



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 8T45 / pdb_00008t45
EMDB ID : EMD-41020
Title : Cryo-EM Analysis of AE1 Structure in 100 mM NaHCO₃ Buffer: Form2
Authors : Su, C.C.
Deposited on : 2023-06-08
Resolution : 2.99 Å(reported)

This is a wwPDB EM Validation Summary 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

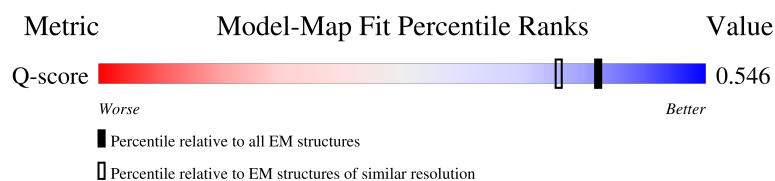
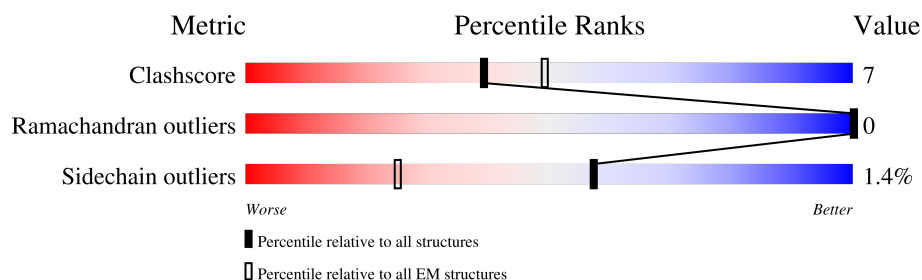
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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	13287 (2.49 - 3.49)

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	911	
1	B	911	

2 Entry composition [i](#)

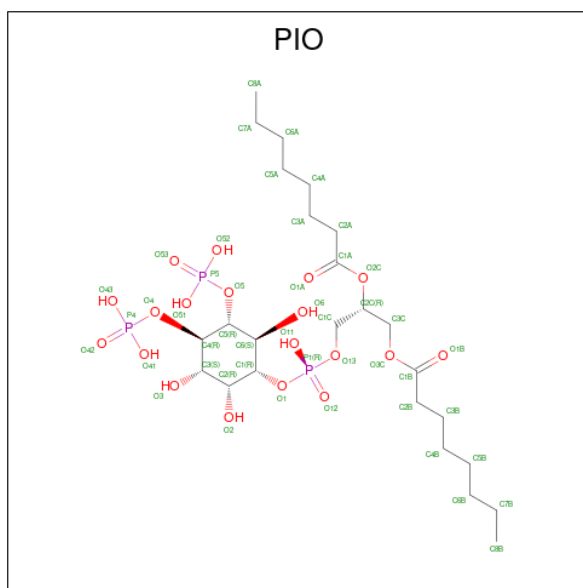
There are 4 unique types of molecules in this entry. The entry contains 7475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3611	2428	570	597	16		
1	B	457	Total	C	N	O	S	0	0
			3607	2427	570	594	16		

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



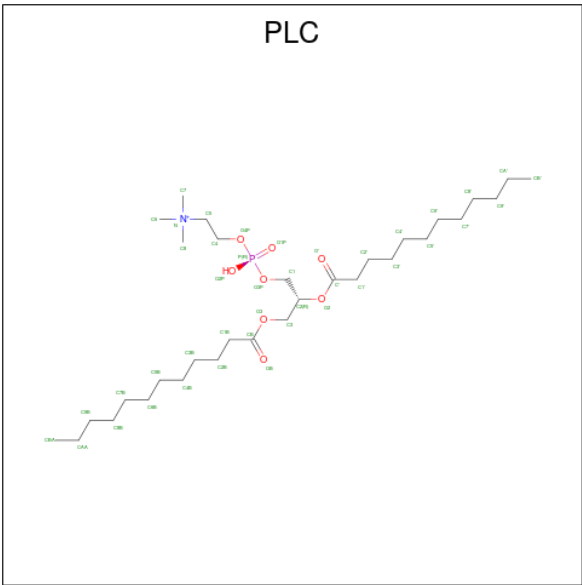
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			47	25	19	3	
2	B	1	Total	C	O	P	0
			44	22	19	3	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			37	28	8	1	
4	A	1	Total	C	O	P	0
			36	27	8	1	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	O	P	0
			36	27	8	1	
4	B	1	Total	C	O	P	0
			29	20	8	1	

Frequency	Percentage
Daily	40%
Weekly	10%
Monthly	50%

T837	F702	V437	GLY	ALA	VAL	SER	LEU	LEU	MET
V849	L706	S443	ASN	GLY	PHE	GLN	GLU	GLU	GLU
V850	A716	A452	GLY	GLU	GLU	GLN	GLU	GLU	GLU
K851	M721	Q457	ASP	SER	HIS	GLN	LEU	LEU	GLU
S852	P722	Q458	ASP	SER	ALA	GLN	GLN	GLN	GLN
T853		L459	PRO	LEU	GLU	GLU	GLU	GLU	MET
L857	T727	G509	PRO	GLU	GLU	GLU	GLU	GLU	MET
A858	T728	V610	GLN	GLN	PHE	GLN	GLU	GLU	GLU
L859	V729	V618	THR	THR	GLU	GLU	LEU	LEU	GLU
P860	R730	F464	GLY	GLY	ASP	VAL	GLU	GLU	GLU
F861	R731	V470	GLN	CYS	THR	GLU	GLU	GLU	GLU
V862	S731	F471	LEU	SER	SER	LEU	LEU	LEU	GLN
L863	V732	V640	PHE	LEU	LEU	PRO	LEU	LEU	GLU
L864	T733	S641	GLY	VAL	VAL	VAL	GLU	GLU	GLU
L865	T733	N642	GLY	LEU	PRO	CYS	GLU	GLU	TYR
V872	H734	F476	LEU	PRO	ILE	GLU	GLU	GLU	GLU
	ALA	S644	VAL	PRO	THR	GLN	ASP	GLN	ASP
R879	ASN	A645	ARG	THR	PHE	GLY	GLN	GLN	PRO
	ALA	R646	ASP	ALA	ASP	ASP	ILE	ILE	PRO
	LEU	G647	ILE	PRO	PHE	GLY	ARG	GLU	GLU
D889	VAL	S510	ARG	ARG	VAL	LEU	THR	GLN	GLN
A890	MET	R656	ARG	ARG	GLU	GLU	GLY	GLY	SER
L891	GLY	F511	TYR	TYR	GLN	GLN	GLY	GLY	GLN
ALA	LYS	I512	PRO	PRO	ALA	PRO	HIS	GLU	MET
THR	ALA	V513	TYR	LEU	LEU	GLU	SER	GLY	GLY
PHE	SER	R514	THR	SER	LEU	ALA	PRO	LEU	GLU
ASP	THR	I661	THR	LEU	SER	LEU	SER	LEU	PRO
GLU	PRO	W662	ASP	ASP	LEU	GLY	GLY	GLY	PRO
GLU	GLY	Q521	SER	VAL	LEU	ILE	ILE	ARG	ALA
GLY	ALA	I531	ASP	VAL	VAL	VAL	ASP	ALA	ALA
ARG	ALA	E535	THR	PRO	PRO	PRO	THR	LEU	HIS
ASP	GLN	L673	ASP	ARG	ARG	GLN	ILE	LEU	ALA
GLU	I753	E681	PHE	LEU	LEU	LEU	PRO	SER	THR
TYR	Q754	S882	GLY	S402	LEU	GLY	PRO	THR	ALA
ASP	E755	Q883	ALA	P403	LEU	ALA	ASP	THR	THR
GLU		I684	ARG	ARG	ARG	ALA	GLY	TRP	ALA
VAL		T685	ARG	ARG	ARG	ALA	GLY	TRP	ASP
ALA	Q759	T686	THR	TYR	TYR	THR	GLY	SER	TYR
VAL	R760	L687	THR	GLN	THR	THR	LEU	LEU	HIS
MET		L687	THR	GLN	THR	THR	LEU	LEU	THR
PRO	V766	ILE	THR	SER	SER	VAL	GLU	GLU	THR
VAL		V560	THR	SER	SER	GLU	LEU	LEU	THR
	I783	P561	SER	PRO	GLU	VAL	GLY	ARG	HIS
	P784	L565	PRO	ALA	ARG	ARG	GLY	GLY	PRO
	L785	L567	GLU	LYS	VAL	VAL	VAL	VAL	GLY
	A786	P568	ARG	PRO	PHE	ARG	VAL	VAL	THR
	I791	N569	LYS	ASP	PHE	ALA	LYS	LYS	THR
		MET	THR	SER	ARG	ASP	ARG	PHO	HIS
	R808	VAL	VAL	PHE	THR	PHE	VAL	VAL	THR
	I809	LYS	GLY	TYR	THR	GLN	THR	THR	TYR
				VAL	VAL	THR	VAL	VAL	GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.013	Depositor
Minimum map value	-1.814	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PLC, PIO

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	0.11	0/3704	0.23	0/5041
1	B	0.11	0/3700	0.24	0/5035
All	All	0.11	0/7404	0.24	0/10076

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

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	3611	0	3788	54	0
1	B	3607	0	3803	54	0
2	A	47	0	44	2	0
2	B	44	0	35	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	73	0	102	1	0
4	B	65	0	85	2	0
All	All	7475	0	7883	110	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 7.

The worst 5 of 110 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:B:646:ARG:NH1	1:B:647:GLY:O	2.25	0.70
1:B:443:SER:HB2	1:B:721:MET:HB3	1.74	0.69
1:B:490:ARG:NH2	1:B:721:MET:O	2.26	0.68
1:A:673:LEU:HB3	1:A:860:PRO:HG2	1.75	0.68
1:B:592:LYS:HB2	1:B:606:GLY:HA3	1.79	0.65

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	454/911 (50%)	445 (98%)	9 (2%)	0	100	100
1	B	451/911 (50%)	437 (97%)	14 (3%)	0	100	100
All	All	905/1822 (50%)	882 (98%)	23 (2%)	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	396/786 (50%)	392 (99%)	4 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	399/786 (51%)	392 (98%)	7 (2%)	51	77
All	All	795/1572 (51%)	784 (99%)	11 (1%)	57	80

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	729	VAL
1	B	837	THR
1	B	872	VAL
1	B	864	ILE
1	B	437	VAL

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	564	GLN
1	B	564	GLN
1	B	683	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
4	PLC	B	1003	-	35,35,41	0.67	1 (2%)	38,40,49	1.04	2 (5%)
2	PIO	B	1002	-	44,44,47	1.25	6 (13%)	59,62,65	1.10	3 (5%)
4	PLC	B	1004	-	28,28,41	0.74	1 (3%)	31,33,49	1.16	2 (6%)
4	PLC	A	1004	-	35,35,41	0.66	1 (2%)	38,40,49	1.11	3 (7%)
4	PLC	A	1003	-	36,36,41	0.57	0	39,41,49	0.52	0
3	NAG	B	1001	1	14,14,15	0.42	0	17,19,21	0.45	0
3	NAG	A	1002	1	14,14,15	0.22	0	17,19,21	0.45	0
2	PIO	A	1001	-	47,47,47	1.20	7 (14%)	62,65,65	1.04	5 (8%)

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
4	PLC	B	1003	-	-	4/37/37/45	-
2	PIO	B	1002	-	-	12/41/65/68	0/1/1/1
4	PLC	B	1004	-	-	9/30/30/45	-
4	PLC	A	1004	-	-	11/37/37/45	-
4	PLC	A	1003	-	-	8/40/40/45	-
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	PIO	A	1001	-	-	25/44/68/68	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PIO	P5-O5	3.28	1.65	1.59
2	B	1002	PIO	P5-O5	3.26	1.65	1.59
2	B	1002	PIO	P4-O4	3.23	1.65	1.59
2	A	1001	PIO	P4-O4	3.20	1.65	1.59
4	A	1004	PLC	P-O4P	2.81	1.65	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	PLC	O4P-P-O3P	-5.06	93.49	106.67
4	B	1004	PLC	O4P-P-O3P	-5.05	93.51	106.67
4	B	1003	PLC	O4P-P-O3P	-5.04	93.53	106.67
2	B	1002	PIO	O2C-C1A-C2A	4.32	120.82	111.48
2	A	1001	PIO	O2C-C1A-C2A	3.60	119.26	111.48

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

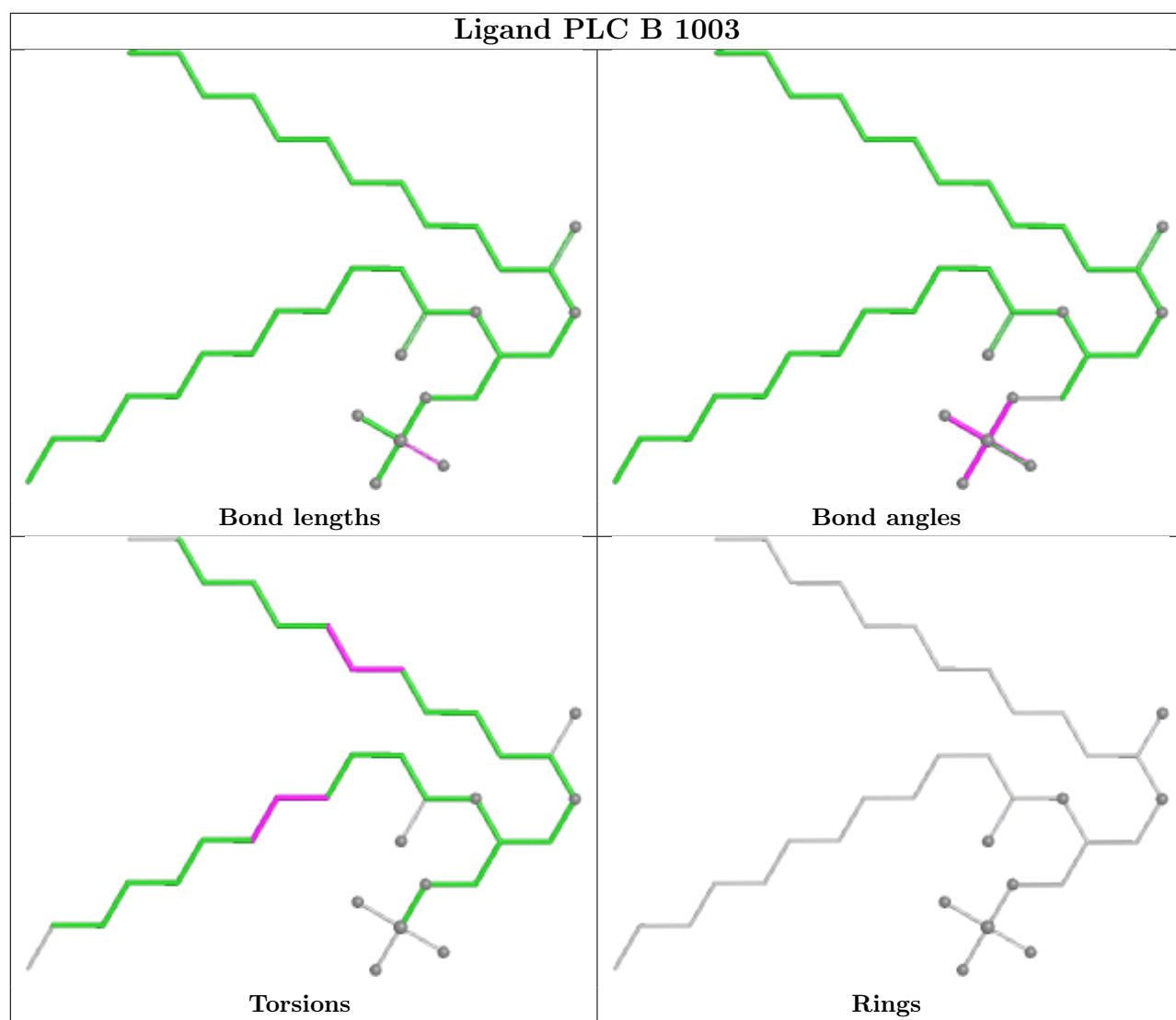
Mol	Chain	Res	Type	Atoms
2	A	1001	PIO	C2-C1-O1-P1
2	A	1001	PIO	C1-O1-P1-O13
2	B	1002	PIO	O1A-C1A-O2C-C2C
2	B	1002	PIO	C2A-C1A-O2C-C2C
4	A	1004	PLC	C1'-C'-O2-C2

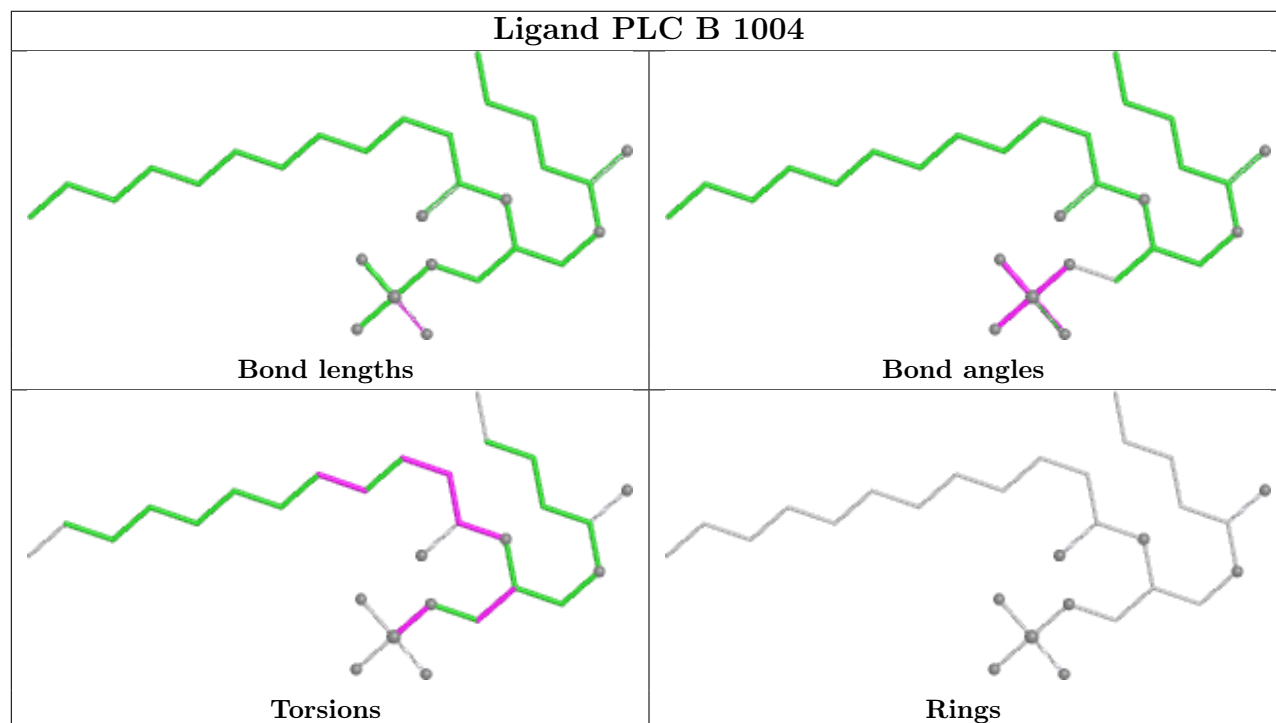
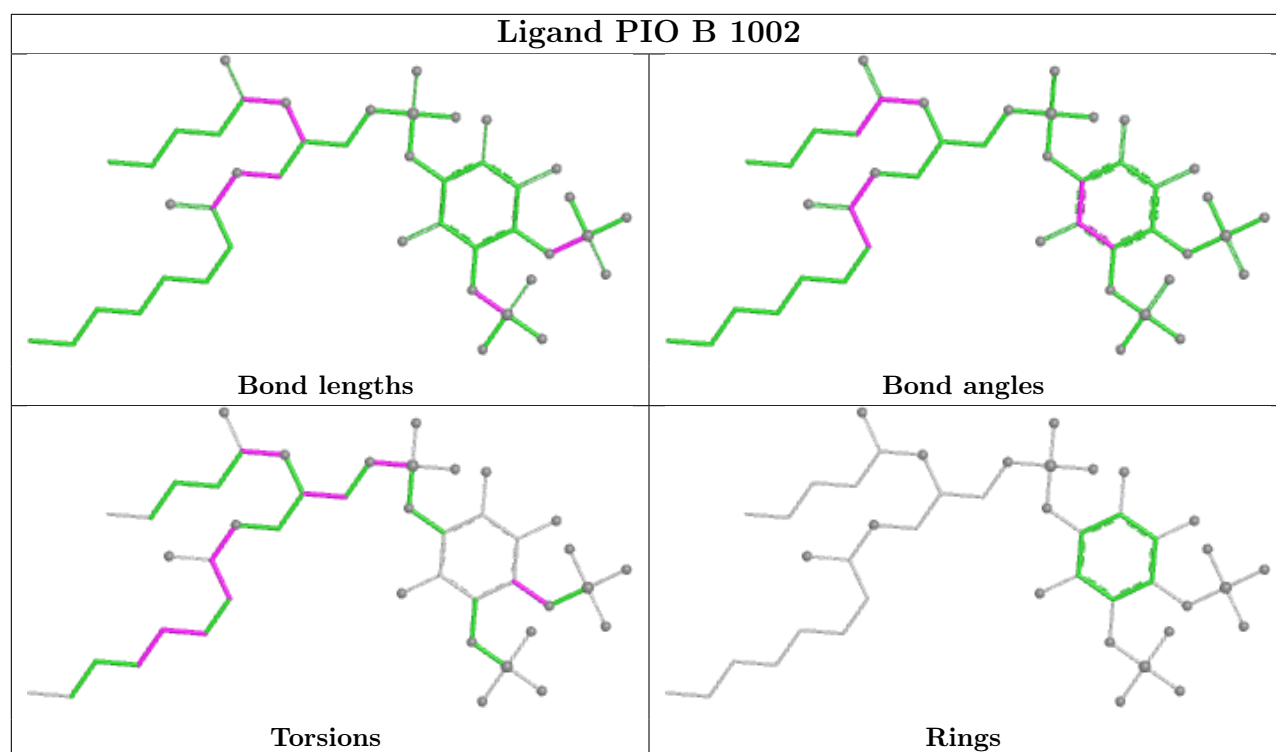
There are no ring outliers.

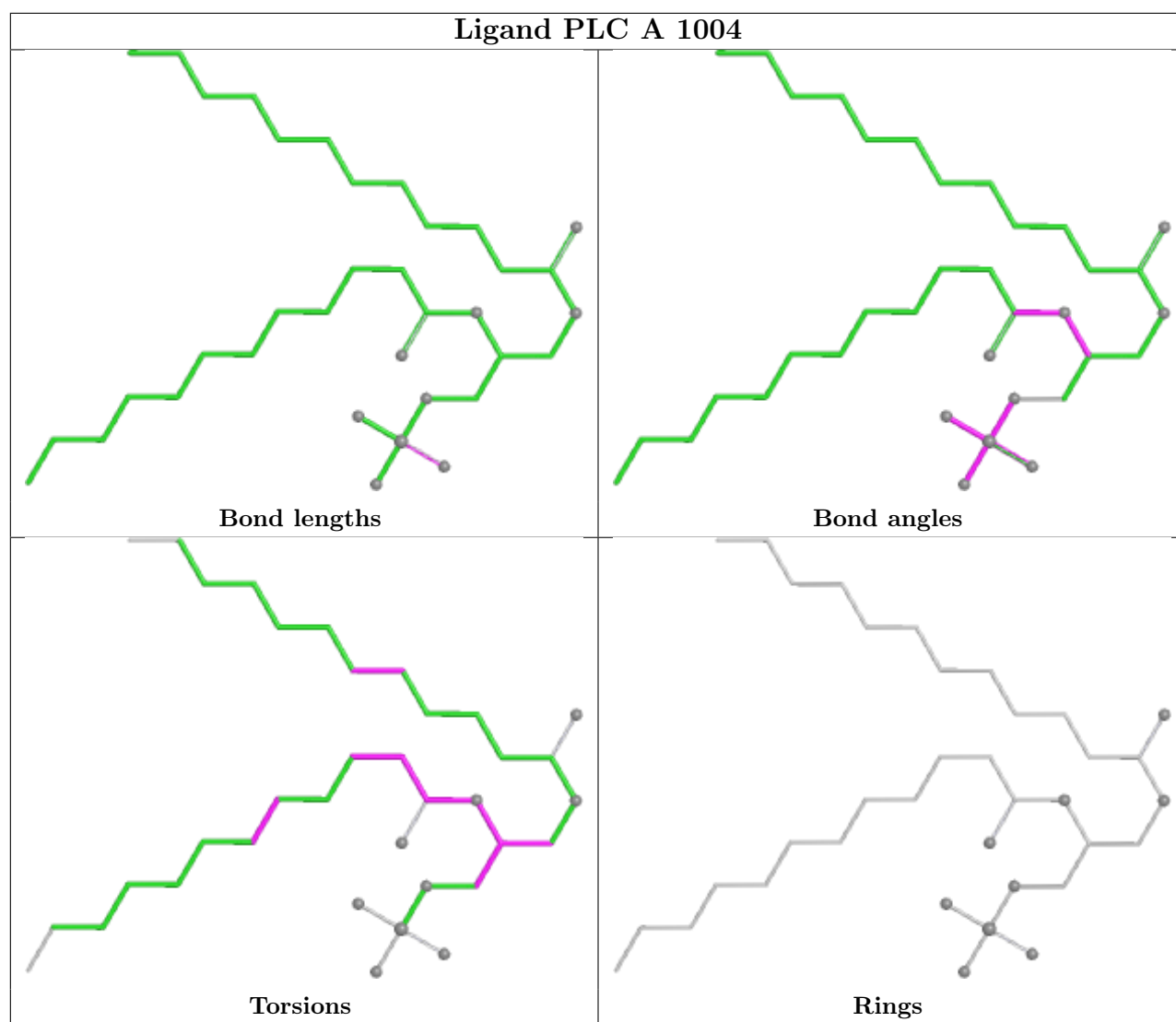
4 monomers are involved in 6 short contacts:

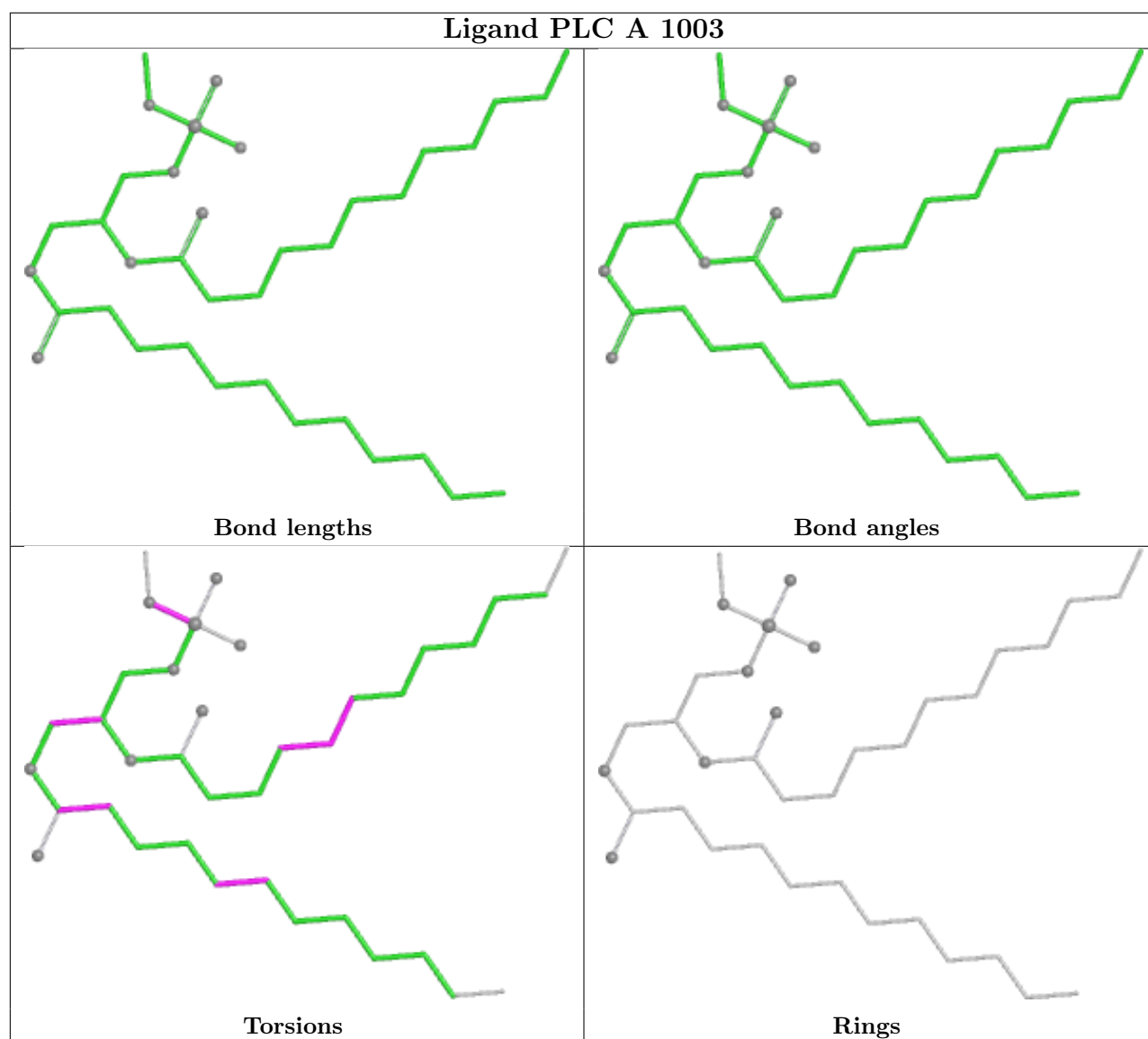
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	PLC	2	0
2	B	1002	PIO	1	0
4	A	1003	PLC	1	0
2	A	1001	PIO	2	0

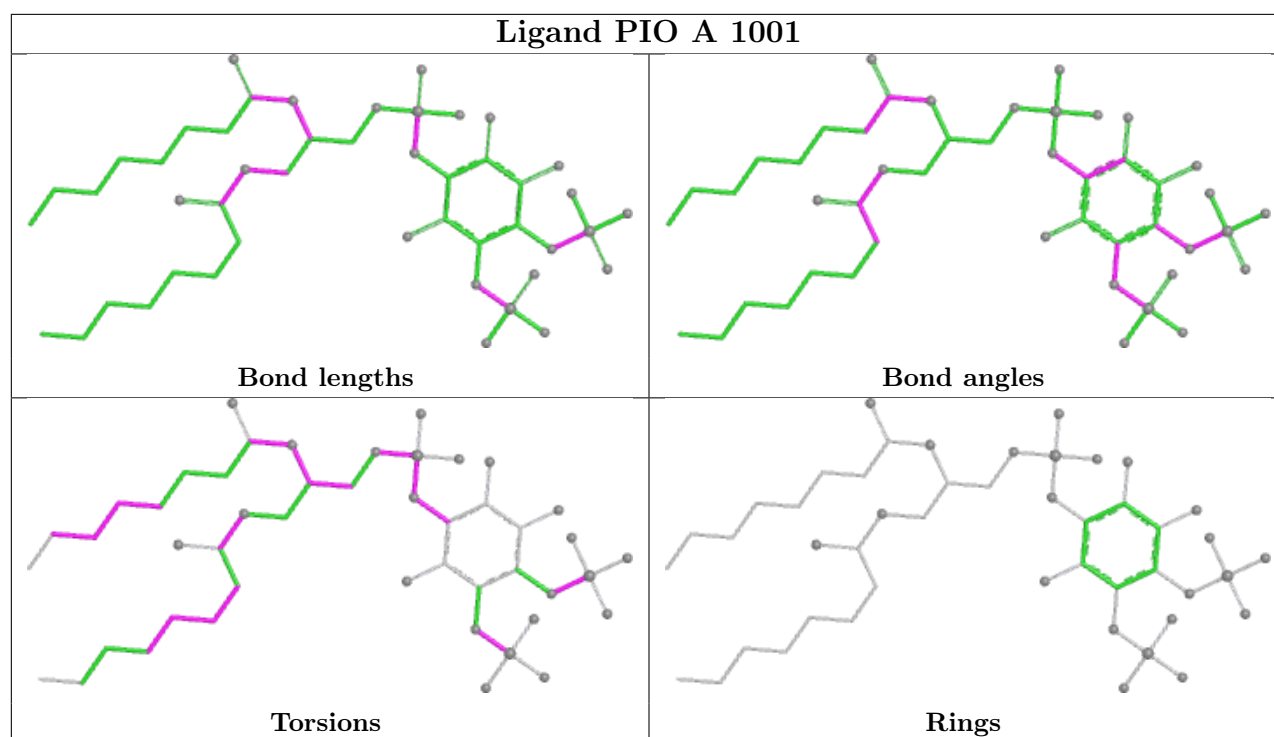
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

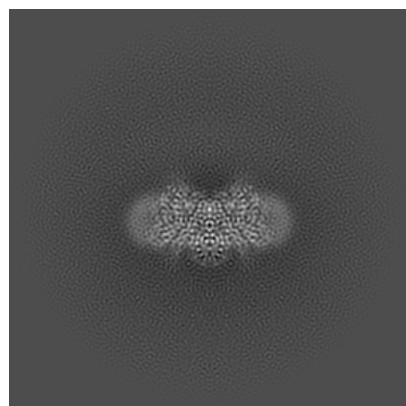
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41020. These allow visual inspection of the internal detail of the map and identification of artifacts.

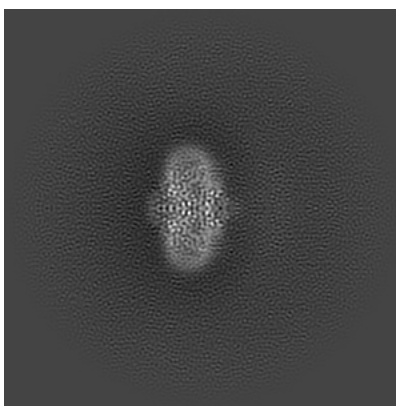
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

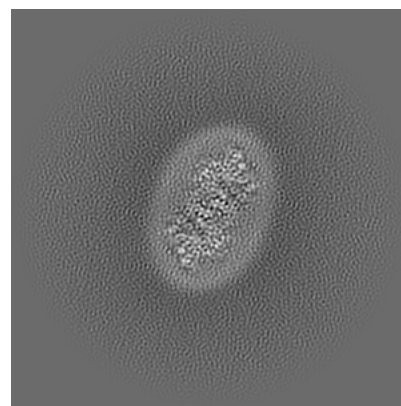
6.1.1 Primary map



X

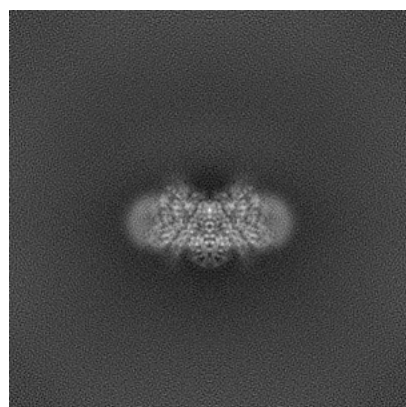


Y

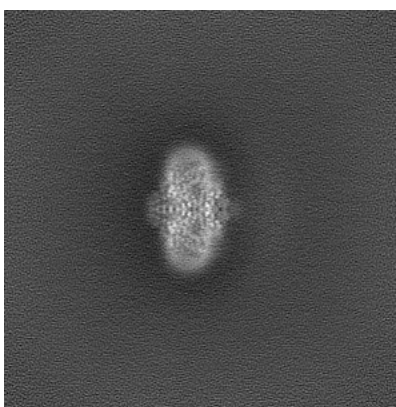


Z

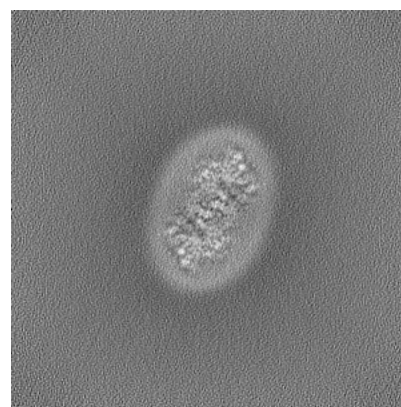
6.1.2 Raw map



X



Y

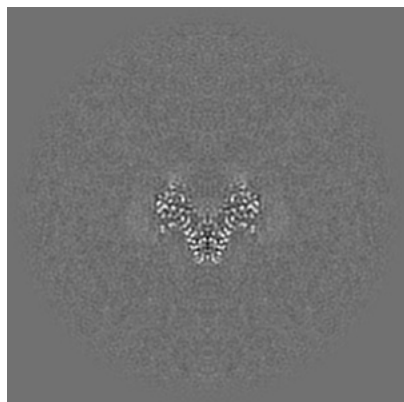


Z

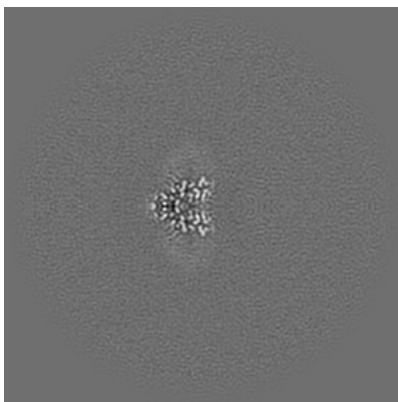
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

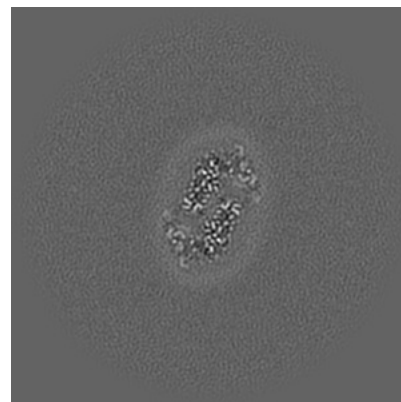
6.2.1 Primary map



X Index: 150

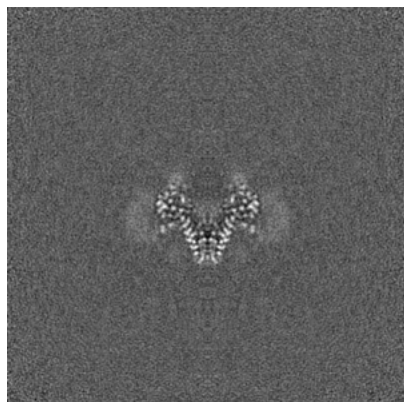


Y Index: 150

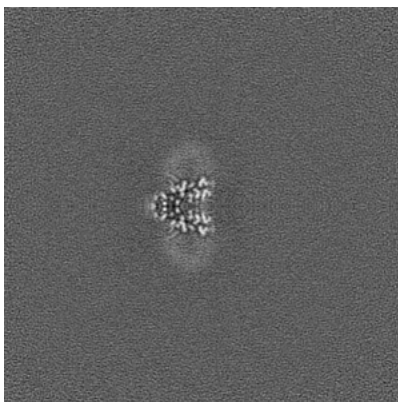


Z Index: 150

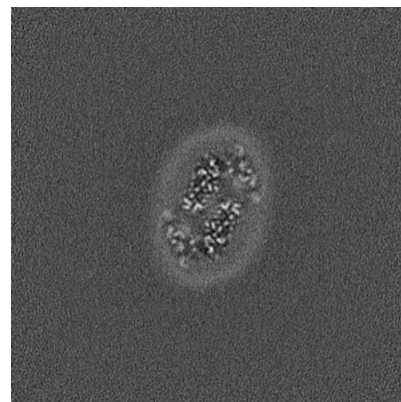
6.2.2 Raw map



X Index: 150



Y Index: 150

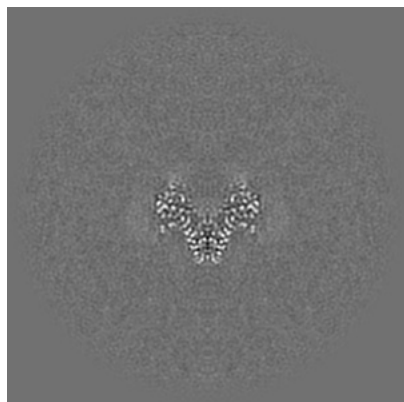


Z Index: 150

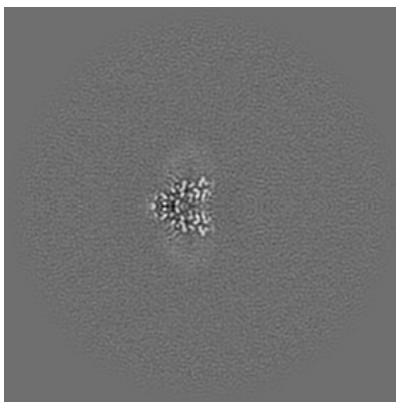
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

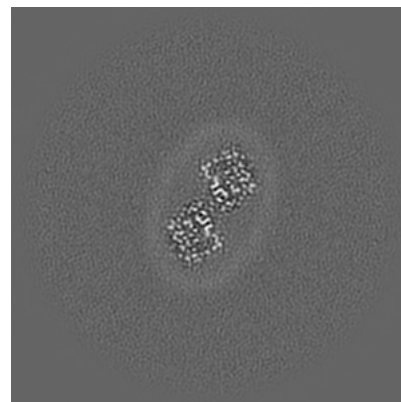
6.3.1 Primary map



X Index: 150

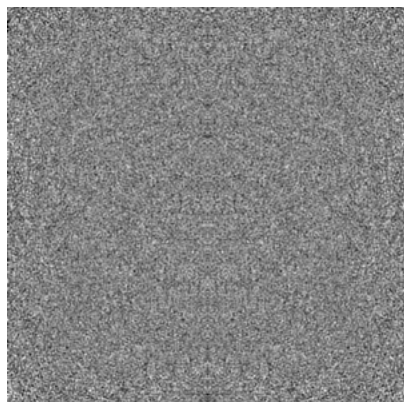


Y Index: 150

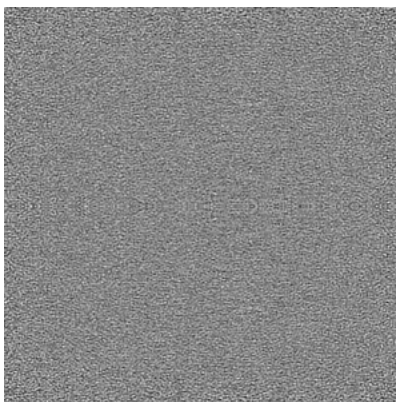


Z Index: 138

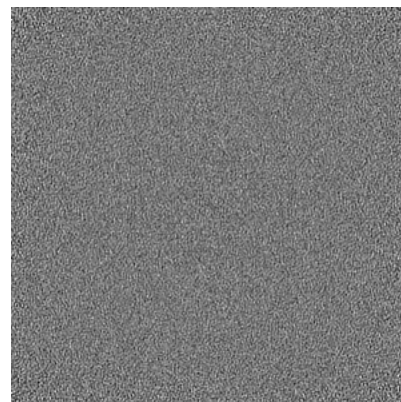
6.3.2 Raw map



X Index: 0



Y Index: 0

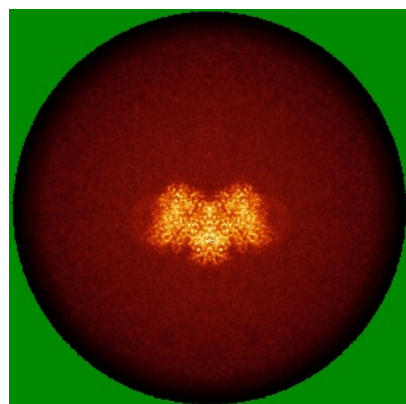


Z Index: 0

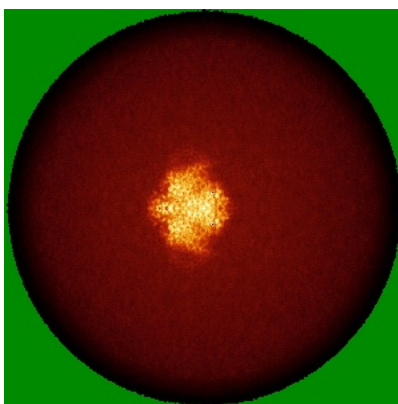
The images above show the largest variance slices of the map in three orthogonal directions.

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

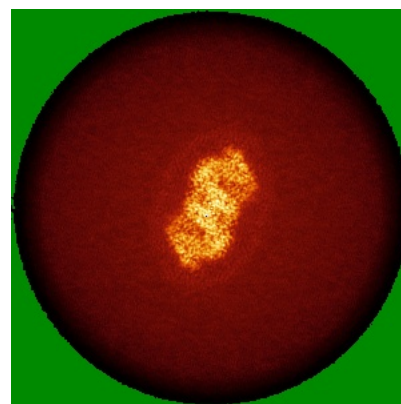
6.4.1 Primary map



X

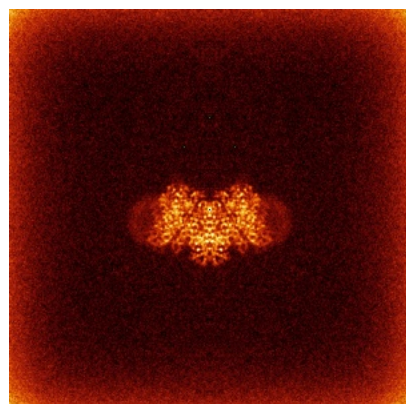


Y

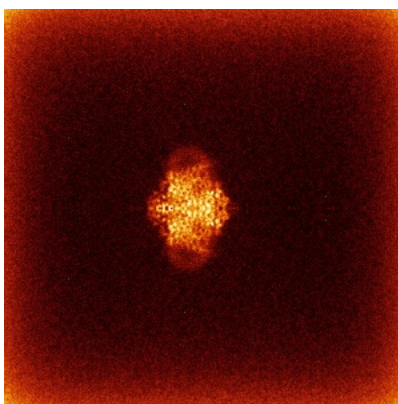


Z

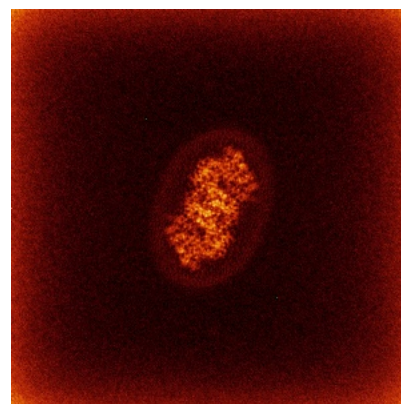
6.4.2 Raw map



X



Y

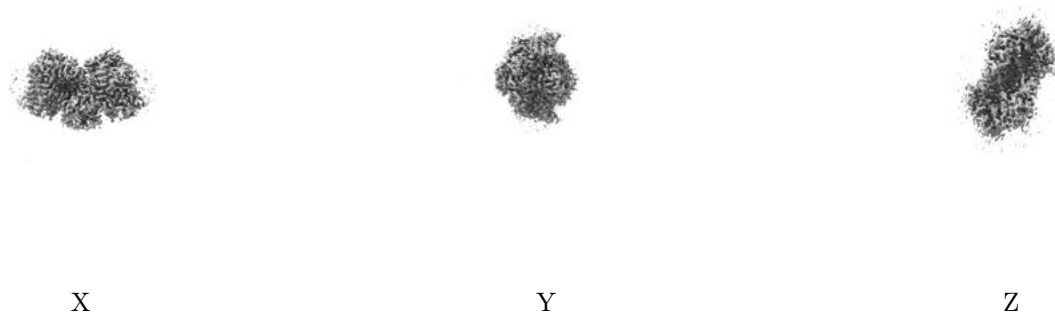


Z

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.

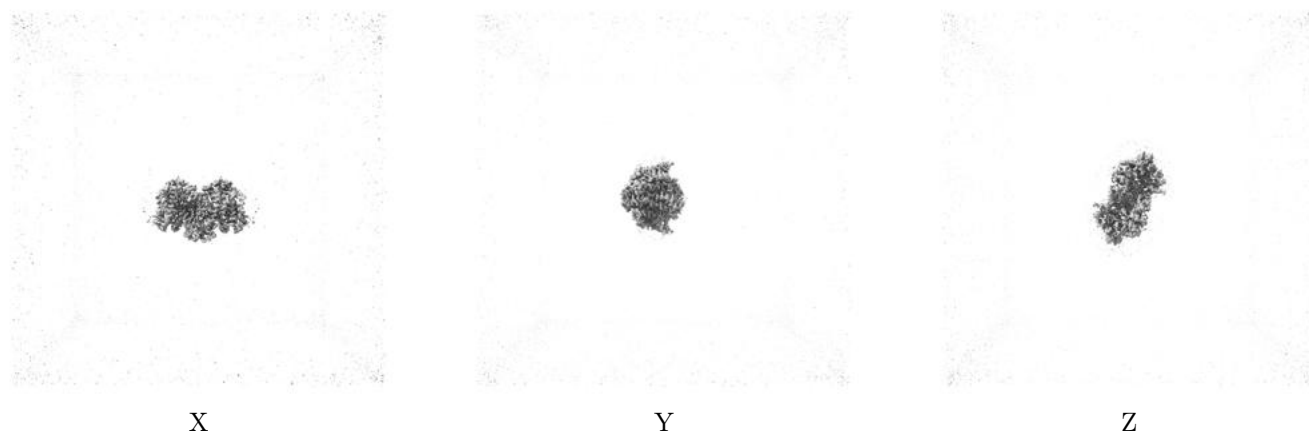
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

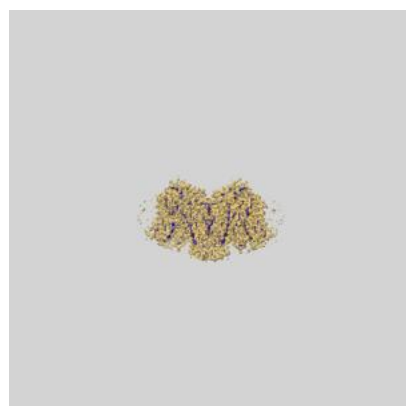
6.6 Mask visualisation [i](#)

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

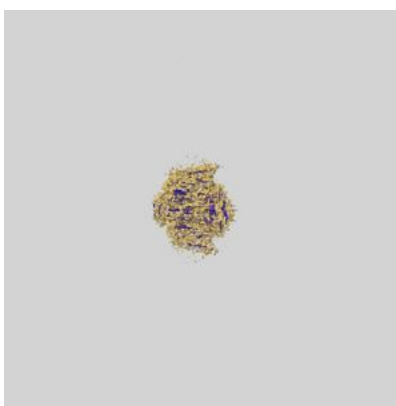
A mask typically either:

- 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_41020_msk_1.map [i](#)



X



Y

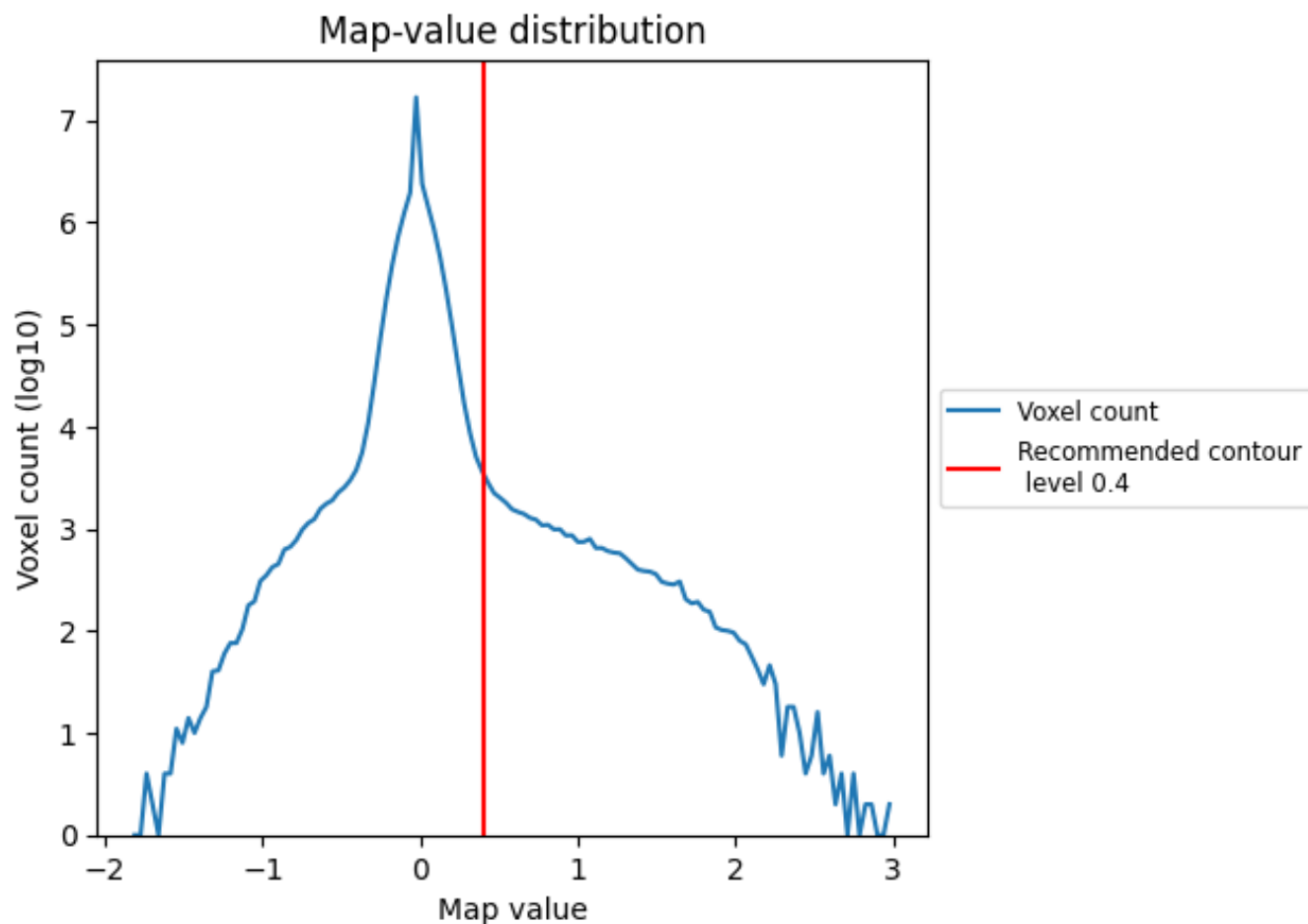


Z

7 Map analysis [i](#)

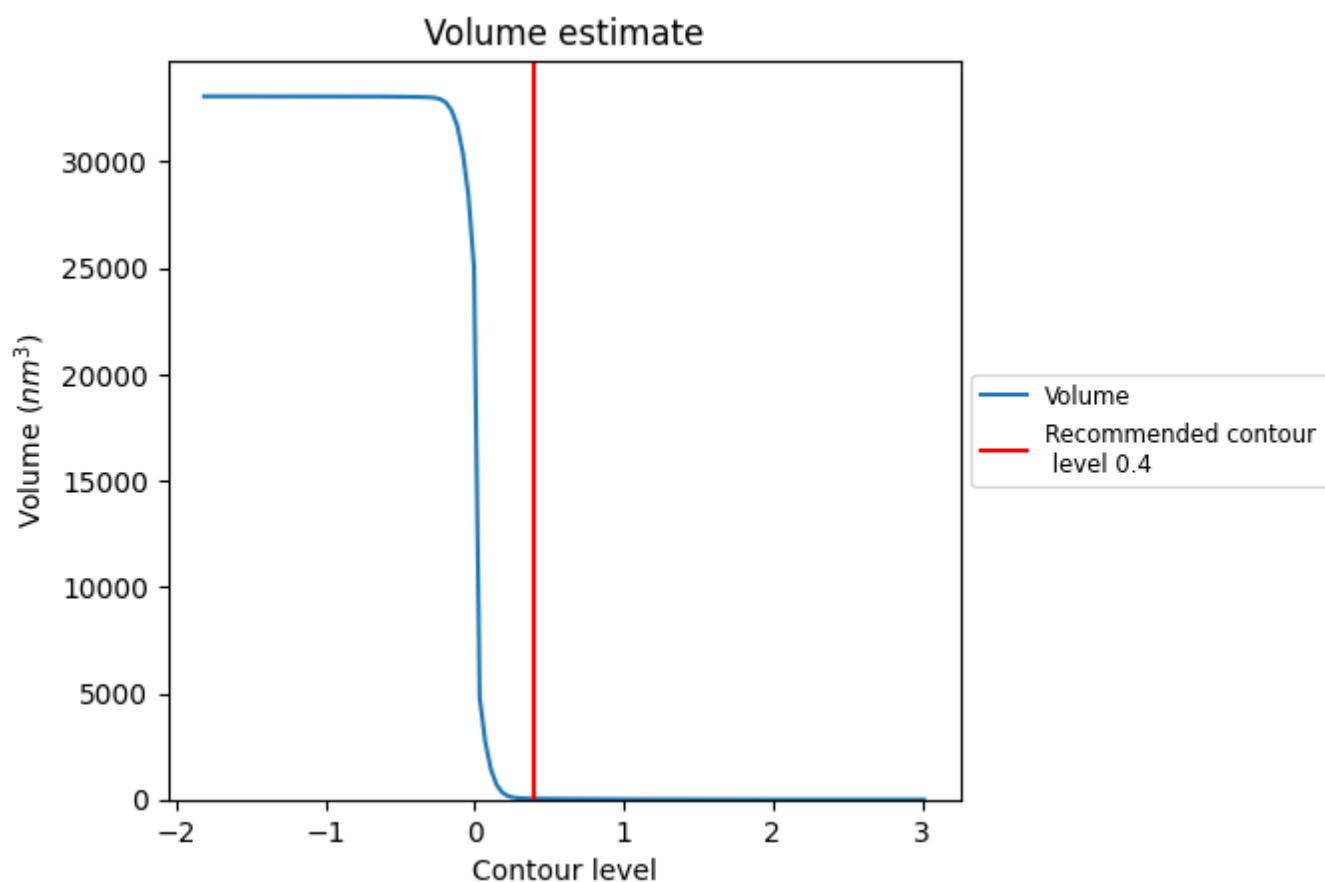
This section contains the results of statistical analysis of the map.

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.

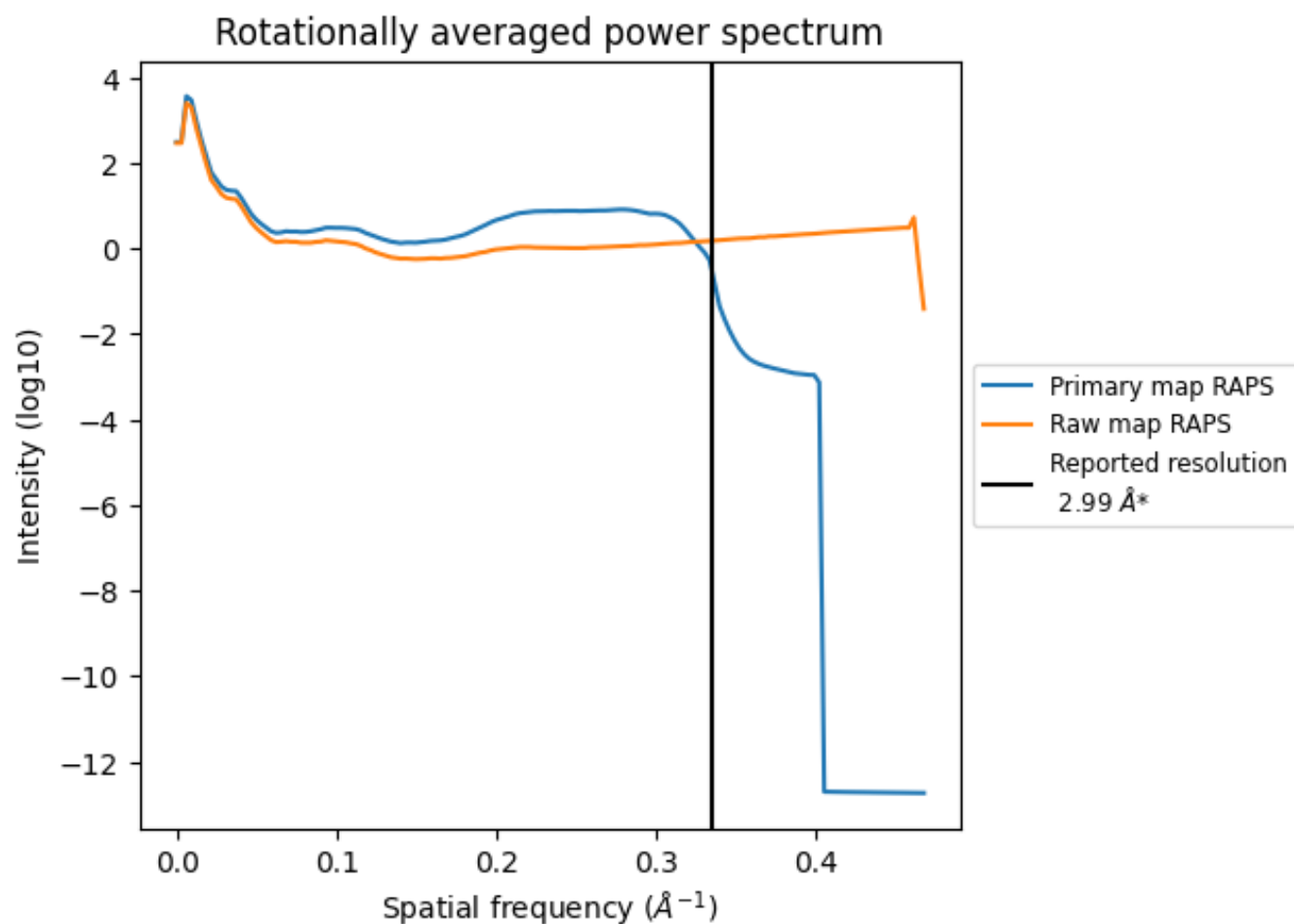
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm³; this corresponds to an approximate mass of 39 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 ⓘ

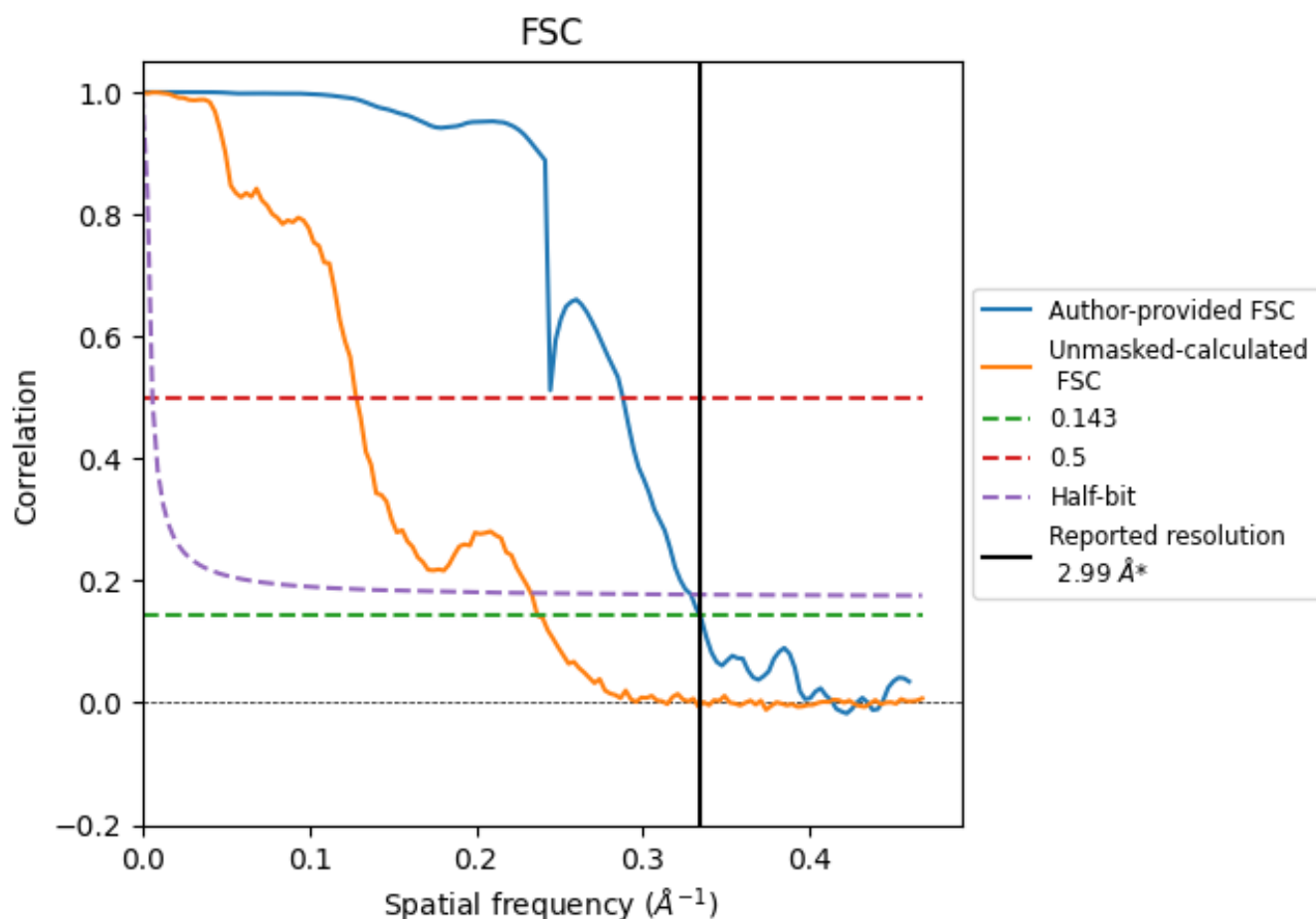


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

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 $0.334 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

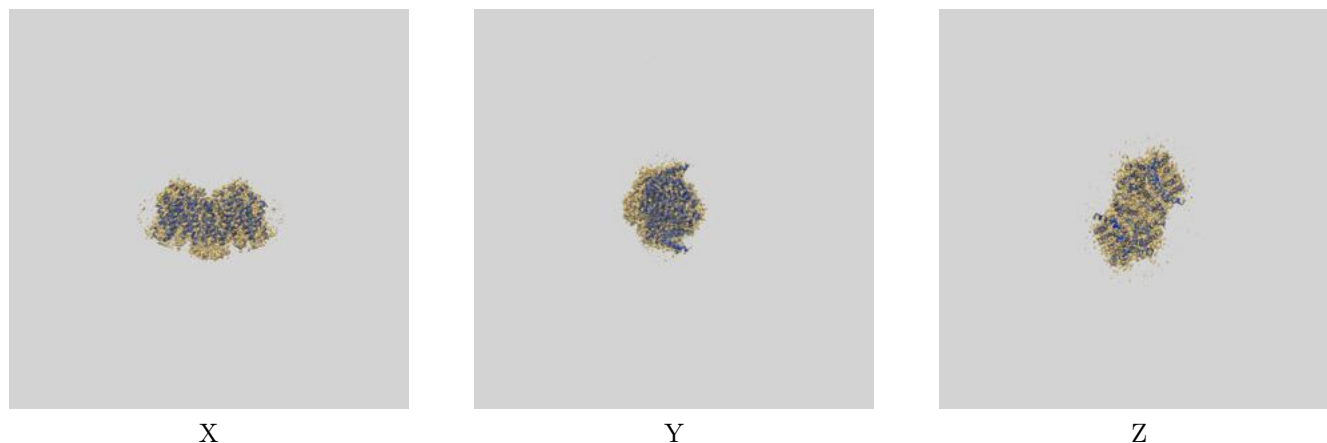
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.47	3.04
Unmasked-calculated*	4.22	7.79	4.29

*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 4.22 differs from the reported value 2.99 by more than 10 %

9 Map-model fit [i](#)

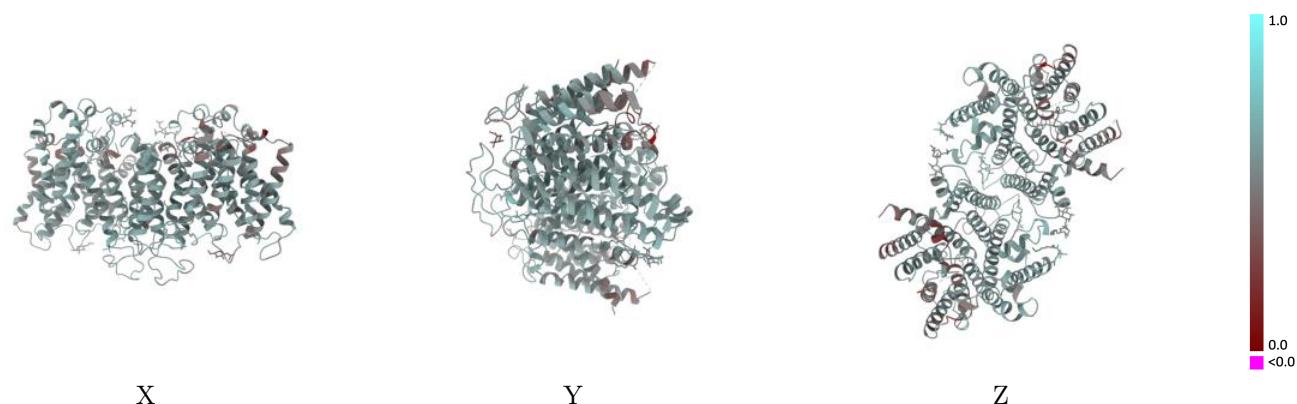
This section contains information regarding the fit between EMDB map EMD-41020 and PDB model 8T45. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



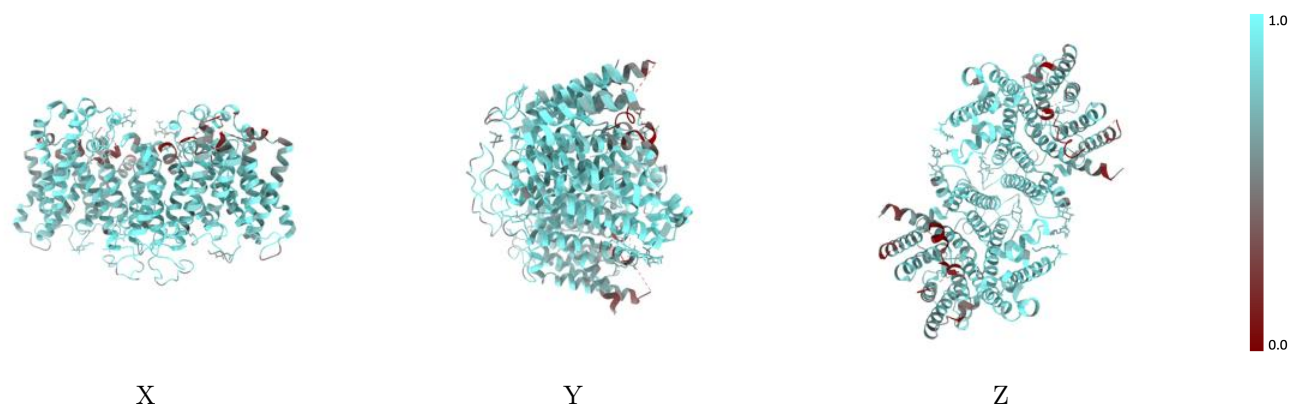
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



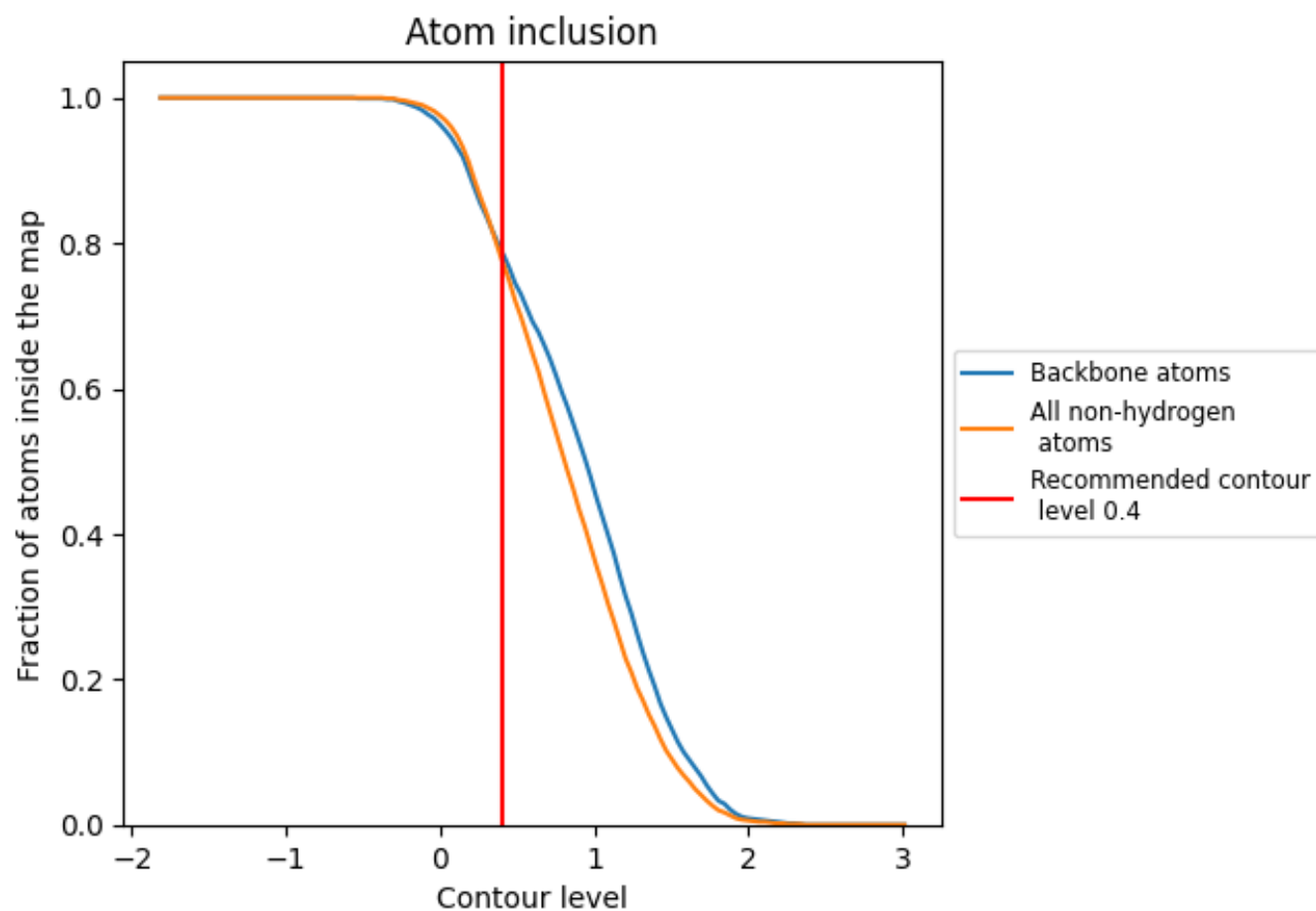
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.5460
A	0.7730	0.5450
B	0.7810	0.5460

