Full wwPDB EM Validation Report

Mar 8, 2026 – 07:12 AM UTC

PDB ID	:	8K9F / pdb_00008k9f
EMDB ID	:	EMD-36985
Title	:	Cryo-EM structure of the photosynthetic alternative complex III from Chloroflexus aurantiacus at 2.9 angstrom
Authors	:	Xu, X.
Deposited on	:	2023-08-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

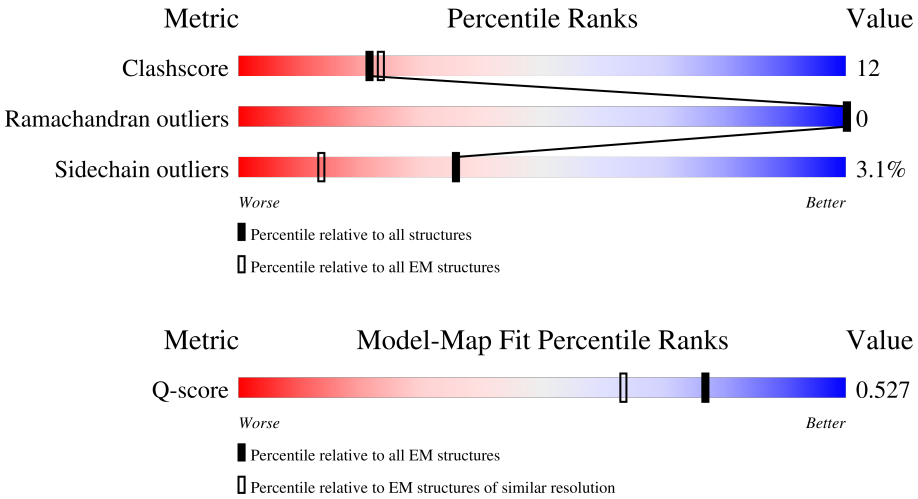
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.90 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	13054 (2.40 - 3.40)

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	219	68% 29%
2	B	1029	73% 19% 8%
3	C	486	69% 23% 8%
4	D	179	68% 30%

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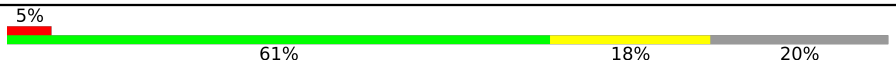
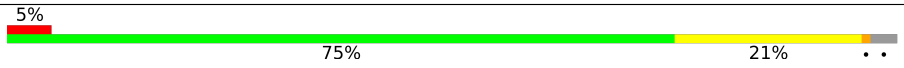
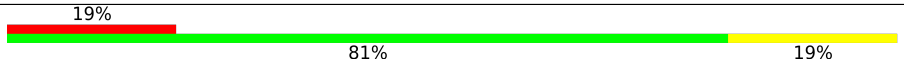
Mol	Chain	Length	Quality of chain
5	E	205	
6	F	411	
7	G	112	
8	I	37	

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
11	F3S	B	1104	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 19906 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 Cytochrome c7-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	218	1763	1129	306	313	15	0	0

- Molecule 2 is a protein called Fe-S-cluster-containing hydrogenase components 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	951	7350	4622	1303	1395	30	0	0

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	449	3655	2476	576	586	17	0	0

- Molecule 4 is a protein called Quinol:cytochrome c oxidoreductase membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	175	1350	884	215	245	6	0	0

- Molecule 5 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	164	1298	822	223	246	7	0	0

- Molecule 6 is a protein called Quinol:cytochrome c oxidoreductase quinone-binding subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	397	3128	2091	506	514	17	0	0

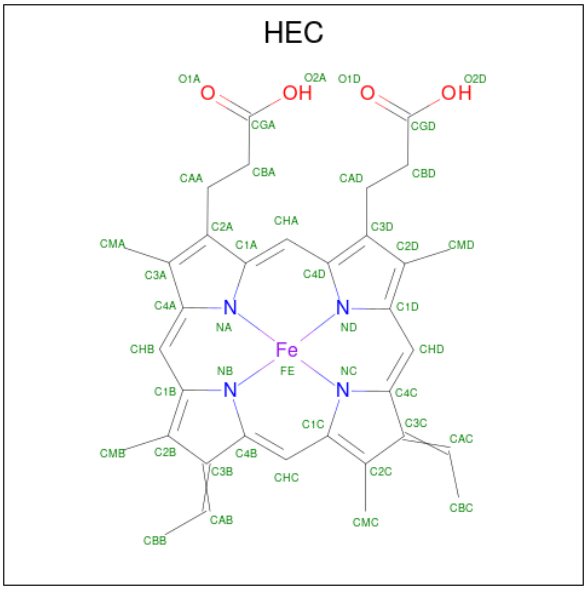
- Molecule 7 is a protein called hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			623	404	108	107	4		

- Molecule 8 is a protein called unknown.

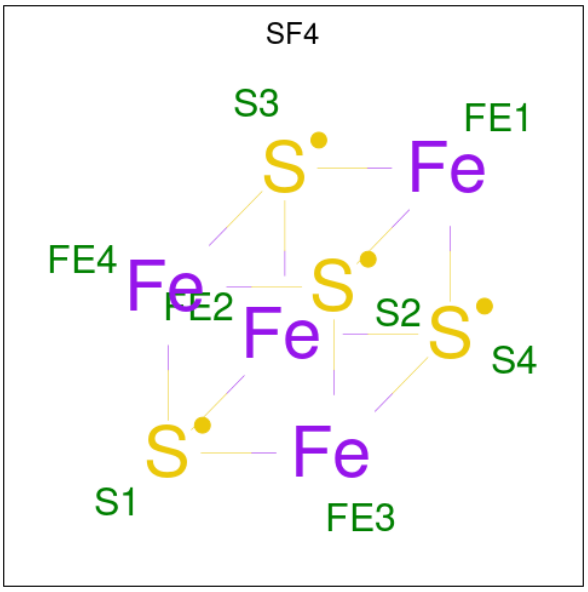
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



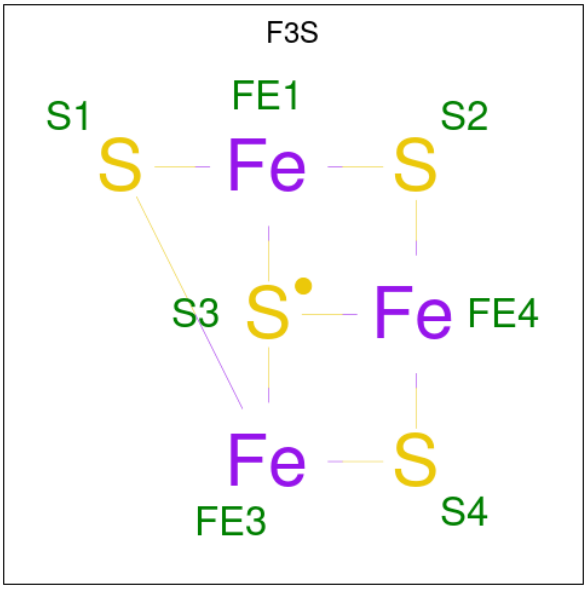
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

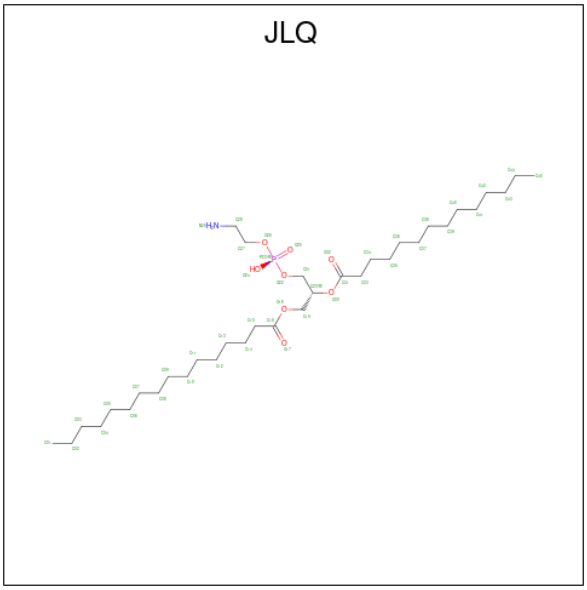


Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

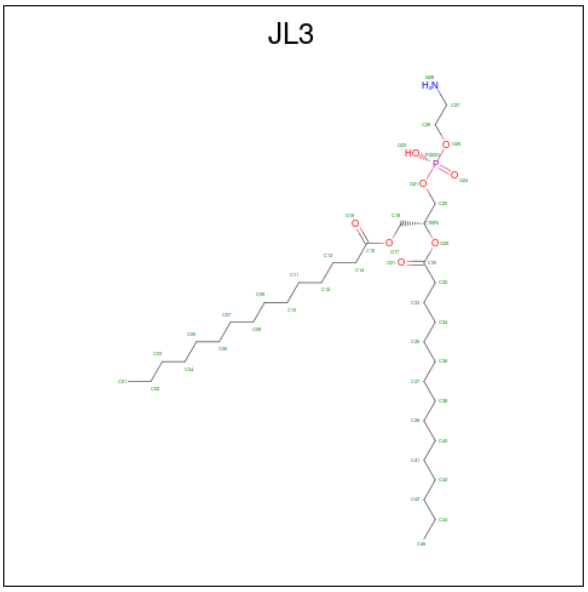
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	Mg	0
			1	1	

- Molecule 13 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (CCD ID: JLQ) (formula: $C_{35}H_{70}NO_8P$).



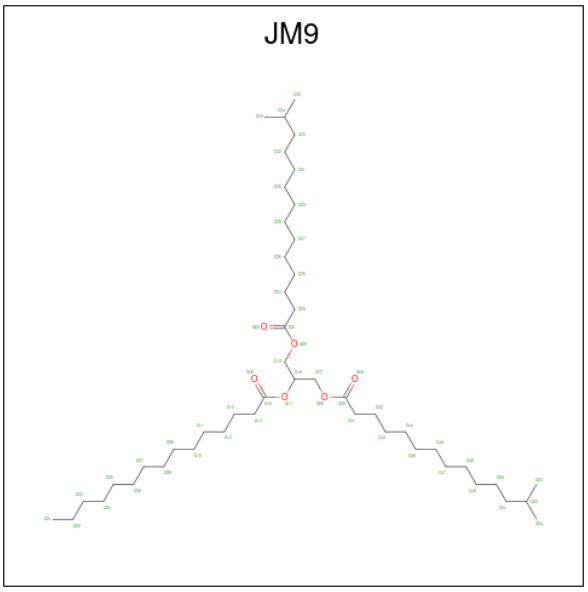
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 14 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (CCD ID: JL3) (formula: $C_{35}H_{70}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 15 is 1,3-bis(13-methyltetradecanoyloxy)propan-2-yl pentadecanoate (CCD ID: JM9) (formula: $C_{48}H_{92}O_6$).



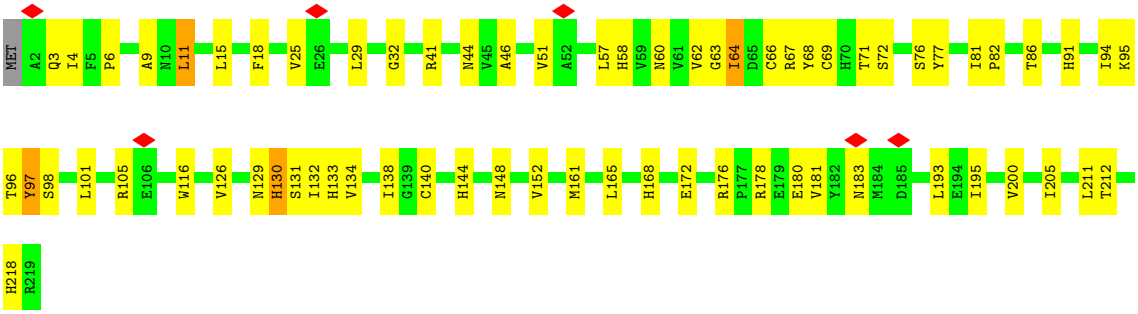
Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	C	O	0
			54	48	6	

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.

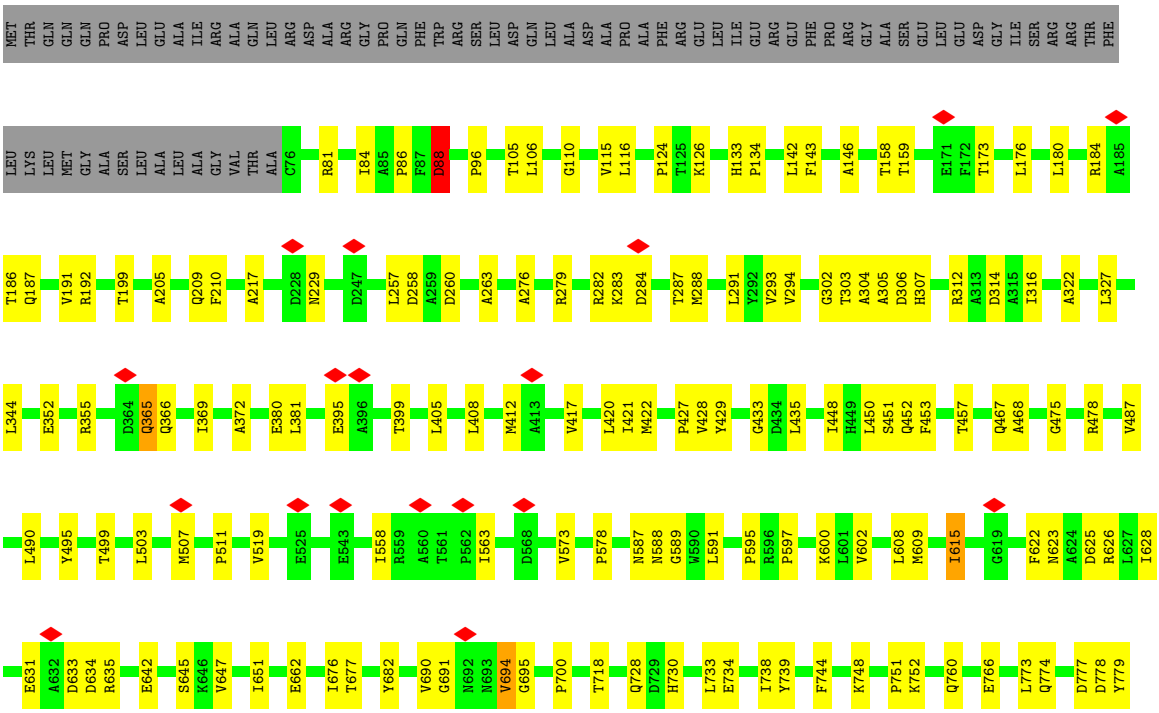
• Molecule 1: Cytochrome c7-like domain-containing protein

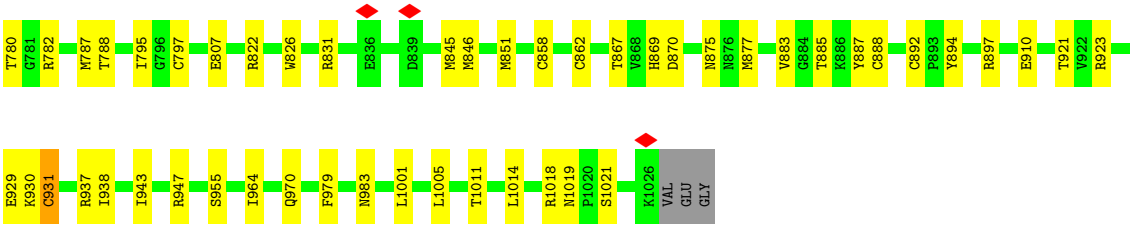
Chain A:



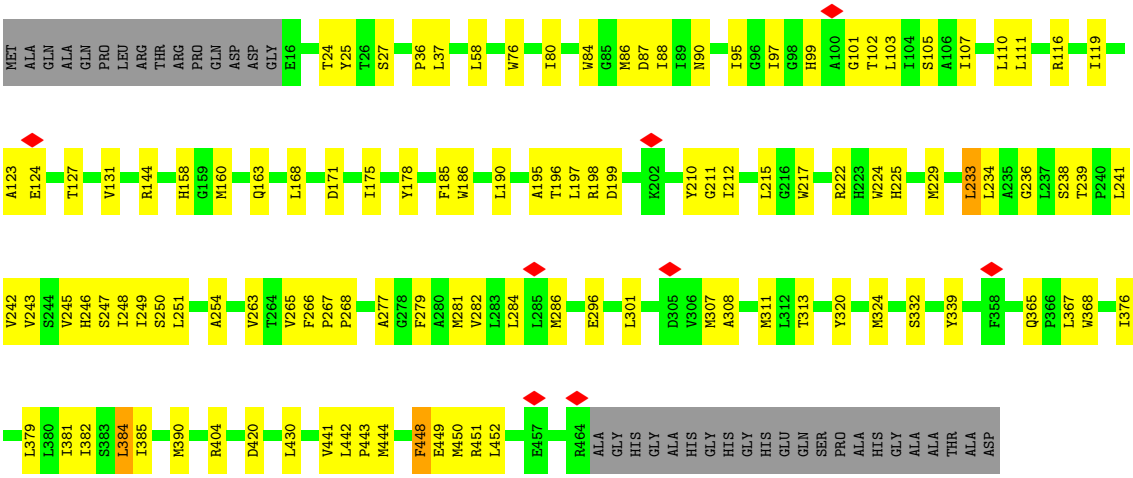
• Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein

Chain B:

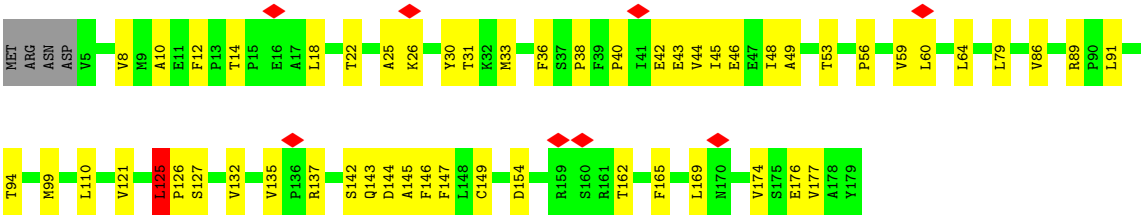




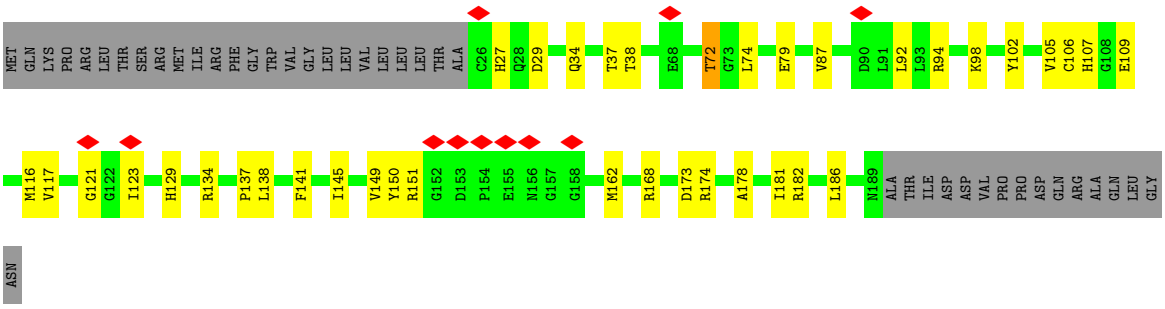
• Molecule 3: Polysulphide reductase NrfD



• Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

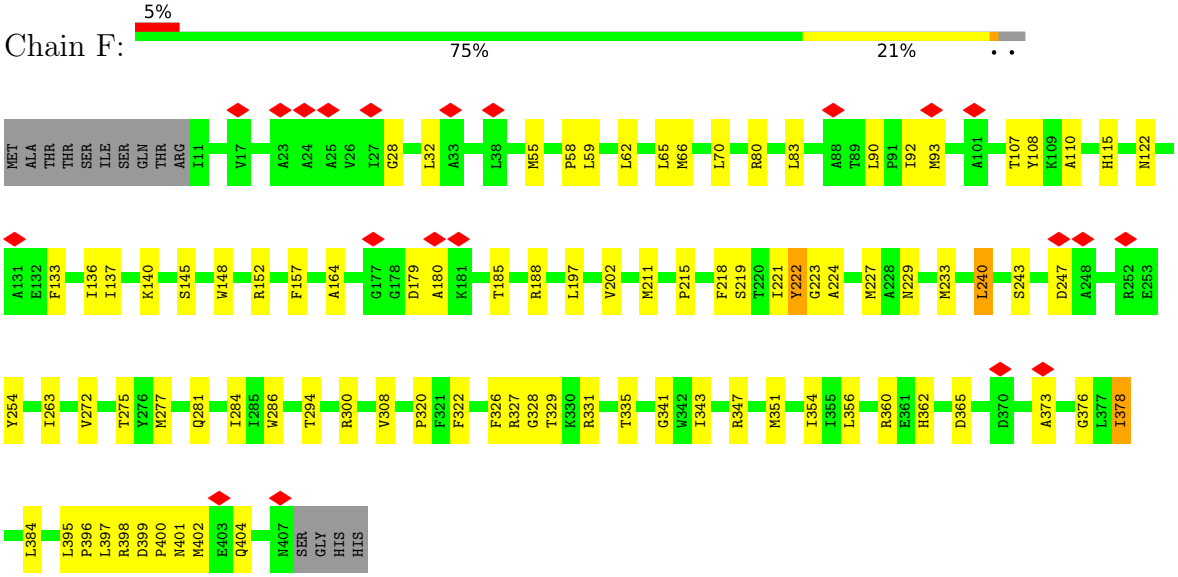


• Molecule 5: Cytochrome c domain-containing protein



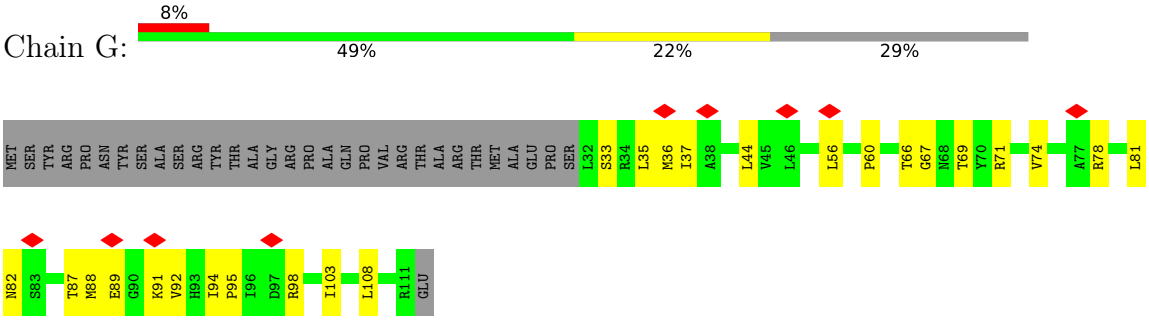
• Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

Chain F:



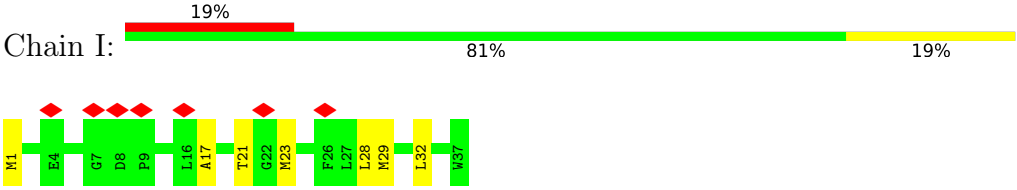
• Molecule 7: hypothetical protein

Chain G:



• Molecule 8: unknown

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103633	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	200.88, 200.88, 200.88	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JLQ, MG, JM9, HEC, F3S, SF4, JL3

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	0.44	0/1812	0.71	0/2472
2	B	0.35	0/7518	0.63	5/10249 (0.0%)
3	C	0.37	0/3787	0.66	1/5179 (0.0%)
4	D	0.44	0/1388	0.84	6/1895 (0.3%)
5	E	0.39	0/1333	0.66	0/1810
6	F	0.38	0/3226	0.72	3/4408 (0.1%)
7	G	0.28	0/635	0.72	0/865
8	I	0.29	0/318	0.70	0/436
All	All	0.37	0/20017	0.68	15/27314 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	883	VAL	N-CA-C	-9.87	101.87	113.42
4	D	99	MET	CA-C-N	8.63	125.68	120.24
4	D	99	MET	C-N-CA	8.63	125.68	120.24
6	F	326	PHE	N-CA-C	8.56	122.11	110.55
2	B	887	TYR	N-CA-C	-8.43	100.73	112.45
6	F	328	GLY	N-CA-C	-7.94	102.80	111.93
3	C	448	PHE	N-CA-C	-7.80	100.46	110.53
2	B	81	ARG	N-CA-C	7.77	120.64	111.71
4	D	125	LEU	N-CA-C	7.71	123.24	112.75
6	F	222	TYR	N-CA-C	-7.07	101.20	110.53
4	D	144	ASP	N-CA-C	6.42	122.83	113.40
4	D	125	LEU	CA-C-N	-6.12	112.18	119.84
4	D	125	LEU	C-N-CA	-6.12	112.18	119.84
2	B	88	ASP	N-CA-C	-5.27	106.91	113.55
2	B	1005	LEU	N-CA-C	-5.26	101.20	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1714	70	0
2	B	7350	0	7178	144	0
3	C	3655	0	3688	101	0
4	D	1350	0	1341	47	0
5	E	1298	0	1229	48	0
6	F	3128	0	3175	67	0
7	G	623	0	660	21	0
8	I	305	0	302	7	0
9	A	215	0	152	30	0
9	E	43	0	31	15	0
10	B	24	0	0	1	0
11	B	7	0	0	10	0
12	B	1	0	0	0	0
13	C	45	0	0	0	0
14	F	45	0	0	4	0
15	F	54	0	0	6	0
All	All	19906	0	19470	457	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 (457) 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:66:CYS:CB	9:A:304:HEC:HAB	1.07	1.51
1:A:66:CYS:HB3	9:A:304:HEC:CAB	1.03	1.47
5:E:106:CYS:SG	9:E:301:HEC:CAC	2.18	1.31
6:F:145:SER:HG	6:F:148:TRP:CD1	1.69	1.10
4:D:26:LYS:HE2	4:D:48:ILE:HG22	1.29	1.08
2:B:421:ILE:HD13	2:B:507:MET:HE1	1.37	1.07
1:A:66:CYS:SG	9:A:304:HEC:HAB	1.95	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:LEU:HD12	3:C:107:ILE:HB	1.48	0.95
5:E:106:CYS:SG	9:E:301:HEC:C3C	2.55	0.94
2:B:651:ILE:CG2	2:B:662:GLU:OE2	2.22	0.88
1:A:18:PHE:CD1	7:G:36:MET:HE1	2.09	0.86
6:F:145:SER:OG	6:F:148:TRP:HD1	1.57	0.86
1:A:94:ILE:HD11	5:E:123:ILE:CD1	2.07	0.84
3:C:163:GLN:HE21	4:D:86:VAL:HG21	1.43	0.84
3:C:37:LEU:HD23	3:C:197:LEU:HD22	1.61	0.82
6:F:233:MET:CE	6:F:347:ARG:HB2	2.11	0.81
2:B:862:CYS:HB2	11:B:1104:F3S:S1	2.21	0.80
6:F:145:SER:HG	6:F:148:TRP:HD1	0.80	0.80
6:F:145:SER:OG	6:F:148:TRP:CD1	2.33	0.80
1:A:94:ILE:HD11	5:E:123:ILE:HG13	1.62	0.80
5:E:106:CYS:SG	9:E:301:HEC:HAC	2.20	0.80
5:E:149:VAL:HG11	9:E:301:HEC:CGD	2.12	0.79
3:C:111:LEU:HD22	14:F:501:JL3:C32	2.14	0.78
6:F:329:THR:HA	6:F:335:THR:HG23	1.64	0.78
1:A:15:LEU:HD21	7:G:35:LEU:HD13	1.67	0.77
3:C:242:VAL:HA	3:C:245:VAL:HG12	1.65	0.77
2:B:888:CYS:HB3	11:B:1104:F3S:S1	2.24	0.77
3:C:36:PRO:O	3:C:37:LEU:HG	1.86	0.76
2:B:421:ILE:CD1	2:B:507:MET:HE1	2.15	0.76
4:D:26:LYS:CE	4:D:48:ILE:HG22	2.12	0.76
1:A:94:ILE:HD11	5:E:123:ILE:CG1	2.16	0.75
1:A:66:CYS:HB3	9:A:304:HEC:C3B	2.12	0.75
6:F:362:HIS:HD2	6:F:365:ASP:OD2	1.69	0.75
1:A:66:CYS:CB	9:A:304:HEC:CAB	1.92	0.75
2:B:609:MET:SD	2:B:676:ILE:CD1	2.75	0.74
2:B:862:CYS:SG	11:B:1104:F3S:S3	2.84	0.74
6:F:233:MET:HE2	6:F:347:ARG:CB	2.17	0.74
5:E:105:VAL:HG22	5:E:117:VAL:HG21	1.69	0.74
5:E:145:ILE:HG22	5:E:174:ARG:HD2	1.68	0.74
2:B:651:ILE:HG21	2:B:662:GLU:OE2	1.85	0.73
2:B:405:LEU:HD21	2:B:435:LEU:HD12	1.69	0.73
1:A:11:LEU:O	1:A:15:LEU:HD13	1.88	0.72
2:B:888:CYS:HG	11:B:1104:F3S:FE3	0.46	0.72
3:C:263:VAL:HG12	3:C:265:VAL:HG12	1.71	0.72
4:D:169:LEU:HD12	4:D:169:LEU:O	1.89	0.71
6:F:233:MET:HE2	6:F:347:ARG:HB2	1.73	0.71
4:D:12:PHE:CZ	4:D:169:LEU:HD11	2.25	0.71
5:E:106:CYS:SG	9:E:301:HEC:C2C	2.79	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:ILE:CG2	5:E:174:ARG:HD2	2.20	0.70
3:C:311:MET:HE3	3:C:367:LEU:HD11	1.72	0.70
1:A:101:LEU:HD21	9:A:305:HEC:HMA1	1.73	0.70
5:E:149:VAL:HG11	9:E:301:HEC:O2D	1.91	0.70
2:B:421:ILE:HD13	2:B:507:MET:CE	2.19	0.69
2:B:322:ALA:HB1	2:B:344:LEU:HD21	1.74	0.69
3:C:103:LEU:HD12	3:C:107:ILE:CB	2.23	0.68
6:F:329:THR:HA	6:F:335:THR:CG2	2.23	0.68
1:A:94:ILE:HD11	5:E:123:ILE:HD11	1.75	0.68
2:B:797:CYS:N	10:B:1101:SF4:S2	2.66	0.68
6:F:92:ILE:HG21	6:F:384:LEU:CD1	2.24	0.68
4:D:12:PHE:CE1	4:D:169:LEU:CD1	2.77	0.68
2:B:405:LEU:HD21	2:B:435:LEU:CD1	2.25	0.67
6:F:362:HIS:CD2	6:F:365:ASP:OD2	2.47	0.67
1:A:18:PHE:CE1	7:G:36:MET:HE1	2.30	0.67
1:A:94:ILE:CD1	5:E:123:ILE:HG13	2.25	0.67
1:A:133:HIS:HE1	9:A:302:HEC:NA	1.83	0.67
4:D:36:PHE:HB2	4:D:147:PHE:HB2	1.75	0.67
2:B:405:LEU:CD2	2:B:435:LEU:CD1	2.72	0.66
3:C:245:VAL:HG13	3:C:246:HIS:CD2	2.31	0.66
5:E:149:VAL:CG1	9:E:301:HEC:O1D	2.44	0.66
6:F:233:MET:HE1	6:F:347:ARG:HB2	1.77	0.66
3:C:311:MET:HE3	3:C:367:LEU:CD1	2.25	0.66
5:E:123:ILE:HG22	9:E:301:HEC:HMD2	1.78	0.66
6:F:327:ARG:HG2	15:F:502:JM9:C37	2.25	0.65
9:A:302:HEC:O2A	9:A:302:HEC:O1D	2.15	0.65
3:C:103:LEU:HD23	3:C:279:PHE:HE2	1.62	0.65
3:C:233:LEU:HD21	4:D:59:VAL:HG11	1.80	0.64
6:F:133:PHE:O	6:F:133:PHE:CD2	2.50	0.64
2:B:322:ALA:CB	2:B:344:LEU:HD21	2.27	0.64
1:A:165:LEU:HD22	1:A:212:THR:HG22	1.79	0.64
4:D:12:PHE:HZ	4:D:169:LEU:HD11	1.61	0.64
1:A:18:PHE:CG	7:G:36:MET:HE1	2.32	0.63
2:B:421:ILE:CD1	2:B:507:MET:CE	2.76	0.63
2:B:176:LEU:HD11	2:B:507:MET:HG2	1.81	0.63
3:C:250:SER:OG	3:C:266:PHE:HB3	1.98	0.63
5:E:72:THR:HG23	5:E:74:LEU:H	1.63	0.63
2:B:192:ARG:HG3	2:B:417:VAL:HG22	1.81	0.62
2:B:862:CYS:CB	11:B:1104:F3S:S1	2.87	0.62
2:B:888:CYS:CB	11:B:1104:F3S:S1	2.86	0.62
2:B:199:THR:HB	2:B:478:ARG:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:VAL:HG11	2:B:302:GLY:HA2	1.83	0.61
2:B:124:PRO:HG3	2:B:490:LEU:HB2	1.81	0.61
3:C:277:ALA:HB2	3:C:390:MET:HG3	1.82	0.61
5:E:87:VAL:HG11	7:G:108:LEU:HD23	1.82	0.61
2:B:180:LEU:HB3	2:B:184:ARG:HH21	1.66	0.61
6:F:185:THR:HG22	6:F:188:ARG:HH21	1.65	0.61
7:G:94:ILE:HG23	7:G:98:ARG:HH11	1.65	0.61
3:C:86:MET:O	3:C:90:ASN:ND2	2.33	0.60
3:C:263:VAL:CG1	3:C:265:VAL:HG12	2.32	0.60
1:A:71:THR:HG21	5:E:168:ARG:HG2	1.83	0.60
4:D:18:LEU:HD22	4:D:146:PHE:HB3	1.84	0.60
1:A:144:HIS:CE1	9:A:303:HEC:ND	2.70	0.60
3:C:119:ILE:HG12	3:C:286:MET:HE1	1.84	0.60
6:F:272:VAL:CG1	15:F:502:JM9:C31	2.79	0.60
3:C:163:GLN:HE21	4:D:86:VAL:CG2	2.13	0.60
7:G:94:ILE:HG23	7:G:98:ARG:NH1	2.17	0.60
3:C:110:LEU:HD11	3:C:236:GLY:HA2	1.84	0.59
2:B:773:LEU:HG	6:F:294:THR:HG23	1.82	0.59
6:F:272:VAL:HG11	15:F:502:JM9:C31	2.32	0.59
2:B:623:ASN:HD22	2:B:626:ARG:HG3	1.67	0.59
2:B:877:MET:HB2	2:B:930:LYS:HE3	1.85	0.59
2:B:609:MET:SD	2:B:676:ILE:HD12	2.43	0.59
3:C:282:VAL:HG13	3:C:286:MET:SD	2.42	0.59
3:C:163:GLN:NE2	4:D:86:VAL:HG21	2.13	0.59
5:E:149:VAL:HG11	9:E:301:HEC:O1D	2.01	0.59
5:E:129:HIS:HB3	5:E:134:ARG:HH21	1.68	0.59
6:F:92:ILE:HG21	6:F:384:LEU:HD11	1.85	0.59
1:A:101:LEU:CD2	9:A:305:HEC:HMA1	2.32	0.58
2:B:306:ASP:O	2:B:1018:ARG:NH2	2.36	0.58
2:B:774:GLN:NE2	6:F:286:TRP:O	2.37	0.58
7:G:69:THR:HG23	7:G:71:ARG:H	1.67	0.58
2:B:888:CYS:SG	11:B:1104:F3S:S1	3.01	0.58
6:F:356:LEU:O	6:F:360:ARG:HB2	2.04	0.58
3:C:245:VAL:HG13	3:C:246:HIS:HD2	1.68	0.58
1:A:161:MET:HG3	9:A:301:HEC:C1D	2.34	0.57
2:B:421:ILE:HA	2:B:448:ILE:HB	1.86	0.57
2:B:662:GLU:OE2	2:B:718:THR:HG21	2.04	0.57
1:A:81:ILE:HG22	2:B:86:PRO:HB3	1.86	0.57
2:B:733:LEU:HD12	2:B:733:LEU:O	2.04	0.57
5:E:149:VAL:CG1	9:E:301:HEC:O2D	2.52	0.57
1:A:134:VAL:HB	1:A:180:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HD13	2:B:591:LEU:HD22	1.85	0.57
2:B:408:LEU:HG	2:B:412:MET:HE2	1.86	0.57
2:B:888:CYS:SG	11:B:1104:F3S:S4	3.01	0.57
2:B:142:LEU:HD13	2:B:591:LEU:CD2	2.35	0.57
5:E:105:VAL:CG2	5:E:117:VAL:HG21	2.35	0.57
3:C:76:TRP:CD1	3:C:420:ASP:OD1	2.58	0.57
3:C:175:ILE:HD11	3:C:249:ILE:HD11	1.86	0.57
2:B:826:TRP:NE1	2:B:929:GLU:OE1	2.38	0.56
1:A:67:ARG:CZ	1:A:181:VAL:HG21	2.35	0.56
3:C:87:ASP:OD1	3:C:87:ASP:N	2.38	0.56
3:C:97:ILE:HG12	3:C:281:MET:HG3	1.86	0.56
5:E:105:VAL:O	5:E:106:CYS:SG	2.62	0.56
2:B:133:HIS:ND1	2:B:134:PRO:O	2.39	0.56
3:C:103:LEU:HA	3:C:107:ILE:HD12	1.88	0.56
2:B:822:ARG:NH2	3:C:76:TRP:O	2.39	0.55
8:I:17:ALA:O	8:I:21:THR:OG1	2.23	0.55
5:E:27:HIS:HD2	5:E:29:ASP:CG	2.15	0.55
5:E:27:HIS:HD2	5:E:29:ASP:OD2	1.89	0.55
5:E:149:VAL:CG1	9:E:301:HEC:CGD	2.82	0.55
3:C:103:LEU:HD23	3:C:279:PHE:CE2	2.40	0.55
2:B:260:ASP:HB2	2:B:263:ALA:HB3	1.88	0.55
3:C:251:LEU:HA	3:C:254:ALA:HB3	1.87	0.55
1:A:77:TYR:HH	5:E:38:THR:HG1	1.52	0.55
4:D:12:PHE:CZ	4:D:169:LEU:CD1	2.90	0.55
2:B:312:ARG:NH2	2:B:314:ASP:OD2	2.39	0.55
3:C:196:THR:HG22	4:D:142:SER:HB2	1.88	0.55
6:F:92:ILE:HG21	6:F:384:LEU:HD13	1.88	0.55
2:B:276:ALA:HA	2:B:279:ARG:HB2	1.88	0.55
6:F:362:HIS:HB2	6:F:365:ASP:CG	2.32	0.55
2:B:608:LEU:HB2	2:B:677:THR:HB	1.88	0.54
4:D:12:PHE:HE1	4:D:169:LEU:CD1	2.17	0.54
2:B:739:TYR:HD2	2:B:846:MET:HE2	1.73	0.54
1:A:6:PRO:HD2	1:A:9:ALA:HB2	1.88	0.54
1:A:29:LEU:HD23	8:I:32:LEU:HD22	1.88	0.54
3:C:242:VAL:HA	3:C:245:VAL:CG1	2.35	0.54
1:A:161:MET:HG3	9:A:301:HEC:ND	2.22	0.54
2:B:427:PRO:HD2	2:B:457:THR:HG21	1.90	0.54
4:D:26:LYS:HA	4:D:30:TYR:H	1.73	0.54
2:B:322:ALA:HB1	2:B:344:LEU:CD2	2.38	0.54
5:E:149:VAL:HG13	9:E:301:HEC:O1D	2.07	0.54
3:C:37:LEU:O	3:C:37:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:HG21	2:B:845:MET:HG2	1.91	0.53
2:B:609:MET:CE	2:B:676:ILE:HD12	2.38	0.53
2:B:779:TYR:HA	2:B:782:ARG:HD2	1.91	0.53
3:C:265:VAL:HA	6:F:221:ILE:HD13	1.91	0.53
3:C:36:PRO:C	3:C:37:LEU:HG	2.34	0.53
3:C:339:TYR:HE2	3:C:404:ARG:HD3	1.74	0.53
2:B:730:HIS:NE2	2:B:734:GLU:OE1	2.40	0.53
3:C:37:LEU:HD12	3:C:37:LEU:C	2.34	0.53
4:D:169:LEU:HD12	4:D:169:LEU:C	2.33	0.53
5:E:79:GLU:HB3	5:E:137:PRO:HG2	1.90	0.53
6:F:401:ASN:ND2	6:F:404:GLN:OE1	2.42	0.52
2:B:88:ASP:OD1	2:B:88:ASP:N	2.30	0.52
2:B:826:TRP:HE1	2:B:929:GLU:HB3	1.73	0.52
3:C:111:LEU:HD23	14:F:501:JL3:C12	2.40	0.52
3:C:105:SER:O	3:C:116:ARG:NH2	2.43	0.52
4:D:125:LEU:O	4:D:127:SER:N	2.43	0.52
3:C:449:GLU:HA	3:C:452:LEU:HB3	1.92	0.52
2:B:682:TYR:HB3	2:B:695:GLY:HA3	1.91	0.52
2:B:738:ILE:HG22	2:B:846:MET:HE1	1.92	0.52
1:A:32:GLY:HA3	8:I:32:LEU:HD21	1.92	0.52
2:B:405:LEU:CD2	2:B:435:LEU:HD11	2.40	0.52
6:F:229:ASN:ND2	6:F:351:MET:SD	2.83	0.52
4:D:45:ILE:HA	4:D:49:ALA:HB3	1.92	0.52
4:D:132:VAL:HA	4:D:177:VAL:HG21	1.91	0.52
3:C:190:LEU:HD21	3:C:442:LEU:HD13	1.92	0.51
6:F:80:ARG:HD2	6:F:396:PRO:HG2	1.92	0.51
6:F:233:MET:HE2	6:F:347:ARG:HB3	1.91	0.51
6:F:179:ASP:OD2	6:F:398:ARG:NH1	2.33	0.51
2:B:352:GLU:HG3	2:B:355:ARG:HE	1.75	0.51
4:D:31:THR:O	4:D:154:ASP:OD1	2.27	0.51
5:E:178:ALA:HA	5:E:181:ILE:HD12	1.92	0.51
3:C:215:LEU:HB3	4:D:126:PRO:HA	1.93	0.51
2:B:475:GLY:HA2	2:B:519:VAL:HG11	1.93	0.51
3:C:186:TRP:O	3:C:190:LEU:HB2	2.10	0.51
2:B:173:THR:HG21	2:B:511:PRO:HB3	1.93	0.51
5:E:94:ARG:NE	5:E:173:ASP:OD2	2.40	0.51
2:B:851:MET:HA	2:B:1011:THR:HB	1.92	0.51
3:C:111:LEU:HG	14:F:501:JL3:C11	2.40	0.51
6:F:32:LEU:HD21	6:F:373:ALA:HB2	1.93	0.50
6:F:136:ILE:O	6:F:140:LYS:NZ	2.41	0.50
1:A:116:TRP:CE3	9:A:304:HEC:HBD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:SER:OG	2:B:453:PHE:O	2.22	0.50
6:F:254:TYR:HB2	6:F:395:LEU:HD21	1.92	0.50
6:F:240:LEU:O	6:F:243:SER:OG	2.29	0.50
2:B:631:GLU:HA	2:B:634:ASP:HB2	1.94	0.50
5:E:150:TYR:O	5:E:151:ARG:HG3	2.11	0.50
3:C:222:ARG:NH1	4:D:33:MET:O	2.45	0.50
1:A:211:LEU:HD21	9:A:302:HEC:O1D	2.12	0.50
1:A:58:HIS:O	1:A:63:GLY:N	2.39	0.50
2:B:142:LEU:HD12	2:B:143:PHE:N	2.26	0.49
6:F:58:PRO:HB2	6:F:90:LEU:HD22	1.94	0.49
2:B:210:PHE:CZ	2:B:507:MET:HE2	2.46	0.49
3:C:195:ALA:HB2	3:C:217:TRP:HB3	1.94	0.49
3:C:242:VAL:CA	3:C:245:VAL:HG12	2.40	0.49
2:B:322:ALA:CB	2:B:344:LEU:CD2	2.91	0.49
2:B:778:ASP:OD2	2:B:780:THR:OG1	2.31	0.49
5:E:182:ARG:HG2	7:G:108:LEU:HD11	1.93	0.49
1:A:60:ASN:O	7:G:69:THR:OG1	2.31	0.49
2:B:158:THR:HA	2:B:495:TYR:HB3	1.94	0.49
2:B:380:GLU:HG2	2:B:381:LEU:HD23	1.95	0.49
1:A:66:CYS:SG	9:A:304:HEC:CAB	2.84	0.49
3:C:268:PRO:HG2	6:F:221:ILE:HD11	1.94	0.49
5:E:109:GLU:OE1	7:G:78:ARG:NH1	2.46	0.49
2:B:858:CYS:HB3	2:B:892:CYS:HB2	1.95	0.49
2:B:937:ARG:NH1	2:B:970:GLN:OE1	2.41	0.49
1:A:161:MET:O	1:A:165:LEU:HB2	2.13	0.48
2:B:642:GLU:O	2:B:645:SER:OG	2.30	0.48
6:F:137:ILE:HG12	6:F:215:PRO:HB2	1.94	0.48
7:G:82:ASN:HA	7:G:95:PRO:HB3	1.95	0.48
2:B:578:PRO:HB2	2:B:597:PRO:HD2	1.95	0.48
2:B:625:ASP:HA	2:B:628:ILE:HG12	1.96	0.48
2:B:938:ILE:HA	2:B:964:ILE:HD13	1.95	0.48
4:D:56:PRO:HA	4:D:59:VAL:HG12	1.95	0.48
4:D:79:LEU:HD22	4:D:91:LEU:HA	1.94	0.48
2:B:304:ALA:HB2	2:B:795:ILE:HG22	1.96	0.48
2:B:744:PHE:O	2:B:748:LYS:HB2	2.14	0.48
2:B:779:TYR:O	2:B:983:ASN:ND2	2.45	0.48
3:C:25:TYR:HB3	3:C:451:ARG:HD3	1.94	0.48
5:E:107:HIS:CE1	9:E:301:HEC:NA	2.82	0.48
5:E:182:ARG:HA	5:E:182:ARG:HD3	1.72	0.48
3:C:160:MET:HB3	3:C:160:MET:HE3	1.74	0.48
3:C:198:ARG:HD3	3:C:211:GLY:HA2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:162:MET:HE1	9:E:301:HEC:C1A	2.44	0.48
1:A:66:CYS:CB	9:A:304:HEC:C3B	2.80	0.48
6:F:272:VAL:HG13	15:F:502:JM9:C31	2.43	0.48
6:F:180:ALA:HA	6:F:400:PRO:HB3	1.95	0.47
2:B:587:ASN:ND2	2:B:690:VAL:O	2.46	0.47
6:F:300:ARG:NH2	6:F:354:ILE:O	2.43	0.47
4:D:135:VAL:HG12	4:D:137:ARG:H	1.80	0.47
6:F:247:ASP:O	6:F:247:ASP:OD1	2.33	0.47
2:B:142:LEU:HD12	2:B:142:LEU:C	2.39	0.47
2:B:429:TYR:OH	2:B:682:TYR:O	2.29	0.47
2:B:633:ASP:N	2:B:633:ASP:OD1	2.47	0.47
3:C:217:TRP:HE3	4:D:125:LEU:HD21	1.80	0.47
4:D:33:MET:HE2	4:D:48:ILE:HG21	1.95	0.47
6:F:223:GLY:O	6:F:227:MET:N	2.42	0.47
2:B:327:LEU:HD13	2:B:381:LEU:HD21	1.96	0.47
3:C:365:GLN:HA	3:C:368:TRP:HD1	1.80	0.47
3:C:441:VAL:HG13	3:C:442:LEU:HG	1.96	0.47
6:F:65:LEU:HB2	6:F:83:LEU:HB3	1.97	0.47
2:B:369:ILE:HG21	2:B:563:ILE:HA	1.97	0.47
3:C:210:TYR:OH	3:C:441:VAL:O	2.32	0.47
1:A:44:ASN:HB3	7:G:60:PRO:HD3	1.97	0.46
5:E:138:LEU:HA	5:E:141:PHE:HD2	1.80	0.46
7:G:87:THR:OG1	7:G:88:MET:N	2.46	0.46
1:A:68:TYR:HD1	5:E:102:TYR:HA	1.79	0.46
1:A:176:ARG:O	1:A:178:ARG:N	2.46	0.46
1:A:69:CYS:HB3	1:A:82:PRO:HG3	1.97	0.46
7:G:89:GLU:OE2	7:G:89:GLU:N	2.47	0.46
2:B:283:LYS:HG3	2:B:751:PRO:HG3	1.97	0.46
1:A:62:VAL:HG13	5:E:117:VAL:HG22	1.98	0.46
4:D:94:THR:HG22	4:D:94:THR:O	2.16	0.46
1:A:91:HIS:NE2	9:A:305:HEC:O1A	2.49	0.46
3:C:320:TYR:O	3:C:324:MET:HG2	2.16	0.46
3:C:448:PHE:CE1	3:C:449:GLU:HG2	2.50	0.46
6:F:320:PRO:HB3	6:F:343:ILE:HD11	1.97	0.46
6:F:327:ARG:HH21	6:F:331:ARG:HE	1.63	0.46
2:B:615:ILE:HD11	2:B:622:PHE:HB2	1.97	0.46
2:B:870:ASP:OD1	2:B:870:ASP:N	2.49	0.46
3:C:101:GLY:HA2	3:C:123:ALA:HB1	1.98	0.46
4:D:25:ALA:HA	4:D:165:PHE:HZ	1.81	0.46
6:F:224:ALA:HA	6:F:227:MET:HB2	1.98	0.46
4:D:26:LYS:HE2	4:D:48:ILE:CG2	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HA	3:C:171:ASP:HB2	1.98	0.46
4:D:10:ALA:HA	4:D:174:VAL:HG12	1.98	0.46
1:A:138:ILE:HG21	9:A:302:HEC:HBC2	1.98	0.45
3:C:225:HIS:O	3:C:229:MET:HB3	2.16	0.45
3:C:107:ILE:HG12	3:C:239:THR:HG23	1.98	0.45
4:D:53:THR:HA	8:I:1:MET:HE2	1.97	0.45
3:C:307:MET:HE2	3:C:307:MET:HB3	1.72	0.45
2:B:691:GLY:HA2	2:B:694:VAL:HB	1.98	0.45
1:A:218:HIS:CD2	9:A:301:HEC:NC	2.79	0.45
2:B:110:GLY:O	2:B:199:THR:OG1	2.34	0.45
2:B:191:VAL:HG13	2:B:217:ALA:HB2	1.98	0.45
3:C:103:LEU:CD1	3:C:107:ILE:CD1	2.95	0.45
1:A:200:VAL:HA	1:A:205:ILE:HD12	1.99	0.45
3:C:95:ILE:HG21	3:C:249:ILE:HG13	1.99	0.45
3:C:163:GLN:NE2	4:D:86:VAL:CG2	2.77	0.45
3:C:248:ILE:HA	3:C:251:LEU:HB2	1.98	0.45
6:F:108:TYR:C	6:F:110:ALA:H	2.24	0.45
6:F:277:MET:HE2	6:F:277:MET:HB2	1.81	0.45
6:F:399:ASP:HB3	6:F:402:MET:HG2	1.98	0.45
3:C:250:SER:HG	3:C:266:PHE:HB3	1.81	0.45
4:D:64:LEU:HD21	6:F:322:PHE:HE1	1.81	0.45
2:B:921:THR:O	2:B:923:ARG:NH1	2.50	0.44
3:C:111:LEU:CD2	14:F:501:JL3:C12	2.95	0.44
6:F:55:MET:HE1	6:F:157:PHE:HE1	1.82	0.44
7:G:91:LYS:HG3	7:G:92:VAL:HG12	2.00	0.44
3:C:110:LEU:HA	3:C:110:LEU:HD23	1.83	0.44
4:D:43:GLU:HA	4:D:46:GLU:HB3	2.00	0.44
5:E:123:ILE:CG2	9:E:301:HEC:HMD2	2.47	0.44
2:B:142:LEU:HD11	2:B:143:PHE:CE1	2.52	0.44
2:B:199:THR:HG22	2:B:395:GLU:HA	1.99	0.44
7:G:66:THR:OG1	7:G:67:GLY:N	2.45	0.44
2:B:229:ASN:ND2	2:B:366:GLN:O	2.50	0.44
2:B:282:ARG:HB2	2:B:284:ASP:OD1	2.18	0.44
1:A:58:HIS:HE1	9:A:305:HEC:NA	1.99	0.44
3:C:448:PHE:C	3:C:450:MET:H	2.25	0.44
4:D:12:PHE:CE1	4:D:169:LEU:HD13	2.50	0.44
1:A:98:SER:H	1:A:105:ARG:HH12	1.65	0.44
2:B:307:HIS:CE1	2:B:1021:SER:H	2.35	0.44
3:C:247:SER:HB3	3:C:267:PRO:HB3	2.00	0.44
1:A:25:VAL:HG13	8:I:29:MET:HE2	2.00	0.44
1:A:72:SER:HB2	2:B:96:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:MET:HG2	2:B:1019:ASN:HB2	2.00	0.44
2:B:894:TYR:HE2	2:B:1001:LEU:HB3	1.83	0.44
6:F:221:ILE:HG21	6:F:281:GLN:HB2	1.99	0.44
1:A:211:LEU:HD11	9:A:302:HEC:HBD2	2.00	0.44
3:C:103:LEU:HD12	3:C:107:ILE:CD1	2.48	0.43
3:C:144:ARG:NH1	5:E:29:ASP:OD2	2.50	0.43
1:A:18:PHE:CE1	7:G:36:MET:CE	3.01	0.43
2:B:105:THR:HB	2:B:487:VAL:HG22	2.00	0.43
2:B:126:LYS:HE3	2:B:807:GLU:HB2	1.99	0.43
2:B:405:LEU:HD23	2:B:435:LEU:HD11	1.99	0.43
2:B:826:TRP:CE3	2:B:931:CYS:HA	2.52	0.43
3:C:199:ASP:OD2	4:D:142:SER:OG	2.36	0.43
3:C:284:LEU:HD11	3:C:384:LEU:HA	2.00	0.43
3:C:332:SER:HB2	6:F:218:PHE:CE2	2.53	0.43
2:B:589:GLY:HA2	2:B:690:VAL:HG11	2.01	0.43
3:C:197:LEU:HD11	3:C:443:PRO:HD3	2.00	0.43
6:F:62:LEU:HD13	6:F:164:ALA:HB2	2.00	0.43
15:F:502:JM9:O20	15:F:502:JM9:C15	2.65	0.43
1:A:148:ASN:ND2	1:A:183:ASN:OD1	2.52	0.43
3:C:254:ALA:HB1	6:F:284:ILE:HG12	2.01	0.43
3:C:282:VAL:HG12	3:C:307:MET:HE1	2.00	0.43
4:D:8:VAL:HG22	4:D:176:GLU:HG3	2.00	0.43
2:B:365:GLN:H	2:B:365:GLN:HG2	1.48	0.43
3:C:102:THR:HG21	3:C:178:TYR:HE1	1.83	0.43
3:C:282:VAL:CG1	3:C:286:MET:SD	3.07	0.43
6:F:133:PHE:O	6:F:133:PHE:CG	2.69	0.43
2:B:433:GLY:HA3	2:B:700:PRO:HA	1.99	0.43
2:B:420:LEU:HG	2:B:422:MET:HE2	2.01	0.43
3:C:229:MET:HE2	3:C:229:MET:HB2	1.77	0.43
1:A:94:ILE:HG23	5:E:121:GLY:HA3	2.00	0.43
6:F:58:PRO:HG3	6:F:93:MET:HG3	2.00	0.43
6:F:240:LEU:HD11	6:F:341:GLY:HA2	2.01	0.43
6:F:272:VAL:HA	6:F:275:THR:HG22	2.00	0.43
1:A:3:GLN:HG3	1:A:4:ILE:HD13	2.01	0.43
1:A:195:ILE:HD12	1:A:195:ILE:HA	1.95	0.42
2:B:955:SER:O	2:B:955:SER:OG	2.34	0.42
3:C:24:THR:HG23	3:C:27:SER:H	1.84	0.42
3:C:58:LEU:HD12	3:C:430:LEU:HA	2.01	0.42
2:B:450:LEU:HD13	2:B:503:LEU:HD22	2.01	0.42
3:C:224:TRP:CE3	4:D:40:PRO:HG3	2.53	0.42
4:D:60:LEU:HB2	15:F:502:JM9:C44	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:304:HEC:HBC1	9:A:305:HEC:HMC2	2.01	0.42
2:B:651:ILE:HG22	2:B:662:GLU:OE2	2.15	0.42
2:B:910:GLU:H	2:B:910:GLU:CD	2.27	0.42
3:C:103:LEU:HD13	3:C:107:ILE:HD13	2.02	0.42
9:A:303:HEC:HHA	9:A:303:HEC:HAA1	1.57	0.42
3:C:376:ILE:HD13	3:C:376:ILE:HA	1.82	0.42
6:F:28:GLY:HA3	6:F:376:GLY:HA3	2.02	0.42
8:I:23:MET:SD	8:I:23:MET:N	2.92	0.42
2:B:421:ILE:HG12	2:B:507:MET:SD	2.59	0.42
3:C:124:GLU:HB3	3:C:186:TRP:HD1	1.84	0.42
8:I:28:LEU:HD23	8:I:28:LEU:HA	1.87	0.42
2:B:450:LEU:HG	2:B:467:GLN:HB2	2.02	0.42
2:B:787:MET:HE2	2:B:979:PHE:HB2	2.01	0.42
3:C:238:SER:HA	3:C:241:LEU:HB3	2.01	0.42
6:F:378:ILE:HD13	6:F:378:ILE:HA	1.81	0.42
1:A:132:ILE:HB	2:B:943:ILE:HG23	2.02	0.42
3:C:233:LEU:HD11	4:D:59:VAL:HG11	2.02	0.42
3:C:308:ALA:HB2	3:C:379:LEU:HD11	2.00	0.42
4:D:22:THR:HG21	4:D:44:VAL:HG12	2.01	0.42
6:F:59:LEU:HD13	6:F:202:VAL:HG23	2.01	0.42
7:G:33:SER:O	7:G:37:ILE:HG12	2.20	0.42
3:C:163:GLN:NE2	4:D:86:VAL:CB	2.83	0.41
1:A:77:TYR:HA	1:A:130:HIS:H	1.85	0.41
3:C:243:VAL:O	3:C:247:SER:OG	2.25	0.41
4:D:36:PHE:HE2	4:D:149:CYS:HB3	1.85	0.41
6:F:219:SER:HB3	6:F:222:TYR:HB2	2.02	0.41
1:A:95:LYS:HG3	9:A:305:HEC:O2A	2.20	0.41
2:B:312:ARG:HE	2:B:312:ARG:HB3	1.61	0.41
3:C:163:GLN:NE2	4:D:86:VAL:HB	2.36	0.41
1:A:46:ALA:HB1	1:A:152:VAL:HB	2.02	0.41
2:B:106:LEU:HD12	2:B:115:VAL:HG11	2.02	0.41
2:B:258:ASP:OD2	2:B:366:GLN:NE2	2.48	0.41
2:B:405:LEU:HG	2:B:435:LEU:HD13	2.02	0.41
2:B:867:THR:OG1	2:B:875:ASN:OD1	2.37	0.41
7:G:81:LEU:HD23	7:G:81:LEU:HA	1.90	0.41
2:B:260:ASP:OD1	2:B:260:ASP:N	2.53	0.41
2:B:877:MET:SD	2:B:897:ARG:NH2	2.94	0.41
6:F:62:LEU:O	6:F:66:MET:HG3	2.20	0.41
2:B:279:ARG:HD3	2:B:279:ARG:HA	1.85	0.41
2:B:316:ILE:HD13	2:B:316:ILE:HA	1.86	0.41
4:D:38:PRO:HD3	4:D:145:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:138:LEU:HD22	5:E:182:ARG:HH21	1.86	0.41
1:A:168:HIS:CD2	9:A:302:HEC:NC	2.86	0.41
2:B:885:THR:HG23	11:B:1104:F3S:S2	2.60	0.41
6:F:59:LEU:HD23	6:F:59:LEU:HA	1.82	0.41
6:F:211:MET:HE2	6:F:211:MET:HB3	1.75	0.41
1:A:96:THR:OG1	1:A:97:TYR:N	2.54	0.41
2:B:146:ALA:O	2:B:588:ASN:ND2	2.49	0.41
5:E:98:LYS:HD3	5:E:98:LYS:HA	1.93	0.41
6:F:70:LEU:HD23	6:F:70:LEU:HA	1.95	0.41
1:A:126:VAL:HG13	9:A:301:HEC:HHD	2.02	0.41
1:A:211:LEU:HD21	9:A:302:HEC:HBD2	2.03	0.41
9:A:301:HEC:HAA2	3:C:158:HIS:NE2	2.36	0.41
2:B:369:ILE:HD12	2:B:372:ALA:HB3	2.03	0.41
2:B:777:ASP:OD2	2:B:782:ARG:NH1	2.54	0.41
5:E:186:LEU:HD22	7:G:103:ILE:HD13	2.02	0.41
1:A:64:ILE:HG12	9:A:305:HEC:HBC2	2.03	0.41
2:B:291:LEU:HB3	2:B:305:ALA:HA	2.02	0.41
2:B:468:ALA:HB3	2:B:499:THR:HG22	2.03	0.41
1:A:57:LEU:CD2	9:A:305:HEC:HHA	2.50	0.40
1:A:129:ASN:HB3	1:A:132:ILE:HG22	2.02	0.40
3:C:99:HIS:HB2	3:C:246:HIS:CE1	2.55	0.40
1:A:131:SER:HB3	2:B:947:ARG:HH21	1.86	0.40
2:B:186:THR:OG1	2:B:187:GLN:N	2.54	0.40
2:B:452:GLN:HB2	2:B:467:GLN:HB3	2.03	0.40
2:B:595:PRO:HA	2:B:602:VAL:HG12	2.03	0.40
2:B:635:ARG:HD2	2:B:635:ARG:HA	1.92	0.40
3:C:301:LEU:HD23	3:C:301:LEU:HA	1.91	0.40
3:C:381:ILE:O	3:C:385:ILE:HD12	2.21	0.40
2:B:205:ALA:O	2:B:209:GLN:HG3	2.21	0.40
2:B:728:GLN:OE1	2:B:831:ARG:NH2	2.54	0.40
2:B:760:GLN:HE22	2:B:766:GLU:HG2	1.86	0.40
5:E:34:GLN:H	5:E:34:GLN:HG3	1.47	0.40
1:A:72:SER:OG	1:A:76:SER:OG	2.26	0.40
2:B:885:THR:OG1	11:B:1104:F3S:S1	2.79	0.40
3:C:84:TRP:CG	3:C:88:ILE:HG13	2.55	0.40
1:A:41:ARG:HE	1:A:41:ARG:HB3	1.71	0.40
2:B:372:ALA:HB1	2:B:558:ILE:HG12	2.04	0.40
2:B:600:LYS:HA	2:B:600:LYS:HD3	1.84	0.40
2:B:1001:LEU:HD23	2:B:1001:LEU:HA	1.86	0.40
3:C:80:ILE:HD12	3:C:80:ILE:HA	1.78	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	216/219 (99%)	202 (94%)	14 (6%)	0	100	100
2	B	949/1029 (92%)	888 (94%)	61 (6%)	0	100	100
3	C	447/486 (92%)	425 (95%)	22 (5%)	0	100	100
4	D	173/179 (97%)	158 (91%)	15 (9%)	0	100	100
5	E	162/205 (79%)	149 (92%)	13 (8%)	0	100	100
6	F	395/411 (96%)	370 (94%)	25 (6%)	0	100	100
7	G	78/112 (70%)	72 (92%)	6 (8%)	0	100	100
8	I	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	2455/2678 (92%)	2297 (94%)	158 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	198/199 (100%)	189 (96%)	9 (4%)	24	58
2	B	768/830 (92%)	749 (98%)	19 (2%)	42	74
3	C	382/405 (94%)	371 (97%)	11 (3%)	37	71
4	D	143/147 (97%)	135 (94%)	8 (6%)	19	50
5	E	136/171 (80%)	132 (97%)	4 (3%)	37	71
6	F	318/330 (96%)	308 (97%)	10 (3%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	69/95 (73%)	66 (96%)	3 (4%)	26 60
8	I	32/32 (100%)	32 (100%)	0	100 100
All	All	2046/2209 (93%)	1982 (97%)	64 (3%)	36 69

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	51	VAL
1	A	64	ILE
1	A	86	THR
1	A	97	TYR
1	A	130	HIS
1	A	140	CYS
1	A	172	GLU
1	A	193	LEU
2	B	84	ILE
2	B	88	ASP
2	B	116	LEU
2	B	159	THR
2	B	257	LEU
2	B	287	THR
2	B	294	VAL
2	B	365	GLN
2	B	399	THR
2	B	428	VAL
2	B	573	VAL
2	B	615	ILE
2	B	647	VAL
2	B	694	VAL
2	B	752	LYS
2	B	788	THR
2	B	869	HIS
2	B	931	CYS
2	B	1014	LEU
3	C	127	THR
3	C	131	VAL
3	C	185	PHE
3	C	212	ILE
3	C	233	LEU
3	C	234	LEU

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Mol	Chain	Res	Type
3	C	296	GLU
3	C	313	THR
3	C	382	ILE
3	C	384	LEU
3	C	444	MET
4	D	14	THR
4	D	42	GLU
4	D	89	ARG
4	D	110	LEU
4	D	121	VAL
4	D	125	LEU
4	D	143	GLN
4	D	162	THR
5	E	37	THR
5	E	72	THR
5	E	92	LEU
5	E	116	MET
6	F	107	THR
6	F	115	HIS
6	F	122	ASN
6	F	152	ARG
6	F	197	LEU
6	F	240	LEU
6	F	263	ILE
6	F	308	VAL
6	F	378	ILE
6	F	397	LEU
7	G	44	LEU
7	G	56	LEU
7	G	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	56	GLN
1	A	129	ASN
1	A	130	HIS
2	B	100	GLN
2	B	365	GLN
2	B	383	ASN
2	B	400	ASN

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Mol	Chain	Res	Type
2	B	587	ASN
2	B	623	ASN
2	B	760	GLN
2	B	817	GLN
3	C	90	ASN
3	C	113	GLN
3	C	163	GLN
4	D	78	ASN
4	D	143	GLN
5	E	27	HIS
5	E	34	GLN
5	E	160	GLN
6	F	13	GLN
6	F	18	GLN
6	F	122	ASN
6	F	174	GLN
6	F	229	ASN
6	F	332	ASN
6	F	362	HIS

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

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
15	JM9	F	502	-	53,53,53	1.25	8 (15%)	58,58,58	1.86	13 (22%)
9	HEC	A	305	1	46,50,50	1.97	10 (21%)	58,82,82	2.15	16 (27%)
9	HEC	A	302	1	46,50,50	2.04	11 (23%)	58,82,82	2.59	16 (27%)
10	SF4	B	1103	2	0,12,12	-	-	-		
9	HEC	A	304	1	46,50,50	1.99	10 (21%)	58,82,82	2.59	18 (31%)
9	HEC	A	301	1	46,50,50	2.04	9 (19%)	58,82,82	2.71	22 (37%)
10	SF4	B	1101	2	0,12,12	-	-	-		
10	SF4	B	1102	2	0,12,12	-	-	-		
11	F3S	B	1104	2	0,9,9	-	-	-		
13	JLQ	C	501	-	44,44,44	0.99	4 (9%)	47,49,49	1.22	5 (10%)
9	HEC	A	303	1	46,50,50	2.13	10 (21%)	58,82,82	2.59	22 (37%)
14	JL3	F	501	-	44,44,44	1.01	5 (11%)	47,49,49	0.91	3 (6%)
9	HEC	E	301	5	46,50,50	1.95	10 (21%)	58,82,82	2.31	17 (29%)

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
15	JM9	F	502	-	-	28/56/56/56	-
9	HEC	A	305	1	-	9/14/54/54	-
9	HEC	A	302	1	-	12/14/54/54	-
10	SF4	B	1103	2	-	-	0/6/5/5
9	HEC	A	304	1	-	5/14/54/54	-
9	HEC	A	301	1	-	10/14/54/54	-
10	SF4	B	1101	2	-	-	0/6/5/5
10	SF4	B	1102	2	-	-	0/6/5/5
13	JLQ	C	501	-	-	28/48/48/48	-
11	F3S	B	1104	2	-	-	0/3/3/3
9	HEC	A	303	1	-	4/14/54/54	-
14	JL3	F	501	-	-	28/48/48/48	-
9	HEC	E	301	5	-	9/14/54/54	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEC	CAC-C3C	7.18	1.58	1.35
9	A	304	HEC	CAB-C3B	6.94	1.57	1.35
9	A	304	HEC	CAC-C3C	6.49	1.56	1.35
9	A	305	HEC	CAC-C3C	6.44	1.55	1.35
9	A	301	HEC	CAB-C3B	6.29	1.55	1.35
9	A	302	HEC	CAB-C3B	6.20	1.55	1.35
9	E	301	HEC	CAC-C3C	6.20	1.55	1.35
9	E	301	HEC	CAB-C3B	6.15	1.55	1.35
9	A	302	HEC	CAC-C3C	6.02	1.54	1.35
9	A	305	HEC	CAB-C3B	5.98	1.54	1.35
9	A	303	HEC	CAB-C3B	5.88	1.54	1.35
9	A	301	HEC	C3D-C2D	5.82	1.54	1.38
9	A	301	HEC	CAC-C3C	5.75	1.53	1.35
9	A	302	HEC	C3D-C2D	5.55	1.53	1.38
9	E	301	HEC	C3D-C2D	5.19	1.52	1.38
9	A	305	HEC	C3D-C2D	5.05	1.52	1.38
9	A	301	HEC	C1C-NC	-3.91	1.32	1.39
9	A	303	HEC	C1A-C2A	-3.78	1.38	1.45
9	A	303	HEC	C3D-C2D	3.65	1.48	1.38
9	A	304	HEC	C3D-C2D	3.59	1.48	1.38
9	A	303	HEC	CHA-C4D	-3.59	1.31	1.39
9	A	302	HEC	C2A-C3A	3.53	1.44	1.36
15	F	502	JM9	O17-C18	-3.44	1.38	1.46
9	A	303	HEC	C3B-C2B	-3.20	1.30	1.41
15	F	502	JM9	O16-C15	3.12	1.31	1.22
9	A	303	HEC	O2D-CGD	-3.10	1.20	1.30
14	F	501	JL3	O29-C19	-2.96	1.39	1.46
9	A	303	HEC	C2A-C3A	-2.89	1.30	1.36
15	F	502	JM9	O20-C21	2.87	1.41	1.33
15	F	502	JM9	O20-C19	-2.86	1.38	1.45
15	F	502	JM9	C14-C15	2.85	1.59	1.50
9	A	304	HEC	C2A-C3A	2.80	1.42	1.36
9	A	304	HEC	CHA-C1A	-2.80	1.32	1.38
9	A	301	HEC	C3B-C2B	-2.79	1.31	1.41
9	A	304	HEC	C3B-C2B	-2.65	1.32	1.41
9	E	301	HEC	C3B-C2B	-2.64	1.32	1.41
9	A	305	HEC	CHA-C4D	-2.63	1.33	1.39
9	E	301	HEC	CMC-C2C	2.61	1.56	1.50
9	A	304	HEC	C3C-C2C	-2.58	1.32	1.41
9	A	302	HEC	C3B-C2B	-2.56	1.32	1.41
9	A	305	HEC	C3B-C2B	-2.56	1.32	1.41
9	E	301	HEC	CMD-C2D	2.51	1.55	1.50
9	A	303	HEC	CHA-C1A	-2.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	501	JL3	O17-C18	-2.45	1.39	1.45
13	C	501	JLQ	O18-C19	-2.43	1.39	1.45
13	C	501	JLQ	O30-C31	2.40	1.41	1.34
9	A	301	HEC	CHC-C4B	-2.40	1.33	1.38
9	A	305	HEC	CHD-C1D	-2.40	1.34	1.39
9	A	302	HEC	CMC-C2C	2.40	1.55	1.50
13	C	501	JLQ	O18-C16	2.36	1.40	1.33
9	A	301	HEC	C2A-C3A	2.36	1.41	1.36
15	F	502	JM9	O38-C37	-2.33	1.40	1.45
14	F	501	JL3	O17-C15	2.31	1.40	1.33
9	A	303	HEC	C3C-C2C	-2.29	1.33	1.41
9	A	305	HEC	C2A-C3A	-2.29	1.31	1.36
13	C	501	JLQ	O30-C20	-2.26	1.41	1.46
9	A	302	HEC	CHA-C4D	-2.24	1.34	1.39
9	A	304	HEC	CHC-C1C	-2.23	1.34	1.39
9	E	301	HEC	CHC-C1C	-2.22	1.34	1.39
9	E	301	HEC	CMA-C3A	2.19	1.55	1.50
9	A	302	HEC	CMB-C2B	2.18	1.55	1.50
9	E	301	HEC	CHC-C4B	-2.16	1.34	1.38
9	A	304	HEC	CHA-C4D	-2.13	1.34	1.39
9	A	305	HEC	O2A-CGA	-2.11	1.23	1.30
14	F	501	JL3	O29-C30	2.10	1.40	1.34
9	E	301	HEC	C3C-C2C	-2.08	1.34	1.41
9	A	301	HEC	C3C-C2C	-2.07	1.34	1.41
9	A	302	HEC	C3C-C2C	-2.07	1.34	1.41
15	F	502	JM9	C23-C21	2.06	1.56	1.50
14	F	501	JL3	P22-O23	-2.05	1.45	1.55
9	A	304	HEC	CMC-C2C	2.04	1.55	1.50
9	A	302	HEC	CAD-C3D	2.04	1.56	1.51
15	F	502	JM9	C19-C18	2.03	1.57	1.50
9	A	305	HEC	C3C-C2C	-2.03	1.34	1.41
9	A	301	HEC	C3B-C4B	-2.02	1.42	1.46
9	A	302	HEC	O1D-CGD	2.01	1.28	1.22
9	A	305	HEC	CMB-C2B	2.01	1.54	1.50

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	305	HEC	CBB-CAB-C3B	-8.55	110.35	127.43
9	E	301	HEC	CBB-CAB-C3B	-8.25	110.94	127.43
9	A	301	HEC	CBB-CAB-C3B	-8.09	111.26	127.43
9	A	302	HEC	CBB-CAB-C3B	-8.07	111.31	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	304	HEC	C2A-C1A-NA	7.48	117.54	110.32
9	A	304	HEC	CMD-C2D-C1D	7.43	136.73	125.42
9	A	303	HEC	CMD-C2D-C1D	7.38	136.66	125.42
9	A	303	HEC	CHA-C1A-NA	7.07	132.15	124.45
9	A	303	HEC	CBB-CAB-C3B	-6.65	114.14	127.43
9	A	304	HEC	CHA-C1A-C2A	-6.57	114.49	124.86
9	A	304	HEC	CBB-CAB-C3B	-6.39	114.66	127.43
9	A	301	HEC	CBC-CAC-C3C	-6.33	114.79	127.43
9	A	302	HEC	C2A-C1A-NA	6.26	116.36	110.32
9	A	303	HEC	CHA-C1A-C2A	-6.23	115.02	124.86
9	A	301	HEC	CAD-CBD-CGD	-6.12	97.44	113.67
9	A	304	HEC	C1A-C2A-C3A	-6.11	99.07	107.11
9	A	302	HEC	C1A-C2A-C3A	-6.09	99.09	107.11
9	A	302	HEC	CBC-CAC-C3C	-6.04	115.36	127.43
9	E	301	HEC	CAD-CBD-CGD	5.98	129.53	113.67
9	E	301	HEC	CBC-CAC-C3C	-5.92	115.60	127.43
9	A	302	HEC	CMC-C2C-C1C	-5.84	116.52	125.42
9	A	302	HEC	CHA-C1A-C2A	-5.31	116.48	124.86
15	F	502	JM9	C12-C13-C14	5.26	132.46	113.13
13	C	501	JLQ	O30-C31-C33	5.25	122.84	111.48
9	A	301	HEC	C1A-C2A-C3A	-5.14	100.34	107.11
9	A	303	HEC	C1D-C2D-C3D	-5.13	100.94	106.82
9	A	301	HEC	C2A-C1A-NA	5.08	115.22	110.32
15	F	502	JM9	C37-O38-C39	5.07	135.66	117.12
15	F	502	JM9	C18-O17-C15	-5.04	105.72	117.80
9	A	301	HEC	CHA-C1A-C2A	-4.95	117.04	124.86
15	F	502	JM9	C37-C18-C19	4.72	122.78	111.78
9	A	305	HEC	C3D-C4D-ND	4.68	115.35	110.15
9	A	302	HEC	C3D-C4D-ND	4.65	115.31	110.15
9	E	301	HEC	CMC-C2C-C1C	-4.65	118.35	125.42
9	A	301	HEC	CAA-C2A-C1A	4.51	134.03	124.85
9	A	301	HEC	C2C-C1C-NC	4.29	117.01	110.14
9	E	301	HEC	O2D-CGD-CBD	4.16	127.15	114.00
15	F	502	JM9	C13-C12-C11	-4.12	93.53	114.37
9	A	301	HEC	CHC-C1C-C2C	-4.09	115.56	127.43
9	A	304	HEC	CMD-C2D-C3D	-3.99	117.15	125.62
9	A	305	HEC	O2A-CGA-O1A	-3.89	113.32	123.33
9	A	301	HEC	CAD-C3D-C4D	3.82	132.39	124.94
9	A	305	HEC	CMC-C2C-C1C	-3.80	119.63	125.42
9	A	304	HEC	CAA-C2A-C1A	3.65	132.27	124.85
9	A	301	HEC	CBA-CAA-C2A	-3.52	102.79	112.53
9	A	305	HEC	CAA-CBA-CGA	3.50	122.96	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	305	HEC	CBC-CAC-C3C	-3.50	120.43	127.43
9	A	301	HEC	CHC-C4B-C3B	-3.50	119.31	125.21
9	A	303	HEC	CMC-C2C-C1C	-3.49	120.11	125.42
9	A	303	HEC	CBC-CAC-C3C	-3.49	120.46	127.43
9	A	304	HEC	CBC-CAC-C3C	-3.43	120.57	127.43
15	F	502	JM9	O20-C21-C23	3.40	122.21	111.83
9	E	301	HEC	C1D-C2D-C3D	-3.35	102.98	106.82
9	A	305	HEC	CAD-CBD-CGD	-3.34	104.80	113.67
9	E	301	HEC	CHC-C4B-C3B	-3.33	119.60	125.21
9	E	301	HEC	O1D-CGD-CBD	-3.30	112.63	123.09
14	F	501	JL3	O29-C30-C32	3.29	118.60	111.48
9	A	303	HEC	C3D-C4D-ND	3.26	113.77	110.15
9	A	301	HEC	CMC-C2C-C3C	3.18	134.04	126.55
9	A	301	HEC	CMC-C2C-C1C	-3.16	120.60	125.42
9	A	303	HEC	C4B-NB-C1B	-3.16	100.67	105.82
9	A	303	HEC	CAA-C2A-C1A	-3.15	118.44	124.85
9	A	304	HEC	CBD-CAD-C3D	-3.11	103.92	112.53
9	A	302	HEC	C4B-NB-C1B	-3.10	100.76	105.82
9	A	304	HEC	CAA-CBA-CGA	-3.10	105.45	113.67
9	A	303	HEC	CMA-C3A-C4A	3.08	130.15	124.73
9	A	304	HEC	CMC-C2C-C1C	-3.04	120.80	125.42
9	A	301	HEC	CHA-C1A-NA	3.00	127.72	124.45
9	A	301	HEC	C1C-CHC-C4B	-3.00	115.41	124.66
9	A	305	HEC	C4C-NC-C1C	-2.99	100.94	105.82
9	A	302	HEC	C4D-C3D-C2D	-2.99	102.24	106.87
9	A	304	HEC	CHA-C1A-NA	2.99	127.71	124.45
9	E	301	HEC	CHC-C1C-C2C	-2.96	118.84	127.43
15	F	502	JM9	O38-C39-O40	-2.95	116.24	123.63
9	A	304	HEC	C4B-NB-C1B	-2.89	101.11	105.82
9	A	305	HEC	C2D-C1D-ND	2.88	114.76	110.14
9	E	301	HEC	CHC-C4B-NB	2.87	127.58	124.45
15	F	502	JM9	O20-C19-C18	2.84	116.58	108.40
9	A	302	HEC	CHC-C1C-C2C	-2.82	119.25	127.43
9	E	301	HEC	CMC-C2C-C3C	2.74	132.99	126.55
9	A	305	HEC	C4D-C3D-C2D	-2.72	102.66	106.87
9	A	305	HEC	CHD-C4C-C3C	-2.72	120.63	125.21
13	C	501	JLQ	O18-C16-C15	2.67	119.97	111.83
15	F	502	JM9	C12-C11-C10	2.65	127.78	114.37
9	A	305	HEC	C4B-NB-C1B	-2.65	101.50	105.82
15	F	502	JM9	O38-C39-C41	2.64	119.88	111.83
9	A	302	HEC	C1B-CHB-C4A	-2.64	116.52	124.66
9	A	302	HEC	CAD-C3D-C2D	2.64	132.99	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	303	HEC	C1B-CHB-C4A	-2.62	116.57	124.66
9	E	301	HEC	C4C-NC-C1C	-2.61	101.56	105.82
9	A	303	HEC	CHD-C1D-ND	-2.60	119.14	123.86
14	F	501	JL3	O17-C15-C14	2.58	119.71	111.83
15	F	502	JM9	O17-C15-O16	-2.57	117.71	123.70
9	A	302	HEC	CAA-C2A-C1A	2.56	130.06	124.85
9	A	304	HEC	CHD-C4C-C3C	2.56	129.53	125.21
9	A	303	HEC	CAA-C2A-C3A	2.55	132.65	127.87
14	F	501	JL3	O23-P22-O24	-2.54	100.61	112.44
9	A	302	HEC	CHC-C4B-C3B	-2.52	120.96	125.21
9	A	303	HEC	CAD-CBD-CGD	-2.51	107.02	113.67
9	A	302	HEC	CHA-C1A-NA	2.47	127.15	124.45
9	A	304	HEC	CHD-C4C-NC	-2.45	121.78	124.45
9	A	304	HEC	CHC-C1C-C2C	-2.45	120.32	127.43
13	C	501	JLQ	C21-C20-C19	-2.44	106.11	111.78
9	A	303	HEC	C2D-C1D-ND	2.43	114.05	110.14
9	A	301	HEC	C4B-NB-C1B	-2.43	101.86	105.82
9	A	303	HEC	C2A-C1A-NA	2.43	112.67	110.32
9	E	301	HEC	C2C-C1C-NC	2.42	114.03	110.14
9	A	305	HEC	O1D-CGD-CBD	-2.42	115.42	123.09
9	E	301	HEC	C1C-CHC-C4B	-2.41	117.22	124.66
9	E	301	HEC	CMD-C2D-C1D	2.39	129.05	125.42
9	A	305	HEC	O2A-CGA-CBA	2.39	121.54	114.00
9	A	305	HEC	C1D-C2D-C3D	-2.38	104.09	106.82
9	A	301	HEC	CAA-CBA-CGA	-2.36	107.40	113.67
9	A	303	HEC	C4A-NA-C1A	-2.35	101.99	105.82
9	A	301	HEC	CHC-C4B-NB	2.34	127.01	124.45
13	C	501	JLQ	O30-C31-O32	-2.34	118.22	123.70
9	A	303	HEC	CHC-C4B-C3B	-2.34	121.26	125.21
13	C	501	JLQ	O24-P23-O25	-2.34	101.54	112.44
9	A	304	HEC	C4A-NA-C1A	-2.33	102.02	105.82
15	F	502	JM9	O20-C21-O22	-2.32	117.82	123.63
9	A	303	HEC	O2D-CGD-CBD	2.30	121.26	114.00
9	A	302	HEC	C4C-NC-C1C	-2.28	102.10	105.82
9	A	301	HEC	CAD-C3D-C2D	-2.20	122.14	127.07
9	A	305	HEC	CMD-C2D-C3D	2.18	130.26	125.62
15	F	502	JM9	O17-C15-C14	2.17	116.18	111.48
9	A	304	HEC	CHC-C4B-C3B	-2.14	121.60	125.21
9	A	303	HEC	O1D-CGD-CBD	-2.12	116.36	123.09
9	E	301	HEC	O2A-CGA-CBA	2.06	120.50	114.00
9	A	301	HEC	C4C-NC-C1C	-2.04	102.49	105.82
9	E	301	HEC	C2A-C1A-NA	2.04	112.29	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	303	HEC	CMC-C2C-C3C	-2.04	121.75	126.55
9	A	301	HEC	C4A-C3A-C2A	2.02	109.97	106.97

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	HEC	C2C-C3C-CAC-CBC
9	A	301	HEC	C4C-C3C-CAC-CBC
9	A	302	HEC	C2C-C3C-CAC-CBC
9	A	302	HEC	C4C-C3C-CAC-CBC
9	A	303	HEC	C2C-C3C-CAC-CBC
9	A	303	HEC	C4C-C3C-CAC-CBC
9	A	305	HEC	C2A-CAA-CBA-CGA
9	A	305	HEC	C2C-C3C-CAC-CBC
9	A	305	HEC	C4C-C3C-CAC-CBC
9	E	301	HEC	C2C-C3C-CAC-CBC
9	E	301	HEC	C4C-C3C-CAC-CBC
9	E	301	HEC	C3D-CAD-CBD-CGD
13	C	501	JLQ	C21-O22-P23-O25
13	C	501	JLQ	C21-O22-P23-O26
13	C	501	JLQ	C27-O26-P23-O22
13	C	501	JLQ	C27-O26-P23-O24
13	C	501	JLQ	C27-O26-P23-O25
13	C	501	JLQ	O30-C20-C21-O22
13	C	501	JLQ	O32-C31-O30-C20
14	F	501	JL3	O17-C18-C19-O29
15	F	502	JM9	O17-C18-C37-O38
13	C	501	JLQ	C33-C31-O30-C20
9	A	302	HEC	C3A-C2A-CAA-CBA
9	A	302	HEC	C1A-C2A-CAA-CBA
9	A	301	HEC	C3D-CAD-CBD-CGD
9	A	302	HEC	C2A-CAA-CBA-CGA
9	A	303	HEC	C3D-CAD-CBD-CGD
13	C	501	JLQ	C15-C16-O18-C19
14	F	501	JL3	C14-C15-O17-C18
15	F	502	JM9	C12-C13-C14-C15
14	F	501	JL3	O16-C15-O17-C18
15	F	502	JM9	C48-C49-C50-C51
13	C	501	JLQ	O17-C16-O18-C19
15	F	502	JM9	C44-C45-C46-C47
15	F	502	JM9	C50-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
9	A	302	HEC	C2D-C3D-CAD-CBD
14	F	501	JL3	C32-C33-C34-C35
15	F	502	JM9	C30-C31-C32-C33
14	F	501	JL3	C40-C41-C42-C43
14	F	501	JL3	C35-C36-C37-C38
15	F	502	JM9	C21-C23-C24-C25
14	F	501	JL3	C41-C42-C43-C44
15	F	502	JM9	C09-C10-C11-C12
13	C	501	JLQ	C09-C10-C11-C12
15	F	502	JM9	C43-C44-C45-C46
13	C	501	JLQ	C08-C09-C10-C11
14	F	501	JL3	C36-C37-C38-C39
15	F	502	JM9	C10-C11-C12-C13
14	F	501	JL3	C11-C12-C13-C14
15	F	502	JM9	C50-C51-C52-C54
15	F	502	JM9	C14-C15-O17-C18
15	F	502	JM9	C23-C21-O20-C19
15	F	502	JM9	C46-C47-C48-C49
13	C	501	JLQ	C39-C40-C41-C42
14	F	501	JL3	C33-C34-C35-C36
13	C	501	JLQ	C04-C05-C06-C07
15	F	502	JM9	O16-C15-O17-C18
14	F	501	JL3	C10-C11-C12-C13
13	C	501	JLQ	O18-C19-C20-C21
15	F	502	JM9	C24-C25-C26-C27
14	F	501	JL3	C09-C10-C11-C12
15	F	502	JM9	C29-C30-C31-C32
13	C	501	JLQ	C07-C08-C09-C10
13	C	501	JLQ	C01-C02-C03-C04
15	F	502	JM9	O22-C21-O20-C19
9	A	302	HEC	C4D-C3D-CAD-CBD
13	C	501	JLQ	C19-C20-C21-O22
13	C	501	JLQ	C13-C14-C15-C16
14	F	501	JL3	C38-C39-C40-C41
14	F	501	JL3	C12-C13-C14-C15
15	F	502	JM9	C01-C02-C03-C04
13	C	501	JLQ	O18-C19-C20-O30
14	F	501	JL3	C18-C19-C20-O21
9	A	301	HEC	C4D-C3D-CAD-CBD
13	C	501	JLQ	C06-C07-C08-C09
14	F	501	JL3	C04-C05-C06-C07
13	C	501	JLQ	C19-C20-O30-C31

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Mol	Chain	Res	Type	Atoms
14	F	501	JL3	O29-C19-C20-O21
15	F	502	JM9	C19-C18-C37-O38
15	F	502	JM9	C45-C46-C47-C48
15	F	502	JM9	C27-C28-C29-C30
9	A	301	HEC	C4B-C3B-CAB-CBB
9	A	302	HEC	C4B-C3B-CAB-CBB
9	A	304	HEC	C4B-C3B-CAB-CBB
9	E	301	HEC	C4B-C3B-CAB-CBB
14	F	501	JL3	C37-C38-C39-C40
13	C	501	JLQ	C02-C03-C04-C05
15	F	502	JM9	C11-C12-C13-C14
14	F	501	JL3	O17-C18-C19-C20
9	A	301	HEC	C2B-C3B-CAB-CBB
9	A	302	HEC	C2B-C3B-CAB-CBB
9	A	304	HEC	C2B-C3B-CAB-CBB
9	A	305	HEC	C2B-C3B-CAB-CBB
9	E	301	HEC	C2B-C3B-CAB-CBB
13	C	501	JLQ	C21-O22-P23-O24
14	F	501	JL3	C26-O25-P22-O24
14	F	501	JL3	C42-C43-C44-C45
13	C	501	JLQ	C38-C39-C40-C41
15	F	502	JM9	C32-C33-C34-C35
14	F	501	JL3	C07-C08-C09-C10
9	A	301	HEC	C2A-CAA-CBA-CGA
15	F	502	JM9	C32-C33-C34-C36
9	A	305	HEC	CAD-CBD-CGD-O2D
9	A	302	HEC	CAD-CBD-CGD-O1D
9	A	305	HEC	CAD-CBD-CGD-O1D
9	A	301	HEC	CAD-CBD-CGD-O1D
9	A	302	HEC	CAD-CBD-CGD-O2D
15	F	502	JM9	C39-C41-C42-C43
9	A	301	HEC	CAD-CBD-CGD-O2D
9	A	302	HEC	C3D-CAD-CBD-CGD
9	A	304	HEC	CAD-CBD-CGD-O2D
13	C	501	JLQ	C36-C37-C38-C39
9	E	301	HEC	CAA-CBA-CGA-O2A
9	E	301	HEC	CAA-CBA-CGA-O1A
9	E	301	HEC	CAD-CBD-CGD-O1D
9	A	304	HEC	CAD-CBD-CGD-O1D
14	F	501	JL3	C19-C20-O21-P22
15	F	502	JM9	C08-C09-C10-C11
15	F	502	JM9	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	F	501	JL3	O29-C30-C32-C33
13	C	501	JLQ	C14-C15-C16-O18
13	C	501	JLQ	C40-C41-C42-C43
9	A	304	HEC	C3D-CAD-CBD-CGD
9	A	305	HEC	CAA-CBA-CGA-O1A
14	F	501	JL3	C13-C14-C15-O17
14	F	501	JL3	C05-C06-C07-C08
14	F	501	JL3	O31-C30-C32-C33
9	A	303	HEC	C4B-C3B-CAB-CBB
9	A	305	HEC	C4B-C3B-CAB-CBB
14	F	501	JL3	C13-C14-C15-O16
9	A	301	HEC	CAA-CBA-CGA-O2A
9	A	305	HEC	CAA-CBA-CGA-O2A
9	E	301	HEC	CAD-CBD-CGD-O2D

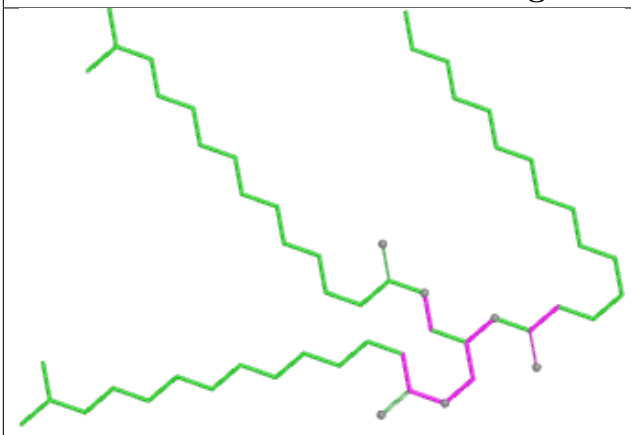
There are no ring outliers.

10 monomers are involved in 66 short contacts:

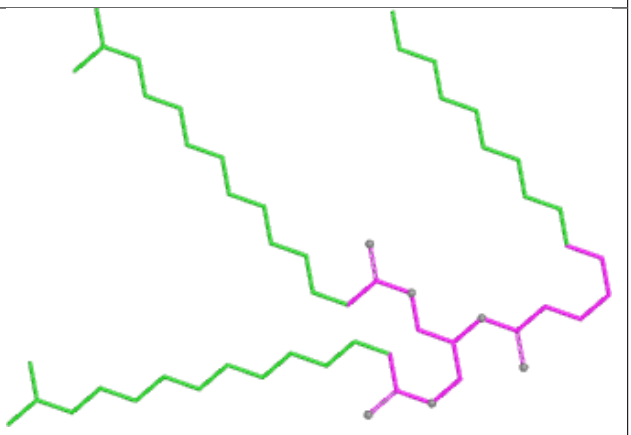
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	502	JM9	6	0
9	A	305	HEC	8	0
9	A	302	HEC	7	0
9	A	304	HEC	9	0
9	A	301	HEC	5	0
10	B	1101	SF4	1	0
11	B	1104	F3S	10	0
9	A	303	HEC	2	0
14	F	501	JL3	4	0
9	E	301	HEC	15	0

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.

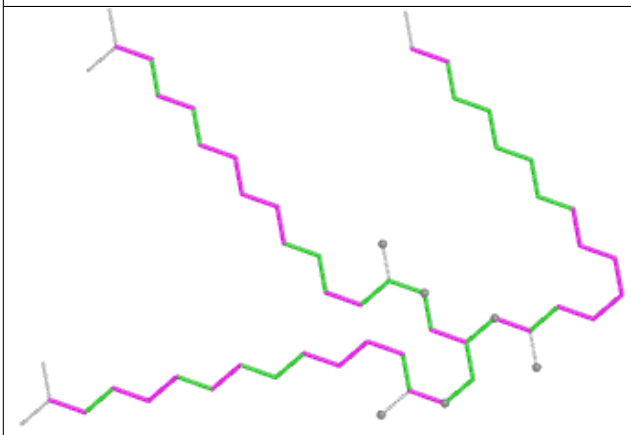
Ligand JM9 F 502



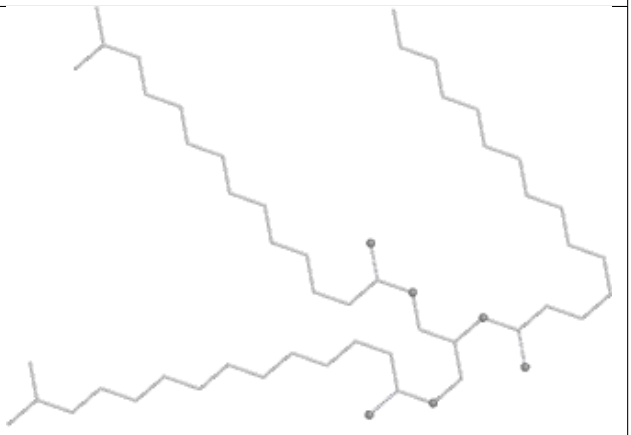
Bond lengths



Bond angles

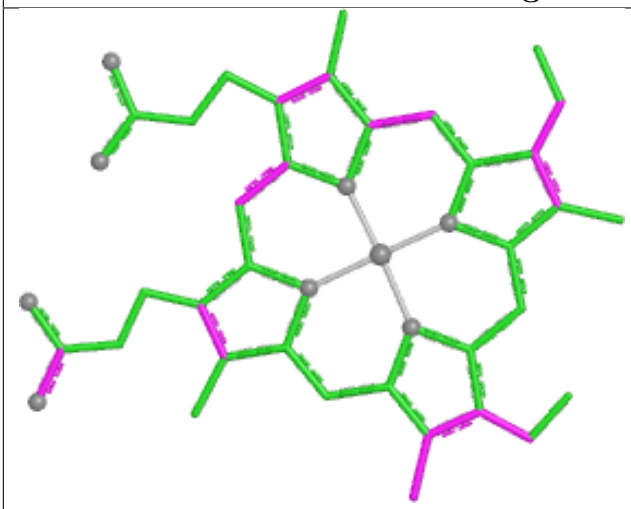


Torsions

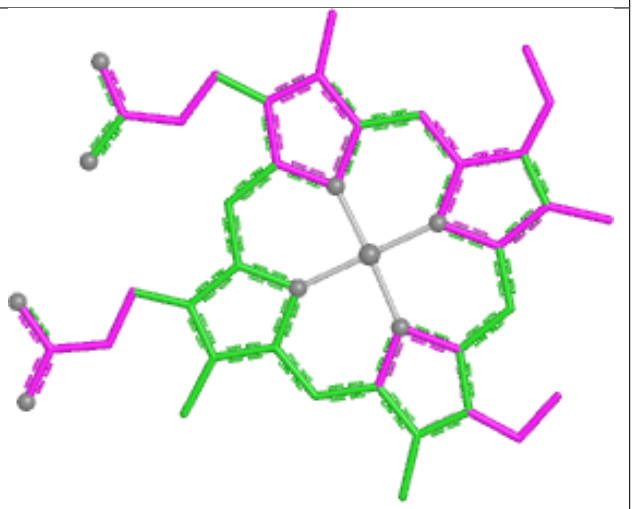


Rings

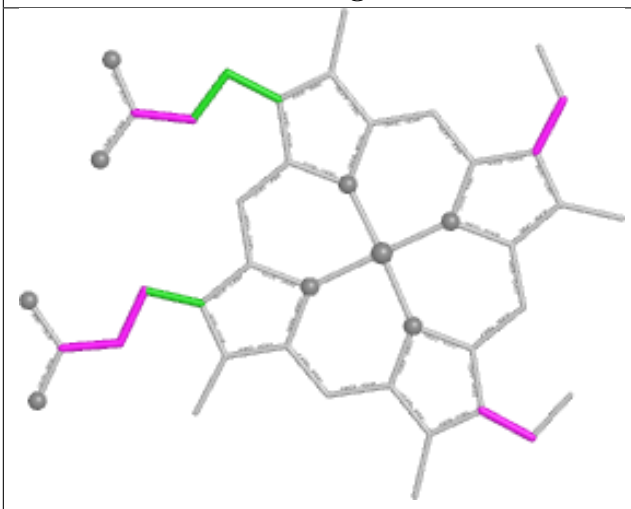
Ligand HEC A 305



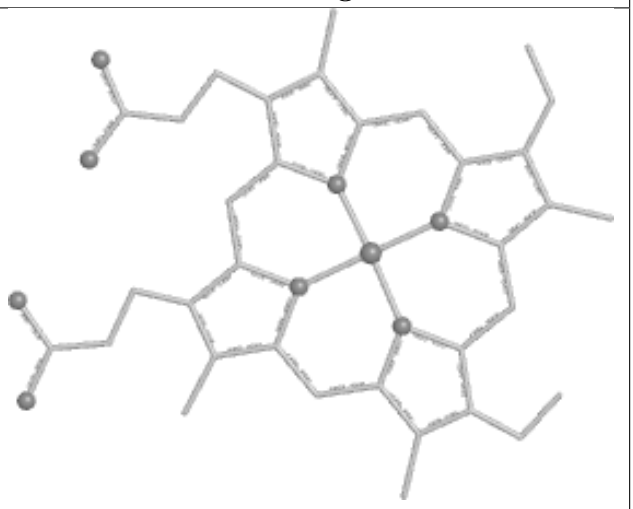
Bond lengths



Bond angles

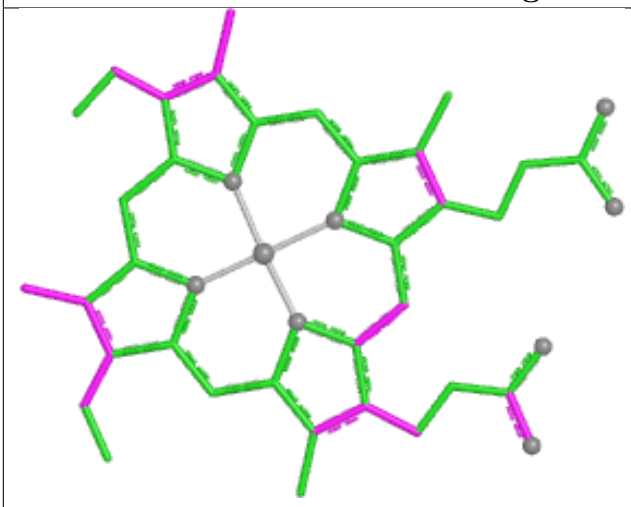


Torsions

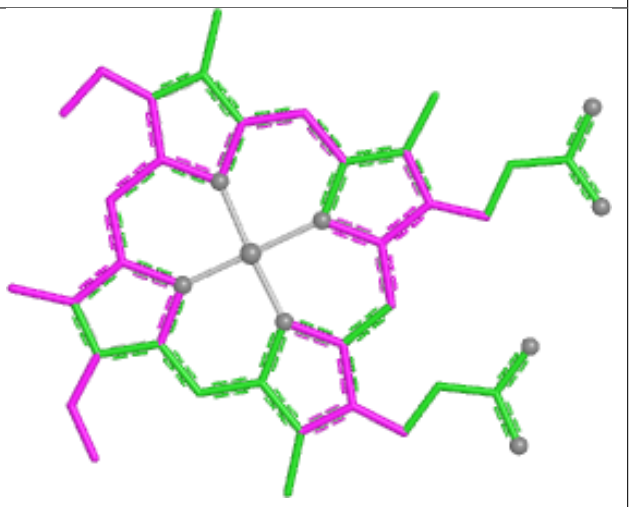


Rings

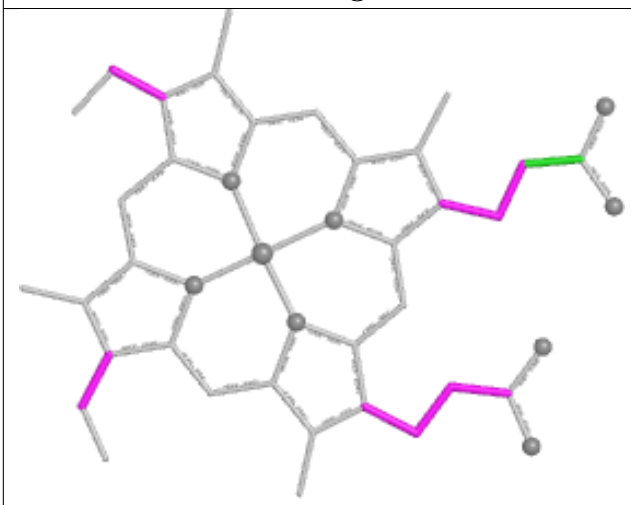
Ligand HEC A 302



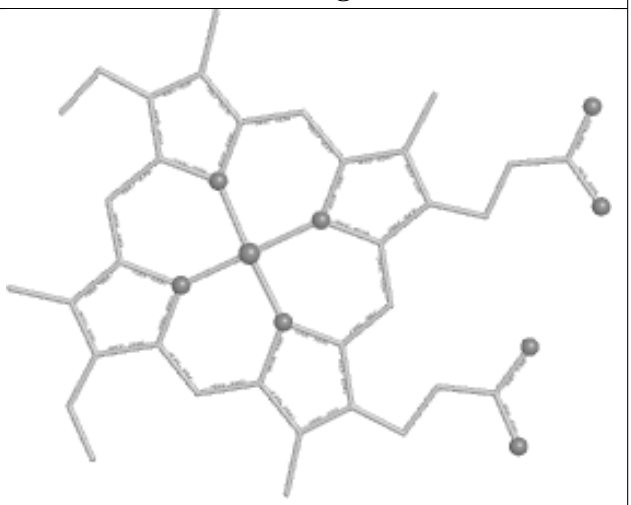
Bond lengths



Bond angles

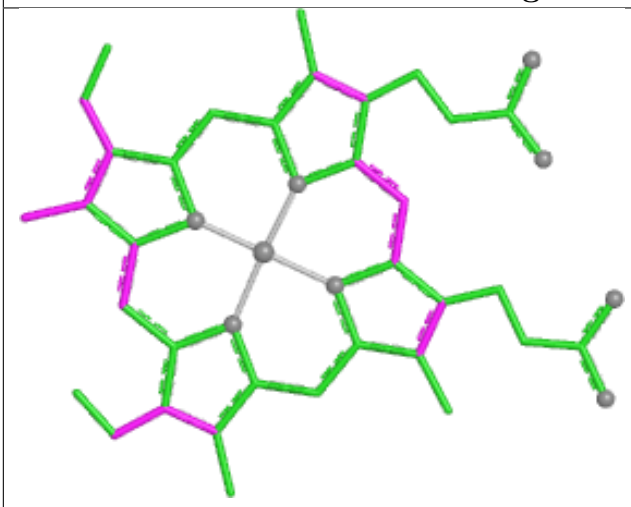


Torsions



Rings

Ligand HEC A 304



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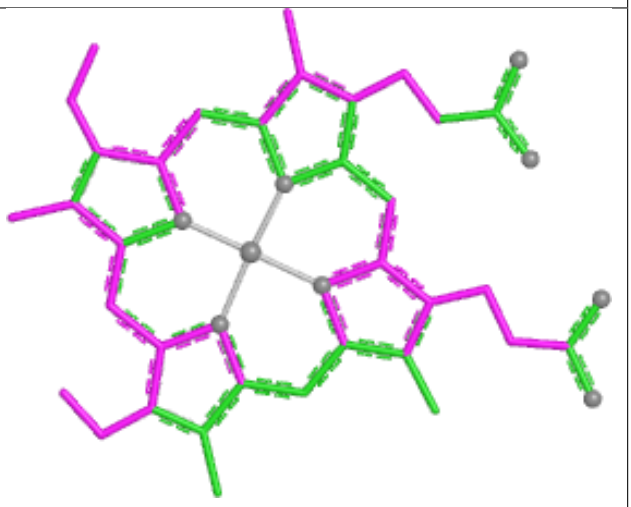
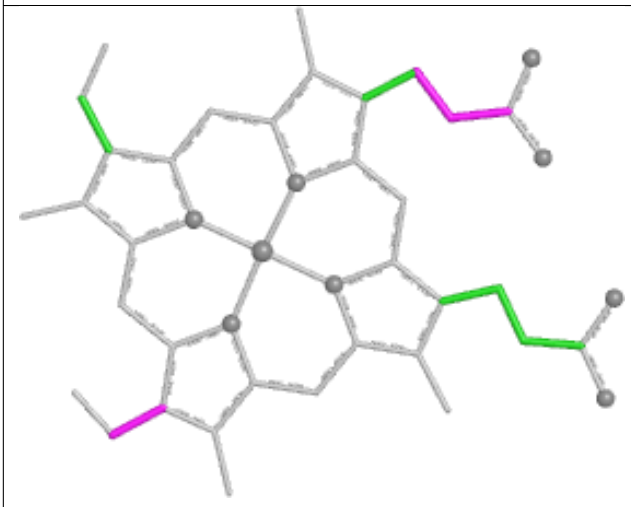
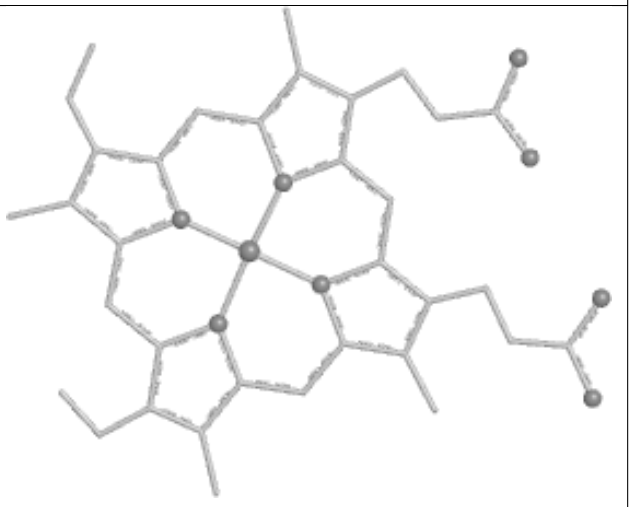


Bond angles

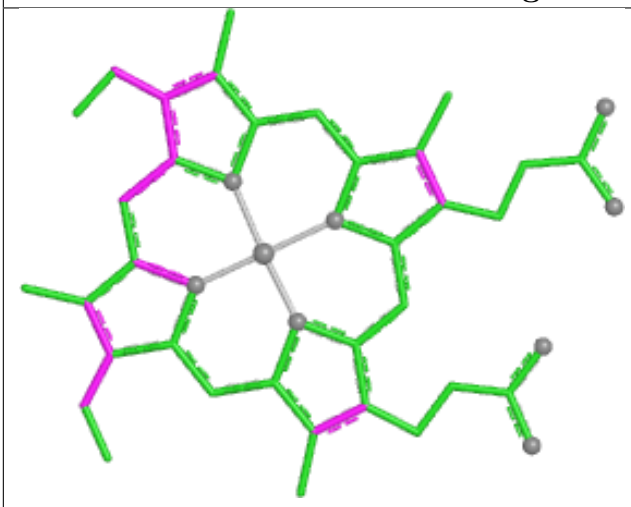


Torsions



Rings

Ligand HEC A 301



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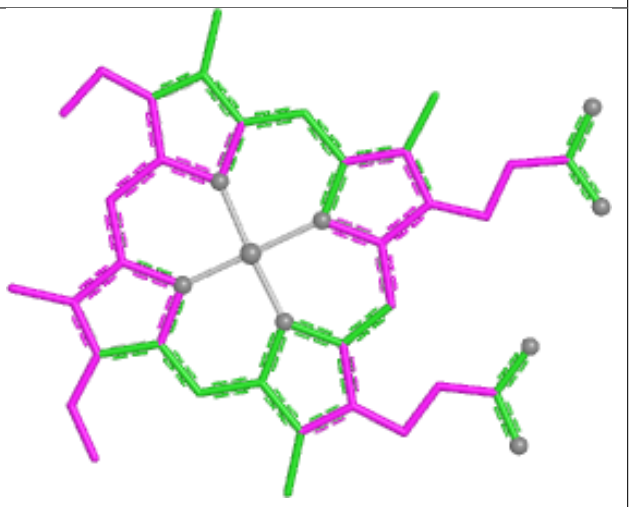
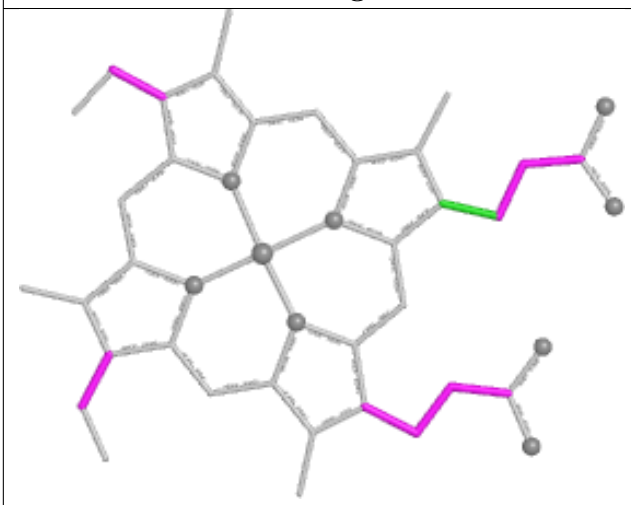


Bond angles



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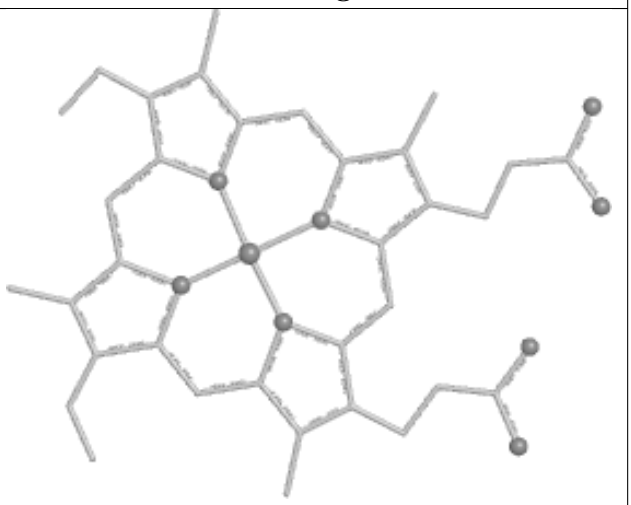
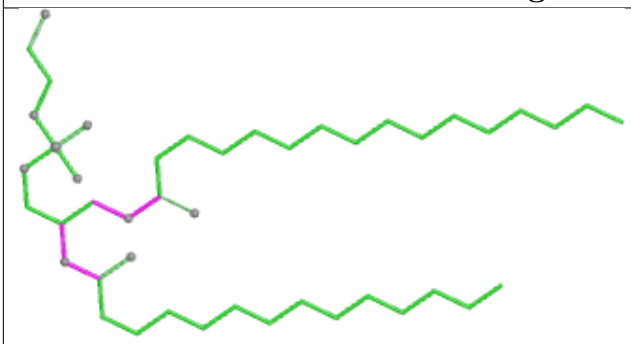


Rings

Ligand JLQ C 501



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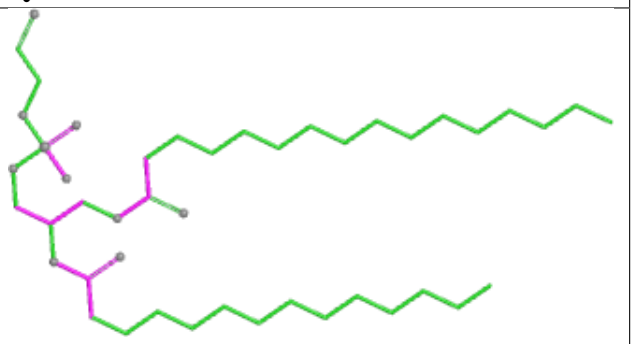
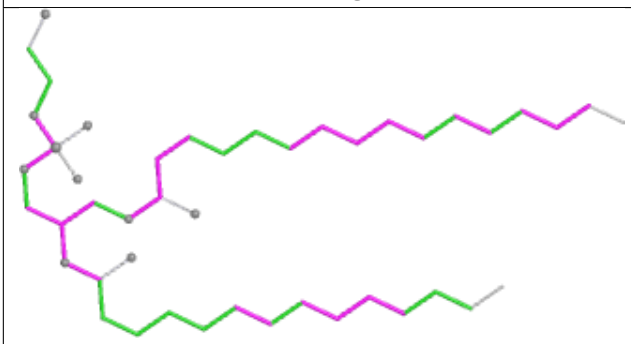


Bond angles



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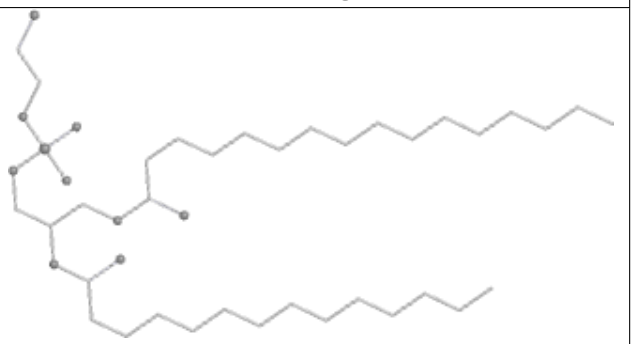
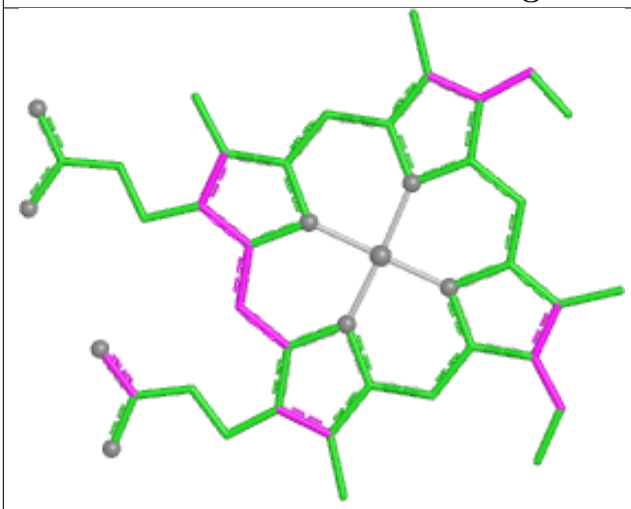
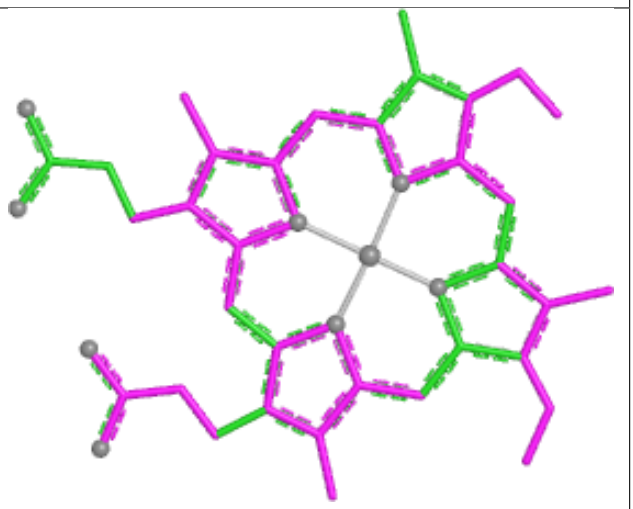


Rings

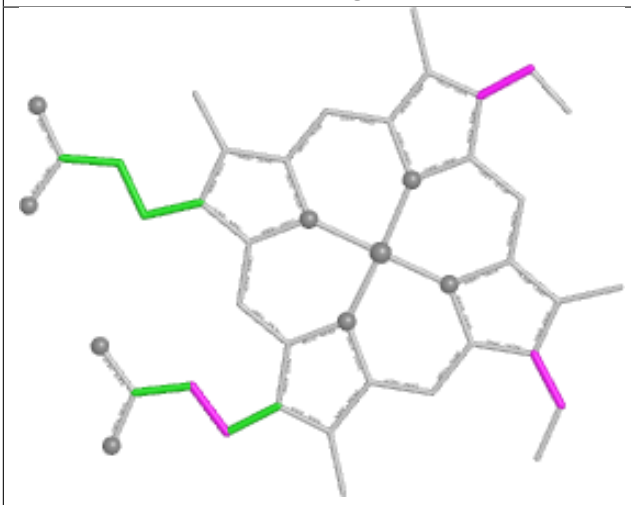
Ligand HEC A 303



Bond lengths



Bond angles



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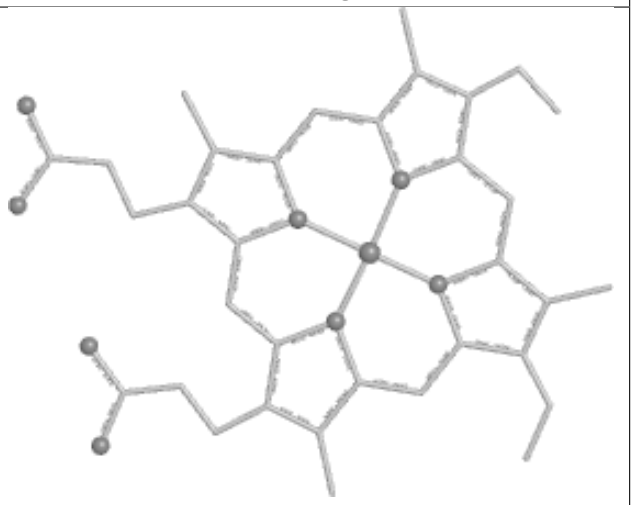
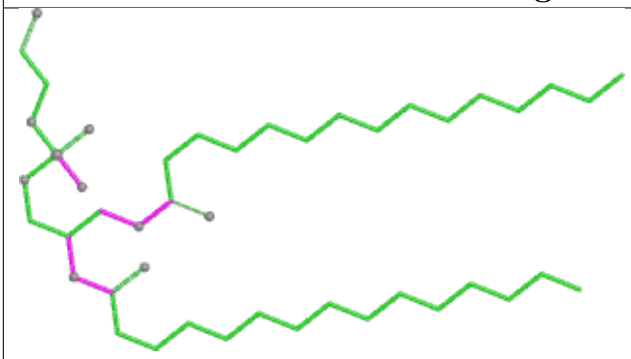


Rings

Ligand JL3 F 501



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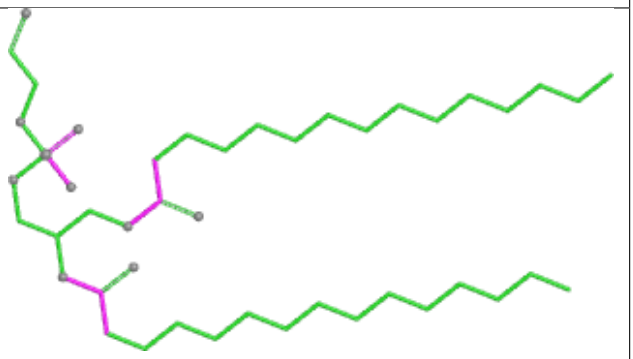
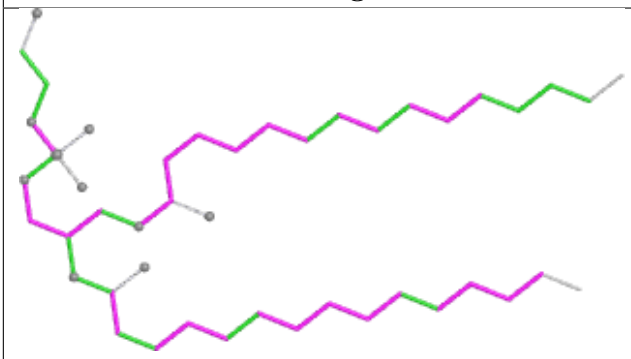


Bond angles



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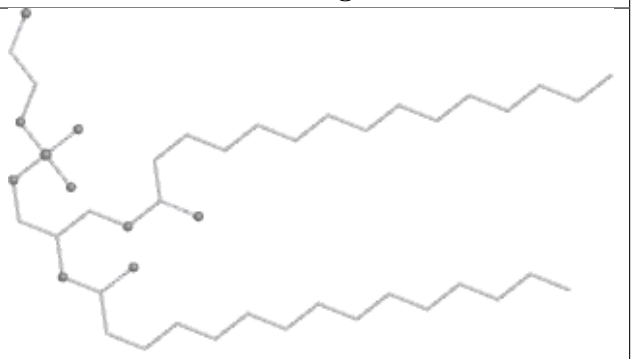
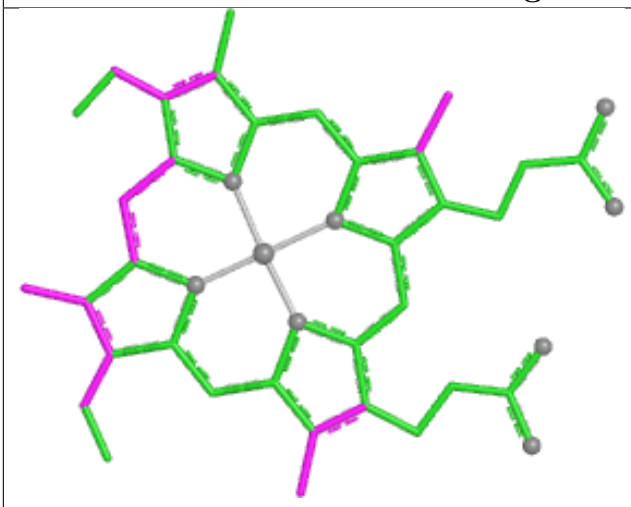
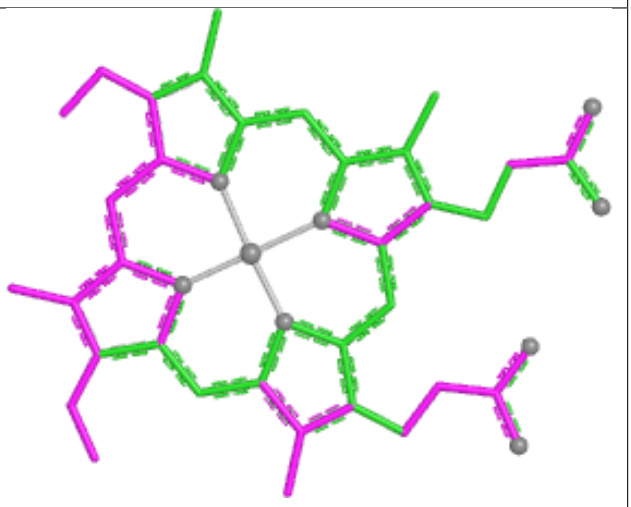


Rings

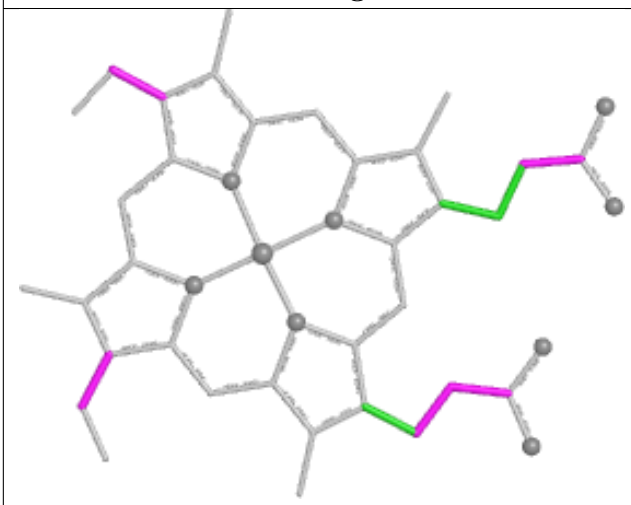
Ligand HEC E 301



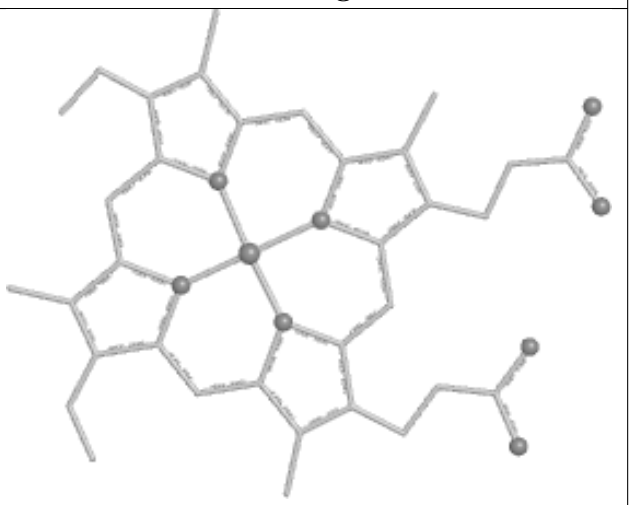
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

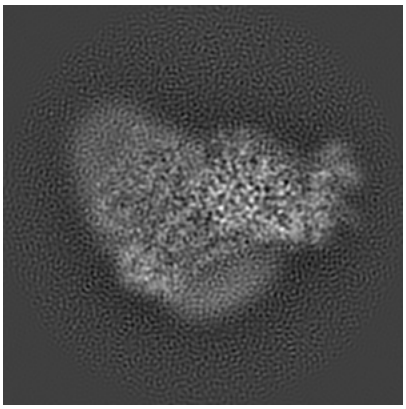
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36985. These allow visual inspection of the internal detail of the map and identification of artifacts.

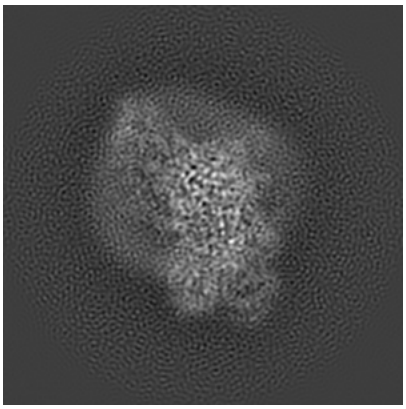
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

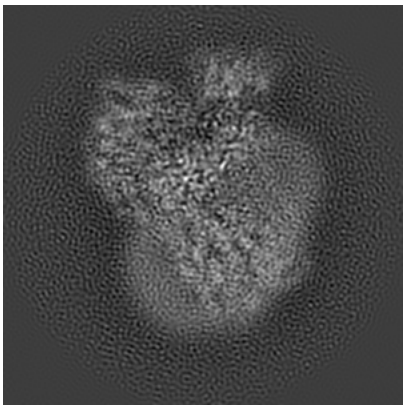
6.1.1 Primary map



X

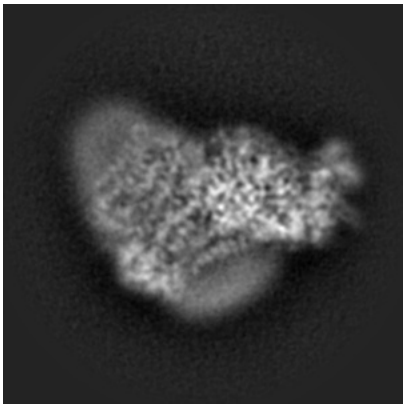


Y

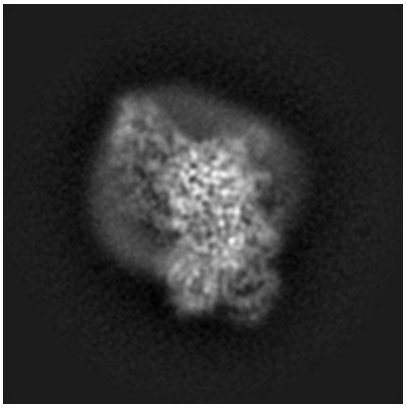


Z

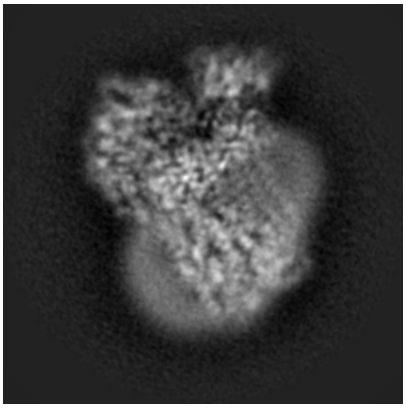
6.1.2 Raw map



X



Y

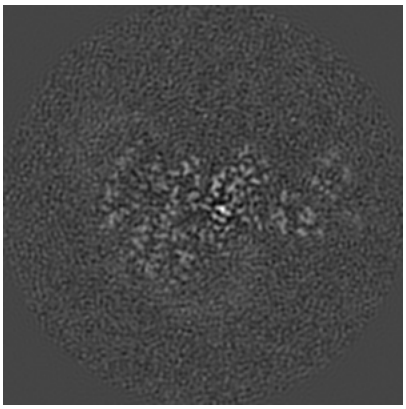


Z

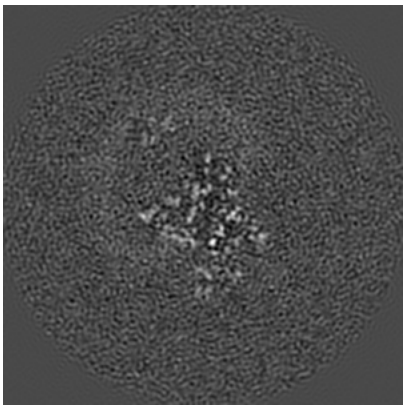
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

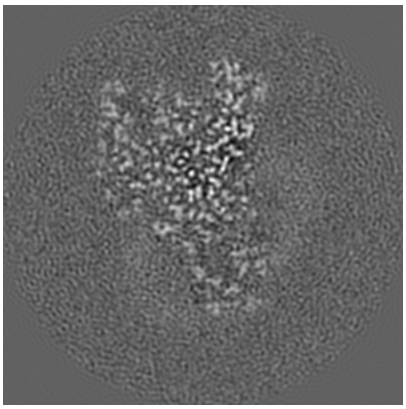
6.2.1 Primary map



X Index: 108

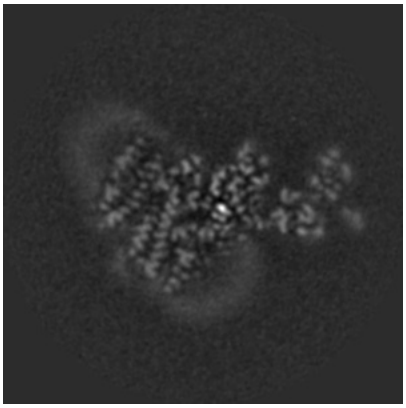


Y Index: 108

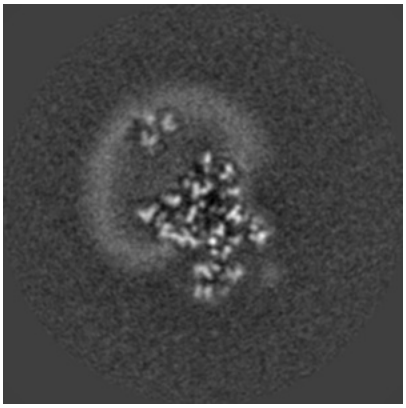


Z Index: 108

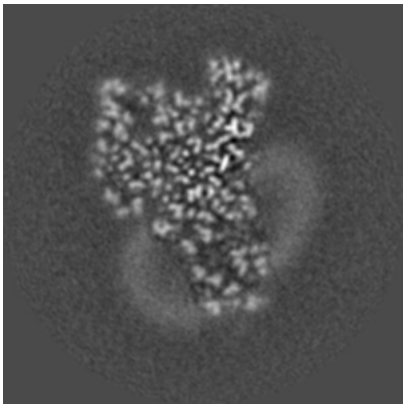
6.2.2 Raw map



X Index: 108



Y Index: 108

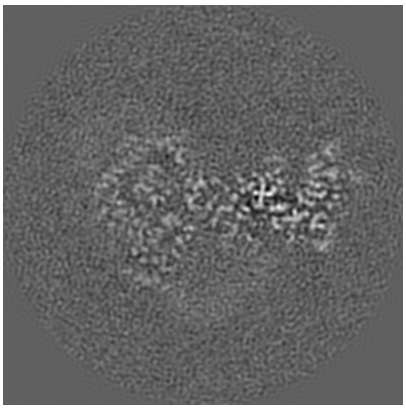


Z Index: 108

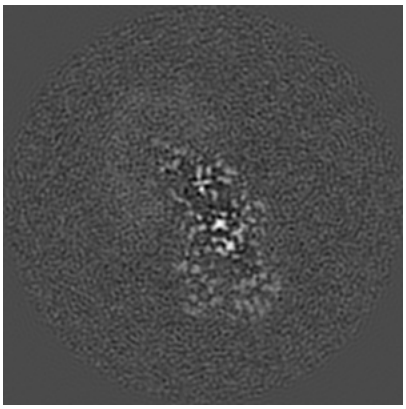
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

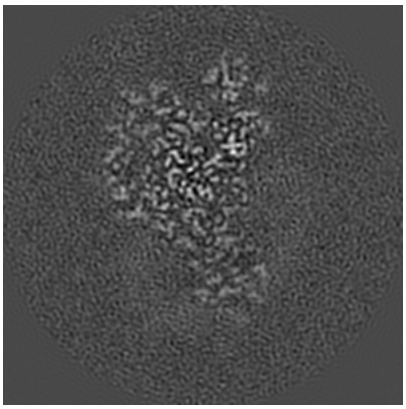
6.3.1 Primary map



X Index: 123

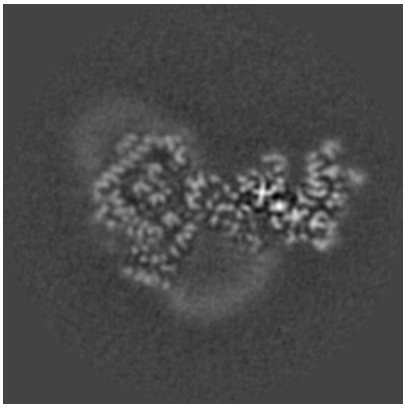


Y Index: 131

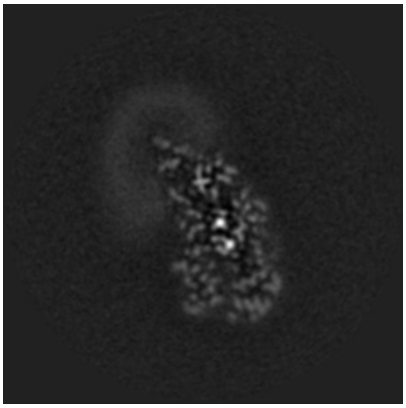


Z Index: 114

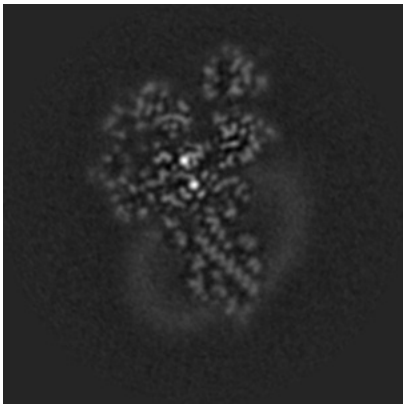
6.3.2 Raw map



X Index: 123



Y Index: 131

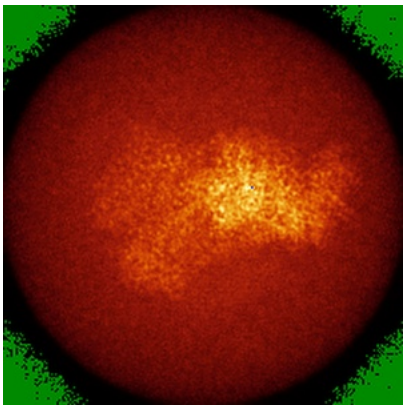


Z Index: 117

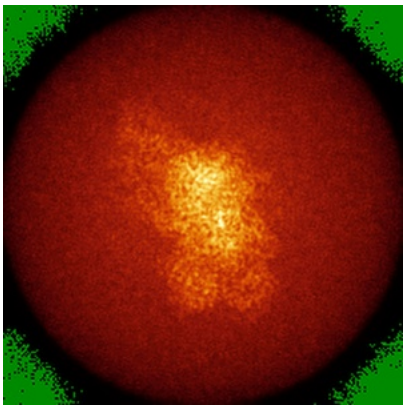
The images above show the largest variance slices of the map in three orthogonal directions.

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

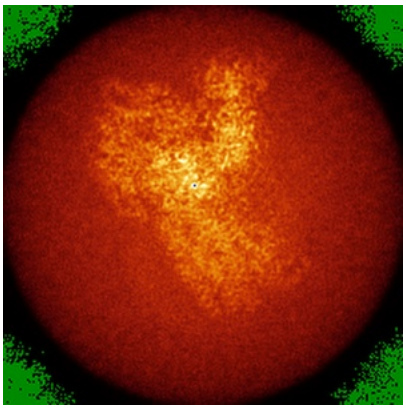
6.4.1 Primary map



X

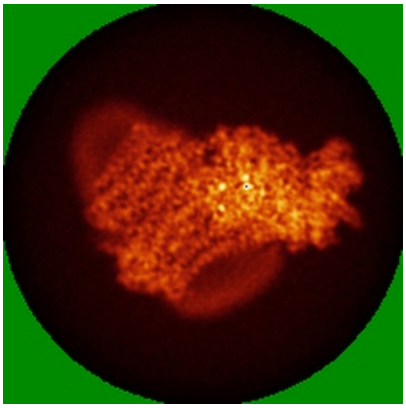


Y

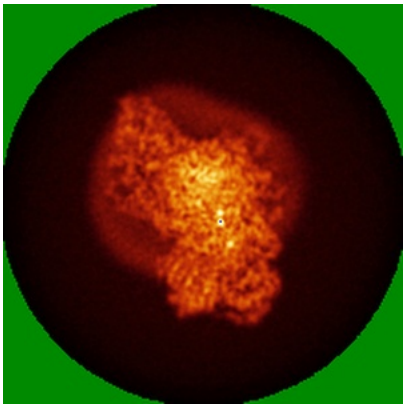


Z

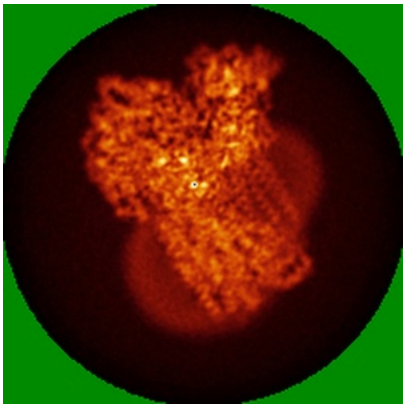
6.4.2 Raw map



X



Y

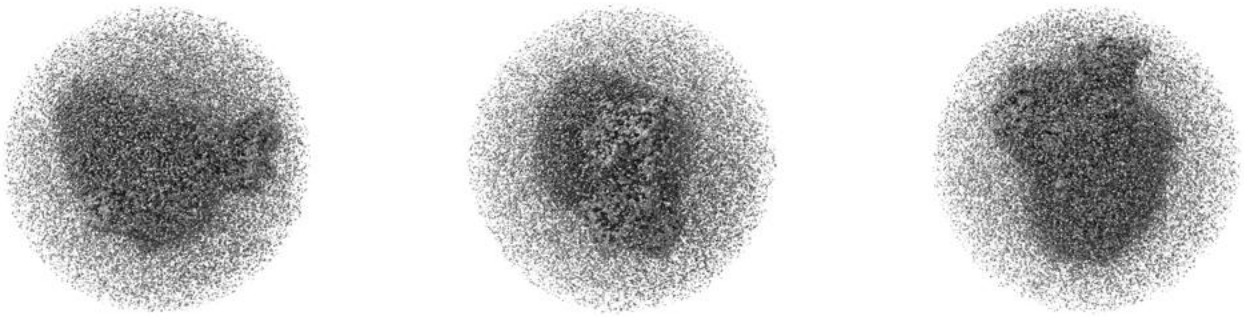


Z

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 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

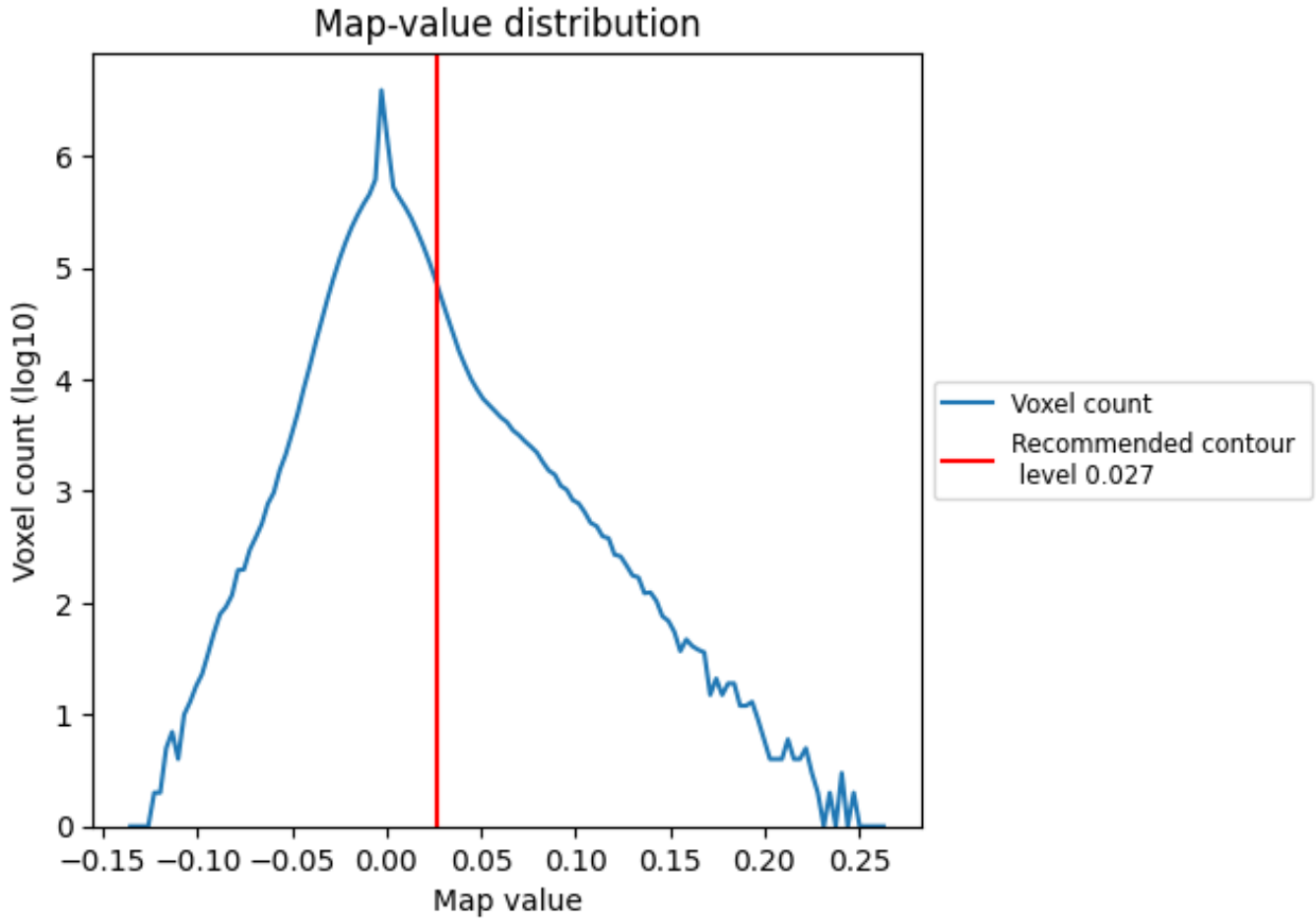
6.6 Mask visualisation (i)

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

7 Map analysis

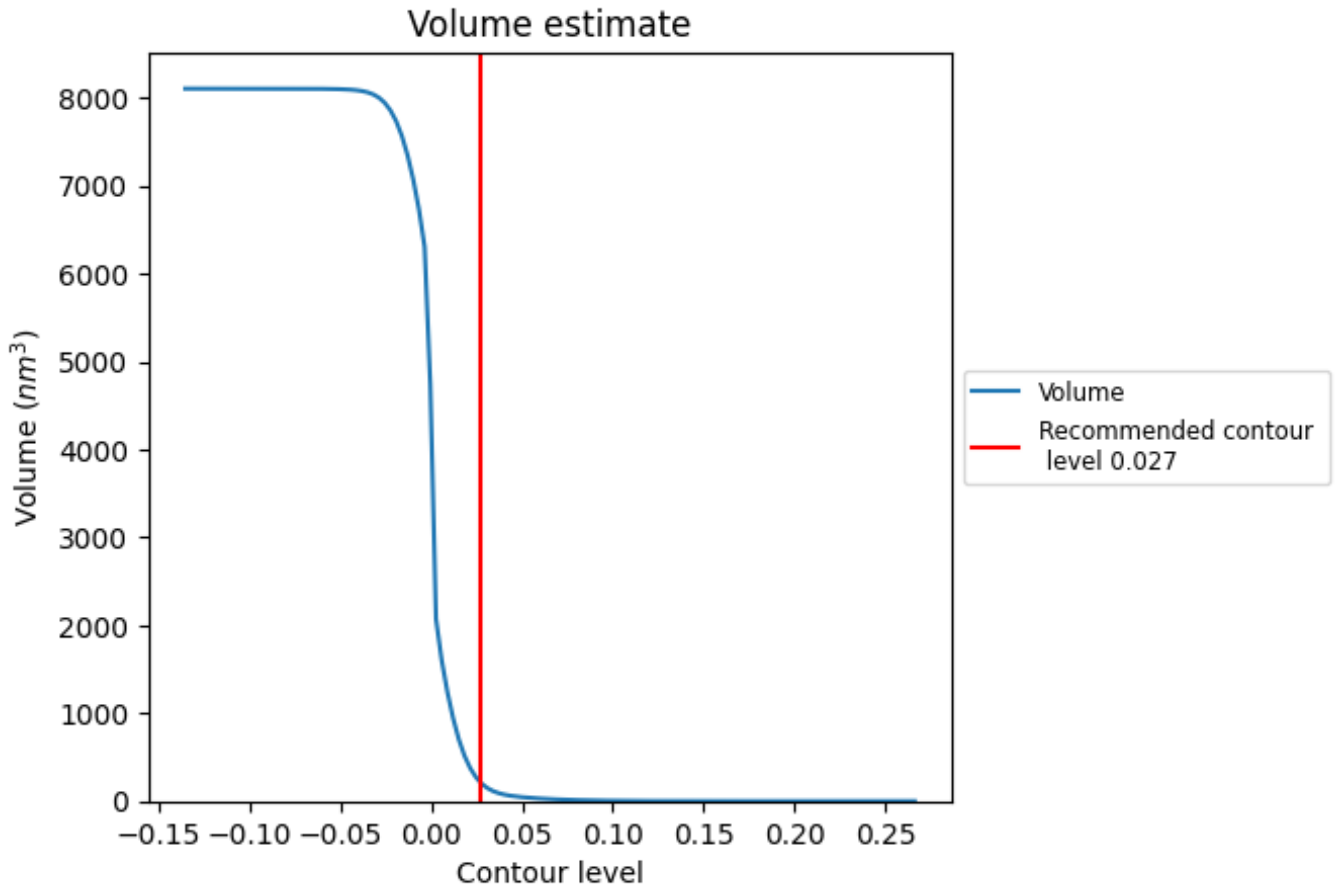
This section contains the results of statistical analysis of the map.

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.

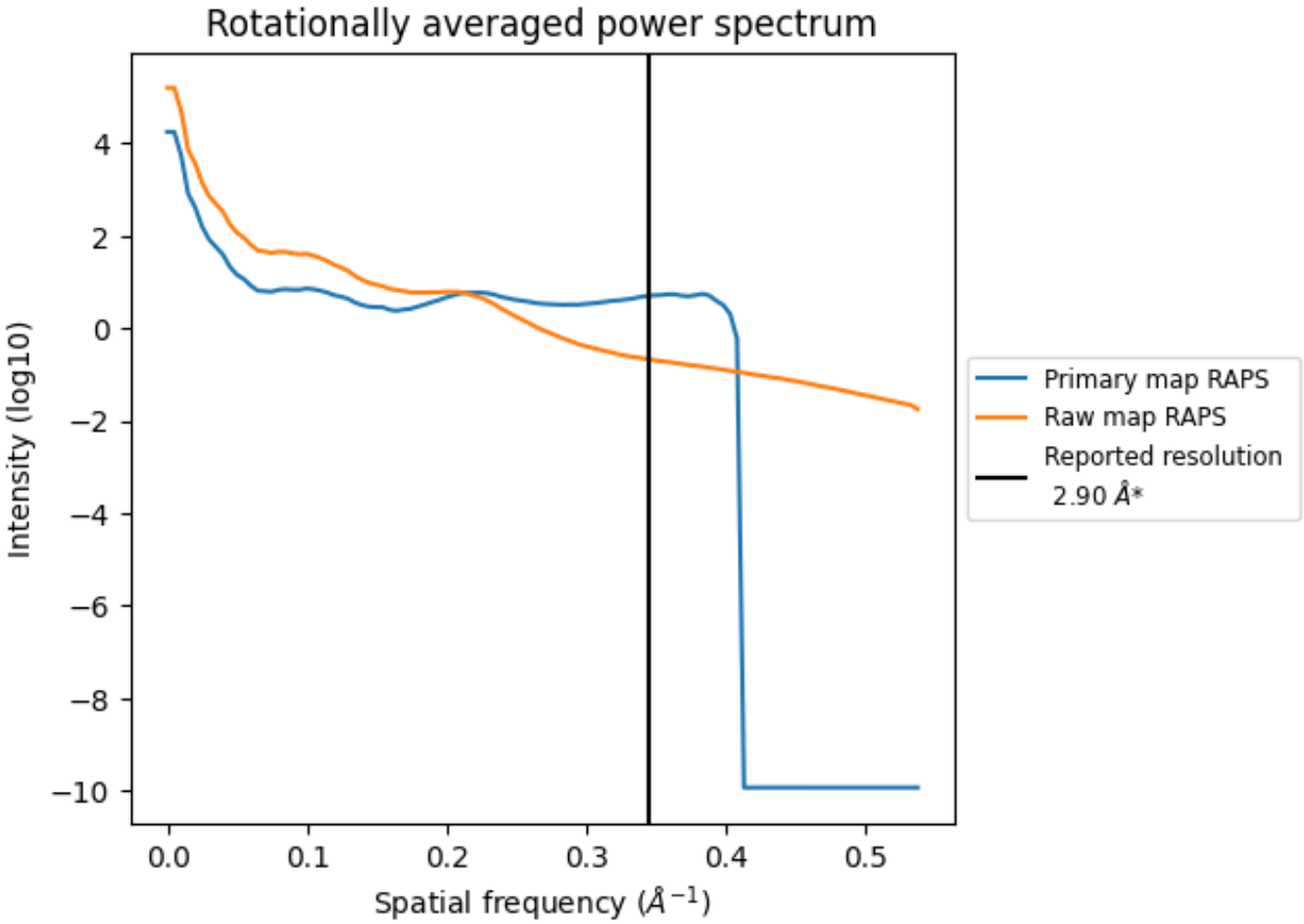
7.2 Volume estimate



The volume at the recommended contour level is 216 nm^3; this corresponds to an approximate mass of 195 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)

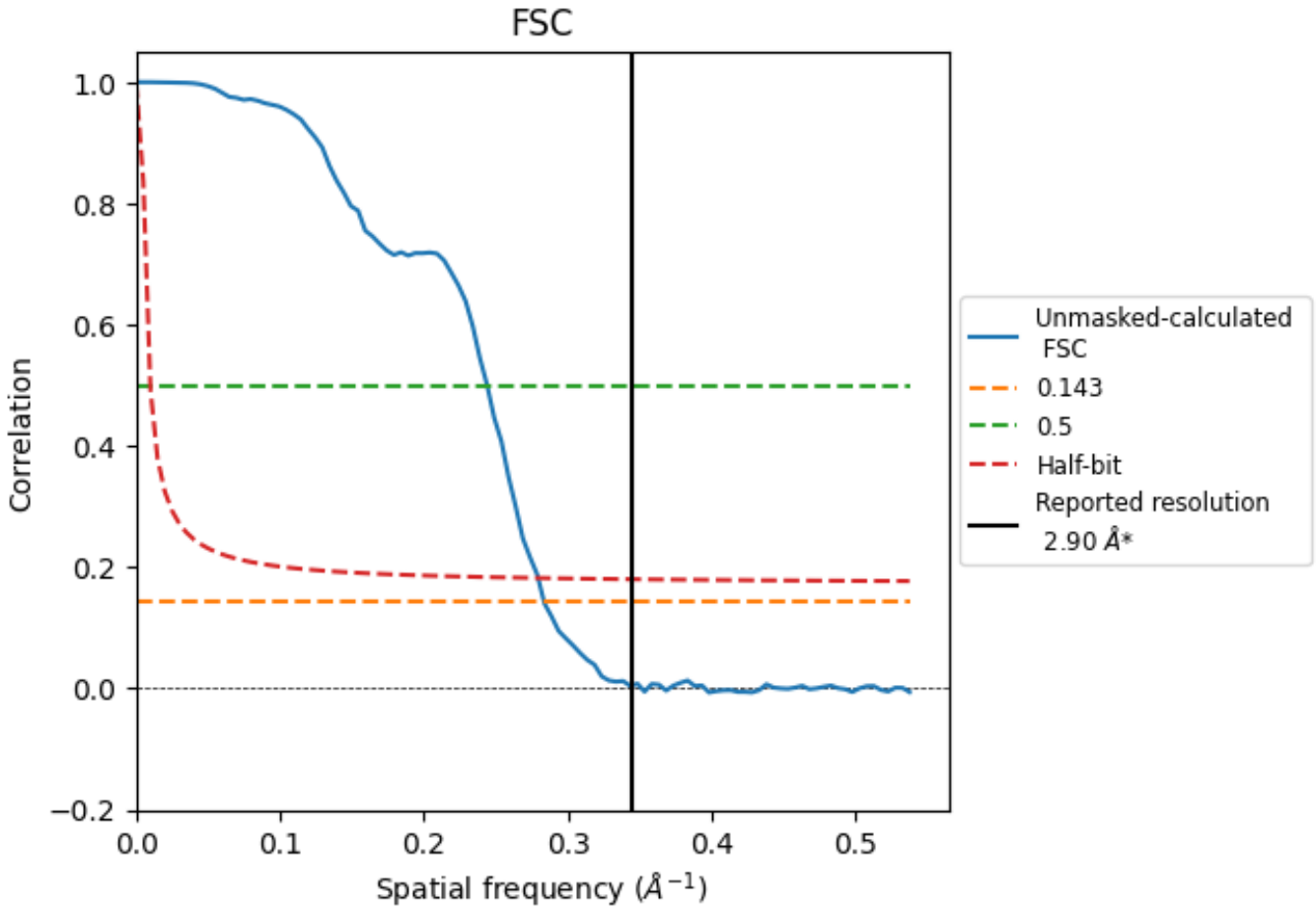


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

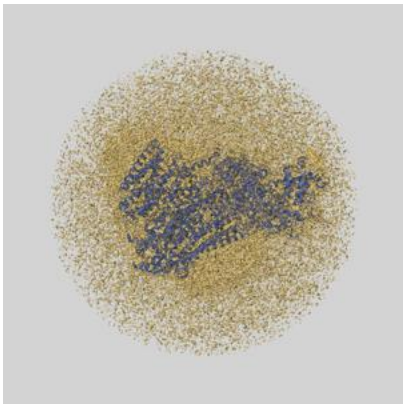
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.10	3.58

*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 3.53 differs from the reported value 2.9 by more than 10 %

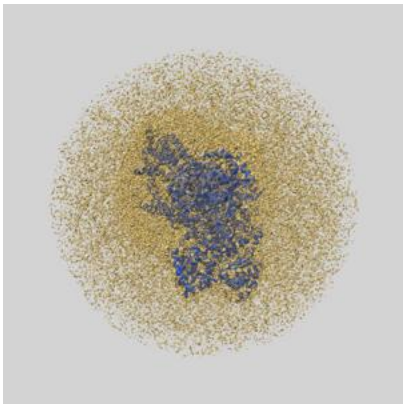
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36985 and PDB model 8K9F. Per-residue inclusion information can be found in section 3 on page 9.

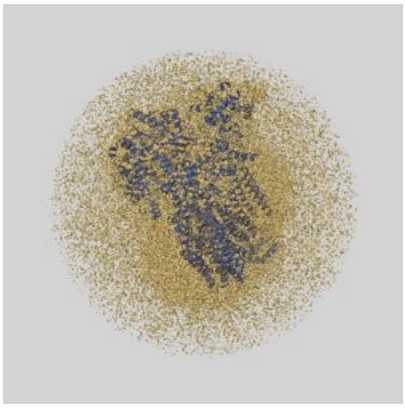
9.1 Map-model overlay



X



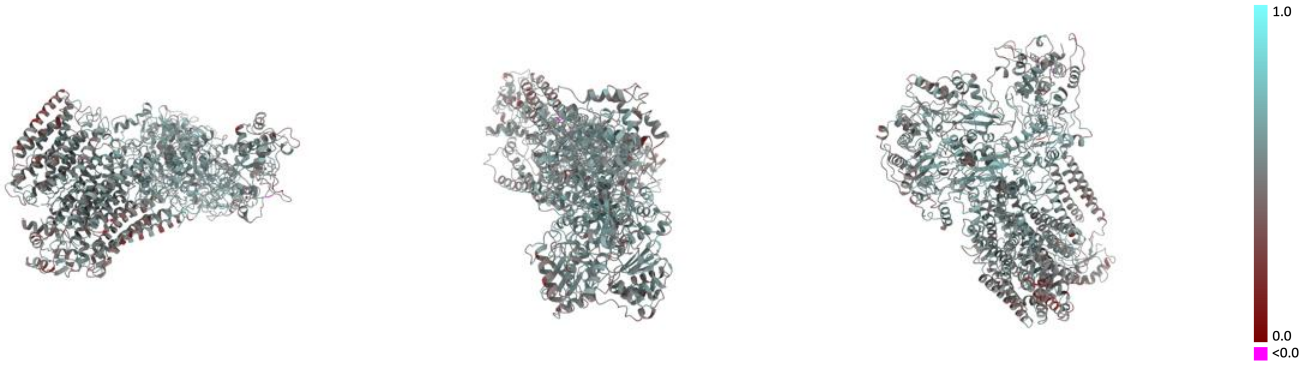
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

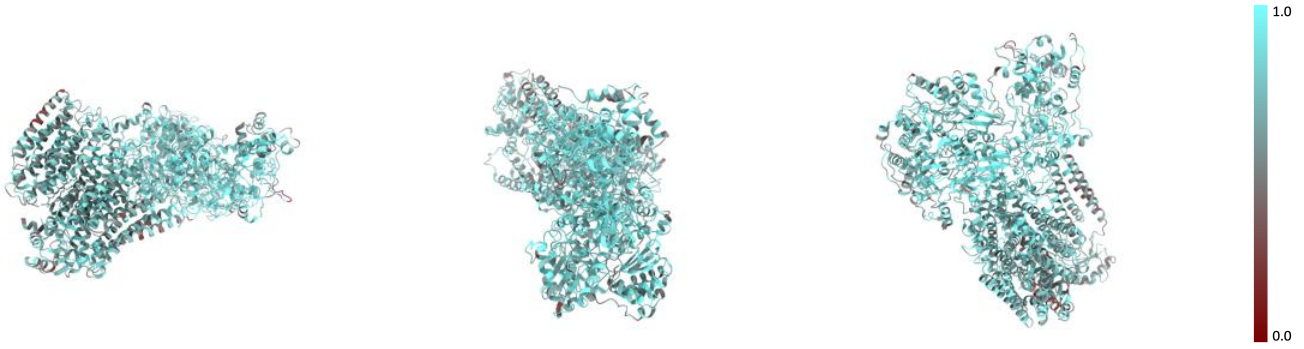
9.2 Q-score mapped to coordinate model (i)



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.

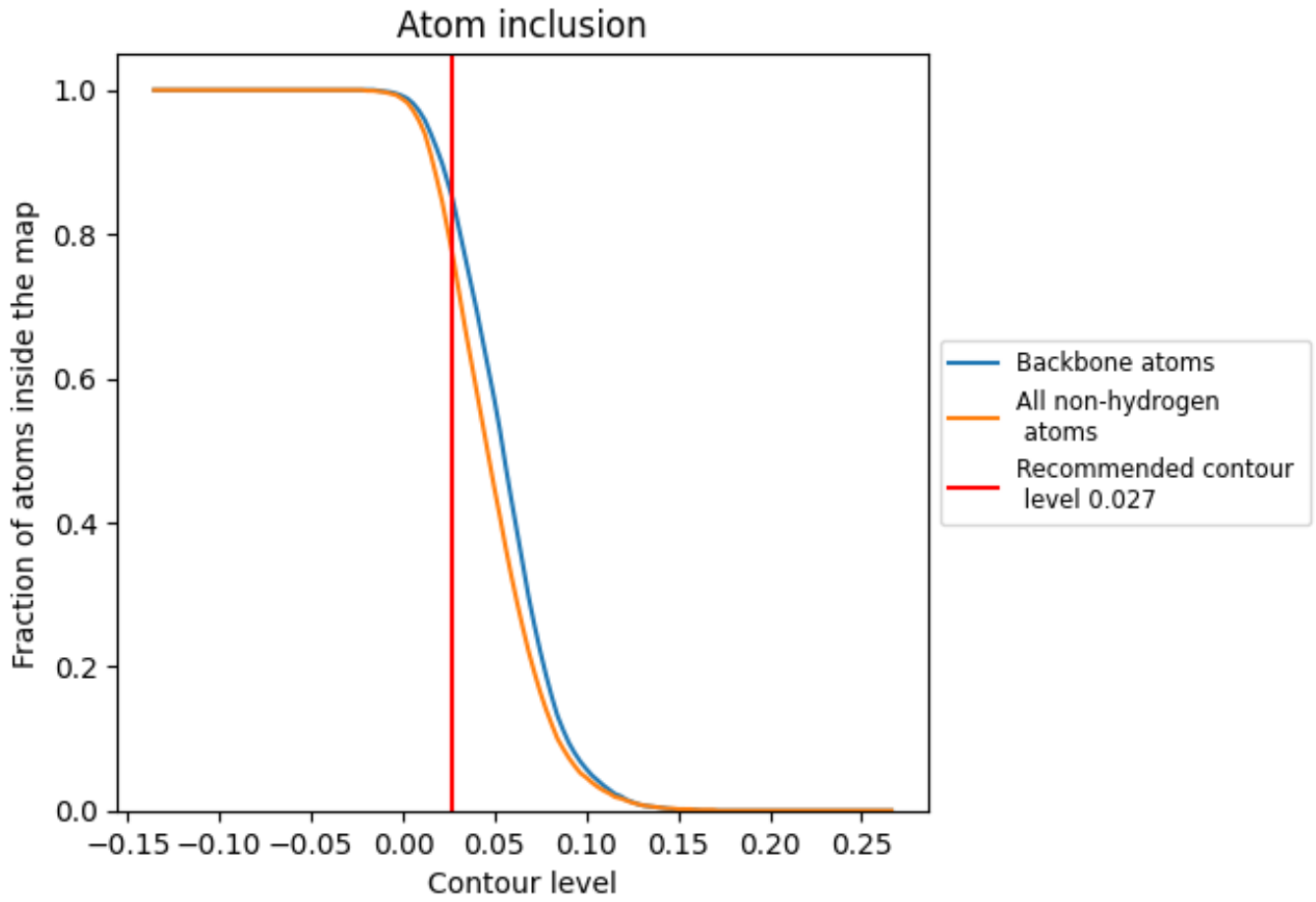
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5270
A	0.8340	0.5520
B	0.8130	0.5490
C	0.7630	0.5320
D	0.7070	0.4900
E	0.7680	0.5020
F	0.7190	0.5000
G	0.6780	0.4620
I	0.5780	0.4370