD12	2:B:71:LYS:N	2.25	0.51
13:B:304:MQ7:H393	13:B:304:MQ7:H341	1.92	0.51
9:I:85:PRO:C	9:I:86:HIS:HD2	2.19	0.51
2:b:26:GLU:HG3	3:c:30:TYR:CD1	2.46	0.51
1:a:62:PRO:HG2	1:a:109:TRP:CD2	2.46	0.51
2:b:213:ILE:HD13	13:b:304:MQ7:H192	1.92	0.51
2:B:43:CYS:SG	3:C:48:VAL:HG11	2.50	0.51
2:B:105:MET:HE1	2:B:132:ILE:HG22	1.93	0.50
2:B:123:GLU:O	2:B:127:ILE:HG12	2.10	0.50
9:i:15:GLU:O	9:i:19:LEU:HD22	2.12	0.50
1:A:36:ALA:HA	2:B:64:MET:HE1	1.94	0.50
3:c:59:LEU:HD22	14:e:101:PEE:H20	1.93	0.50
5:E:47:THR:HG22	5:E:49:ARG:H	1.76	0.50
2:b:105:MET:HE1	2:b:136:MET:HB3	1.94	0.50
3:C:220:LYS:HE2	3:C:243:GLU:HA	1.94	0.50
1:a:119:PHE:HB2	1:a:128:TYR:HB2	1.94	0.50
9:I:61:ALA:HB3	9:I:71:VAL:HG23	1.92	0.50
3:c:72:ASP:OD1	3:c:74:THR:HG22	2.12	0.50
3:c:210:VAL:HG13	3:c:254:ALA:HB3	1.92	0.50
1:a:83:SER:HB3	1:a:98:PRO:HG2	1.93	0.50
3:c:93:LEU:HD12	13:c:301:MQ7:H7	1.93	0.49
1:A:18:THR:OG1	8:H:22:PHE:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:TYR:O	2:B:76:SER:HB3	2.12	0.49
1:a:41:LEU:HB3	8:h:41:LEU:HD21	1.94	0.49
3:C:3:ARG:HE	3:C:4:GLY:H	1.60	0.49
3:C:93:LEU:O	3:C:99:ALA:HB2	2.12	0.49
1:a:22:GLY:HA3	8:h:25:SER:OG	2.13	0.49
2:b:195:ILE:HA	2:b:199:PHE:HD2	1.76	0.49
12:b:303:HEM:HBC2	12:b:303:HEM:HMC2	1.94	0.49
3:c:145:ALA:HB2	14:c:303:PEE:H67	1.94	0.49
9:i:30:ARG:HD3	9:i:41:TYR:HE1	1.78	0.49
9:i:54:LEU:HD13	9:i:104:SER:HB3	1.94	0.49
2:B:15:ILE:HG22	2:B:15:ILE:O	2.13	0.49
3:C:31:PRO:HG2	9:I:82:HIS:CD2	2.48	0.49
9:I:85:PRO:C	9:I:86:HIS:CD2	2.91	0.49
2:b:125:ASN:HD21	2:b:215:ILE:HG13	1.77	0.49
11:b:301:HEC:CHC	3:c:45:GLU:HB3	2.43	0.49
2:b:216:ARG:HG2	11:b:301:HEC:HBA2	1.94	0.48
13:c:301:MQ7:H412	13:c:301:MQ7:H391	1.56	0.48
16:b:305:CDL:H761	16:b:305:CDL:HB62	1.94	0.48
1:A:16:THR:HG21	5:E:52:ILE:HG12	1.95	0.48
1:A:96:LEU:HD11	1:A:144:LEU:HB3	1.95	0.48
1:a:37:LEU:O	1:a:41:LEU:HD12	2.14	0.48
13:B:304:MQ7:O1	3:C:82:PRO:HB3	2.13	0.48
9:I:19:LEU:HD11	9:I:74:LEU:HD11	1.95	0.48
1:A:162:LYS:NZ	1:A:163:PRO:HD2	2.28	0.48
3:C:132:PRO:HB2	7:G:29:GLU:HG3	1.96	0.48
1:A:118:LYS:HE2	1:A:127:LEU:HD11	1.95	0.48
13:B:305:MQ7:H32	13:B:305:MQ7:H27	1.96	0.48
3:C:42:LEU:HA	3:C:45:GLU:HG3	1.96	0.48
3:c:26:ASP:HB3	3:c:29:GLU:HG2	1.96	0.48
1:A:32:MET:HE2	2:B:93:MET:HE1	1.95	0.48
1:A:41:LEU:HB3	8:H:41:LEU:HD21	1.95	0.48
3:C:2:HIS:O	3:C:5:LYS:HG3	2.14	0.48
1:a:62:PRO:HG3	1:a:87:PHE:HD2	1.79	0.48
3:c:98:ALA:HB1	3:c:106:GLY:HA3	1.96	0.48
3:c:105:VAL:HG11	4:d:42:TRP:HZ3	1.79	0.48
2:B:126:TRP:CE3	12:B:303:HEM:HMD1	2.49	0.48
2:B:164:GLU:O	2:B:164:GLU:HG3	2.12	0.48
3:c:234:VAL:HG11	11:c:302:HEC:HAB	1.95	0.48
2:B:105:MET:HG3	12:B:303:HEM:O2D	2.15	0.47
2:B:210:ALA:HB1	13:B:305:MQ7:H262	1.96	0.47
1:a:99:ILE:HD12	1:a:105:CYS:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:23:MET:SD	9:i:41:TYR:HD2	2.37	0.47
1:A:100:CYS:HB3	1:A:107:VAL:CG1	2.44	0.47
1:a:52:VAL:HG12	1:a:53:VAL:HG23	1.95	0.47
3:C:211:ASP:H	3:C:253:THR:HA	1.79	0.47
2:B:150:MET:HG3	3:C:69:ARG:HG3	1.96	0.47
3:C:7:MET:SD	3:C:16:PRO:HB3	2.55	0.47
16:b:305:CDL:HB61	16:b:305:CDL:H712	1.60	0.47
2:B:141:PHE:CG	13:B:304:MQ7:H152	2.50	0.47
14:c:303:PEE:H49	14:c:303:PEE:H8	1.44	0.47
1:a:109:TRP:CE2	1:a:110:ASN:HB2	2.50	0.47
16:b:305:CDL:H191	16:b:305:CDL:H801	1.96	0.47
3:c:220:LYS:HA	3:c:242:LEU:HD11	1.96	0.47
13:c:301:MQ7:H291	13:c:301:MQ7:H311	1.64	0.47
2:B:20:ARG:O	2:B:24:ASP:HB2	2.14	0.46
3:c:120:LEU:HD13	4:d:28:LEU:HD21	1.97	0.46
3:c:82:PRO:HB3	13:c:301:MQ7:O1	2.15	0.46
3:c:183:GLY:HA3	3:c:248:PHE:HB3	1.97	0.46
3:C:192:CYS:C	3:C:195:CYS:HB3	2.41	0.46
3:C:207:PRO:HD2	11:C:301:HEC:HHA	1.97	0.46
1:A:82:ARG:HG2	1:A:82:ARG:HH11	1.80	0.46
1:A:124:HIS:CG	10:A:201:FES:S2	2.83	0.46
3:C:124:LEU:HD11	4:D:32:LEU:HD13	1.97	0.46
2:B:154:PHE:HB3	3:C:80:PRO:HB3	1.98	0.46
8:H:2:ASN:HB3	8:H:5:GLU:HB3	1.97	0.46
3:C:26:ASP:HB3	3:C:29:GLU:HG3	1.97	0.46
2:B:145:LEU:HA	2:B:152:ALA:HB1	1.98	0.46
13:B:304:MQ7:H341	13:B:304:MQ7:H362	1.74	0.46
3:C:120:LEU:HA	3:C:123:PHE:HD2	1.81	0.46
3:C:222:ILE:HG23	3:C:227:LYS:HB2	1.98	0.46
8:h:4:PHE:HE2	9:i:38:ARG:HG2	1.81	0.46
9:i:30:ARG:HD3	9:i:41:TYR:CE1	2.50	0.46
3:C:39:PRO:HG2	3:C:40:ASN:OD1	2.16	0.46
11:b:301:HEC:HMC3	3:c:48:VAL:HB	1.98	0.46
1:A:83:SER:HB3	1:A:98:PRO:HG2	1.98	0.46
2:B:65:TYR:HB2	2:B:80:LEU:HD12	1.96	0.46
3:c:2:HIS:H	3:c:2:HIS:HD2	1.63	0.46
3:C:192:CYS:CA	3:C:195:CYS:HB3	2.46	0.45
2:B:41:VAL:O	2:B:111:ARG:HD3	2.16	0.45
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.73	0.45
13:B:305:MQ7:H201	2:b:18:MET:SD	2.56	0.45
1:a:62:PRO:HG3	1:a:87:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:126:ARG:HE	3:c:126:ARG:HB2	1.47	0.45
9:I:86:HIS:HB2	3:c:2:HIS:HA	1.98	0.45
1:A:68:LYS:NZ	1:A:81:SER:HB3	2.31	0.45
3:C:82:PRO:HG2	3:C:87:LEU:HD23	1.98	0.45
2:b:192:PHE:O	2:b:196:HIS:HB3	2.17	0.45
2:B:70:ILE:H	2:B:70:ILE:HG13	1.58	0.45
1:A:65:PHE:CE1	1:A:86:VAL:HB	2.52	0.45
2:B:35:HIS:HE1	9:I:31:ALA:HB1	1.82	0.45
3:C:192:CYS:HA	3:C:195:CYS:HB3	1.99	0.45
5:e:18:MET:HG3	14:e:101:PEE:H60	1.99	0.45
1:A:22:GLY:HA3	8:H:25:SER:OG	2.17	0.45
2:B:119:LYS:NZ	3:C:125:ASP:OD1	2.39	0.45
3:C:14:ARG:NH2	2:b:219:GLY:HA2	2.32	0.45
1:A:114:LYS:HB3	1:A:114:LYS:HE2	1.72	0.45
3:C:110:MET:HE1	4:D:43:PHE:CG	2.52	0.45
11:B:301:HEC:HHC	11:B:301:HEC:HAB	1.75	0.44
4:d:44:THR:O	4:d:48:VAL:HG12	2.16	0.44
11:b:301:HEC:C2C	3:c:45:GLU:HB3	2.48	0.44
2:B:62:LEU:HD22	2:B:80:LEU:HD11	1.98	0.44
2:B:132:ILE:HG21	12:B:303:HEM:CBA	2.43	0.44
11:B:301:HEC:HBA1	11:B:301:HEC:HMA3	1.99	0.44
2:b:153:LEU:HD22	3:c:71:ALA:HB1	2.00	0.44
2:B:17:PRO:HG3	3:C:20:LYS:HG3	1.99	0.44
2:B:204:LEU:O	2:B:208:MET:HB2	2.18	0.44
2:b:1:MET:HE3	2:b:5:ILE:HD11	1.99	0.44
2:b:33:PRO:HA	2:b:36:HIS:O	2.17	0.44
2:B:164:GLU:OE1	2:B:174:LYS:HD3	2.17	0.44
9:I:86:HIS:CG	3:c:2:HIS:HA	2.53	0.44
9:I:54:LEU:HD13	9:I:104:SER:HB3	2.00	0.44
1:A:68:LYS:HA	1:A:80:GLU:O	2.18	0.44
3:C:183:GLY:HA3	3:C:248:PHE:HB3	1.99	0.44
5:E:2:ASN:O	5:E:42:SER:HB2	2.17	0.44
1:a:69:ILE:HD11	1:a:82:ARG:HE	1.83	0.44
16:b:305:CDL:H592	16:b:305:CDL:H561	1.82	0.44
5:e:2:ASN:O	5:e:42:SER:HB2	2.18	0.44
12:B:303:HEM:HHD	12:B:303:HEM:CBC	2.46	0.43
13:B:304:MQ7:H8	3:C:90:TYR:CD1	2.45	0.43
3:C:23:ILE:HD12	8:H:11:LYS:HD2	2.00	0.43
13:b:304:MQ7:H162	13:b:304:MQ7:H12	1.82	0.43
4:d:1:MET:O	4:d:4:VAL:HG12	2.18	0.43
1:A:55:VAL:HG23	1:A:58:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HA	3:C:43:LEU:HD13	2.00	0.43
2:B:139:LEU:HG	2:B:200:LEU:HB3	2.00	0.43
2:b:213:ILE:O	2:b:217:LYS:HG3	2.19	0.43
3:c:1:MET:CB	3:c:14:ARG:HD2	2.49	0.43
3:C:117:ALA:HB1	14:C:302:PEE:H51	2.00	0.43
3:C:177:ILE:HD11	3:C:252:THR:HG23	2.00	0.43
1:a:88:LYS:HA	1:a:93:ILE:HA	2.01	0.43
3:c:110:MET:HB2	3:c:111:PRO:HD3	2.00	0.43
1:A:100:CYS:HA	1:A:144:LEU:HD21	2.01	0.43
2:B:15:ILE:H	2:B:15:ILE:CD1	2.31	0.43
2:B:63:THR:O	2:b:190:THR:HG22	2.19	0.43
3:c:183:GLY:HA3	3:c:248:PHE:CG	2.54	0.43
1:A:73:ASP:OD2	2:b:185:GLY:HA3	2.18	0.43
2:B:123:GLU:CG	3:C:122:PRO:HB2	2.49	0.43
8:h:4:PHE:CE2	9:i:38:ARG:HG2	2.53	0.43
2:b:112:VAL:HG11	12:b:303:HEM:HMD2	2.01	0.43
3:c:141:MET:HE2	4:d:13:PHE:HB3	2.01	0.43
9:i:108:ILE:O	9:i:111:ILE:HG13	2.19	0.43
1:A:68:LYS:HE3	1:A:68:LYS:HB3	1.87	0.43
7:G:13:PHE:O	7:G:17:ILE:HG12	2.19	0.43
9:i:45:PHE:HE2	9:i:104:SER:OG	2.02	0.43
2:B:33:PRO:O	5:E:3:ARG:HG2	2.18	0.43
2:B:212:PHE:CE2	11:B:301:HEC:HBA2	2.54	0.43
8:H:4:PHE:CE1	9:I:38:ARG:HG2	2.54	0.43
2:b:214:MET:O	2:b:218:GLN:HG3	2.19	0.43
1:A:84:ALA:HA	1:A:98:PRO:HD3	2.01	0.42
2:B:126:TRP:O	2:B:130:VAL:HG23	2.18	0.42
2:B:214:MET:O	2:B:218:GLN:HG3	2.18	0.42
2:B:63:THR:HG21	2:b:198:PHE:HE2	1.83	0.42
2:b:29:GLU:HG3	3:c:33:LYS:CB	2.49	0.42
3:c:183:GLY:HA3	3:c:248:PHE:CB	2.49	0.42
9:i:28:LEU:HG	9:i:43:LYS:HB2	2.02	0.42
9:i:114:MET:O	9:i:118:VAL:HG23	2.20	0.42
3:c:92:LEU:HD22	14:c:303:PEE:H81	1.99	0.42
3:c:129:GLU:O	3:c:135:ARG:HD2	2.19	0.42
3:c:222:ILE:HG12	3:c:227:LYS:HB2	2.01	0.42
2:b:29:GLU:HG3	3:c:33:LYS:HB2	2.01	0.42
2:b:136:MET:CE	12:b:303:HEM:HBB1	2.49	0.42
3:c:39:PRO:HG2	3:c:40:ASN:OD1	2.19	0.42
3:c:105:VAL:HA	3:c:109:ILE:HB	2.01	0.42
9:I:18:TRP:HH2	9:I:118:VAL:HB	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:113:PHE:CZ	14:c:303:PEE:H19	2.54	0.42
2:B:15:ILE:H	2:B:15:ILE:HD12	1.83	0.42
2:B:18:MET:O	2:B:22:ILE:HG23	2.20	0.42
1:a:60:LYS:HE3	1:a:88:LYS:HG2	2.00	0.42
3:c:192:CYS:HB2	3:c:195:CYS:HB2	1.73	0.42
9:i:18:TRP:NE1	9:i:118:VAL:HG21	2.35	0.42
1:a:64:ARG:HB2	1:a:85:TRP:CH2	2.53	0.42
2:b:127:ILE:HD11	3:c:123:PHE:CE2	2.55	0.42
2:B:198:PHE:HE2	2:b:63:THR:HG21	1.85	0.42
2:B:220:ILE:CG1	11:B:301:HEC:HBB2	2.50	0.42
2:B:89:ILE:HD11	3:C:61:ILE:HG13	2.00	0.42
2:B:213:ILE:O	2:B:217:LYS:HG3	2.19	0.42
3:C:55:GLY:HA2	5:E:31:PHE:CZ	2.55	0.41
1:A:88:LYS:HA	1:A:93:ILE:HA	2.02	0.41
14:C:302:PEE:H49	14:C:302:PEE:H54	1.85	0.41
1:a:120:PHE:HE1	1:a:125:TYR:HA	1.84	0.41
1:A:49:MET:HE1	1:A:158:LEU:O	2.19	0.41
1:A:147:TYR:HA	1:A:160:LYS:O	2.20	0.41
3:C:215:LYS:HB2	3:C:218:GLU:HG3	2.01	0.41
14:C:302:PEE:H7	14:C:302:PEE:O1P	2.21	0.41
14:a:202:PEE:H16	14:a:202:PEE:H22	1.86	0.41
1:A:150:GLU:HG2	1:A:157:TYR:HB2	2.02	0.41
2:B:79:TYR:CD1	2:B:83:GLU:HG3	2.56	0.41
2:B:194:ALA:CB	2:b:64:MET:HG2	2.51	0.41
2:b:27:VAL:HA	2:b:28:PRO:HD3	1.97	0.41
3:c:31:PRO:HA	9:i:55:ARG:NH1	2.36	0.41
9:i:29:ILE:HD13	9:i:31:ALA:HB3	2.01	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.77	0.41
3:C:69:ARG:HG2	3:C:169:GLY:HA2	2.02	0.41
5:E:44:LEU:HD23	5:E:44:LEU:HA	1.90	0.41
2:B:14:ASP:O	2:B:15:ILE:C	2.63	0.41
2:b:18:MET:HE2	2:b:18:MET:HB3	1.70	0.41
1:A:97:SER:HA	1:A:147:TYR:CE2	2.56	0.41
1:A:128:TYR:CE2	1:A:144:LEU:HG	2.56	0.41
2:B:120:LYS:HA	2:B:121:PRO:HA	1.88	0.41
8:H:9:GLN:HA	9:I:38:ARG:NH1	2.36	0.41
3:c:32:GLY:HA2	9:i:42:ASP:OD2	2.21	0.41
1:A:47:GLN:HE22	1:A:160:LYS:N	2.18	0.41
3:C:30:TYR:HA	3:C:31:PRO:HD3	1.87	0.41
1:a:118:LYS:HD3	1:a:128:TYR:O	2.21	0.41
2:b:35:HIS:CE1	9:i:31:ALA:HB1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:213:ILE:HG22	13:b:304:MQ7:H243	2.03	0.41
3:c:247:LYS:HG3	3:c:248:PHE:N	2.36	0.41
8:H:6:LYS:HB3	8:H:6:LYS:HE2	1.87	0.41
13:b:304:MQ7:H112	13:b:304:MQ7:H2M1	1.84	0.41
5:e:2:ASN:ND2	5:e:45:ASN:HA	2.36	0.41
3:C:47:MET:HE3	5:E:8:LEU:HD11	2.03	0.40
2:B:1:MET:HE2	2:B:1:MET:HB2	1.88	0.40
2:b:139:LEU:HG	2:b:200:LEU:HB3	2.02	0.40
1:a:17:LEU:HD11	3:c:42:LEU:HG	2.03	0.40
1:a:98:PRO:HA	1:a:107:VAL:HG22	2.04	0.40
1:a:120:PHE:CE1	1:a:125:TYR:HA	2.57	0.40
3:c:55:GLY:HA2	5:e:31:PHE:CZ	2.56	0.40
3:c:90:TYR:CD1	13:c:301:MQ7:H8	2.45	0.40
9:i:20:ASP:O	9:i:24:GLU:HB2	2.22	0.40
9:I:26:LYS:HA	9:I:26:LYS:HD3	1.86	0.40
1:a:67:PHE:CE1	1:a:82:ARG:HB2	2.56	0.40
2:b:71:LYS:HZ2	2:b:71:LYS:HG2	1.70	0.40
2:b:112:VAL:HG13	2:b:117:ALA:HB3	2.02	0.40
5:e:2:ASN:HD21	5:e:45:ASN:HA	1.86	0.40
2:B:136:MET:HE2	2:B:136:MET:HB2	2.00	0.40
2:B:175:THR:HG22	1:a:39:PRO:HB2	2.02	0.40
3:C:210:VAL:HA	3:C:252:THR:HG22	2.04	0.40
3:c:82:PRO:HG2	3:c:87:LEU:HD23	2.03	0.40
5:e:24:MET:HE1	14:e:101:PEE:H13	2.03	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%)	149 (92%)	12 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	156/167 (93%)	140 (90%)	16 (10%)	0	100	100
2	B	222/224 (99%)	214 (96%)	6 (3%)	2 (1%)	14	30
2	b	222/224 (99%)	218 (98%)	4 (2%)	0	100	100
3	C	253/255 (99%)	230 (91%)	23 (9%)	0	100	100
3	c	253/255 (99%)	241 (95%)	12 (5%)	0	100	100
4	D	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
4	d	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
5	E	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
5	e	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
7	G	27/29 (93%)	22 (82%)	5 (18%)	0	100	100
7	g	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
8	H	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
8	h	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
9	I	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
9	i	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	14	30
All	All	1897/1954 (97%)	1791 (94%)	103 (5%)	3 (0%)	44	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	ILE
2	B	16	THR
9	i	85	PRO

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%)	137 (96%)	5 (4%)	32	59
1	a	139/144 (96%)	134 (96%)	5 (4%)	31	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	188/188 (100%)	179 (95%)	9 (5%)	23 47
2	b	188/188 (100%)	182 (97%)	6 (3%)	34 62
3	C	205/205 (100%)	200 (98%)	5 (2%)	43 70
3	c	205/205 (100%)	199 (97%)	6 (3%)	37 65
4	D	45/46 (98%)	43 (96%)	2 (4%)	25 50
4	d	45/46 (98%)	42 (93%)	3 (7%)	15 33
5	E	66/67 (98%)	63 (96%)	3 (4%)	24 50
5	e	66/67 (98%)	63 (96%)	3 (4%)	24 50
7	G	25/25 (100%)	24 (96%)	1 (4%)	28 55
7	g	25/25 (100%)	25 (100%)	0	100 100
8	H	37/37 (100%)	34 (92%)	3 (8%)	11 24
8	h	37/37 (100%)	35 (95%)	2 (5%)	20 42
9	I	100/101 (99%)	96 (96%)	4 (4%)	28 55
9	i	100/101 (99%)	96 (96%)	4 (4%)	28 55
All	All	1613/1626 (99%)	1552 (96%)	61 (4%)	30 56

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	52	VAL
1	A	75	TRP
1	A	108	ASN
1	A	129	GLU
2	B	43	CYS
2	B	70	ILE
2	B	80	LEU
2	B	88	GLN
2	B	99	SER
2	B	161	GLN
2	B	182	ASP
2	B	221	SER
2	B	224	LEU
3	C	7	MET
3	C	8	LYS
3	C	89	LEU
3	C	101	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	128	THR
4	D	19	LEU
4	D	32	LEU
5	E	1	MET
5	E	29	LEU
5	E	50	MET
7	G	3	THR
8	H	1	MET
8	H	11	LYS
8	H	32	LEU
9	I	12	VAL
9	I	22	LEU
9	I	108	ILE
9	I	120	MET
1	a	41	LEU
1	a	77	GLU
1	a	100	CYS
1	a	125	TYR
1	a	156	LEU
2	b	2	LEU
2	b	38	SER
2	b	67	VAL
2	b	71	LYS
2	b	80	LEU
2	b	197	VAL
3	c	1	MET
3	c	2	HIS
3	c	126	ARG
3	c	128	THR
3	c	141	MET
3	c	234	VAL
4	d	1	MET
4	d	19	LEU
4	d	32	LEU
5	e	29	LEU
5	e	36	ILE
5	e	50	MET
8	h	1	MET
8	h	32	LEU
9	i	19	LEU
9	i	40	THR
9	i	88	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	120	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	32	ASN
2	B	35	HIS
2	B	82	ASN
2	B	88	GLN
2	B	125	ASN
2	B	161	GLN
2	B	172	GLN
2	B	218	GLN
3	C	160	HIS
4	D	26	ASN
4	D	50	ASN
8	H	7	ASN
8	H	9	GLN
9	I	73	GLN
9	I	82	HIS
9	I	86	HIS
1	a	70	ASN
2	b	35	HIS
2	b	82	ASN
2	b	125	ASN
3	c	2	HIS
3	c	63	HIS
3	c	190	GLN
5	e	34	GLN
8	h	7	ASN
8	h	9	GLN
9	i	82	HIS
9	i	109	GLN
9	i	119	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
12	HEM	b	302	2	50,50,50	1.66	9 (18%)	67,82,82	1.62	12 (17%)
12	HEM	B	302	2	50,50,50	1.67	9 (18%)	67,82,82	1.70	15 (22%)
14	PEE	e	101	-	33,33,50	0.38	0	36,38,55	0.48	0
13	MQ7	b	304	-	49,49,49	0.40	0	61,63,63	0.84	2 (3%)
11	HEC	c	302	3	50,50,50	3.85	32 (64%)	68,82,82	9.13	31 (45%)
14	PEE	a	202	-	39,39,50	0.37	0	42,44,55	0.51	0
10	FES	a	201	1	0,4,4	-	-	-		
11	HEC	C	301	-	50,50,50	3.05	29 (58%)	68,82,82	2.24	27 (39%)
13	MQ7	B	305	-	49,49,49	0.39	0	61,63,63	0.61	1 (1%)
13	MQ7	B	304	-	49,49,49	0.43	1 (2%)	61,63,63	0.54	1 (1%)
14	PEE	c	303	-	46,46,50	0.39	0	49,51,55	0.42	0
16	CDL	b	305	-	97,97,99	0.28	0	103,109,111	0.40	0
15	PC1	E	101	-	36,36,53	0.61	0	42,44,61	0.67	1 (2%)
11	HEC	B	301	2	50,50,50	2.89	26 (52%)	68,82,82	2.76	26 (38%)
14	PEE	C	302	-	43,43,50	0.39	0	46,48,55	0.50	1 (2%)
10	FES	A	201	1	0,4,4	-	-	-		
12	HEM	b	303	2	50,50,50	1.72	10 (20%)	67,82,82	1.50	12 (17%)
11	HEC	b	301	2	50,50,50	2.78	26 (52%)	68,82,82	2.56	30 (44%)
12	HEM	B	303	2	50,50,50	1.79	13 (26%)	67,82,82	2.13	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	MQ7	c	301	-	49,49,49	0.42	0	61,63,63	0.50	1 (1%)

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
12	HEM	b	302	2	-	7/14/54/54	-
12	HEM	B	302	2	-	7/14/54/54	-
14	PEE	e	101	-	-	7/37/37/54	-
13	MQ7	b	304	-	-	7/41/61/61	0/2/2/2
11	HEC	c	302	3	1/1/3/7	10/14/54/54	-
14	PEE	a	202	-	-	15/43/43/54	-
10	FES	a	201	1	-	-	0/1/1/1
11	HEC	C	301	-	1/1/3/7	7/14/54/54	-
13	MQ7	B	305	-	-	10/41/61/61	0/2/2/2
13	MQ7	B	304	-	-	12/41/61/61	0/2/2/2
14	PEE	c	303	-	-	11/50/50/54	-
16	CDL	b	305	-	-	20/108/108/110	-
15	PC1	E	101	-	-	11/40/40/57	-
11	HEC	B	301	2	1/1/3/7	12/14/54/54	-
14	PEE	C	302	-	-	11/47/47/54	-
10	FES	A	201	1	-	-	0/1/1/1
12	HEM	b	303	2	-	0/14/54/54	-
11	HEC	b	301	2	1/1/3/7	9/14/54/54	-
12	HEM	B	303	2	-	8/14/54/54	-
13	MQ7	c	301	-	-	15/41/61/61	0/2/2/2

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	302	HEC	CAC-C3C	9.94	1.76	1.51
11	c	302	HEC	CMC-C2C	9.61	1.70	1.50
11	c	302	HEC	C3B-C2B	5.70	1.49	1.36
11	B	301	HEC	C2A-C3A	5.70	1.49	1.36
11	C	301	HEC	C3B-C2B	5.61	1.48	1.36
11	c	302	HEC	CHA-C1A	5.59	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	302	HEC	C3D-C2D	5.58	1.48	1.36
11	c	302	HEC	CHD-C1D	5.57	1.49	1.38
11	c	302	HEC	CHC-C4B	5.52	1.49	1.38
11	C	301	HEC	C2A-C3A	5.50	1.48	1.36
11	c	302	HEC	C2A-C3A	5.49	1.48	1.36
12	B	302	HEM	FE-NB	5.40	2.11	1.94
11	C	301	HEC	C3D-C2D	5.36	1.48	1.36
11	c	302	HEC	CHB-C4A	5.33	1.48	1.38
12	b	302	HEM	FE-NB	5.32	2.11	1.94
11	C	301	HEC	CHA-C1A	5.30	1.48	1.38
11	C	301	HEC	CHB-C4A	5.26	1.48	1.38
12	b	303	HEM	FE-NB	5.20	2.10	1.94
11	B	301	HEC	C3D-C2D	5.20	1.48	1.36
11	C	301	HEC	CHC-C4B	5.17	1.48	1.38
11	C	301	HEC	CHD-C1D	5.15	1.48	1.38
11	c	302	HEC	C4C-C3C	5.01	1.54	1.44
11	c	302	HEC	CHD-C4C	5.00	1.50	1.39
11	b	301	HEC	CHD-C1D	4.98	1.48	1.38
11	b	301	HEC	C2A-C3A	4.95	1.47	1.36
11	B	301	HEC	CHB-C4A	4.93	1.48	1.38
11	b	301	HEC	FE-NB	4.91	2.10	1.94
11	c	302	HEC	C3C-C2C	-4.89	1.26	1.38
11	B	301	HEC	C3B-C2B	4.84	1.47	1.36
11	B	301	HEC	FE-ND	4.80	2.09	1.94
11	B	301	HEC	CHA-C1A	4.78	1.47	1.38
11	B	301	HEC	CHD-C1D	4.78	1.48	1.38
11	B	301	HEC	FE-NB	4.76	2.09	1.94
11	b	301	HEC	FE-ND	4.76	2.09	1.94
11	C	301	HEC	FE-NB	4.71	2.09	1.94
11	b	301	HEC	C3D-C2D	4.68	1.46	1.36
11	B	301	HEC	FE-NA	4.66	2.10	1.95
11	C	301	HEC	FE-ND	4.65	2.09	1.94
11	B	301	HEC	FE-NC	4.65	2.10	1.95
11	b	301	HEC	CHA-C1A	4.60	1.47	1.38
11	b	301	HEC	C3B-C2B	4.60	1.46	1.36
11	c	302	HEC	CHC-C1C	4.59	1.49	1.39
11	c	302	HEC	C1C-NC	-4.53	1.31	1.39
12	B	303	HEM	FE-NB	4.50	2.08	1.94
11	c	302	HEC	CHA-C4D	4.48	1.49	1.39
11	b	301	HEC	FE-NA	4.48	2.09	1.95
11	c	302	HEC	FE-NB	4.41	2.08	1.94
11	b	301	HEC	CHB-C4A	4.36	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	302	HEC	FE-ND	4.31	2.08	1.94
12	B	303	HEM	FE-NC	4.31	2.09	1.95
11	b	301	HEC	FE-NC	4.30	2.09	1.95
11	C	301	HEC	CHA-C4D	4.30	1.49	1.39
11	C	301	HEC	FE-NC	4.29	2.09	1.95
11	C	301	HEC	FE-NA	4.26	2.09	1.95
11	c	302	HEC	CHB-C1B	4.25	1.48	1.39
12	b	303	HEM	FE-NC	4.24	2.09	1.95
12	B	302	HEM	FE-NC	4.21	2.09	1.95
12	b	302	HEM	FE-NC	4.20	2.09	1.95
11	C	301	HEC	CHD-C4C	4.15	1.48	1.39
11	C	301	HEC	CHB-C1B	4.12	1.48	1.39
12	b	303	HEM	C1B-NB	-4.09	1.33	1.40
11	c	302	HEC	FE-NA	4.09	2.08	1.95
11	C	301	HEC	CHC-C1C	4.06	1.48	1.39
11	B	301	HEC	C4B-NB	-4.03	1.33	1.40
11	c	302	HEC	FE-NC	4.03	2.08	1.95
11	b	301	HEC	CHD-C4C	4.01	1.48	1.39
12	B	303	HEM	C1B-NB	-3.98	1.33	1.40
11	c	302	HEC	C4C-NC	-3.98	1.32	1.39
11	B	301	HEC	CHD-C4C	3.94	1.48	1.39
11	b	301	HEC	C4B-NB	-3.84	1.33	1.40
11	B	301	HEC	CHB-C1B	3.78	1.47	1.39
11	C	301	HEC	C3C-C2C	3.78	1.48	1.38
11	B	301	HEC	CHA-C4D	3.70	1.47	1.39
11	b	301	HEC	CHA-C4D	3.69	1.47	1.39
12	b	302	HEM	C4D-ND	-3.68	1.33	1.40
11	B	301	HEC	CHC-C4B	3.67	1.45	1.38
12	b	302	HEM	C1B-NB	-3.58	1.34	1.40
12	B	302	HEM	C4D-ND	-3.58	1.34	1.40
12	b	303	HEM	C4D-ND	-3.51	1.34	1.40
11	c	302	HEC	C1C-C2C	3.50	1.51	1.43
12	B	303	HEM	C4D-ND	-3.48	1.34	1.40
11	b	301	HEC	CHB-C1B	3.44	1.47	1.39
11	b	301	HEC	CHC-C4B	3.43	1.45	1.38
12	B	302	HEM	C1B-NB	-3.41	1.34	1.40
11	B	301	HEC	C3C-C2C	3.27	1.47	1.38
11	b	301	HEC	C3C-C2C	3.21	1.47	1.38
11	c	302	HEC	C4B-NB	-3.20	1.34	1.40
11	c	302	HEC	C1D-ND	-3.17	1.34	1.40
11	C	301	HEC	C4B-NB	-3.16	1.34	1.40
12	B	303	HEM	C4B-NB	-3.03	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	HEC	C1D-ND	-3.00	1.35	1.40
11	b	301	HEC	C1C-NC	-2.99	1.34	1.39
12	b	303	HEM	C1C-C2C	-2.98	1.39	1.45
11	B	301	HEC	C1D-ND	-2.96	1.35	1.40
11	b	301	HEC	CHC-C1C	2.95	1.46	1.39
12	b	302	HEM	C1C-C2C	-2.91	1.39	1.45
12	B	303	HEM	FE-ND	-2.82	1.86	1.94
11	b	301	HEC	C4C-C3C	2.75	1.50	1.44
11	B	301	HEC	C1B-C2B	2.72	1.50	1.44
12	B	302	HEM	C1C-C2C	-2.70	1.40	1.45
11	C	301	HEC	C1C-C2C	2.69	1.49	1.43
11	b	301	HEC	C1D-ND	-2.68	1.35	1.40
11	B	301	HEC	CHC-C1C	2.67	1.45	1.39
11	b	301	HEC	C4A-NA	-2.67	1.34	1.39
12	B	303	HEM	C1A-C2A	-2.64	1.39	1.44
12	B	302	HEM	C3C-C4C	-2.63	1.41	1.46
11	c	302	HEC	C4A-NA	-2.61	1.34	1.39
11	B	301	HEC	C1A-NA	-2.60	1.34	1.39
12	b	302	HEM	C3C-C4C	-2.59	1.41	1.46
11	C	301	HEC	C4D-C3D	2.57	1.49	1.45
12	B	303	HEM	C1B-C2B	-2.56	1.39	1.44
11	c	302	HEC	C1A-NA	-2.56	1.34	1.39
11	B	301	HEC	C4C-NC	-2.56	1.34	1.39
11	c	302	HEC	C4D-C3D	2.55	1.49	1.45
11	b	301	HEC	C1B-C2B	2.55	1.49	1.44
12	B	303	HEM	C1D-ND	-2.51	1.33	1.38
11	B	301	HEC	C1C-NC	-2.50	1.34	1.39
11	C	301	HEC	C1A-NA	-2.48	1.34	1.39
11	C	301	HEC	C4A-NA	-2.47	1.35	1.39
11	C	301	HEC	C4C-NC	-2.47	1.35	1.39
11	b	301	HEC	C1A-NA	-2.46	1.35	1.39
12	b	303	HEM	FE-ND	-2.46	1.87	1.94
11	C	301	HEC	C1B-C2B	2.45	1.49	1.44
12	b	302	HEM	FE-ND	-2.44	1.87	1.94
12	B	303	HEM	C3C-C4C	-2.44	1.41	1.46
11	c	302	HEC	C1A-C2A	2.38	1.49	1.45
12	b	303	HEM	C1D-ND	-2.37	1.34	1.38
12	b	303	HEM	C4B-NB	-2.34	1.34	1.38
12	B	302	HEM	FE-ND	-2.34	1.87	1.94
11	c	302	HEC	C4B-C3B	2.33	1.49	1.45
12	b	303	HEM	C3C-C4C	-2.31	1.42	1.46
11	c	302	HEC	C1D-C2D	2.29	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	302	HEC	C1B-C2B	2.29	1.49	1.44
12	b	302	HEM	C4B-NB	-2.28	1.34	1.38
11	C	301	HEC	C1A-C2A	2.27	1.49	1.45
11	B	301	HEC	C4A-NA	-2.27	1.35	1.39
11	C	301	HEC	C1D-C2D	2.24	1.49	1.44
11	B	301	HEC	C4C-C3C	2.24	1.49	1.44
11	C	301	HEC	C4B-C3B	2.23	1.48	1.45
11	b	301	HEC	C1A-C2A	2.22	1.49	1.45
11	B	301	HEC	C1A-C2A	2.22	1.49	1.45
11	C	301	HEC	C1C-NC	-2.21	1.35	1.39
12	B	303	HEM	C3D-C2D	-2.19	1.32	1.36
11	B	301	HEC	C4D-ND	-2.17	1.34	1.38
11	b	301	HEC	C1B-NB	-2.17	1.34	1.38
12	b	302	HEM	O2A-CGA	-2.15	1.23	1.30
12	B	302	HEM	O2A-CGA	-2.14	1.23	1.30
12	B	303	HEM	C1A-NA	-2.13	1.35	1.39
12	B	302	HEM	C3B-C4B	2.11	1.49	1.44
11	C	301	HEC	C4C-C3C	2.11	1.48	1.44
12	B	303	HEM	O2A-CGA	-2.08	1.23	1.30
12	b	303	HEM	O2D-CGD	-2.08	1.23	1.30
13	B	304	MQ7	C3-C2	2.06	1.38	1.35
11	b	301	HEC	C1D-C2D	2.03	1.48	1.44
11	c	302	HEC	C4D-ND	-2.03	1.34	1.38

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	c	302	HEC	CAC-C3C-C2C	-52.72	43.48	126.89
11	c	302	HEC	CMC-C2C-C3C	-46.67	26.64	125.62
11	c	302	HEC	CAC-C3C-C4C	13.66	143.70	124.91
11	c	302	HEC	CBC-CAC-C3C	12.34	145.87	112.42
11	B	301	HEC	C1B-C2B-C3B	-6.86	99.77	106.98
11	c	302	HEC	CMC-C2C-C1C	6.62	135.50	125.42
11	B	301	HEC	C1C-C2C-C3C	-6.33	99.57	106.82
11	b	301	HEC	C1B-C2B-C3B	-6.26	100.39	106.98
11	B	301	HEC	C2A-C1A-NA	6.10	116.21	110.32
11	c	302	HEC	C3C-C4C-NC	5.89	116.69	110.15
12	B	303	HEM	CHC-C4B-NB	5.83	130.70	124.42
11	c	302	HEC	C1B-C2B-C3B	-5.63	101.06	106.98
11	C	301	HEC	C1B-C2B-C3B	-5.62	101.07	106.98
11	b	301	HEC	C2B-C1B-NB	5.42	116.17	109.90
11	b	301	HEC	C2A-C1A-NA	5.26	115.39	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	303	HEM	CAD-C3D-C4D	5.10	133.58	124.70
11	B	301	HEC	C3D-C4D-ND	5.08	115.26	110.35
11	C	301	HEC	C1C-C2C-C3C	-5.05	101.03	106.82
11	b	301	HEC	CMC-C2C-C3C	5.05	136.34	125.62
11	B	301	HEC	C2C-C1C-NC	5.02	118.19	110.14
12	b	302	HEM	CHC-C4B-NB	5.00	129.80	124.42
11	b	301	HEC	C3D-C4D-ND	4.99	115.17	110.35
11	B	301	HEC	C2B-C1B-NB	4.91	115.58	109.90
11	B	301	HEC	CAB-C3B-C4B	-4.83	118.50	124.79
12	B	303	HEM	CAD-CBD-CGD	-4.79	100.95	113.67
11	B	301	HEC	C3B-C4B-NB	4.71	115.34	110.17
11	B	301	HEC	CAB-C3B-C2B	4.58	135.97	127.56
11	b	301	HEC	C3B-C4B-NB	4.56	115.18	110.17
12	B	303	HEM	C3B-C4B-NB	-4.56	106.19	109.47
11	C	301	HEC	CBB-CAB-C3B	4.54	124.73	112.42
11	C	301	HEC	CBC-CAC-C3C	4.52	124.67	112.42
11	c	302	HEC	CBB-CAB-C3B	4.44	124.44	112.42
11	b	301	HEC	CAC-C3C-C4C	4.43	131.01	124.91
11	B	301	HEC	CBC-CAC-C3C	4.43	124.43	112.42
11	C	301	HEC	C2B-C1B-NB	4.39	114.98	109.90
12	B	303	HEM	CAD-C3D-C2D	-4.33	119.75	127.87
11	c	302	HEC	C4C-C3C-C2C	-4.30	100.22	106.87
11	B	301	HEC	C2D-C1D-ND	4.17	114.64	109.84
11	b	301	HEC	C2D-C1D-ND	4.15	114.61	109.84
11	c	302	HEC	C2B-C1B-NB	4.14	114.68	109.90
12	b	302	HEM	CHD-C1D-ND	4.13	128.87	124.42
11	B	301	HEC	CBB-CAB-C3B	4.11	123.57	112.42
11	B	301	HEC	CMC-C2C-C3C	4.10	134.33	125.62
12	B	302	HEM	CHA-C4D-ND	4.09	129.43	124.37
12	B	303	HEM	C1B-NB-C4B	4.08	110.04	105.21
11	b	301	HEC	C1C-C2C-C3C	-4.02	102.22	106.82
11	b	301	HEC	C2C-C1C-NC	4.01	116.58	110.14
12	B	302	HEM	CHD-C1D-ND	3.97	128.69	124.42
12	b	302	HEM	CHA-C4D-ND	3.95	129.25	124.37
11	B	301	HEC	C1A-C2A-C3A	-3.93	101.93	107.11
12	B	303	HEM	CHB-C1B-NB	3.92	129.22	124.37
11	C	301	HEC	C2A-C1A-NA	3.86	114.05	110.32
11	B	301	HEC	C1D-C2D-C3D	-3.82	102.96	106.98
12	B	302	HEM	CHB-C1B-NB	3.78	129.04	124.37
11	b	301	HEC	C1D-C2D-C3D	-3.77	103.02	106.98
11	C	301	HEC	C3D-C4D-ND	3.74	113.97	110.35
11	C	301	HEC	C1D-C2D-C3D	-3.74	103.05	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	301	HEC	C2D-C1D-ND	3.73	114.13	109.84
12	b	302	HEM	CBD-CAD-C3D	-3.72	102.24	112.53
12	B	302	HEM	CHC-C4B-NB	3.70	128.41	124.42
12	b	303	HEM	CHB-C1B-NB	3.64	128.87	124.37
11	b	301	HEC	CBC-CAC-C3C	3.63	122.25	112.42
11	b	301	HEC	CHC-C1C-C2C	-3.62	116.91	127.43
11	B	301	HEC	CHC-C4B-C3B	-3.61	118.57	125.23
12	B	302	HEM	C3B-C4B-NB	-3.61	106.88	109.47
11	b	301	HEC	C1A-C2A-C3A	-3.60	102.36	107.11
12	B	303	HEM	CHD-C1D-ND	3.54	128.23	124.42
11	c	302	HEC	CHD-C4C-NC	-3.53	117.46	123.86
12	b	303	HEM	CHC-C4B-NB	3.51	128.19	124.42
12	b	303	HEM	CHA-C4D-ND	3.49	128.68	124.37
13	b	304	MQ7	C11-C3-C2	-3.49	118.91	124.89
11	b	301	HEC	CBB-CAB-C3B	3.46	121.81	112.42
12	B	303	HEM	C4A-CHB-C1B	-3.45	118.14	126.25
11	c	302	HEC	C1D-C2D-C3D	-3.41	103.39	106.98
11	c	302	HEC	C2A-C1A-NA	3.36	113.57	110.32
11	b	301	HEC	C3A-C4A-NA	3.36	115.86	109.64
11	c	302	HEC	CHA-C1A-NA	-3.35	120.80	124.45
13	b	304	MQ7	C11-C3-C4	3.35	122.11	118.58
12	B	302	HEM	CBD-CAD-C3D	-3.35	103.28	112.53
11	c	302	HEC	CHB-C1B-NB	-3.29	120.88	124.42
12	B	303	HEM	CBB-CAB-C3B	-3.28	111.12	127.53
12	B	303	HEM	CMD-C2D-C1D	3.28	130.16	125.03
11	c	302	HEC	CHB-C4A-NA	-3.23	120.93	124.45
11	C	301	HEC	C1A-C2A-C3A	-3.17	102.93	107.11
11	B	301	HEC	C3A-C4A-NA	3.17	115.50	109.64
11	c	302	HEC	CHA-C4D-ND	-3.16	121.02	124.42
11	C	301	HEC	CHB-C1B-NB	-3.16	121.03	124.42
12	B	302	HEM	C1B-NB-C4B	3.15	108.94	105.21
11	c	302	HEC	C4C-NC-C1C	-3.12	100.74	105.82
11	C	301	HEC	CHA-C4D-ND	-3.10	121.08	124.42
11	C	301	HEC	C2C-C1C-NC	3.10	115.11	110.14
12	b	302	HEM	C1B-NB-C4B	3.08	108.85	105.21
11	c	302	HEC	C3D-C4D-ND	3.06	113.31	110.35
12	b	303	HEM	CHD-C1D-ND	3.03	127.69	124.42
11	B	301	HEC	C4D-C3D-C2D	-3.02	102.50	106.89
11	B	301	HEC	CHC-C1C-C2C	-3.01	118.68	127.43
11	c	302	HEC	C1A-C2A-C3A	-3.00	103.16	107.11
11	B	301	HEC	CHB-C1B-NB	-2.99	121.21	124.42
11	C	301	HEC	CMC-C2C-C3C	2.98	131.94	125.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	301	HEC	CHA-C1A-NA	-2.96	121.23	124.45
12	b	302	HEM	CHB-C1B-NB	2.96	128.03	124.37
11	B	301	HEC	C4A-C3A-C2A	-2.95	102.59	106.97
12	B	303	HEM	C4D-ND-C1D	2.92	108.66	105.21
11	c	302	HEC	C2D-C1D-ND	2.88	113.15	109.84
12	B	302	HEM	CHD-C4C-NC	2.88	127.59	124.45
11	b	301	HEC	C4A-C3A-C2A	-2.88	102.69	106.97
12	B	303	HEM	CAA-CBA-CGA	-2.87	106.04	113.67
11	B	301	HEC	CAA-C2A-C3A	2.87	133.25	127.87
12	b	303	HEM	C1B-NB-C4B	2.87	108.60	105.21
11	b	301	HEC	CBD-CAD-C3D	-2.84	104.69	112.53
12	b	302	HEM	CHD-C4C-NC	2.79	127.49	124.45
11	c	302	HEC	C4A-C3A-C2A	-2.78	102.84	106.97
11	b	301	HEC	CMD-C2D-C1D	2.78	129.37	125.03
11	C	301	HEC	C4A-C3A-C2A	-2.72	102.94	106.97
11	c	302	HEC	C4D-C3D-C2D	-2.70	102.97	106.89
11	C	301	HEC	C4D-C3D-C2D	-2.69	102.97	106.89
12	B	302	HEM	CAA-CBA-CGA	-2.69	106.53	113.67
11	b	301	HEC	C4D-C3D-C2D	-2.69	102.98	106.89
11	c	302	HEC	CHD-C1D-ND	-2.67	121.06	124.37
11	B	301	HEC	CMB-C2B-C1B	2.67	129.20	125.03
12	B	303	HEM	O2D-CGD-CBD	2.66	122.42	114.00
11	C	301	HEC	CHB-C4A-NA	-2.64	121.58	124.45
11	b	301	HEC	CMC-C2C-C1C	-2.61	121.44	125.42
12	B	303	HEM	C4C-CHD-C1D	-2.59	120.51	126.02
13	B	305	MQ7	C11-C3-C2	-2.56	120.50	124.89
11	B	301	HEC	C3C-C4C-NC	2.51	112.94	110.15
11	c	302	HEC	CHC-C4B-NB	-2.50	121.28	124.37
12	b	303	HEM	CHB-C1B-C2B	-2.48	119.89	126.95
11	C	301	HEC	C3B-C4B-NB	2.48	112.89	110.17
12	b	302	HEM	CHD-C1D-C2D	-2.45	121.16	125.03
11	C	301	HEC	C3C-C4C-NC	2.45	112.87	110.15
12	B	302	HEM	CHA-C4D-C3D	-2.44	120.73	125.23
11	C	301	HEC	C3A-C4A-NA	2.43	114.13	109.64
11	C	301	HEC	CAD-C3D-C4D	2.40	128.87	124.70
12	B	303	HEM	CHB-C1B-C2B	-2.37	120.20	126.95
11	c	302	HEC	C3A-C4A-NA	2.37	114.03	109.64
12	B	303	HEM	CHA-C4D-ND	2.36	127.28	124.37
12	B	302	HEM	CHD-C1D-C2D	-2.35	121.32	125.03
12	b	302	HEM	CHA-C4D-C3D	-2.35	120.90	125.23
11	B	301	HEC	CHA-C1A-NA	-2.31	121.94	124.45
11	C	301	HEC	CAC-C3C-C2C	2.29	130.51	126.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	301	HEC	CAB-C3B-C2B	2.29	131.77	127.56
12	b	303	HEM	C3B-C4B-NB	-2.28	107.83	109.47
11	c	302	HEC	CHC-C1C-NC	-2.28	119.73	123.86
12	b	302	HEM	CAA-CBA-CGA	-2.27	107.65	113.67
12	B	302	HEM	C4C-CHD-C1D	-2.26	121.21	126.02
12	b	303	HEM	C1A-CHA-C4D	-2.26	120.94	126.25
12	b	303	HEM	C4C-CHD-C1D	-2.25	121.23	126.02
11	C	301	HEC	CHD-C1D-ND	-2.25	121.58	124.37
11	c	302	HEC	CMB-C2B-C3B	2.25	132.23	126.15
11	c	302	HEC	CAD-C3D-C4D	2.23	128.58	124.70
11	b	301	HEC	CHC-C4B-C3B	-2.23	121.12	125.23
11	C	301	HEC	CHC-C4B-NB	-2.22	121.62	124.37
12	B	302	HEM	CHB-C1B-C2B	-2.21	120.66	126.95
12	b	302	HEM	C4C-CHD-C1D	-2.19	121.36	126.02
11	b	301	HEC	CHA-C4D-C3D	-2.18	121.60	124.77
11	b	301	HEC	CAA-C2A-C1A	2.17	129.27	124.85
11	b	301	HEC	CHA-C1A-NA	-2.17	122.09	124.45
12	B	302	HEM	CAB-C3B-C2B	-2.17	121.39	128.43
11	b	301	HEC	CHB-C1B-C2B	-2.13	121.67	125.03
12	b	303	HEM	CAD-CBD-CGD	-2.12	108.03	113.67
12	B	303	HEM	O1D-CGD-CBD	-2.12	116.37	123.09
11	c	302	HEC	CMA-C3A-C4A	2.12	128.45	124.73
11	b	301	HEC	CHB-C1B-NB	-2.10	122.16	124.42
12	b	303	HEM	O2A-CGA-CBA	2.09	120.61	114.00
11	c	302	HEC	C2C-C1C-NC	2.09	113.49	110.14
15	E	101	PC1	O12-P-O14	2.09	122.14	112.44
11	C	301	HEC	CMB-C2B-C3B	2.06	131.73	126.15
12	b	302	HEM	C3B-C4B-NB	-2.05	108.00	109.47
11	b	301	HEC	CHB-C4A-C3A	-2.05	121.23	125.49
12	b	303	HEM	C4B-C3B-C2B	-2.05	105.40	107.28
11	B	301	HEC	CMA-C3A-C2A	2.04	131.68	126.15
12	B	302	HEM	O2D-CGD-CBD	2.04	120.45	114.00
11	b	301	HEC	CMB-C2B-C1B	2.04	128.22	125.03
11	C	301	HEC	CMD-C2D-C1D	2.02	128.19	125.03
12	B	303	HEM	O2A-CGA-CBA	2.02	120.38	114.00
13	c	301	MQ7	C11-C3-C2	-2.01	121.44	124.89
13	B	304	MQ7	C11-C3-C2	-2.01	121.45	124.89
14	C	302	PEE	O2-C2-C1	2.00	115.54	108.34

All (4) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

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

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	302	HEM	C2C-C3C-CAC-CBC
12	B	303	HEM	C2B-C3B-CAB-CBB
12	B	303	HEM	C2D-C3D-CAD-CBD
12	B	303	HEM	C4D-C3D-CAD-CBD
12	b	302	HEM	C2C-C3C-CAC-CBC
13	B	305	MQ7	C39-C38-C40-C41
13	b	304	MQ7	C12-C11-C3-C2
13	b	304	MQ7	C12-C11-C3-C4
14	C	302	PEE	C4-O4P-P-O3P
14	C	302	PEE	C4-O4P-P-O1P
14	a	202	PEE	C1-O3P-P-O1P
14	a	202	PEE	C1-O3P-P-O4P
14	a	202	PEE	C5-C4-O4P-P
14	a	202	PEE	O5-C30-O3-C3
14	a	202	PEE	C31-C30-O3-C3
14	c	303	PEE	C1-O3P-P-O4P
14	c	303	PEE	O5-C30-O3-C3
14	c	303	PEE	C31-C30-O3-C3
14	e	101	PEE	C4-O4P-P-O1P
14	e	101	PEE	C5-C4-O4P-P
15	E	101	PC1	C11-O13-P-O11
15	E	101	PC1	C1-O11-P-O14
16	b	305	CDL	C1-CA2-OA2-PA1
16	b	305	CDL	CA2-OA2-PA1-OA4
16	b	305	CDL	CA2-OA2-PA1-OA5
16	b	305	CDL	CB3-OB5-PB2-OB4
16	b	305	CDL	OB7-CB5-OB6-CB4
16	b	305	CDL	C51-CB5-OB6-CB4
16	b	305	CDL	OB9-CB7-OB8-CB6
16	b	305	CDL	C71-CB7-OB8-CB6
11	C	301	HEC	C4B-C3B-CAB-CBB
11	b	301	HEC	C2C-C3C-CAC-CBC
11	B	301	HEC	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	301	HEC	C4C-C3C-CAC-CBC
11	b	301	HEC	C4C-C3C-CAC-CBC
11	c	302	HEC	C4C-C3C-CAC-CBC
11	B	301	HEC	C4B-C3B-CAB-CBB
11	b	301	HEC	C4B-C3B-CAB-CBB
11	c	302	HEC	C4B-C3B-CAB-CBB
11	C	301	HEC	C2B-C3B-CAB-CBB
11	c	302	HEC	C2B-C3B-CAB-CBB
11	B	301	HEC	C2B-C3B-CAB-CBB
11	b	301	HEC	C2B-C3B-CAB-CBB
11	B	301	HEC	C2C-C3C-CAC-CBC
11	C	301	HEC	C2C-C3C-CAC-CBC
11	c	302	HEC	C2C-C3C-CAC-CBC
13	B	305	MQ7	C37-C38-C40-C41
11	B	301	HEC	C3A-C2A-CAA-CBA
11	B	301	HEC	C1A-C2A-CAA-CBA
13	B	304	MQ7	C34-C33-C35-C36
13	b	304	MQ7	C39-C38-C40-C41
13	c	301	MQ7	C29-C28-C30-C31
13	c	301	MQ7	C39-C38-C40-C41
13	B	304	MQ7	C32-C33-C35-C36
13	b	304	MQ7	C37-C38-C40-C41
13	c	301	MQ7	C27-C28-C30-C31
13	c	301	MQ7	C37-C38-C40-C41
13	B	304	MQ7	C18-C20-C21-C22
13	B	305	MQ7	C33-C35-C36-C37
13	c	301	MQ7	C13-C15-C16-C17
13	c	301	MQ7	C28-C30-C31-C32
11	B	301	HEC	C2A-CAA-CBA-CGA
11	B	301	HEC	C3D-CAD-CBD-CGD
11	c	302	HEC	C3D-CAD-CBD-CGD
12	B	303	HEM	C2A-CAA-CBA-CGA
14	c	303	PEE	C2-C1-O3P-P
15	E	101	PC1	C31-C32-C33-C34
12	B	302	HEM	C2A-CAA-CBA-CGA
12	b	302	HEM	C2A-CAA-CBA-CGA
14	a	202	PEE	C10-C11-C12-C13
14	a	202	PEE	C13-C14-C15-C16
12	B	303	HEM	C3D-CAD-CBD-CGD
12	B	302	HEM	C4C-C3C-CAC-CBC
12	B	303	HEM	C4B-C3B-CAB-CBB
12	b	302	HEM	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	101	PEE	O2-C2-C3-O3
16	b	305	CDL	CB4-CB3-OB5-PB2
13	c	301	MQ7	C38-C40-C41-C42
14	c	303	PEE	C14-C15-C16-C17
14	C	302	PEE	C10-C11-C12-C13
13	B	304	MQ7	C24-C23-C25-C26
13	c	301	MQ7	C24-C23-C25-C26
11	b	301	HEC	C2A-CAA-CBA-CGA
11	c	302	HEC	C2A-CAA-CBA-CGA
16	b	305	CDL	OB5-CB3-CB4-CB6
14	e	101	PEE	C1-C2-C3-O3
14	a	202	PEE	C2-C1-O3P-P
14	C	302	PEE	O2-C2-C3-O3
13	B	304	MQ7	C22-C23-C25-C26
16	b	305	CDL	C33-C34-C35-C36
15	E	101	PC1	C27-C28-C29-C2A
14	a	202	PEE	C12-C13-C14-C15
14	a	202	PEE	C16-C17-C18-C19
13	c	301	MQ7	C22-C23-C25-C26
14	e	101	PEE	C36-C37-C38-C39
16	b	305	CDL	OB5-CB3-CB4-OB6
14	c	303	PEE	C5-C4-O4P-P
15	E	101	PC1	C12-C11-O13-P
16	b	305	CDL	OA6-CA4-CA6-OA8
15	E	101	PC1	O13-C11-C12-N
16	b	305	CDL	C38-C39-C40-C41
14	a	202	PEE	C34-C35-C36-C37
14	a	202	PEE	O2-C2-C3-O3
14	C	302	PEE	C4-O4P-P-O2P
14	a	202	PEE	C1-O3P-P-O2P
14	c	303	PEE	C1-O3P-P-O1P
15	E	101	PC1	C11-O13-P-O14
16	b	305	CDL	CB3-OB5-PB2-OB2
13	B	305	MQ7	C34-C33-C35-C36
14	c	303	PEE	C18-C19-C20-C21
13	B	305	MQ7	C23-C25-C26-C27
13	b	304	MQ7	C28-C30-C31-C32
15	E	101	PC1	C21-C22-C23-C24
14	C	302	PEE	C16-C17-C18-C19
13	b	304	MQ7	C15-C16-C17-C18
13	c	301	MQ7	C14-C13-C15-C16
13	B	305	MQ7	C32-C33-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	304	MQ7	C14-C13-C15-C16
13	B	305	MQ7	C14-C13-C15-C16
13	B	305	MQ7	C12-C13-C15-C16
14	c	303	PEE	C16-C17-C18-C19
11	B	301	HEC	C4D-C3D-CAD-CBD
14	a	202	PEE	C36-C37-C38-C39
13	c	301	MQ7	C12-C13-C15-C16
14	C	302	PEE	C2-C1-O3P-P
11	c	302	HEC	CAD-CBD-CGD-O2D
13	B	305	MQ7	C29-C28-C30-C31
11	b	301	HEC	CAA-CBA-CGA-O1A
12	B	302	HEM	CAD-CBD-CGD-O2D
12	b	302	HEM	CAD-CBD-CGD-O1D
12	b	302	HEM	CAD-CBD-CGD-O2D
14	C	302	PEE	C12-C13-C14-C15
11	b	301	HEC	CAD-CBD-CGD-O1D
12	B	302	HEM	CAD-CBD-CGD-O1D
14	a	202	PEE	C18-C19-C20-C21
16	b	305	CDL	C56-C57-C58-C59
11	b	301	HEC	CAD-CBD-CGD-O2D
12	B	302	HEM	CAA-CBA-CGA-O1A
12	b	302	HEM	CAA-CBA-CGA-O1A
13	c	301	MQ7	C19-C18-C20-C21
14	c	303	PEE	C31-C32-C33-C34
14	C	302	PEE	C18-C19-C20-C21
13	B	304	MQ7	C12-C13-C15-C16
13	B	304	MQ7	C27-C28-C30-C31
13	B	305	MQ7	C27-C28-C30-C31
13	c	301	MQ7	C17-C18-C20-C21
11	b	301	HEC	CAA-CBA-CGA-O2A
12	B	303	HEM	CAD-CBD-CGD-O1D
13	c	301	MQ7	C35-C36-C37-C38
11	c	302	HEC	CAD-CBD-CGD-O1D
13	B	304	MQ7	C29-C28-C30-C31
12	B	303	HEM	CAD-CBD-CGD-O2D
15	E	101	PC1	C32-C33-C34-C35
11	B	301	HEC	C2D-C3D-CAD-CBD
11	c	302	HEC	CAA-CBA-CGA-O2A
12	b	302	HEM	CAA-CBA-CGA-O2A
12	B	302	HEM	CAA-CBA-CGA-O2A
14	c	303	PEE	C3-C2-O2-C10
14	e	101	PEE	C1-C2-O2-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	c	302	HEC	CAA-CBA-CGA-O1A
13	c	301	MQ7	C40-C41-C42-C43
15	E	101	PC1	O21-C2-C3-O31
16	b	305	CDL	C51-C52-C53-C54
13	B	304	MQ7	C33-C35-C36-C37
11	C	301	HEC	CAA-CBA-CGA-O2A
11	C	301	HEC	C3D-CAD-CBD-CGD
14	C	302	PEE	O2-C10-C11-C12
11	B	301	HEC	CAD-CBD-CGD-O2D
11	C	301	HEC	CAA-CBA-CGA-O1A
15	E	101	PC1	C26-C27-C28-C29
13	B	304	MQ7	C3-C11-C12-C13
13	b	304	MQ7	C40-C41-C42-C43
11	B	301	HEC	CAD-CBD-CGD-O1D
16	b	305	CDL	C81-C82-C83-C84
16	b	305	CDL	CA3-CA4-CA6-OA8
16	b	305	CDL	CB3-CB4-CB6-OB8
13	B	304	MQ7	C25-C26-C27-C28
14	C	302	PEE	C33-C34-C35-C36
14	e	101	PEE	O3-C30-C31-C32

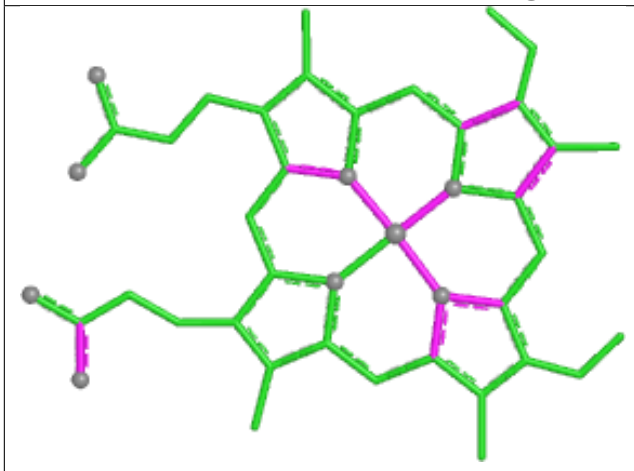
There are no ring outliers.

17 monomers are involved in 85 short contacts:

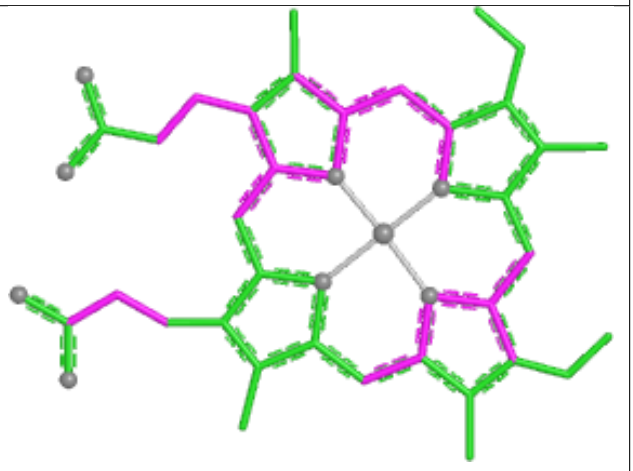
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	302	HEM	1	0
14	e	101	PEE	4	0
13	b	304	MQ7	7	0
11	c	302	HEC	1	0
14	a	202	PEE	2	0
11	C	301	HEC	2	0
13	B	305	MQ7	5	0
13	B	304	MQ7	7	0
14	c	303	PEE	7	0
16	b	305	CDL	7	0
11	B	301	HEC	6	0
14	C	302	PEE	3	0
10	A	201	FES	5	0
12	b	303	HEM	3	0
11	b	301	HEC	6	0
12	B	303	HEM	11	0
13	c	301	MQ7	8	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.

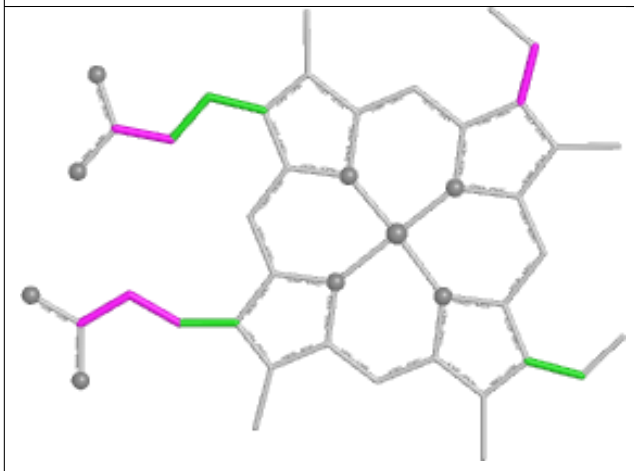
Ligand HEM b 302



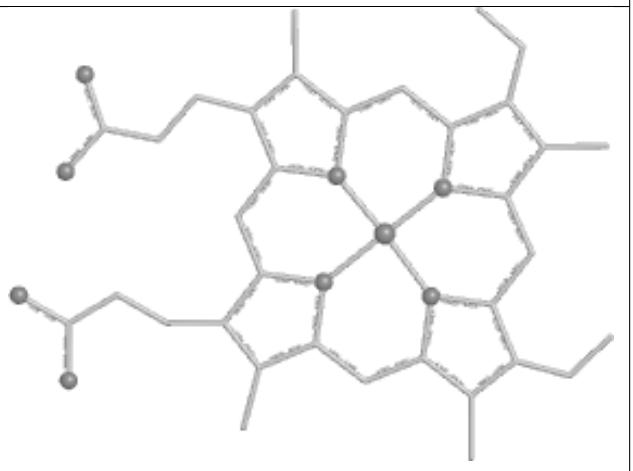
Bond lengths



Bond angles

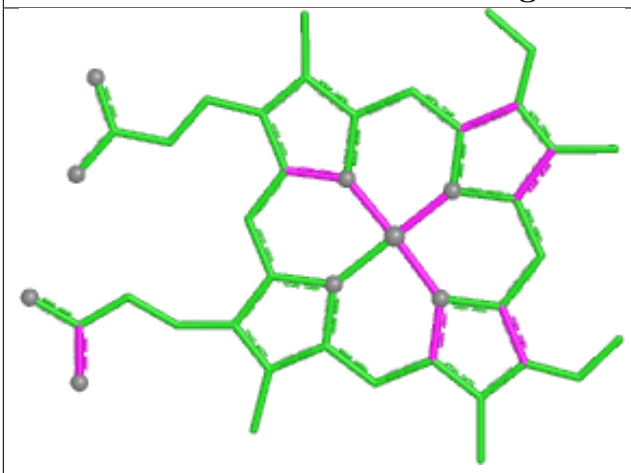


Torsions

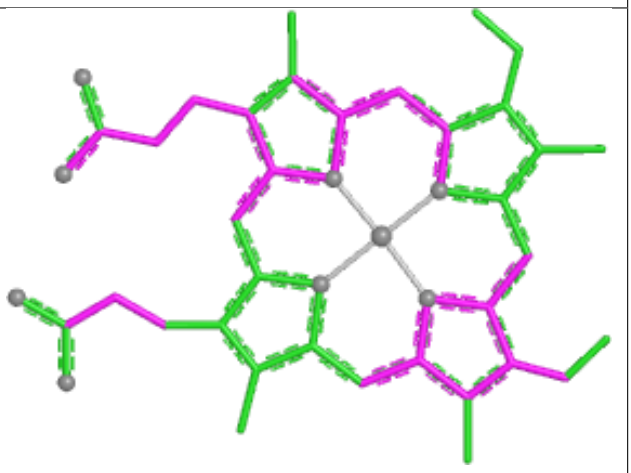


Rings

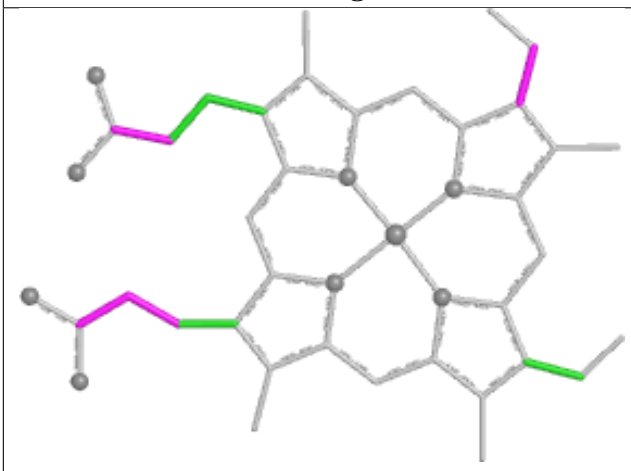
Ligand HEM B 302



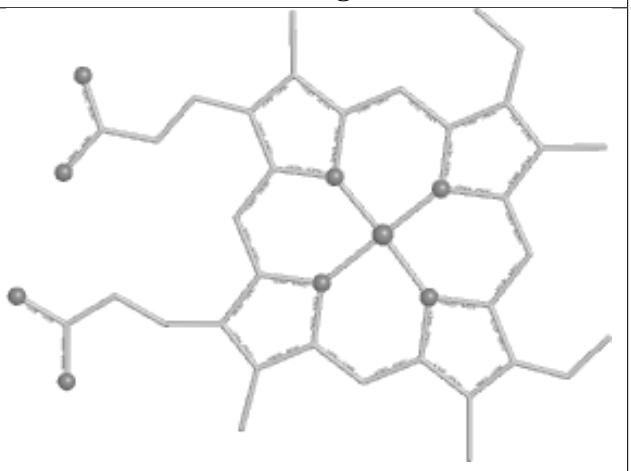
Bond lengths



Bond angles

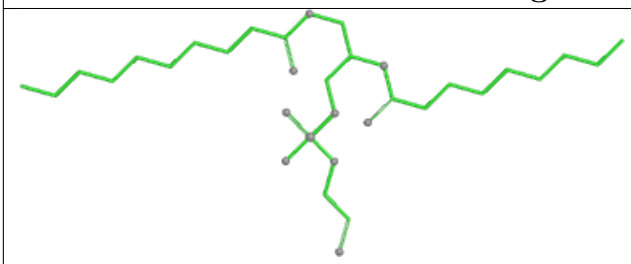


Torsions

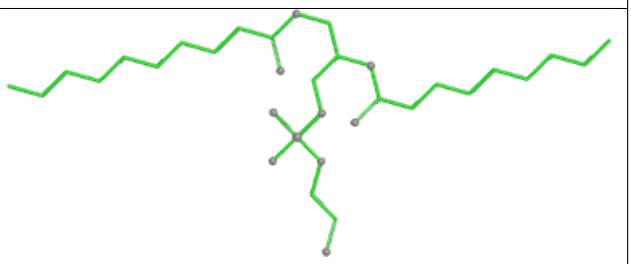


Rings

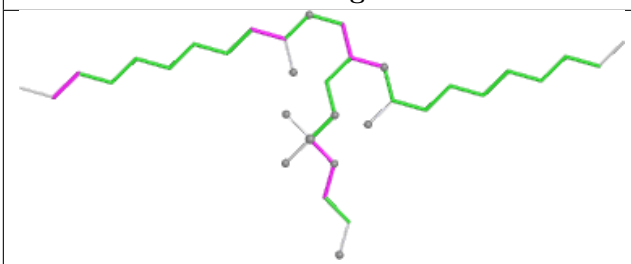
Ligand PEE e 101



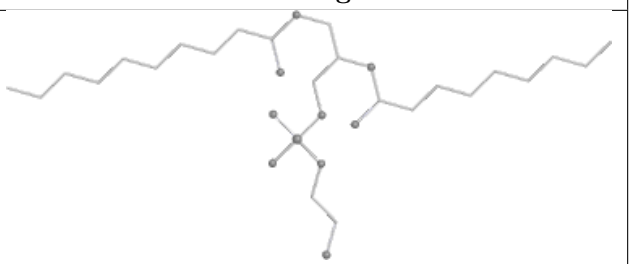
Bond lengths



Bond angles



Torsions

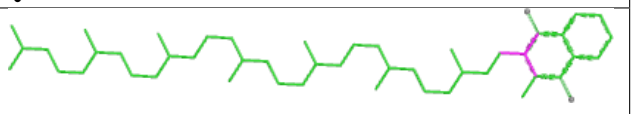


Rings

Ligand MQ7 b 304



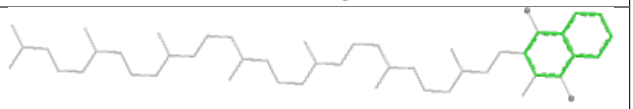
Bond lengths



Bond angles

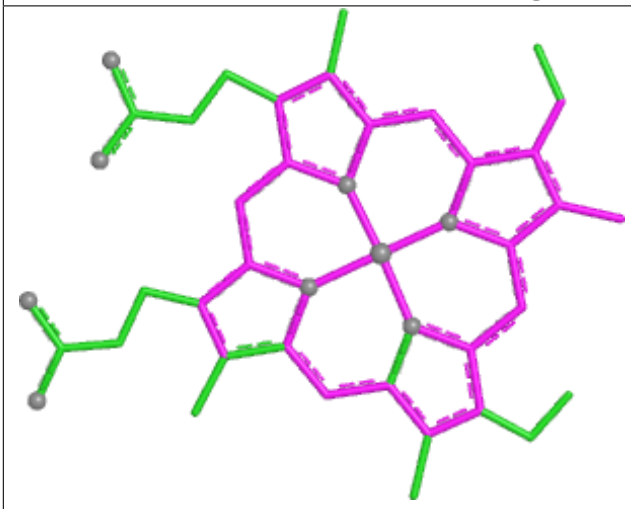


Torsions

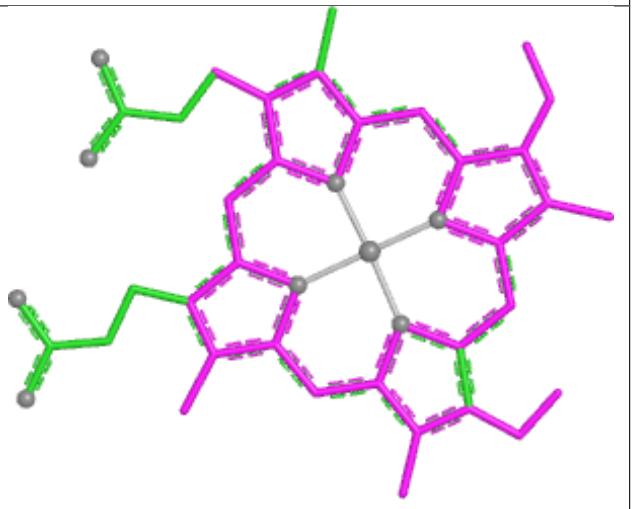


Rings

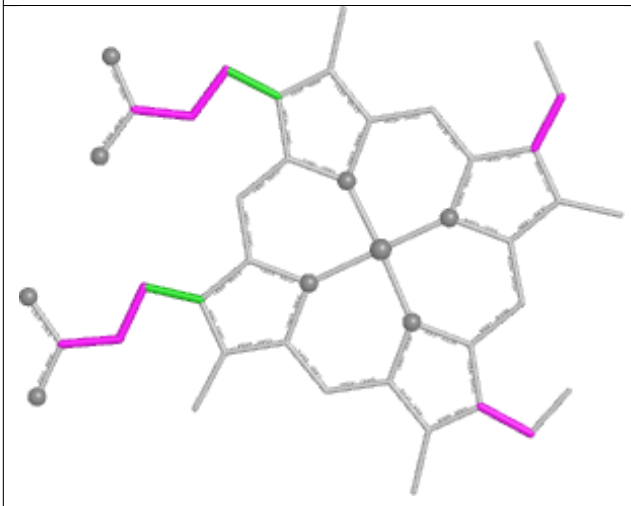
Ligand HEC c 302



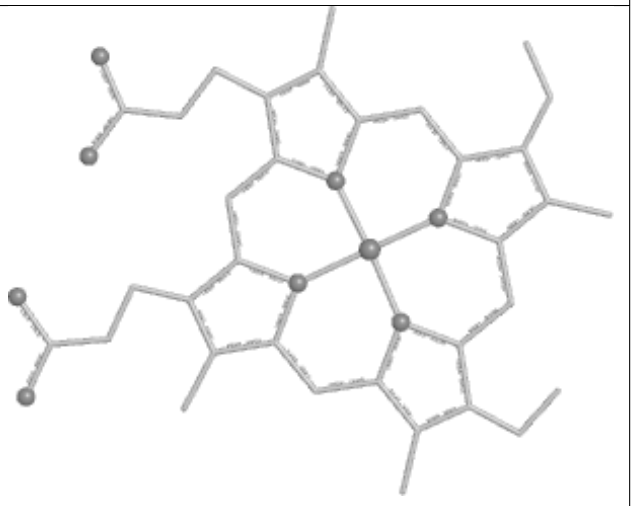
Bond lengths



Bond angles

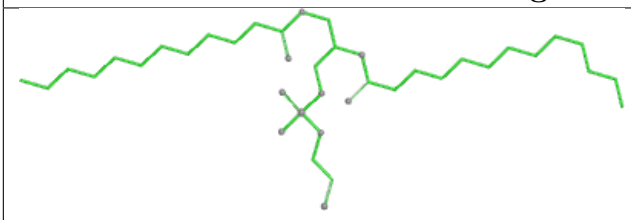


Torsions

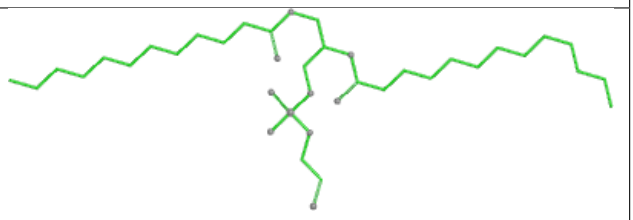


Rings

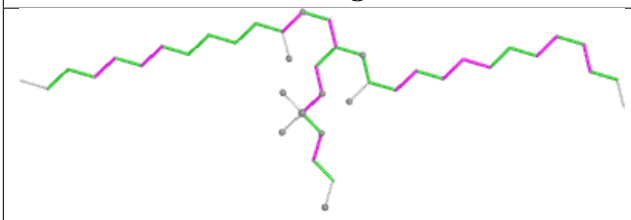
Ligand PEE a 202



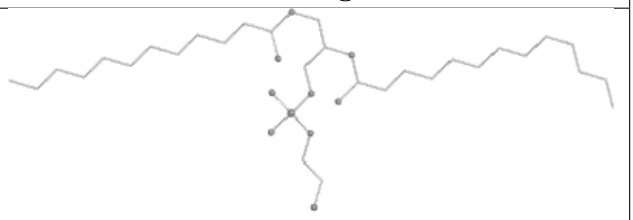
Bond lengths



Bond angles

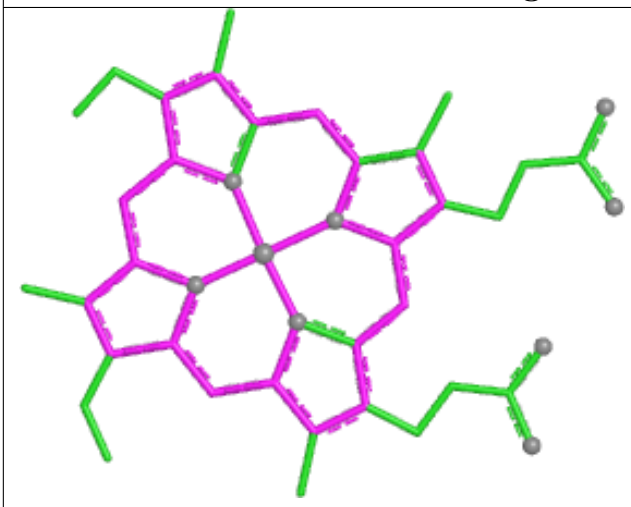


Torsions

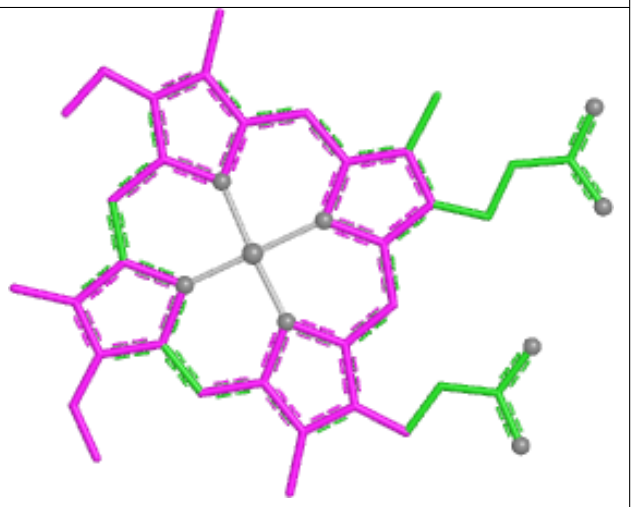


Rings

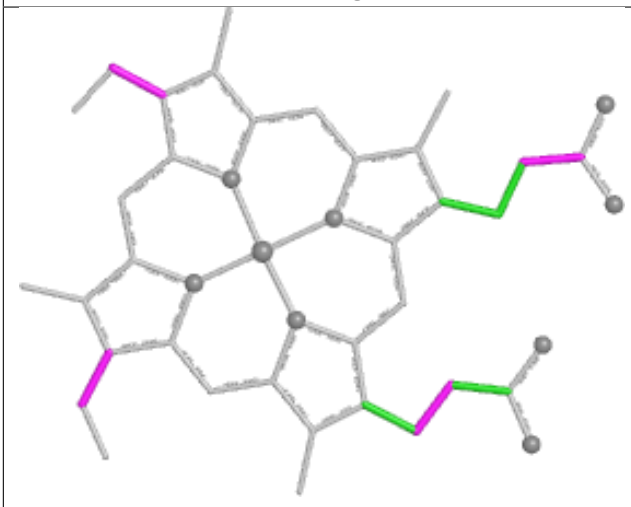
Ligand HEC C 301



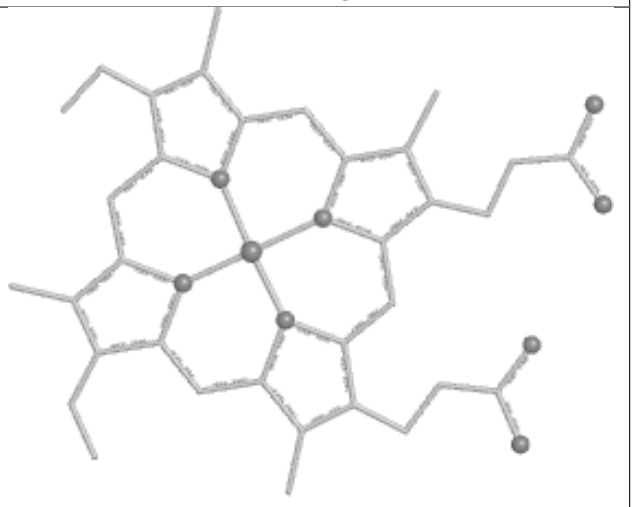
Bond lengths



Bond angles

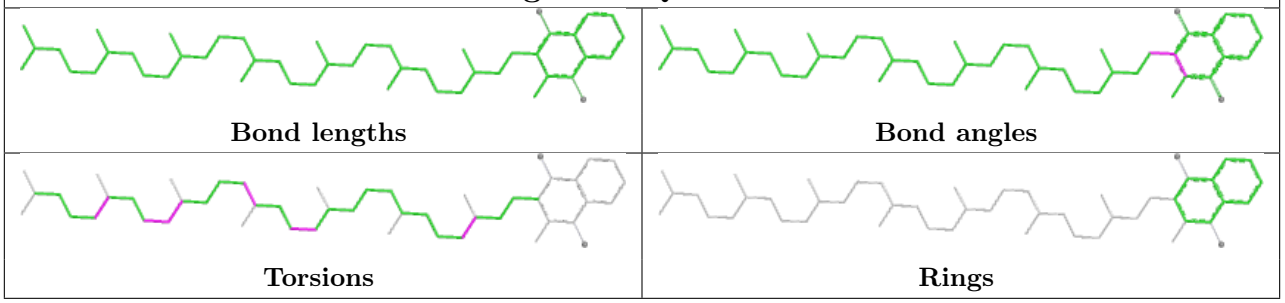


Torsions

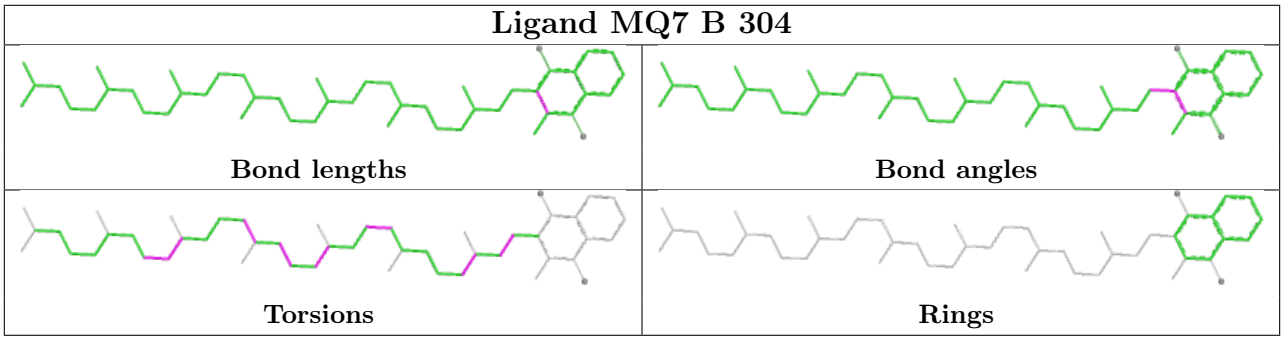


Rings

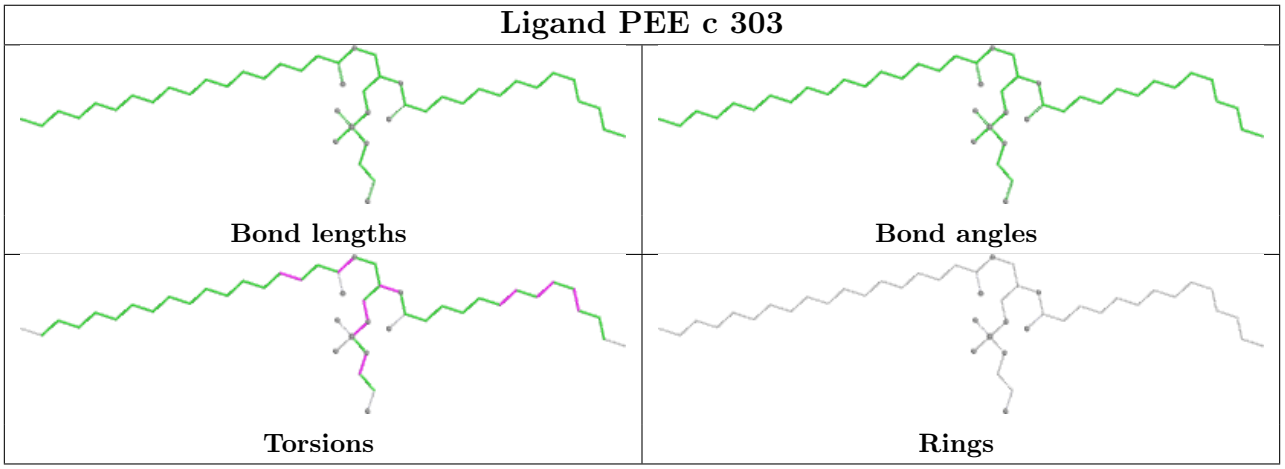
Ligand MQ7 B 305



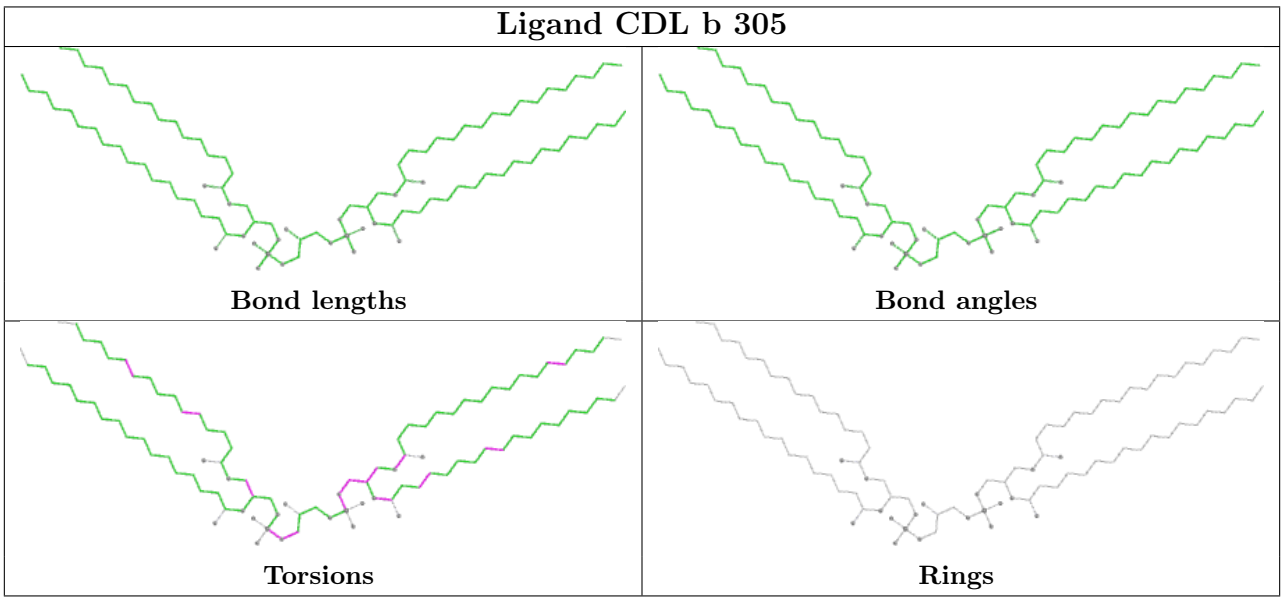
Ligand MQ7 B 304



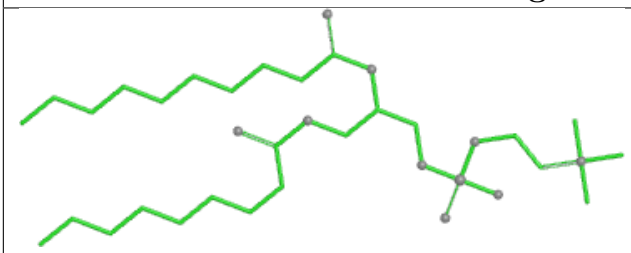
Ligand PEE c 303



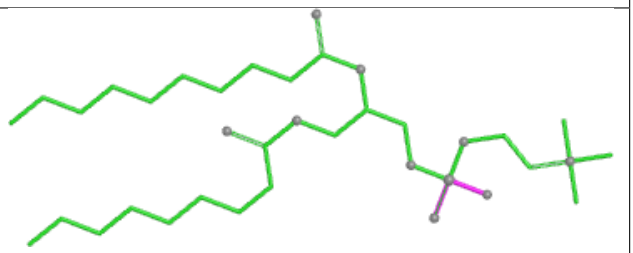
Ligand CDL b 305



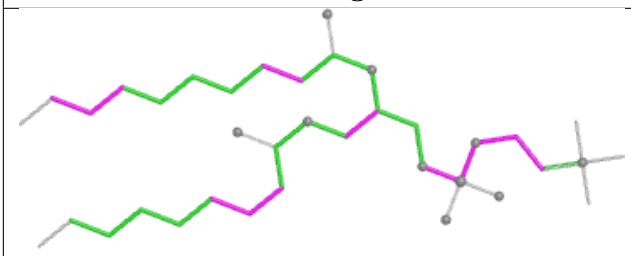
Ligand PC1 E 101



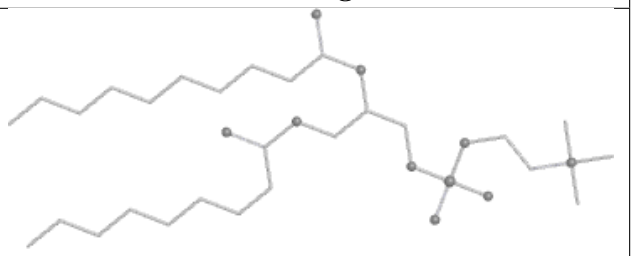
Bond lengths



Bond angles

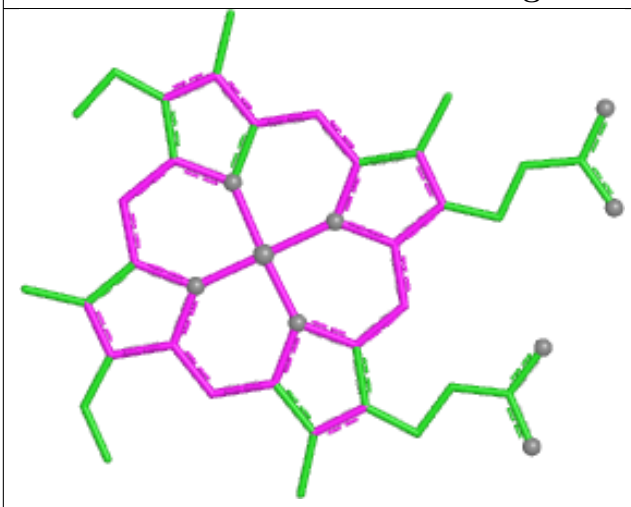


Torsions

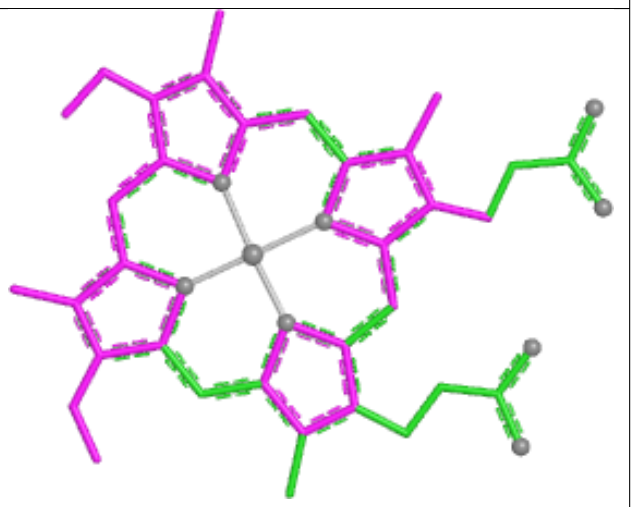


Rings

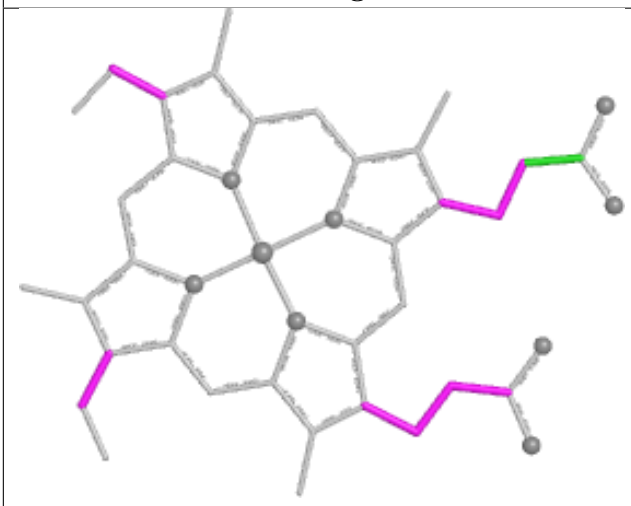
Ligand HEC B 301



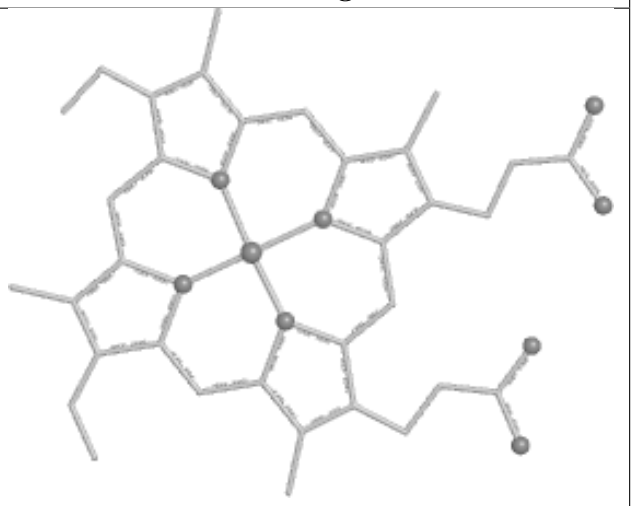
Bond lengths



Bond angles

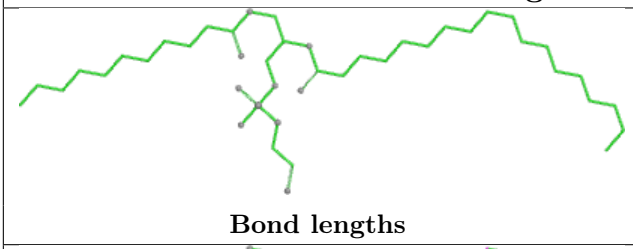


Torsions

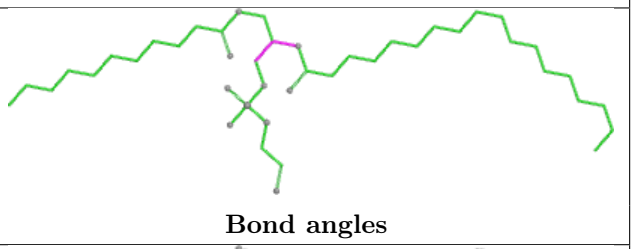


Rings

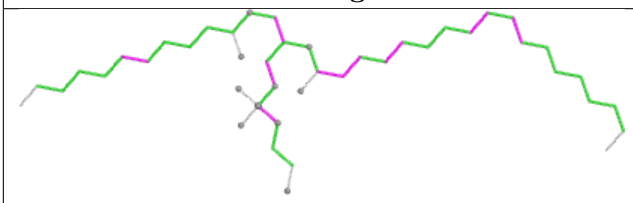
Ligand PEE C 302



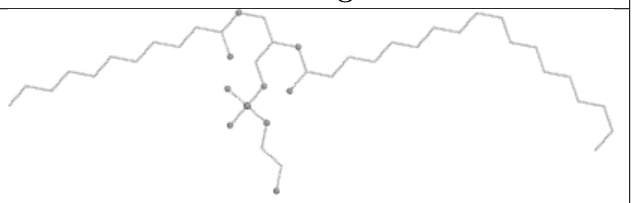
Bond lengths



Bond angles

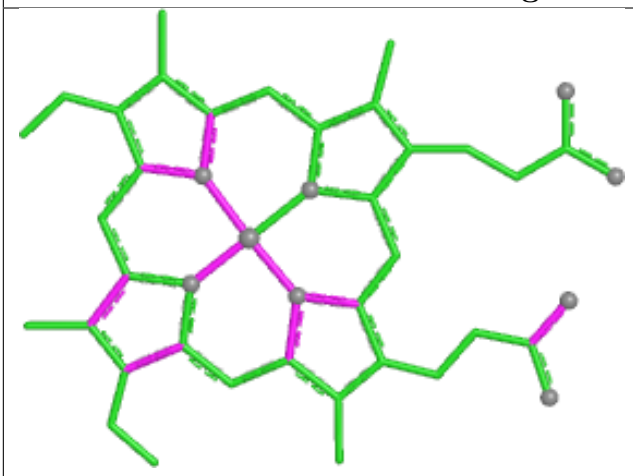


Torsions

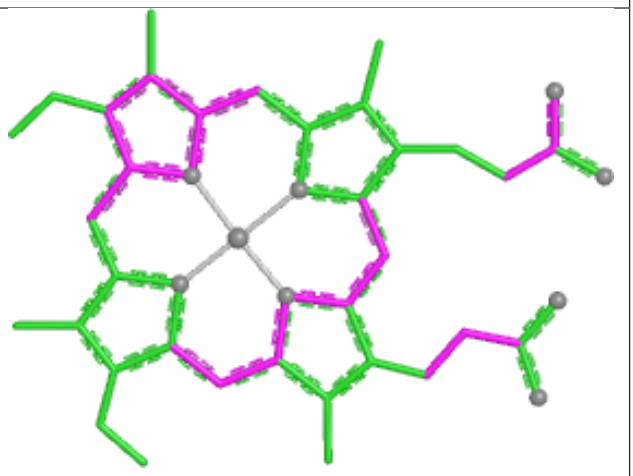


Rings

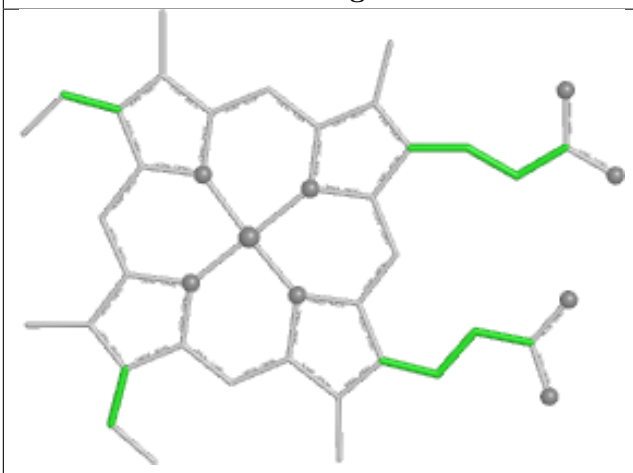
Ligand HEM b 303



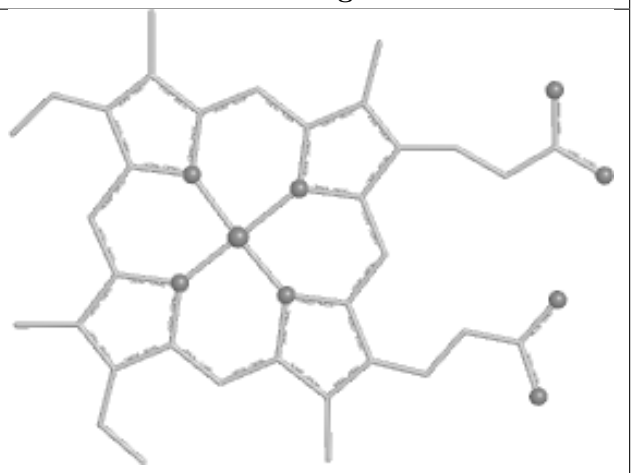
Bond lengths



Bond angles

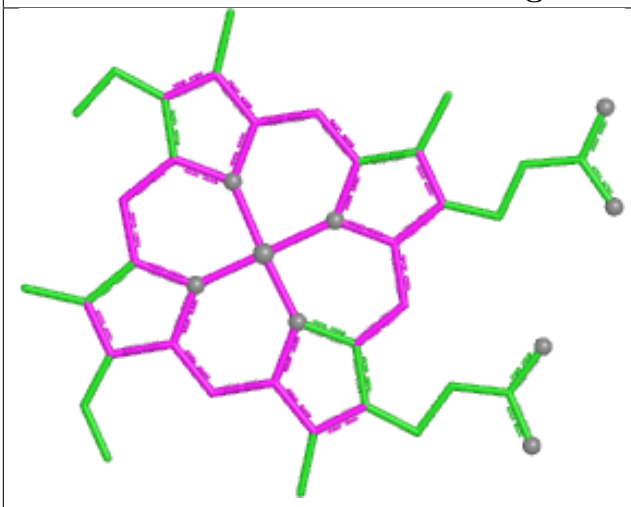


Torsions

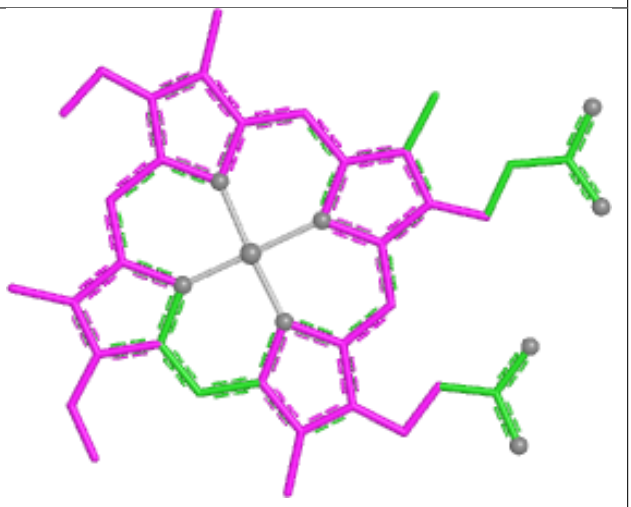


Rings

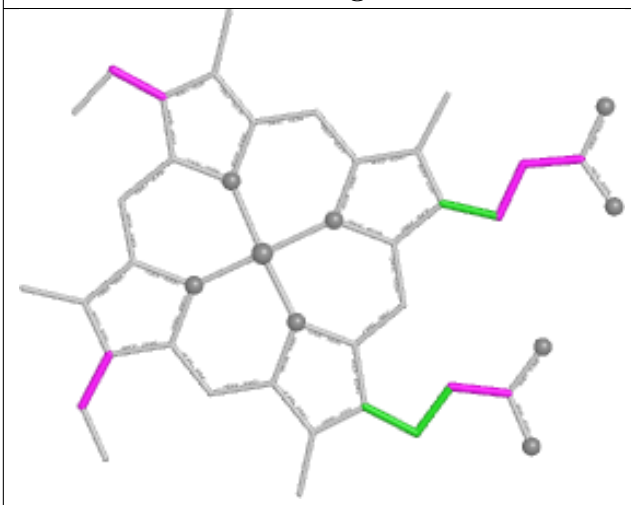
Ligand HEC b 301



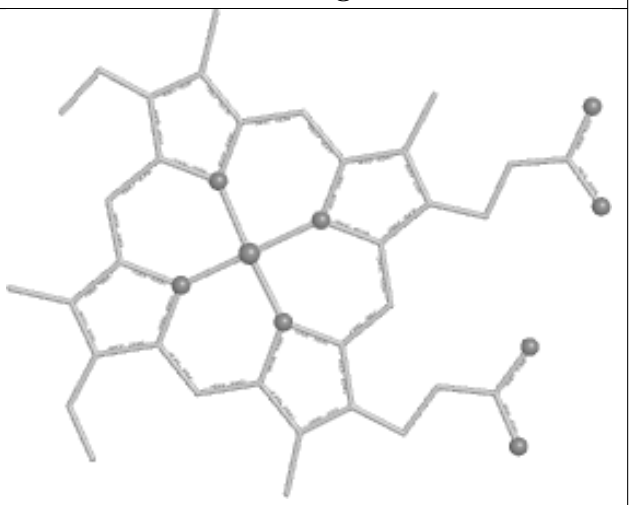
Bond lengths



Bond angles

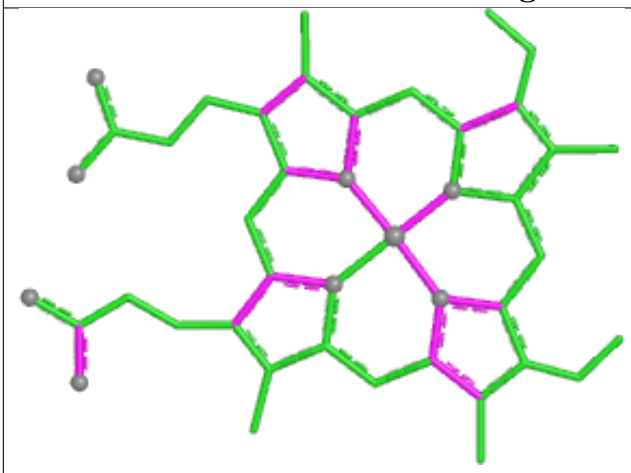


Torsions

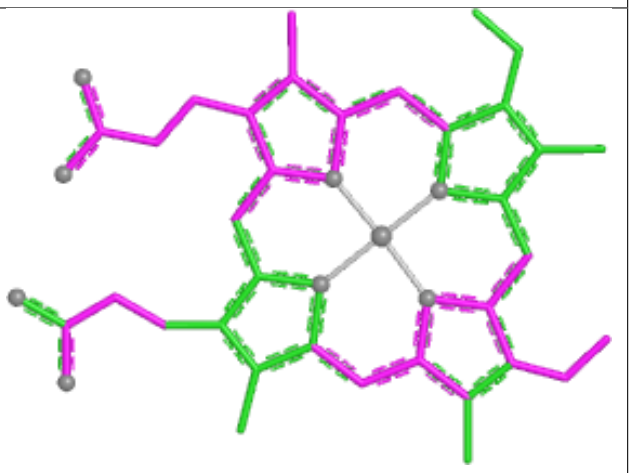


Rings

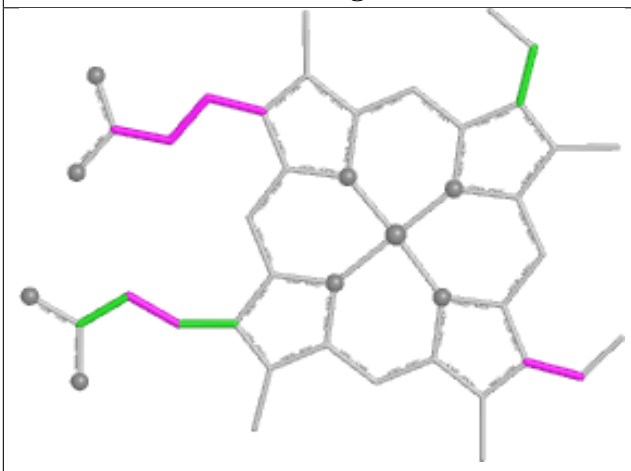
Ligand HEM B 303



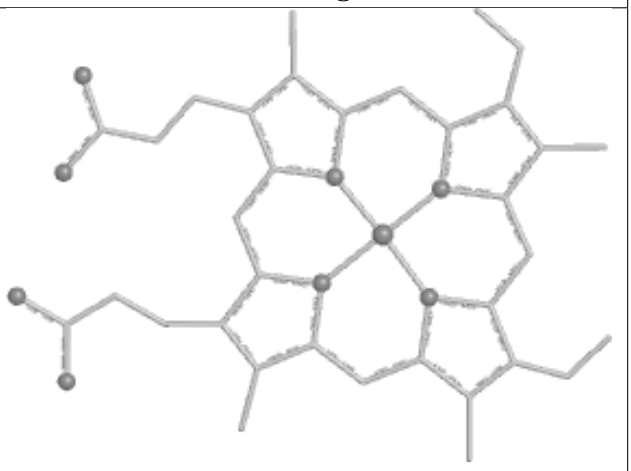
Bond lengths



Bond angles

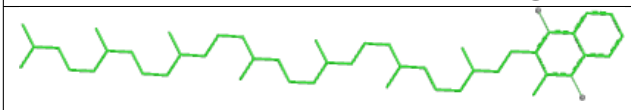


Torsions

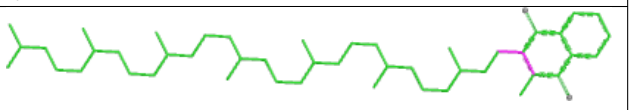


Rings

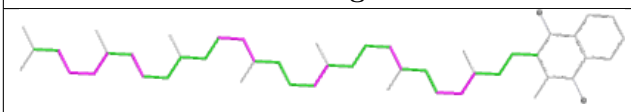
Ligand MQ7 c 301



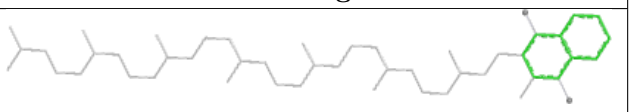
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

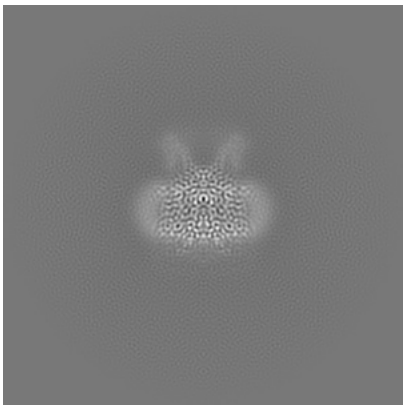
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70331. These allow visual inspection of the internal detail of the map and identification of artifacts.

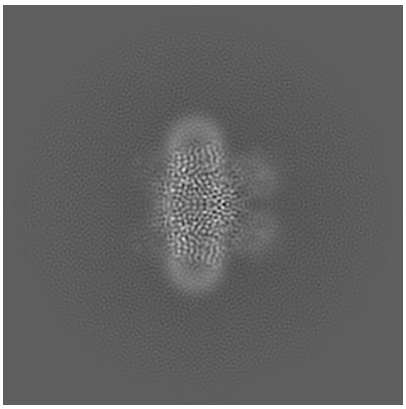
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

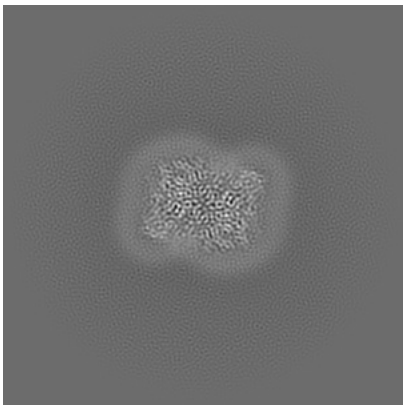
6.1.1 Primary map



X

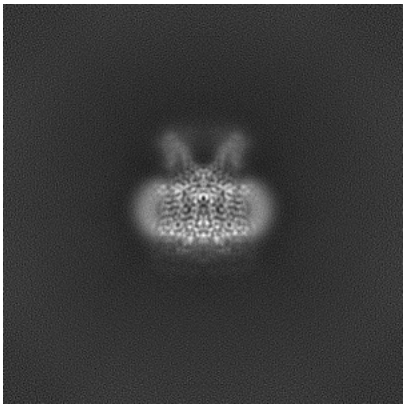


Y

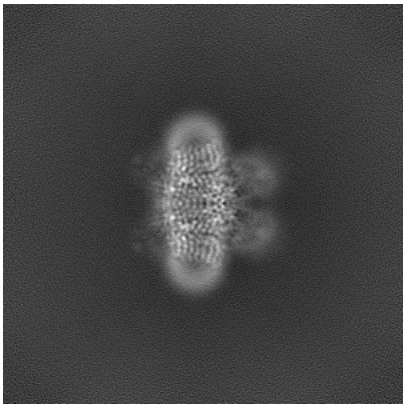


Z

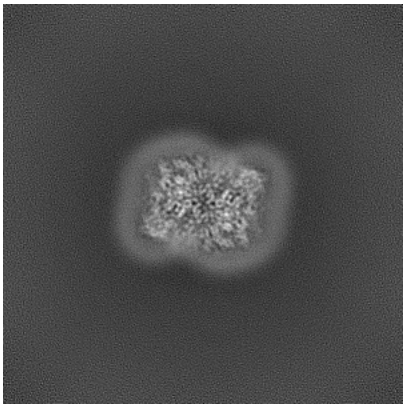
6.1.2 Raw map



X



Y

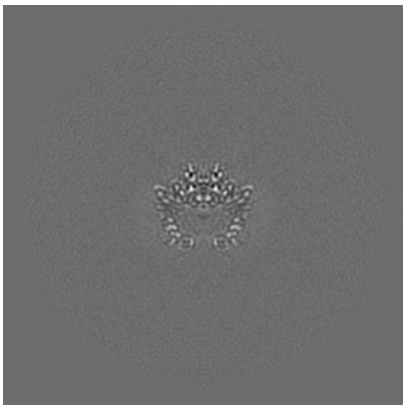


Z

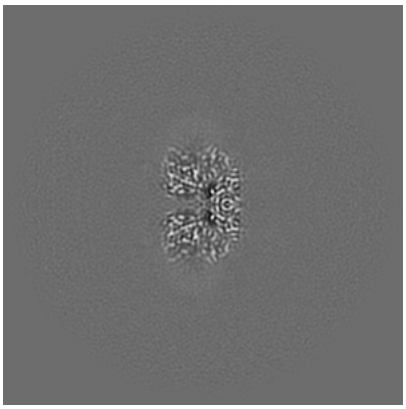
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

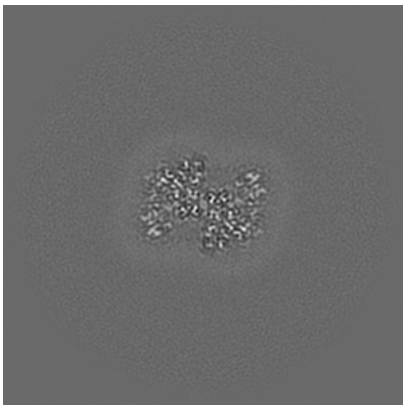
6.2.1 Primary map



X Index: 180

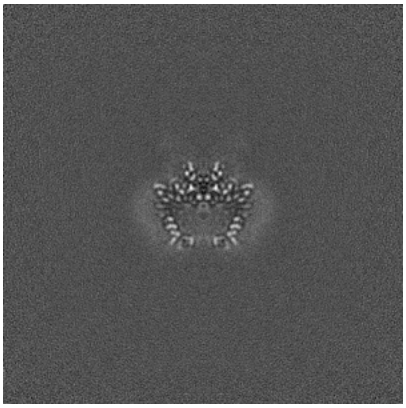


Y Index: 180

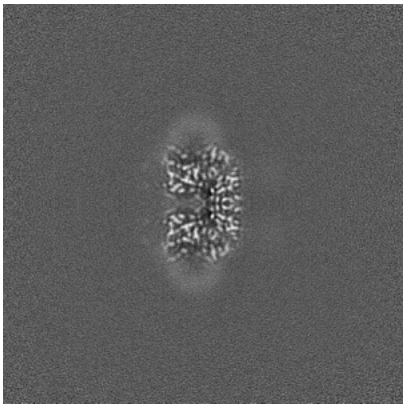


Z Index: 180

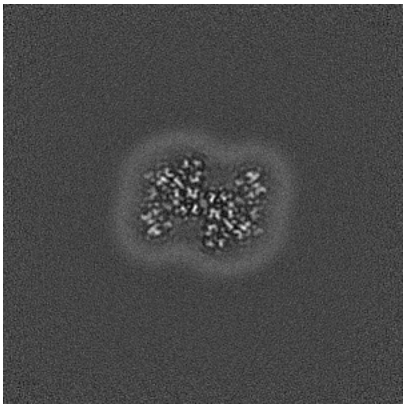
6.2.2 Raw map



X Index: 180



Y Index: 180

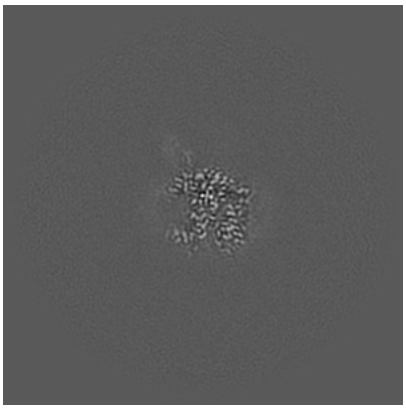


Z Index: 180

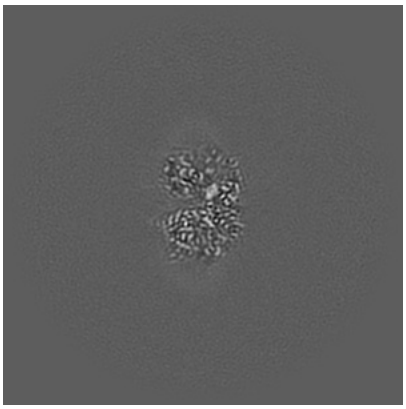
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

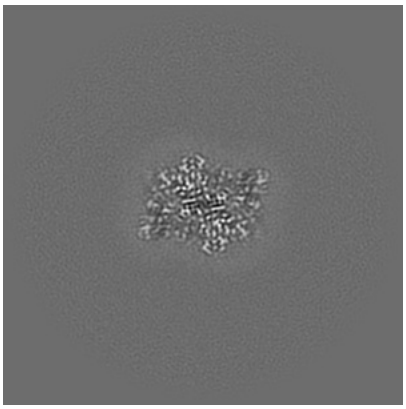
6.3.1 Primary map



X Index: 168

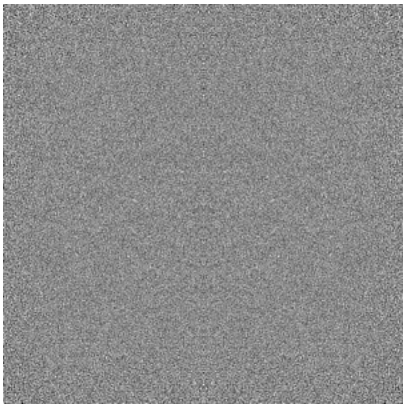


Y Index: 177

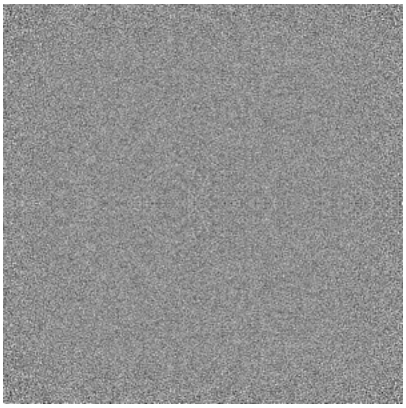


Z Index: 190

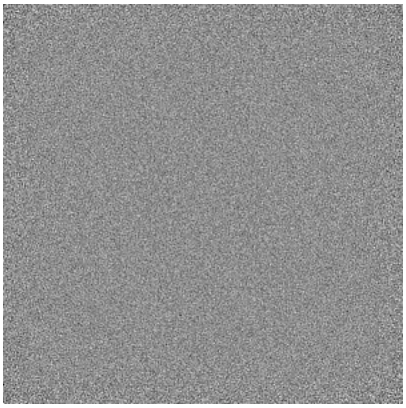
6.3.2 Raw map



X Index: 0



Y Index: 0

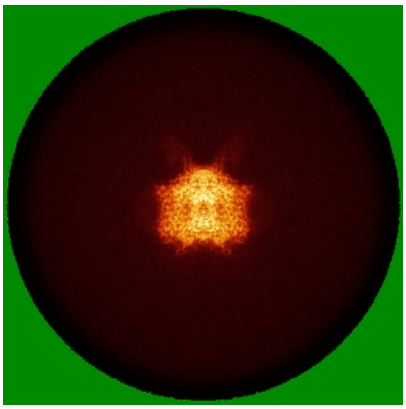


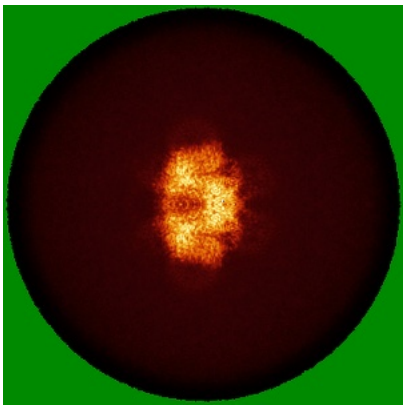
Z Index: 0

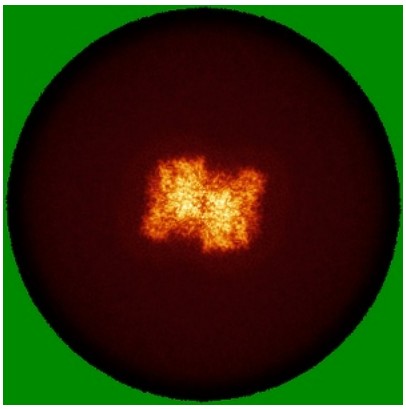
The images above show the largest variance slices of the map in three orthogonal directions.

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

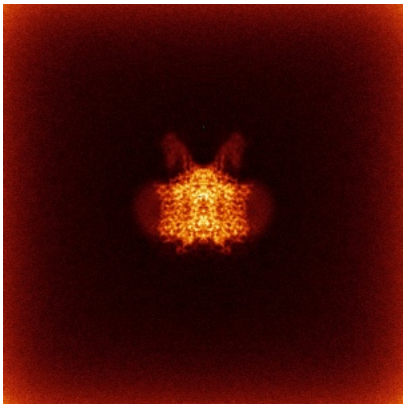
6.4.1 Primary map

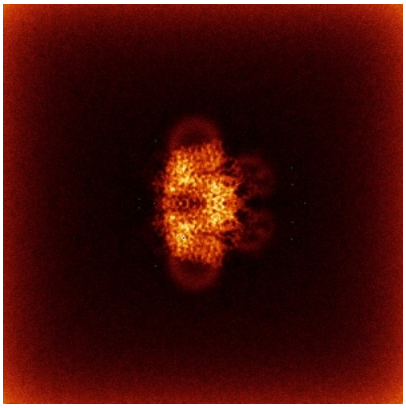

X

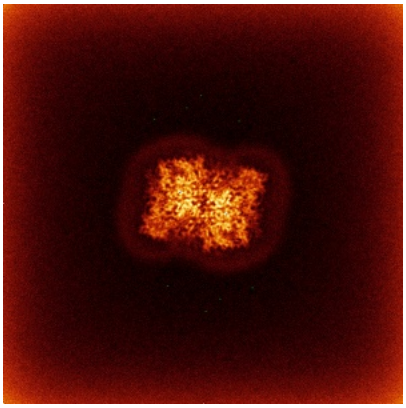

Y


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 0.35. 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.

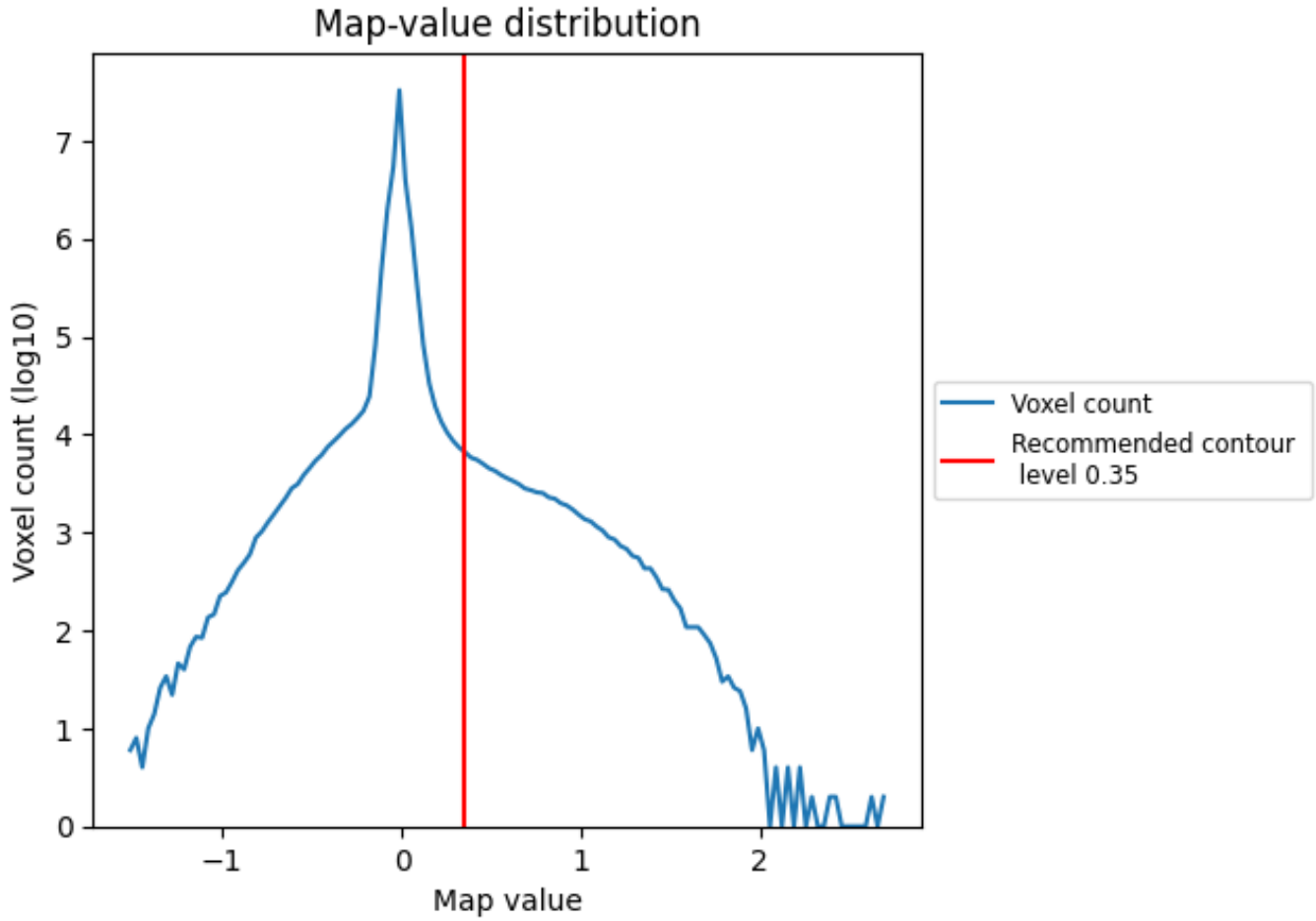
6.6 Mask visualisation (i)

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

7 Map analysis

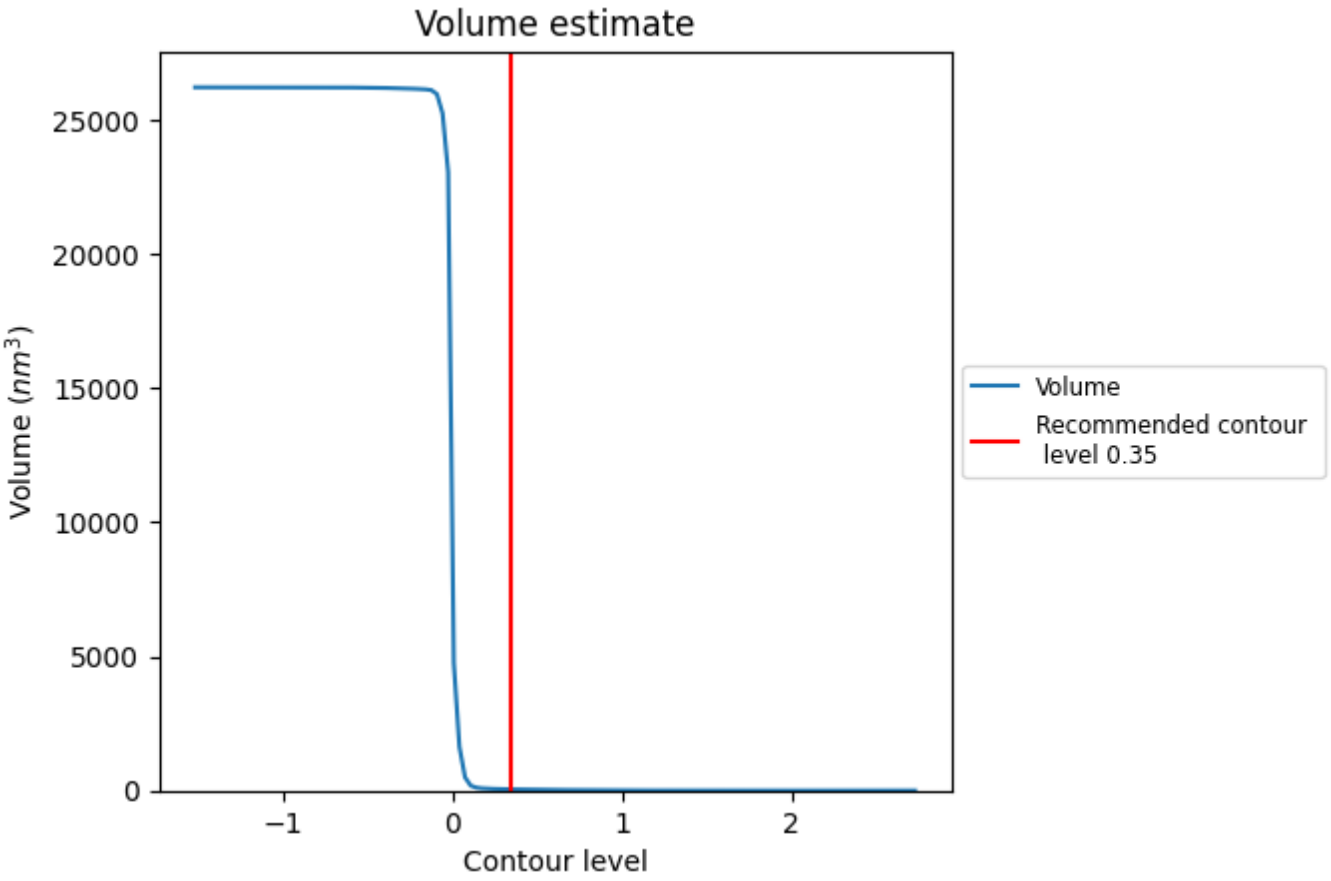
This section contains the results of statistical analysis of the map.

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.

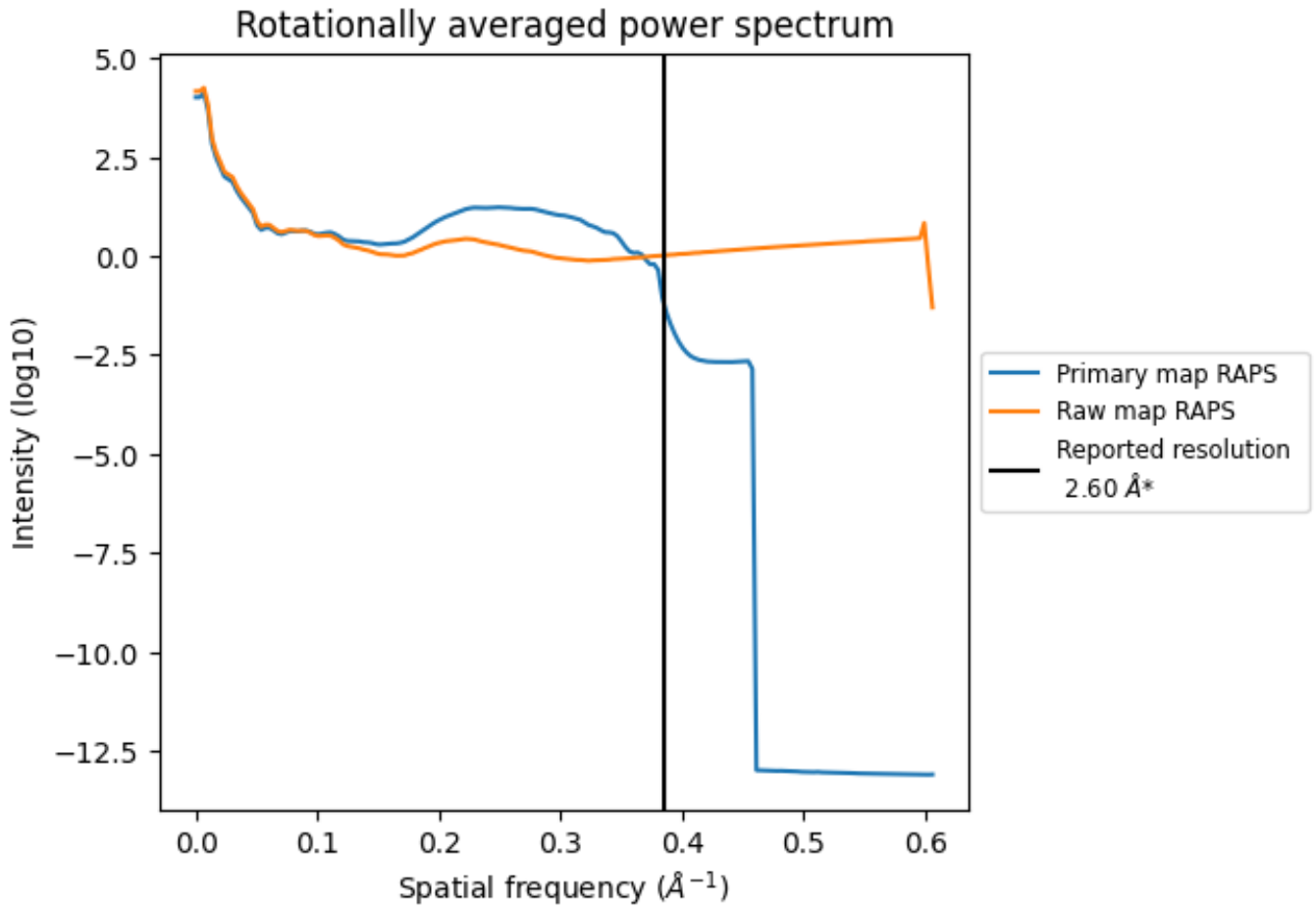
7.2 Volume estimate



The volume at the recommended contour level is 45 nm^3; this corresponds to an approximate mass of 41 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)

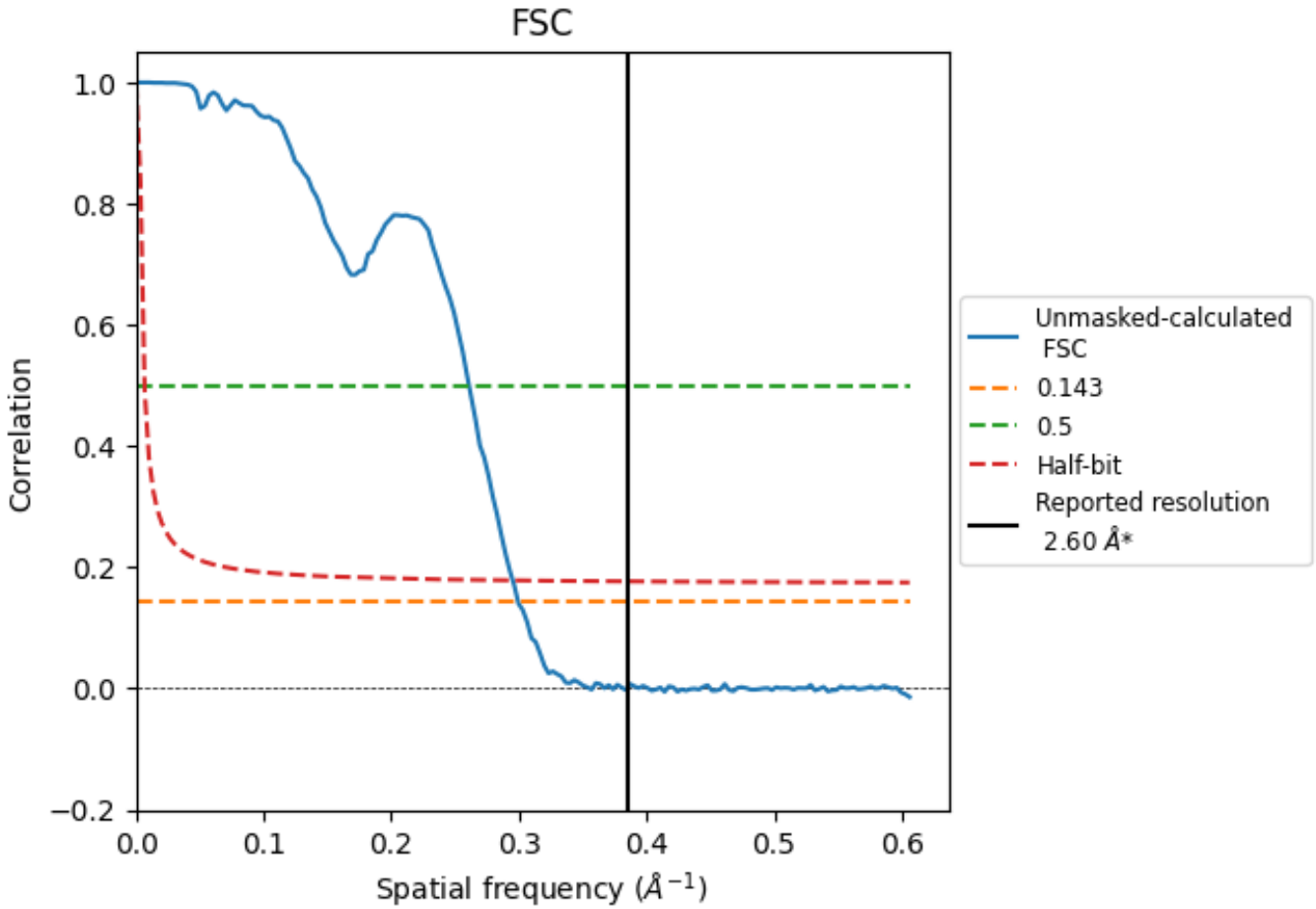


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

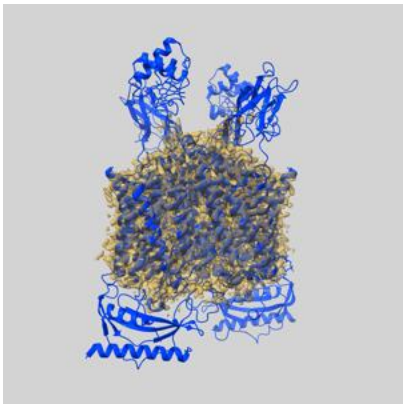
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.83	3.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.6 by more than 10 %

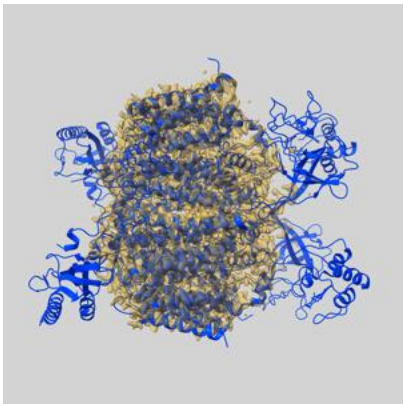
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70331 and PDB model 9OCT. Per-residue inclusion information can be found in section 3 on page 11.

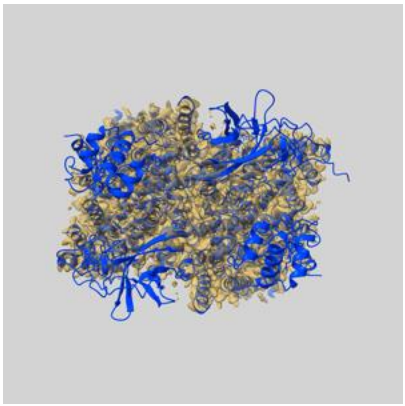
9.1 Map-model overlay



X



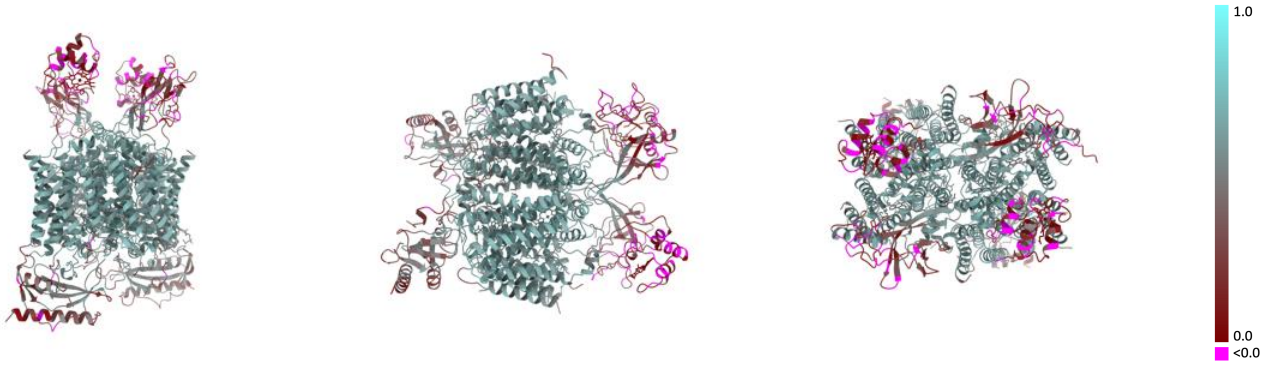
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

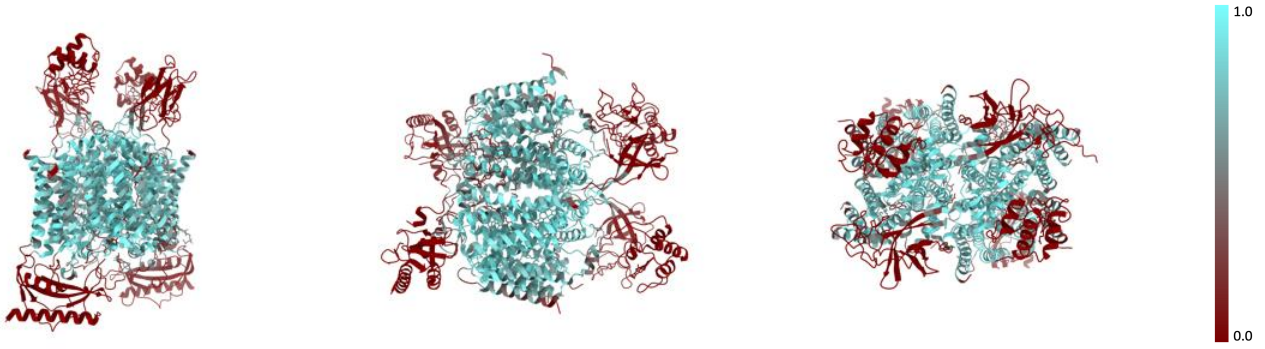
9.2 Q-score mapped to coordinate model (i)



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.

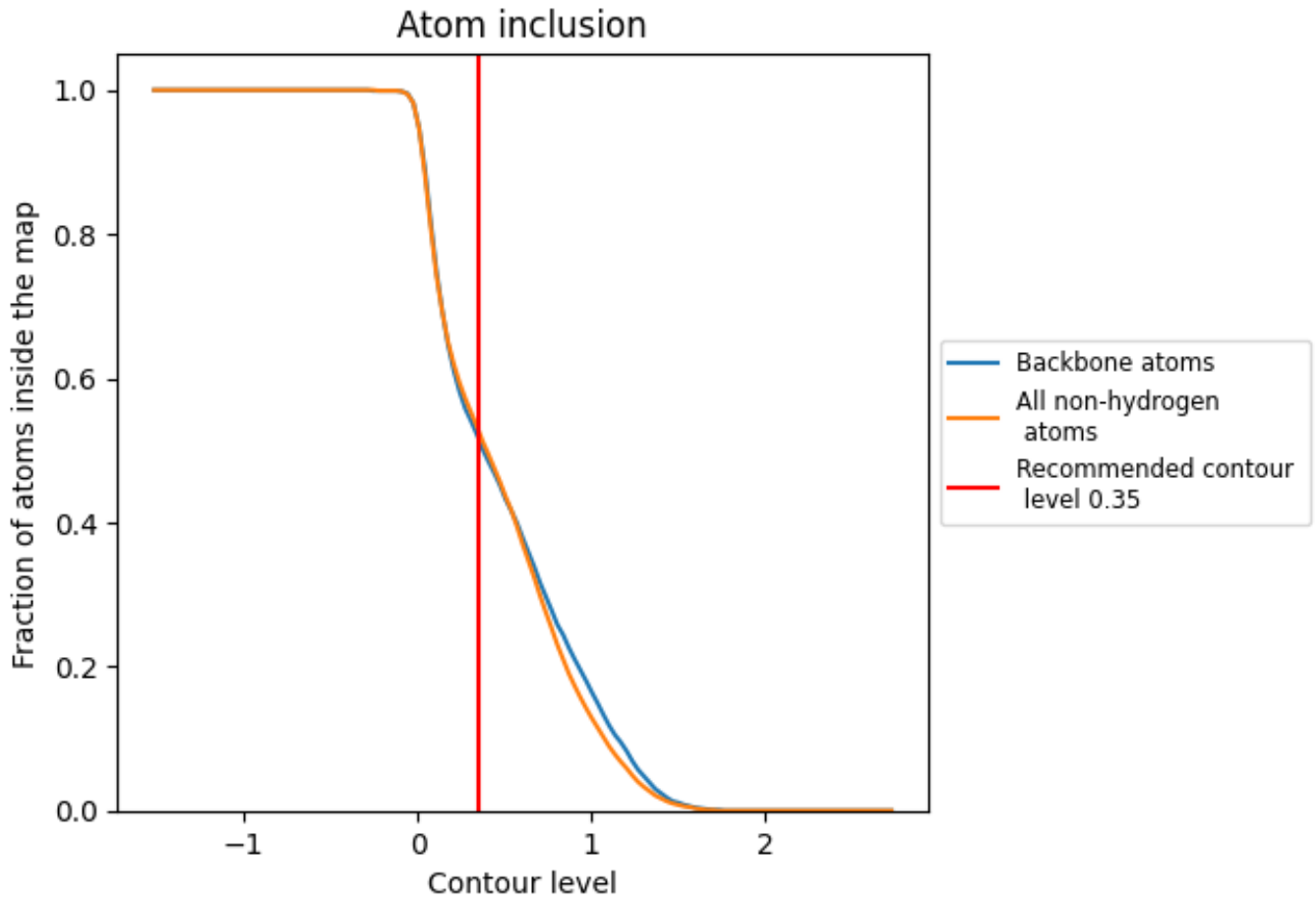
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 53% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5280	0.4880
A	0.2400	0.3240
B	0.8500	0.6220
C	0.5000	0.4400
D	0.6450	0.5510
E	0.8220	0.6190
F	0.4910	0.5720
G	0.6180	0.5200
H	0.5500	0.5000
I	0.0030	0.3590
a	0.2560	0.3350
b	0.8300	0.6190
c	0.4930	0.4340
d	0.6900	0.5850
e	0.8290	0.6250
f	0.4820	0.5670
g	0.6590	0.5690
h	0.5470	0.4930
i	0.0020	0.3930

