



wwPDB EM Validation Summary Report ⓘ

May 19, 2026 – 10:23 am BST

PDB ID : 8OMA / pdb_00008oma
EMDB ID : EMD-16972
Title : MutSbeta bound to 61bp homoduplex DNA
Authors : Lee, J.-H.; Thomsen, M.; Daub, H.; Steinbacher, S.; Sztyler, A.; Thieulin-Pardo, G.; Neudegger, T.; Plotnikov, N.; Iyer, R.R.; Wilkinson, H.; Monteagudo, E.; Felsenfeld, D.P.; Haque, T.; Finley, M.; Dominguez, C.; Vogt, T.F.; Prasad, B.C.
Deposited on : 2023-03-31
Resolution : 3.29 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 : 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) : 2.49

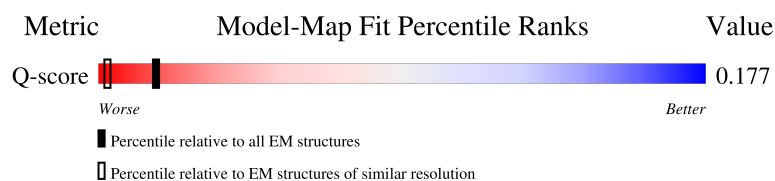
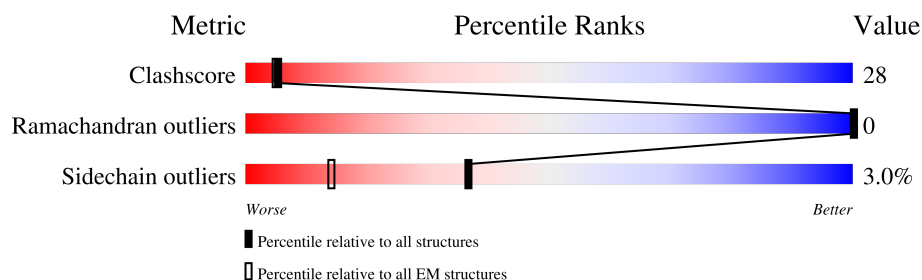
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

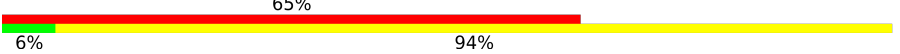
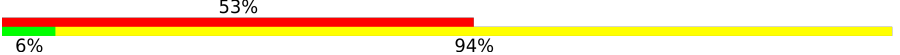
The reported resolution of this entry is 3.29 Å.

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	14466 (2.79 - 3.79)

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	C	17	
2	D	17	
3	A	934	

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Mol	Chain	Length	Quality of chain
4	B	1137	27%23%49%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11379 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 DNA chain called DNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	17	Total	C	N	O	P	0	0
			351	167	64	103	17		

- Molecule 2 is a DNA chain called DNA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	17	Total	C	N	O	P	0	0
			346	165	63	101	17		

- Molecule 3 is a protein called DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	760	Total	C	N	O	S	0	0
			5990	3790	1017	1151	32		

- Molecule 4 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	577	Total	C	N	O	S	0	0
			4629	2957	798	854	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	949	ARG	GLN	variant	UNP P20585

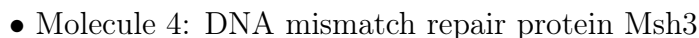
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total Mg 1 1	0



E1094	G1095	M1098	T1099	K1102	R1103	L1104	K1105	Y1106	F1107	A1108	K1109	M1113	H1114	N1115	A1116	Q1117	D1118	L1119	Q1120	ALA	K1121	ALA	GLU	GLN	E1124	GLU	PHE	ASN	MET	GLU	GLU	THR	GLN	THR	SER	LEU	LEU	HIS																		
P1013	V1014	C1015	E1016	L1017	E1018	Q1024	N1027	Y1028	H1029	M1030	V1034	S1035	GLU	ASP	GLU	GLU	SER	LVS	LEU	ASP	PRO	GLY	GLY	ALA	ALA	GLU	GLN	PRO	D1051	F1055	L1056	GLU	Y1057	T1060	R1061	G1062	I1063	S1067	I1068	G1069	L1070	N1071	V1072	K1073	A1074	L1075	V1078	I1082	S1090	K1091	E1092	L1093				
Q947	G948	R949	S950	T951	F952	N953	E954	E955	L956	T957	D958	T959	A960	E961	T962	L963	R964	K965	A966	T967	Q968	S969	S970	L971	V972	L973	L974	D975	E976	R979	G980	T981	S982	T983	H984	D985	G986	I987	A988	T989	A990	Y991	A992	T993	L994	F997	S1003	L1004	T1005	L1006	F1007	V1008	T1009	H1010	N1011	P1012
Q874	D875	Q876	Y877	V878	P879	N880	N881	T882	D883	E889	R890	V891	M892	T893	I894	T895	G896	P897	N898	M899	K902	S903	Y905	I906	K907	Q908	L911	I912	T913	I914	Q917	I918	G919	S920	Y921	V922	P923	T928	I929	V932	I935	F936	T937	R938	A941	A942	D943	N944	I945	Y946						
F780	H781	S782	P783	F784	I785	V786	Y789	R790	N793	Q794	L795	R796	E797	D802	E806	F810	I811	E812	K813	H817	Y818	V825	L828	D832	F835	K839	V840	A841	R848	P849	R855	K856	I857	V858	I859	G862	R863	H864	P865	V866	I867	D868	V869	L870												
L706	F709	I712	K713	K716	D717	E718	I719	Q720	G721	V722	I723	D724	E725	I726	R727	M728	H729	L730	Q731	E732	I733	R734	K735	I736	L737	A742	Q743	Y744	V747	Q750	E751	F752	M753	I754	E755	I756	V761	S762	C763	I764	P765	T766	D767	W768	V769	K770	V771	G772	S773	T774	R779					
I621	L625	C626	S627	I628	Y629	H630	C633	E637	F638	F639	L640	I641	V642	K643	H647	L648	E651	F652	I656	P657	I663	Q664	S665	D666	T670	P676	E677	L678	L679	V682	E683	H684	Y685	L686	K687	I688	L689	M690	E691	Q692	A693	A694	K695	V696	G697	D698	K704	D705								
T541	L542	R543	E546	I547	L548	Q549	N550	Q551	T552	D553	M554	K555	T556	K557	G558	S559	L560	V563	L564	D565	H566	T567	F571	L576	K577	T581	Q582	P583	L584	L587	I590	R593	L594	D595	A596	V600	L601	H602	S603	GLU	S605	F608	E612	L615	L618											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.168	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	292.544, 292.544, 292.544	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9142, 0.9142, 0.9142	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: ATP, MG

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	C	0.33	0/393	0.64	0/605
2	D	0.31	0/387	0.63	0/594
3	A	0.49	0/6075	0.90	0/8184
4	B	0.52	0/4717	0.90	0/6369
All	All	0.49	0/11572	0.88	0/15752

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	938	ARG	Sidechain

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	C	351	0	193	27	0
2	D	346	0	192	25	0
3	A	5990	0	6061	366	0
4	B	4629	0	4714	290	0
5	A	31	0	12	5	0
5	B	31	0	12	5	0
6	B	1	0	0	0	0
All	All	11379	0	11184	637	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 28.

The worst 5 of 637 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)
4:B:938:ARG:HD3	4:B:958:ASP:HB2	1.30	1.12
4:B:938:ARG:CD	4:B:958:ASP:HB2	1.82	1.09
3:A:167:ASP:O	3:A:171:ARG:HA	1.61	1.00
4:B:615:LEU:HD11	4:B:828:LEU:HD21	1.43	0.98
4:B:590:ILE:HD11	4:B:917:GLN:HA	1.51	0.92

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	
3	A	750/934 (80%)	698 (93%)	52 (7%)	0	100	100
4	B	571/1137 (50%)	519 (91%)	52 (9%)	0	100	100
All	All	1321/2071 (64%)	1217 (92%)	104 (8%)	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	
3	A	665/808 (82%)	646 (97%)	19 (3%)	37	62
4	B	515/998 (52%)	499 (97%)	16 (3%)	35	60
All	All	1180/1806 (65%)	1145 (97%)	35 (3%)	37	61

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	866	VAL
4	B	895	THR
4	B	1027	ASN
3	A	663	MET
3	A	644	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	864	HIS
4	B	874	GLN
4	B	1058	GLN
4	B	908	GLN
4	B	1027	ASN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	ATP	A	2000	-	29,33,33	0.61	0	44,52,52	0.46	0
5	ATP	B	2000	6	29,33,33	0.53	0	44,52,52	0.53	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
5	ATP	A	2000	-	-	1/22/38/38	0/3/3/3
5	ATP	B	2000	6	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

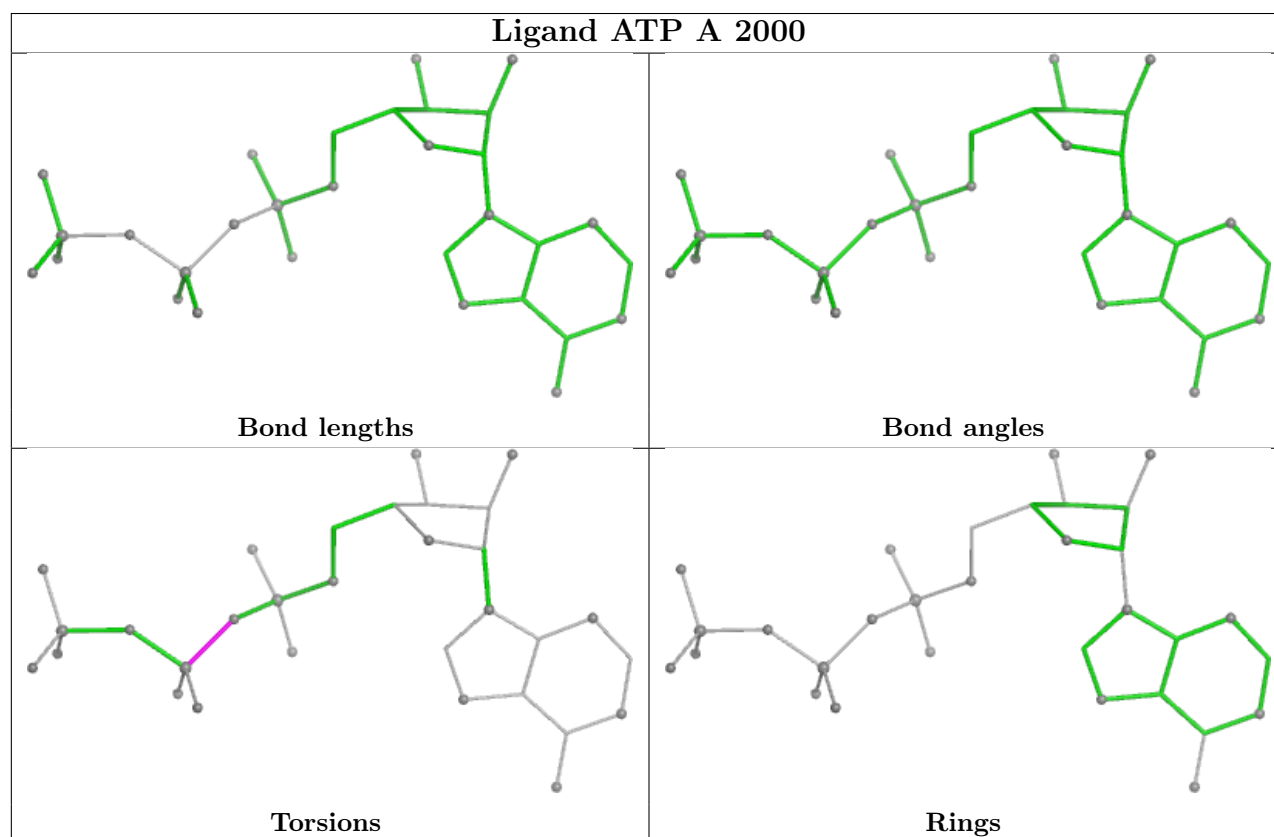
Mol	Chain	Res	Type	Atoms
5	B	2000	ATP	C5'-O5'-PA-O3A
5	B	2000	ATP	C3'-C4'-C5'-O5'
5	B	2000	ATP	O4'-C4'-C5'-O5'
5	B	2000	ATP	C5'-O5'-PA-O1A
5	A	2000	ATP	PA-O3A-PB-O2B

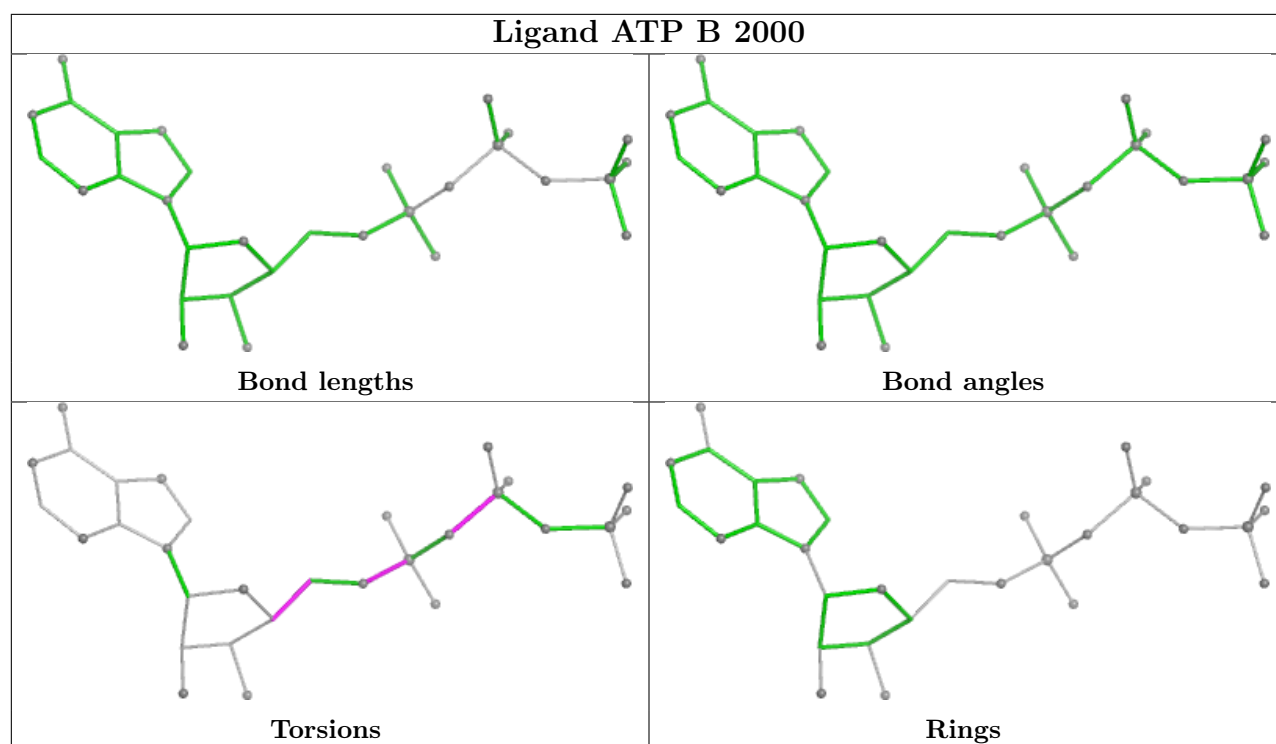
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2000	ATP	5	0
5	B	2000	ATP	5	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-16972. These allow visual inspection of the internal detail of the map and identification of artifacts.

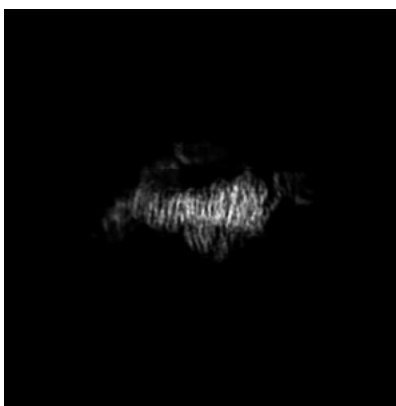
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

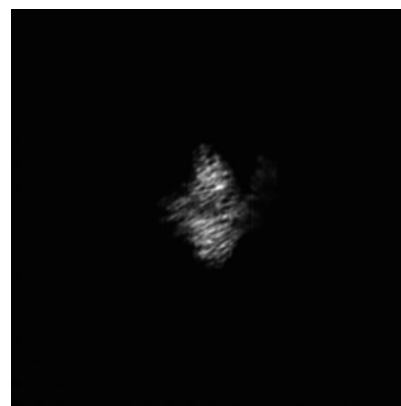
6.1.1 Primary map



X

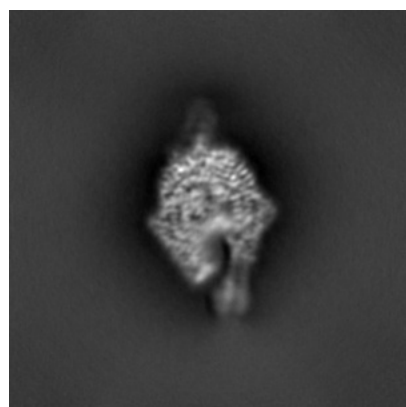


Y

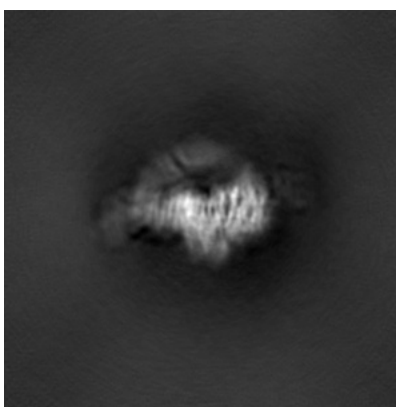


Z

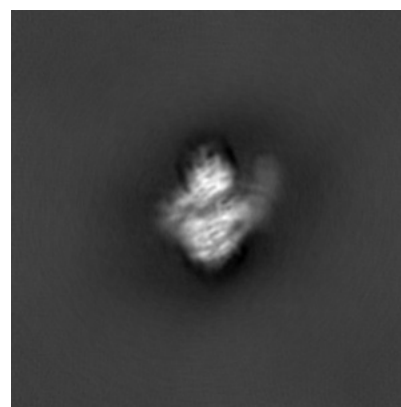
6.1.2 Raw map



X



Y

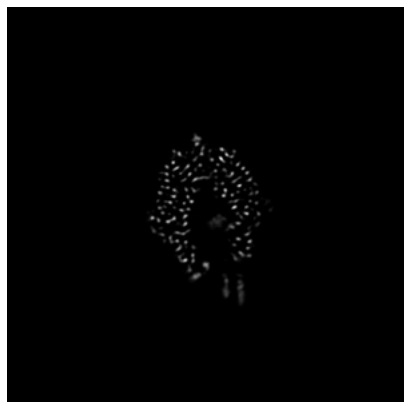


Z

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

6.2 Central slices [i](#)

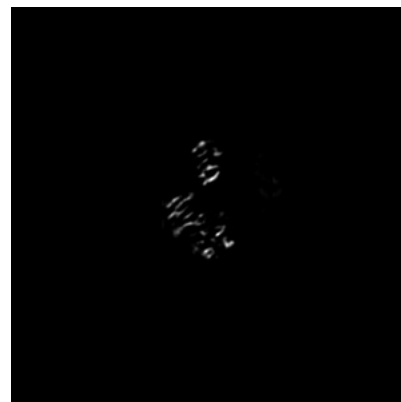
6.2.1 Primary map



X Index: 160

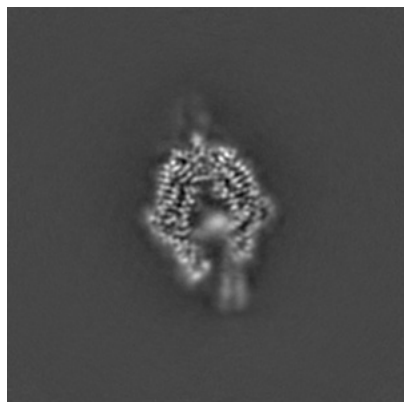


Y Index: 160

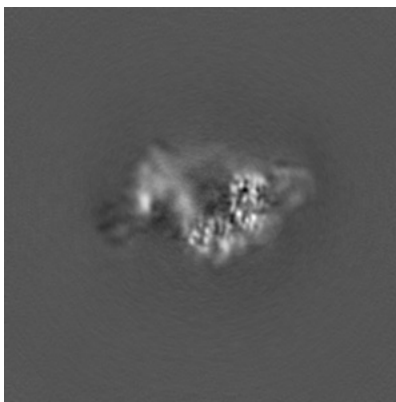


Z Index: 160

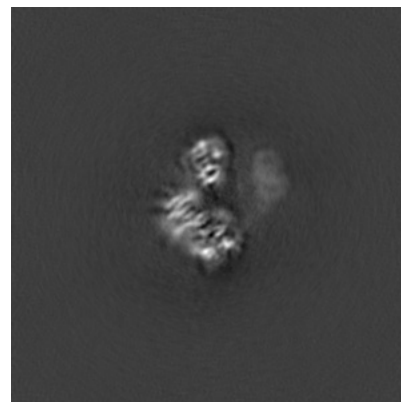
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 155

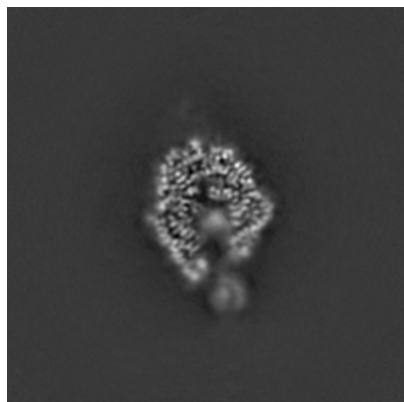


Y Index: 154

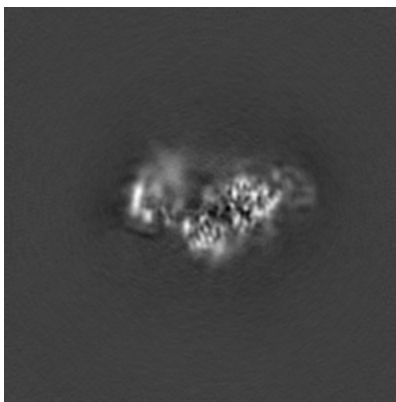


Z Index: 173

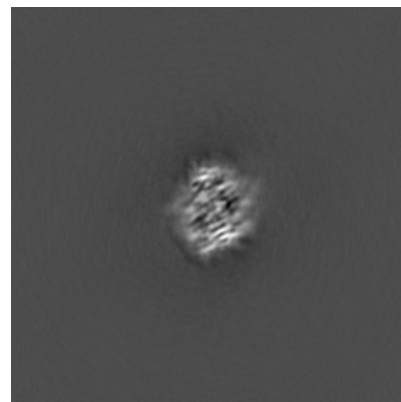
6.3.2 Raw map



X Index: 155



Y Index: 153



Z Index: 192

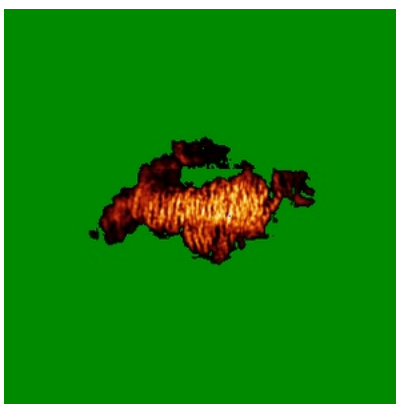
The images above show the largest variance slices of the map in three orthogonal directions.

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

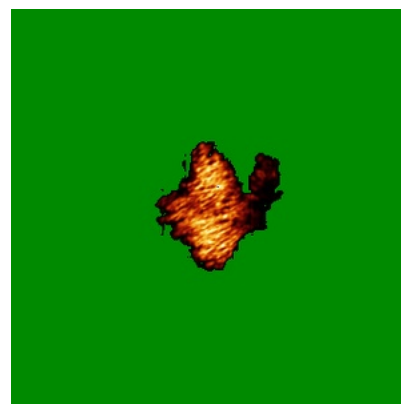
6.4.1 Primary map



X

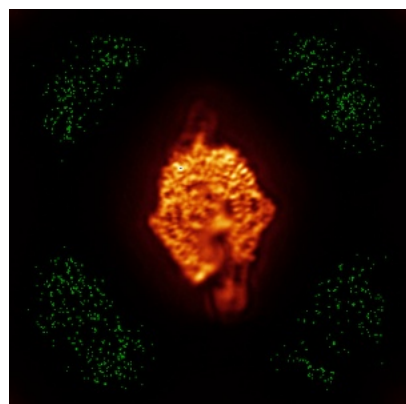


Y

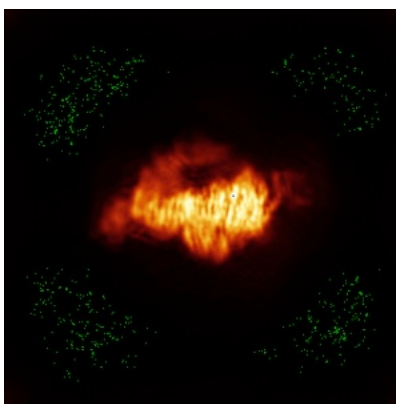


Z

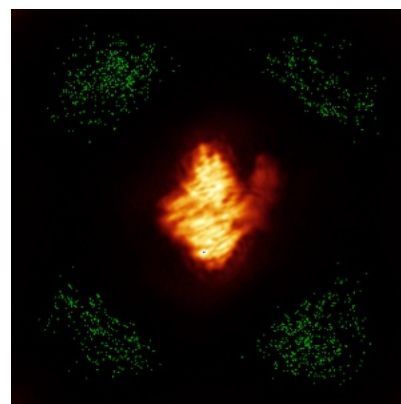
6.4.2 Raw map



X



Y

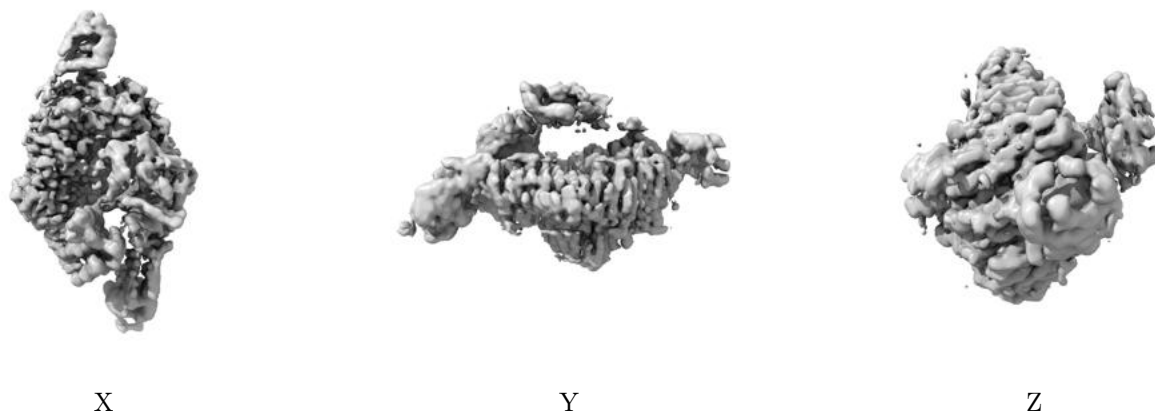


Z

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 0.01. 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.

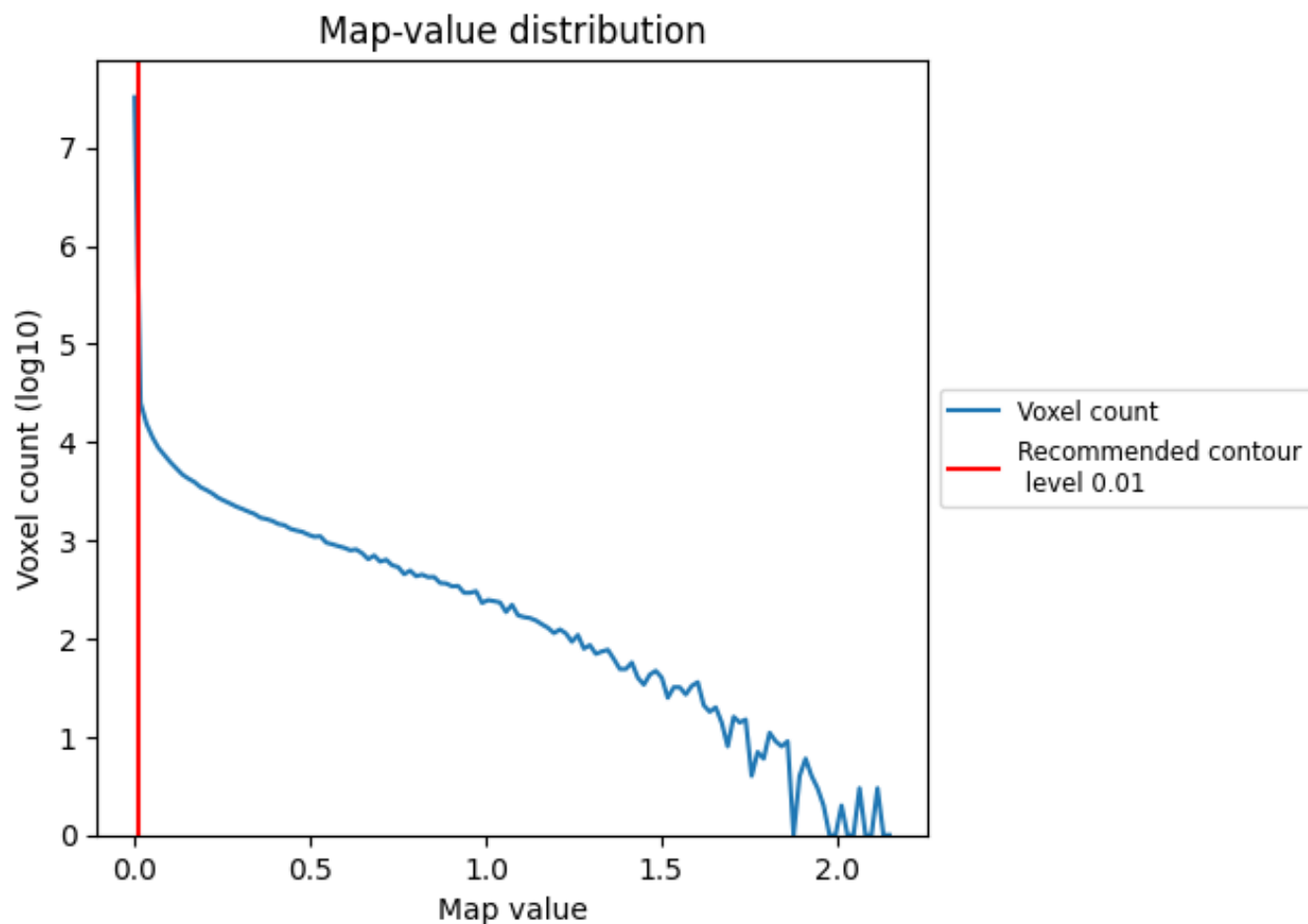
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

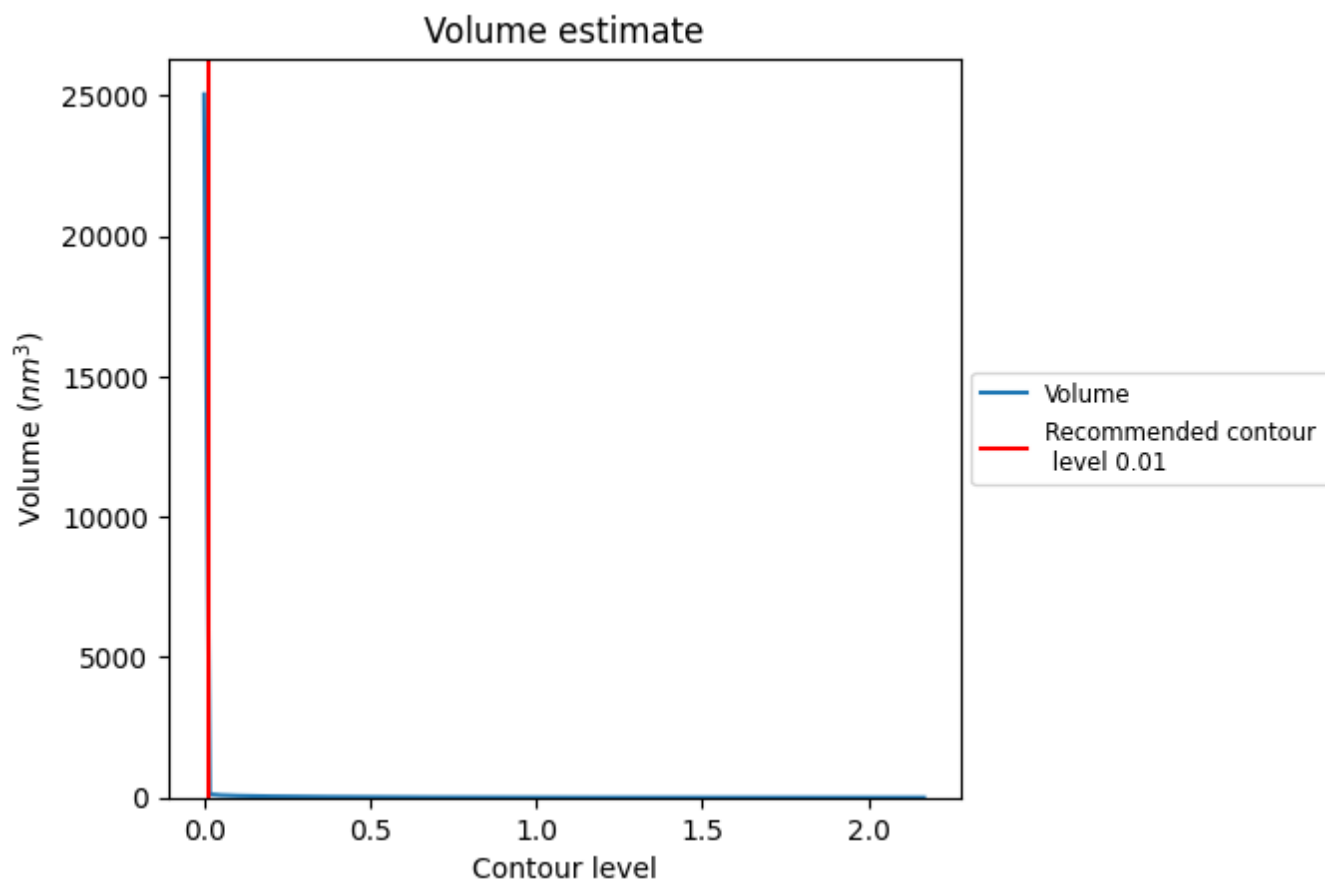
This section contains the results of statistical analysis of the map.

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.

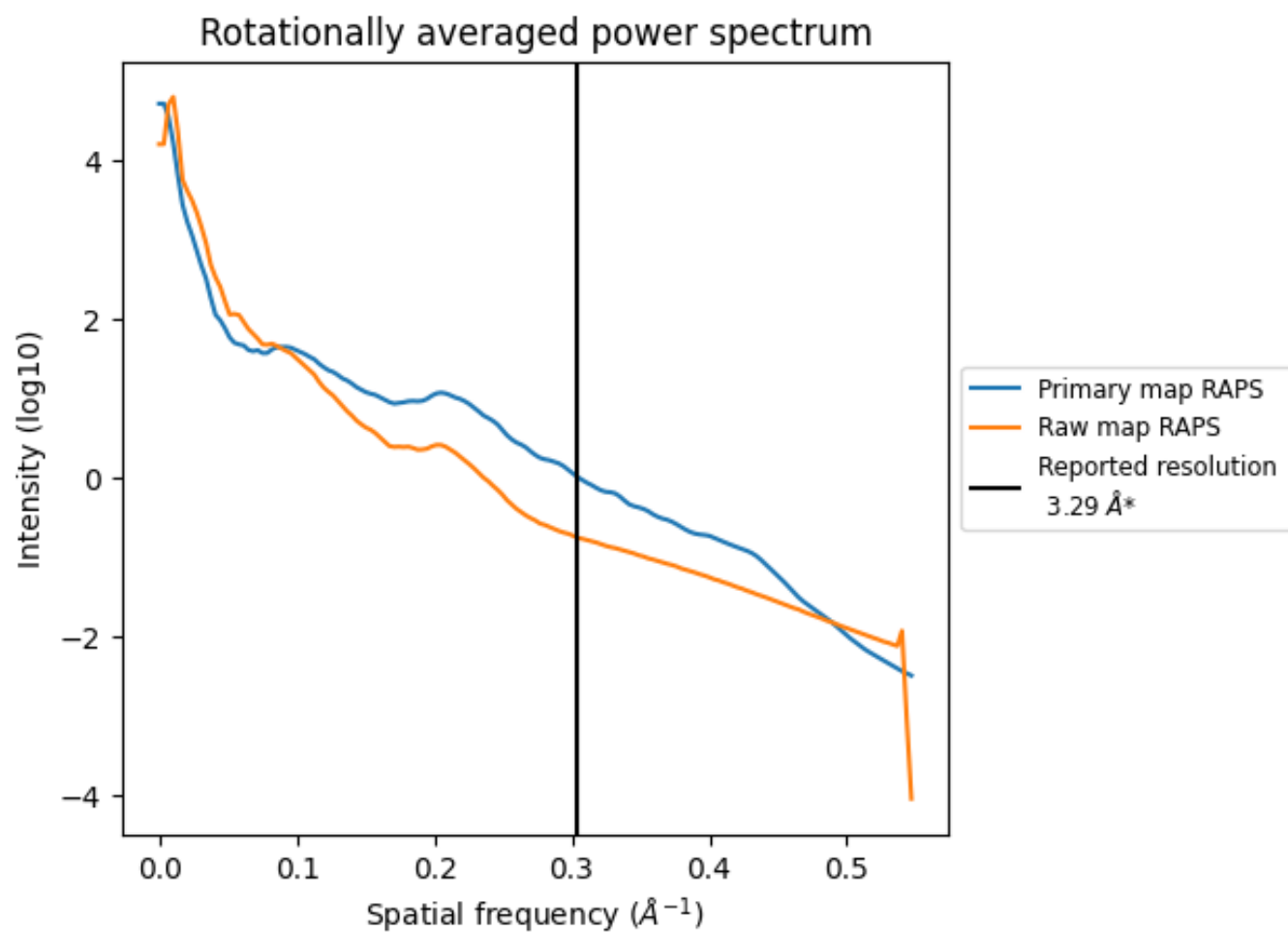
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7732 nm³; this corresponds to an approximate mass of 6985 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 ⓘ

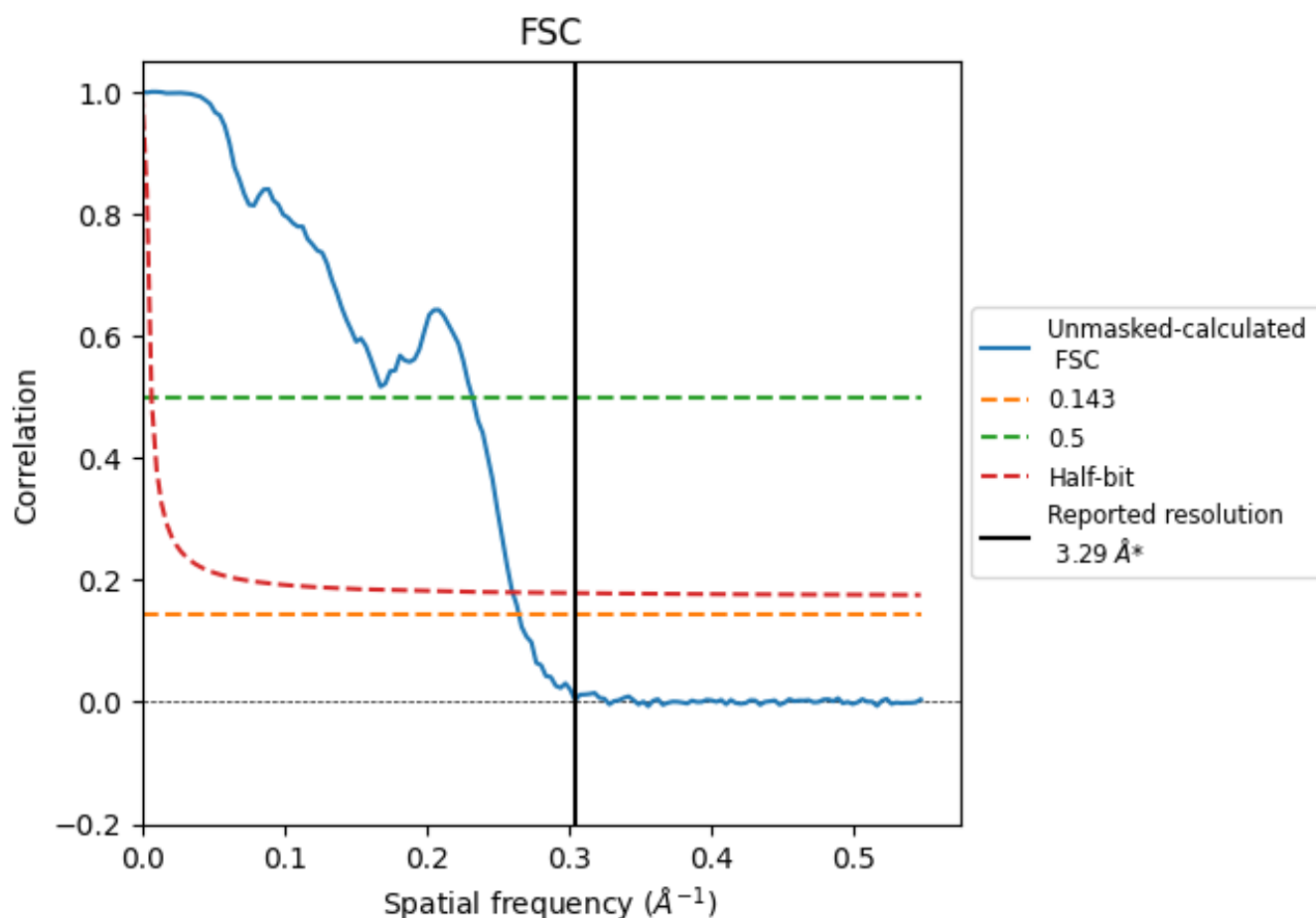


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

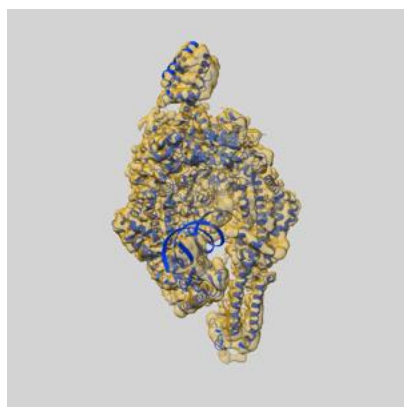
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	4.31	3.84

*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 3.78 differs from the reported value 3.29 by more than 10 %

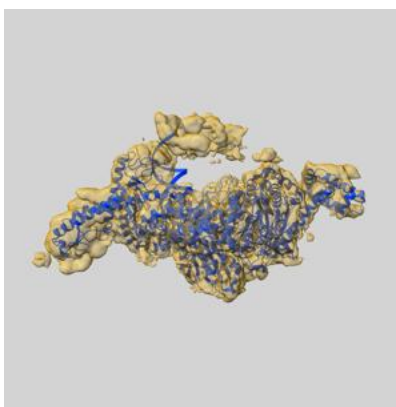
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16972 and PDB model 8OMA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

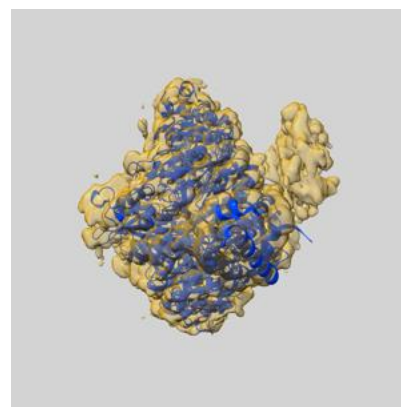
9.1 Map-model overlay [i](#)



X



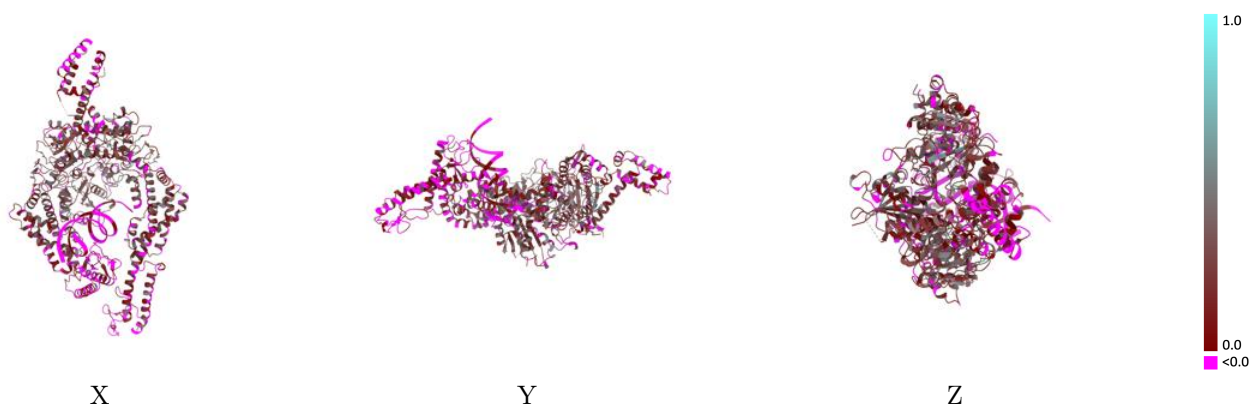
Y



Z

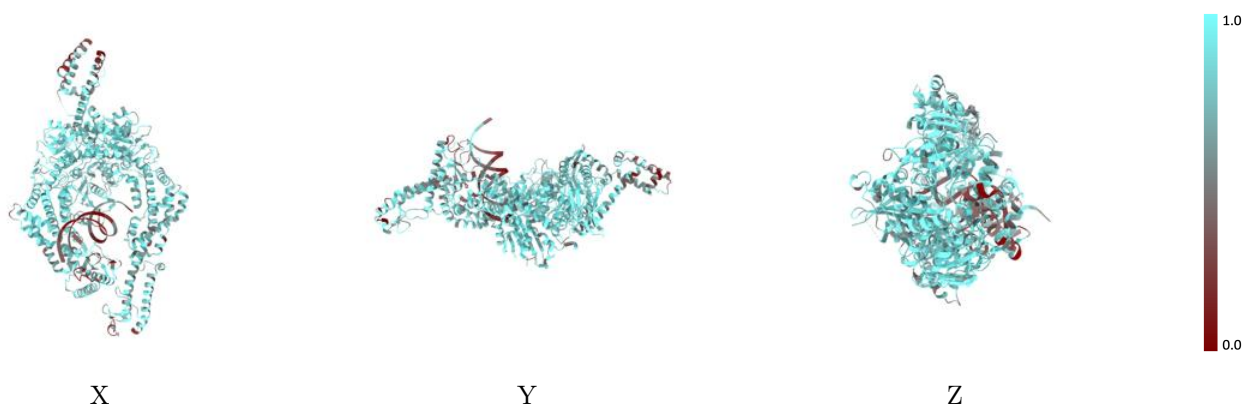
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



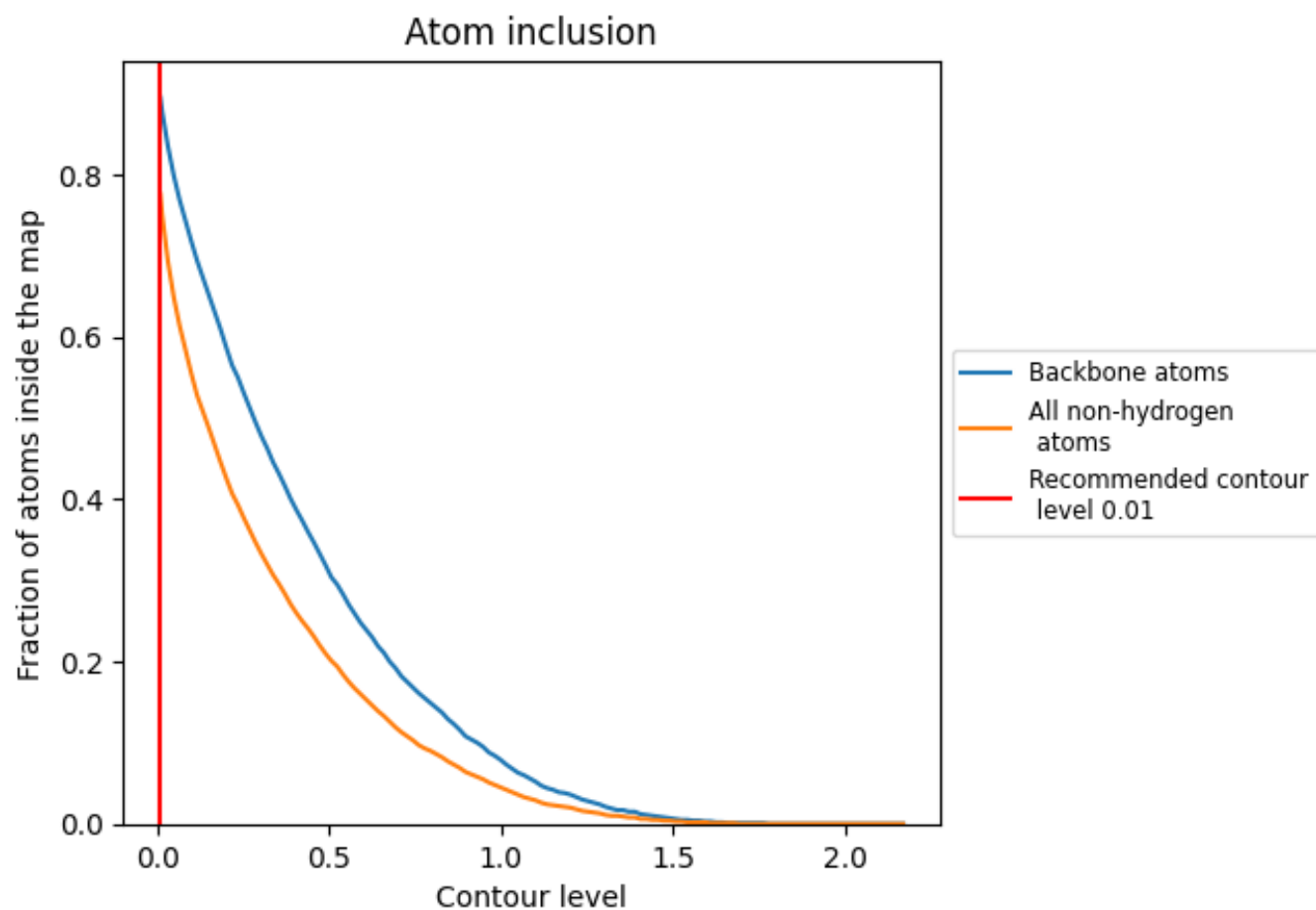
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.1770
A	0.8050	0.1890
B	0.8030	0.1970
C	0.3130	-0.0560
D	0.3840	-0.0580

