



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:09 pm BST

PDB ID : 6S6V / pdb_00006s6v
EMDB ID : EMD-10107
Title : Resting state of the E. coli Mre11-Rad50 (SbcCD) head complex bound to ATPgS
Authors : Kaeshammer, L.; Saathoff, J.H.; Gut, F.; Bartho, J.; Alt, A.; Kessler, B.; Lammens, K.; Hopfner, K.P.
Deposited on : 2019-07-03
Resolution : 3.50 Å (reported)
Based on initial models : 4M0V, 3QF7

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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

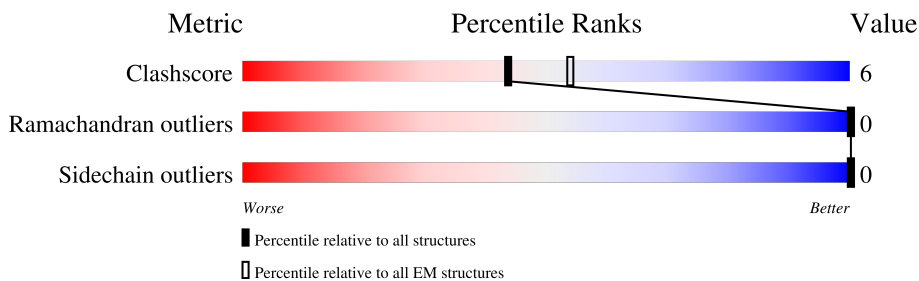
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	407	
1	B	407	
2	C	1048	
2	D	1048	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11820 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 Nuclease SbcCD subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	386	Total	C	N	O	S	0	0
			3047	1921	542	575	9		
1	B	385	Total	C	N	O	S	0	0
			3041	1918	540	574	9		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	GLY	-	expression tag	UNP C3TMC7
A	402	HIS	-	expression tag	UNP C3TMC7
A	403	HIS	-	expression tag	UNP C3TMC7
A	404	HIS	-	expression tag	UNP C3TMC7
A	405	HIS	-	expression tag	UNP C3TMC7
A	406	HIS	-	expression tag	UNP C3TMC7
A	407	HIS	-	expression tag	UNP C3TMC7
B	401	GLY	-	expression tag	UNP C3TMC7
B	402	HIS	-	expression tag	UNP C3TMC7
B	403	HIS	-	expression tag	UNP C3TMC7
B	404	HIS	-	expression tag	UNP C3TMC7
B	405	HIS	-	expression tag	UNP C3TMC7
B	406	HIS	-	expression tag	UNP C3TMC7
B	407	HIS	-	expression tag	UNP C3TMC7

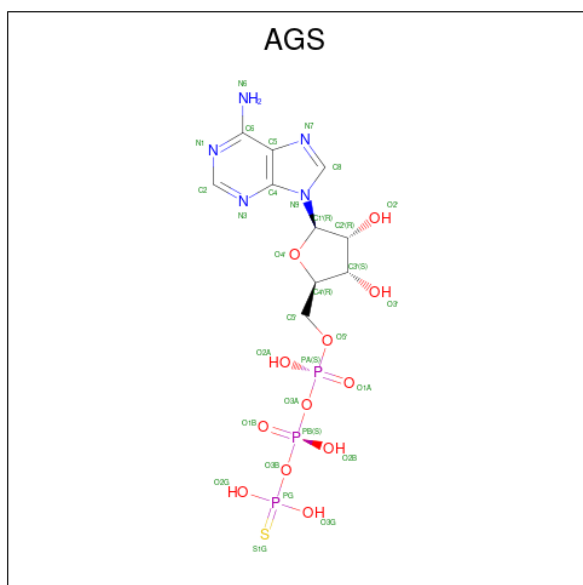
- Molecule 2 is a protein called Nuclease SbcCD subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	364	Total	C	N	O	S	0	0
			2836	1789	494	545	8		
2	D	363	Total	C	N	O	S	0	0
			2828	1785	493	542	8		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mn	0
			2	2	
3	B	2	Total	Mn	0
			2	2	

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

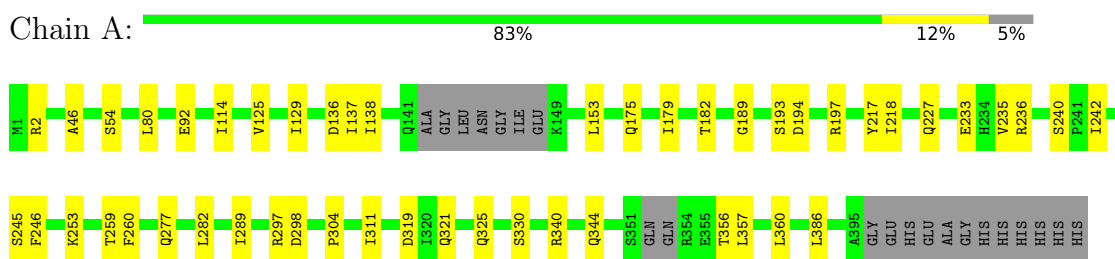
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

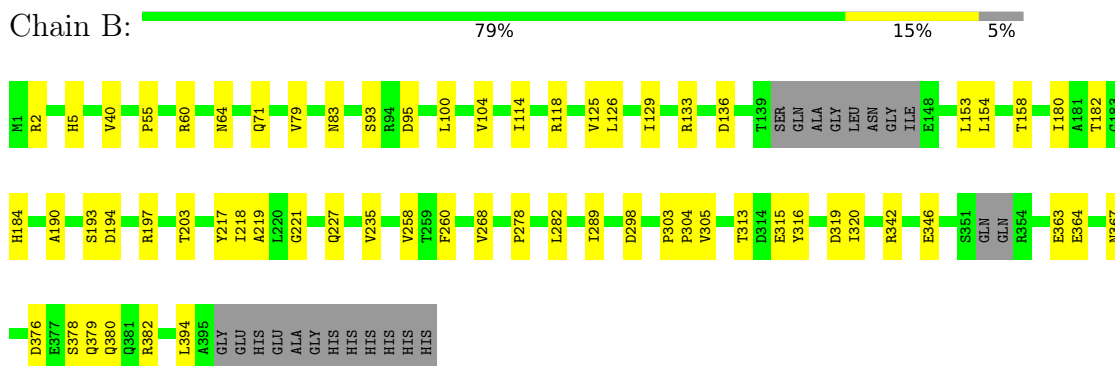
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

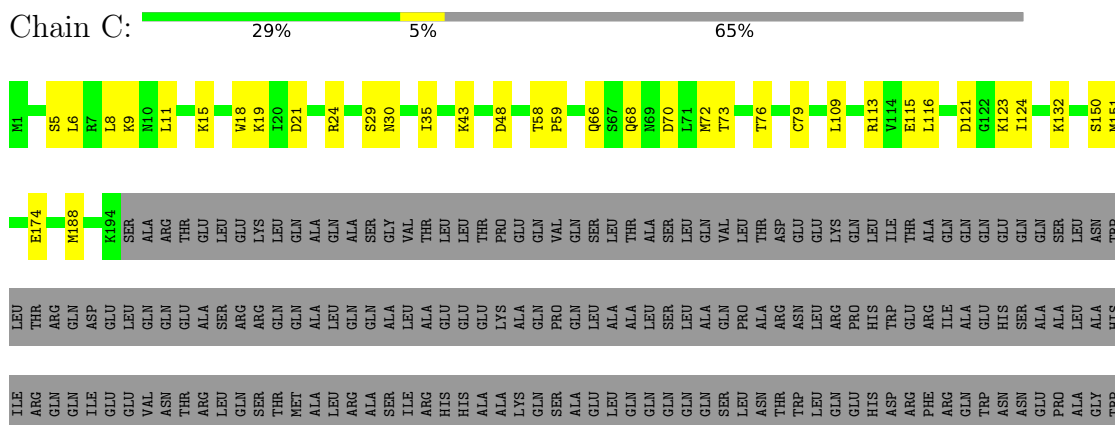
• Molecule 1: Nuclease SbcCD subunit D



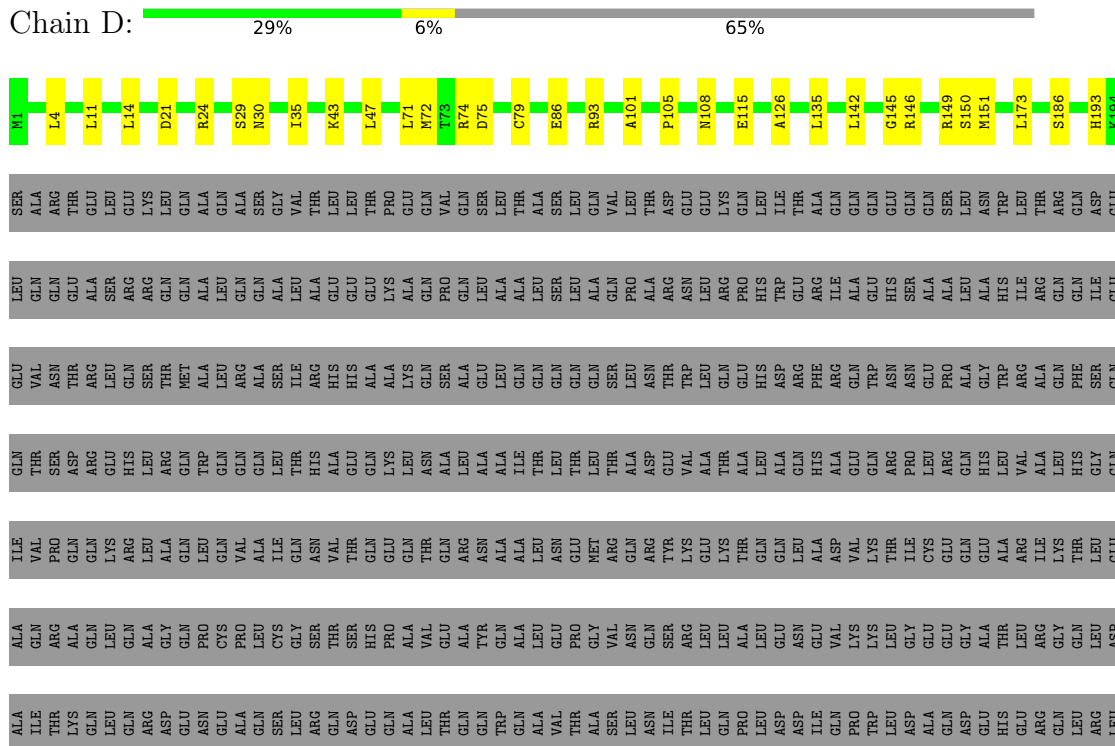
• Molecule 1: Nuclease SbcCD subunit D



• Molecule 2: Nuclease SbcCD subunit C



- Molecule 2: Nuclease SbcCD subunit C



I1033	GLN ASP	GLN ALA	THR LEU	GLN SER
Y1038	ASP ASN	THR LEU	GLN GLN	TRP ARG
K1040	ARG GLN	VAL THR	VAL GLN	GLN HIS
E1042	GLN GLN	THR ALA	ALA GLN	LEU GLN
F1045	GLN THR	ALA GLU	ALA GLN	GLY ILE
K1048	MET GLN	THR ALA	SER LEU	ALA HIS
	GLN ILE	GLN HIS	LYS ALA	ASN GLN
	ALA GLN	GLN ARG	ALA PHE	GLN ILE
	MET THR	HIS ARG	GLN PHE	ILE GLN
	GLN VAL	PRO ASP	THR ALA	TYP GLN
	GLN GLU	ASP GLY	THR LEU	GLN GLN
	ASP W880	LEU LEU	GLN SER	ILE GLU
	S889	THR VAL	PHE ASP	ARG GLN
	L904	THR VAL	ASP ASP	GLN SER
	V908	GLU GLN	GLN GLN	LEU GLU
N912	ILE GLN	ILE GLN	ALA PHE	THR HIS
D947	GLN GLU	GLN LEU	LEU ALA	CYS THR
V971	S972	LEU ALA	LEU MET	GLU VAL
R976	R976	GLN THR	ASP GLU	VAL LEU
F981	F981	HIS GLN	GLU THR	THR LEU
G985	G985	LYS LEU	THR LEU	ASN GLN
T988	T988	ARG GLU	THR LEU	TRP GLN
D995	D995	ASN THR	GLN GLU	ASP GLU
T996	T996	GLN THR	VAL HIS	GLU GLU
D999	D999	SER SER	GLN CYS	GLU SER
		GLY GLN	LYS GLN	TRP THR
I1014	I1014	GLU ILE	ASN LEU	LEU ALA
E1018	E1018	THR ARG	LEU HIS	ALA THR
K1021	K1021	GLN GLN	ASN GLN	ARG GLN
O1027	O1027	LEU TYR	ARG GLN	GLU ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	142229	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 ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: MN, MG, AGS

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	0.41	0/3112	0.54	0/4238
1	B	0.41	0/3106	0.54	0/4230
2	C	0.45	0/2877	0.57	0/3880
2	D	0.46	0/2869	0.60	0/3869
All	All	0.43	0/11964	0.56	0/16217

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	3047	0	3011	32	0
1	B	3041	0	3004	46	0
2	C	2836	0	2871	37	0
2	D	2828	0	2866	39	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	C	31	0	11	2	0
4	D	31	0	11	1	0
5	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	11820	0	11774	147	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 6.

The worst 5 of 147 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:5:HIS:CE1	1:B:219:ALA:HB1	1.71	1.24
1:B:5:HIS:CE1	1:B:219:ALA:CB	2.45	1.00
1:B:5:HIS:NE2	1:B:219:ALA:HB1	1.96	0.80
2:D:1041:LEU:HD12	2:D:1042:GLU:N	1.97	0.78
1:A:125:VAL:O	1:A:179:ILE:HA	1.88	0.72

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	380/407 (93%)	351 (92%)	29 (8%)	0	100	100
1	B	379/407 (93%)	350 (92%)	29 (8%)	0	100	100
2	C	360/1048 (34%)	332 (92%)	28 (8%)	0	100	100
2	D	359/1048 (34%)	330 (92%)	29 (8%)	0	100	100
All	All	1478/2910 (51%)	1363 (92%)	115 (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	
1	A	334/350 (95%)	334 (100%)	0	100	100
1	B	333/350 (95%)	333 (100%)	0	100	100
2	C	304/897 (34%)	304 (100%)	0	100	100
2	D	303/897 (34%)	303 (100%)	0	100	100
All	All	1274/2494 (51%)	1274 (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. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	193	HIS
2	C	69	ASN
1	B	384	GLN
1	B	367	ASN
2	C	56	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 8 ligands modelled in this entry, 6 are 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
4	AGS	C	1101	2,5	26,33,33	0.85	0	26,52,52	0.93	2 (7%)
4	AGS	D	1101	2,5	26,33,33	0.80	0	26,52,52	1.02	2 (7%)

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	AGS	C	1101	2,5	-	6/17/38/38	0/3/3/3
4	AGS	D	1101	2,5	-	7/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1101	AGS	PA-O3A-PB	-2.83	123.11	132.83
4	C	1101	AGS	PA-O3A-PB	-2.37	124.69	132.83
4	C	1101	AGS	C5-C6-N6	2.26	123.79	120.35
4	D	1101	AGS	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1101	AGS	PB-O3B-PG-O2G
4	D	1101	AGS	PB-O3B-PG-O3G
4	D	1101	AGS	C5'-O5'-PA-O1A
4	D	1101	AGS	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

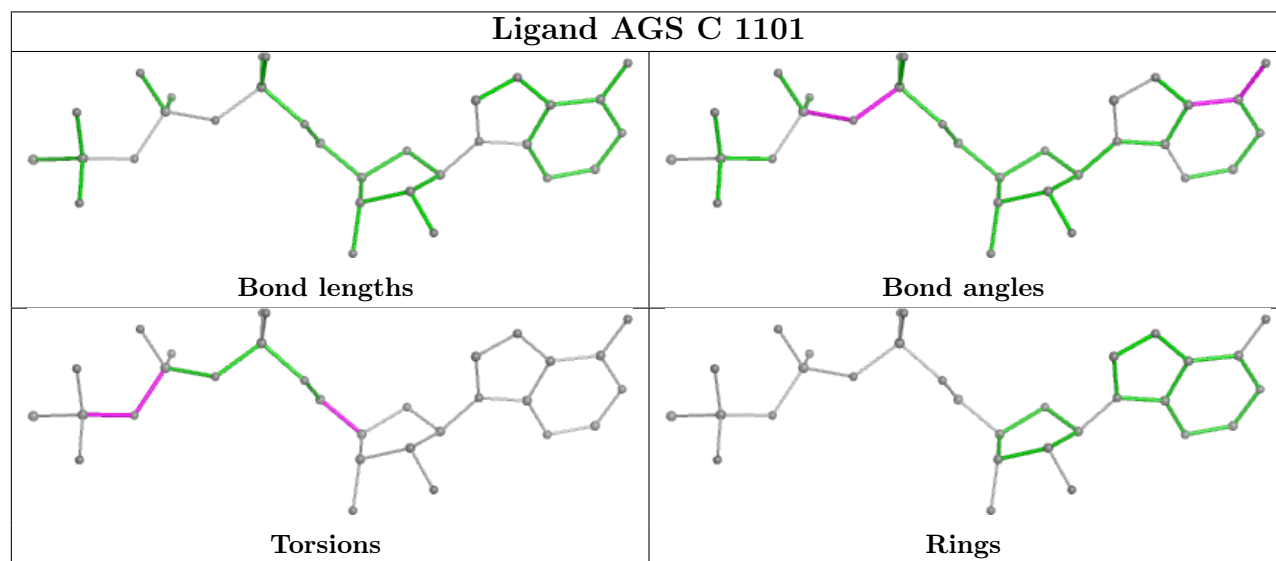
Mol	Chain	Res	Type	Atoms
4	D	1101	AGS	C3'-C4'-C5'-O5'

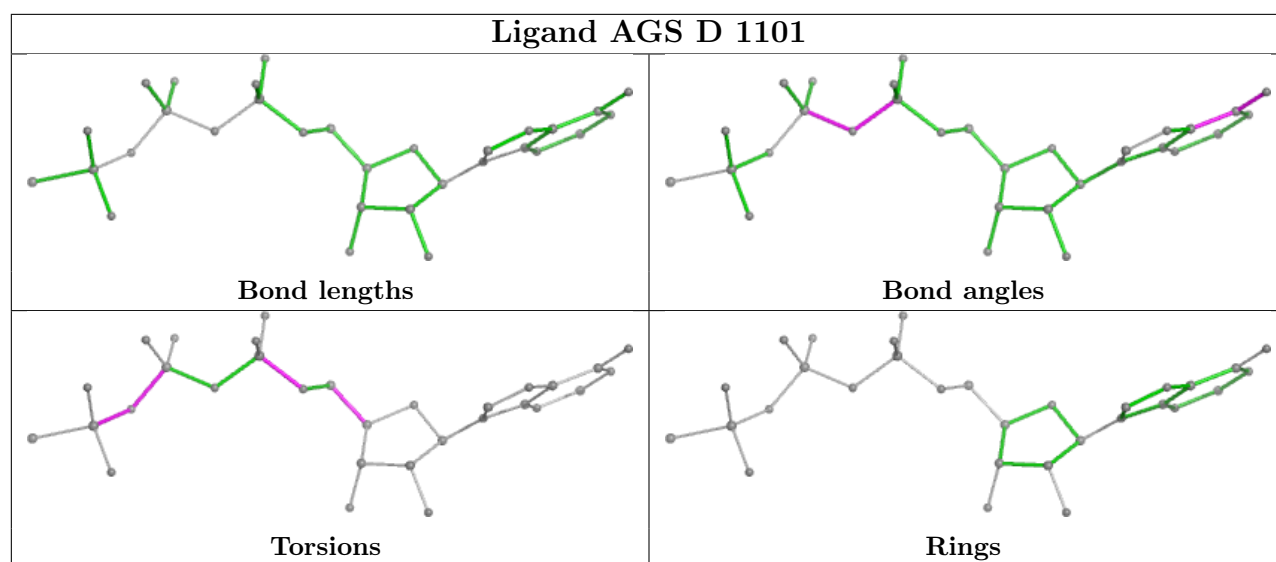
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1101	AGS	2	0
4	D	1101	AGS	1	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.

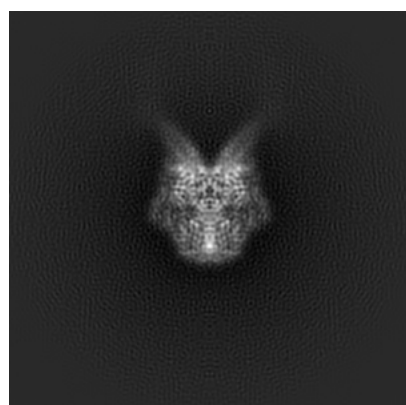
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10107. These allow visual inspection of the internal detail of the map and identification of artifacts.

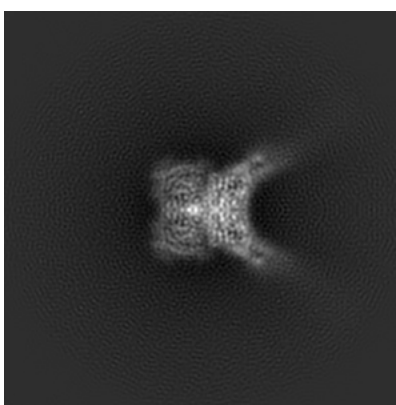
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

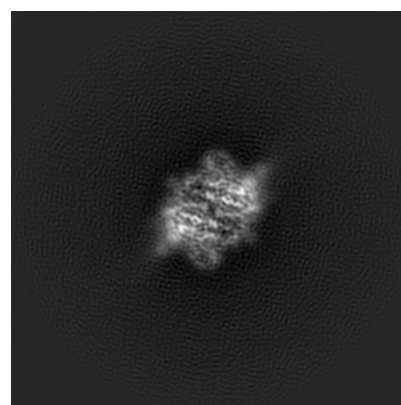
6.1.1 Primary map



X



Y

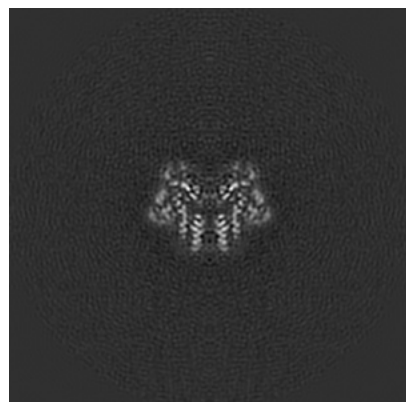


Z

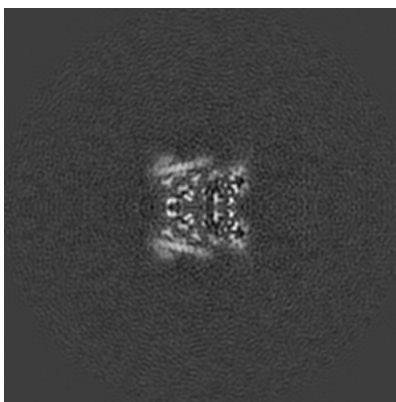
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

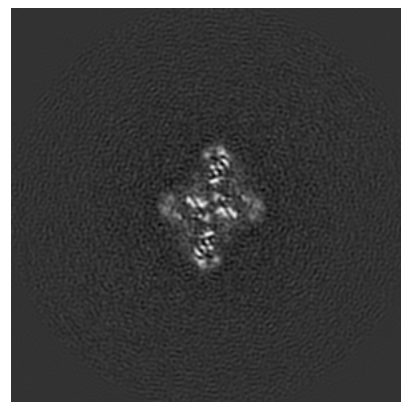
6.2.1 Primary map



X Index: 150



Y Index: 150

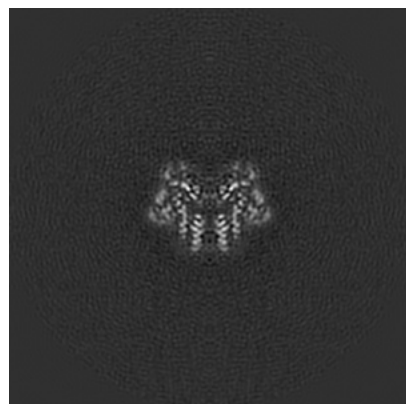


Z Index: 150

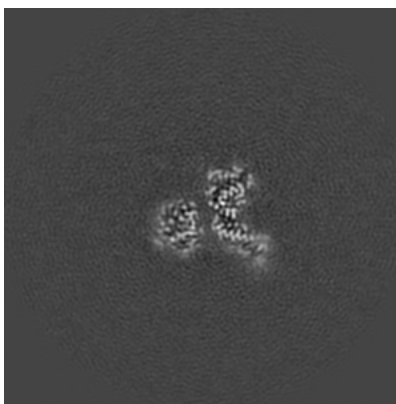
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

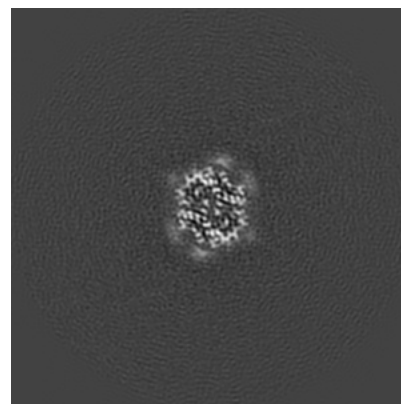
6.3.1 Primary map



X Index: 150



Y Index: 137

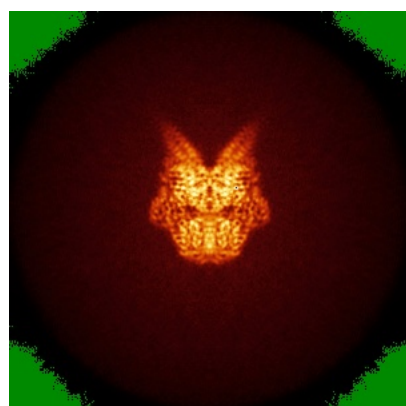


Z Index: 167

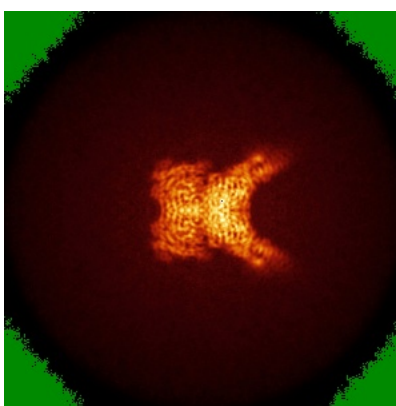
The images above show the largest variance slices of the map in three orthogonal directions.

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

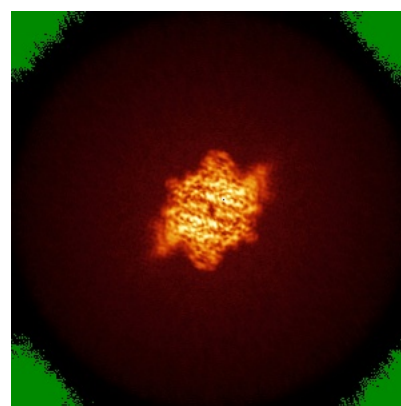
6.4.1 Primary map



X



Y

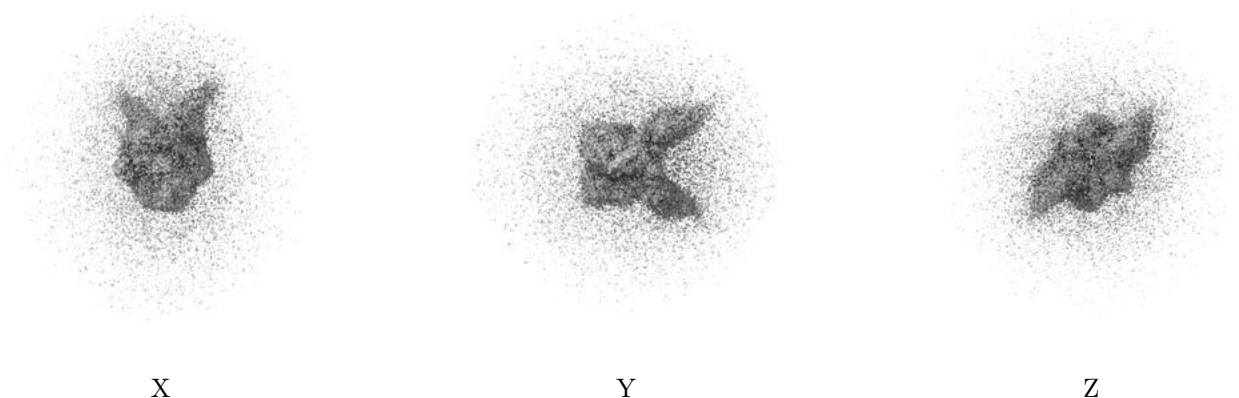


Z

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 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

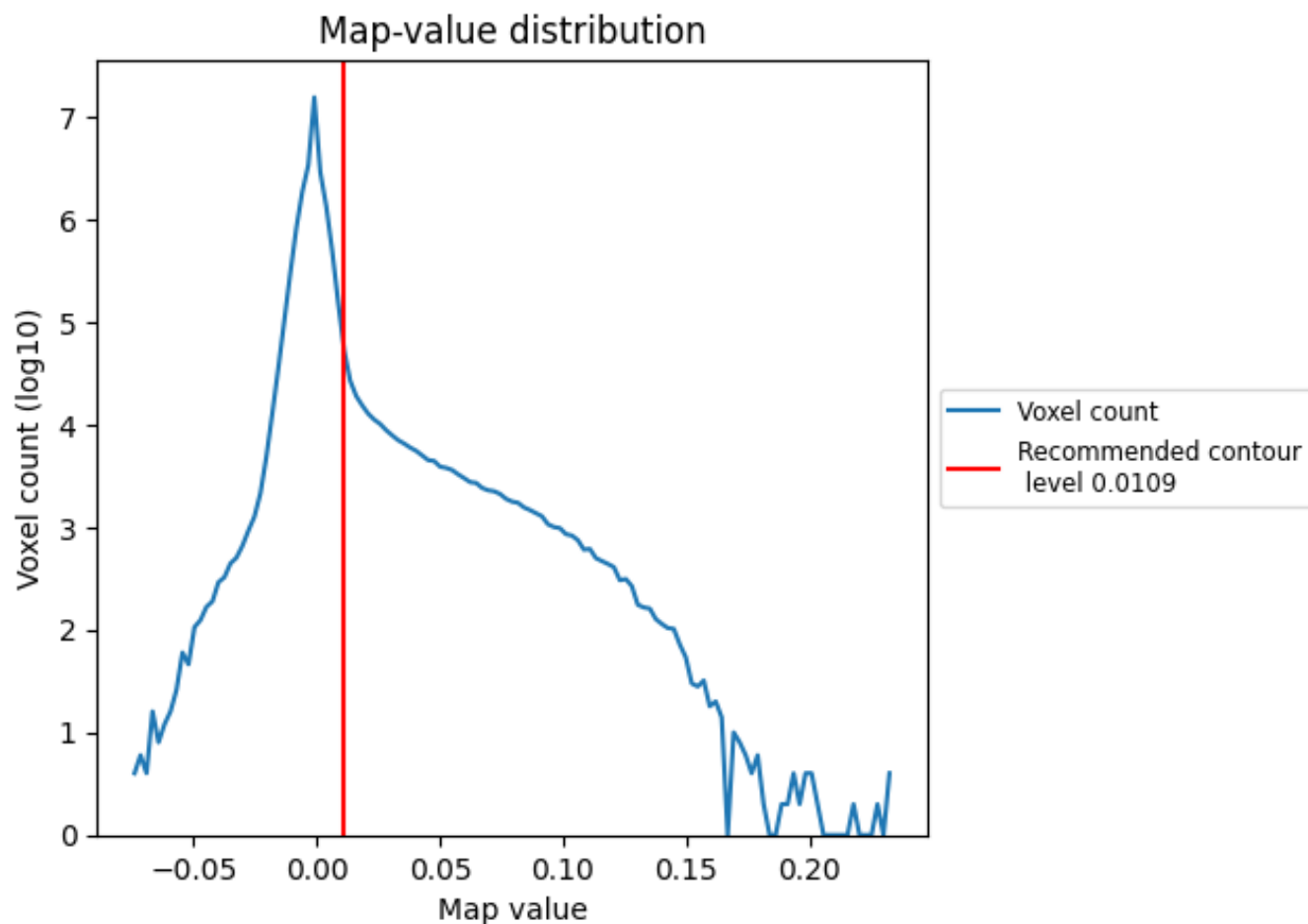
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

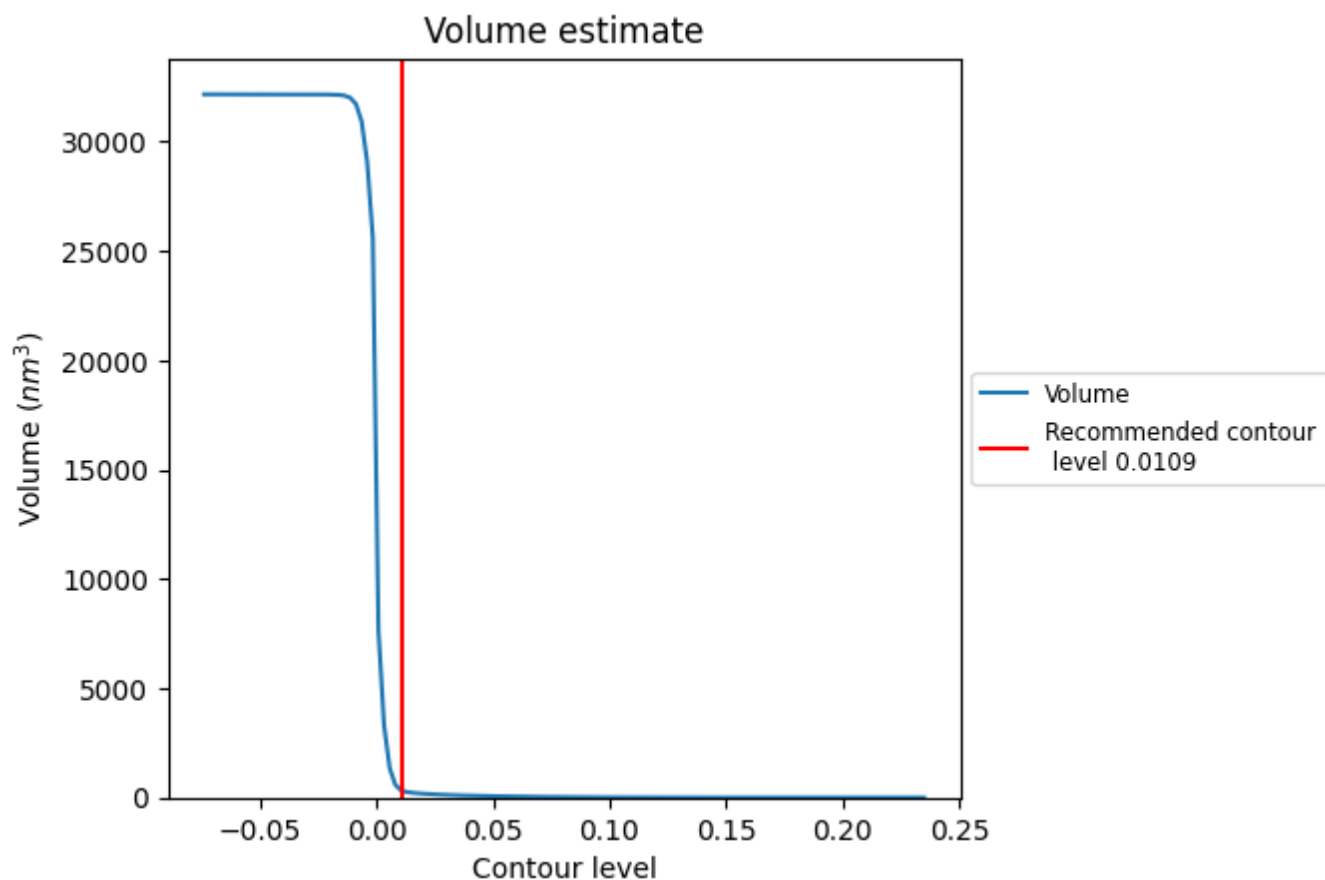
This section contains the results of statistical analysis of the map.

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.

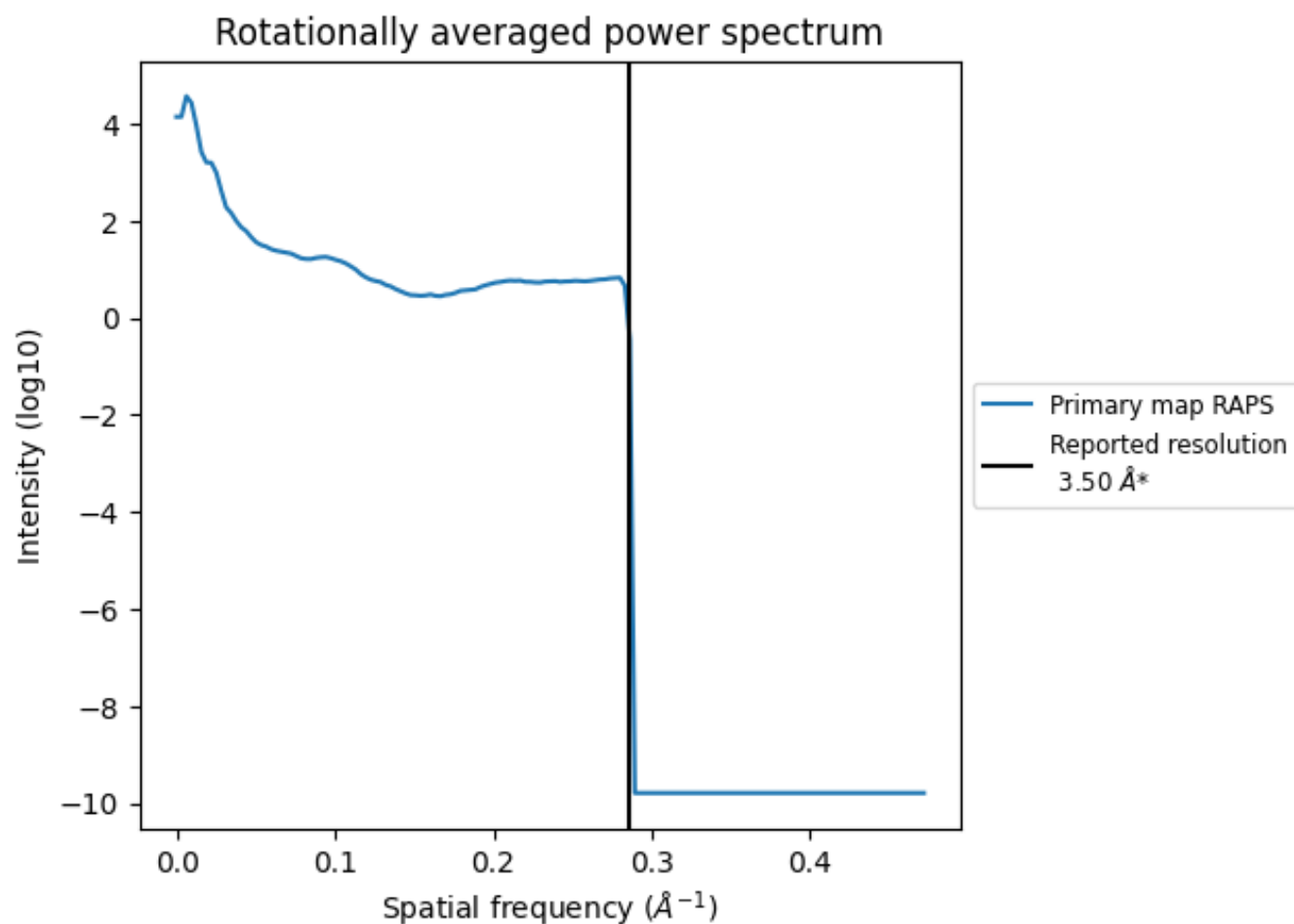
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 324 nm³; this corresponds to an approximate mass of 293 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 0.286 Å⁻¹

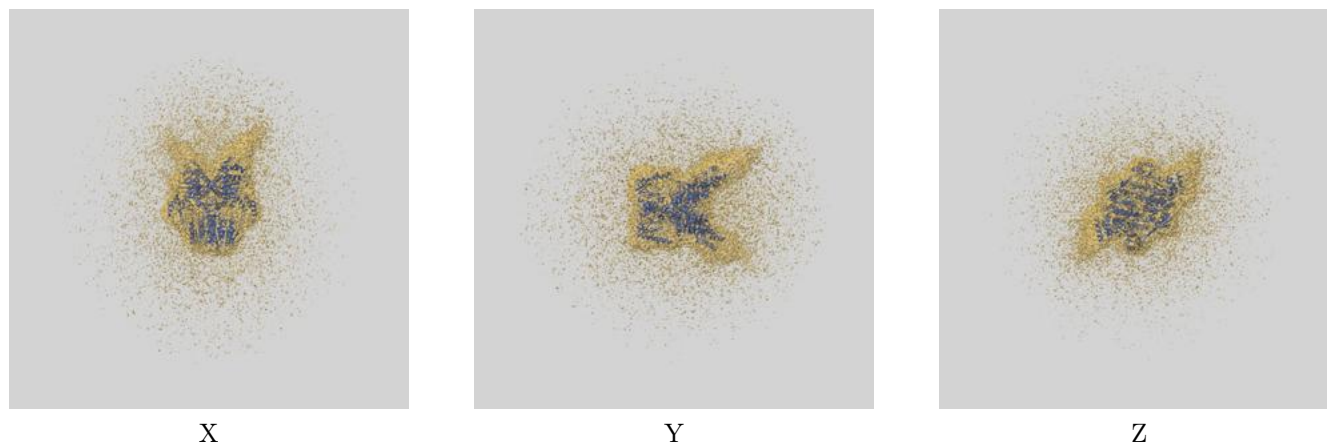
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

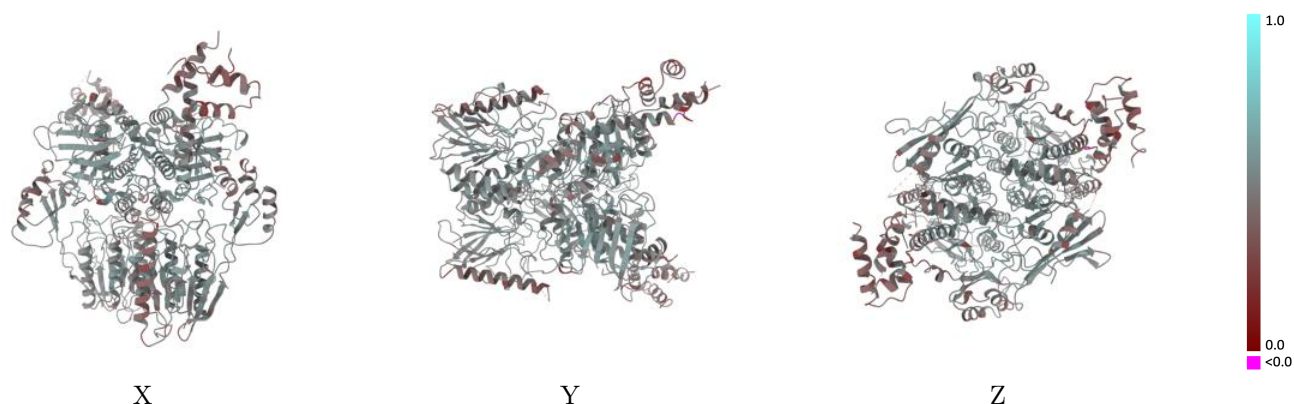
This section contains information regarding the fit between EMDB map EMD-10107 and PDB model 6S6V. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



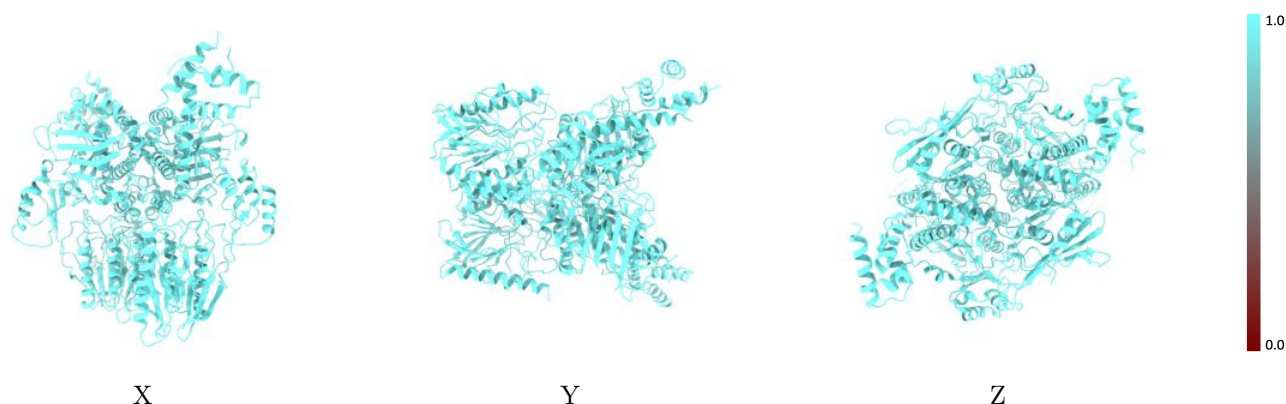
The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



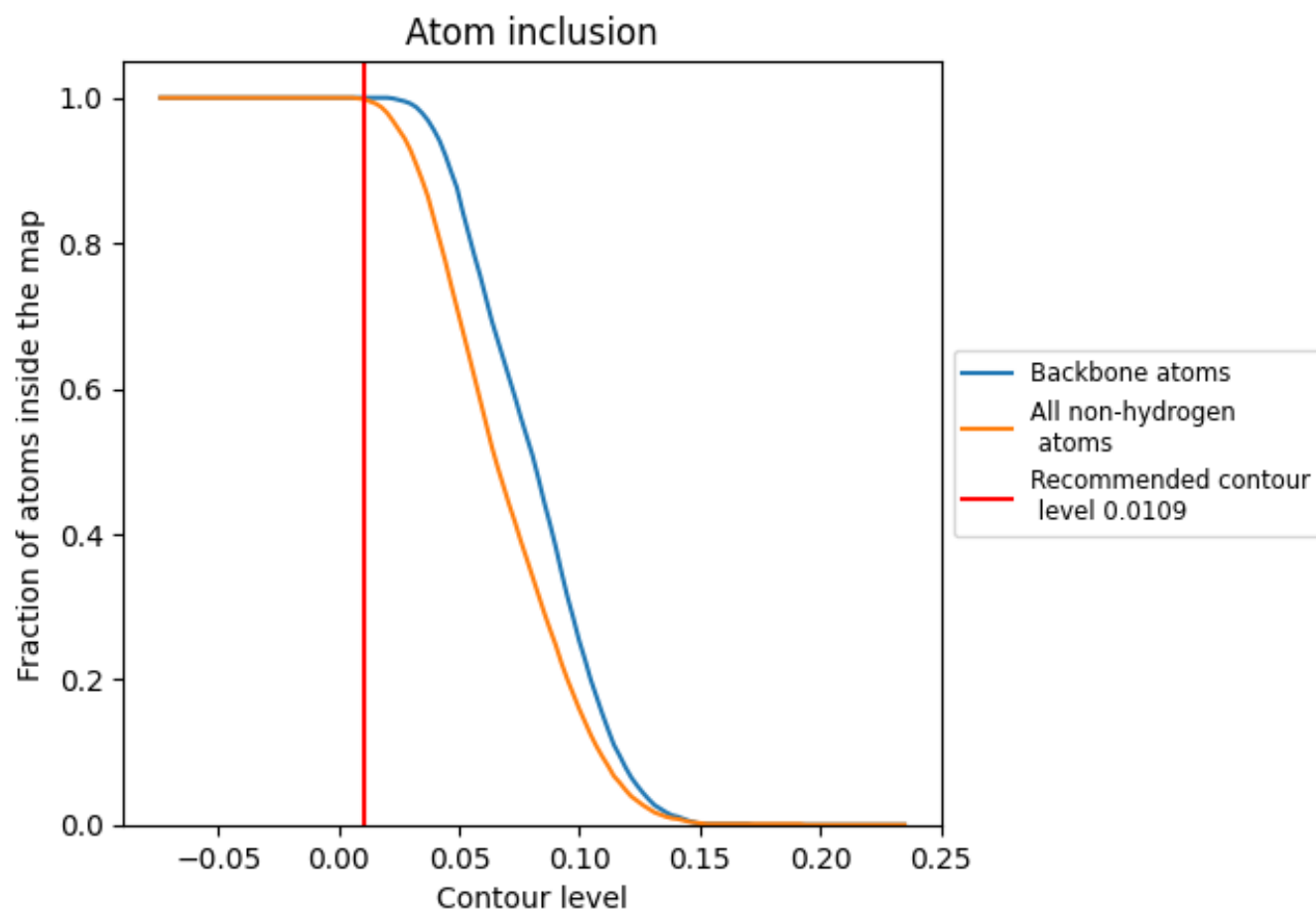
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0109).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9980	<div></div> 0.4860
A	<div></div> 0.9980	<div></div> 0.4680
B	<div></div> 0.9980	<div></div> 0.4690
C	<div></div> 0.9970	<div></div> 0.5050
D	<div></div> 0.9980	<div></div> 0.5010

