Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 02:35 AM JST

PDB ID	:	6LOE / pdb_00006loe
EMDB ID	:	EMD-0937
Title	:	Cryo-EM structure of the dithionite-reduced photosynthetic alternative complex III from Roseiflexus castenholzii
Authors	:	Shi, Y.; Xin, Y.Y.; Wang, C.; Blankenship, R.E.; Sun, F.; Xu, X.L.
Deposited on	:	2020-01-05
Resolution	:	3.50 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:

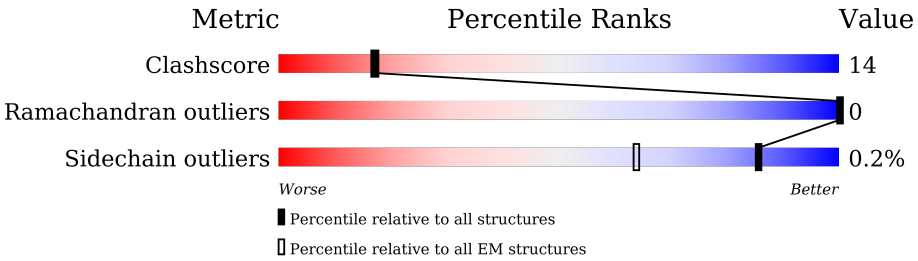
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

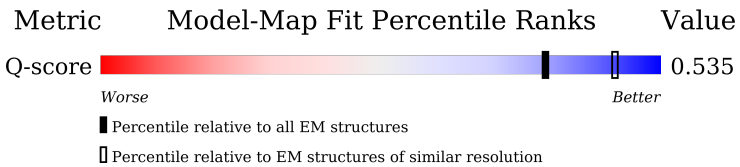
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	226	69% 28%
2	B	933	5% 65% 34%
3	C	471	66% 31%
4	D	192	11% 65% 26% 9%

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Mol	Chain	Length	Quality of chain
5	E	162	7% 72% 26%
6	F	414	71% 24% 5%

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
7	HEC	A	301	X	-	-	-
7	HEC	A	302	X	-	-	-
7	HEC	A	303	X	-	-	-
7	HEC	A	304	X	-	-	-
7	HEC	A	305	X	-	-	-
7	HEC	E	201	X	-	-	-
8	SF4	B	1101	-	-	X	-
8	SF4	B	1102	-	-	X	-
8	SF4	B	1103	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 18785 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 MULTIHEME_CYTC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	218	1763	1123	322	303	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	929	7176	4519	1264	1358	35	0	0

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	456	3728	2531	589	595	13	0	0

- Molecule 4 is a protein called Uncharacterized protein ActD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	174	1348	884	218	239	7	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	158	1253	783	234	230	6	0	0

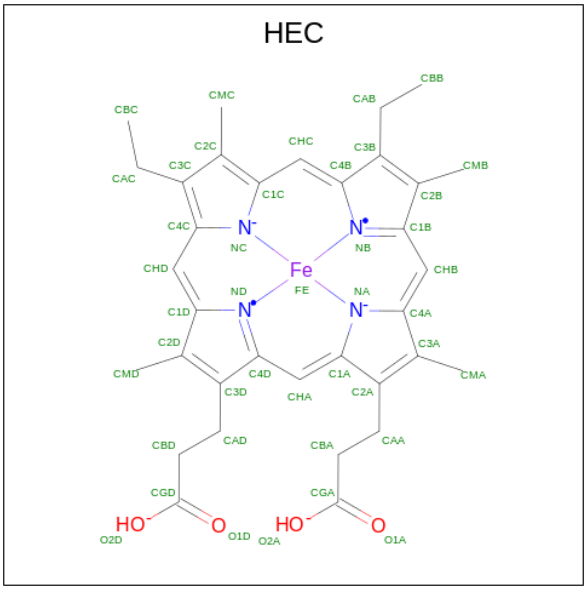
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	32	ACE	-	acetylation	UNP A7NJ91

- Molecule 6 is a protein called Uncharacterized protein ActF.

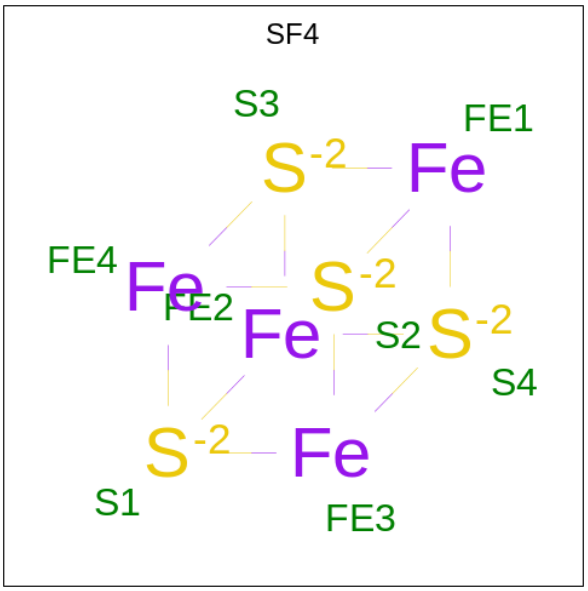
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	395	3159	2130	512	503	14	0	0

- Molecule 7 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



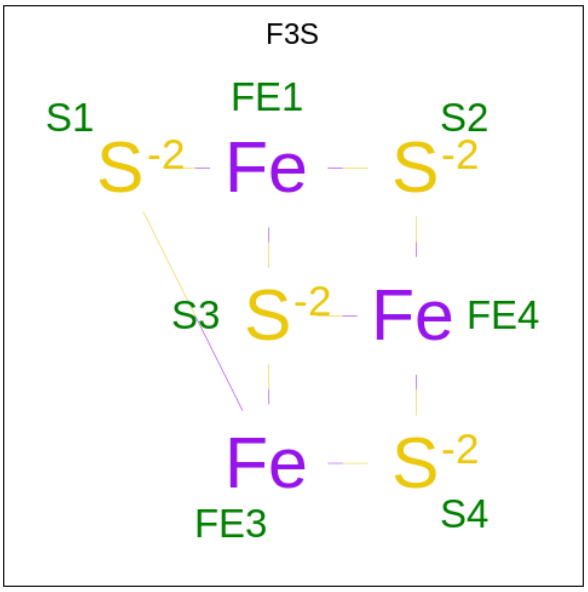
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
7	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	A	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	E	1	43	34	1	4	4	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



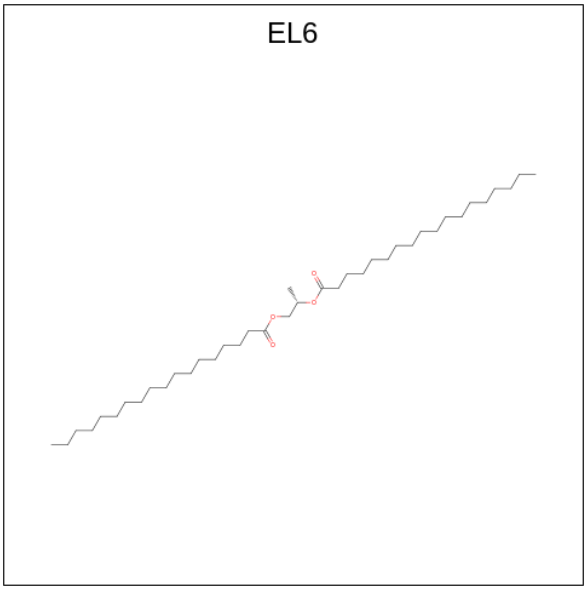
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
8	B	1	8	4	4	0
8	B	1	8	4	4	0
8	B	1	8	4	4	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is [(2S)-2-octadecanoyloxypropyl] octadecanoate (CCD ID: EL6) (formula: $C_{39}H_{76}O_4$).



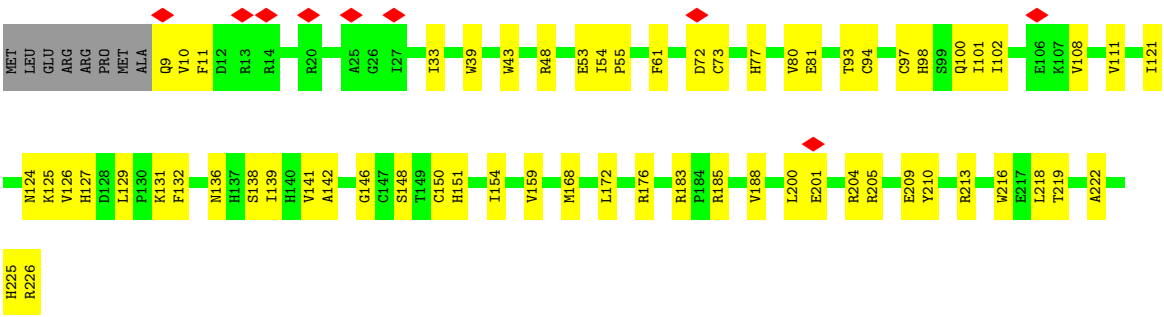
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	B	1	26	22	4	0
			Total	C	O	
10	E	1	43	39	4	0

3 Residue-property plots (i)

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

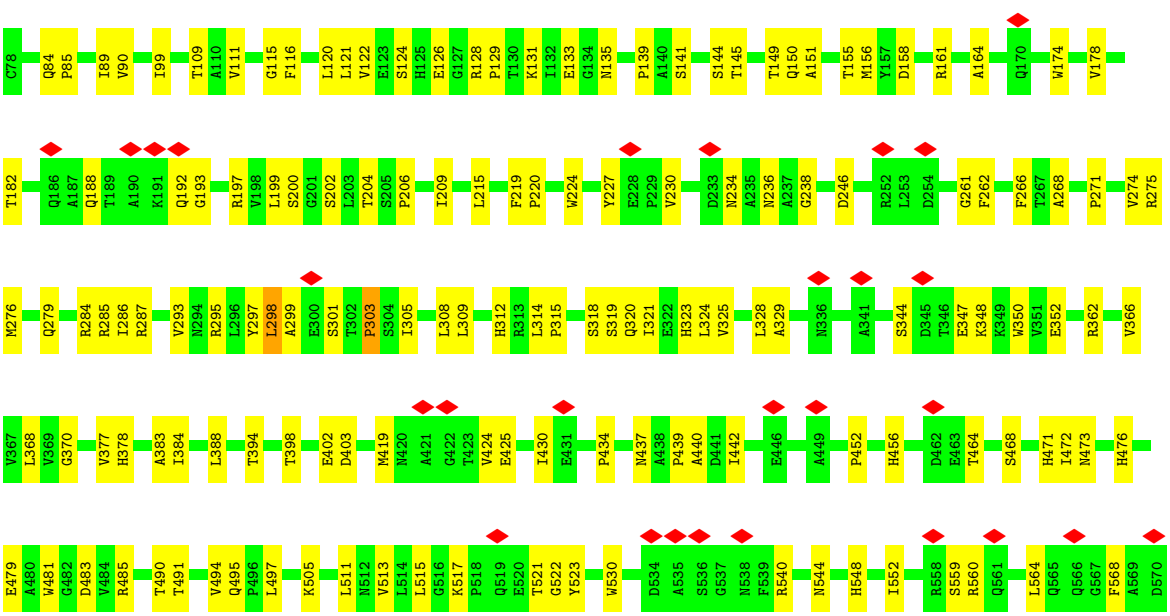
• Molecule 1: MULTIHEME_CYTC domain-containing protein

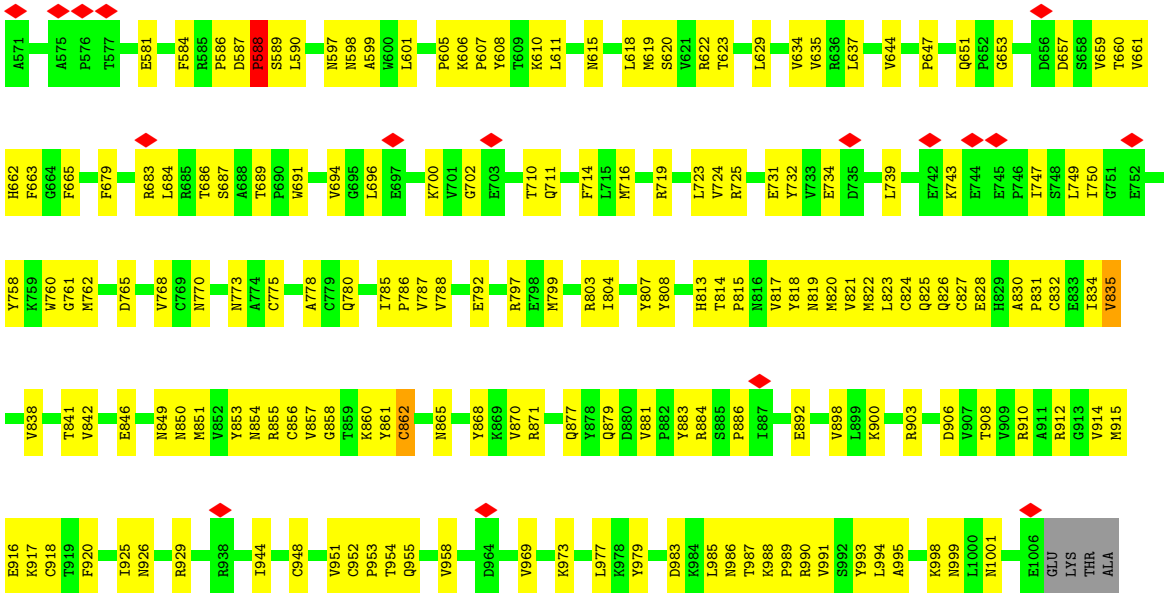
Chain A: 69% 28%



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

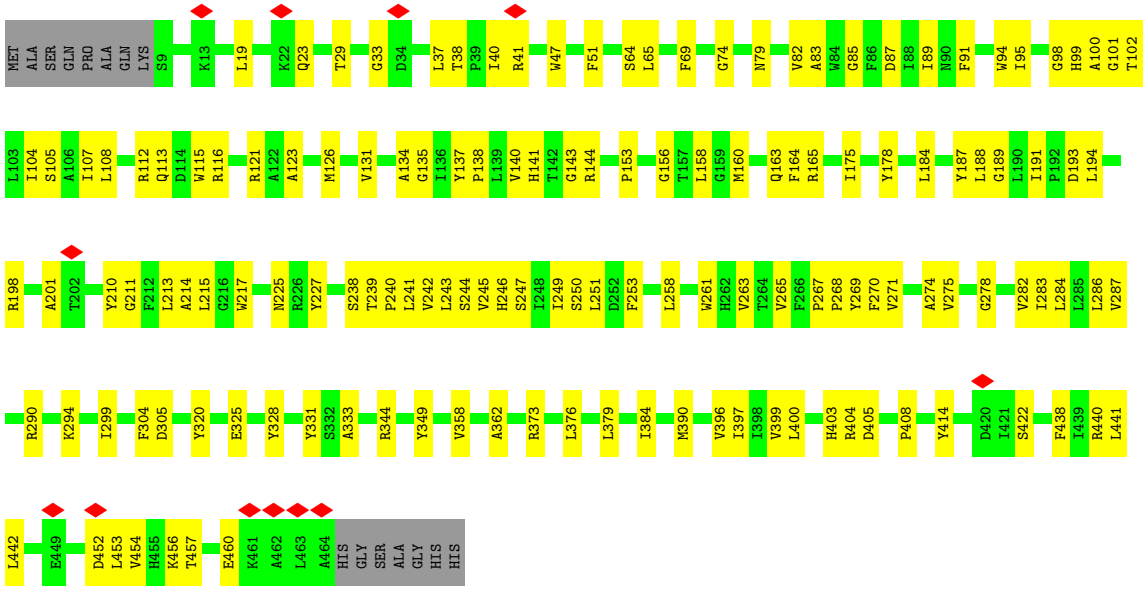
Chain B: 5% 65% 34%





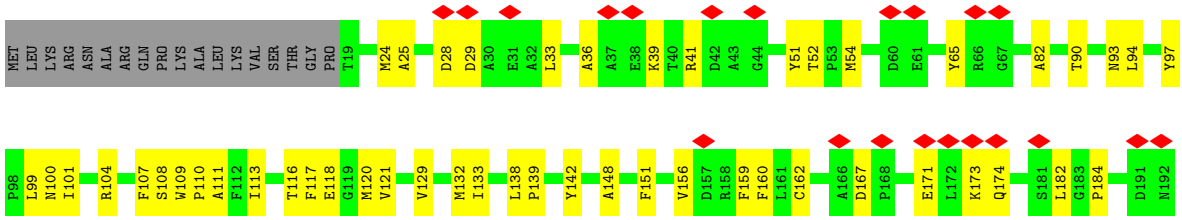
- Molecule 3: Polysulphide reductase NrfD

Chain C:



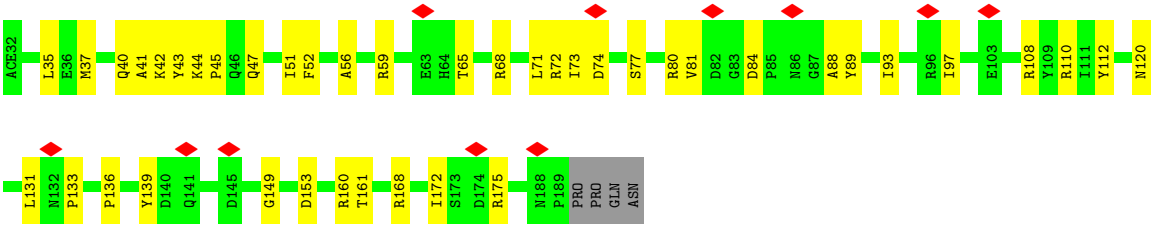
- Molecule 4: Uncharacterized protein ActD

Chain D:



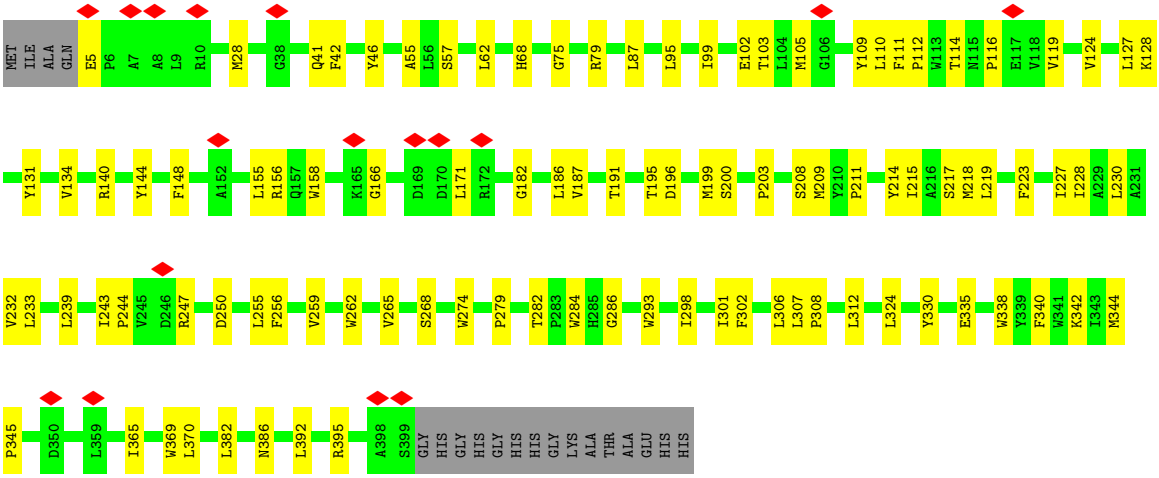
• Molecule 5: Cytochrome c domain-containing protein

Chain E:



• Molecule 6: Uncharacterized protein ActF

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	207633	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 ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0321	Depositor
Map size (Å)	224.63998, 224.63998, 224.63998	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, F3S, EL6, HEC, SF4

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	0.23	0/1820	0.46	0/2479
2	B	0.31	0/7337	0.55	6/10002 (0.1%)
3	C	0.25	0/3869	0.44	0/5299
4	D	0.19	0/1389	0.44	0/1892
5	E	0.31	0/1280	0.59	1/1738 (0.1%)
6	F	0.21	0/3265	0.37	0/4460
All	All	0.27	0/18960	0.49	7/25870 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	588	PRO	N-CA-CB	-8.50	93.89	103.15
2	B	588	PRO	CB-CA-C	-7.35	100.77	113.20
2	B	588	PRO	CA-C-N	6.14	128.99	120.63
2	B	588	PRO	C-N-CA	6.14	128.99	120.63
2	B	298	LEU	N-CA-C	5.82	120.51	113.41
2	B	303	PRO	N-CA-CB	-5.77	98.08	103.27
5	E	80	ARG	CB-CA-C	5.35	120.76	109.79

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	1688	54	0
2	B	7176	0	7049	248	0
3	C	3728	0	3740	116	0
4	D	1348	0	1319	47	0
5	E	1253	0	1227	40	0
6	F	3159	0	3214	70	0
7	A	215	0	148	19	0
7	E	43	0	30	2	0
8	B	24	0	0	9	0
9	B	7	0	0	0	0
10	B	26	0	0	0	0
10	E	43	0	0	0	0
All	All	18785	0	18415	511	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 14.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:ASP:HB2	2:B:662:HIS:HB3	1.57	0.86
1:A:146:GLY:HA2	1:A:188:VAL:HG13	1.61	0.83
2:B:952:CYS:SG	8:B:1101:SF4:S3	2.75	0.83
2:B:124:SER:HB2	2:B:497:LEU:HD23	1.64	0.78
3:C:184:LEU:HB3	4:D:129:VAL:HG21	1.66	0.76
2:B:851:MET:SD	2:B:871:ARG:NH2	2.59	0.74
2:B:716:MET:HG3	2:B:723:LEU:HD12	1.69	0.73
2:B:834:ILE:HA	3:C:163:GLN:HE22	1.53	0.72
2:B:383:ALA:HA	2:B:564:LEU:HD21	1.70	0.71
2:B:762:MET:HB3	2:B:991:VAL:HG12	1.73	0.71
3:C:95:ILE:HG21	3:C:249:ILE:HD13	1.72	0.70
2:B:158:ASP:OD2	2:B:597:ASN:ND2	2.25	0.70
3:C:113:GLN:OE1	3:C:115:TRP:NE1	2.26	0.69
3:C:349:TYR:HB2	3:C:400:LEU:HD13	1.74	0.69
2:B:653:GLY:HA2	2:B:815:PRO:HD2	1.75	0.68
2:B:308:LEU:HG	2:B:819:ASN:HD21	1.57	0.68
2:B:131:LYS:NZ	2:B:133:GLU:OE1	2.24	0.67
2:B:826:GLN:NE2	2:B:918:CYS:O	2.26	0.67
3:C:38:THR:O	3:C:440:ARG:NH2	2.28	0.67
2:B:548:HIS:NE2	5:E:68:ARG:O	2.28	0.66
3:C:19:LEU:HD12	3:C:23:GLN:HG3	1.77	0.66
6:F:166:GLY:HA2	6:F:386:ASN:HD22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:SER:HB3	2:B:430:ILE:HD12	1.78	0.66
2:B:129:PRO:HB3	2:B:497:LEU:HD22	1.79	0.65
1:A:81:GLU:OE2	5:E:108:ARG:NH2	2.30	0.64
6:F:103:THR:HG22	6:F:134:VAL:HG13	1.79	0.64
2:B:151:ALA:HB3	2:B:601:LEU:HD23	1.79	0.64
2:B:586:PRO:HA	2:B:663:PHE:HB2	1.78	0.64
2:B:200:SER:OG	2:B:224:TRP:NE1	2.29	0.64
2:B:634:VAL:HB	2:B:702:GLY:HA3	1.79	0.64
2:B:832:CYS:SG	2:B:871:ARG:NH1	2.69	0.64
4:D:148:ALA:HB3	4:D:151:PHE:HB2	1.79	0.64
2:B:325:VAL:HG11	2:B:377:VAL:HG13	1.80	0.64
6:F:244:PRO:HG2	6:F:247:ARG:HB2	1.79	0.63
2:B:608:TYR:HE2	2:B:817:VAL:HG21	1.63	0.63
1:A:148:SER:HB2	1:A:183:ARG:HH22	1.64	0.63
6:F:284:TRP:HZ2	6:F:342:LYS:HG3	1.63	0.63
1:A:77:HIS:CE1	7:A:304:HEC:ND	2.68	0.62
2:B:197:ARG:HD3	2:B:424:VAL:HG22	1.81	0.62
4:D:113:ILE:HA	4:D:116:THR:HG22	1.81	0.62
2:B:842:VAL:HG12	4:D:101:ILE:HD12	1.82	0.61
2:B:483:ASP:HA	2:B:494:VAL:H	1.64	0.61
3:C:79:ASN:HD21	3:C:414:TYR:H	1.47	0.61
2:B:948:CYS:HB3	8:B:1102:SF4:S2	2.40	0.61
2:B:908:THR:O	2:B:910:ARG:NH1	2.34	0.61
4:D:33:LEU:HD22	4:D:159:PHE:HB3	1.82	0.61
3:C:138:PRO:HA	3:C:141:HIS:HD2	1.65	0.61
2:B:193:GLY:HA3	2:B:219:PHE:HB3	1.83	0.61
2:B:832:CYS:SG	8:B:1103:SF4:S1	2.99	0.61
2:B:723:LEU:HD11	3:C:408:PRO:HD2	1.82	0.60
3:C:188:LEU:HD11	4:D:132:MET:HE3	1.81	0.60
4:D:82:ALA:HB2	4:D:120:MET:HB2	1.81	0.60
6:F:227:ILE:HG21	6:F:324:LEU:HG	1.83	0.60
1:A:139:ILE:HG21	7:A:302:HEC:HAA2	1.82	0.60
3:C:305:ASP:OD1	3:C:373:ARG:NH1	2.35	0.60
2:B:912:ARG:NH2	3:C:69:PHE:O	2.34	0.60
3:C:153:PRO:HG3	3:C:164:PHE:HZ	1.66	0.60
2:B:293:VAL:HB	2:B:999:ASN:HD22	1.65	0.60
2:B:828:GLU:HG2	2:B:990:ARG:HH21	1.66	0.60
5:E:160:ARG:NH1	7:E:201:HEC:O2D	2.32	0.59
5:E:43:TYR:HA	5:E:47:GLN:HE21	1.67	0.59
2:B:370:GLY:O	2:B:378:HIS:NE2	2.34	0.59
3:C:217:TRP:HA	4:D:138:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:GLN:NE2	2:B:993:TYR:OH	2.31	0.59
3:C:137:TYR:HA	3:C:140:VAL:HG12	1.83	0.59
3:C:163:GLN:HG3	4:D:101:ILE:HD13	1.83	0.59
3:C:261:TRP:NE1	3:C:397:ILE:O	2.35	0.59
1:A:222:ALA:O	2:B:926:ASN:ND2	2.36	0.58
6:F:209:MET:HE2	6:F:265:VAL:HA	1.85	0.58
2:B:725:ARG:NH1	2:B:739:LEU:O	2.36	0.58
5:E:72:ARG:HE	5:E:172:ILE:HD11	1.68	0.58
3:C:105:SER:O	3:C:116:ARG:NH1	2.29	0.58
7:A:301:HEC:HMA3	2:B:855:ARG:HD3	1.85	0.58
4:D:24:MET:HE2	4:D:160:PHE:HB3	1.86	0.58
1:A:176:ARG:HE	4:D:97:TYR:HD1	1.49	0.58
2:B:958:VAL:HG12	2:B:969:VAL:HG22	1.86	0.58
6:F:215:ILE:HA	6:F:218:MET:HE2	1.85	0.58
2:B:831:PRO:O	2:B:865:ASN:ND2	2.37	0.57
2:B:588:PRO:HG2	2:B:607:PRO:HD2	1.86	0.57
2:B:860:LYS:HG3	3:C:83:ALA:HB1	1.84	0.57
5:E:72:ARG:HG3	5:E:77:SER:HB3	1.86	0.57
2:B:495:GLN:HE21	5:E:65:THR:HB	1.68	0.57
2:B:236:ASN:ND2	2:B:402:GLU:OE2	2.36	0.57
2:B:832:CYS:HG	8:B:1103:SF4:FE2	1.21	0.57
2:B:188:GLN:NE2	2:B:425:GLU:OE1	2.37	0.57
3:C:263:VAL:HG21	3:C:325:GLU:HG3	1.86	0.57
2:B:926:ASN:OD1	2:B:929:ARG:NH2	2.37	0.57
6:F:62:LEU:HD22	6:F:219:LEU:HD21	1.86	0.57
1:A:213:ARG:NH2	7:A:302:HEC:O2A	2.38	0.57
6:F:140:ARG:NH1	6:F:196:ASP:OD1	2.38	0.57
3:C:246:HIS:HD2	3:C:270:PHE:HB3	1.70	0.57
2:B:209:ILE:HG12	2:B:403:ASP:HB3	1.86	0.56
2:B:599:ALA:HB1	2:B:787:VAL:HG11	1.87	0.56
3:C:112:ARG:NH2	6:F:250:ASP:OD1	2.38	0.56
3:C:165:ARG:NH2	4:D:93:ASN:OD1	2.34	0.56
1:A:93:THR:HA	5:E:168:ARG:HH21	1.70	0.56
2:B:434:PRO:HD2	2:B:464:THR:HG21	1.88	0.56
3:C:87:ASP:OD1	3:C:87:ASP:N	2.37	0.56
4:D:171:GLU:HB2	4:D:174:GLN:HB3	1.87	0.56
2:B:285:ARG:NH2	2:B:954:THR:O	2.39	0.56
1:A:39:TRP:HA	1:A:43:TRP:HB2	1.87	0.56
3:C:290:ARG:HD2	3:C:304:PHE:HE2	1.71	0.56
2:B:786:PRO:HG2	2:B:799:MET:HG3	1.88	0.56
1:A:142:ALA:O	1:A:185:ARG:NE	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:MET:HB3	5:E:40:GLN:HE21	1.70	0.56
2:B:178:VAL:HG13	2:B:513:VAL:HG13	1.88	0.55
3:C:64:SER:OG	3:C:422:SER:OG	2.23	0.55
2:B:161:ARG:NH1	2:B:479:GLU:OE2	2.38	0.55
2:B:637:LEU:HB3	2:B:696:LEU:HD11	1.88	0.55
1:A:200:LEU:O	1:A:201:GLU:HG3	2.06	0.55
2:B:320:GLN:HA	2:B:323:HIS:CE1	2.41	0.55
3:C:283:ILE:HG21	3:C:379:LEU:HG	1.89	0.55
6:F:41:GLN:HE22	6:F:344:MET:HE1	1.72	0.55
1:A:218:LEU:HD11	7:A:302:HEC:HBD1	1.89	0.55
2:B:262:PHE:HZ	2:B:328:LEU:HD13	1.71	0.55
6:F:55:ALA:HB1	6:F:218:MET:HG2	1.87	0.55
4:D:109:TRP:CD1	4:D:110:PRO:HD3	2.41	0.54
4:D:133:ILE:HG12	4:D:138:LEU:HD23	1.89	0.54
2:B:842:VAL:HG11	4:D:99:LEU:HD13	1.88	0.54
3:C:104:ILE:HA	3:C:108:LEU:HD12	1.90	0.54
2:B:383:ALA:HB2	2:B:568:PHE:HZ	1.71	0.54
3:C:121:ARG:NH2	3:C:189:GLY:O	2.41	0.54
6:F:75:GLY:O	6:F:79:ARG:N	2.40	0.54
6:F:95:LEU:HD13	6:F:365:ILE:HG23	1.90	0.54
6:F:308:PRO:HG3	6:F:330:TYR:HE2	1.72	0.54
2:B:227:TYR:OH	2:B:437:ASN:O	2.25	0.54
2:B:587:ASP:HB3	2:B:590:LEU:O	2.08	0.54
6:F:57:SER:HB2	6:F:369:TRP:HE1	1.72	0.54
5:E:93:ILE:HG21	5:E:97:ILE:HD11	1.90	0.54
6:F:256:PHE:HB2	6:F:312:LEU:HB3	1.90	0.54
2:B:618:LEU:HB2	2:B:660:THR:HG22	1.88	0.54
3:C:175:ILE:HD11	3:C:249:ILE:HD11	1.90	0.54
2:B:635:VAL:HA	2:B:700:LYS:HA	1.90	0.53
5:E:136:PRO:HD3	7:E:201:HEC:HAD2	1.90	0.53
1:A:55:PRO:O	1:A:124:ASN:ND2	2.41	0.53
2:B:724:VAL:HB	2:B:820:MET:HB2	1.89	0.53
3:C:287:VAL:HG13	3:C:376:LEU:HD13	1.91	0.53
2:B:145:THR:OG1	2:B:150:GLN:OE1	2.17	0.53
6:F:131:TYR:O	6:F:140:ARG:NH2	2.42	0.53
2:B:615:ASN:HB2	2:B:665:PHE:CG	2.44	0.53
3:C:238:SER:HA	3:C:241:LEU:HB3	1.91	0.53
6:F:195:THR:HA	6:F:199:MET:HB3	1.91	0.53
2:B:823:LEU:HD11	2:B:991:VAL:HG11	1.91	0.53
2:B:846:GLU:OE2	2:B:929:ARG:NE	2.40	0.53
3:C:65:LEU:HD22	3:C:140:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:LEU:HB2	3:C:261:TRP:HB2	1.91	0.53
6:F:196:ASP:O	6:F:200:SER:OG	2.26	0.53
2:B:204:THR:HG22	2:B:402:GLU:HB3	1.90	0.52
5:E:84:ASP:N	5:E:84:ASP:OD1	2.42	0.52
6:F:111:PHE:O	6:F:114:THR:OG1	2.27	0.52
2:B:312:HIS:CE1	2:B:1001:ASN:H	2.27	0.52
1:A:100:GLN:HE21	5:E:131:LEU:HD22	1.73	0.52
2:B:286:ILE:O	2:B:287:ARG:NH1	2.42	0.52
3:C:243:LEU:HD13	3:C:271:VAL:HG11	1.89	0.52
2:B:344:SER:HB3	2:B:347:GLU:HB2	1.92	0.52
2:B:822:MET:HE2	2:B:868:TYR:HB3	1.92	0.52
2:B:366:VAL:HB	2:B:394:THR:HG21	1.90	0.52
3:C:102:THR:OG1	3:C:242:VAL:HG11	2.09	0.52
3:C:240:PRO:HB2	4:D:117:PHE:HZ	1.74	0.52
3:C:333:ALA:HB1	6:F:127:LEU:HD12	1.91	0.52
2:B:139:PRO:HG2	2:B:490:THR:HG21	1.92	0.52
2:B:111:VAL:HG11	2:B:149:THR:HG23	1.92	0.52
2:B:320:GLN:O	2:B:324:LEU:N	2.42	0.52
2:B:540:ARG:O	2:B:544:ASN:ND2	2.38	0.52
2:B:835:VAL:HG13	2:B:835:VAL:O	2.10	0.52
5:E:71:LEU:HG	5:E:73:ILE:HG12	1.91	0.52
3:C:99:HIS:NE2	3:C:246:HIS:HB2	2.25	0.52
5:E:120:ASN:O	5:E:139:TYR:OH	2.20	0.52
6:F:233:LEU:HD13	6:F:382:LEU:HD21	1.91	0.52
2:B:747:ILE:HG21	6:F:286:GLY:HA3	1.91	0.52
2:B:749:LEU:HD12	6:F:274:TRP:HA	1.91	0.52
2:B:456:HIS:O	2:B:472:ILE:N	2.41	0.51
2:B:719:ARG:NH2	3:C:405:ASP:O	2.42	0.51
2:B:855:ARG:O	2:B:855:ARG:HG3	2.10	0.51
3:C:460:GLU:OE1	6:F:395:ARG:NH2	2.40	0.51
4:D:36:ALA:HB1	4:D:182:LEU:HD23	1.92	0.51
5:E:44:LYS:HD2	5:E:45:PRO:HD2	1.92	0.51
2:B:268:ALA:HA	2:B:305:ILE:HD11	1.92	0.51
2:B:155:THR:OG1	2:B:598:ASN:ND2	2.43	0.51
3:C:95:ILE:O	3:C:99:HIS:ND1	2.40	0.51
3:C:40:ILE:O	3:C:41:ARG:HG2	2.10	0.51
4:D:25:ALA:HB1	4:D:184:PRO:HB3	1.93	0.51
2:B:295:ARG:NH1	2:B:999:ASN:OD1	2.43	0.51
1:A:72:ASP:OD1	5:E:110:ARG:NH1	2.42	0.51
3:C:82:VAL:HG11	3:C:414:TYR:HB2	1.93	0.51
3:C:100:ALA:HB2	3:C:275:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:761:GLY:HA2	2:B:990:ARG:HG3	1.92	0.51
2:B:314:LEU:HD21	2:B:347:GLU:HG2	1.91	0.51
1:A:176:ARG:HG2	1:A:219:THR:HG21	1.92	0.50
2:B:589:SER:HB3	2:B:601:LEU:O	2.10	0.50
3:C:101:GLY:HA2	3:C:123:ALA:HB1	1.91	0.50
3:C:194:LEU:HD21	3:C:442:LEU:HD22	1.93	0.50
2:B:851:MET:HB2	2:B:917:LYS:HE3	1.93	0.50
2:B:862:CYS:SG	2:B:915:MET:SD	3.09	0.50
3:C:453:LEU:O	3:C:457:THR:OG1	2.26	0.50
1:A:54:ILE:HB	1:A:126:VAL:HG12	1.94	0.50
2:B:303:PRO:HG3	2:B:651:GLN:HG2	1.94	0.50
2:B:425:GLU:HA	2:B:452:PRO:HD2	1.92	0.50
2:B:491:THR:HG23	2:B:552:ILE:HB	1.93	0.50
2:B:689:THR:O	2:B:689:THR:OG1	2.28	0.50
6:F:158:TRP:HB3	6:F:171:LEU:HD11	1.92	0.50
2:B:765:ASP:HA	2:B:994:LEU:HB2	1.94	0.50
2:B:910:ARG:NE	2:B:916:GLU:OE1	2.44	0.50
2:B:831:PRO:HD3	2:B:987:THR:HG22	1.93	0.50
6:F:298:ILE:HA	6:F:301:ILE:HD12	1.94	0.50
2:B:760:TRP:CD1	2:B:846:GLU:HB3	2.47	0.50
3:C:85:GLY:HA3	3:C:414:TYR:CZ	2.46	0.50
3:C:178:TYR:HB2	3:C:245:VAL:HG21	1.94	0.50
3:C:253:PHE:O	3:C:261:TRP:HB3	2.12	0.50
3:C:98:GLY:O	3:C:178:TYR:OH	2.29	0.50
6:F:182:GLY:O	6:F:186:LEU:N	2.43	0.50
2:B:246:ASP:O	2:B:560:ARG:NH2	2.45	0.49
2:B:287:ARG:O	2:B:732:TYR:OH	2.29	0.49
2:B:973:LYS:NZ	2:B:990:ARG:O	2.44	0.49
3:C:29:THR:HG21	4:D:156:VAL:HG13	1.94	0.49
2:B:199:LEU:HD23	2:B:434:PRO:HG3	1.95	0.49
3:C:403:HIS:CD2	3:C:404:ARG:HG3	2.48	0.49
2:B:778:ALA:HB2	2:B:951:VAL:HG11	1.95	0.49
3:C:198:ARG:HD3	3:C:211:GLY:HA2	1.94	0.49
3:C:333:ALA:HB3	6:F:124:VAL:HG13	1.93	0.49
2:B:122:VAL:HB	2:B:497:LEU:HD21	1.95	0.49
2:B:629:LEU:HD21	2:B:700:LYS:HB2	1.95	0.49
2:B:797:ARG:NH1	3:C:74:GLY:O	2.32	0.49
3:C:225:ASN:HD22	4:D:65:TYR:HD2	1.60	0.49
2:B:84:GLN:HA	5:E:35:LEU:HD21	1.95	0.49
3:C:244:SER:HA	3:C:247:SER:HB3	1.94	0.49
2:B:881:VAL:HG13	2:B:886:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ALA:HB3	3:C:278:GLY:HA3	1.95	0.49
7:A:301:HEC:HBB2	4:D:97:TYR:HE2	1.77	0.49
3:C:94:TRP:HB3	3:C:134:ALA:HB2	1.95	0.49
3:C:126:MET:HE2	3:C:282:VAL:HG22	1.95	0.49
4:D:29:ASP:OD1	4:D:29:ASP:N	2.46	0.48
1:A:185:ARG:N	1:A:210:TYR:OH	2.47	0.48
2:B:581:GLU:HB2	2:B:694:VAL:HG12	1.95	0.48
2:B:605:PRO:O	2:B:773:ASN:ND2	2.46	0.48
2:B:644:VAL:HB	2:B:684:LEU:HD21	1.94	0.48
2:B:315:PRO:HG3	2:B:814:THR:HG22	1.96	0.48
2:B:925:ILE:HA	2:B:944:ILE:HD13	1.94	0.48
3:C:210:TYR:OH	3:C:441:LEU:O	2.28	0.48
4:D:28:ASP:OD1	4:D:28:ASP:N	2.45	0.48
6:F:144:TYR:HB3	6:F:148:PHE:CE2	2.49	0.48
2:B:540:ARG:HE	5:E:84:ASP:HB3	1.79	0.48
2:B:584:PHE:N	2:B:691:TRP:O	2.46	0.48
4:D:109:TRP:CG	4:D:110:PRO:HD3	2.48	0.48
5:E:81:VAL:HG22	5:E:88:ALA:H	1.78	0.48
6:F:46:TYR:OH	6:F:95:LEU:O	2.30	0.48
2:B:298:LEU:HG	2:B:298:LEU:O	2.14	0.48
6:F:255:LEU:O	6:F:259:VAL:HG23	2.14	0.48
2:B:164:ALA:N	2:B:473:ASN:HD21	2.11	0.47
3:C:265:VAL:HB	6:F:208:SER:HB2	1.96	0.47
2:B:121:LEU:N	2:B:133:GLU:O	2.46	0.47
2:B:827:CYS:HB3	2:B:987:THR:HB	1.96	0.47
3:C:107:ILE:HG12	3:C:239:THR:HG23	1.96	0.47
1:A:141:VAL:HG13	1:A:188:VAL:HG11	1.97	0.47
2:B:440:ALA:HB2	2:B:683:ARG:HA	1.95	0.47
2:B:615:ASN:HB3	2:B:679:PHE:HB3	1.97	0.47
2:B:856:CYS:O	3:C:144:ARG:NH1	2.42	0.47
2:B:977:LEU:HB3	2:B:995:ALA:H	1.79	0.47
5:E:149:GLY:O	5:E:153:ASP:N	2.46	0.47
1:A:94:CYS:HA	7:A:305:HEC:HHC	1.97	0.47
1:A:151:HIS:HB3	1:A:154:ILE:HD11	1.95	0.47
2:B:731:GLU:HA	2:B:734:GLU:HG2	1.96	0.47
3:C:29:THR:O	3:C:33:GLY:N	2.42	0.47
1:A:102:ILE:HG13	1:A:108:VAL:HG11	1.95	0.47
1:A:127:HIS:HD2	7:A:304:HEC:HAA1	1.79	0.47
2:B:620:SER:HB3	2:B:623:THR:HG22	1.97	0.47
3:C:138:PRO:HA	3:C:141:HIS:CD2	2.49	0.47
2:B:224:TRP:HH2	2:B:511:LEU:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ASP:N	2:B:403:ASP:OD1	2.43	0.47
2:B:827:CYS:HB2	2:B:830:ALA:HA	1.97	0.47
5:E:108:ARG:HD2	5:E:112:TYR:HE2	1.80	0.47
6:F:302:PHE:HA	6:F:306:LEU:HB2	1.97	0.47
1:A:131:LYS:HD3	5:E:44:LYS:HG3	1.96	0.47
2:B:99:ILE:HD12	2:B:126:GLU:HA	1.96	0.47
2:B:481:TRP:CD1	2:B:523:TYR:HB2	2.49	0.47
4:D:133:ILE:HG23	4:D:138:LEU:HB3	1.97	0.47
2:B:158:ASP:OD1	2:B:883:TYR:OH	2.30	0.47
2:B:517:LYS:HE3	2:B:517:LYS:HB2	1.78	0.47
2:B:725:ARG:HD2	2:B:739:LEU:HD13	1.96	0.46
2:B:824:CYS:H	2:B:918:CYS:HB3	1.80	0.46
2:B:877:GLN:HG2	2:B:892:GLU:HB2	1.96	0.46
2:B:879:GLN:O	2:B:884:ARG:NH1	2.43	0.46
2:B:914:VAL:HG23	3:C:144:ARG:HD2	1.98	0.46
2:B:952:CYS:HG	8:B:1101:SF4:FE2	1.29	0.46
6:F:214:TYR:O	6:F:218:MET:N	2.45	0.46
2:B:321:ILE:HA	2:B:324:LEU:HB3	1.97	0.46
2:B:723:LEU:HD13	2:B:807:TYR:CZ	2.50	0.46
2:B:584:PHE:HB3	2:B:663:PHE:CZ	2.51	0.46
6:F:187:VAL:O	6:F:191:THR:HG23	2.15	0.46
1:A:111:VAL:HG12	1:A:121:ILE:HD11	1.97	0.46
1:A:136:ASN:HD22	1:A:226:ARG:HH22	1.63	0.46
4:D:90:THR:HG23	4:D:94:LEU:HD13	1.97	0.46
6:F:102:GLU:HA	6:F:105:MET:HG2	1.98	0.46
1:A:148:SER:C	1:A:150:CYS:H	2.23	0.46
1:A:216:TRP:CZ2	4:D:100:ASN:HB2	2.51	0.46
2:B:634:VAL:HA	2:B:647:PRO:HA	1.97	0.46
2:B:825:GLN:HB3	2:B:989:PRO:HB3	1.97	0.46
6:F:128:LYS:NZ	6:F:203:PRO:O	2.36	0.46
2:B:90:VAL:HG21	5:E:56:ALA:HA	1.98	0.46
2:B:439:PRO:HG2	2:B:442:ILE:HD12	1.98	0.46
3:C:37:LEU:HD13	3:C:201:ALA:HA	1.98	0.46
3:C:390:MET:HE3	3:C:390:MET:HB3	1.79	0.46
1:A:98:HIS:HE1	7:A:305:HEC:ND	2.10	0.46
2:B:301:SER:HB3	2:B:318:SER:HB2	1.98	0.46
2:B:456:HIS:ND1	2:B:471:HIS:HD2	2.14	0.46
2:B:804:ILE:HA	2:B:821:VAL:HA	1.97	0.46
3:C:286:LEU:HD22	3:C:299:ILE:HD13	1.98	0.46
6:F:28:MET:HE1	6:F:46:TYR:HE1	1.80	0.46
1:A:168:MET:HE1	3:C:160:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LYS:HA	2:B:505:LYS:HD3	1.77	0.46
3:C:121:ARG:NH1	3:C:193:ASP:OD2	2.44	0.46
3:C:320:TYR:CE1	6:F:191:THR:HG21	2.51	0.46
1:A:129:LEU:HD12	7:A:303:HEC:HBD2	1.99	0.45
2:B:141:SER:HB2	2:B:144:SER:O	2.16	0.45
2:B:284:ARG:HG3	2:B:768:VAL:HG12	1.98	0.45
2:B:834:ILE:HG21	4:D:104:ARG:CZ	2.46	0.45
2:B:828:GLU:HB2	2:B:988:LYS:HB2	1.98	0.45
2:B:898:VAL:HG22	5:E:51:ILE:HD12	1.98	0.45
1:A:125:LYS:HB2	2:B:89:ILE:HG12	1.98	0.45
2:B:309:LEU:HG	2:B:770:ASN:HB3	1.98	0.45
2:B:803:ARG:O	2:B:822:MET:N	2.35	0.45
2:B:824:CYS:N	2:B:870:VAL:HG11	2.32	0.45
4:D:94:LEU:HD11	4:D:107:PHE:HB2	1.98	0.45
7:A:304:HEC:HHA	7:A:304:HEC:HBA1	1.99	0.45
2:B:605:PRO:HB2	2:B:610:LYS:HD2	1.98	0.45
6:F:191:THR:HG22	6:F:211:PRO:HB2	1.99	0.45
2:B:788:VAL:HG12	2:B:792:GLU:HB2	1.98	0.45
6:F:102:GLU:OE1	6:F:109:TYR:N	2.50	0.45
1:A:81:GLU:HA	1:A:138:SER:HA	1.98	0.45
1:A:101:ILE:HG22	1:A:102:ILE:HG23	1.99	0.45
2:B:780:GLN:HG2	2:B:785:ILE:HB	1.98	0.45
1:A:132:PHE:HB3	5:E:40:GLN:HE22	1.82	0.45
3:C:247:SER:O	3:C:251:LEU:HG	2.17	0.45
6:F:262:TRP:HZ2	6:F:338:TRP:CD1	2.35	0.45
2:B:215:LEU:HD13	2:B:515:LEU:HD12	1.99	0.45
5:E:74:ASP:OD1	5:E:74:ASP:N	2.49	0.45
1:A:205:ARG:NH1	1:A:209:GLU:OE1	2.51	0.44
3:C:131:VAL:O	3:C:135:GLY:N	2.40	0.44
5:E:52:PHE:CD2	5:E:59:ARG:HD3	2.52	0.44
2:B:115:GLY:O	2:B:204:THR:OG1	2.34	0.44
2:B:319:SER:OG	2:B:581:GLU:OE1	2.33	0.44
3:C:453:LEU:HA	3:C:456:LYS:HB2	1.99	0.44
1:A:61:PHE:CZ	7:A:304:HEC:HBC2	2.51	0.44
2:B:398:THR:HG22	2:B:559:SER:HA	1.99	0.44
6:F:124:VAL:HG12	6:F:128:LYS:HE3	2.00	0.44
1:A:53:GLU:HB3	1:A:159:VAL:HB	2.00	0.44
2:B:714:PHE:HB3	2:B:808:TYR:HD2	1.82	0.44
2:B:854:ASN:OD1	2:B:855:ARG:N	2.51	0.44
1:A:172:LEU:HD22	1:A:219:THR:HB	1.99	0.44
1:A:97:CYS:HB3	1:A:101:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:SER:O	2:B:202:SER:OG	2.36	0.44
2:B:266:PHE:HD2	2:B:276:MET:HB3	1.83	0.44
2:B:605:PRO:HG3	2:B:710:THR:HG21	1.99	0.44
2:B:303:PRO:HG3	2:B:651:GLN:CG	2.47	0.44
2:B:623:THR:O	2:B:623:THR:OG1	2.35	0.44
2:B:623:THR:HB	2:B:657:ASP:H	1.83	0.44
2:B:858:GLY:C	3:C:143:GLY:H	2.26	0.44
3:C:227:TYR:HA	4:D:132:MET:HE2	1.98	0.44
2:B:619:MET:HG2	2:B:659:VAL:HG12	2.00	0.43
2:B:749:LEU:HG	6:F:282:THR:HG23	1.99	0.43
2:B:954:THR:OG1	8:B:1101:SF4:S3	2.76	0.43
3:C:191:ILE:HG22	3:C:217:TRP:HB2	2.00	0.43
3:C:244:SER:OG	4:D:118:GLU:OE2	2.28	0.43
4:D:108:SER:HB2	6:F:274:TRP:CH2	2.53	0.43
1:A:73:CYS:HA	7:A:304:HEC:HHC	1.99	0.43
2:B:906:ASP:OD1	2:B:906:ASP:N	2.51	0.43
6:F:87:LEU:HD11	6:F:156:ARG:HG2	1.99	0.43
6:F:293:TRP:CD2	6:F:345:PRO:HG3	2.53	0.43
1:A:225:HIS:CE1	7:A:301:HEC:ND	2.87	0.43
2:B:835:VAL:O	2:B:835:VAL:CG1	2.67	0.43
3:C:284:LEU:HD21	3:C:384:ILE:HG12	2.00	0.43
6:F:307:LEU:HB3	6:F:308:PRO:HD3	1.99	0.43
2:B:760:TRP:CH2	2:B:944:ILE:HD12	2.54	0.43
2:B:853:TYR:HB3	2:B:914:VAL:HG11	2.00	0.43
3:C:246:HIS:CD2	3:C:270:PHE:HB3	2.53	0.43
6:F:284:TRP:CZ2	6:F:342:LYS:HG3	2.49	0.43
2:B:299:ALA:HB2	2:B:350:TRP:CH2	2.53	0.43
3:C:250:SER:HB2	3:C:270:PHE:HB2	2.00	0.43
2:B:824:CYS:SG	2:B:917:LYS:HD2	2.58	0.43
2:B:983:ASP:OD1	2:B:983:ASP:N	2.44	0.43
3:C:358:VAL:HA	3:C:362:ALA:HB3	2.00	0.43
2:B:743:LYS:HD2	2:B:743:LYS:HA	1.85	0.43
2:B:948:CYS:CB	8:B:1102:SF4:S2	3.02	0.43
4:D:167:ASP:N	4:D:167:ASP:OD1	2.51	0.43
5:E:133:PRO:HG2	5:E:161:THR:HG21	2.00	0.43
2:B:109:THR:O	2:B:120:LEU:N	2.52	0.43
2:B:178:VAL:O	2:B:182:THR:OG1	2.26	0.43
2:B:234:ASN:O	2:B:238:GLY:N	2.50	0.43
2:B:419:MET:HG3	2:B:424:VAL:HG21	2.01	0.43
2:B:985:LEU:HA	6:F:279:PRO:HD2	2.01	0.43
3:C:294:LYS:HA	3:C:294:LYS:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:230:LEU:HD22	6:F:239:LEU:HD11	2.00	0.43
2:B:868:TYR:HB2	2:B:870:VAL:HG23	2.01	0.43
3:C:452:ASP:C	3:C:454:VAL:H	2.26	0.43
4:D:24:MET:HE3	4:D:162:CYS:HB2	2.01	0.43
1:A:11:PHE:O	4:D:142:TYR:HB2	2.19	0.43
2:B:661:VAL:HG12	2:B:679:PHE:HZ	1.84	0.43
2:B:832:CYS:SG	2:B:849:ASN:ND2	2.92	0.43
3:C:165:ARG:HA	4:D:111:ALA:HB1	2.01	0.43
3:C:265:VAL:HA	6:F:209:MET:HB2	2.01	0.43
5:E:88:ALA:O	5:E:89:TYR:HB2	2.19	0.43
1:A:222:ALA:HB2	2:B:850:ASN:ND2	2.34	0.42
7:A:301:HEC:HBB2	4:D:97:TYR:CE2	2.53	0.42
5:E:77:SER:HA	5:E:172:ILE:HG12	2.00	0.42
6:F:42:PHE:O	6:F:46:TYR:N	2.47	0.42
2:B:230:VAL:HG13	2:B:691:TRP:HH2	1.84	0.42
2:B:622:ARG:HH21	2:B:813:HIS:CG	2.37	0.42
3:C:215:LEU:HB3	4:D:139:PRO:HA	2.01	0.42
4:D:138:LEU:HD12	4:D:138:LEU:HA	1.85	0.42
2:B:491:THR:HG21	2:B:530:TRP:CH2	2.54	0.42
3:C:187:TYR:OH	3:C:213:LEU:O	2.28	0.42
2:B:464:THR:O	2:B:468:SER:N	2.41	0.42
3:C:267:PRO:HG2	6:F:268:SER:HB3	1.99	0.42
6:F:68:HIS:HD2	6:F:155:LEU:HD22	1.83	0.42
2:B:135:ASN:OD1	5:E:68:ARG:NH2	2.52	0.42
2:B:297:TYR:HB3	2:B:350:TRP:CZ2	2.54	0.42
3:C:191:ILE:HG23	3:C:214:ALA:HA	2.01	0.42
3:C:194:LEU:HD13	3:C:213:LEU:HB3	2.01	0.42
2:B:329:ALA:HB2	2:B:384:ILE:HD11	2.02	0.42
2:B:986:ASN:HB2	6:F:279:PRO:HG3	2.01	0.42
2:B:998:LYS:HE3	2:B:998:LYS:HB2	1.72	0.42
2:B:206:PRO:HD3	2:B:485:ARG:HB2	2.00	0.42
4:D:39:LYS:C	4:D:41:ARG:H	2.28	0.42
6:F:112:PRO:HG2	6:F:203:PRO:HG3	2.01	0.42
2:B:131:LYS:HE2	2:B:150:GLN:NE2	2.35	0.42
3:C:265:VAL:O	3:C:269:TYR:HB3	2.19	0.42
5:E:72:ARG:HA	5:E:77:SER:HB2	2.00	0.42
6:F:99:ILE:HG23	6:F:110:LEU:HD13	2.01	0.42
2:B:456:HIS:HD1	2:B:471:HIS:HD2	1.68	0.42
2:B:584:PHE:HB2	2:B:691:TRP:HA	2.01	0.42
5:E:40:GLN:OE1	5:E:42:LYS:HE3	2.20	0.42
1:A:9:GLN:NE2	4:D:142:TYR:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:818:TYR:HE1	2:B:998:LYS:HD2	1.85	0.42
2:B:622:ARG:HE	2:B:622:ARG:HB2	1.69	0.41
3:C:241:LEU:HD13	4:D:121:VAL:HG11	2.02	0.41
3:C:376:LEU:HD23	3:C:376:LEU:HA	1.91	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.89	0.41
7:A:301:HEC:HMB3	7:A:301:HEC:HBB3	2.02	0.41
2:B:724:VAL:HA	2:B:979:TYR:OH	2.19	0.41
2:B:861:TYR:HD1	2:B:861:TYR:O	2.03	0.41
6:F:392:LEU:HD12	6:F:395:ARG:HE	1.85	0.41
1:A:9:GLN:HG2	1:A:10:VAL:O	2.20	0.41
3:C:278:GLY:O	3:C:282:VAL:HG23	2.20	0.41
4:D:52:THR:OG1	4:D:54:MET:O	2.35	0.41
6:F:223:PHE:O	6:F:227:ILE:HG13	2.21	0.41
2:B:85:PRO:HD3	5:E:35:LEU:HD21	2.03	0.41
2:B:275:ARG:HE	2:B:279:GLN:NE2	2.18	0.41
2:B:879:GLN:HG3	2:B:903:ARG:HH22	1.85	0.41
3:C:99:HIS:HB2	3:C:274:ALA:HB1	2.02	0.41
3:C:286:LEU:HA	3:C:286:LEU:HD23	1.83	0.41
3:C:325:GLU:CD	3:C:344:ARG:HH12	2.29	0.41
2:B:838:VAL:HG21	2:B:857:VAL:HG13	2.02	0.41
3:C:328:TYR:HA	3:C:331:TYR:HB3	2.02	0.41
5:E:172:ILE:HA	5:E:175:ARG:HB2	2.02	0.41
6:F:230:LEU:HB3	6:F:243:ILE:HD11	2.03	0.41
6:F:370:LEU:HD23	6:F:370:LEU:HA	1.90	0.41
1:A:98:HIS:HE1	7:A:305:HEC:C4D	2.34	0.41
2:B:128:ARG:NH2	5:E:43:TYR:O	2.54	0.41
2:B:174:TRP:CD2	2:B:505:LYS:HG3	2.56	0.41
2:B:274:VAL:HG13	2:B:953:PRO:HB3	2.02	0.41
2:B:285:ARG:HH22	2:B:955:GLN:HB2	1.84	0.41
2:B:305:ILE:HA	2:B:308:LEU:HD23	2.02	0.41
2:B:584:PHE:HA	2:B:661:VAL:HG22	2.02	0.41
2:B:714:PHE:HB3	2:B:808:TYR:CD2	2.55	0.41
2:B:775:CYS:CB	8:B:1101:SF4:S4	3.08	0.41
2:B:775:CYS:HB3	8:B:1101:SF4:S4	2.61	0.41
3:C:241:LEU:O	3:C:245:VAL:N	2.52	0.41
2:B:362:ARG:HE	2:B:388:LEU:HA	1.86	0.41
2:B:606:LYS:HG2	2:B:611:LEU:O	2.20	0.41
2:B:861:TYR:O	2:B:861:TYR:CD1	2.74	0.41
3:C:47:TRP:O	3:C:51:PHE:N	2.43	0.41
3:C:194:LEU:HB2	3:C:214:ALA:HB2	2.02	0.41
1:A:48:ARG:NH2	7:A:301:HEC:O2D	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:HB2	2:B:271:PRO:HB3	2.01	0.41
2:B:156:MET:HB2	2:B:476:HIS:ND1	2.35	0.41
2:B:192:GLN:HG2	2:B:220:PRO:HD2	2.03	0.41
2:B:491:THR:HG21	2:B:530:TRP:HH2	1.86	0.41
2:B:548:HIS:HB2	5:E:71:LEU:HD13	2.02	0.41
2:B:686:THR:O	2:B:687:SER:OG	2.36	0.41
2:B:826:GLN:HG3	2:B:920:PHE:CE2	2.56	0.41
2:B:900:LYS:HG2	5:E:41:ALA:HB1	2.03	0.41
3:C:121:ARG:HG2	3:C:438:PHE:CZ	2.55	0.41
3:C:396:VAL:HG13	3:C:400:LEU:HD23	2.02	0.41
3:C:452:ASP:O	3:C:453:LEU:HB3	2.21	0.41
6:F:5:GLU:N	6:F:5:GLU:OE2	2.54	0.41
1:A:33:ILE:HD13	1:A:33:ILE:HA	1.91	0.41
1:A:80:VAL:O	1:A:81:GLU:HG2	2.21	0.41
2:B:120:LEU:HD21	2:B:149:THR:HG21	2.03	0.41
2:B:521:THR:OG1	2:B:522:GLY:N	2.54	0.41
2:B:853:TYR:O	5:E:37:MET:HE1	2.20	0.41
3:C:126:MET:HE3	3:C:126:MET:HB3	1.86	0.41
4:D:173:LYS:HE3	4:D:173:LYS:HB3	1.85	0.41
1:A:201:GLU:HA	1:A:204:ARG:HB2	2.03	0.40
2:B:348:LYS:O	2:B:352:GLU:HG2	2.21	0.40
3:C:91:PHE:CD1	3:C:138:PRO:HD3	2.56	0.40
3:C:265:VAL:O	3:C:268:PRO:HD2	2.20	0.40
2:B:610:LYS:HG3	2:B:711:GLN:HB2	2.02	0.40
3:C:89:ILE:HD11	3:C:399:VAL:HG23	2.04	0.40
4:D:51:TYR:HE1	4:D:162:CYS:HB3	1.86	0.40
6:F:228:ILE:O	6:F:232:VAL:HG23	2.21	0.40
1:A:61:PHE:HZ	7:A:304:HEC:HBC2	1.87	0.40
2:B:758:TYR:HB3	2:B:760:TRP:CE2	2.57	0.40
6:F:217:SER:OG	6:F:335:GLU:OE1	2.37	0.40
2:B:261:GLY:HA2	2:B:368:LEU:O	2.22	0.40
2:B:485:ARG:HA	2:B:491:THR:HA	2.03	0.40
2:B:750:ILE:HD13	4:D:104:ARG:CZ	2.50	0.40
3:C:156:GLY:C	3:C:158:LEU:H	2.29	0.40
3:C:304:PHE:HB3	3:C:379:LEU:HD23	2.03	0.40
6:F:116:PRO:HA	6:F:119:VAL:HG22	2.02	0.40
6:F:338:TRP:CZ2	6:F:342:LYS:HE3	2.56	0.40
6:F:340:PHE:O	6:F:345:PRO:HD3	2.21	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	216/226 (96%)	178 (82%)	38 (18%)	0	100	100
2	B	927/933 (99%)	816 (88%)	111 (12%)	0	100	100
3	C	454/471 (96%)	418 (92%)	36 (8%)	0	100	100
4	D	172/192 (90%)	156 (91%)	16 (9%)	0	100	100
5	E	156/162 (96%)	141 (90%)	15 (10%)	0	100	100
6	F	393/414 (95%)	378 (96%)	15 (4%)	0	100	100
All	All	2318/2398 (97%)	2087 (90%)	231 (10%)	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	191/198 (96%)	191 (100%)	0	100	100
2	B	763/766 (100%)	759 (100%)	4 (0%)	81	80
3	C	384/394 (98%)	384 (100%)	0	100	100
4	D	135/150 (90%)	135 (100%)	0	100	100
5	E	131/135 (97%)	131 (100%)	0	100	100
6	F	320/332 (96%)	320 (100%)	0	100	100
All	All	1924/1975 (97%)	1920 (100%)	4 (0%)	85	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	588	PRO
2	B	835	VAL
2	B	841	THR
2	B	862	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	100	GLN
1	A	127	HIS
1	A	136	ASN
1	A	156	GLN
1	A	199	GLN
2	B	214	GLN
2	B	221	GLN
2	B	248	HIS
2	B	279	GLN
2	B	294	ASN
2	B	456	HIS
2	B	467	GLN
2	B	471	HIS
2	B	495	GLN
2	B	602	GLN
2	B	625	ASN
2	B	756	ASN
2	B	773	ASN
2	B	800	HIS
2	B	813	HIS
2	B	816	ASN
2	B	877	GLN
2	B	955	GLN
2	B	975	GLN
2	B	986	ASN
3	C	79	ASN
3	C	141	HIS
3	C	163	GLN
3	C	225	ASN
3	C	246	HIS
3	C	334	ASN
5	E	40	GLN

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Mol	Chain	Res	Type
5	E	47	GLN
5	E	122	ASN
5	E	157	ASN
6	F	41	GLN
6	F	44	HIS
6	F	67	ASN
6	F	68	HIS
6	F	249	HIS
6	F	348	HIS
6	F	353	HIS
6	F	386	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
8	SF4	B	1101	2	0,12,12	-	-	-		
9	F3S	B	1104	2	0,9,9	-	-	-		
7	HEC	A	304	1	50,50,50	1.68	6 (12%)	68,82,82	1.38	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SF4	B	1102	2	0,12,12	-	-	-		
7	HEC	A	302	1	50,50,50	1.71	5 (10%)	68,82,82	1.44	7 (10%)
7	HEC	A	303	1	50,50,50	1.59	5 (10%)	68,82,82	1.31	5 (7%)
7	HEC	E	201	5	50,50,50	1.71	5 (10%)	68,82,82	1.43	8 (11%)
7	HEC	A	301	1	50,50,50	1.67	5 (10%)	68,82,82	1.48	10 (14%)
10	EL6	B	1105	-	25,25,42	1.24	4 (16%)	27,27,44	1.41	3 (11%)
10	EL6	E	202	-	42,42,42	0.97	4 (9%)	44,44,44	1.21	3 (6%)
8	SF4	B	1103	2	0,12,12	-	-	-		
7	HEC	A	305	1	50,50,50	1.71	5 (10%)	68,82,82	1.37	5 (7%)

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
8	SF4	B	1101	2	-	-	0/6/5/5
9	F3S	B	1104	2	-	-	0/3/3/3
7	HEC	A	304	1	1/1/3/7	6/14/54/54	-
8	SF4	B	1102	2	-	-	0/6/5/5
7	HEC	A	302	1	1/1/3/7	6/14/54/54	-
7	HEC	A	303	1	1/1/3/7	4/14/54/54	-
7	HEC	E	201	5	1/1/3/7	2/14/54/54	-
7	HEC	A	301	1	1/1/3/7	2/14/54/54	-
10	EL6	B	1105	-	-	11/26/26/43	-
10	EL6	E	202	-	-	12/43/43/43	-
8	SF4	B	1103	2	-	-	0/6/5/5
7	HEC	A	305	1	1/1/3/7	3/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	305	HEC	C3D-C2D	7.95	1.53	1.36
7	A	302	HEC	C3D-C2D	7.83	1.53	1.36
7	A	304	HEC	C3D-C2D	7.71	1.53	1.36
7	A	301	HEC	C3D-C2D	7.71	1.53	1.36
7	E	201	HEC	C3D-C2D	7.67	1.53	1.36
7	A	303	HEC	C3D-C2D	7.46	1.52	1.36
7	E	201	HEC	FE-ND	4.40	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	201	HEC	FE-NB	4.05	2.07	1.94
7	A	301	HEC	FE-ND	4.05	2.07	1.94
10	B	1105	EL6	O21-C2	-4.02	1.40	1.47
10	E	202	EL6	O21-C2	-3.99	1.40	1.47
7	A	302	HEC	FE-NB	3.84	2.06	1.94
7	A	302	HEC	FE-ND	3.71	2.06	1.94
7	A	305	HEC	FE-ND	3.67	2.06	1.94
7	A	305	HEC	FE-NB	3.50	2.05	1.94
7	A	304	HEC	FE-ND	3.37	2.05	1.94
7	A	304	HEC	FE-NB	3.31	2.05	1.94
7	A	301	HEC	FE-NB	3.29	2.05	1.94
7	A	303	HEC	FE-NB	3.12	2.04	1.94
7	A	303	HEC	FE-ND	3.06	2.04	1.94
7	A	304	HEC	FE-NA	2.99	2.05	1.95
7	A	305	HEC	FE-NA	2.99	2.05	1.95
7	A	305	HEC	FE-NC	2.80	2.04	1.95
7	A	302	HEC	FE-NA	2.66	2.04	1.95
7	A	301	HEC	FE-NA	2.49	2.03	1.95
7	A	302	HEC	FE-NC	2.45	2.03	1.95
7	A	304	HEC	FE-NC	2.42	2.03	1.95
10	B	1105	EL6	O31-C31	2.33	1.40	1.33
7	A	303	HEC	FE-NA	2.33	2.03	1.95
7	E	201	HEC	FE-NC	2.33	2.03	1.95
10	E	202	EL6	O31-C31	2.29	1.40	1.33
10	E	202	EL6	O31-C3	-2.29	1.39	1.45
10	B	1105	EL6	O31-C3	-2.24	1.40	1.45
7	E	201	HEC	FE-NA	2.23	2.02	1.95
7	A	301	HEC	FE-NC	2.17	2.02	1.95
7	A	304	HEC	CMA-C3A	2.16	1.55	1.50
10	E	202	EL6	O21-C21	2.12	1.40	1.34
10	B	1105	EL6	O21-C21	2.11	1.40	1.34
7	A	303	HEC	FE-NC	2.00	2.01	1.95

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	301	HEC	C1D-ND-C4D	6.50	111.79	105.07
7	A	305	HEC	C1D-ND-C4D	6.27	111.55	105.07
7	A	302	HEC	C1D-ND-C4D	6.26	111.54	105.07
7	A	304	HEC	C1D-ND-C4D	5.96	111.23	105.07
7	E	201	HEC	C1D-ND-C4D	5.94	111.21	105.07
7	A	303	HEC	C1D-ND-C4D	5.36	110.61	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	1105	EL6	O21-C21-C22	3.94	119.99	111.50
10	E	202	EL6	O21-C21-C22	3.78	119.64	111.50
7	E	201	HEC	CAD-C3D-C4D	3.24	130.31	124.66
7	A	302	HEC	C2A-C1A-NA	-2.84	107.56	110.32
7	A	301	HEC	CAB-C3B-C4B	-2.73	121.27	124.81
7	A	302	HEC	CAA-C2A-C3A	-2.72	122.81	127.88
7	E	201	HEC	CMC-C2C-C1C	-2.71	121.24	125.37
10	E	202	EL6	O31-C31-C32	2.69	120.34	111.91
10	B	1105	EL6	O31-C31-C32	2.68	120.31	111.91
7	A	302	HEC	C4A-NA-C1A	2.63	107.92	105.35
10	B	1105	EL6	C2-O21-C21	-2.57	114.57	117.88
7	E	201	HEC	C4A-NA-C1A	2.55	107.85	105.35
7	A	304	HEC	C2A-C1A-NA	-2.52	107.87	110.32
7	A	305	HEC	C2A-C1A-NA	-2.50	107.89	110.32
7	A	305	HEC	C4A-NA-C1A	2.48	107.78	105.35
7	A	302	HEC	CAA-CBA-CGA	-2.43	108.38	113.60
7	A	303	HEC	CAA-CBA-CGA	-2.41	108.41	113.60
7	E	201	HEC	C2A-C1A-NA	-2.36	108.03	110.32
7	A	304	HEC	CAD-CBD-CGD	-2.32	108.61	113.60
7	A	303	HEC	CBD-CAD-C3D	-2.32	106.19	112.63
7	E	201	HEC	CAD-CBD-CGD	-2.31	108.63	113.60
7	A	304	HEC	CBD-CAD-C3D	-2.31	106.22	112.63
7	A	304	HEC	C4A-NA-C1A	2.30	107.61	105.35
7	A	305	HEC	C4B-NB-C1B	2.29	107.43	105.07
7	A	302	HEC	CAA-C2A-C1A	2.28	129.20	124.89
7	A	301	HEC	CHB-C4A-NA	2.26	126.88	124.44
7	A	301	HEC	C4C-NC-C1C	2.25	107.55	105.35
7	A	301	HEC	C2A-C1A-NA	-2.25	108.14	110.32
7	A	305	HEC	CAD-CBD-CGD	-2.23	108.81	113.60
7	A	303	HEC	C4A-NA-C1A	2.22	107.52	105.35
7	A	304	HEC	C4B-NB-C1B	2.15	107.29	105.07
7	A	301	HEC	C3C-C4C-NC	-2.15	107.75	110.15
10	E	202	EL6	C2-O21-C21	-2.15	115.12	117.88
7	E	201	HEC	C4B-NB-C1B	2.13	107.27	105.07
7	A	301	HEC	CMD-C2D-C1D	2.12	128.26	125.04
7	A	304	HEC	CHB-C1B-NB	2.12	126.72	124.42
7	A	303	HEC	C4B-NB-C1B	2.11	107.25	105.07
7	A	301	HEC	CBA-CAA-C2A	-2.09	106.83	112.63
7	A	301	HEC	CAB-C3B-C2B	2.08	131.09	127.53
7	E	201	HEC	CAA-CBA-CGA	-2.06	109.17	113.60
7	A	301	HEC	CAD-CBD-CGD	-2.05	109.19	113.60
7	A	302	HEC	CAD-C3D-C4D	2.04	128.23	124.66

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	301	HEC	NA
7	A	302	HEC	NA
7	A	303	HEC	NA
7	A	304	HEC	NA
7	A	305	HEC	NA
7	E	201	HEC	NA

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1105	EL6	O21-C2-C3-O31
10	E	202	EL6	O21-C2-C3-O31
7	A	301	HEC	C2B-C3B-CAB-CBB
7	A	301	HEC	C4B-C3B-CAB-CBB
10	E	202	EL6	C31-C32-C33-C34
7	A	303	HEC	C3D-CAD-CBD-CGD
10	B	1105	EL6	C35-C36-C37-C38
10	E	202	EL6	C37-C38-C39-C3A
10	E	202	EL6	C3B-C3C-C3D-C3E
10	E	202	EL6	C28-C29-C2A-C2B
7	A	302	HEC	C1A-C2A-CAA-CBA
10	E	202	EL6	C2B-C2C-C2D-C2E
7	A	304	HEC	C1A-C2A-CAA-CBA
10	B	1105	EL6	C26-C27-C28-C29
10	E	202	EL6	C27-C28-C29-C2A
10	E	202	EL6	C29-C2A-C2B-C2C
7	A	302	HEC	C3A-C2A-CAA-CBA
7	A	304	HEC	C3D-CAD-CBD-CGD
10	B	1105	EL6	C32-C31-O31-C3
10	B	1105	EL6	C1-C2-C3-O31
10	E	202	EL6	C1-C2-C3-O31
10	B	1105	EL6	C33-C34-C35-C36
10	B	1105	EL6	C34-C35-C36-C37
7	A	304	HEC	C3A-C2A-CAA-CBA
10	B	1105	EL6	O32-C31-O31-C3
7	A	302	HEC	C2C-C3C-CAC-CBC
10	E	202	EL6	C34-C35-C36-C37
10	B	1105	EL6	C36-C37-C38-C39
7	A	304	HEC	C2C-C3C-CAC-CBC
7	A	305	HEC	C3D-CAD-CBD-CGD
10	B	1105	EL6	C32-C33-C34-C35
7	A	302	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
7	A	304	HEC	CAA-CBA-CGA-O2A
7	A	305	HEC	C2C-C3C-CAC-CBC
7	A	304	HEC	CAA-CBA-CGA-O1A
7	A	303	HEC	C2C-C3C-CAC-CBC
10	E	202	EL6	C2C-C2D-C2E-C2F
7	A	302	HEC	C4B-C3B-CAB-CBB
7	A	302	HEC	C2B-C3B-CAB-CBB
7	E	201	HEC	CAD-CBD-CGD-O2D
7	A	303	HEC	CAD-CBD-CGD-O1D
10	E	202	EL6	O21-C21-C22-C23
7	E	201	HEC	CAD-CBD-CGD-O1D
7	A	303	HEC	CAD-CBD-CGD-O2D
10	B	1105	EL6	C31-C32-C33-C34
7	A	305	HEC	C2D-C3D-CAD-CBD

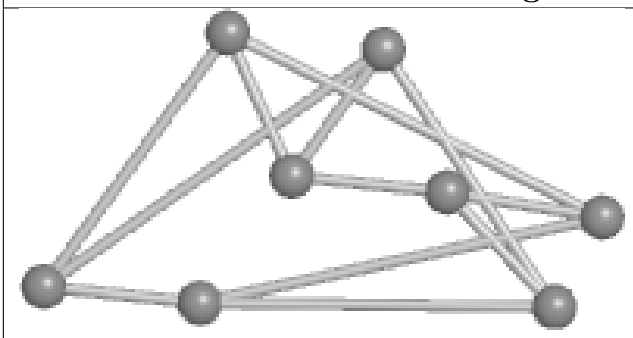
There are no ring outliers.

9 monomers are involved in 30 short contacts:

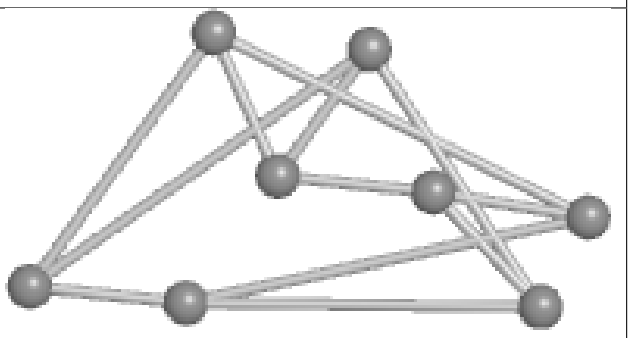
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1101	SF4	5	0
7	A	304	HEC	6	0
8	B	1102	SF4	2	0
7	A	302	HEC	3	0
7	A	303	HEC	1	0
7	E	201	HEC	2	0
7	A	301	HEC	6	0
8	B	1103	SF4	2	0
7	A	305	HEC	3	0

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.

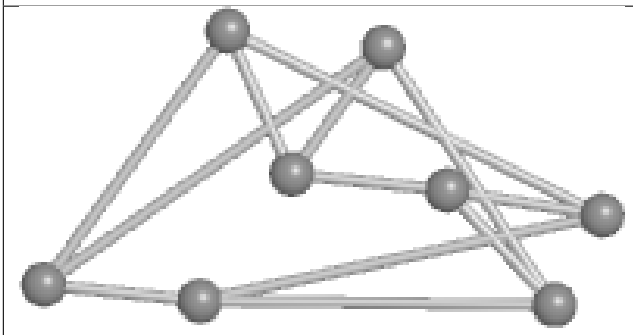
Ligand SF4 B 1101



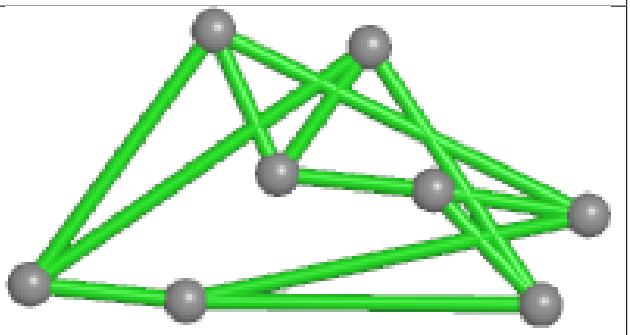
Bond lengths



Bond angles

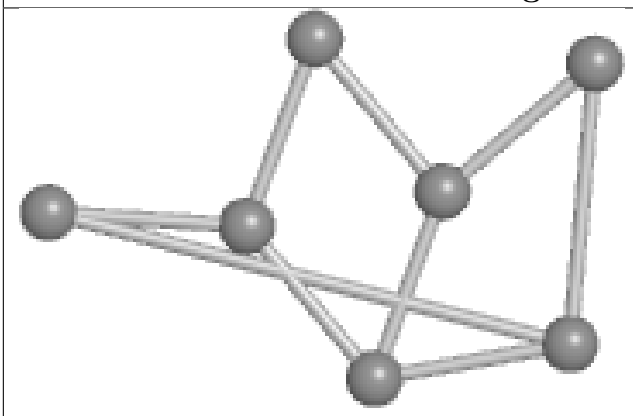


Torsions

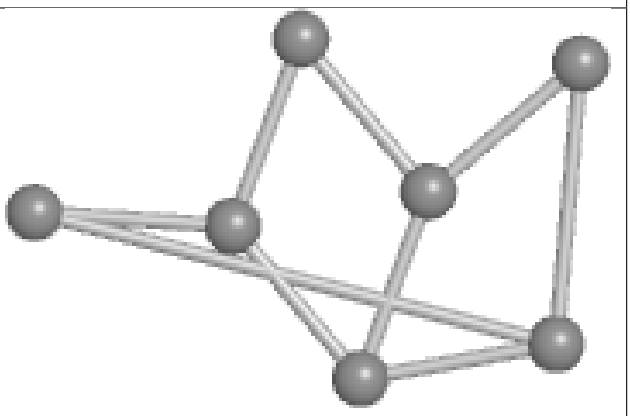


Rings

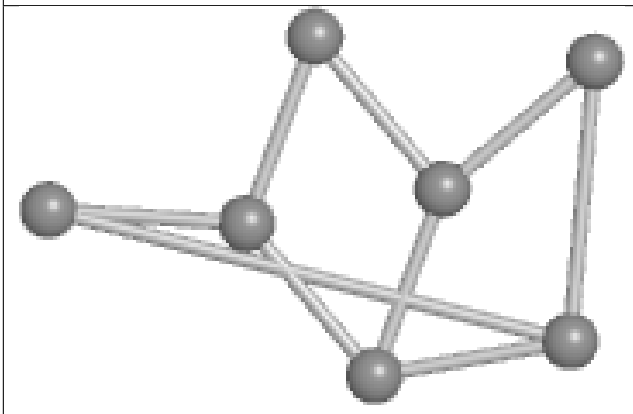
Ligand F3S B 1104



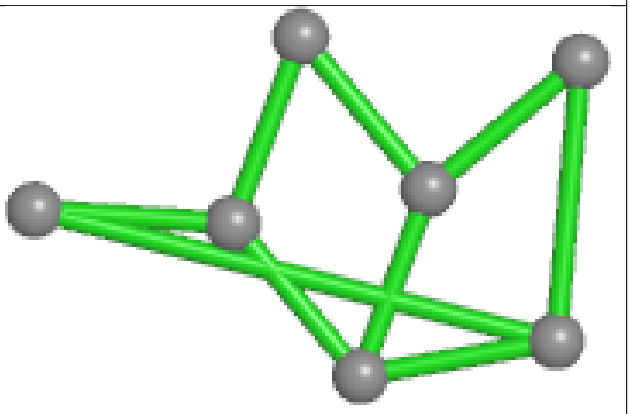
Bond lengths



Bond angles

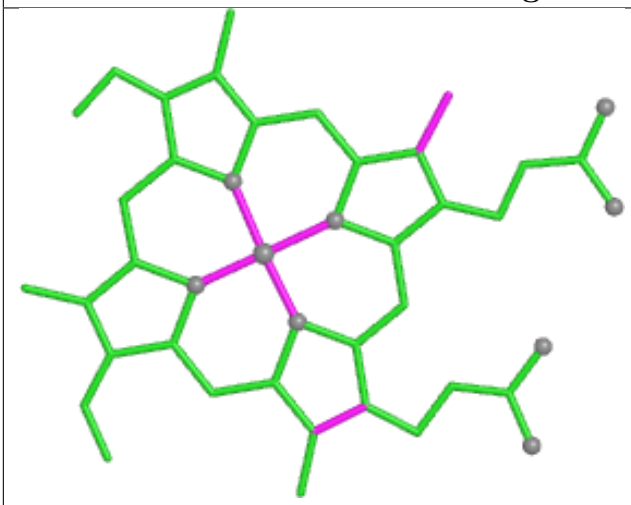


Torsions

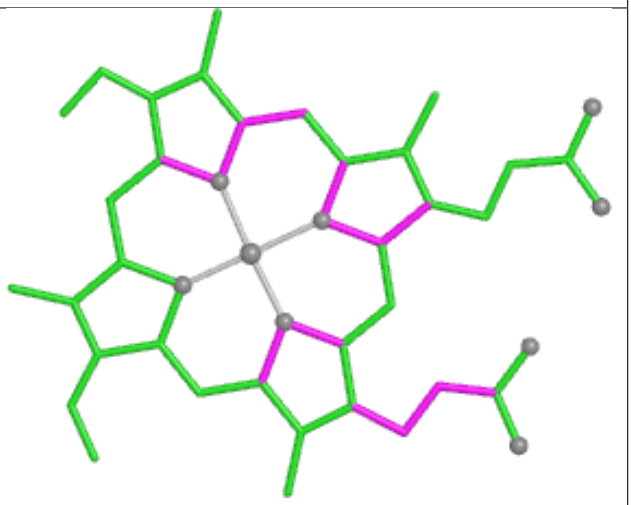


Rings

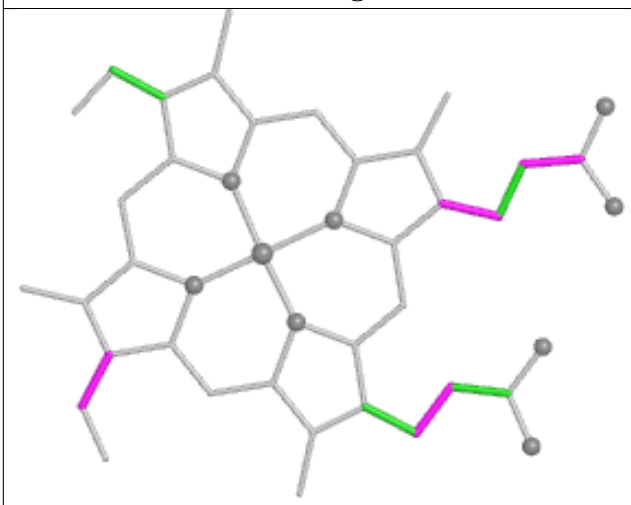
Ligand HEC A 304



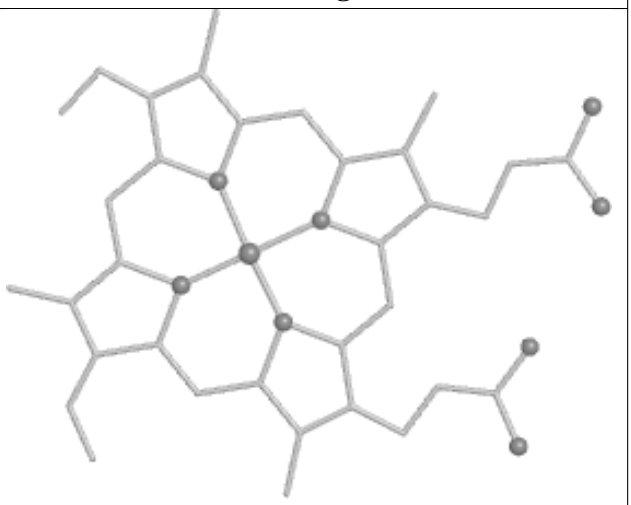
Bond lengths



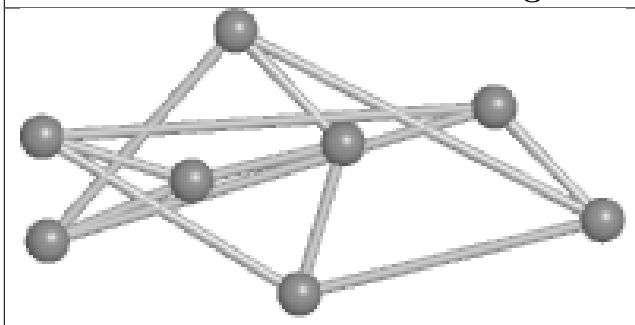
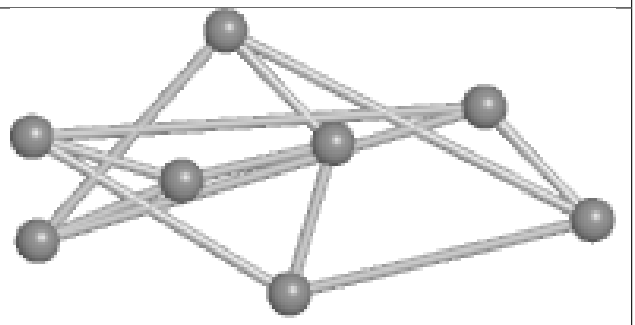
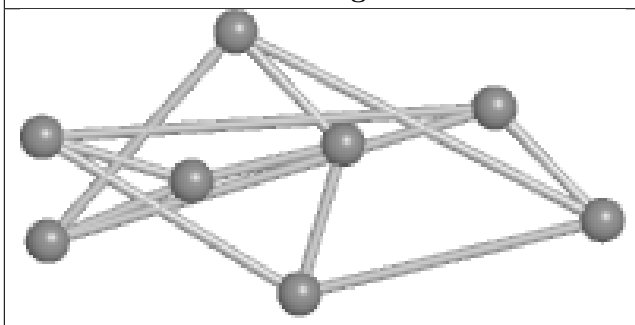
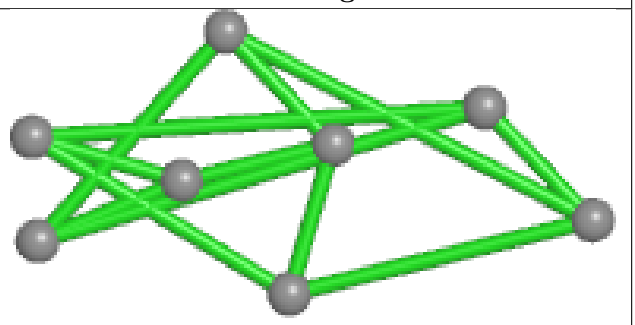
Bond angles



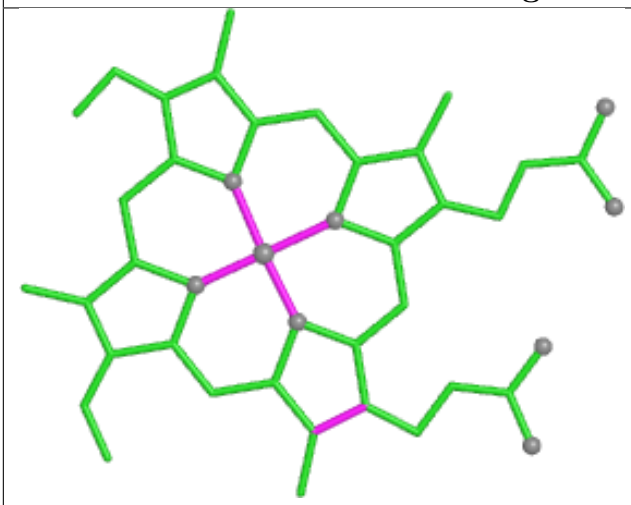
Torsions



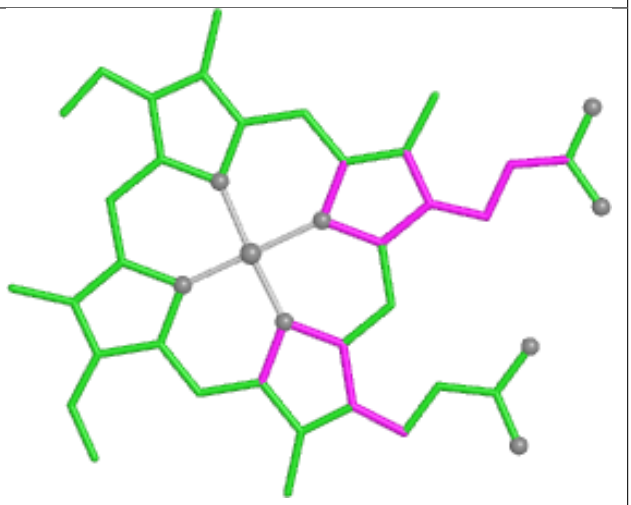
Rings

Ligand SF4 B 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

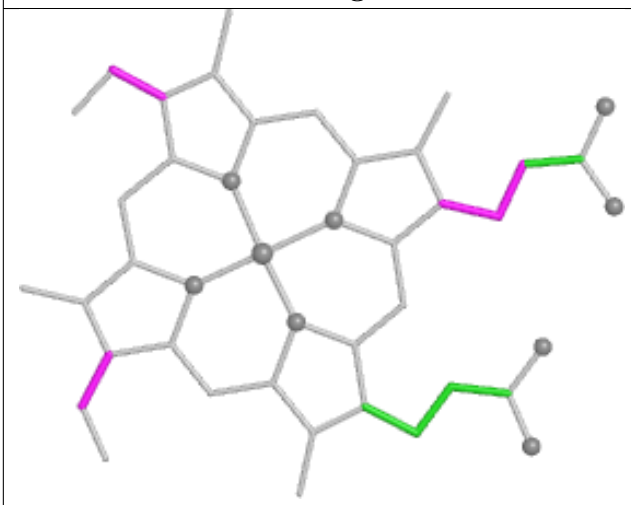
Ligand HEC A 302



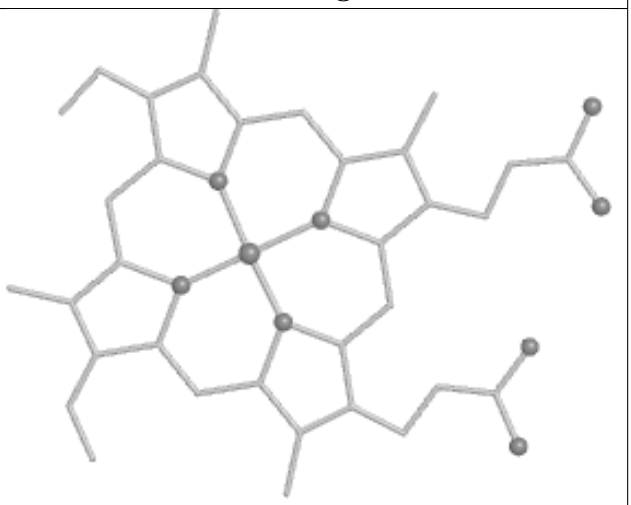
Bond lengths



Bond angles

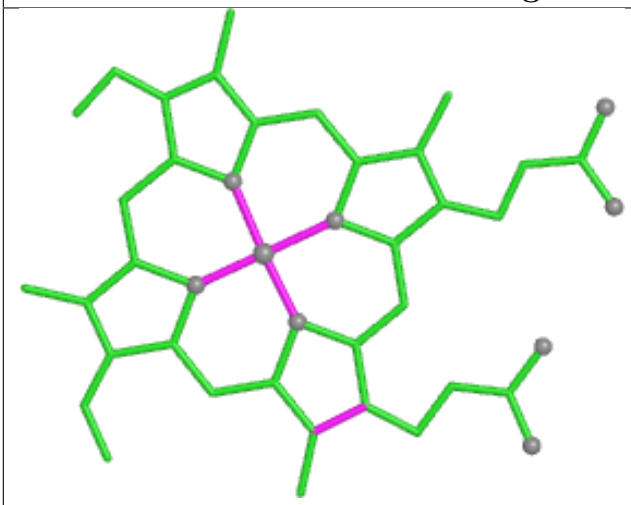


Torsions

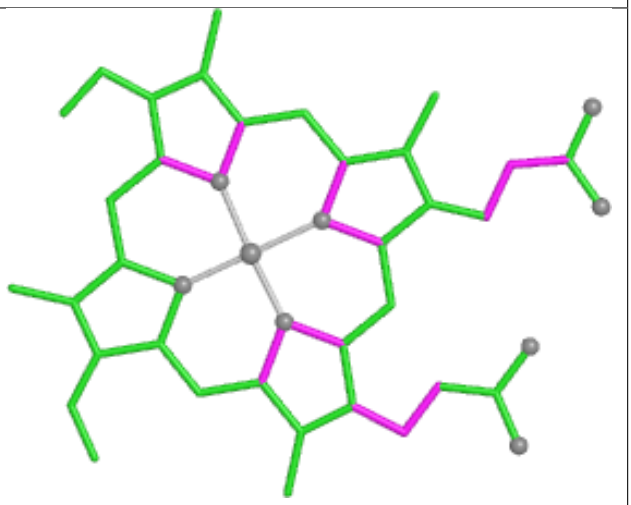


Rings

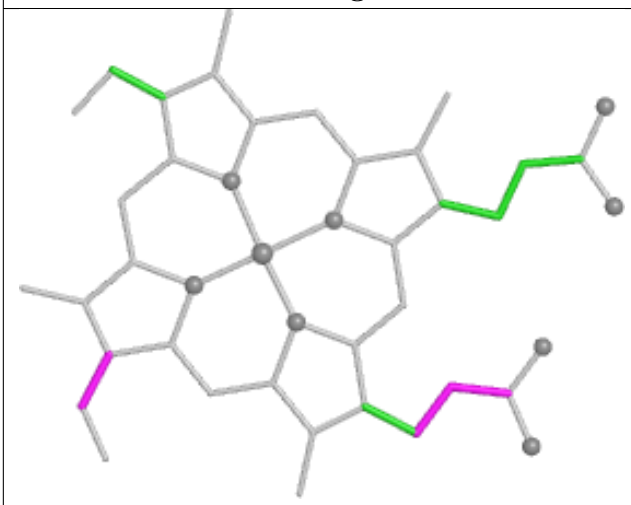
Ligand HEC A 303



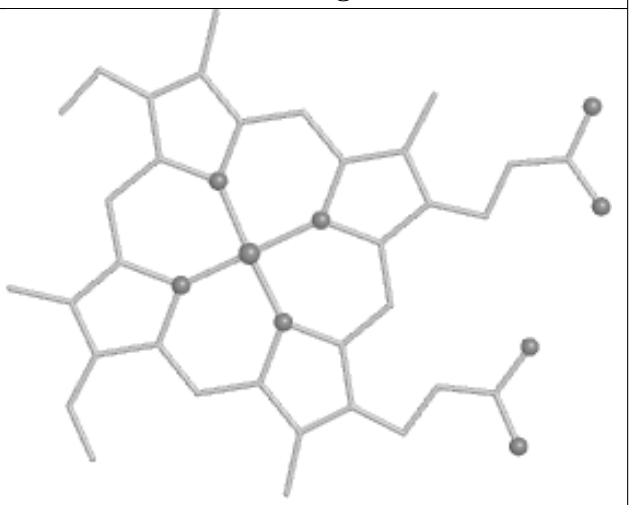
Bond lengths



Bond angles

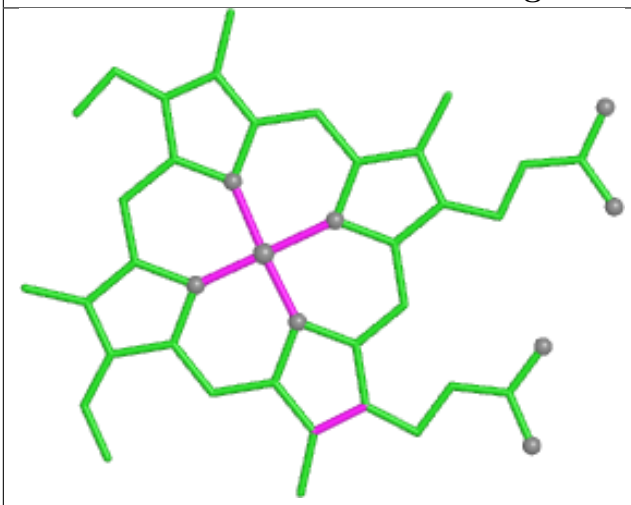


Torsions

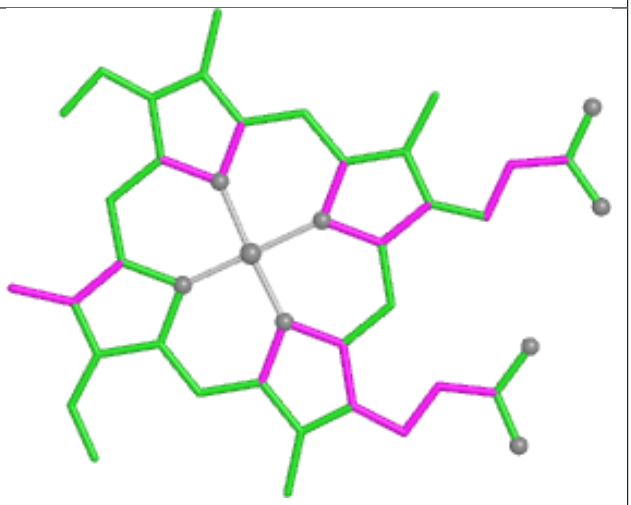


Rings

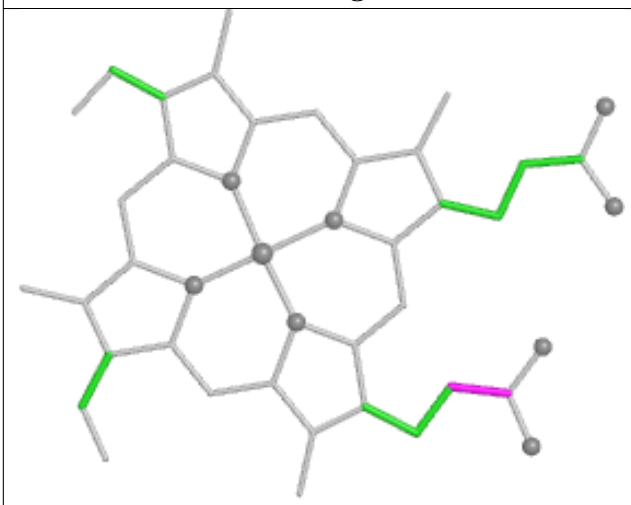
Ligand HEC E 201



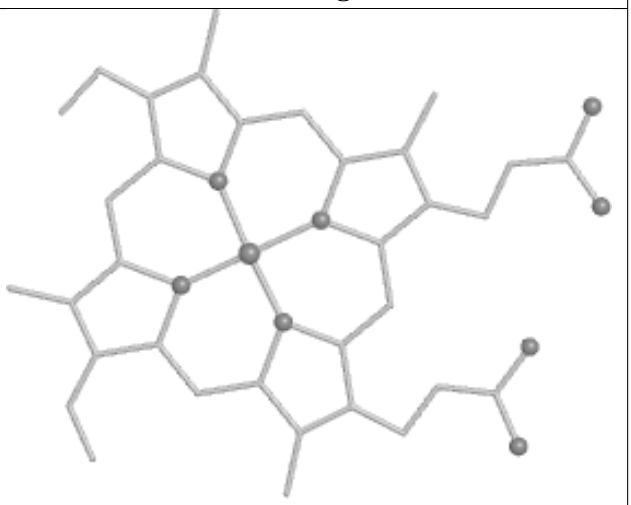
Bond lengths



Bond angles

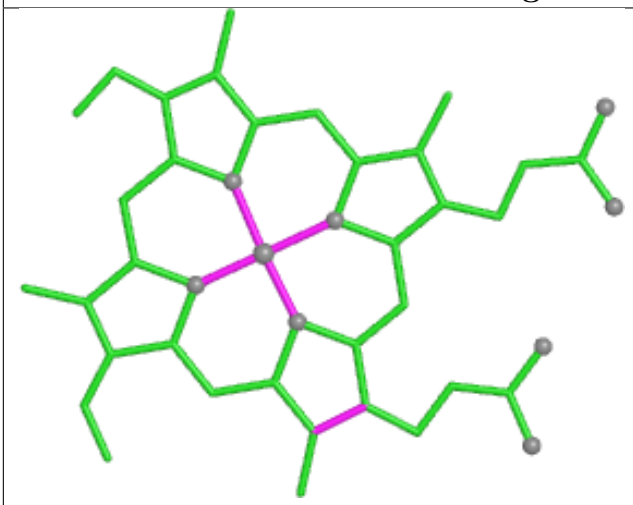


Torsions

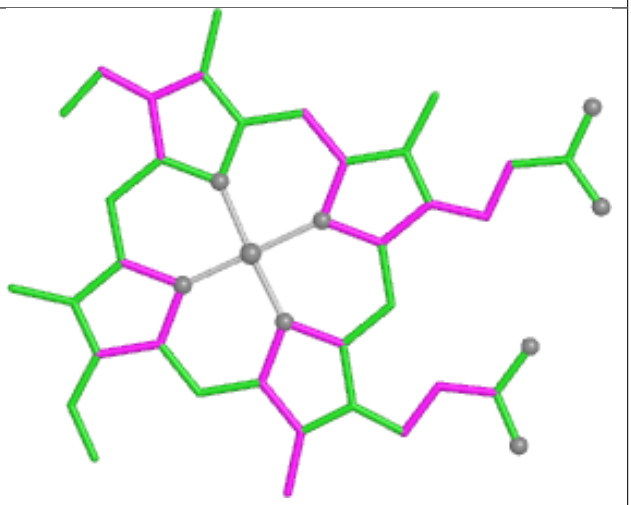


Rings

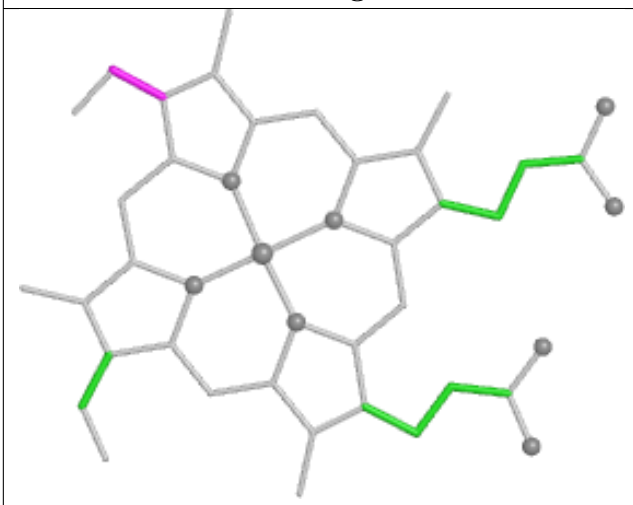
Ligand HEC A 301



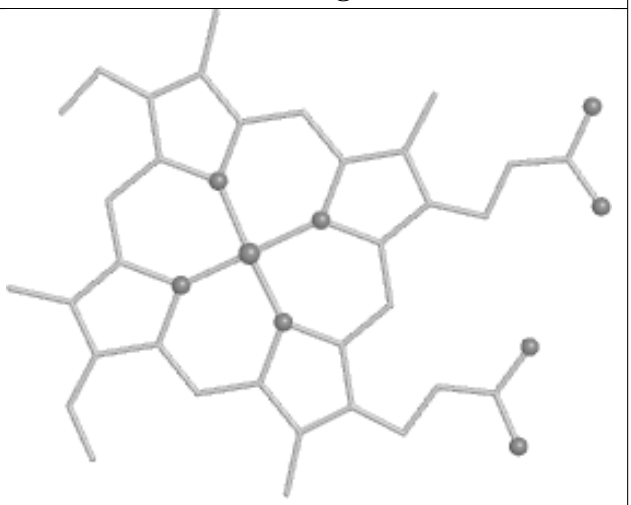
Bond lengths



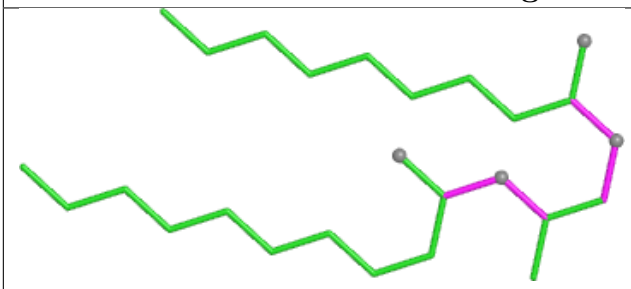
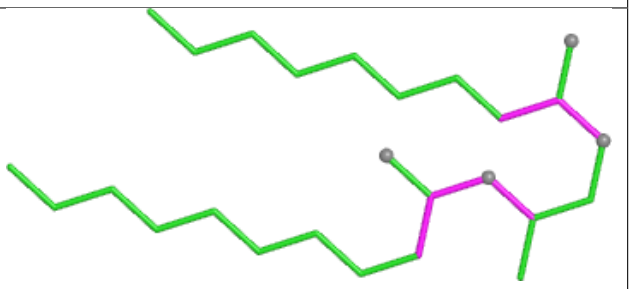
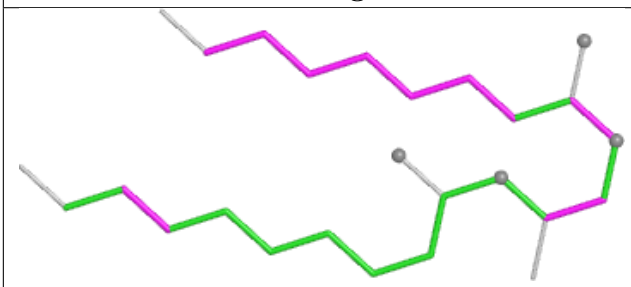
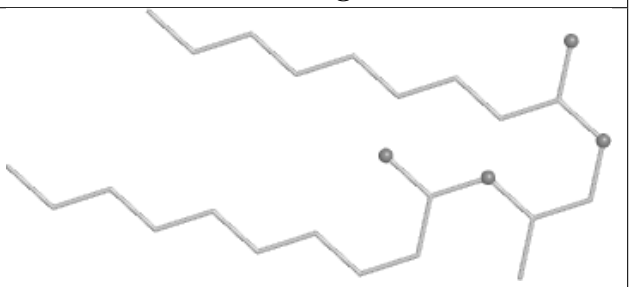
Bond angles

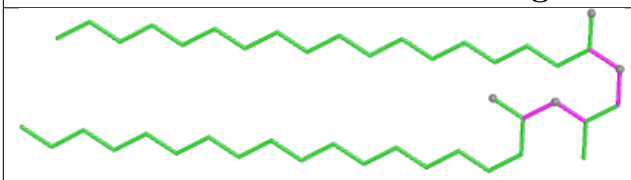
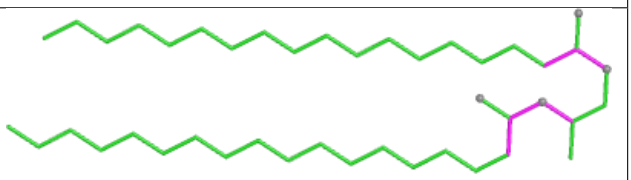
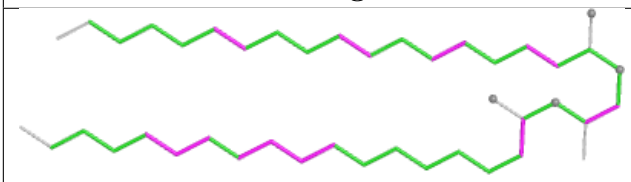
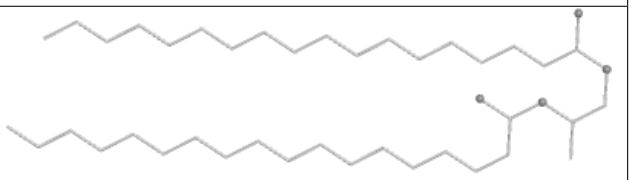


Torsions

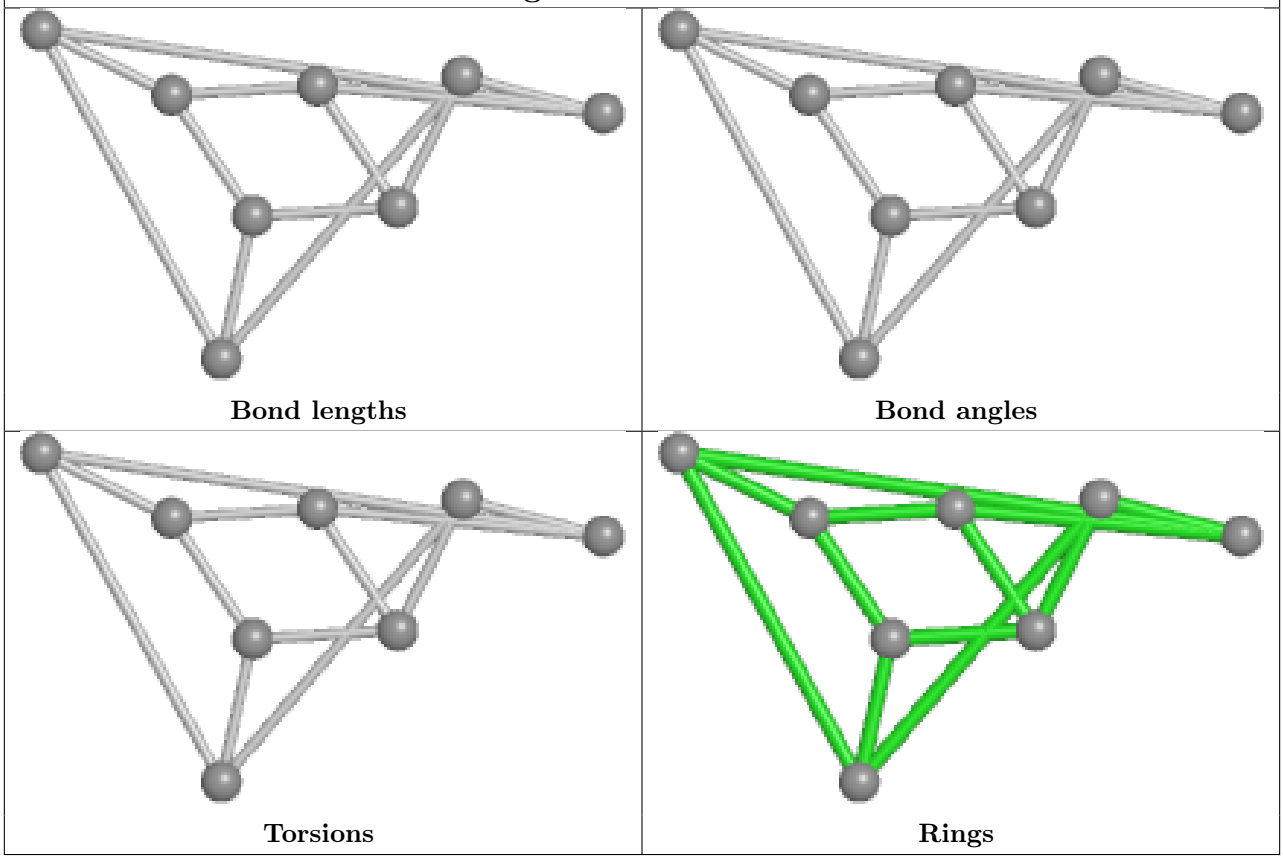


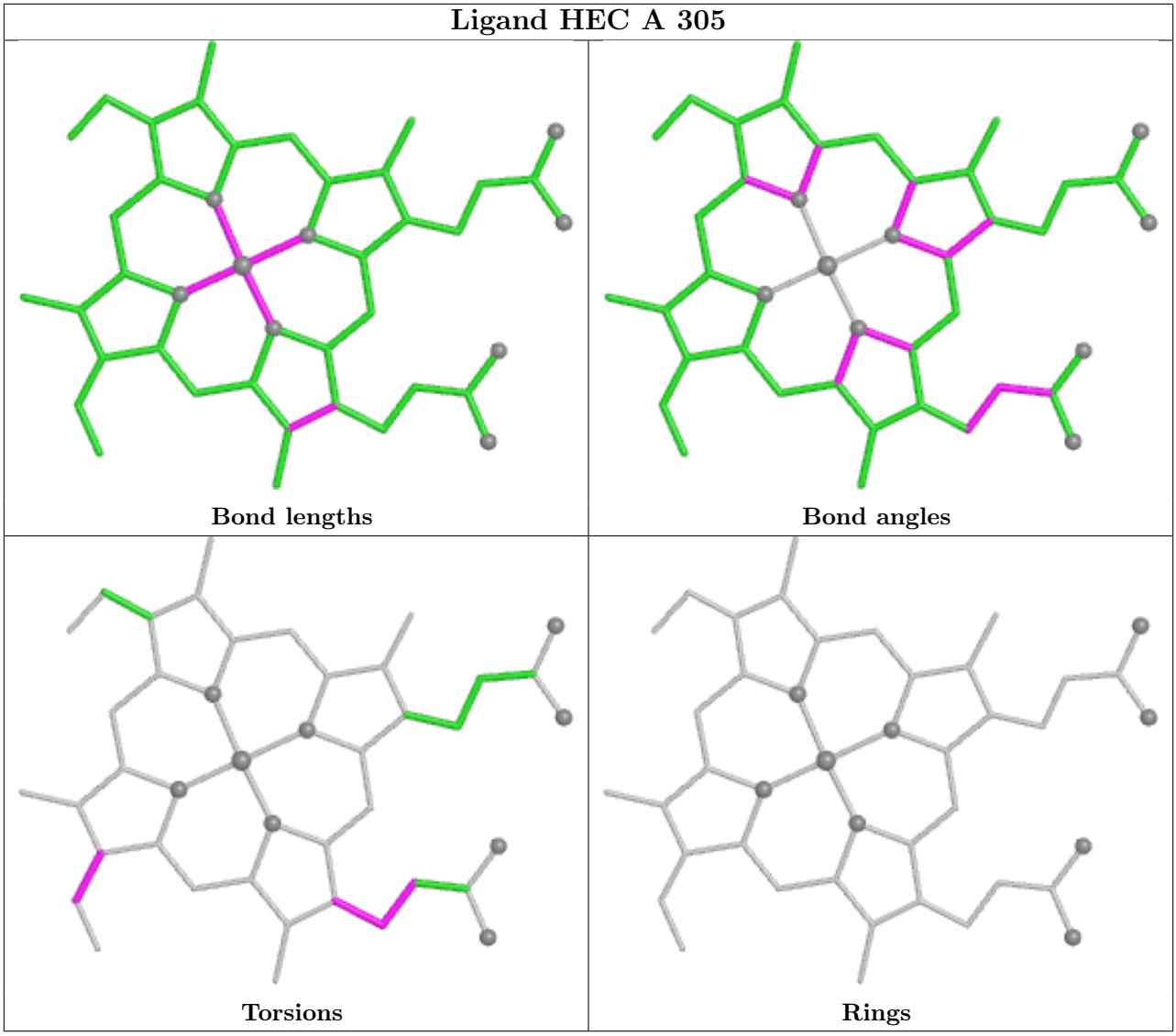
Rings

Ligand EL6 B 1105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EL6 E 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 B 1103





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.

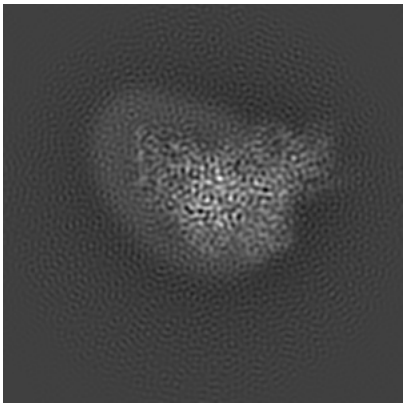
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0937. These allow visual inspection of the internal detail of the map and identification of artifacts.

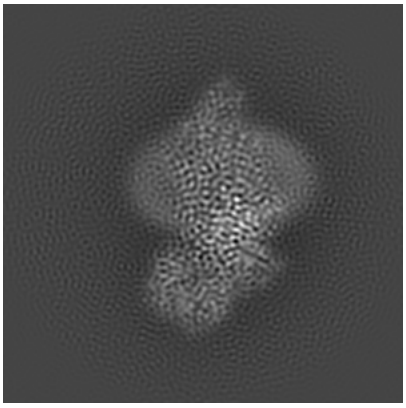
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

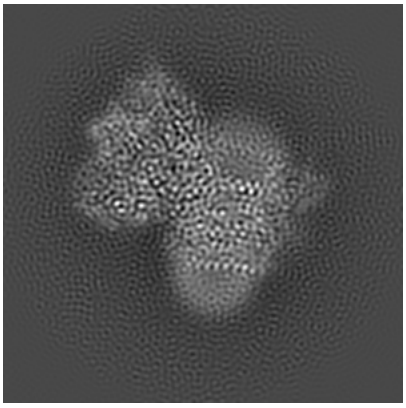
6.1.1 Primary map



X



Y

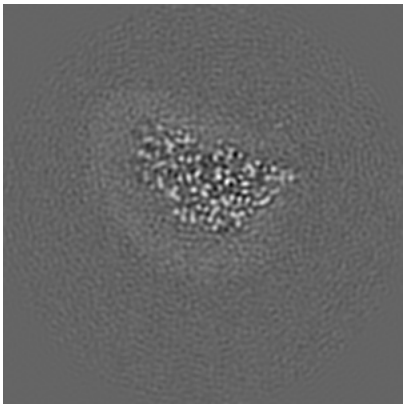


Z

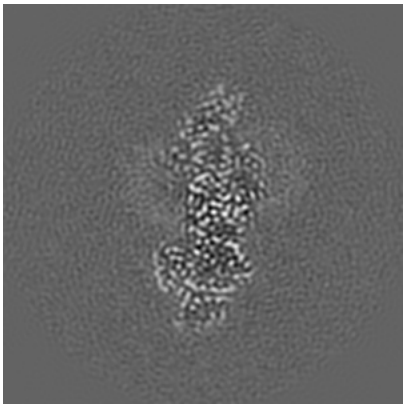
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

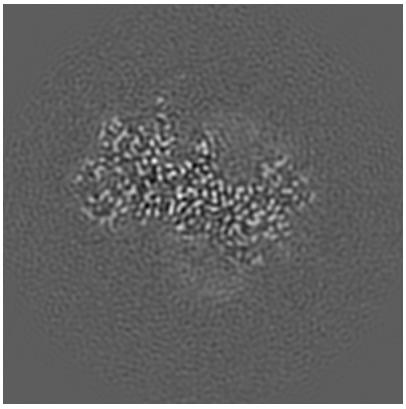
6.2.1 Primary map



X Index: 108



Y Index: 108

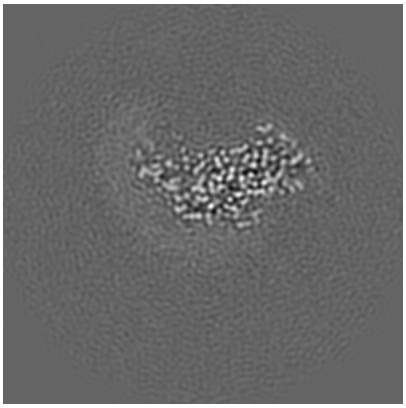


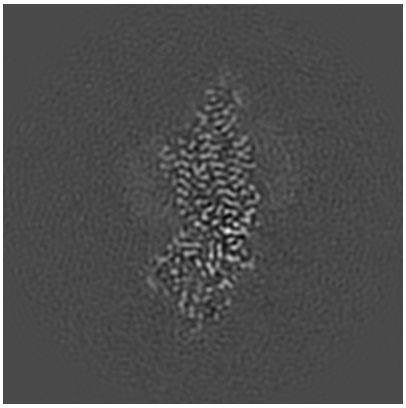
Z Index: 108

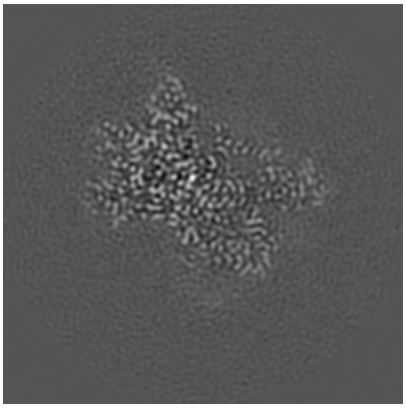
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 99

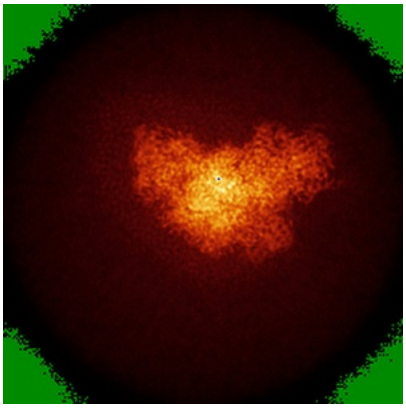

Y Index: 115

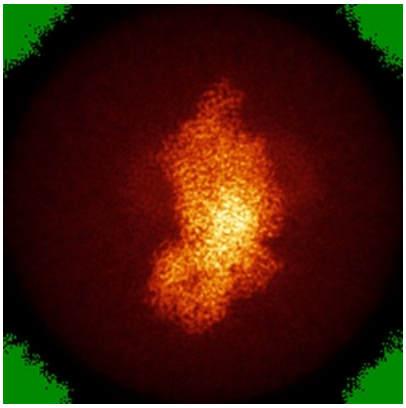

Z Index: 117

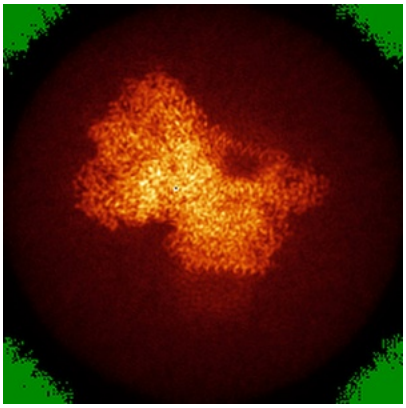
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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 0.0321. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

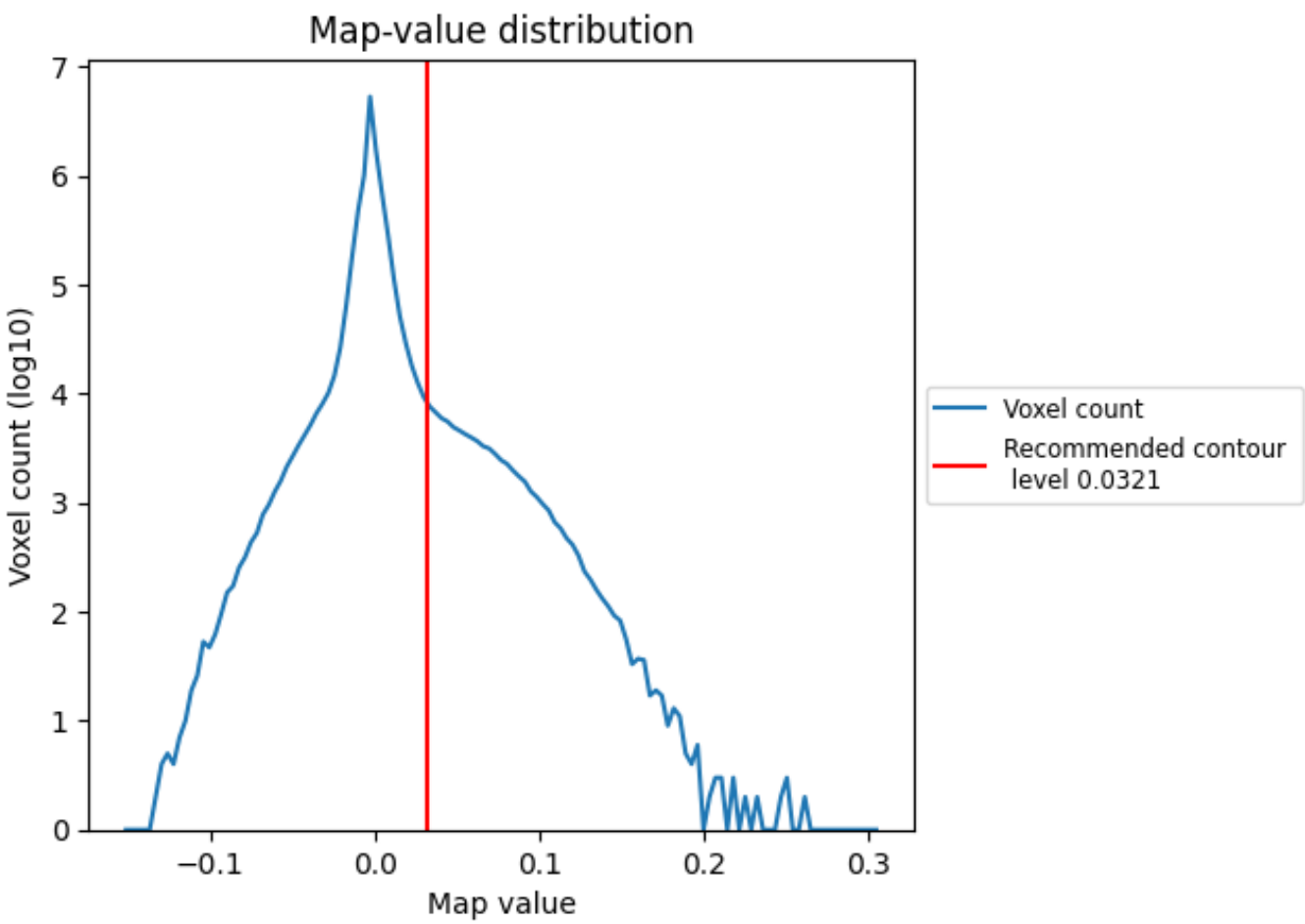
6.6 Mask visualisation (i)

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

7 Map analysis (i)

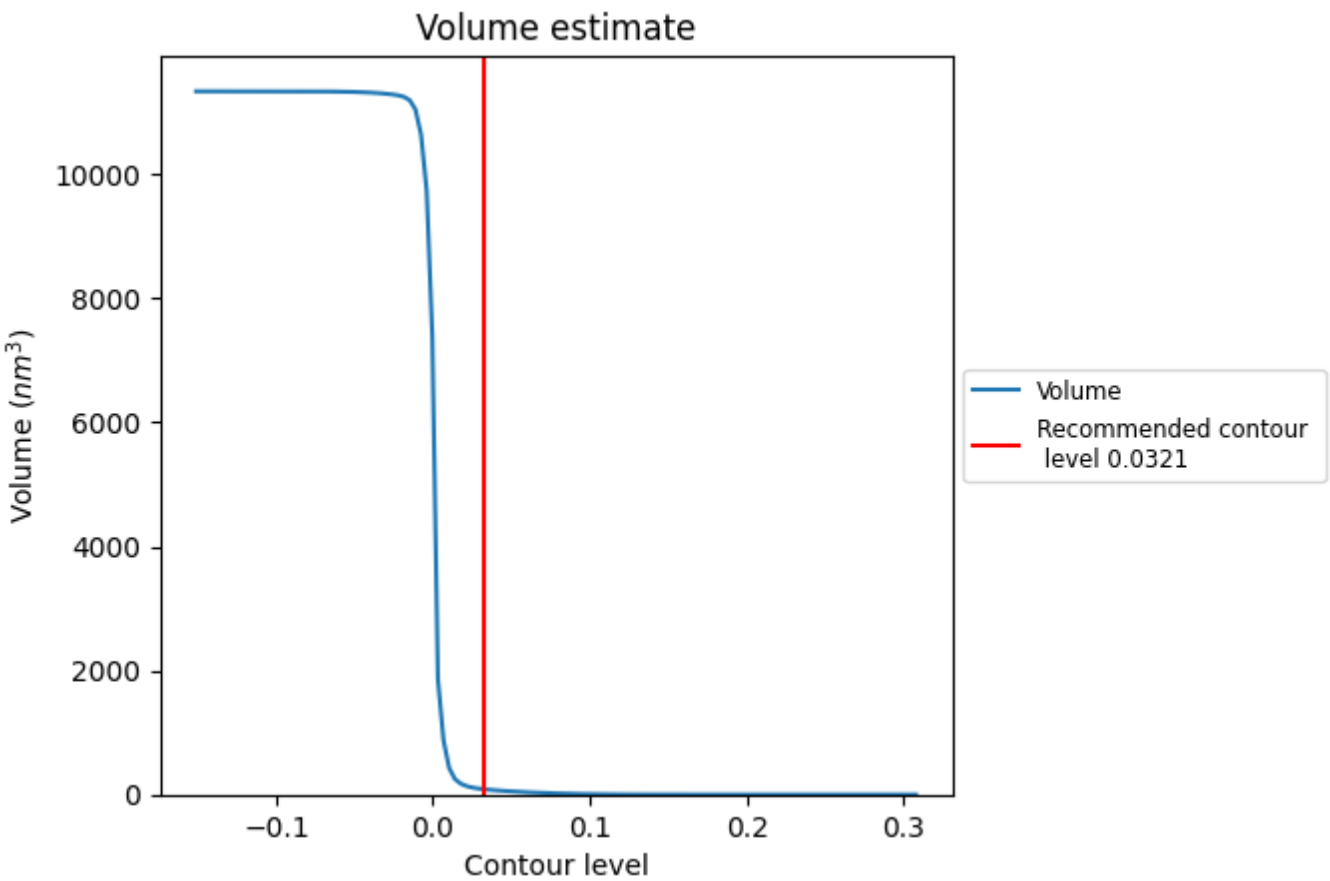
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

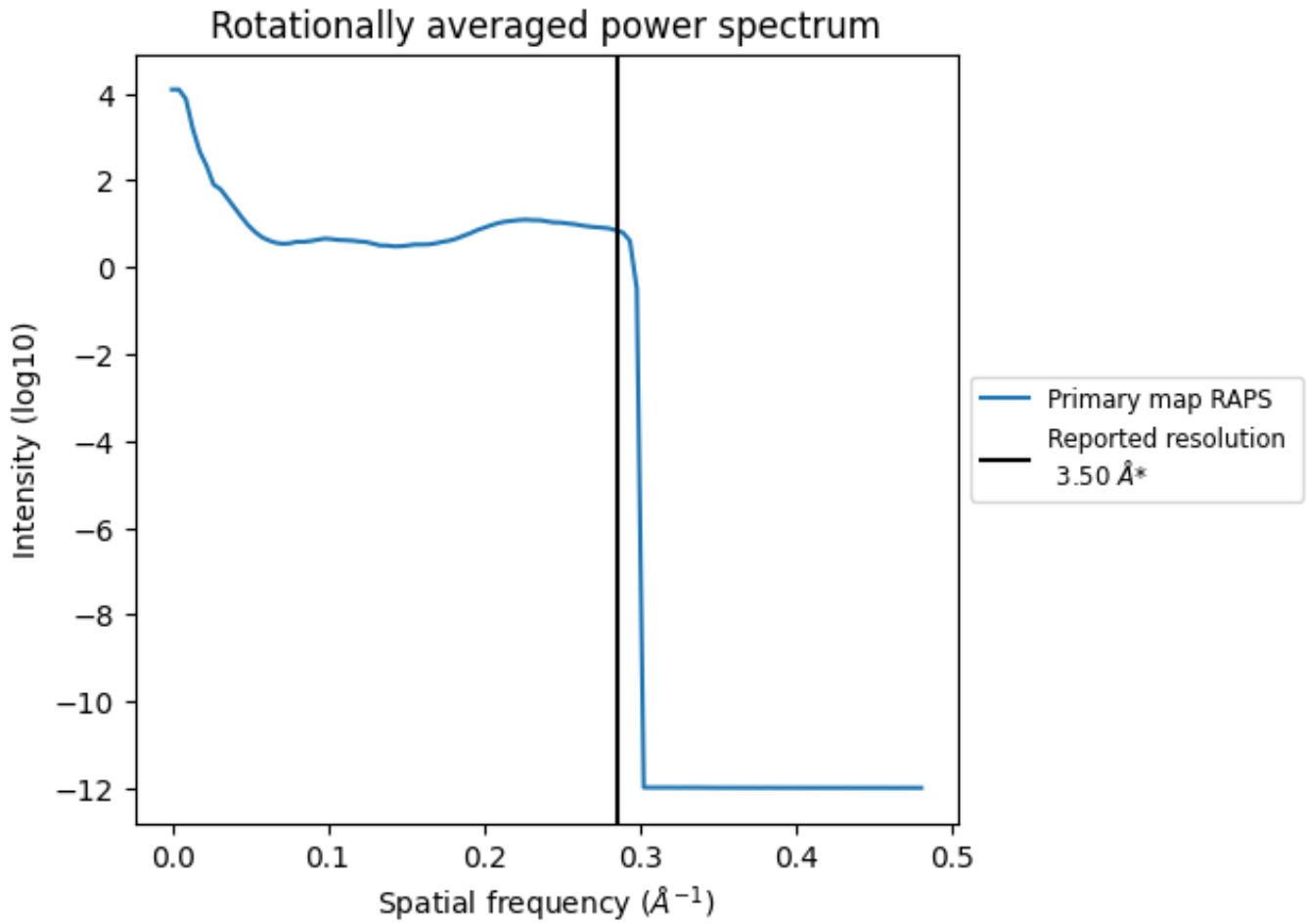
7.2 Volume estimate (i)



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 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 0.286 Å^{-1}

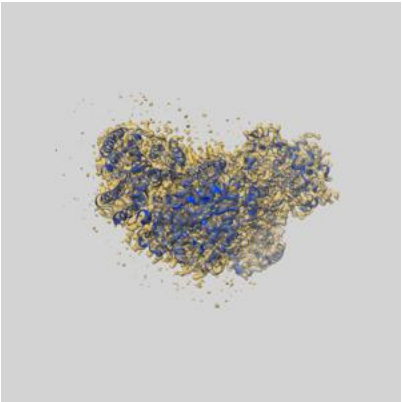
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

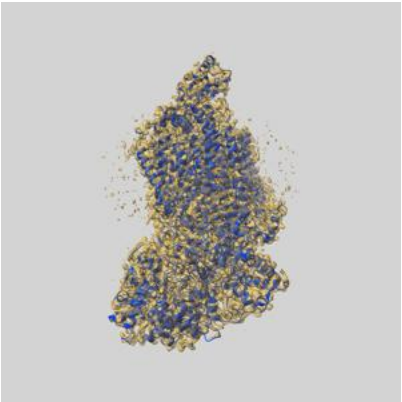
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0937 and PDB model 6LOE. Per-residue inclusion information can be found in section 3 on page 8.

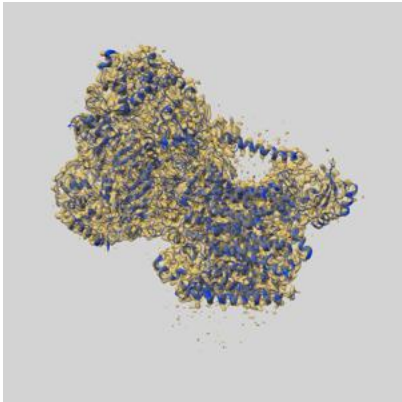
9.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0321 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

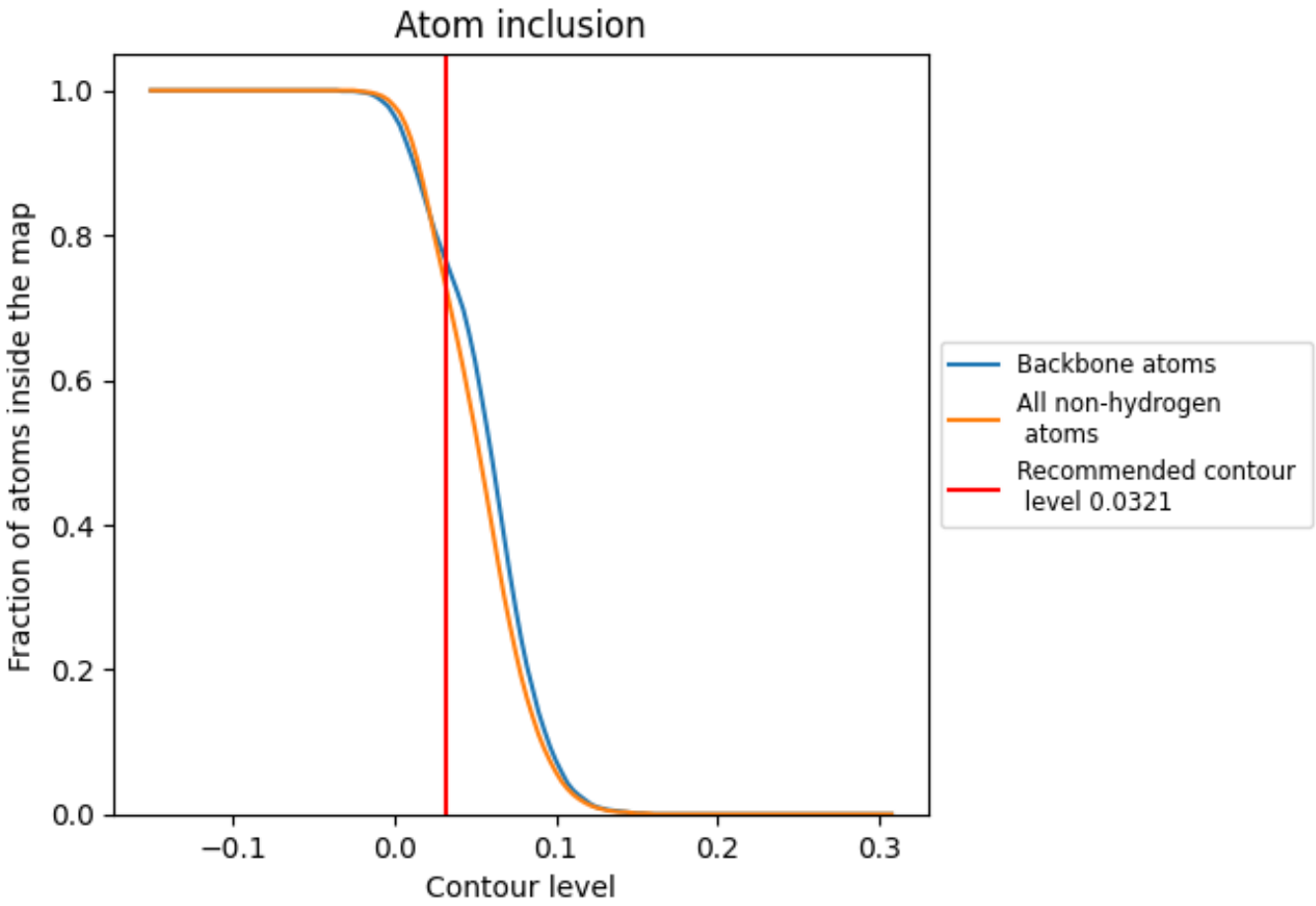
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0321).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0321) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.5350
A	0.7500	0.5360
B	0.7280	0.5390
C	0.7540	0.5360
D	0.6610	0.5210
E	0.6850	0.5290
F	0.7150	0.5360