



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:46 AM EDT

PDB ID : 6BTM / pdb_00006btm
EMDB ID : EMD-7286
Title : Structure of Alternative Complex III from *Flavobacterium johnsoniae* (Wild Type)
Authors : Sun, C.; Benlekbir, S.; Venkatakrisnan, P.; Yuhang, W.; Tajkhorshid, E.; Rubinstein, J.L.; Gennis, R.B.
Deposited on : 2017-12-07
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

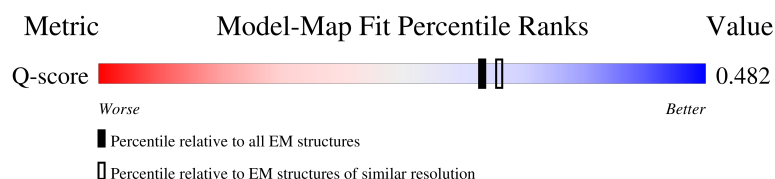
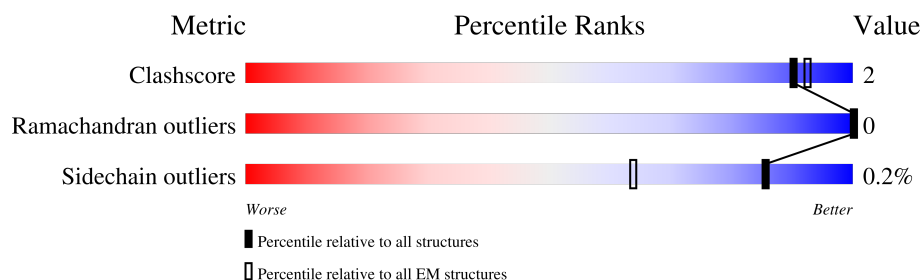
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



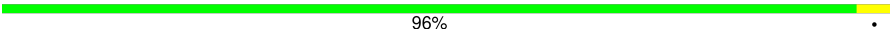
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	444	 45% 5% 50%
2	B	949	 95% 5%
3	C	466	 96% ..
4	D	174	 90% 9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	162	 96%
6	F	464	 86% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	HEC	A	1001	X	-	-	-
7	HEC	A	1002	X	-	-	-
7	HEC	A	1003	X	-	-	-
7	HEC	A	1004	X	-	-	-
7	HEC	E	201	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18934 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 Alternative Complex III subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	221	Total	C	N	O	S	0	0
			1737	1107	296	318	16		

- Molecule 2 is a protein called Alternative Complex III subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	949	Total	C	N	O	S	0	0
			7214	4523	1258	1396	37		

- Molecule 3 is a protein called Alternative Complex III subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	457	Total	C	N	O	S	0	0
			3697	2480	590	611	16		

- Molecule 4 is a protein called Alternative Complex III subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	172	Total	C	N	O	S	0	0
			1363	886	220	245	12		

- Molecule 5 is a protein called Alternative Complex III subunit E.

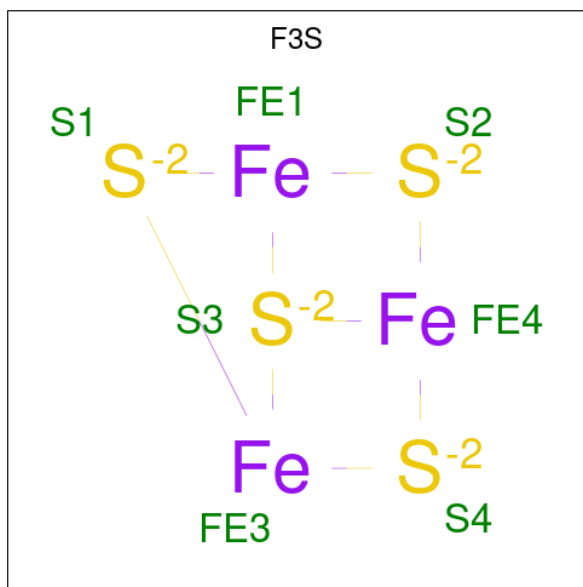
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	162	Total	C	N	O	S	0	0
			1269	804	211	249	5		

- Molecule 6 is a protein called Alternative Complex III subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	402	Total	C	N	O	S	0	0
			3300	2249	503	533	15		

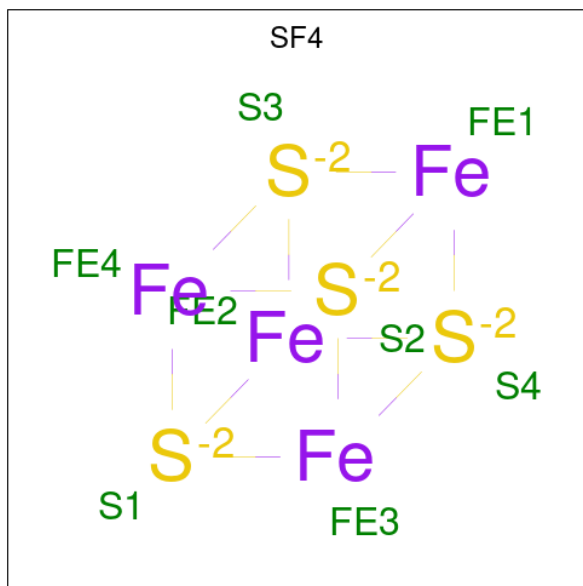
- # HEC
-
- The chemical structure shows a central iron atom (Fe) coordinated by six nitrogen atoms (N) in a hexagonal arrangement. Each nitrogen atom is part of a 1,4,7-triazacyclononane ring. The rings are substituted with ethyl groups (C2C, C3C, C4C, C1C, C2B, C3B, C4B, C1B, C2A, C3A, C4A, C1A) and methyl groups (C2D, C3D, C4D, C1D, C2E, C3E, C4E, C1E). The iron atom is also coordinated by two water molecules (H2O) in the axial positions, represented by O1D and O2A. The overall structure is highly symmetrical.

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



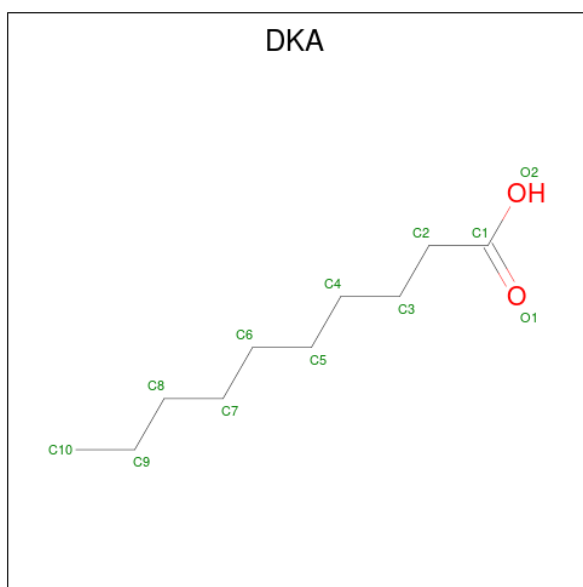
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



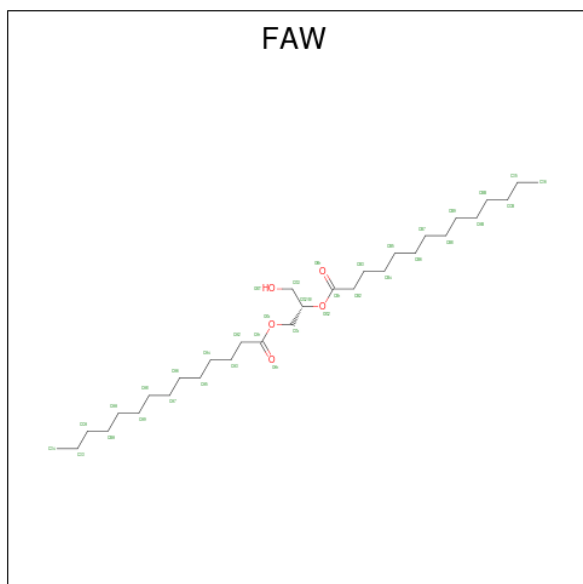
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 10 is DECANOIC ACID (CCD ID: DKA) (formula: $\text{C}_{10}\text{H}_{20}\text{O}_2$).



Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	C	O	0
			11	10	1	
10	E	1	Total	C	O	0
			8	7	1	

- Molecule 11 is (2S)-3-hydroxypropane-1,2-diyl ditetradecanoate (CCD ID: FAW) (formula: $C_{31}H_{60}O_5$).



Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			35	31	4	

Continued on next page...

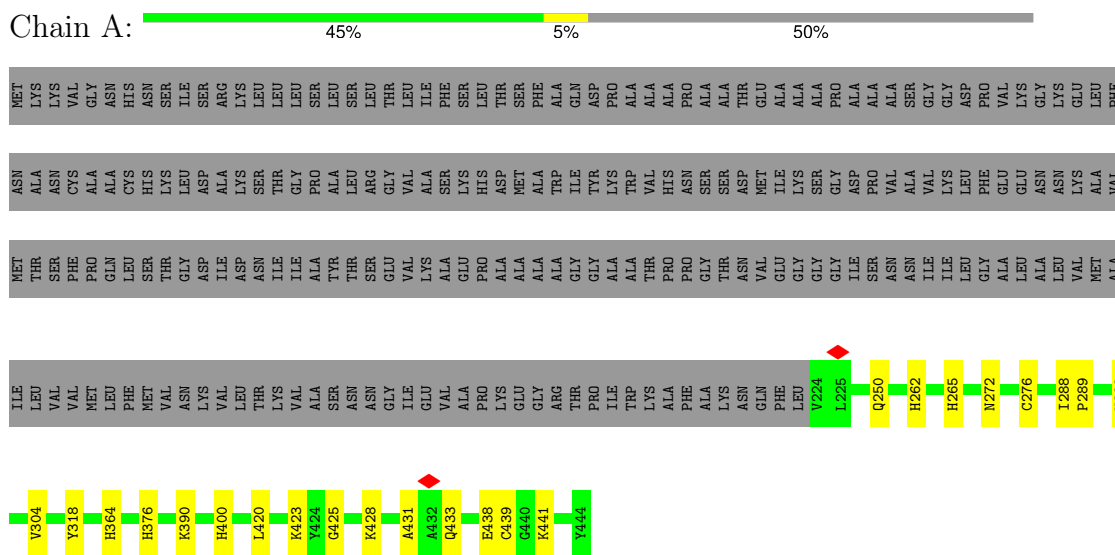
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	E	1	27	23	4	0

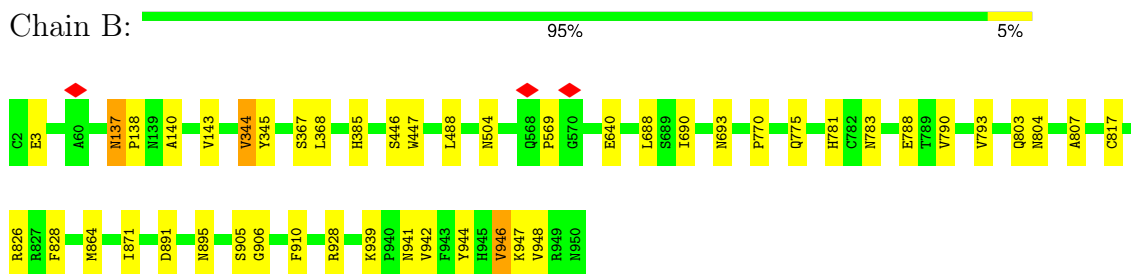
3 Residue-property plots

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.

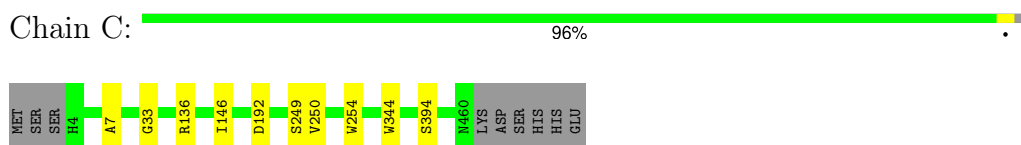
• Molecule 1: Alternative Complex III subunit A



• Molecule 2: Alternative Complex III subunit B



• Molecule 3: Alternative Complex III subunit C



• Molecule 4: Alternative Complex III subunit D

Chain D:

90%

9%



• Molecule 5: Alternative Complex III subunit E

Chain E:

96%

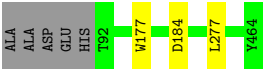


• Molecule 6: Alternative Complex III subunit F

Chain F:

86%

13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164239	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 ($e^-/\text{\AA}^2$)	61	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	5.341	Depositor
Minimum map value	-1.606	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.39	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/1782	0.55	0/2414
2	B	0.45	1/7354 (0.0%)	0.81	7/9967 (0.1%)
3	C	0.51	0/3827	0.83	8/5240 (0.2%)
4	D	0.61	0/1401	0.89	6/1904 (0.3%)
5	E	0.20	0/1300	0.56	2/1755 (0.1%)
6	F	0.49	0/3417	0.78	2/4649 (0.0%)
All	All	0.46	1/19081 (0.0%)	0.78	25/25929 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	VAL	C-O	-5.23	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	ASN	CA-C-N	6.64	126.89	119.32
2	B	137	ASN	C-N-CA	6.64	126.89	119.32
4	D	35	THR	CA-C-N	6.01	125.63	119.56
4	D	35	THR	C-N-CA	6.01	125.63	119.56
3	C	33	GLY	CA-C-N	5.83	126.32	120.14
3	C	33	GLY	C-N-CA	5.83	126.32	120.14
4	D	126	TRP	CA-C-N	5.78	126.17	119.47
4	D	126	TRP	C-N-CA	5.78	126.17	119.47
3	C	136	ARG	CA-C-N	5.45	125.12	119.56
3	C	136	ARG	C-N-CA	5.45	125.12	119.56
3	C	7	ALA	CA-C-N	5.41	125.50	119.87
3	C	7	ALA	C-N-CA	5.41	125.50	119.87
6	F	184	ASP	CA-C-N	5.16	125.61	120.04
6	F	184	ASP	C-N-CA	5.16	125.61	120.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	146	ILE	CA-C-N	5.15	125.44	119.93
3	C	146	ILE	C-N-CA	5.15	125.44	119.93
5	E	57	SER	CA-C-N	5.13	131.34	121.54
5	E	57	SER	C-N-CA	5.13	131.34	121.54
2	B	344	VAL	CA-C-N	5.06	131.20	121.54
2	B	344	VAL	C-N-CA	5.06	131.20	121.54
2	B	140	ALA	N-CA-C	5.02	117.42	109.24
4	D	49	ALA	CA-C-N	5.02	124.95	119.78
4	D	49	ALA	C-N-CA	5.02	124.95	119.78
2	B	504	ASN	CA-C-N	5.01	124.67	119.56
2	B	504	ASN	C-N-CA	5.01	124.67	119.56

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	1737	0	1668	17	0
2	B	7214	0	7067	26	0
3	C	3697	0	3683	4	0
4	D	1363	0	1330	11	0
5	E	1269	0	1196	7	0
6	F	3300	0	3298	2	0
7	A	215	0	150	8	0
7	E	43	0	30	0	0
8	B	7	0	0	0	0
9	B	8	0	0	0	0
10	B	11	0	19	1	0
10	E	8	0	10	1	0
11	B	35	0	0	0	0
11	E	27	0	0	0	0
All	All	18934	0	18451	63	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 2.

All (63) 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)
4:D:57:ALA:O	4:D:60:TYR:N	2.22	0.72
3:C:192:ASP:OD2	4:D:139:THR:HG21	1.94	0.67
4:D:138:THR:HA	4:D:141:ASP:O	1.99	0.63
2:B:817:CYS:SG	2:B:826:ARG:NH1	2.74	0.61
1:A:364:HIS:HD1	7:A:1002:HEC:HBB2	1.65	0.60
4:D:57:ALA:O	4:D:58:PHE:C	2.44	0.60
1:A:262:HIS:HE1	7:A:1001:HEC:NA	2.00	0.59
2:B:788:GLU:OE2	2:B:804:ASN:ND2	2.33	0.59
1:A:272:ASN:HD22	5:E:88:ILE:HA	1.69	0.57
1:A:265:HIS:CD2	7:A:1000:HEC:NB	2.73	0.56
1:A:298:HIS:CD2	7:A:1000:HEC:NC	2.73	0.56
10:B:1103:DKA:H21	5:E:10:TYR:HB3	1.88	0.55
4:D:36:PRO:HB3	4:D:139:THR:O	2.05	0.55
1:A:438:GLU:OE1	1:A:441:LYS:NZ	2.40	0.54
2:B:828:PHE:HB2	2:B:864:MET:HE2	1.90	0.54
2:B:803:GLN:HG2	2:B:871:ILE:HD11	1.90	0.54
2:B:688:LEU:HB3	2:B:942:VAL:HG22	1.89	0.54
1:A:420:LEU:HA	1:A:423:LYS:HB2	1.89	0.53
1:A:250:GLN:HE21	1:A:390:LYS:HB3	1.74	0.52
1:A:376:HIS:CE1	7:A:1002:HEC:NA	2.79	0.51
4:D:137:ARG:O	4:D:141:ASP:O	2.30	0.49
2:B:946:VAL:HG12	2:B:948:VAL:HG22	1.94	0.49
3:C:254:TRP:NE1	3:C:394:SER:OG	2.46	0.49
3:C:344:TRP:CD1	3:C:344:TRP:H	2.30	0.49
3:C:249:SER:OG	3:C:250:VAL:N	2.44	0.49
2:B:775:GLN:HE21	2:B:944:TYR:HE2	1.60	0.48
1:A:439:CYS:HB3	2:B:807:ALA:HB2	1.95	0.48
5:E:146:ALA:HA	5:E:149:ARG:HE	1.78	0.48
6:F:177:TRP:CD1	6:F:177:TRP:H	2.31	0.48
4:D:141:ASP:HB3	4:D:142:HIS:HD2	1.78	0.48
6:F:277:LEU:HG	6:F:277:LEU:O	2.14	0.48
1:A:304:VAL:HG12	7:A:1000:HEC:HAA2	1.96	0.47
1:A:420:LEU:O	1:A:425:GLY:N	2.46	0.47
4:D:57:ALA:O	4:D:59:LEU:N	2.47	0.47
2:B:928:ARG:NH2	2:B:946:VAL:O	2.48	0.46
2:B:640:GLU:HG2	2:B:947:LYS:HB3	1.97	0.46
1:A:276:CYS:HB3	1:A:289:PRO:HG3	1.98	0.46
2:B:783:ASN:HB2	2:B:939:LYS:HB2	1.98	0.45
5:E:31:PHE:HE2	5:E:36:GLU:HG3	1.82	0.45
1:A:304:VAL:HG11	1:A:318:TYR:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:891:ASP:O	2:B:895:ASN:ND2	2.50	0.45
1:A:400:HIS:HB3	1:A:431:ALA:HB2	1.99	0.44
1:A:428:LYS:HD2	1:A:433:GLN:HB3	1.99	0.44
4:D:53:LEU:HD23	4:D:53:LEU:HA	1.65	0.44
2:B:367:SER:OG	2:B:368:LEU:N	2.51	0.43
1:A:288:ILE:HD12	7:A:1001:HEC:HAD2	2.00	0.43
2:B:3:GLU:HA	5:E:10:TYR:HD1	1.83	0.43
2:B:693:ASN:HD21	2:B:948:VAL:HG23	1.84	0.42
2:B:385:HIS:O	2:B:385:HIS:CD2	2.72	0.42
2:B:446:SER:OG	2:B:447:TRP:N	2.52	0.42
2:B:488:LEU:C	2:B:488:LEU:HD12	2.45	0.42
2:B:137:ASN:HA	2:B:138:PRO:HD2	1.74	0.42
2:B:688:LEU:HD23	2:B:910:PHE:HD1	1.85	0.41
4:D:139:THR:OG1	4:D:140:ASP:N	2.53	0.41
2:B:569:PRO:HB3	2:B:770:PRO:HD2	2.01	0.41
2:B:3:GLU:HA	5:E:10:TYR:CD1	2.55	0.41
4:D:36:PRO:CB	4:D:139:THR:O	2.69	0.41
2:B:905:SER:OG	2:B:906:GLY:N	2.53	0.41
7:A:1002:HEC:HHC	7:A:1002:HEC:HBB3	2.03	0.41
2:B:344:VAL:O	2:B:345:TYR:HB3	2.20	0.41
2:B:690:ILE:HD13	2:B:944:TYR:HE1	1.85	0.41
2:B:781:HIS:O	2:B:941:ASN:ND2	2.53	0.41
5:E:10:TYR:HE2	10:E:202:DKA:H32	1.87	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	219/444 (49%)	199 (91%)	20 (9%)	0	100	100
2	B	947/949 (100%)	864 (91%)	83 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	455/466 (98%)	436 (96%)	19 (4%)	0	100	100
4	D	170/174 (98%)	158 (93%)	12 (7%)	0	100	100
5	E	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
6	F	398/464 (86%)	379 (95%)	19 (5%)	0	100	100
All	All	2349/2659 (88%)	2178 (93%)	171 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	185/359 (52%)	185 (100%)	0	100	100
2	B	769/772 (100%)	766 (100%)	3 (0%)	84	83
3	C	391/402 (97%)	391 (100%)	0	100	100
4	D	148/151 (98%)	148 (100%)	0	100	100
5	E	131/134 (98%)	131 (100%)	0	100	100
6	F	351/392 (90%)	351 (100%)	0	100	100
All	All	1975/2210 (89%)	1972 (100%)	3 (0%)	85	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	790	VAL
2	B	793	VAL
2	B	946	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	GLN
1	A	343	GLN
1	A	352	ASN
1	A	417	HIS
2	B	242	GLN
2	B	571	GLN
2	B	781	HIS
2	B	801	GLN
2	B	803	GLN
2	B	895	ASN
3	C	336	ASN
4	D	95	ASN
4	D	142	HIS
6	F	94	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEC	E	201	5	50,50,50	1.68	5 (10%)	68,82,82	1.18	3 (4%)
7	HEC	A	1002	1	50,50,50	1.73	8 (16%)	68,82,82	1.87	14 (20%)
9	SF4	B	1102	2	0,12,12	-	-	-	-	-
7	HEC	A	1003	1	50,50,50	1.69	6 (12%)	68,82,82	1.44	8 (11%)
7	HEC	A	1000	1	50,50,50	1.69	7 (14%)	68,82,82	1.34	4 (5%)
11	FAW	B	1104	2	34,34,35	1.12	3 (8%)	36,36,37	1.43	4 (11%)
10	DKA	E	202	5	6,7,11	0.27	0	5,6,11	0.58	0
7	HEC	A	1004	1	50,50,50	1.69	5 (10%)	68,82,82	2.13	16 (23%)
7	HEC	A	1001	1	50,50,50	1.74	5 (10%)	68,82,82	1.47	9 (13%)
11	FAW	E	203	5	26,26,35	1.30	3 (11%)	28,28,37	1.49	3 (10%)
10	DKA	B	1103	2	9,10,11	0.23	0	8,9,11	0.65	0
8	F3S	B	1101	2	0,9,9	-	-	-	-	-

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
7	HEC	E	201	5	1/1/3/7	2/14/54/54	-
7	HEC	A	1002	1	1/1/3/7	6/14/54/54	-
9	SF4	B	1102	2	-	-	0/6/5/5
7	HEC	A	1003	1	1/1/3/7	3/14/54/54	-
7	HEC	A	1000	1	-	4/14/54/54	-
11	FAW	B	1104	2	-	8/35/35/37	-
10	DKA	E	202	5	-	3/5/5/9	-
7	HEC	A	1004	1	1/1/3/7	2/14/54/54	-
7	HEC	A	1001	1	1/1/3/7	8/14/54/54	-
11	FAW	E	203	5	-	9/27/27/37	-
10	DKA	B	1103	2	-	0/8/8/9	-
8	F3S	B	1101	2	-	-	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1000	HEC	C3D-C2D	7.92	1.53	1.36
7	E	201	HEC	C3D-C2D	7.75	1.53	1.36
7	A	1003	HEC	C3D-C2D	7.69	1.53	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1002	HEC	C3D-C2D	7.67	1.53	1.36
7	A	1001	HEC	C3D-C2D	7.65	1.53	1.36
7	A	1004	HEC	C3D-C2D	7.12	1.52	1.36
11	E	203	FAW	OG1-CA1	4.28	1.45	1.33
7	A	1004	HEC	FE-NA	4.19	2.09	1.95
11	B	1104	FAW	OG1-CA1	4.17	1.45	1.33
11	E	203	FAW	OG2-CB1	4.09	1.45	1.34
7	A	1001	HEC	FE-NA	3.94	2.08	1.95
11	B	1104	FAW	OG2-CB1	3.94	1.45	1.34
7	A	1001	HEC	FE-NB	3.89	2.06	1.94
7	E	201	HEC	FE-NB	3.88	2.06	1.94
7	A	1003	HEC	FE-NB	3.69	2.06	1.94
7	A	1002	HEC	FE-NB	3.44	2.05	1.94
7	A	1003	HEC	FE-ND	3.39	2.05	1.94
7	E	201	HEC	FE-ND	3.36	2.05	1.94
7	A	1004	HEC	FE-NC	3.10	2.05	1.95
7	A	1004	HEC	FE-NB	2.98	2.04	1.94
7	A	1000	HEC	FE-NC	2.94	2.04	1.95
7	A	1001	HEC	FE-ND	2.93	2.03	1.94
7	A	1000	HEC	FE-NA	2.88	2.04	1.95
7	A	1000	HEC	FE-ND	2.78	2.03	1.94
7	A	1002	HEC	FE-ND	2.70	2.03	1.94
11	B	1104	FAW	OG2-CG2	-2.58	1.42	1.47
7	A	1003	HEC	FE-NA	2.56	2.03	1.95
7	A	1002	HEC	FE-NA	2.51	2.03	1.95
7	A	1000	HEC	FE-NB	2.45	2.02	1.94
7	E	201	HEC	FE-NC	2.45	2.03	1.95
11	E	203	FAW	OG2-CG2	-2.40	1.43	1.47
7	A	1003	HEC	FE-NC	2.28	2.02	1.95
7	A	1002	HEC	CMC-C2C	2.18	1.55	1.50
7	A	1001	HEC	FE-NC	2.16	2.02	1.95
7	E	201	HEC	FE-NA	2.12	2.02	1.95
7	A	1000	HEC	C3B-C2B	-2.09	1.32	1.36
7	A	1002	HEC	CHC-C4B	-2.08	1.34	1.38
7	A	1002	HEC	CHC-C1C	-2.07	1.34	1.39
7	A	1004	HEC	C3B-C2B	-2.06	1.32	1.36
7	A	1002	HEC	C2A-C3A	-2.04	1.32	1.36
7	A	1000	HEC	CMC-C2C	2.03	1.54	1.50
7	A	1003	HEC	C3B-C2B	-2.00	1.32	1.36

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1004	HEC	CAC-C3C-C4C	6.46	133.79	124.91
7	A	1002	HEC	CMC-C2C-C1C	-5.95	116.35	125.42
7	A	1004	HEC	C1D-ND-C4D	5.87	112.16	105.21
7	A	1002	HEC	C1D-ND-C4D	5.49	111.71	105.21
7	A	1001	HEC	C1D-ND-C4D	5.41	111.62	105.21
7	A	1000	HEC	C1D-ND-C4D	5.37	111.57	105.21
7	A	1003	HEC	C1D-ND-C4D	5.35	111.55	105.21
7	A	1004	HEC	CHA-C4D-ND	5.06	129.87	124.42
7	A	1004	HEC	CMC-C2C-C1C	-4.99	117.82	125.42
7	E	201	HEC	C1D-ND-C4D	4.96	111.08	105.21
11	B	1104	FAW	CG2-OG2-CB1	-4.79	110.87	117.78
7	A	1002	HEC	CAB-C3B-C4B	4.67	130.86	124.79
7	A	1004	HEC	CAC-C3C-C2C	-4.55	119.70	126.89
11	B	1104	FAW	OG2-CB1-CB2	4.45	121.10	111.48
11	E	203	FAW	CG2-OG2-CB1	-4.42	111.41	117.78
7	A	1004	HEC	CHD-C4C-C3C	4.30	134.72	125.30
7	A	1001	HEC	CAD-C3D-C4D	4.11	131.87	124.70
11	E	203	FAW	OG2-CB1-CB2	3.96	120.05	111.48
7	A	1004	HEC	C2D-C1D-ND	-3.79	105.48	109.84
7	A	1004	HEC	CHC-C1C-NC	3.46	130.14	123.86
7	A	1002	HEC	CHC-C1C-NC	3.44	130.09	123.86
7	A	1002	HEC	CMC-C2C-C3C	3.35	132.73	125.62
7	A	1002	HEC	CAC-C3C-C4C	3.20	129.32	124.91
7	A	1001	HEC	CMC-C2C-C1C	-3.19	120.56	125.42
7	A	1004	HEC	C3C-C4C-NC	-3.12	106.69	110.15
7	A	1002	HEC	CHB-C4A-NA	3.03	127.75	124.45
7	A	1004	HEC	CHA-C4D-C3D	-3.02	120.37	124.77
7	A	1002	HEC	CHC-C1C-C2C	-3.01	118.68	127.43
7	A	1004	HEC	CHD-C4C-NC	-2.96	118.49	123.86
7	A	1003	HEC	CAC-C3C-C4C	2.90	128.91	124.91
7	A	1002	HEC	CHA-C4D-ND	2.89	127.53	124.42
11	B	1104	FAW	OG1-CA1-CA2	2.77	120.29	111.83
7	A	1002	HEC	CHD-C4C-C3C	2.76	131.34	125.30
7	A	1004	HEC	CHD-C1D-ND	2.74	127.76	124.37
7	A	1003	HEC	CHC-C1C-NC	2.65	128.66	123.86
11	E	203	FAW	OG1-CA1-CA2	2.60	119.76	111.83
7	A	1004	HEC	CMD-C2D-C1D	2.59	129.08	125.03
7	A	1001	HEC	CAA-C2A-C3A	-2.55	123.08	127.87
7	A	1002	HEC	CHD-C1D-ND	2.52	127.48	124.37
7	A	1000	HEC	C2A-C1A-NA	-2.49	107.92	110.32
7	A	1000	HEC	CAA-CBA-CGA	-2.41	107.28	113.67
11	B	1104	FAW	OG2-CB1-OB1	-2.40	118.08	123.70
7	A	1001	HEC	CBC-CAC-C3C	2.40	118.93	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	HEC	CAA-C2A-C1A	2.38	129.69	124.85
7	A	1003	HEC	CAB-C3B-C4B	2.34	127.84	124.79
7	A	1004	HEC	CBB-CAB-C3B	-2.34	106.08	112.42
7	E	201	HEC	C2A-C1A-NA	-2.30	108.10	110.32
7	A	1002	HEC	CBB-CAB-C3B	2.28	118.61	112.42
7	A	1003	HEC	CMC-C2C-C1C	-2.20	122.07	125.42
7	A	1003	HEC	C3C-C4C-NC	-2.17	107.75	110.15
7	A	1002	HEC	C1B-C2B-C3B	2.15	109.25	106.98
7	A	1003	HEC	C2A-C1A-NA	-2.15	108.25	110.32
7	E	201	HEC	CBA-CAA-C2A	-2.14	106.63	112.53
7	A	1001	HEC	CHD-C1D-ND	2.11	126.98	124.37
7	A	1001	HEC	CAD-C3D-C2D	-2.08	123.97	127.87
7	A	1000	HEC	CMC-C2C-C1C	-2.07	122.27	125.42
7	A	1004	HEC	C4D-C3D-C2D	-2.07	103.89	106.89
7	A	1002	HEC	CAB-C3B-C2B	-2.06	123.77	127.56
7	A	1004	HEC	CHC-C1C-C2C	-2.06	121.44	127.43
7	A	1003	HEC	CHA-C4D-ND	2.05	126.63	124.42
7	A	1001	HEC	CBD-CAD-C3D	2.01	118.10	112.53

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1001	HEC	NA
7	A	1002	HEC	NA
7	A	1003	HEC	NA
7	A	1004	HEC	NA
7	E	201	HEC	NA

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	202	DKA	O1-C1-C2-C3
11	B	1104	FAW	OG1-CG1-CG2-CG3
11	B	1104	FAW	OG1-CG1-CG2-OG2
11	E	203	FAW	CG1-CG2-OG2-CB1
11	E	203	FAW	OB1-CB1-OG2-CG2
11	E	203	FAW	CB2-CB1-OG2-CG2
7	A	1004	HEC	C4C-C3C-CAC-CBC
7	A	1004	HEC	C2C-C3C-CAC-CBC
7	A	1002	HEC	C2B-C3B-CAB-CBB
11	B	1104	FAW	CA2-CA1-OG1-CG1
11	B	1104	FAW	CB2-CB1-OG2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1002	HEC	C3D-CAD-CBD-CGD
11	B	1104	FAW	OA1-CA1-OG1-CG1
7	A	1001	HEC	C2C-C3C-CAC-CBC
11	B	1104	FAW	OB1-CB1-OG2-CG2
11	E	203	FAW	CA2-CA1-OG1-CG1
7	A	1002	HEC	C4B-C3B-CAB-CBB
7	A	1000	HEC	C2A-CAA-CBA-CGA
11	E	203	FAW	CB1-CB2-CB3-CB4
11	E	203	FAW	OA1-CA1-OG1-CG1
7	A	1001	HEC	C2D-C3D-CAD-CBD
7	A	1002	HEC	C2A-CAA-CBA-CGA
7	A	1001	HEC	C4D-C3D-CAD-CBD
7	A	1001	HEC	C4C-C3C-CAC-CBC
11	B	1104	FAW	CBB-CAB-CB9-CB8
7	A	1001	HEC	C1A-C2A-CAA-CBA
10	E	202	DKA	C2-C3-C4-C5
7	A	1001	HEC	C3A-C2A-CAA-CBA
11	E	203	FAW	CG3-CG2-OG2-CB1
7	A	1003	HEC	C3D-CAD-CBD-CGD
7	A	1000	HEC	C2C-C3C-CAC-CBC
7	A	1003	HEC	CAA-CBA-CGA-O2A
11	B	1104	FAW	CA3-CA4-CA5-CA6
11	E	203	FAW	CB6-CB7-CB8-CB9
7	A	1003	HEC	CAA-CBA-CGA-O1A
7	E	201	HEC	CAD-CBD-CGD-O2D
7	A	1000	HEC	CAA-CBA-CGA-O2A
7	E	201	HEC	CAD-CBD-CGD-O1D
7	A	1000	HEC	CAA-CBA-CGA-O1A
10	E	202	DKA	C1-C2-C3-C4
7	A	1002	HEC	CAA-CBA-CGA-O2A
7	A	1001	HEC	CAA-CBA-CGA-O2A
7	A	1002	HEC	CAA-CBA-CGA-O1A
7	A	1001	HEC	CAA-CBA-CGA-O1A
11	E	203	FAW	OG1-CA1-CA2-CA3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

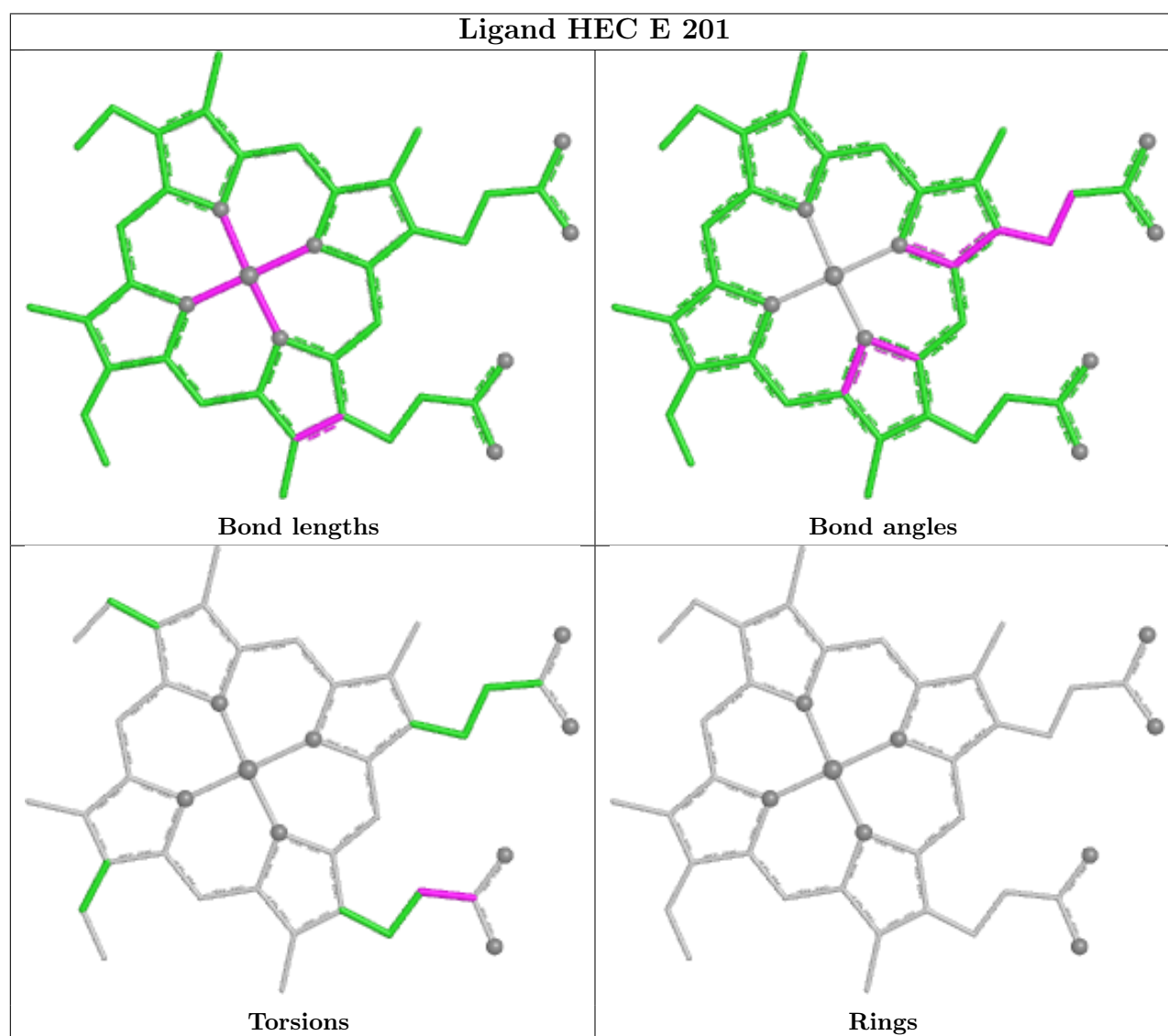
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1002	HEC	3	0
7	A	1000	HEC	3	0
10	E	202	DKA	1	0

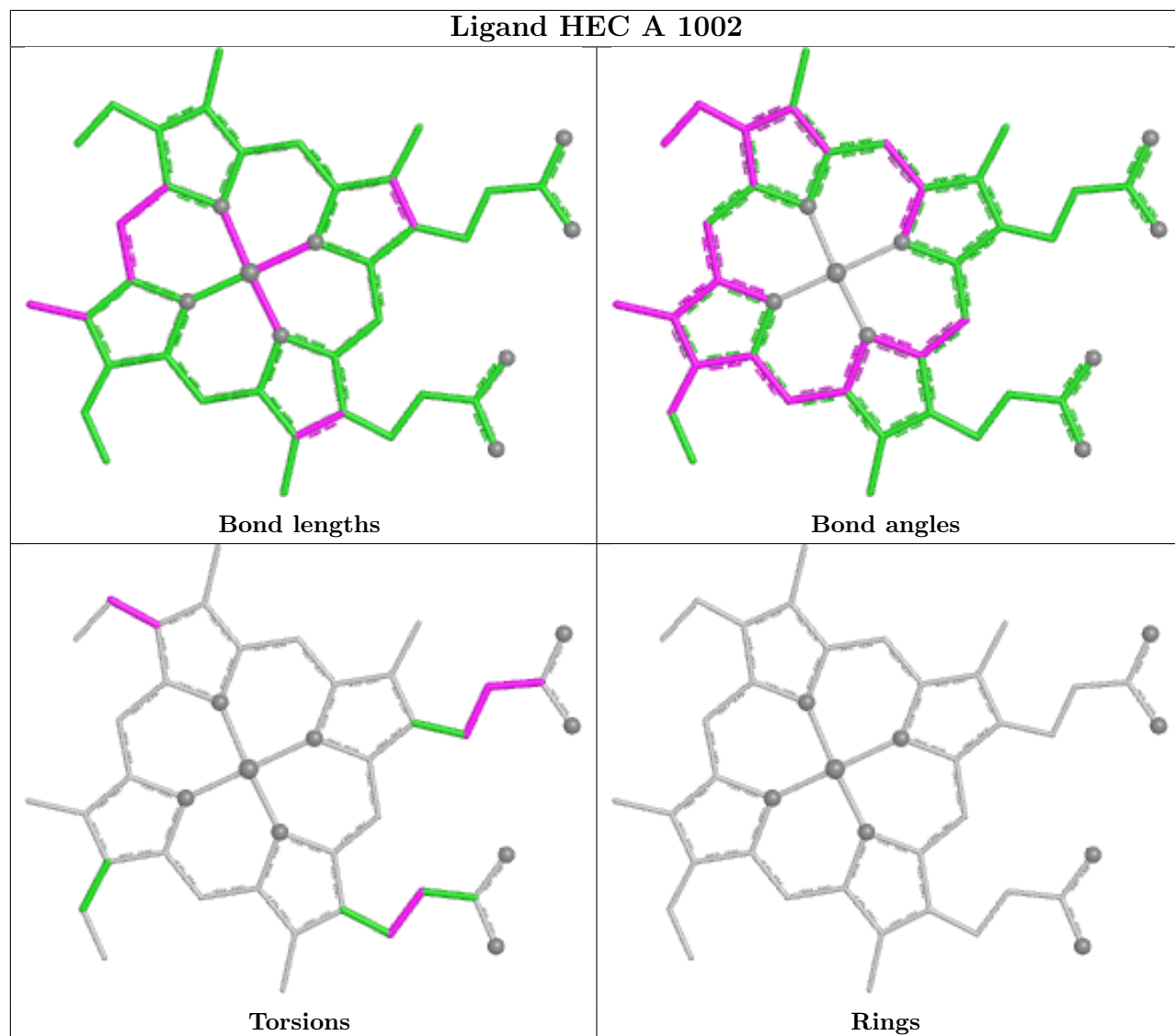
Continued on next page...

Continued from previous page...

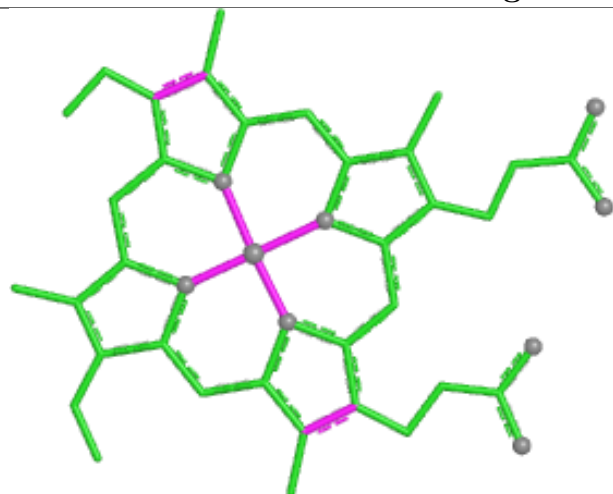
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	HEC	2	0
10	B	1103	DKA	1	0

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.

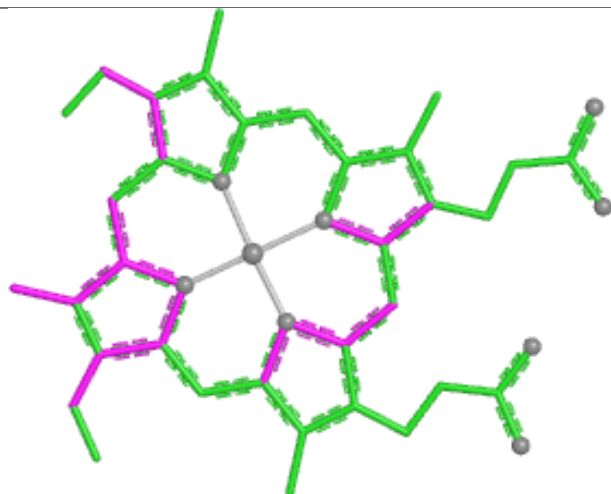




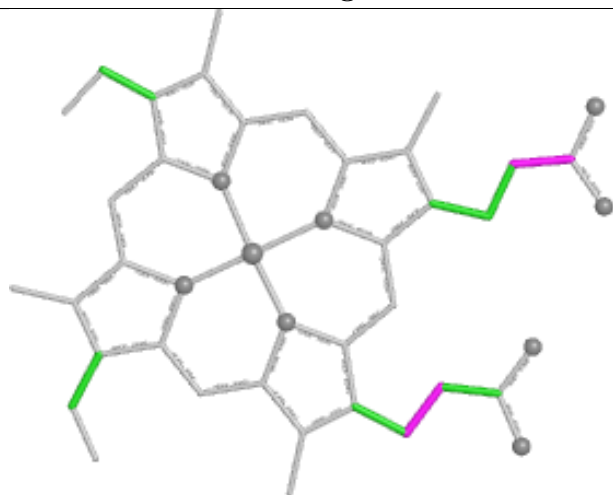
Ligand HEC A 1003



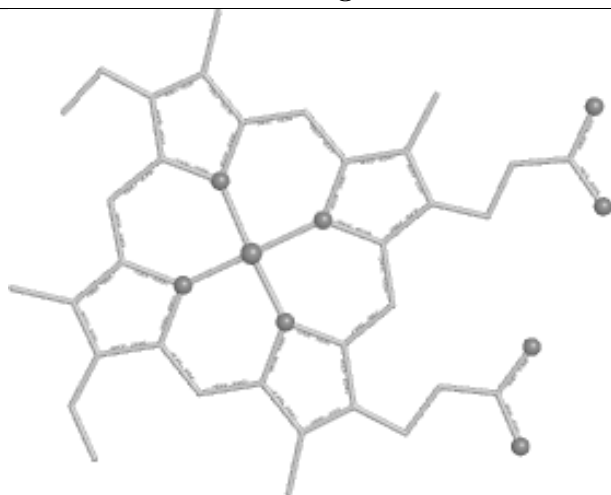
Bond lengths



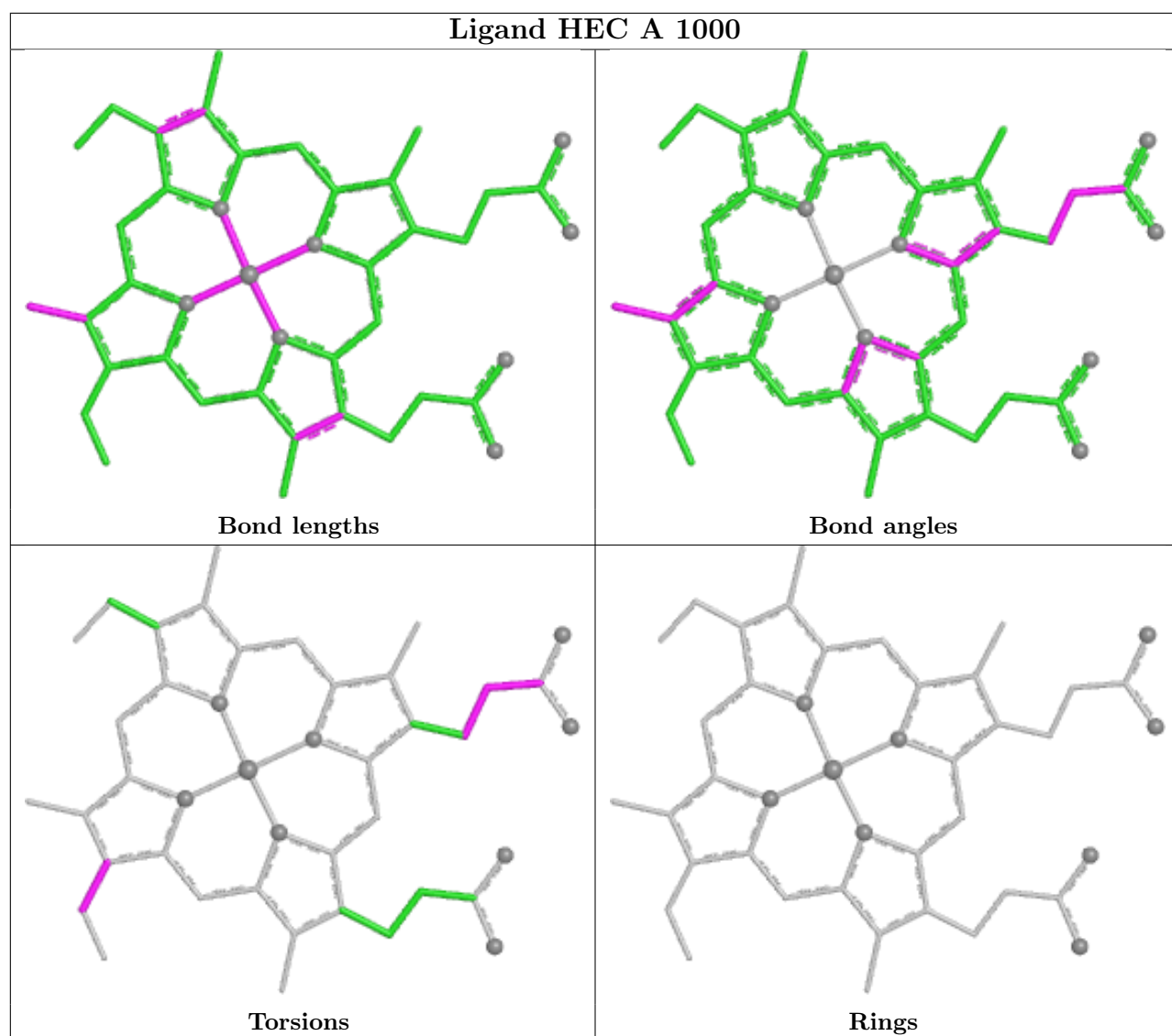
Bond angles

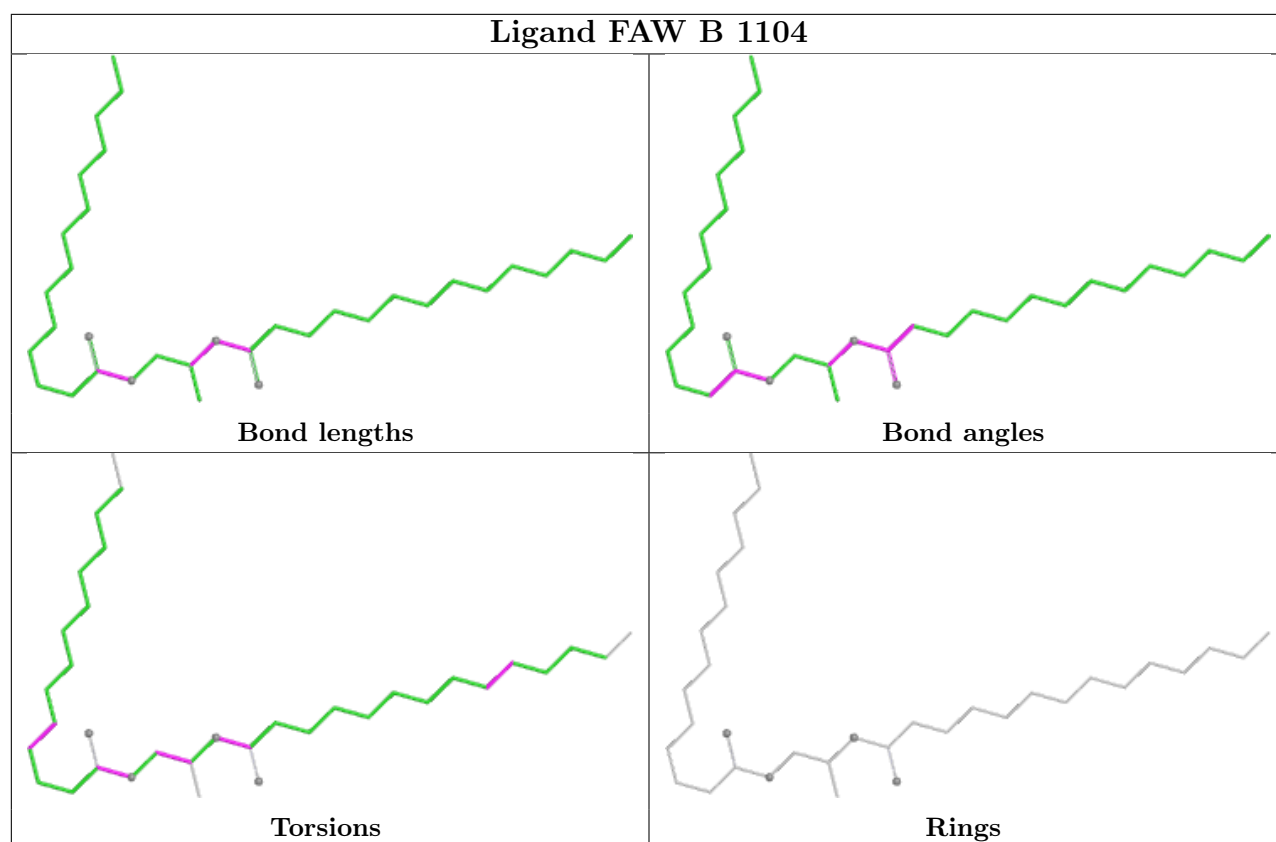


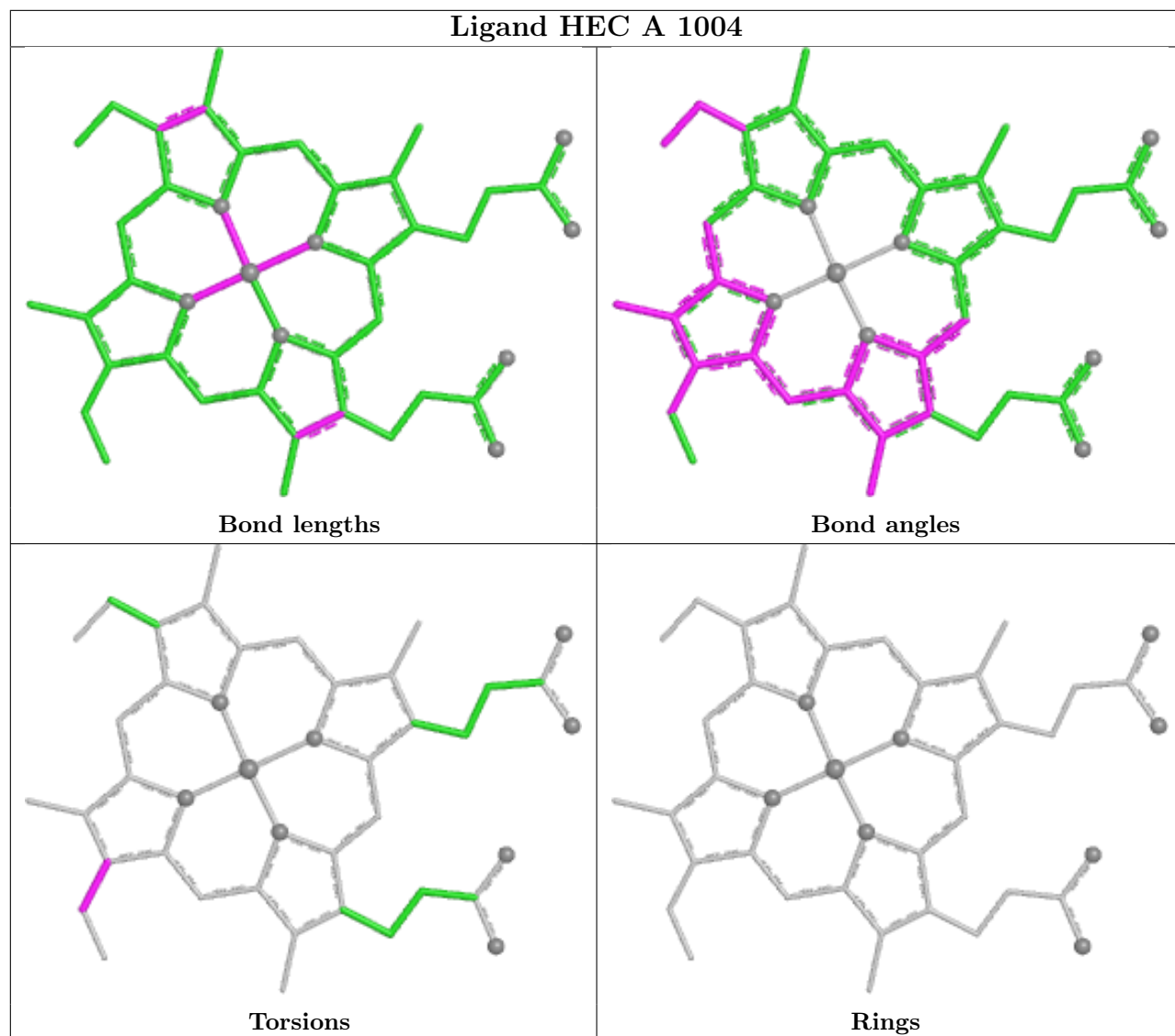
Torsions

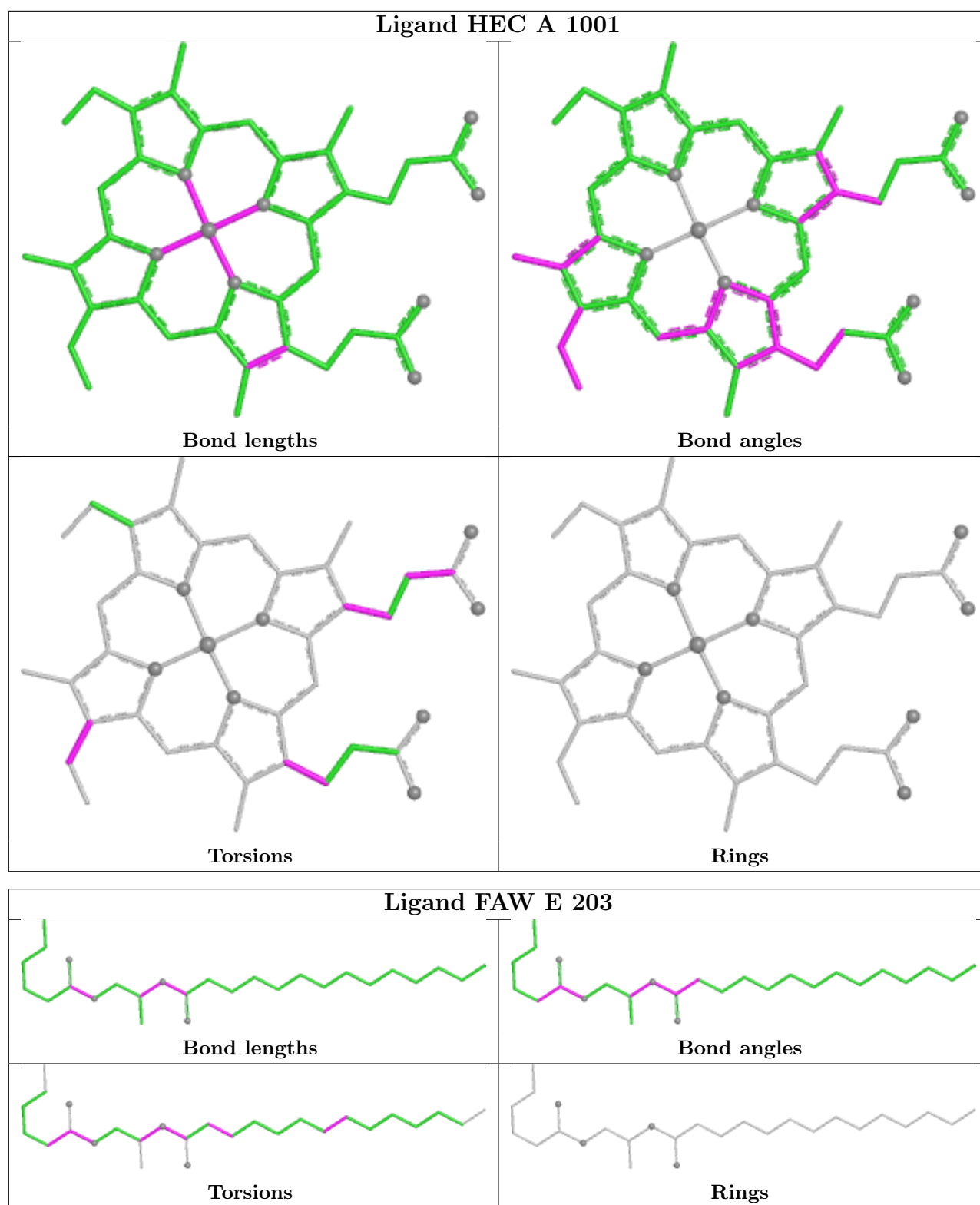


Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

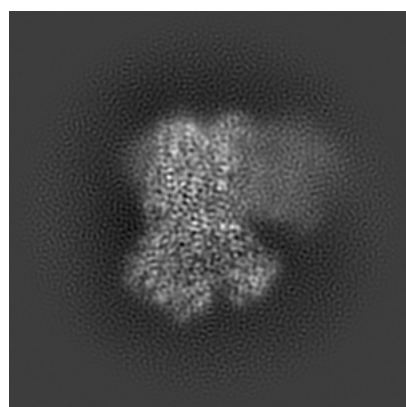
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7286. These allow visual inspection of the internal detail of the map and identification of artifacts.

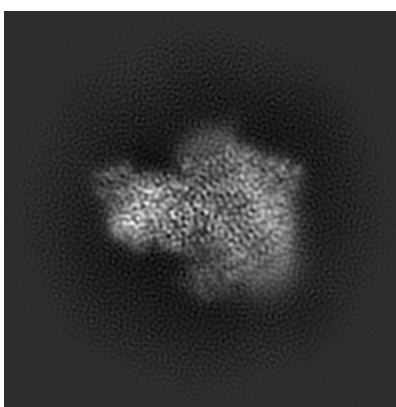
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

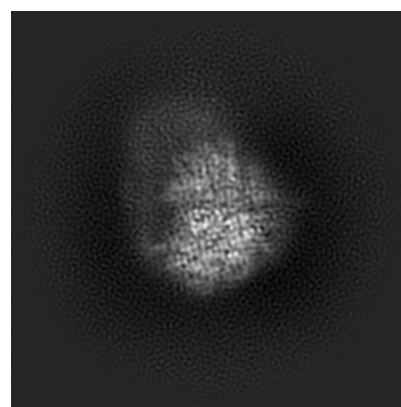
6.1.1 Primary map



X



Y

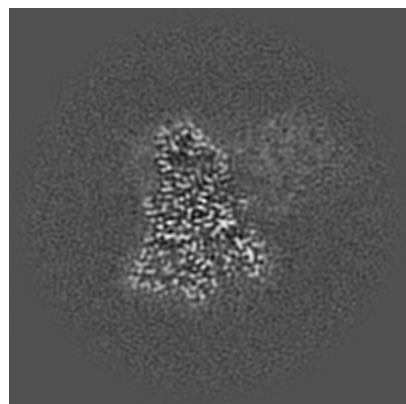


Z

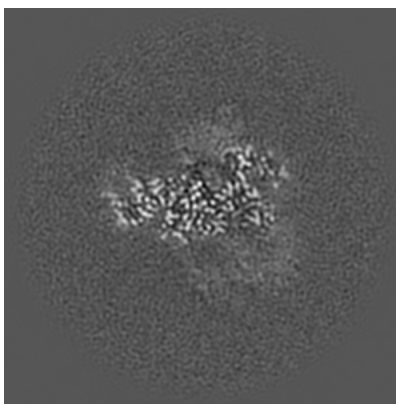
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

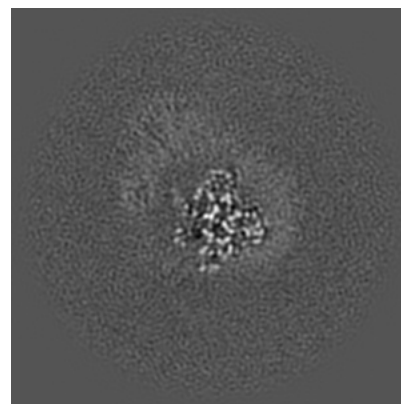
6.2.1 Primary map



X Index: 128



Y Index: 128

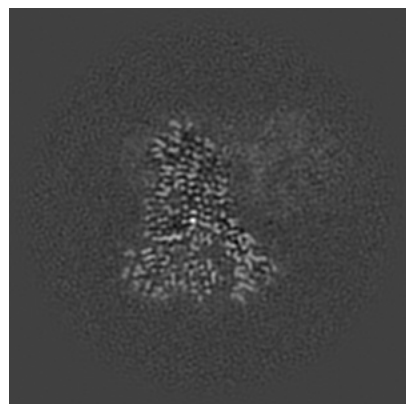


Z Index: 128

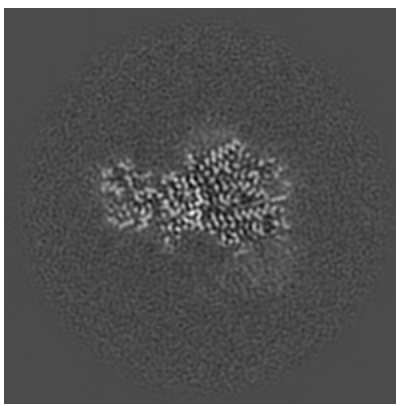
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

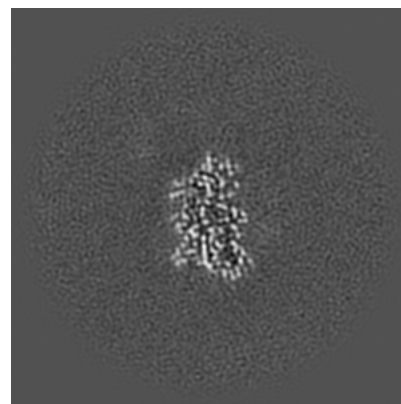
6.3.1 Primary map



X Index: 123



Y Index: 119

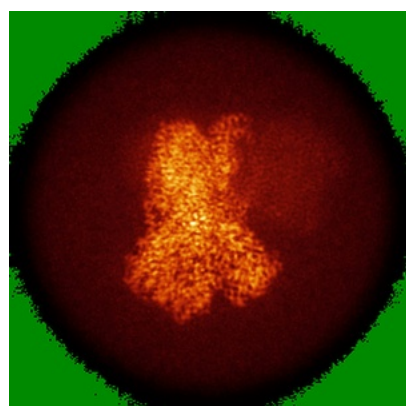


Z Index: 108

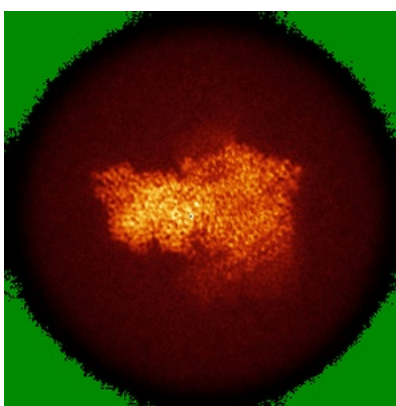
The images above show the largest variance slices of the map in three orthogonal directions.

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

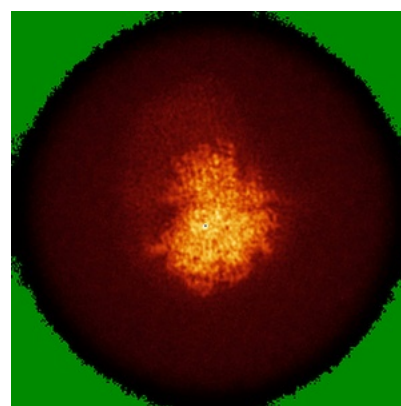
6.4.1 Primary map



X



Y

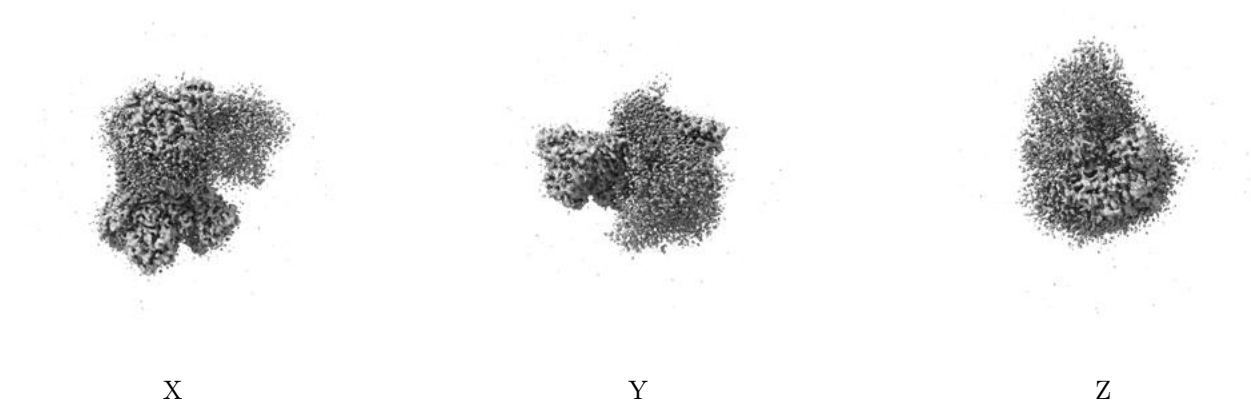


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

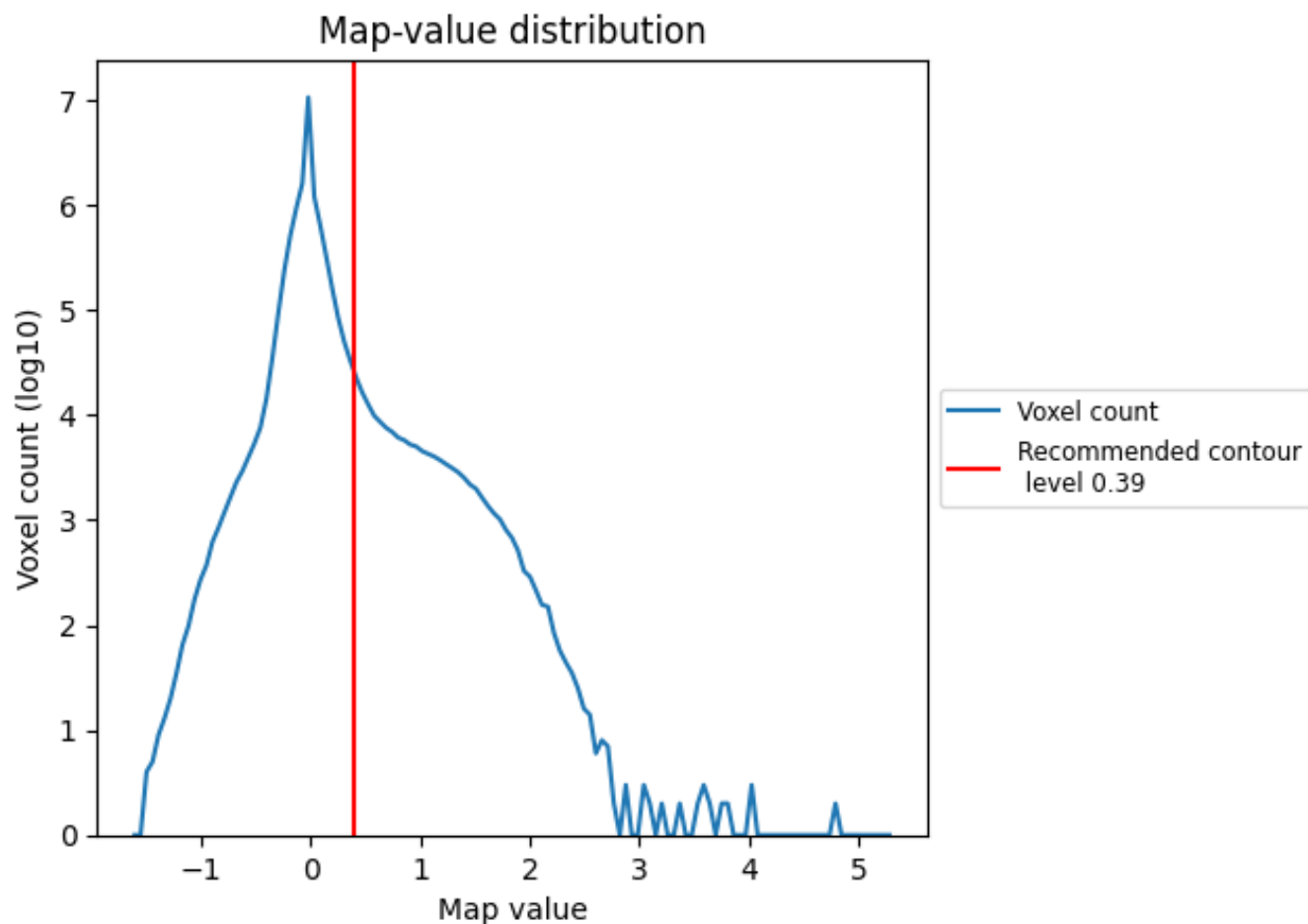
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

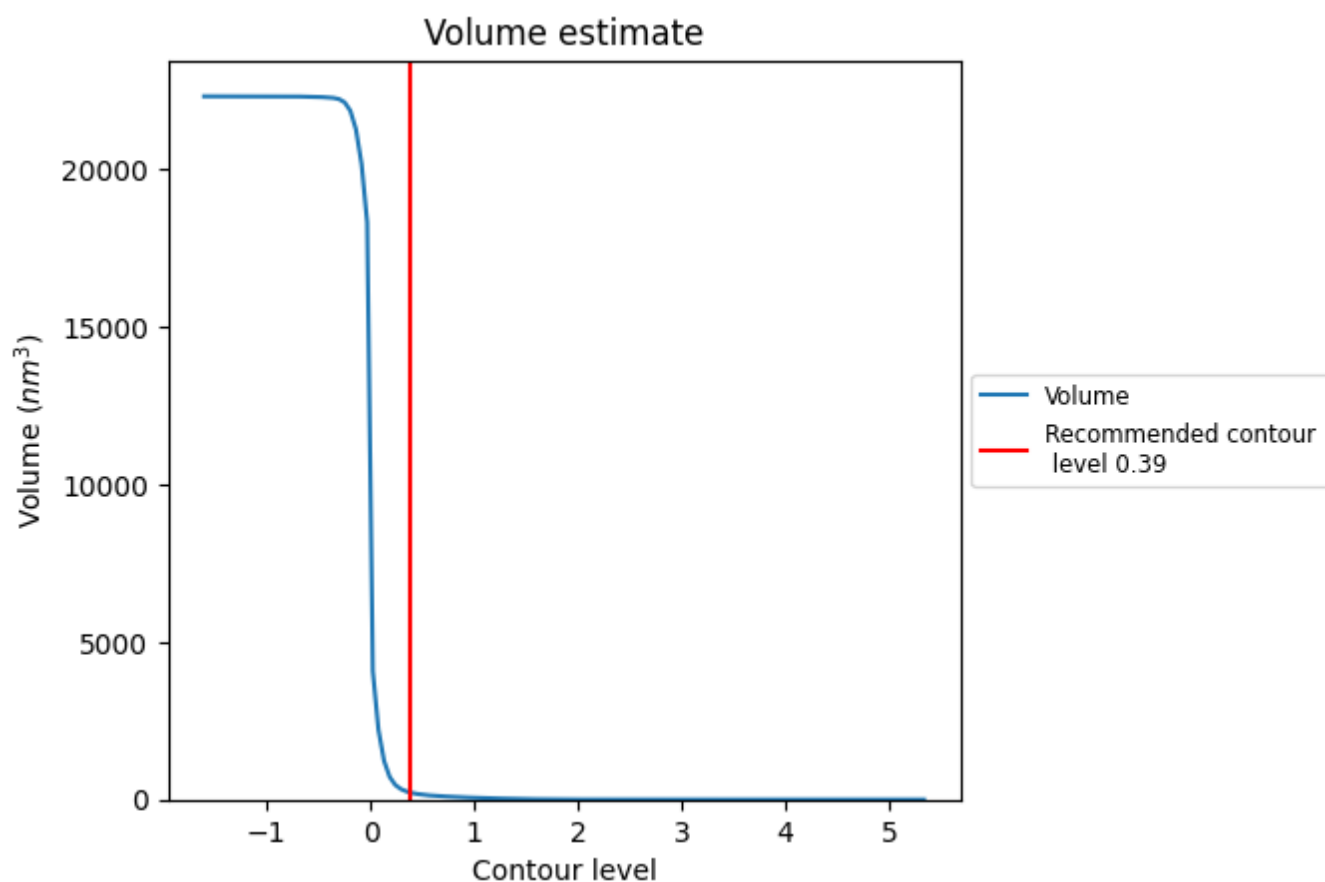
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

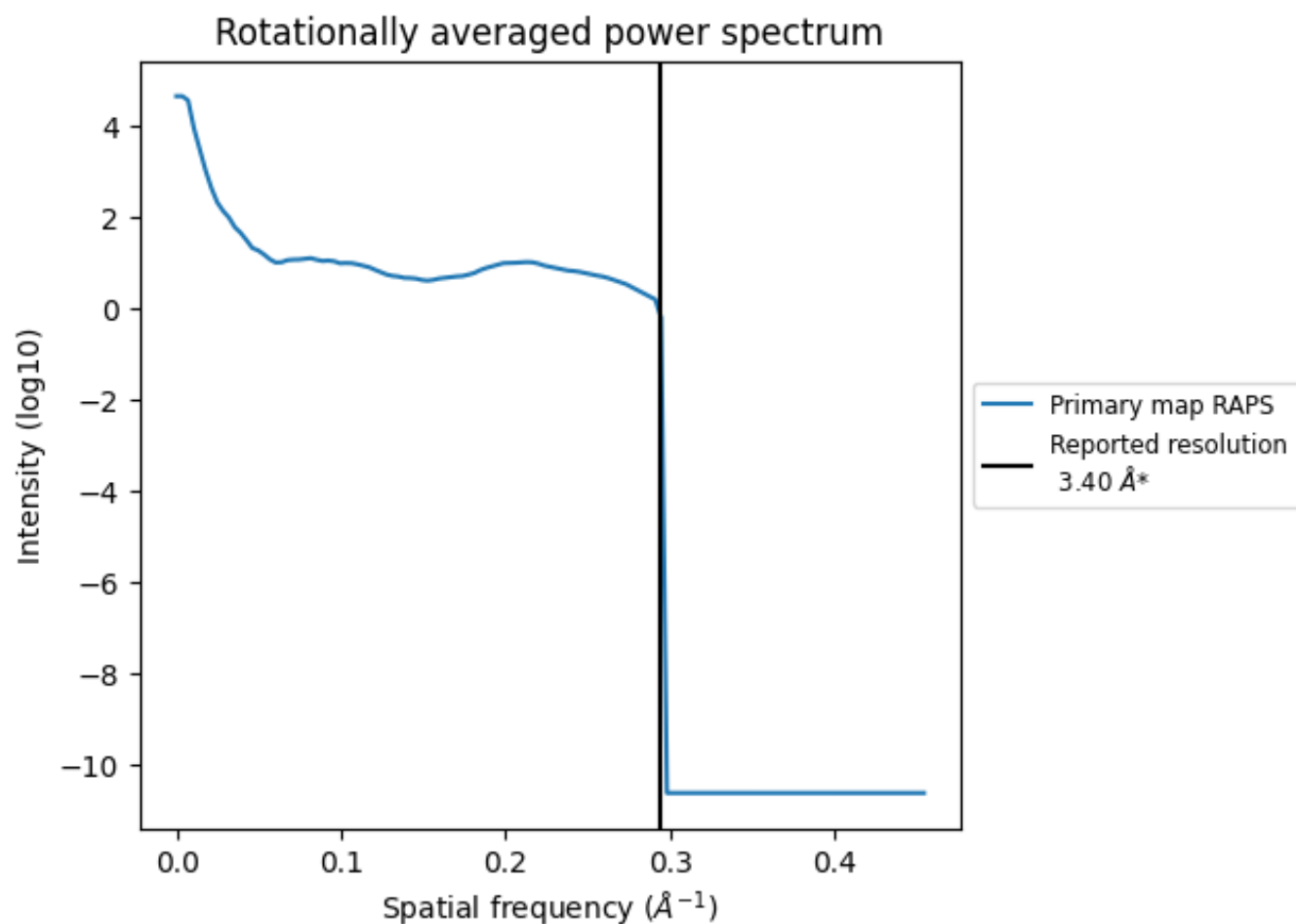
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 0.294 $\text{\AA}^{-1}$

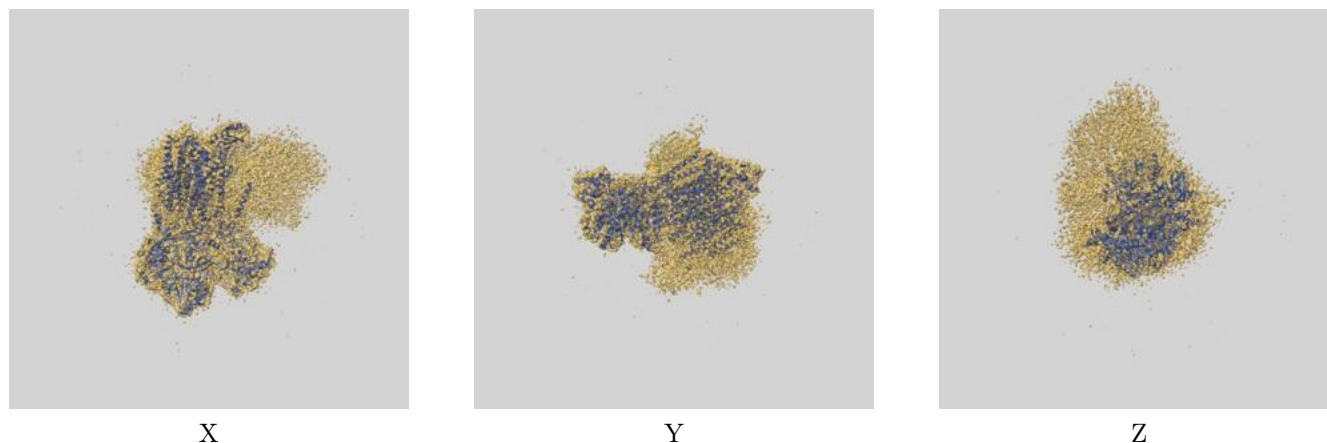
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

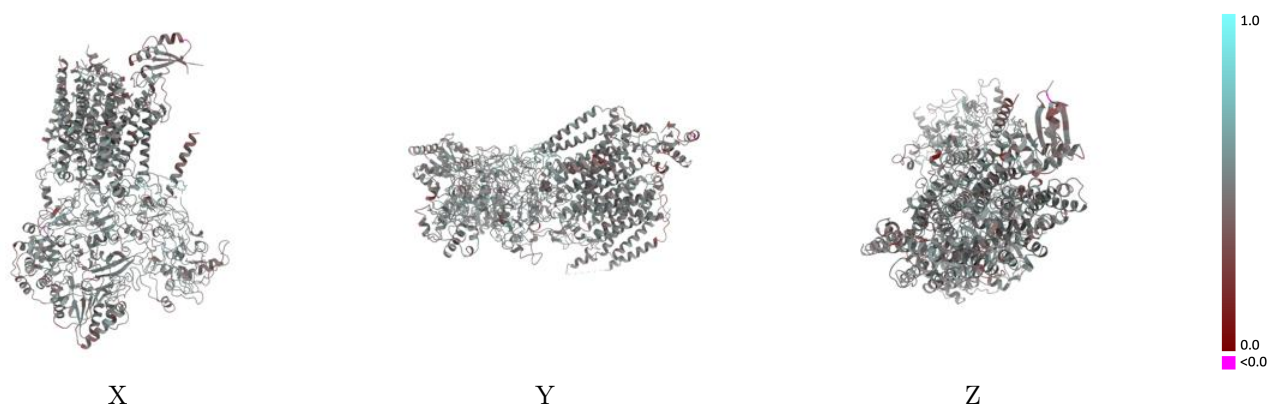
This section contains information regarding the fit between EMDB map EMD-7286 and PDB model 6BTM. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



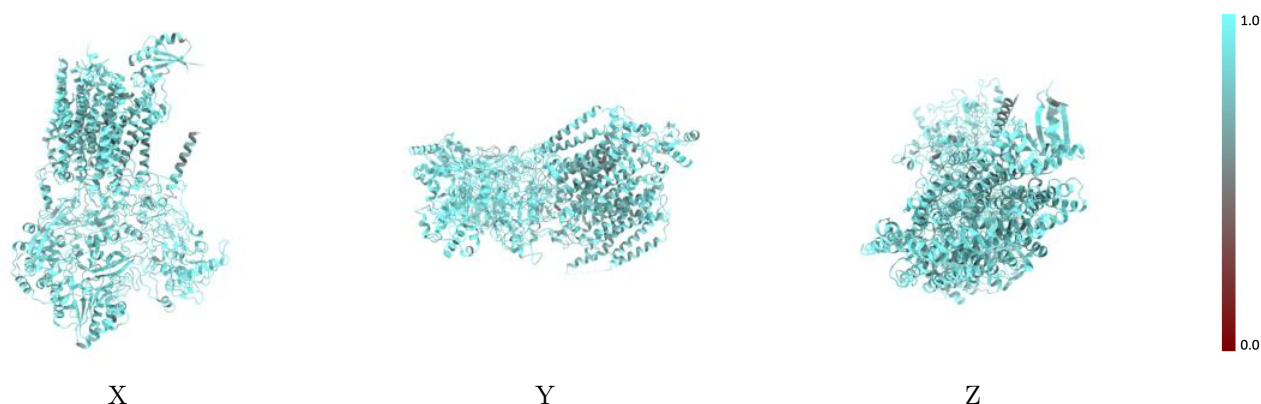
The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



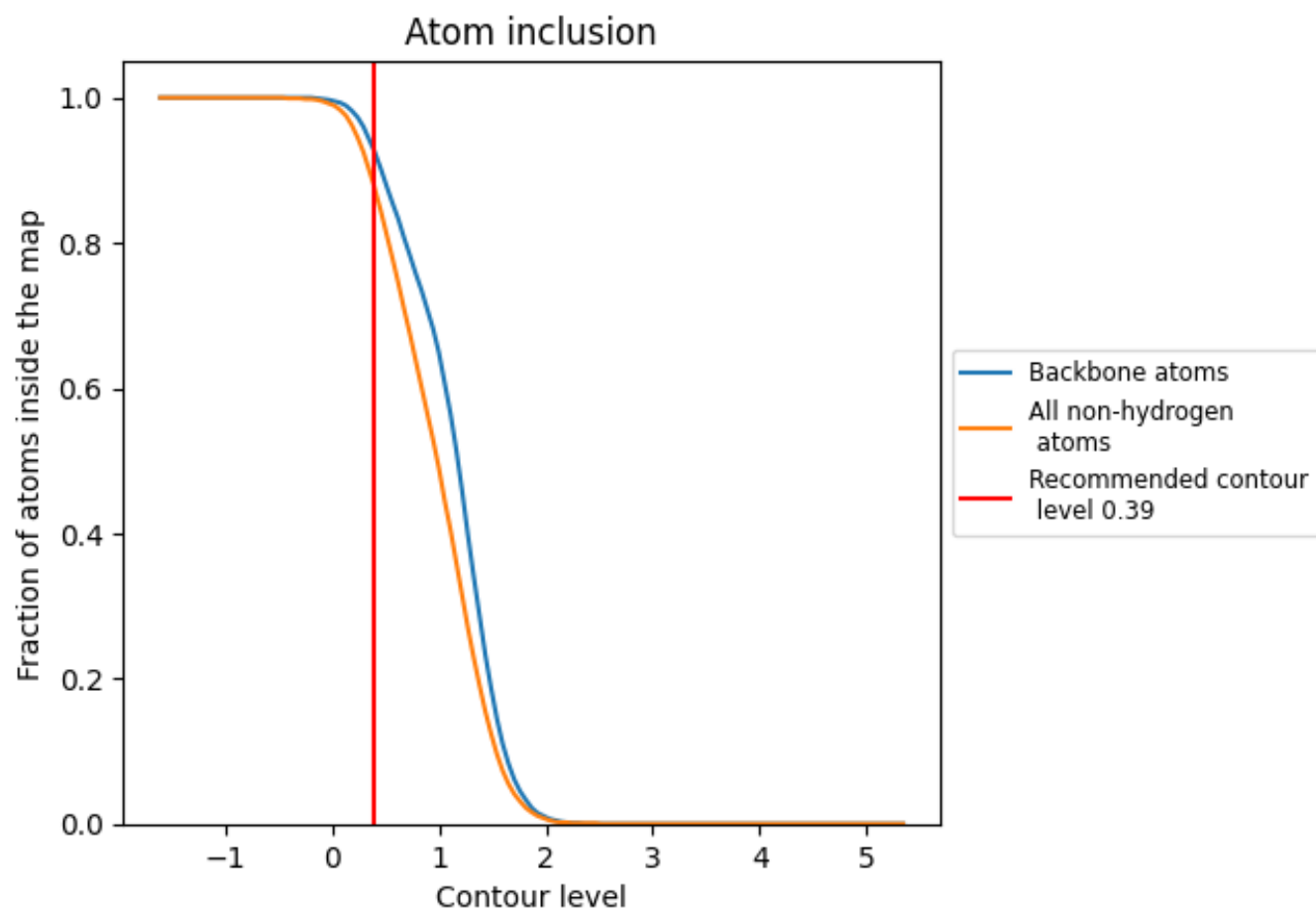
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.39).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.4820
A	0.8820	0.4800
B	0.8870	0.4830
C	0.8780	0.4900
D	0.8570	0.4590
E	0.9040	0.4900
F	0.8670	0.4760

1.0

0.0

<0.0