



Full wwPDB EM Validation Report ⓘ

Sep 22, 2025 – 12:16 PM JST

PDB ID : 9M88 / pdb_00009m88
EMDB ID : EMD-63702
Title : PGS fused GPR3 dimer with antagonist AF64394
Authors : Geng, C.; Jun, X.
Deposited on : 2025-03-11
Resolution : 3.10 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

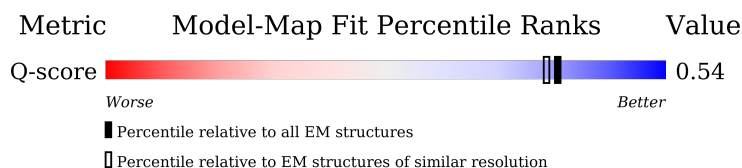
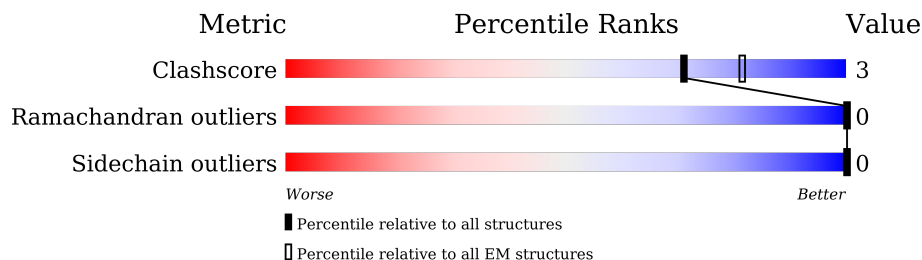
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	640	
1	B	640	
2	C	196	
2	D	196	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7137 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.

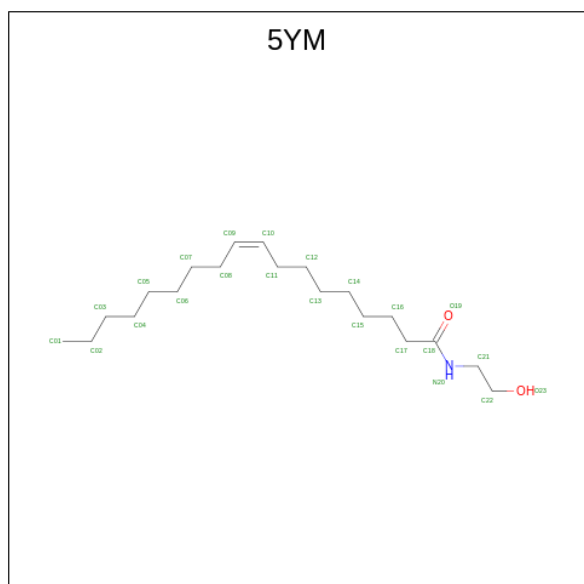
- Molecule 1 is a protein called GPR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	S	0	0
			1886	1254	295	321	16		
1	B	254	Total	C	N	O	S	0	0
			1897	1262	298	322	15		

- Molecule 2 is a protein called Glycogen synthase.

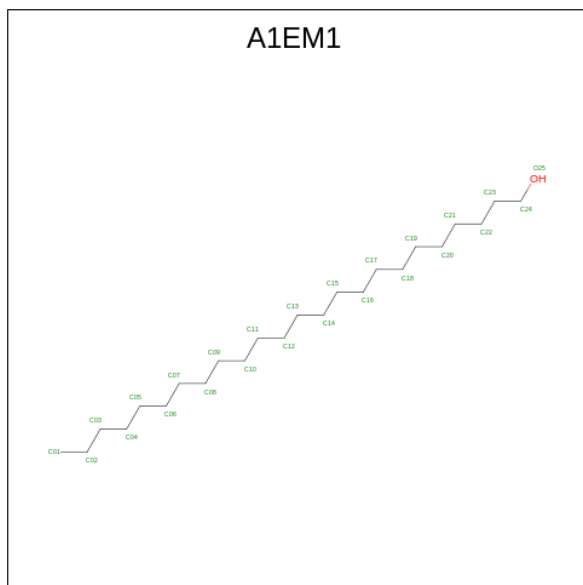
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	195	Total	C	N	O	S	0	0
			1431	918	233	273	7		
2	D	196	Total	C	N	O	S	0	0
			1435	920	234	274	7		

- Molecule 3 is (Z)-N-(2-hydroxyethyl)octadec-9-enamide (CCD ID: 5YM) (formula: $C_{20}H_{39}NO_2$) (labeled as "Ligand of Interest" by depositor).



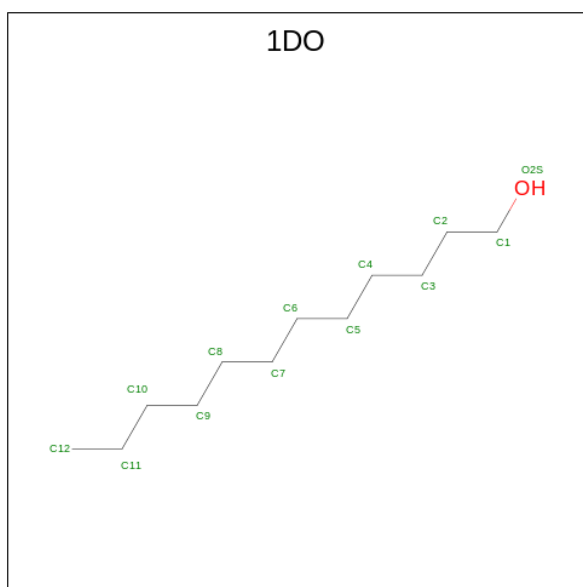
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			23	20	1	2	
3	B	1	Total	C	N	O	0
			23	20	1	2	

- Molecule 4 is tetracosan-1-ol (CCD ID: A1EM1) (formula: $C_{24}H_{50}O$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			25	24	1	
4	B	1	Total	C	O	0
			25	24	1	

- Molecule 5 is 1-DODECANOL (CCD ID: 1DO) (formula: $C_{12}H_{26}O$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			13	12	1	
5	A	1	Total	C	O	0
			13	12	1	
5	A	1	Total	C	O	0
			13	12	1	
5	A	1	Total	C	O	0
			13	12	1	
5	B	1	Total	C	O	0
			13	12	1	
5	B	1	Total	C	O	0
			13	12	1	
5	B	1	Total	C	O	0
			13	12	1	
5	B	1	Total	C	O	0
			13	12	1	

- Molecule 6 is [(2R)-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-decanoyloxy-propyl] dodecanoate (CCD ID: A1EM3) (formula: C₂₇H₅₄NO₈P).

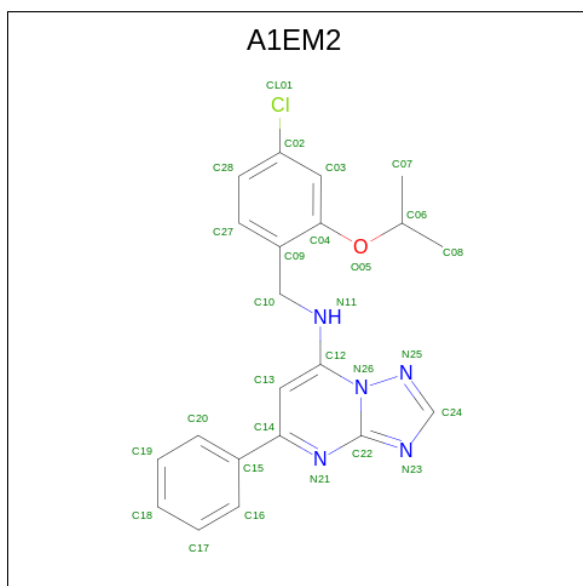


- Molecule 7 is icosan-1-ol (CCD ID: A1EQ8) (formula: $C_{20}H_{42}O$).



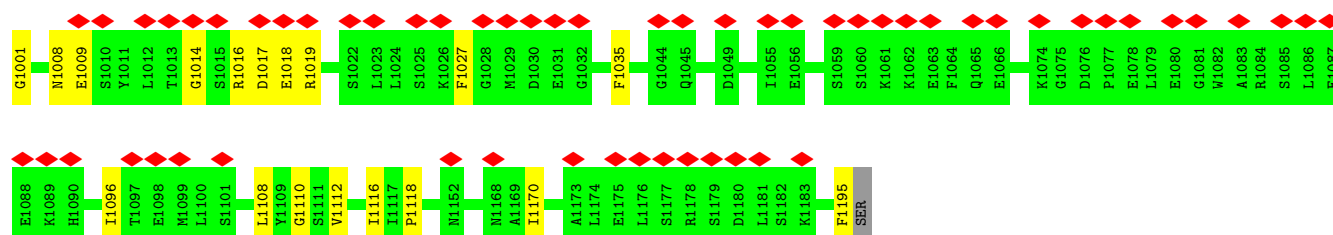
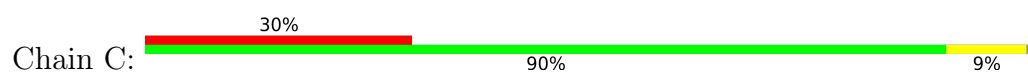
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			21	20	1	
7	B	1	Total	C	O	0
			21	20	1	
7	B	1	Total	C	O	0
			21	20	1	
7	B	1	Total	C	O	0
			21	20	1	

- Molecule 8 is N-[(4-chloranyl-2-propan-2-yloxy-phenyl)methyl]-5-phenyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (CCD ID: A1EM2) (formula: $C_{21}H_{20}ClN_5O$) (labeled as "Ligand of Interest" by depositor).

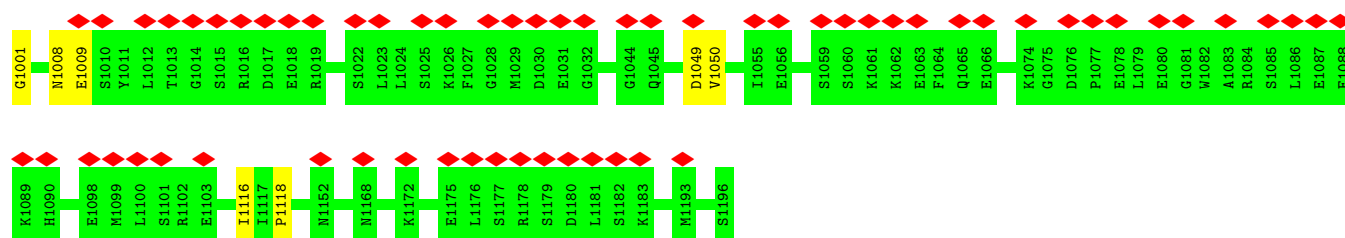


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Cl	N	O	0
			28	21	1	5	1	
8	B	1	Total	C	Cl	N	O	0
			28	21	1	5	1	

- Molecule 2: Glycogen synthase



- Molecule 2: Glycogen synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.12	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.916	Depositor
Minimum map value	-7.178	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	0.844	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EM1, A1EM3, 1DO, 5YM, A1EQ8, A1EM2

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	0.31	2/1931 (0.1%)	0.43	0/2650
1	B	0.27	1/1942 (0.1%)	0.41	0/2664
2	C	0.14	0/1455	0.26	0/1968
2	D	0.10	0/1459	0.25	0/1973
All	All	0.23	3/6787 (0.0%)	0.36	0/9255

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	GLN	C-O	-5.47	1.17	1.24
1	A	280	TYR	C-O	-5.43	1.17	1.24
1	B	86	ASP	C-O	-5.21	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1949	17	0
1	B	1897	0	1960	18	0
2	C	1431	0	1355	10	0
2	D	1435	0	1365	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	0	0	0
3	B	23	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
5	A	52	0	104	0	0
5	B	52	0	104	1	0
6	A	74	0	0	4	0
6	B	74	0	0	3	0
7	A	21	0	0	0	0
7	B	63	0	0	0	0
8	A	28	0	0	0	0
8	B	28	0	0	0	0
All	All	7137	0	6837	46	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 3.

All (46) 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:170:LEU:HD21	6:A:406:A1EM3:C02	2.02	0.89
2:C:1014:GLY:O	2:C:1019:ARG:NH1	2.12	0.82
1:A:221:CYS:O	2:D:1001:GLY:N	2.14	0.80
1:B:221:CYS:O	2:C:1001:GLY:N	2.14	0.80
1:B:170:LEU:HD11	6:B:410:A1EM3:C17	2.14	0.76
1:A:170:LEU:HD21	6:A:406:A1EM3:C01	2.18	0.73
1:A:174:ALA:HB1	6:A:406:A1EM3:P19	2.30	0.70
1:A:144:TYR:O	1:A:149:THR:OG1	2.07	0.70
1:A:174:ALA:HB1	6:A:406:A1EM3:O22	1.93	0.68
2:C:1116:ILE:HG22	2:C:1118:PRO:HD3	1.76	0.66
2:D:1116:ILE:HG22	2:D:1118:PRO:HD3	1.76	0.66
1:A:179:ASP:OD1	1:A:180:GLY:N	2.33	0.60
1:B:172:VAL:HG12	1:B:172:VAL:O	2.01	0.59
1:B:49:ILE:HD11	5:B:406:1DO:H8C2	1.88	0.54
1:B:243:ARG:N	2:C:1195:PHE:O	2.41	0.54
2:C:1008:ASN:OD1	2:C:1009:GLU:N	2.41	0.54
2:C:1017:ASP:OD1	2:C:1018:GLU:N	2.40	0.54
1:B:174:ALA:HB2	6:B:410:A1EM3:N25	2.23	0.54
2:C:1108:LEU:O	2:C:1112:VAL:HG22	2.08	0.53
1:B:182:THR:O	1:B:183:THR:HG22	2.08	0.53
1:B:182:THR:C	1:B:183:THR:HG22	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:O	1:B:183:THR:CG2	2.60	0.50
1:B:192:LYS:O	1:B:196:VAL:HG23	2.13	0.48
1:A:257:ALA:O	1:A:261:LEU:HD13	2.14	0.48
1:B:170:LEU:CD1	6:B:410:A1EM3:C17	2.90	0.48
1:B:165:LEU:O	1:B:165:LEU:HD23	2.14	0.47
1:A:128:LEU:O	1:A:132:VAL:HG23	2.15	0.46
1:A:170:LEU:HD12	1:A:194:HIS:CE1	2.50	0.46
1:A:188:TYR:HB3	1:A:189:PRO:HD3	1.99	0.45
2:C:1035:PHE:HE2	2:C:1170:ILE:HG23	1.81	0.45
1:A:195:LEU:HB3	1:A:267:CYS:SG	2.58	0.44
1:A:165:LEU:HD23	1:A:165:LEU:O	2.17	0.43
1:A:169:LEU:HD12	1:A:169:LEU:C	2.43	0.43
1:B:195:LEU:HB3	1:B:267:CYS:SG	2.58	0.43
1:B:182:THR:O	1:B:182:THR:HG22	2.19	0.42
1:B:108:MET:HG2	1:B:112:LEU:HD12	2.02	0.42
2:C:1027:PHE:CE1	2:C:1096:ILE:HD11	2.54	0.42
1:B:188:TYR:HB3	1:B:189:PRO:HD3	2.02	0.42
1:A:50:SER:HB3	1:A:287:THR:HG21	2.02	0.42
2:C:1016:ARG:NE	2:C:1110:GLY:O	2.52	0.41
1:A:184:CYS:SG	1:A:188:TYR:O	2.78	0.41
1:B:170:LEU:HD22	1:B:170:LEU:N	2.36	0.41
1:B:177:CYS:SG	1:B:184:CYS:N	2.94	0.41
2:D:1049:ASP:OD1	2:D:1050:VAL:N	2.54	0.41
2:D:1008:ASN:OD1	2:D:1009:GLU:N	2.55	0.40
1:A:183:THR:HG23	1:A:183:THR:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	250/640 (39%)	242 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	250/640 (39%)	239 (96%)	11 (4%)	0	100	100
2	C	193/196 (98%)	189 (98%)	4 (2%)	0	100	100
2	D	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	887/1672 (53%)	860 (97%)	27 (3%)	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	199/525 (38%)	199 (100%)	0	100	100
1	B	199/525 (38%)	199 (100%)	0	100	100
2	C	139/165 (84%)	139 (100%)	0	100	100
2	D	141/165 (86%)	141 (100%)	0	100	100
All	All	678/1380 (49%)	678 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	B	193	ASN
1	B	215	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](#)

22 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
8	A1EM2	B	401	-	26,31,31	1.77	6 (23%)	32,43,43	1.32	3 (9%)
8	A1EM2	A	410	-	26,31,31	1.78	6 (23%)	32,43,43	1.33	3 (9%)
5	1DO	A	404	-	12,12,12	0.32	0	11,11,11	0.24	0
5	1DO	B	406	-	12,12,12	0.23	0	11,11,11	0.39	0
7	A1EQ8	A	409	-	20,20,20	0.21	0	19,19,19	0.75	0
7	A1EQ8	B	411	-	20,20,20	0.22	0	19,19,19	0.43	0
6	A1EM3	A	405	-	36,36,36	1.27	5 (13%)	39,41,41	1.19	3 (7%)
5	1DO	B	408	-	12,12,12	0.26	0	11,11,11	0.44	0
4	A1EM1	B	404	-	24,24,24	0.26	0	23,23,23	0.36	0
7	A1EQ8	B	412	-	20,20,20	0.24	0	19,19,19	0.62	0
6	A1EM3	B	409	-	36,36,36	1.32	6 (16%)	39,41,41	1.66	6 (15%)
4	A1EM1	A	402	-	24,24,24	0.26	0	23,23,23	0.40	0
5	1DO	B	405	-	12,12,12	0.19	0	11,11,11	0.39	0
6	A1EM3	B	410	-	36,36,36	1.24	4 (11%)	39,41,41	1.01	3 (7%)
5	1DO	A	408	-	12,12,12	0.26	0	11,11,11	0.39	0
6	A1EM3	A	406	-	36,36,36	1.23	4 (11%)	39,41,41	0.86	1 (2%)
3	5YM	B	403	-	22,22,22	1.29	2 (9%)	22,22,22	1.90	5 (22%)
5	1DO	A	407	-	12,12,12	0.23	0	11,11,11	0.48	0
7	A1EQ8	B	402	-	20,20,20	0.20	0	19,19,19	0.72	0
5	1DO	B	407	-	12,12,12	0.26	0	11,11,11	0.40	0
5	1DO	A	403	-	12,12,12	0.27	0	11,11,11	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5YM	A	401	-	22,22,22	1.29	2 (9%)	22,22,22	1.90	5 (22%)

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
8	A1EM2	B	401	-	-	1/13/13/13	0/4/4/4
8	A1EM2	A	410	-	-	3/13/13/13	0/4/4/4
5	1DO	A	404	-	-	3/10/10/10	-
5	1DO	B	406	-	-	4/10/10/10	-
7	A1EQ8	A	409	-	-	8/18/18/18	-
7	A1EQ8	B	411	-	-	9/18/18/18	-
6	A1EM3	A	405	-	-	15/40/40/40	-
5	1DO	B	408	-	-	6/10/10/10	-
4	A1EM1	B	404	-	-	8/22/22/22	-
7	A1EQ8	B	412	-	-	7/18/18/18	-
6	A1EM3	B	409	-	-	14/40/40/40	-
4	A1EM1	A	402	-	-	12/22/22/22	-
5	1DO	B	405	-	-	5/10/10/10	-
6	A1EM3	B	410	-	-	19/40/40/40	-
5	1DO	A	408	-	-	5/10/10/10	-
6	A1EM3	A	406	-	-	15/40/40/40	-
3	5YM	B	403	-	-	7/21/21/21	-
5	1DO	A	407	-	-	3/10/10/10	-
7	A1EQ8	B	402	-	-	5/18/18/18	-
5	1DO	B	407	-	-	4/10/10/10	-
5	1DO	A	403	-	-	6/10/10/10	-
3	5YM	A	401	-	-	7/21/21/21	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	5YM	C18-N20	4.29	1.43	1.33
3	B	403	5YM	C18-N20	4.25	1.43	1.33
8	A	410	A1EM2	C12-N11	4.16	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	401	A1EM2	C12-N11	4.11	1.47	1.37
3	B	403	5YM	O19-C18	-3.93	1.15	1.23
3	A	401	5YM	O19-C18	-3.93	1.15	1.23
6	A	406	A1EM3	O26-C01	-3.51	1.37	1.46
8	A	410	A1EM2	C15-C14	3.45	1.54	1.48
6	B	410	A1EM3	O26-C01	-3.44	1.38	1.46
8	B	401	A1EM2	C15-C14	3.43	1.54	1.48
8	A	410	A1EM2	O05-C04	3.15	1.43	1.37
8	B	401	A1EM2	O05-C04	3.14	1.43	1.37
6	B	409	A1EM3	O05-C04	-3.09	1.13	1.22
8	A	410	A1EM2	C10-C09	3.00	1.60	1.50
8	B	401	A1EM2	C10-C09	2.99	1.60	1.50
6	B	409	A1EM3	O26-C27	2.94	1.42	1.34
6	A	405	A1EM3	O26-C27	2.93	1.42	1.34
6	B	409	A1EM3	O26-C01	-2.88	1.39	1.46
6	A	406	A1EM3	O26-C27	2.85	1.42	1.34
6	A	405	A1EM3	O03-C04	2.81	1.41	1.33
6	A	405	A1EM3	O26-C01	-2.78	1.39	1.46
6	B	410	A1EM3	O26-C27	2.75	1.42	1.34
6	B	410	A1EM3	O03-C04	2.75	1.41	1.33
8	A	410	A1EM2	C22-N23	2.71	1.39	1.35
8	B	401	A1EM2	C22-N23	2.67	1.39	1.35
6	B	409	A1EM3	P19-O18	2.56	1.69	1.59
6	A	406	A1EM3	O03-C04	2.53	1.40	1.33
6	B	409	A1EM3	O28-C27	-2.52	1.15	1.22
6	A	405	A1EM3	P19-O18	2.48	1.69	1.59
6	A	406	A1EM3	O03-C02	-2.27	1.40	1.45
6	B	409	A1EM3	O03-C04	2.18	1.39	1.33
8	A	410	A1EM2	C13-C14	-2.16	1.35	1.39
6	A	405	A1EM3	O05-C04	-2.16	1.16	1.22
8	B	401	A1EM2	C13-C14	-2.11	1.36	1.39
6	B	410	A1EM3	P19-O18	2.01	1.67	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	5YM	C17-C18-N20	5.48	125.64	116.42
3	B	403	5YM	C17-C18-N20	5.44	125.58	116.42
6	B	409	A1EM3	O03-C04-C06	5.28	128.49	111.91
6	B	409	A1EM3	O26-C27-C29	4.99	122.25	111.50
8	A	410	A1EM2	N11-C12-N26	4.14	119.55	116.65
6	A	405	A1EM3	O03-C04-C06	3.97	124.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	401	A1EM2	N11-C12-N26	3.94	119.41	116.65
3	B	403	5YM	C16-C17-C18	-3.62	103.11	113.26
6	B	409	A1EM3	C01-O26-C27	3.60	126.64	117.79
3	A	401	5YM	C16-C17-C18	-3.58	103.21	113.26
6	A	405	A1EM3	O26-C27-C29	3.53	119.11	111.50
6	B	409	A1EM3	O03-C04-O05	-3.51	114.72	123.59
3	A	401	5YM	O19-C18-C17	-3.20	116.17	122.02
3	A	401	5YM	C21-N20-C18	-3.15	116.99	122.84
3	B	403	5YM	C21-N20-C18	-3.15	117.00	122.84
3	B	403	5YM	O19-C18-C17	-3.15	116.26	122.02
6	B	410	A1EM3	O26-C27-C29	2.85	117.65	111.50
8	B	401	A1EM2	C13-C14-N21	-2.74	119.73	122.23
8	A	410	A1EM2	C13-C14-N21	-2.73	119.74	122.23
3	B	403	5YM	O19-C18-N20	-2.58	118.15	123.01
3	A	401	5YM	O19-C18-N20	-2.56	118.19	123.01
6	B	409	A1EM3	O21-P19-O20	-2.46	100.09	112.24
6	B	409	A1EM3	O26-C01-C17	-2.35	99.88	108.40
8	A	410	A1EM2	C10-N11-C12	-2.35	119.58	123.26
6	B	410	A1EM3	O03-C04-C06	2.26	118.99	111.91
8	B	401	A1EM2	C10-N11-C12	-2.13	119.93	123.26
6	B	410	A1EM3	C02-O03-C04	-2.12	109.25	117.12
6	A	405	A1EM3	O26-C01-C02	-2.12	100.73	108.40
6	A	406	A1EM3	O26-C27-C29	2.04	115.90	111.50

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	5YM	N20-C21-C22-O23
6	A	405	A1EM3	C17-O18-P19-O20
6	A	405	A1EM3	O22-C23-C24-N25
6	A	406	A1EM3	C17-O18-P19-O22
6	A	406	A1EM3	C24-C23-O22-P19
6	B	409	A1EM3	O22-C23-C24-N25
6	B	410	A1EM3	C23-O22-P19-O18
6	B	410	A1EM3	C23-O22-P19-O20
6	B	410	A1EM3	O26-C01-C17-O18
6	B	410	A1EM3	O28-C27-O26-C01
6	B	410	A1EM3	C29-C27-O26-C01
6	B	410	A1EM3	C06-C04-O03-C02
6	B	410	A1EM3	O05-C04-O03-C02
6	B	410	A1EM3	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
6	A	406	A1EM3	C04-C06-C07-C08
6	A	405	A1EM3	C17-O18-P19-O22
6	B	409	A1EM3	C17-O18-P19-O22
4	B	404	A1EM1	C18-C19-C20-C21
6	A	406	A1EM3	C07-C08-C09-C10
6	A	406	A1EM3	C09-C10-C11-C12
5	B	405	1DO	C2-C3-C4-C5
7	B	411	A1EQ8	C14-C15-C16-C17
3	A	401	5YM	C12-C13-C14-C15
4	A	402	A1EM1	C07-C08-C09-C10
3	B	403	5YM	C12-C13-C14-C15
5	A	403	1DO	C4-C5-C6-C7
7	B	411	A1EQ8	C07-C08-C09-C10
3	A	401	5YM	N20-C21-C22-O23
4	B	404	A1EM1	C14-C15-C16-C17
3	A	401	5YM	C13-C14-C15-C16
4	B	404	A1EM1	C06-C07-C08-C09
3	B	403	5YM	C13-C14-C15-C16
6	A	405	A1EM3	C09-C10-C11-C12
6	A	406	A1EM3	O22-C23-C24-N25
5	A	403	1DO	C6-C7-C8-C9
6	B	409	A1EM3	C33-C34-C35-C36
6	B	409	A1EM3	O28-C27-O26-C01
7	B	411	A1EQ8	C06-C07-C08-C09
6	B	409	A1EM3	C29-C27-O26-C01
5	A	403	1DO	C11-C10-C9-C8
6	B	410	A1EM3	C10-C11-C12-C13
6	B	409	A1EM3	C09-C10-C11-C12
4	A	402	A1EM1	C02-C03-C04-C05
5	B	407	1DO	C3-C4-C5-C6
5	A	408	1DO	C1-C2-C3-C4
6	B	410	A1EM3	C31-C32-C33-C34
6	A	405	A1EM3	C31-C32-C33-C34
7	B	411	A1EQ8	C13-C14-C15-C16
6	A	405	A1EM3	O26-C01-C02-O03
6	A	406	A1EM3	O26-C01-C02-O03
6	B	409	A1EM3	C06-C07-C08-C09
5	A	403	1DO	C1-C2-C3-C4
6	B	410	A1EM3	C02-C01-C17-O18
5	B	405	1DO	O2S-C1-C2-C3
3	B	403	5YM	C06-C07-C08-C09
5	A	408	1DO	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
7	B	411	A1EQ8	C16-C17-C18-C19
4	B	404	A1EM1	C15-C16-C17-C18
5	A	407	1DO	O2S-C1-C2-C3
5	B	406	1DO	O2S-C1-C2-C3
6	B	410	A1EM3	C27-C29-C30-C31
4	A	402	A1EM1	C15-C16-C17-C18
7	B	402	A1EQ8	C01-C02-C03-C04
7	B	402	A1EQ8	C13-C14-C15-C16
4	A	402	A1EM1	C12-C13-C14-C15
6	A	405	A1EM3	C06-C04-O03-C02
5	B	405	1DO	C11-C10-C9-C8
6	A	406	A1EM3	C31-C32-C33-C34
4	B	404	A1EM1	C12-C13-C14-C15
4	A	402	A1EM1	C22-C23-C24-O25
7	B	402	A1EQ8	C05-C06-C07-C08
5	A	408	1DO	C3-C4-C5-C6
5	B	405	1DO	C6-C7-C8-C9
5	A	408	1DO	C9-C10-C11-C12
6	A	405	A1EM3	C17-C01-C02-O03
4	B	404	A1EM1	C09-C10-C11-C12
6	A	405	A1EM3	C13-C14-C15-C16
4	A	402	A1EM1	C10-C11-C12-C13
5	A	404	1DO	C4-C5-C6-C7
5	A	404	1DO	C7-C8-C9-C10
6	A	405	A1EM3	O05-C04-O03-C02
7	B	411	A1EQ8	C02-C03-C04-C05
3	A	401	5YM	C06-C07-C08-C09
5	B	408	1DO	C5-C6-C7-C8
6	A	405	A1EM3	C34-C35-C36-C37
7	A	409	A1EQ8	C16-C17-C18-C19
6	A	406	A1EM3	C08-C09-C10-C11
7	A	409	A1EQ8	C11-C12-C13-C14
7	B	412	A1EQ8	C13-C14-C15-C16
7	B	412	A1EQ8	C16-C17-C18-C19
7	B	412	A1EQ8	C11-C12-C13-C14
6	B	409	A1EM3	C02-C01-C17-O18
7	A	409	A1EQ8	C02-C03-C04-C05
6	B	410	A1EM3	C08-C09-C10-C11
6	A	406	A1EM3	C13-C14-C15-C16
7	B	411	A1EQ8	C11-C12-C13-C14
5	B	407	1DO	C1-C2-C3-C4
7	A	409	A1EQ8	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	B	403	5YM	C04-C05-C06-C07
5	B	408	1DO	C3-C4-C5-C6
7	B	411	A1EQ8	C12-C13-C14-C15
8	A	410	A1EM2	C08-C06-O05-C04
7	A	409	A1EQ8	C03-C04-C05-C06
5	B	408	1DO	C7-C8-C9-C10
6	A	405	A1EM3	C17-O18-P19-O21
6	B	409	A1EM3	C17-O18-P19-O20
6	B	409	A1EM3	C17-O18-P19-O21
3	A	401	5YM	C04-C05-C06-C07
7	B	412	A1EQ8	C08-C09-C10-C11
5	A	408	1DO	C6-C7-C8-C9
6	B	409	A1EM3	C30-C31-C32-C33
5	A	403	1DO	O2S-C1-C2-C3
6	B	409	A1EM3	O26-C01-C17-O18
6	A	405	A1EM3	C30-C31-C32-C33
7	B	402	A1EQ8	C15-C16-C17-C18
4	B	404	A1EM1	C01-C02-C03-C04
6	A	406	A1EM3	C27-C29-C30-C31
4	A	402	A1EM1	C11-C12-C13-C14
6	A	406	A1EM3	C17-C01-C02-O03
5	B	407	1DO	C11-C10-C9-C8
6	B	409	A1EM3	C29-C30-C31-C32
6	A	406	A1EM3	C11-C12-C13-C14
4	A	402	A1EM1	C09-C10-C11-C12
6	B	410	A1EM3	C12-C13-C14-C15
5	B	406	1DO	C2-C3-C4-C5
5	B	408	1DO	C4-C5-C6-C7
7	A	409	A1EQ8	C05-C06-C07-C08
6	A	406	A1EM3	C23-O22-P19-O18
6	B	410	A1EM3	C17-O18-P19-O22
4	B	404	A1EM1	C20-C21-C22-C23
5	B	408	1DO	O2S-C1-C2-C3
6	B	410	A1EM3	C04-C06-C07-C08
7	B	411	A1EQ8	C09-C10-C11-C12
5	B	406	1DO	C11-C10-C9-C8
4	A	402	A1EM1	C21-C22-C23-C24
4	A	402	A1EM1	C13-C14-C15-C16
7	B	412	A1EQ8	C07-C08-C09-C10
5	A	407	1DO	C3-C4-C5-C6
6	A	405	A1EM3	C17-C01-O26-C27
5	B	407	1DO	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	A	405	A1EM3	C10-C11-C12-C13
5	A	404	1DO	C5-C6-C7-C8
5	B	405	1DO	C5-C6-C7-C8
7	B	412	A1EQ8	C10-C11-C12-C13
7	B	412	A1EQ8	C06-C07-C08-C09
4	A	402	A1EM1	C19-C20-C21-C22
8	B	401	A1EM2	C04-C09-C10-N11
5	B	408	1DO	C1-C2-C3-C4
7	A	409	A1EQ8	C06-C07-C08-C09
3	A	401	5YM	C09-C10-C11-C12
3	B	403	5YM	C09-C10-C11-C12
3	B	403	5YM	C01-C02-C03-C04
5	A	403	1DO	C5-C6-C7-C8
7	A	409	A1EQ8	C07-C08-C09-C10
6	B	410	A1EM3	O26-C27-C29-C30
8	A	410	A1EM2	C04-C09-C10-N11
8	A	410	A1EM2	C03-C04-O05-C06
6	B	409	A1EM3	C07-C08-C09-C10
4	A	402	A1EM1	C03-C04-C05-C06
6	B	410	A1EM3	O28-C27-C29-C30
6	B	410	A1EM3	C17-O18-P19-O20
3	A	401	5YM	C01-C02-C03-C04
5	B	406	1DO	C5-C6-C7-C8
6	A	406	A1EM3	O03-C04-C06-C07
5	A	407	1DO	C6-C7-C8-C9
7	B	402	A1EQ8	C18-C19-C20-O21

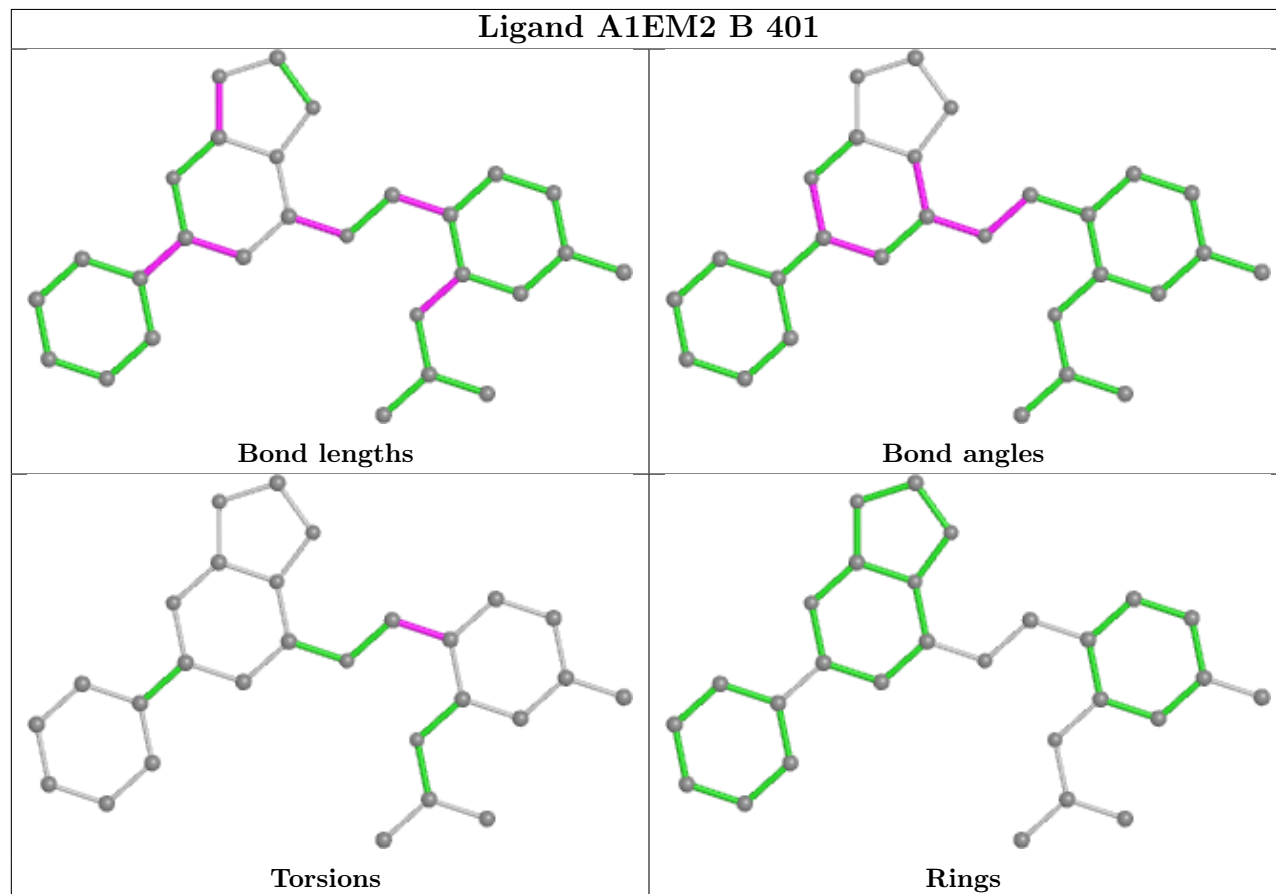
There are no ring outliers.

3 monomers are involved in 8 short contacts:

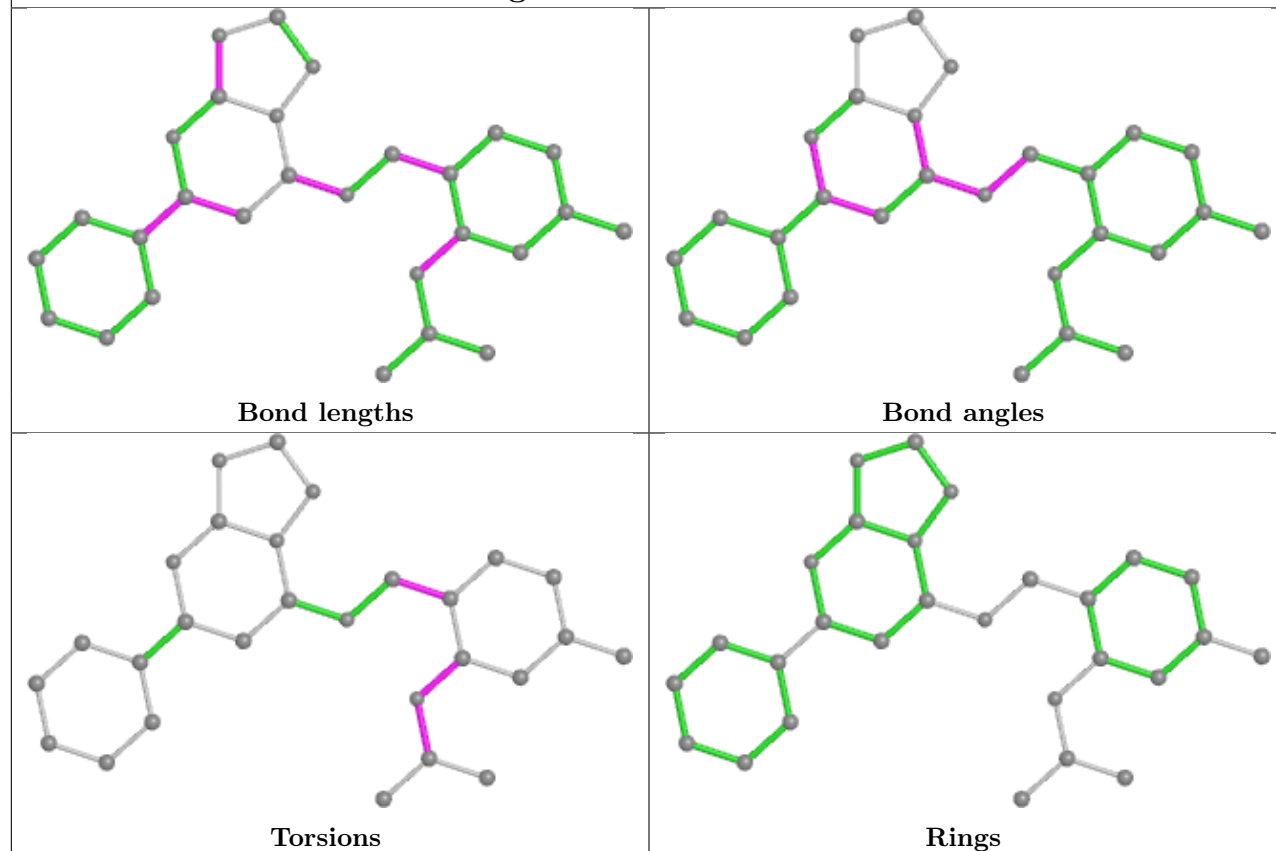
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	1DO	1	0
6	B	410	A1EM3	3	0
6	A	406	A1EM3	4	0

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

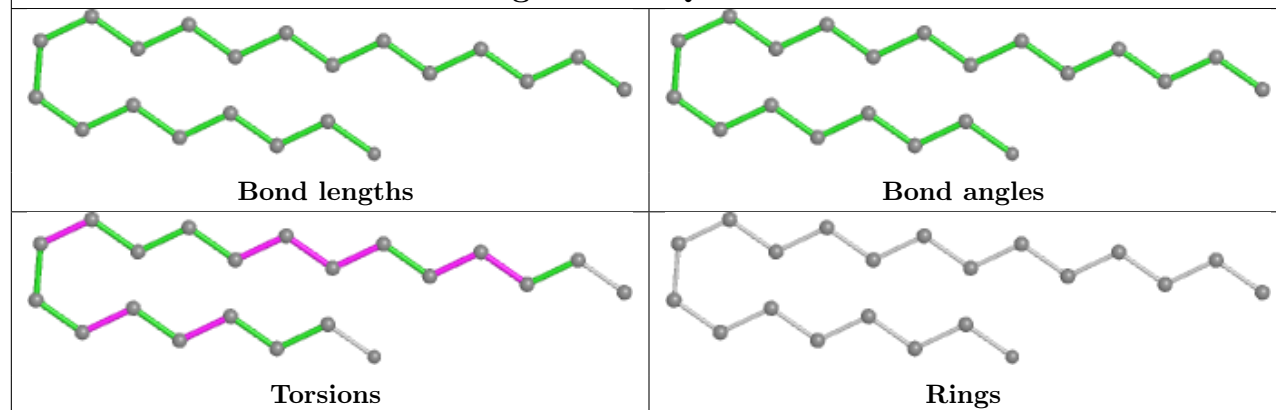
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

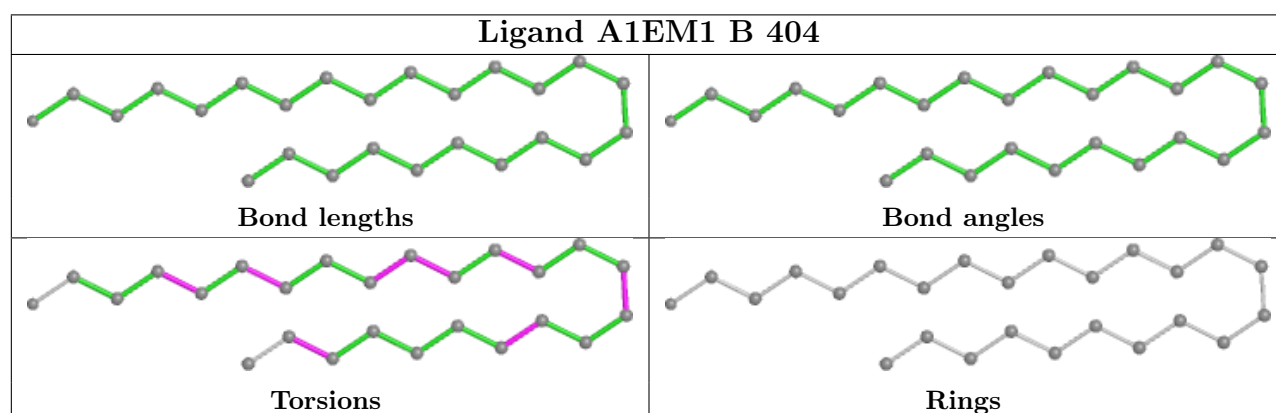
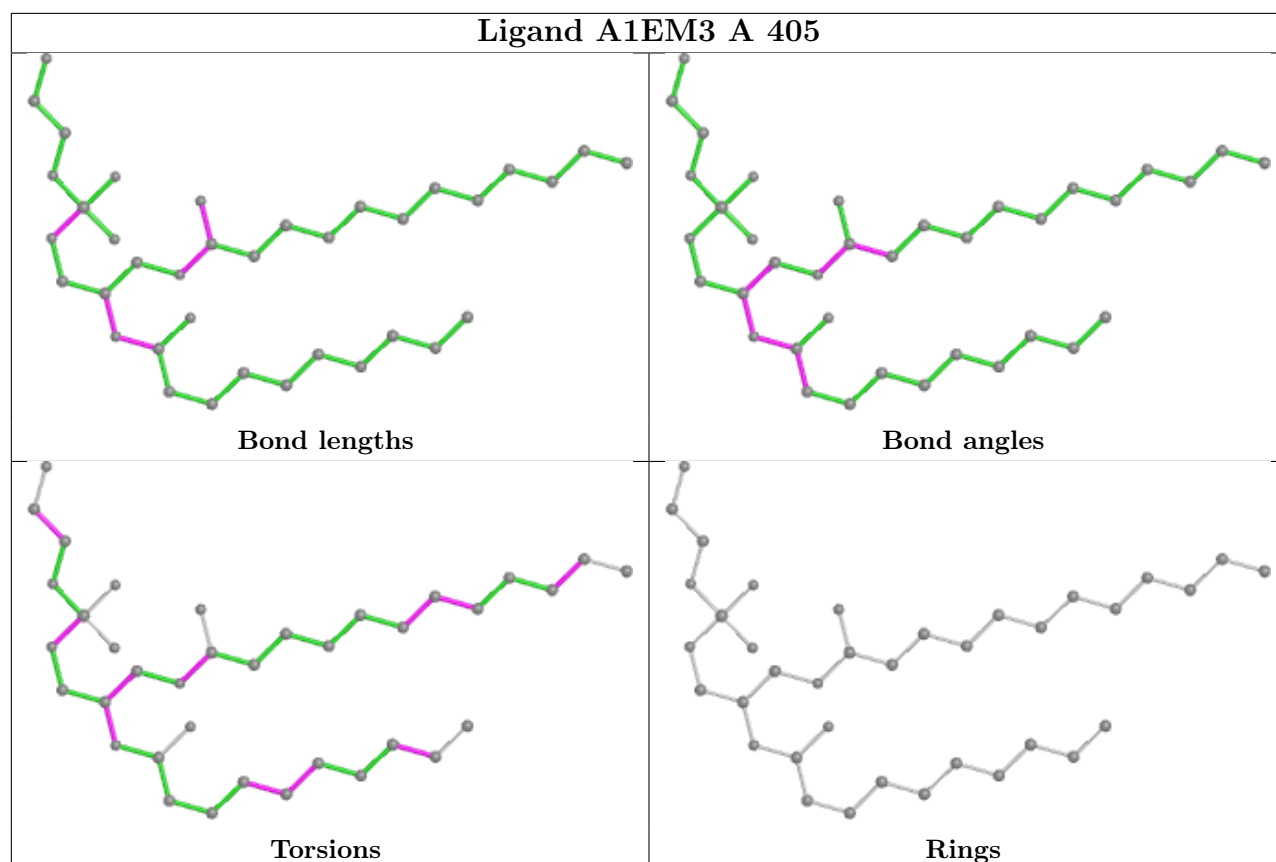
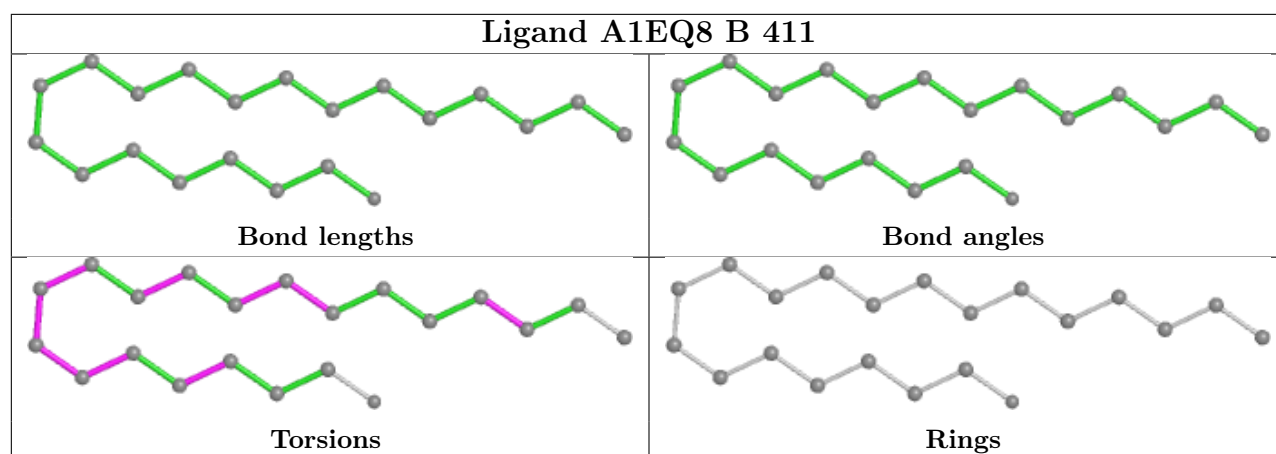


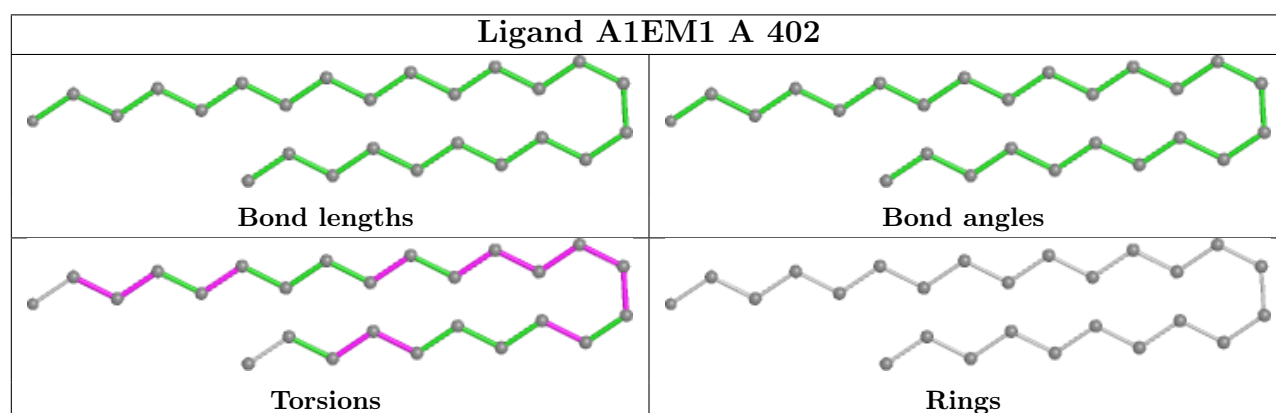
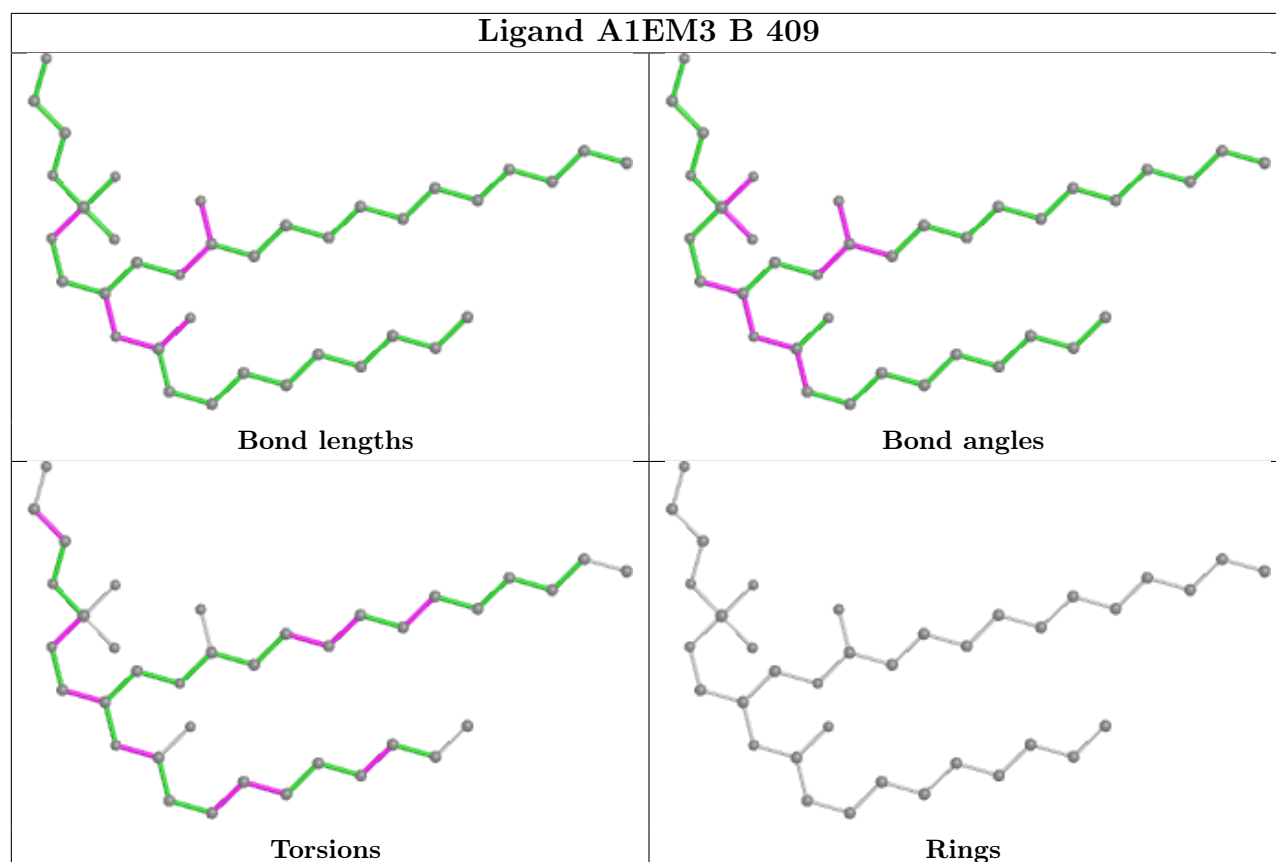
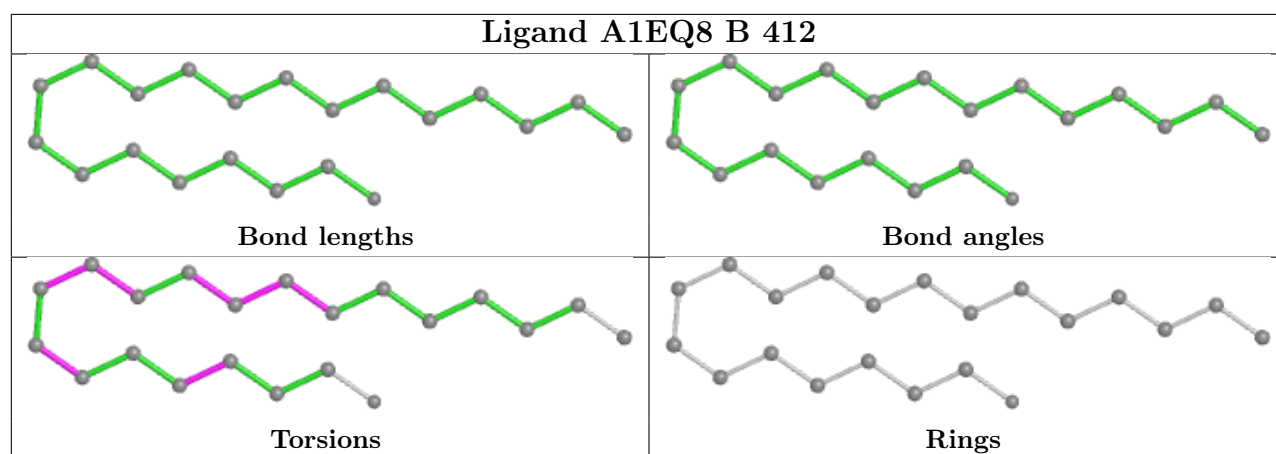
Ligand A1EM2 A 410

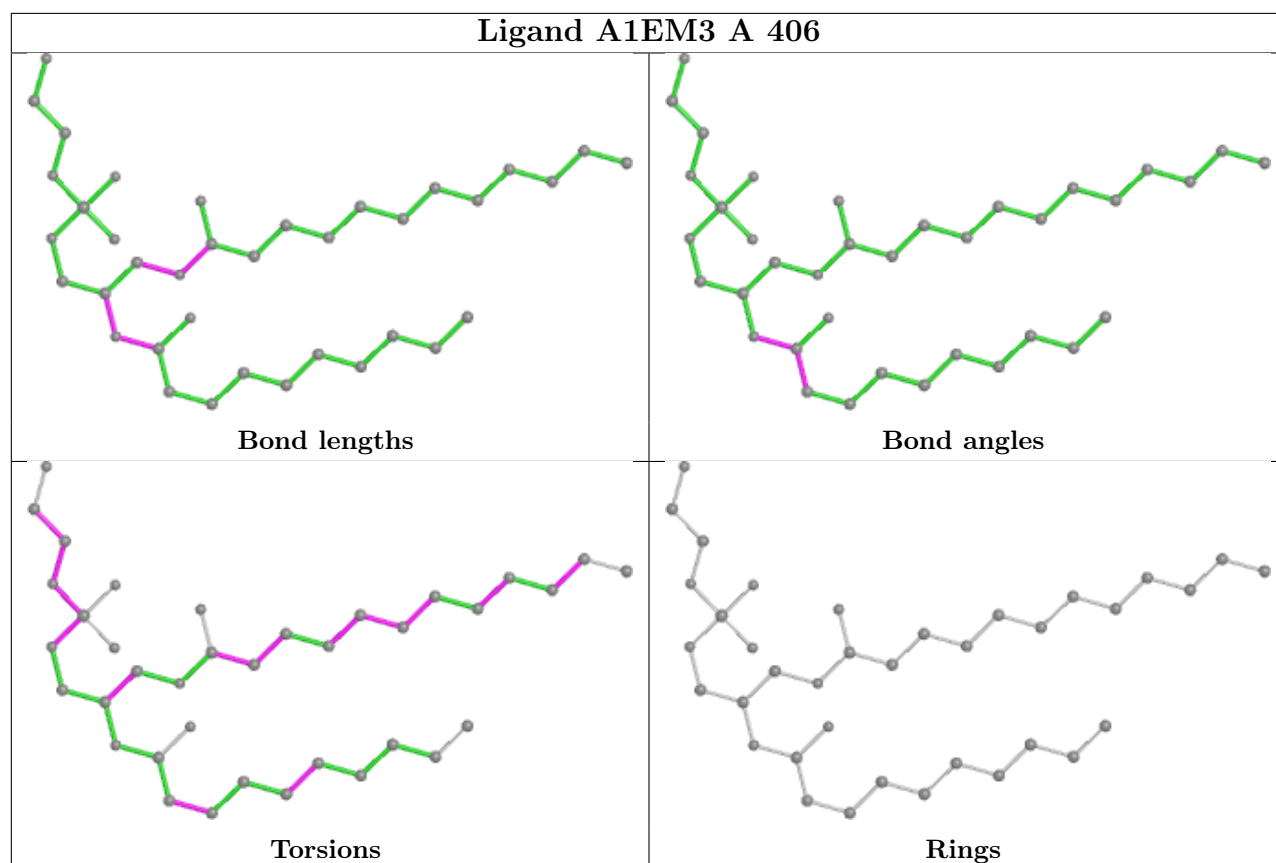
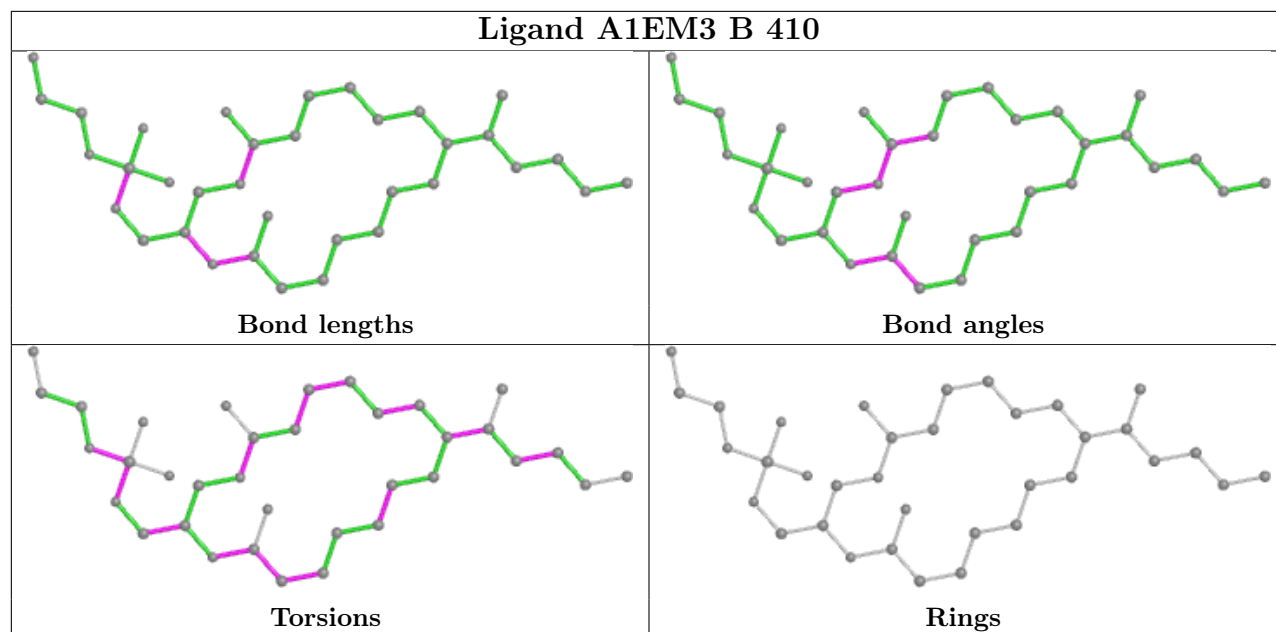


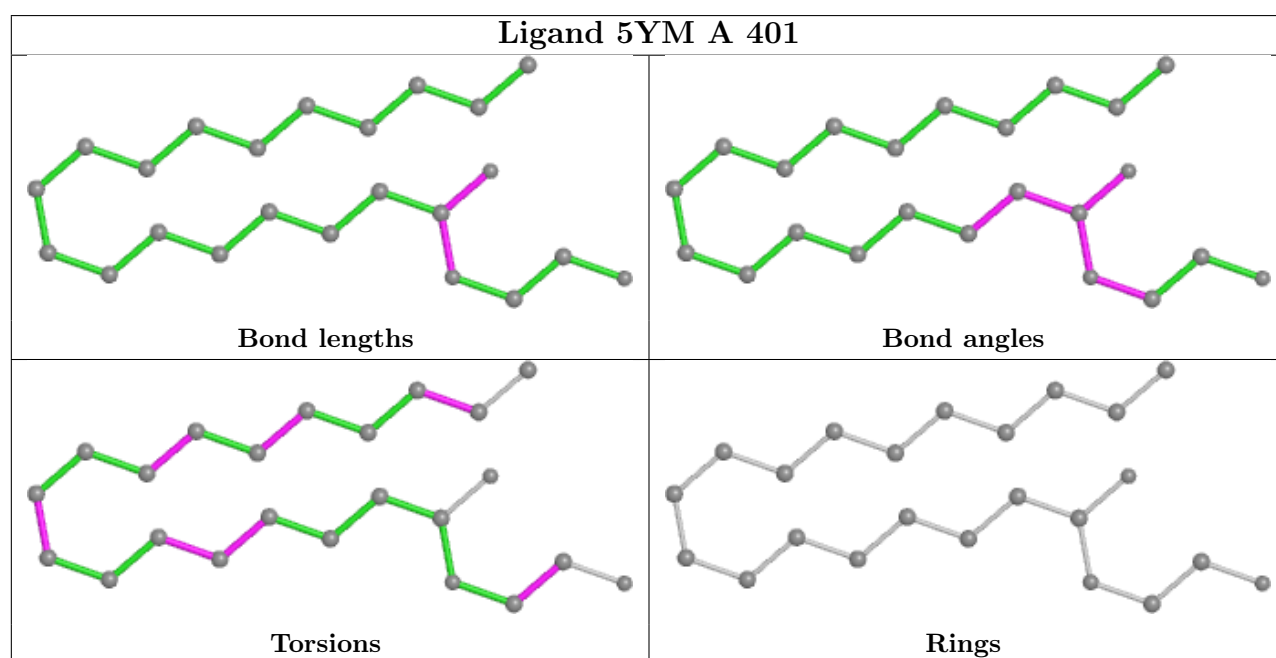
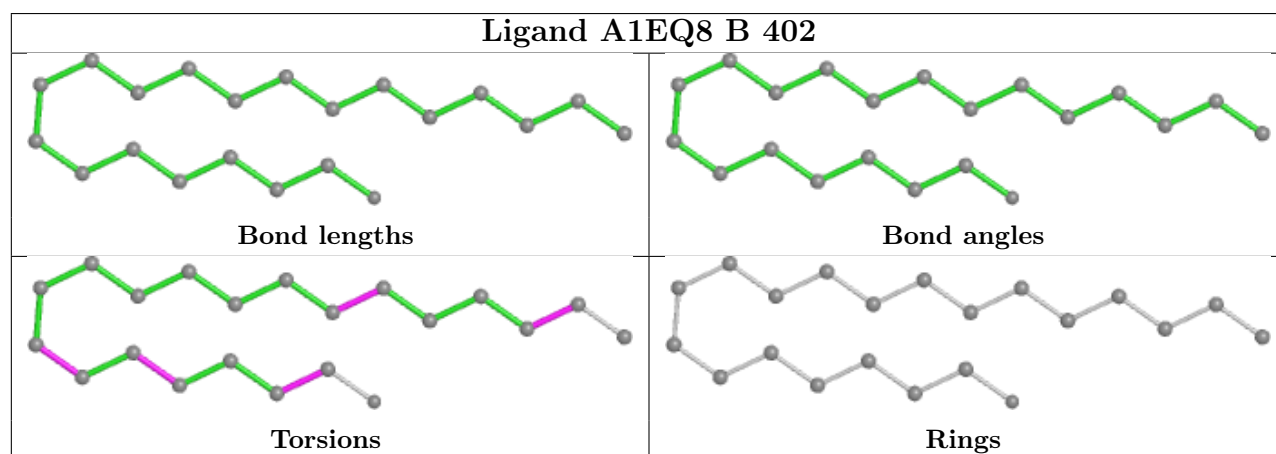
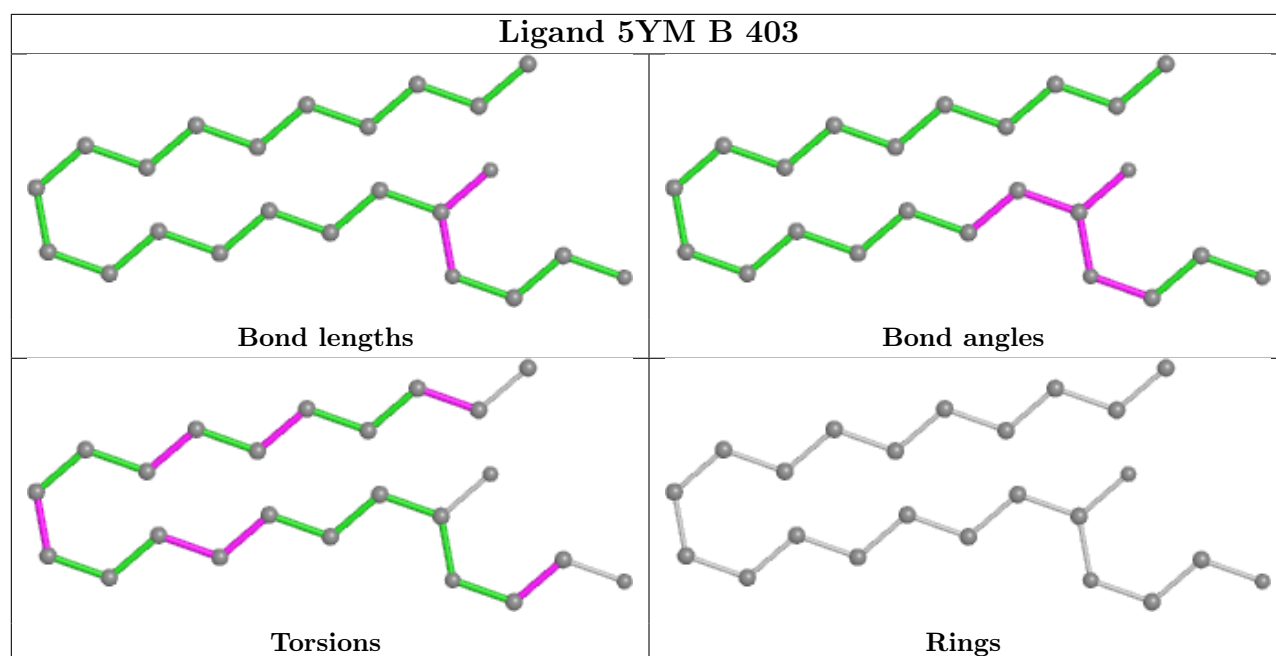
Ligand A1EQ8 A 409











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.

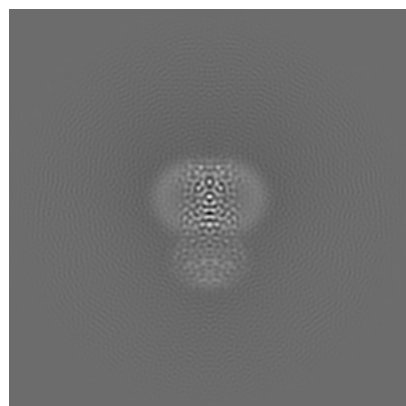
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63702. These allow visual inspection of the internal detail of the map and identification of artifacts.

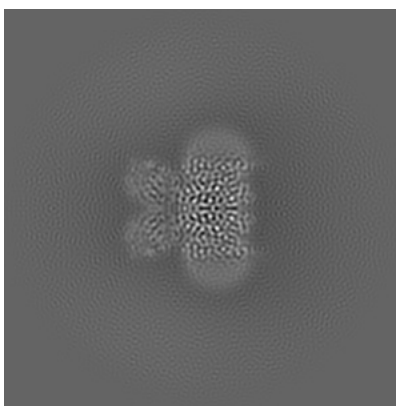
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

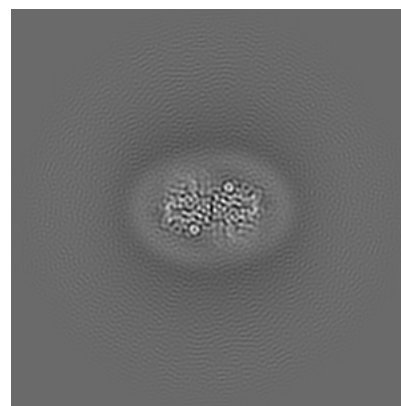
6.1.1 Primary map



X

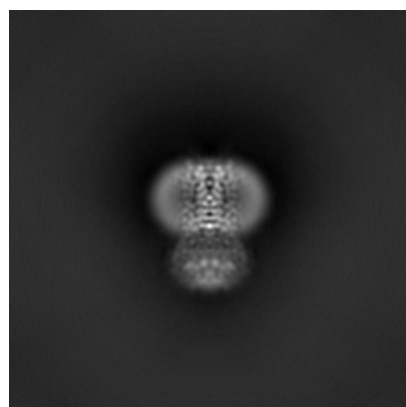


Y

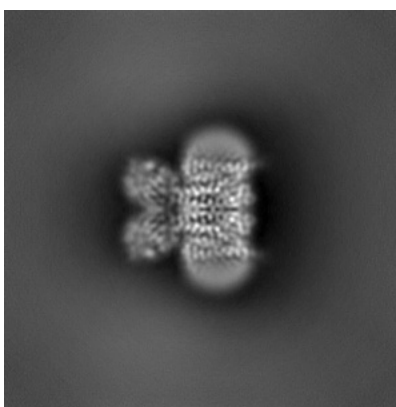


Z

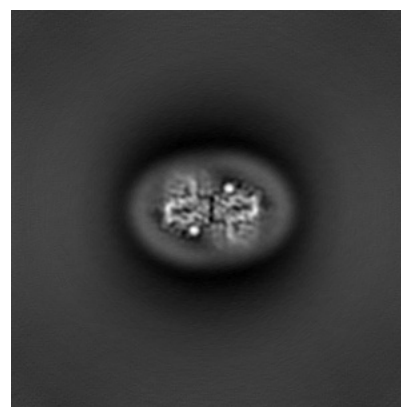
6.1.2 Raw map



X



Y

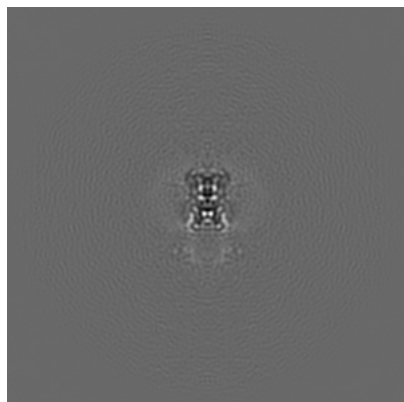


Z

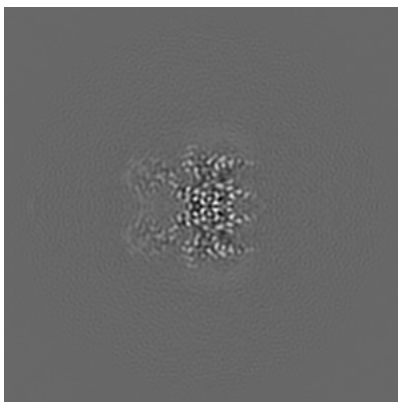
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

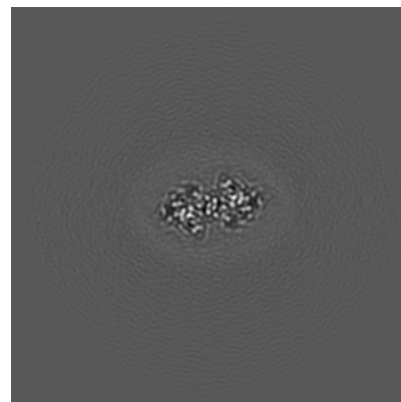
6.2.1 Primary map



X Index: 160

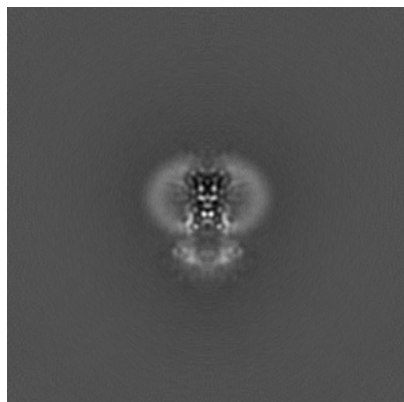


Y Index: 160

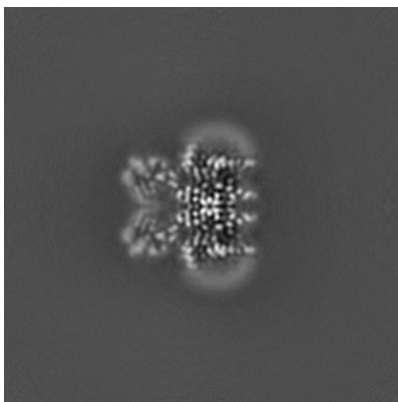


Z Index: 160

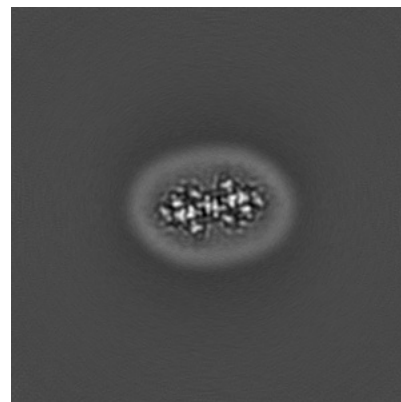
6.2.2 Raw map



X Index: 160



Y Index: 160

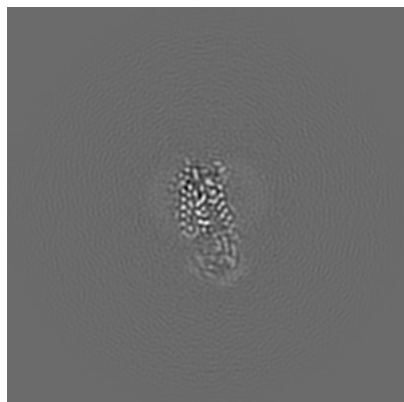


Z Index: 160

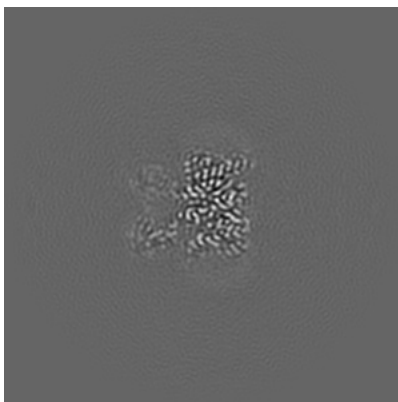
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

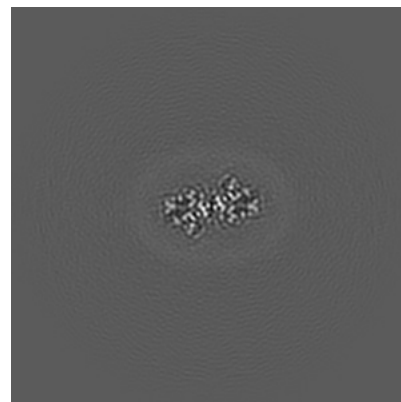
6.3.1 Primary map



X Index: 146

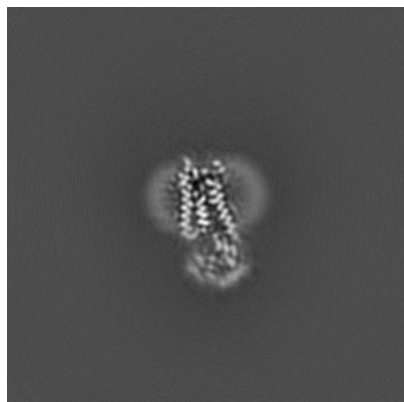


Y Index: 166

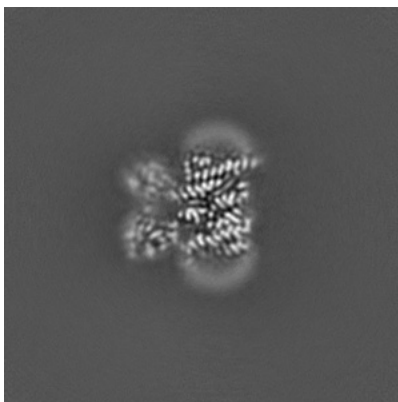


Z Index: 170

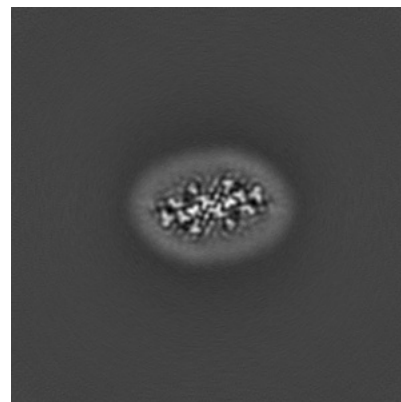
6.3.2 Raw map



X Index: 146



Y Index: 166

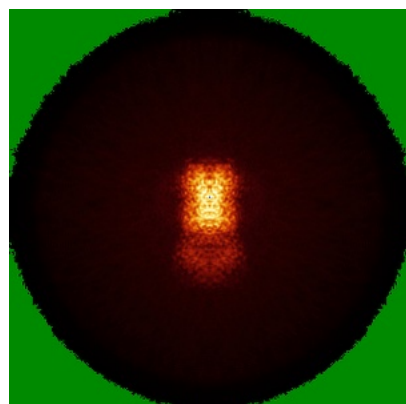


Z Index: 153

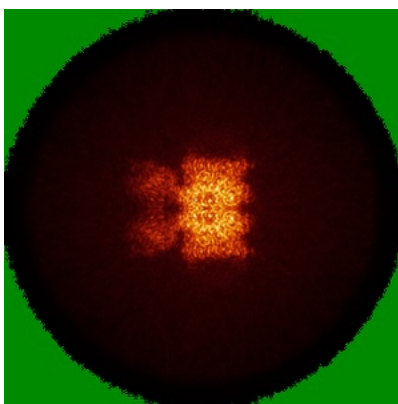
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

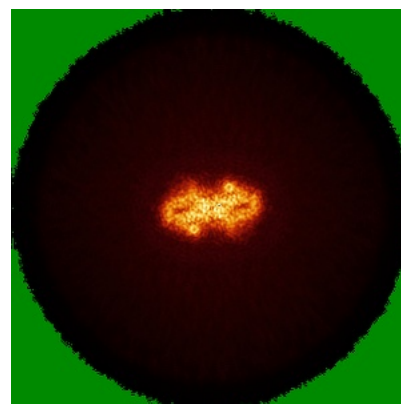
6.4.1 Primary map



X

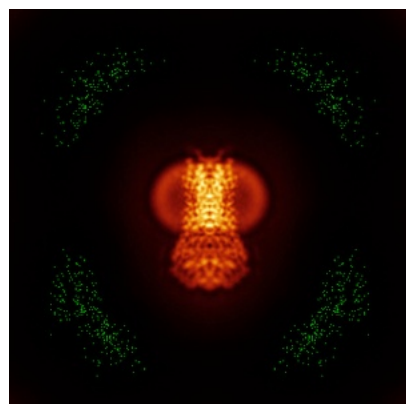


Y

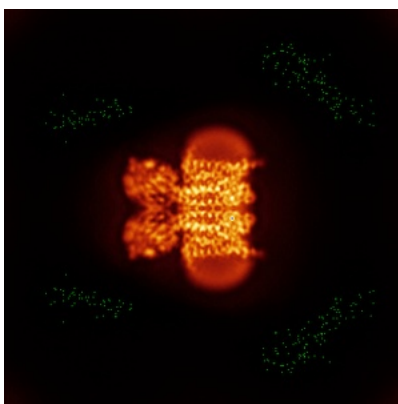


Z

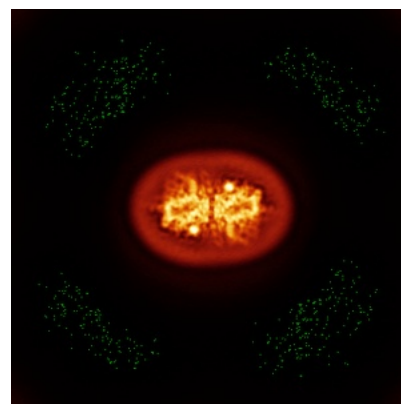
6.4.2 Raw map



X



Y

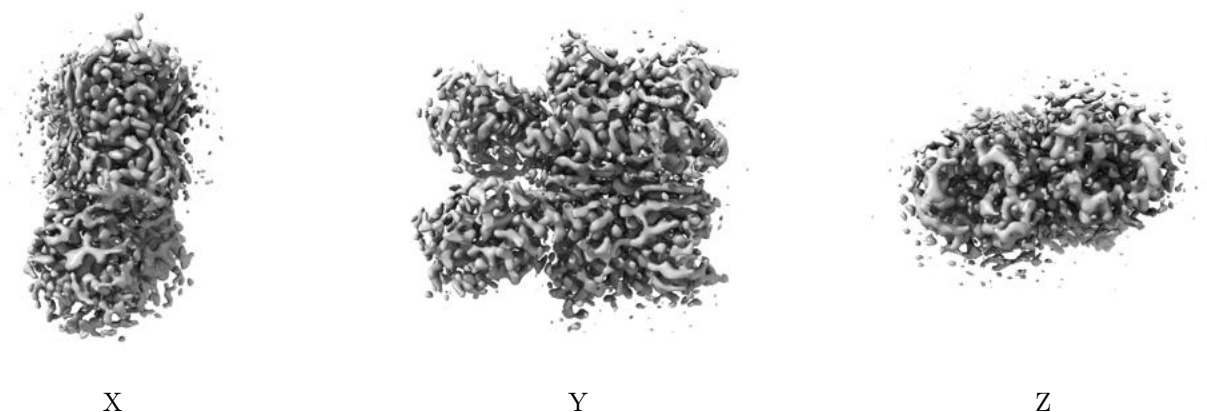


Z

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

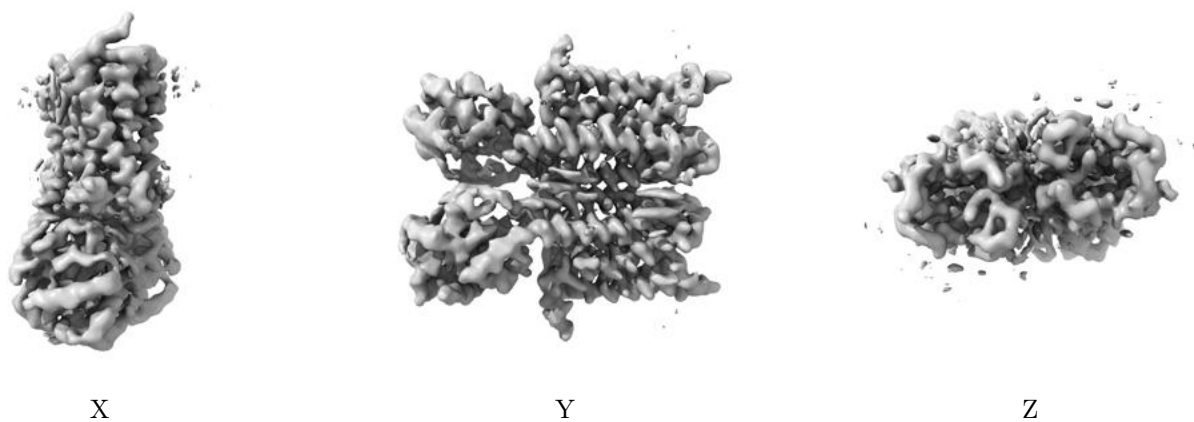
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.844. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

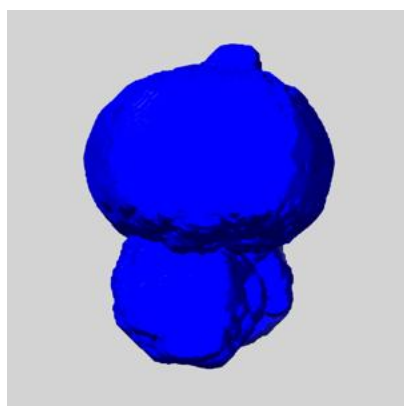
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

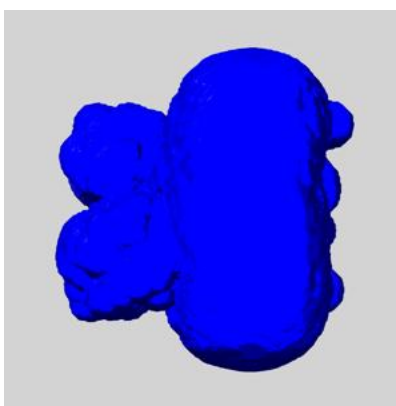
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_63702_msk_1.map [i](#)



X



Y

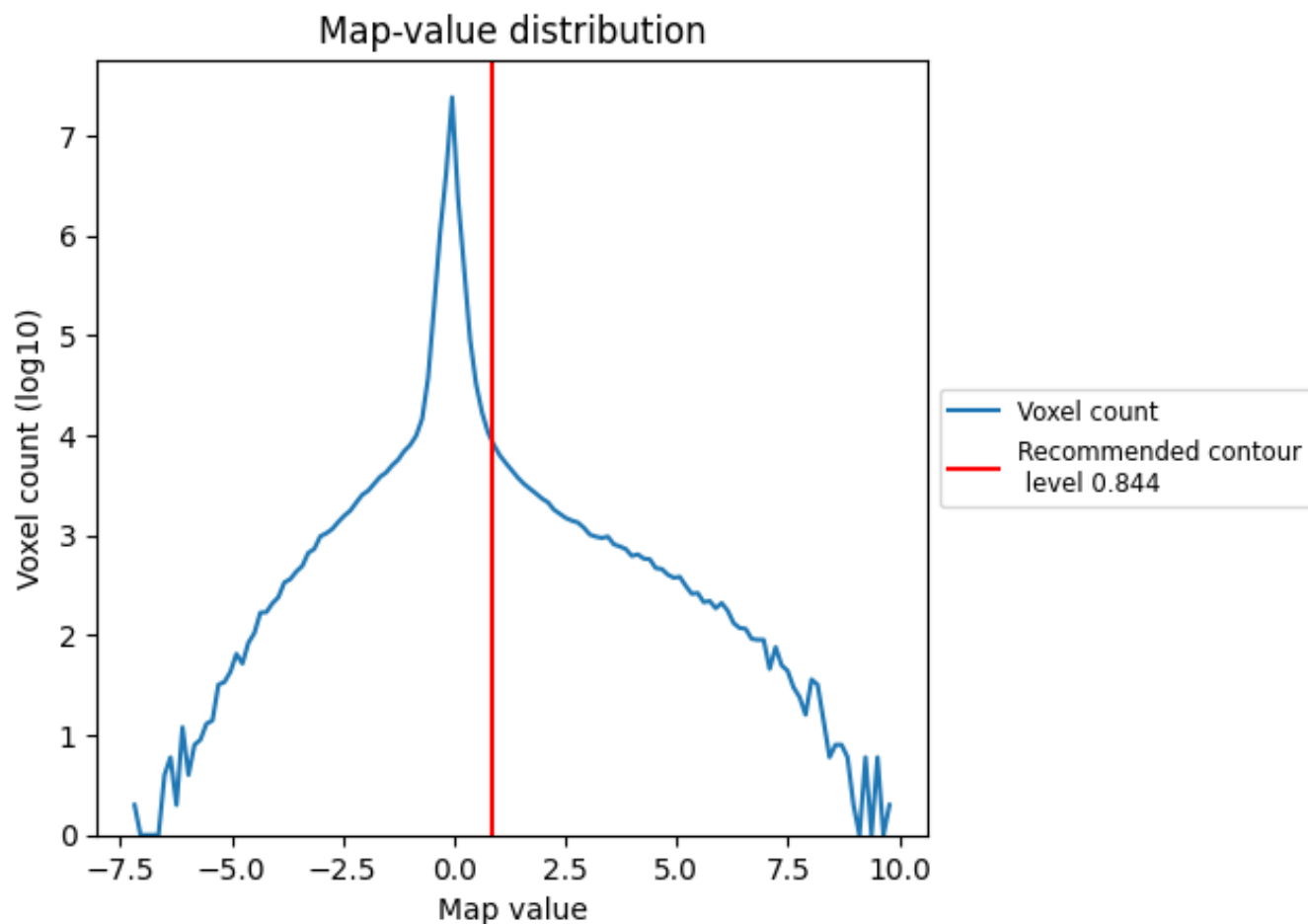


Z

7 Map analysis [i](#)

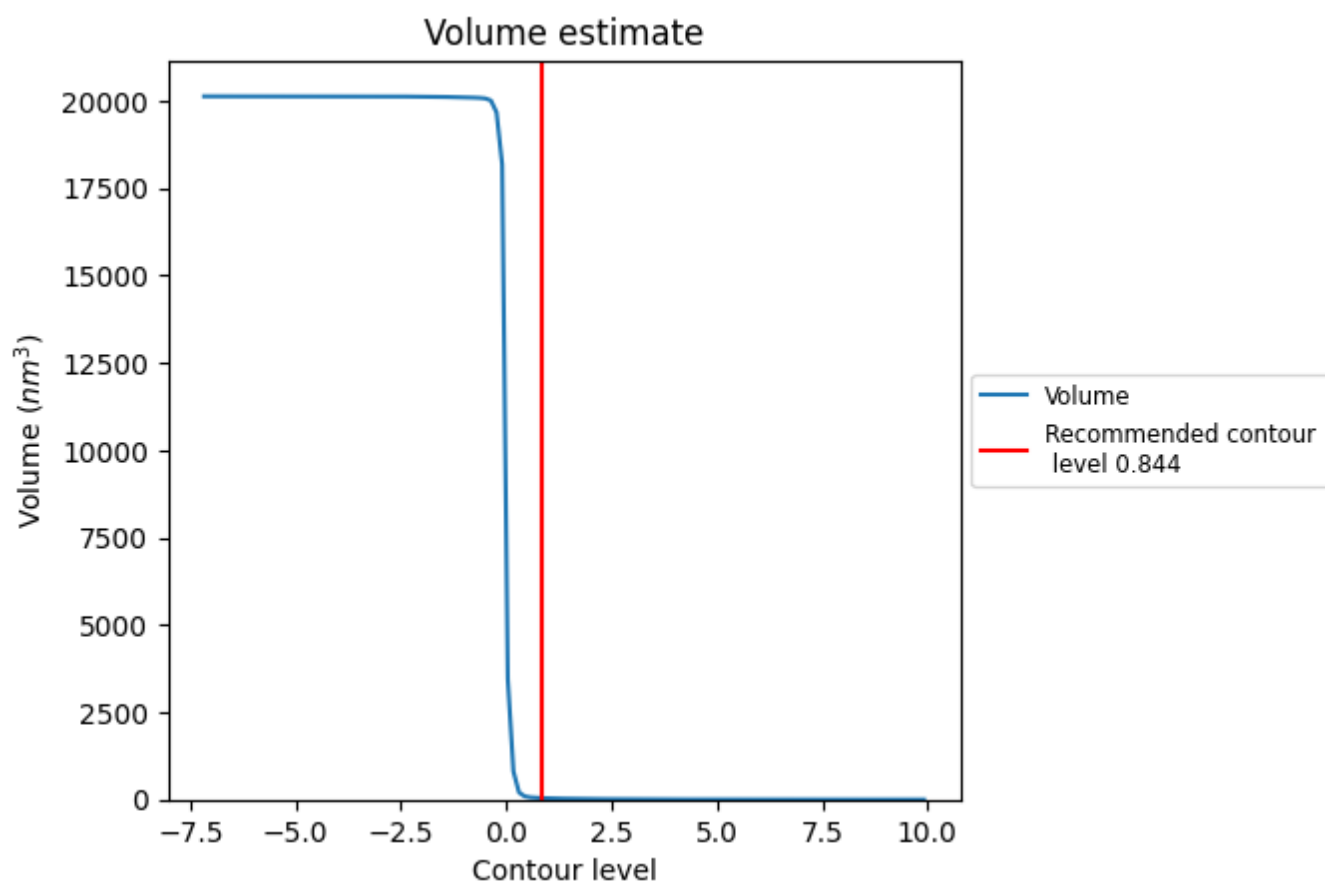
This section contains the results of statistical analysis of the map.

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.

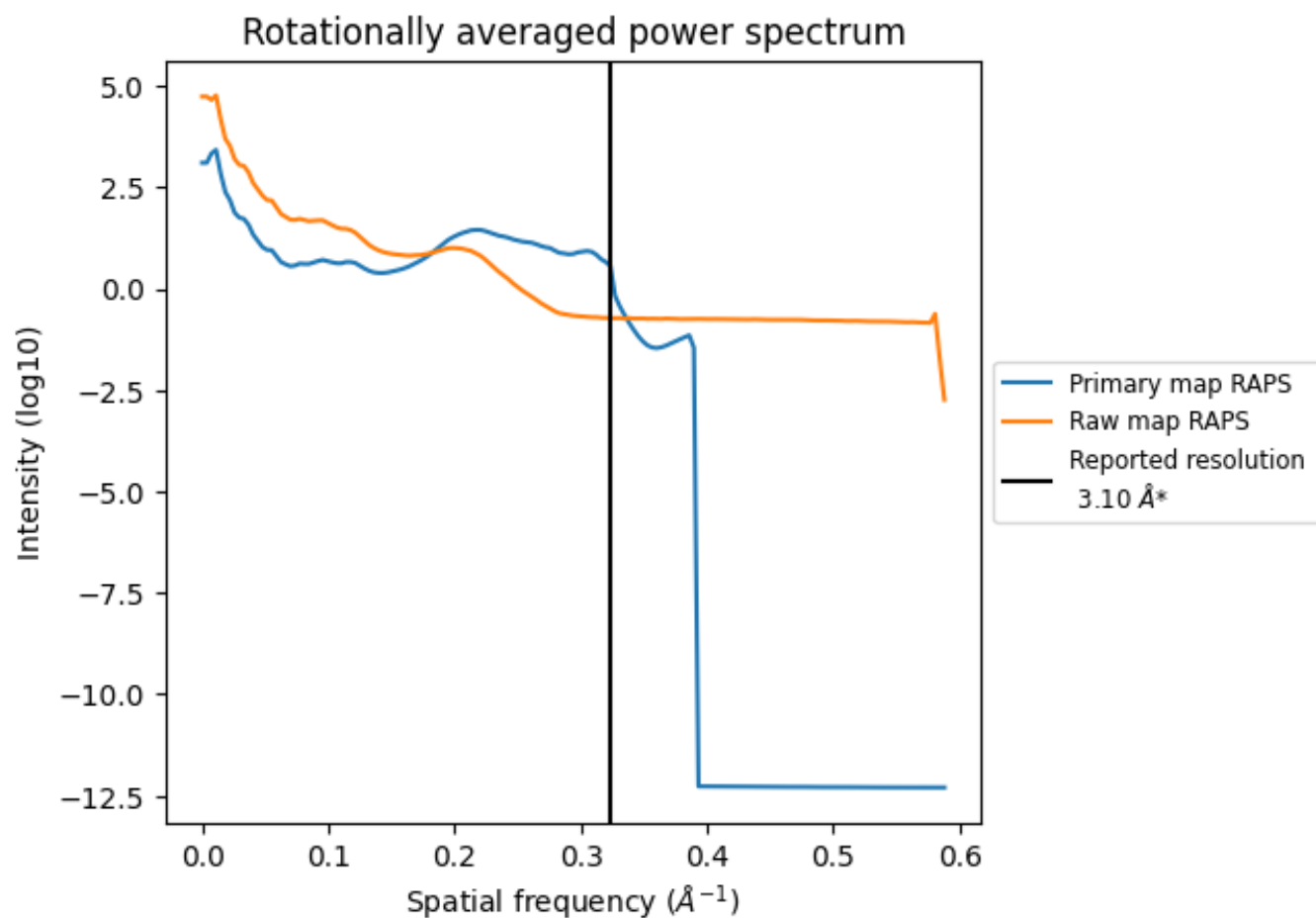
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm³; this corresponds to an approximate mass of 37 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 ⓘ

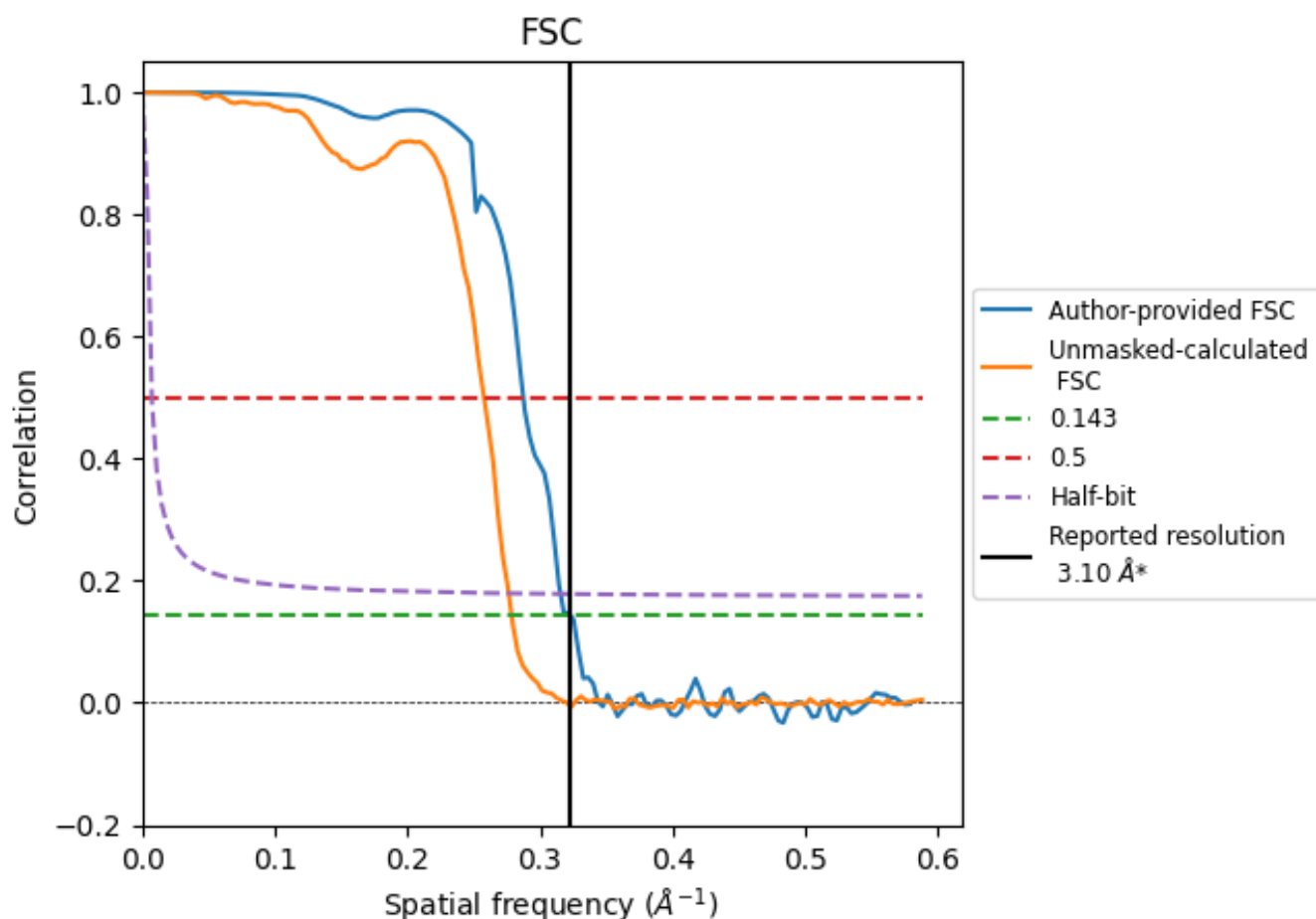


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

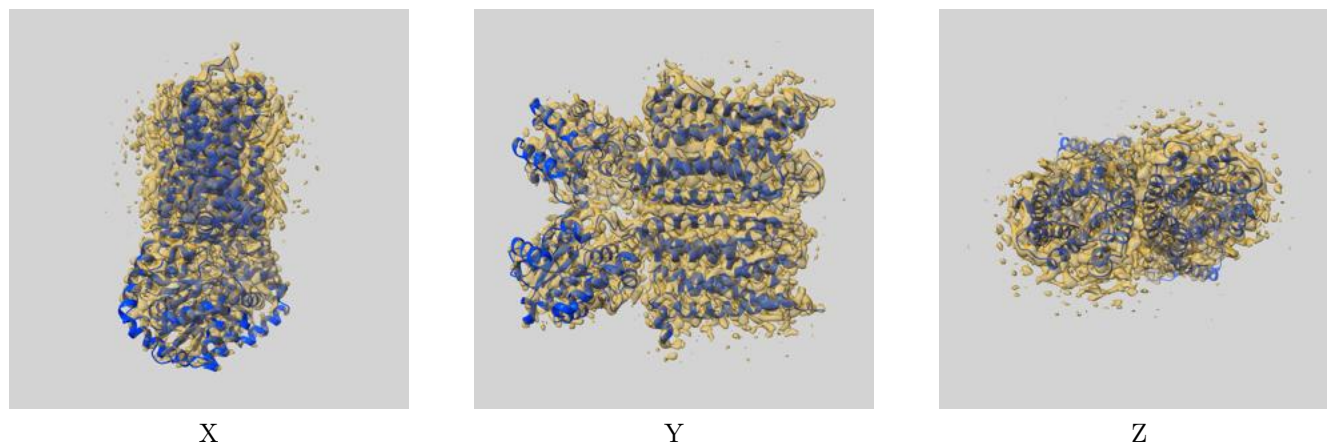
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.48	3.17
Unmasked-calculated*	3.59	3.88	3.62

*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 3.59 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

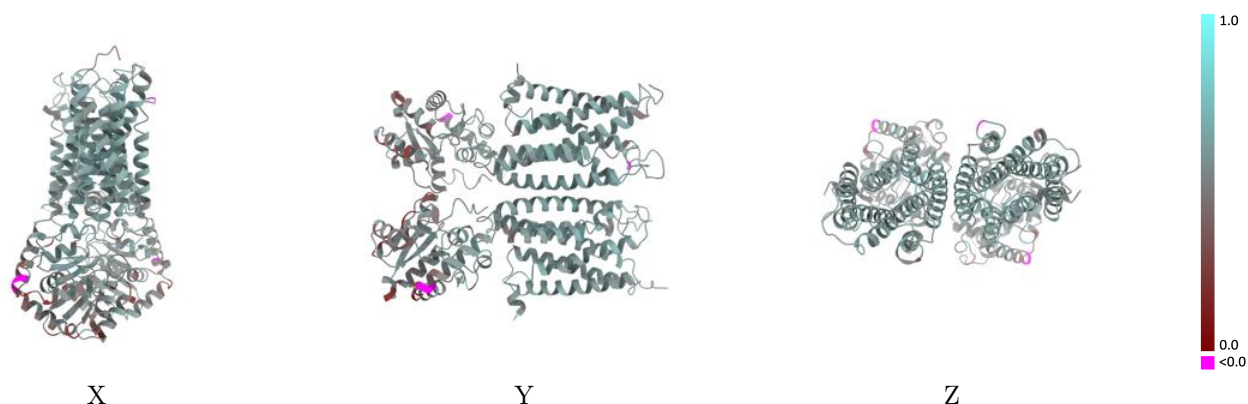
This section contains information regarding the fit between EMDB map EMD-63702 and PDB model 9M88. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



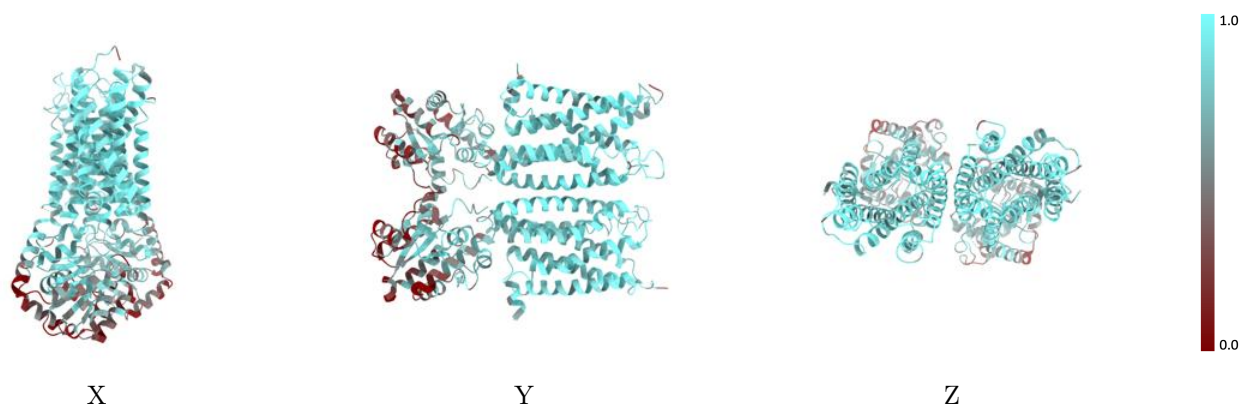
The images above show the 3D surface view of the map at the recommended contour level 0.844 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



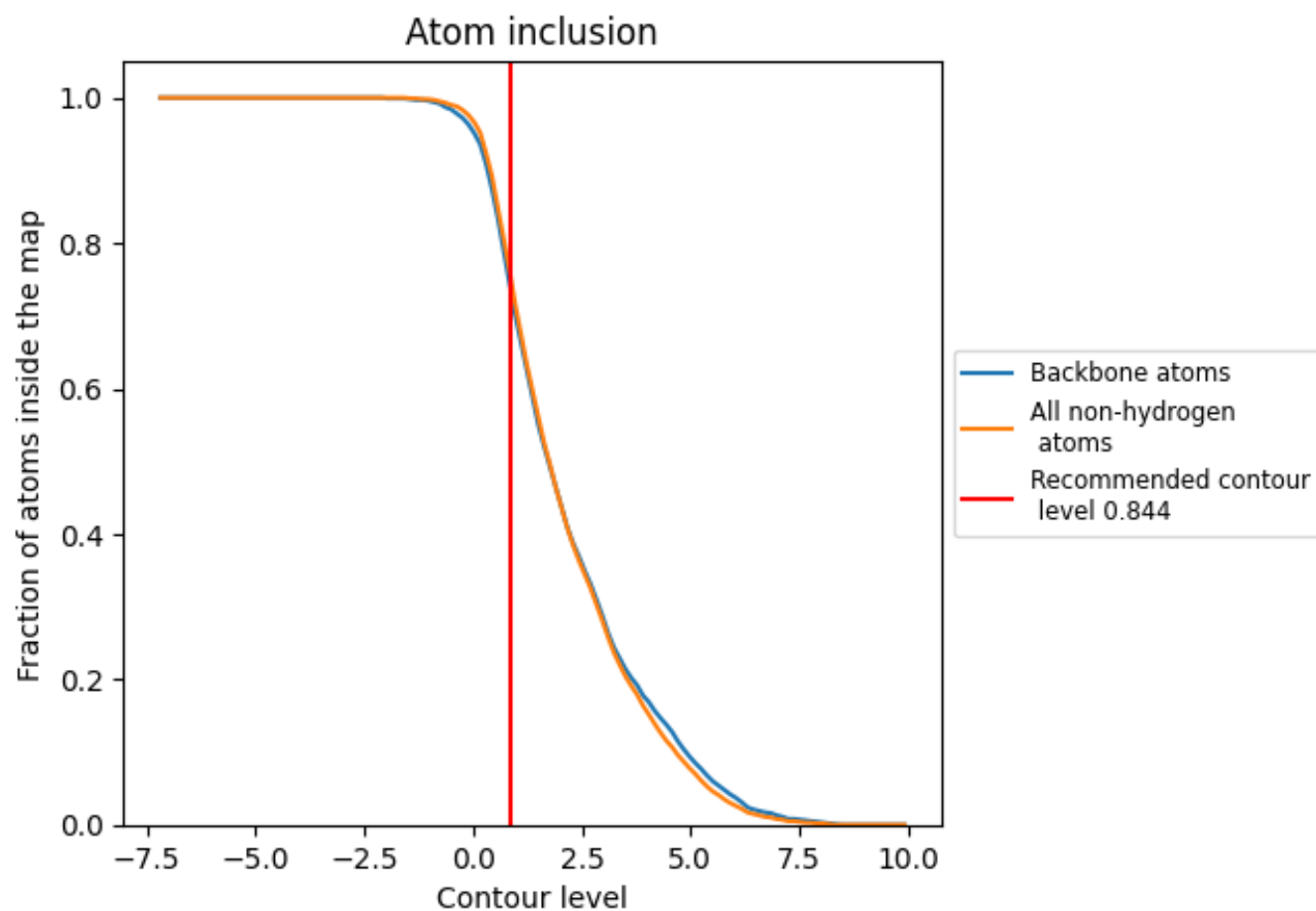
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.844).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.844) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7620	<div></div> 0.5400
A	<div></div> 0.8820	<div></div> 0.5760
B	<div></div> 0.8860	<div></div> 0.5770
C	<div></div> 0.5840	<div></div> 0.4840
D	<div></div> 0.5770	<div></div> 0.4860

