



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:26 AM UTC

PDB ID : 8D9M / pdb_00008d9m
EMDB ID : EMD-27266
Title : Cryo-EM of the OmcZ nanowires from *Geobacter sulfurreducens*
Authors : Wang, F.; Chan, C.H.; Mustafa, K.; Hochbaum, A.I.; Bond, D.R.; Egelman, E.H.
Deposited on : 2022-06-10
Resolution : 4.20 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.dev132
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) : 2.49

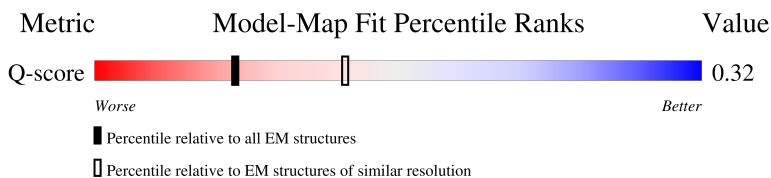
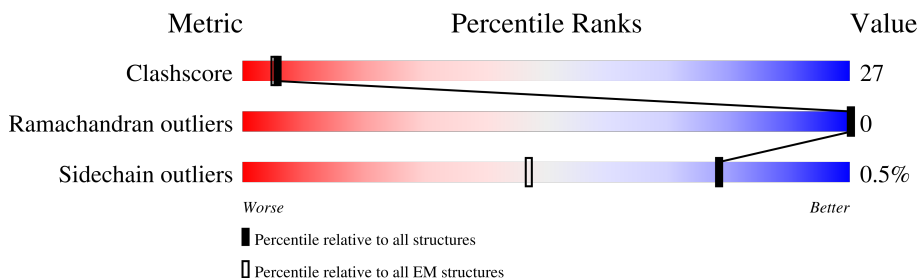
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

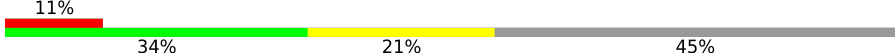
The reported resolution of this entry is 4.20 Å.

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	5410 (3.70 - 4.70)

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.

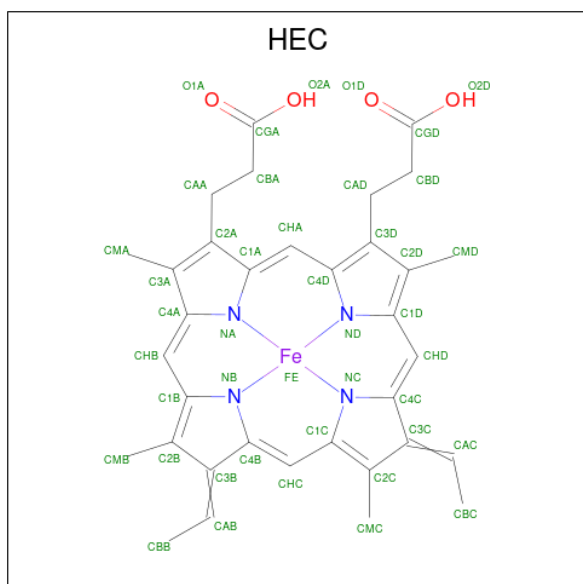
Mol	Chain	Length	Quality of chain
1	A	473	

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	258	Total	C	N	O	S	0	0
			1937	1196	348	375	18		

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-158.2°, rise=58.1 Å, axial sym=C1	Depositor
Number of segments used	92170	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 ($e^-/\text{Å}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.127	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: 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	0.21	0/1996	0.48	0/2739

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	1796	113	0
2	A	344	0	246	62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2281	0	2042	117	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 27.

All (117) 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)
1:A:77:CYS:SG	2:A:601:HEC:HAB	1.29	1.70
1:A:131:CYS:CB	2:A:604:HEC:HAB	1.14	1.55
1:A:131:CYS:HB3	2:A:604:HEC:CAB	1.35	1.51
1:A:50:CYS:SG	2:A:603:HEC:CAB	2.04	1.45
1:A:275:CYS:SG	2:A:608:HEC:CAC	2.05	1.44
1:A:217:CYS:SG	2:A:606:HEC:CAC	2.08	1.42
1:A:53:CYS:SG	2:A:603:HEC:CAC	2.13	1.34
1:A:131:CYS:SG	2:A:604:HEC:CAB	2.16	1.34
1:A:131:CYS:SG	2:A:604:HEC:HAB	1.66	1.33
1:A:77:CYS:SG	2:A:601:HEC:CAB	2.17	1.31
1:A:217:CYS:SG	2:A:606:HEC:HAC	1.71	1.26
1:A:53:CYS:SG	2:A:603:HEC:C3C	2.36	1.13
1:A:131:CYS:CB	2:A:604:HEC:CAB	1.96	1.08
1:A:77:CYS:CB	2:A:601:HEC:HAB	2.00	0.91
1:A:53:CYS:SG	2:A:603:HEC:HAC	2.19	0.83
1:A:121:HIS:HD1	1:A:209:THR:HB	1.44	0.81
1:A:131:CYS:HB3	2:A:604:HEC:HAB	0.82	0.80
1:A:37:ILE:HG21	1:A:135:HIS:HB2	1.67	0.77
1:A:131:CYS:HB3	2:A:604:HEC:C3B	2.13	0.77
1:A:256:PRO:HA	1:A:267:GLY:HA2	1.70	0.74
1:A:53:CYS:SG	2:A:603:HEC:C2C	2.77	0.73
1:A:180:ALA:HB3	2:A:607:HEC:HMC1	1.72	0.71
1:A:131:CYS:CB	2:A:604:HEC:C3B	2.70	0.70
1:A:151:TYR:H	1:A:227:ARG:HH22	1.39	0.69
1:A:150:THR:HA	1:A:227:ARG:HH12	1.58	0.69
1:A:121:HIS:CE1	2:A:604:HEC:NA	2.61	0.68
1:A:250:ASN:ND2	1:A:259:GLU:OE2	2.28	0.67
1:A:275:CYS:HB2	2:A:608:HEC:C3C	2.26	0.65
1:A:217:CYS:HG	2:A:606:HEC:HAC	1.58	0.63
1:A:51:LEU:HB2	2:A:603:HEC:HMC1	1.80	0.62
1:A:275:CYS:CB	2:A:608:HEC:CAC	2.77	0.62
1:A:275:CYS:CB	2:A:608:HEC:C3C	2.79	0.61
1:A:56:SER:HB3	1:A:59:VAL:HB	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:HIS:HD2	2:A:604:HEC:C4C	2.16	0.59
1:A:138:PHE:O	1:A:237:SER:OG	2.20	0.59
1:A:161:SER:OG	1:A:176:GLN:OE1	2.16	0.59
1:A:38:TYR:CZ	1:A:197:ARG:HD2	2.39	0.58
1:A:261:LEU:HB3	1:A:268:ASN:HD22	1.68	0.57
1:A:77:CYS:CB	2:A:601:HEC:CAB	2.73	0.57
1:A:183:GLN:HG2	1:A:184:ALA:H	1.69	0.57
2:A:604:HEC:HBA2	2:A:605:HEC:HBD2	1.87	0.57
1:A:219:ASN:H	1:A:228:GLN:HG3	1.70	0.57
1:A:218:HIS:ND1	1:A:228:GLN:OE1	2.31	0.56
1:A:185:ALA:HB3	1:A:199:ILE:HB	1.88	0.55
1:A:77:CYS:HB3	2:A:601:HEC:HHC	1.88	0.55
1:A:147:TYR:CD2	1:A:149:PRO:HD3	2.41	0.55
1:A:87:THR:H	1:A:90:THR:HG1	1.53	0.54
2:A:605:HEC:HHA	2:A:605:HEC:HBD1	1.88	0.54
1:A:47:LYS:HE3	2:A:602:HEC:HBB1	1.89	0.54
1:A:61:VAL:HG12	2:A:601:HEC:HBD2	1.89	0.54
1:A:226:ILE:O	1:A:230:GLU:HG3	2.08	0.54
1:A:182:HIS:CE1	2:A:607:HEC:ND	2.76	0.54
1:A:54:HIS:NE2	2:A:603:HEC:C1D	2.68	0.54
1:A:120:HIS:CE1	2:A:603:HEC:NB	2.69	0.53
1:A:217:CYS:CB	2:A:606:HEC:CAC	2.86	0.53
1:A:135:HIS:HD2	2:A:604:HEC:NC	1.95	0.53
1:A:54:HIS:HD2	2:A:603:HEC:NC	2.00	0.52
1:A:261:LEU:HD12	1:A:270:TRP:CD1	2.44	0.51
1:A:217:CYS:CB	2:A:606:HEC:C3C	2.88	0.51
1:A:121:HIS:ND1	1:A:209:THR:HB	2.20	0.51
1:A:234:GLY:O	1:A:238:LEU:HG	2.10	0.50
1:A:275:CYS:HB2	2:A:608:HEC:C2C	2.42	0.49
1:A:217:CYS:SG	2:A:606:HEC:C3C	2.95	0.49
1:A:46:THR:HG23	1:A:49:ASP:H	1.78	0.49
1:A:236:ASN:OD1	1:A:237:SER:N	2.45	0.49
1:A:217:CYS:HB2	2:A:606:HEC:C3C	2.43	0.49
1:A:52:GLU:HA	1:A:55:VAL:HB	1.95	0.49
2:A:607:HEC:HHA	2:A:607:HEC:HBD2	1.94	0.49
1:A:274:GLY:HA2	1:A:280:PHE:CZ	2.48	0.48
1:A:111:CYS:HB2	2:A:602:HEC:HHC	1.96	0.48
1:A:275:CYS:SG	2:A:608:HEC:C3C	2.94	0.48
1:A:200:PHE:HB3	1:A:204:ASP:HB2	1.96	0.48
1:A:239:HIS:HE1	2:A:608:HEC:ND	2.12	0.48
1:A:207:HIS:NE2	2:A:606:HEC:C4B	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:C	1:A:91:GLY:HA3	2.40	0.47
1:A:200:PHE:HD2	1:A:204:ASP:HB3	1.79	0.47
1:A:245:SER:OG	1:A:259:GLU:OE1	2.26	0.47
1:A:159:MET:HG2	1:A:175:VAL:HG13	1.95	0.47
1:A:217:CYS:SG	2:A:606:HEC:CBC	2.98	0.47
1:A:146:HIS:NE2	1:A:148:ILE:HD11	2.30	0.47
1:A:233:HIS:CD2	2:A:605:HEC:NC	2.83	0.46
1:A:54:HIS:HD2	2:A:603:HEC:C1C	2.29	0.46
1:A:241:ILE:HD11	1:A:265:HIS:CE1	2.50	0.46
1:A:150:THR:HA	1:A:227:ARG:NH1	2.29	0.46
1:A:206:HIS:HE1	2:A:605:HEC:C1A	2.27	0.46
1:A:77:CYS:SG	2:A:601:HEC:CBB	3.00	0.46
1:A:93:HIS:CE1	2:A:601:HEC:ND	2.84	0.46
1:A:109:ARG:NH2	2:A:601:HEC:O1A	2.48	0.46
1:A:151:TYR:H	1:A:227:ARG:NH2	2.12	0.45
1:A:159:MET:N	1:A:160:PRO:HD3	2.31	0.45
1:A:233:HIS:HB3	1:A:238:LEU:HD21	1.98	0.45
2:A:605:HEC:HMC3	2:A:605:HEC:HBC3	1.98	0.45
1:A:77:CYS:CB	2:A:601:HEC:HHC	2.46	0.45
1:A:275:CYS:SG	2:A:608:HEC:CBC	2.96	0.45
1:A:203:GLN:O	1:A:207:HIS:HB2	2.17	0.45
1:A:111:CYS:HB2	2:A:602:HEC:CHC	2.46	0.45
1:A:202:ASN:HA	1:A:205:THR:OG1	2.17	0.44
1:A:156:VAL:O	1:A:156:VAL:HG13	2.18	0.44
1:A:183:GLN:H	1:A:183:GLN:CD	2.25	0.44
1:A:132:LYS:HD3	1:A:139:ILE:O	2.17	0.44
1:A:49:ASP:OD1	1:A:193:THR:HG21	2.19	0.43
1:A:161:SER:HA	1:A:180:ALA:HB2	2.01	0.43
1:A:65:HIS:HE1	2:A:601:HEC:C4D	2.32	0.43
1:A:163:ARG:NH1	1:A:179:GLU:O	2.40	0.42
1:A:146:HIS:HD2	1:A:234:GLY:HA3	1.85	0.42
1:A:30:PRO:HA	1:A:183:GLN:NE2	2.35	0.42
1:A:270:TRP:CH2	1:A:280:PHE:HB3	2.54	0.42
1:A:219:ASN:H	1:A:228:GLN:CG	2.32	0.42
1:A:268:ASN:OD1	1:A:269:ASN:N	2.50	0.41
1:A:39:ASP:OD1	1:A:197:ARG:NH2	2.52	0.41
1:A:30:PRO:HA	1:A:183:GLN:HE22	1.86	0.41
1:A:162:GLY:H	1:A:173:VAL:HG23	1.84	0.41
1:A:92:CYS:SG	2:A:602:HEC:HMD1	2.61	0.41
1:A:241:ILE:HG13	1:A:241:ILE:O	2.20	0.41
1:A:132:LYS:HG3	1:A:136:GLY:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:O	1:A:257:GLY:N	2.51	0.40
1:A:206:HIS:HB3	2:A:606:HEC:HHD	2.02	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	256/473 (54%)	212 (83%)	44 (17%)	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	222/389 (57%)	221 (100%)	1 (0%)	81	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	273	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	HEC	A	601	1	46,50,50	1.89	6 (13%)	58,82,82	2.03	8 (13%)
2	HEC	A	604	1	46,50,50	1.86	5 (10%)	58,82,82	1.76	7 (12%)
2	HEC	A	605	1	46,50,50	1.85	6 (13%)	58,82,82	1.77	5 (8%)
2	HEC	A	608	1	46,50,50	1.85	6 (13%)	58,82,82	1.68	4 (6%)
2	HEC	A	603	1	46,50,50	1.86	5 (10%)	58,82,82	1.60	7 (12%)
2	HEC	A	602	1	46,50,50	1.86	7 (15%)	58,82,82	1.87	4 (6%)
2	HEC	A	607	1	46,50,50	1.84	6 (13%)	58,82,82	1.96	6 (10%)
2	HEC	A	606	1	46,50,50	1.86	6 (13%)	58,82,82	1.85	4 (6%)

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
2	HEC	A	601	1	-	8/14/54/54	-
2	HEC	A	604	1	-	8/14/54/54	-
2	HEC	A	605	1	-	11/14/54/54	-
2	HEC	A	608	1	-	4/14/54/54	-
2	HEC	A	603	1	-	4/14/54/54	-
2	HEC	A	602	1	-	11/14/54/54	-
2	HEC	A	607	1	-	9/14/54/54	-
2	HEC	A	606	1	-	6/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	HEC	CAB-C3B	6.40	1.55	1.35
2	A	604	HEC	CAC-C3C	6.27	1.55	1.35
2	A	603	HEC	CAC-C3C	6.25	1.55	1.35
2	A	601	HEC	CAB-C3B	6.25	1.55	1.35
2	A	602	HEC	CAB-C3B	6.24	1.55	1.35
2	A	605	HEC	CAC-C3C	6.18	1.55	1.35
2	A	607	HEC	CAB-C3B	6.18	1.55	1.35
2	A	604	HEC	CAB-C3B	6.17	1.55	1.35
2	A	606	HEC	CAC-C3C	6.17	1.55	1.35
2	A	601	HEC	CAC-C3C	6.12	1.54	1.35
2	A	608	HEC	CAB-C3B	6.10	1.54	1.35
2	A	608	HEC	CAC-C3C	6.06	1.54	1.35
2	A	607	HEC	CAC-C3C	6.06	1.54	1.35
2	A	603	HEC	CAB-C3B	6.05	1.54	1.35
2	A	605	HEC	CAB-C3B	6.05	1.54	1.35
2	A	602	HEC	CAC-C3C	6.04	1.54	1.35
2	A	603	HEC	C3D-C2D	5.60	1.53	1.38
2	A	602	HEC	C3D-C2D	5.59	1.53	1.38
2	A	608	HEC	C3D-C2D	5.58	1.53	1.38
2	A	604	HEC	C3D-C2D	5.56	1.53	1.38
2	A	605	HEC	C3D-C2D	5.54	1.53	1.38
2	A	607	HEC	C3D-C2D	5.53	1.53	1.38
2	A	606	HEC	C3D-C2D	5.50	1.53	1.38
2	A	601	HEC	C3D-C2D	5.44	1.53	1.38
2	A	601	HEC	CMB-C2B	2.63	1.56	1.50
2	A	604	HEC	CMC-C2C	2.38	1.55	1.50
2	A	605	HEC	CMC-C2C	2.26	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	HEC	C3B-C2B	-2.26	1.33	1.41
2	A	602	HEC	C3C-C2C	-2.24	1.33	1.41
2	A	603	HEC	CMC-C2C	2.23	1.55	1.50
2	A	602	HEC	C3B-C2B	-2.17	1.33	1.41
2	A	607	HEC	C3C-C2C	-2.16	1.33	1.41
2	A	605	HEC	C3B-C2B	-2.16	1.33	1.41
2	A	601	HEC	C3C-C2C	-2.15	1.33	1.41
2	A	608	HEC	C3C-C2C	-2.14	1.33	1.41
2	A	606	HEC	C3B-C2B	-2.14	1.33	1.41
2	A	607	HEC	C3B-C2B	-2.11	1.34	1.41
2	A	601	HEC	CMC-C2C	2.10	1.55	1.50
2	A	606	HEC	CMC-C2C	2.10	1.55	1.50
2	A	603	HEC	C3B-C2B	-2.08	1.34	1.41
2	A	602	HEC	CMC-C2C	2.05	1.55	1.50
2	A	602	HEC	CMB-C2B	2.04	1.55	1.50
2	A	606	HEC	CMB-C2B	2.04	1.55	1.50
2	A	608	HEC	C3B-C2B	-2.02	1.34	1.41
2	A	608	HEC	CMB-C2B	2.01	1.54	1.50
2	A	605	HEC	CMB-C2B	2.00	1.54	1.50
2	A	607	HEC	CMB-C2B	2.00	1.54	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	HEC	CBB-CAB-C3B	-9.83	107.79	127.43
2	A	601	HEC	CBB-CAB-C3B	-9.14	109.17	127.43
2	A	605	HEC	CBB-CAB-C3B	-8.63	110.18	127.43
2	A	602	HEC	CBB-CAB-C3B	-8.61	110.23	127.43
2	A	606	HEC	CBB-CAB-C3B	-8.49	110.46	127.43
2	A	602	HEC	CBC-CAC-C3C	-8.42	110.61	127.43
2	A	601	HEC	CBC-CAC-C3C	-7.75	111.94	127.43
2	A	607	HEC	CBC-CAC-C3C	-7.75	111.94	127.43
2	A	604	HEC	CBB-CAB-C3B	-7.70	112.05	127.43
2	A	606	HEC	CBC-CAC-C3C	-7.54	112.36	127.43
2	A	608	HEC	CBC-CAC-C3C	-7.44	112.56	127.43
2	A	608	HEC	CBB-CAB-C3B	-6.56	114.32	127.43
2	A	604	HEC	CBC-CAC-C3C	-6.37	114.70	127.43
2	A	603	HEC	CBC-CAC-C3C	-6.26	114.93	127.43
2	A	605	HEC	CBC-CAC-C3C	-5.83	115.78	127.43
2	A	603	HEC	CBB-CAB-C3B	-5.12	117.21	127.43
2	A	601	HEC	CAD-C3D-C4D	4.23	133.20	124.94
2	A	603	HEC	CMC-C2C-C1C	-3.46	120.15	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEC	CMC-C2C-C1C	-3.44	120.19	125.42
2	A	606	HEC	C4D-ND-C1D	3.41	111.37	105.82
2	A	603	HEC	C4D-ND-C1D	3.27	111.16	105.82
2	A	601	HEC	C4D-ND-C1D	3.25	111.12	105.82
2	A	605	HEC	C4D-ND-C1D	3.17	110.99	105.82
2	A	607	HEC	C4D-ND-C1D	3.07	110.83	105.82
2	A	608	HEC	C4D-ND-C1D	3.05	110.79	105.82
2	A	604	HEC	C4D-ND-C1D	3.01	110.72	105.82
2	A	602	HEC	C4D-ND-C1D	2.98	110.68	105.82
2	A	605	HEC	CMC-C2C-C1C	-2.67	121.35	125.42
2	A	603	HEC	CHC-C4B-NB	2.36	127.02	124.45
2	A	601	HEC	C2A-C1A-NA	-2.35	108.06	110.32
2	A	604	HEC	CAA-CBA-CGA	-2.32	107.50	113.67
2	A	605	HEC	CAD-C3D-C4D	2.29	129.41	124.94
2	A	601	HEC	CHB-C4A-NA	2.24	126.89	124.45
2	A	606	HEC	C2A-C1A-NA	-2.23	108.17	110.32
2	A	601	HEC	CHA-C1A-NA	2.20	126.85	124.45
2	A	601	HEC	CAD-C3D-C2D	-2.19	122.17	127.07
2	A	604	HEC	C2A-C1A-NA	-2.12	108.27	110.32
2	A	607	HEC	CHA-C1A-NA	2.11	126.75	124.45
2	A	603	HEC	C2A-C1A-NA	-2.10	108.30	110.32
2	A	603	HEC	CHA-C1A-NA	2.09	126.73	124.45
2	A	607	HEC	CHD-C4C-NC	2.06	126.69	124.45
2	A	602	HEC	C2A-C1A-NA	-2.03	108.36	110.32
2	A	604	HEC	CMC-C2C-C3C	2.01	131.29	126.55
2	A	607	HEC	CAD-C3D-C4D	2.01	128.87	124.94
2	A	608	HEC	CMB-C2B-C1B	-2.01	122.36	125.42

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C2C-C3C-CAC-CBC
2	A	601	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C2B-C3B-CAB-CBB
2	A	602	HEC	C4B-C3B-CAB-CBB
2	A	602	HEC	C2C-C3C-CAC-CBC
2	A	602	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C3D-CAD-CBD-CGD
2	A	603	HEC	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	603	HEC	C4B-C3B-CAB-CBB
2	A	603	HEC	C2C-C3C-CAC-CBC
2	A	603	HEC	C4C-C3C-CAC-CBC
2	A	604	HEC	C2B-C3B-CAB-CBB
2	A	604	HEC	C4B-C3B-CAB-CBB
2	A	604	HEC	C2C-C3C-CAC-CBC
2	A	604	HEC	C4C-C3C-CAC-CBC
2	A	605	HEC	C2B-C3B-CAB-CBB
2	A	605	HEC	C4B-C3B-CAB-CBB
2	A	605	HEC	C2C-C3C-CAC-CBC
2	A	605	HEC	C4C-C3C-CAC-CBC
2	A	605	HEC	C4D-C3D-CAD-CBD
2	A	606	HEC	C2B-C3B-CAB-CBB
2	A	606	HEC	C4B-C3B-CAB-CBB
2	A	606	HEC	C2C-C3C-CAC-CBC
2	A	606	HEC	C4C-C3C-CAC-CBC
2	A	607	HEC	C2B-C3B-CAB-CBB
2	A	607	HEC	C2C-C3C-CAC-CBC
2	A	607	HEC	C4C-C3C-CAC-CBC
2	A	608	HEC	C2B-C3B-CAB-CBB
2	A	608	HEC	C4B-C3B-CAB-CBB
2	A	608	HEC	C2C-C3C-CAC-CBC
2	A	608	HEC	C4C-C3C-CAC-CBC
2	A	601	HEC	C4D-C3D-CAD-CBD
2	A	604	HEC	C3D-CAD-CBD-CGD
2	A	607	HEC	C2A-CAA-CBA-CGA
2	A	601	HEC	C2D-C3D-CAD-CBD
2	A	607	HEC	C4D-C3D-CAD-CBD
2	A	602	HEC	C2D-C3D-CAD-CBD
2	A	605	HEC	C2D-C3D-CAD-CBD
2	A	607	HEC	C2D-C3D-CAD-CBD
2	A	602	HEC	C4D-C3D-CAD-CBD
2	A	607	HEC	C4B-C3B-CAB-CBB
2	A	605	HEC	C1A-C2A-CAA-CBA
2	A	601	HEC	CAA-CBA-CGA-O2A
2	A	602	HEC	CAA-CBA-CGA-O2A
2	A	606	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O1A
2	A	607	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	CAD-CBD-CGD-O2D
2	A	604	HEC	C2D-C3D-CAD-CBD
2	A	604	HEC	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

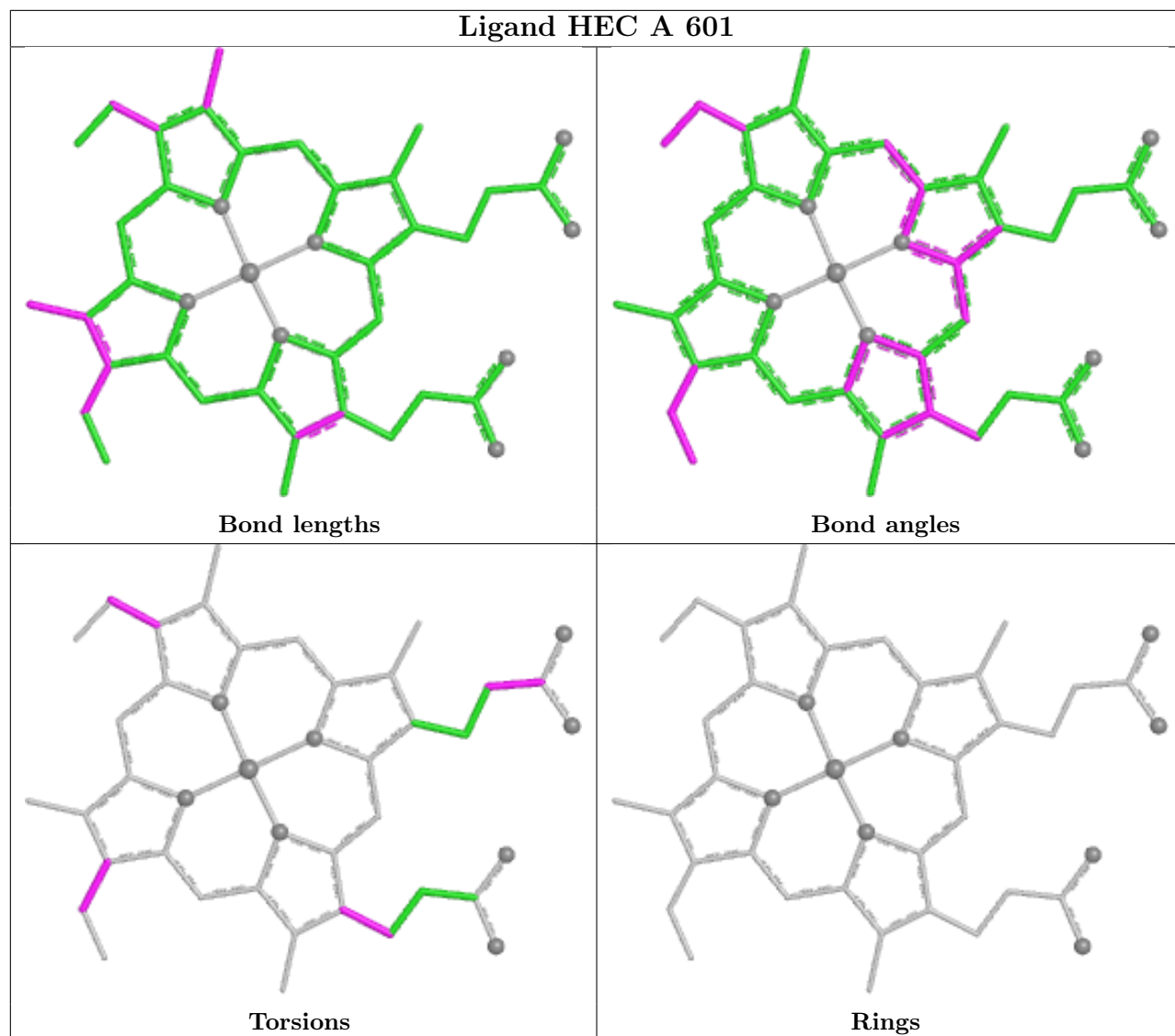
Mol	Chain	Res	Type	Atoms
2	A	602	HEC	CAA-CBA-CGA-O1A
2	A	606	HEC	CAA-CBA-CGA-O1A
2	A	607	HEC	CAA-CBA-CGA-O1A
2	A	602	HEC	CAD-CBD-CGD-O1D
2	A	605	HEC	C3A-C2A-CAA-CBA
2	A	602	HEC	CAD-CBD-CGD-O2D
2	A	605	HEC	CAD-CBD-CGD-O2D
2	A	605	HEC	CAA-CBA-CGA-O2A
2	A	605	HEC	CAA-CBA-CGA-O1A

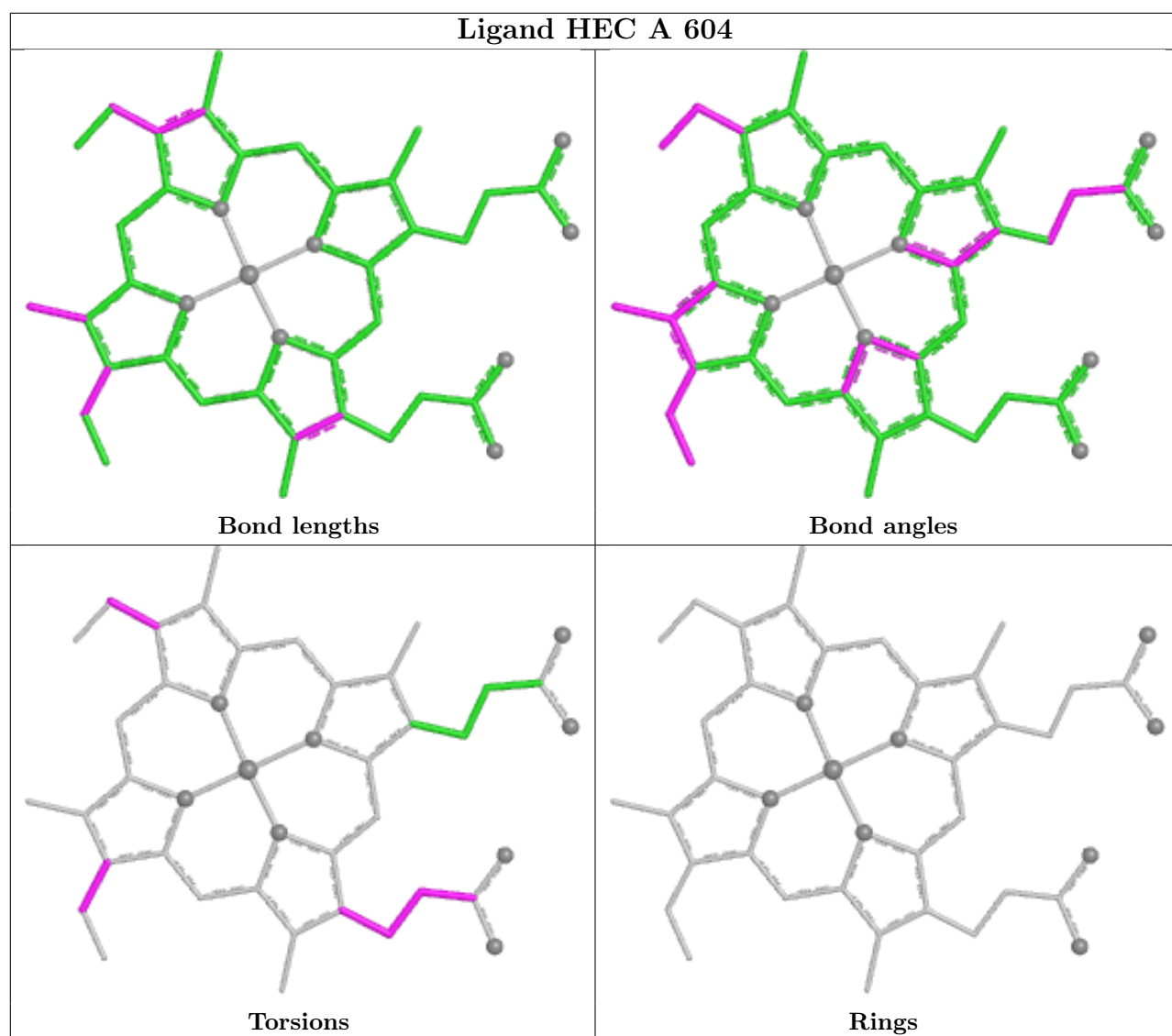
There are no ring outliers.

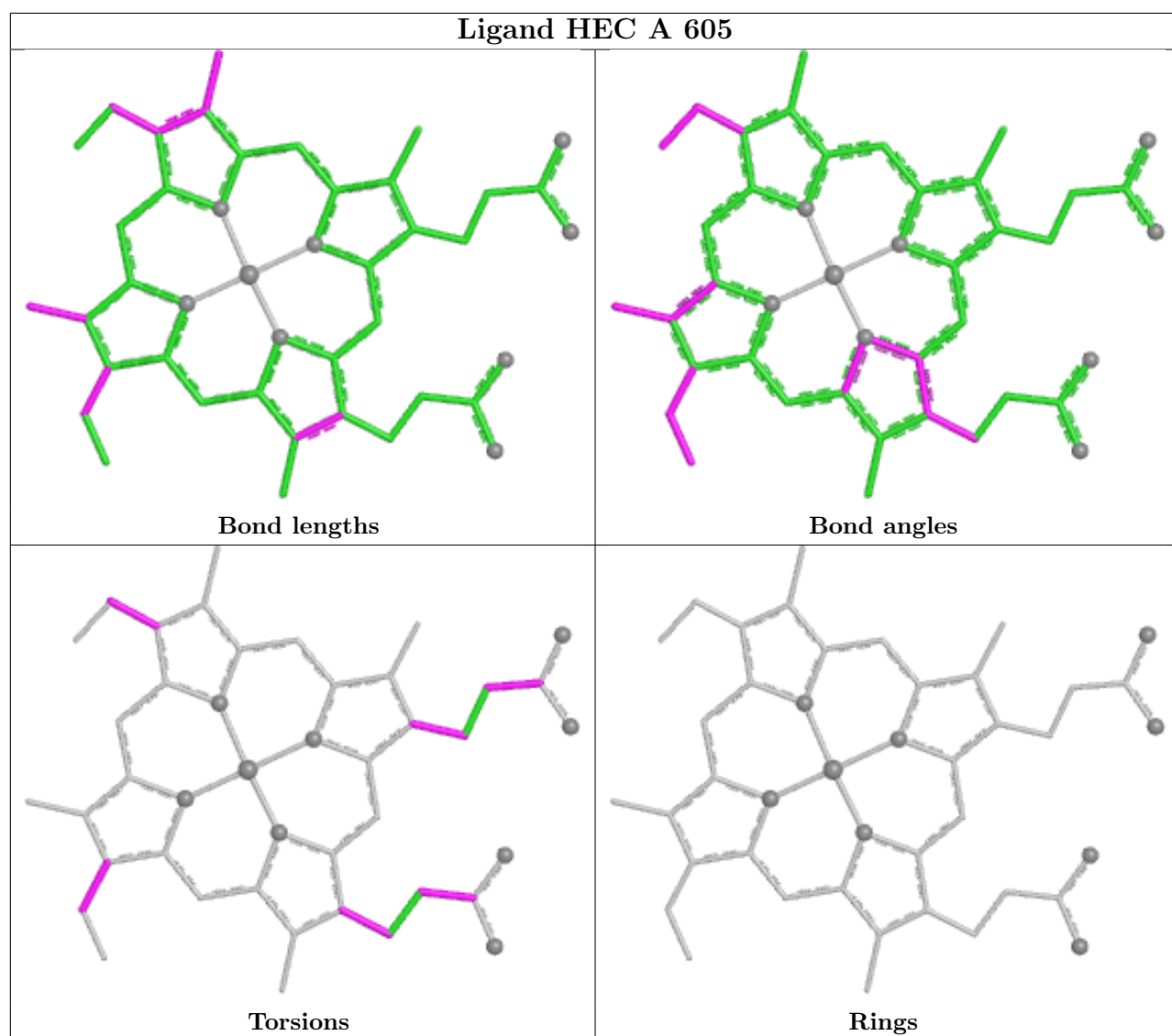
8 monomers are involved in 62 short contacts:

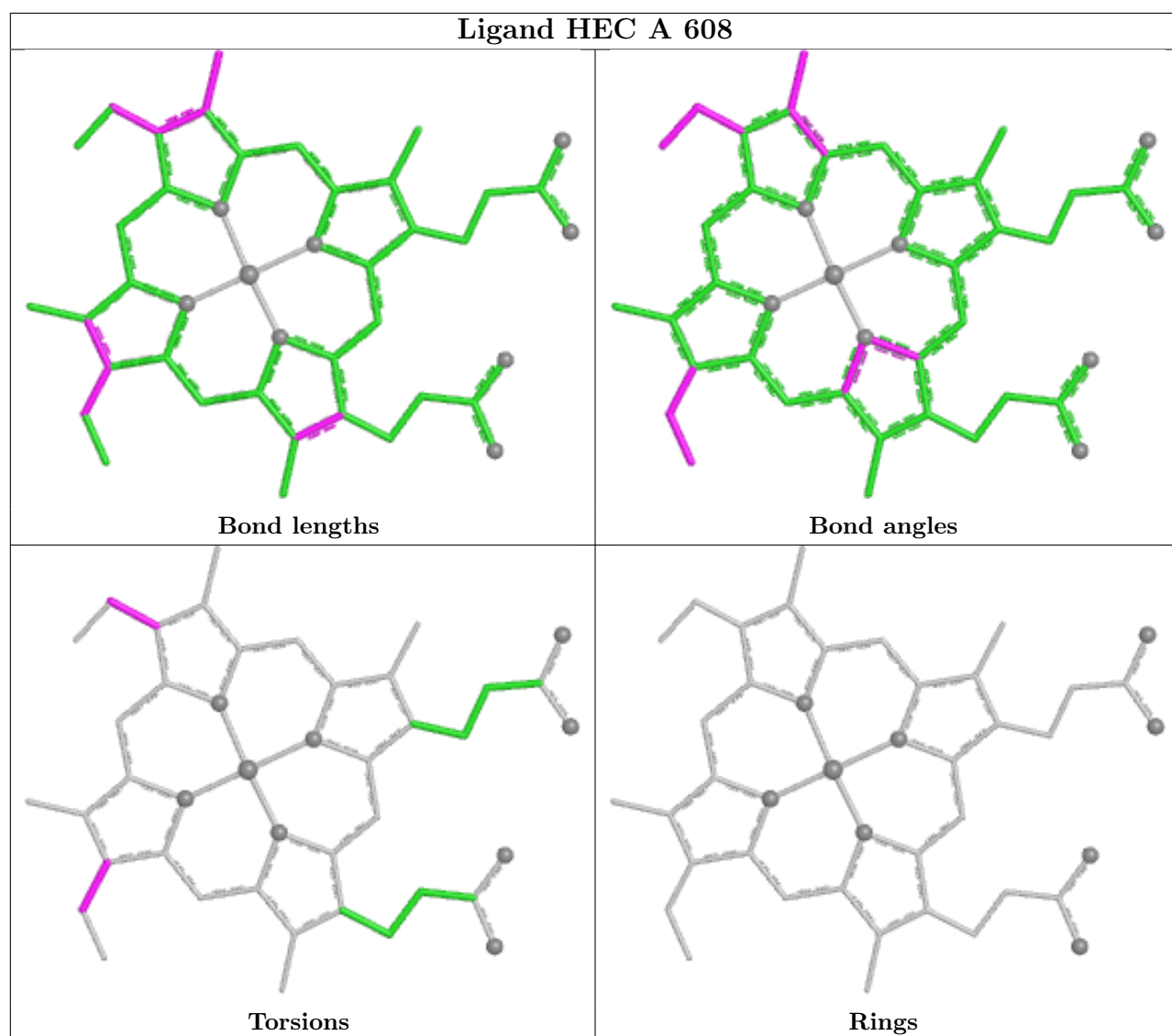
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	11	0
2	A	604	HEC	12	0
2	A	605	HEC	5	0
2	A	608	HEC	8	0
2	A	603	HEC	10	0
2	A	602	HEC	4	0
2	A	607	HEC	3	0
2	A	606	HEC	10	0

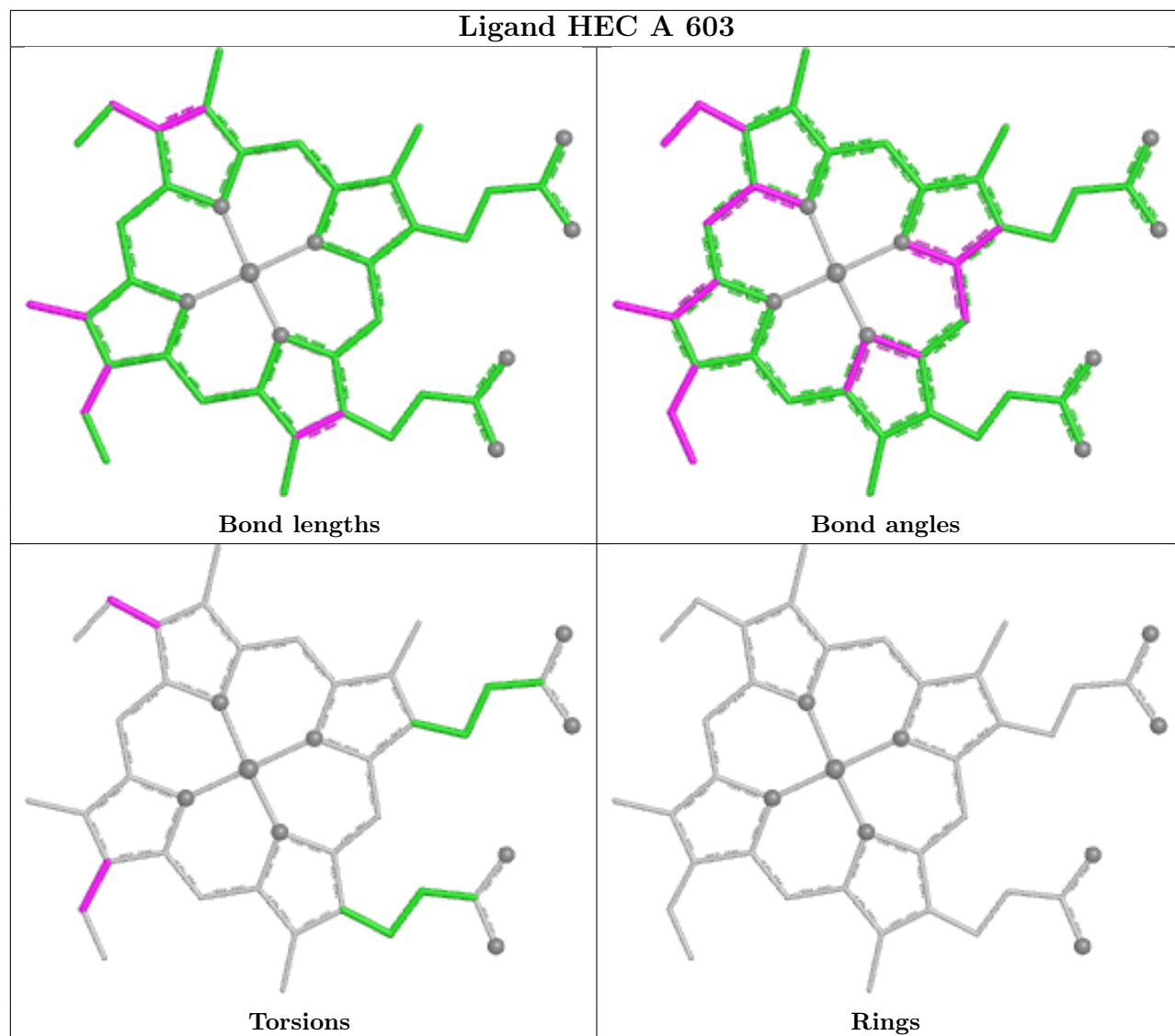
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

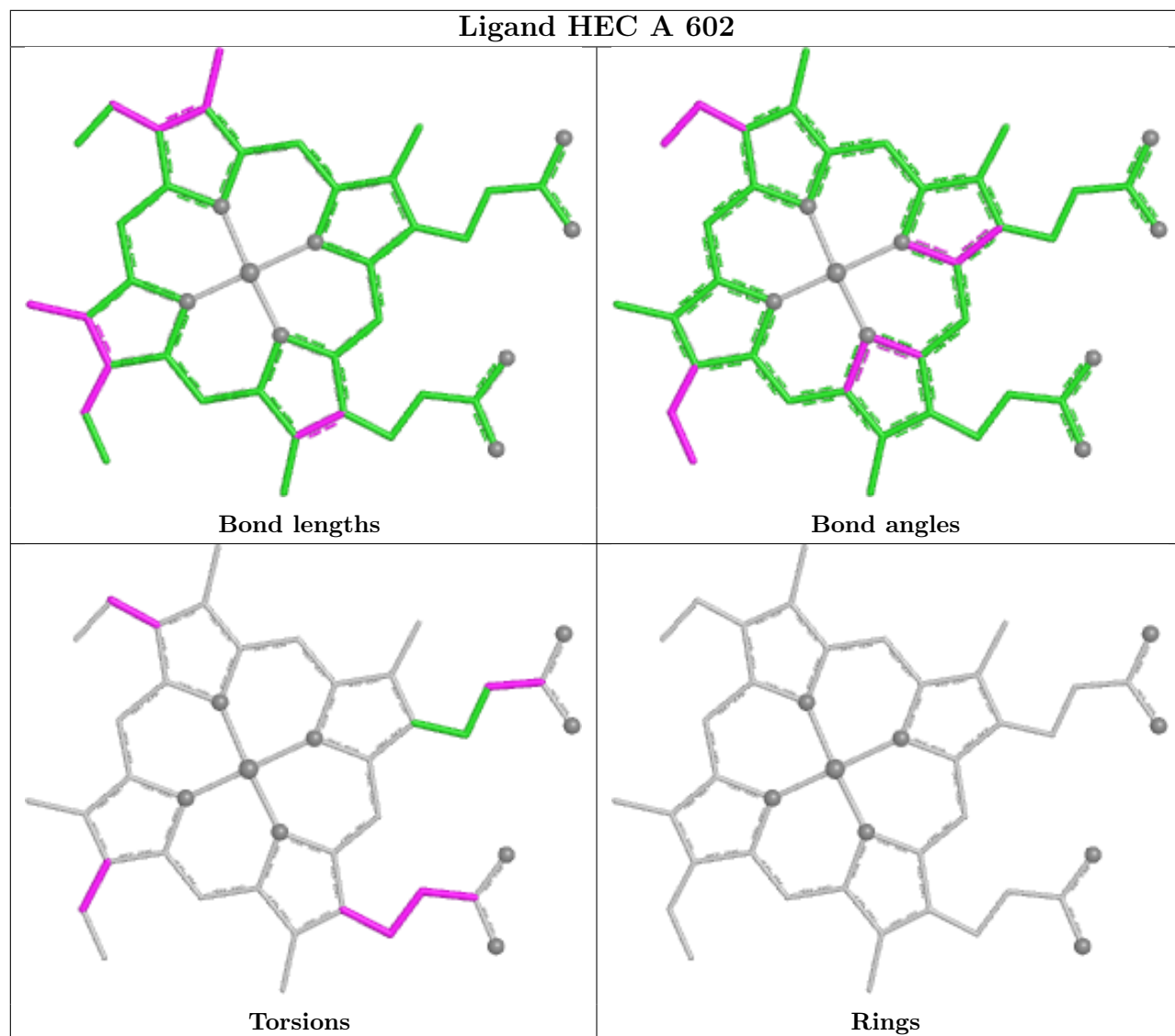


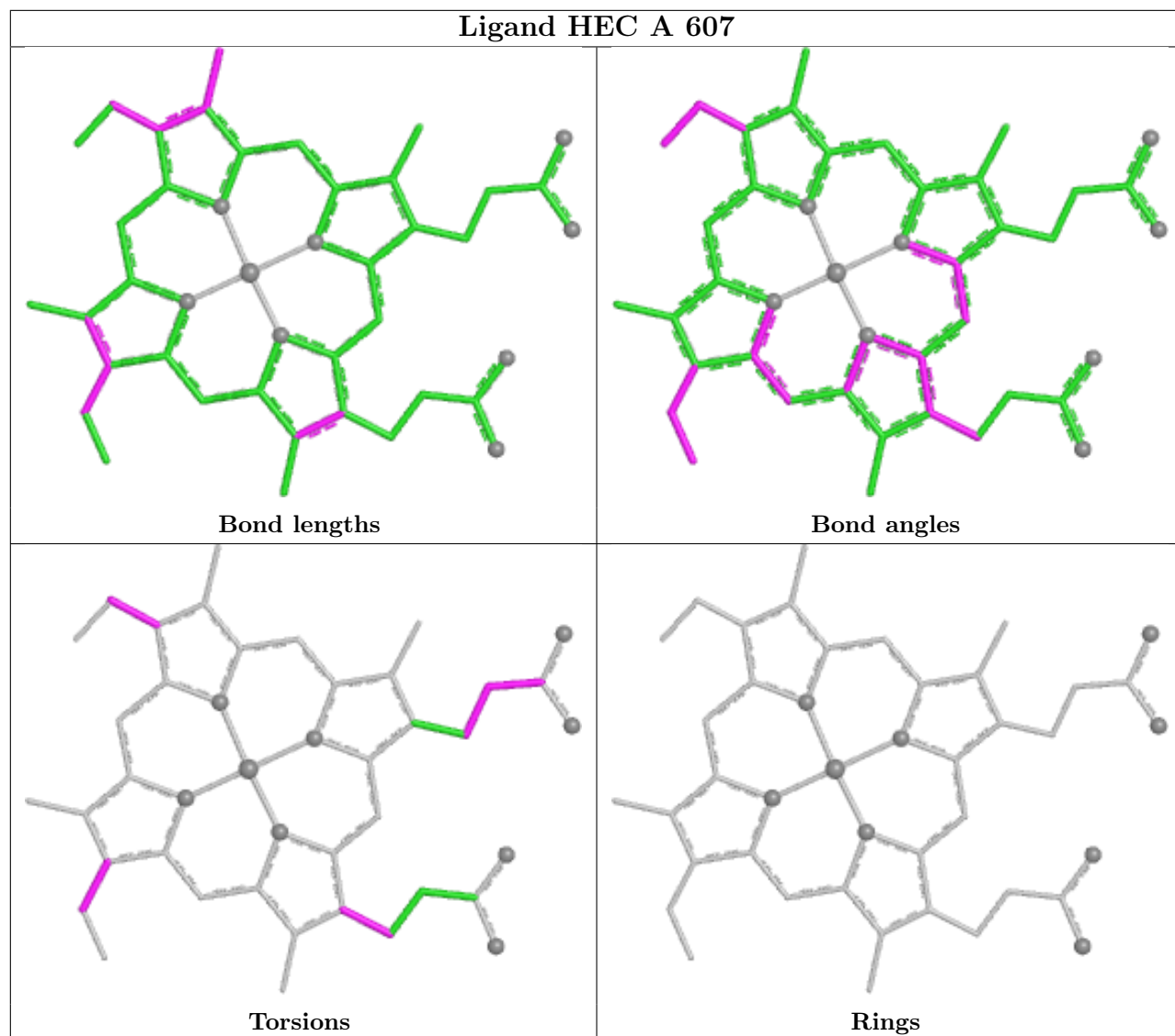


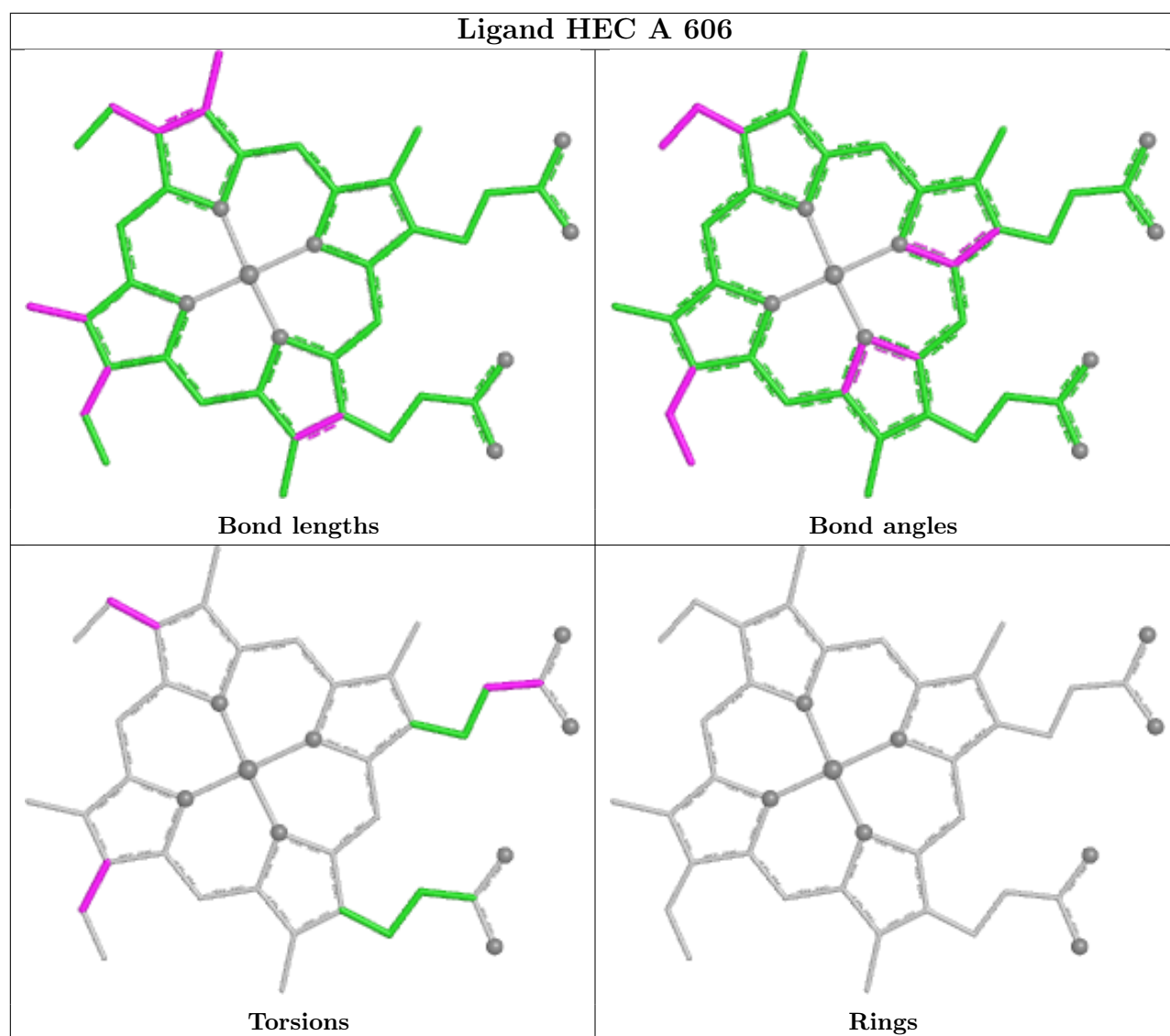












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

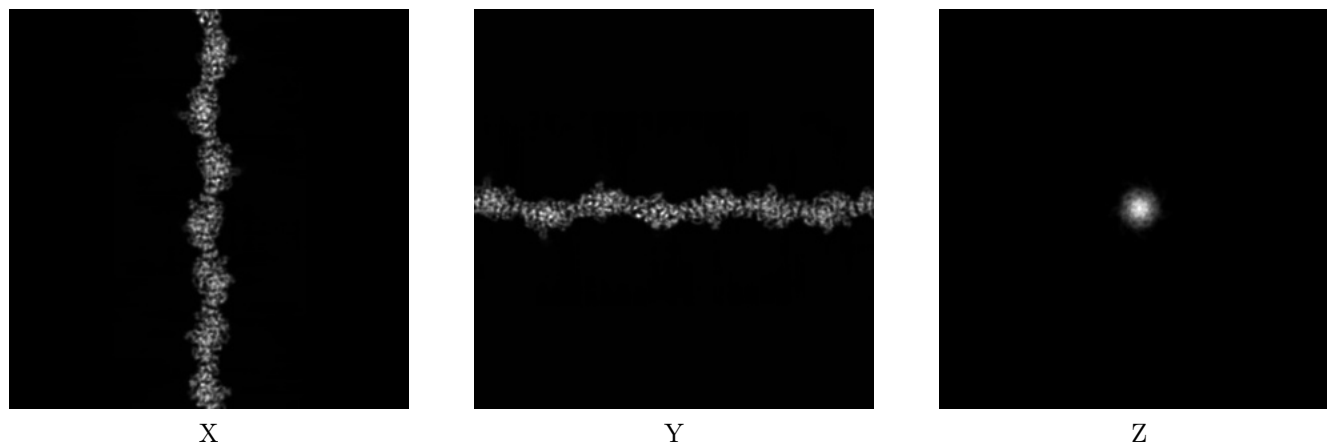
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27266. These allow visual inspection of the internal detail of the map and identification of artifacts.

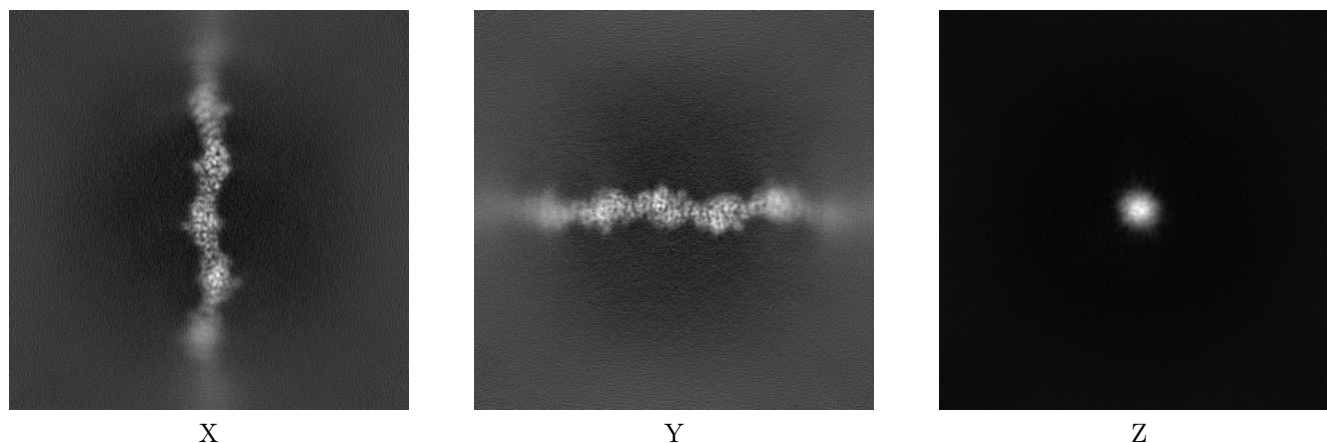
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



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

6.2 Central slices [i](#)

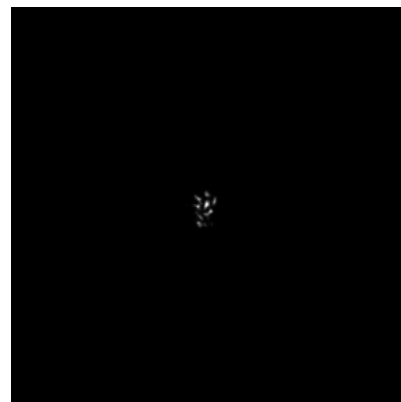
6.2.1 Primary map



X Index: 192

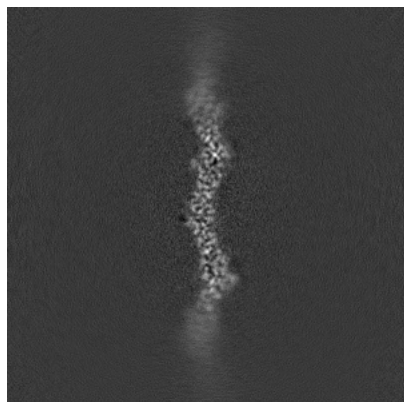


Y Index: 192

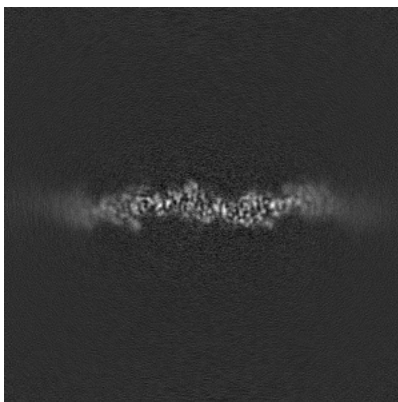


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

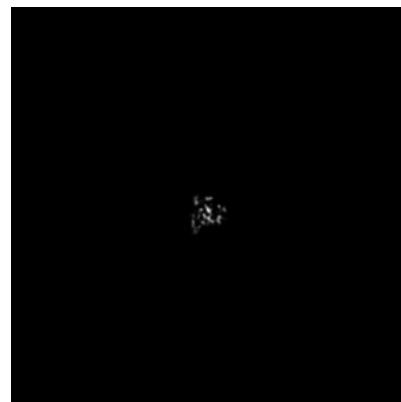
6.3.1 Primary map



X Index: 192

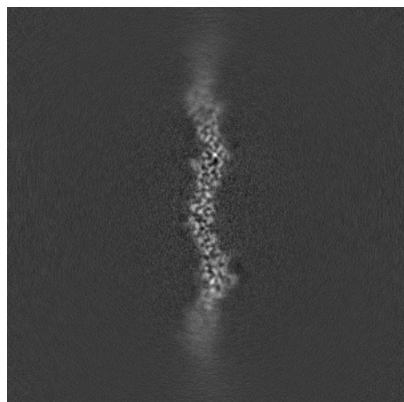


Y Index: 191

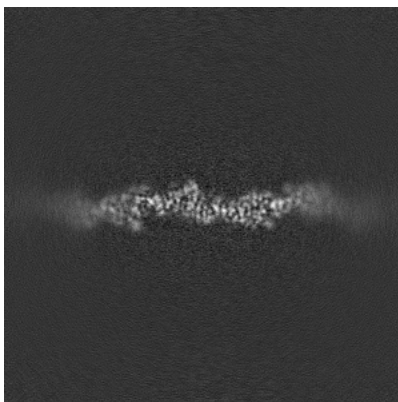


Z Index: 172

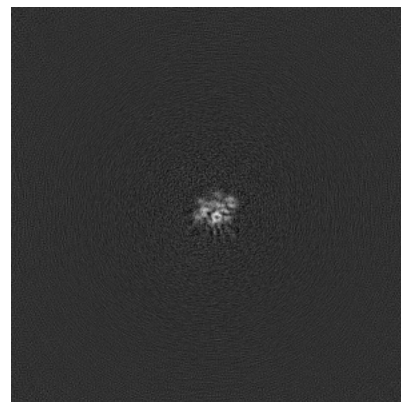
6.3.2 Raw map



X Index: 191



Y Index: 193

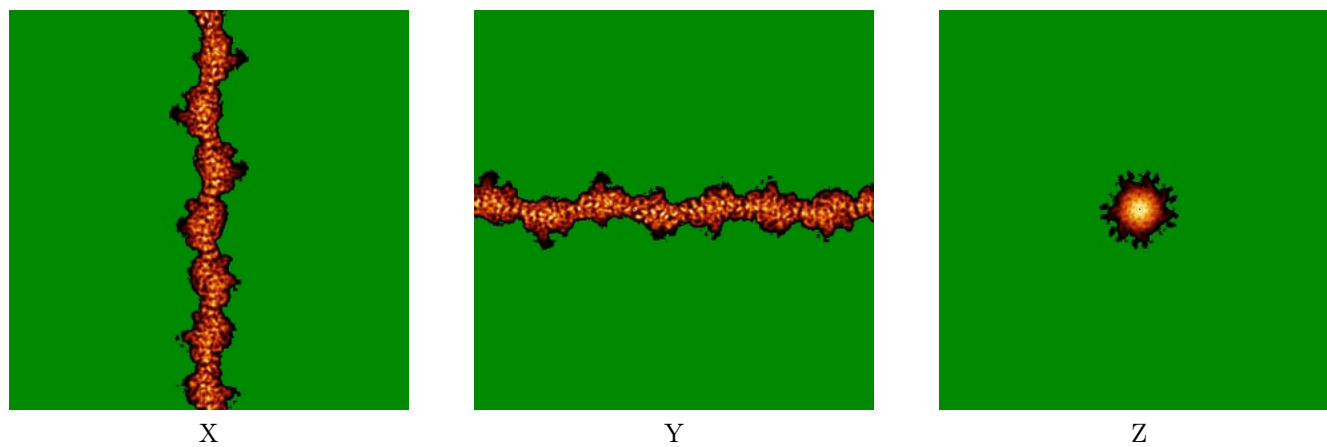


Z Index: 182

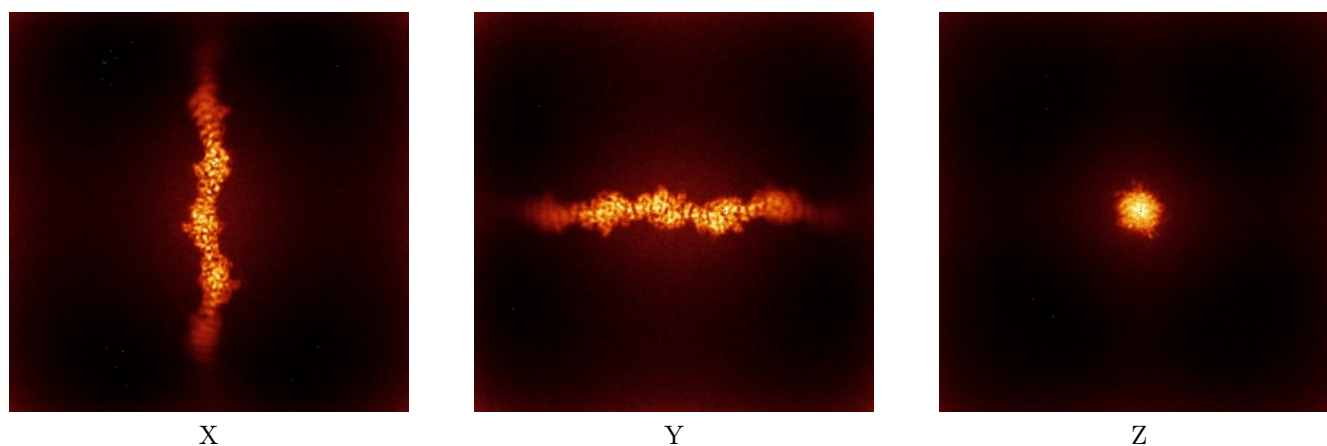
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

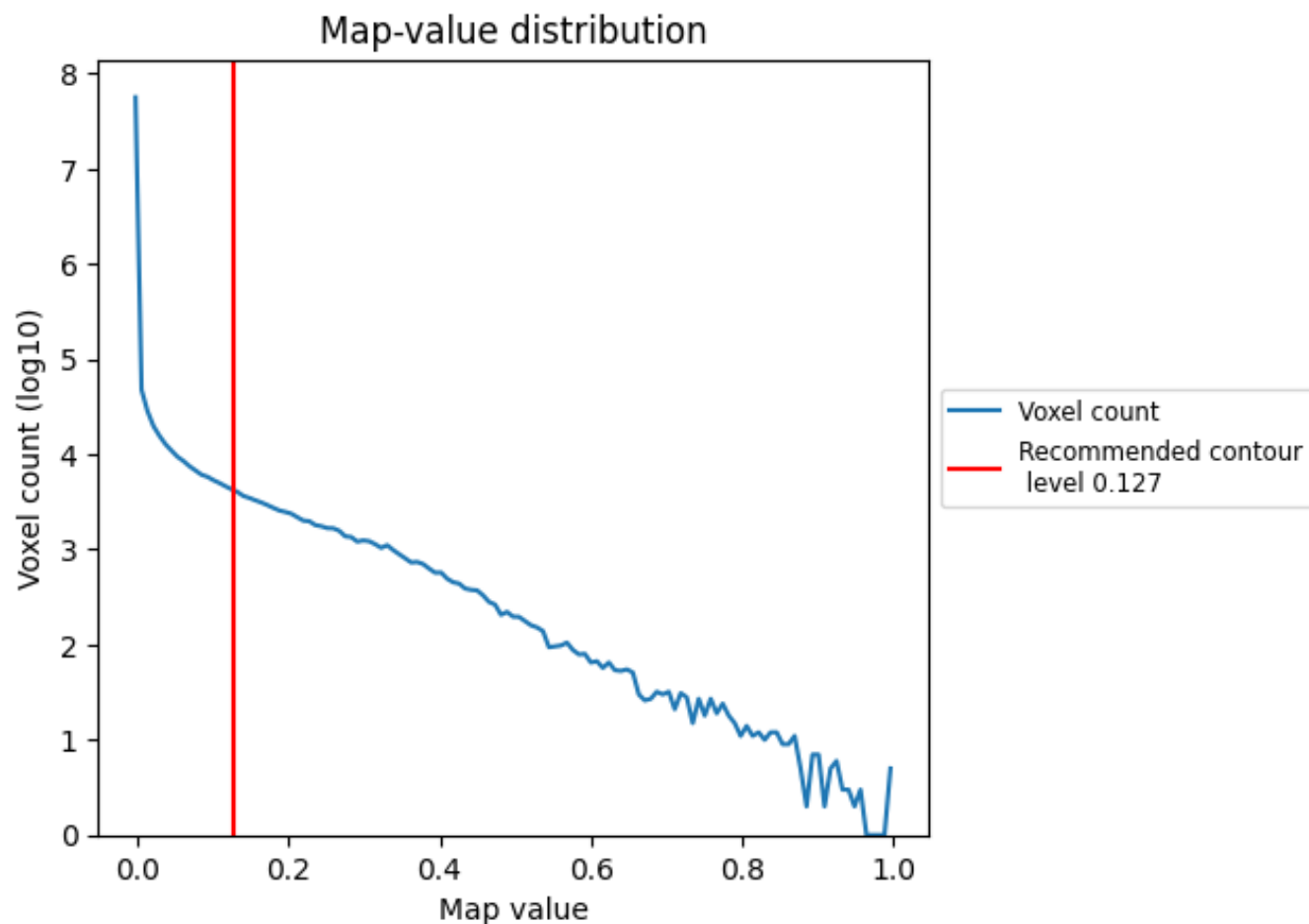
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

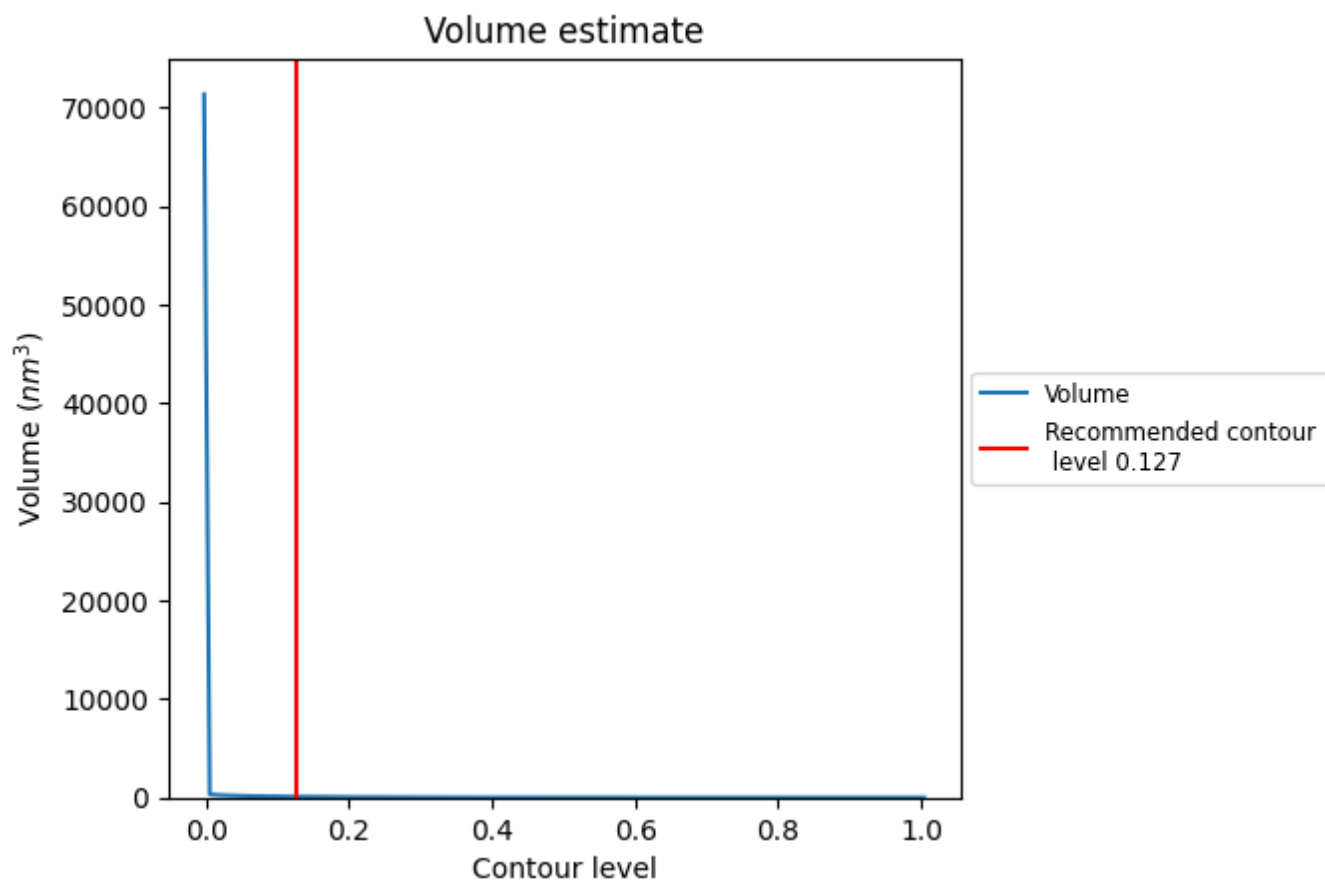
This section contains the results of statistical analysis of the map.

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.

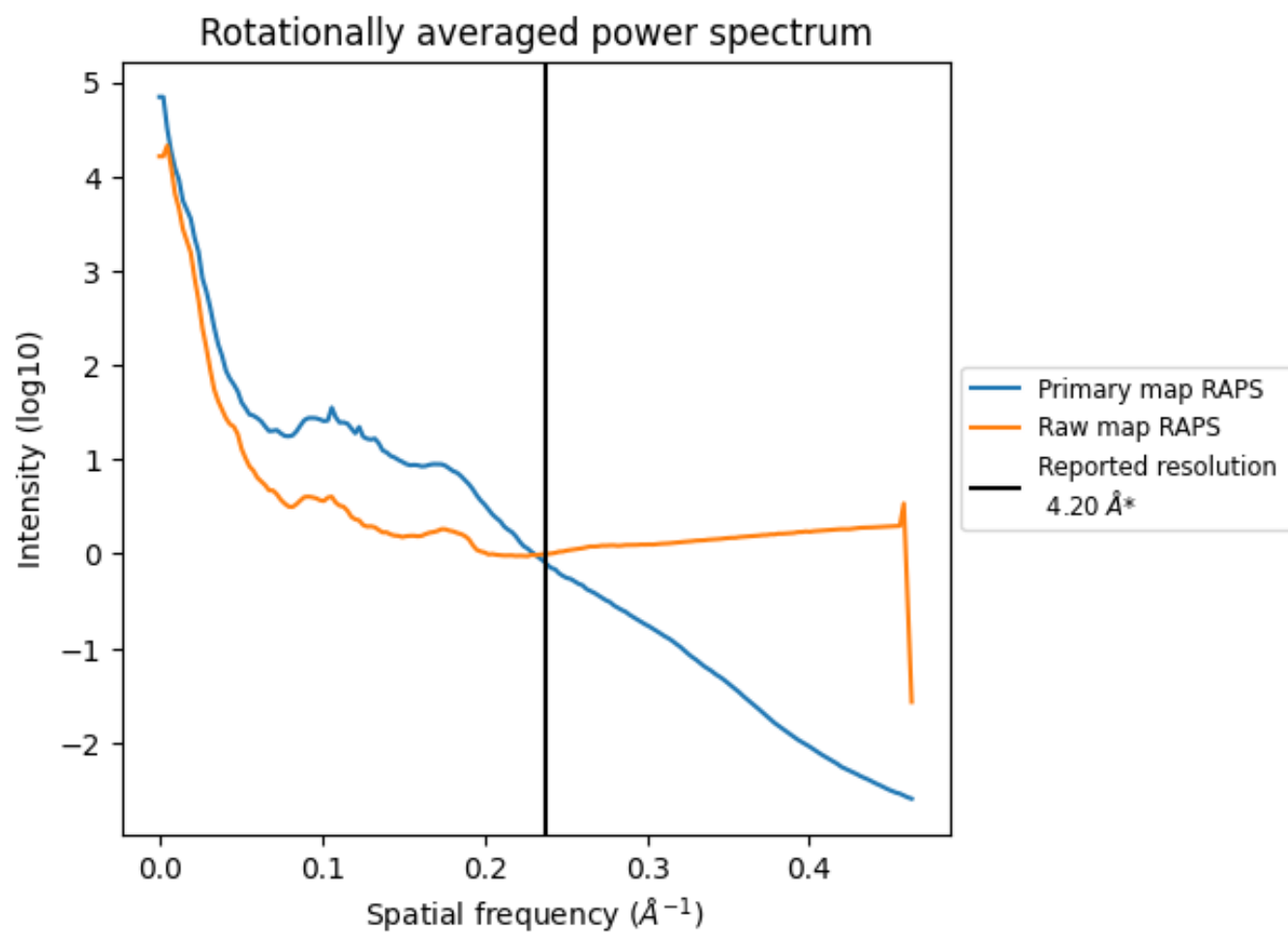
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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 ⓘ

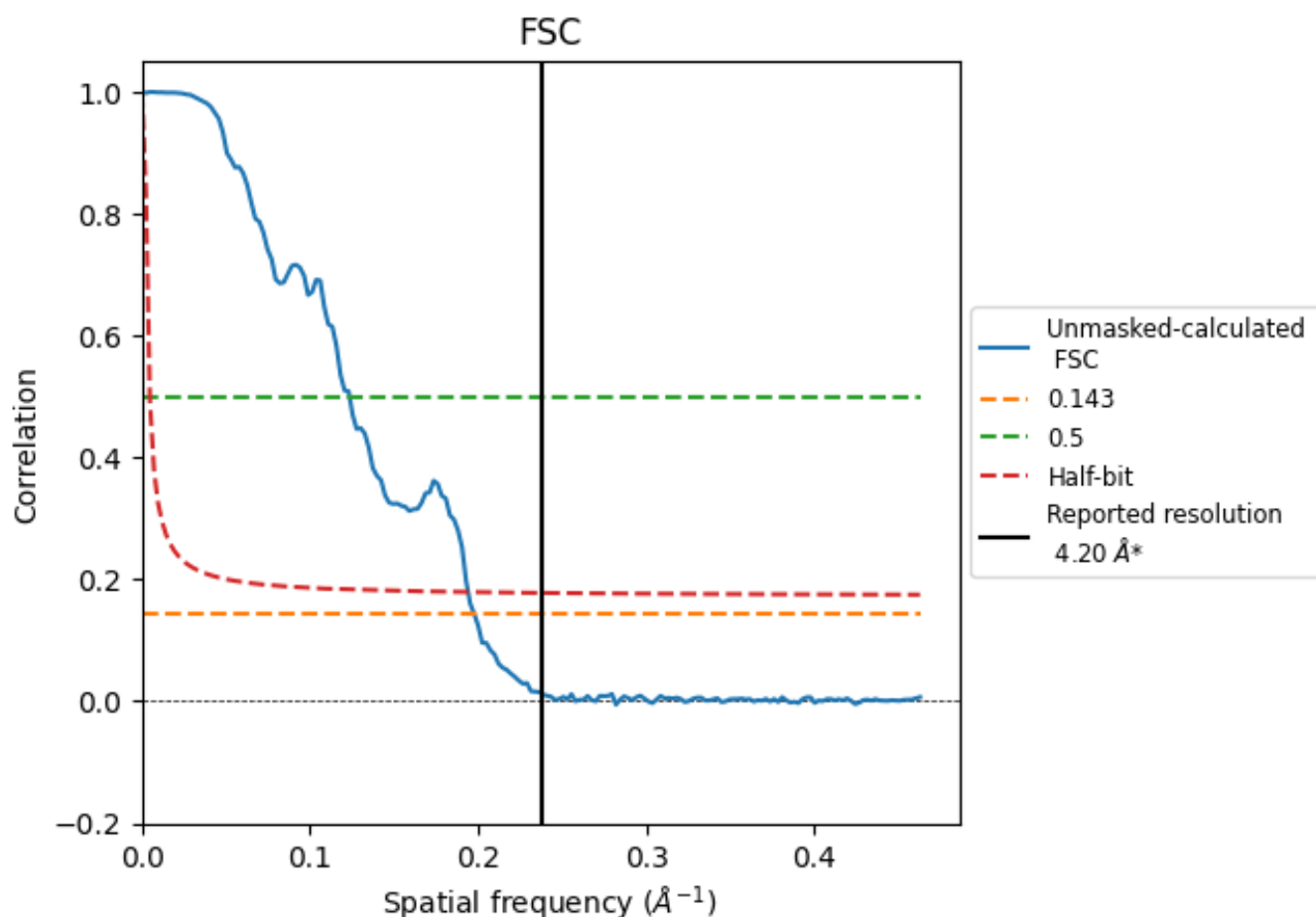


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.06	8.10	5.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.06 differs from the reported value 4.2 by more than 10 %

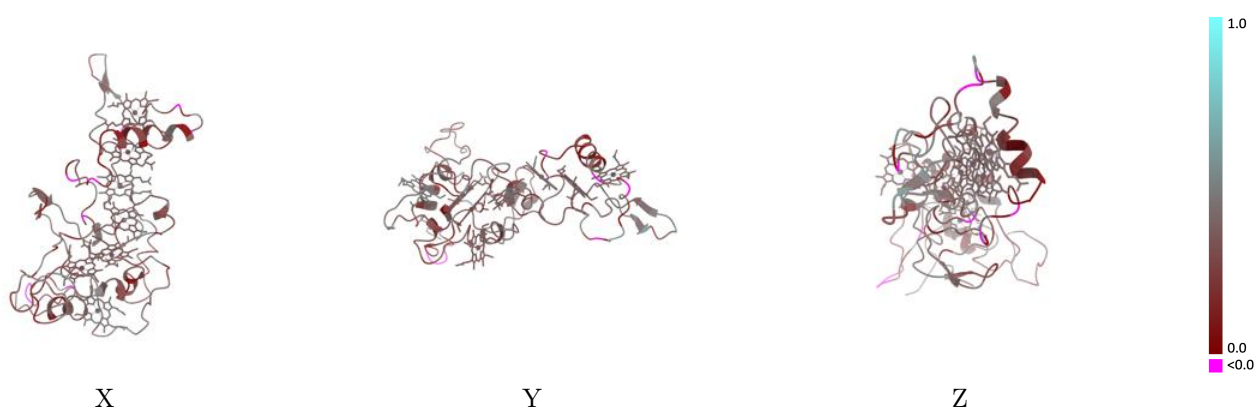
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27266 and PDB model 8D9M. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

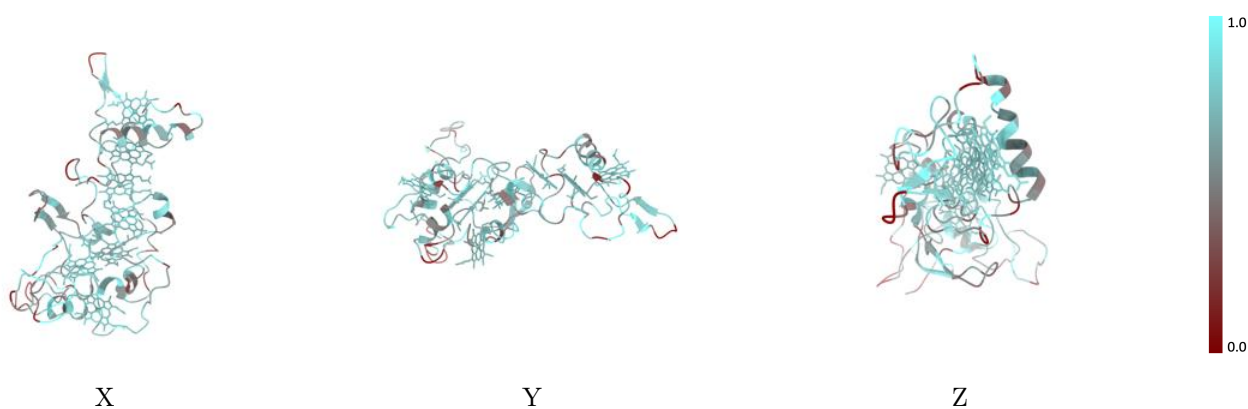
This section was not generated.

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



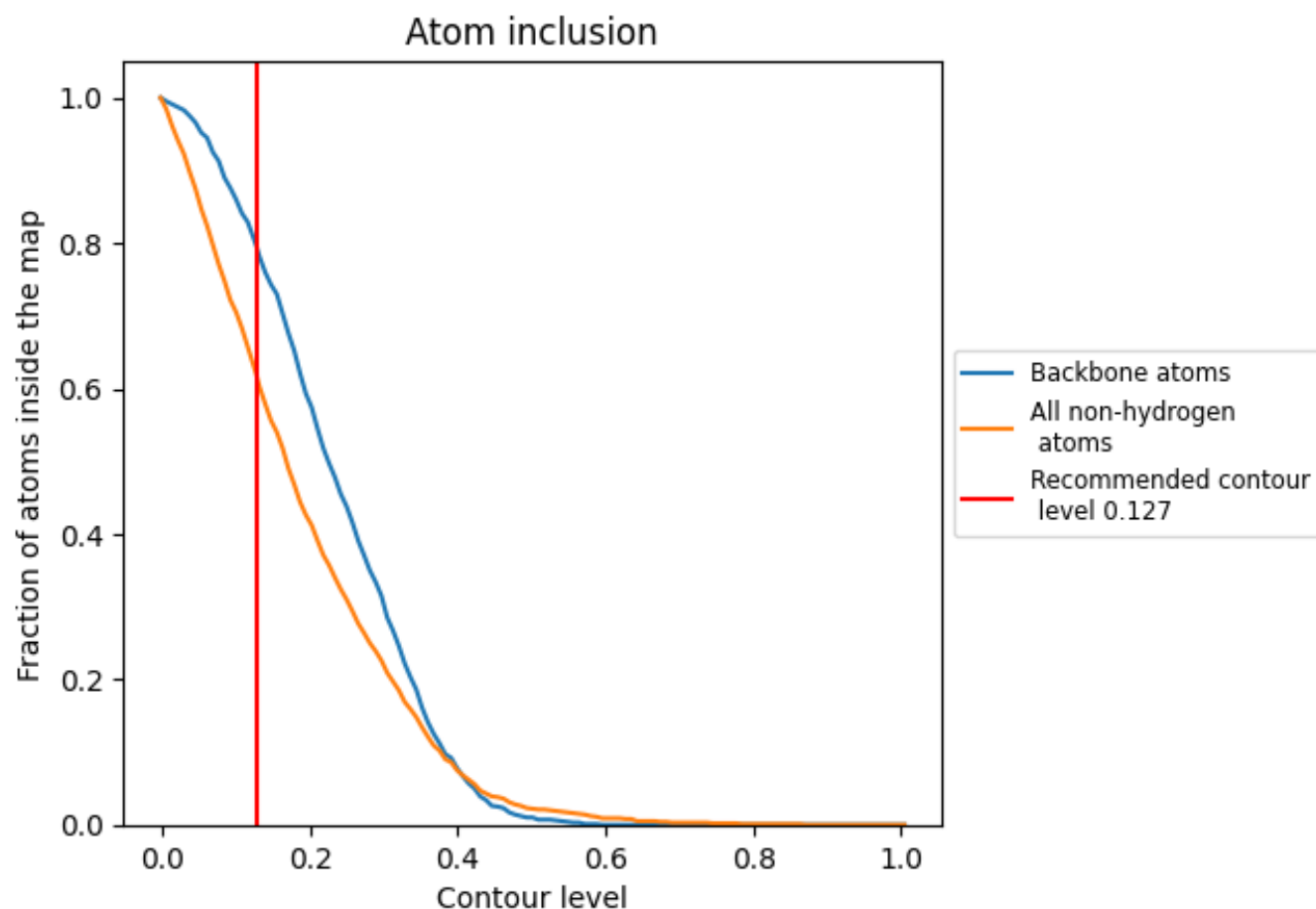
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.127).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 62% 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 (0.127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.3200
A	0.6200	0.3200

