



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2023 – 01:55 PM EST

PDB ID : 8DTI
EMDB ID : EMD-27699
Title : Cryo-EM structure of Arabidopsis SPY in complex with GDP-fucose
Authors : Kumar, S.; Zhou, Y.; Dillard, L.; Borgnia, M.J.; Bartesaghi, A.; Zhou, P.
Deposited on : 2022-07-25
Resolution : 3.80 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

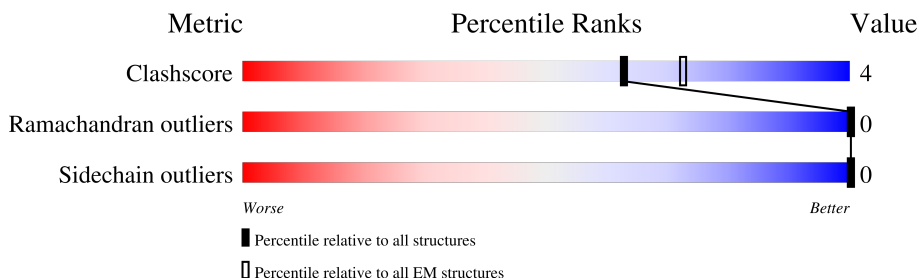
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	946	
1	B	946	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9455 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 Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	629	4684	2990	790	872	32	0	0
1	B	629	4695	2996	794	874	31	0	0

There are 64 discrepancies between the modelled and reference sequences:

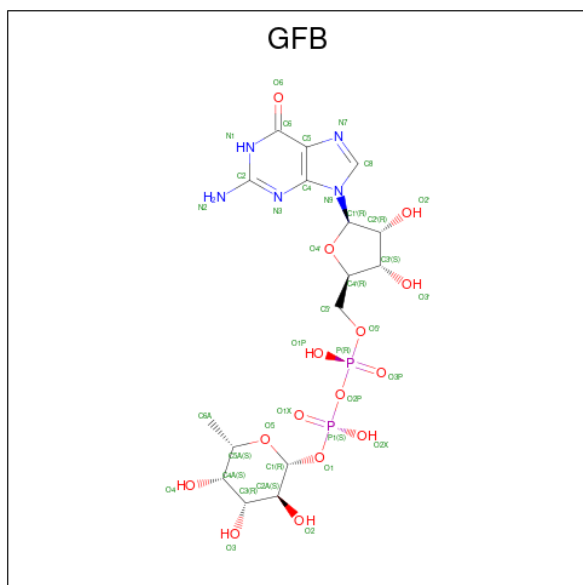
Chain	Residue	Modelled	Actual	Comment	Reference
A	915	GLY	-	expression tag	UNP Q96301
A	916	GLY	-	expression tag	UNP Q96301
A	917	SER	-	expression tag	UNP Q96301
A	918	GLU	-	expression tag	UNP Q96301
A	919	ASN	-	expression tag	UNP Q96301
A	920	LEU	-	expression tag	UNP Q96301
A	921	TYR	-	expression tag	UNP Q96301
A	922	PHE	-	expression tag	UNP Q96301
A	923	GLN	-	expression tag	UNP Q96301
A	924	GLY	-	expression tag	UNP Q96301
A	925	GLY	-	expression tag	UNP Q96301
A	926	SER	-	expression tag	UNP Q96301
A	927	HIS	-	expression tag	UNP Q96301
A	928	HIS	-	expression tag	UNP Q96301
A	929	HIS	-	expression tag	UNP Q96301
A	930	HIS	-	expression tag	UNP Q96301
A	931	HIS	-	expression tag	UNP Q96301
A	932	HIS	-	expression tag	UNP Q96301
A	933	HIS	-	expression tag	UNP Q96301
A	934	HIS	-	expression tag	UNP Q96301
A	935	HIS	-	expression tag	UNP Q96301
A	936	HIS	-	expression tag	UNP Q96301
A	937	GLY	-	expression tag	UNP Q96301
A	938	GLY	-	expression tag	UNP Q96301
A	939	TRP	-	expression tag	UNP Q96301

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Chain	Residue	Modelled	Actual	Comment	Reference
A	940	SER	-	expression tag	UNP Q96301
A	941	HIS	-	expression tag	UNP Q96301
A	942	PRO	-	expression tag	UNP Q96301
A	943	GLN	-	expression tag	UNP Q96301
A	944	PHE	-	expression tag	UNP Q96301
A	945	GLU	-	expression tag	UNP Q96301
A	946	LYS	-	expression tag	UNP Q96301
B	915	GLY	-	expression tag	UNP Q96301
B	916	GLY	-	expression tag	UNP Q96301
B	917	SER	-	expression tag	UNP Q96301
B	918	GLU	-	expression tag	UNP Q96301
B	919	ASN	-	expression tag	UNP Q96301
B	920	LEU	-	expression tag	UNP Q96301
B	921	TYR	-	expression tag	UNP Q96301
B	922	PHE	-	expression tag	UNP Q96301
B	923	GLN	-	expression tag	UNP Q96301
B	924	GLY	-	expression tag	UNP Q96301
B	925	GLY	-	expression tag	UNP Q96301
B	926	SER	-	expression tag	UNP Q96301
B	927	HIS	-	expression tag	UNP Q96301
B	928	HIS	-	expression tag	UNP Q96301
B	929	HIS	-	expression tag	UNP Q96301
B	930	HIS	-	expression tag	UNP Q96301
B	931	HIS	-	expression tag	UNP Q96301
B	932	HIS	-	expression tag	UNP Q96301
B	933	HIS	-	expression tag	UNP Q96301
B	934	HIS	-	expression tag	UNP Q96301
B	935	HIS	-	expression tag	UNP Q96301
B	936	HIS	-	expression tag	UNP Q96301
B	937	GLY	-	expression tag	UNP Q96301
B	938	GLY	-	expression tag	UNP Q96301
B	939	TRP	-	expression tag	UNP Q96301
B	940	SER	-	expression tag	UNP Q96301
B	941	HIS	-	expression tag	UNP Q96301
B	942	PRO	-	expression tag	UNP Q96301
B	943	GLN	-	expression tag	UNP Q96301
B	944	PHE	-	expression tag	UNP Q96301
B	945	GLU	-	expression tag	UNP Q96301
B	946	LYS	-	expression tag	UNP Q96301

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-BETA-L-FUCOPYRANOSE (three-letter code: GFB) (formula: C₁₆H₂₅N₅O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
2	A	1	Total	C	N	O	P	0
			38	16	5	15	2	
2	B	1	Total	C	N	O	P	0
			38	16	5	15	2	

HIS	ASP	M402	D740	SER	HIS
LYS	PRO	L403	T748	ARG	HIS
GLU	HIS	G404	E752	VAL	GLY
GLY	TYR	M415	Y755	THR	TRP
ARG	ALA	Y420	T762	GLY	HIS
LEU	PRO	G434	L785	GLU	PRO
VAL	ALA	R437	L438	ALA	GLN
GLU	TYR	L438	E790	THR	PHE
ALA	ASN	M441	D791	SER	GLU
GLY	LEU	I485	E792	LEU	LYS
TYR	VAL	F500	Y793	LYS	ALA
TRP	VAL	1501	V794	ALA	ASN
GLN	VAL	E502	L796	GLY	GLY
LEU	ASP	A503	L800	SER	SER
ALA	TYR	P504	L810	PRO	VAL
ILE	ASN	Y518	L814	SER	PRO
LEU	LEU	D560	R815	LEU	LEU
VAL	ALA	I564	A836	PRO	THR
LEU	CYS	V587	M840	THR	GLN
THR	TYR	P595	K848	SER	PRO
GLY	LYS	T598	GLY	LEU	LEU
ASP	ALA	G599	VAL	ARG	LYS
LEU	ALA	L600	PRO	VAL	ARG
LEU	LEU	R606	SER	THR	MET
GLY	LEU	L633	LEU	ARG	PRO
THR	THR	T636	LEU	THR	ASP
SER	SER	E640	LEU	LEU	ASP
LEU	SER	S684	GLN	GLN	LEU
LEU	LEU	R685	LYS	ASN	LEU
LYS	LYS	K689	TYR	LYS	TYR
LEU	ALA	R715	VAL	VAL	PHE
LEU	ALA	V716	HIS	GLN	GLY
LEU	ALA	D717	ASP	GLY	GLY
LEU	ASN	I722	ASP	ASP	SER
LEU	ASN	D346	PRO	PRO	HIS
LYS	ASN	Y318	ILE	ILE	HIS
GLY	THR	D346	ILE	HIS	HIS
GLY	GLN	N371	SER	HIS	HIS
ILE	LYS	D380	LYS	HIS	HIS
LYS	TYR	N381	ASP	LEU	HIS
TYR	GLU	A381	GLY	GLY	HIS
GLU	ALA		PRO	PRO	HIS
ALA	LEU				
LEU	LYS				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182947	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 ($e^-/\text{\AA}^2$)	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	56.301	Depositor
Minimum map value	-41.943	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.976	Depositor
Recommended contour level	5.4	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GFB

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	0.27	0/4797	0.45	0/6561
1	B	0.27	0/4808	0.45	0/6573
All	All	0.27	0/9605	0.45	0/13134

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	4684	0	4388	41	0
1	B	4695	0	4404	41	0
2	A	38	0	23	2	0
2	B	38	0	23	2	0
All	All	9455	0	8838	80	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 4.

The worst 5 of 80 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:684:SER:OG	1:B:715:ARG:NH2	2.28	0.66
1:A:684:SER:OG	1:A:715:ARG:NH2	2.29	0.66
1:A:346:ASP:OD2	1:B:252:ASN:ND2	2.31	0.64
1:A:722:ILE:O	2:A:1001:GFB:N1	2.31	0.63
1:B:722:ILE:O	2:B:1001:GFB:N1	2.31	0.63

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	627/946 (66%)	609 (97%)	18 (3%)	0	100	100
1	B	627/946 (66%)	609 (97%)	18 (3%)	0	100	100
All	All	1254/1892 (66%)	1218 (97%)	36 (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	466/800 (58%)	466 (100%)	0	100	100
1	B	467/800 (58%)	467 (100%)	0	100	100
All	All	933/1600 (58%)	933 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	HIS
1	B	508	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GFB	A	1001	-	34,41,41	2.66	13 (38%)	45,64,64	1.44	9 (20%)
2	GFB	B	1001	-	34,41,41	2.66	13 (38%)	45,64,64	1.45	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GFB	A	1001	-	-	4/17/57/57	0/4/4/4
2	GFB	B	1001	-	-	4/17/57/57	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GFB	C2-N2	6.46	1.49	1.34
2	B	1001	GFB	C2-N2	6.44	1.49	1.34
2	A	1001	GFB	C4-N3	5.52	1.50	1.37
2	B	1001	GFB	C4-N3	5.51	1.50	1.37
2	A	1001	GFB	O4'-C4'	-5.30	1.33	1.45

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GFB	O2P-P1-O1	3.50	109.54	102.48
2	B	1001	GFB	O2P-P1-O1	3.49	109.52	102.48
2	B	1001	GFB	C5-C6-N1	3.31	119.79	113.95
2	A	1001	GFB	C5-C6-N1	3.30	119.77	113.95
2	B	1001	GFB	P1-O2P-P	-3.00	122.53	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	GFB	O5-C1-O1-P1
2	B	1001	GFB	O5-C1-O1-P1
2	A	1001	GFB	P1-O2P-P-O5'
2	B	1001	GFB	P1-O2P-P-O5'
2	A	1001	GFB	O4'-C4'-C5'-O5'

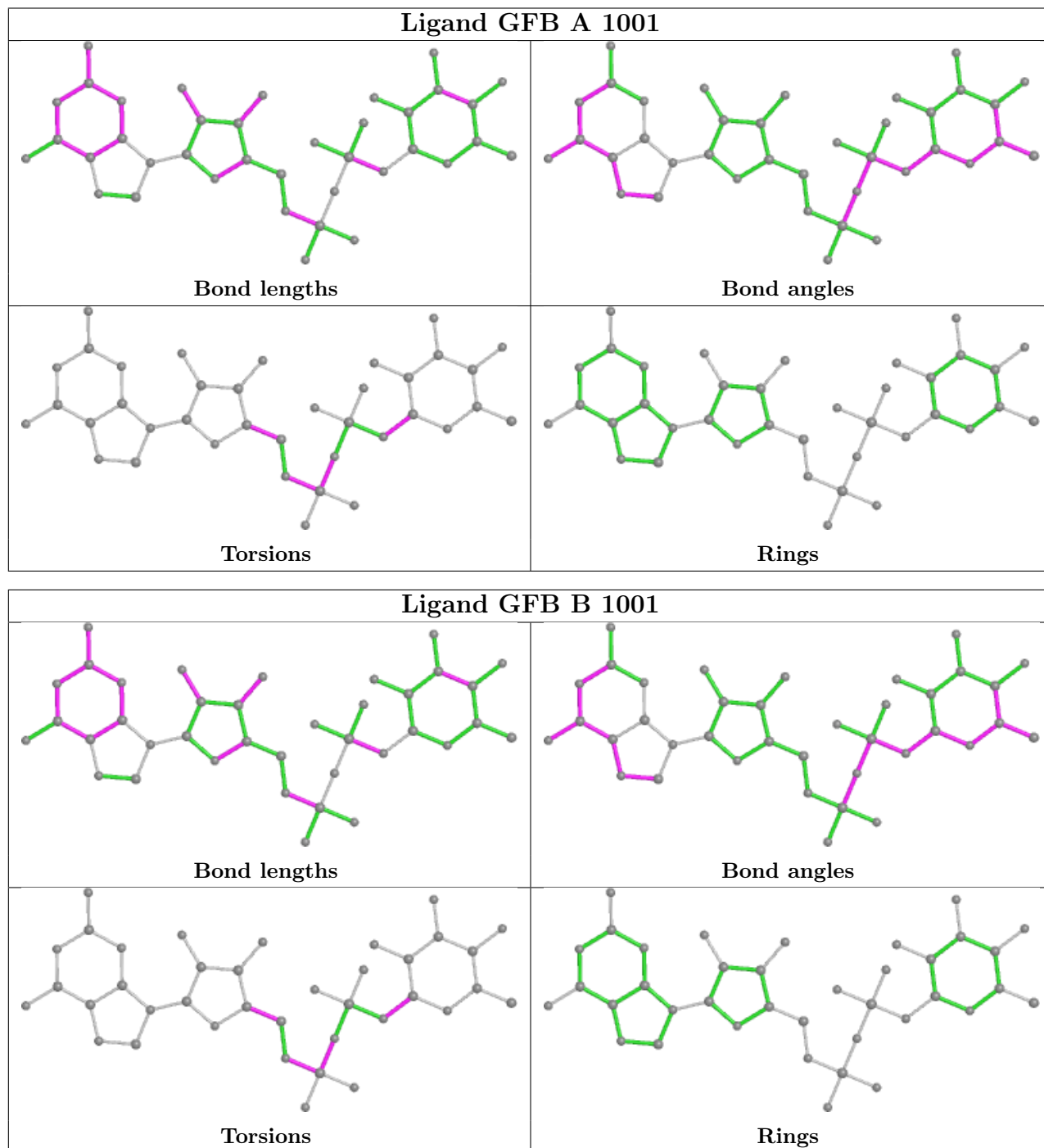
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GFB	2	0
2	B	1001	GFB	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.

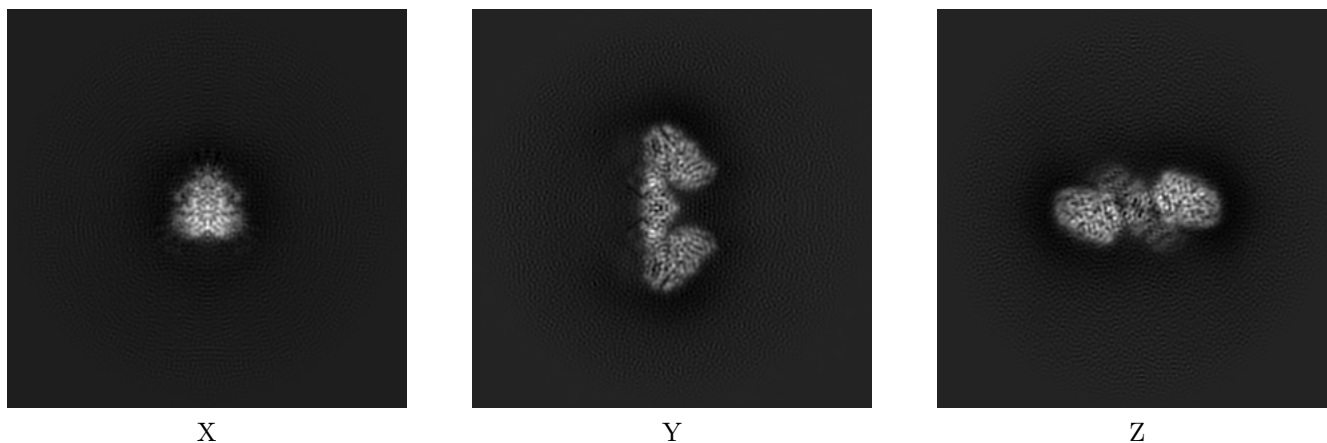
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27699. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

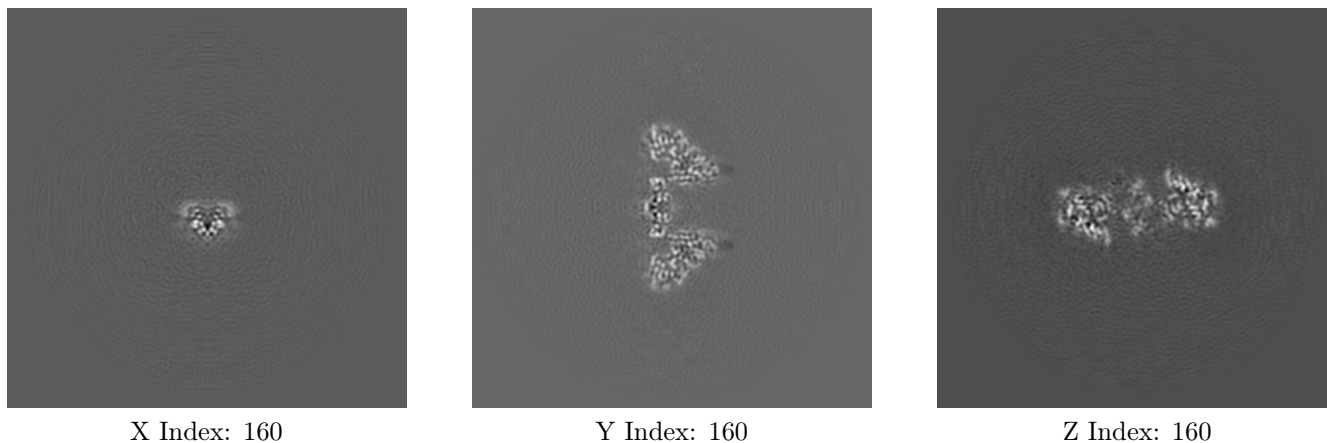
6.1.1 Primary map



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

6.2 Central slices [i](#)

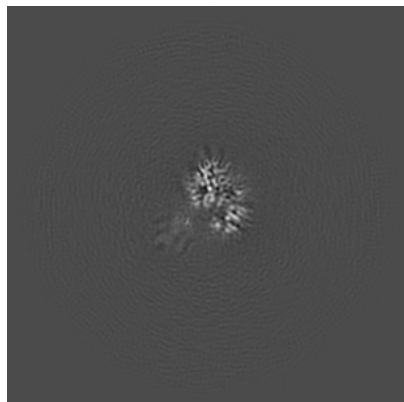
6.2.1 Primary map



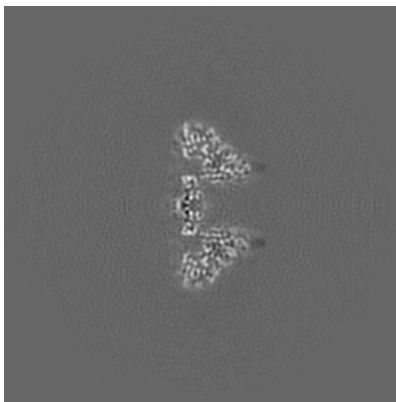
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

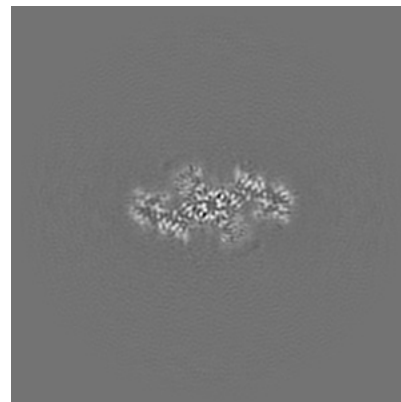
6.3.1 Primary map



X Index: 188



Y Index: 160

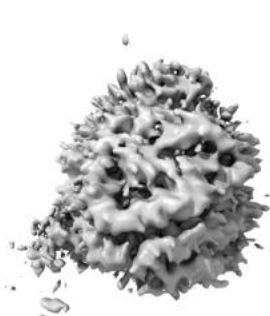


Z Index: 149

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

6.4 Orthogonal surface views [i](#)

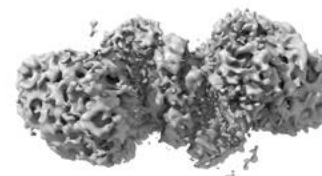
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

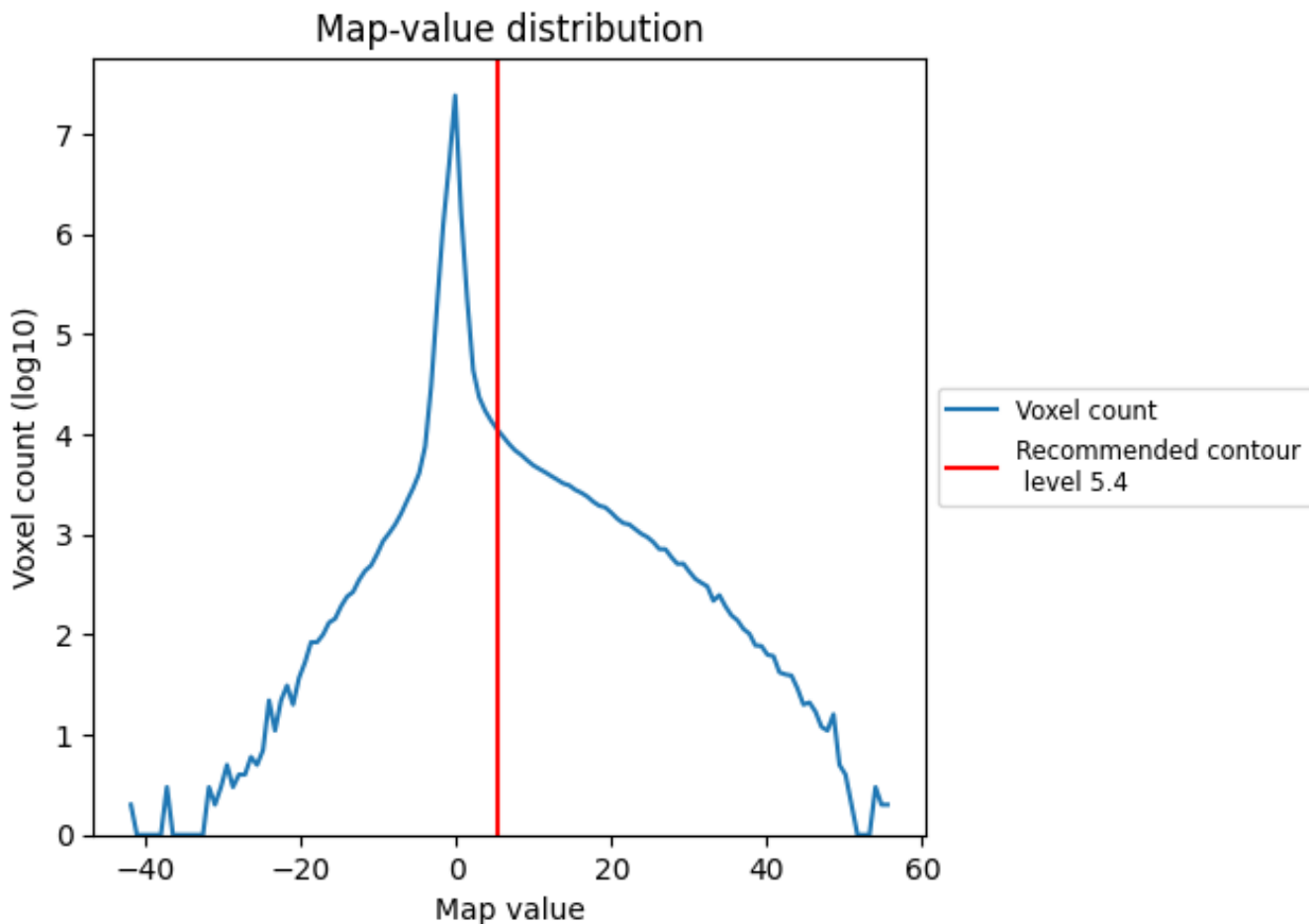
6.5 Mask visualisation

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

7 Map analysis [i](#)

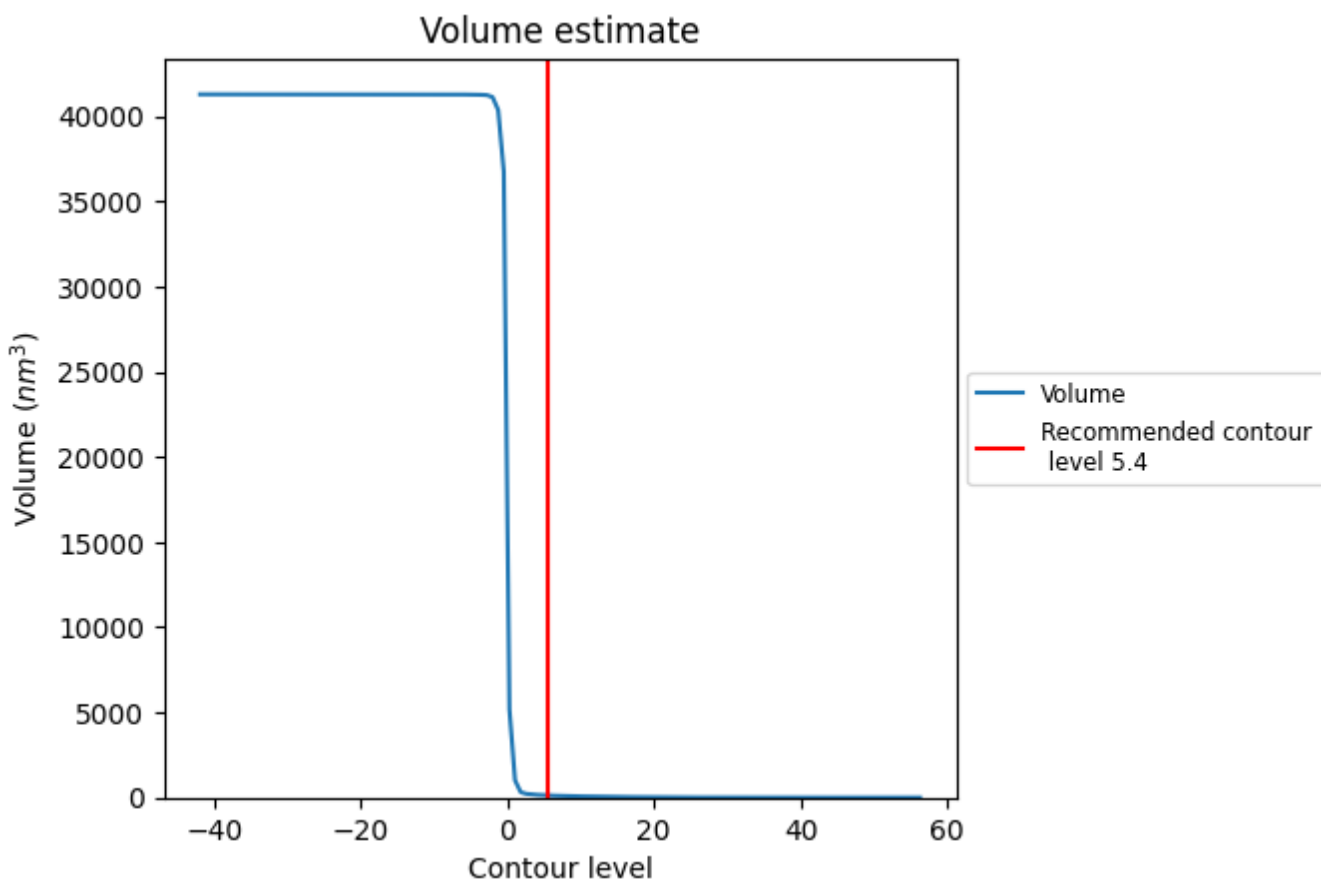
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

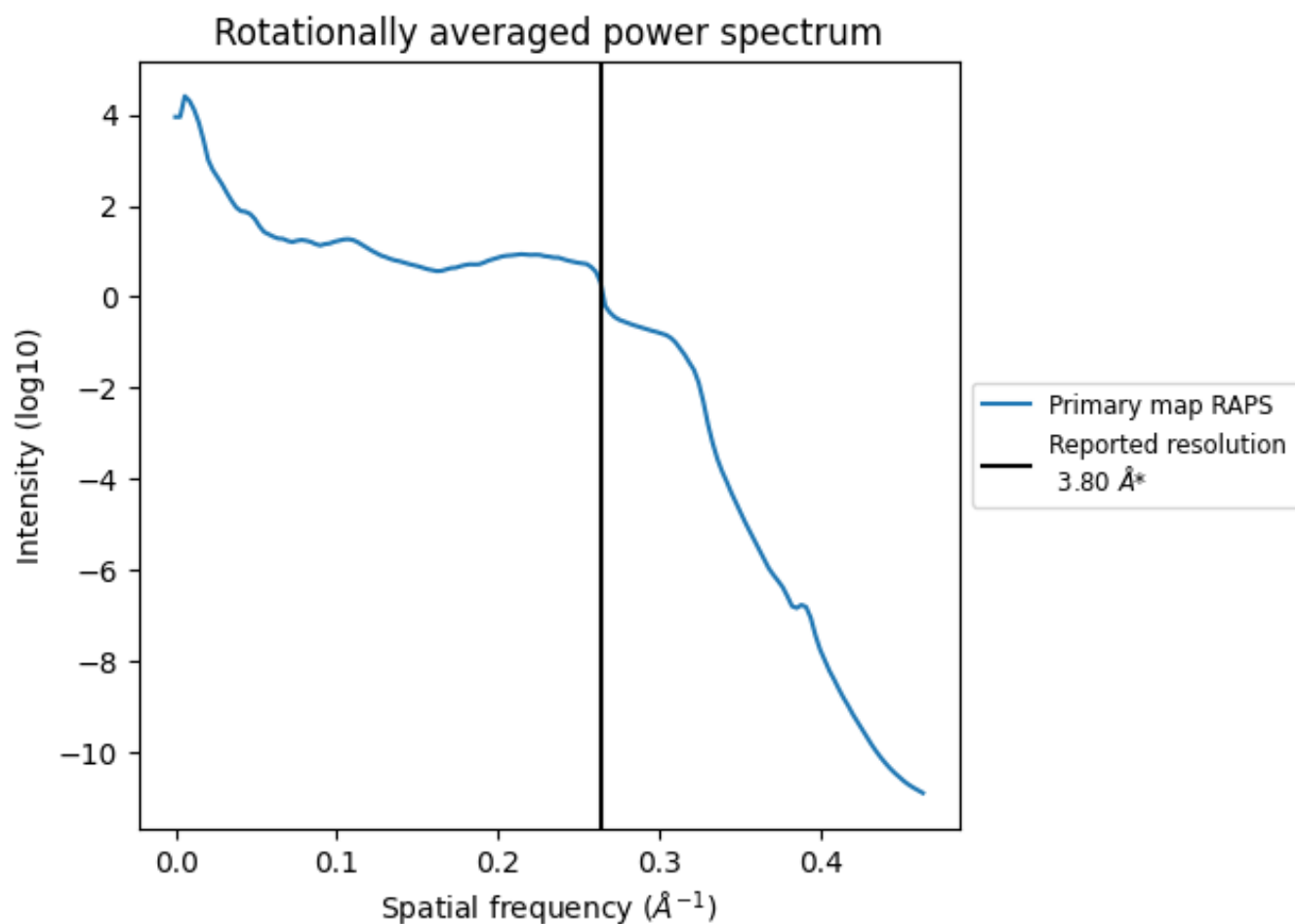
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

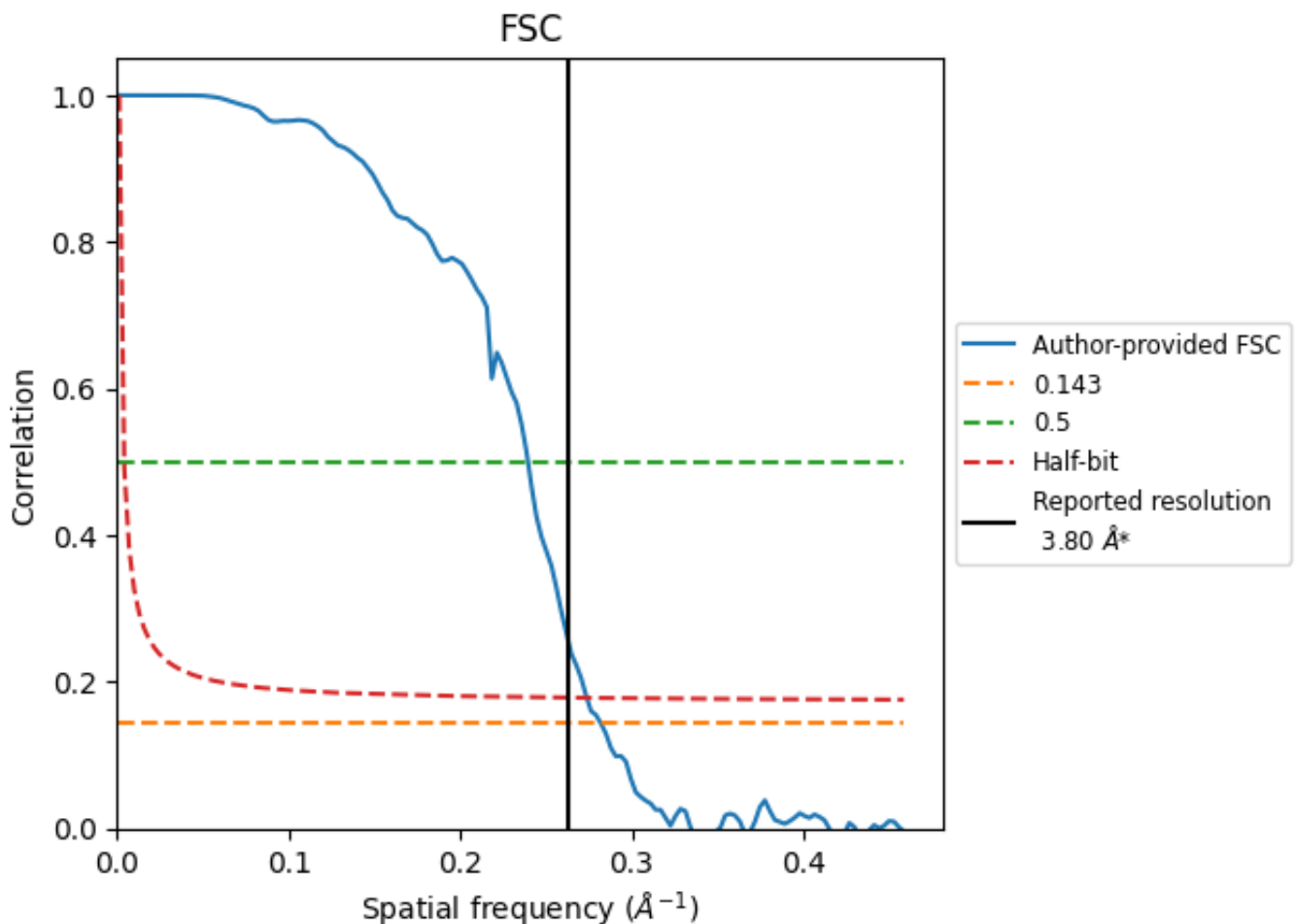


*Reported resolution corresponds to spatial frequency of 0.263\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

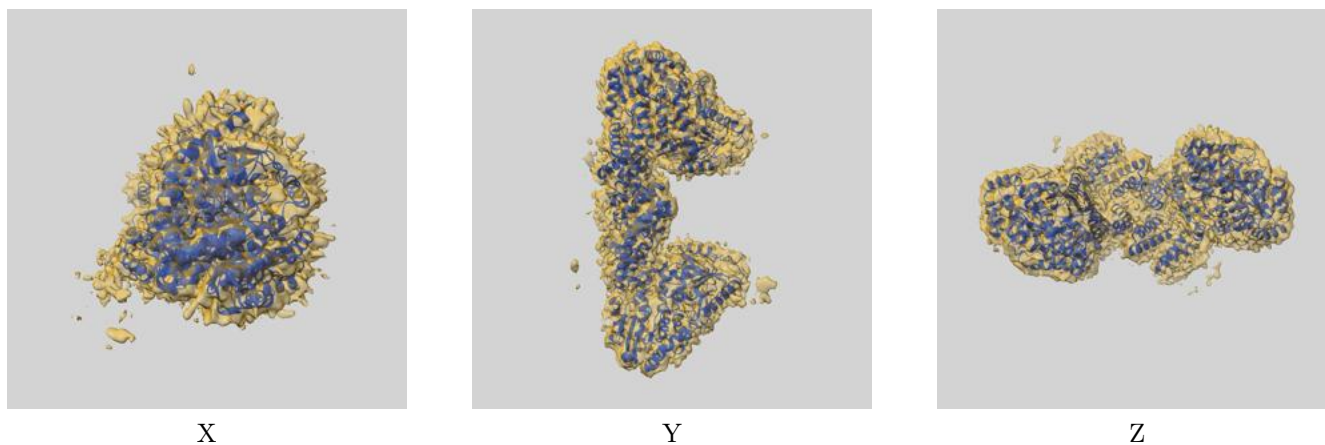
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.55	4.18	3.65
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

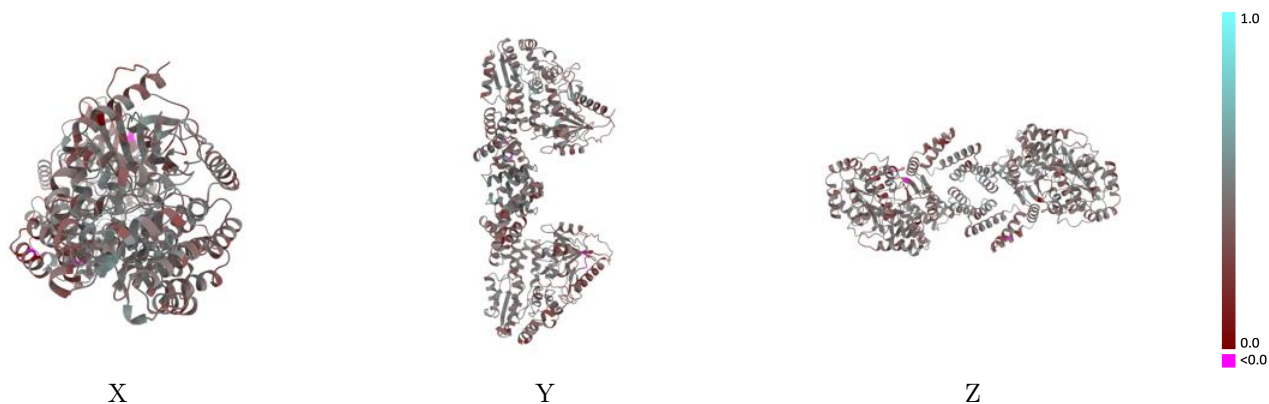
This section contains information regarding the fit between EMDB map EMD-27699 and PDB model 8DTI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



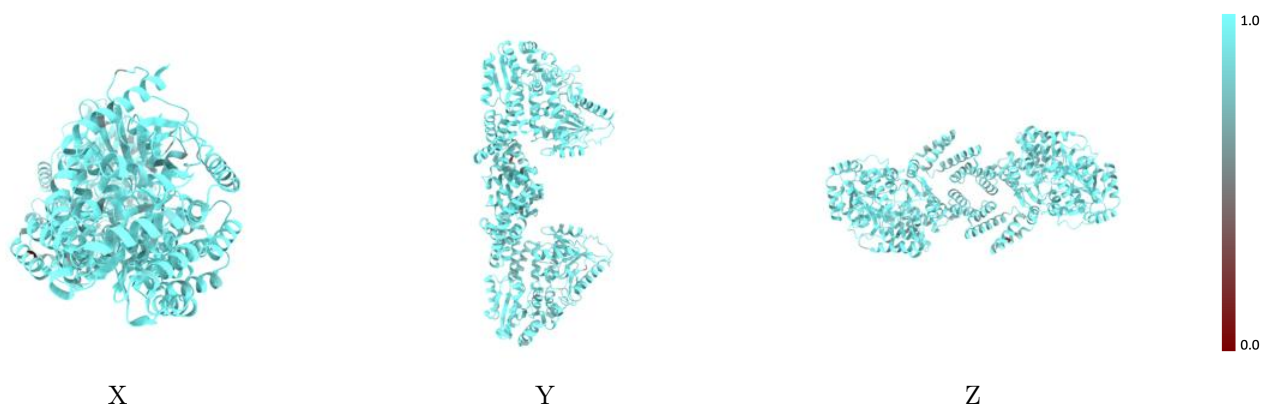
The images above show the 3D surface view of the map at the recommended contour level 5.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



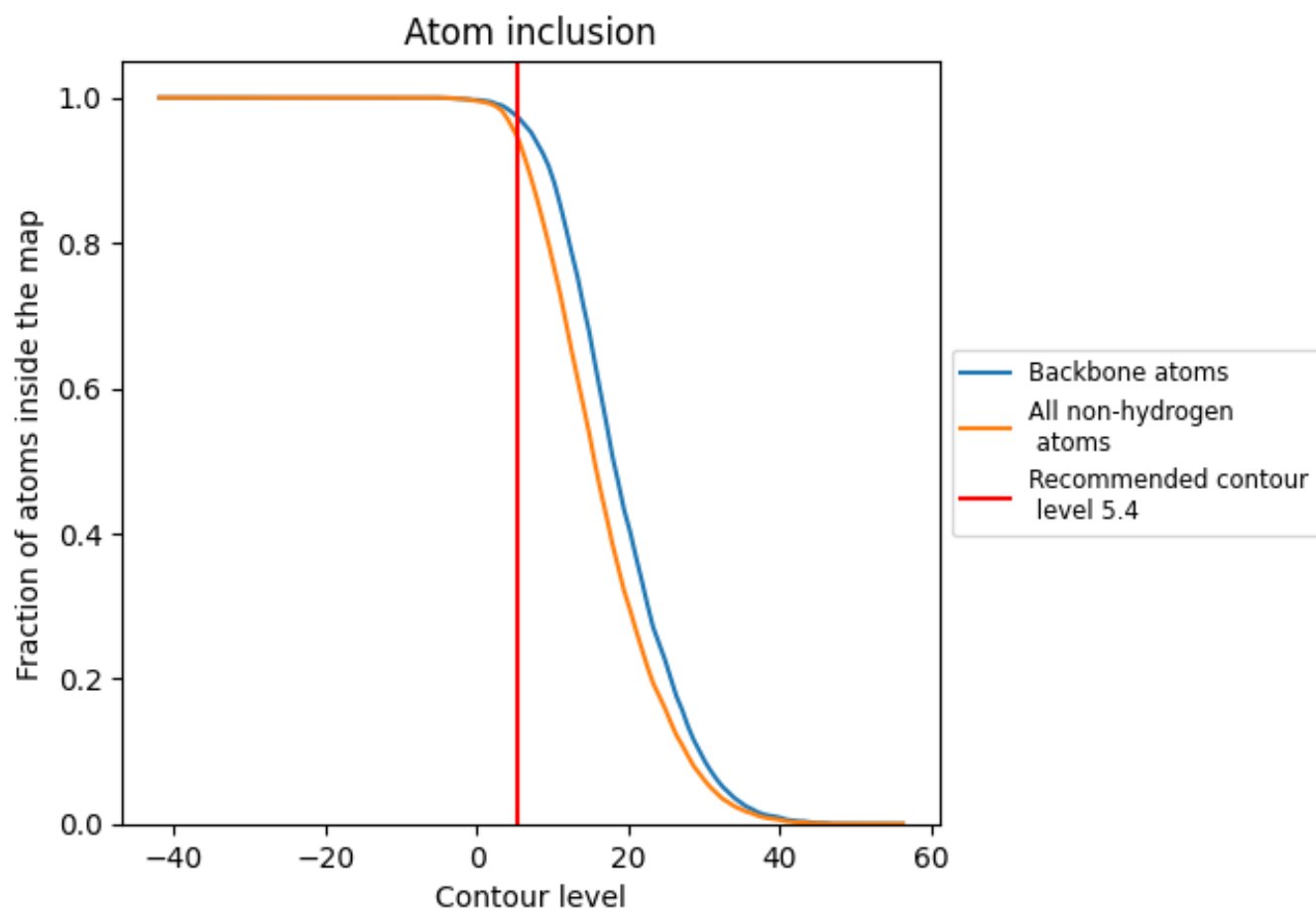
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.4).







9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (5.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.4120
A	 0.9352	 0.4020
B	 0.9549	 0.4210

