



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 07:47 PM JST

PDB ID : 6KLS / pdb\_00006kls  
EMDB ID : EMD-0716  
Title : Hyperthermophilic respiratory Complex III  
Authors : Fei, S.; Hartmut, M.; Yun, Z.; Guohong, P.; Guoliang, Z.; Hui, Z.; Shuangbo, Z.; Xiaoyun, P.; Yan, Z.  
Deposited on : 2019-07-30  
Resolution : 3.30 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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

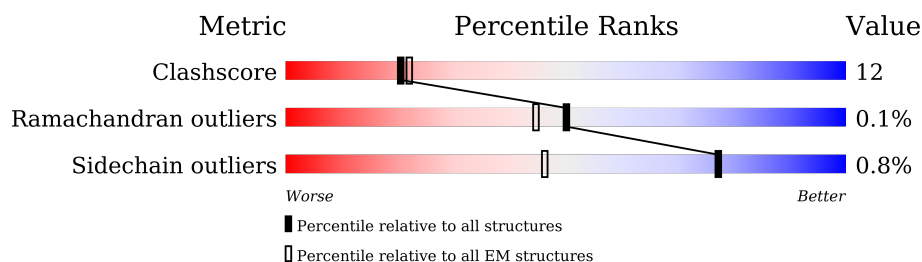
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	181	<div> <div>41%</div> <div> <div>51%</div> <div>23%</div> <div>•</div> <div>26%</div> </div> </div>
1	D	181	<div> <div>41%</div> <div> <div>51%</div> <div>22%</div> <div>•</div> <div>26%</div> </div> </div>
2	B	410	<div> <div>10%</div> <div> <div>73%</div> <div>23%</div> <div>•</div> </div> </div>
2	E	410	<div> <div>10%</div> <div> <div>73%</div> <div>23%</div> <div>•</div> </div> </div>
3	C	240	<div> <div>23%</div> <div> <div>70%</div> <div>28%</div> <div>•</div> </div> </div>
3	F	240	<div> <div>23%</div> <div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>

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
6	DLX	B	504	-	X	-	-
6	DLX	C	301	-	X	-	-
6	DLX	E	504	-	X	-	-
6	DLX	F	301	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13011 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 Rieske-I iron sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1012	668	169	169	6		
1	D	134	Total	C	N	O	S	0	0
			1012	668	169	169	6		

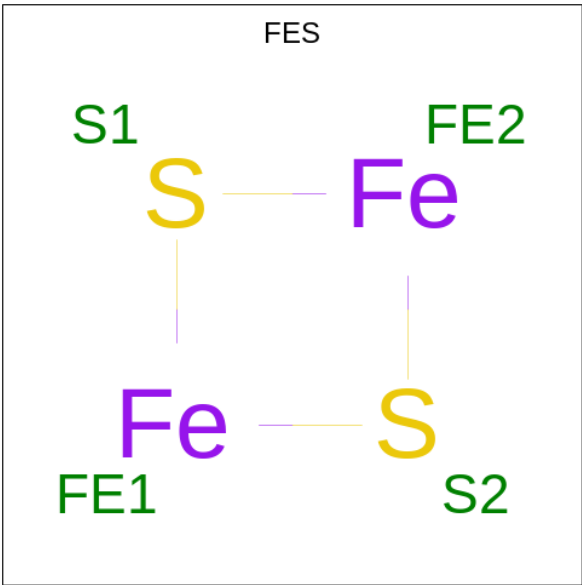
- Molecule 2 is a protein called cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	395	Total	C	N	O	S	0	0
			3226	2208	491	515	12		
2	E	395	Total	C	N	O	S	0	0
			3226	2208	491	515	12		

- Molecule 3 is a protein called Cytochrome c.

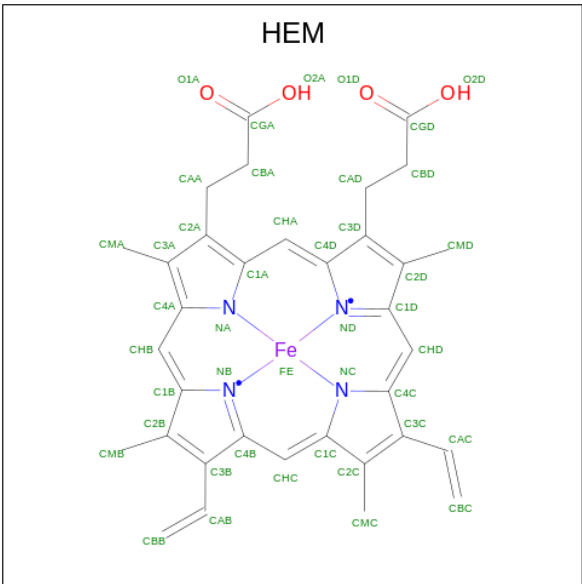
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	236	Total	C	N	O	S	0	0
			1917	1263	312	334	8		
3	F	236	Total	C	N	O	S	0	0
			1917	1263	312	334	8		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



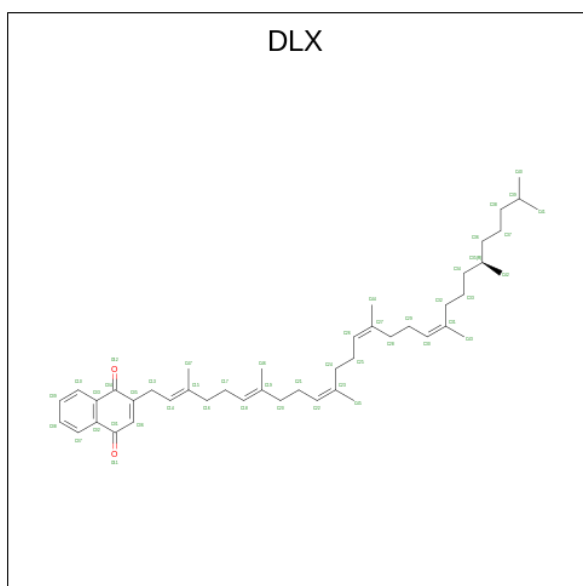
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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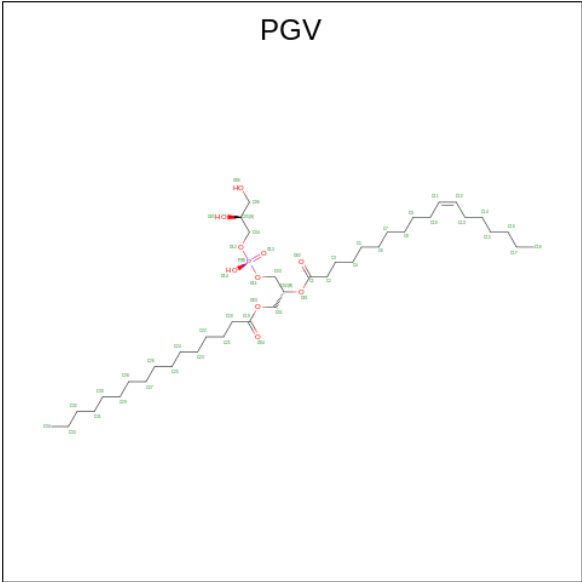
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 6 is 2-[(2 {E},6 {E},10 {Z},14 {Z},18 {Z},23 {R})-3,7,11,15,19,23,27-heptamethylotacosa-2,6,10,14,18-pentaenyl]naphthalene-1,4-dione (CCD ID: DLX) (formula: C<sub>45</sub>H<sub>66</sub>O<sub>2</sub>).



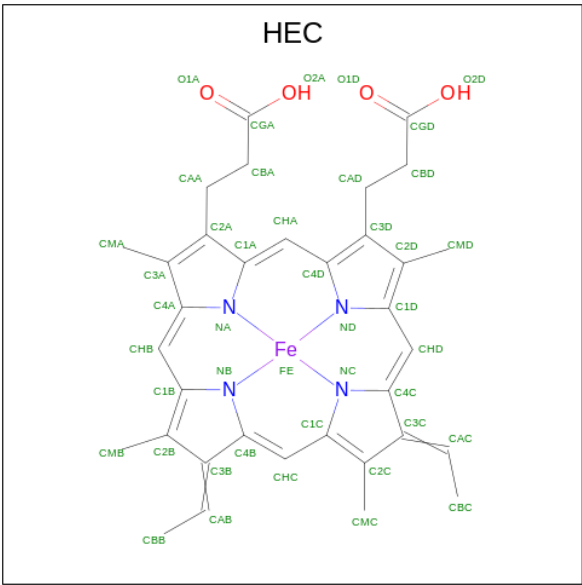
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			47	45	2	
6	B	1	Total	C	O	0
			47	45	2	
6	C	1	Total	C	O	0
			47	45	2	
6	E	1	Total	C	O	0
			47	45	2	
6	E	1	Total	C	O	0
			47	45	2	
6	F	1	Total	C	O	0
			47	45	2	

- Molecule 7 is (1R)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	O	P	0
			51	40	10	1	
7	B	1	Total	C	O	P	0
			51	40	10	1	
7	E	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 8 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

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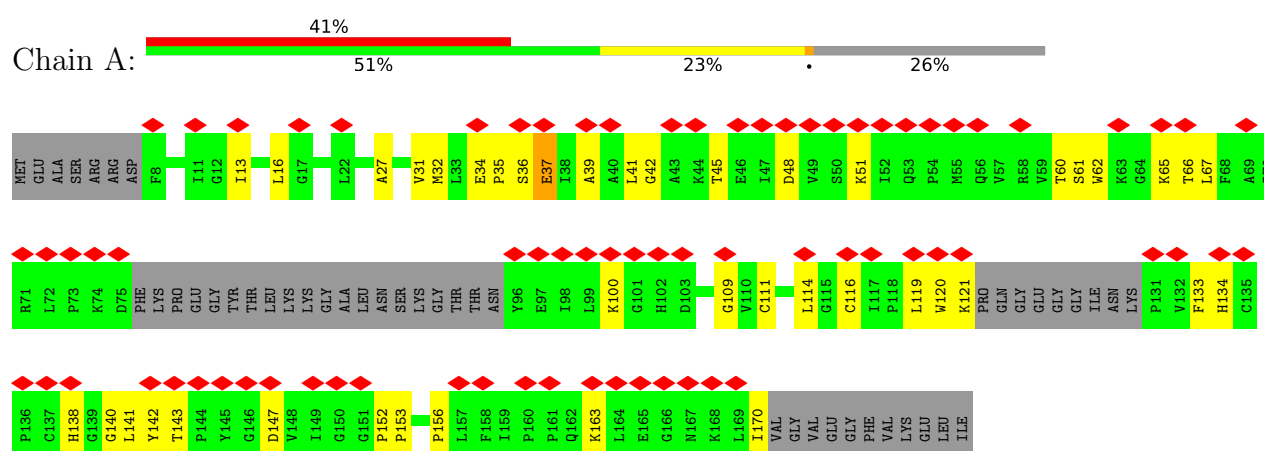
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
8	F	1	43	34	1	4	4	0



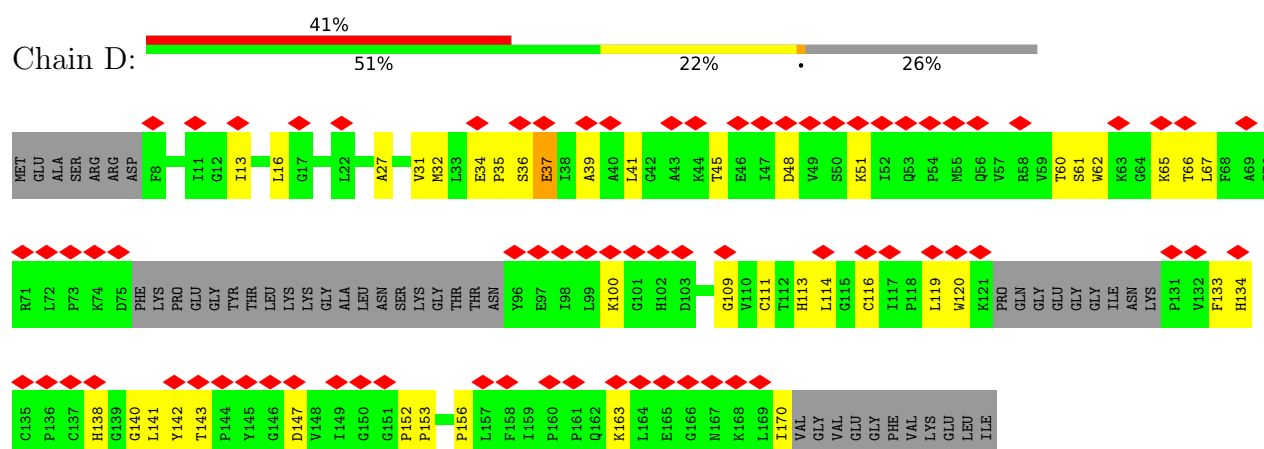
### 3 Residue-property plots

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.

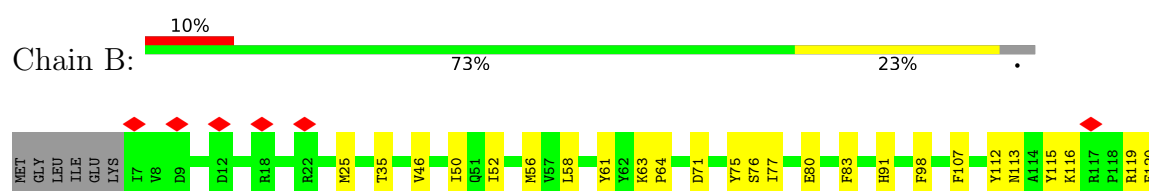
#### • Molecule 1: Rieske-I iron sulfur protein

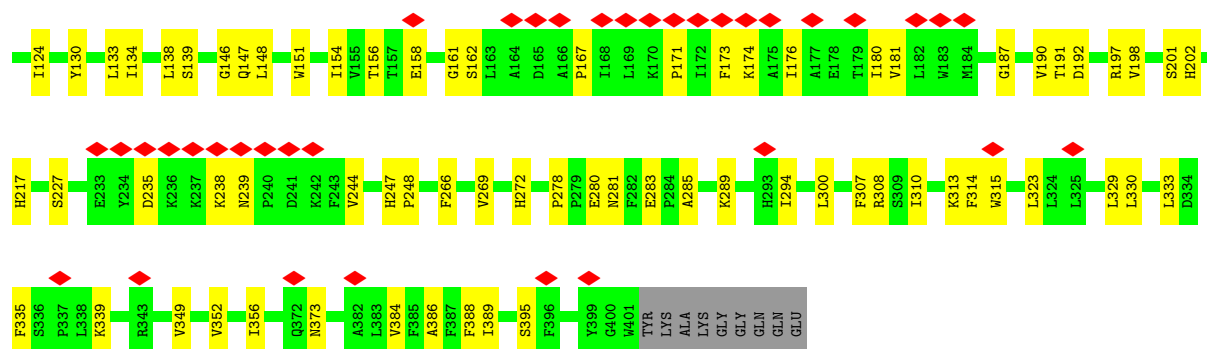


#### • Molecule 1: Rieske-I iron sulfur protein

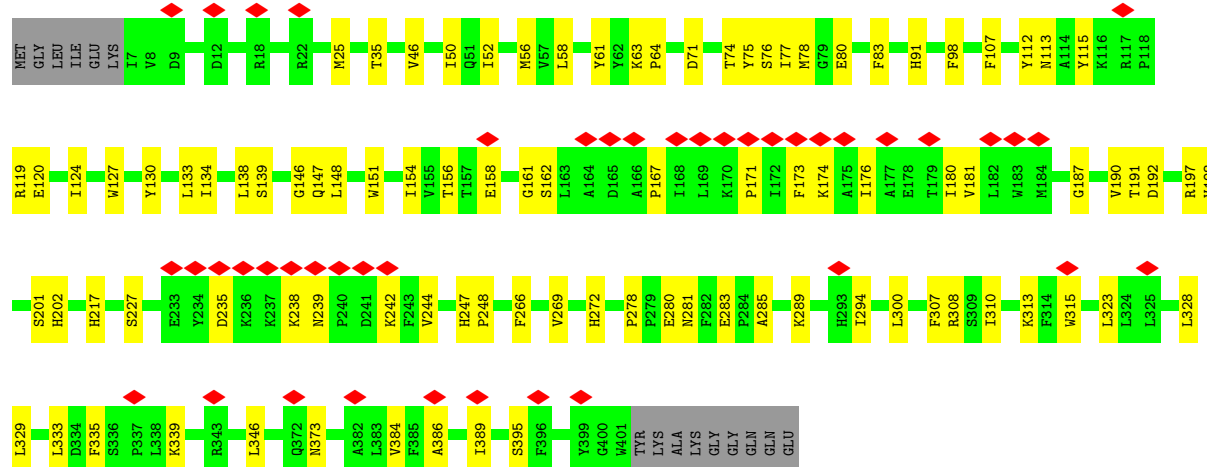


#### • Molecule 2: cytochrome b subunit

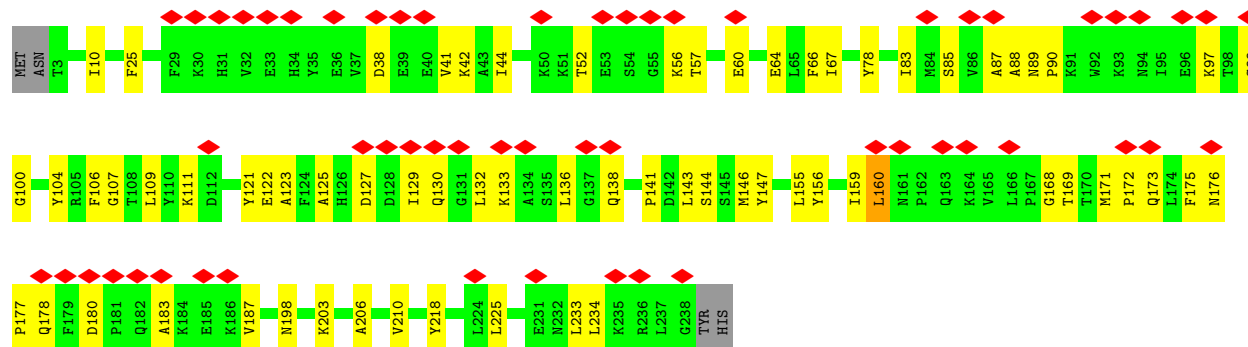




• Molecule 2: cytochrome b subunit

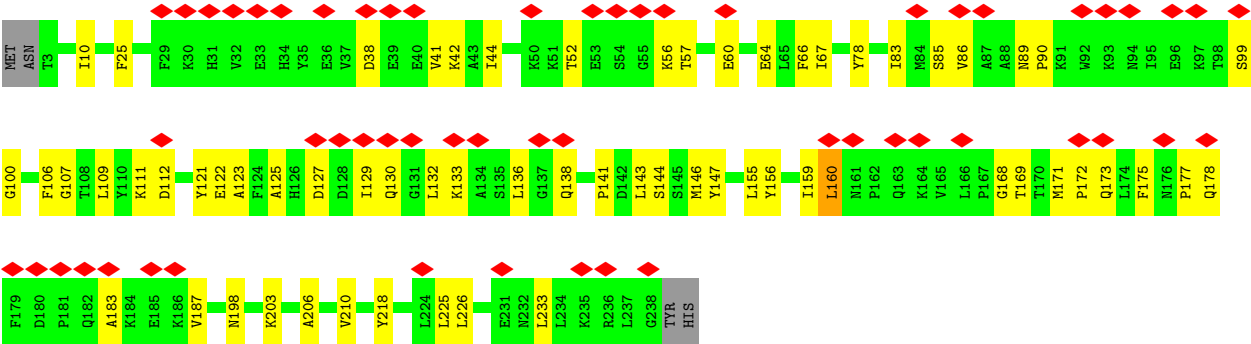


• Molecule 3: Cytochrome c



• Molecule 3: Cytochrome c





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93622	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	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	0.283	Depositor
Minimum map value	-0.198	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.055	Depositor
Map size ( $\text{\AA}$ )	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, DLX, HEM, FES, 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	0.28	0/1039	0.48	0/1410
1	D	0.26	0/1039	0.48	0/1410
2	B	0.28	0/3346	0.44	0/4570
2	E	0.28	0/3346	0.44	0/4570
3	C	0.27	0/1974	0.48	0/2674
3	F	0.27	0/1974	0.48	0/2674
All	All	0.27	0/12718	0.46	0/17308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1012	0	1055	38	0
1	D	1012	0	1055	34	0
2	B	3226	0	3280	66	0
2	E	3226	0	3280	65	0
3	C	1917	0	1929	51	0
3	F	1917	0	1929	50	0
4	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	1	0
5	B	86	0	60	7	0
5	E	86	0	60	7	0
6	B	94	0	0	13	0
6	C	47	0	0	0	0
6	E	94	0	0	8	0
6	F	47	0	0	0	0
7	B	102	0	151	15	0
7	E	51	0	75	1	0
8	C	43	0	29	9	0
8	F	43	0	29	8	0
All	All	13011	0	12932	309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (309) 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)
3:C:168:GLY:O	1:D:138:HIS:HD2	1.12	1.28
3:C:168:GLY:O	1:D:138:HIS:CD2	1.99	1.14
1:A:114:LEU:HD12	1:A:138:HIS:HE1	1.16	1.05
6:B:503:DLX:C23	7:B:506:PGV:H341	1.90	1.01
1:A:138:HIS:CD2	3:F:168:GLY:O	2.14	1.00
1:A:138:HIS:HB2	4:A:501:FES:S1	2.06	0.96
3:F:159:ILE:CD1	8:F:302:HEC:HMB2	1.99	0.93
3:C:159:ILE:CD1	8:C:302:HEC:HMB2	1.98	0.93
1:D:138:HIS:HB2	4:D:501:FES:S1	2.10	0.91
1:A:114:LEU:HD12	1:A:138:HIS:CE1	2.06	0.91
3:C:159:ILE:HD13	8:C:302:HEC:HMB2	1.53	0.89
3:F:159:ILE:HD13	8:F:302:HEC:HMB2	1.54	0.89
1:D:114:LEU:HD12	1:D:138:HIS:HE1	1.39	0.88
1:D:114:LEU:HD12	1:D:138:HIS:CE1	2.09	0.87
6:B:503:DLX:C24	7:B:506:PGV:C33	2.60	0.80
1:A:138:HIS:HD2	3:F:168:GLY:O	1.66	0.78
5:B:501:HEM:HHC	5:B:501:HEM:HBB2	1.66	0.77
5:E:501:HEM:HHC	5:E:501:HEM:HBB2	1.66	0.76
1:A:48:ASP:HB3	1:A:51:LYS:HG3	1.67	0.74
1:D:48:ASP:HB3	1:D:51:LYS:HG3	1.67	0.74
2:E:238:LYS:HD3	2:E:239:ASN:H	1.53	0.74
5:B:501:HEM:HBC2	5:B:501:HEM:HHH	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:335:PHE:O	2:E:395:SER:OG	2.06	0.73
2:B:335:PHE:O	2:B:395:SER:OG	2.06	0.73
5:E:501:HEM:HBC2	5:E:501:HEM:HHD	1.70	0.73
2:B:238:LYS:HD3	2:B:239:ASN:H	1.52	0.73
3:F:159:ILE:HD11	8:F:302:HEC:HMB2	1.75	0.69
2:E:167:PRO:HD2	2:E:171:PRO:HA	1.75	0.68
2:B:167:PRO:HD2	2:B:171:PRO:HA	1.75	0.66
2:B:248:PRO:HG3	3:C:233:LEU:HD22	1.77	0.66
1:A:140:GLY:HA2	1:A:152:PRO:HD2	1.78	0.66
3:C:159:ILE:HD11	8:C:302:HEC:HMB2	1.74	0.65
6:B:503:DLX:C24	7:B:506:PGV:H331	2.25	0.65
2:E:248:PRO:HG3	3:F:233:LEU:HD22	1.77	0.65
3:F:129:ILE:HD11	3:F:133:LYS:HB3	1.78	0.65
2:E:310:ILE:HG21	2:E:315:TRP:HD1	1.62	0.65
3:F:177:PRO:O	3:F:178:GLN:HG2	1.97	0.64
1:D:62:TRP:HB2	1:D:67:LEU:HD22	1.79	0.64
1:D:140:GLY:HA2	1:D:152:PRO:HD2	1.78	0.64
3:C:129:ILE:HD11	3:C:133:LYS:HB3	1.78	0.64
2:B:310:ILE:HG21	2:B:315:TRP:HD1	1.62	0.64
3:C:177:PRO:O	3:C:178:GLN:HG2	1.97	0.64
3:C:169:THR:HG22	3:C:171:MET:H	1.62	0.64
1:A:134:HIS:HB3	1:A:141:LEU:HD23	1.79	0.64
1:A:62:TRP:HB2	1:A:67:LEU:HD22	1.79	0.64
1:D:134:HIS:HB3	1:D:141:LEU:HD23	1.79	0.63
7:B:506:PGV:H171	6:E:503:DLX:C24	2.29	0.63
3:C:41:VAL:HG23	3:C:42:LYS:H	1.62	0.62
3:F:169:THR:HG22	3:F:171:MET:H	1.62	0.62
3:F:41:VAL:HG23	3:F:42:LYS:H	1.63	0.62
1:D:13:ILE:HG22	3:F:225:LEU:HB3	1.82	0.62
3:C:160:LEU:HB3	3:C:187:VAL:HG21	1.81	0.62
3:F:160:LEU:HB3	3:F:187:VAL:HG21	1.81	0.61
1:A:13:ILE:HG22	3:C:225:LEU:HB3	1.82	0.61
6:B:503:DLX:C45	7:B:506:PGV:H341	2.30	0.60
7:B:506:PGV:H183	6:E:503:DLX:C46	2.32	0.59
2:B:162:SER:HB2	2:B:313:LYS:HB3	1.85	0.59
6:B:503:DLX:C23	7:B:506:PGV:C34	2.75	0.59
2:E:162:SER:HB2	2:E:313:LYS:HB3	1.85	0.59
2:B:113:ASN:ND2	2:B:339:LYS:O	2.32	0.58
2:E:113:ASN:ND2	2:E:339:LYS:O	2.32	0.58
2:B:187:GLY:HA3	1:D:39:ALA:HB1	1.85	0.58
5:B:502:HEM:HMC2	5:B:502:HEM:HBC2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLU:OE2	1:D:36:SER:OG	2.21	0.58
3:C:147:TYR:HB3	3:C:198:ASN:HD22	1.69	0.58
3:C:160:LEU:O	3:C:173:GLN:NE2	2.37	0.58
1:A:34:GLU:OE2	1:A:36:SER:OG	2.21	0.57
3:F:147:TYR:HB3	3:F:198:ASN:HD22	1.69	0.57
3:F:160:LEU:O	3:F:173:GLN:NE2	2.37	0.57
1:D:31:VAL:HG22	2:E:83:PHE:HB2	1.87	0.57
2:B:238:LYS:HD3	2:B:239:ASN:N	2.19	0.57
2:E:154:ILE:O	2:E:158:GLU:HG2	2.05	0.57
2:B:154:ILE:O	2:B:158:GLU:HG2	2.05	0.56
2:B:192:ASP:OD1	2:E:63:LYS:HE3	2.05	0.56
1:D:27:ALA:O	1:D:31:VAL:HG23	2.06	0.56
1:A:39:ALA:HB1	2:E:187:GLY:HA3	1.87	0.56
1:D:35:PRO:HB2	1:D:39:ALA:HB2	1.87	0.56
1:A:35:PRO:HB2	1:A:39:ALA:HB2	1.87	0.56
1:A:31:VAL:HG22	2:B:83:PHE:HB2	1.87	0.56
6:B:503:DLX:C24	7:B:506:PGV:H332	2.34	0.56
1:A:60:THR:HG22	1:A:61:SER:H	1.71	0.55
1:A:27:ALA:O	1:A:31:VAL:HG23	2.06	0.55
2:E:238:LYS:HD3	2:E:239:ASN:N	2.19	0.55
2:B:63:LYS:HE3	2:E:192:ASP:OD1	2.06	0.55
2:E:148:LEU:HD23	2:E:280:GLU:HG2	1.88	0.55
6:E:503:DLX:C30	6:E:503:DLX:C44	2.85	0.55
2:B:181:VAL:HA	2:B:187:GLY:HA2	1.89	0.54
1:D:60:THR:HG22	1:D:61:SER:H	1.71	0.54
2:B:148:LEU:HD23	2:B:280:GLU:HG2	1.88	0.54
6:B:503:DLX:C44	6:B:503:DLX:C30	2.85	0.54
6:E:503:DLX:C26	6:E:503:DLX:C45	2.85	0.54
3:C:175:PHE:HB3	3:C:183:ALA:HB1	1.90	0.53
2:E:181:VAL:HA	2:E:187:GLY:HA2	1.88	0.53
3:C:52:THR:OG1	3:C:56:LYS:O	2.24	0.53
2:B:35:THR:HG21	2:B:112:TYR:OH	2.09	0.53
2:E:35:THR:HG21	2:E:112:TYR:OH	2.09	0.53
2:B:138:LEU:HD11	2:B:156:THR:HG21	1.90	0.53
3:F:175:PHE:HB3	3:F:183:ALA:HB1	1.90	0.53
6:B:503:DLX:C45	6:B:503:DLX:C26	2.85	0.52
1:D:41:LEU:HD11	3:F:111:LYS:HE3	1.91	0.52
2:E:76:SER:HA	2:E:80:GLU:HB2	1.90	0.52
2:E:138:LEU:HD11	2:E:156:THR:HG21	1.91	0.52
2:B:76:SER:HA	2:B:80:GLU:HB2	1.90	0.52
2:B:139:SER:OG	2:B:202:HIS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:SER:OG	2:E:202:HIS:HB2	2.09	0.52
3:C:172:PRO:HD3	8:C:302:HEC:HBC3	1.92	0.52
3:F:52:THR:OG1	3:F:56:LYS:O	2.24	0.51
1:A:41:LEU:HD11	3:C:111:LYS:HE3	1.91	0.51
2:B:138:LEU:HD12	2:B:300:LEU:HD11	1.92	0.51
2:B:161:GLY:HA3	2:B:180:ILE:HD11	1.93	0.51
3:F:83:ILE:O	3:F:89:ASN:HB2	2.11	0.51
3:C:83:ILE:O	3:C:89:ASN:HB2	2.11	0.50
2:E:173:PHE:HA	2:E:176:ILE:HG12	1.94	0.50
5:E:502:HEM:HBC2	5:E:502:HEM:HMC1	1.93	0.50
3:F:172:PRO:HD3	8:F:302:HEC:HBC3	1.92	0.50
2:E:154:ILE:HD11	2:E:190:VAL:HG21	1.93	0.50
2:E:91:HIS:NE2	5:E:501:HEM:ND	2.60	0.50
2:E:138:LEU:HD12	2:E:300:LEU:HD11	1.92	0.50
6:B:503:DLX:C24	7:B:506:PGV:H341	2.41	0.50
2:B:91:HIS:NE2	5:B:501:HEM:ND	2.60	0.50
2:B:173:PHE:HA	2:B:176:ILE:HG12	1.94	0.50
2:E:161:GLY:HA3	2:E:180:ILE:HD11	1.93	0.49
6:B:503:DLX:C32	6:B:503:DLX:C42	2.90	0.49
2:B:154:ILE:HD11	2:B:190:VAL:HG21	1.93	0.49
2:B:272:HIS:CE1	3:C:25:PHE:HB3	2.48	0.49
6:E:503:DLX:C42	6:E:503:DLX:C32	2.90	0.49
3:C:146:MET:HG2	8:C:302:HEC:HMA3	1.95	0.49
3:C:206:ALA:O	3:C:210:VAL:HG23	2.13	0.49
3:F:206:ALA:O	3:F:210:VAL:HG23	2.13	0.48
3:C:87:ALA:HA	3:C:88:ALA:HA	1.61	0.48
2:E:107:PHE:HE2	7:E:505:PGV:H291	1.78	0.48
3:F:146:MET:HG2	8:F:302:HEC:HMA3	1.95	0.48
2:E:323:LEU:HD11	2:E:384:VAL:HG12	1.96	0.48
2:E:71:ASP:O	2:E:75:TYR:HB3	2.14	0.48
2:E:238:LYS:CD	2:E:239:ASN:H	2.26	0.48
2:E:98:PHE:CE2	2:E:133:LEU:HD11	2.49	0.48
1:D:143:THR:HG22	1:D:147:ASP:O	2.14	0.47
3:F:130:GLN:HG2	3:F:132:LEU:HG	1.96	0.47
2:E:272:HIS:CE1	3:F:25:PHE:HB3	2.48	0.47
1:A:45:THR:HG21	1:A:62:TRP:HD1	1.79	0.47
7:B:506:PGV:H22	6:E:504:DLX:C13	2.44	0.47
2:B:107:PHE:HE2	7:B:505:PGV:H291	1.78	0.47
2:B:71:ASP:O	2:B:75:TYR:HB3	2.14	0.47
2:E:151:TRP:HB3	2:E:294:ILE:HG12	1.97	0.47
1:D:45:THR:HG21	1:D:62:TRP:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:CYS:HB3	1:A:116:CYS:H	1.80	0.47
2:B:98:PHE:CE2	2:B:133:LEU:HD11	2.49	0.47
3:C:99:SER:N	3:C:100:GLY:HA3	2.30	0.47
1:D:100:LYS:HD2	1:D:100:LYS:HA	1.61	0.47
3:F:78:TYR:CD2	3:F:144:SER:HB3	2.50	0.47
1:A:143:THR:HG22	1:A:147:ASP:O	2.14	0.46
3:C:172:PRO:HD3	8:C:302:HEC:CBC	2.46	0.46
2:B:323:LEU:HD11	2:B:384:VAL:HG12	1.96	0.46
2:E:307:PHE:O	2:E:308:ARG:HG3	2.15	0.46
5:B:502:HEM:HMB1	5:B:502:HEM:HBB2	1.96	0.46
1:D:111:CYS:HB3	1:D:116:CYS:H	1.80	0.46
2:E:146:GLY:O	2:E:285:ALA:HB2	2.16	0.46
3:F:89:ASN:ND2	3:F:125:ALA:HB1	2.31	0.46
3:F:109:LEU:HD23	3:F:109:LEU:H	1.81	0.46
2:B:307:PHE:O	2:B:308:ARG:HG3	2.15	0.46
2:B:120:GLU:O	2:B:124:ILE:HG12	2.16	0.46
3:C:106:PHE:HA	3:C:107:GLY:HA2	1.65	0.46
3:F:99:SER:N	3:F:100:GLY:HA3	2.30	0.46
3:C:130:GLN:HG2	3:C:132:LEU:HG	1.96	0.46
5:E:502:HEM:HMB1	5:E:502:HEM:HBB2	1.96	0.46
2:B:58:LEU:HD13	5:B:501:HEM:HBD1	1.97	0.46
2:E:386:ALA:HA	2:E:389:ILE:HG12	1.98	0.46
3:F:172:PRO:HD3	8:F:302:HEC:CBC	2.46	0.46
2:B:151:TRP:HB3	2:B:294:ILE:HG12	1.97	0.46
3:C:78:TYR:CD2	3:C:144:SER:HB3	2.50	0.46
2:E:58:LEU:HD13	5:E:501:HEM:HBD1	1.97	0.46
2:E:120:GLU:O	2:E:124:ILE:HG12	2.16	0.46
2:B:146:GLY:O	2:B:285:ALA:HB2	2.15	0.45
1:A:100:LYS:HD2	1:A:100:LYS:HA	1.61	0.45
1:D:120:TRP:HA	1:D:133:PHE:HB2	1.98	0.45
3:C:89:ASN:ND2	3:C:125:ALA:HB1	2.31	0.45
1:A:16:LEU:HG	3:C:218:TYR:CE1	2.52	0.45
1:A:152:PRO:N	1:A:153:PRO:HD2	2.32	0.45
1:D:16:LEU:HG	3:F:218:TYR:CE1	2.52	0.45
1:D:163:LYS:HB2	1:D:170:ILE:HG13	1.98	0.45
2:E:329:LEU:O	2:E:333:LEU:N	2.50	0.45
3:F:121:TYR:O	3:F:122:GLU:HG2	2.17	0.45
2:E:235:ASP:OD2	2:E:239:ASN:HB2	2.17	0.45
1:A:36:SER:O	1:A:37:GLU:HG3	2.17	0.45
2:B:329:LEU:O	2:B:333:LEU:N	2.50	0.45
3:C:57:THR:OG1	3:C:60:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:SER:HB2	2:E:198:VAL:HG13	1.99	0.45
3:C:109:LEU:H	3:C:109:LEU:HD23	1.81	0.45
1:D:65:LYS:HA	1:D:66:THR:HA	1.58	0.45
3:F:160:LEU:CD1	3:F:160:LEU:C	2.85	0.45
1:A:111:CYS:SG	1:A:142:TYR:OH	2.69	0.44
1:A:120:TRP:HA	1:A:133:PHE:HB2	1.98	0.44
2:B:116:LYS:O	2:B:119:ARG:N	2.44	0.44
2:B:386:ALA:HA	2:B:389:ILE:HG12	1.98	0.44
3:C:121:TYR:O	3:C:122:GLU:HG2	2.17	0.44
3:C:160:LEU:CD1	3:C:160:LEU:C	2.85	0.44
1:A:163:LYS:HB2	1:A:170:ILE:HG13	1.99	0.44
6:B:503:DLX:C24	7:B:506:PGV:C34	2.95	0.44
2:E:61:TYR:HB2	2:E:77:ILE:HD11	1.99	0.44
2:B:235:ASP:OD2	2:B:239:ASN:HB2	2.17	0.44
3:F:57:THR:OG1	3:F:60:GLU:HG3	2.17	0.44
1:D:152:PRO:N	1:D:153:PRO:HD2	2.32	0.44
6:E:503:DLX:C42	6:E:503:DLX:C38	2.96	0.44
3:C:60:GLU:O	3:C:64:GLU:HG2	2.18	0.44
8:C:302:HEC:HBA2	8:C:302:HEC:HHA	2.00	0.44
1:D:36:SER:O	1:D:37:GLU:HG3	2.17	0.44
2:B:61:TYR:HB2	2:B:77:ILE:HD11	1.99	0.43
3:F:38:ASP:HB2	3:F:156:TYR:CE2	2.53	0.43
6:B:503:DLX:C42	6:B:503:DLX:C38	2.96	0.43
3:C:41:VAL:HB	3:C:44:ILE:HG12	2.01	0.43
3:C:159:ILE:HD13	8:C:302:HEC:CMB	2.38	0.43
1:A:66:THR:OG1	1:A:109:GLY:O	2.36	0.43
2:B:278:PRO:HG2	2:B:281:ASN:HB2	2.00	0.43
1:D:66:THR:OG1	1:D:109:GLY:O	2.36	0.43
3:C:38:ASP:HB2	3:C:156:TYR:CE2	2.53	0.43
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.90	0.43
2:E:130:TYR:CZ	2:E:134:ILE:HD11	2.54	0.43
2:B:139:SER:HB2	2:B:198:VAL:HG13	1.99	0.43
2:B:52:ILE:O	2:B:56:MET:HG3	2.19	0.43
3:C:64:GLU:HA	3:C:67:ILE:HG12	2.01	0.42
3:F:64:GLU:HA	3:F:67:ILE:HG12	2.00	0.42
2:B:217:HIS:NE2	5:B:502:HEM:ND	2.67	0.42
3:F:60:GLU:O	3:F:64:GLU:HG2	2.18	0.42
3:F:130:GLN:OE1	3:F:130:GLN:N	2.52	0.42
3:F:41:VAL:HB	3:F:44:ILE:HG12	2.00	0.42
2:B:247:HIS:CE1	2:B:248:PRO:HB3	2.55	0.42
2:B:289:LYS:HE2	1:D:114:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:503:DLX:C22	7:B:506:PGV:H341	2.45	0.42
2:E:52:ILE:O	2:E:56:MET:HG3	2.19	0.42
2:E:191:THR:OG1	2:E:192:ASP:N	2.52	0.42
2:E:266:PHE:HA	2:E:269:VAL:HB	2.00	0.42
2:E:278:PRO:HG2	2:E:281:ASN:HB2	2.00	0.42
2:E:308:ARG:HH22	2:E:373:ASN:ND2	2.18	0.42
8:F:302:HEC:HBA2	8:F:302:HEC:HHA	2.00	0.42
2:B:130:TYR:CZ	2:B:134:ILE:HD11	2.54	0.42
3:C:130:GLN:OE1	3:C:130:GLN:N	2.52	0.42
3:F:155:LEU:O	3:F:159:ILE:HG13	2.20	0.42
3:C:155:LEU:O	3:C:159:ILE:HG13	2.19	0.42
1:D:111:CYS:SG	1:D:142:TYR:OH	2.69	0.42
1:D:147:ASP:HA	1:D:156:PRO:HB3	2.01	0.42
2:E:113:ASN:HA	2:E:115:TYR:CE2	2.55	0.42
2:E:201:SER:OG	2:E:202:HIS:N	2.53	0.42
1:A:32:MET:O	2:E:197:ARG:HD3	2.20	0.42
1:A:119:LEU:O	1:A:133:PHE:HB2	2.19	0.42
2:B:113:ASN:HA	2:B:115:TYR:CE2	2.55	0.42
2:B:266:PHE:HA	2:B:269:VAL:HB	2.01	0.42
7:B:506:PGV:H131	7:B:506:PGV:H101	1.83	0.42
3:C:136:LEU:HD21	8:C:302:HEC:HAC	2.02	0.42
2:E:119:ARG:CZ	2:E:227:SER:HB3	2.50	0.42
2:E:217:HIS:NE2	5:E:502:HEM:ND	2.67	0.42
2:B:25:MET:HB3	2:B:247:HIS:HB2	2.02	0.42
2:B:197:ARG:HD3	1:D:32:MET:O	2.20	0.42
3:C:85:SER:O	3:C:85:SER:OG	2.38	0.42
2:B:191:THR:OG1	2:B:192:ASP:N	2.52	0.41
2:B:201:SER:OG	2:B:202:HIS:N	2.53	0.41
2:B:244:VAL:HG13	2:B:244:VAL:O	2.20	0.41
3:C:89:ASN:N	3:C:90:PRO:HD2	2.35	0.41
2:B:64:PRO:HD2	2:E:64:PRO:HD2	2.02	0.41
3:C:97:LYS:HA	3:C:97:LYS:HD3	1.78	0.41
2:E:46:VAL:O	2:E:50:ILE:HG12	2.21	0.41
2:E:247:HIS:CE1	2:E:248:PRO:HB3	2.54	0.41
3:F:112:ASP:OD1	3:F:112:ASP:N	2.53	0.41
3:F:171:MET:HA	3:F:172:PRO:HD3	1.94	0.41
2:B:238:LYS:CD	2:B:239:ASN:H	2.26	0.41
3:C:138:GLN:HB3	1:D:116:CYS:SG	2.60	0.41
3:F:226:LEU:HD23	3:F:226:LEU:HA	1.95	0.41
1:A:41:LEU:HA	1:A:42:GLY:HA2	1.68	0.41
1:A:114:LEU:HD22	2:E:289:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ILE:HD13	2:B:315:TRP:CD1	2.56	0.41
1:A:121:LYS:HE2	1:A:121:LYS:HB2	1.91	0.41
1:D:119:LEU:O	1:D:133:PHE:HB2	2.19	0.41
3:F:89:ASN:N	3:F:90:PRO:HD2	2.35	0.41
1:A:65:LYS:HA	1:A:66:THR:HA	1.58	0.41
2:B:294:ILE:HD12	2:B:294:ILE:HA	1.91	0.41
3:C:234:LEU:HD23	3:C:234:LEU:HA	1.93	0.41
3:F:136:LEU:HD21	8:F:302:HEC:HAC	2.02	0.41
3:F:106:PHE:HA	3:F:107:GLY:HA2	1.65	0.41
2:B:46:VAL:O	2:B:50:ILE:HG12	2.21	0.41
2:B:119:ARG:CZ	2:B:227:SER:HB3	2.50	0.41
2:B:147:GLN:N	2:B:283:GLU:O	2.54	0.41
2:B:349:VAL:O	2:B:352:VAL:HG12	2.21	0.41
2:B:356:ILE:HD13	2:B:356:ILE:HA	1.96	0.41
7:B:506:PGV:C18	6:E:503:DLX:C46	2.98	0.41
2:E:25:MET:HB3	2:E:247:HIS:HB2	2.02	0.41
2:E:113:ASN:HB2	2:E:339:LYS:O	2.21	0.41
2:E:127:TRP:CD2	2:E:328:LEU:HG	2.56	0.41
1:A:147:ASP:HA	1:A:156:PRO:HB3	2.01	0.41
2:E:242:LYS:HE2	2:E:242:LYS:HB2	1.95	0.41
2:E:154:ILE:HD13	2:E:154:ILE:HA	1.91	0.40
3:F:123:ALA:HA	3:F:127:ASP:HB2	2.02	0.40
3:C:104:TYR:HA	3:C:109:LEU:HA	2.03	0.40
3:C:176:ASN:O	3:C:180:ASP:HB2	2.22	0.40
2:E:74:THR:O	2:E:78:MET:HB2	2.21	0.40
2:E:244:VAL:O	2:E:244:VAL:HG13	2.20	0.40
3:F:85:SER:HA	3:F:86:VAL:HA	1.83	0.40
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.82	0.40
2:B:113:ASN:HB2	2:B:339:LYS:O	2.21	0.40
3:C:66:PHE:CE1	3:C:143:LEU:HD12	2.57	0.40
3:C:123:ALA:HA	3:C:127:ASP:HB2	2.02	0.40
2:E:147:GLN:N	2:E:283:GLU:O	2.54	0.40
2:E:346:LEU:HD12	2:E:346:LEU:HA	1.96	0.40
2:B:308:ARG:HH22	2:B:373:ASN:ND2	2.18	0.40
2:B:330:LEU:HD12	2:B:388:PHE:HE1	1.87	0.40
1:A:116:CYS:SG	3:F:138:GLN:HB3	2.62	0.40
2:B:167:PRO:HB3	2:B:314:PHE:CE2	2.57	0.40
2:E:310:ILE:HD13	2:E:315:TRP:CD1	2.56	0.40
3:F:41:VAL:HG23	3:F:42:LYS:N	2.34	0.40
3:F:66:PHE:CE1	3:F:143:LEU:HD12	2.57	0.40
3:F:132:LEU:O	3:F:136:LEU:HB2	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	128/181 (71%)	111 (87%)	17 (13%)	0	100	100
1	D	128/181 (71%)	111 (87%)	17 (13%)	0	100	100
2	B	393/410 (96%)	358 (91%)	35 (9%)	0	100	100
2	E	393/410 (96%)	359 (91%)	34 (9%)	0	100	100
3	C	234/240 (98%)	204 (87%)	29 (12%)	1 (0%)	30	61
3	F	234/240 (98%)	204 (87%)	29 (12%)	1 (0%)	30	61
All	All	1510/1662 (91%)	1347 (89%)	161 (11%)	2 (0%)	50	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	141	PRO
3	F	141	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/145 (74%)	107 (99%)	1 (1%)	75	85
1	D	108/145 (74%)	106 (98%)	2 (2%)	52	72
2	B	339/350 (97%)	338 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	339/350 (97%)	338 (100%)	1 (0%)	91	94
3	C	206/210 (98%)	203 (98%)	3 (2%)	60	77
3	F	206/210 (98%)	203 (98%)	3 (2%)	60	77
All	All	1306/1410 (93%)	1295 (99%)	11 (1%)	77	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
2	B	174	LYS
3	C	10	ILE
3	C	160	LEU
3	C	203	LYS
1	D	37	GLU
1	D	113	HIS
2	E	174	LYS
3	F	10	ILE
3	F	160	LEU
3	F	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	24	GLN
2	B	51	GLN
2	B	96	ASN
2	B	147	GLN
2	B	373	ASN
3	C	176	ASN
3	C	198	ASN
2	E	24	GLN
2	E	51	GLN
2	E	96	ASN
2	E	147	GLN
2	E	373	ASN
3	F	176	ASN
3	F	198	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

17 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	$\# Z  > 2$
5	HEM	B	502	2	41,50,50	1.43	3 (7%)	45,82,82	1.38	8 (17%)
6	DLX	B	503	-	48,48,48	1.57	6 (12%)	59,61,61	1.64	14 (23%)
6	DLX	C	301	-	48,48,48	4.54	27 (56%)	59,61,61	3.15	23 (38%)
6	DLX	E	503	-	48,48,48	1.58	6 (12%)	59,61,61	1.65	14 (23%)
5	HEM	E	501	2	41,50,50	1.51	3 (7%)	45,82,82	1.49	5 (11%)
5	HEM	E	502	2	41,50,50	1.44	3 (7%)	45,82,82	1.38	8 (17%)
7	PGV	B	505	2	50,50,50	1.20	3 (6%)	53,56,56	0.88	2 (3%)
5	HEM	B	501	2	41,50,50	1.51	3 (7%)	45,82,82	1.49	5 (11%)
4	FES	D	501	1	0,4,4	-	-	-	-	-
6	DLX	F	301	-	48,48,48	4.54	27 (56%)	59,61,61	3.16	23 (38%)
8	HEC	C	302	3	32,50,50	2.20	3 (9%)	24,82,82	1.43	3 (12%)
6	DLX	E	504	-	48,48,48	4.57	27 (56%)	59,61,61	3.15	22 (37%)
8	HEC	F	302	3	32,50,50	2.19	3 (9%)	24,82,82	1.43	4 (16%)
7	PGV	E	505	2	50,50,50	1.20	4 (8%)	53,56,56	0.87	2 (3%)
4	FES	A	501	1	0,4,4	-	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PGV	B	506	-	50,50,50	0.88	3 (6%)	53,56,56	0.87	3 (5%)
6	DLX	B	504	-	48,48,48	4.57	27 (56%)	59,61,61	3.15	22 (37%)

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
5	HEM	B	502	2	-	0/12/54/54	-
6	DLX	B	503	-	-	10/41/57/57	0/2/2/2
6	DLX	C	301	-	-	23/41/57/57	0/2/2/2
6	DLX	E	503	-	-	10/41/57/57	0/2/2/2
5	HEM	E	501	2	-	2/12/54/54	-
5	HEM	E	502	2	-	0/12/54/54	-
7	PGV	B	505	2	-	20/55/55/55	-
5	HEM	B	501	2	-	2/12/54/54	-
8	HEC	C	302	3	-	4/10/54/54	-
8	HEC	F	302	3	-	4/10/54/54	-
4	FES	D	501	1	-	-	0/1/1/1
6	DLX	E	504	-	-	22/41/57/57	0/2/2/2
7	PGV	E	505	2	-	20/55/55/55	-
6	DLX	F	301	-	-	23/41/57/57	0/2/2/2
7	PGV	B	506	-	-	35/55/55/55	-
6	DLX	B	504	-	-	22/41/57/57	0/2/2/2
4	FES	A	501	1	-	-	0/1/1/1

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	DLX	C30-C31	13.87	1.66	1.33
6	E	504	DLX	C30-C31	13.87	1.66	1.33
6	F	301	DLX	C30-C31	13.79	1.66	1.33
6	C	301	DLX	C30-C31	13.76	1.66	1.33
6	E	504	DLX	C22-C23	11.32	1.60	1.33
6	B	504	DLX	C22-C23	11.32	1.60	1.33
6	F	301	DLX	C22-C23	11.23	1.59	1.33
6	C	301	DLX	C22-C23	11.22	1.59	1.33
6	C	301	DLX	C26-C27	10.59	1.58	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	DLX	C26-C27	10.57	1.58	1.33
6	E	504	DLX	C26-C27	10.57	1.58	1.33
6	F	301	DLX	C26-C27	10.56	1.58	1.33
6	B	504	DLX	O11-C01	9.55	1.45	1.24
6	E	504	DLX	O11-C01	9.53	1.45	1.24
6	C	301	DLX	O11-C01	9.50	1.45	1.24
6	F	301	DLX	O11-C01	9.50	1.45	1.24
6	B	504	DLX	C18-C19	9.10	1.54	1.33
6	E	504	DLX	C18-C19	9.08	1.54	1.33
6	F	301	DLX	C18-C19	9.03	1.54	1.33
6	C	301	DLX	C18-C19	9.00	1.54	1.33
6	E	504	DLX	C14-C15	8.40	1.53	1.33
6	B	504	DLX	C14-C15	8.35	1.53	1.33
6	C	301	DLX	C14-C15	8.34	1.53	1.33
6	F	301	DLX	C14-C15	8.33	1.53	1.33
6	C	301	DLX	C32-C31	6.52	1.64	1.51
6	F	301	DLX	C32-C31	6.49	1.64	1.51
6	B	504	DLX	C32-C31	6.42	1.64	1.51
6	E	504	DLX	C32-C31	6.42	1.64	1.51
8	C	302	HEC	C2B-C3B	-6.38	1.34	1.40
8	C	302	HEC	C3C-C2C	-6.38	1.34	1.40
8	F	302	HEC	C3C-C2C	-6.38	1.34	1.40
8	F	302	HEC	C2B-C3B	-6.36	1.34	1.40
6	B	504	DLX	O12-C04	5.96	1.35	1.23
6	E	504	DLX	O12-C04	5.96	1.35	1.23
6	F	301	DLX	O12-C04	5.92	1.35	1.23
6	C	301	DLX	O12-C04	5.89	1.35	1.23
6	E	504	DLX	C13-C05	5.42	1.56	1.51
6	B	504	DLX	C13-C05	5.40	1.56	1.51
8	F	302	HEC	C3D-C2D	5.35	1.53	1.37
8	C	302	HEC	C3D-C2D	5.33	1.53	1.37
6	E	503	DLX	C02-C01	-5.25	1.39	1.48
6	C	301	DLX	C13-C05	5.20	1.56	1.51
6	F	301	DLX	C13-C05	5.20	1.56	1.51
6	B	503	DLX	C02-C01	-5.20	1.39	1.48
6	E	503	DLX	C05-C04	-5.10	1.38	1.48
6	B	503	DLX	C05-C04	-5.08	1.38	1.48
6	E	503	DLX	C03-C04	-5.07	1.38	1.48
6	B	503	DLX	C03-C04	-5.07	1.38	1.48
5	B	501	HEM	C3C-C2C	-5.01	1.33	1.40
5	E	501	HEM	C3C-C2C	-5.01	1.33	1.40
6	E	504	DLX	C29-C30	4.56	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	DLX	C29-C30	4.55	1.65	1.50
6	C	301	DLX	C05-C04	-4.54	1.39	1.48
6	F	301	DLX	C05-C04	-4.54	1.39	1.48
6	C	301	DLX	C29-C30	4.53	1.65	1.50
6	F	301	DLX	C29-C30	4.53	1.65	1.50
6	E	504	DLX	C05-C04	-4.47	1.39	1.48
6	B	504	DLX	C05-C04	-4.42	1.39	1.48
6	C	301	DLX	C28-C27	4.25	1.60	1.51
6	F	301	DLX	C28-C27	4.25	1.60	1.51
6	B	504	DLX	C28-C27	4.19	1.60	1.51
6	E	504	DLX	C28-C27	4.19	1.60	1.51
6	B	504	DLX	C43-C31	3.90	1.60	1.50
6	E	504	DLX	C43-C31	3.90	1.60	1.50
6	C	301	DLX	C43-C31	3.88	1.60	1.50
6	F	301	DLX	C43-C31	3.86	1.60	1.50
5	B	502	HEM	C3C-C2C	-3.86	1.35	1.40
5	E	502	HEM	C3C-C2C	-3.85	1.35	1.40
5	E	502	HEM	C3C-CAC	3.71	1.55	1.47
5	B	502	HEM	C3C-CAC	3.70	1.55	1.47
7	B	505	PGV	O03-C19	3.66	1.44	1.33
7	E	505	PGV	O03-C19	3.63	1.44	1.33
6	C	301	DLX	C44-C27	3.46	1.59	1.50
6	F	301	DLX	C44-C27	3.46	1.59	1.50
5	E	501	HEM	C3C-CAC	3.44	1.54	1.47
5	B	501	HEM	C3C-CAC	3.44	1.54	1.47
6	E	504	DLX	C28-C29	3.40	1.65	1.53
6	B	504	DLX	C28-C29	3.39	1.65	1.53
6	B	504	DLX	C44-C27	3.38	1.59	1.50
6	F	301	DLX	C28-C29	3.37	1.65	1.53
6	B	504	DLX	C10-C03	3.37	1.45	1.39
6	E	504	DLX	C10-C03	3.37	1.45	1.39
6	E	504	DLX	C44-C27	3.36	1.59	1.50
6	C	301	DLX	C28-C29	3.36	1.64	1.53
6	B	504	DLX	C13-C14	3.31	1.55	1.50
6	B	504	DLX	C25-C26	3.30	1.61	1.50
6	F	301	DLX	C13-C14	3.29	1.55	1.50
6	E	504	DLX	C13-C14	3.29	1.55	1.50
6	E	504	DLX	C25-C26	3.28	1.61	1.50
6	C	301	DLX	C10-C03	3.27	1.45	1.39
6	C	301	DLX	C13-C14	3.26	1.55	1.50
6	F	301	DLX	C25-C26	3.25	1.61	1.50
6	C	301	DLX	C25-C26	3.24	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	301	DLX	C10-C03	3.23	1.45	1.39
7	B	505	PGV	O01-C1	3.16	1.43	1.34
7	E	505	PGV	O01-C1	3.16	1.43	1.34
6	E	504	DLX	C16-C15	3.15	1.57	1.51
6	B	504	DLX	C16-C15	3.15	1.57	1.51
6	F	301	DLX	C06-C05	3.13	1.42	1.34
6	B	504	DLX	C06-C05	3.11	1.42	1.34
6	E	504	DLX	C06-C05	3.11	1.42	1.34
6	C	301	DLX	C06-C05	3.10	1.42	1.34
6	F	301	DLX	C16-C15	3.04	1.57	1.51
6	C	301	DLX	C16-C15	3.03	1.57	1.51
6	B	503	DLX	C06-C01	-2.94	1.38	1.44
6	E	504	DLX	C07-C02	2.93	1.44	1.39
6	B	504	DLX	C07-C02	2.92	1.44	1.39
6	E	503	DLX	C06-C01	-2.90	1.38	1.44
5	B	502	HEM	CAB-C3B	2.86	1.55	1.47
5	E	502	HEM	CAB-C3B	2.84	1.55	1.47
6	C	301	DLX	C07-C02	2.83	1.44	1.39
6	C	301	DLX	C24-C23	2.83	1.57	1.51
6	F	301	DLX	C07-C02	2.82	1.44	1.39
6	E	504	DLX	C24-C23	2.82	1.57	1.51
5	B	501	HEM	CAB-C3B	2.78	1.55	1.47
6	F	301	DLX	C24-C23	2.78	1.57	1.51
5	E	501	HEM	CAB-C3B	2.78	1.55	1.47
6	B	504	DLX	C24-C23	2.78	1.57	1.51
6	E	504	DLX	C06-C01	-2.63	1.39	1.44
6	F	301	DLX	C06-C01	-2.62	1.39	1.44
6	B	504	DLX	C06-C01	-2.61	1.39	1.44
6	C	301	DLX	C06-C01	-2.61	1.39	1.44
6	B	504	DLX	C03-C04	-2.56	1.43	1.48
6	E	504	DLX	C03-C04	-2.55	1.43	1.48
6	E	504	DLX	C17-C18	2.54	1.58	1.50
6	B	503	DLX	O11-C01	-2.52	1.18	1.24
6	B	504	DLX	C17-C18	2.51	1.58	1.50
6	E	503	DLX	O11-C01	-2.51	1.18	1.24
6	C	301	DLX	C03-C04	-2.48	1.43	1.48
6	F	301	DLX	C03-C04	-2.48	1.43	1.48
6	C	301	DLX	C17-C18	2.48	1.58	1.50
6	F	301	DLX	C17-C18	2.48	1.58	1.50
7	B	506	PGV	O01-C02	-2.46	1.40	1.46
6	B	504	DLX	C21-C22	2.42	1.58	1.50
6	E	504	DLX	C21-C22	2.42	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	506	PGV	O03-C19	2.41	1.40	1.33
6	C	301	DLX	C02-C01	-2.40	1.44	1.48
6	E	504	DLX	C02-C01	-2.36	1.44	1.48
6	F	301	DLX	C02-C01	-2.35	1.44	1.48
6	B	504	DLX	C02-C01	-2.34	1.44	1.48
6	C	301	DLX	C21-C22	2.32	1.58	1.50
6	F	301	DLX	C21-C22	2.32	1.58	1.50
6	B	503	DLX	O12-C04	-2.24	1.18	1.23
6	E	503	DLX	O12-C04	-2.23	1.18	1.23
7	B	505	PGV	O01-C02	-2.09	1.41	1.46
7	E	505	PGV	O01-C02	-2.09	1.41	1.46
7	B	506	PGV	O01-C1	2.09	1.40	1.34
7	E	505	PGV	C20-C19	2.00	1.56	1.50

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	DLX	C13-C14-C15	-8.66	112.37	126.79
6	C	301	DLX	C13-C14-C15	-8.65	112.39	126.79
6	E	504	DLX	C13-C14-C15	-8.51	112.63	126.79
6	B	504	DLX	C13-C14-C15	-8.50	112.64	126.79
6	F	301	DLX	C17-C18-C19	-6.74	111.43	127.66
6	C	301	DLX	C17-C18-C19	-6.72	111.48	127.66
6	C	301	DLX	C21-C22-C23	-6.58	111.83	127.66
6	F	301	DLX	C21-C22-C23	-6.56	111.86	127.66
6	B	504	DLX	C17-C18-C19	-6.45	112.12	127.66
6	E	504	DLX	C17-C18-C19	-6.45	112.12	127.66
6	F	301	DLX	C25-C26-C27	-6.29	112.52	127.66
6	C	301	DLX	C25-C26-C27	-6.28	112.53	127.66
6	B	504	DLX	C21-C22-C23	-6.28	112.54	127.66
6	E	504	DLX	C21-C22-C23	-6.27	112.57	127.66
6	E	504	DLX	C29-C30-C31	-6.18	112.78	127.66
6	B	504	DLX	C29-C30-C31	-6.17	112.81	127.66
6	C	301	DLX	C29-C30-C31	-6.10	112.97	127.66
6	E	504	DLX	C25-C26-C27	-6.09	112.99	127.66
6	F	301	DLX	C29-C30-C31	-6.09	112.99	127.66
6	B	504	DLX	C25-C26-C27	-6.09	113.00	127.66
6	C	301	DLX	C16-C15-C14	-5.85	109.29	121.12
6	F	301	DLX	C16-C15-C14	-5.84	109.29	121.12
6	F	301	DLX	C46-C19-C18	-5.71	109.03	123.68
6	C	301	DLX	C46-C19-C18	-5.69	109.08	123.68
6	B	504	DLX	C46-C19-C18	-5.66	109.16	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	504	DLX	C46-C19-C18	-5.65	109.18	123.68
6	B	504	DLX	C20-C19-C18	-5.65	109.68	121.12
6	F	301	DLX	C20-C19-C18	-5.65	109.69	121.12
6	C	301	DLX	C20-C19-C18	-5.64	109.70	121.12
6	E	504	DLX	C20-C19-C18	-5.64	109.71	121.12
6	E	504	DLX	C16-C15-C14	-5.64	109.71	121.12
6	B	504	DLX	C16-C15-C14	-5.63	109.72	121.12
6	B	504	DLX	C47-C15-C14	-5.44	109.72	123.68
6	E	504	DLX	C47-C15-C14	-5.43	109.75	123.68
6	F	301	DLX	C47-C15-C14	-5.42	109.77	123.68
6	C	301	DLX	C47-C15-C14	-5.41	109.81	123.68
6	B	504	DLX	C32-C31-C30	-5.28	110.44	121.12
6	E	504	DLX	C32-C31-C30	-5.28	110.44	121.12
6	C	301	DLX	C45-C23-C22	-5.07	110.67	123.68
6	F	301	DLX	C45-C23-C22	-5.07	110.67	123.68
6	F	301	DLX	C32-C31-C30	-5.02	110.95	121.12
6	C	301	DLX	C32-C31-C30	-5.01	110.97	121.12
6	B	504	DLX	C45-C23-C22	-4.94	111.00	123.68
6	B	504	DLX	C28-C27-C26	-4.94	111.11	121.12
6	E	504	DLX	C43-C31-C30	-4.94	111.01	123.68
6	E	504	DLX	C45-C23-C22	-4.94	111.01	123.68
6	E	504	DLX	C28-C27-C26	-4.94	111.12	121.12
6	B	504	DLX	C43-C31-C30	-4.94	111.01	123.68
6	E	504	DLX	C44-C27-C26	-4.92	111.05	123.68
6	B	504	DLX	C44-C27-C26	-4.91	111.07	123.68
6	B	504	DLX	C24-C23-C22	-4.89	111.22	121.12
6	E	504	DLX	C24-C23-C22	-4.88	111.24	121.12
6	F	301	DLX	C43-C31-C30	-4.83	111.28	123.68
6	C	301	DLX	C43-C31-C30	-4.83	111.29	123.68
6	F	301	DLX	C24-C23-C22	-4.69	111.63	121.12
6	C	301	DLX	C24-C23-C22	-4.68	111.65	121.12
6	B	503	DLX	C13-C14-C15	-4.61	119.12	126.79
6	E	503	DLX	C13-C14-C15	-4.60	119.14	126.79
6	C	301	DLX	C44-C27-C26	-4.60	111.88	123.68
6	F	301	DLX	C44-C27-C26	-4.59	111.89	123.68
6	C	301	DLX	C28-C27-C26	-4.54	111.93	121.12
6	F	301	DLX	C28-C27-C26	-4.53	111.95	121.12
6	E	503	DLX	C13-C05-C04	4.06	120.17	116.88
7	B	505	PGV	O01-C1-C2	4.02	120.17	111.50
6	B	503	DLX	C13-C05-C04	4.00	120.13	116.88
7	E	505	PGV	O01-C1-C2	3.99	120.10	111.50
7	B	506	PGV	O01-C1-C2	3.97	120.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	504	DLX	C13-C05-C04	3.80	119.96	116.88
6	F	301	DLX	C13-C05-C04	3.75	119.93	116.88
6	E	504	DLX	C13-C05-C04	3.74	119.92	116.88
6	E	503	DLX	C17-C18-C19	-3.73	118.67	127.66
6	B	503	DLX	C17-C18-C19	-3.72	118.70	127.66
6	C	301	DLX	C13-C05-C04	3.71	119.89	116.88
6	F	301	DLX	C46-C19-C20	-3.64	109.15	115.27
6	B	504	DLX	C47-C15-C16	-3.62	109.18	115.27
6	C	301	DLX	C46-C19-C20	-3.62	109.18	115.27
6	F	301	DLX	C47-C15-C16	-3.62	109.18	115.27
6	C	301	DLX	C47-C15-C16	-3.61	109.19	115.27
6	E	504	DLX	C47-C15-C16	-3.60	109.21	115.27
6	E	504	DLX	C46-C19-C20	-3.55	109.31	115.27
6	B	504	DLX	C46-C19-C20	-3.53	109.33	115.27
5	E	501	HEM	C4B-CHC-C1C	3.34	126.97	122.56
5	B	501	HEM	C4B-CHC-C1C	3.31	126.92	122.56
5	B	501	HEM	C1B-NB-C4B	3.07	108.25	105.07
6	B	503	DLX	C21-C22-C23	-3.05	120.33	127.66
6	E	503	DLX	C21-C22-C23	-3.05	120.33	127.66
5	E	501	HEM	C1B-NB-C4B	3.04	108.21	105.07
6	B	503	DLX	C47-C15-C16	2.96	120.26	115.27
6	E	503	DLX	C47-C15-C16	2.96	120.26	115.27
6	E	503	DLX	C45-C23-C24	2.96	120.25	115.27
8	C	302	HEC	CMC-C2C-C1C	-2.95	123.93	128.46
6	B	503	DLX	C45-C23-C24	2.94	120.22	115.27
8	F	302	HEC	CMC-C2C-C1C	-2.94	123.95	128.46
6	E	503	DLX	C13-C05-C06	-2.91	119.47	123.30
6	B	503	DLX	C13-C05-C06	-2.87	119.53	123.30
6	B	503	DLX	C44-C27-C28	2.87	120.09	115.27
6	E	503	DLX	C44-C27-C28	2.85	120.06	115.27
6	E	503	DLX	C46-C19-C20	2.80	119.99	115.27
5	B	502	HEM	C4D-ND-C1D	2.79	107.95	105.07
6	B	503	DLX	C46-C19-C20	2.78	119.95	115.27
6	E	504	DLX	C44-C27-C28	-2.78	110.59	115.27
5	E	502	HEM	C4D-ND-C1D	2.78	107.94	105.07
6	B	504	DLX	C44-C27-C28	-2.76	110.62	115.27
5	B	501	HEM	C3B-C2B-C1B	2.74	108.52	106.49
5	E	501	HEM	C3B-C2B-C1B	2.74	108.52	106.49
5	B	502	HEM	C1B-NB-C4B	2.69	107.85	105.07
7	B	505	PGV	O03-C19-C20	2.67	120.29	111.91
7	E	505	PGV	O03-C19-C20	2.67	120.28	111.91
5	E	502	HEM	C1B-NB-C4B	2.64	107.81	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	503	DLX	C29-C30-C31	-2.64	121.31	127.66
6	B	503	DLX	C29-C30-C31	-2.63	121.34	127.66
6	B	503	DLX	C25-C26-C27	-2.62	121.34	127.66
6	E	503	DLX	C25-C26-C27	-2.61	121.37	127.66
5	E	501	HEM	C4D-ND-C1D	2.59	107.75	105.07
6	B	504	DLX	C03-C04-C05	2.59	120.13	116.62
5	B	501	HEM	C4C-CHD-C1D	2.59	125.97	122.56
6	B	504	DLX	C43-C31-C32	-2.58	110.94	115.27
5	B	501	HEM	C4D-ND-C1D	2.57	107.73	105.07
7	B	506	PGV	O03-C19-C20	2.57	119.97	111.91
5	E	501	HEM	C4C-CHD-C1D	2.56	125.94	122.56
6	E	504	DLX	C03-C04-C05	2.56	120.09	116.62
6	E	504	DLX	C43-C31-C32	-2.54	111.00	115.27
6	E	503	DLX	C43-C31-C32	2.52	119.52	115.27
6	F	301	DLX	C03-C04-C05	2.51	120.02	116.62
6	C	301	DLX	C03-C04-C05	2.48	119.98	116.62
6	B	503	DLX	C43-C31-C32	2.48	119.44	115.27
6	E	503	DLX	C03-C04-C05	2.48	119.98	116.62
6	B	503	DLX	C03-C04-C05	2.47	119.97	116.62
6	C	301	DLX	C44-C27-C28	-2.42	111.20	115.27
6	F	301	DLX	C44-C27-C28	-2.42	111.20	115.27
5	B	502	HEM	CMC-C2C-C3C	2.42	129.20	124.68
5	E	502	HEM	CMC-C2C-C3C	2.41	129.19	124.68
6	F	301	DLX	C13-C05-C06	-2.41	120.13	123.30
6	C	301	DLX	C13-C05-C06	-2.40	120.15	123.30
6	E	504	DLX	C13-C05-C06	-2.35	120.21	123.30
6	B	504	DLX	C13-C05-C06	-2.33	120.24	123.30
5	E	502	HEM	C4B-CHC-C1C	2.32	125.62	122.56
6	F	301	DLX	O12-C04-C05	-2.32	119.49	121.96
5	B	502	HEM	C4B-CHC-C1C	2.31	125.61	122.56
6	C	301	DLX	C43-C31-C32	-2.31	111.38	115.27
8	F	302	HEC	CMB-C2B-C1B	-2.31	124.92	128.46
8	C	302	HEC	CMB-C2B-C1B	-2.31	124.92	128.46
6	F	301	DLX	C43-C31-C32	-2.29	111.42	115.27
6	C	301	DLX	O12-C04-C05	-2.28	119.53	121.96
5	B	502	HEM	CAD-CBD-CGD	-2.26	108.75	113.60
5	E	502	HEM	CAD-CBD-CGD	-2.24	108.79	113.60
8	C	302	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
5	B	502	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
8	F	302	HEC	C1D-C2D-C3D	-2.17	105.48	107.00
5	E	502	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
5	E	502	HEM	C4C-CHD-C1D	2.14	125.38	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	HEM	C4C-CHD-C1D	2.13	125.37	122.56
5	B	502	HEM	C3D-C4D-ND	-2.13	107.79	110.17
5	E	502	HEM	C3D-C4D-ND	-2.13	107.80	110.17
7	B	506	PGV	C02-O01-C1	-2.07	112.70	117.79
6	B	503	DLX	O12-C04-C05	-2.05	119.77	121.96
6	E	503	DLX	O12-C04-C05	-2.04	119.78	121.96
8	F	302	HEC	CAD-CBD-CGD	-2.01	108.12	113.76

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	503	DLX	C45-C23-C24-C25
6	B	503	DLX	C22-C23-C24-C25
6	B	504	DLX	C29-C30-C31-C32
6	B	504	DLX	C25-C26-C27-C44
6	B	504	DLX	C45-C23-C24-C25
6	B	504	DLX	C21-C22-C23-C45
6	B	504	DLX	C21-C22-C23-C24
6	B	504	DLX	C17-C18-C19-C46
6	B	504	DLX	C13-C14-C15-C47
6	C	301	DLX	C29-C30-C31-C43
6	C	301	DLX	C25-C26-C27-C44
6	C	301	DLX	C45-C23-C24-C25
6	C	301	DLX	C21-C22-C23-C45
6	C	301	DLX	C21-C22-C23-C24
6	C	301	DLX	C17-C18-C19-C46
6	C	301	DLX	C17-C18-C19-C20
6	C	301	DLX	C13-C14-C15-C47
6	E	503	DLX	C45-C23-C24-C25
6	E	503	DLX	C22-C23-C24-C25
6	E	504	DLX	C29-C30-C31-C32
6	E	504	DLX	C25-C26-C27-C44
6	E	504	DLX	C45-C23-C24-C25
6	E	504	DLX	C21-C22-C23-C45
6	E	504	DLX	C21-C22-C23-C24
6	E	504	DLX	C17-C18-C19-C46
6	E	504	DLX	C13-C14-C15-C47
6	F	301	DLX	C29-C30-C31-C43
6	F	301	DLX	C25-C26-C27-C44
6	F	301	DLX	C45-C23-C24-C25
6	F	301	DLX	C21-C22-C23-C45

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Mol	Chain	Res	Type	Atoms
6	F	301	DLX	C21-C22-C23-C24
6	F	301	DLX	C17-C18-C19-C46
6	F	301	DLX	C17-C18-C19-C20
6	F	301	DLX	C13-C14-C15-C47
7	B	505	PGV	C04-O12-P-O14
7	B	505	PGV	O03-C01-C02-O01
7	B	505	PGV	C04-C05-C06-O06
7	B	506	PGV	C03-O11-P-O13
7	B	506	PGV	C03-O11-P-O14
7	B	506	PGV	C04-O12-P-O13
7	B	506	PGV	C2-C1-O01-C02
7	E	505	PGV	C04-O12-P-O14
7	E	505	PGV	O03-C01-C02-O01
7	E	505	PGV	C04-C05-C06-O06
8	C	302	HEC	C1A-C2A-CAA-CBA
8	F	302	HEC	C1A-C2A-CAA-CBA
7	B	506	PGV	O02-C1-O01-C02
6	B	504	DLX	C43-C31-C32-C33
6	E	504	DLX	C43-C31-C32-C33
6	B	504	DLX	C25-C26-C27-C28
6	B	504	DLX	C17-C18-C19-C20
6	E	504	DLX	C25-C26-C27-C28
6	E	504	DLX	C17-C18-C19-C20
6	B	503	DLX	C31-C32-C33-C34
6	E	503	DLX	C31-C32-C33-C34
5	B	501	HEM	C3D-CAD-CBD-CGD
5	E	501	HEM	C3D-CAD-CBD-CGD
6	B	504	DLX	C19-C20-C21-C22
6	B	504	DLX	C15-C16-C17-C18
6	C	301	DLX	C23-C24-C25-C26
6	C	301	DLX	C15-C16-C17-C18
6	E	504	DLX	C19-C20-C21-C22
6	E	504	DLX	C15-C16-C17-C18
6	F	301	DLX	C23-C24-C25-C26
6	F	301	DLX	C15-C16-C17-C18
6	C	301	DLX	C25-C26-C27-C28
6	F	301	DLX	C25-C26-C27-C28
6	B	503	DLX	C19-C20-C21-C22
6	E	503	DLX	C19-C20-C21-C22
6	C	301	DLX	C36-C37-C38-C39
6	F	301	DLX	C36-C37-C38-C39
7	B	505	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
7	B	506	PGV	C04-O12-P-O11
7	E	505	PGV	C04-O12-P-O11
7	B	506	PGV	C2-C3-C4-C5
7	B	506	PGV	C5-C6-C7-C8
7	B	506	PGV	C29-C30-C31-C32
6	C	301	DLX	C47-C15-C16-C17
6	F	301	DLX	C47-C15-C16-C17
7	B	506	PGV	C04-C05-C06-O06
7	B	506	PGV	C23-C24-C25-C26
7	B	506	PGV	C24-C25-C26-C27
7	B	506	PGV	C6-C7-C8-C9
7	B	506	PGV	C27-C28-C29-C30
7	B	505	PGV	C28-C29-C30-C31
7	E	505	PGV	C28-C29-C30-C31
6	B	503	DLX	C37-C38-C39-C40
6	E	503	DLX	C37-C38-C39-C40
6	C	301	DLX	C26-C27-C28-C29
6	F	301	DLX	C26-C27-C28-C29
7	B	506	PGV	O05-C05-C06-O06
7	B	506	PGV	C7-C8-C9-C10
6	B	503	DLX	C37-C38-C39-C41
6	E	503	DLX	C37-C38-C39-C41
6	C	301	DLX	C13-C14-C15-C16
6	F	301	DLX	C13-C14-C15-C16
7	B	506	PGV	C1-C2-C3-C4
7	B	506	PGV	C14-C15-C16-C17
7	B	505	PGV	C25-C26-C27-C28
7	E	505	PGV	C25-C26-C27-C28
7	B	506	PGV	C19-C20-C21-C22
5	B	501	HEM	C4B-C3B-CAB-CBB
5	E	501	HEM	C4B-C3B-CAB-CBB
6	B	503	DLX	C04-C05-C13-C14
6	C	301	DLX	C04-C05-C13-C14
6	E	503	DLX	C04-C05-C13-C14
6	F	301	DLX	C04-C05-C13-C14
6	C	301	DLX	C33-C34-C35-C42
6	F	301	DLX	C33-C34-C35-C42
7	B	506	PGV	C03-O11-P-O12
6	B	504	DLX	C05-C13-C14-C15
6	E	504	DLX	C05-C13-C14-C15
6	C	301	DLX	C14-C15-C16-C17
6	F	301	DLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	B	505	PGV	O03-C01-C02-C03
7	B	506	PGV	O03-C01-C02-C03
7	E	505	PGV	O03-C01-C02-C03
7	B	506	PGV	C15-C16-C17-C18
7	B	505	PGV	O05-C05-C06-O06
7	E	505	PGV	O05-C05-C06-O06
7	B	506	PGV	C31-C32-C33-C34
7	B	505	PGV	C21-C22-C23-C24
7	E	505	PGV	C21-C22-C23-C24
7	B	505	PGV	C20-C19-O03-C01
7	E	505	PGV	C20-C19-O03-C01
6	C	301	DLX	C43-C31-C32-C33
6	F	301	DLX	C43-C31-C32-C33
6	B	504	DLX	C33-C34-C35-C36
6	C	301	DLX	C33-C34-C35-C36
6	E	504	DLX	C33-C34-C35-C36
6	F	301	DLX	C33-C34-C35-C36
7	B	506	PGV	C28-C29-C30-C31
6	C	301	DLX	C29-C30-C31-C32
6	F	301	DLX	C29-C30-C31-C32
7	B	506	PGV	C01-C02-C03-O11
6	B	504	DLX	C14-C15-C16-C17
6	E	504	DLX	C14-C15-C16-C17
7	B	505	PGV	C19-C20-C21-C22
7	E	505	PGV	C19-C20-C21-C22
7	B	506	PGV	C26-C27-C28-C29
7	B	505	PGV	C26-C27-C28-C29
7	E	505	PGV	C26-C27-C28-C29
7	B	506	PGV	O01-C02-C03-O11
7	B	505	PGV	O04-C19-O03-C01
7	E	505	PGV	O04-C19-O03-C01
6	B	503	DLX	C36-C37-C38-C39
6	E	503	DLX	C36-C37-C38-C39
7	B	505	PGV	C11-C10-C9-C8
7	E	505	PGV	C11-C10-C9-C8
7	B	506	PGV	C13-C14-C15-C16
6	B	503	DLX	C06-C05-C13-C14
6	E	503	DLX	C06-C05-C13-C14
7	B	506	PGV	O03-C01-C02-O01
7	B	505	PGV	C04-O12-P-O13
7	B	506	PGV	C04-O12-P-O14
7	E	505	PGV	C04-O12-P-O13

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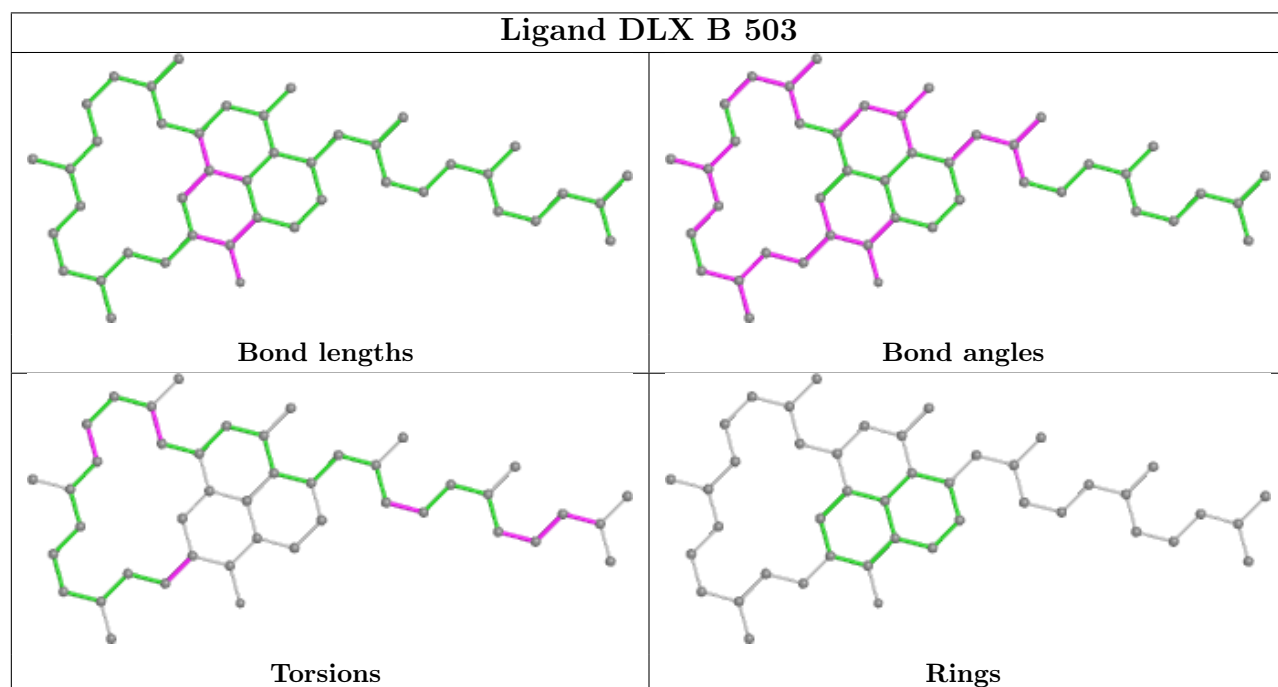
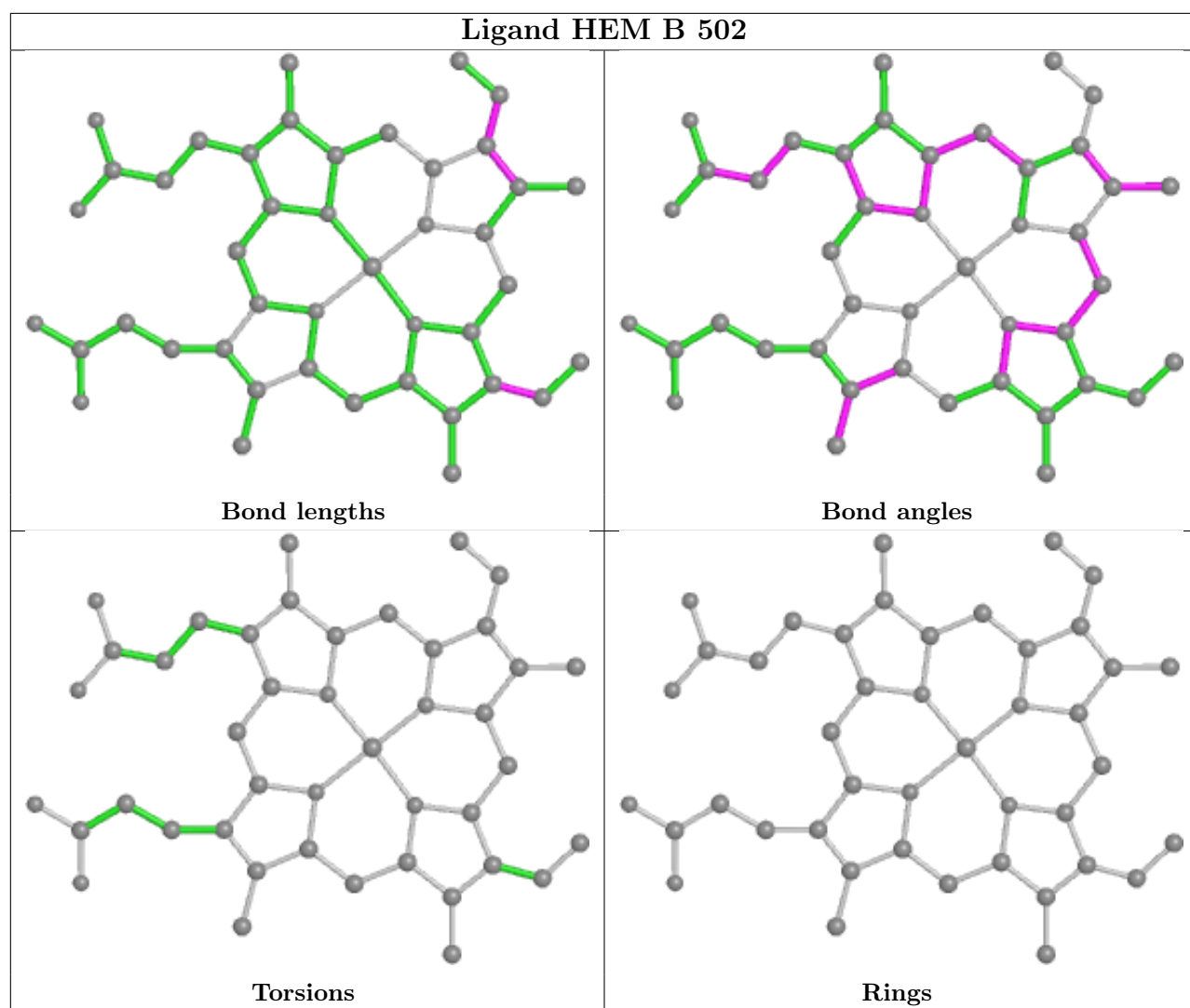
Mol	Chain	Res	Type	Atoms
8	C	302	HEC	C3A-C2A-CAA-CBA
8	F	302	HEC	C3A-C2A-CAA-CBA
6	B	504	DLX	C42-C35-C36-C37
6	B	504	DLX	C33-C34-C35-C42
6	E	504	DLX	C42-C35-C36-C37
6	E	504	DLX	C33-C34-C35-C42
6	B	504	DLX	C44-C27-C28-C29
6	E	504	DLX	C44-C27-C28-C29
7	B	506	PGV	O12-C04-C05-C06
7	B	506	PGV	C12-C13-C14-C15
6	B	504	DLX	C27-C28-C29-C30
6	E	504	DLX	C27-C28-C29-C30
7	B	506	PGV	C21-C22-C23-C24
7	B	506	PGV	C20-C21-C22-C23
6	C	301	DLX	C06-C05-C13-C14
6	F	301	DLX	C06-C05-C13-C14
6	E	504	DLX	C35-C36-C37-C38
6	B	504	DLX	C35-C36-C37-C38
6	E	503	DLX	C35-C36-C37-C38
6	B	503	DLX	C35-C36-C37-C38
7	B	505	PGV	O03-C19-C20-C21
7	E	505	PGV	O03-C19-C20-C21
7	B	505	PGV	O01-C1-C2-C3
7	E	505	PGV	O01-C1-C2-C3
6	B	504	DLX	C28-C29-C30-C31
6	E	504	DLX	C28-C29-C30-C31
7	E	505	PGV	C22-C23-C24-C25
7	B	505	PGV	C22-C23-C24-C25
7	B	505	PGV	O04-C19-C20-C21
7	E	505	PGV	O04-C19-C20-C21
6	B	504	DLX	C32-C33-C34-C35
6	E	504	DLX	C32-C33-C34-C35
8	C	302	HEC	CAA-CBA-CGA-O1A
8	F	302	HEC	CAA-CBA-CGA-O1A
6	C	301	DLX	C16-C17-C18-C19
6	F	301	DLX	C16-C17-C18-C19
7	B	505	PGV	C20-C21-C22-C23
7	E	505	PGV	C20-C21-C22-C23
8	C	302	HEC	CAA-CBA-CGA-O2A
7	B	506	PGV	O12-C04-C05-O05
8	F	302	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

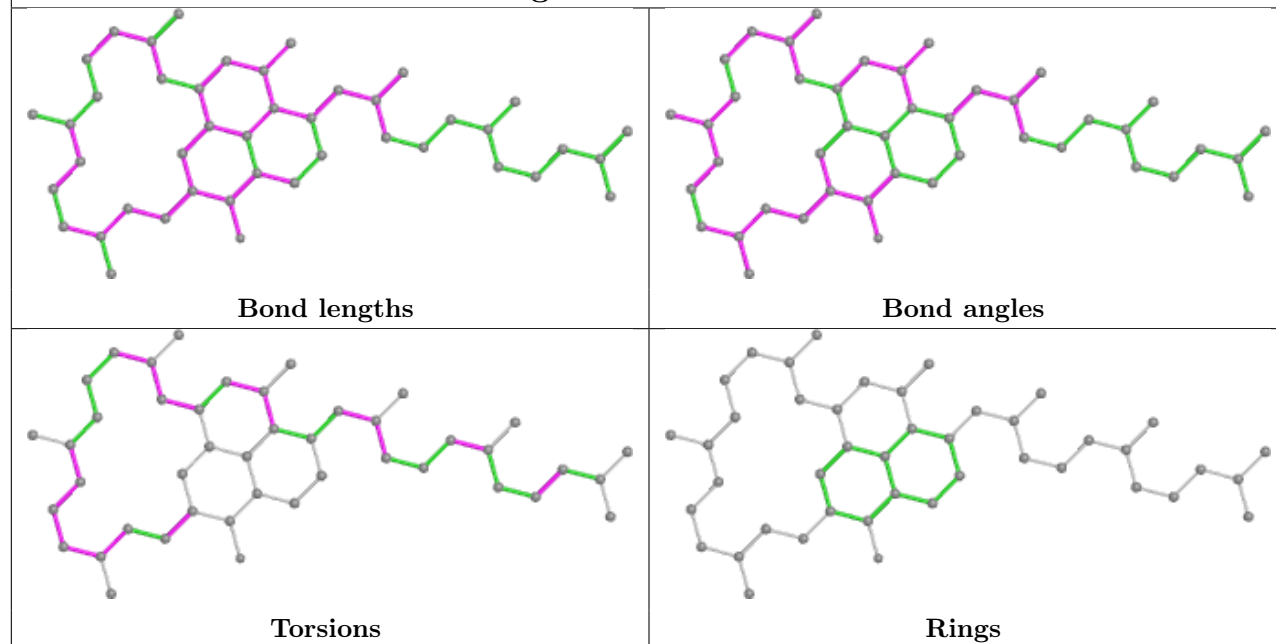
14 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	HEM	3	0
6	B	503	DLX	13	0
6	E	503	DLX	7	0
5	E	501	HEM	4	0
5	E	502	HEM	3	0
7	B	505	PGV	1	0
5	B	501	HEM	4	0
4	D	501	FES	1	0
8	C	302	HEC	9	0
6	E	504	DLX	1	0
8	F	302	HEC	8	0
7	E	505	PGV	1	0
4	A	501	FES	1	0
7	B	506	PGV	14	0

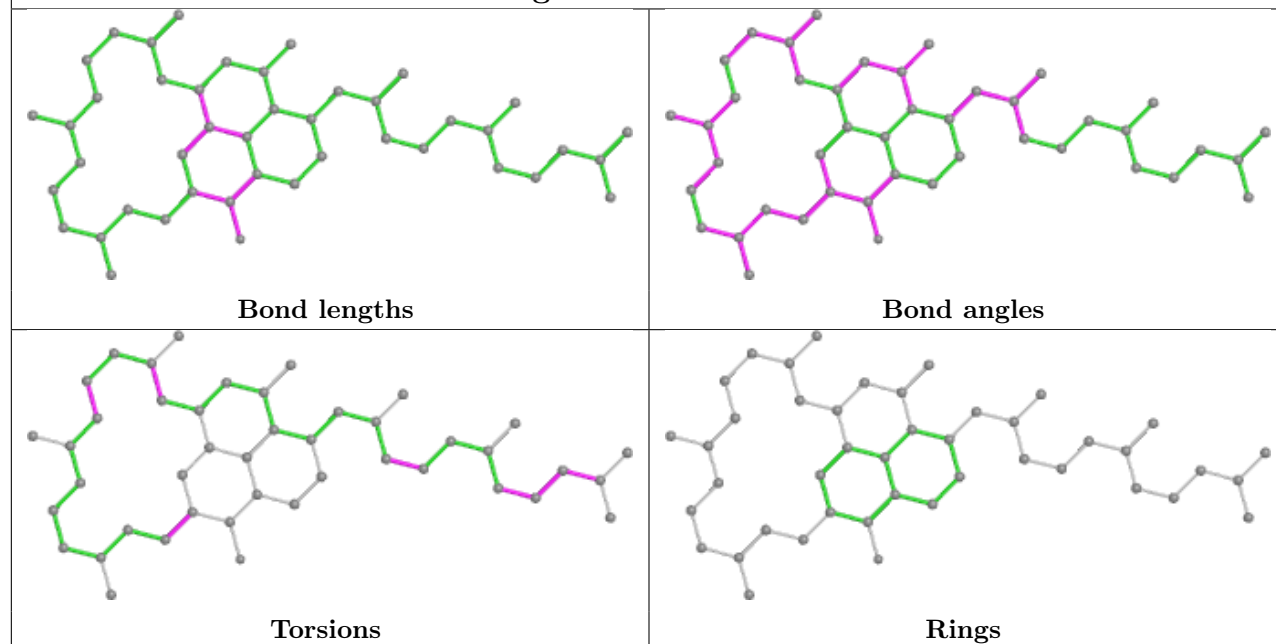
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



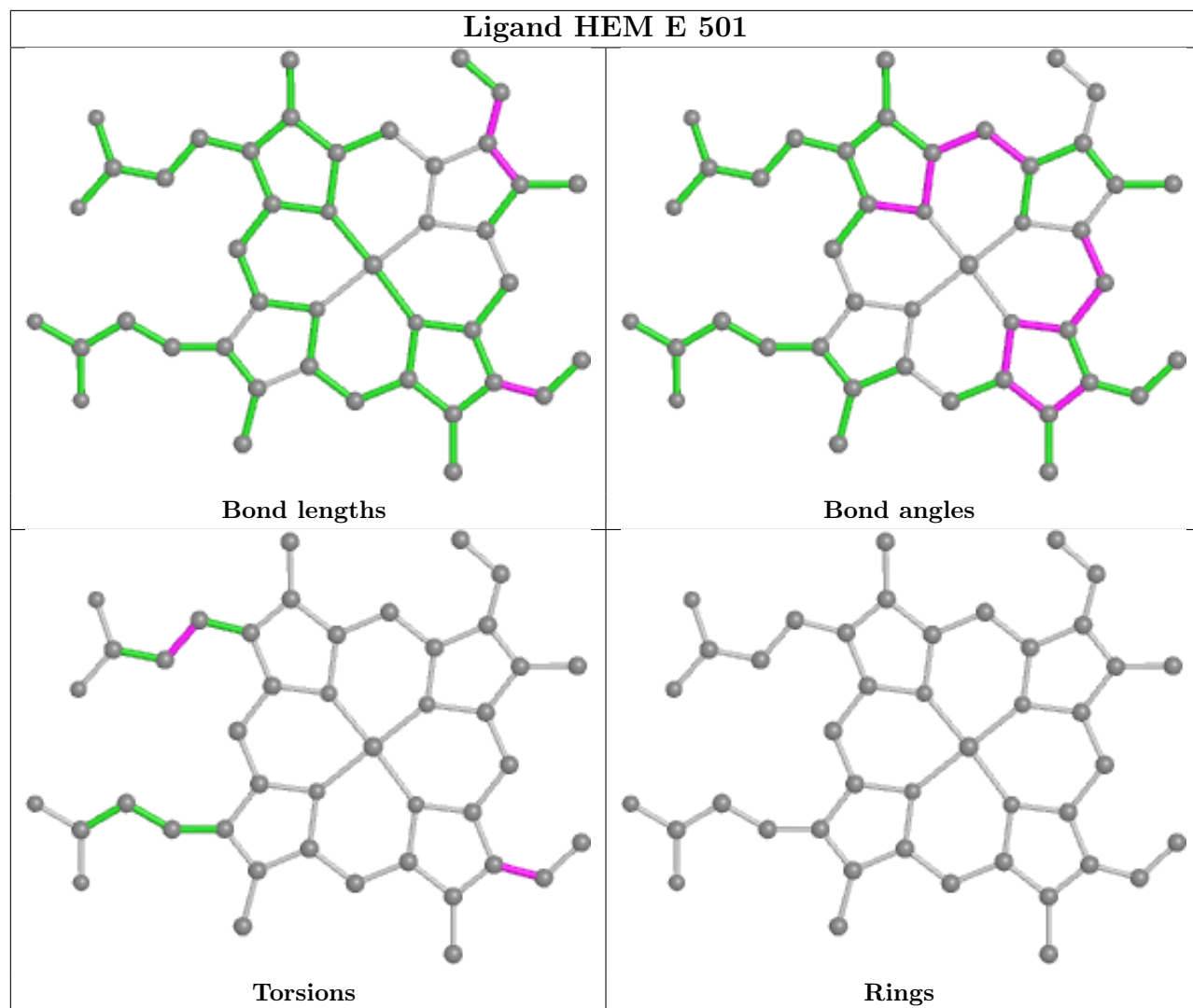
## Ligand DLX C 301

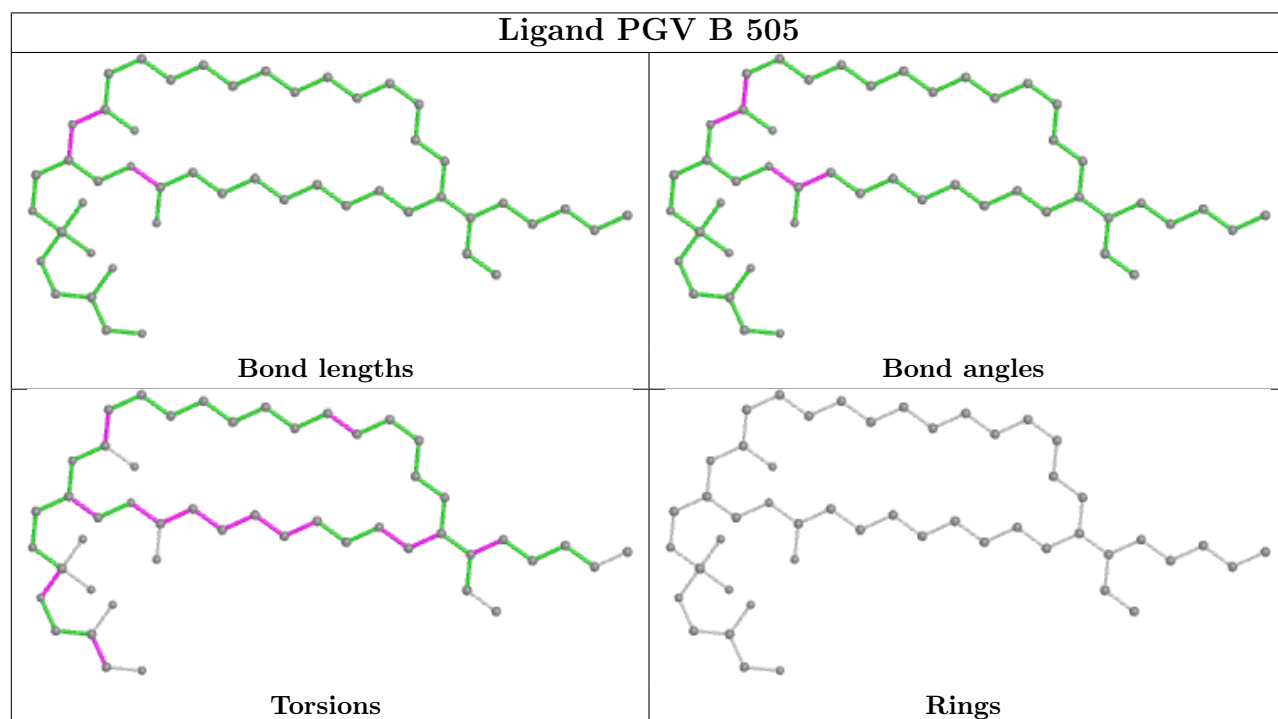
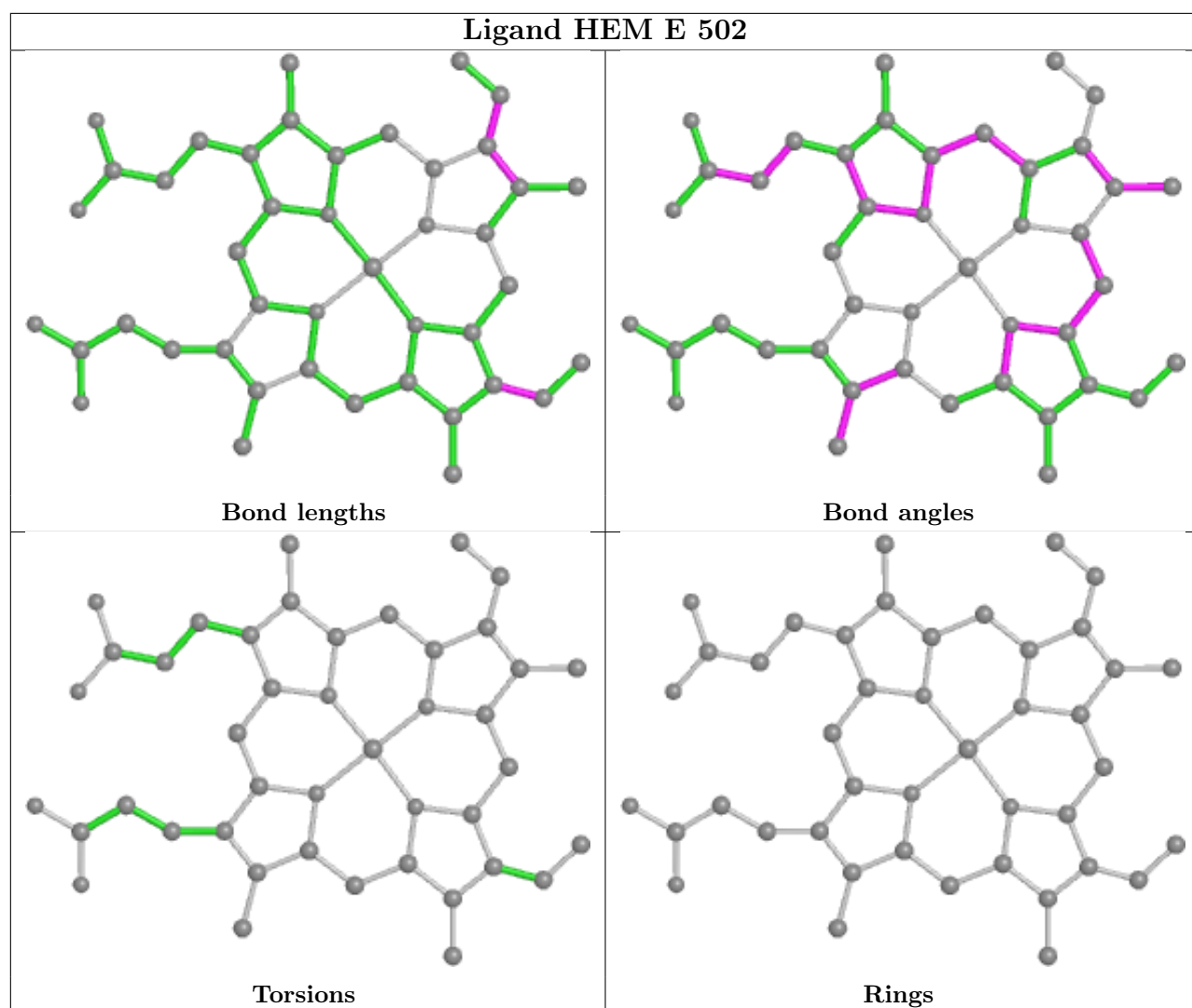


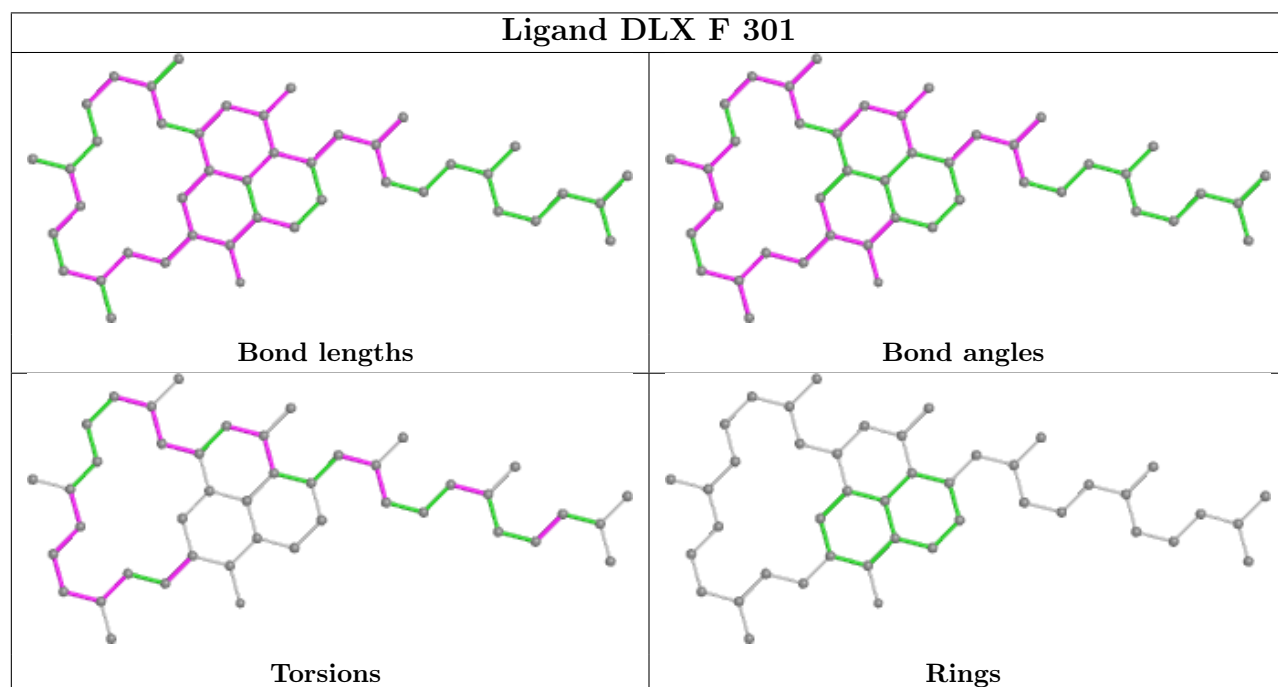
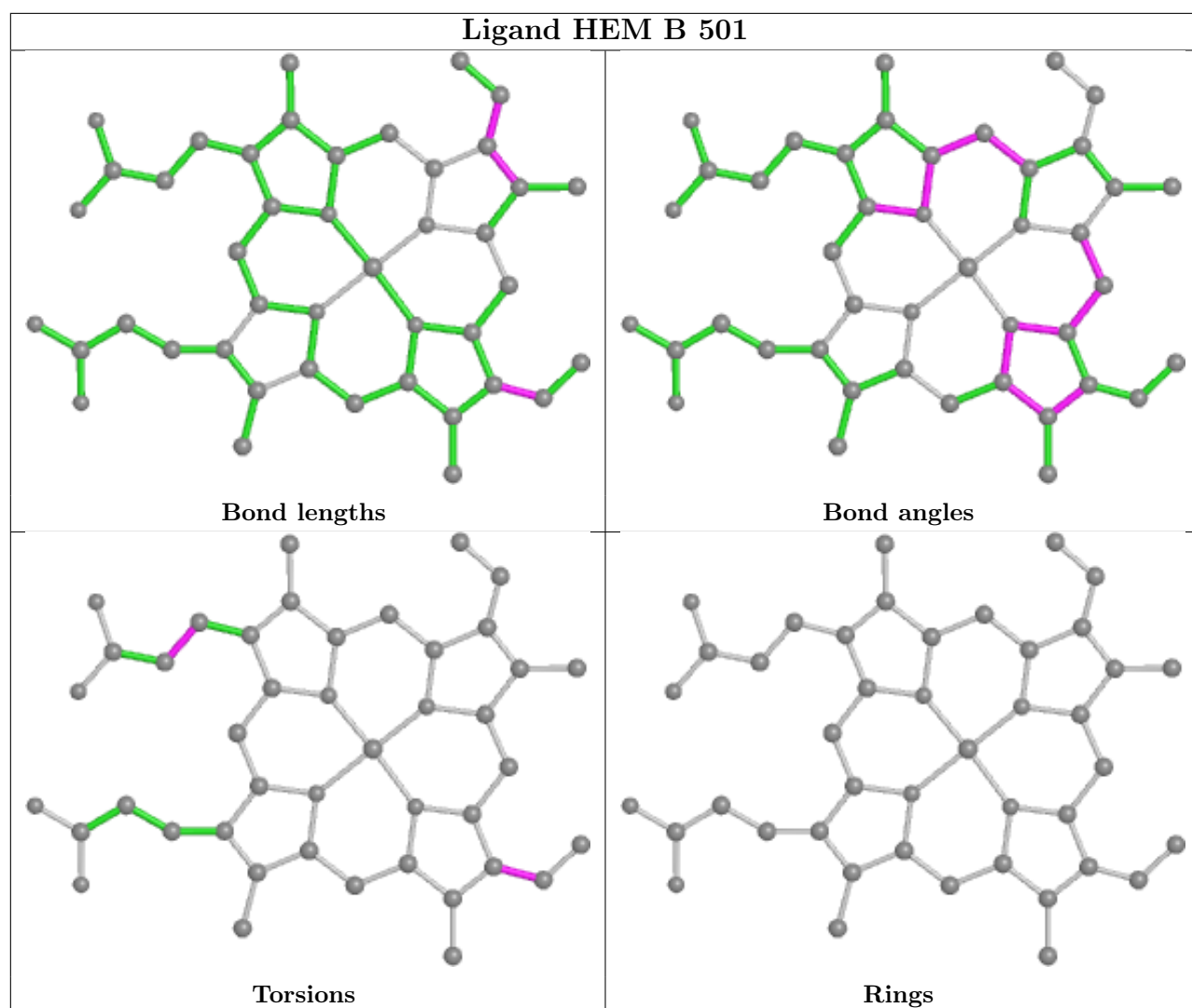
## Ligand DLX E 503

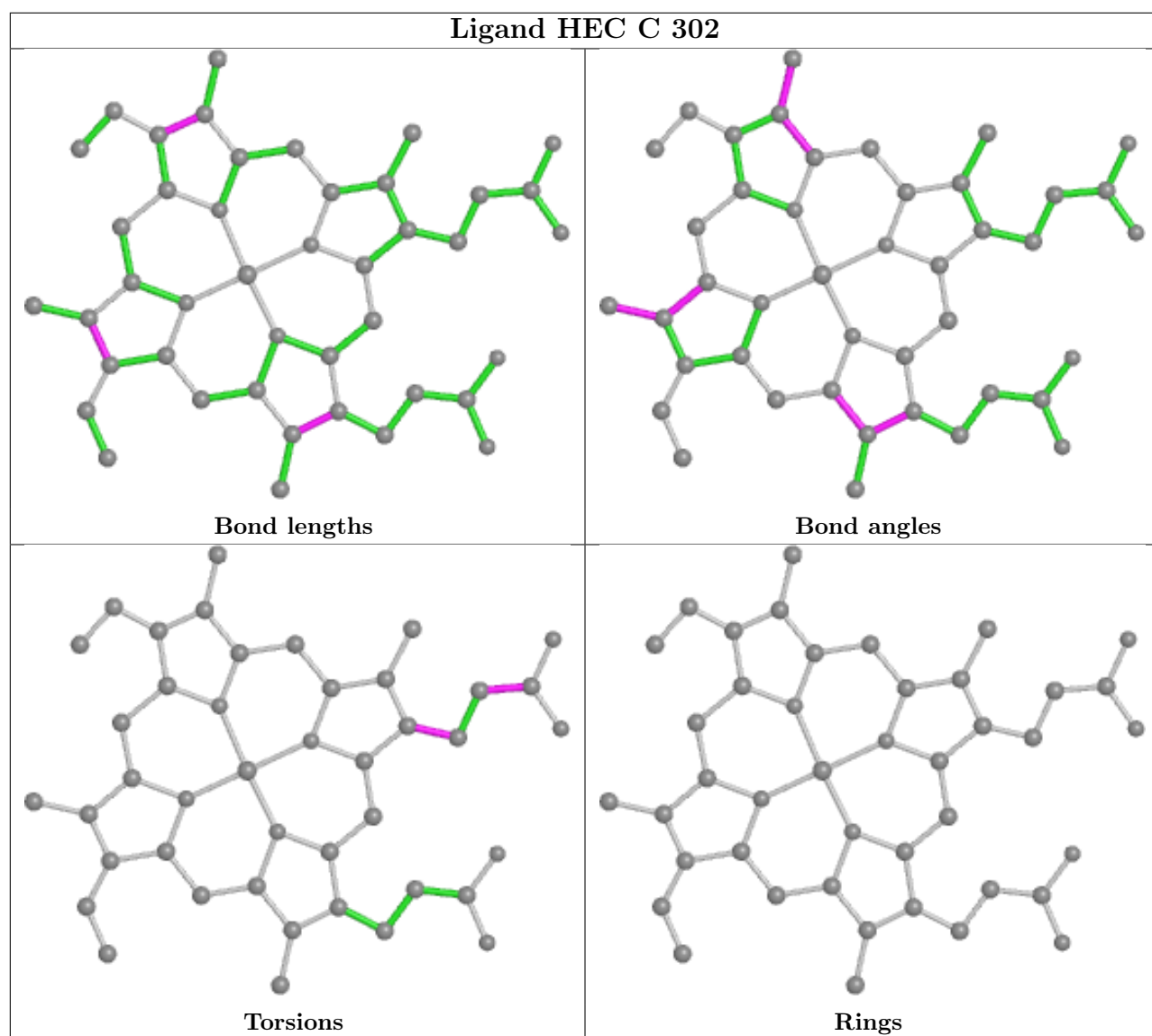


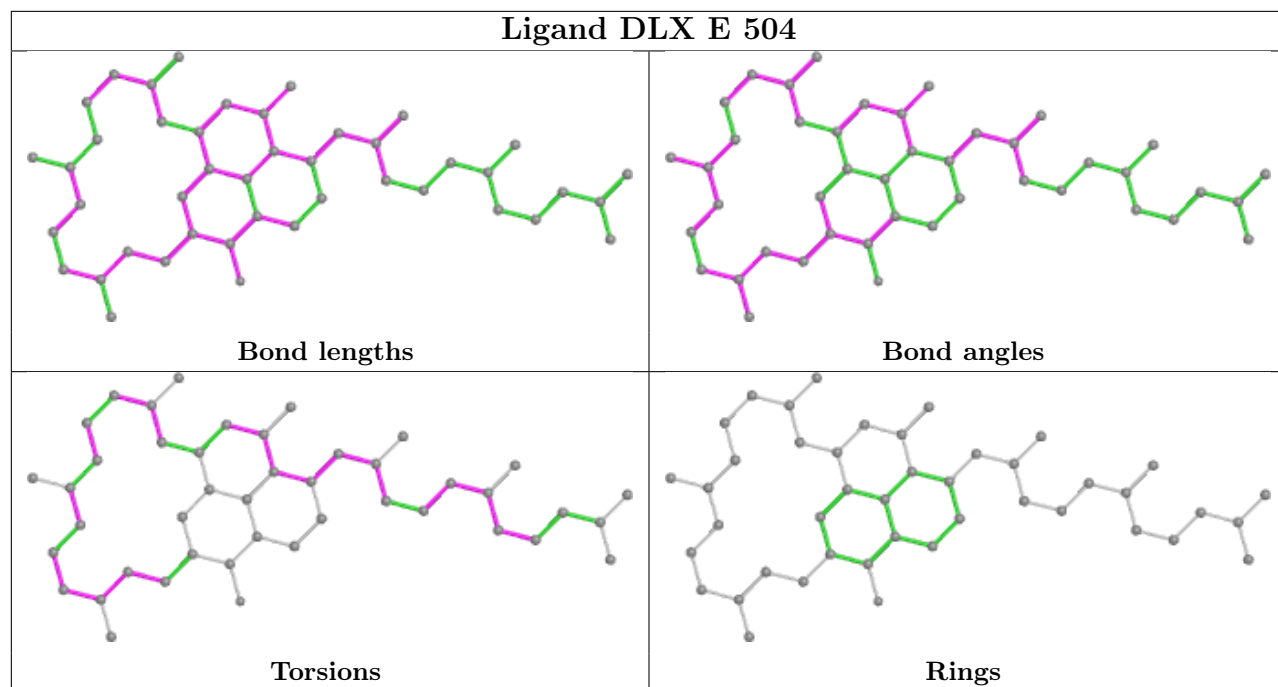




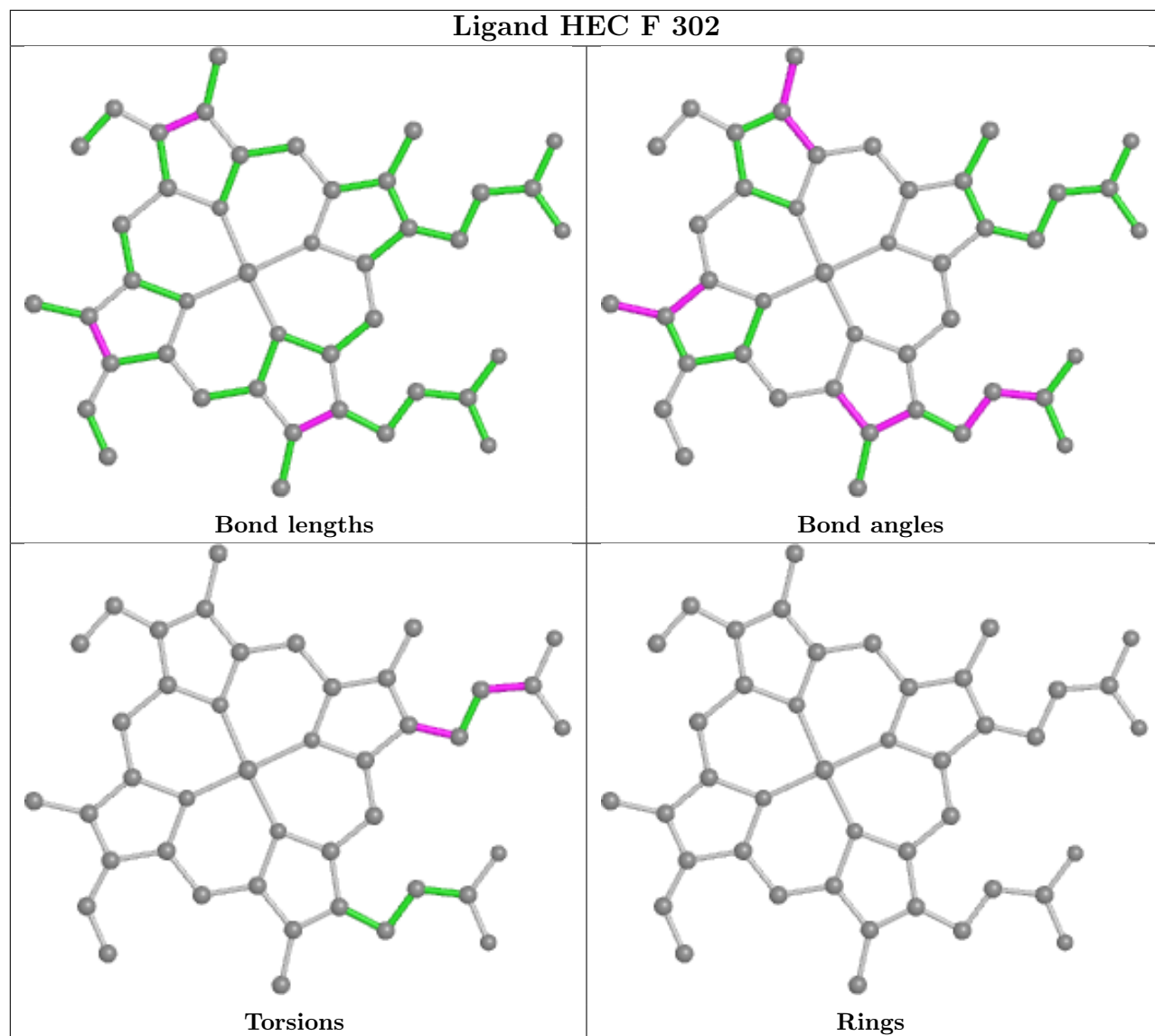


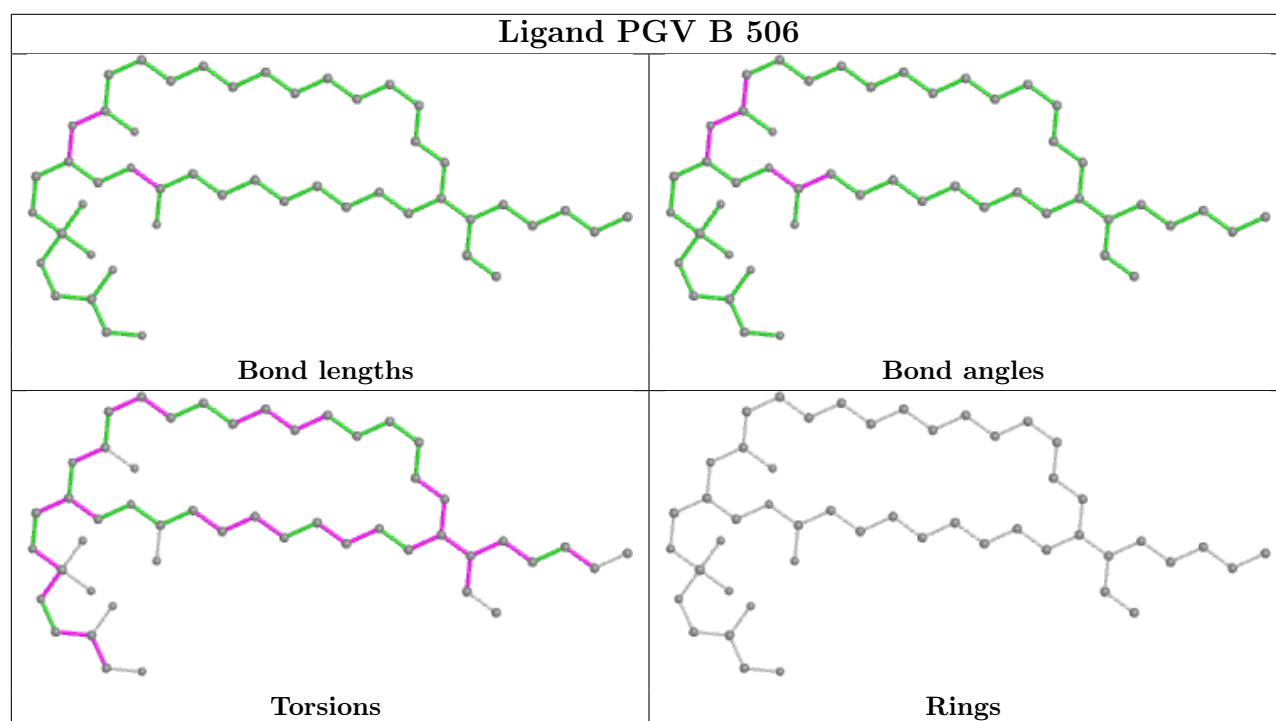
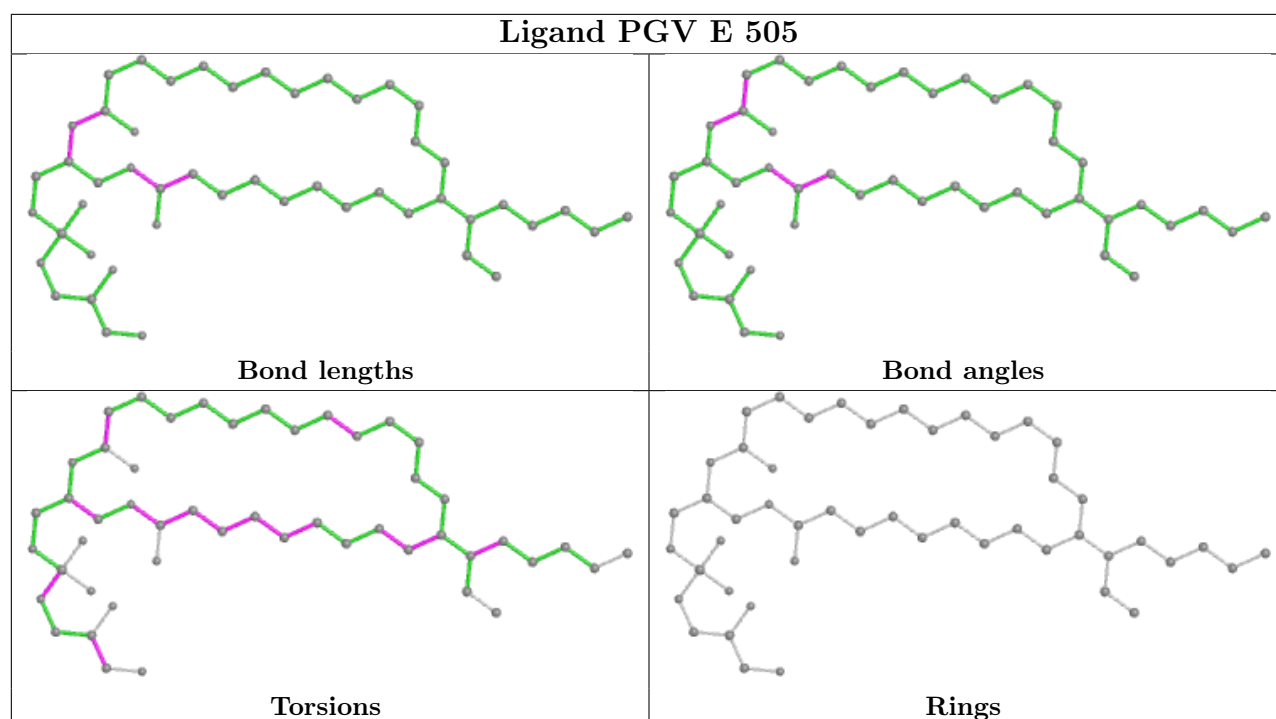


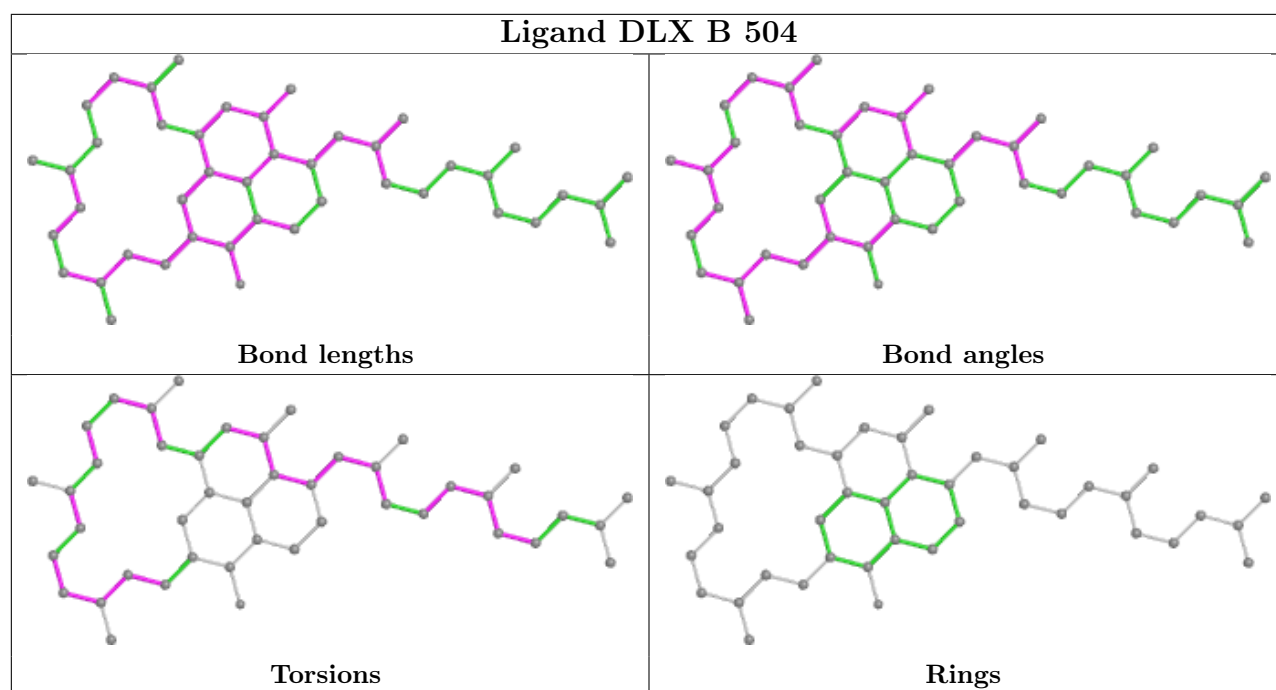




## Ligand HEC F 302







## 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.



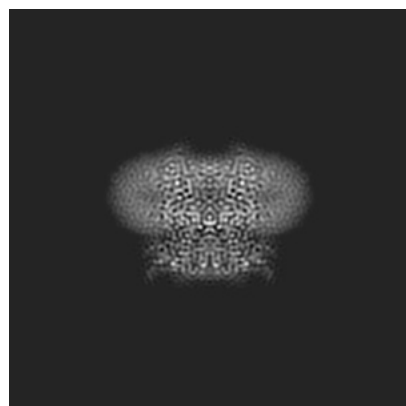
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0716. These allow visual inspection of the internal detail of the map and identification of artifacts.

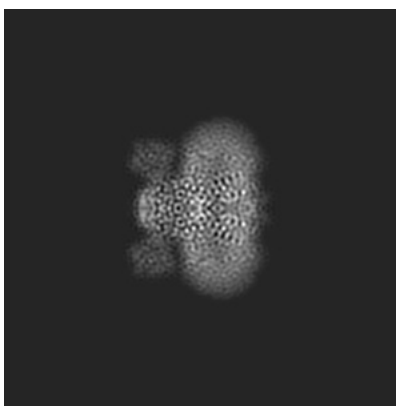
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

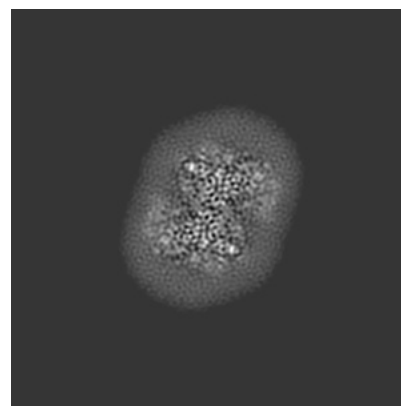
#### 6.1.1 Primary map



X

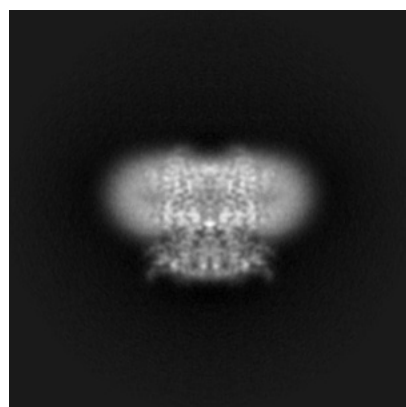


Y

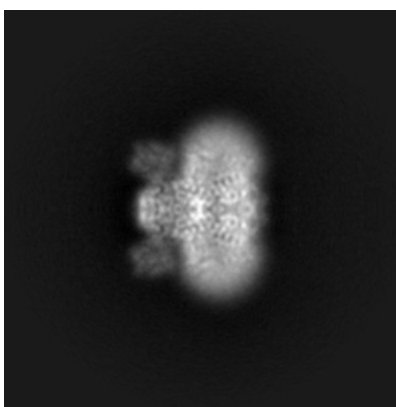


Z

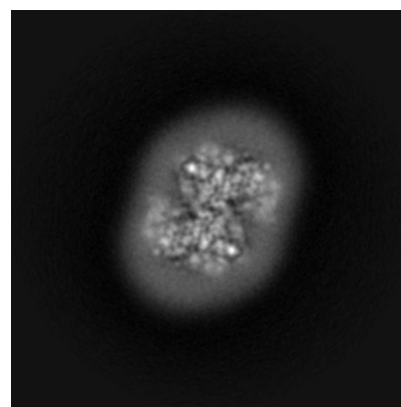
#### 6.1.2 Raw map



X



Y

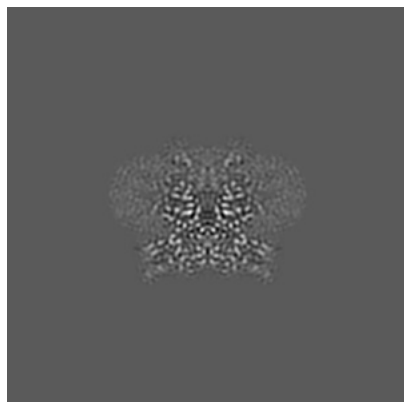


Z

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

## 6.2 Central slices [i](#)

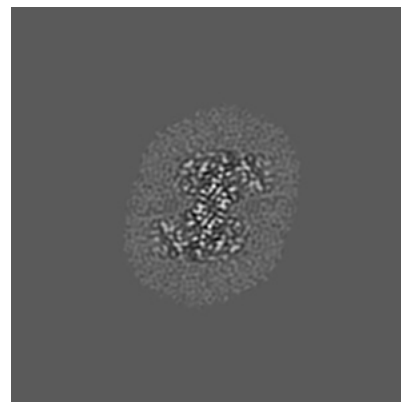
### 6.2.1 Primary map



X Index: 128

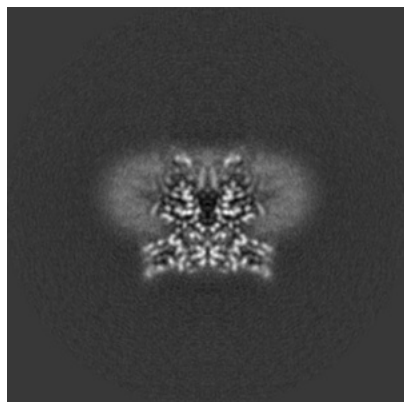


Y Index: 128

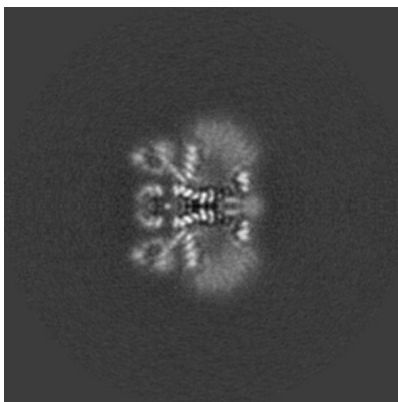


Z Index: 128

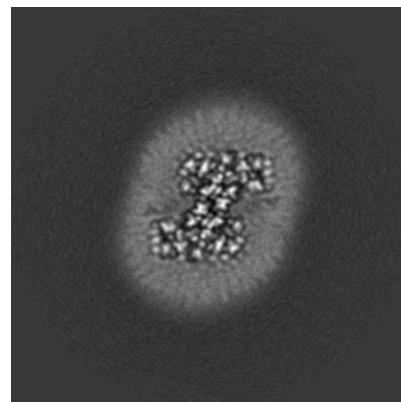
### 6.2.2 Raw map



X Index: 128



Y Index: 128

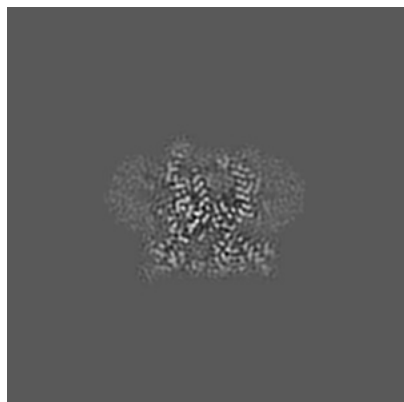


Z Index: 128

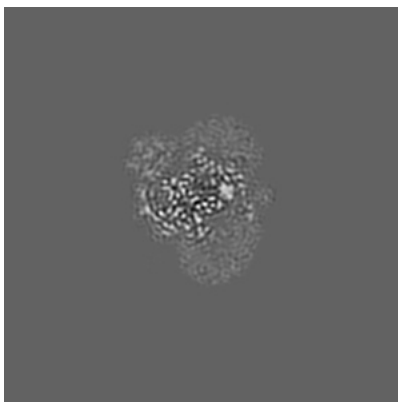
The images above show central slices of the map in three orthogonal directions.

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

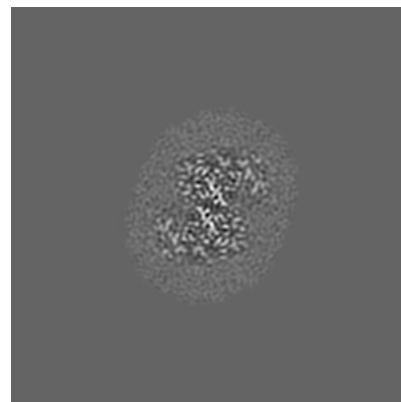
### 6.3.1 Primary map



X Index: 123

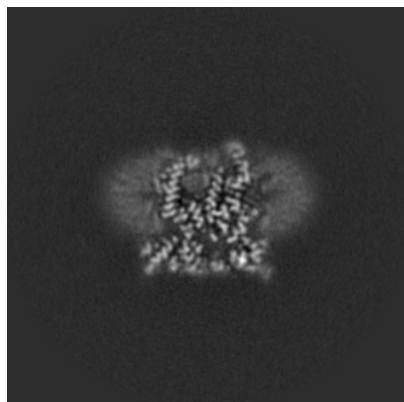


Y Index: 141

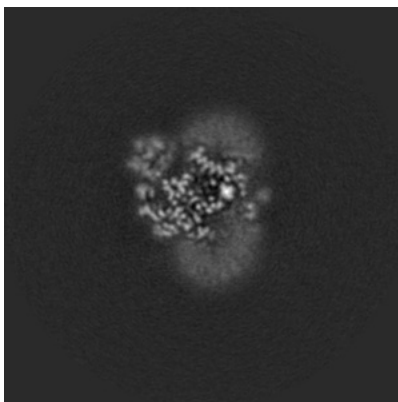


Z Index: 124

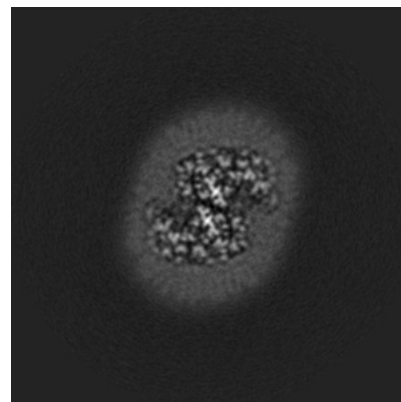
### 6.3.2 Raw map



X Index: 133



Y Index: 141

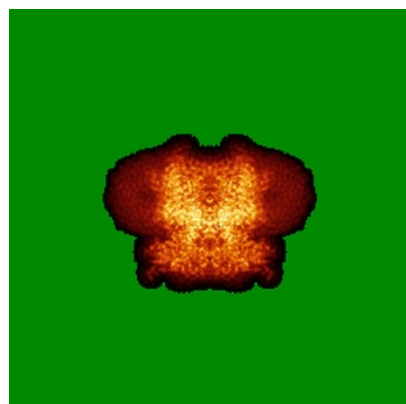


Z Index: 124

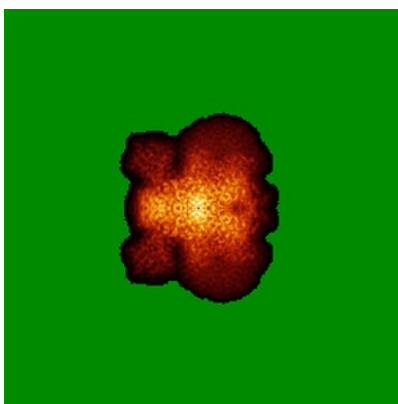
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

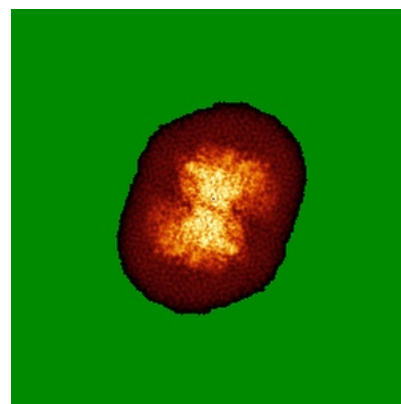
### 6.4.1 Primary map



X

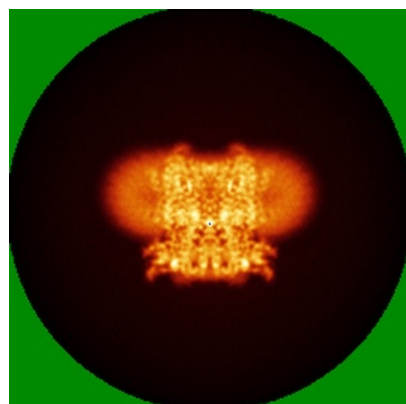


Y

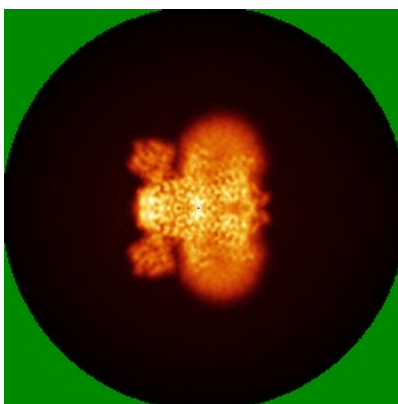


Z

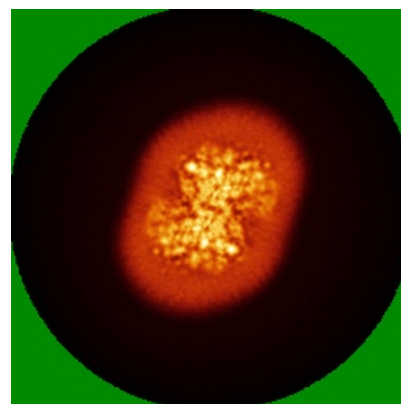
### 6.4.2 Raw map



X



Y

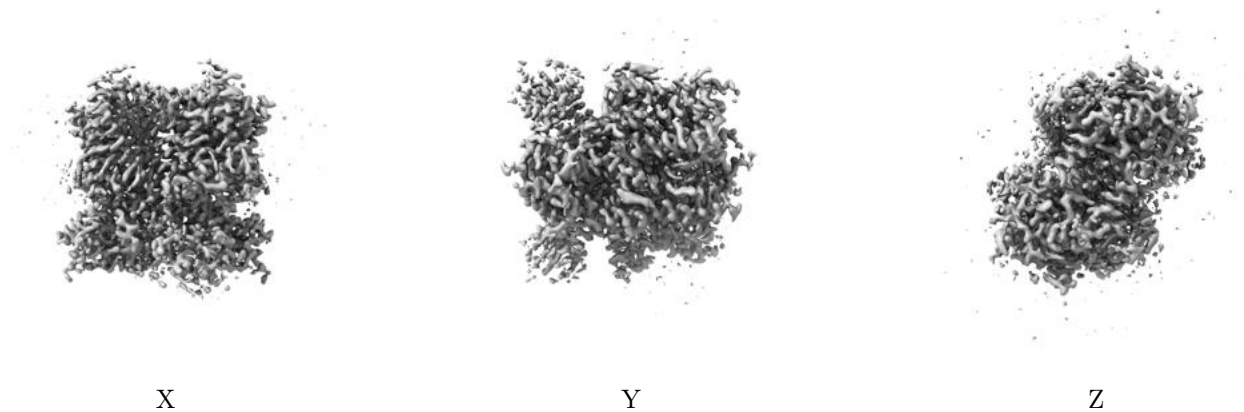


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

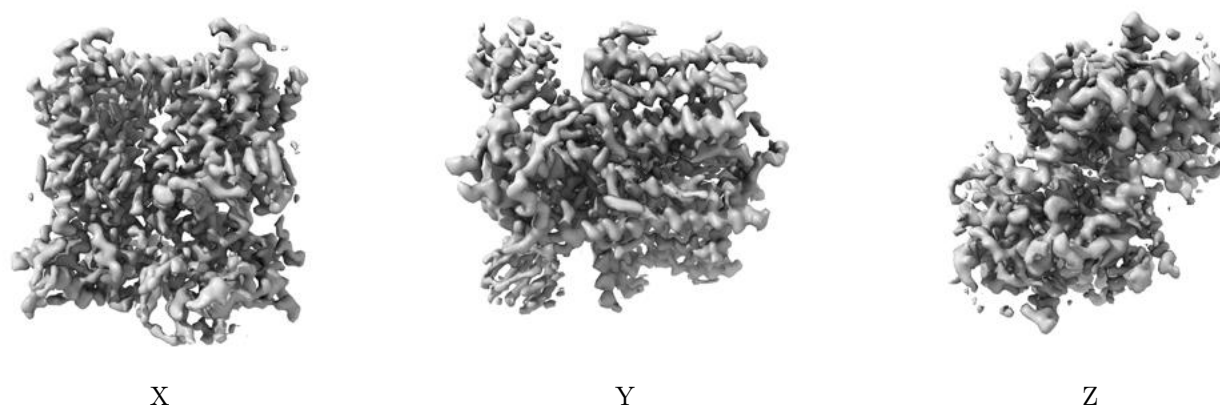
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

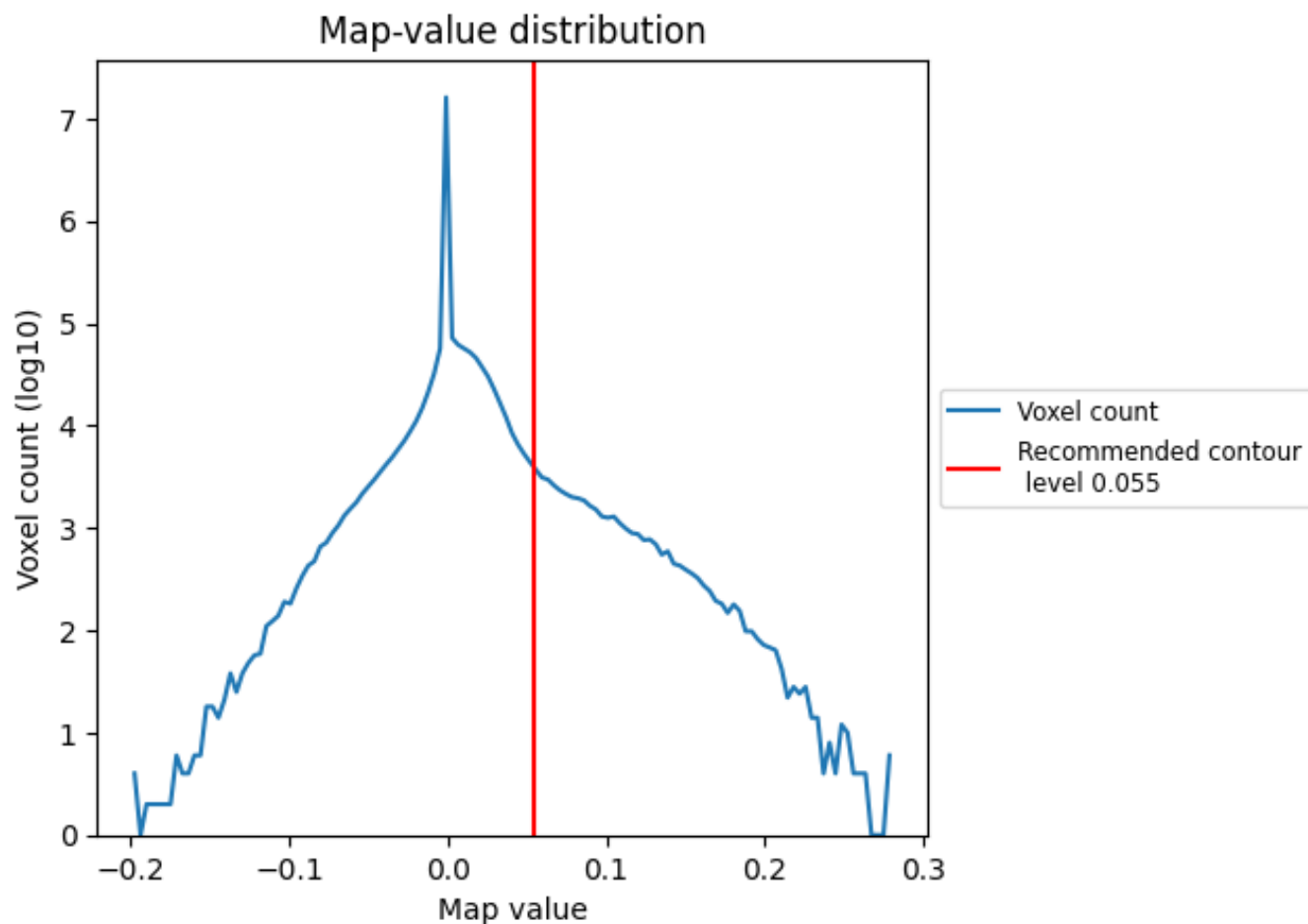
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

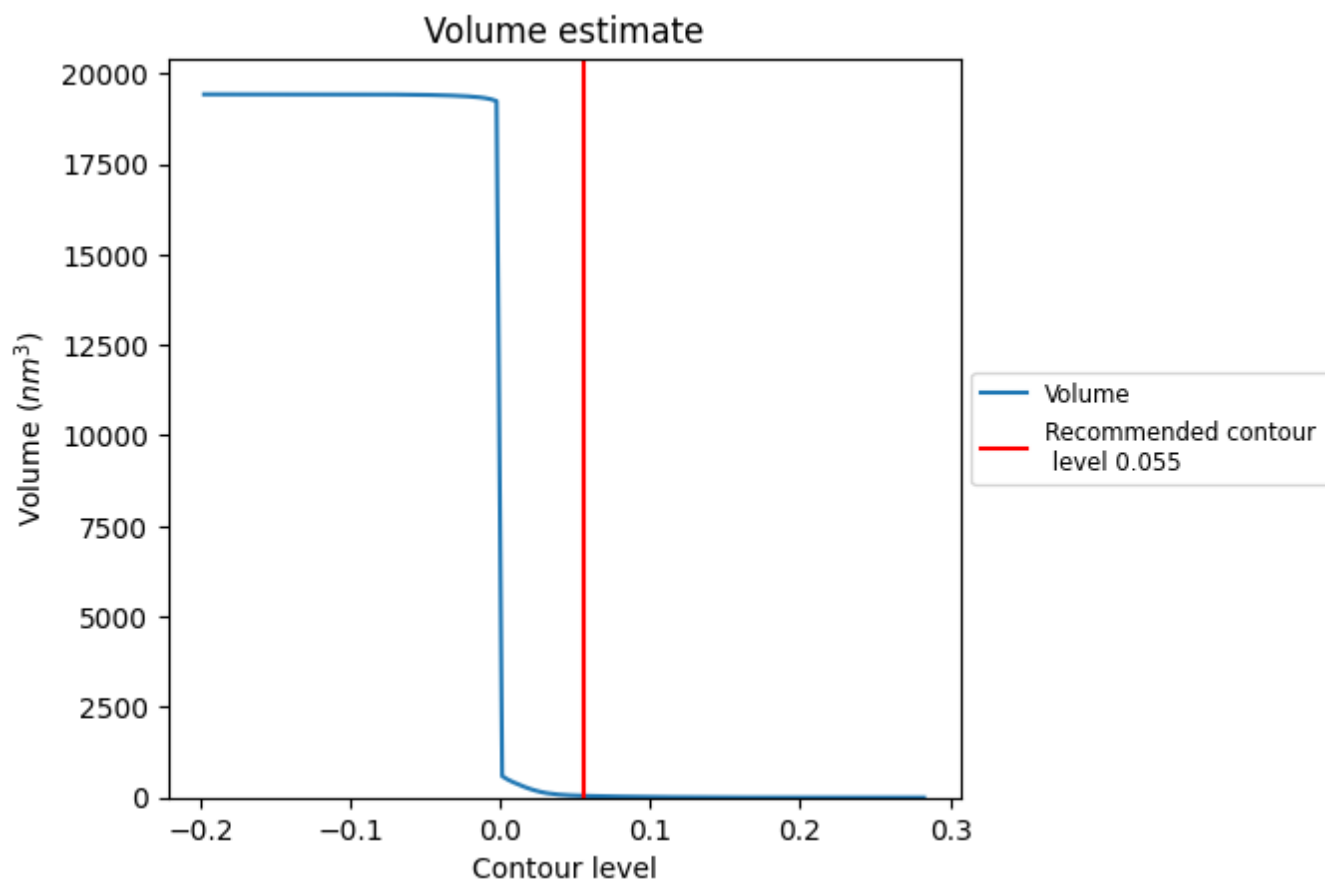
This section contains the results of statistical analysis of the map.

### 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.

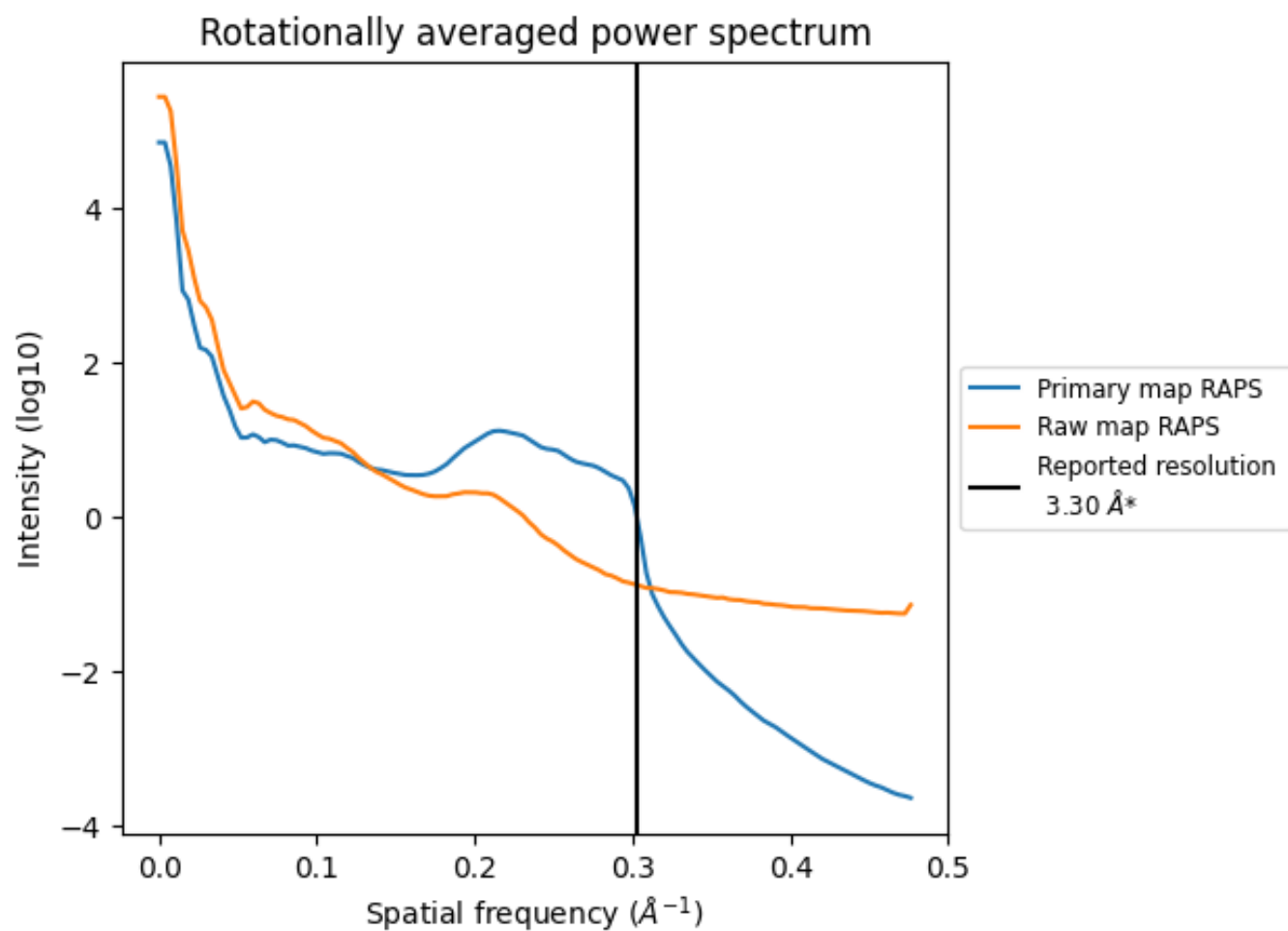
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48  $\text{nm}^3$ ; this corresponds to an approximate mass of 44 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 ⓘ



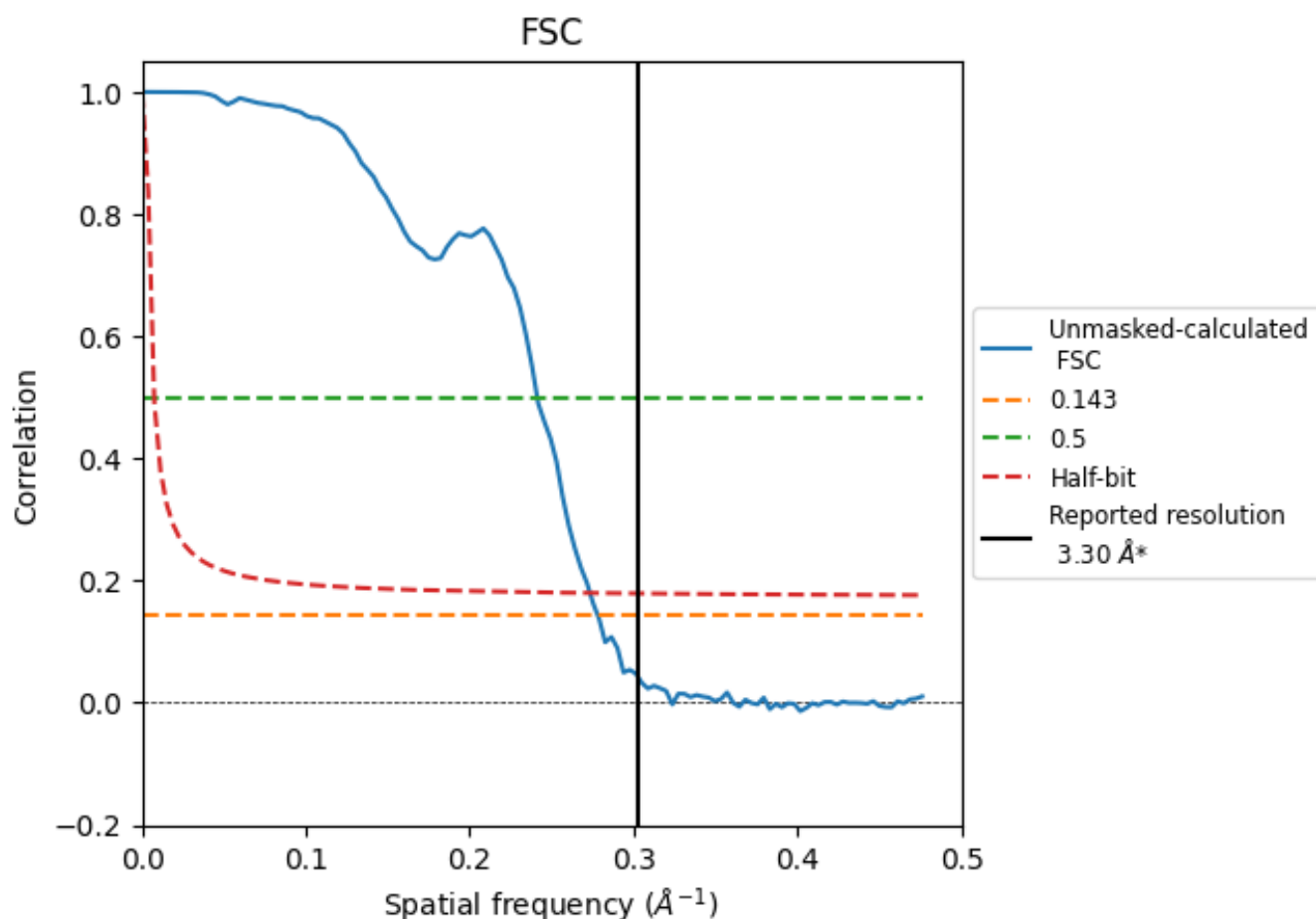
\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

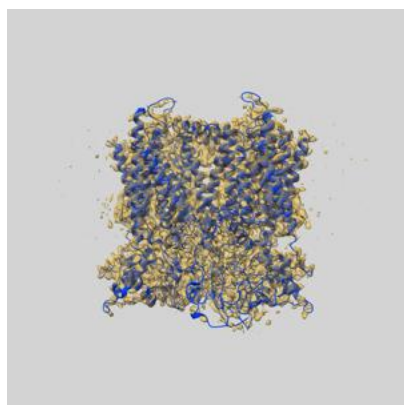
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.15	3.66

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

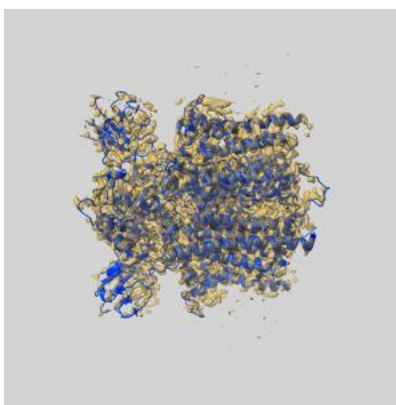
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0716 and PDB model 6KLS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

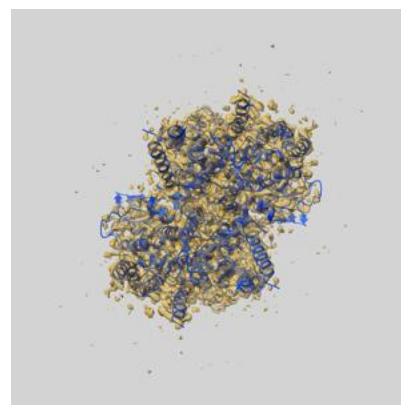
### 9.1 Map-model overlay [i](#)



X



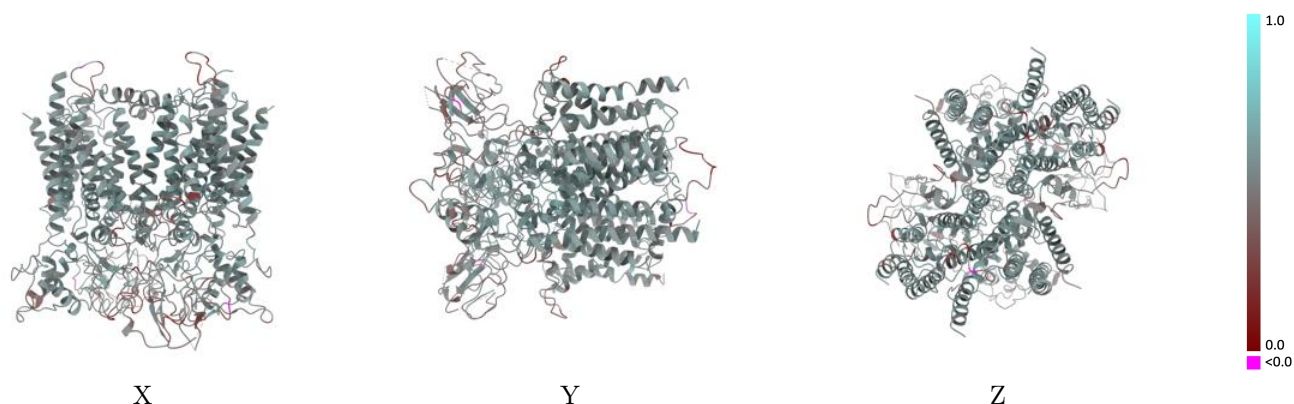
Y



Z

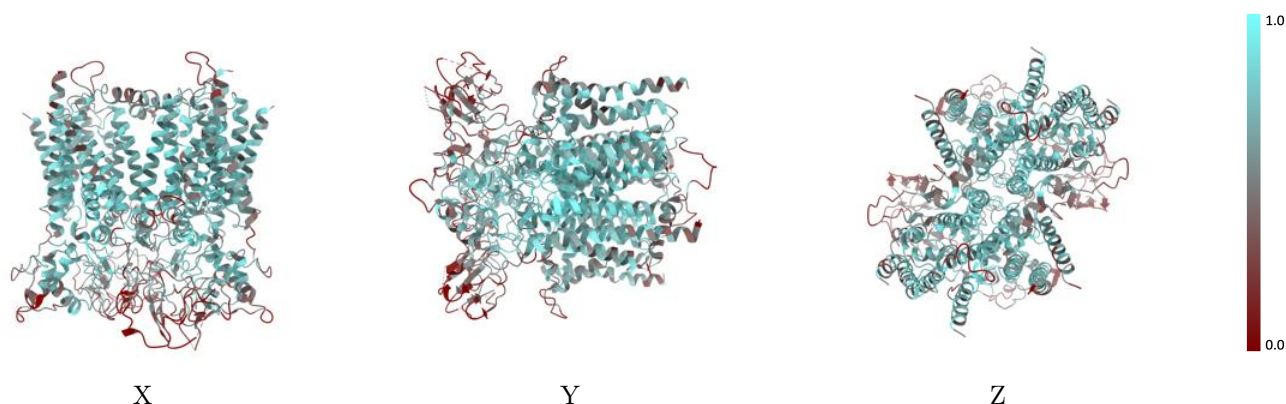
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



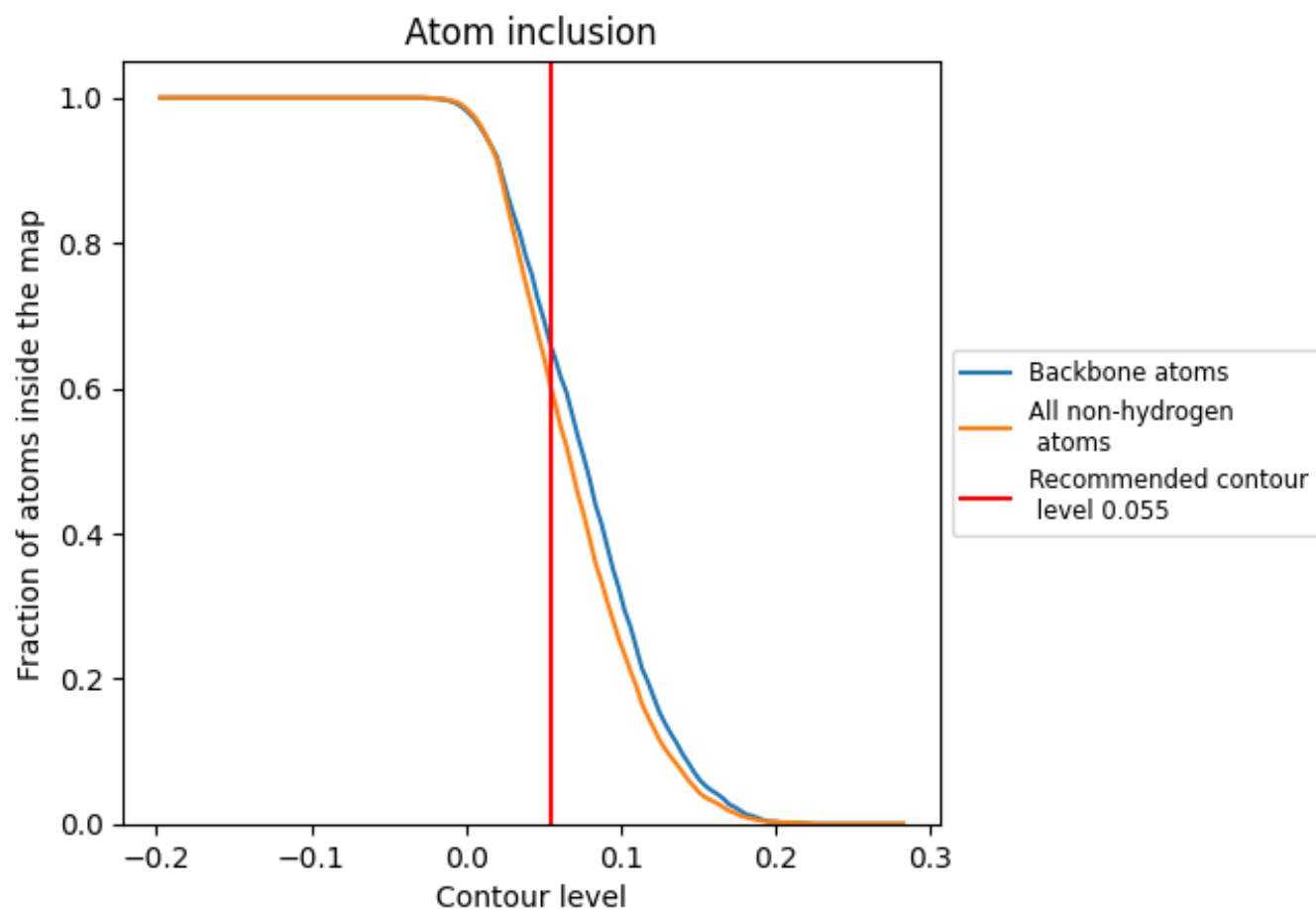
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 60% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6000	<div></div> 0.5150
A	<div></div> 0.3380	<div></div> 0.4600
B	<div></div> 0.6810	<div></div> 0.5350
C	<div></div> 0.5900	<div></div> 0.5080
D	<div></div> 0.3390	<div></div> 0.4590
E	<div></div> 0.6830	<div></div> 0.5360
F	<div></div> 0.5900	<div></div> 0.5080

1.0

0.0

<0.0