



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 10:42 AM EST

PDB ID : 6BTM
EMDB ID : EMD-7286
Title : Structure of Alternative Complex III from *Flavobacterium johnsoniae* (Wild Type)
Authors : Sun, C.; Benlekbir, S.; Venkatakrishnan, 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.

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

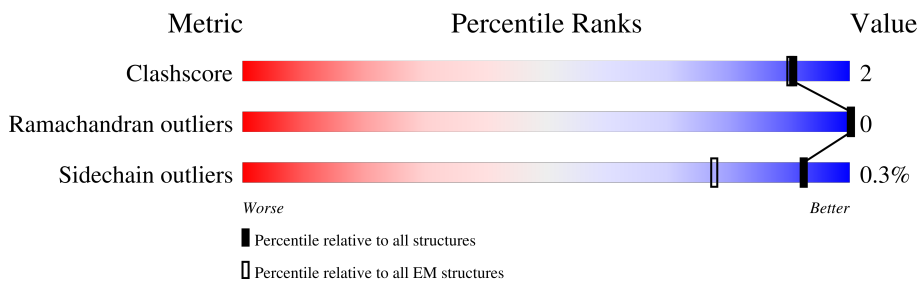
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 44% 6% 50%
2	B	948	 95% 5%
3	C	466	 97% ..
4	D	174	 92% 7% .
5	E	161	 96% ..
6	F	464	 86% . 13%

2 Entry composition [i](#)

There are 10 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
			Total	C	N	O	S		
1	A	221	1737	1107	296	318	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	948	7208	4520	1257	1395	36	0	0

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

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

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

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

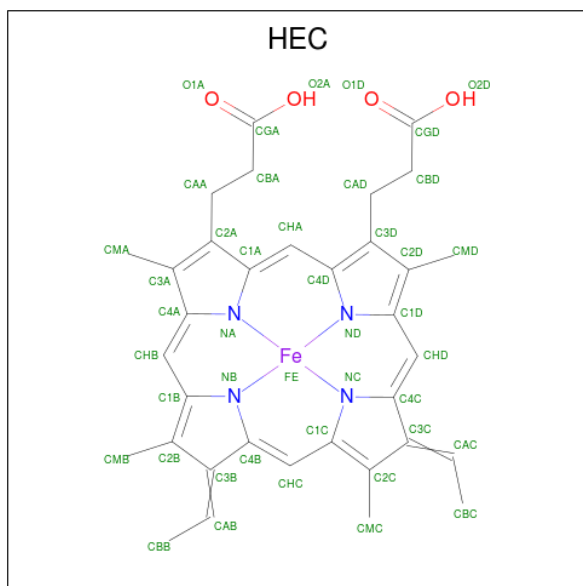
- Molecule 5 is a protein called Alternative Complex III subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	161	1263	801	210	248	4	0	0

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

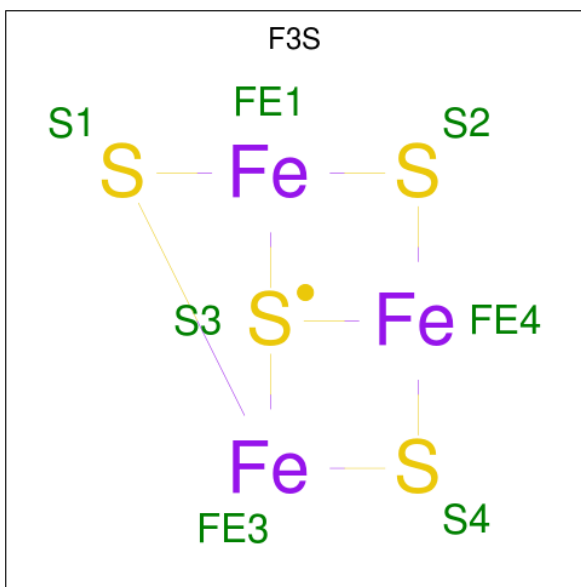
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	402	3300	2249	503	533	15	0	0

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



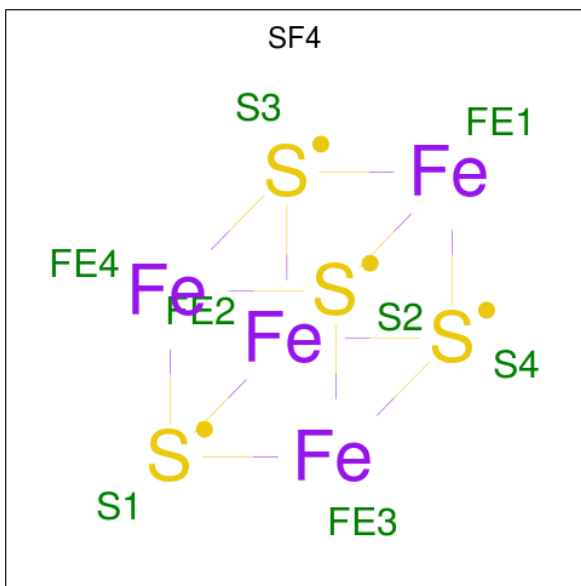
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
7	A	1	Total	C	Fe	N	O	0
			215	170	5	20	20	
7	A	1	Total	C	Fe	N	O	0
			215	170	5	20	20	
7	A	1	Total	C	Fe	N	O	0
			215	170	5	20	20	
7	A	1	Total	C	Fe	N	O	0
			215	170	5	20	20	
7	A	1	Total	C	Fe	N	O	0
			215	170	5	20	20	
7	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



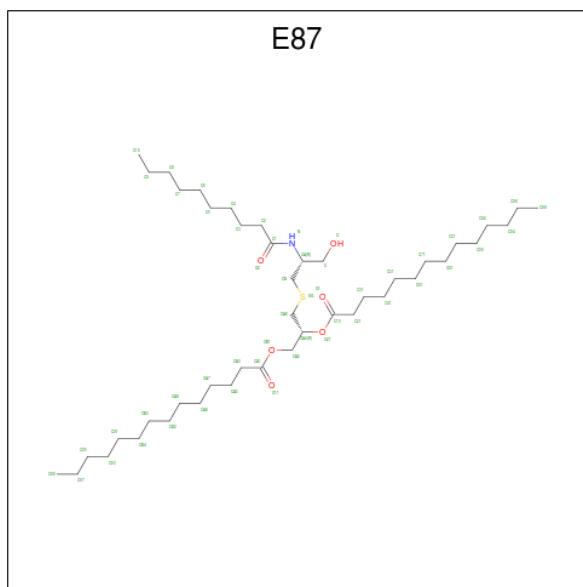
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



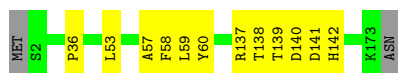
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 10 is (2R)-3-{[(2R)-2-(decanoylamino)-3-hydroxypropyl]sulfanyl}propane-1,2-diyl ditetradecanoate (three-letter code: E87) (formula: $\text{C}_{44}\text{H}_{85}\text{NO}_6\text{S}$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
10	B	1	52	44	1	6	1	0
10	E	1	41	33	1	6	1	0

Chain D:  92% 7%




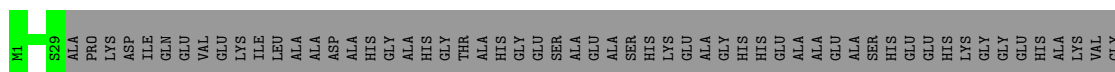
- Molecule 5: Alternative Complex III subunit E

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, E87, HEC, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/1782	0.59	2/2414 (0.1%)
2	B	0.47	1/7348 (0.0%)	0.66	9/9959 (0.1%)
3	C	0.51	0/3827	0.58	0/5240
4	D	0.57	0/1401	0.63	0/1904
5	E	0.29	0/1294	0.55	0/1747
6	F	0.50	0/3417	0.60	2/4649 (0.0%)
All	All	0.47	1/19069 (0.0%)	0.62	13/25913 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	413	TYR	CB-CG	-5.92	1.42	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	TYR	CB-CG-CD1	-9.37	115.38	121.00
1	A	420	LEU	CA-CB-CG	7.29	132.06	115.30
2	B	884	TYR	CB-CG-CD2	-7.01	116.80	121.00
2	B	413	TYR	CB-CG-CD2	6.20	124.72	121.00
1	A	356	PHE	CB-CG-CD2	-6.01	116.59	120.80
2	B	590	TYR	CB-CG-CD2	-5.77	117.54	121.00
2	B	884	TYR	CB-CG-CD1	5.67	124.40	121.00
2	B	1014	VAL	CG1-CB-CG2	-5.45	102.18	110.90
6	F	111	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	B	252	PHE	CB-CG-CD2	-5.34	117.06	120.80
2	B	650	TYR	CB-CG-CD2	-5.32	117.81	121.00
2	B	821	LEU	CA-CB-CG	5.07	126.97	115.30
6	F	286	PHE	CB-CG-CD1	5.03	124.32	120.80

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	18	0
2	B	7208	0	7063	24	0
3	C	3697	0	3683	3	0
4	D	1363	0	1330	11	0
5	E	1263	0	1192	5	0
6	F	3300	0	3298	1	0
7	A	215	0	150	9	0
7	E	43	0	30	0	0
8	B	7	0	0	0	0
9	B	8	0	0	0	0
10	B	52	0	0	0	0
10	E	41	0	0	0	0
All	All	18934	0	18414	58	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 (58) 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:885:CYS:SG	2:B:894:ARG:NH1	2.74	0.61
1:A:364:HIS:HD1	7:A:1002:HEC:HBB2	1.65	0.60
1:A:262:HIS:HE1	7:A:1001:HEC:NA	2.00	0.59
2:B:856:GLU:OE2	2:B:872:ASN:ND2	2.33	0.59
1:A:272:ASN:HD22	5:E:106: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
4:D:57:ALA:O	4:D:58:PHE:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:871:GLN:HG2	2:B:939:ILE:HD11	1.90	0.54
2:B:756:LEU:HB3	2:B:1010: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
1:A:379:VAL:HG21	7:A:1001:HEC:HMB2	1.93	0.50
4:D:137:ARG:O	4:D:141:ASP:O	2.30	0.49
2:B:1014:VAL:HG12	2:B:1016:VAL:HG22	1.94	0.49
3:C:249:SER:OG	3:C:250:VAL:N	2.44	0.49
2:B:843:GLN:HE21	2:B:1012:TYR:HE2	1.60	0.48
1:A:439:CYS:HB3	2:B:875:ALA:HB2	1.95	0.48
5:E:164:ALA:HA	5:E:167:ARG:HE	1.78	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:996:ARG:NH2	2:B:1014:VAL:O	2.48	0.46
2:B:708:GLU:HG2	2:B:1015:LYS:HB3	1.97	0.46
1:A:276:CYS:HB3	1:A:289:PRO:HG3	1.98	0.46
3:C:254:TRP:NE1	3:C:394:SER:OG	2.46	0.45
2:B:851:ASN:HB2	2:B:1007:LYS:HB2	1.98	0.45
5:E:49:PHE:HE2	5:E:54:GLU:HG3	1.82	0.45
1:A:304:VAL:HG11	1:A:318:TYR:HB3	1.99	0.45
2:B:959:ASP:O	2:B:963: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:435:SER:OG	2:B:436:LEU:N	2.51	0.43
1:A:288:ILE:HD12	7:A:1001:HEC:HAD2	2.00	0.43
2:B:71:GLU:HA	5:E:28:TYR:HD1	1.83	0.43
2:B:761:ASN:HD21	2:B:1016:VAL:HG23	1.84	0.42
2:B:453:HIS:CD2	2:B:453:HIS:O	2.72	0.42
2:B:514:SER:OG	2:B:515:TRP:N	2.52	0.42
2:B:205:ASN:HA	2:B:206:PRO:HD2	1.74	0.42
2:B:756:LEU:HD23	2:B:978:PHE:HD1	1.85	0.41
4:D:139:THR:OG1	4:D:140:ASP:N	2.53	0.41
2:B:637:PRO:HB3	2:B:838:PRO:HD2	2.01	0.41
2:B:71:GLU:HA	5:E:28:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:PRO:CB	4:D:139:THR:O	2.69	0.41
2:B:973:SER:OG	2:B:974:GLY:N	2.53	0.41
7:A:1002:HEC:HHC	7:A:1002:HEC:HBB3	2.03	0.41
2:B:412:VAL:O	2:B:413:TYR:HB3	2.20	0.41
2:B:758:ILE:HD13	2:B:1012:TYR:HE1	1.85	0.41
2:B:849:HIS:O	2:B:1009:ASN:ND2	2.53	0.41

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	946/948 (100%)	863 (91%)	83 (9%)	0	100	100
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	159/161 (99%)	141 (89%)	18 (11%)	0	100	100
6	F	398/464 (86%)	379 (95%)	19 (5%)	0	100	100
All	All	2347/2657 (88%)	2176 (93%)	171 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/359 (52%)	184 (100%)	1 (0%)	88	94
2	B	768/771 (100%)	764 (100%)	4 (0%)	88	94
3	C	391/402 (97%)	391 (100%)	0	100	100
4	D	148/151 (98%)	148 (100%)	0	100	100
5	E	130/133 (98%)	129 (99%)	1 (1%)	81	91
6	F	351/392 (90%)	351 (100%)	0	100	100
All	All	1973/2208 (89%)	1967 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LYS
2	B	788	ARG
2	B	800	ARG
2	B	872	ASN
2	B	927	ARG
5	E	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	752	HIS
2	B	849	HIS
2	B	869	GLN
2	B	963	ASN
4	D	142	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEC	A	1001	1	32,50,50	2.16	4 (12%)	24,82,82	1.80	4 (16%)
7	HEC	A	1002	1	32,50,50	2.34	5 (15%)	24,82,82	2.39	4 (16%)
10	E87	B	1103	2	50,51,51	1.09	3 (6%)	49,55,55	1.41	6 (12%)
10	E87	E	202	5	39,40,51	1.25	3 (7%)	38,44,55	1.39	5 (13%)
7	HEC	A	1000	1	32,50,50	2.39	3 (9%)	24,82,82	1.57	3 (12%)
7	HEC	A	1003	1	32,50,50	2.32	3 (9%)	24,82,82	1.61	4 (16%)
9	SF4	B	1102	2	0,12,12	-	-	-	-	-
8	F3S	B	1101	2	0,9,9	-	-	-	-	-
7	HEC	A	1004	1	32,50,50	2.36	6 (18%)	24,82,82	1.95	5 (20%)
7	HEC	E	201	5	32,50,50	2.20	3 (9%)	24,82,82	1.69	5 (20%)

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	A	1001	1	-	6/10/54/54	-
7	HEC	A	1002	1	-	4/10/54/54	-
10	E87	B	1103	2	-	12/56/56/56	-
10	E87	E	202	5	-	14/45/45/56	-
7	HEC	A	1000	1	-	3/10/54/54	-
7	HEC	A	1003	1	-	3/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	1102	2	-	-	0/6/5/5
8	F3S	B	1101	2	-	-	0/3/3/3
7	HEC	A	1004	1	-	0/10/54/54	-
7	HEC	E	201	5	-	2/10/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1000	HEC	C2B-C3B	-8.13	1.32	1.40
7	A	1004	HEC	C2B-C3B	-8.07	1.32	1.40
7	A	1003	HEC	C2B-C3B	-7.94	1.32	1.40
7	A	1002	HEC	C2B-C3B	-7.91	1.32	1.40
7	A	1000	HEC	C3C-C2C	-6.70	1.33	1.40
7	E	201	HEC	C3C-C2C	-6.57	1.33	1.40
7	A	1004	HEC	C3C-C2C	-6.47	1.34	1.40
7	E	201	HEC	C2B-C3B	-6.46	1.34	1.40
7	A	1001	HEC	C2B-C3B	-6.45	1.34	1.40
7	A	1003	HEC	C3C-C2C	-6.27	1.34	1.40
7	A	1002	HEC	C3C-C2C	-6.02	1.34	1.40
7	A	1001	HEC	C3C-C2C	-5.62	1.34	1.40
7	A	1000	HEC	C3D-C2D	5.46	1.53	1.37
7	E	201	HEC	C3D-C2D	5.34	1.53	1.37
7	A	1003	HEC	C3D-C2D	5.29	1.53	1.37
7	A	1002	HEC	C3D-C2D	5.27	1.53	1.37
7	A	1001	HEC	C3D-C2D	5.26	1.53	1.37
7	A	1004	HEC	C3D-C2D	4.88	1.52	1.37
10	E	202	E87	OB1-CA1	4.27	1.45	1.33
10	B	1103	E87	OB1-CA1	4.16	1.45	1.33
10	B	1103	E87	O-C	-4.14	1.25	1.42
10	E	202	E87	O21-C15	4.09	1.45	1.34
10	E	202	E87	O-C	-4.07	1.25	1.42
10	B	1103	E87	O21-C15	3.94	1.45	1.34
7	A	1004	HEC	C3C-C4C	2.74	1.48	1.43
7	A	1001	HEC	CAD-C3D	2.71	1.56	1.52
7	A	1002	HEC	C3C-C4C	2.56	1.47	1.43
7	A	1002	HEC	C1C-CHC	-2.23	1.34	1.41
7	A	1004	HEC	C4D-ND	2.05	1.40	1.36
7	A	1004	HEC	C1D-ND	2.05	1.40	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1002	HEC	CMC-C2C-C1C	-7.88	116.35	128.46
7	A	1004	HEC	CMC-C2C-C1C	-6.93	117.82	128.46
7	A	1002	HEC	CMC-C2C-C3C	5.87	132.73	125.82
10	B	1103	E87	CA6-SG-CB	5.67	111.76	102.13
7	A	1001	HEC	CMC-C2C-C1C	-5.14	120.56	128.46
10	B	1103	E87	O21-C15-C21	4.46	121.10	111.50
7	A	1003	HEC	CMC-C2C-C1C	-4.16	122.07	128.46
7	A	1000	HEC	CMC-C2C-C1C	-4.03	122.27	128.46
10	E	202	E87	O21-C15-C21	3.97	120.05	111.50
10	E	202	E87	CA6-SG-CB	3.70	108.42	102.13
7	E	201	HEC	CMC-C2C-C1C	-3.65	122.85	128.46
7	E	201	HEC	CBA-CAA-C2A	-3.55	106.63	112.60
7	A	1001	HEC	CBD-CAD-C3D	3.21	118.10	112.62
7	A	1002	HEC	CBD-CAD-C3D	-3.11	107.31	112.62
7	A	1001	HEC	CMC-C2C-C3C	3.10	129.47	125.82
10	E	202	E87	O-C-CA	3.03	119.77	111.95
7	A	1001	HEC	CMB-C2B-C1B	-3.02	123.82	128.46
7	A	1004	HEC	CBA-CAA-C2A	-2.89	107.74	112.60
10	B	1103	E87	CA4-O21-C15	-2.81	110.87	117.79
7	E	201	HEC	CMB-C2B-C1B	-2.72	124.29	128.46
10	B	1103	E87	OB1-CA1-CA3	2.67	120.29	111.91
7	A	1003	HEC	CMC-C2C-C3C	2.63	128.91	125.82
10	E	202	E87	CA4-O21-C15	-2.59	111.41	117.79
7	A	1003	HEC	CBA-CAA-C2A	-2.57	108.27	112.60
7	A	1002	HEC	CBA-CAA-C2A	-2.51	108.38	112.60
10	E	202	E87	OB1-CA1-CA3	2.50	119.76	111.91
7	A	1004	HEC	C1D-C2D-C3D	2.47	108.71	107.00
7	E	201	HEC	C1D-C2D-C3D	-2.41	105.32	107.00
10	B	1103	E87	O21-C15-O1	-2.33	118.08	123.70
7	A	1000	HEC	CAA-CBA-CGA	-2.31	107.28	113.76
7	A	1004	HEC	C3C-C4C-NC	-2.25	106.69	110.94
10	B	1103	E87	O-C-CA	2.22	117.68	111.95
7	E	201	HEC	CBD-CAD-C3D	-2.20	108.87	112.62
7	A	1000	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
7	A	1003	HEC	CBD-CAD-C3D	-2.11	109.02	112.62
7	A	1004	HEC	C2B-C3B-C4B	2.01	108.53	106.35

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1001	HEC	C2D-C3D-CAD-CBD
7	A	1001	HEC	C4D-C3D-CAD-CBD

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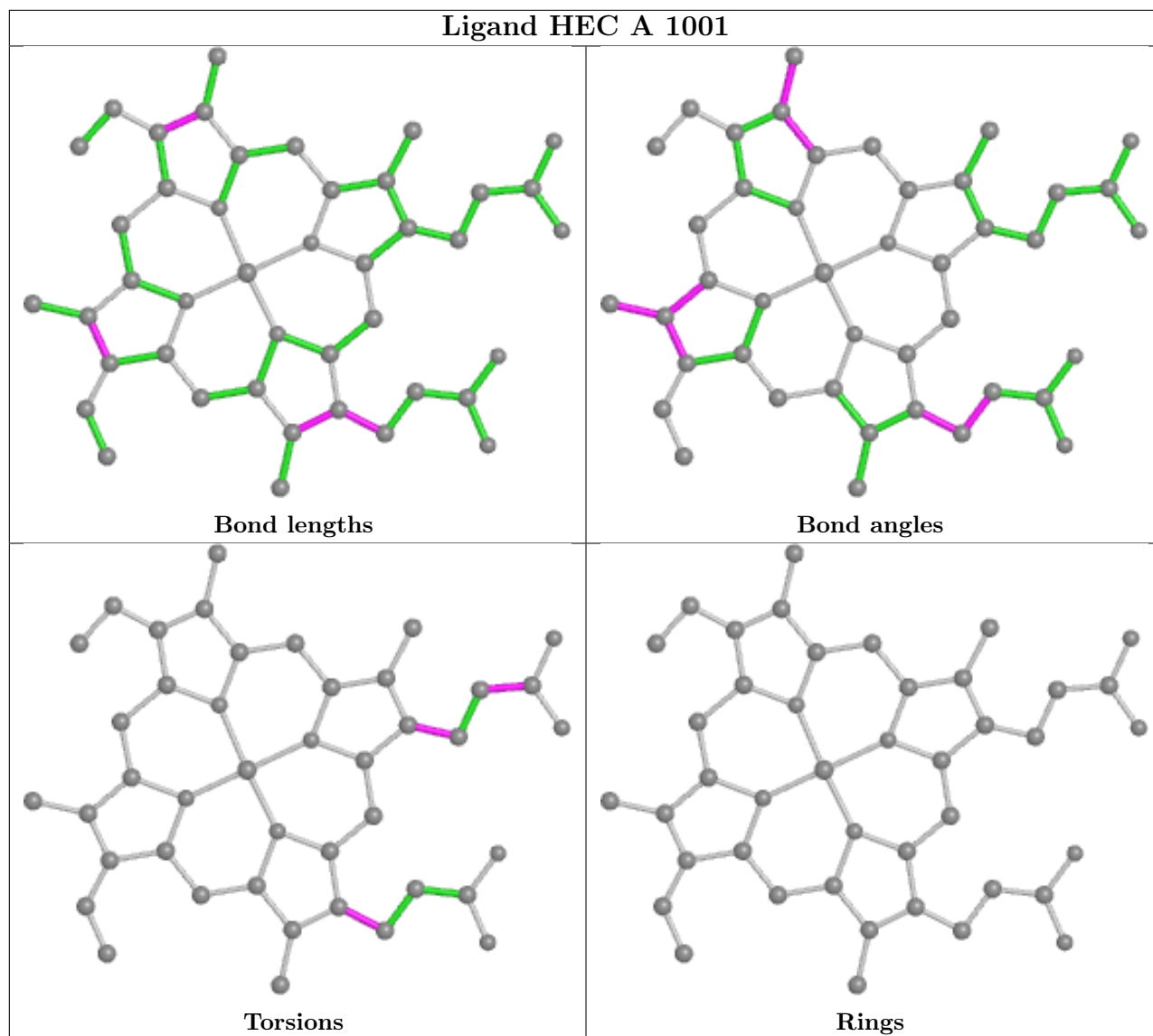
Mol	Chain	Res	Type	Atoms
7	A	1002	HEC	C3D-CAD-CBD-CGD
10	E	202	E87	C2-C1-N-CA
10	E	202	E87	O2-C1-N-CA
10	E	202	E87	O-C-CA-N
10	E	202	E87	O-C-CA-CB
10	E	202	E87	CA-CB-SG-CA6
10	E	202	E87	O1-C15-O21-CA4
10	E	202	E87	C21-C15-O21-CA4
10	B	1103	E87	CA3-CA1-OB1-CA2
10	B	1103	E87	C21-C15-O21-CA4
10	B	1103	E87	C2-C1-N-CA
10	B	1103	E87	O11-CA1-OB1-CA2
10	B	1103	E87	O2-C1-N-CA
10	B	1103	E87	O1-C15-O21-CA4
10	E	202	E87	CA3-CA1-OB1-CA2
7	A	1000	HEC	C2A-CAA-CBA-CGA
7	A	1002	HEC	C2A-CAA-CBA-CGA
10	E	202	E87	C15-C21-C31-C41
10	E	202	E87	O11-CA1-OB1-CA2
10	B	1103	E87	O-C-CA-N
10	B	1103	E87	C92-C90-CC1-C81
10	B	1103	E87	OB1-CA2-CA4-O21
7	A	1003	HEC	C3D-CAD-CBD-CGD
10	E	202	E87	C2-C3-C4-C5
7	A	1001	HEC	C1A-C2A-CAA-CBA
7	A	1001	HEC	C3A-C2A-CAA-CBA
7	A	1003	HEC	CAA-CBA-CGA-O2A
10	B	1103	E87	CA5-CA7-CA8-CA9
7	A	1003	HEC	CAA-CBA-CGA-O1A
10	E	202	E87	C61-C71-C81-CC1
7	E	201	HEC	CAD-CBD-CGD-O2D
10	B	1103	E87	O-C-CA-CB
7	E	201	HEC	CAD-CBD-CGD-O1D
7	A	1000	HEC	CAA-CBA-CGA-O2A
10	E	202	E87	C1-C2-C3-C4
10	B	1103	E87	OB1-CA2-CA4-CA6
7	A	1000	HEC	CAA-CBA-CGA-O1A
7	A	1002	HEC	CAA-CBA-CGA-O2A
7	A	1001	HEC	CAA-CBA-CGA-O2A
10	E	202	E87	OB1-CA1-CA3-CA5
7	A	1001	HEC	CAA-CBA-CGA-O1A
7	A	1002	HEC	CAA-CBA-CGA-O1A

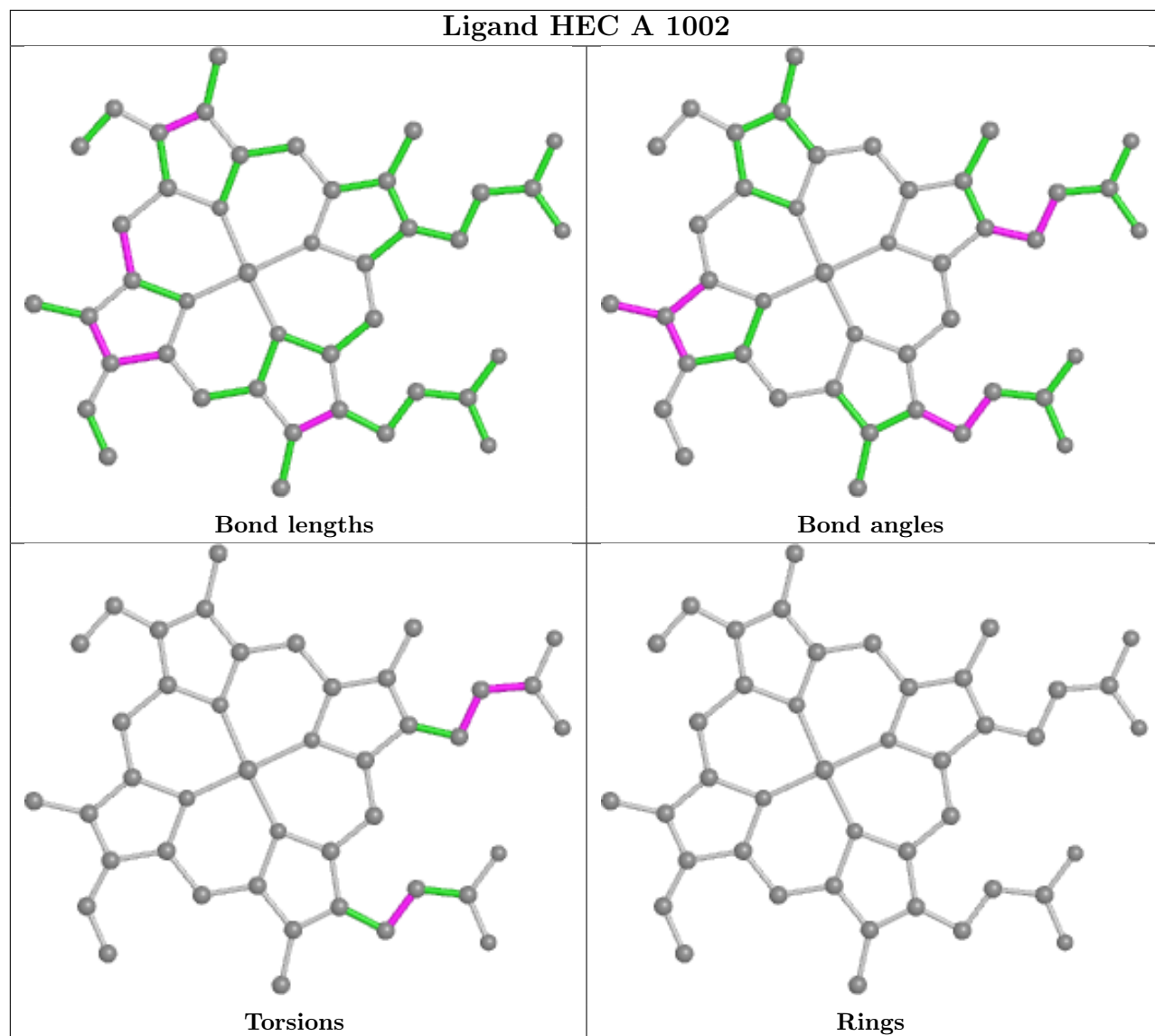
There are no ring outliers.

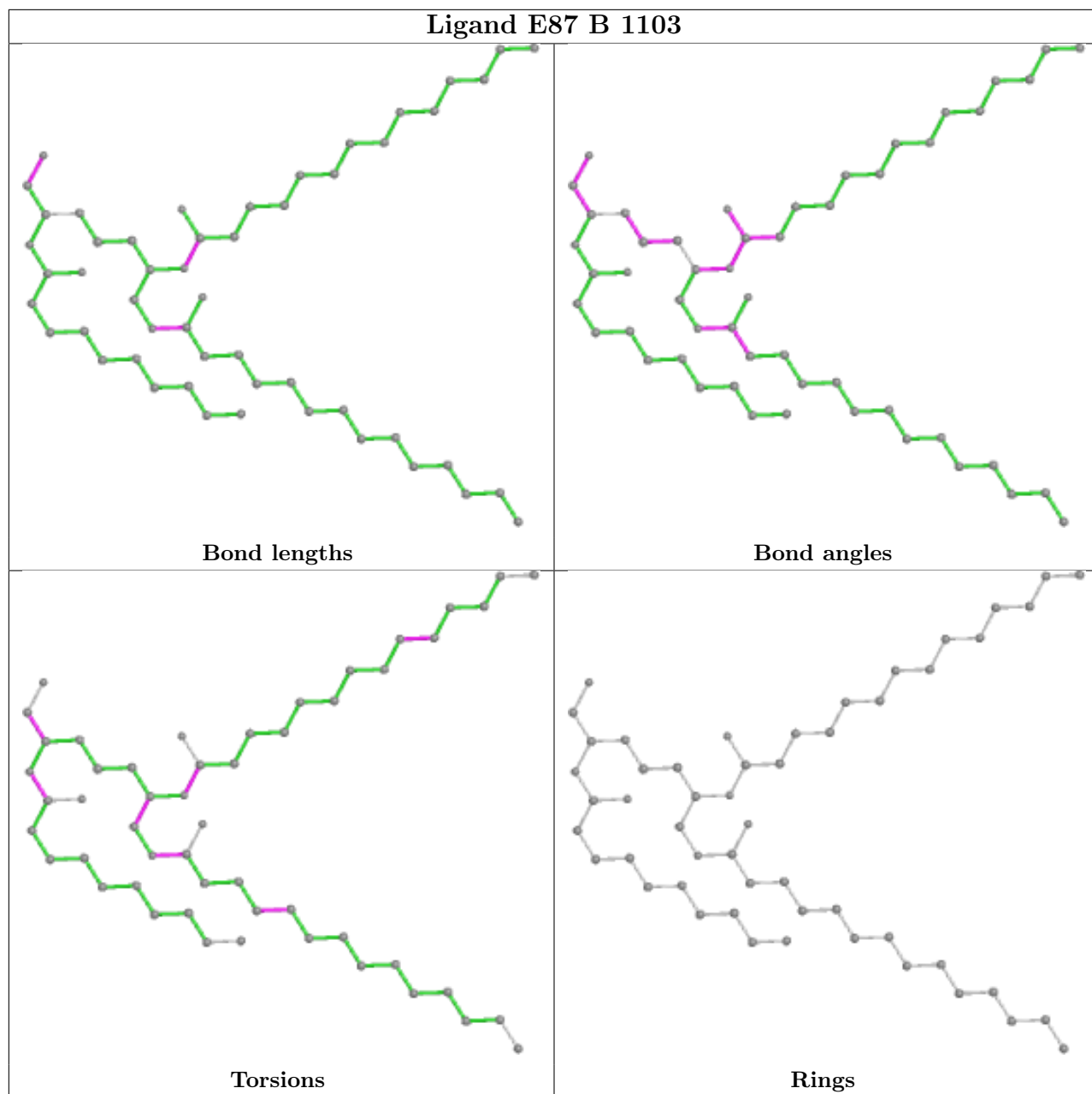
3 monomers are involved in 9 short contacts:

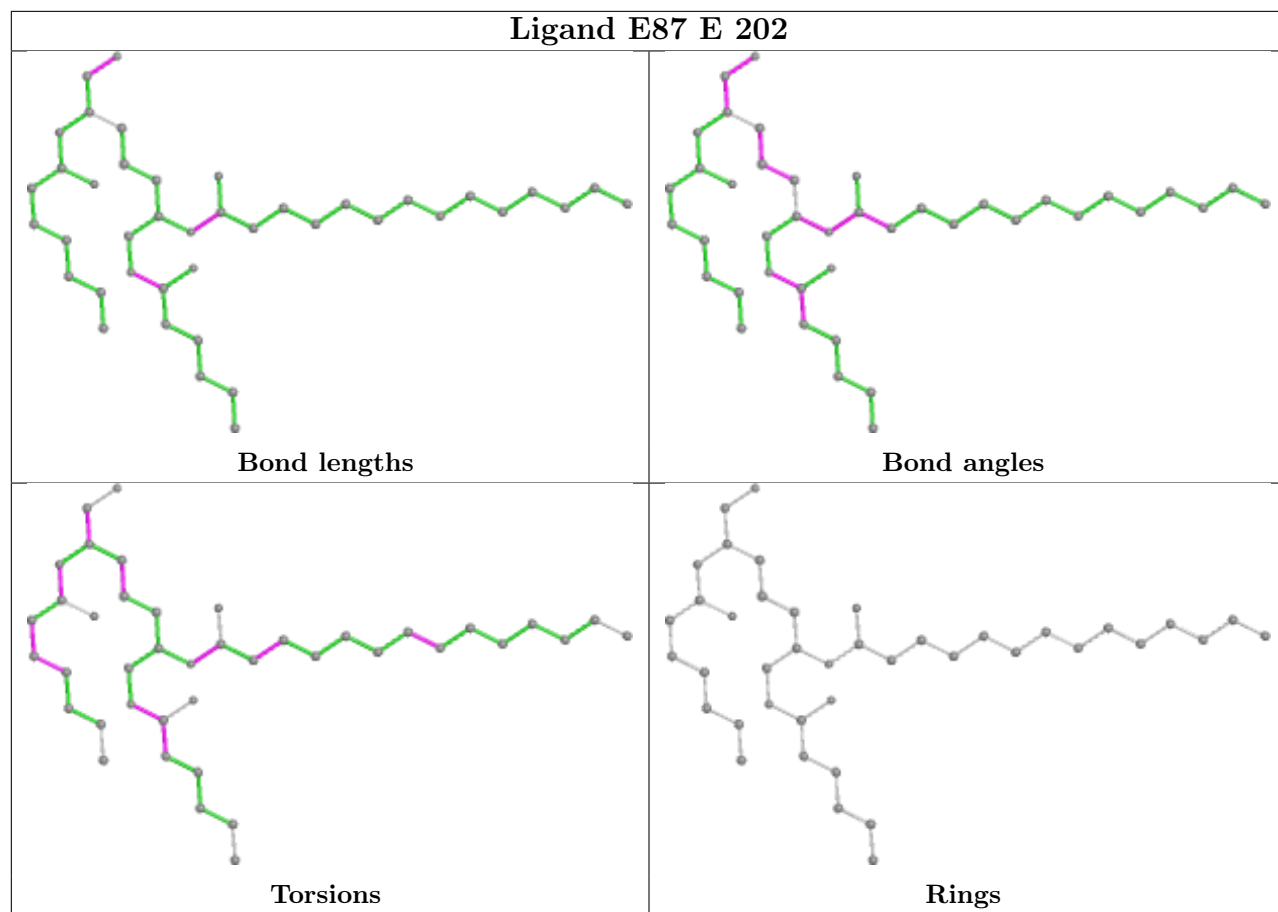
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	HEC	3	0
7	A	1002	HEC	3	0
7	A	1000	HEC	3	0

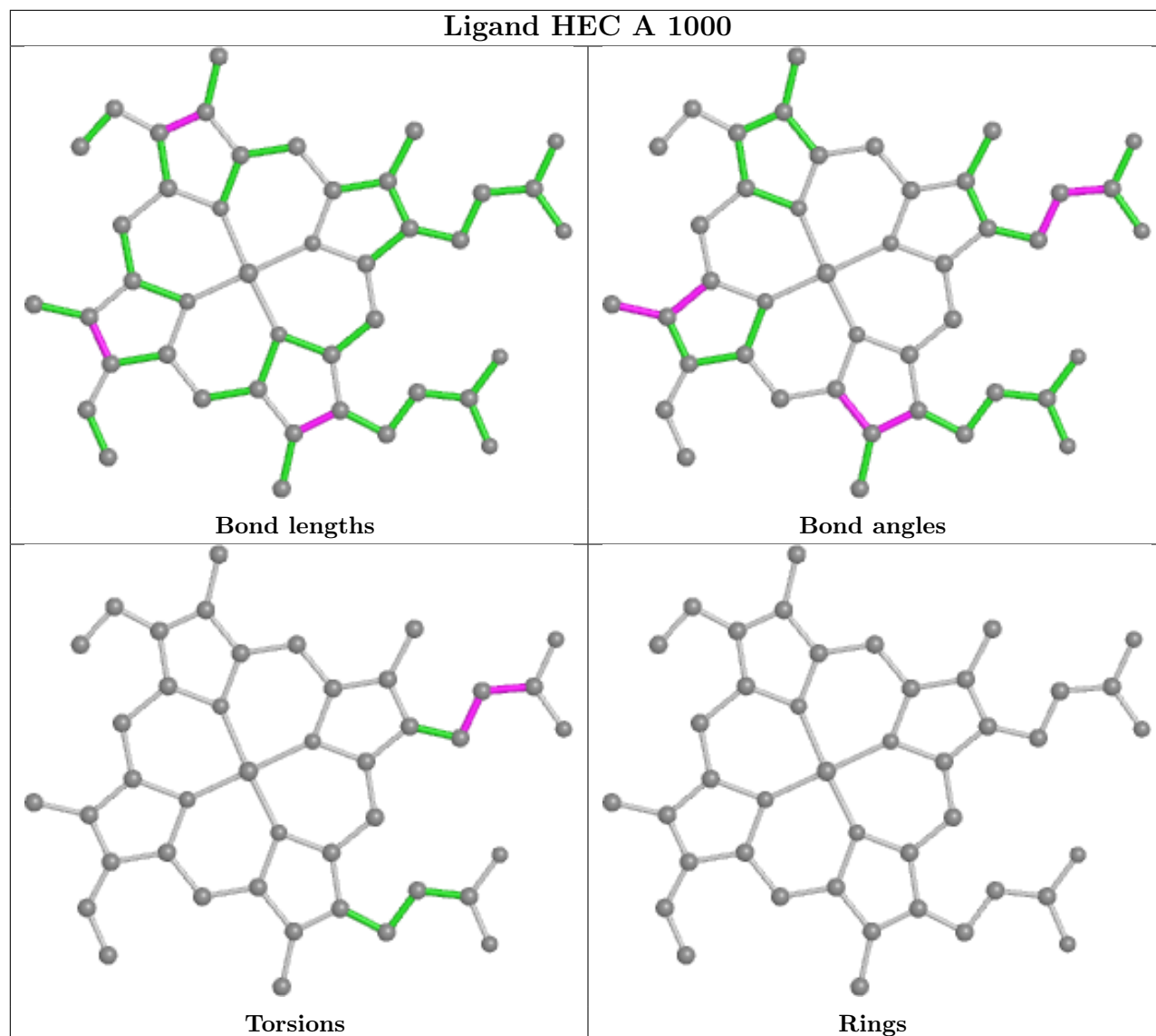
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

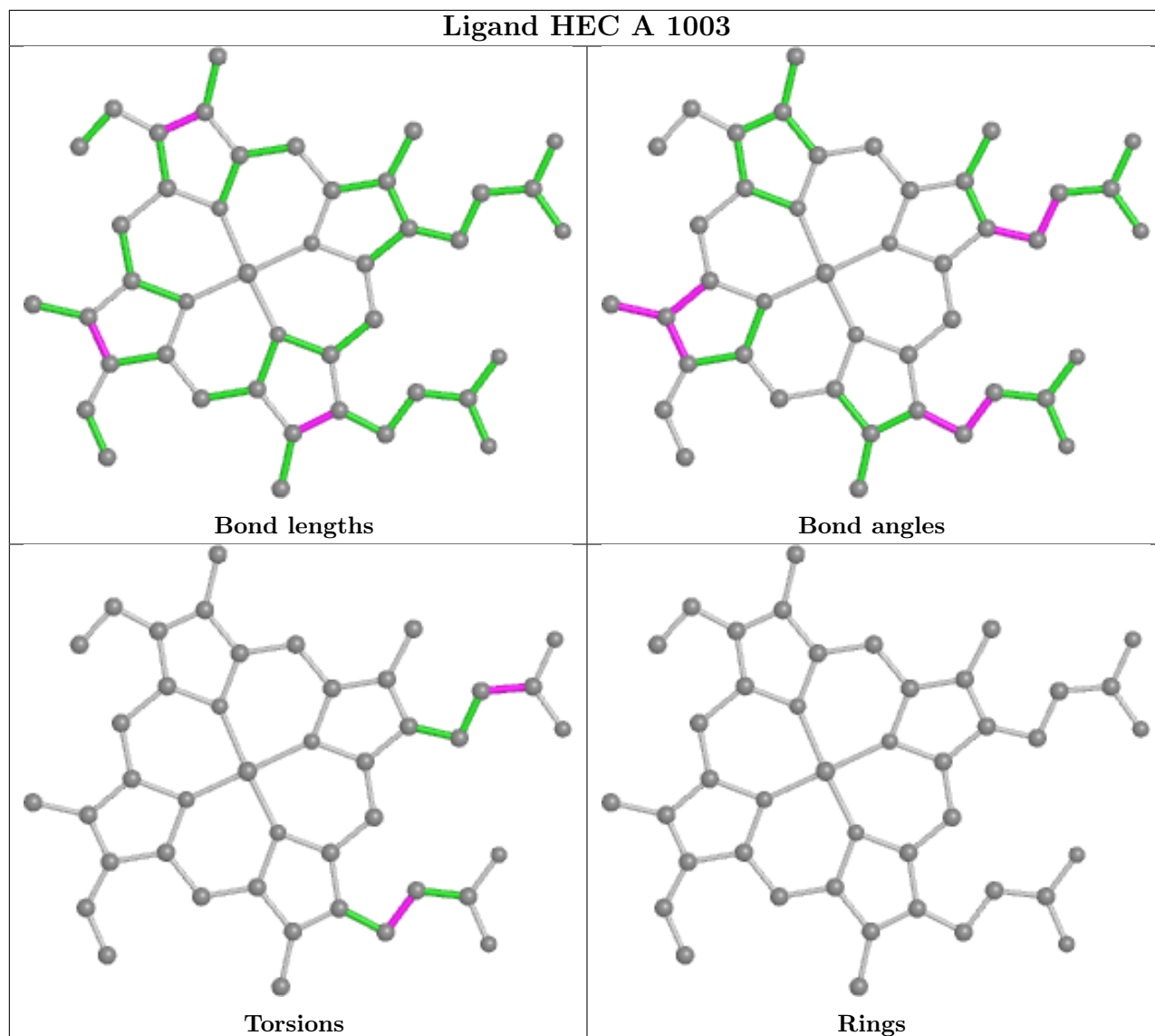


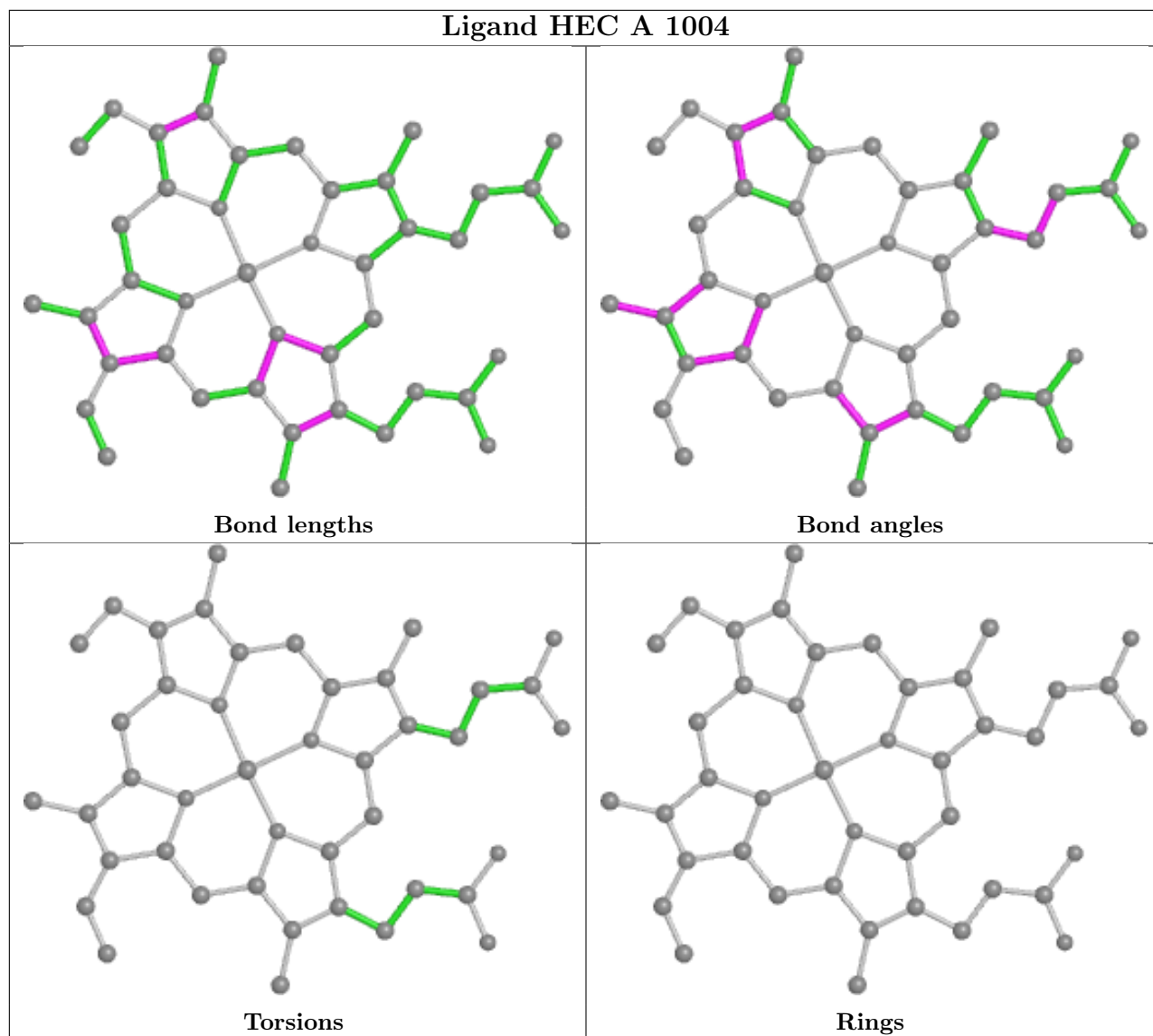


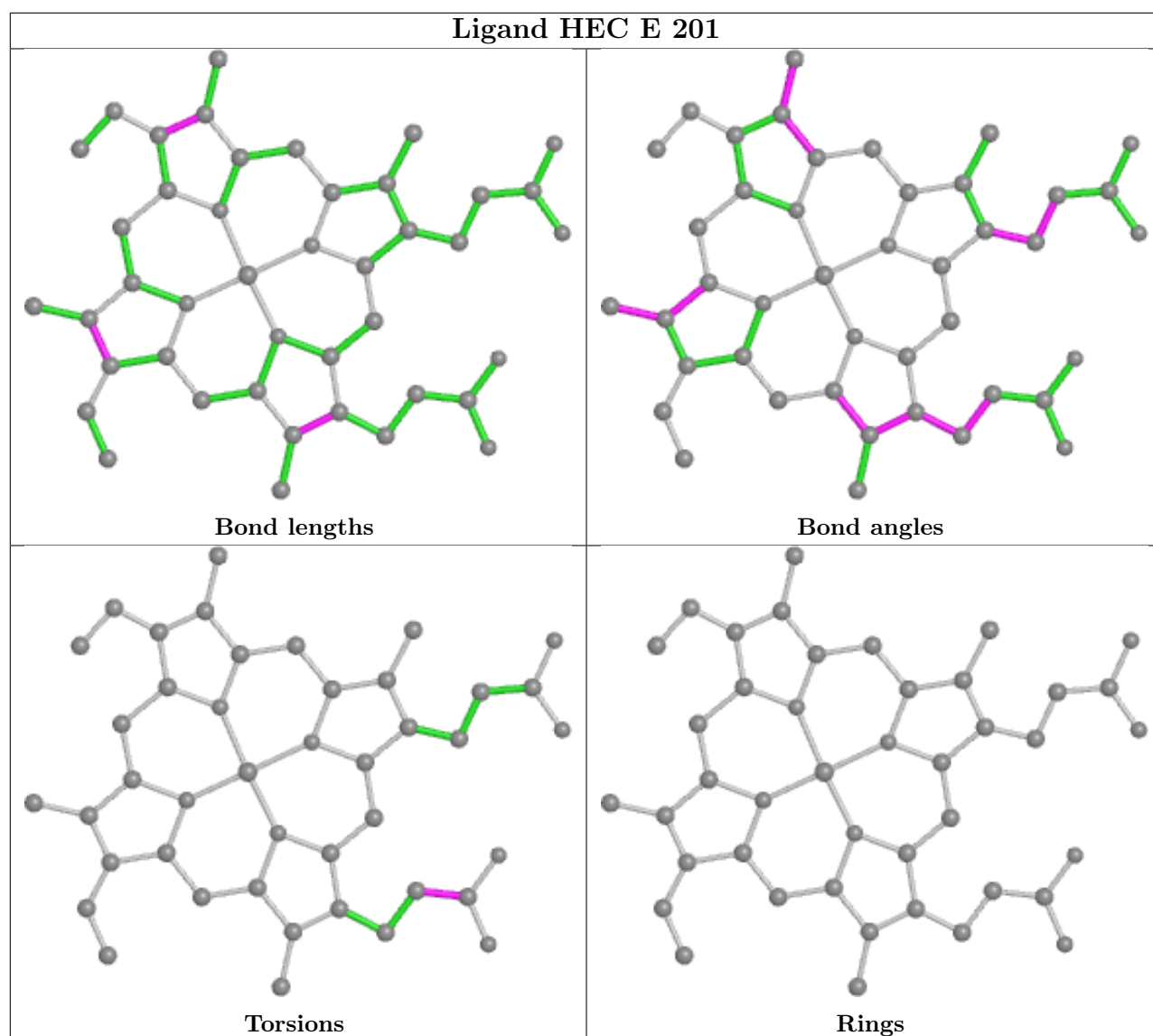












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

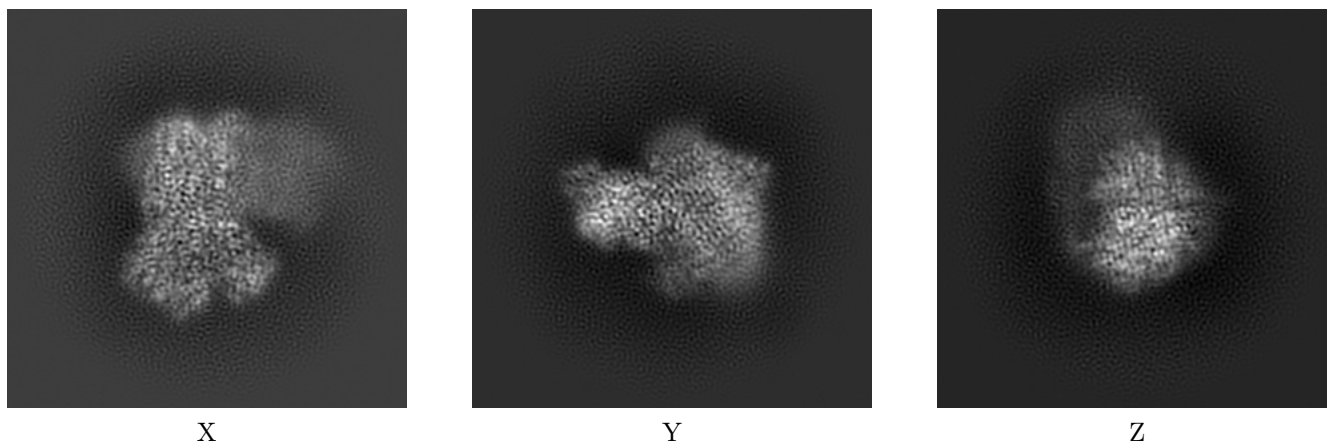
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-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](#)

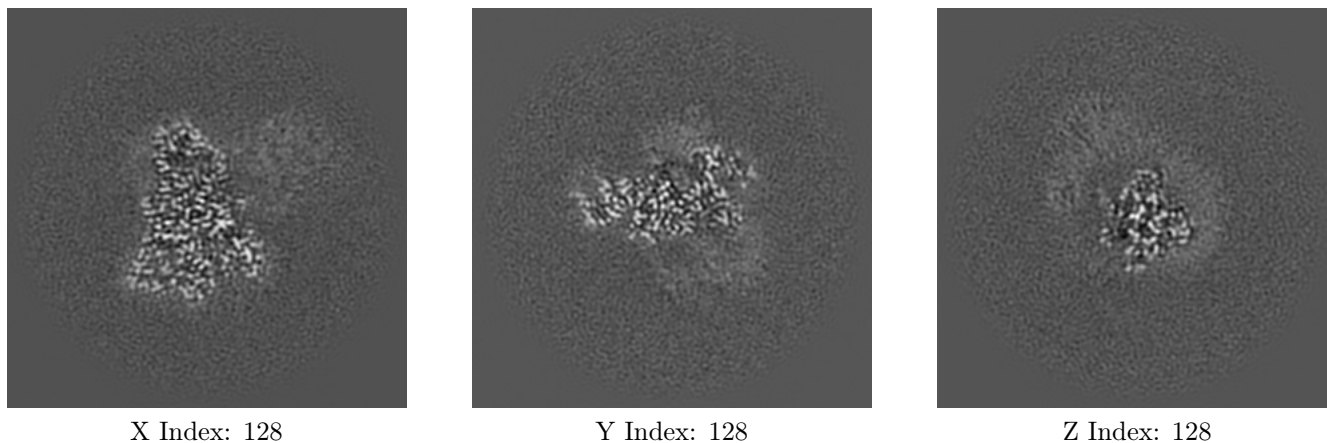
6.1.1 Primary map



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

6.2 Central slices [i](#)

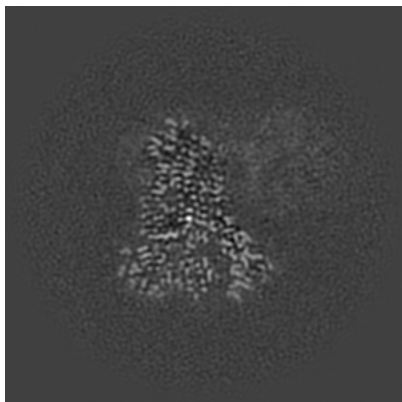
6.2.1 Primary map



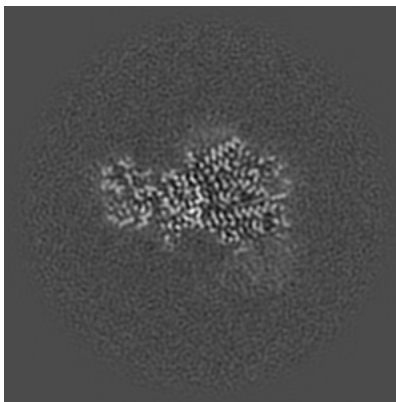
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

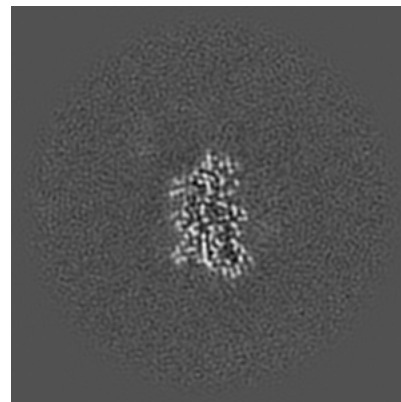
6.3.1 Primary map



X Index: 123



Y Index: 119



Z Index: 108

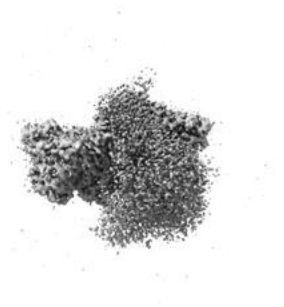
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

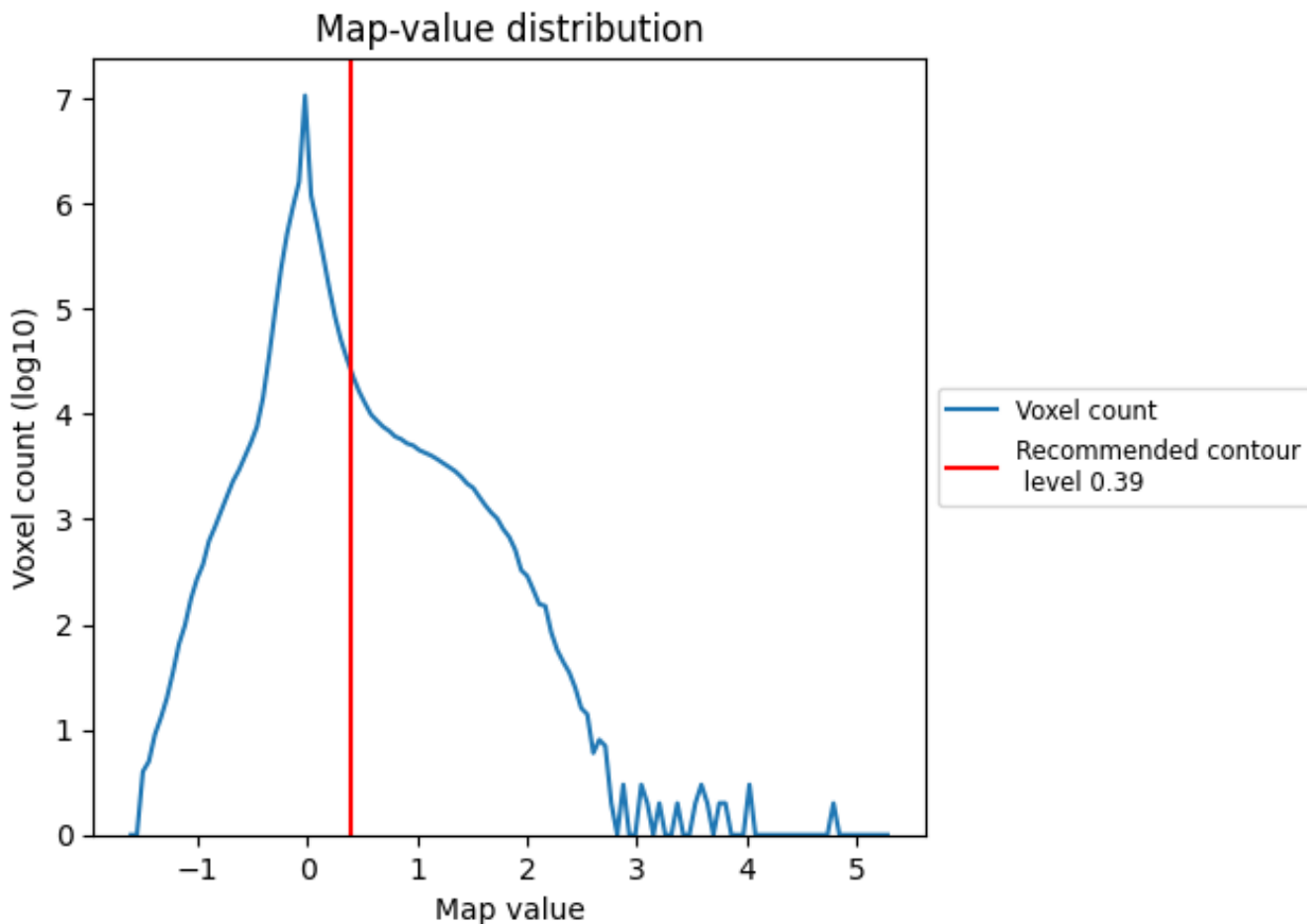
6.5 Mask visualisation

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

7 Map analysis [i](#)

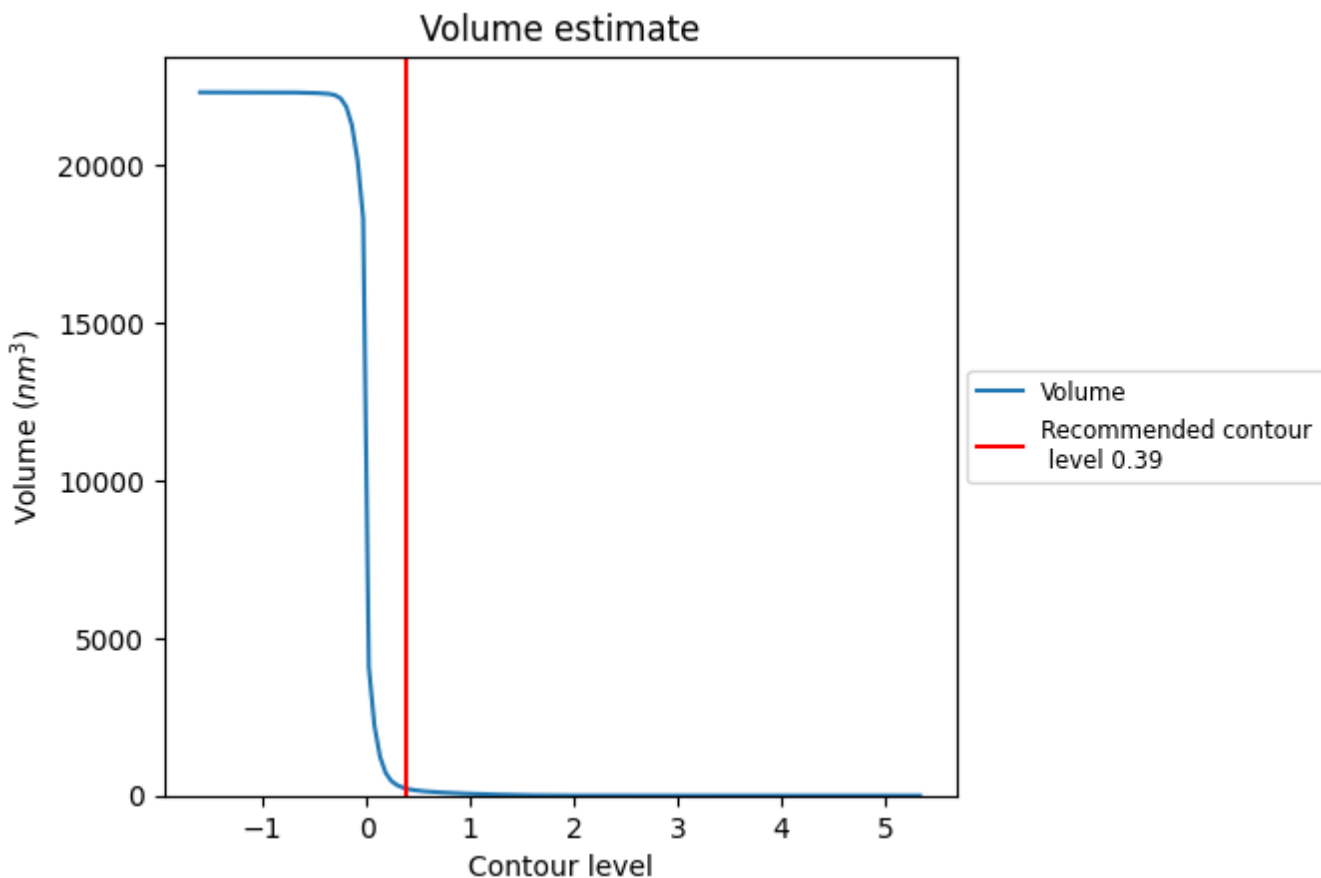
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

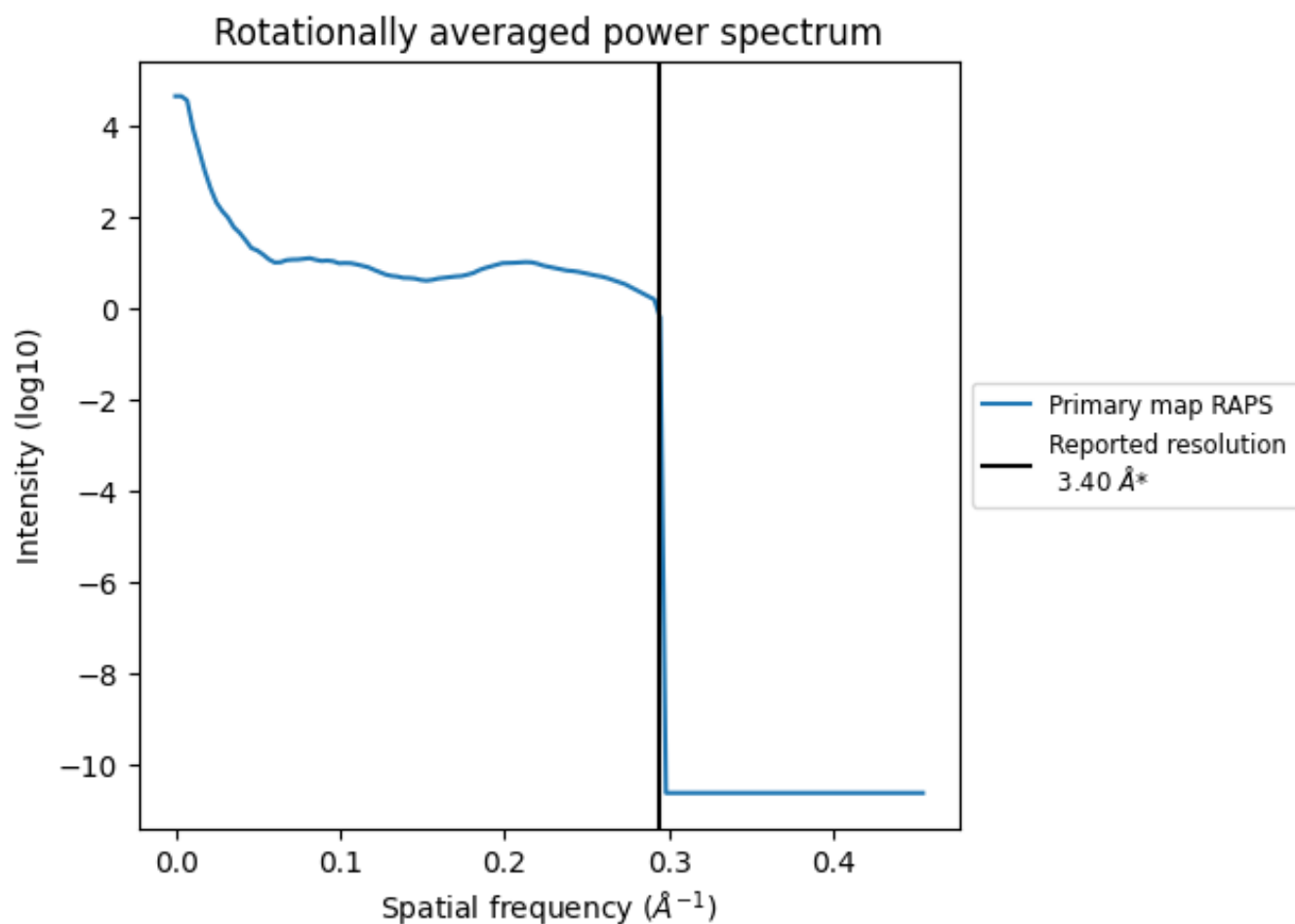
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

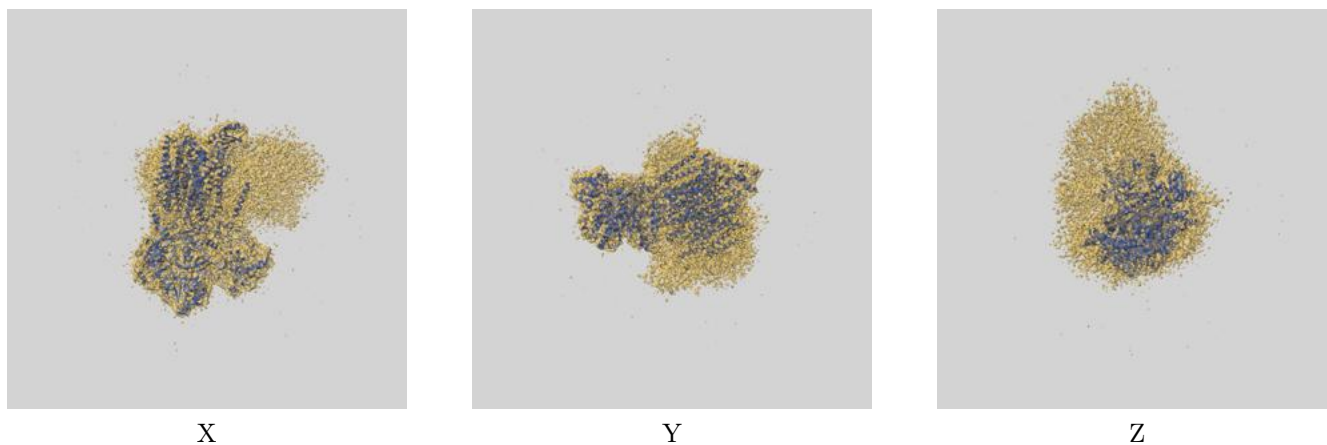
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

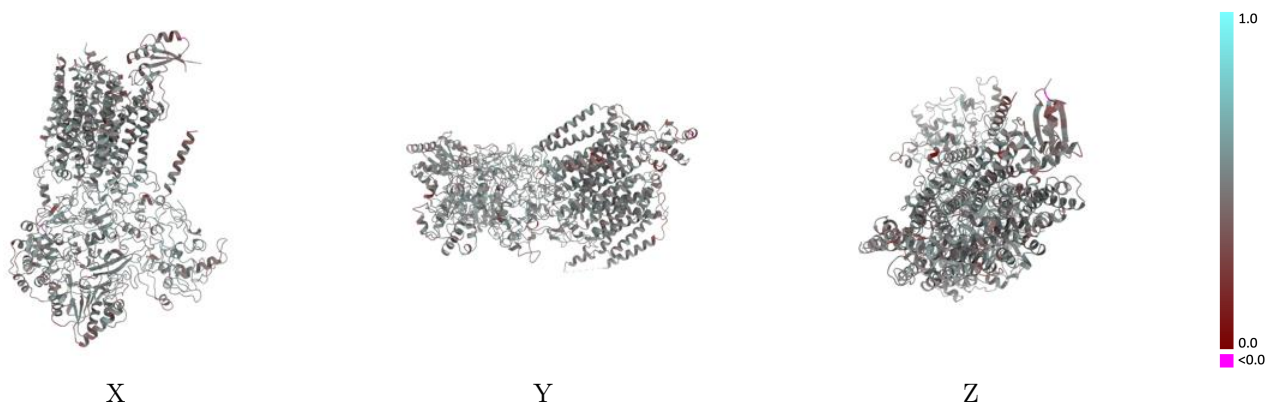
This section contains information regarding the fit between EMDB map EMD-7286 and PDB model 6BTM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



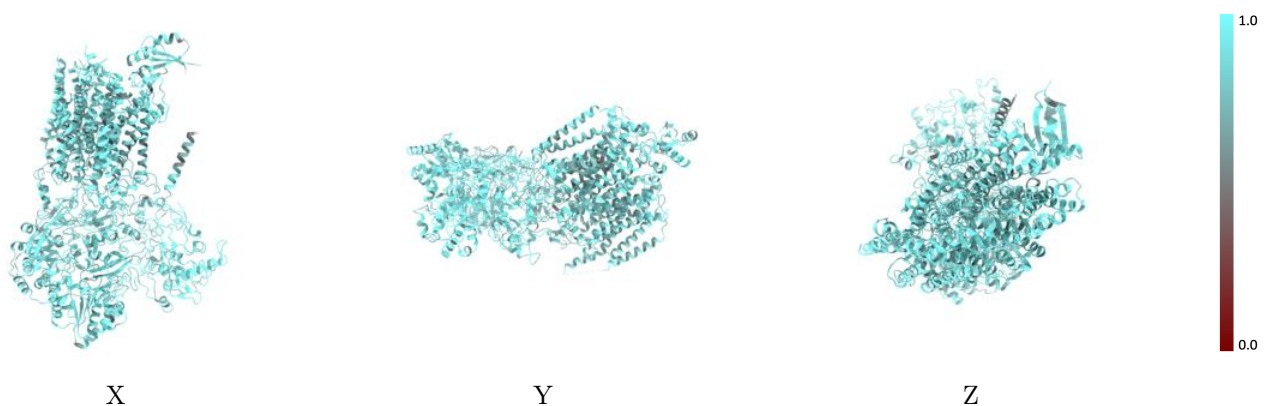
The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



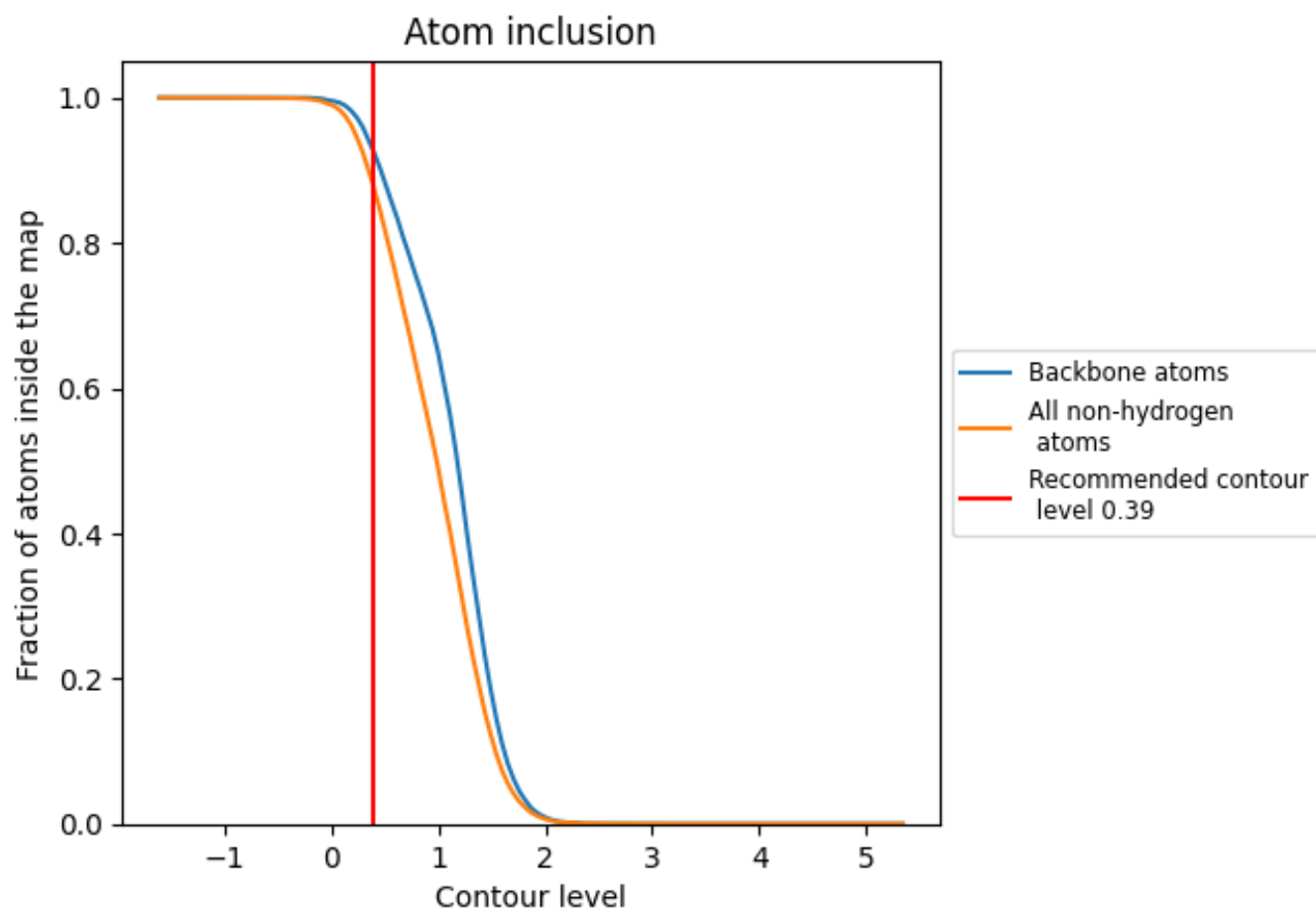
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8804	 0.4820
A	 0.8820	 0.4800
B	 0.8871	 0.4830
C	 0.8778	 0.4900
D	 0.8574	 0.4590
E	 0.9039	 0.4900
F	 0.8672	 0.4760

