Full wwPDB EM Validation Report

Oct 26, 2026 – 06:45 PM EDT

PDB ID	:	9OCZ / pdb_00009ocz
EMDB ID	:	EMD-70336
Title	:	Cryo-EM structure of the CIII2 without YlbA from Bacillus subtilis
Authors	:	Zong, Y.; Zheng, W.; Gu, M.; Zhang, K.; Zhu, J.
Deposited on	:	2025-04-25
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

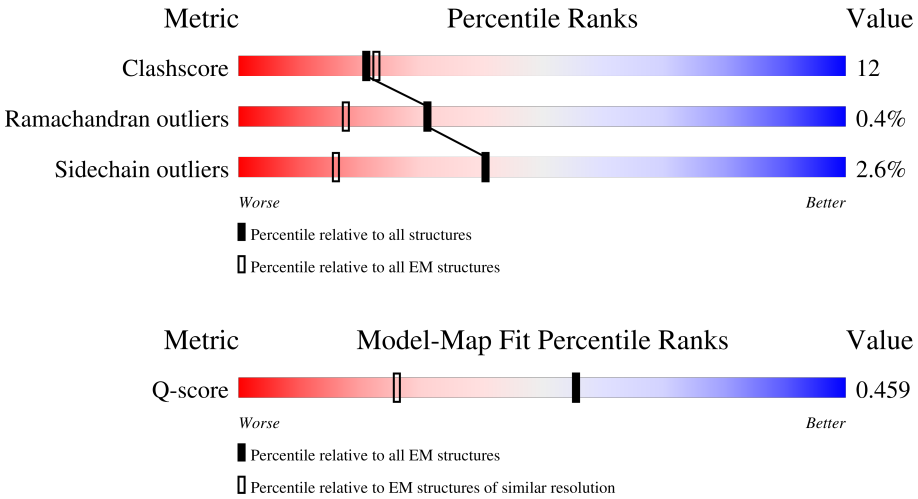
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.80 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.



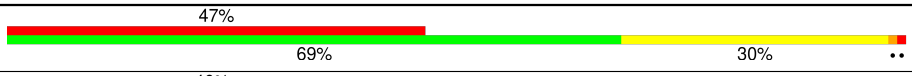
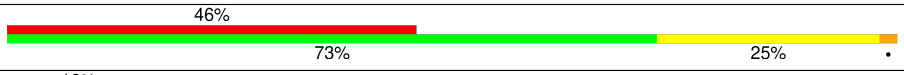
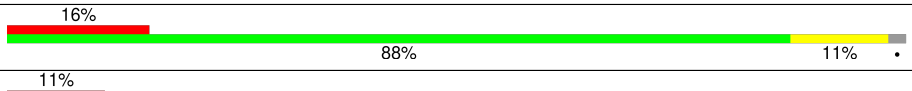
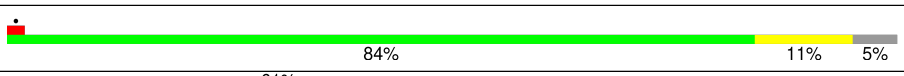
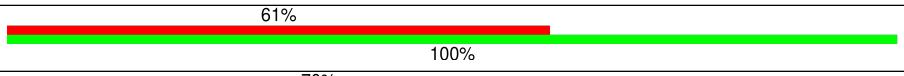
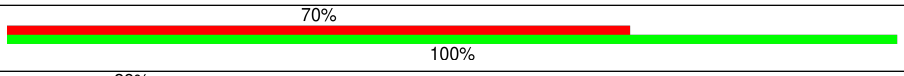
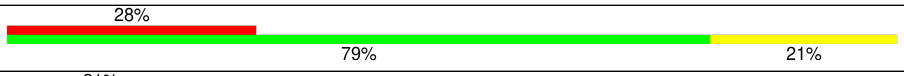
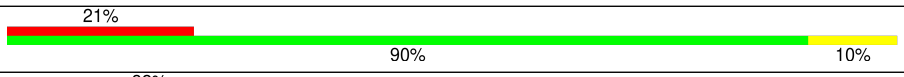
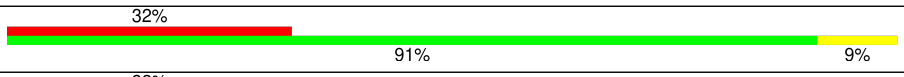
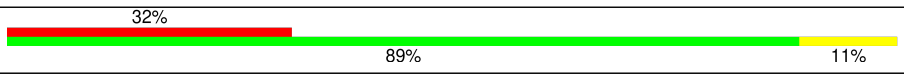
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	71% 72% 24%
1	a	167	69% 62% 32% 5%
2	B	224	68% 30%
2	b	224	71% 28%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEC	B	301	X	-	-	-
10	HEC	C	301	X	-	-	-
10	HEC	b	301	X	-	-	-
10	HEC	c	302	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Menaquinol:cytochrome c reductase iron-sulfur subunit.

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

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

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

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

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

- Molecule 4 is a protein called YqgW.

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

- Molecule 5 is a protein called YqgY.

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

- Molecule 6 is a protein called QcrF.

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

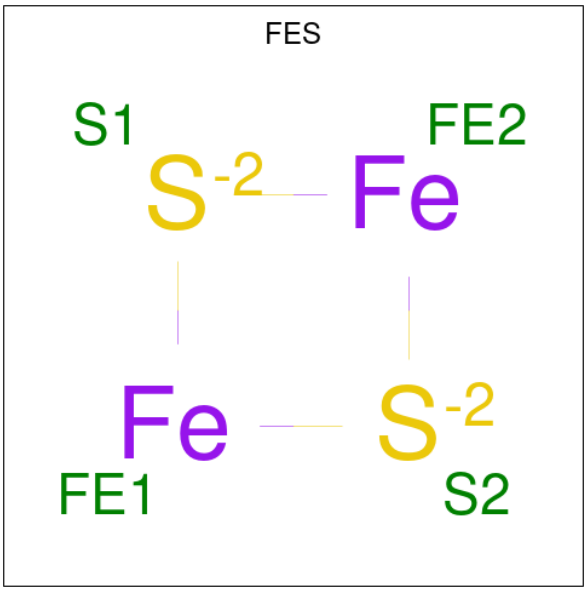
- Molecule 7 is a protein called QcrG.

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

- Molecule 8 is a protein called YqzM.

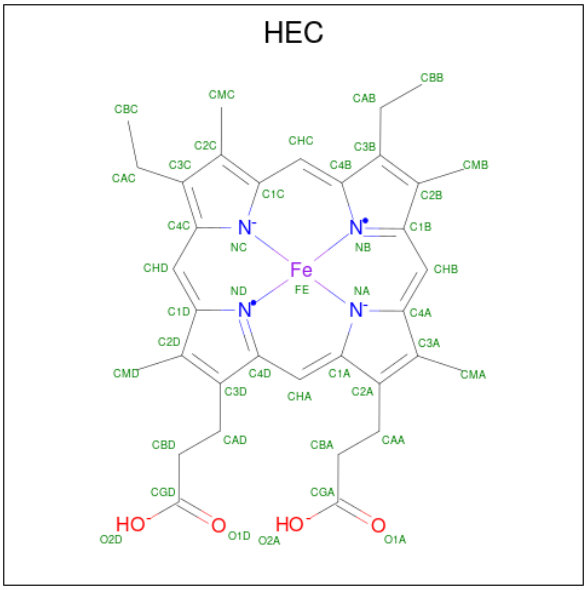
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	44	Total	C	N	O	S	0	0
			342	223	55	62	2		
8	h	44	Total	C	N	O	S	0	0
			342	223	55	62	2		

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



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

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



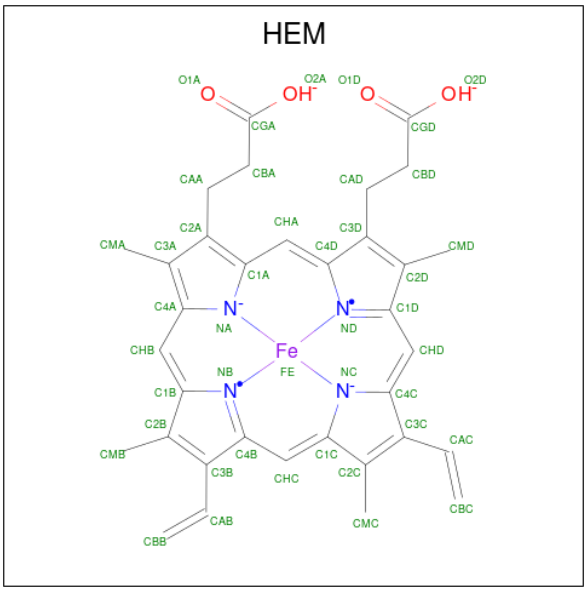
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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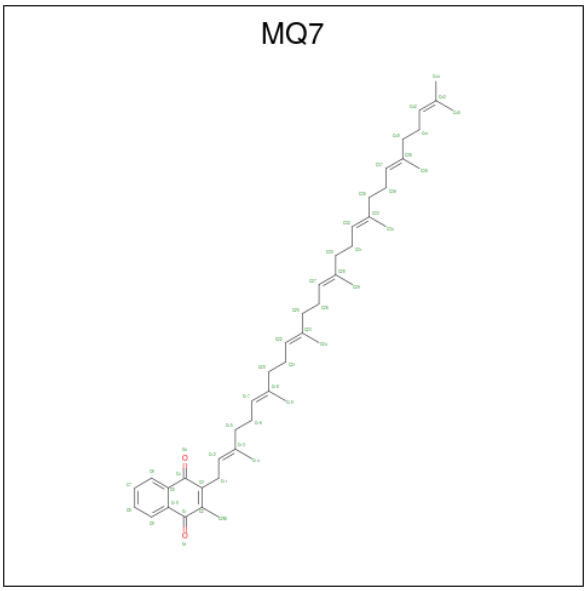
Mol	Chain	Residues	Atoms					AltConf
10	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



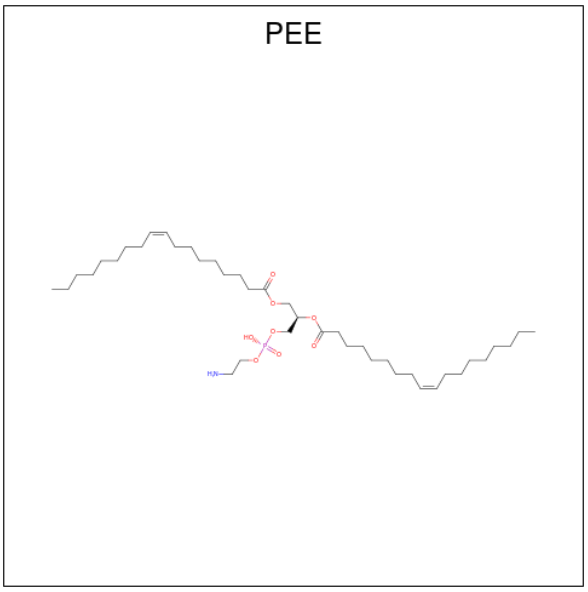
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



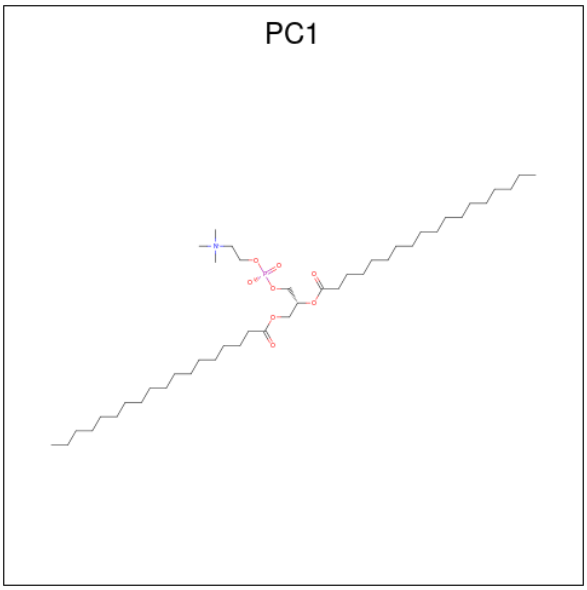
Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C O 48 46 2	0
12	B	1	Total C O 48 46 2	0
12	b	1	Total C O 48 46 2	0
12	c	1	Total C O 48 46 2	0

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



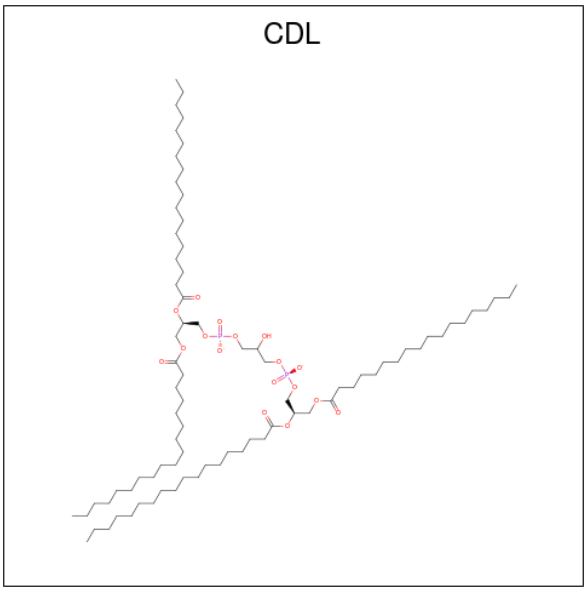
Mol	Chain	Residues	Atoms					AltConf
13	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
13	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
13	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	e	1	Total	C	N	O	P	0
			34	24	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf
14	E	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



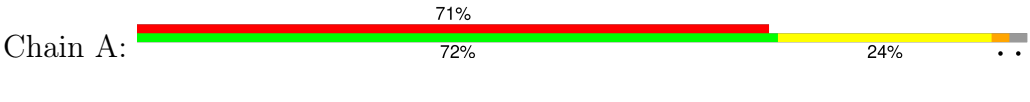
Mol	Chain	Residues	Atoms				AltConf
15	b	1	Total	C	O	P	0
			98	79	17	2	

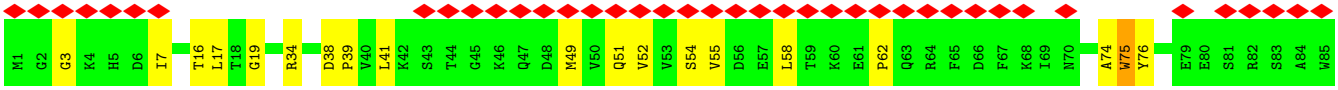
3 Residue-property plots (i)

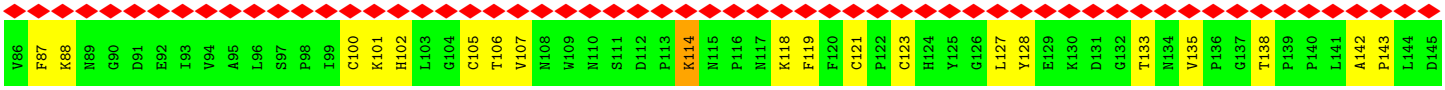
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

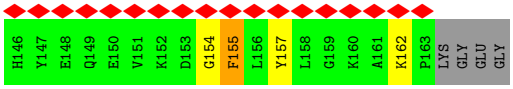
• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain A:





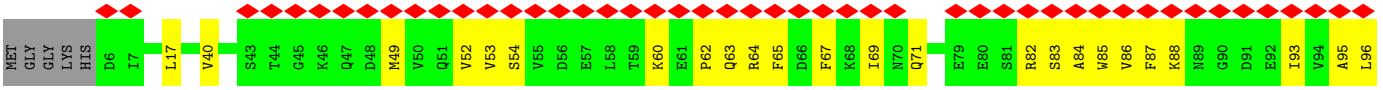




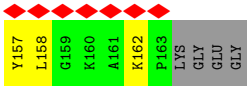
• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain a:





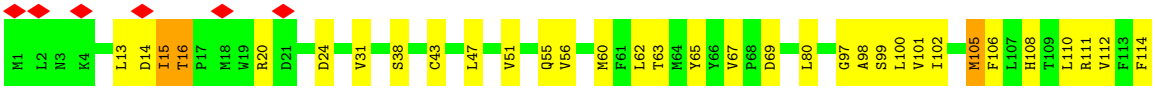


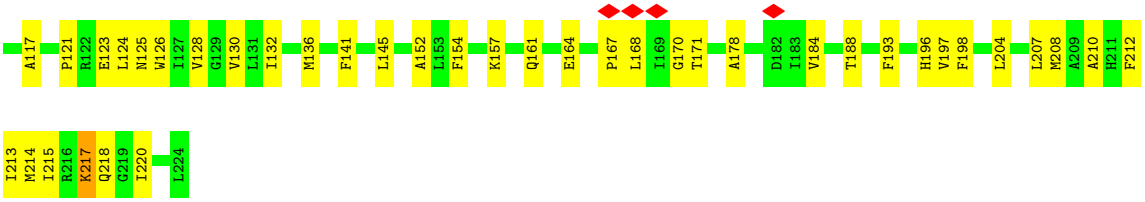


• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain B:



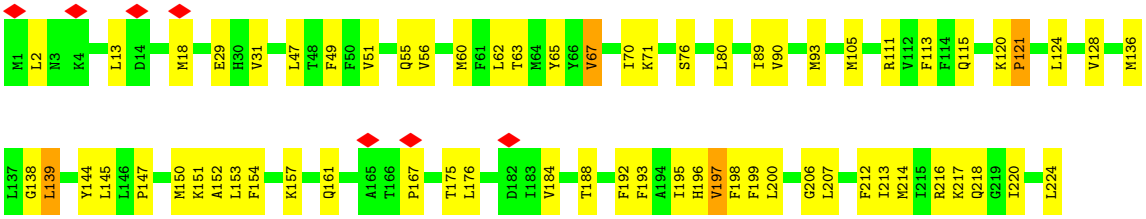




• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain b:

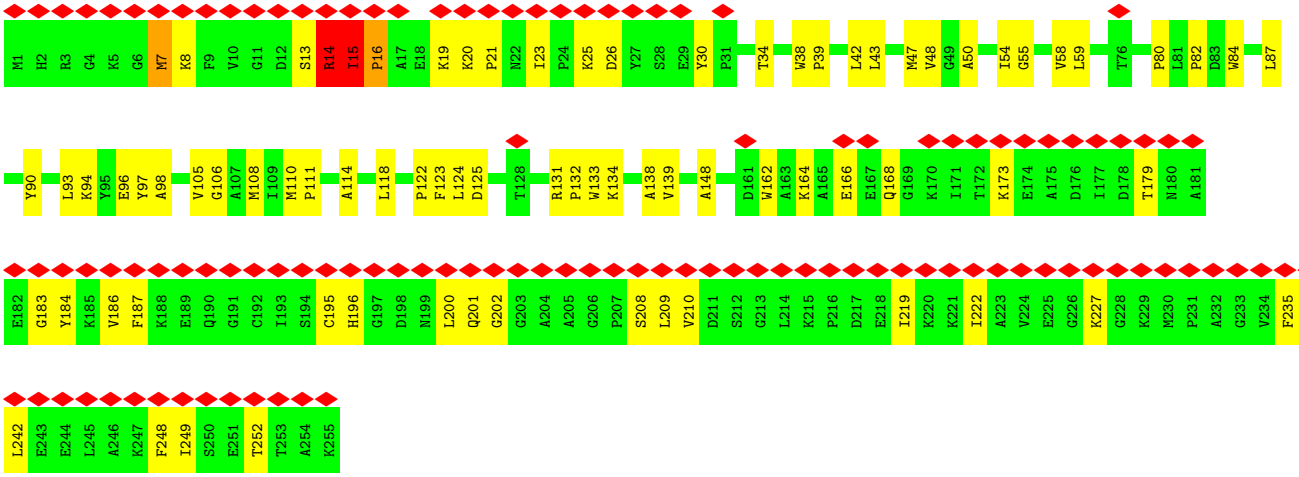




• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain C:

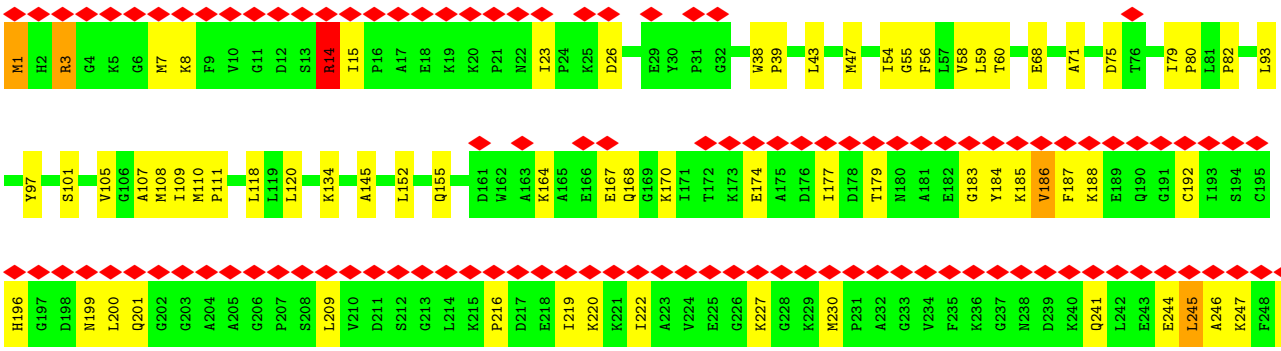




• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

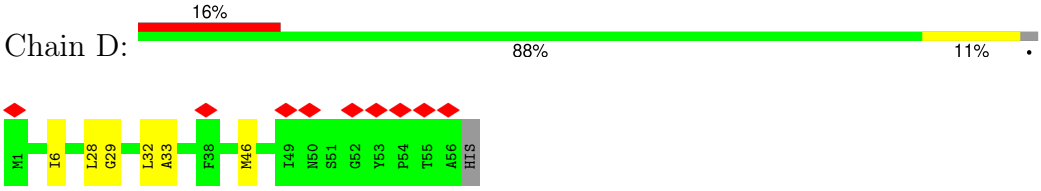
Chain c:





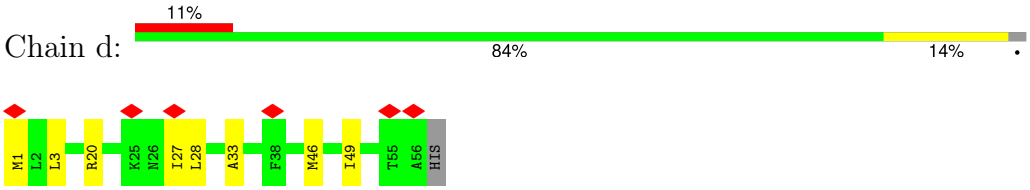
• Molecule 4: YqgW

Chain D:



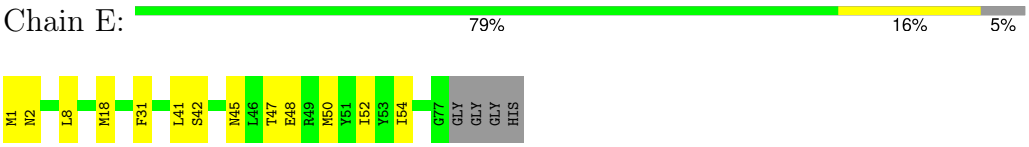
• Molecule 4: YqgW

Chain d:



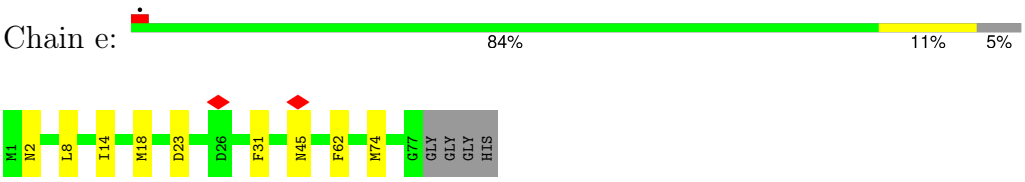
• Molecule 5: YqgY

Chain E:



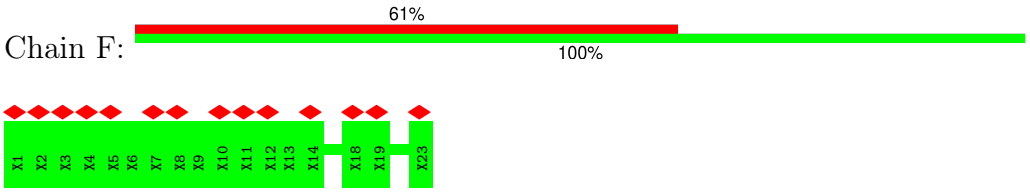
• Molecule 5: YqgY

Chain e:



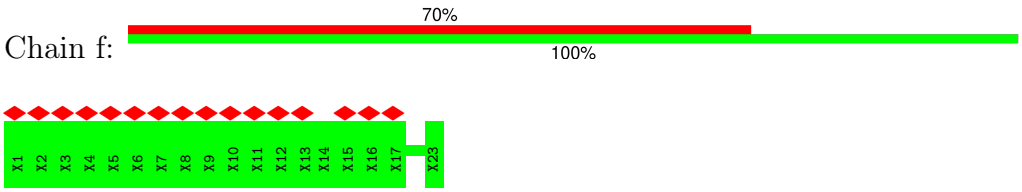
• Molecule 6: QcrF

Chain F:



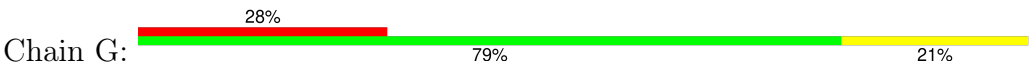
• Molecule 6: QcrF

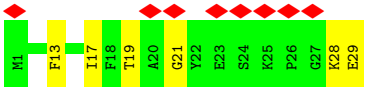
Chain f:



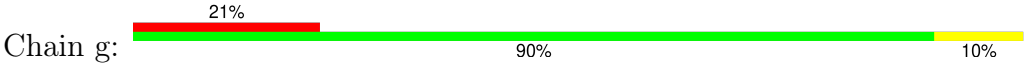
• Molecule 7: QcrG

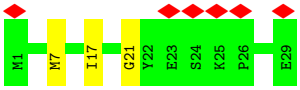
Chain G:



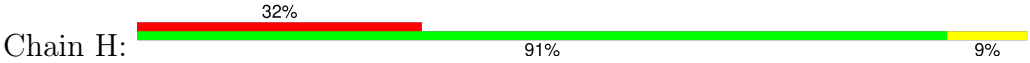


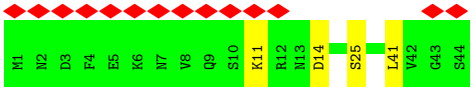
• Molecule 7: QcrG



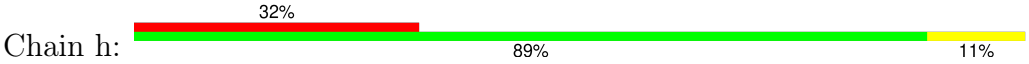


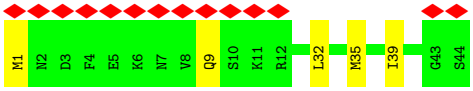
• Molecule 8: YqzM





• Molecule 8: YqzM





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96392	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	2.205	Depositor
Minimum map value	-1.441	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.31	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: PC1, PEE, MQ7, FES, HEM, HEC, CDL

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	0.14	0/1326	0.38	0/1796
1	a	0.15	0/1290	0.38	0/1750
2	B	0.19	0/1863	0.40	0/2533
2	b	0.18	0/1863	0.40	1/2533 (0.0%)
3	C	0.23	0/2040	0.44	1/2759 (0.0%)
3	c	0.20	0/2040	0.41	1/2759 (0.0%)
4	D	0.11	0/444	0.24	0/605
4	d	0.13	0/444	0.35	0/605
5	E	0.11	0/667	0.24	0/900
5	e	0.12	0/667	0.29	0/900
7	G	0.12	0/224	0.32	0/299
7	g	0.12	0/224	0.31	0/299
8	H	0.15	0/349	0.44	0/468
8	h	0.14	0/349	0.32	0/468
All	All	0.18	0/13790	0.39	3/18674 (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
3	C	0	1
3	c	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	120	LYS	O-C-N	-7.12	114.97	121.30
3	c	14	ARG	CB-CA-C	-6.08	102.12	111.66
3	C	16	PRO	CB-CA-C	-5.75	102.07	111.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	14	ARG	Sidechain
3	c	14	ARG	Sidechain
3	c	3	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1290	0	1254	34	0
1	a	1255	0	1216	39	0
2	B	1804	0	1813	66	0
2	b	1804	0	1813	51	0
3	C	1986	0	1999	76	0
3	c	1986	0	1997	61	0
4	D	433	0	462	6	0
4	d	433	0	463	8	0
5	E	645	0	642	11	0
5	e	645	0	642	9	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	2	0
8	H	342	0	334	4	0
8	h	342	0	334	4	0
9	A	4	0	0	1	0
9	a	4	0	0	1	0
10	B	43	0	31	3	0
10	C	43	0	32	1	0
10	b	43	0	31	1	0
10	c	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	86	0	60	10	0
11	b	86	0	60	2	0
12	B	96	0	128	17	0
12	b	48	0	64	3	0
12	c	48	0	64	7	0
13	D	46	0	64	5	0
13	a	40	0	54	0	0
13	d	51	0	78	5	0
13	e	34	0	42	3	0
14	E	41	0	56	11	0
15	b	98	0	149	8	0
All	All	14489	0	14444	343	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 12.

All (343) 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:100:CYS:SG	1:A:105:CYS:HB2	1.87	1.13
3:C:15:ILE:H	3:C:16:PRO:HD2	1.34	0.92
3:C:14:ARG:HB3	3:C:16:PRO:HD2	1.55	0.87
1:A:105:CYS:HB3	1:A:123:CYS:SG	2.17	0.83
3:c:219:ILE:HG21	3:c:249:ILE:HD11	1.61	0.83
3:c:183:GLY:HA2	3:c:244:GLU:HB3	1.63	0.81
1:A:41:LEU:HB3	8:H:41:LEU:HD21	1.63	0.79
3:c:164:LYS:O	3:c:168:GLN:HB2	1.83	0.79
2:B:20:ARG:HH21	3:C:26:ASP:HA	1.47	0.77
5:e:2:ASN:HD21	5:e:45:ASN:HA	1.51	0.76
2:b:154:PHE:HB3	3:c:80:PRO:HB3	1.68	0.75
2:b:90:VAL:HA	2:b:93:MET:HE2	1.69	0.73
3:C:210:VAL:HA	3:C:252:THR:HG22	1.71	0.73
3:c:79:ILE:H	3:c:168:GLN:NE2	1.88	0.72
3:C:196:HIS:HB3	3:C:209:LEU:HD11	1.73	0.70
1:a:96:LEU:HD23	1:a:144:LEU:HB2	1.74	0.69
3:c:59:LEU:HD22	13:e:101:PEE:H24	1.74	0.69
15:b:305:CDL:H762	15:b:305:CDL:HA61	1.74	0.68
3:c:43:LEU:O	3:c:47:MET:HG3	1.93	0.68
2:B:65:TYR:HB2	2:B:80:LEU:HD12	1.76	0.68
2:B:154:PHE:HB3	3:C:80:PRO:HB3	1.75	0.68
2:B:97:GLY:O	2:B:101:VAL:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:49:MET:HE2	1:a:49:MET:HA	1.73	0.67
3:c:167:GLU:HA	3:c:170:LYS:HD2	1.77	0.67
11:B:303:HEM:HBC2	11:B:303:HEM:HHD	1.76	0.66
5:E:1:MET:HG3	5:E:48:GLU:HG3	1.78	0.66
3:c:105:VAL:HA	3:c:109:ILE:HB	1.77	0.65
11:B:303:HEM:O1D	11:B:303:HEM:HHA	1.96	0.65
2:b:62:LEU:HD22	2:b:80:LEU:HD11	1.77	0.64
3:C:16:PRO:HD3	2:b:121:PRO:HD3	1.79	0.64
2:b:206:GLY:HA3	12:c:301:MQ7:H401	1.79	0.64
2:b:207:LEU:HD11	12:c:301:MQ7:H32	1.78	0.64
3:C:43:LEU:O	3:C:47:MET:HG3	1.98	0.64
5:E:18:MET:HE3	14:E:101:PC1:H331	1.80	0.64
2:B:20:ARG:NH2	3:C:26:ASP:HA	2.12	0.64
2:B:193:PHE:O	2:B:197:VAL:HB	1.99	0.63
1:A:58:LEU:HB2	1:A:88:LYS:HE3	1.81	0.63
10:B:301:HEC:HBC1	3:C:48:VAL:HG21	1.81	0.62
3:C:164:LYS:O	3:C:168:GLN:HG2	1.99	0.62
3:c:105:VAL:HG12	3:c:109:ILE:HD12	1.80	0.62
1:a:49:MET:SD	1:a:157:TYR:HB3	2.40	0.62
2:B:217:LYS:HB3	3:c:15:ILE:HD11	1.81	0.61
1:a:147:TYR:HB2	1:a:158:LEU:HG	1.83	0.61
15:b:305:CDL:H191	15:b:305:CDL:H801	1.84	0.60
3:c:1:MET:HG2	3:c:14:ARG:HD2	1.83	0.60
3:C:15:ILE:H	3:C:16:PRO:CD	2.11	0.60
3:C:25:LYS:HG2	8:H:11:LYS:HE3	1.84	0.60
2:B:56:VAL:O	2:B:60:MET:HG3	2.03	0.59
5:e:18:MET:HB3	13:e:101:PEE:H18	1.84	0.59
1:A:54:SER:HA	1:A:155:PHE:HA	1.84	0.59
1:a:54:SER:HA	1:a:155:PHE:HA	1.83	0.59
12:B:305:MQ7:H242	2:b:13:LEU:HD13	1.85	0.59
3:C:200:LEU:HA	3:C:209:LEU:HD13	1.84	0.59
1:a:119:PHE:HB2	1:a:128:TYR:HB2	1.85	0.59
1:A:3:GLY:HA3	1:A:7:ILE:HG12	1.85	0.58
1:a:52:VAL:HG13	1:a:65:PHE:HD2	1.68	0.58
2:b:193:PHE:O	2:b:197:VAL:HB	2.04	0.58
3:C:50:ALA:O	3:C:54:ILE:HG12	2.03	0.58
2:B:13:LEU:HD21	2:b:214:MET:HG2	1.85	0.58
3:C:186:VAL:HG22	3:C:241:GLN:HE21	1.69	0.58
2:b:145:LEU:HA	2:b:152:ALA:HB1	1.87	0.57
3:C:7:MET:HG2	3:C:8:LYS:H	1.69	0.57
3:c:23:ILE:HG22	8:h:9:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:LYS:HE3	3:C:19:LYS:HE2	1.87	0.57
12:B:304:MQ7:H8	3:C:90:TYR:HD1	1.70	0.57
3:C:114:ALA:HB2	13:D:101:PEE:H70	1.87	0.57
1:a:96:LEU:HG	1:a:146:HIS:HB3	1.86	0.57
2:B:125:ASN:HD21	2:B:215:ILE:HG13	1.70	0.56
5:e:18:MET:HE2	13:e:101:PEE:H54	1.86	0.56
1:A:17:LEU:HD21	3:C:42:LEU:HD23	1.87	0.56
2:B:184:VAL:HG13	2:B:188:THR:HG21	1.87	0.56
4:D:33:ALA:HB2	13:D:101:PEE:H49	1.86	0.56
3:c:152:LEU:HD21	4:d:3:LEU:HD22	1.88	0.56
3:c:167:GLU:O	3:c:167:GLU:HG3	2.05	0.56
3:c:222:ILE:HG12	3:c:227:LYS:HD3	1.86	0.56
2:b:184:VAL:HG13	2:b:188:THR:HG21	1.87	0.56
2:b:56:VAL:O	2:b:60:MET:HG3	2.05	0.55
2:b:111:ARG:HH22	11:b:303:HEM:HBD1	1.70	0.55
3:C:59:LEU:HD13	14:E:101:PC1:H351	1.88	0.55
2:b:192:PHE:O	2:b:196:HIS:HB3	2.06	0.55
2:B:108:HIS:CE1	2:B:111:ARG:HE	2.25	0.55
5:E:18:MET:HG3	14:E:101:PC1:H291	1.89	0.55
2:b:213:ILE:O	2:b:217:LYS:HG3	2.07	0.55
2:B:157:LYS:O	2:B:161:GLN:HG2	2.07	0.55
2:b:89:ILE:HG13	5:e:74:MET:HE1	1.87	0.55
3:C:124:LEU:HD23	4:D:29:GLY:HA2	1.88	0.54
3:C:219:ILE:HA	3:C:222:ILE:HB	1.88	0.54
3:c:145:ALA:HB2	13:d:101:PEE:H67	1.88	0.54
3:c:120:LEU:HD13	4:d:28:LEU:HD21	1.89	0.54
1:a:84:ALA:HA	1:a:98:PRO:HD3	1.90	0.54
5:E:18:MET:HB3	14:E:101:PC1:H371	1.88	0.53
3:c:227:LYS:O	3:c:230:MET:HG2	2.09	0.53
2:B:145:LEU:HA	2:B:152:ALA:HB1	1.90	0.53
11:B:302:HEM:HHC	11:B:302:HEM:HBB2	1.89	0.53
4:d:46:MET:HA	4:d:46:MET:HE2	1.91	0.53
3:C:14:ARG:HH11	3:C:14:ARG:HB2	1.74	0.53
3:c:222:ILE:HG23	3:c:227:LYS:HB2	1.89	0.53
2:B:108:HIS:HD2	11:B:303:HEM:CHA	2.22	0.53
2:B:214:MET:HE2	12:B:305:MQ7:H261	1.91	0.53
3:c:244:GLU:HA	3:c:247:LYS:HB2	1.89	0.53
3:C:138:ALA:HB2	13:D:101:PEE:H3	1.91	0.52
1:a:96:LEU:HA	1:a:146:HIS:HA	1.90	0.52
3:c:79:ILE:H	3:c:168:GLN:HE22	1.57	0.52
3:C:30:TYR:HB3	3:C:34:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:86:VAL:HG12	1:a:93:ILE:HD11	1.92	0.52
3:c:184:TYR:HA	3:c:187:PHE:CE1	2.44	0.52
3:c:186:VAL:HG22	3:c:241:GLN:HG2	1.92	0.52
1:a:88:LYS:HA	1:a:93:ILE:HD12	1.91	0.52
1:a:102:HIS:HB3	9:a:201:FES:S1	2.50	0.52
11:B:303:HEM:HHA	11:B:303:HEM:CGD	2.40	0.52
1:a:71:GLN:HE21	1:a:82:ARG:HH22	1.58	0.51
3:c:93:LEU:HD12	12:c:301:MQ7:H7	1.92	0.51
2:b:111:ARG:HA	7:g:17:ILE:HG23	1.91	0.51
1:A:49:MET:HG3	1:A:157:TYR:HB3	1.92	0.51
2:B:124:LEU:HD21	12:B:305:MQ7:H302	1.93	0.51
15:b:305:CDL:H182	15:b:305:CDL:H772	1.93	0.51
2:b:111:ARG:HH11	2:b:115:GLN:NE2	2.08	0.51
2:b:157:LYS:O	2:b:161:GLN:HG2	2.11	0.51
2:B:132:ILE:HG21	11:B:303:HEM:HBA2	1.92	0.51
2:B:214:MET:HG2	12:B:305:MQ7:H241	1.93	0.51
15:b:305:CDL:H851	15:b:305:CDL:H381	1.92	0.51
2:b:224:LEU:HD12	7:g:21:GLY:HA3	1.93	0.50
2:B:47:LEU:O	2:B:51:VAL:HG23	2.11	0.50
1:a:52:VAL:HG12	1:a:53:VAL:HG13	1.91	0.50
3:c:177:ILE:HD11	3:c:184:TYR:CZ	2.46	0.50
3:c:184:TYR:O	3:c:188:LYS:HB3	2.12	0.50
2:B:69:ASP:HB2	2:b:67:VAL:HG11	1.92	0.50
2:B:196:HIS:HE1	11:B:302:HEM:C4C	2.29	0.50
2:b:195:ILE:HA	2:b:199:PHE:HD2	1.76	0.50
3:C:59:LEU:HD22	14:E:101:PC1:H362	1.93	0.50
1:a:98:PRO:HA	1:a:107:VAL:HG22	1.94	0.50
12:b:304:MQ7:H291	12:b:304:MQ7:H32	1.92	0.50
3:c:199:ASN:HD22	3:c:201:GLN:HE22	1.59	0.50
2:b:128:VAL:HG21	2:b:214:MET:HE1	1.93	0.50
2:B:62:LEU:HD22	2:B:80:LEU:HD11	1.93	0.50
3:C:16:PRO:HG3	2:b:121:PRO:HG3	1.92	0.50
3:C:98:ALA:HB1	3:C:106:GLY:HA3	1.93	0.50
2:B:193:PHE:HE1	11:B:302:HEM:HMA3	1.76	0.50
2:b:151:LYS:HB2	3:c:68:GLU:OE2	2.12	0.50
3:c:93:LEU:HD21	3:c:107:ALA:HB2	1.93	0.50
1:A:102:HIS:HB3	9:A:201:FES:S1	2.52	0.49
1:a:83:SER:HB3	1:a:98:PRO:HG2	1.94	0.49
2:B:99:SER:HB3	3:C:84:TRP:HE1	1.76	0.49
3:C:15:ILE:N	3:C:16:PRO:HD2	2.16	0.49
3:C:96:GLU:CD	3:C:96:GLU:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:67:PHE:CE2	1:a:158:LEU:HD23	2.46	0.49
1:a:101:LYS:HE2	1:a:145:ASP:H	1.78	0.49
2:B:207:LEU:HD23	12:B:305:MQ7:H361	1.95	0.49
1:A:119:PHE:HB2	1:A:128:TYR:HB2	1.95	0.49
2:b:167:PRO:HD3	3:c:108:MET:HG3	1.95	0.49
2:B:105:MET:HE1	2:B:136:MET:CB	2.43	0.49
2:B:212:PHE:HE1	11:B:303:HEM:HHB	1.77	0.49
3:C:202:GLY:HA3	3:C:208:SER:HA	1.94	0.49
1:a:118:LYS:HD3	1:a:128:TYR:O	2.14	0.48
2:b:105:MET:HE1	2:b:136:MET:HB3	1.95	0.48
2:b:214:MET:O	2:b:218:GLN:HG3	2.12	0.48
3:C:132:PRO:HB2	7:G:29:GLU:HG3	1.94	0.48
1:A:51:GLN:H	1:A:51:GLN:CD	2.21	0.48
2:B:123:GLU:HG2	3:C:122:PRO:HB2	1.95	0.48
5:E:2:ASN:O	5:E:42:SER:HB2	2.13	0.48
2:B:112:VAL:HG13	2:B:117:ALA:HB3	1.95	0.48
3:c:155:GLN:NE2	4:d:1:MET:HE1	2.28	0.48
3:c:82:PRO:HB3	12:c:301:MQ7:O1	2.13	0.48
1:A:133:THR:HG22	1:A:143:PRO:HB3	1.96	0.47
1:A:39:PRO:HB2	2:b:175:THR:HG22	1.96	0.47
2:B:128:VAL:O	2:B:132:ILE:HG13	2.14	0.47
2:b:49:PHE:HD2	10:b:301:HEC:HMB2	1.79	0.47
3:c:118:LEU:HD13	13:d:101:PEE:H31	1.97	0.47
1:A:106:THR:O	1:A:121:CYS:HB2	2.15	0.47
2:B:101:VAL:O	2:B:105:MET:HB2	2.15	0.47
3:C:219:ILE:HG21	3:C:249:ILE:HG21	1.96	0.47
2:B:220:ILE:HB	10:B:301:HEC:HBB2	1.97	0.47
2:b:153:LEU:HD22	3:c:71:ALA:HB1	1.97	0.47
3:c:187:PHE:HB2	3:c:245:LEU:HD23	1.97	0.47
2:B:13:LEU:HD13	12:b:304:MQ7:H242	1.97	0.47
14:E:101:PC1:H381	14:E:101:PC1:H352	1.75	0.47
8:h:1:MET:HE2	8:h:1:MET:HB2	1.84	0.47
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.79	0.47
1:a:71:GLN:NE2	1:a:82:ARG:HH22	2.12	0.47
3:c:186:VAL:HG11	3:c:244:GLU:HB2	1.97	0.47
2:B:31:VAL:HG21	10:B:301:HEC:HBB1	1.96	0.46
2:B:124:LEU:HG	2:B:214:MET:HE1	1.96	0.46
3:C:23:ILE:O	3:C:23:ILE:HG13	2.15	0.46
3:c:56:PHE:O	3:c:60:THR:HG23	2.15	0.46
1:A:16:THR:HG21	5:E:52:ILE:HG12	1.97	0.46
1:A:62:PRO:HA	1:A:87:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:PHE:HE2	2:b:63:THR:HG21	1.81	0.46
3:C:47:MET:HE3	5:E:8:LEU:HD11	1.97	0.46
2:B:20:ARG:HD2	2:B:20:ARG:HA	1.66	0.46
2:B:210:ALA:HB1	12:B:305:MQ7:H262	1.98	0.46
3:C:184:TYR:HA	3:C:187:PHE:HB3	1.96	0.46
3:c:38:TRP:HB3	3:c:39:PRO:HD3	1.98	0.46
1:A:135:VAL:O	1:A:138:THR:HG22	2.15	0.45
3:c:110:MET:HB2	3:c:111:PRO:HD3	1.98	0.45
15:b:305:CDL:H561	15:b:305:CDL:H592	1.80	0.45
1:a:123:CYS:SG	1:a:124:HIS:N	2.90	0.45
3:c:196:HIS:CE1	3:c:209:LEU:HD12	2.52	0.45
1:A:118:LYS:HE2	1:A:127:LEU:HD11	1.97	0.45
2:B:100:LEU:HD11	14:E:101:PC1:H3B1	1.98	0.45
1:a:138:THR:OG1	1:a:140:PRO:HD2	2.17	0.45
1:A:114:LYS:HB3	1:A:114:LYS:HE2	1.67	0.45
2:B:126:TRP:O	2:B:130:VAL:HG23	2.17	0.45
1:a:60:LYS:HA	1:a:88:LYS:HB3	1.98	0.45
3:c:7:MET:HG3	3:c:8:LYS:H	1.82	0.45
1:A:76:TYR:HE1	2:b:71:LYS:HE3	1.81	0.45
1:A:76:TYR:CD2	2:b:70:ILE:HG21	2.52	0.45
3:C:173:LYS:O	3:C:201:GLN:HG3	2.16	0.45
1:a:148:GLU:HB3	1:a:162:LYS:HD2	1.97	0.45
2:b:139:LEU:HG	2:b:200:LEU:HB3	1.98	0.45
12:B:304:MQ7:H362	12:B:304:MQ7:H341	1.64	0.45
2:B:63:THR:HG21	2:b:198:PHE:HE2	1.81	0.45
12:B:305:MQ7:H162	12:B:305:MQ7:H141	1.38	0.45
3:C:94:LYS:HE3	3:C:94:LYS:HB2	1.78	0.45
14:E:101:PC1:H321	14:E:101:PC1:H32	1.67	0.44
2:B:141:PHE:CG	12:B:304:MQ7:H152	2.52	0.44
1:a:62:PRO:HG3	1:a:87:PHE:HB2	1.98	0.44
1:a:17:LEU:HA	3:c:43:LEU:HD13	2.00	0.44
1:A:51:GLN:HB3	1:A:157:TYR:CE1	2.53	0.44
1:A:55:VAL:HG12	1:A:154:GLY:HA2	2.00	0.44
2:B:43:CYS:SG	3:C:48:VAL:HG11	2.58	0.44
2:B:178:ALA:HA	2:B:188:THR:HG23	1.99	0.44
3:c:184:TYR:HA	3:c:187:PHE:CD1	2.53	0.44
5:E:2:ASN:HD21	5:E:45:ASN:HA	1.83	0.44
1:a:64:ARG:HB2	1:a:85:TRP:CH2	2.53	0.44
2:b:47:LEU:O	2:b:51:VAL:HG23	2.17	0.44
14:E:101:PC1:H361	14:E:101:PC1:H332	1.57	0.44
1:a:52:VAL:HG21	1:a:158:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:305:CDL:H761	15:b:305:CDL:HB62	1.99	0.44
4:d:33:ALA:HB2	13:d:101:PEE:H48	1.98	0.44
12:B:304:MQ7:O1	3:C:82:PRO:HB3	2.17	0.44
7:G:13:PHE:O	7:G:17:ILE:HG12	2.18	0.44
3:C:82:PRO:HG2	3:C:87:LEU:HD23	1.99	0.43
15:b:305:CDL:HB61	15:b:305:CDL:H712	1.66	0.43
3:C:105:VAL:O	3:C:110:MET:HG3	2.18	0.43
3:C:124:LEU:HD11	4:D:32:LEU:HD13	2.00	0.43
1:a:86:VAL:HG13	1:a:95:ALA:HB2	1.99	0.43
3:c:26:ASP:HB2	8:h:9:GLN:OE1	2.18	0.43
3:C:38:TRP:HB3	3:C:39:PRO:HD3	1.99	0.43
3:C:97:TYR:CE2	4:D:46:MET:HB3	2.53	0.43
3:c:199:ASN:HD22	3:c:201:GLN:NE2	2.16	0.43
2:B:210:ALA:O	2:B:214:MET:HG3	2.18	0.43
8:H:11:LYS:HB3	8:H:11:LYS:HE2	1.71	0.43
2:b:150:MET:HE1	3:c:75:ASP:HB3	1.99	0.43
3:c:55:GLY:HA2	5:e:31:PHE:CZ	2.53	0.43
1:A:107:VAL:HG13	1:A:121:CYS:HB3	2.00	0.43
2:B:15:ILE:HG22	2:B:15:ILE:O	2.17	0.43
1:a:127:LEU:HD12	1:a:135:VAL:HG21	2.00	0.43
1:A:19:GLY:HA2	8:H:25:SER:OG	2.19	0.43
3:C:183:GLY:HA3	3:C:248:PHE:CG	2.54	0.43
3:C:219:ILE:H	3:C:219:ILE:HG13	1.68	0.43
5:E:41:LEU:HD13	5:E:54:ILE:HG21	2.01	0.43
3:c:179:THR:O	3:c:185:LYS:HB2	2.18	0.43
2:B:14:ASP:HB3	2:b:217:LYS:HZ1	1.84	0.43
12:B:305:MQ7:H261	12:B:305:MQ7:H241	1.71	0.43
3:C:148:ALA:HB2	4:D:6:ILE:HG21	1.99	0.43
3:c:174:GLU:HA	3:c:199:ASN:ND2	2.33	0.43
1:A:107:VAL:HG22	1:A:121:CYS:HB3	2.01	0.43
2:B:204:LEU:O	2:B:208:MET:HG3	2.18	0.43
3:C:13:SER:O	3:C:14:ARG:C	2.62	0.43
2:b:212:PHE:O	2:b:216:ARG:HG3	2.19	0.43
3:c:134:LYS:HD3	3:c:134:LYS:HA	1.84	0.43
2:B:14:ASP:OD1	2:b:217:LYS:HE3	2.19	0.43
2:B:105:MET:HE1	2:B:136:MET:HB3	2.00	0.43
2:B:114:PHE:CD1	3:C:139:VAL:HG13	2.54	0.43
2:B:213:ILE:HG23	12:B:305:MQ7:H151	2.01	0.43
3:C:179:THR:HG22	3:C:184:TYR:HE2	1.84	0.43
1:a:93:ILE:HG12	1:a:156:LEU:HD13	2.01	0.43
2:b:65:TYR:O	2:b:76:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:219:ILE:HA	3:c:222:ILE:HB	2.00	0.43
2:B:217:LYS:HD2	12:B:305:MQ7:H202	2.00	0.42
3:C:118:LEU:HB2	13:D:101:PEE:H25	2.01	0.42
4:d:20:ARG:HB3	13:d:101:PEE:N	2.33	0.42
3:C:20:LYS:N	3:C:21:PRO:HD3	2.33	0.42
3:C:222:ILE:HG12	3:C:227:LYS:HD3	2.00	0.42
3:C:235:PHE:CE2	3:C:242:LEU:HD11	2.55	0.42
1:a:128:TYR:CE2	1:a:140:PRO:HB3	2.53	0.42
2:B:111:ARG:HA	7:G:17:ILE:HG23	2.01	0.42
2:b:144:TYR:O	2:b:147:PRO:HD2	2.20	0.42
1:A:101:LYS:HE3	1:A:142:ALA:HB3	2.01	0.42
2:B:106:PHE:O	2:B:110:LEU:HG	2.19	0.42
2:B:121:PRO:HB2	2:B:218:GLN:NE2	2.35	0.42
3:C:195:CYS:HB3	10:C:301:HEC:HHC	2.02	0.42
7:G:19:THR:HG22	7:G:21:GLY:H	1.85	0.42
3:c:200:LEU:HD21	3:c:249:ILE:HG22	2.01	0.42
2:B:15:ILE:H	2:B:15:ILE:HD12	1.84	0.42
2:B:167:PRO:HD3	3:C:108:MET:HG3	2.01	0.42
1:a:128:TYR:CZ	1:a:140:PRO:HB3	2.55	0.42
1:a:96:LEU:HD22	1:a:132:GLY:HA3	2.00	0.42
1:a:109:TRP:CE2	1:a:110:ASN:HB2	2.55	0.42
3:c:183:GLY:O	3:c:187:PHE:HD1	2.03	0.42
2:B:13:LEU:HB2	2:B:15:ILE:HD13	2.02	0.42
2:B:98:ALA:O	2:B:102:ILE:HG12	2.20	0.42
3:C:134:LYS:HB3	3:C:134:LYS:HE3	1.81	0.42
3:c:54:ILE:HG12	5:e:62:PHE:CD2	2.55	0.42
3:c:58:VAL:HG11	5:e:31:PHE:HE2	1.85	0.42
12:c:301:MQ7:H311	12:c:301:MQ7:H291	1.70	0.42
3:C:183:GLY:HA3	3:C:248:PHE:CD1	2.55	0.42
3:c:220:LYS:HG3	3:c:246:ALA:HB2	2.01	0.42
3:C:13:SER:HA	3:C:20:LYS:HD3	2.02	0.41
3:C:131:ARG:HD2	3:C:133:TRP:CZ2	2.54	0.41
1:a:63:GLN:HE22	1:a:65:PHE:HB2	1.84	0.41
3:c:47:MET:HE3	5:e:8:LEU:HD11	2.02	0.41
1:A:74:ALA:O	1:A:75:TRP:CE3	2.73	0.41
2:B:20:ARG:O	2:B:24:ASP:HB2	2.20	0.41
2:B:164:GLU:HA	2:B:170:GLY:O	2.20	0.41
14:E:101:PC1:H242	14:E:101:PC1:C31	2.50	0.41
1:a:112:ASP:HB2	1:a:120:PHE:HB2	2.01	0.41
2:B:15:ILE:H	2:B:15:ILE:CD1	2.33	0.41
12:B:304:MQ7:H7	3:C:93:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:PRO:HD3	2:b:121:PRO:CD	2.49	0.41
3:C:125:ASP:HB2	13:D:101:PEE:H2	2.03	0.41
2:b:124:LEU:HD21	12:b:304:MQ7:H293	2.02	0.41
3:c:187:PHE:HB3	3:c:245:LEU:HA	2.03	0.41
1:A:76:TYR:CE2	2:b:70:ILE:HG12	2.55	0.41
3:C:8:LYS:HD3	3:C:8:LYS:HA	1.82	0.41
3:C:55:GLY:HA2	5:E:31:PHE:CZ	2.55	0.41
3:C:110:MET:HB2	3:C:111:PRO:HD3	2.02	0.41
2:b:113:PHE:CZ	13:d:101:PEE:H19	2.54	0.41
3:C:58:VAL:HG11	5:E:31:PHE:HE2	1.86	0.41
3:C:219:ILE:HD13	3:C:249:ILE:HG22	2.03	0.41
1:A:34:ARG:HD2	1:A:34:ARG:O	2.21	0.41
1:A:49:MET:HG3	1:A:157:TYR:CD2	2.56	0.41
2:B:55:GLN:HG2	11:B:302:HEM:C2C	2.55	0.41
3:C:19:LYS:C	3:C:21:PRO:HD3	2.45	0.41
3:C:123:PHE:CD2	15:b:305:CDL:H351	2.56	0.41
3:c:216:PRO:HA	3:c:219:ILE:HD12	2.03	0.41
4:d:27:ILE:HD12	4:d:27:ILE:HA	1.90	0.41
1:A:34:ARG:NH1	1:A:41:LEU:HD12	2.36	0.41
12:B:305:MQ7:H192	2:b:18:MET:SD	2.61	0.41
3:C:162:TRP:O	3:C:166:GLU:HG3	2.21	0.41
1:a:114:LYS:HD2	1:a:125:TYR:OH	2.21	0.41
2:b:31:VAL:HG11	2:b:220:ILE:HG21	2.03	0.41
2:b:138:GLY:HA3	12:c:301:MQ7:H243	2.03	0.41
3:c:97:TYR:CE2	4:d:46:MET:HB3	2.56	0.40
1:A:38:ASP:N	1:A:39:PRO:HD2	2.36	0.40
2:B:14:ASP:O	2:B:15:ILE:C	2.65	0.40
12:B:304:MQ7:H412	12:B:304:MQ7:H391	1.78	0.40
4:D:28:LEU:HD12	4:D:28:LEU:HA	1.87	0.40
2:b:55:GLN:HG2	11:b:302:HEM:C2C	2.57	0.40
8:h:35:MET:O	8:h:39:ILE:HD12	2.21	0.40
5:e:14:ILE:HD13	5:e:14:ILE:HA	1.92	0.40
14:E:101:PC1:H361	14:E:101:PC1:H281	2.03	0.40
12:c:301:MQ7:H391	12:c:301:MQ7:H412	1.53	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%)	152 (94%)	9 (6%)	0	100 100
1	a	156/167 (93%)	146 (94%)	10 (6%)	0	100 100
2	B	222/224 (99%)	214 (96%)	5 (2%)	3 (1%)	9 30
2	b	222/224 (99%)	219 (99%)	3 (1%)	0	100 100
3	C	253/255 (99%)	230 (91%)	21 (8%)	2 (1%)	16 44
3	c	253/255 (99%)	229 (90%)	23 (9%)	1 (0%)	30 60
4	D	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
4	d	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
5	E	75/81 (93%)	73 (97%)	2 (3%)	0	100 100
5	e	75/81 (93%)	75 (100%)	0	0	100 100
7	G	27/29 (93%)	21 (78%)	6 (22%)	0	100 100
7	g	27/29 (93%)	27 (100%)	0	0	100 100
8	H	42/44 (96%)	39 (93%)	3 (7%)	0	100 100
8	h	42/44 (96%)	40 (95%)	2 (5%)	0	100 100
All	All	1663/1714 (97%)	1568 (94%)	89 (5%)	6 (0%)	31 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	ILE
2	B	16	THR
3	C	7	MET
3	C	15	ILE
2	B	168	LEU
3	c	3	ARG

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%)	138 (97%)	4 (3%)	38	73
1	a	139/144 (96%)	134 (96%)	5 (4%)	31	66
2	B	188/188 (100%)	182 (97%)	6 (3%)	34	70
2	b	188/188 (100%)	181 (96%)	7 (4%)	30	65
3	C	205/205 (100%)	203 (99%)	2 (1%)	68	88
3	c	205/205 (100%)	200 (98%)	5 (2%)	43	77
4	D	45/46 (98%)	45 (100%)	0	100	100
4	d	45/46 (98%)	44 (98%)	1 (2%)	45	78
5	E	66/67 (98%)	64 (97%)	2 (3%)	36	72
5	e	66/67 (98%)	65 (98%)	1 (2%)	57	84
7	G	25/25 (100%)	24 (96%)	1 (4%)	28	63
7	g	25/25 (100%)	24 (96%)	1 (4%)	28	63
8	H	37/37 (100%)	36 (97%)	1 (3%)	39	74
8	h	37/37 (100%)	36 (97%)	1 (3%)	39	74
All	All	1413/1424 (99%)	1376 (97%)	37 (3%)	41	75

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	75	TRP
1	A	114	LYS
1	A	155	PHE
2	B	16	THR
2	B	38	SER
2	B	67	VAL
2	B	105	MET
2	B	171	THR
2	B	217	LYS
3	C	14	ARG

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Mol	Chain	Res	Type
3	C	15	ILE
5	E	47	THR
5	E	50	MET
7	G	28	LYS
8	H	14	ASP
1	a	40	VAL
1	a	69	ILE
1	a	121	CYS
1	a	140	PRO
1	a	156	LEU
2	b	2	LEU
2	b	29	GLU
2	b	67	VAL
2	b	121	PRO
2	b	139	LEU
2	b	176	LEU
2	b	197	VAL
3	c	1	MET
3	c	101	SER
3	c	186	VAL
3	c	192	CYS
3	c	245	LEU
4	d	49	ILE
5	e	23	ASP
7	g	7	MET
8	h	32	LEU

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

Mol	Chain	Res	Type
1	A	63	GLN
1	A	149	GLN
2	B	55	GLN
2	B	81	GLN
2	B	82	ASN
2	B	88	GLN
2	B	108	HIS
2	B	218	GLN
3	C	91	GLN
3	C	155	GLN
3	C	160	HIS
3	C	241	GLN

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Mol	Chain	Res	Type
4	D	24	ASN
4	D	50	ASN
5	E	34	GLN
8	H	7	ASN
1	a	63	GLN
1	a	71	GLN
2	b	32	ASN
2	b	55	GLN
2	b	115	GLN
2	b	218	GLN
3	c	91	GLN
3	c	155	GLN
3	c	168	GLN
3	c	196	HIS
3	c	199	ASN
5	e	34	GLN
8	h	9	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	MQ7	B	304	-	49,49,49	0.39	0	61,63,63	0.52	1 (1%)
11	HEM	b	302	2	50,50,50	1.57	8 (16%)	67,82,82	1.64	12 (17%)
13	PEE	D	101	-	45,45,50	0.31	0	48,50,55	0.42	0
12	MQ7	b	304	-	49,49,49	0.39	0	61,63,63	0.61	1 (1%)
12	MQ7	c	301	-	49,49,49	0.39	0	61,63,63	0.51	1 (1%)
10	HEC	c	302	-	50,50,50	3.84	33 (66%)	68,82,82	9.13	29 (42%)
13	PEE	e	101	-	33,33,50	0.33	0	36,38,55	0.74	0
10	HEC	C	301	-	50,50,50	3.06	29 (58%)	68,82,82	2.27	28 (41%)
13	PEE	a	202	-	39,39,50	0.33	0	42,44,55	0.43	0
14	PC1	E	101	-	40,40,53	0.55	0	46,48,61	0.57	1 (2%)
13	PEE	d	101	-	50,50,50	0.30	0	53,55,55	0.37	0
15	CDL	b	305	-	97,97,99	0.27	0	103,109,111	0.42	0
9	FES	A	201	1	0,4,4	-	-	-		
10	HEC	B	301	2	50,50,50	2.89	28 (56%)	68,82,82	2.57	27 (39%)
12	MQ7	B	305	-	49,49,49	0.38	0	61,63,63	0.50	0
10	HEC	b	301	2	50,50,50	2.86	26 (52%)	68,82,82	2.52	26 (38%)
9	FES	a	201	1	0,4,4	-	-	-		
11	HEM	B	302	2	50,50,50	1.58	9 (18%)	67,82,82	1.65	13 (19%)
11	HEM	b	303	2	50,50,50	1.61	9 (18%)	67,82,82	1.52	13 (19%)
11	HEM	B	303	2	50,50,50	1.62	8 (16%)	67,82,82	1.70	13 (19%)

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	MQ7	B	304	-	-	12/41/61/61	0/2/2/2
11	HEM	b	302	2	-	9/14/54/54	-
13	PEE	D	101	-	-	1/49/49/54	-
12	MQ7	b	304	-	-	9/41/61/61	0/2/2/2
12	MQ7	c	301	-	-	15/41/61/61	0/2/2/2
10	HEC	c	302	-	1/1/3/7	7/14/54/54	-
13	PEE	e	101	-	-	9/37/37/54	-
10	HEC	C	301	-	1/1/3/7	8/14/54/54	-
13	PEE	a	202	-	-	7/43/43/54	-
14	PC1	E	101	-	-	18/44/44/57	-
13	PEE	d	101	-	-	7/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	b	305	-	-	18/108/108/110	-
9	FES	A	201	1	-	-	0/1/1/1
10	HEC	B	301	2	1/1/3/7	11/14/54/54	-
12	MQ7	B	305	-	-	30/41/61/61	0/2/2/2
10	HEC	b	301	2	1/1/3/7	9/14/54/54	-
9	FES	a	201	1	-	-	0/1/1/1
11	HEM	B	302	2	-	7/14/54/54	-
11	HEM	b	303	2	-	2/14/54/54	-
11	HEM	B	303	2	-	4/14/54/54	-

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	302	HEC	CAC-C3C	9.94	1.76	1.51
10	c	302	HEC	CMC-C2C	9.38	1.70	1.50
10	c	302	HEC	C3B-C2B	5.76	1.49	1.36
10	c	302	HEC	CHB-C4A	5.73	1.49	1.38
10	C	301	HEC	C3B-C2B	5.61	1.48	1.36
10	c	302	HEC	CHA-C1A	5.58	1.49	1.38
10	c	302	HEC	C3D-C2D	5.53	1.48	1.36
10	c	302	HEC	CHD-C1D	5.47	1.49	1.38
10	c	302	HEC	C2A-C3A	5.46	1.48	1.36
10	c	302	HEC	CHC-C4B	5.39	1.49	1.38
10	C	301	HEC	C3D-C2D	5.38	1.48	1.36
11	B	302	HEM	FE-NB	5.38	2.11	1.94
10	B	301	HEC	C2A-C3A	5.36	1.48	1.36
10	C	301	HEC	C2A-C3A	5.36	1.48	1.36
10	C	301	HEC	CHB-C4A	5.33	1.48	1.38
11	b	302	HEM	FE-NB	5.31	2.11	1.94
10	C	301	HEC	CHA-C1A	5.26	1.48	1.38
11	b	303	HEM	FE-NB	5.23	2.11	1.94
10	C	301	HEC	CHD-C1D	5.21	1.48	1.38
10	B	301	HEC	C3B-C2B	5.19	1.48	1.36
10	C	301	HEC	CHC-C4B	5.16	1.48	1.38
10	b	301	HEC	C3B-C2B	5.11	1.47	1.36
10	B	301	HEC	FE-ND	5.09	2.10	1.94
10	b	301	HEC	FE-NB	5.06	2.10	1.94
10	c	302	HEC	C4C-C3C	5.05	1.54	1.44
10	B	301	HEC	C3D-C2D	5.04	1.47	1.36
10	B	301	HEC	FE-NB	5.04	2.10	1.94
10	b	301	HEC	C2A-C3A	5.02	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	301	HEC	FE-ND	4.97	2.10	1.94
10	B	301	HEC	CHB-C4A	4.95	1.48	1.38
10	b	301	HEC	C3D-C2D	4.94	1.47	1.36
10	c	302	HEC	CHD-C4C	4.91	1.50	1.39
10	b	301	HEC	CHB-C4A	4.82	1.47	1.38
10	c	302	HEC	C3C-C2C	-4.80	1.26	1.38
10	B	301	HEC	CHA-C1A	4.79	1.47	1.38
10	b	301	HEC	CHD-C1D	4.79	1.48	1.38
10	b	301	HEC	CHA-C1A	4.74	1.47	1.38
10	B	301	HEC	FE-NC	4.73	2.10	1.95
11	B	303	HEM	FE-NB	4.70	2.09	1.94
10	b	301	HEC	FE-NC	4.66	2.10	1.95
10	C	301	HEC	FE-ND	4.66	2.09	1.94
10	C	301	HEC	FE-NB	4.66	2.09	1.94
10	c	302	HEC	C1C-NC	-4.63	1.30	1.39
10	b	301	HEC	FE-NA	4.63	2.10	1.95
10	B	301	HEC	FE-NA	4.61	2.10	1.95
10	c	302	HEC	CHA-C4D	4.50	1.49	1.39
10	c	302	HEC	CHB-C1B	4.47	1.49	1.39
10	B	301	HEC	CHD-C1D	4.46	1.47	1.38
10	c	302	HEC	FE-NB	4.42	2.08	1.94
10	c	302	HEC	FE-ND	4.39	2.08	1.94
10	c	302	HEC	CHC-C1C	4.37	1.49	1.39
10	C	301	HEC	CHA-C4D	4.30	1.49	1.39
10	C	301	HEC	FE-NC	4.29	2.09	1.95
10	B	301	HEC	CHC-C4B	4.28	1.47	1.38
10	C	301	HEC	FE-NA	4.27	2.09	1.95
10	C	301	HEC	CHB-C1B	4.23	1.48	1.39
11	b	302	HEM	FE-NC	4.20	2.09	1.95
11	B	302	HEM	FE-NC	4.19	2.09	1.95
10	C	301	HEC	CHC-C1C	4.18	1.48	1.39
10	b	301	HEC	CHC-C4B	4.16	1.46	1.38
10	C	301	HEC	CHD-C4C	4.15	1.48	1.39
11	b	303	HEM	FE-NC	4.06	2.08	1.95
10	c	302	HEC	C4C-NC	-4.05	1.32	1.39
11	B	303	HEM	FE-NC	4.03	2.08	1.95
10	c	302	HEC	FE-NA	4.02	2.08	1.95
10	c	302	HEC	FE-NC	3.96	2.08	1.95
10	b	301	HEC	CHD-C4C	3.93	1.48	1.39
10	b	301	HEC	CHA-C4D	3.89	1.48	1.39
10	B	301	HEC	CHB-C1B	3.83	1.47	1.39
10	C	301	HEC	C3C-C2C	3.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	HEC	CHD-C4C	3.80	1.47	1.39
11	B	303	HEM	C1B-NB	-3.73	1.33	1.40
10	b	301	HEC	CHB-C1B	3.72	1.47	1.39
10	B	301	HEC	CHA-C4D	3.72	1.47	1.39
11	B	303	HEM	C4D-ND	-3.66	1.33	1.40
11	b	303	HEM	C1B-NB	-3.63	1.34	1.40
10	B	301	HEC	CHC-C1C	3.42	1.47	1.39
10	B	301	HEC	C3C-C2C	3.41	1.47	1.38
11	b	303	HEM	C4D-ND	-3.36	1.34	1.40
10	c	302	HEC	C1C-C2C	3.35	1.51	1.43
11	b	302	HEM	C1B-NB	-3.33	1.34	1.40
10	b	301	HEC	CHC-C1C	3.32	1.46	1.39
11	B	302	HEM	C1B-NB	-3.28	1.34	1.40
11	b	302	HEM	C4D-ND	-3.23	1.34	1.40
10	c	302	HEC	C4B-NB	-3.20	1.34	1.40
10	c	302	HEC	C1D-ND	-3.19	1.34	1.40
10	b	301	HEC	C3C-C2C	3.17	1.47	1.38
10	b	301	HEC	C4B-NB	-3.16	1.34	1.40
11	B	302	HEM	C4D-ND	-3.16	1.34	1.40
10	B	301	HEC	C4B-NB	-3.12	1.34	1.40
10	C	301	HEC	C4B-NB	-3.09	1.34	1.40
10	C	301	HEC	C1D-ND	-3.06	1.34	1.40
10	B	301	HEC	C1D-ND	-2.94	1.35	1.40
11	B	303	HEM	FE-ND	-2.91	1.85	1.94
11	b	303	HEM	C1C-C2C	-2.81	1.39	1.45
10	C	301	HEC	C1C-C2C	2.74	1.49	1.43
10	b	301	HEC	C1D-ND	-2.72	1.35	1.40
10	b	301	HEC	C4C-C3C	2.71	1.50	1.44
10	c	302	HEC	C4D-C3D	2.63	1.49	1.45
10	c	302	HEC	C1B-C2B	2.60	1.49	1.44
10	C	301	HEC	C4D-C3D	2.58	1.49	1.45
10	C	301	HEC	C4C-NC	-2.53	1.34	1.39
10	B	301	HEC	C1B-C2B	2.53	1.49	1.44
10	C	301	HEC	C1B-C2B	2.52	1.49	1.44
10	c	302	HEC	C1A-NA	-2.52	1.34	1.39
10	C	301	HEC	C1A-NA	-2.49	1.34	1.39
10	c	302	HEC	C4A-NA	-2.49	1.34	1.39
10	C	301	HEC	C4A-NA	-2.48	1.35	1.39
10	b	301	HEC	C1B-C2B	2.46	1.49	1.44
11	b	303	HEM	FE-ND	-2.44	1.87	1.94
11	B	302	HEM	C1C-C2C	-2.42	1.40	1.45
10	B	301	HEC	C1C-C2C	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	302	HEM	FE-ND	-2.41	1.87	1.94
11	B	303	HEM	C4B-NB	-2.40	1.34	1.38
11	B	303	HEM	C1D-ND	-2.39	1.34	1.38
11	B	303	HEM	C1C-C2C	-2.37	1.40	1.45
10	b	301	HEC	C1A-NA	-2.37	1.35	1.39
11	b	302	HEM	C1C-C2C	-2.36	1.40	1.45
11	B	302	HEM	FE-ND	-2.36	1.87	1.94
10	B	301	HEC	C4C-NC	-2.35	1.35	1.39
10	B	301	HEC	C1A-NA	-2.33	1.35	1.39
10	b	301	HEC	C1C-NC	-2.32	1.35	1.39
10	B	301	HEC	C4D-C3D	2.31	1.49	1.45
10	C	301	HEC	C1A-C2A	2.30	1.49	1.45
10	c	302	HEC	C1A-C2A	2.26	1.49	1.45
10	b	301	HEC	C4D-C3D	2.25	1.48	1.45
11	B	302	HEM	C3B-C4B	2.25	1.49	1.44
10	b	301	HEC	C4A-NA	-2.24	1.35	1.39
10	C	301	HEC	C1D-C2D	2.23	1.49	1.44
10	c	302	HEC	C1D-C2D	2.22	1.49	1.44
10	B	301	HEC	C4A-NA	-2.21	1.35	1.39
10	C	301	HEC	C4B-C3B	2.21	1.48	1.45
10	b	301	HEC	C1D-C2D	2.20	1.49	1.44
11	B	302	HEM	C3C-C4C	-2.20	1.42	1.46
10	C	301	HEC	C1C-NC	-2.18	1.35	1.39
10	B	301	HEC	C4C-C3C	2.17	1.48	1.44
10	b	301	HEC	C1A-C2A	2.16	1.49	1.45
11	b	302	HEM	C3C-C4C	-2.16	1.42	1.46
11	b	303	HEM	C3C-C4C	-2.16	1.42	1.46
10	c	302	HEC	C4B-C3B	2.15	1.48	1.45
11	b	303	HEM	C1D-ND	-2.12	1.34	1.38
11	b	303	HEM	C4B-NB	-2.11	1.34	1.38
10	c	302	HEC	C4D-ND	-2.11	1.34	1.38
10	C	301	HEC	C4C-C3C	2.09	1.48	1.44
10	B	301	HEC	C1D-C2D	2.06	1.48	1.44
10	B	301	HEC	C1C-NC	-2.04	1.35	1.39
10	c	302	HEC	C4A-C3A	2.03	1.49	1.45
10	B	301	HEC	C1A-C2A	2.02	1.48	1.45
11	B	302	HEM	C1D-ND	-2.01	1.34	1.38
11	b	302	HEM	C1D-ND	-2.00	1.34	1.38

All (165) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	c	302	HEC	CAC-C3C-C2C	-52.38	44.02	126.89
10	c	302	HEC	CMC-C2C-C3C	-46.99	25.96	125.62
10	c	302	HEC	CAC-C3C-C4C	13.92	144.07	124.91
10	c	302	HEC	CBC-CAC-C3C	12.22	145.55	112.42
10	c	302	HEC	CMC-C2C-C1C	6.25	134.93	125.42
10	B	301	HEC	C1B-C2B-C3B	-6.14	100.52	106.98
10	b	301	HEC	C1B-C2B-C3B	-6.06	100.60	106.98
10	c	302	HEC	C3C-C4C-NC	5.82	116.60	110.15
10	B	301	HEC	C2A-C1A-NA	5.67	115.79	110.32
10	C	301	HEC	C1B-C2B-C3B	-5.61	101.08	106.98
10	B	301	HEC	C1C-C2C-C3C	-5.53	100.48	106.82
10	b	301	HEC	C2B-C1B-NB	5.44	116.19	109.90
10	c	302	HEC	C1B-C2B-C3B	-5.41	101.29	106.98
10	B	301	HEC	C3D-C4D-ND	5.29	115.47	110.35
10	B	301	HEC	C2B-C1B-NB	5.28	116.00	109.90
10	b	301	HEC	C2A-C1A-NA	5.27	115.41	110.32
10	B	301	HEC	C2D-C1D-ND	5.08	115.68	109.84
11	b	302	HEM	CHC-C4B-NB	5.04	129.84	124.42
10	C	301	HEC	C1C-C2C-C3C	-4.99	101.10	106.82
10	b	301	HEC	CAC-C3C-C4C	4.88	131.63	124.91
10	b	301	HEC	C3D-C4D-ND	4.88	115.07	110.35
11	B	303	HEM	CHC-C4B-NB	4.79	129.58	124.42
10	C	301	HEC	CBC-CAC-C3C	4.57	124.80	112.42
10	c	302	HEC	CBB-CAB-C3B	4.55	124.76	112.42
10	C	301	HEC	CBB-CAB-C3B	4.55	124.75	112.42
11	B	303	HEM	C1B-NB-C4B	4.55	110.59	105.21
10	b	301	HEC	C2D-C1D-ND	4.53	115.05	109.84
10	B	301	HEC	CBC-CAC-C3C	4.46	124.52	112.42
10	b	301	HEC	C1C-C2C-C3C	-4.44	101.73	106.82
10	c	302	HEC	C4C-C3C-C2C	-4.41	100.04	106.87
10	b	301	HEC	CBC-CAC-C3C	4.39	124.33	112.42
11	B	302	HEM	CHD-C1D-ND	4.37	129.13	124.42
11	b	303	HEM	CHC-C4B-NB	4.37	129.12	124.42
11	b	302	HEM	CHD-C1D-ND	4.34	129.09	124.42
10	C	301	HEC	C2B-C1B-NB	4.32	114.89	109.90
10	B	301	HEC	CBB-CAB-C3B	4.30	124.09	112.42
10	B	301	HEC	C2C-C1C-NC	4.19	116.86	110.14
10	b	301	HEC	C3B-C4B-NB	4.18	114.76	110.17
10	B	301	HEC	C1D-C2D-C3D	-4.18	102.58	106.98
10	b	301	HEC	CBB-CAB-C3B	4.17	123.72	112.42
11	B	303	HEM	C3B-C4B-NB	-4.12	106.51	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	302	HEM	CHC-C4B-NB	4.11	128.84	124.42
10	b	301	HEC	C1D-C2D-C3D	-4.03	102.74	106.98
10	b	301	HEC	C2C-C1C-NC	4.01	116.56	110.14
10	C	301	HEC	C2A-C1A-NA	3.93	114.12	110.32
10	B	301	HEC	C3B-C4B-NB	3.88	114.43	110.17
11	b	302	HEM	CHA-C4D-ND	3.84	129.12	124.37
11	B	302	HEM	CHA-C4D-ND	3.81	129.08	124.37
10	c	302	HEC	CHB-C1B-NB	-3.75	120.39	124.42
10	C	301	HEC	C1D-C2D-C3D	-3.73	103.06	106.98
11	B	302	HEM	CHB-C1B-NB	3.72	128.97	124.37
10	c	302	HEC	CHA-C4D-ND	-3.72	120.42	124.42
10	C	301	HEC	C3D-C4D-ND	3.70	113.92	110.35
10	C	301	HEC	C2D-C1D-ND	3.69	114.08	109.84
10	c	302	HEC	C2B-C1B-NB	3.68	114.16	109.90
10	c	302	HEC	C1D-C2D-C3D	-3.62	103.17	106.98
10	B	301	HEC	C1A-C2A-C3A	-3.53	102.46	107.11
11	b	303	HEM	CHD-C1D-ND	3.48	128.17	124.42
11	b	302	HEM	CHB-C1B-NB	3.47	128.66	124.37
10	c	302	HEC	CHD-C4C-NC	-3.47	117.57	123.86
11	b	303	HEM	CHA-C4D-ND	3.43	128.60	124.37
10	b	301	HEC	C1A-C2A-C3A	-3.43	102.60	107.11
10	B	301	HEC	C3C-C4C-NC	3.39	113.91	110.15
11	b	303	HEM	CHB-C1B-NB	3.38	128.54	124.37
11	B	303	HEM	C4D-ND-C1D	3.29	109.10	105.21
10	B	301	HEC	CMC-C2C-C3C	3.28	132.57	125.62
10	C	301	HEC	CHB-C1B-NB	-3.26	120.91	124.42
10	C	301	HEC	CHA-C4D-ND	-3.26	120.92	124.42
10	c	302	HEC	C2A-C1A-NA	3.24	113.45	110.32
11	B	303	HEM	CHB-C1B-NB	3.23	128.36	124.37
10	c	302	HEC	CHA-C1A-NA	-3.18	120.99	124.45
10	C	301	HEC	C1A-C2A-C3A	-3.18	102.92	107.11
10	c	302	HEC	CHB-C4A-NA	-3.16	121.01	124.45
10	c	302	HEC	C2D-C1D-ND	3.14	113.45	109.84
11	b	303	HEM	C1B-NB-C4B	3.14	108.92	105.21
10	C	301	HEC	CHA-C1A-NA	-3.12	121.05	124.45
10	C	301	HEC	CHB-C4A-NA	-3.11	121.07	124.45
10	B	301	HEC	C3A-C4A-NA	3.10	115.37	109.64
12	b	304	MQ7	C11-C3-C2	-3.09	119.59	124.89
10	b	301	HEC	C3A-C4A-NA	3.08	115.34	109.64
10	c	302	HEC	C1A-C2A-C3A	-3.07	103.06	107.11
10	b	301	HEC	CMC-C2C-C3C	3.05	132.10	125.62
11	b	302	HEM	C1B-NB-C4B	3.05	108.82	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	303	HEM	CAD-C3D-C4D	3.03	129.97	124.70
11	B	302	HEM	C1B-NB-C4B	3.03	108.79	105.21
11	B	303	HEM	C4A-CHB-C1B	-3.02	119.14	126.25
10	c	302	HEC	C4C-NC-C1C	-3.01	100.91	105.82
11	B	303	HEM	CHD-C1D-ND	3.01	127.67	124.42
10	c	302	HEC	C3D-C4D-ND	3.00	113.25	110.35
10	C	301	HEC	C2C-C1C-NC	2.97	114.91	110.14
10	B	301	HEC	C4A-C3A-C2A	-2.96	102.58	106.97
10	B	301	HEC	C4D-C3D-C2D	-2.94	102.62	106.89
10	C	301	HEC	CMC-C2C-C3C	2.87	131.71	125.62
10	b	301	HEC	C4A-C3A-C2A	-2.83	102.77	106.97
10	b	301	HEC	CHC-C1C-C2C	-2.79	119.31	127.43
11	B	302	HEM	C3B-C4B-NB	-2.74	107.50	109.47
11	b	302	HEM	CHD-C4C-NC	2.73	127.42	124.45
10	b	301	HEC	C4D-C3D-C2D	-2.72	102.93	106.89
10	C	301	HEC	C4D-C3D-C2D	-2.71	102.95	106.89
11	B	303	HEM	C4C-CHD-C1D	-2.71	120.27	126.02
11	B	302	HEM	CHD-C1D-C2D	-2.68	120.80	125.03
10	b	301	HEC	C3C-C4C-NC	2.67	113.11	110.15
10	C	301	HEC	C4A-C3A-C2A	-2.66	103.02	106.97
10	B	301	HEC	CAB-C3B-C2B	2.64	132.41	127.56
11	b	303	HEM	C4C-CHD-C1D	-2.63	120.42	126.02
11	B	302	HEM	CHD-C4C-NC	2.63	127.31	124.45
10	C	301	HEC	CAD-C3D-C4D	2.62	129.27	124.70
10	c	302	HEC	C4D-C3D-C2D	-2.61	103.09	106.89
11	b	302	HEM	CHD-C1D-C2D	-2.61	120.91	125.03
10	c	302	HEC	CHD-C1D-ND	-2.57	121.19	124.37
10	b	301	HEC	CBD-CAD-C3D	-2.56	105.47	112.53
10	C	301	HEC	CHD-C1D-ND	-2.54	121.23	124.37
10	c	302	HEC	CAD-C3D-C4D	2.51	129.07	124.70
11	B	303	HEM	C4C-NC-C1C	2.48	109.87	105.82
10	C	301	HEC	CAC-C3C-C2C	2.44	130.76	126.89
10	C	301	HEC	C3C-C4C-NC	2.44	112.86	110.15
10	b	301	HEC	CMD-C2D-C1D	2.44	128.84	125.03
10	c	302	HEC	C4A-C3A-C2A	-2.44	103.36	106.97
14	E	101	PC1	O12-P-O14	2.44	123.78	112.44
10	B	301	HEC	CHC-C1C-C2C	-2.43	120.37	127.43
10	B	301	HEC	CHA-C1A-C2A	-2.43	121.03	124.86
11	b	302	HEM	CBD-CAD-C3D	-2.41	105.87	112.53
10	c	302	HEC	CHC-C4B-NB	-2.41	121.39	124.37
12	B	304	MQ7	C11-C3-C2	-2.40	120.77	124.89
10	C	301	HEC	C3B-C4B-NB	2.40	112.81	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	301	HEC	CAA-CBA-CGA	-2.40	107.31	113.67
10	C	301	HEC	C3A-C4A-NA	2.37	114.02	109.64
10	b	301	HEC	CAB-C3B-C2B	2.37	131.91	127.56
10	C	301	HEC	CMA-C3A-C4A	2.35	128.86	124.73
11	b	303	HEM	C3B-C4B-NB	-2.35	107.78	109.47
11	b	302	HEM	CHA-C4D-C3D	-2.33	120.94	125.23
11	B	302	HEM	CHA-C4D-C3D	-2.32	120.94	125.23
10	c	302	HEC	CHC-C1C-NC	-2.32	119.66	123.86
11	b	302	HEM	C1A-CHA-C4D	-2.31	120.82	126.25
11	b	303	HEM	C1A-CHA-C4D	-2.30	120.83	126.25
11	b	303	HEM	C4A-CHB-C1B	-2.25	120.95	126.25
11	b	302	HEM	C3B-C4B-NB	-2.25	107.85	109.47
10	c	302	HEC	CMA-C3A-C4A	2.24	128.66	124.73
10	C	301	HEC	CMD-C2D-C1D	2.23	128.52	125.03
10	C	301	HEC	CHC-C4B-NB	-2.21	121.63	124.37
11	B	302	HEM	C1A-CHA-C4D	-2.21	121.05	126.25
11	B	302	HEM	CHB-C1B-C2B	-2.20	120.69	126.95
12	c	301	MQ7	C11-C3-C2	-2.20	121.12	124.89
10	B	301	HEC	CHC-C4B-C3B	-2.19	121.19	125.23
11	B	302	HEM	C4C-CHD-C1D	-2.17	121.40	126.02
10	b	301	HEC	CHB-C1B-C2B	-2.17	121.60	125.03
11	b	303	HEM	CHB-C1B-C2B	-2.17	120.78	126.95
10	b	301	HEC	CAD-C3D-C4D	2.12	128.40	124.70
11	b	302	HEM	CHB-C1B-C2B	-2.12	120.92	126.95
10	B	301	HEC	CAD-C3D-C4D	2.12	128.39	124.70
11	B	303	HEM	O2A-CGA-CBA	2.10	120.64	114.00
11	B	302	HEM	CBD-CAD-C3D	-2.10	106.72	112.53
10	B	301	HEC	CAA-C2A-C3A	2.10	131.80	127.87
10	C	301	HEC	CMB-C2B-C3B	2.09	131.79	126.15
10	c	302	HEC	C2C-C1C-NC	2.08	113.47	110.14
11	b	303	HEM	CHA-C4D-C3D	-2.07	121.42	125.23
10	B	301	HEC	CHB-C1B-NB	-2.06	122.20	124.42
11	B	303	HEM	CAD-C3D-C2D	-2.06	124.00	127.87
10	b	301	HEC	CHB-C1B-NB	-2.06	122.21	124.42
10	B	301	HEC	CHB-C1B-C2B	-2.05	121.80	125.03
11	B	303	HEM	CBB-CAB-C3B	-2.03	117.36	127.53
10	b	301	HEC	CMA-C3A-C4A	2.03	128.31	124.73
11	b	303	HEM	O2A-CGA-CBA	2.01	120.35	114.00
10	B	301	HEC	CMB-C2B-C3B	2.01	131.59	126.15
11	b	303	HEM	CHD-C1D-C2D	-2.00	121.87	125.03

All (4) chirality outliers are listed below:

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

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	301	HEC	C1A-C2A-CAA-CBA
10	B	301	HEC	C3A-C2A-CAA-CBA
11	B	302	HEM	C2C-C3C-CAC-CBC
11	B	302	HEM	C4C-C3C-CAC-CBC
11	B	303	HEM	C2B-C3B-CAB-CBB
11	B	303	HEM	C4B-C3B-CAB-CBB
11	b	302	HEM	C2C-C3C-CAC-CBC
12	B	305	MQ7	C11-C12-C13-C14
12	B	305	MQ7	C11-C12-C13-C15
12	B	305	MQ7	C28-C30-C31-C32
13	a	202	PEE	C2-C1-O3P-P
13	a	202	PEE	C4-O4P-P-O1P
14	E	101	PC1	C11-O13-P-O11
14	E	101	PC1	C1-O11-P-O14
14	E	101	PC1	O21-C2-C3-O31
14	E	101	PC1	O32-C31-O31-C3
14	E	101	PC1	C32-C31-O31-C3
15	b	305	CDL	C1-CA2-OA2-PA1
15	b	305	CDL	CA2-OA2-PA1-OA4
15	b	305	CDL	CA2-OA2-PA1-OA5
15	b	305	CDL	OB7-CB5-OB6-CB4
15	b	305	CDL	C51-CB5-OB6-CB4
15	b	305	CDL	OB9-CB7-OB8-CB6
15	b	305	CDL	C71-CB7-OB8-CB6
10	b	301	HEC	C2C-C3C-CAC-CBC
12	B	305	MQ7	C41-C42-C43-C44
12	B	305	MQ7	C41-C42-C43-C45
10	C	301	HEC	C4B-C3B-CAB-CBB
10	c	302	HEC	C4B-C3B-CAB-CBB
10	B	301	HEC	C4C-C3C-CAC-CBC
10	C	301	HEC	C4C-C3C-CAC-CBC
10	b	301	HEC	C4C-C3C-CAC-CBC
10	c	302	HEC	C4C-C3C-CAC-CBC
10	B	301	HEC	C4B-C3B-CAB-CBB
10	b	301	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	B	301	HEC	C2B-C3B-CAB-CBB
10	C	301	HEC	C2B-C3B-CAB-CBB
10	b	301	HEC	C2B-C3B-CAB-CBB
10	c	302	HEC	C2B-C3B-CAB-CBB
10	B	301	HEC	C2C-C3C-CAC-CBC
10	C	301	HEC	C2C-C3C-CAC-CBC
10	c	302	HEC	C2C-C3C-CAC-CBC
12	B	304	MQ7	C39-C38-C40-C41
12	B	305	MQ7	C39-C38-C40-C41
12	B	305	MQ7	C37-C38-C40-C41
12	B	305	MQ7	C26-C27-C28-C29
12	B	305	MQ7	C31-C32-C33-C34
12	B	305	MQ7	C26-C27-C28-C30
12	B	305	MQ7	C31-C32-C33-C35
12	B	304	MQ7	C34-C33-C35-C36
12	B	305	MQ7	C14-C13-C15-C16
12	b	304	MQ7	C39-C38-C40-C41
12	c	301	MQ7	C29-C28-C30-C31
12	c	301	MQ7	C39-C38-C40-C41
12	B	304	MQ7	C32-C33-C35-C36
12	B	305	MQ7	C12-C13-C15-C16
12	b	304	MQ7	C37-C38-C40-C41
12	c	301	MQ7	C27-C28-C30-C31
12	c	301	MQ7	C37-C38-C40-C41
12	B	305	MQ7	C13-C15-C16-C17
12	B	305	MQ7	C33-C35-C36-C37
12	c	301	MQ7	C13-C15-C16-C17
12	c	301	MQ7	C38-C40-C41-C42
10	B	301	HEC	C3D-CAD-CBD-CGD
12	B	305	MQ7	C36-C37-C38-C39
12	B	304	MQ7	C37-C38-C40-C41
12	b	304	MQ7	C13-C15-C16-C17
13	d	101	PEE	C30-C31-C32-C33
10	c	302	HEC	C2A-CAA-CBA-CGA
11	B	302	HEM	C2A-CAA-CBA-CGA
12	B	305	MQ7	C16-C17-C18-C19
14	E	101	PC1	C33-C34-C35-C36
11	b	302	HEM	C2A-CAA-CBA-CGA
14	E	101	PC1	C32-C33-C34-C35
11	B	303	HEM	C2A-CAA-CBA-CGA
12	B	305	MQ7	C36-C37-C38-C40
11	B	303	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	b	302	HEM	C4C-C3C-CAC-CBC
15	b	305	CDL	OA6-CA4-CA6-OA8
12	B	305	MQ7	C34-C33-C35-C36
12	B	305	MQ7	C27-C28-C30-C31
12	B	305	MQ7	C29-C28-C30-C31
12	B	305	MQ7	C32-C33-C35-C36
14	E	101	PC1	C35-C36-C37-C38
15	b	305	CDL	C33-C34-C35-C36
13	d	101	PEE	C34-C35-C36-C37
15	b	305	CDL	CB4-CB3-OB5-PB2
12	b	304	MQ7	C14-C13-C15-C16
14	E	101	PC1	C37-C38-C39-C3A
14	E	101	PC1	C1-C2-C3-O31
15	b	305	CDL	CA3-CA4-CA6-OA8
12	B	305	MQ7	C19-C18-C20-C21
12	b	304	MQ7	C12-C13-C15-C16
10	b	301	HEC	C2A-CAA-CBA-CGA
12	b	304	MQ7	C28-C30-C31-C32
13	d	101	PEE	C38-C39-C40-C41
12	b	304	MQ7	C12-C11-C3-C2
14	E	101	PC1	C39-C3A-C3B-C3C
12	c	301	MQ7	C24-C23-C25-C26
11	b	303	HEM	C2C-C3C-CAC-CBC
13	e	101	PEE	O3P-C1-C2-O2
12	B	304	MQ7	C33-C35-C36-C37
12	B	305	MQ7	C23-C25-C26-C27
12	B	305	MQ7	C17-C18-C20-C21
12	b	304	MQ7	C12-C11-C3-C4
13	a	202	PEE	C5-C4-O4P-P
13	e	101	PEE	C5-C4-O4P-P
14	E	101	PC1	C12-C11-O13-P
13	a	202	PEE	O2-C2-C3-O3
14	E	101	PC1	O13-C11-C12-N
12	B	304	MQ7	C24-C23-C25-C26
13	e	101	PEE	O3P-C1-C2-C3
15	b	305	CDL	OB5-CB3-CB4-OB6
14	E	101	PC1	C23-C24-C25-C26
12	B	304	MQ7	C22-C23-C25-C26
12	c	301	MQ7	C22-C23-C25-C26
13	d	101	PEE	C36-C37-C38-C39
13	a	202	PEE	C10-C11-C12-C13
13	d	101	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
13	d	101	PEE	C4-O4P-P-O1P
13	e	101	PEE	C4-O4P-P-O1P
14	E	101	PC1	C11-O13-P-O14
15	b	305	CDL	CB2-OB2-PB2-OB3
14	E	101	PC1	C2-C1-O11-P
13	e	101	PEE	C1-C2-O2-C10
12	c	301	MQ7	C28-C30-C31-C32
13	D	101	PEE	C36-C37-C38-C39
13	a	202	PEE	C36-C37-C38-C39
14	E	101	PC1	C24-C25-C26-C27
12	B	304	MQ7	C29-C28-C30-C31
15	b	305	CDL	OB5-CB3-CB4-CB6
13	e	101	PEE	O2-C2-C3-O3
13	d	101	PEE	C33-C34-C35-C36
10	c	302	HEC	CAD-CBD-CGD-O2D
11	b	302	HEM	CAD-CBD-CGD-O1D
12	c	301	MQ7	C19-C18-C20-C21
11	b	302	HEM	CAD-CBD-CGD-O2D
11	b	302	HEM	CAA-CBA-CGA-O1A
15	b	305	CDL	C56-C57-C58-C59
10	c	302	HEC	CAD-CBD-CGD-O1D
11	B	302	HEM	CAA-CBA-CGA-O1A
12	B	304	MQ7	C27-C28-C30-C31
12	c	301	MQ7	C17-C18-C20-C21
10	C	301	HEC	CAA-CBA-CGA-O2A
11	b	302	HEM	CAA-CBA-CGA-O2A
14	E	101	PC1	C34-C35-C36-C37
12	B	304	MQ7	C14-C13-C15-C16
12	c	301	MQ7	C14-C13-C15-C16
12	c	301	MQ7	C12-C13-C15-C16
10	C	301	HEC	C4D-C3D-CAD-CBD
10	b	301	HEC	CAD-CBD-CGD-O2D
11	B	302	HEM	CAA-CBA-CGA-O2A
12	B	305	MQ7	C24-C23-C25-C26
12	B	304	MQ7	C12-C13-C15-C16
10	C	301	HEC	CAA-CBA-CGA-O1A
10	b	301	HEC	CAA-CBA-CGA-O2A
11	B	302	HEM	CAD-CBD-CGD-O1D
10	b	301	HEC	CAA-CBA-CGA-O1A
11	B	302	HEM	CAD-CBD-CGD-O2D
15	b	305	CDL	C51-C52-C53-C54
12	B	305	MQ7	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
10	B	301	HEC	C2A-CAA-CBA-CGA
15	b	305	CDL	C32-C31-CA7-OA8
12	B	305	MQ7	C16-C17-C18-C20
10	b	301	HEC	CAD-CBD-CGD-O1D
11	b	302	HEM	C2B-C3B-CAB-CBB
10	B	301	HEC	CAD-CBD-CGD-O2D
12	c	301	MQ7	C40-C41-C42-C43
12	B	305	MQ7	C20-C21-C22-C23
12	c	301	MQ7	C30-C31-C32-C33
12	B	305	MQ7	C38-C40-C41-C42
11	b	302	HEM	C4B-C3B-CAB-CBB
11	b	303	HEM	C4C-C3C-CAC-CBC
10	B	301	HEC	CAD-CBD-CGD-O1D
12	b	304	MQ7	C40-C41-C42-C43
13	e	101	PEE	O3-C30-C31-C32
13	e	101	PEE	C3-C2-O2-C10
12	B	304	MQ7	C3-C11-C12-C13
10	C	301	HEC	CAD-CBD-CGD-O2D
13	e	101	PEE	O5-C30-C31-C32
10	B	301	HEC	C2D-C3D-CAD-CBD
15	b	305	CDL	C40-C41-C42-C43
13	a	202	PEE	C11-C12-C13-C14

There are no ring outliers.

18 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	304	MQ7	6	0
11	b	302	HEM	1	0
13	D	101	PEE	5	0
12	b	304	MQ7	3	0
12	c	301	MQ7	7	0
13	e	101	PEE	3	0
10	C	301	HEC	1	0
14	E	101	PC1	11	0
13	d	101	PEE	5	0
15	b	305	CDL	8	0
9	A	201	FES	1	0
10	B	301	HEC	3	0
12	B	305	MQ7	11	0
10	b	301	HEC	1	0
9	a	201	FES	1	0

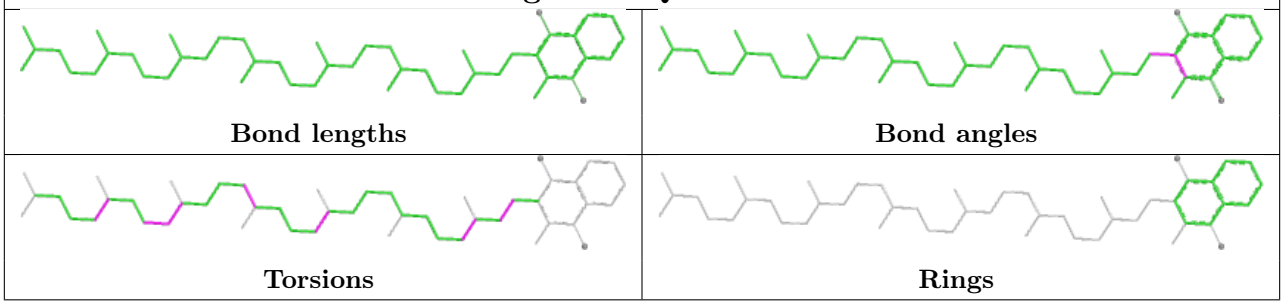
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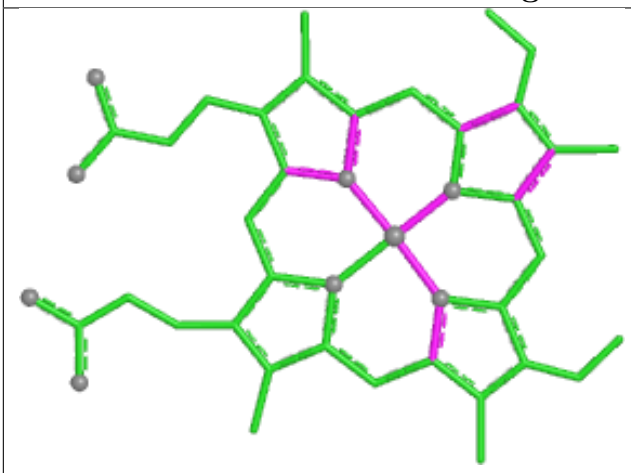
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	302	HEM	4	0
11	b	303	HEM	1	0
11	B	303	HEM	6	0

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.

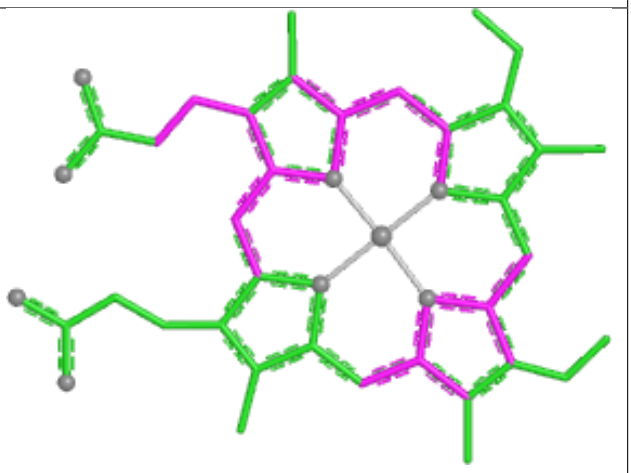
Ligand MQ7 B 304



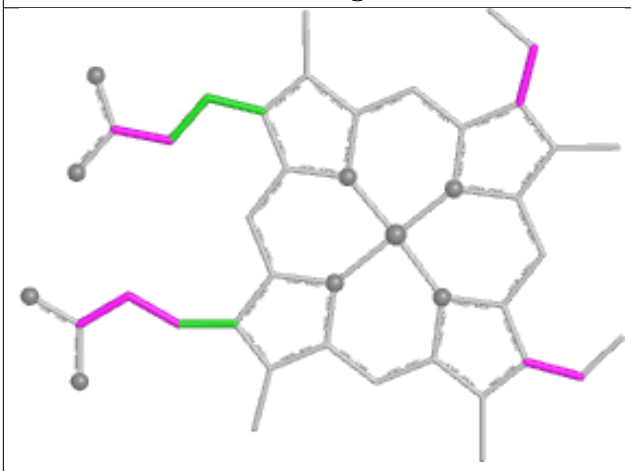
Ligand HEM b 302



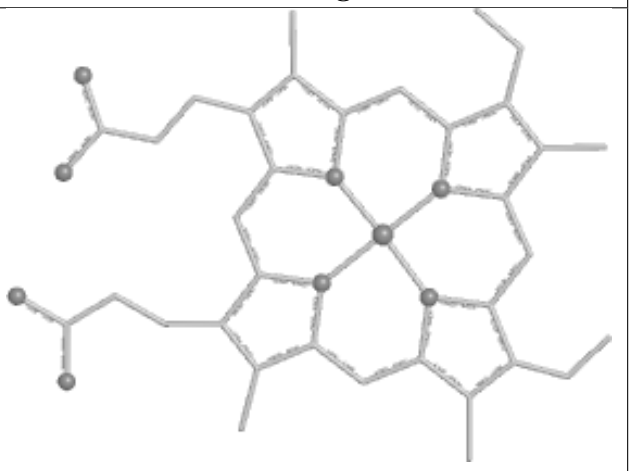
Bond lengths



Bond angles

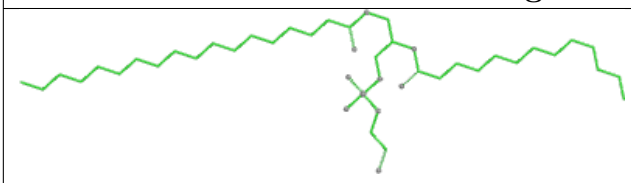


Torsions

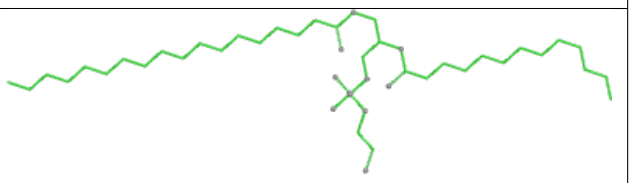


Rings

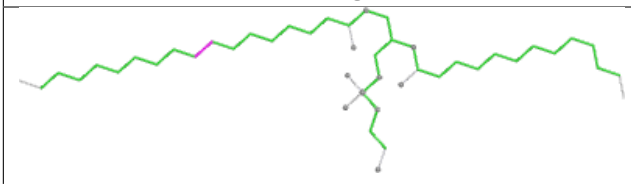
Ligand PEE D 101



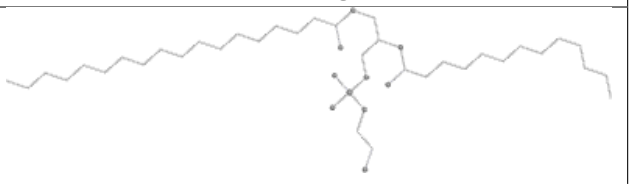
Bond lengths



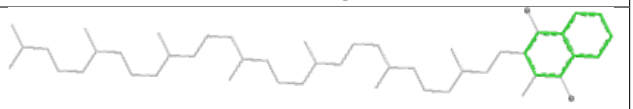
Bond angles

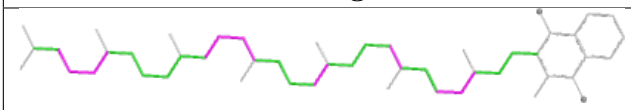
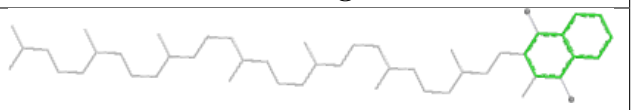


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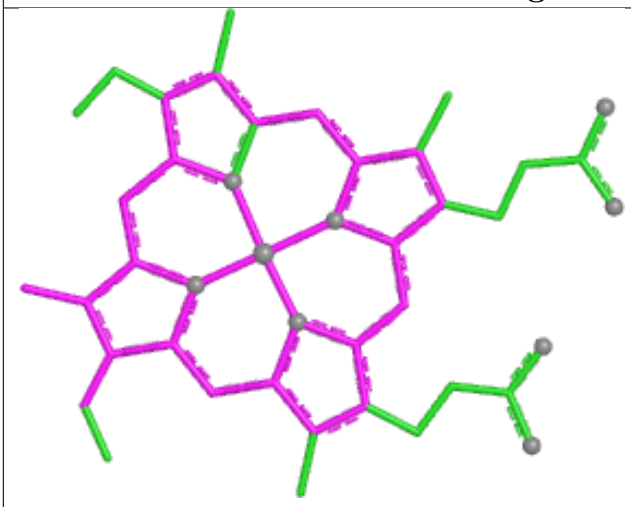


Rings

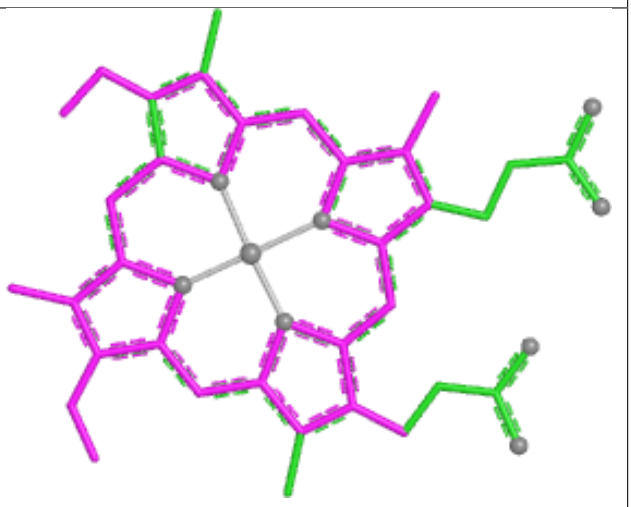
Ligand MQ7 b 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ7 c 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

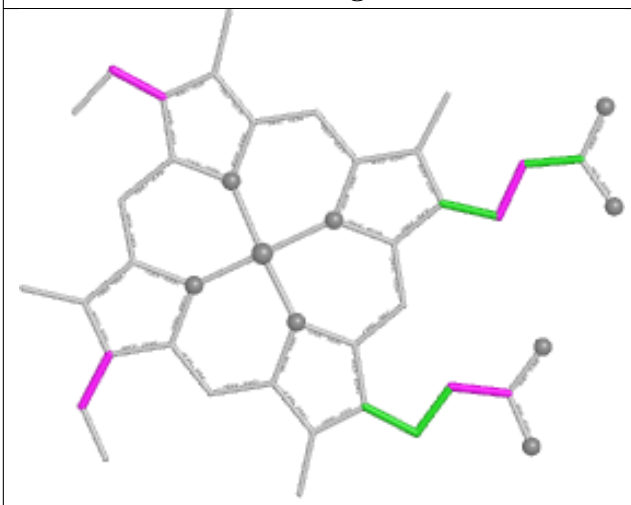
Ligand HEC c 302



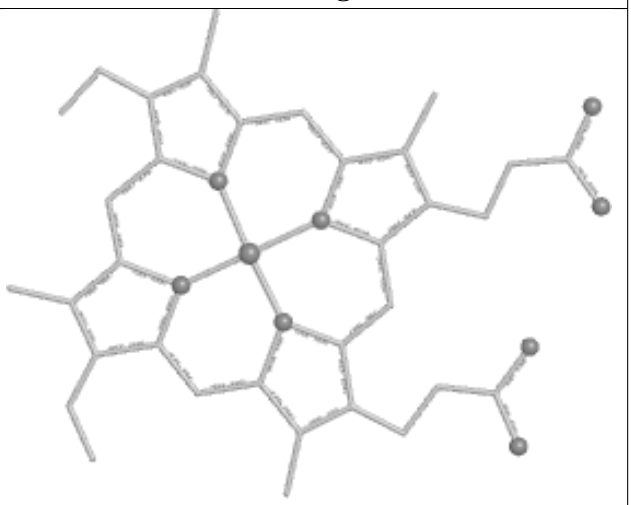
Bond lengths



Bond angles

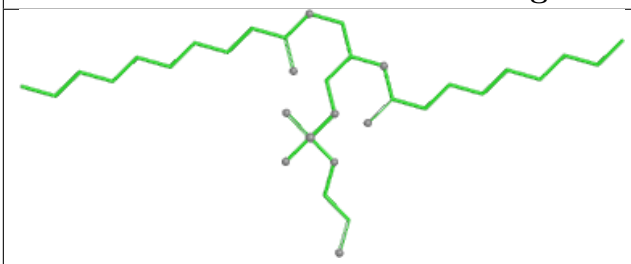


Torsions

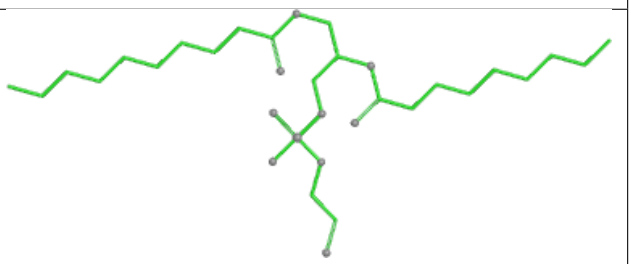


Rings

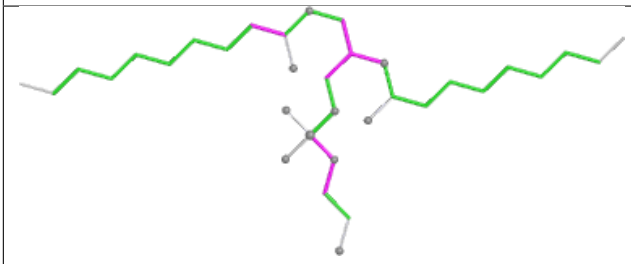
Ligand PEE e 101



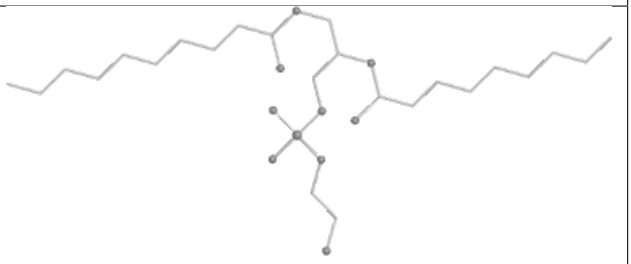
Bond lengths



Bond angles

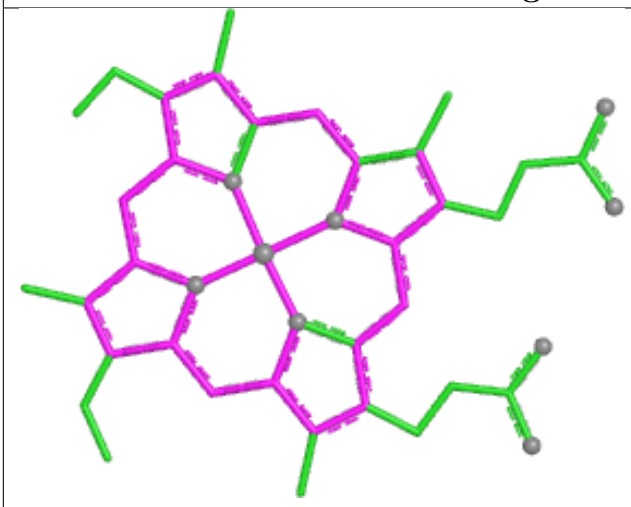


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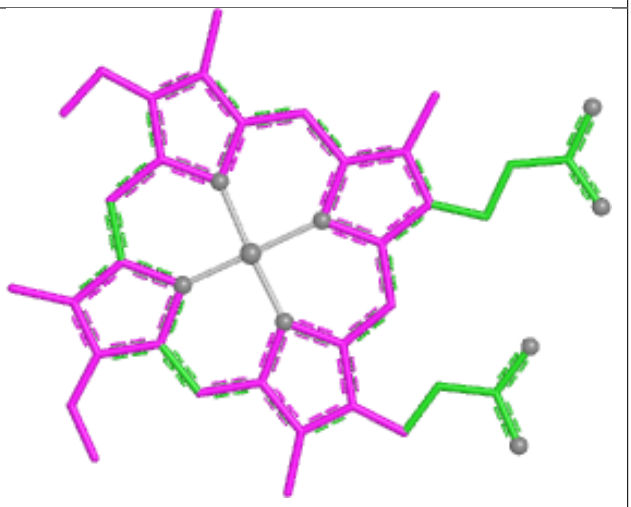


Rings

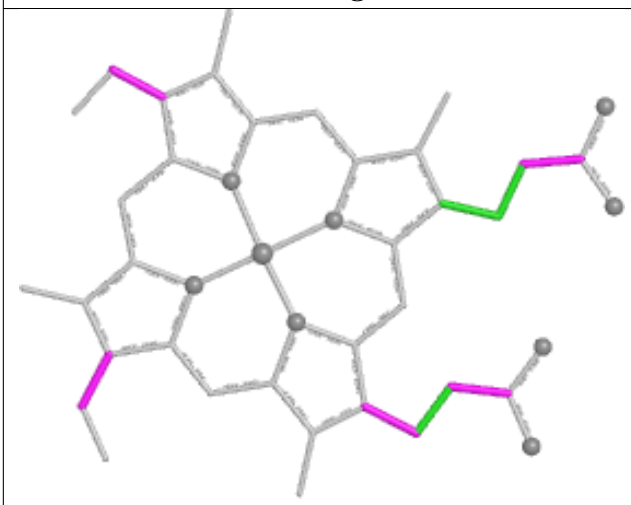
Ligand HEC C 301



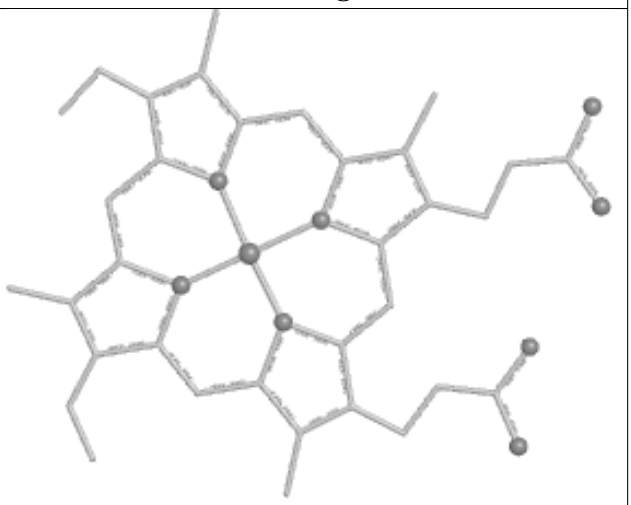
Bond lengths



Bond angles

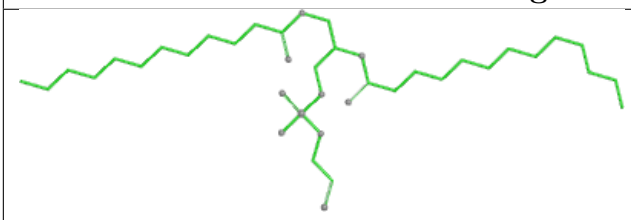


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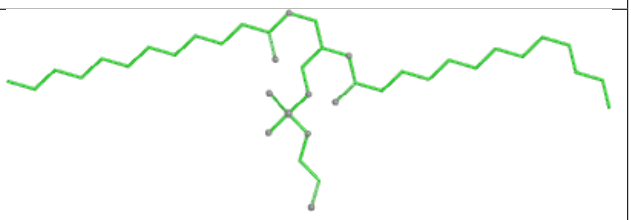


Rings

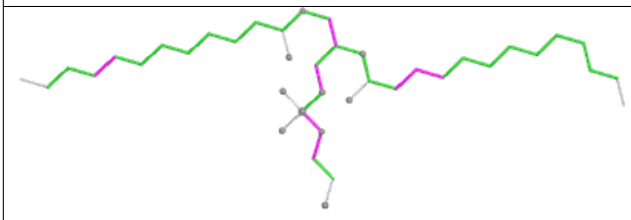
Ligand PEE a 202



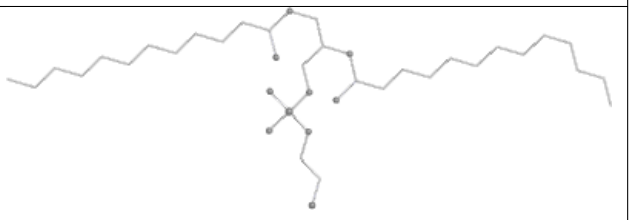
Bond lengths



Bond angles

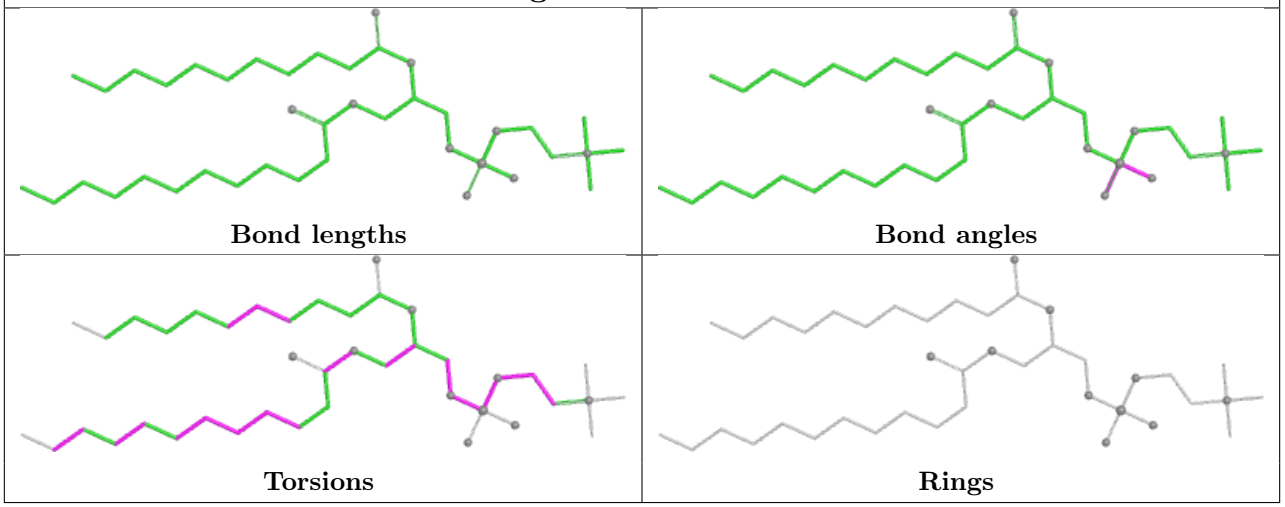


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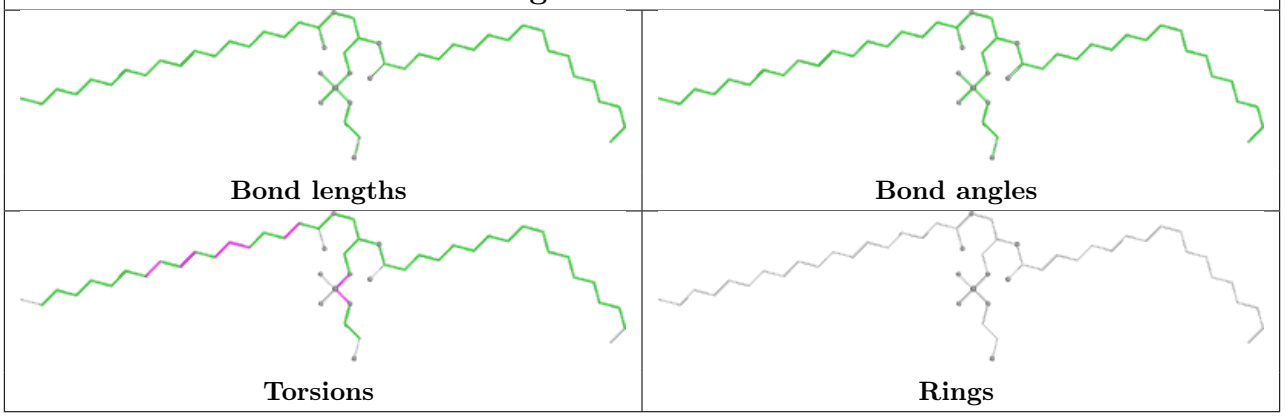


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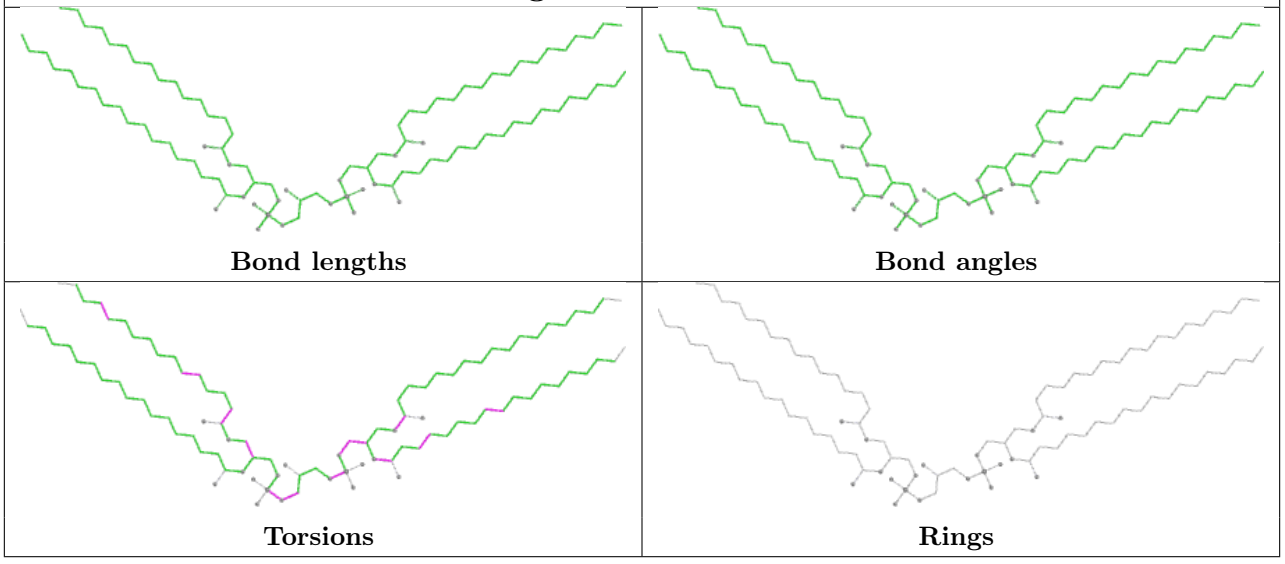
Ligand PC1 E 101



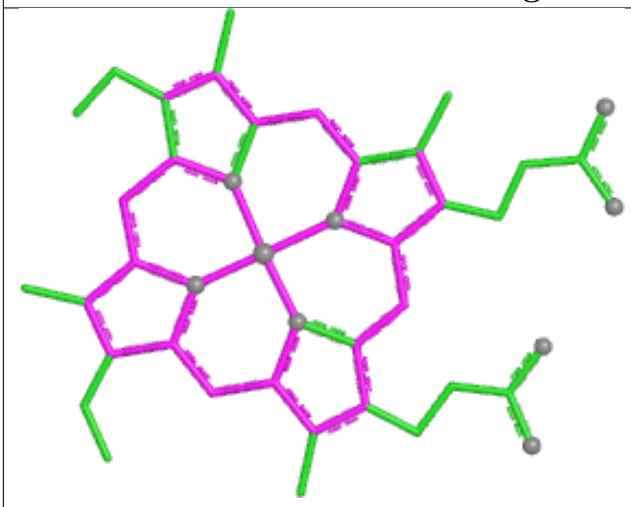
Ligand PEE d 101



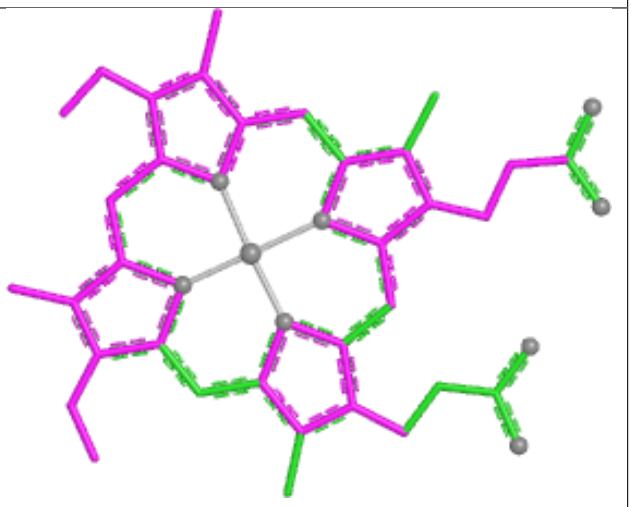
Ligand CDL b 305



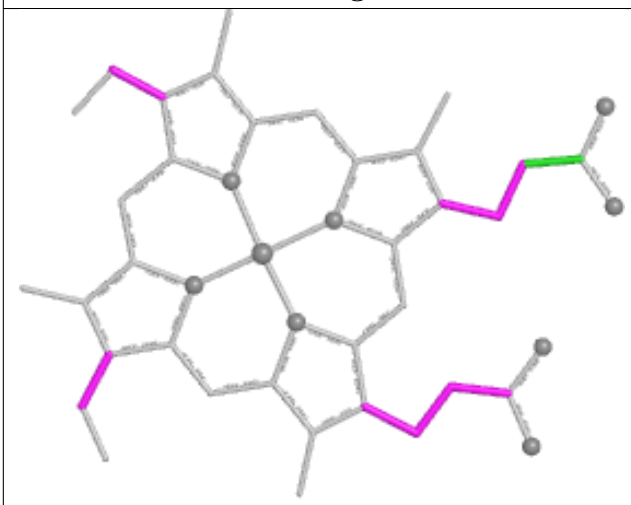
Ligand HEC B 301



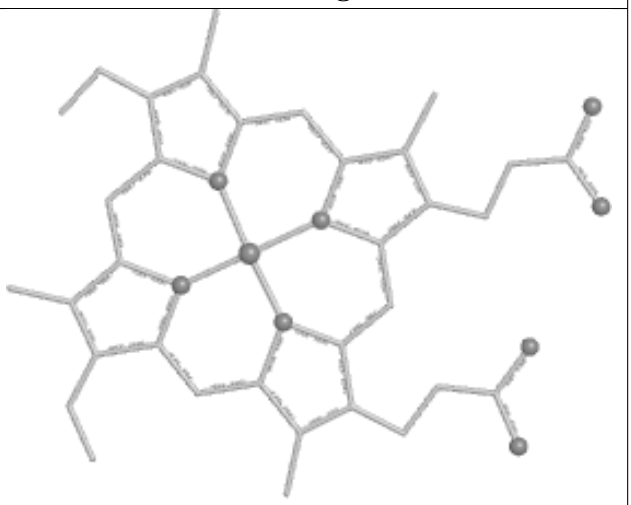
Bond lengths



Bond angles



Torsions



Rings

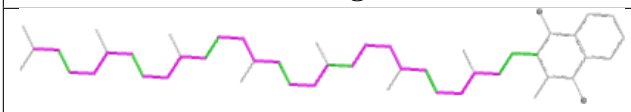
Ligand MQ7 B 305



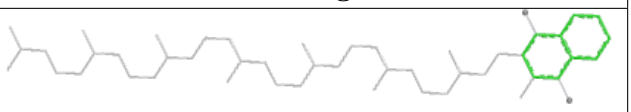
Bond lengths



Bond angles

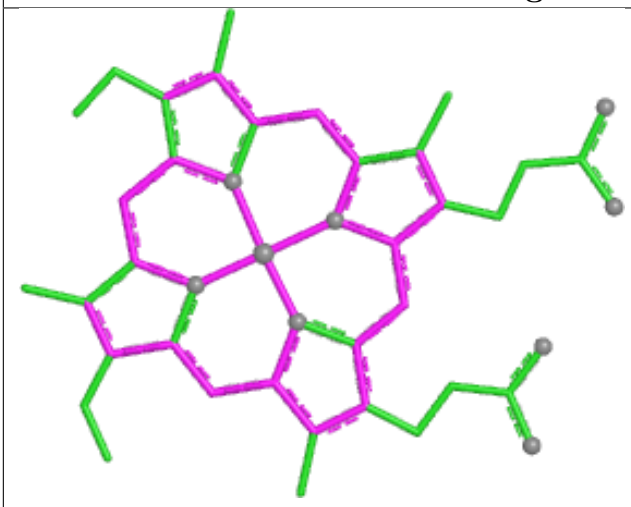


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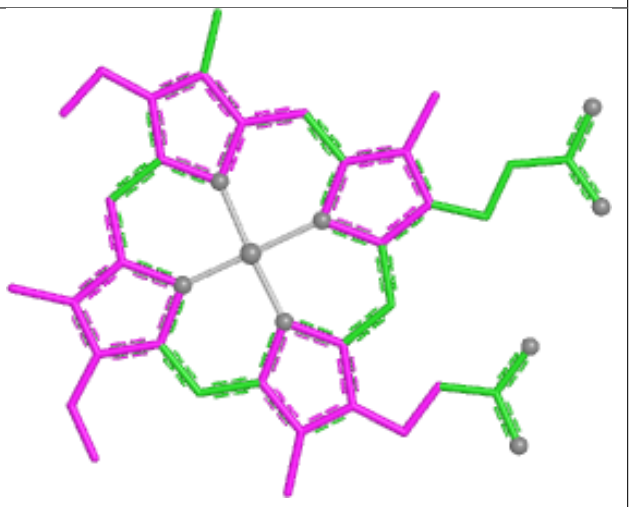


Rings

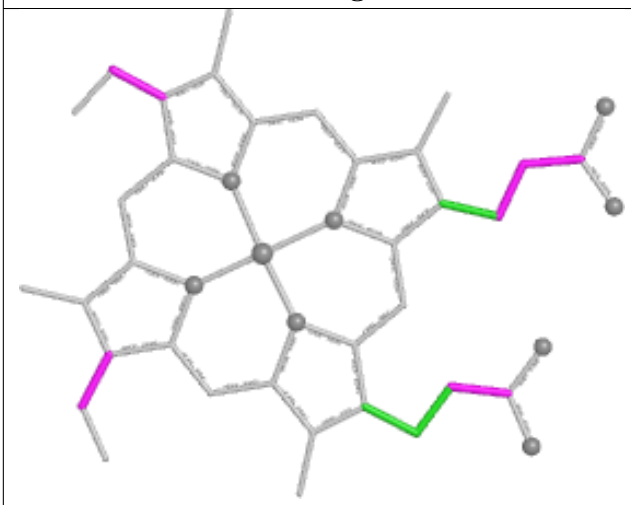
Ligand HEC b 301



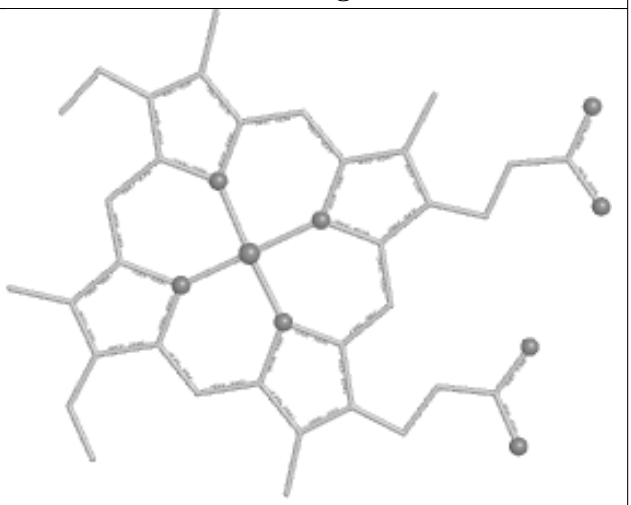
Bond lengths



Bond angles

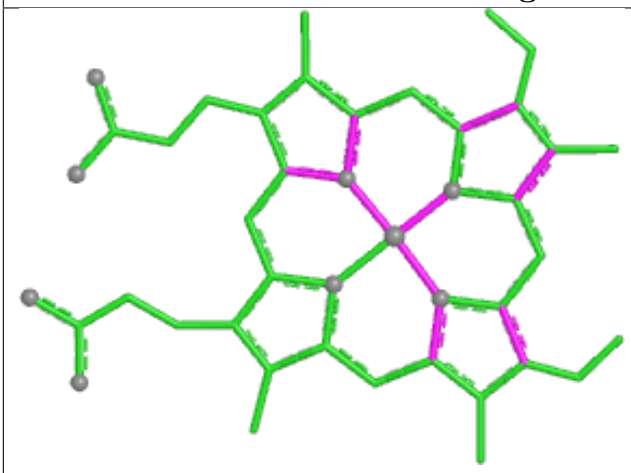


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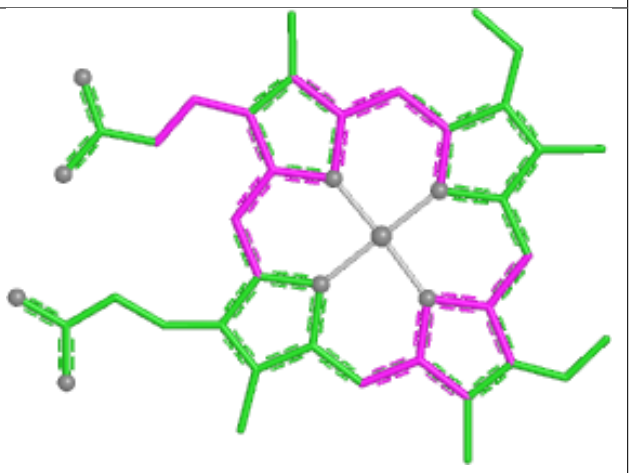


Rings

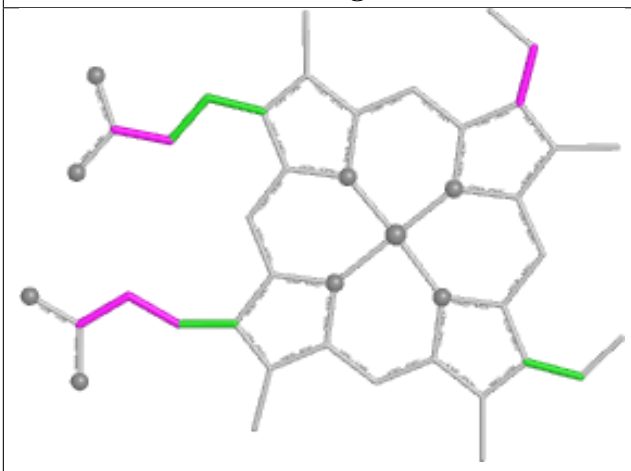
Ligand HEM B 302



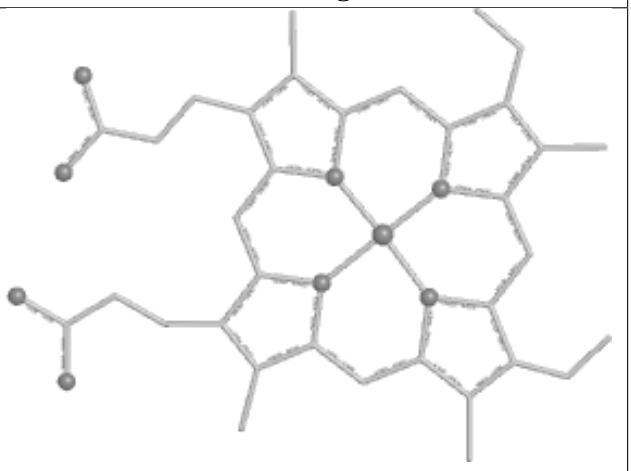
Bond lengths



Bond angles

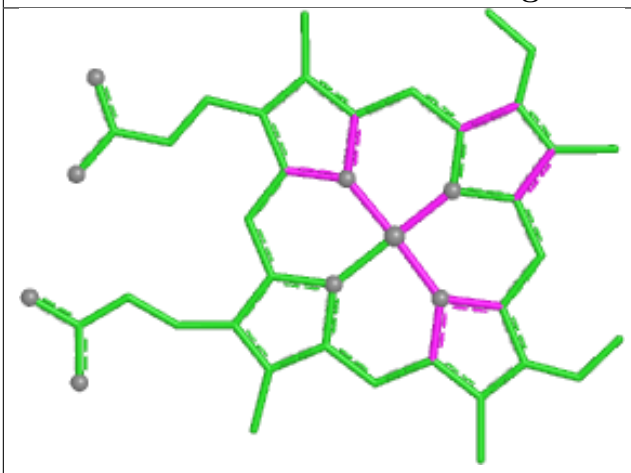


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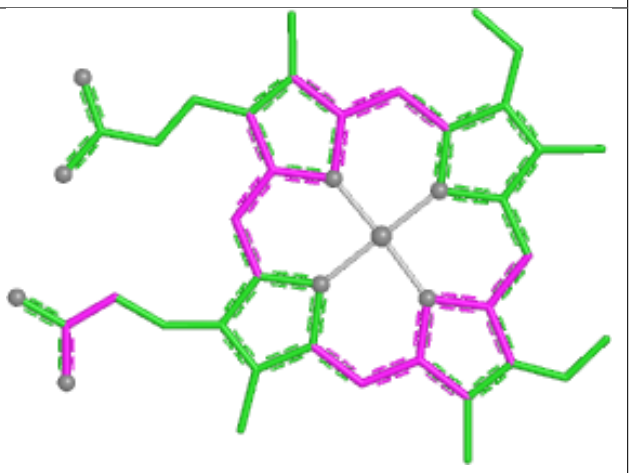


Rings

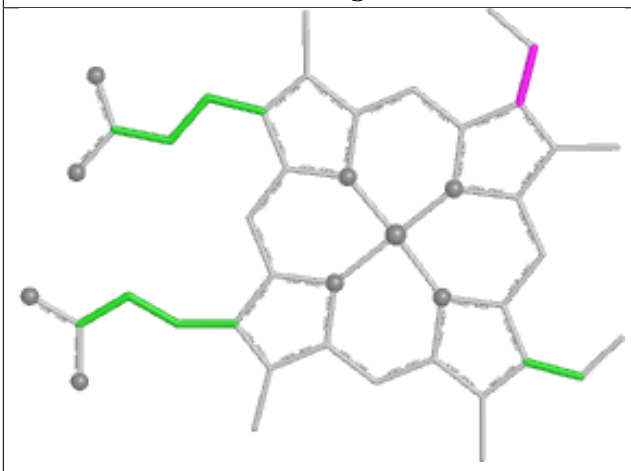
Ligand HEM b 303



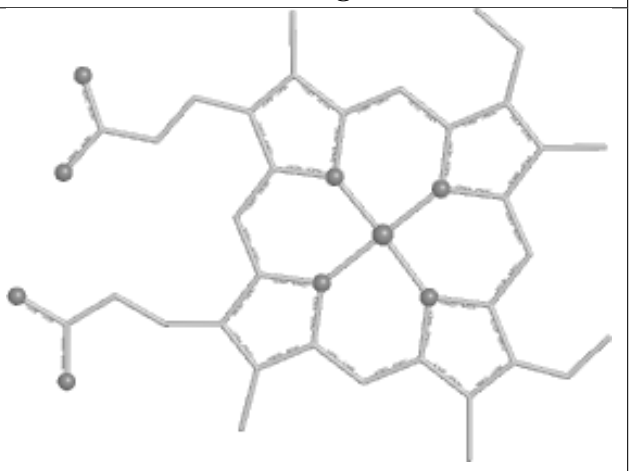
Bond lengths



Bond angles

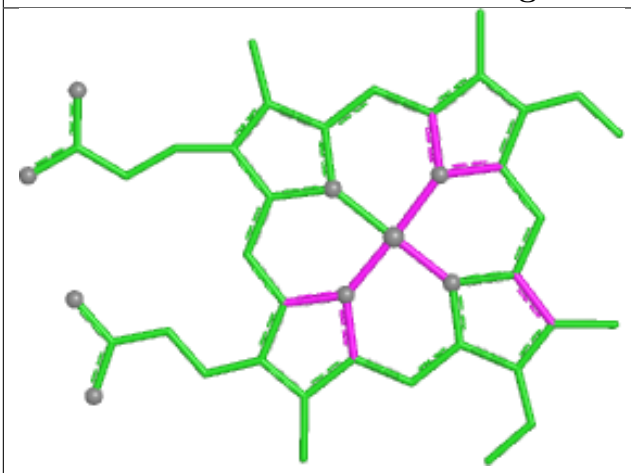


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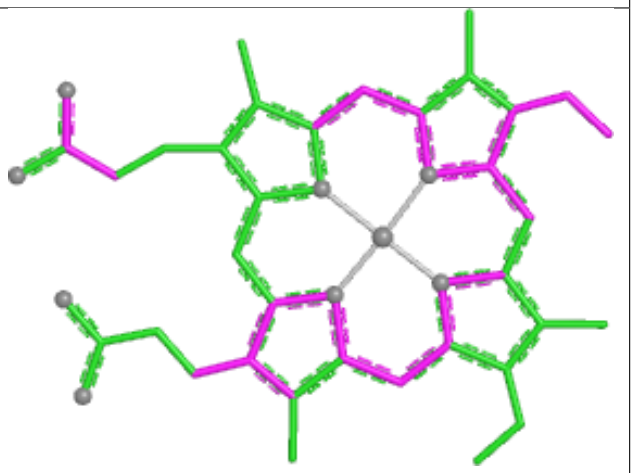


Rings

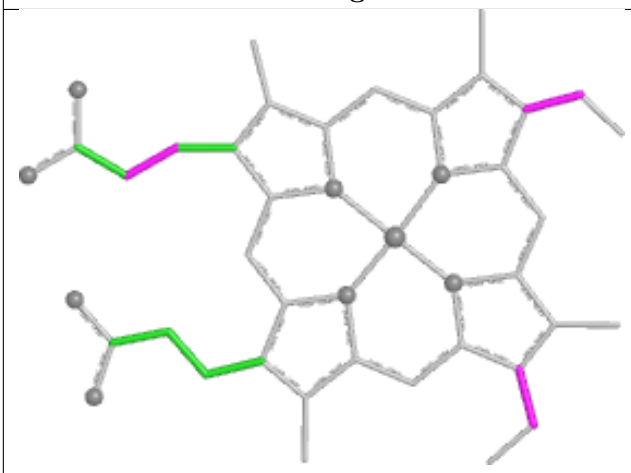
Ligand HEM B 303



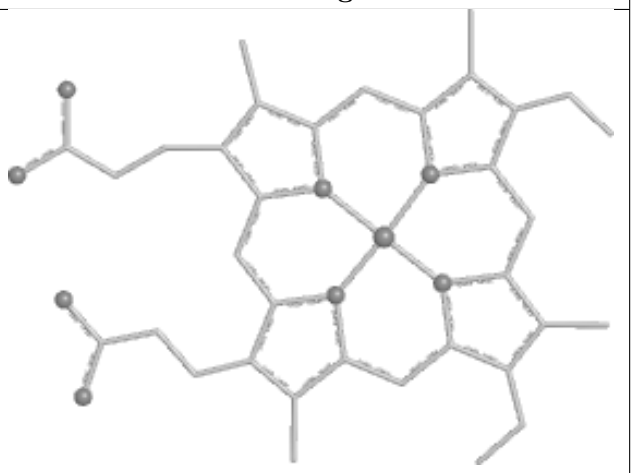
Bond lengths



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.

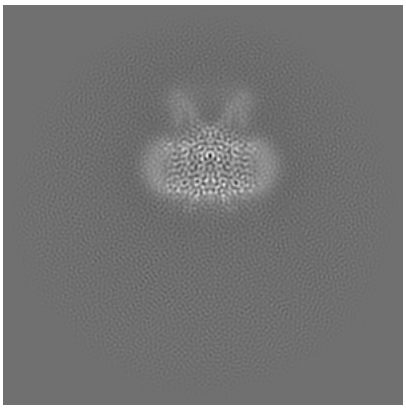
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70336. These allow visual inspection of the internal detail of the map and identification of artifacts.

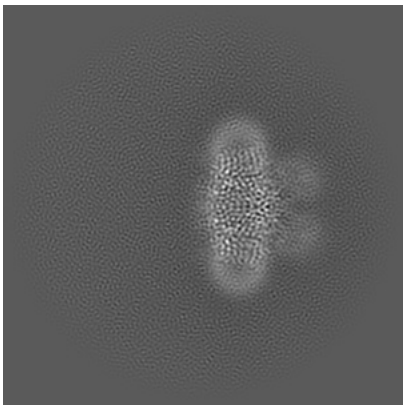
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

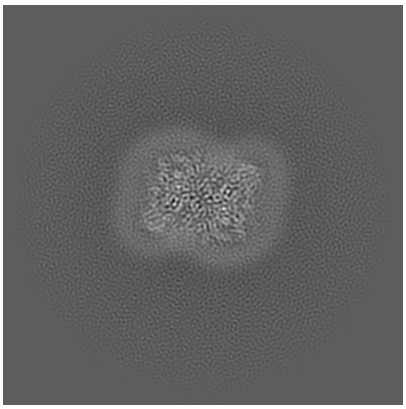
6.1.1 Primary map



X

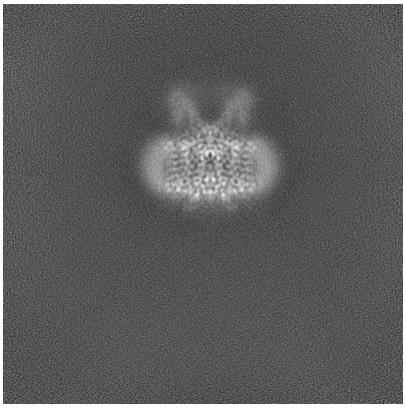


Y

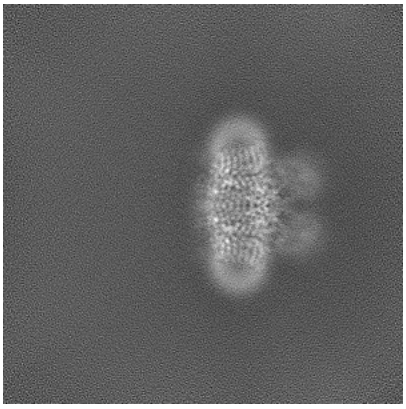


Z

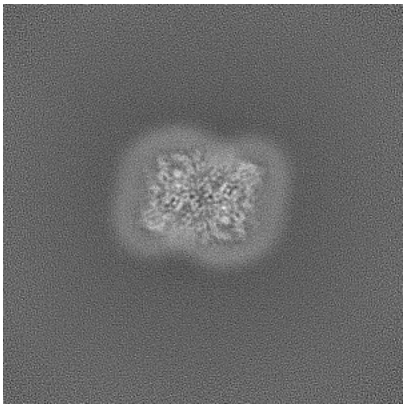
6.1.2 Raw map



X



Y

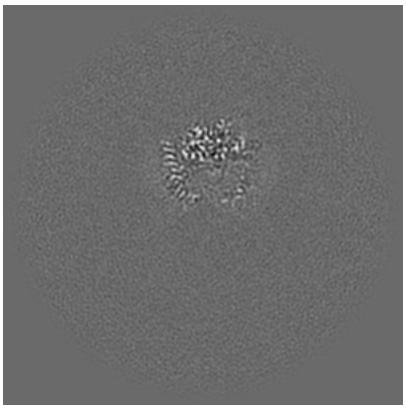


Z

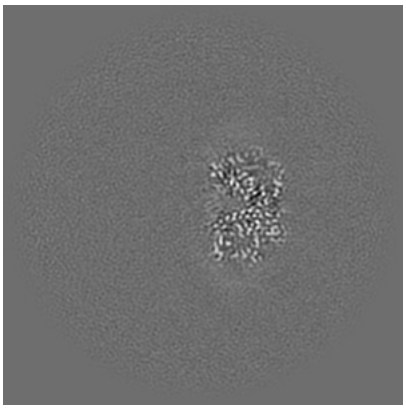
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

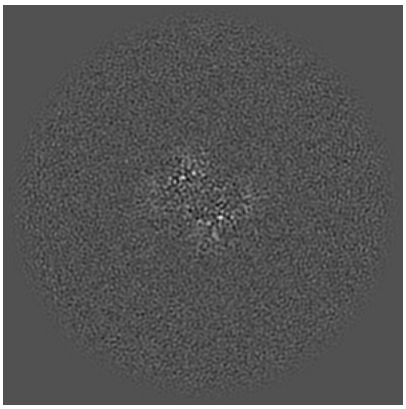
6.2.1 Primary map



X Index: 180

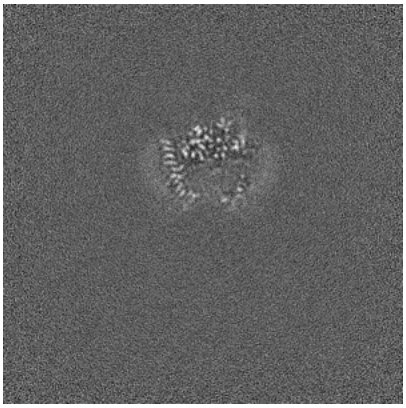


Y Index: 180

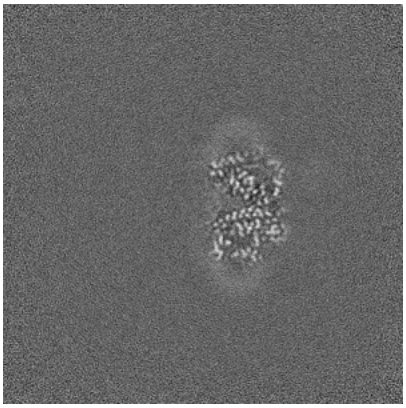


Z Index: 180

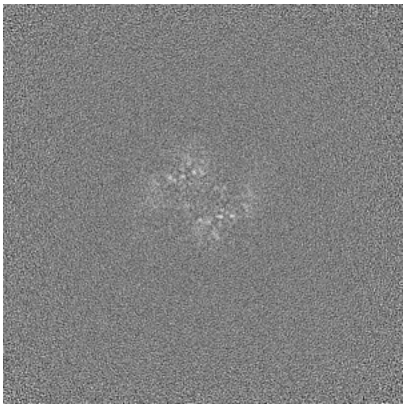
6.2.2 Raw map



X Index: 180



Y Index: 180

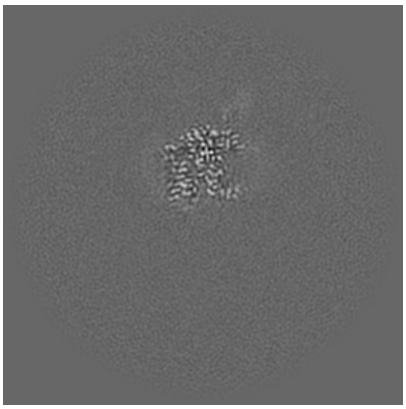


Z Index: 180

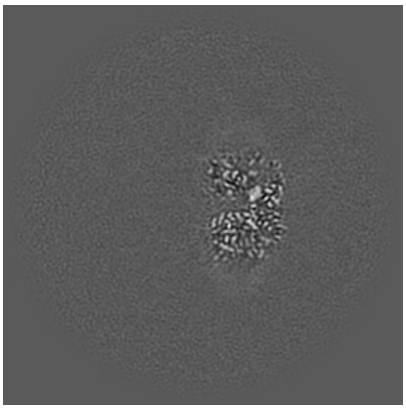
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

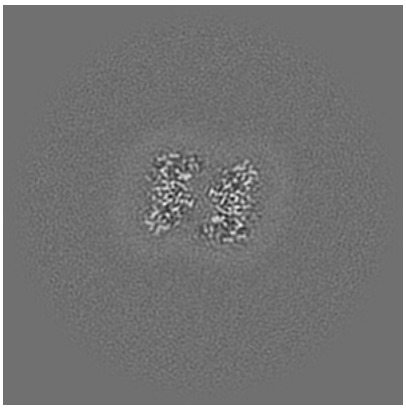
6.3.1 Primary map



X Index: 190

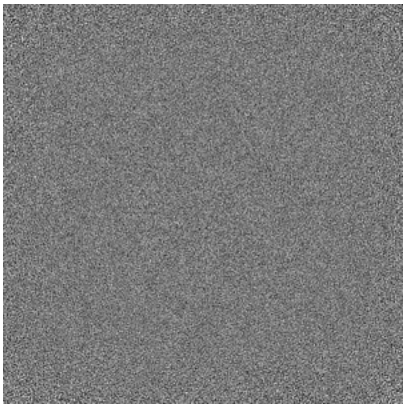


Y Index: 183

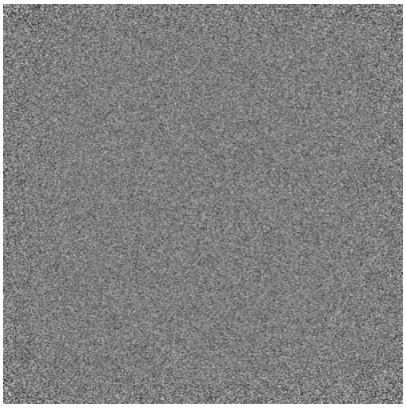


Z Index: 202

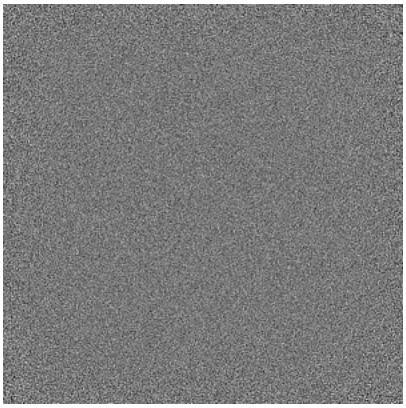
6.3.2 Raw map



X Index: 0



Y Index: 0

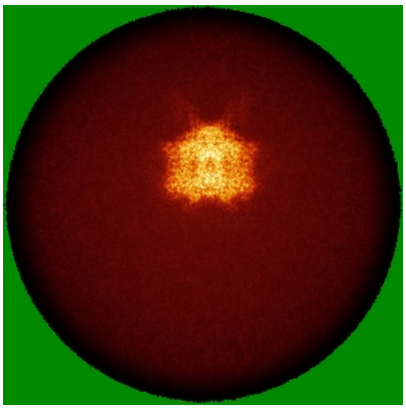


Z Index: 0

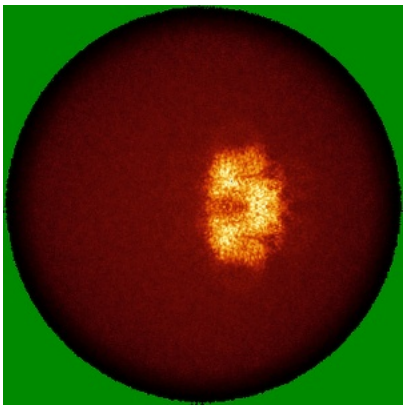
The images above show the largest variance slices of the map in three orthogonal directions.

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

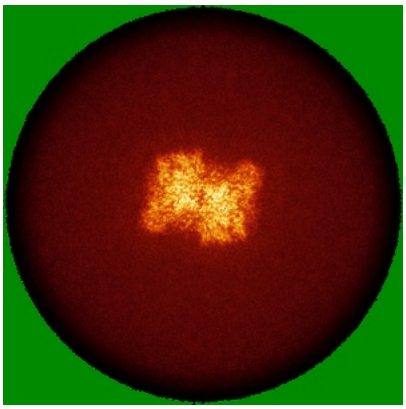
6.4.1 Primary map



X

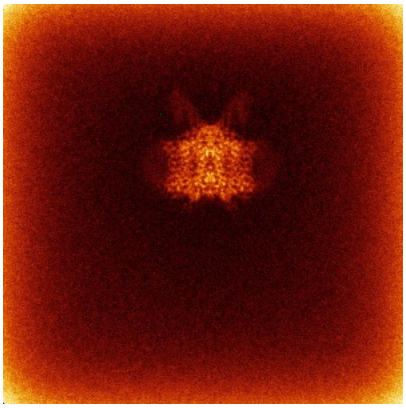


Y

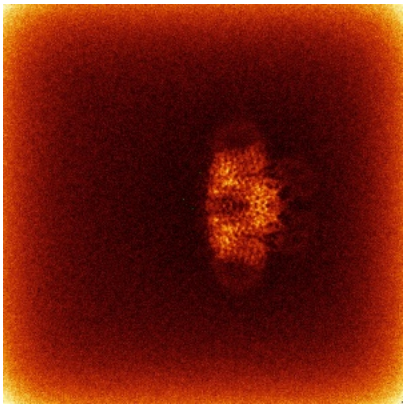


Z

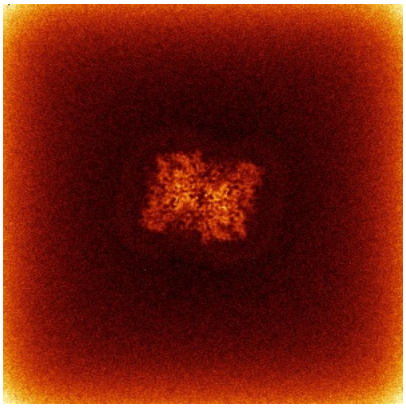
6.4.2 Raw map



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 0.31. 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.

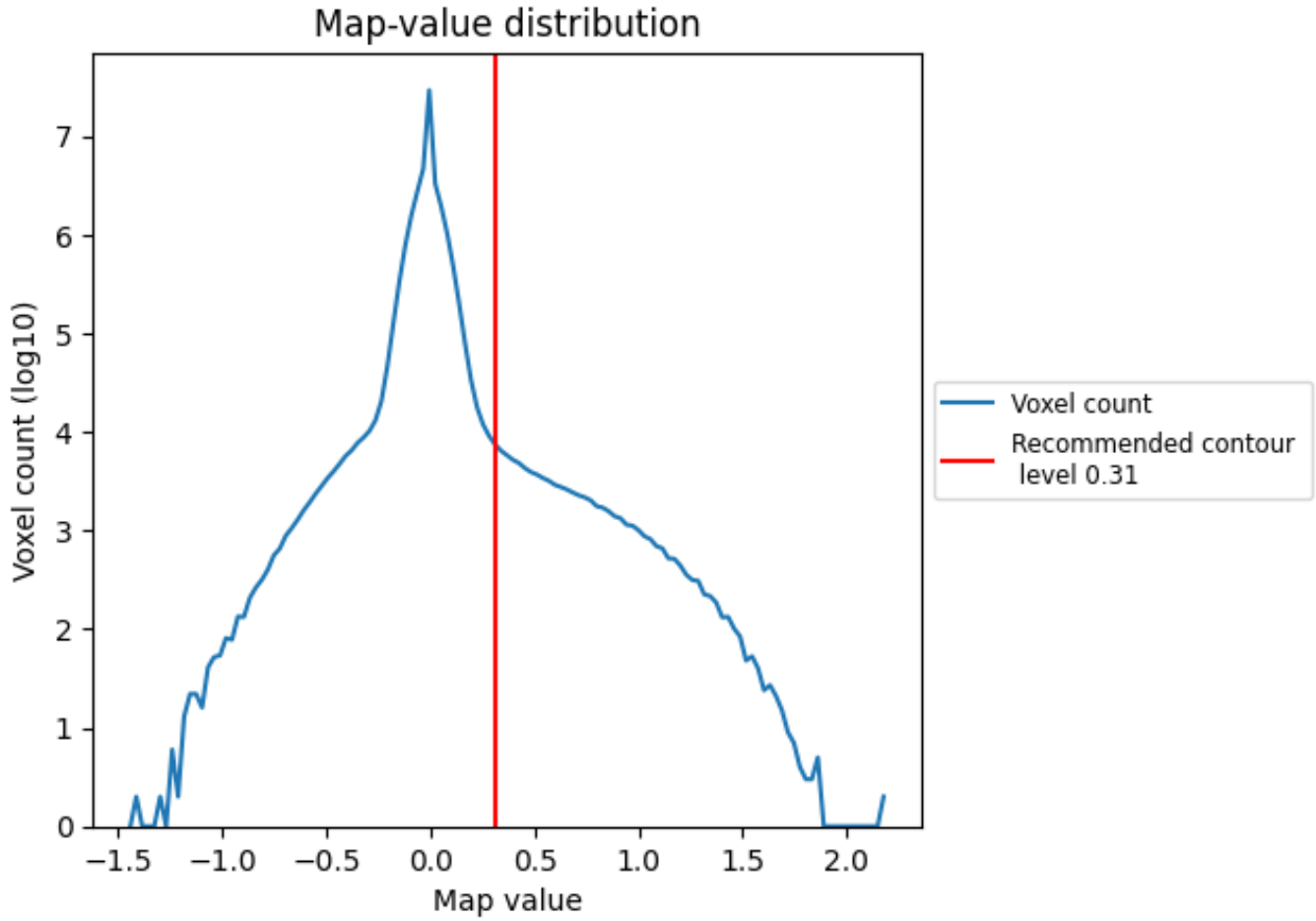
6.6 Mask visualisation (i)

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

7 Map analysis

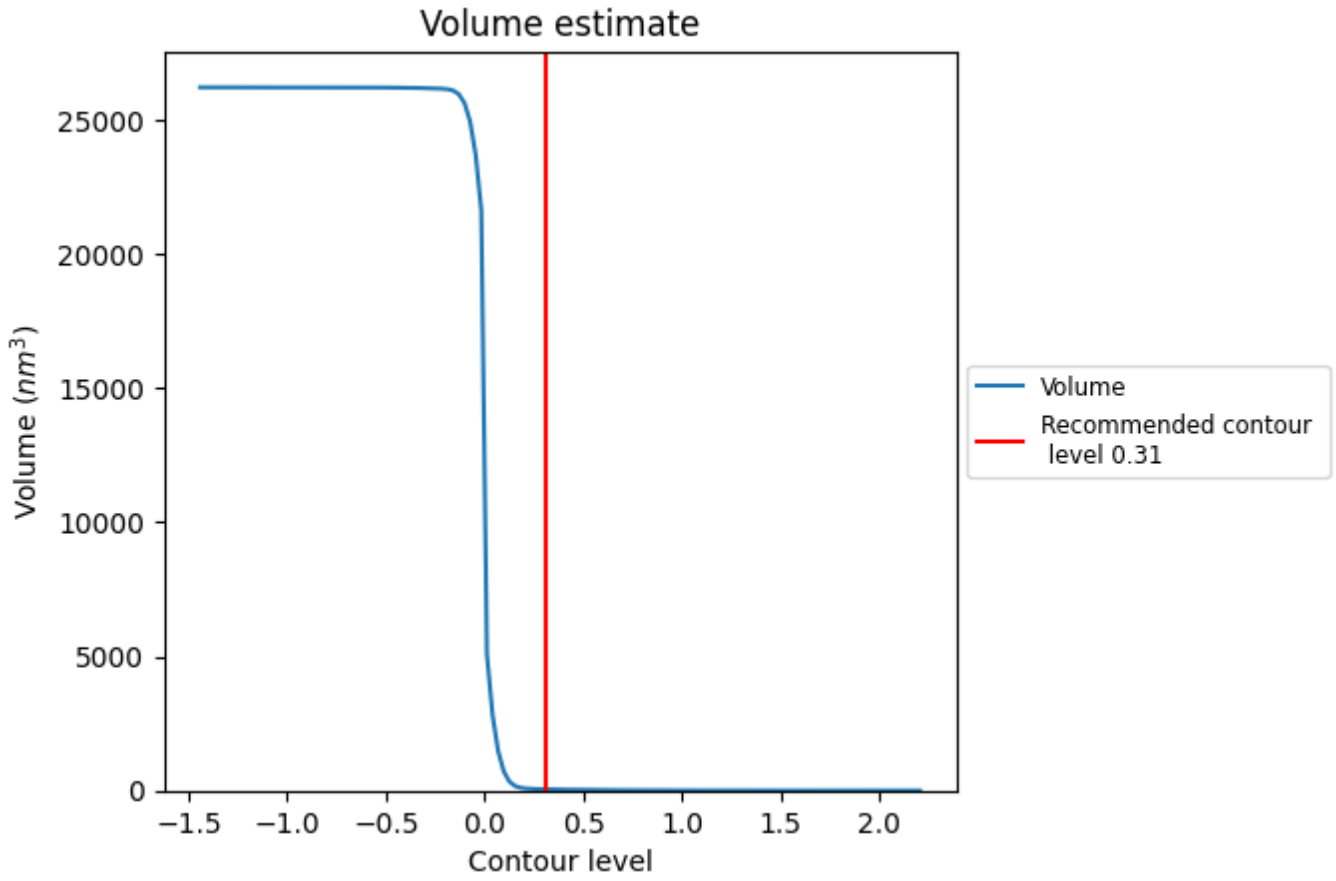
This section contains the results of statistical analysis of the map.

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.

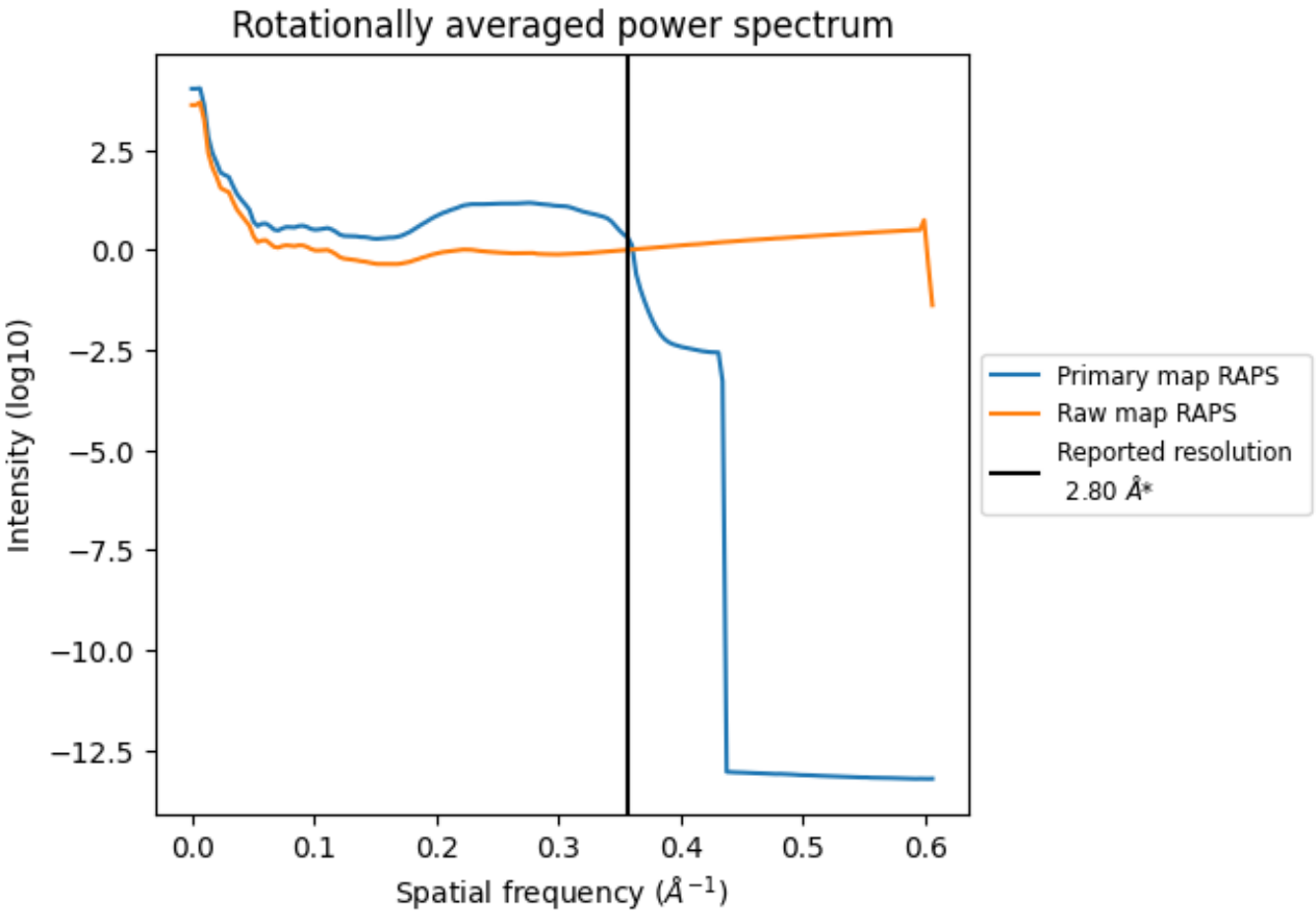
7.2 Volume estimate



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 42 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)

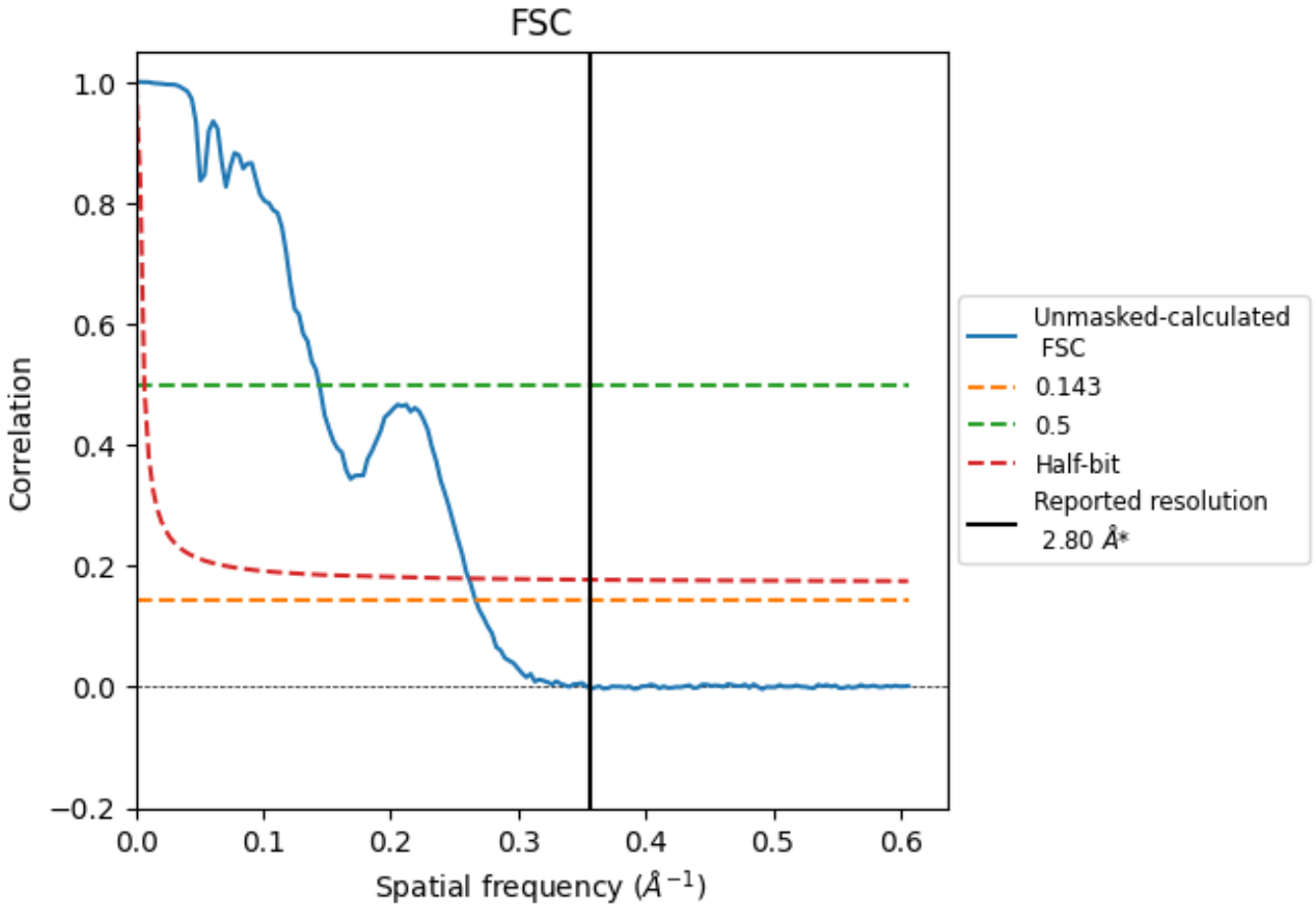


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

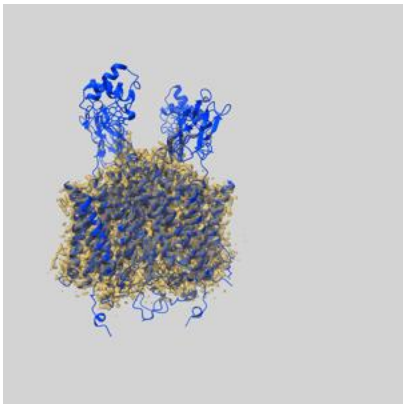
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	6.95	3.83

*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 3.75 differs from the reported value 2.8 by more than 10 %

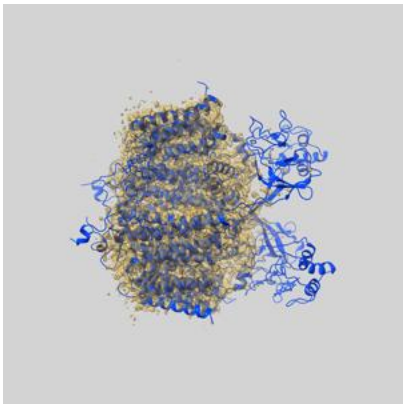
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70336 and PDB model 9OCZ. Per-residue inclusion information can be found in section 3 on page 11.

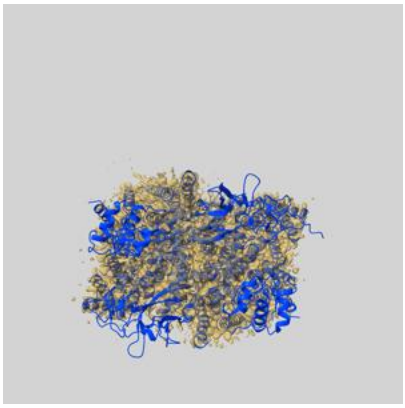
9.1 Map-model overlay



X



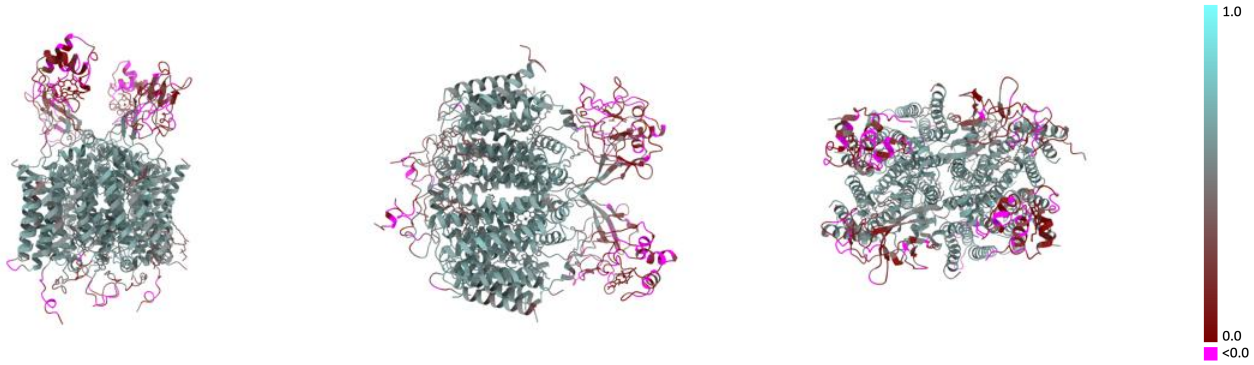
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.31 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.

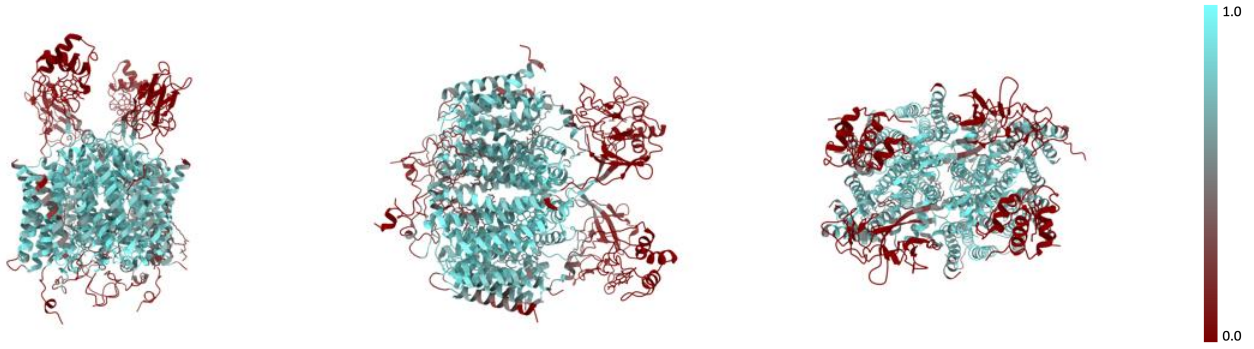
9.2 Q-score mapped to coordinate model (i)



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.

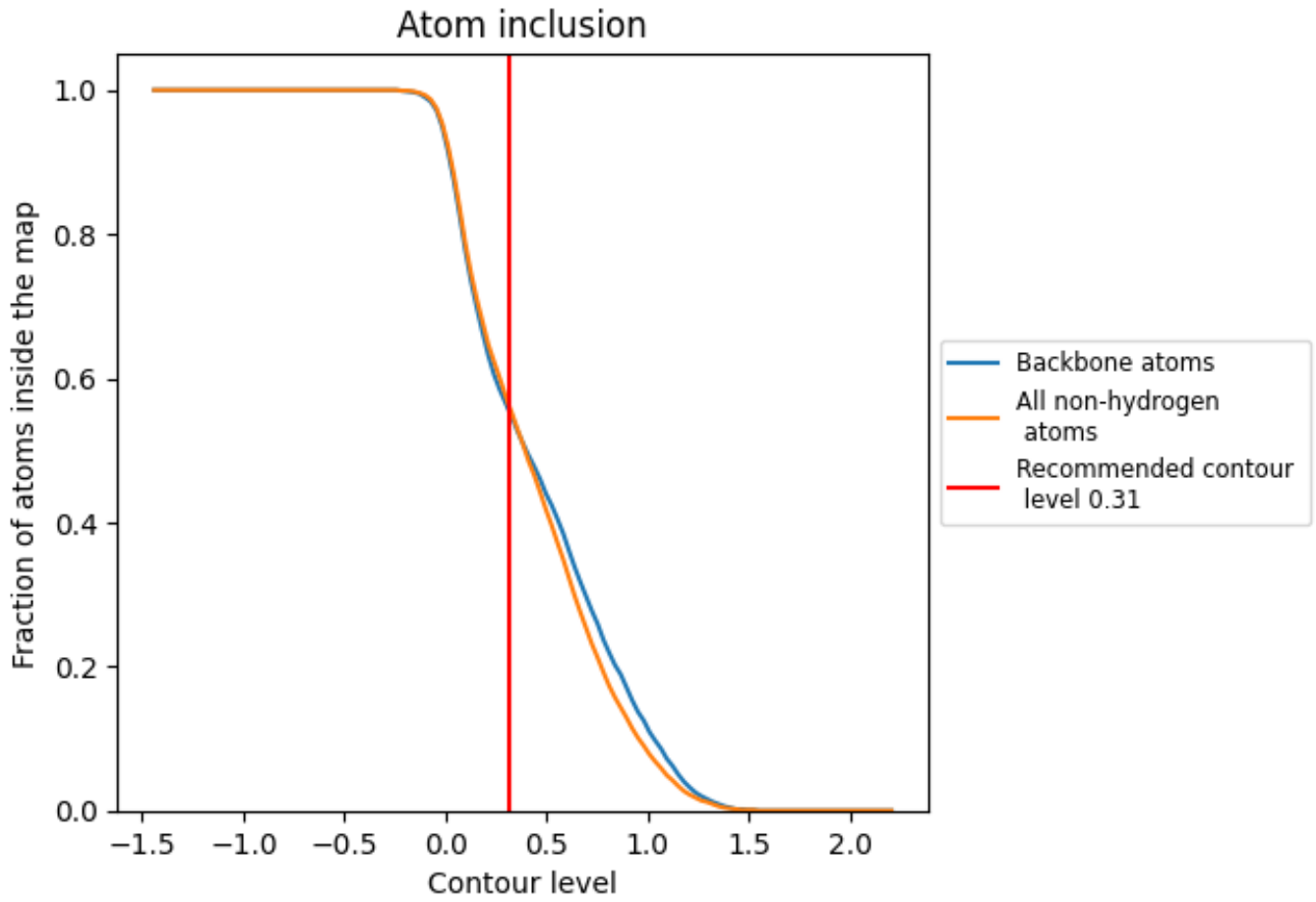
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.31).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.4590
A	0.2340	0.3010
B	0.8120	0.5890
C	0.4330	0.3620
D	0.6570	0.5270
E	0.7980	0.5790
F	0.4210	0.5140
G	0.6050	0.4820
H	0.5180	0.4040
a	0.2380	0.2920
b	0.8000	0.5880
c	0.4440	0.3800
d	0.6850	0.5520
e	0.8010	0.5950
f	0.3510	0.4920
g	0.6180	0.5180
h	0.5210	0.4150

