



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 11:13 am BST

PDB ID : 9R8J / pdb_00009r8j
EMDB ID : EMD-53827
Title : Structure of human NHE9
Authors : Hansen, J.S.; Pike, A.C.W.; Chi, G.; Wolf, G.; Ingles-Prieto, A.; Tranberg-Jensen, J.; Ye, M.; Speedman, D.; Goericke, F.; Sauer, D.B.; Beck, H.; Superti-Furga, G.; Huber, K.V.M.
Deposited on : 2025-05-16
Resolution : 2.83 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

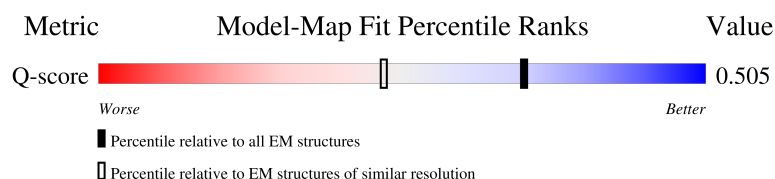
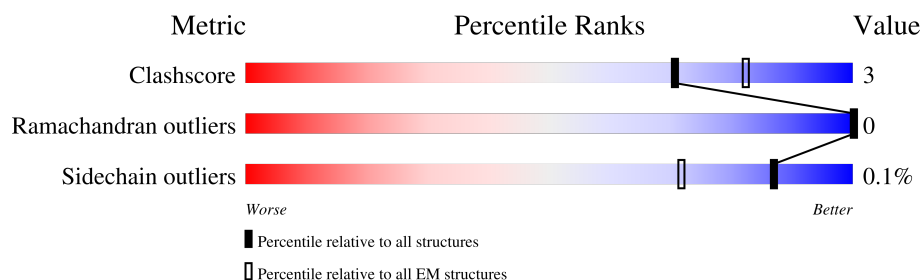
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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	11847 (2.33 - 3.33)

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	716	
1	B	716	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7784 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 Sodium/hydrogen exchanger 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	480	Total	C	N	O	S	0	0
			3725	2477	587	638	23		
1	B	480	Total	C	N	O	S	0	0
			3727	2479	588	637	23		

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	646	ASP	-	expression tag	UNP Q8IVB4
A	647	PRO	-	expression tag	UNP Q8IVB4
A	648	ALA	-	expression tag	UNP Q8IVB4
A	649	PHE	-	expression tag	UNP Q8IVB4
A	650	LEU	-	expression tag	UNP Q8IVB4
A	651	TYR	-	expression tag	UNP Q8IVB4
A	652	LYS	-	expression tag	UNP Q8IVB4
A	653	VAL	-	expression tag	UNP Q8IVB4
A	654	VAL	-	expression tag	UNP Q8IVB4
A	655	ASP	-	expression tag	UNP Q8IVB4
A	656	ILE	-	expression tag	UNP Q8IVB4
A	657	LYS	-	expression tag	UNP Q8IVB4
A	658	ALA	-	expression tag	UNP Q8IVB4
A	659	ALA	-	expression tag	UNP Q8IVB4
A	660	ASP	-	expression tag	UNP Q8IVB4
A	661	ILE	-	expression tag	UNP Q8IVB4
A	662	THR	-	expression tag	UNP Q8IVB4
A	663	SER	-	expression tag	UNP Q8IVB4
A	664	LEU	-	expression tag	UNP Q8IVB4
A	665	TYR	-	expression tag	UNP Q8IVB4
A	666	LYS	-	expression tag	UNP Q8IVB4
A	667	LYS	-	expression tag	UNP Q8IVB4
A	668	VAL	-	expression tag	UNP Q8IVB4
A	669	GLY	-	expression tag	UNP Q8IVB4
A	670	TRP	-	expression tag	UNP Q8IVB4
A	671	SER	-	expression tag	UNP Q8IVB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	672	HIS	-	expression tag	UNP Q8IVB4
A	673	PRO	-	expression tag	UNP Q8IVB4
A	674	GLN	-	expression tag	UNP Q8IVB4
A	675	PHE	-	expression tag	UNP Q8IVB4
A	676	GLU	-	expression tag	UNP Q8IVB4
A	677	LYS	-	expression tag	UNP Q8IVB4
A	678	GLY	-	expression tag	UNP Q8IVB4
A	679	GLY	-	expression tag	UNP Q8IVB4
A	680	GLY	-	expression tag	UNP Q8IVB4
A	681	SER	-	expression tag	UNP Q8IVB4
A	682	GLY	-	expression tag	UNP Q8IVB4
A	683	GLY	-	expression tag	UNP Q8IVB4
A	684	GLY	-	expression tag	UNP Q8IVB4
A	685	SER	-	expression tag	UNP Q8IVB4
A	686	GLY	-	expression tag	UNP Q8IVB4
A	687	GLY	-	expression tag	UNP Q8IVB4
A	688	GLY	-	expression tag	UNP Q8IVB4
A	689	SER	-	expression tag	UNP Q8IVB4
A	690	TRP	-	expression tag	UNP Q8IVB4
A	691	SER	-	expression tag	UNP Q8IVB4
A	692	HIS	-	expression tag	UNP Q8IVB4
A	693	PRO	-	expression tag	UNP Q8IVB4
A	694	GLN	-	expression tag	UNP Q8IVB4
A	695	PHE	-	expression tag	UNP Q8IVB4
A	696	GLU	-	expression tag	UNP Q8IVB4
A	697	LYS	-	expression tag	UNP Q8IVB4
A	698	GLY	-	expression tag	UNP Q8IVB4
A	699	THR	-	expression tag	UNP Q8IVB4
A	700	GLU	-	expression tag	UNP Q8IVB4
A	701	LEU	-	expression tag	UNP Q8IVB4
A	702	GLY	-	expression tag	UNP Q8IVB4
A	703	SER	-	expression tag	UNP Q8IVB4
A	704	THR	-	expression tag	UNP Q8IVB4
A	705	MET	-	expression tag	UNP Q8IVB4
A	706	ALA	-	expression tag	UNP Q8IVB4
A	707	SER	-	expression tag	UNP Q8IVB4
A	708	TYR	-	expression tag	UNP Q8IVB4
A	709	PRO	-	expression tag	UNP Q8IVB4
A	710	TYR	-	expression tag	UNP Q8IVB4
A	711	ASP	-	expression tag	UNP Q8IVB4
A	712	VAL	-	expression tag	UNP Q8IVB4
A	713	PRO	-	expression tag	UNP Q8IVB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	714	ASP	-	expression tag	UNP Q8IVB4
A	715	TYR	-	expression tag	UNP Q8IVB4
A	716	ALA	-	expression tag	UNP Q8IVB4
B	646	ASP	-	expression tag	UNP Q8IVB4
B	647	PRO	-	expression tag	UNP Q8IVB4
B	648	ALA	-	expression tag	UNP Q8IVB4
B	649	PHE	-	expression tag	UNP Q8IVB4
B	650	LEU	-	expression tag	UNP Q8IVB4
B	651	TYR	-	expression tag	UNP Q8IVB4
B	652	LYS	-	expression tag	UNP Q8IVB4
B	653	VAL	-	expression tag	UNP Q8IVB4
B	654	VAL	-	expression tag	UNP Q8IVB4
B	655	ASP	-	expression tag	UNP Q8IVB4
B	656	ILE	-	expression tag	UNP Q8IVB4
B	657	LYS	-	expression tag	UNP Q8IVB4
B	658	ALA	-	expression tag	UNP Q8IVB4
B	659	ALA	-	expression tag	UNP Q8IVB4
B	660	ASP	-	expression tag	UNP Q8IVB4
B	661	ILE	-	expression tag	UNP Q8IVB4
B	662	THR	-	expression tag	UNP Q8IVB4
B	663	SER	-	expression tag	UNP Q8IVB4
B	664	LEU	-	expression tag	UNP Q8IVB4
B	665	TYR	-	expression tag	UNP Q8IVB4
B	666	LYS	-	expression tag	UNP Q8IVB4
B	667	LYS	-	expression tag	UNP Q8IVB4
B	668	VAL	-	expression tag	UNP Q8IVB4
B	669	GLY	-	expression tag	UNP Q8IVB4
B	670	TRP	-	expression tag	UNP Q8IVB4
B	671	SER	-	expression tag	UNP Q8IVB4
B	672	HIS	-	expression tag	UNP Q8IVB4
B	673	PRO	-	expression tag	UNP Q8IVB4
B	674	GLN	-	expression tag	UNP Q8IVB4
B	675	PHE	-	expression tag	UNP Q8IVB4
B	676	GLU	-	expression tag	UNP Q8IVB4
B	677	LYS	-	expression tag	UNP Q8IVB4
B	678	GLY	-	expression tag	UNP Q8IVB4
B	679	GLY	-	expression tag	UNP Q8IVB4
B	680	GLY	-	expression tag	UNP Q8IVB4
B	681	SER	-	expression tag	UNP Q8IVB4
B	682	GLY	-	expression tag	UNP Q8IVB4
B	683	GLY	-	expression tag	UNP Q8IVB4
B	684	GLY	-	expression tag	UNP Q8IVB4

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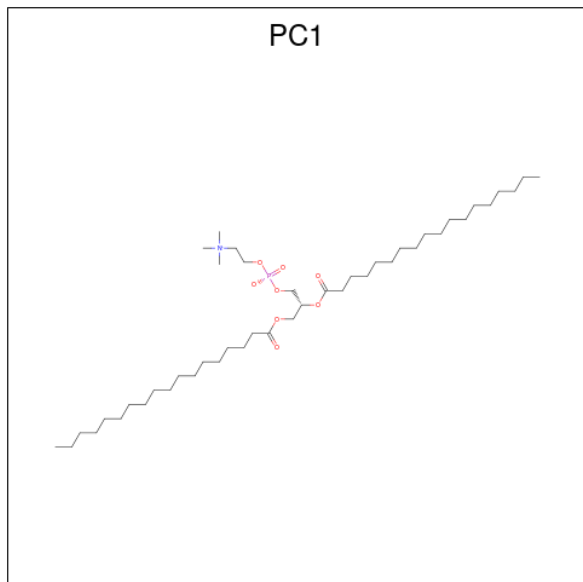
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Chain	Residue	Modelled	Actual	Comment	Reference
B	685	SER	-	expression tag	UNP Q8IVB4
B	686	GLY	-	expression tag	UNP Q8IVB4
B	687	GLY	-	expression tag	UNP Q8IVB4
B	688	GLY	-	expression tag	UNP Q8IVB4
B	689	SER	-	expression tag	UNP Q8IVB4
B	690	TRP	-	expression tag	UNP Q8IVB4
B	691	SER	-	expression tag	UNP Q8IVB4
B	692	HIS	-	expression tag	UNP Q8IVB4
B	693	PRO	-	expression tag	UNP Q8IVB4
B	694	GLN	-	expression tag	UNP Q8IVB4
B	695	PHE	-	expression tag	UNP Q8IVB4
B	696	GLU	-	expression tag	UNP Q8IVB4
B	697	LYS	-	expression tag	UNP Q8IVB4
B	698	GLY	-	expression tag	UNP Q8IVB4
B	699	THR	-	expression tag	UNP Q8IVB4
B	700	GLU	-	expression tag	UNP Q8IVB4
B	701	LEU	-	expression tag	UNP Q8IVB4
B	702	GLY	-	expression tag	UNP Q8IVB4
B	703	SER	-	expression tag	UNP Q8IVB4
B	704	THR	-	expression tag	UNP Q8IVB4
B	705	MET	-	expression tag	UNP Q8IVB4
B	706	ALA	-	expression tag	UNP Q8IVB4
B	707	SER	-	expression tag	UNP Q8IVB4
B	708	TYR	-	expression tag	UNP Q8IVB4
B	709	PRO	-	expression tag	UNP Q8IVB4
B	710	TYR	-	expression tag	UNP Q8IVB4
B	711	ASP	-	expression tag	UNP Q8IVB4
B	712	VAL	-	expression tag	UNP Q8IVB4
B	713	PRO	-	expression tag	UNP Q8IVB4
B	714	ASP	-	expression tag	UNP Q8IVB4
B	715	TYR	-	expression tag	UNP Q8IVB4
B	716	ALA	-	expression tag	UNP Q8IVB4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Na 1 1	0
2	B	1	Total Na 1 1	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
3	B	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



- Molecule 5 is water.

Mol	Chain	Residues	Atoms	AltConf
5	A	7	Total O 7 7	0
5	B	7	Total O 7 7	0

LYS	ALA	TRP
SER	SER	SER
PRO	PRO	HIS
GLN	GLN	PRO
THR	PHE	GLU
PRO	GLU	LYS
GLY	LYS	GLY
GLU	GLY	GLY
ASN	GLY	GLY
ILE	SER	SER
TYR	GLY	GLY
GLU	GLY	GLY
GLY	ASP	GLY
LEU	GLY	GLY
GLY	GLY	GLY
LEU	GLY	GLY
GLY	SER	SER
GLY	TRP	TRP
TYR	SER	SER
GLU	HIS	HIS
LEU	PRO	PRO
LYS	GLN	GLN
LEU	PHE	PHE
GLU	GLU	GLU
GLN	LYS	LYS
THR	GLY	GLY
LEU	THR	THR
GLY	GLU	GLU
GLN	LEU	LEU
SER	GLY	GLY
GLN	SER	SER
LEU	THR	THR
GLN	THR	THR
ASN	MET	MET
ASP	ALA	ALA
PRO	SER	SER
ALA	TYR	TYR
PHE	PRO	PRO
LEU	TYR	TYR
ASP	ASP	ASP
LYS	VAL	VAL
VAL	VAL	VAL
VAL	ASP	ASP
ILE	ILE	ILE
LYS	LYS	LYS
ALA	ALA	ALA
ALA	ALA	ALA
ASP	ASP	ASP
ILE	ILE	ILE
THR	THR	THR
SER	SER	SER
LEU	LEU	LEU
TYR	TYR	TYR
LYS	LYS	LYS
LYS	LYS	LYS
VAL	VAL	VAL
GLY	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212666	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.782	Depositor
Minimum map value	-1.716	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	280.4352, 280.4352, 280.4352	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09545, 1.09545, 1.09545	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: PC1, LMT, NA

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	0.12	0/3829	0.29	0/5210
1	B	0.12	0/3831	0.27	0/5211
All	All	0.12	0/7660	0.28	0/10421

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3725	0	3662	31	0
1	B	3727	0	3668	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	87	0	125	3	0
3	B	85	0	121	2	0
4	A	72	0	105	3	0
4	B	72	0	105	1	0
5	A	7	0	0	1	0
5	B	7	0	0	1	0
All	All	7784	0	7786	54	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 (54) 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:104:TYR:HB3	1:B:104:TYR:HB3	1.65	0.76
1:B:275:VAL:HG22	3:B:802:PC1:H3B1	1.83	0.61
1:A:119:GLN:O	1:A:388:GLN:NE2	2.34	0.61
1:B:441:ARG:NH2	5:B:903:HOH:O	2.35	0.58
1:A:441:ARG:NH2	5:A:901:HOH:O	2.35	0.56
1:A:30:LEU:HD11	1:A:62:MET:HG2	1.87	0.56
1:B:84:VAL:HG12	1:B:85:LYS:HG3	1.88	0.55
1:B:70:THR:HG22	1:B:71:ALA:H	1.72	0.54
1:B:141:PRO:HG3	4:B:805:LMT:H91	1.89	0.54
1:B:245:ALA:HB1	1:B:336:VAL:HG22	1.89	0.54
1:A:141:PRO:HG3	4:A:805:LMT:H91	1.90	0.53
1:A:95:VAL:HG11	1:B:86:LEU:HD23	1.90	0.53
1:B:161:SER:OG	1:B:423:ARG:NH1	2.42	0.51
1:B:30:LEU:HD11	1:B:62:MET:HG2	1.92	0.50
1:A:245:ALA:HB1	1:A:336:VAL:HG22	1.93	0.50
1:B:97:ILE:HG22	1:B:98:THR:HG23	1.95	0.49
1:A:23:GLU:OE1	4:A:804:LMT:O3'	2.26	0.49
1:B:476:PHE:O	1:B:480:THR:OG1	2.29	0.49
1:B:201:PHE:HB3	3:B:802:PC1:H31	1.94	0.48
1:A:171:ALA:HB2	3:A:802:PC1:H3G1	1.96	0.47
1:A:108:ARG:NH2	1:B:103:GLU:OE1	2.49	0.46
1:B:387:PHE:HB3	1:B:390:HIS:NE2	2.31	0.46
1:B:50:HIS:HB2	1:B:218:THR:HG23	1.99	0.45
1:B:481:THR:OG1	1:B:482:PRO:HD3	2.16	0.45
1:A:95:VAL:HG13	1:B:83:CYS:HB2	1.98	0.45
1:B:38:ILE:HG21	1:B:51:GLU:HG2	1.97	0.45
1:A:387:PHE:HD2	1:A:390:HIS:CD2	2.35	0.45
1:A:34:THR:HG22	1:A:38:ILE:HD11	2.00	0.44
1:A:138:LEU:HB3	1:A:376:ILE:HD11	2.00	0.44
1:B:324:PHE:HB2	1:B:338:VAL:CG1	2.48	0.44
1:B:413:TYR:HB2	1:B:414:PRO:HD3	2.01	0.43
1:A:38:ILE:HD13	1:A:51:GLU:HG2	1.98	0.43
1:A:52:THR:HB	1:A:377:PHE:CD2	2.53	0.43
1:A:387:PHE:HB3	1:A:390:HIS:NE2	2.34	0.43
1:B:125:GLU:HG2	1:B:388:GLN:HE22	1.83	0.43
1:A:108:ARG:HG2	1:A:109:GLU:N	2.34	0.43
1:A:324:PHE:HB2	1:A:338:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:HIS:CG	1:A:51:GLU:N	2.86	0.43
1:A:143:ILE:HG13	1:A:335:ILE:HG23	2.01	0.43
1:A:50:HIS:HB2	1:A:218:THR:HG23	2.00	0.42
1:A:200:HIS:HB3	1:A:264:ASN:ND2	2.33	0.42
3:A:806:PC1:H232	3:A:806:PC1:H341	2.01	0.42
1:B:50:HIS:CG	1:B:51:GLU:N	2.88	0.42
1:A:23:GLU:OE2	1:A:126:LYS:HB3	2.20	0.42
1:A:264:ASN:ND2	3:A:802:PC1:O12	2.52	0.42
1:A:413:TYR:HB2	1:A:414:PRO:HD3	2.02	0.41
1:A:84:VAL:HG12	1:A:85:LYS:HG3	2.02	0.41
1:A:165:TYR:HB3	1:A:239:GLU:HG3	2.03	0.41
1:B:310:MET:SD	1:B:360:ARG:NH1	2.93	0.41
4:A:804:LMT:H92	4:A:804:LMT:H122	1.76	0.41
1:A:239:GLU:OE2	1:A:243:ASN:ND2	2.54	0.41
1:A:18:HIS:O	1:A:22:VAL:HG23	2.21	0.41
1:A:259:PRO:HG2	1:A:262:ASN:O	2.20	0.41
1:B:143:ILE:HG13	1:B:335:ILE:HG23	2.03	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	478/716 (67%)	460 (96%)	18 (4%)	0	100	100
1	B	478/716 (67%)	466 (98%)	12 (2%)	0	100	100
All	All	956/1432 (67%)	926 (97%)	30 (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	383/608 (63%)	382 (100%)	1 (0%)	86	94
1	B	383/608 (63%)	383 (100%)	0	100	100
All	All	766/1216 (63%)	765 (100%)	1 (0%)	87	96

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

Mol	Chain	Res	Type
1	A	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	264	ASN
1	A	347	HIS
1	B	145	HIS
1	B	347	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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
3	PC1	B	802	-	47,47,53	0.31	0	53,55,61	0.27	0
3	PC1	A	806	-	38,38,53	0.33	0	44,46,61	0.27	0
4	LMT	A	803	-	24,24,36	0.54	0	29,29,47	0.67	0
3	PC1	A	802	-	47,47,53	0.30	0	53,55,61	0.27	0
4	LMT	A	805	-	24,24,36	0.53	0	29,29,47	0.60	0
4	LMT	B	805	-	24,24,36	0.53	0	29,29,47	0.58	0
4	LMT	B	803	-	24,24,36	0.54	0	29,29,47	0.68	0
4	LMT	B	804	-	24,24,36	0.52	0	29,29,47	0.56	0
3	PC1	B	806	-	36,36,53	0.34	0	42,44,61	0.31	0
4	LMT	A	804	-	24,24,36	0.53	0	29,29,47	0.55	0

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
3	PC1	B	802	-	-	12/51/51/57	-
3	PC1	A	806	-	-	19/42/42/57	-
4	LMT	A	803	-	-	2/15/35/61	0/1/1/2
3	PC1	A	802	-	-	13/51/51/57	-
4	LMT	A	805	-	-	8/15/35/61	0/1/1/2
4	LMT	B	805	-	-	8/15/35/61	0/1/1/2
4	LMT	B	803	-	-	3/15/35/61	0/1/1/2
4	LMT	B	804	-	-	8/15/35/61	0/1/1/2
3	PC1	B	806	-	-	18/40/40/57	-
4	LMT	A	804	-	-	8/15/35/61	0/1/1/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	PC1	C11-O13-P-O11
3	A	806	PC1	C1-O11-P-O12
3	A	806	PC1	O21-C2-C3-O31
3	B	802	PC1	C11-O13-P-O14
3	B	802	PC1	C1-O11-P-O12
3	B	802	PC1	C1-O11-P-O14
3	B	806	PC1	C11-O13-P-O12
3	B	806	PC1	O21-C2-C3-O31
4	A	804	LMT	O5'-C1'-O1'-C1
4	B	804	LMT	O5'-C1'-O1'-C1
4	B	803	LMT	O5'-C5'-C6'-O6'
4	B	803	LMT	C4'-C5'-C6'-O6'
4	B	805	LMT	O5'-C5'-C6'-O6'
4	A	805	LMT	O5'-C5'-C6'-O6'
3	B	802	PC1	C3E-C3F-C3G-C3H
3	A	802	PC1	C1-O11-P-O13
3	B	802	PC1	C11-O13-P-O11
3	B	802	PC1	C1-O11-P-O13
3	B	806	PC1	C11-O13-P-O11
3	B	806	PC1	C11-C12-N-C13
3	B	806	PC1	C11-C12-N-C14
3	B	806	PC1	C11-C12-N-C15
4	A	804	LMT	C6-C7-C8-C9
4	B	804	LMT	C6-C7-C8-C9
3	B	806	PC1	C28-C29-C2A-C2B
4	A	805	LMT	C2-C3-C4-C5
3	A	806	PC1	C2A-C2B-C2C-C2D
3	B	806	PC1	C24-C25-C26-C27
3	B	802	PC1	C11-C12-N-C13
3	A	806	PC1	C22-C23-C24-C25
3	A	806	PC1	C25-C26-C27-C28
3	B	802	PC1	C38-C39-C3A-C3B
3	A	802	PC1	C11-C12-N-C13
3	A	806	PC1	C31-C32-C33-C34
3	A	806	PC1	C26-C27-C28-C29
4	A	804	LMT	C9-C10-C11-C12
4	B	804	LMT	C9-C10-C11-C12
4	A	804	LMT	C11-C10-C9-C8
4	B	804	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	805	LMT	C2'-C1'-O1'-C1
4	B	805	LMT	C2'-C1'-O1'-C1
3	A	806	PC1	C32-C33-C34-C35
3	A	802	PC1	C3B-C3C-C3D-C3E
4	B	805	LMT	C2-C3-C4-C5
4	A	804	LMT	C5-C6-C7-C8
3	A	806	PC1	C1-C2-C3-O31
4	B	804	LMT	C3-C4-C5-C6
4	B	804	LMT	C5-C6-C7-C8
4	B	805	LMT	C5-C6-C7-C8
4	A	805	LMT	C4'-C5'-C6'-O6'
4	A	804	LMT	C3-C4-C5-C6
4	A	805	LMT	C5-C6-C7-C8
4	B	805	LMT	C4'-C5'-C6'-O6'
3	A	802	PC1	C11-C12-N-C15
3	B	802	PC1	C11-C12-N-C14
3	B	806	PC1	C26-C27-C28-C29
3	A	806	PC1	O11-C1-C2-C3
3	B	806	PC1	C2B-C2C-C2D-C2E
3	B	806	PC1	C1-C2-C3-O31
3	A	806	PC1	C2B-C2C-C2D-C2E
4	A	804	LMT	C4-C5-C6-C7
3	B	802	PC1	C11-C12-N-C15
4	B	804	LMT	C4-C5-C6-C7
3	B	806	PC1	C27-C28-C29-C2A
3	A	806	PC1	C2C-C2D-C2E-C2F
4	B	805	LMT	O1'-C1-C2-C3
3	B	802	PC1	C29-C2A-C2B-C2C
3	A	802	PC1	C11-C12-N-C14
4	A	805	LMT	C11-C10-C9-C8
3	A	802	PC1	C11-O13-P-O12
3	A	802	PC1	C1-O11-P-O12
3	A	802	PC1	C1-O11-P-O14
3	A	806	PC1	C11-C12-N-C15
3	B	802	PC1	C11-O13-P-O12
4	A	805	LMT	C6-C7-C8-C9
3	B	806	PC1	C12-C11-O13-P
3	A	806	PC1	O11-C1-C2-O21
3	A	806	PC1	O31-C31-C32-C33
4	B	805	LMT	C11-C10-C9-C8
3	A	806	PC1	C11-C12-N-C14
4	B	804	LMT	C2-C3-C4-C5

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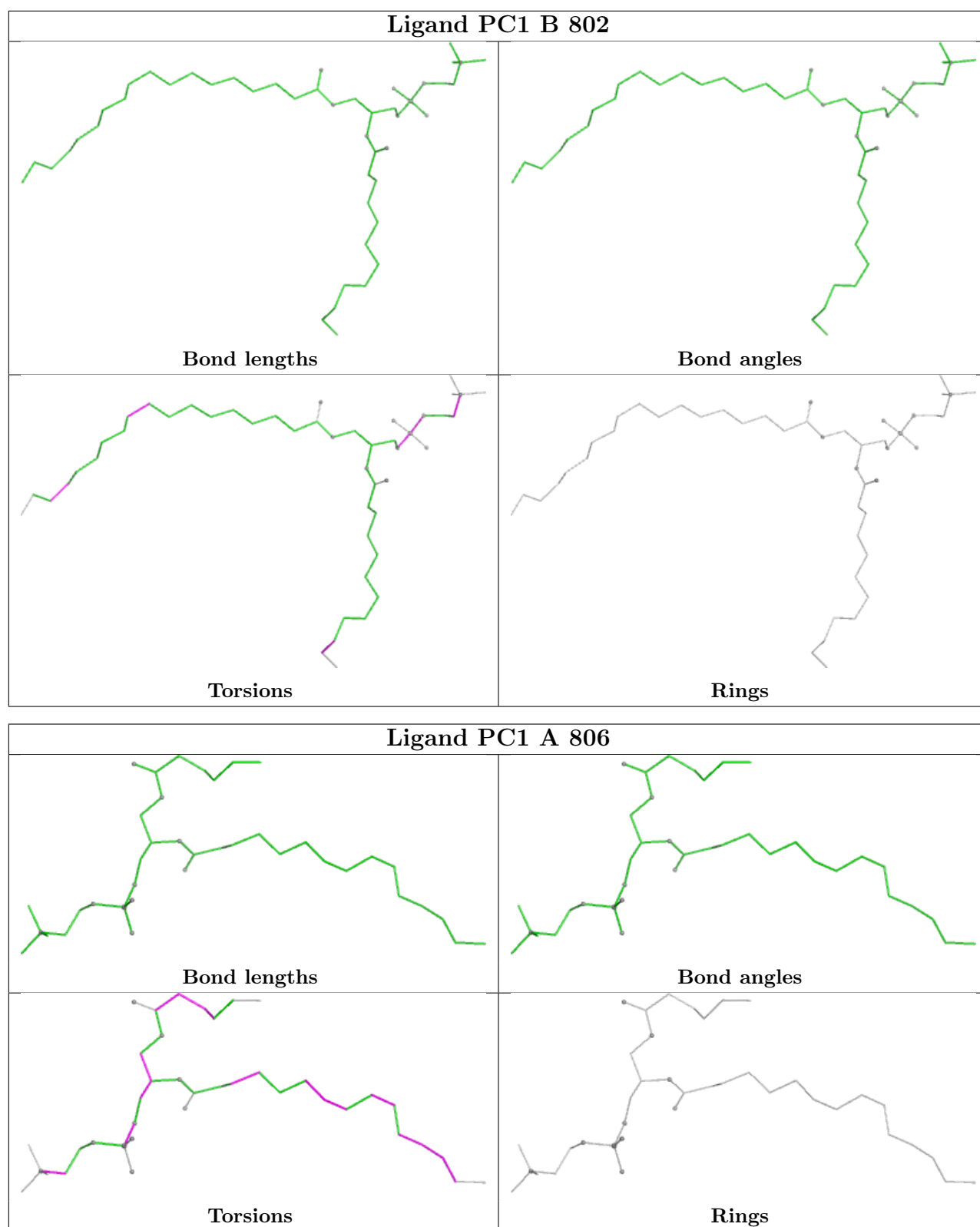
Mol	Chain	Res	Type	Atoms
4	B	805	LMT	C6-C7-C8-C9
4	B	803	LMT	C1-C2-C3-C4
4	A	803	LMT	C5-C6-C7-C8
4	A	805	LMT	O1'-C1-C2-C3
4	A	803	LMT	C3-C4-C5-C6
3	A	802	PC1	C36-C37-C38-C39
3	A	806	PC1	C11-C12-N-C13
4	A	804	LMT	C2-C3-C4-C5
3	B	806	PC1	C29-C2A-C2B-C2C
3	A	806	PC1	C1-O11-P-O14
3	B	806	PC1	C25-C26-C27-C28
3	A	802	PC1	O31-C31-C32-C33
3	B	806	PC1	O21-C21-C22-C23
3	B	806	PC1	C22-C23-C24-C25
3	A	802	PC1	O32-C31-C32-C33
3	B	806	PC1	O22-C21-C22-C23
3	A	802	PC1	C38-C39-C3A-C3B
3	A	806	PC1	C28-C29-C2A-C2B

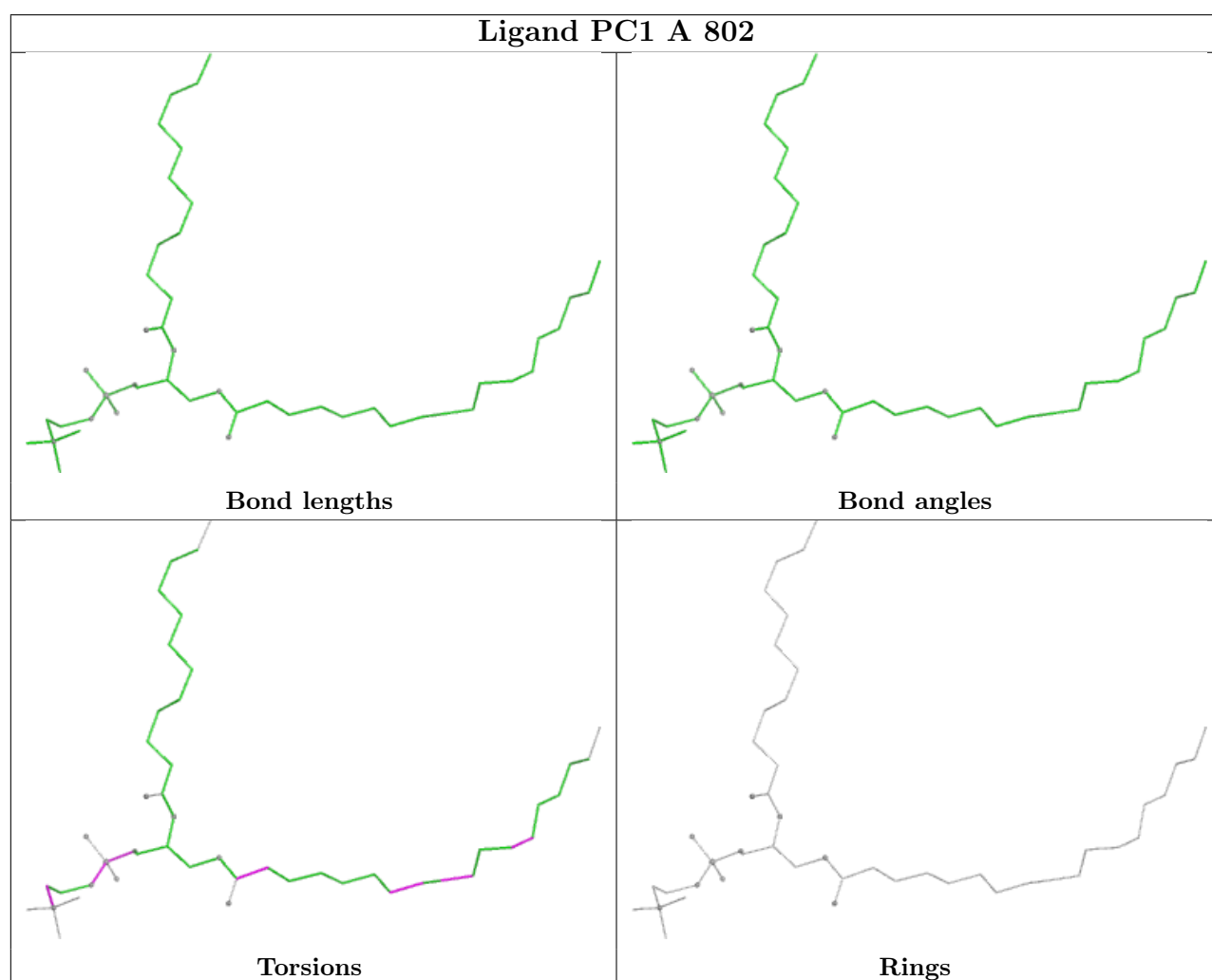
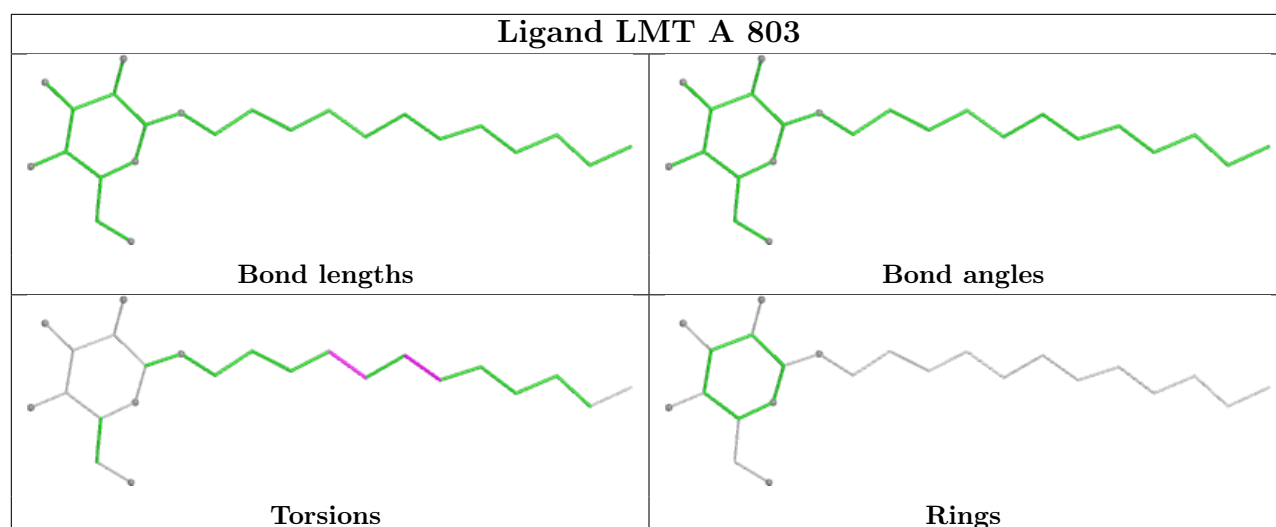
There are no ring outliers.

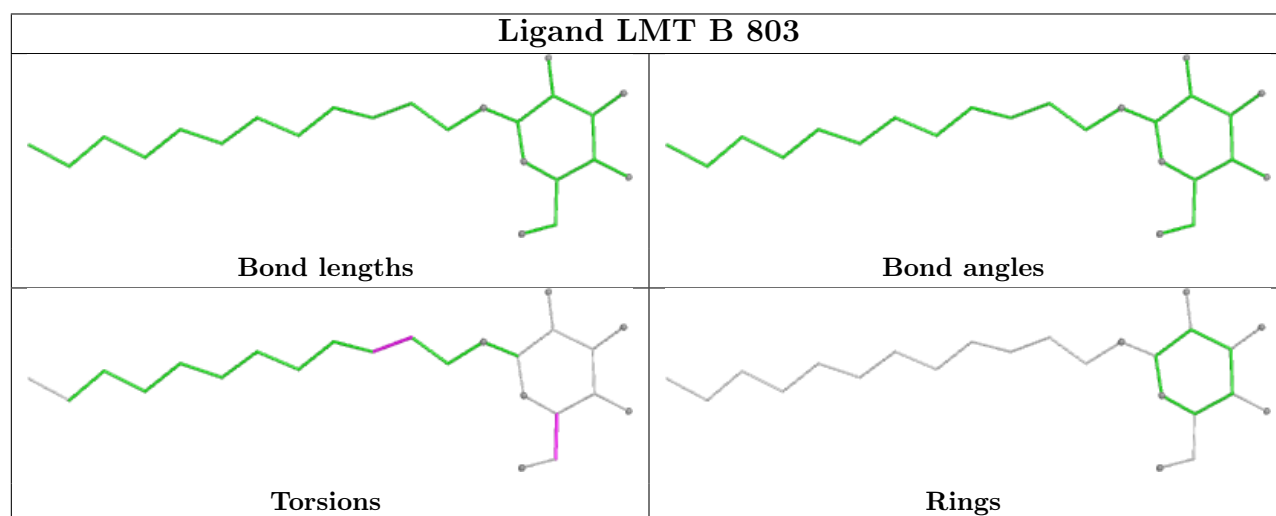
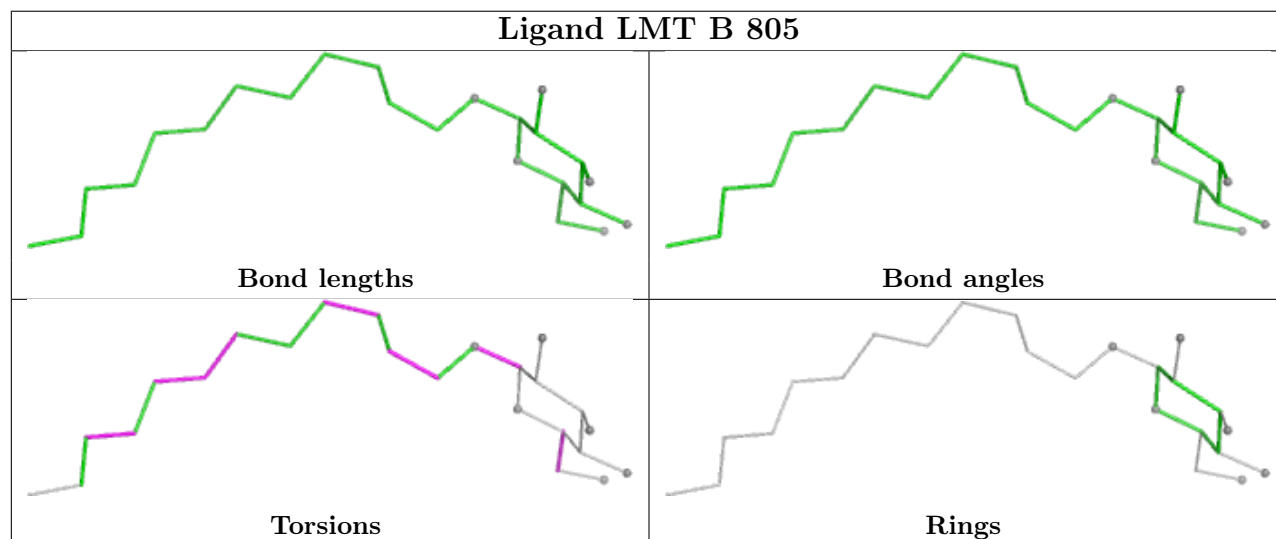
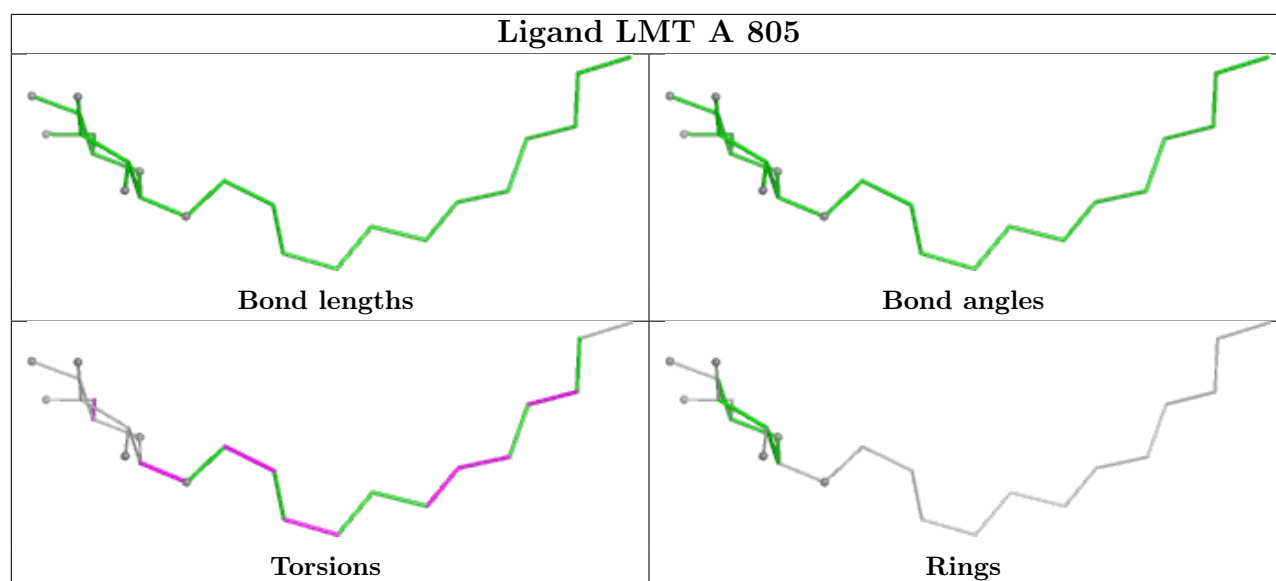
6 monomers are involved in 9 short contacts:

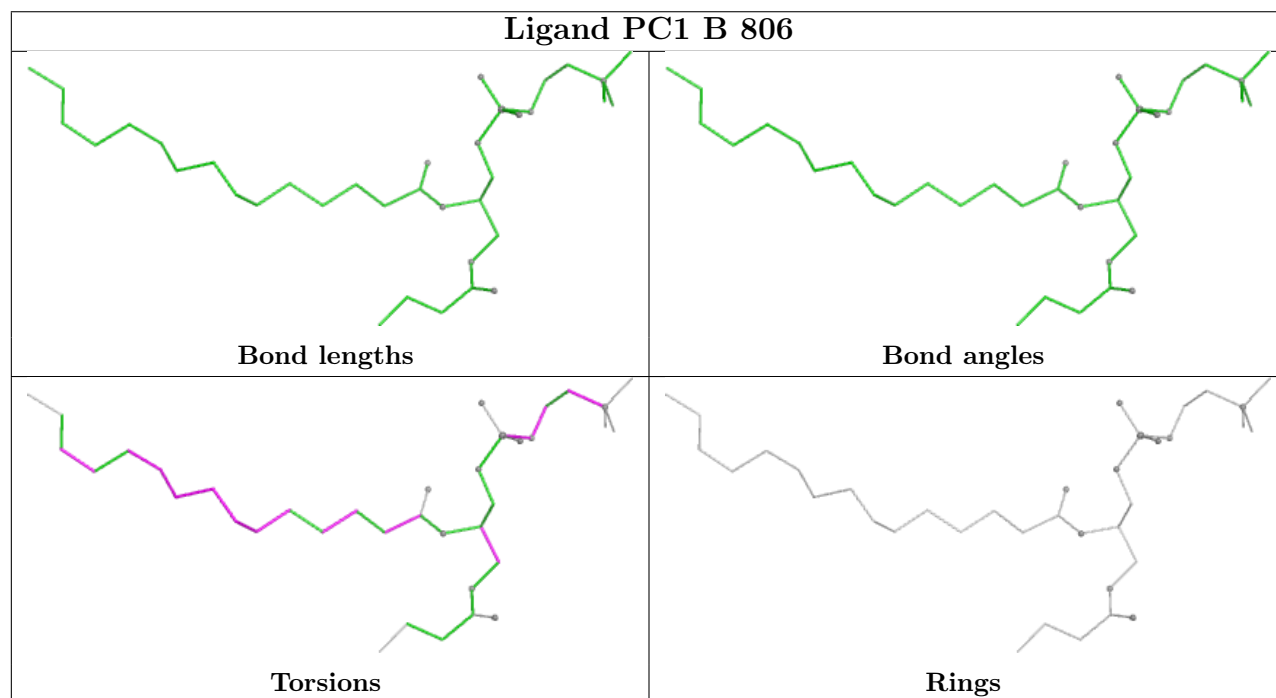
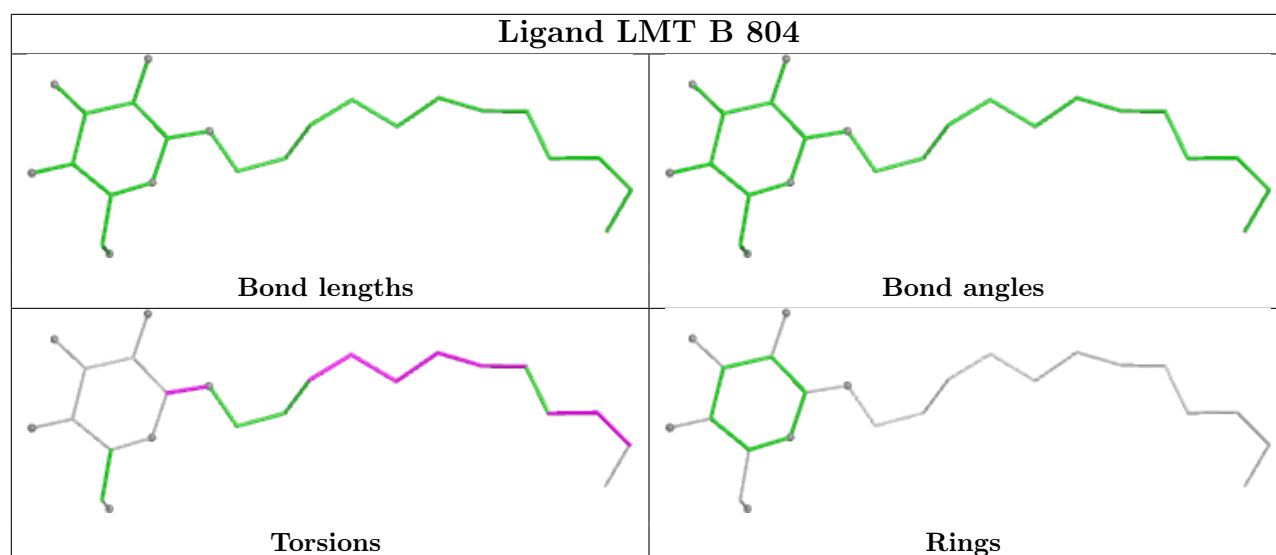
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	PC1	2	0
3	A	806	PC1	1	0
3	A	802	PC1	2	0
4	A	805	LMT	1	0
4	B	805	LMT	1	0
4	A	804	LMT	2	0

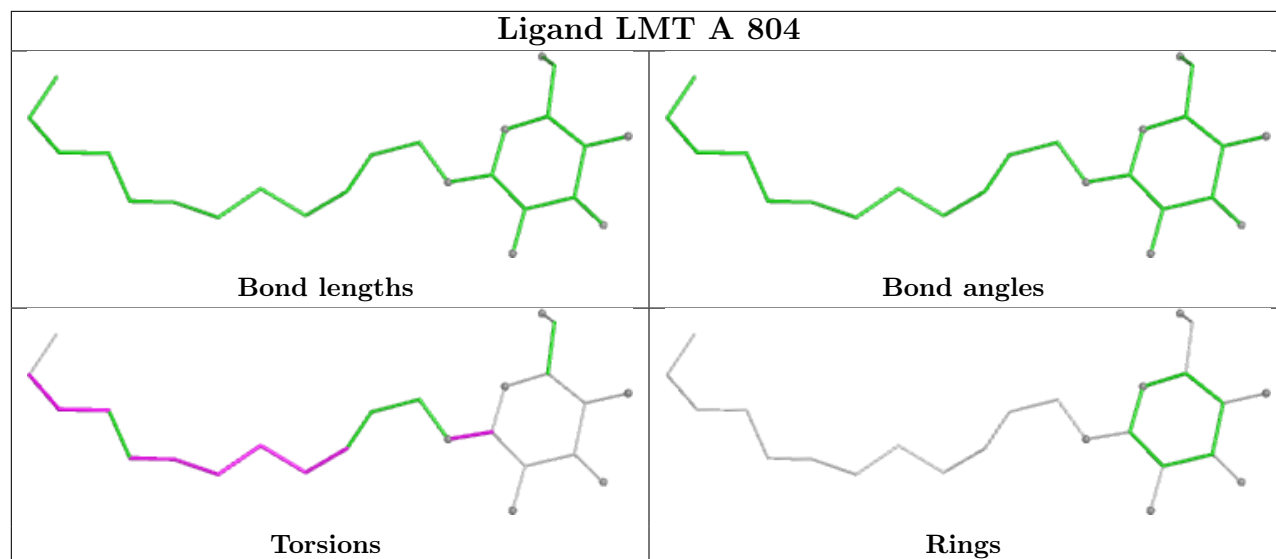
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

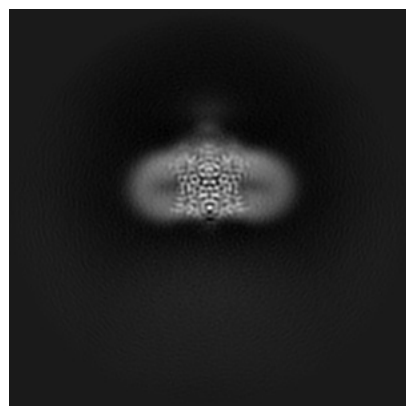
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53827. These allow visual inspection of the internal detail of the map and identification of artifacts.

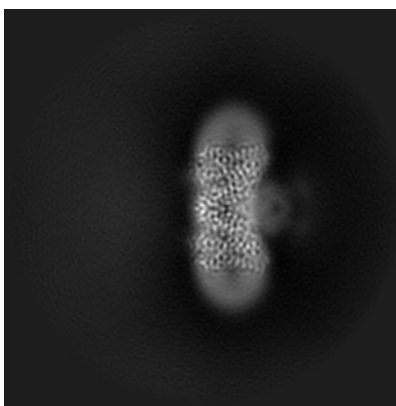
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

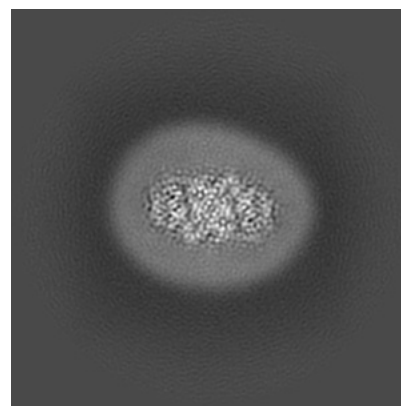
6.1.1 Primary map



X

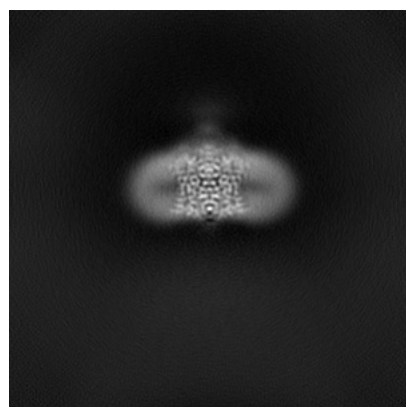


Y

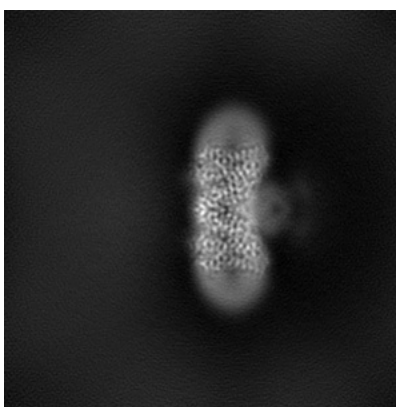


Z

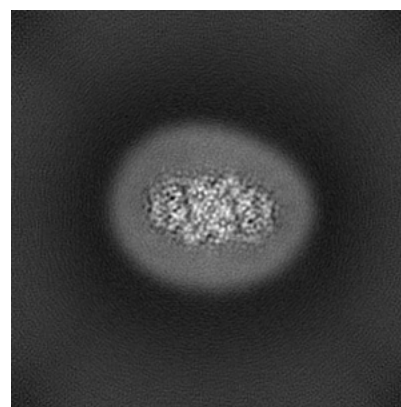
6.1.2 Raw map



X



Y

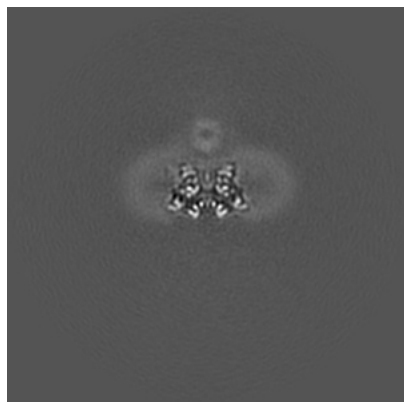


Z

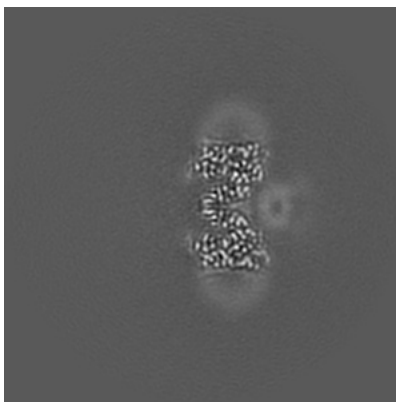
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

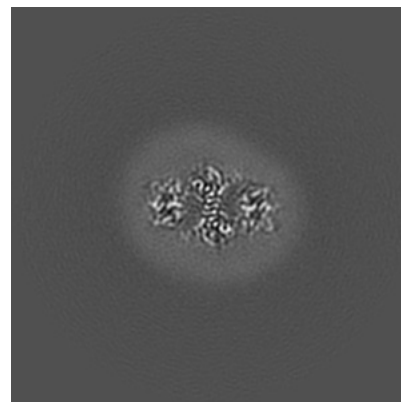
6.2.1 Primary map



X Index: 128

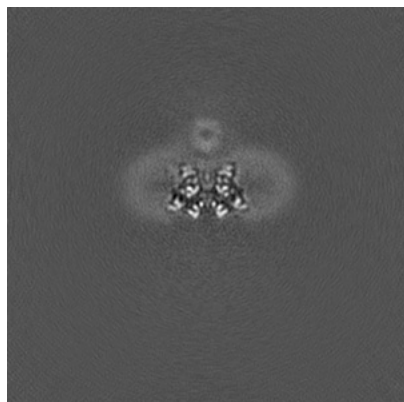


Y Index: 128

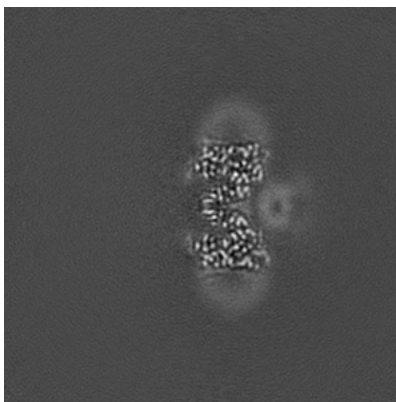


Z Index: 128

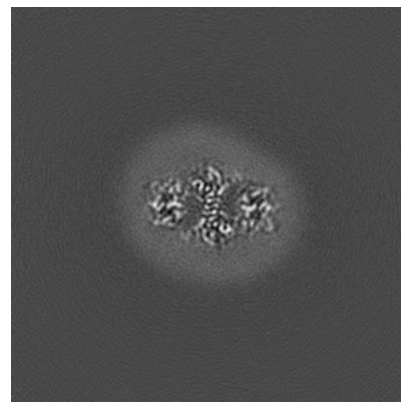
6.2.2 Raw map



X Index: 128



Y Index: 128

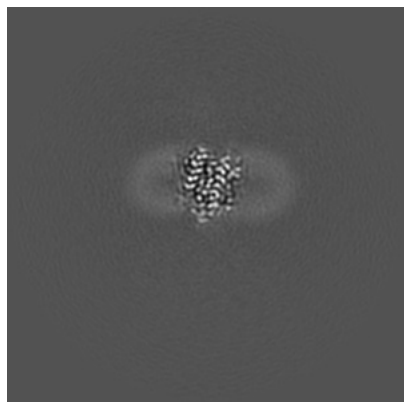


Z Index: 128

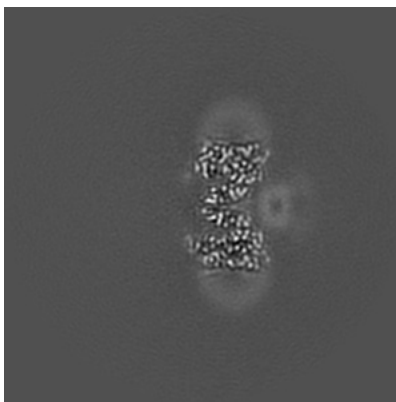
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

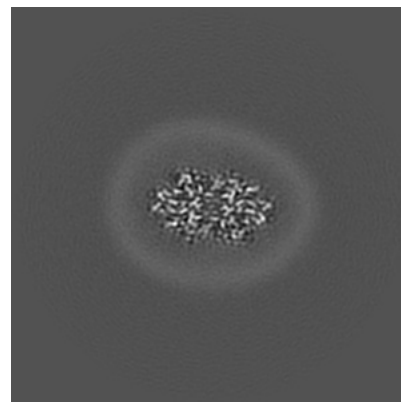
6.3.1 Primary map



X Index: 105

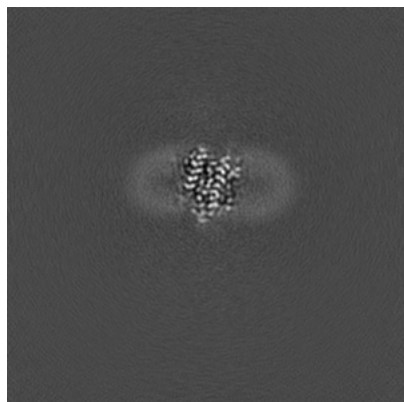


Y Index: 127

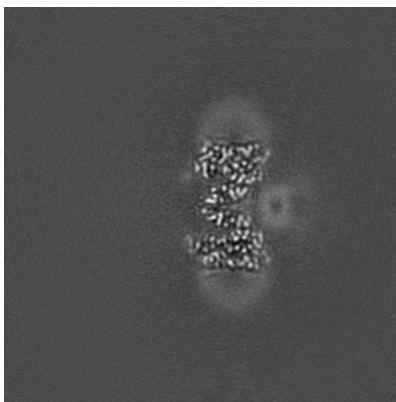


Z Index: 145

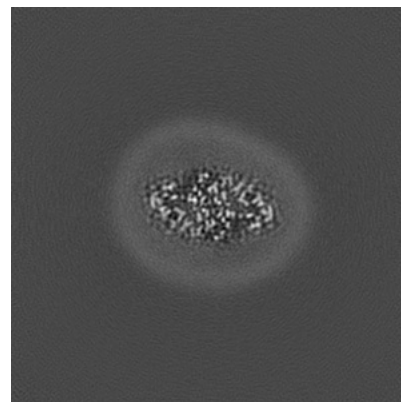
6.3.2 Raw map



X Index: 105



Y Index: 127

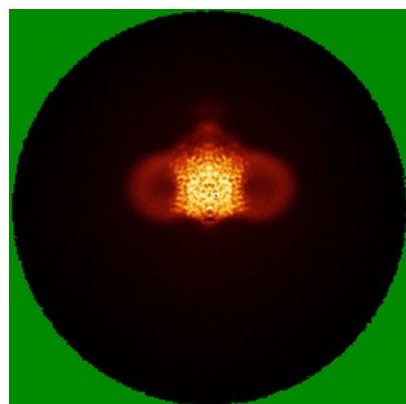


Z Index: 136

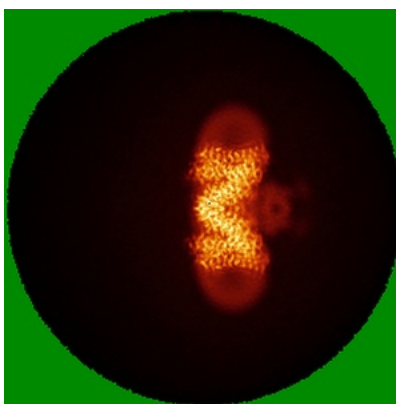
The images above show the largest variance slices of the map in three orthogonal directions.

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

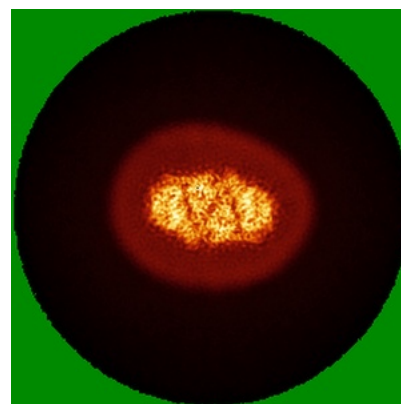
6.4.1 Primary map



X

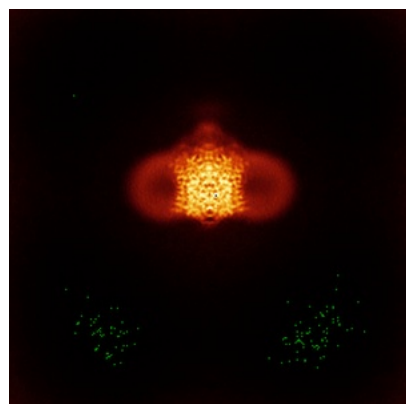


Y

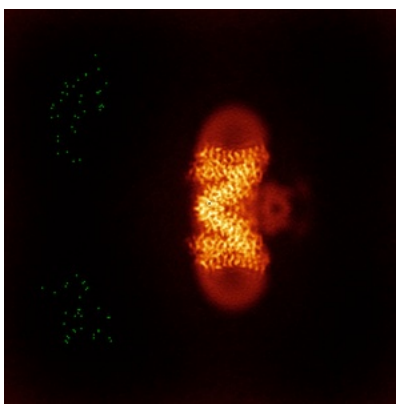


Z

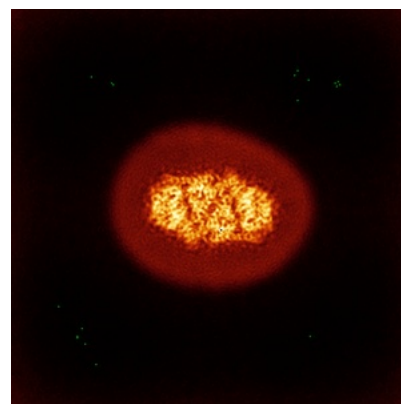
6.4.2 Raw map



X



Y



Z

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

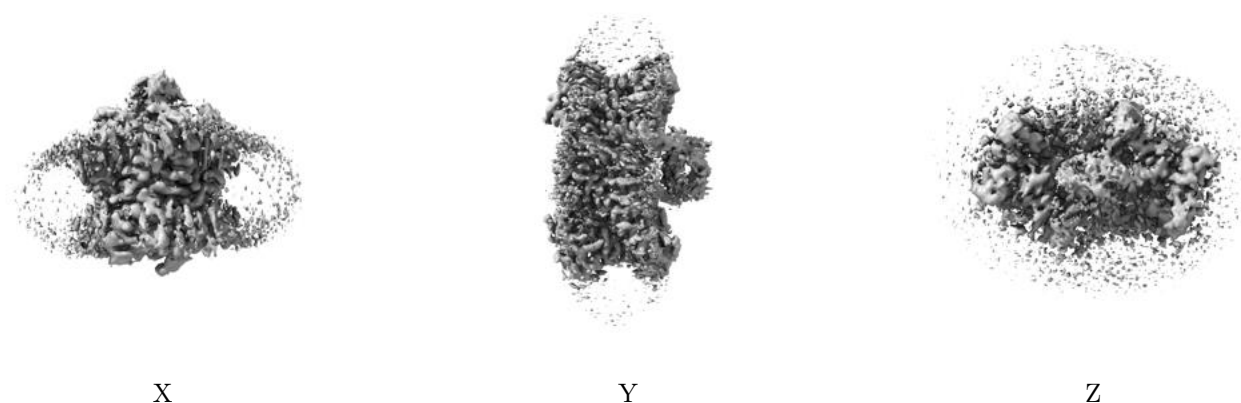
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

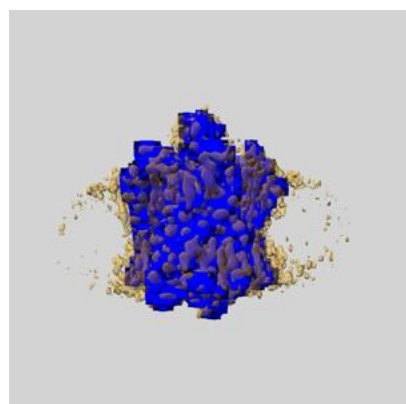
6.6 Mask visualisation [i](#)

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

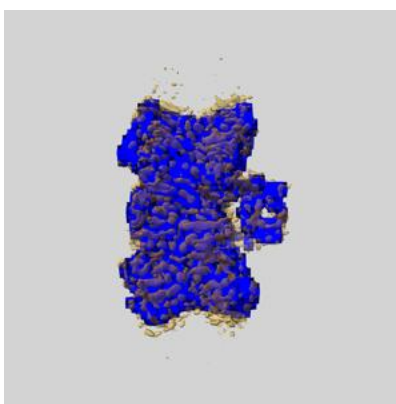
A mask typically either:

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

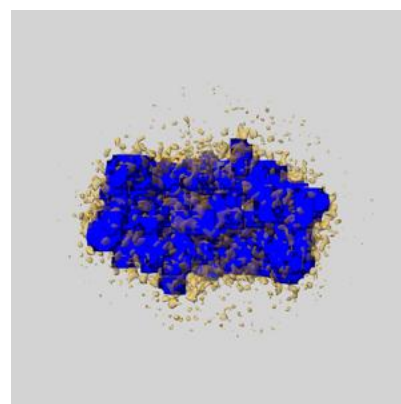
6.6.1 emd_53827_msk_2.map [i](#)



X

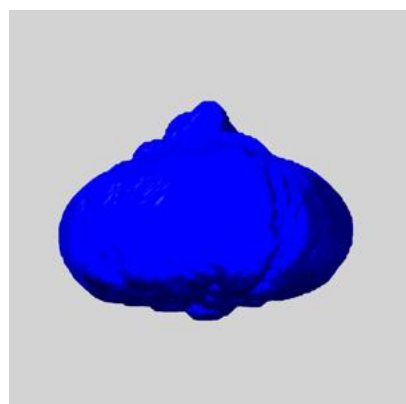


Y

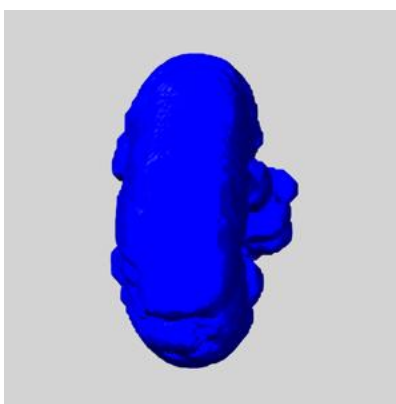


Z

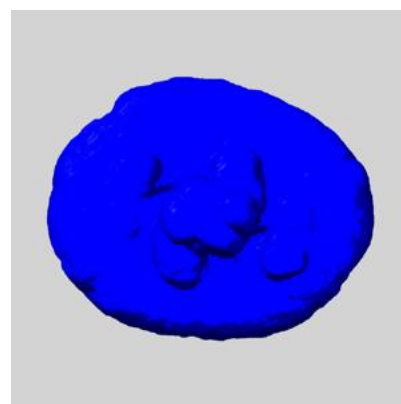
6.6.2 emd_53827_msk_1.map [i](#)



X



Y

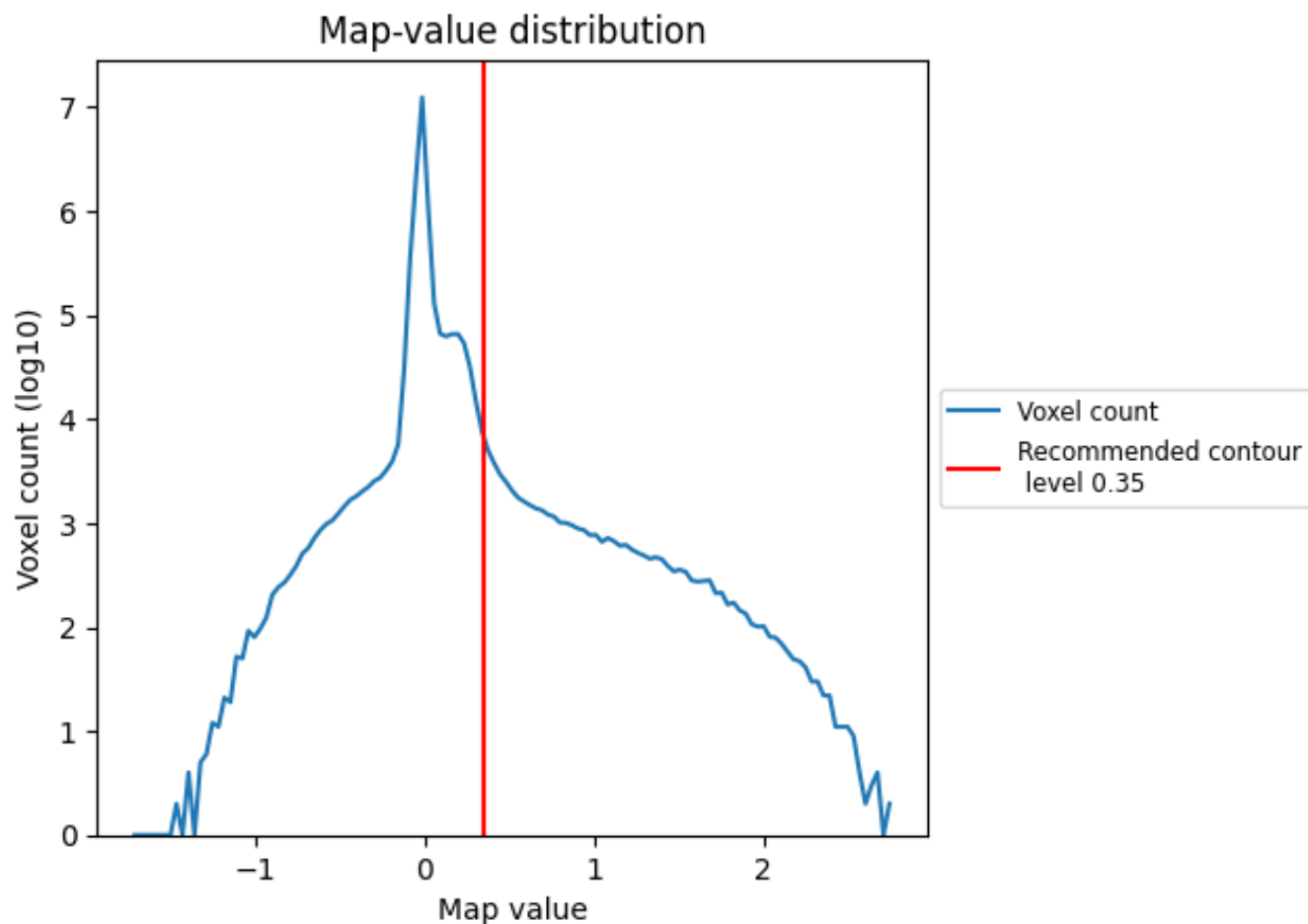


Z

7 Map analysis [i](#)

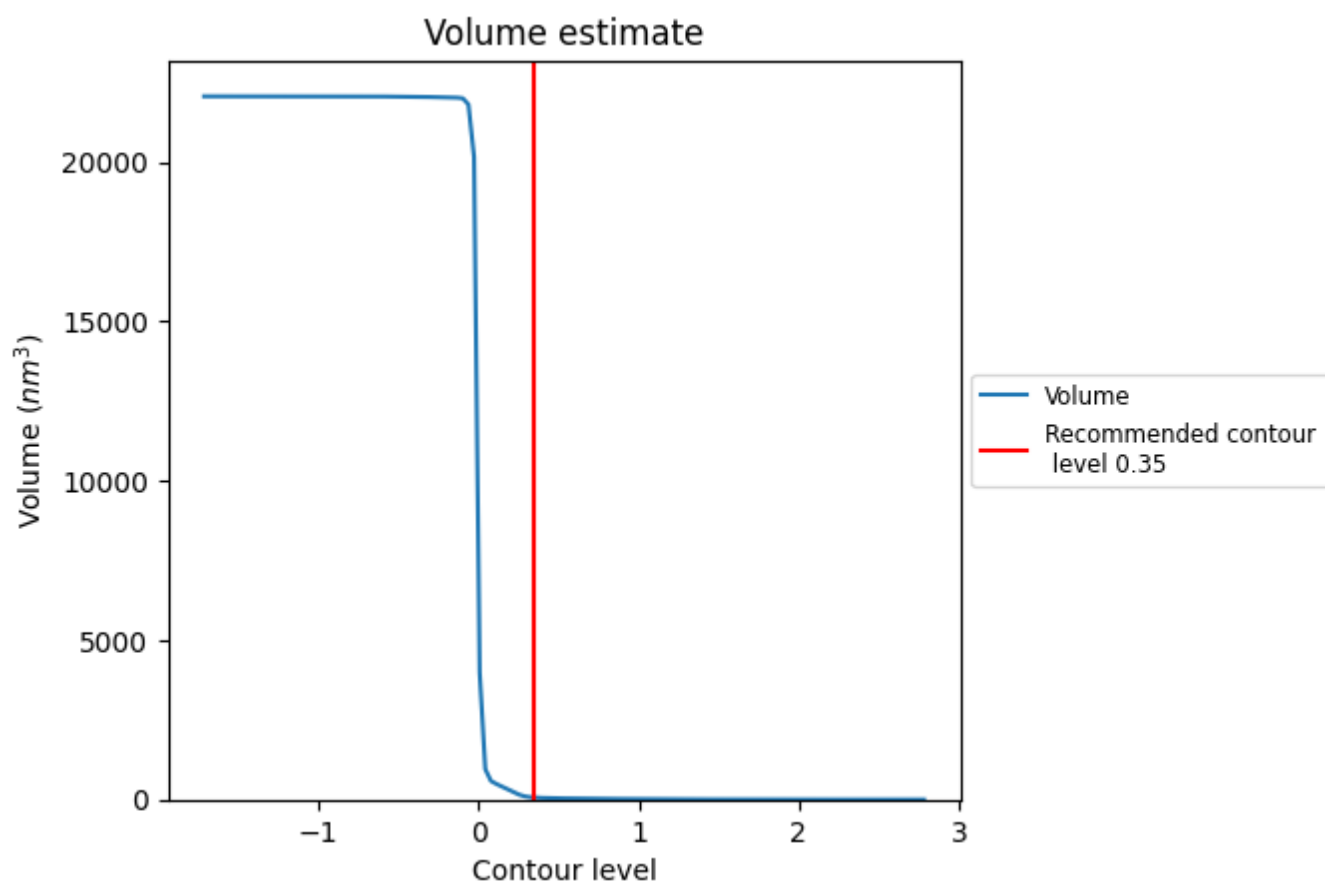
This section contains the results of statistical analysis of the map.

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.

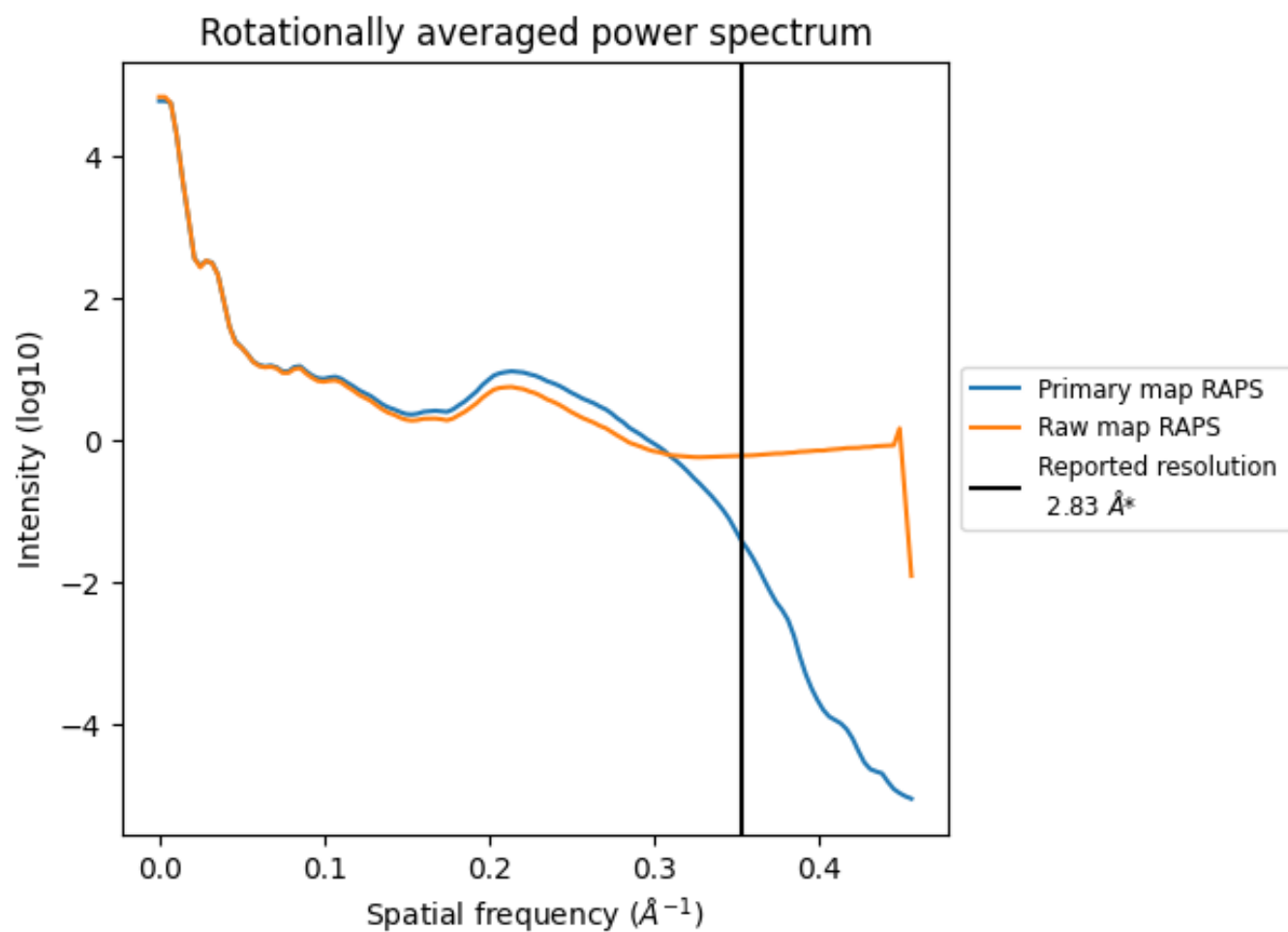
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm³; this corresponds to an approximate mass of 57 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 ⓘ

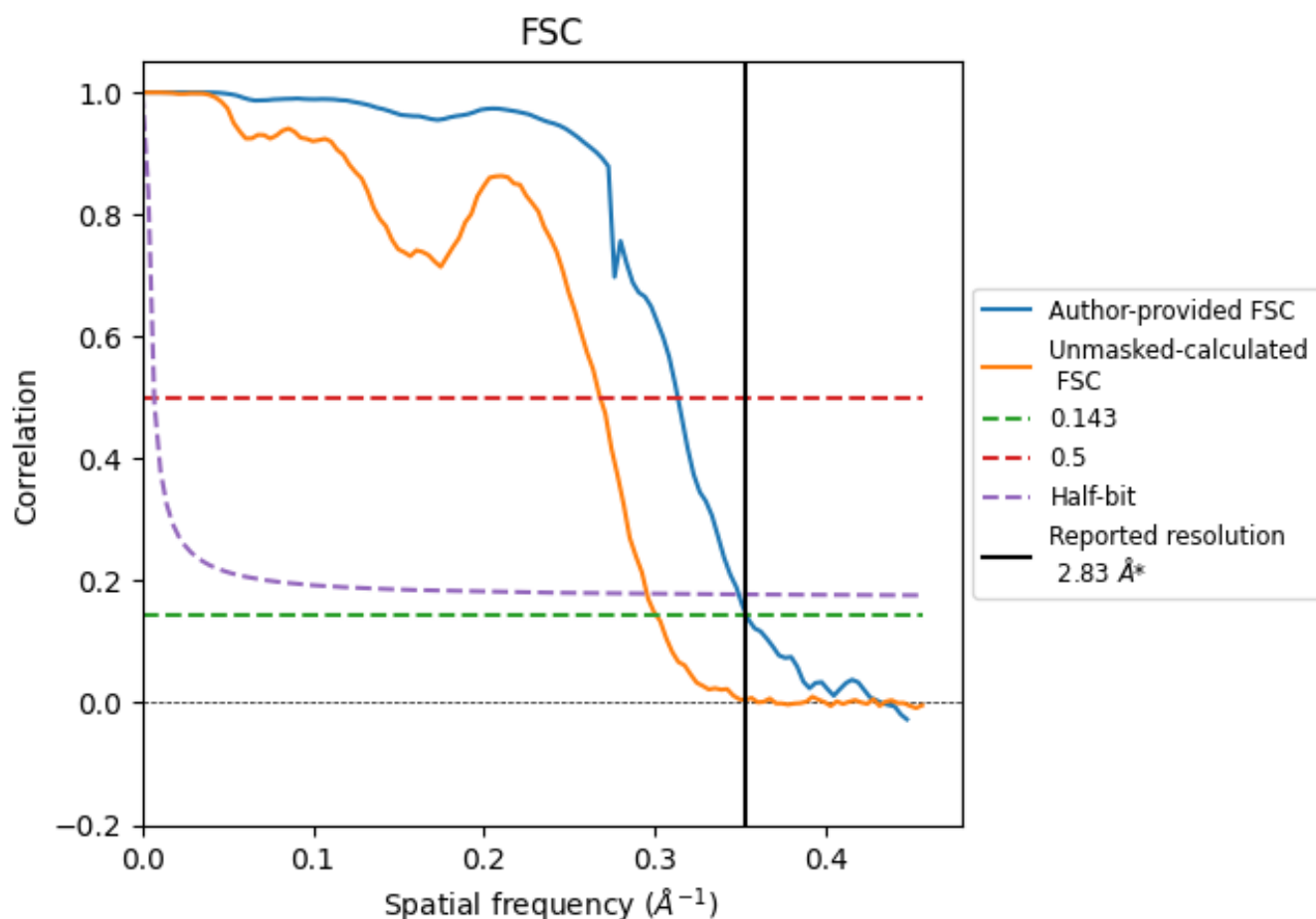


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

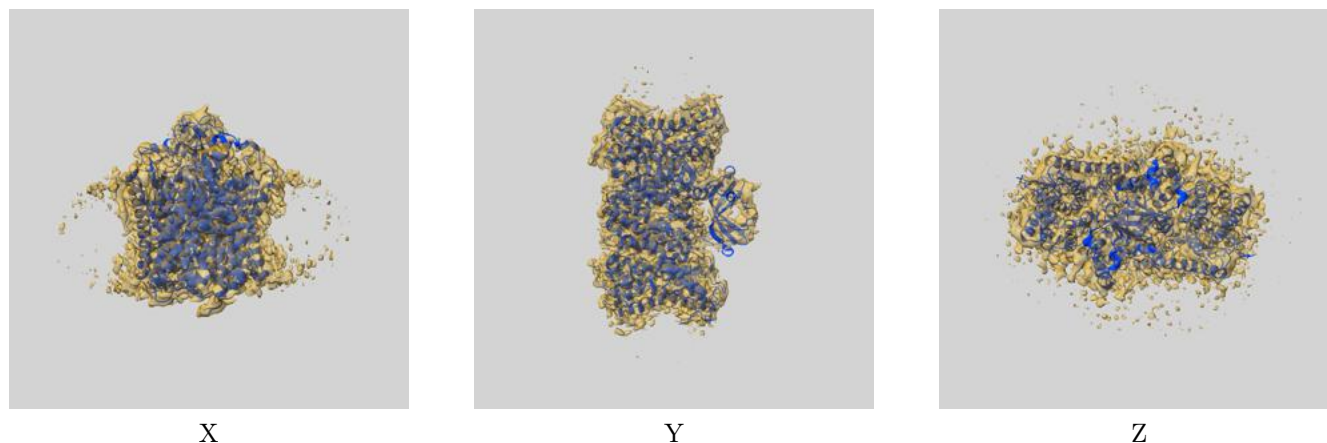
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.19	2.86
Unmasked-calculated*	3.32	3.73	3.39

*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 3.32 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

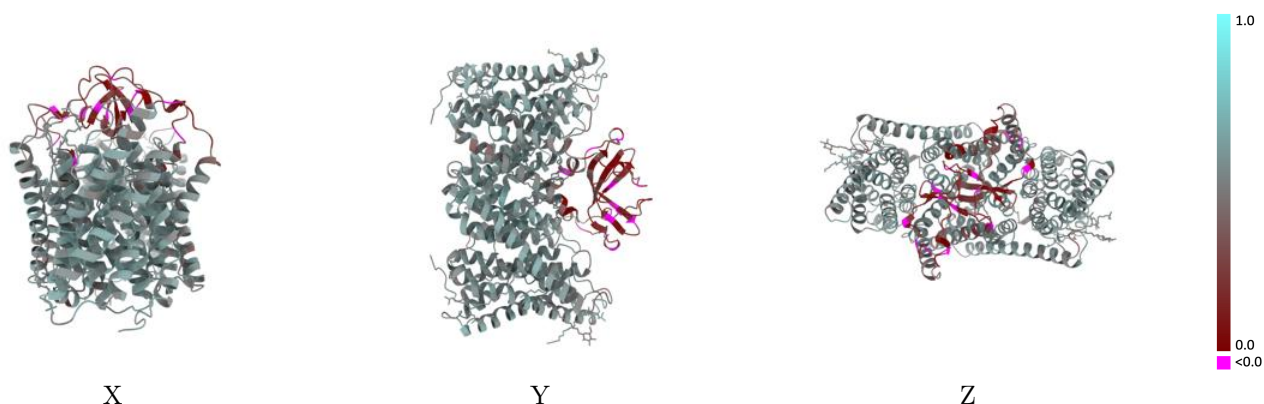
This section contains information regarding the fit between EMDB map EMD-53827 and PDB model 9R8J. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



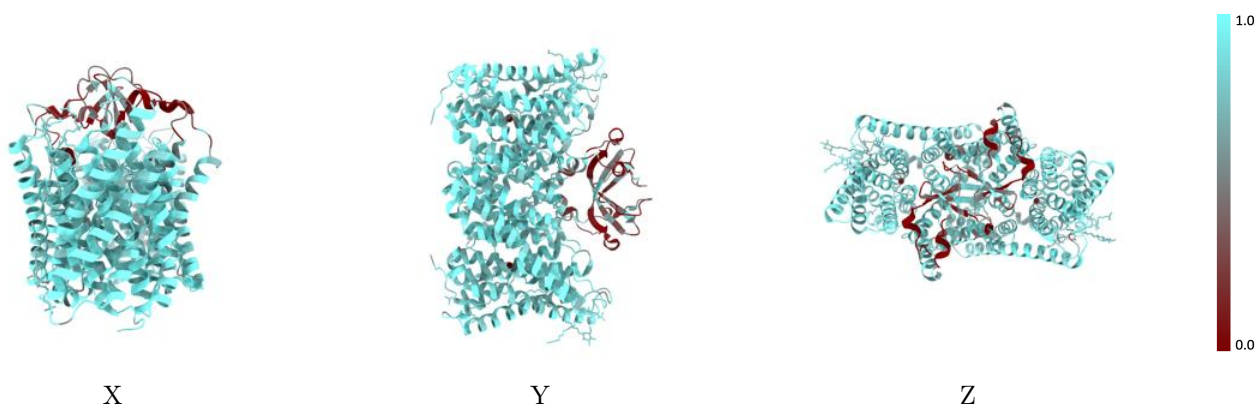
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



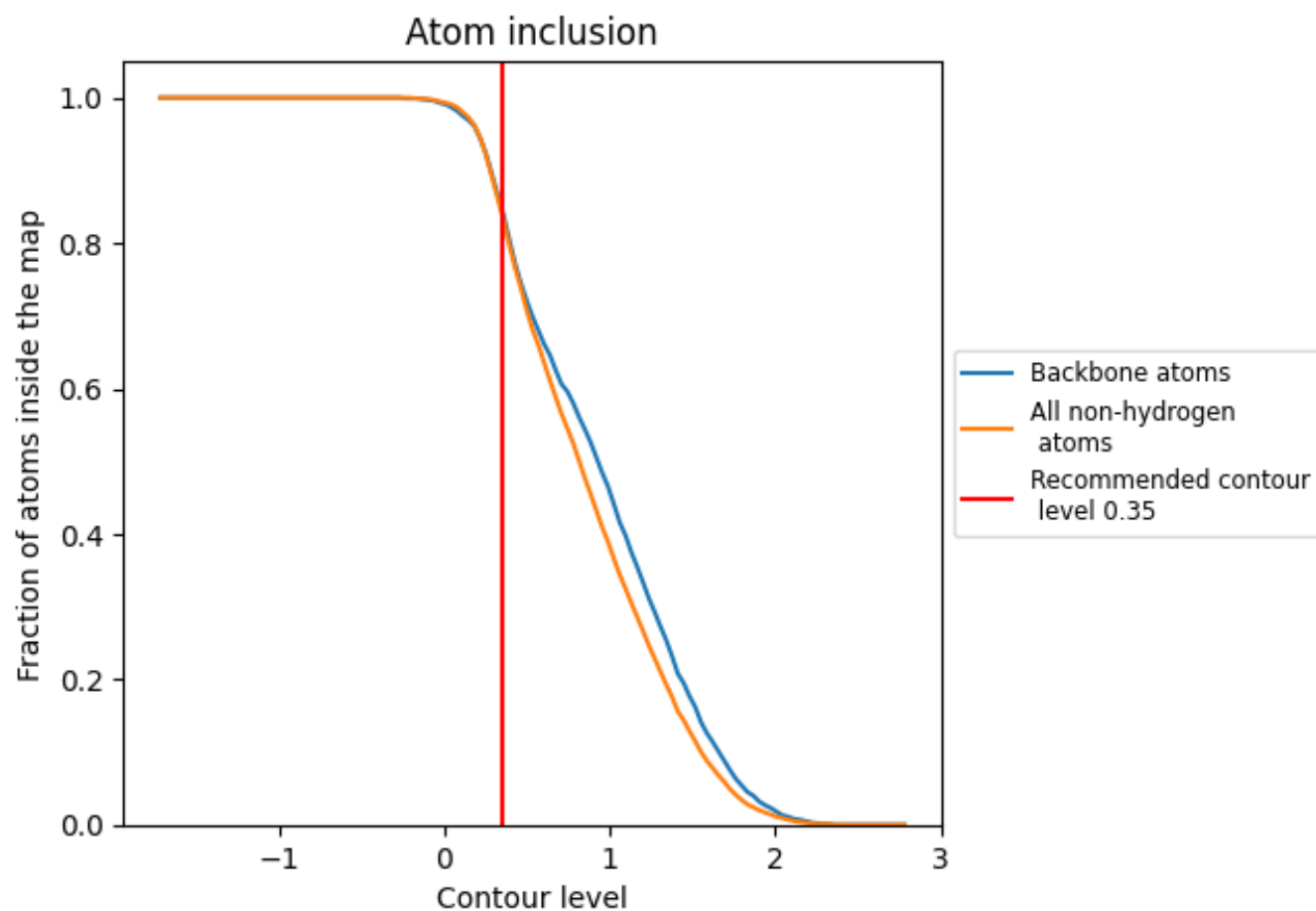
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.5050
A	0.8350	0.5030
B	0.8450	0.5070

