



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:16 pm GMT

PDB ID : 6F0K  
EMDB ID : EMD-4165  
Title : Alternative complex III  
Authors : Sousa, J.S.; Calisto, F.; Mills, D.J.; Pereira, M.M.; Vonck, J.; Kuehlbrandt, W.  
Deposited on : 2017-11-20  
Resolution : 3.87 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

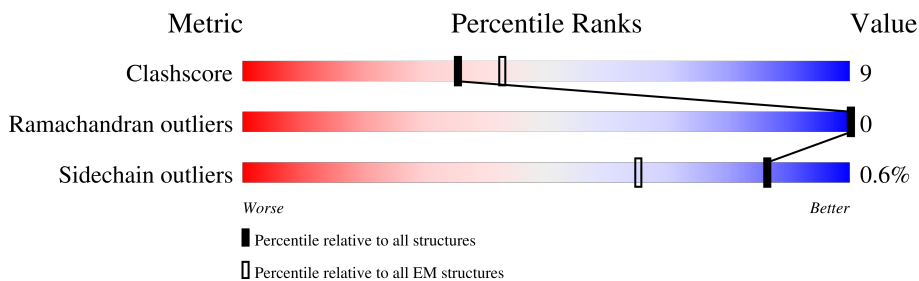
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.87 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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  $\leq 5\%$ . 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	211	25% (red), 75% (green), 22% (yellow), 8% (grey)
2	B	1039	27% (red), 72% (green), 20% (yellow), 8% (grey)
3	C	484	36% (red), 76% (green), 15% (yellow), 8% (grey)
4	D	217	40% (red), 70% (green), 8% (yellow), 21% (grey)
5	E	209	21% (red), 72% (green), 15% (yellow), 13% (grey)
6	F	417	38% (red), 74% (green), 17% (yellow), 8% (grey)
7	H	182	45% (red), 69% (green), 16% (yellow), 14% (grey)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SF4	B	1102	-	-	X	-
10	SF4	B	1103	-	-	X	-
10	SF4	B	1104	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 40046 atoms, of which 19755 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 c family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	207	3253	1057	1583	301	299	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	961	14877	4740	7345	1366	1396	30	0	0

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	445	7234	2447	3617	578	572	20	0	0

- Molecule 4 is a protein called ActD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	171	2656	892	1313	216	229	6	0	0

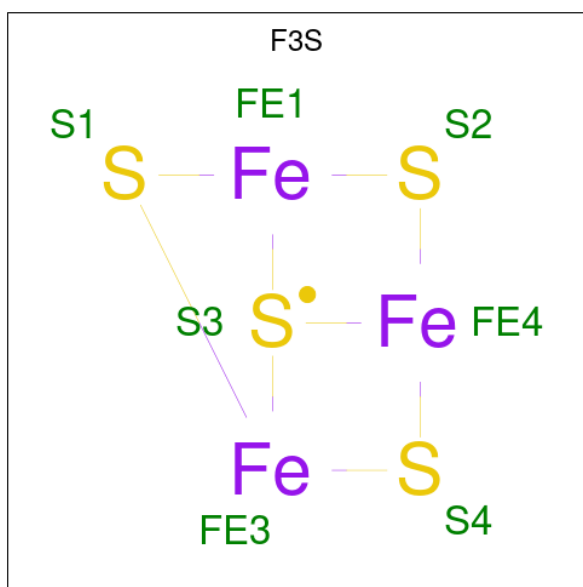
- Molecule 5 is a protein called Quinol:cytochrome c oxidoreductase monoheme cytochrome subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	182	2818	907	1379	265	261	6	0	0

- Molecule 6 is a protein called ActF.

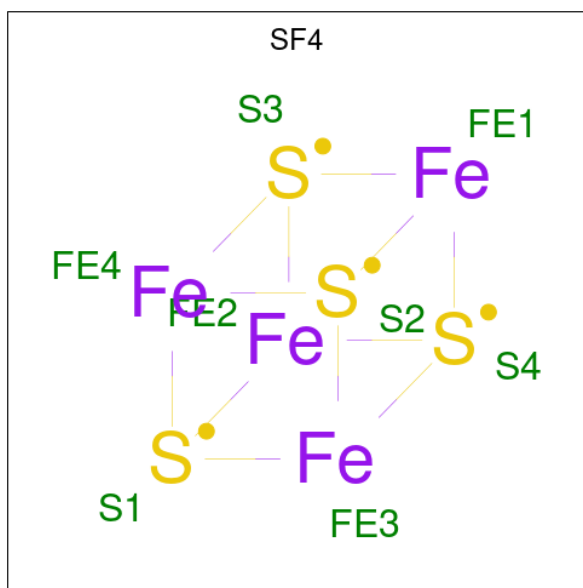
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	382	6308	2158	3141	504	494	11	0	0





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

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).

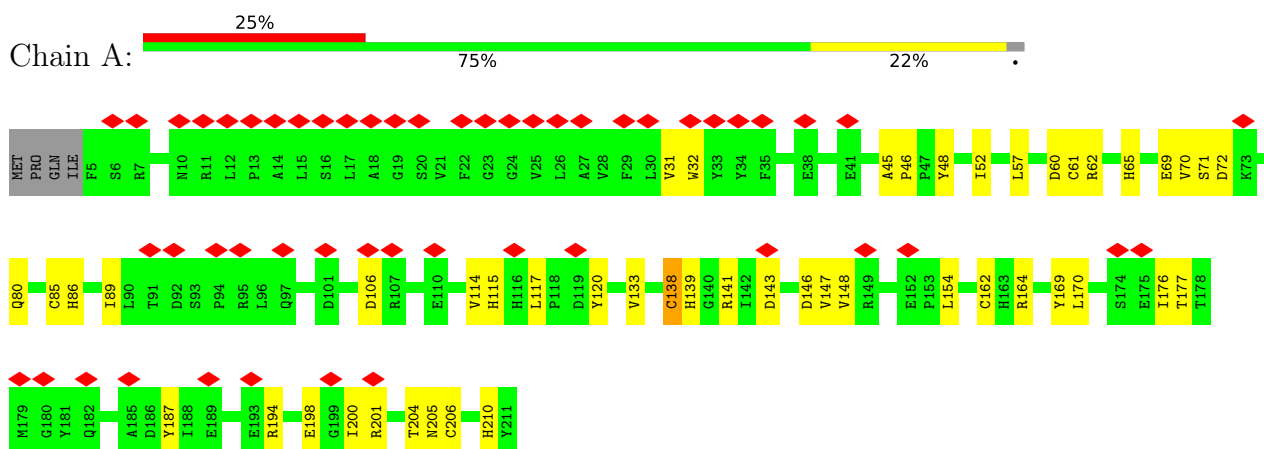


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
10	B	1	24	12	12	0
10	B	1	24	12	12	0
10	B	1	24	12	12	0

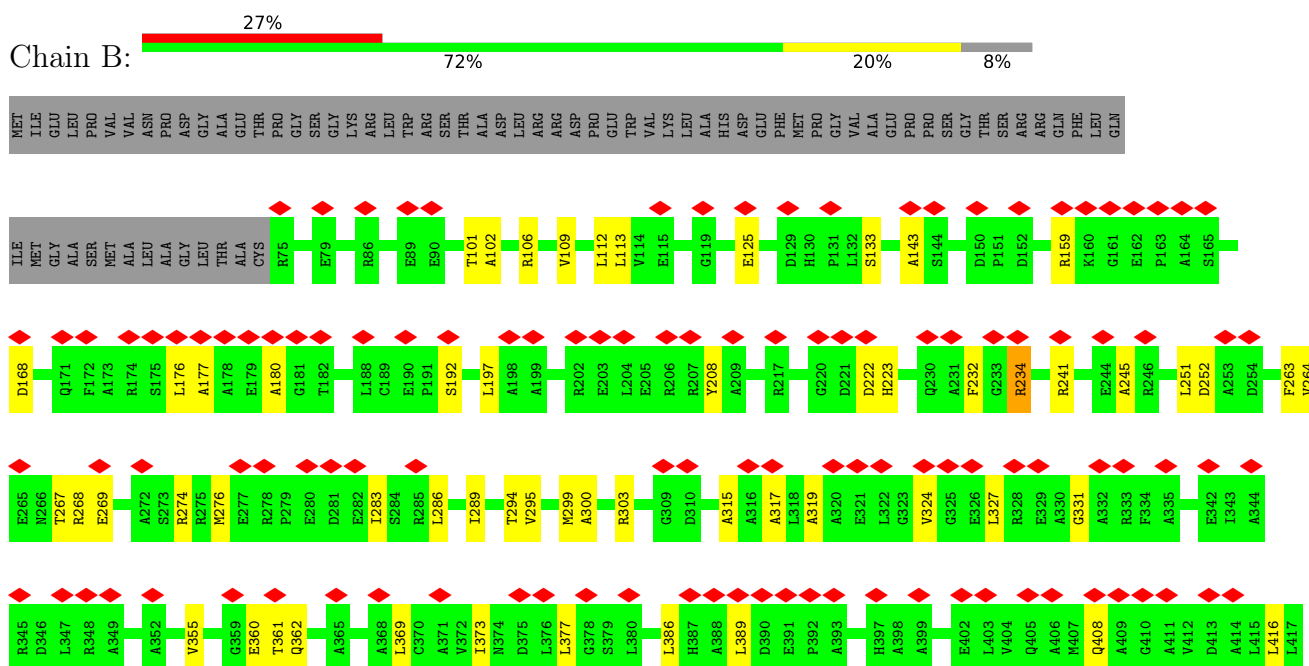
### 3 Residue-property plots

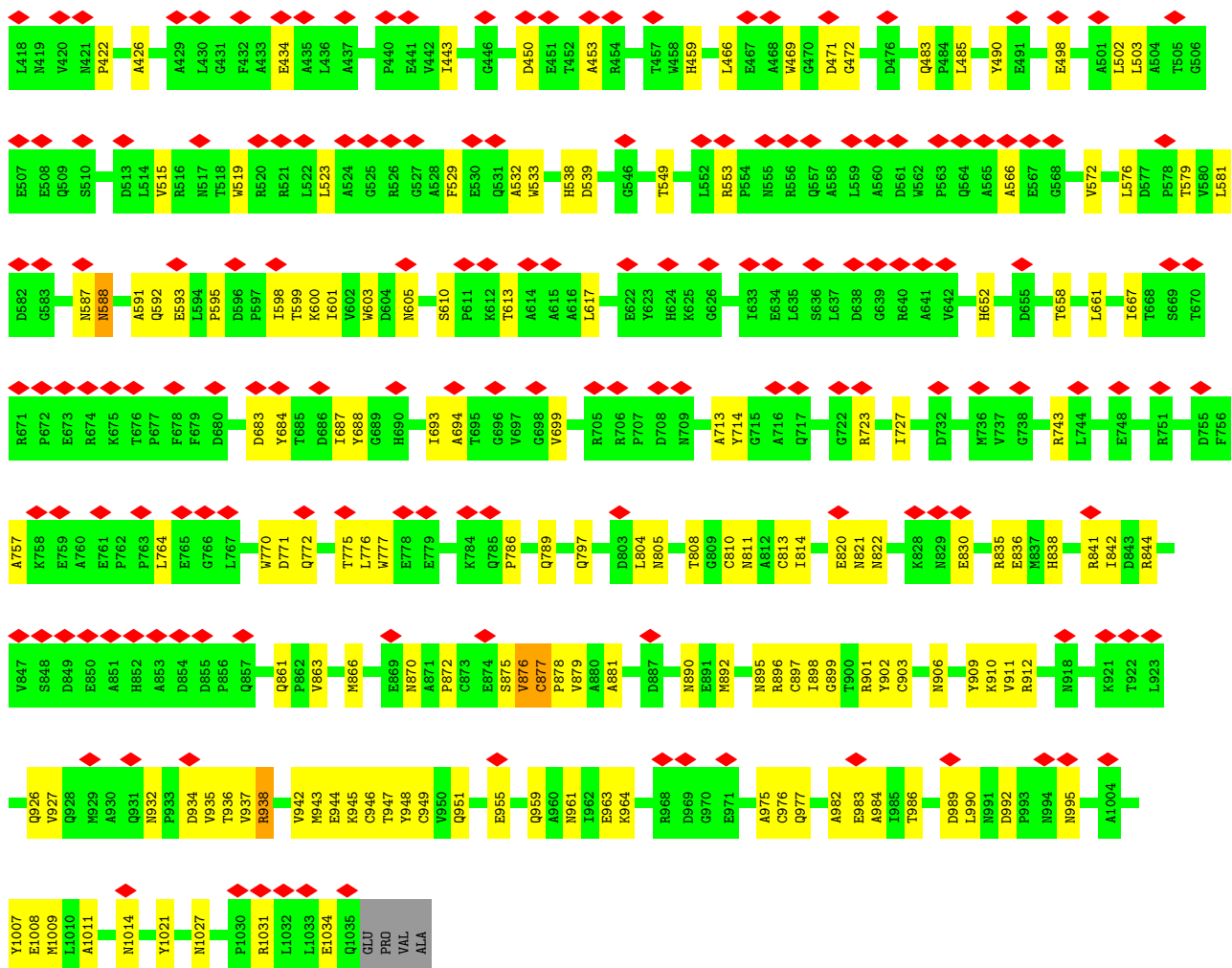
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 c family protein

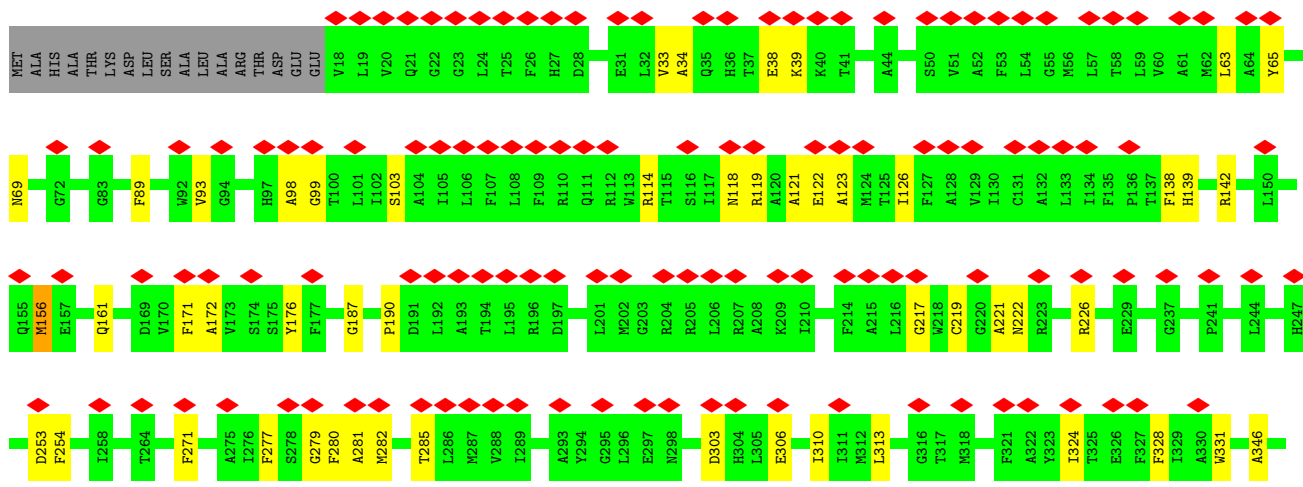
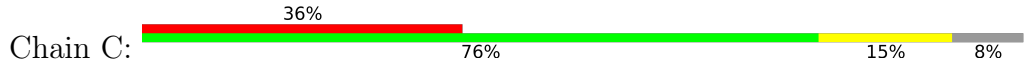


- Molecule 2: Fe-S-cluster-containing hydrogenase

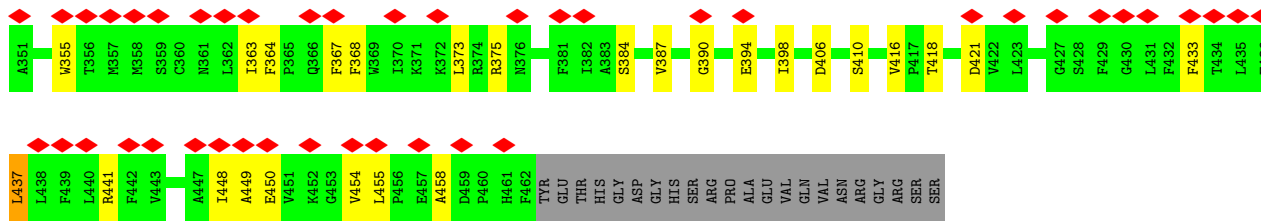




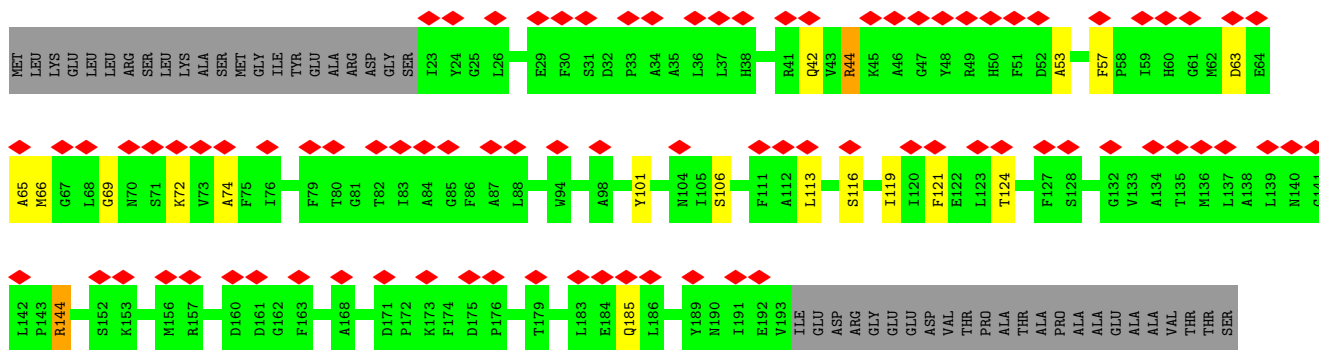
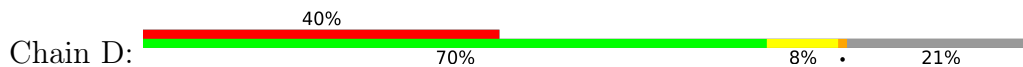
● Molecule 3: Polysulphide reductase NrfD



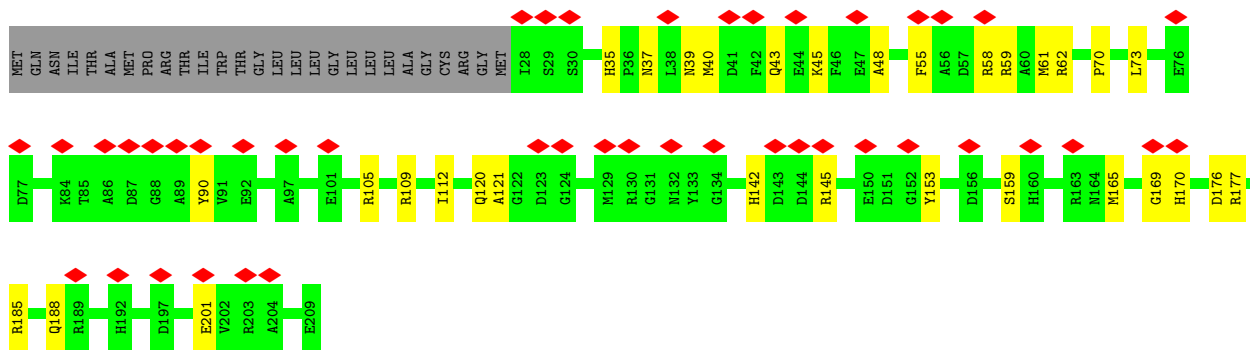




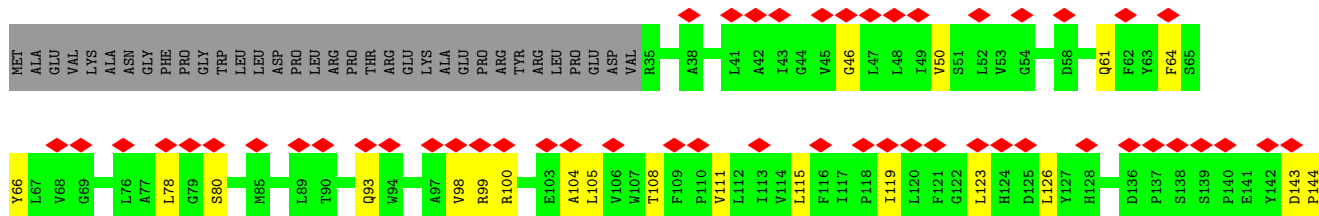
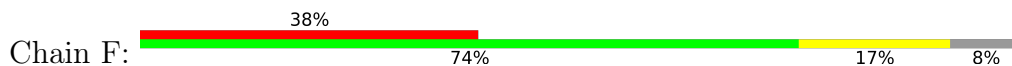
- Molecule 4: ActD

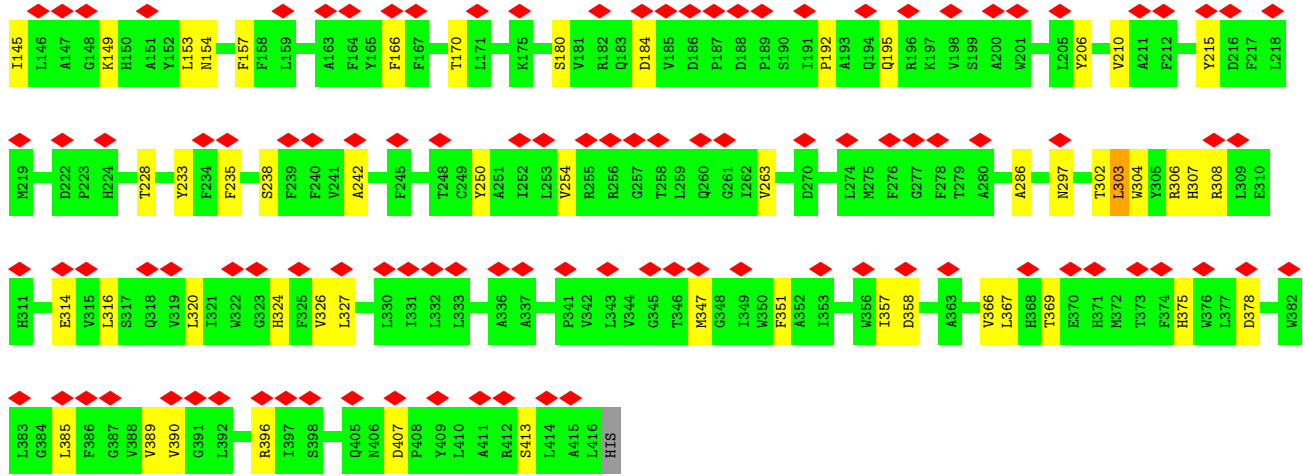


- Molecule 5: Quinol:cytochrome c oxidoreductase monoheme cytochrome subunit

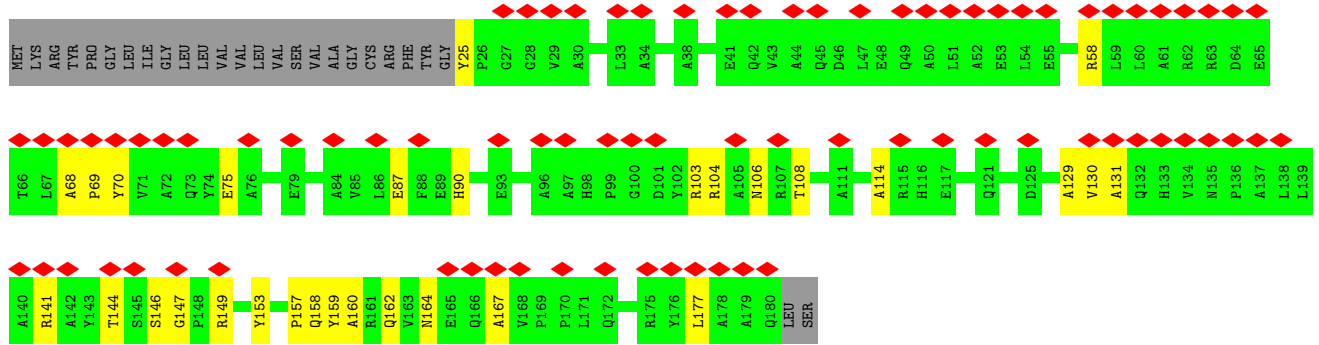


- Molecule 6: ActF





● Molecule 7: ActH



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52386	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 ( $e^-/\text{\AA}^2$ )	72	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	0.331	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	298.08, 298.08, 298.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.035, 1.035, 1.035	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: F3S, SF4, HEC

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	0.55	1/1723 (0.1%)	0.77	3/2349 (0.1%)
2	B	0.56	3/7717 (0.0%)	0.68	0/10526
3	C	0.47	0/3751	0.59	3/5131 (0.1%)
4	D	0.43	0/1390	0.60	0/1895
5	E	0.54	0/1479	0.61	0/2011
6	F	0.47	0/3297	0.62	5/4522 (0.1%)
7	H	0.42	0/1264	0.54	0/1729
All	All	0.51	4/20621 (0.0%)	0.65	11/28163 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	877	CYS	CB-SG	-13.17	1.59	1.82
1	A	206	CYS	CB-SG	-6.69	1.70	1.82
2	B	876	VAL	CB-CG1	-5.66	1.41	1.52
2	B	976	CYS	CB-SG	-5.26	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	CYS	CA-CB-SG	-15.95	85.29	114.00
1	A	85	CYS	CA-CB-SG	10.77	133.38	114.00
1	A	138	CYS	CA-CB-SG	8.25	128.84	114.00
6	F	326	VAL	CG1-CB-CG2	7.50	122.90	110.90
6	F	303	LEU	CB-CG-CD2	7.46	123.68	111.00
6	F	327	LEU	CB-CG-CD1	6.32	121.74	111.00
6	F	303	LEU	CB-CG-CD1	6.16	121.46	111.00
3	C	437	LEU	CB-CG-CD2	5.54	120.42	111.00
6	F	327	LEU	CB-CG-CD2	5.48	120.31	111.00
3	C	437	LEU	CB-CG-CD1	5.13	119.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	226	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	1670	1583	1588	42	0
2	B	7532	7345	7375	157	0
3	C	3617	3617	3627	53	0
4	D	1343	1313	1315	16	0
5	E	1439	1379	1388	23	0
6	F	3167	3141	3142	44	0
7	H	1234	1199	1207	23	0
8	A	215	148	150	35	0
8	E	43	30	31	4	0
9	B	7	0	0	1	0
10	B	24	0	0	7	0
All	All	20291	19755	19823	344	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 9.

All (344) 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:808:THR:HG22	2:B:808:THR:O	1.52	1.04
2:B:295:VAL:HG22	2:B:808:THR:HG22	1.43	1.01
2:B:902:TYR:OH	3:C:253:ASP:O	1.94	0.86
2:B:808:THR:O	2:B:808:THR:CG2	2.23	0.86
4:D:44:ARG:NH1	4:D:65:ALA:O	2.14	0.81
8:A:303:HEC:HMB3	8:A:304:HEC:HMB3	1.63	0.81
2:B:876:VAL:HG21	2:B:906:ASN:HD21	1.46	0.80
2:B:892:MET:SD	2:B:912:ARG:NH1	2.55	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:HD2	8:A:302:HEC:CBC	1.96	0.79
2:B:938:ARG:NE	2:B:944:GLU:OE1	2.17	0.78
4:D:121:PHE:O	4:D:124:THR:OG1	2.01	0.78
6:F:166:PHE:O	6:F:170:THR:OG1	2.03	0.77
1:A:170:LEU:O	1:A:187:TYR:OH	2.02	0.77
2:B:295:VAL:CG2	2:B:808:THR:HG22	2.13	0.77
6:F:100:ARG:NH2	6:F:184:ASP:OD2	2.19	0.76
3:C:103:SER:OG	3:C:118:ASN:OD1	2.03	0.76
2:B:595:PRO:O	2:B:811:ASN:ND2	2.19	0.75
2:B:813:CYS:N	10:B:1104:SF4:S4	2.60	0.73
2:B:295:VAL:CG2	2:B:808:THR:O	2.36	0.73
5:E:176:ASP:OD1	7:H:159:TYR:OH	2.05	0.73
2:B:964:LYS:O	7:H:164:ASN:ND2	2.22	0.72
1:A:169:TYR:HD2	8:A:302:HEC:HBC1	1.54	0.72
2:B:989:ASP:OD1	2:B:995:ASN:ND2	2.23	0.72
3:C:103:SER:OG	3:C:122:GLU:OE2	2.05	0.72
8:A:301:HEC:HMC1	8:A:301:HEC:HBC2	1.71	0.72
2:B:890:ASN:ND2	10:B:1102:SF4:S3	2.63	0.72
3:C:39:LYS:O	3:C:441:ARG:NH2	2.23	0.72
3:C:217:GLY:O	4:D:144:ARG:NH1	2.23	0.71
2:B:299:MET:CB	2:B:808:THR:OG1	2.38	0.71
2:B:890:ASN:O	2:B:945:LYS:NZ	2.18	0.71
2:B:605:ASN:ND2	2:B:699:VAL:O	2.24	0.70
8:E:400:HEC:HBB3	8:E:400:HEC:HMB1	1.72	0.70
5:E:55:PHE:O	5:E:58:ARG:NH1	2.25	0.70
2:B:959:GLN:NE2	2:B:963:GLU:OE2	2.24	0.69
2:B:252:ASP:OD2	2:B:361:THR:OG1	2.07	0.69
3:C:119:ARG:NH2	3:C:187:GLY:O	2.25	0.69
6:F:303:LEU:O	6:F:307:HIS:ND1	2.24	0.69
6:F:180:SER:OG	6:F:195:GLN:NE2	2.26	0.69
8:A:304:HEC:HMC1	8:A:304:HEC:HBC3	1.74	0.68
6:F:215:TYR:OH	6:F:228:THR:O	2.12	0.68
8:A:305:HEC:HMC1	8:A:305:HEC:HBC3	1.76	0.68
2:B:877:CYS:SG	2:B:879:VAL:O	2.52	0.68
1:A:106:ASP:O	5:E:59:ARG:NH1	2.28	0.67
2:B:587:ASN:OD1	2:B:694:ALA:N	2.26	0.67
5:E:159:SER:OG	5:E:177:ARG:NH1	2.28	0.67
2:B:295:VAL:HG22	2:B:808:THR:CG2	2.22	0.67
3:C:303:ASP:OD1	3:C:375:ARG:NH1	2.26	0.67
2:B:811:ASN:OD1	2:B:814:ILE:HD12	1.94	0.67
3:C:99:GLY:HA2	3:C:121:ALA:HB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:301:HEC:HMA1	2:B:896:ARG:HD3	1.77	0.66
2:B:274:ARG:O	2:B:805:ASN:ND2	2.28	0.66
2:B:879:VAL:O	2:B:881:ALA:N	2.28	0.66
2:B:519:TRP:O	2:B:523:LEU:N	2.28	0.66
1:A:169:TYR:CD2	8:A:302:HEC:HBC1	2.30	0.65
4:D:72:LYS:NZ	4:D:74:ALA:HB3	2.12	0.65
2:B:241:ARG:NH2	2:B:269:GLU:OE2	2.30	0.65
2:B:610:SER:OG	2:B:652:HIS:O	2.14	0.65
6:F:61:GLN:NE2	6:F:378:ASP:OD1	2.30	0.64
7:H:58:ARG:NH2	7:H:75:GLU:OE2	2.29	0.64
2:B:770:TRP:NE1	2:B:1011:ALA:O	2.30	0.64
2:B:830:GLU:OE2	2:B:835:ARG:NH2	2.30	0.64
1:A:69:GLU:OE1	7:H:158:GLN:NE2	2.31	0.64
3:C:281:ALA:O	3:C:384:SER:OG	2.14	0.64
6:F:93:GLN:O	6:F:413:SER:OG	2.16	0.64
2:B:820:GLU:O	2:B:932:ASN:ND2	2.32	0.63
2:B:876:VAL:HG21	2:B:906:ASN:ND2	2.13	0.63
3:C:418:THR:N	3:C:421:ASP:OD2	2.30	0.62
1:A:164:ARG:HE	1:A:204:THR:HG23	1.64	0.62
8:E:400:HEC:HBC3	8:E:400:HEC:HMC1	1.81	0.62
7:H:144:THR:OG1	7:H:160:ALA:HB1	1.99	0.62
8:A:302:HEC:CBC	8:A:302:HEC:HMC1	2.30	0.62
6:F:233:TYR:OH	6:F:358:ASP:OD1	2.17	0.61
2:B:113:LEU:O	2:B:125:GLU:N	2.33	0.61
2:B:895:ASN:O	3:C:142:ARG:NH1	2.33	0.61
2:B:866:MET:SD	2:B:866:MET:N	2.73	0.61
1:A:169:TYR:CD2	8:A:302:HEC:CBC	2.82	0.61
2:B:416:LEU:HA	2:B:443:ILE:HG23	1.83	0.61
2:B:159:ARG:NH1	2:B:168:ASP:OD2	2.34	0.61
2:B:600:LYS:HE3	2:B:842:ILE:HG23	1.82	0.60
8:A:301:HEC:HMB1	8:A:301:HEC:HBB2	1.81	0.60
2:B:263:PHE:O	2:B:267:THR:OG1	2.12	0.60
2:B:1009:MET:SD	2:B:1021:TYR:OH	2.56	0.60
3:C:222:ASN:N	4:D:53:ALA:O	2.35	0.60
6:F:144:PRO:O	6:F:149:LYS:NZ	2.28	0.60
3:C:282:MET:O	3:C:285:THR:OG1	2.12	0.60
3:C:310:ILE:HD11	3:C:373:LEU:HD21	1.82	0.60
3:C:363:ILE:O	3:C:367:PHE:N	2.33	0.60
6:F:250:TYR:O	6:F:254:VAL:N	2.35	0.60
1:A:80:GLN:OE1	5:E:170:HIS:NE2	2.36	0.59
2:B:299:MET:HB2	2:B:808:THR:OG1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:ALA:HB3	10:B:1103:SF4:S4	2.43	0.59
2:B:490:TYR:OH	2:B:926:GLN:OE1	2.17	0.59
3:C:433:PHE:O	3:C:437:LEU:HG	2.03	0.59
2:B:897:CYS:SG	2:B:898:ILE:N	2.76	0.58
8:A:305:HEC:HMB1	8:A:305:HEC:HBB3	1.85	0.58
2:B:743:ARG:NH1	2:B:757:ALA:O	2.36	0.58
2:B:949:CYS:N	10:B:1103:SF4:S3	2.75	0.58
2:B:934:ASP:O	2:B:951:GLN:NE2	2.37	0.58
1:A:205:ASN:O	8:A:301:HEC:HMC3	2.03	0.58
4:D:42:GLN:OE1	4:D:185:GLN:NE2	2.36	0.58
6:F:104:ALA:HB1	6:F:396:ARG:HD2	1.86	0.58
2:B:992:ASP:OD2	2:B:995:ASN:ND2	2.37	0.58
8:A:301:HEC:HMA1	2:B:896:ARG:CD	2.33	0.57
2:B:102:ALA:HB1	2:B:109:VAL:CG1	2.34	0.57
2:B:870:ASN:O	4:D:106:SER:OG	2.11	0.57
2:B:286:LEU:HD11	2:B:300:ALA:HB1	1.87	0.57
2:B:268:ARG:NE	2:B:983:GLU:OE2	2.34	0.57
2:B:797:GLN:O	2:B:990:LEU:N	2.38	0.57
2:B:319:ALA:HB1	2:B:324:VAL:HG22	1.87	0.56
2:B:408:GLN:NE2	2:B:434:GLU:OE1	2.38	0.56
3:C:156:MET:SD	3:C:156:MET:N	2.78	0.56
5:E:39:ASN:OD1	5:E:40:MET:N	2.39	0.56
6:F:143:ASP:O	6:F:145:ILE:N	2.39	0.56
2:B:872:PRO:O	2:B:875:SER:OG	2.22	0.56
1:A:169:TYR:HD2	8:A:302:HEC:HBC3	1.69	0.56
2:B:1008:GLU:CG	2:B:1011:ALA:HB2	2.36	0.56
6:F:78:LEU:O	6:F:206:TYR:OH	2.23	0.56
1:A:201:ARG:HD2	7:H:114:ALA:HB2	1.87	0.56
2:B:977:GLN:NE2	2:B:986:THR:O	2.38	0.55
7:H:87:GLU:O	7:H:90:HIS:N	2.39	0.55
2:B:315:ALA:HB1	2:B:369:LEU:HD23	1.89	0.55
5:E:165:MET:SD	8:E:400:HEC:C4C	2.80	0.55
7:H:68:ALA:HB3	7:H:69:PRO:HD3	1.86	0.55
8:A:303:HEC:CMB	8:A:304:HEC:HMB3	2.36	0.55
6:F:119:ILE:O	6:F:123:LEU:N	2.40	0.55
8:A:301:HEC:HAC	8:A:302:HEC:HMB3	1.89	0.54
6:F:154:ASN:O	6:F:157:PHE:N	2.35	0.54
2:B:770:TRP:CD1	2:B:1011:ALA:HB1	2.42	0.54
3:C:65:TYR:O	3:C:69:ASN:ND2	2.41	0.54
2:B:946:CYS:O	2:B:947:THR:OG1	2.22	0.54
6:F:46:GLY:O	6:F:50:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH2	1:A:69:GLU:OE2	2.41	0.53
2:B:579:THR:OG1	2:B:591:ALA:O	2.23	0.53
4:D:113:LEU:O	4:D:116:SER:OG	2.12	0.53
6:F:366:VAL:HG23	6:F:367:LEU:HD12	1.90	0.53
2:B:299:MET:HB3	2:B:808:THR:OG1	2.08	0.53
6:F:66:TYR:OH	6:F:115:LEU:O	2.18	0.53
2:B:1014:ASN:ND2	6:F:297:ASN:O	2.39	0.53
1:A:139:HIS:CE1	8:A:303:HEC:ND	2.77	0.53
5:E:109:ARG:NH1	7:H:158:GLN:OE1	2.40	0.53
2:B:295:VAL:HG23	2:B:808:THR:O	2.07	0.53
2:B:821:ASN:OD1	2:B:935:VAL:HG21	2.09	0.53
3:C:450:GLU:O	3:C:454:VAL:HG12	2.08	0.53
1:A:141:ARG:NH2	1:A:143:ASP:OD1	2.42	0.53
3:C:98:ALA:HB1	3:C:280:PHE:CD1	2.44	0.53
2:B:909:TYR:O	2:B:911:VAL:N	2.42	0.52
5:E:185:ARG:NH1	5:E:188:GLN:OE1	2.43	0.52
1:A:133:VAL:O	1:A:176:ILE:HD11	2.09	0.52
5:E:169:GLY:O	5:E:177:ARG:NH2	2.43	0.52
1:A:65:HIS:CE1	8:A:304:HEC:ND	2.76	0.52
2:B:101:THR:OG1	2:B:112:LEU:HD22	2.10	0.52
2:B:1031:ARG:O	2:B:1034:GLU:N	2.42	0.52
2:B:601:ILE:HD11	2:B:727:ILE:HD11	1.90	0.52
2:B:593:GLU:OE1	2:B:838:HIS:NE2	2.43	0.52
3:C:458:ALA:HB1	4:D:57:PHE:CE2	2.45	0.52
6:F:64:PHE:CE1	6:F:126:LEU:HD13	2.44	0.52
5:E:90:TYR:CE1	5:E:153:TYR:HD1	2.28	0.51
6:F:385:LEU:O	6:F:389:VAL:HG12	2.10	0.51
2:B:903:CYS:N	9:B:1101:F3S:S2	2.83	0.51
6:F:153:LEU:HD12	6:F:153:LEU:O	2.10	0.51
2:B:1007:TYR:N	2:B:1021:TYR:O	2.44	0.51
2:B:112:LEU:HD23	2:B:113:LEU:N	2.26	0.51
1:A:86:HIS:HA	1:A:89:ILE:HG22	1.92	0.51
3:C:34:ALA:O	3:C:38:GLU:N	2.44	0.51
3:C:190:PRO:HB2	3:C:449:ALA:HB2	1.92	0.51
8:A:302:HEC:HMC1	8:A:302:HEC:HBC2	1.93	0.50
2:B:899:GLY:O	2:B:901:ARG:NH1	2.44	0.50
2:B:369:LEU:O	2:B:373:ILE:HG22	2.10	0.50
2:B:963:GLU:OE2	7:H:146:SER:OG	2.22	0.50
2:B:232:PHE:HA	2:B:553:ARG:HB2	1.92	0.50
2:B:315:ALA:HB1	2:B:369:LEU:CD2	2.41	0.50
2:B:901:ARG:NH1	3:C:139:HIS:O	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:HIS:CD2	8:A:301:HEC:NC	2.76	0.50
2:B:588:ASN:O	2:B:592:GLN:N	2.41	0.49
1:A:71:SER:OG	1:A:72:ASP:N	2.45	0.49
2:B:289:ILE:O	2:B:289:ILE:HD12	2.11	0.49
2:B:469:TRP:O	2:B:515:VAL:HG21	2.12	0.49
2:B:982:ALA:O	2:B:984:ALA:N	2.45	0.49
7:H:25:TYR:OH	7:H:103:ARG:NH2	2.45	0.49
2:B:576:LEU:HD13	2:B:581:LEU:HD22	1.93	0.49
8:A:305:HEC:HBC3	8:A:305:HEC:CMC	2.43	0.48
3:C:310:ILE:CD1	3:C:373:LEU:HD21	2.42	0.48
2:B:764:LEU:HD13	6:F:302:THR:HG21	1.95	0.48
3:C:346:ALA:O	3:C:355:TRP:NE1	2.46	0.48
2:B:386:LEU:HD23	2:B:549:THR:HG22	1.94	0.48
2:B:234:ARG:CZ	2:B:553:ARG:HE	2.27	0.48
2:B:841:ARG:NH2	3:C:410:SER:O	2.46	0.48
6:F:235:PHE:O	6:F:238:SER:OG	2.16	0.48
2:B:775:THR:HG21	2:B:777:TRP:CZ2	2.49	0.48
2:B:143:ALA:CB	2:B:591:ALA:HB2	2.44	0.48
2:B:775:THR:HG22	2:B:776:LEU:N	2.28	0.48
3:C:63:LEU:HD21	3:C:138:PHE:CD2	2.49	0.47
6:F:316:LEU:HD11	6:F:357:ILE:HG23	1.95	0.47
2:B:910:LYS:NZ	3:C:406:ASP:OD2	2.37	0.47
6:F:108:THR:O	6:F:111:VAL:N	2.46	0.47
6:F:303:LEU:HD23	6:F:307:HIS:CE1	2.50	0.47
6:F:375:HIS:N	6:F:378:ASP:OD2	2.46	0.47
1:A:201:ARG:CD	7:H:114:ALA:HB2	2.44	0.47
2:B:106:ARG:NH2	2:B:360:GLU:OE2	2.48	0.47
3:C:253:ASP:OD1	3:C:254:PHE:N	2.48	0.47
6:F:64:PHE:CZ	6:F:126:LEU:HD13	2.50	0.47
1:A:138:CYS:SG	8:A:303:HEC:HMC1	2.55	0.47
2:B:319:ALA:HB1	2:B:324:VAL:CG2	2.45	0.47
2:B:373:ILE:O	2:B:377:LEU:N	2.47	0.47
3:C:114:ARG:NH1	3:C:118:ASN:HD22	2.12	0.47
5:E:105:ARG:HH22	7:H:162:GLN:HE22	1.63	0.47
2:B:658:THR:HG23	2:B:658:THR:O	2.15	0.47
6:F:145:ILE:HG23	6:F:149:LYS:HB2	1.96	0.47
2:B:176:LEU:O	2:B:180:ALA:HB2	2.15	0.47
2:B:466:LEU:HD12	2:B:485:LEU:HD12	1.96	0.47
2:B:836:GLU:OE1	2:B:836:GLU:N	2.47	0.47
5:E:70:PRO:HG2	5:E:73:LEU:HD12	1.97	0.47
6:F:98:VAL:HG12	6:F:98:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ASP:OD1	2:B:223:HIS:N	2.49	0.46
2:B:133:SER:HA	2:B:264:VAL:HG11	1.98	0.46
1:A:31:VAL:HG23	1:A:32:TRP:H	1.80	0.46
2:B:688:TYR:CD1	2:B:693:ILE:HD11	2.50	0.46
2:B:529:PHE:O	2:B:533:TRP:N	2.48	0.46
2:B:576:LEU:HD21	2:B:661:LEU:HD12	1.98	0.46
3:C:171:PHE:HD2	4:D:119:ILE:HD12	1.79	0.46
6:F:303:LEU:HD22	6:F:304:TRP:CD1	2.50	0.46
8:A:301:HEC:HMC1	8:A:301:HEC:CBC	2.42	0.46
2:B:688:TYR:HE2	2:B:927:VAL:HG21	1.81	0.46
2:B:450:ASP:OD1	2:B:667:ILE:HD12	2.16	0.46
2:B:599:THR:O	2:B:601:ILE:N	2.47	0.46
1:A:114:VAL:HG21	1:A:148:VAL:HG11	1.98	0.46
8:A:301:HEC:HBB2	4:D:101:TYR:OH	2.16	0.46
3:C:310:ILE:O	3:C:313:LEU:N	2.49	0.46
5:E:177:ARG:NH2	7:H:153:TYR:OH	2.49	0.46
1:A:176:ILE:HG23	1:A:177:THR:HG23	1.98	0.45
2:B:264:VAL:O	2:B:267:THR:N	2.50	0.45
2:B:276:MET:SD	2:B:283:ILE:HD11	2.56	0.45
2:B:319:ALA:HB3	2:B:327:LEU:HD23	1.97	0.45
6:F:308:ARG:O	6:F:314:GLU:N	2.50	0.45
6:F:99:ARG:NH2	6:F:407:ASP:OD1	2.50	0.45
6:F:105:LEU:HD13	6:F:105:LEU:O	2.16	0.45
7:H:70:TYR:OH	7:H:130:VAL:N	2.49	0.45
1:A:57:LEU:HD21	8:A:305:HEC:HMD2	1.99	0.45
2:B:842:ILE:HD11	10:B:1104:SF4:S2	2.56	0.45
3:C:222:ASN:HB2	4:D:53:ALA:HB3	1.98	0.45
2:B:177:ALA:O	2:B:208:TYR:OH	2.33	0.45
2:B:422:PRO:O	2:B:426:ALA:HB3	2.15	0.45
3:C:454:VAL:HG13	3:C:455:LEU:H	1.82	0.45
5:E:35:HIS:NE2	5:E:37:ASN:OD1	2.50	0.45
3:C:390:GLY:O	3:C:394:GLU:N	2.50	0.45
1:A:154:LEU:HD12	8:A:303:HEC:HMD3	1.99	0.44
2:B:276:MET:HG2	2:B:283:ILE:HD11	2.00	0.44
2:B:471:ASP:OD1	2:B:472:GLY:N	2.47	0.44
6:F:347:MET:O	6:F:351:PHE:N	2.47	0.44
2:B:863:VAL:HG13	2:B:863:VAL:O	2.17	0.44
1:A:194:ARG:O	1:A:198:GLU:N	2.48	0.44
1:A:70:VAL:HG12	7:H:157:PRO:HD2	1.98	0.44
6:F:389:VAL:HG13	6:F:390:VAL:HG23	2.00	0.44
1:A:162:CYS:HB2	8:A:302:HEC:HBC3	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:HA	2:B:936:THR:HG22	2.00	0.44
5:E:59:ARG:O	5:E:62:ARG:NH1	2.51	0.44
6:F:192:PRO:O	6:F:195:GLN:N	2.51	0.44
1:A:60:ASP:HB2	5:E:112:ILE:HG22	1.99	0.44
2:B:102:ALA:HB1	2:B:109:VAL:HG12	1.98	0.44
2:B:389:LEU:HD12	2:B:389:LEU:O	2.18	0.44
2:B:866:MET:SD	10:B:1102:SF4:S2	3.16	0.44
2:B:317:ALA:HB2	2:B:331:GLY:O	2.18	0.43
5:E:120:GLN:NE2	5:E:201:GLU:OE2	2.49	0.43
1:A:146:ASP:OD1	1:A:147:VAL:N	2.51	0.43
3:C:99:GLY:CA	3:C:121:ALA:HB1	2.46	0.43
2:B:683:ASP:OD1	2:B:684:TYR:N	2.51	0.43
2:B:1008:GLU:HG3	2:B:1011:ALA:HB2	2.00	0.43
3:C:123:ALA:HA	3:C:126:ILE:HG22	1.99	0.43
3:C:328:PHE:O	3:C:331:TRP:N	2.47	0.43
1:A:164:ARG:NE	1:A:204:THR:HG23	2.31	0.43
6:F:320:LEU:O	6:F:324:HIS:N	2.52	0.43
2:B:361:THR:N	2:B:362:GLN:OE1	2.51	0.43
2:B:771:ASP:OD1	2:B:772:GLN:N	2.49	0.43
3:C:89:PHE:O	3:C:93:VAL:HG12	2.18	0.43
2:B:822:ASN:O	2:B:938:ARG:NH1	2.52	0.42
1:A:45:ALA:HB3	1:A:46:PRO:CD	2.49	0.42
2:B:572:VAL:HG12	2:B:572:VAL:O	2.19	0.42
3:C:364:PHE:O	3:C:368:PHE:N	2.52	0.42
7:H:141:ARG:NE	7:H:167:ALA:O	2.43	0.42
2:B:572:VAL:HB	2:B:713:ALA:HB3	2.01	0.42
3:C:63:LEU:HD21	3:C:138:PHE:CE2	2.55	0.42
1:A:48:TYR:HE1	8:A:305:HEC:HBB2	1.84	0.42
2:B:538:HIS:ND1	2:B:539:ASP:OD1	2.48	0.42
1:A:164:ARG:O	7:H:106:ASN:ND2	2.48	0.42
6:F:78:LEU:HD11	6:F:210:VAL:HG22	2.01	0.42
3:C:277:PHE:CZ	3:C:387:VAL:HG13	2.55	0.42
5:E:165:MET:SD	8:E:400:HEC:C1C	2.85	0.42
2:B:192:SER:CB	2:B:197:LEU:HD12	2.49	0.42
2:B:498:GLU:O	2:B:502:LEU:N	2.50	0.42
3:C:454:VAL:HG13	3:C:455:LEU:N	2.35	0.42
7:H:146:SER:OG	7:H:147:GLY:N	2.51	0.42
8:A:302:HEC:HMC1	8:A:302:HEC:HBC3	2.01	0.42
2:B:613:THR:O	2:B:617:LEU:N	2.53	0.42
2:B:775:THR:HG22	2:B:776:LEU:H	1.85	0.42
2:B:942:VAL:HG12	2:B:943:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:O	1:A:57:LEU:HD13	2.19	0.42
1:A:204:THR:HG22	1:A:204:THR:O	2.20	0.42
2:B:101:THR:HG22	2:B:483:GLN:O	2.20	0.42
2:B:566:ALA:O	2:B:714:TYR:OH	2.16	0.42
4:D:44:ARG:NH1	4:D:66:MET:O	2.52	0.42
4:D:72:LYS:CE	4:D:74:ALA:HB3	2.49	0.42
3:C:33:VAL:HG11	3:C:448:ILE:HD13	2.02	0.41
3:C:172:ALA:O	3:C:176:TYR:N	2.53	0.41
1:A:61:CYS:SG	8:A:304:HEC:HMB1	2.60	0.41
2:B:937:VAL:O	5:E:43:GLN:NE2	2.47	0.41
3:C:98:ALA:HB2	3:C:279:GLY:HA3	2.02	0.41
5:E:48:ALA:HB1	5:E:61:MET:HE1	2.02	0.41
2:B:955:GLU:OE1	7:H:149:ARG:NH1	2.53	0.41
2:B:294:THR:HG22	2:B:295:VAL:H	1.86	0.41
3:C:219:CYS:SG	3:C:221:ALA:HB2	2.60	0.41
3:C:324:ILE:O	3:C:328:PHE:N	2.53	0.41
6:F:80:SER:HB3	6:F:242:ALA:HB1	2.01	0.41
2:B:688:TYR:HD1	2:B:693:ILE:HD11	1.85	0.41
2:B:804:LEU:HD11	2:B:861:GLN:HB3	2.03	0.41
2:B:878:PRO:O	3:C:161:GLN:N	2.49	0.41
2:B:283:ILE:HB	2:B:1027:ASN:HD22	1.85	0.41
2:B:251:LEU:HD11	2:B:315:ALA:HB2	2.01	0.41
2:B:503:LEU:O	2:B:503:LEU:HD13	2.21	0.41
2:B:529:PHE:O	2:B:532:ALA:N	2.53	0.41
2:B:294:THR:HA	2:B:598:ILE:HD11	2.03	0.41
2:B:786:PRO:O	2:B:789:GLN:N	2.54	0.41
3:C:306:GLU:OE2	3:C:373:LEU:HD22	2.19	0.41
5:E:121:ALA:O	5:E:142:HIS:NE2	2.47	0.41
6:F:263:VAL:HG23	6:F:263:VAL:O	2.20	0.41
1:A:115:HIS:O	1:A:117:LEU:N	2.54	0.41
1:A:200:ILE:HD12	8:A:302:HEC:HMD1	2.03	0.41
2:B:245:ALA:HB1	2:B:355:VAL:HG23	2.03	0.41
4:D:63:ASP:OD1	4:D:69:GLY:N	2.54	0.41
4:D:72:LYS:HE3	4:D:74:ALA:HB3	2.03	0.40
7:H:131:ALA:HB2	7:H:177:LEU:HD21	2.02	0.40
8:A:302:HEC:O2D	2:B:961:ASN:ND2	2.51	0.40
2:B:948:TYR:C	10:B:1103:SF4:S3	3.00	0.40
7:H:70:TYR:OH	7:H:129:ALA:HB3	2.20	0.40
8:A:301:HEC:CAC	8:A:302:HEC:HMB3	2.52	0.40
3:C:271:PHE:HZ	3:C:398:ILE:HG21	1.87	0.40
3:C:416:VAL:O	3:C:416:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:TYR:CZ	5:E:153:TYR:HD1	2.39	0.40
2:B:842:ILE:HD12	2:B:842:ILE:HA	1.99	0.40
6:F:233:TYR:HE1	6:F:286:ALA:HB2	1.85	0.40
8:A:302:HEC:HMB1	8:A:302:HEC:HBB3	2.04	0.40
2:B:453:ALA:HB2	2:B:459:HIS:CD2	2.56	0.40
2:B:603:TRP:CZ2	2:B:687:ILE:HD11	2.57	0.40
6:F:306:ARG:NH1	6:F:369:THR:OG1	2.54	0.40
7:H:104:ARG:O	7:H:108:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/211 (97%)	173 (84%)	32 (16%)	0	100	100
2	B	959/1039 (92%)	789 (82%)	170 (18%)	0	100	100
3	C	443/484 (92%)	401 (90%)	42 (10%)	0	100	100
4	D	169/217 (78%)	144 (85%)	25 (15%)	0	100	100
5	E	180/209 (86%)	160 (89%)	20 (11%)	0	100	100
6	F	380/417 (91%)	330 (87%)	50 (13%)	0	100	100
7	H	154/182 (85%)	140 (91%)	14 (9%)	0	100	100
All	All	2490/2759 (90%)	2137 (86%)	353 (14%)	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	184/188 (98%)	184 (100%)	0	100	100
2	B	787/849 (93%)	780 (99%)	7 (1%)	78	87
3	C	375/406 (92%)	374 (100%)	1 (0%)	92	95
4	D	136/171 (80%)	134 (98%)	2 (2%)	65	80
5	E	148/169 (88%)	146 (99%)	2 (1%)	67	81
6	F	329/359 (92%)	329 (100%)	0	100	100
7	H	120/141 (85%)	120 (100%)	0	100	100
All	All	2079/2283 (91%)	2067 (99%)	12 (1%)	86	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	ARG
2	B	303	ARG
2	B	588	ASN
2	B	723	ARG
2	B	810	CYS
2	B	844	ARG
2	B	938	ARG
3	C	156	MET
4	D	44	ARG
4	D	144	ARG
5	E	45	LYS
5	E	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	131	ASN
2	B	142	GLN
2	B	408	GLN
2	B	459	HIS
2	B	592	GLN
2	B	805	ASN

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Mol	Chain	Res	Type
2	B	1027	ASN
3	C	118	ASN
3	C	155	GLN
4	D	42	GLN
4	D	185	GLN
6	F	87	GLN
6	F	88	HIS
6	F	195	GLN
7	H	162	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
10	SF4	B	1102	2	0,12,12	-	-	-		
8	HEC	A	305	1	32,50,50	2.35	6 (18%)	24,82,82	1.82	5 (20%)
8	HEC	A	303	1	32,50,50	2.57	6 (18%)	24,82,82	1.88	8 (33%)
8	HEC	A	304	1	32,50,50	2.18	6 (18%)	24,82,82	1.88	8 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	HEC	E	400	5	32,50,50	2.27	5 (15%)	24,82,82	1.83	9 (37%)
10	SF4	B	1103	2	0,12,12	-	-	-	-	-
9	F3S	B	1101	2	0,9,9	-	-	-	-	-
8	HEC	A	302	1	32,50,50	2.31	6 (18%)	24,82,82	2.41	10 (41%)
10	SF4	B	1104	2	0,12,12	-	-	-	-	-
8	HEC	A	301	1	32,50,50	2.22	7 (21%)	24,82,82	2.21	7 (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
10	SF4	B	1102	2	-	-	0/6/5/5
8	HEC	A	305	1	-	1/10/54/54	-
8	HEC	A	303	1	-	7/10/54/54	-
8	HEC	A	304	1	-	7/10/54/54	-
8	HEC	E	400	5	-	3/10/54/54	-
10	SF4	B	1103	2	-	-	0/6/5/5
9	F3S	B	1101	2	-	-	0/3/3/3
8	HEC	A	302	1	-	7/10/54/54	-
10	SF4	B	1104	2	-	-	0/6/5/5
8	HEC	A	301	1	-	2/10/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	303	HEC	C3C-C2C	-8.76	1.31	1.40
8	A	303	HEC	C2B-C3B	-7.77	1.32	1.40
8	A	302	HEC	C3C-C2C	-7.53	1.32	1.40
8	E	400	HEC	C3C-C2C	-7.27	1.33	1.40
8	A	301	HEC	C3C-C2C	-7.05	1.33	1.40
8	A	305	HEC	C3C-C2C	-7.04	1.33	1.40
8	A	304	HEC	C3C-C2C	-6.20	1.34	1.40
8	A	304	HEC	C2B-C3B	-6.03	1.34	1.40
8	A	305	HEC	C2B-C3B	-5.84	1.34	1.40
8	A	302	HEC	C2B-C3B	-5.66	1.34	1.40
8	E	400	HEC	C2B-C3B	-5.39	1.35	1.40
8	A	301	HEC	CBB-CAB	-4.87	1.31	1.49
8	A	301	HEC	C2B-C3B	-4.70	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	302	HEC	CBB-CAB	-4.66	1.32	1.49
8	E	400	HEC	CBC-CAC	-4.54	1.32	1.49
8	E	400	HEC	CBB-CAB	-4.49	1.32	1.49
8	A	305	HEC	CBB-CAB	-4.45	1.32	1.49
8	A	302	HEC	CBC-CAC	-4.37	1.33	1.49
8	A	305	HEC	CBC-CAC	-4.36	1.33	1.49
8	A	304	HEC	CBC-CAC	-4.35	1.33	1.49
8	A	304	HEC	CBB-CAB	-4.23	1.33	1.49
8	A	301	HEC	CBC-CAC	-4.20	1.33	1.49
8	A	303	HEC	CBB-CAB	-4.01	1.34	1.49
8	A	303	HEC	CBC-CAC	-3.80	1.35	1.49
8	A	305	HEC	C3C-C4C	3.36	1.49	1.43
8	A	305	HEC	CAD-C3D	3.06	1.56	1.52
8	A	303	HEC	C3C-C4C	3.03	1.48	1.43
8	E	400	HEC	CAD-C3D	2.63	1.55	1.52
8	A	302	HEC	CAD-C3D	2.36	1.55	1.52
8	A	301	HEC	C1C-CHC	-2.27	1.34	1.41
8	A	301	HEC	CAD-C3D	2.24	1.55	1.52
8	A	303	HEC	CAD-C3D	2.20	1.55	1.52
8	A	304	HEC	CAD-C3D	2.19	1.55	1.52
8	A	301	HEC	C3C-C4C	2.08	1.46	1.43
8	A	304	HEC	C3C-C4C	2.06	1.46	1.43
8	A	302	HEC	CAA-C2A	2.03	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	301	HEC	CMB-C2B-C1B	-5.44	120.10	128.46
8	A	303	HEC	CMC-C2C-C1C	-4.56	121.46	128.46
8	A	301	HEC	CMD-C2D-C1D	-4.45	121.63	128.46
8	A	305	HEC	CMB-C2B-C1B	-4.04	122.25	128.46
8	A	302	HEC	CMC-C2C-C1C	-3.93	122.43	128.46
8	A	302	HEC	CMA-C3A-C2A	3.89	132.28	124.94
8	A	302	HEC	CBD-CAD-C3D	3.87	119.22	112.62
8	A	305	HEC	CMB-C2B-C3B	3.84	130.34	125.82
8	A	302	HEC	CMC-C2C-C3C	3.78	130.26	125.82
8	A	301	HEC	CMB-C2B-C3B	3.68	130.15	125.82
8	A	302	HEC	CMB-C2B-C1B	-3.67	122.82	128.46
8	A	302	HEC	CBA-CAA-C2A	3.66	118.77	112.60
8	A	302	HEC	CMB-C2B-C3B	3.56	130.00	125.82
8	E	400	HEC	CMC-C2C-C1C	-3.52	123.05	128.46
8	A	302	HEC	CMD-C2D-C1D	-3.43	123.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	304	HEC	CMB-C2B-C1B	-3.33	123.34	128.46
8	E	400	HEC	CMB-C2B-C1B	-3.33	123.34	128.46
8	E	400	HEC	CMC-C2C-C3C	3.31	129.71	125.82
8	A	304	HEC	CMC-C2C-C1C	-3.23	123.50	128.46
8	A	303	HEC	CMB-C2B-C1B	-3.15	123.62	128.46
8	A	303	HEC	C1D-C2D-C3D	3.06	109.12	107.00
8	A	304	HEC	CMB-C2B-C3B	3.00	129.35	125.82
8	A	301	HEC	CMC-C2C-C1C	-3.00	123.86	128.46
8	A	304	HEC	CBA-CAA-C2A	-2.98	107.58	112.60
8	E	400	HEC	CMB-C2B-C3B	2.89	129.22	125.82
8	A	305	HEC	CBD-CAD-C3D	2.88	117.54	112.62
8	A	305	HEC	CMC-C2C-C1C	-2.81	124.15	128.46
8	A	304	HEC	CMD-C2D-C1D	-2.80	124.16	128.46
8	A	304	HEC	CMC-C2C-C3C	2.76	129.06	125.82
8	A	301	HEC	CMC-C2C-C3C	2.76	129.06	125.82
8	A	301	HEC	CMD-C2D-C3D	2.72	130.06	124.94
8	A	305	HEC	CMD-C2D-C1D	-2.68	124.35	128.46
8	A	303	HEC	CMD-C2D-C1D	-2.58	124.50	128.46
8	A	303	HEC	CMC-C2C-C3C	2.56	128.83	125.82
8	E	400	HEC	CBD-CAD-C3D	2.47	116.83	112.62
8	A	302	HEC	CAA-C2A-C3A	2.37	134.06	127.25
8	E	400	HEC	C1D-C2D-C3D	2.28	108.58	107.00
8	A	303	HEC	CMA-C3A-C2A	2.24	129.17	124.94
8	A	303	HEC	CBA-CAA-C2A	2.18	116.28	112.60
8	E	400	HEC	O1D-CGD-CBD	-2.16	116.14	123.08
8	E	400	HEC	O2D-CGD-CBD	2.14	120.90	114.03
8	A	304	HEC	CMA-C3A-C2A	2.12	128.93	124.94
8	A	302	HEC	C1D-C2D-C3D	2.09	108.45	107.00
8	A	301	HEC	O1D-CGD-CBD	-2.06	116.47	123.08
8	E	400	HEC	CMD-C2D-C1D	-2.05	125.31	128.46
8	A	303	HEC	O1D-CGD-CBD	-2.05	116.50	123.08
8	A	304	HEC	O1D-CGD-CBD	-2.03	116.57	123.08

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	302	HEC	C3A-C2A-CAA-CBA
8	A	303	HEC	C1A-C2A-CAA-CBA
8	A	303	HEC	C3A-C2A-CAA-CBA
8	A	303	HEC	C2A-CAA-CBA-CGA
8	A	304	HEC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
8	A	304	HEC	C4D-C3D-CAD-CBD
8	A	304	HEC	C3D-CAD-CBD-CGD
8	A	305	HEC	C3D-CAD-CBD-CGD
8	A	302	HEC	C2A-CAA-CBA-CGA
8	A	302	HEC	C1A-C2A-CAA-CBA
8	A	303	HEC	C3D-CAD-CBD-CGD
8	A	304	HEC	CAD-CBD-CGD-O2D
8	A	304	HEC	CAD-CBD-CGD-O1D
8	E	400	HEC	CAA-CBA-CGA-O1A
8	A	301	HEC	CAD-CBD-CGD-O1D
8	E	400	HEC	CAA-CBA-CGA-O2A
8	A	304	HEC	CAA-CBA-CGA-O2A
8	A	301	HEC	CAD-CBD-CGD-O2D
8	A	304	HEC	CAA-CBA-CGA-O1A
8	E	400	HEC	C2A-CAA-CBA-CGA
8	A	302	HEC	CAA-CBA-CGA-O2A
8	A	302	HEC	CAA-CBA-CGA-O1A
8	A	302	HEC	CAD-CBD-CGD-O1D
8	A	303	HEC	CAA-CBA-CGA-O2A
8	A	302	HEC	CAD-CBD-CGD-O2D
8	A	303	HEC	CAA-CBA-CGA-O1A
8	A	303	HEC	CAD-CBD-CGD-O2D

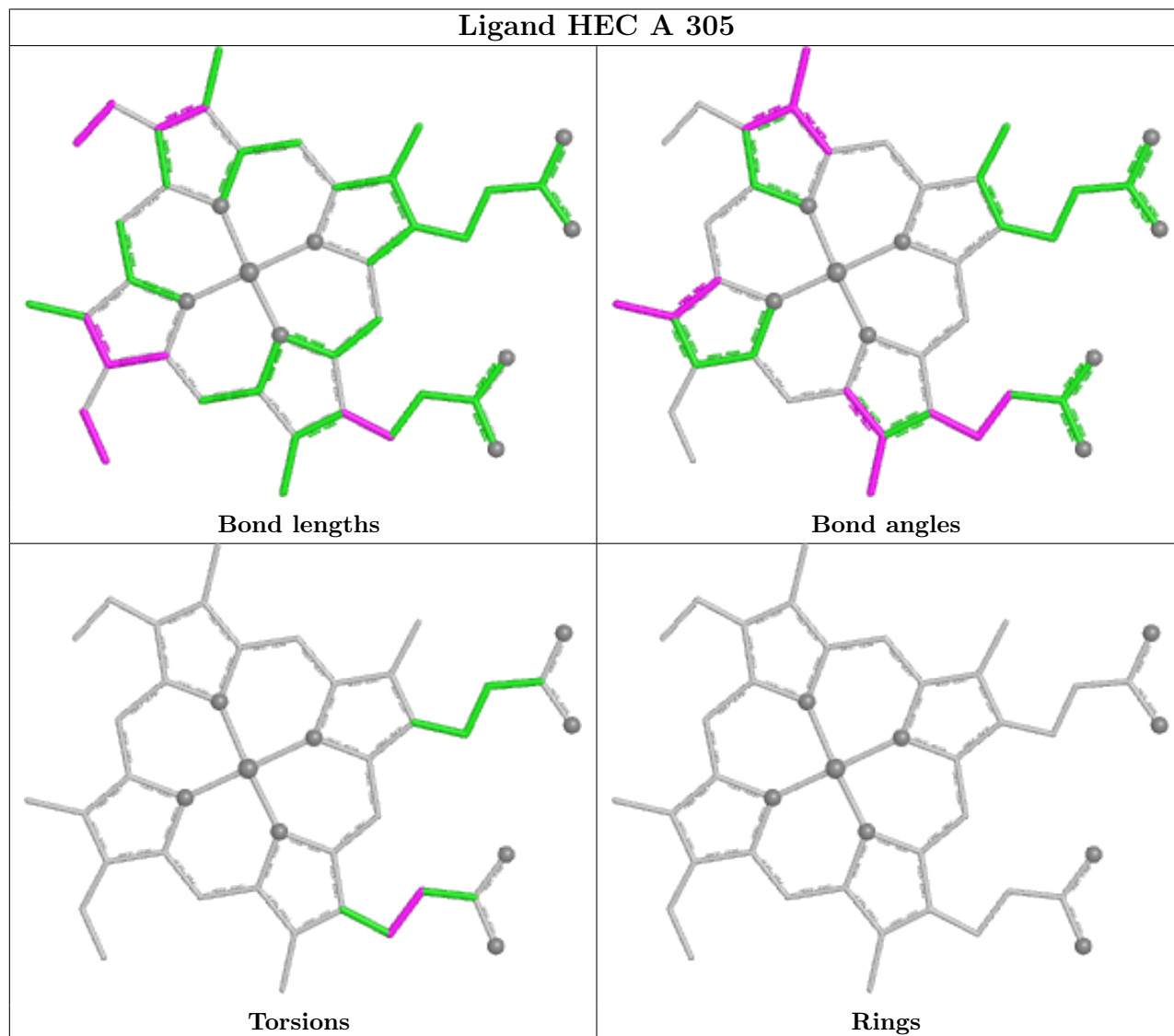
There are no ring outliers.

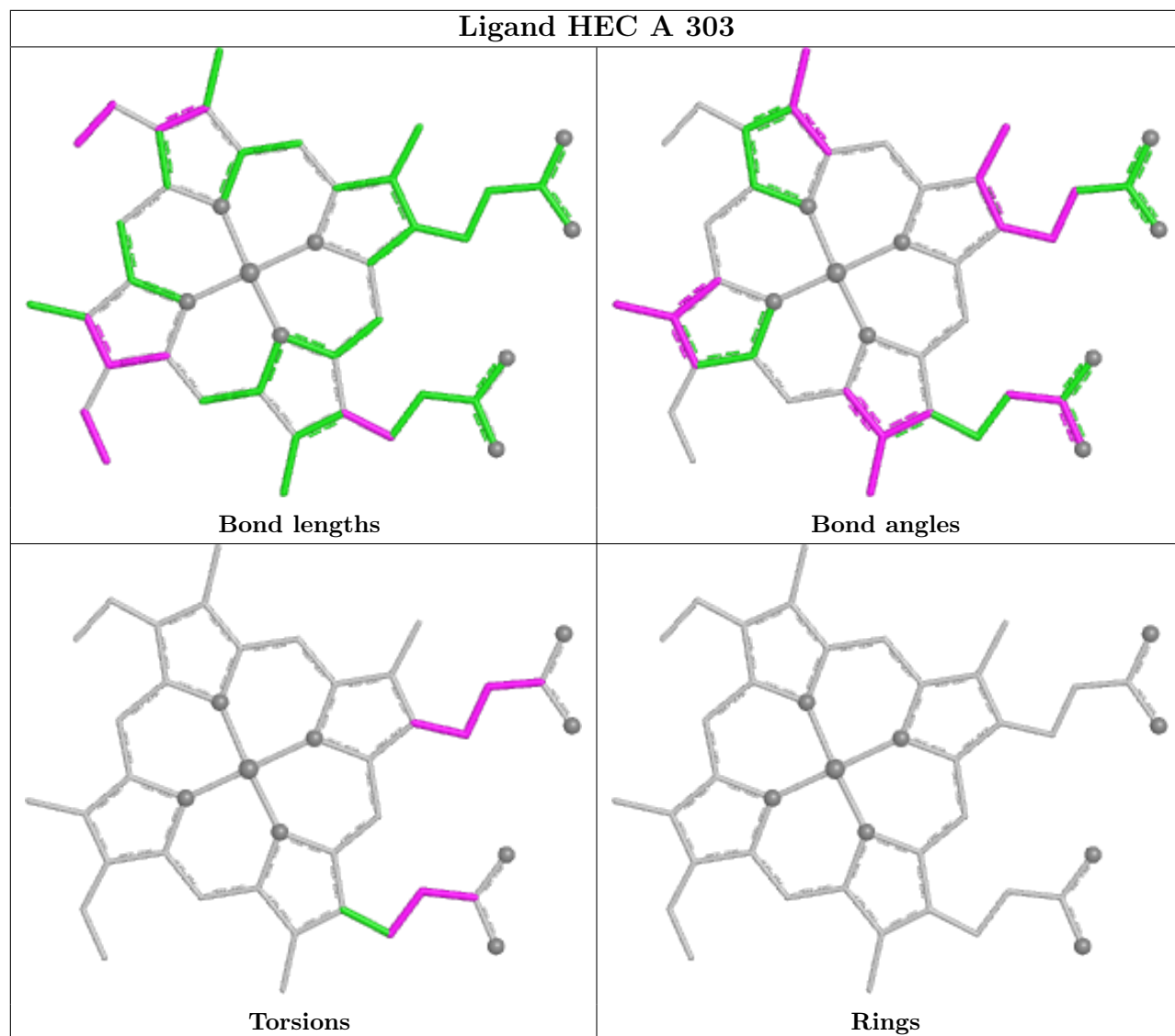
10 monomers are involved in 47 short contacts:

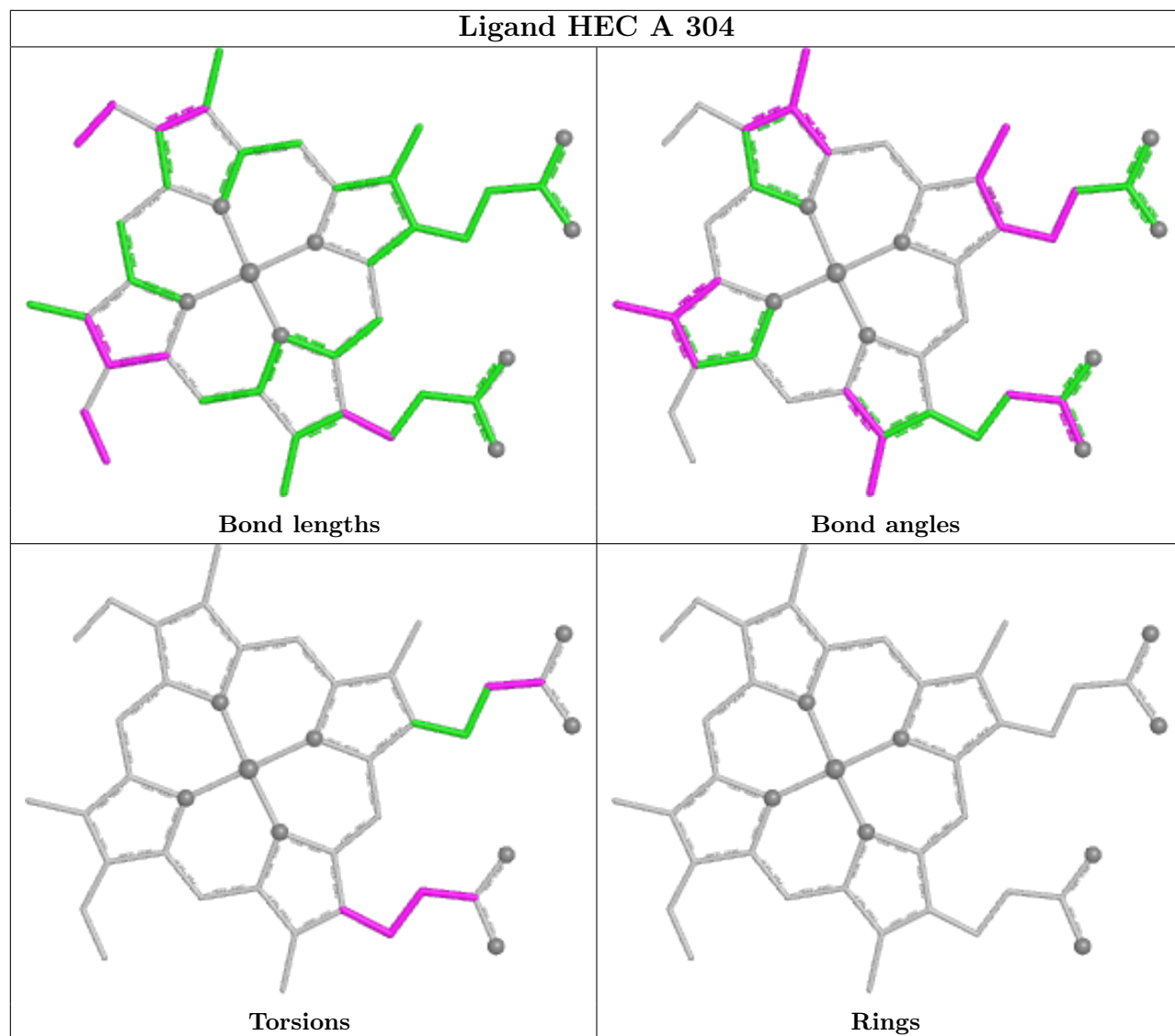
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1102	SF4	2	0
8	A	305	HEC	5	0
8	A	303	HEC	5	0
8	A	304	HEC	5	0
8	E	400	HEC	4	0
10	B	1103	SF4	3	0
9	B	1101	F3S	1	0
8	A	302	HEC	14	0
10	B	1104	SF4	2	0
8	A	301	HEC	10	0

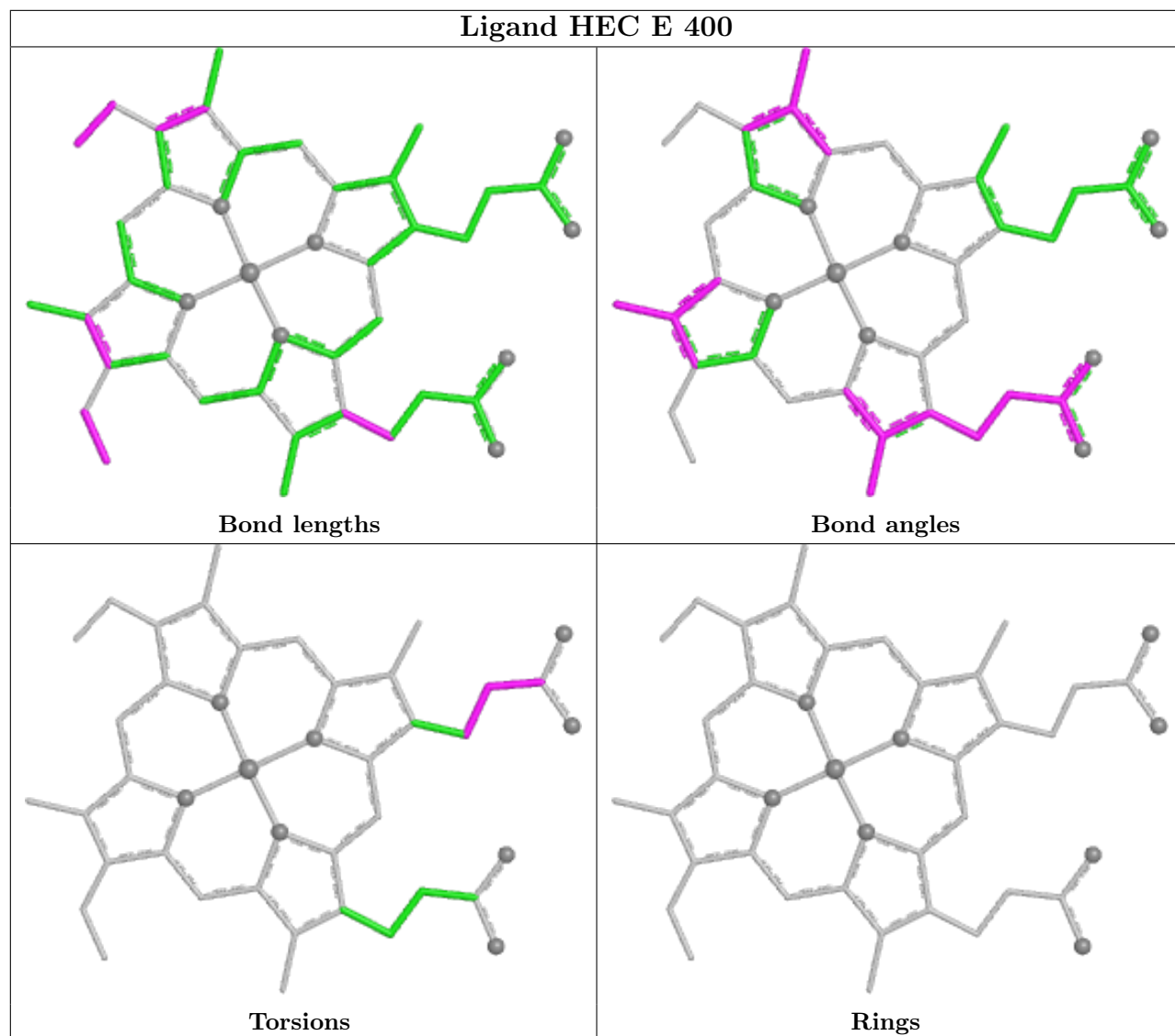
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

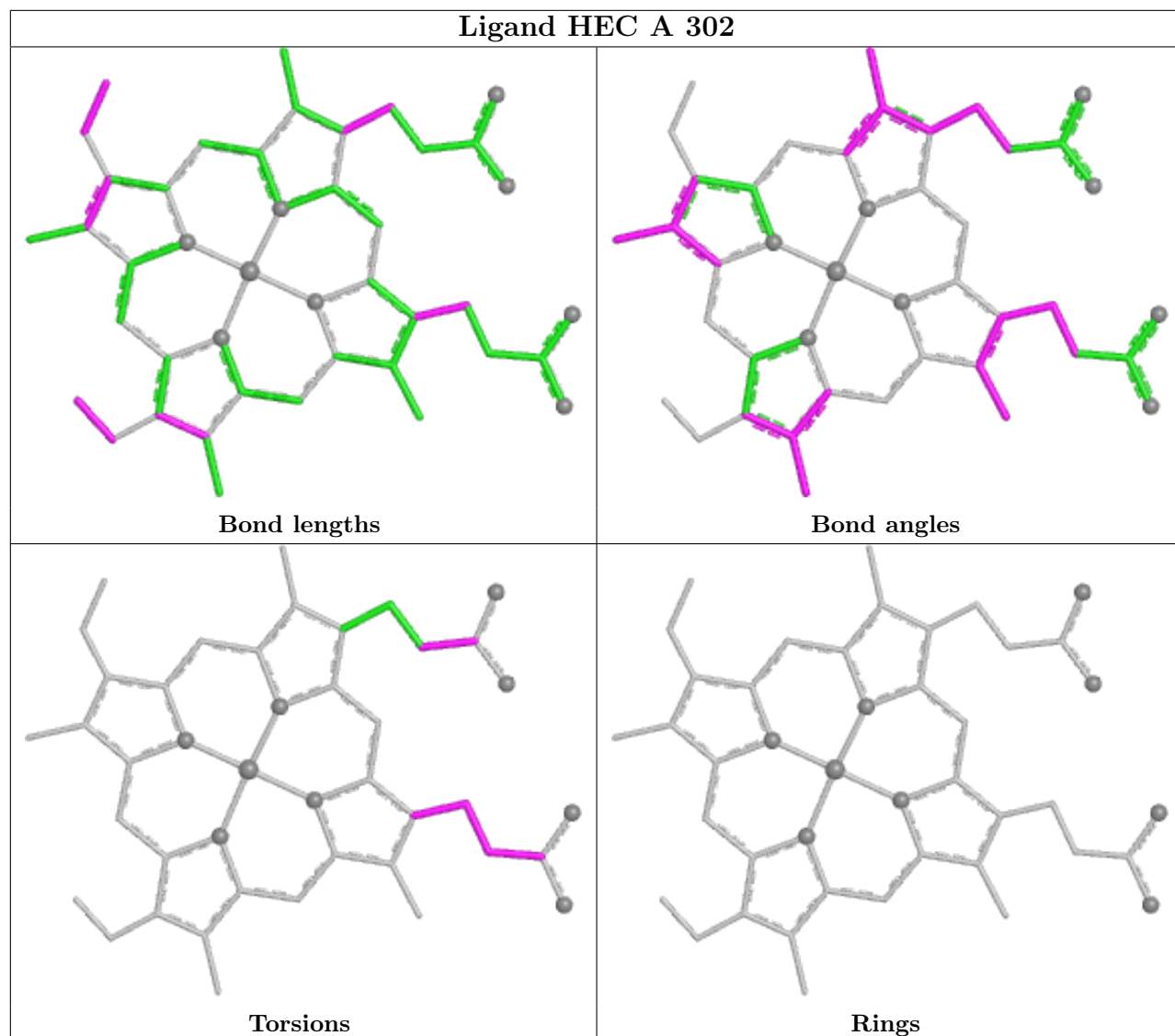


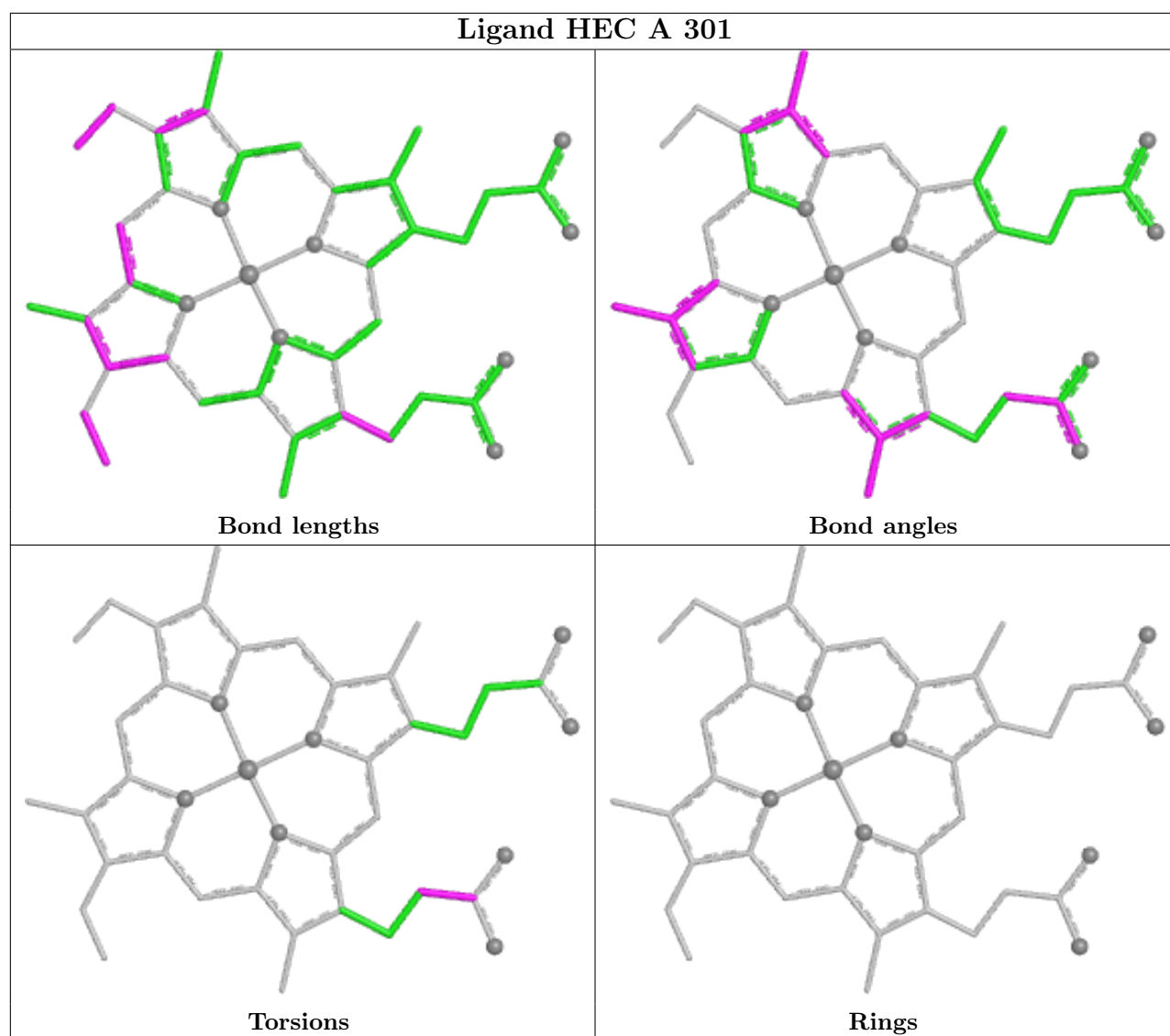












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

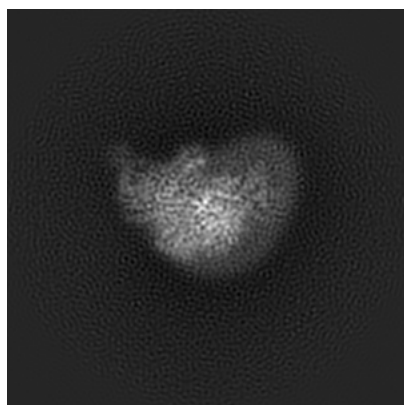
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4165. These allow visual inspection of the internal detail of the map and identification of artifacts.

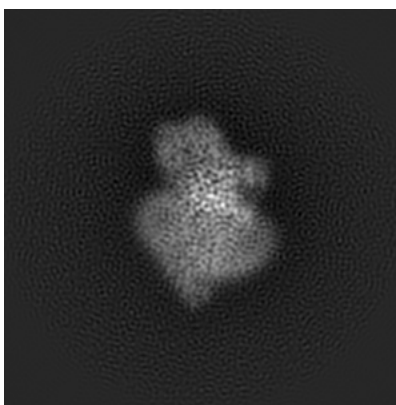
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

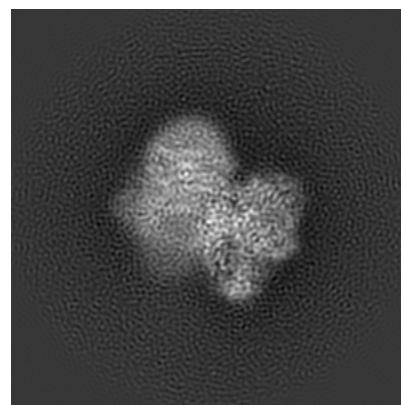
#### 6.1.1 Primary map



X



Y

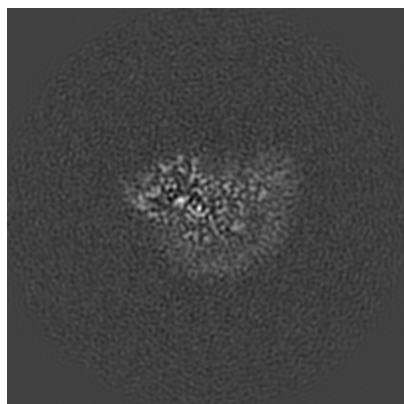


Z

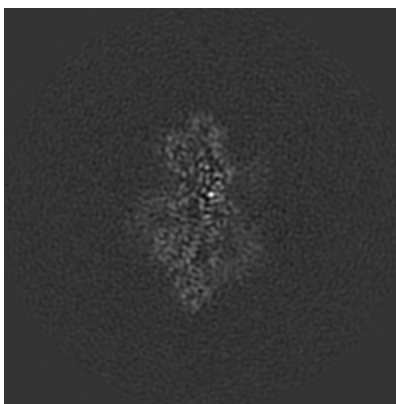
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

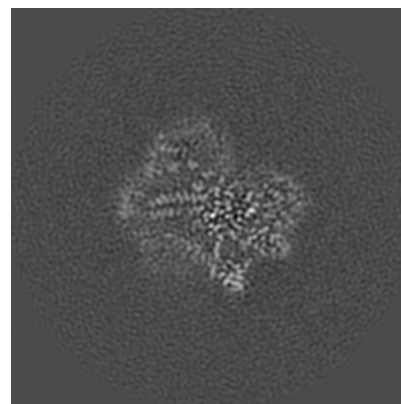
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

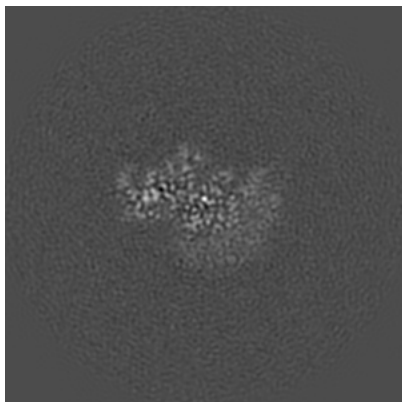


Z Index: 144

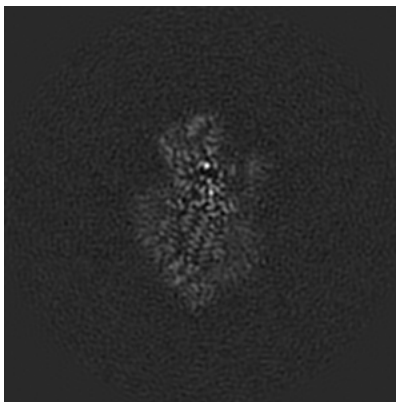
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

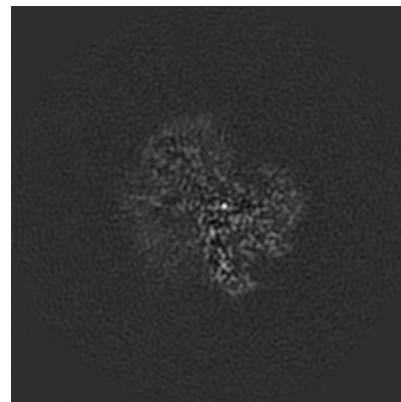
### 6.3.1 Primary map



X Index: 152



Y Index: 142

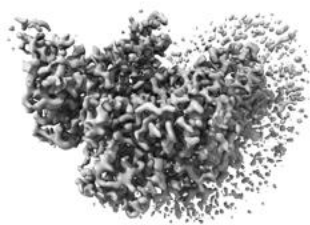


Z Index: 149

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

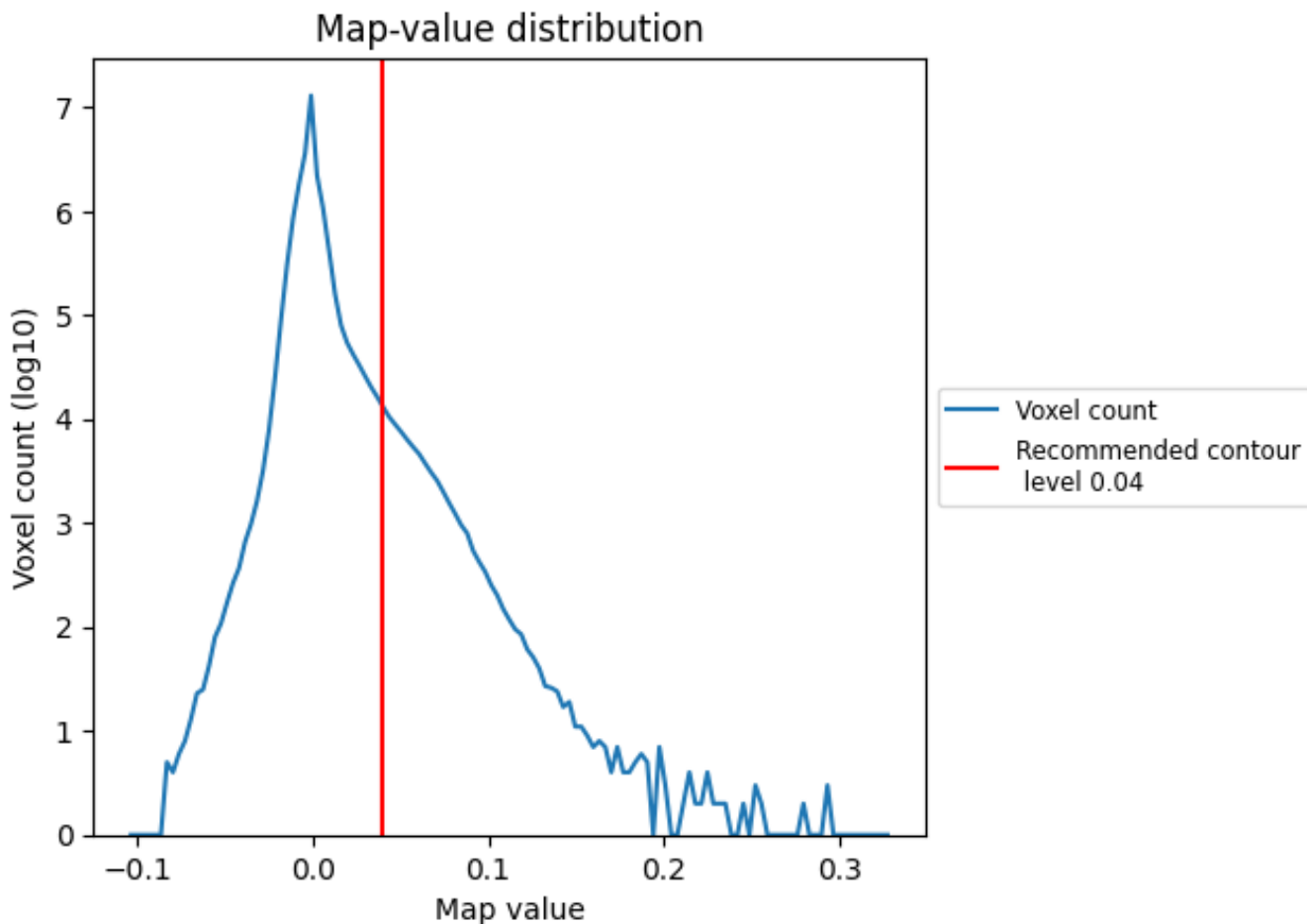
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

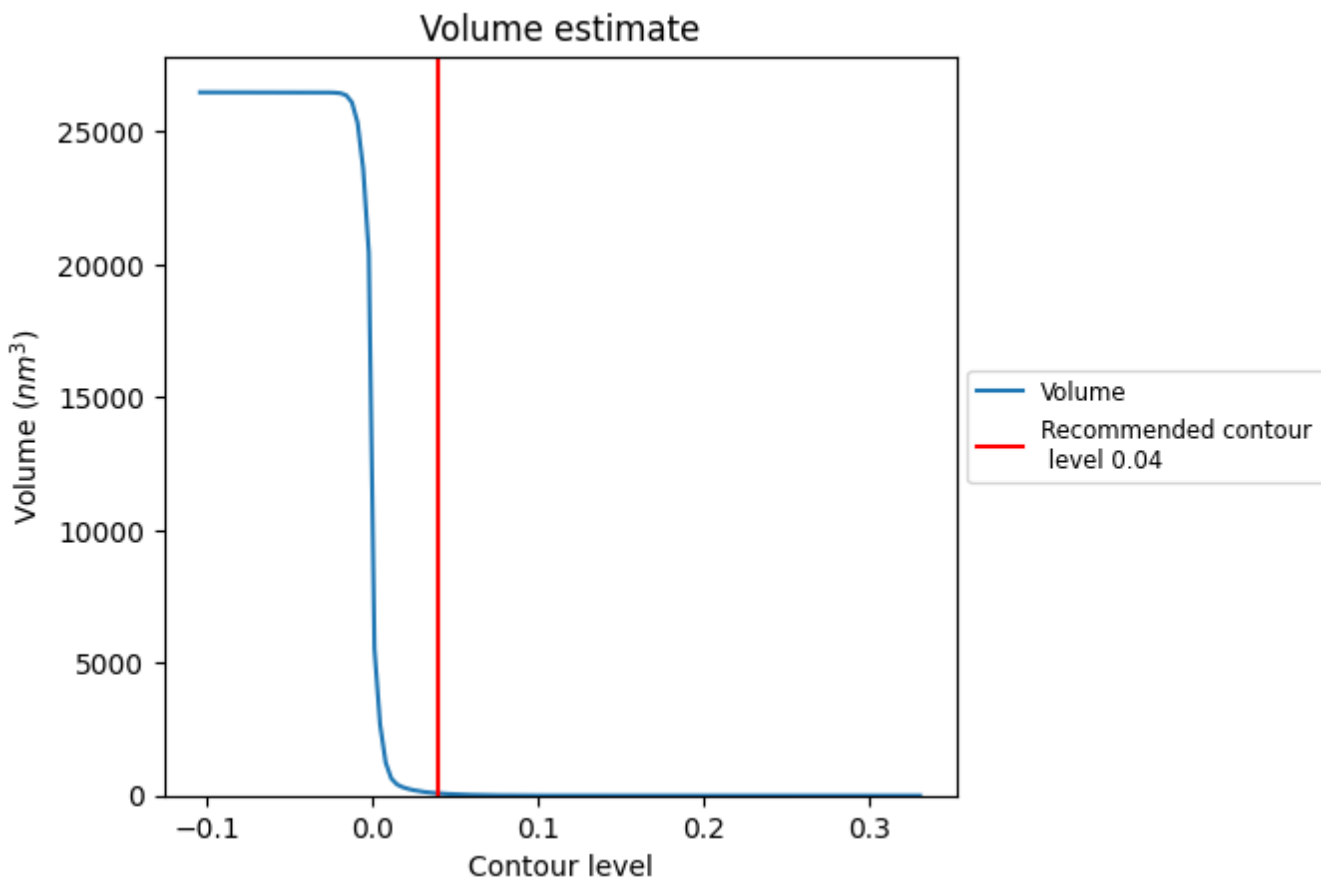
This section contains the results of statistical analysis of the map.

### 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.

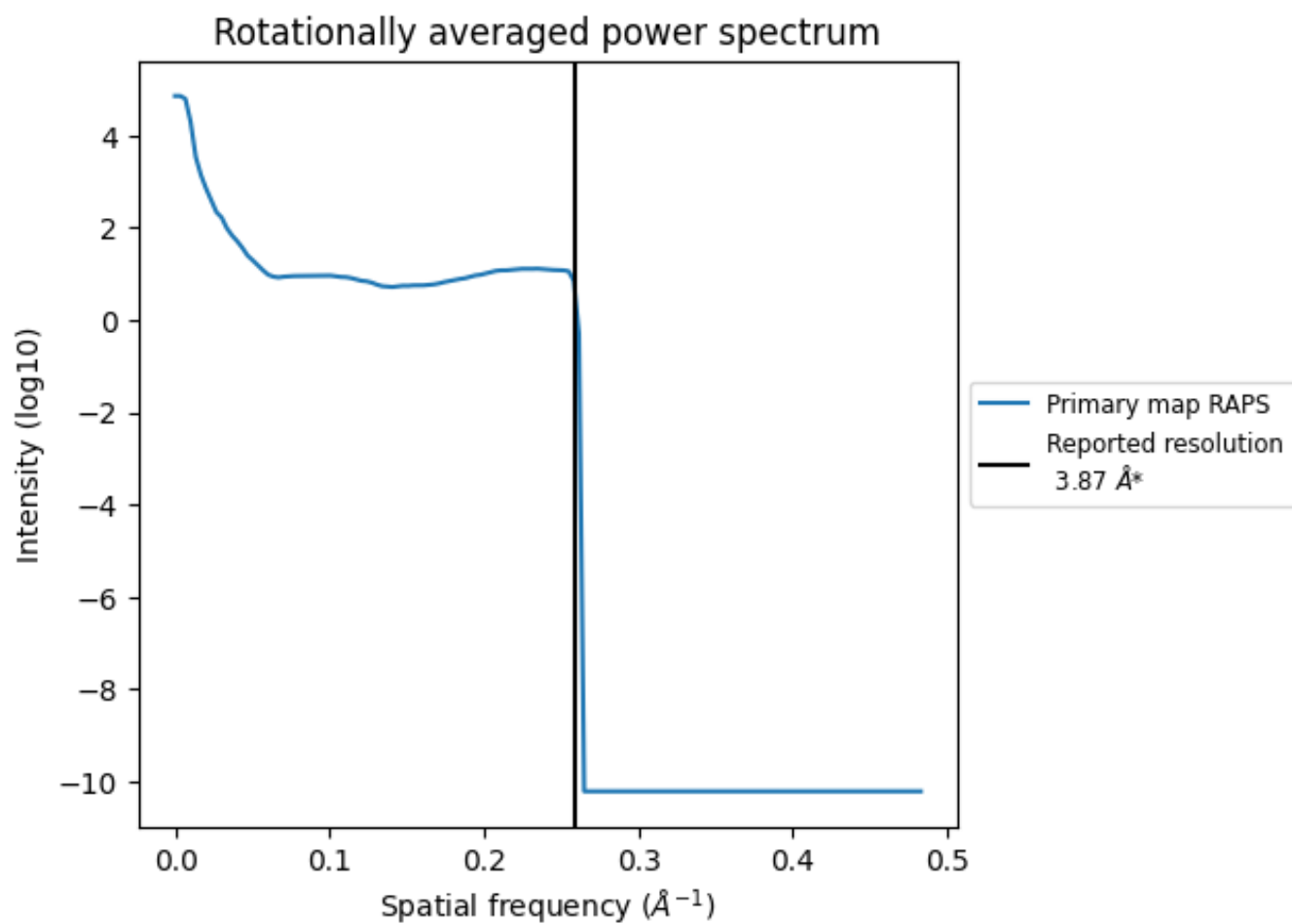
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84  $\text{nm}^3$ ; this corresponds to an approximate mass of 76 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 0.258 Å<sup>-1</sup>



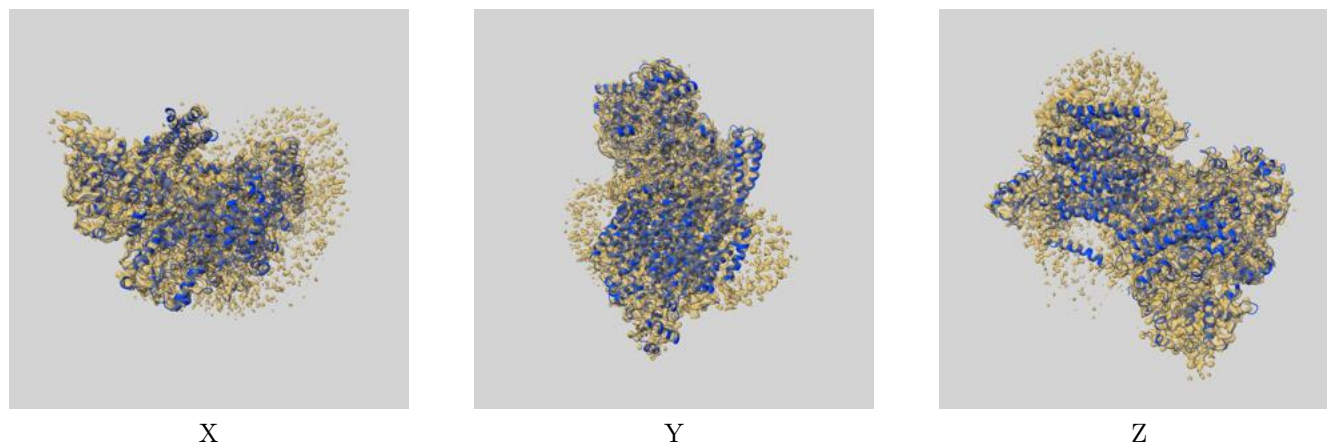
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

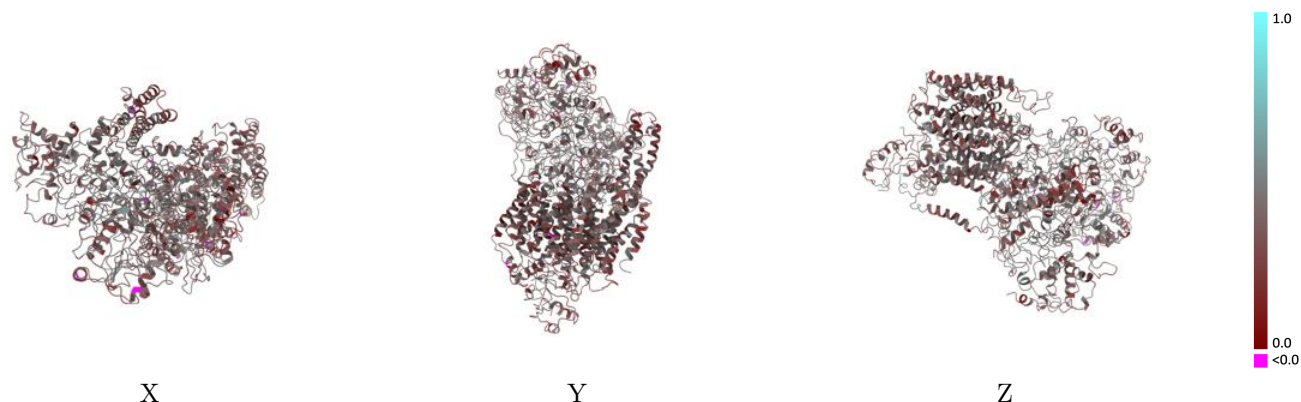
This section contains information regarding the fit between EMDB map EMD-4165 and PDB model 6F0K. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



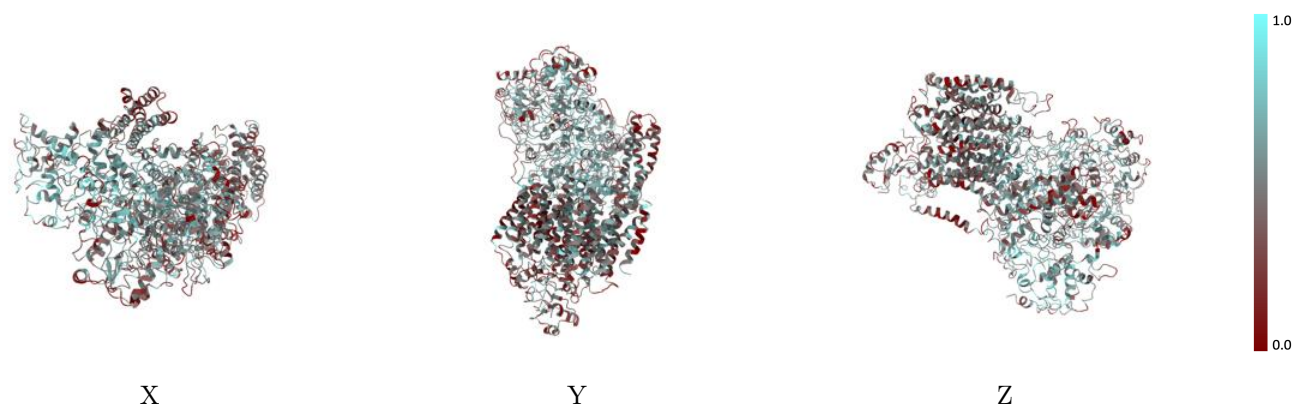
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



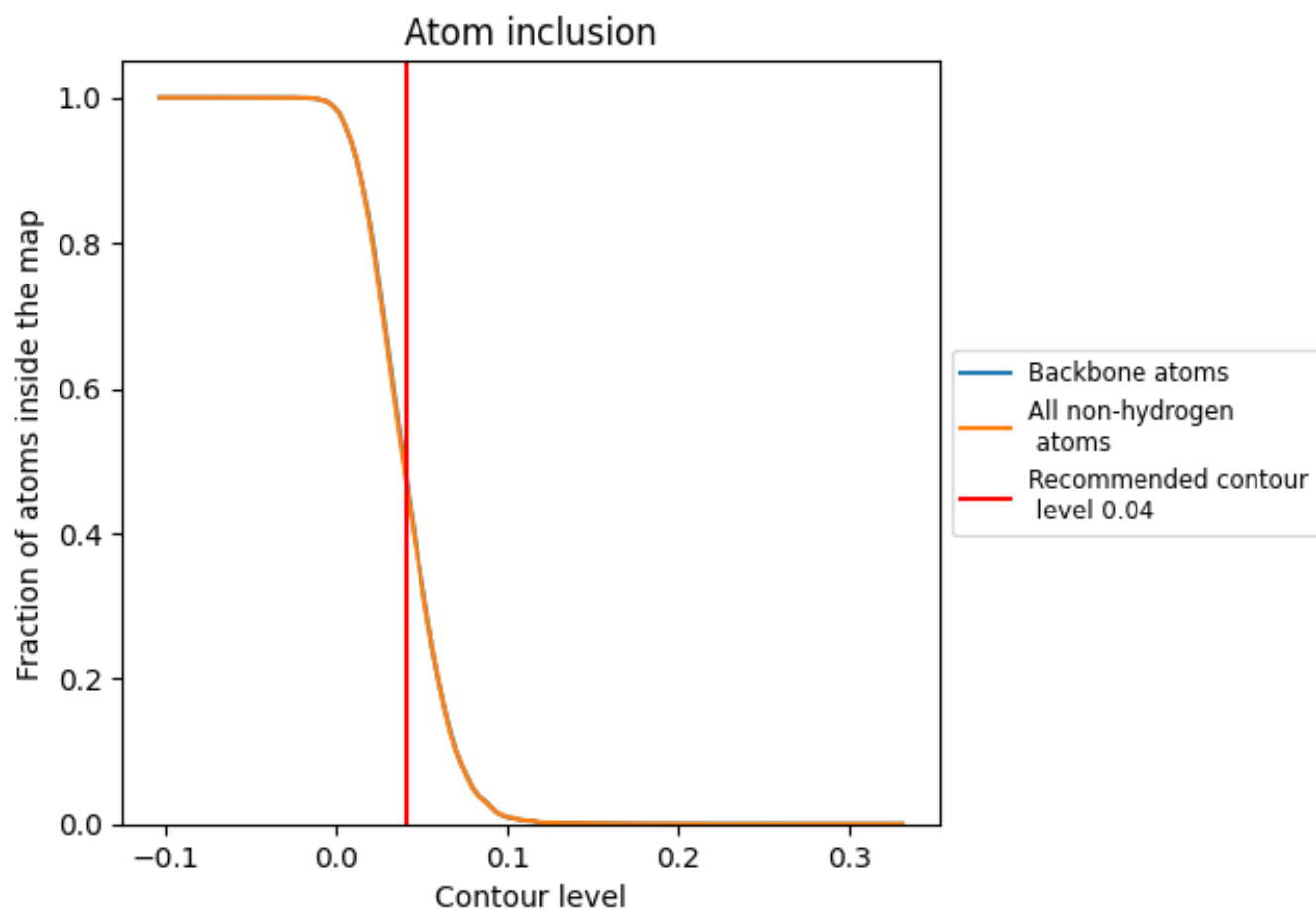
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.04).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 48% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4795	 0.3800
A	 0.5844	 0.4080
B	 0.5224	 0.3950
C	 0.4661	 0.3720
D	 0.4209	 0.3470
E	 0.5488	 0.3870
F	 0.4500	 0.3560
H	 0.4221	 0.3560

