wwPDB EM Validation Summary Report (i)

Apr 2, 2024 – 01:31 PM JST

PDB ID	:	8WBX
EMDB ID	:	EMD-37426
Title	:	Cryo-EM structure of the ABCG25 bound to ABA
Authors	:	Xin, J.; Yan, K.G.
Deposited on	:	2023-09-10
Resolution	:	3.23 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 (i) 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 (1)) were used in the production of this report:

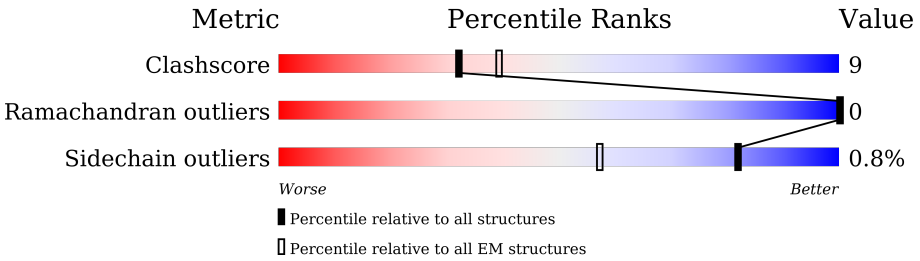
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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 <=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	698	10% 54% 13% 33%
1	B	698	10% 52% 15% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A8S	A	701	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7331 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 ABC transporter G family member 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	467	3656	2397	601	636	22	0	0
1	B	467	3656	2397	601	636	22	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q84TH5
A	-34	ASP	-	expression tag	UNP Q84TH5
A	-33	TYR	-	expression tag	UNP Q84TH5
A	-32	LYS	-	expression tag	UNP Q84TH5
A	-31	ASP	-	expression tag	UNP Q84TH5
A	-30	HIS	-	expression tag	UNP Q84TH5
A	-29	ASP	-	expression tag	UNP Q84TH5
A	-28	GLY	-	expression tag	UNP Q84TH5
A	-27	ASP	-	expression tag	UNP Q84TH5
A	-26	TYR	-	expression tag	UNP Q84TH5
A	-25	LYS	-	expression tag	UNP Q84TH5
A	-24	ASP	-	expression tag	UNP Q84TH5
A	-23	HIS	-	expression tag	UNP Q84TH5
A	-22	ASP	-	expression tag	UNP Q84TH5
A	-21	ILE	-	expression tag	UNP Q84TH5
A	-20	ASP	-	expression tag	UNP Q84TH5
A	-19	TYR	-	expression tag	UNP Q84TH5
A	-18	LYS	-	expression tag	UNP Q84TH5
A	-17	ASP	-	expression tag	UNP Q84TH5
A	-16	ASP	-	expression tag	UNP Q84TH5
A	-15	ASP	-	expression tag	UNP Q84TH5
A	-14	ASP	-	expression tag	UNP Q84TH5
A	-13	LYS	-	expression tag	UNP Q84TH5
A	-12	GLY	-	expression tag	UNP Q84TH5
A	-11	SER	-	expression tag	UNP Q84TH5
A	-10	ASP	-	expression tag	UNP Q84TH5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	LEU	-	expression tag	UNP Q84TH5
A	-8	GLU	-	expression tag	UNP Q84TH5
A	-7	VAL	-	expression tag	UNP Q84TH5
A	-6	LEU	-	expression tag	UNP Q84TH5
A	-5	PHE	-	expression tag	UNP Q84TH5
A	-4	GLN	-	expression tag	UNP Q84TH5
A	-3	GLY	-	expression tag	UNP Q84TH5
A	-2	PRO	-	expression tag	UNP Q84TH5
A	-1	GLY	-	expression tag	UNP Q84TH5
A	0	SER	-	expression tag	UNP Q84TH5
B	-35	MET	-	initiating methionine	UNP Q84TH5
B	-34	ASP	-	expression tag	UNP Q84TH5
B	-33	TYR	-	expression tag	UNP Q84TH5
B	-32	LYS	-	expression tag	UNP Q84TH5
B	-31	ASP	-	expression tag	UNP Q84TH5
B	-30	HIS	-	expression tag	UNP Q84TH5
B	-29	ASP	-	expression tag	UNP Q84TH5
B	-28	GLY	-	expression tag	UNP Q84TH5
B	-27	ASP	-	expression tag	UNP Q84TH5
B	-26	TYR	-	expression tag	UNP Q84TH5
B	-25	LYS	-	expression tag	UNP Q84TH5
B	-24	ASP	-	expression tag	UNP Q84TH5
B	-23	HIS	-	expression tag	UNP Q84TH5
B	-22	ASP	-	expression tag	UNP Q84TH5
B	-21	ILE	-	expression tag	UNP Q84TH5
B	-20	ASP	-	expression tag	UNP Q84TH5
B	-19	TYR	-	expression tag	UNP Q84TH5
B	-18	LYS	-	expression tag	UNP Q84TH5
B	-17	ASP	-	expression tag	UNP Q84TH5
B	-16	ASP	-	expression tag	UNP Q84TH5
B	-15	ASP	-	expression tag	UNP Q84TH5
B	-14	ASP	-	expression tag	UNP Q84TH5
B	-13	LYS	-	expression tag	UNP Q84TH5
B	-12	GLY	-	expression tag	UNP Q84TH5
B	-11	SER	-	expression tag	UNP Q84TH5
B	-10	ASP	-	expression tag	UNP Q84TH5
B	-9	LEU	-	expression tag	UNP Q84TH5
B	-8	GLU	-	expression tag	UNP Q84TH5
B	-7	VAL	-	expression tag	UNP Q84TH5
B	-6	LEU	-	expression tag	UNP Q84TH5
B	-5	PHE	-	expression tag	UNP Q84TH5
B	-4	GLN	-	expression tag	UNP Q84TH5

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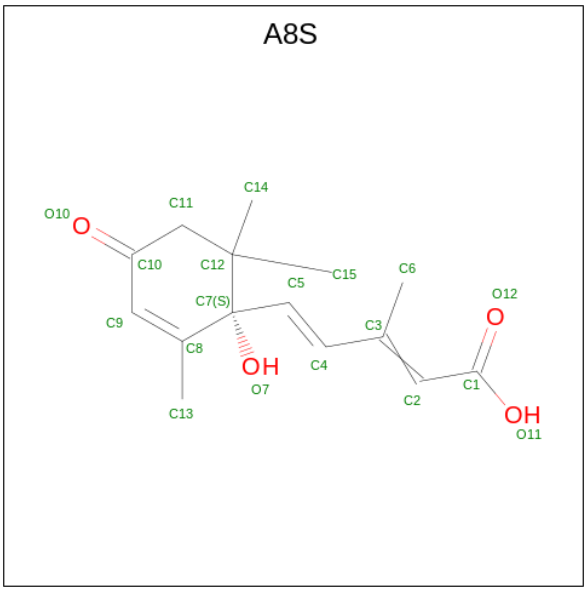
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q84TH5
B	-2	PRO	-	expression tag	UNP Q84TH5
B	-1	GLY	-	expression tag	UNP Q84TH5
B	0	SER	-	expression tag	UNP Q84TH5

- Molecule 2 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methyl penta-2,4-dienoic acid (three-letter code: A8S) (formula: $C_{15}H_{20}O_4$) (labeled as "Ligand of Interest" by depositor).



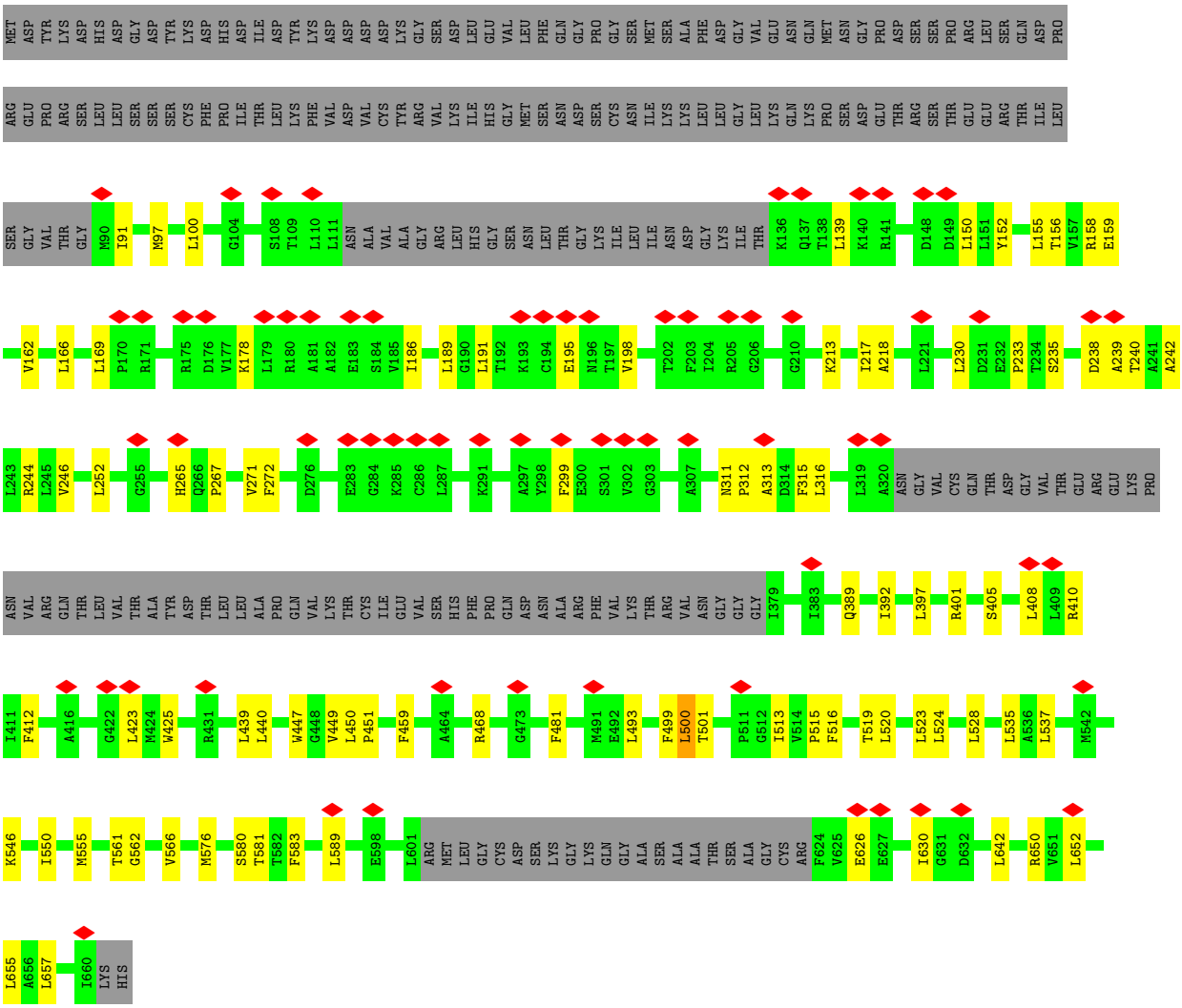
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	19	15	4	0

3 Residue-property plots (i)

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.

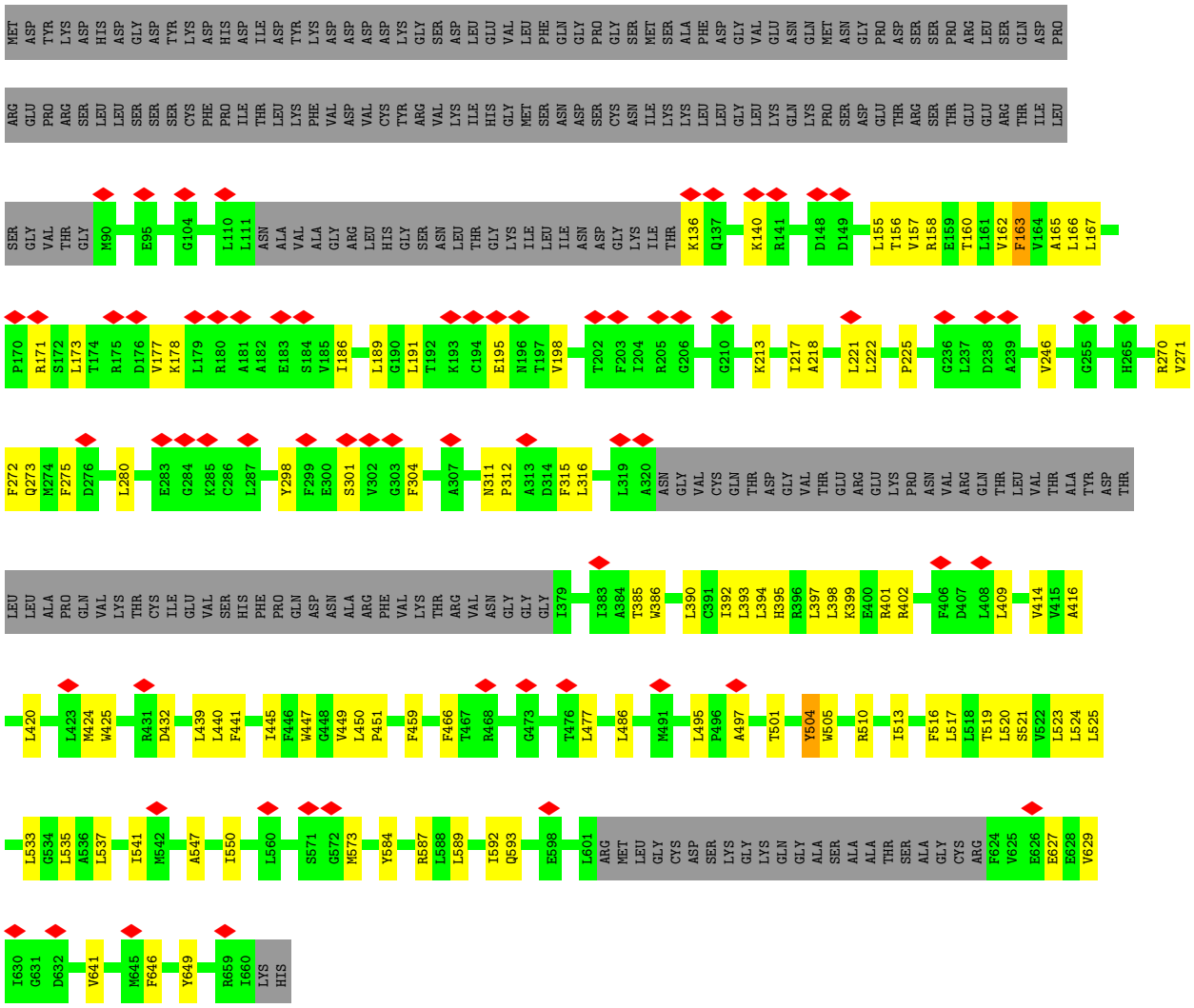
• Molecule 1: ABC transporter G family member 25

Chain A: 10% 54% 13% 33%



• Molecule 1: ABC transporter G family member 25

Chain B: 10% 52% 15% 33%


MET ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP LYS LYS GLY SER ASP LEU GLU VAL LEU PHE GLN GLY PRO GLY SER MET SER ALA PHE ASP GLY VAL GLU ASN GLN MET ASN GLY PRO ASP SER SER PRO ARG LEU SER GLN ASP PRO
ARG GLU PRO ARG SER LEU LEU SER SER SER CYS PHE PRO ILE THR LEU LYS PHE VAL ASP VAL CYS TYR ARG VAL LYS ILE HIS GLY MET SER ASN ASP SER CYS ASN ILE LYS LYS LEU LEU GLY LEU LYS GLN LYS PRO SER ASP GLU THR ARG SER THR GLU GLU ARG THR ILE LEU
SER GLY VAL THR GLY M90 E95 G104 L110 L111 ASN ALA VAL ALA GLY ARG LEU HIS GLY SER ASN LEU THR GLY LYS ILE LEU ILE ASN ASP SER GLY LYS ILE THR K136 Q137 K140 R141 D148 D149 L155 T156 V157 R158 E159 T160 L161 V162 F163 V164 A165 L166 L167
P170 R171 S172 L173 T174 R175 D176 V177 K178 L179 R180 A181 A182 E183 S184 V185 I186 L189 G190 L191 T192 K193 C194 E195 N196 T197 V198 T202 F203 I204 R205 G206 G210 K213 I217 A218 L221 L222 P225 G236 L237 D238 A239 V246 G255 H265 R270 V271
F272 Q273 M274 F275 D276 L280 E283 G284 K285 C286 L287 Y298 F299 E300 S301 V302 G303 F304 A307 N311 P312 A313 D314 F315 L316 L319 A320 ASN GLY VAL CYS GLN THR ASP GLY VAL THR GLU ARG GLU LYS PRO ASN VAL ARG GLN THR LEU VAL THR ALA TYR ASP THR
LEU LEU ALA PRO GLN VAL LYS THR CYS ILE GLU VAL SER HIS PHE PRO GLN ASP ASN ALA ARG PHE VAL LYS THR ARG VAL ASN GLY GLY GLY I379 I383 A384 I385 W386 L390 C391 I392 L393 L394 H395 R396 L397 L398 K399 E400 R401 R402 F406 D407 L408 L409 V414 V415 A416
L420 L423 M424 W425 R431 D432 L439 L440 F441 I445 F446 W447 G448 V449 L450 P451 F459 F466 T467 R468 G473 T476 L477 L486 M491 L495 P496 A497 T501 Y504 W505 R510 I513 F516 L517 L518 T519 L520 S521 V522 L523 L524 L525
L533 G534 L535 A536 L537 I541 M542 A547 I550 L560 S571 G572 M573 Y584 R587 L588 L589 I592 Q593 E598 L601 ARG MET LEU GLY CYS ASP SER LYS GLY LYS GLN GLY ALA SER ALA ALA THR SER ALA GLY CYS ARG F624 V625 E626 E627 E628 V629
I630 G631 D632 V641 M645 F646 Y649 R659 I660 LYS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53233	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.447	Depositor
Minimum map value	-1.748	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: A8S

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	0/3738	0.50	0/5068
1	B	0.26	0/3738	0.51	0/5068
All	All	0.26	0/7476	0.51	0/10136

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	3656	0	3763	72	0
1	B	3656	0	3763	72	0
2	A	19	0	19	12	0
All	All	7331	0	7545	140	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 9.

The worst 5 of 140 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:THR:HG22	1:B:424:MET:HE1	1.43	0.97
1:A:481:PHE:HZ	1:A:650:ARG:HB3	1.30	0.93
1:B:521:SER:HA	1:B:524:LEU:CD2	2.05	0.86
1:A:561:THR:HG22	1:B:424:MET:CE	2.06	0.84
1:A:405:SER:HB2	1:A:410:ARG:HD2	1.67	0.77

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	459/698 (66%)	451 (98%)	8 (2%)	0	100	100
1	B	459/698 (66%)	452 (98%)	7 (2%)	0	100	100
All	All	918/1396 (66%)	903 (98%)	15 (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	397/595 (67%)	395 (100%)	2 (0%)	88	94
1	B	397/595 (67%)	393 (99%)	4 (1%)	76	88
All	All	794/1190 (67%)	788 (99%)	6 (1%)	82	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	504	TYR
1	B	627	GLU
1	B	646	PHE
1	A	642	LEU
1	A	500	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	A8S	A	701	-	17,19,19	0.96	1 (5%)	17,29,29	1.62	3 (17%)

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	A8S	A	701	-	-	0/10/34/34	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A8S	O11-C1	-2.03	1.25	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	A8S	C8-C9-C10	-3.45	120.30	123.82
2	A	701	A8S	O11-C1-C2	2.26	120.51	113.50
2	A	701	A8S	C5-C4-C3	-2.07	122.32	125.53

There are no chirality outliers.

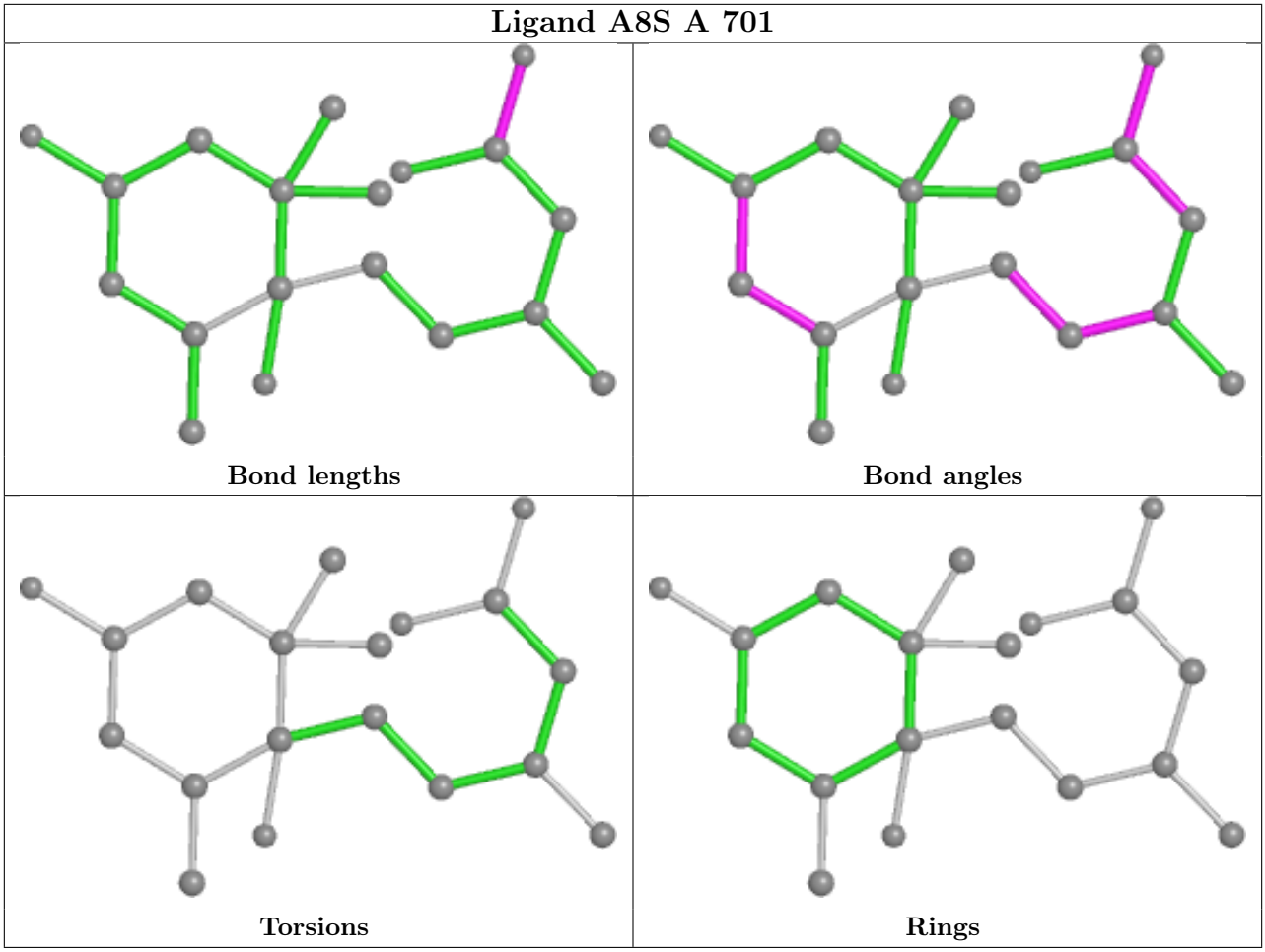
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	A8S	12	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 then 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.

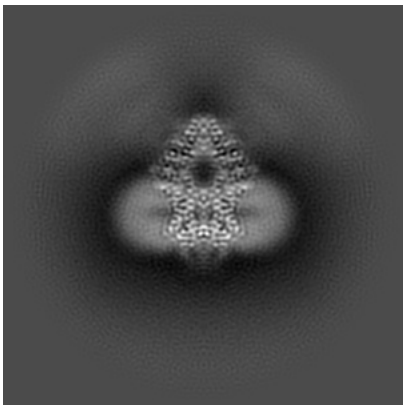
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37426. These allow visual inspection of the internal detail of the map and identification of artifacts.

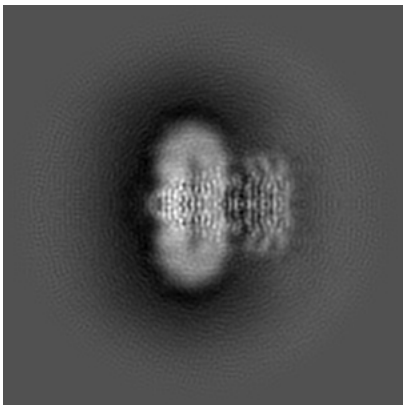
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

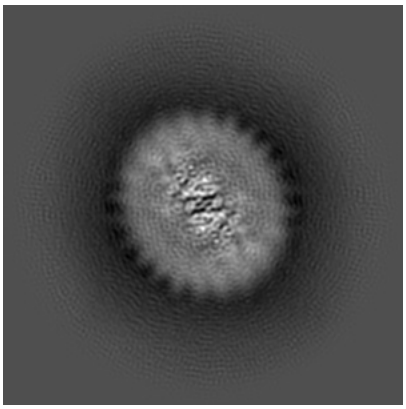
6.1.1 Primary map



X

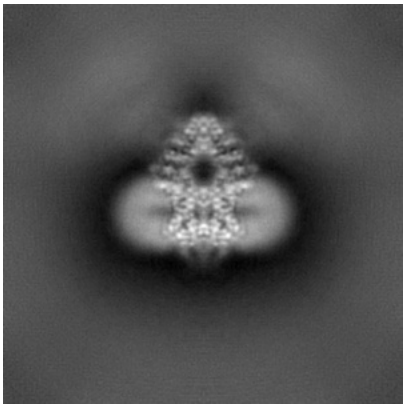


Y

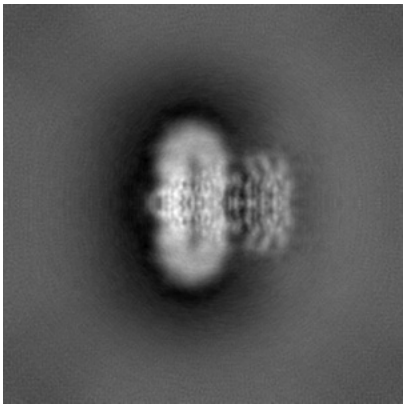


Z

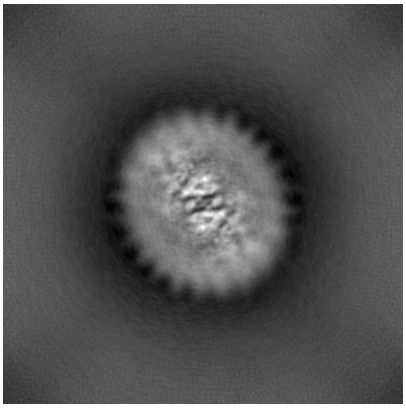
6.1.2 Raw map



X



Y

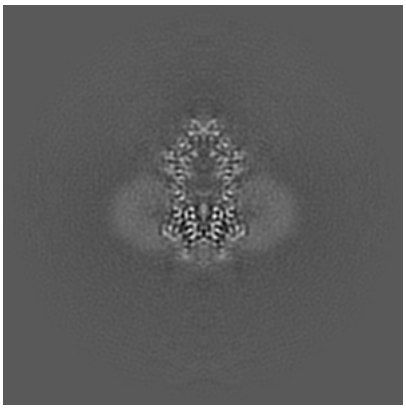


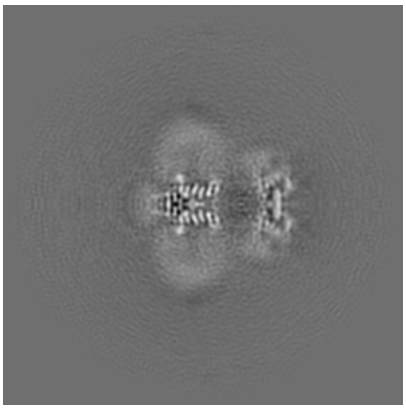
Z

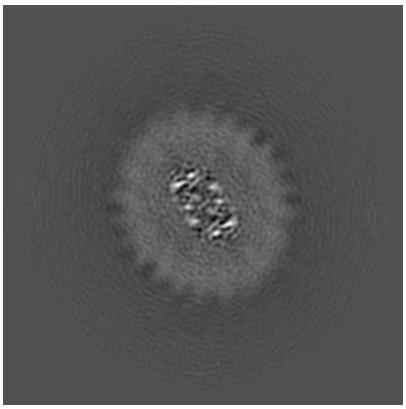
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

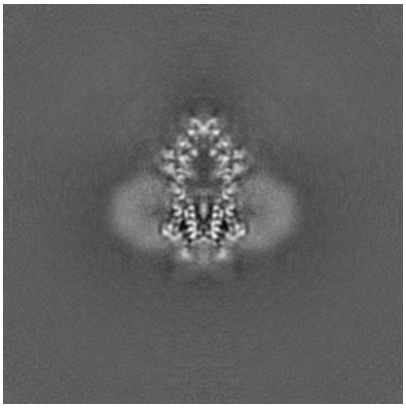
6.2.1 Primary map

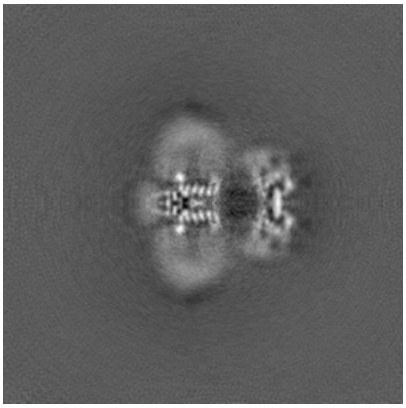

X Index: 128

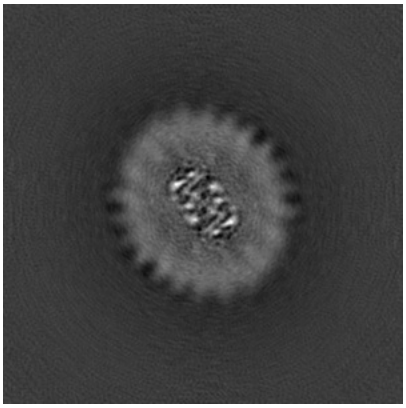

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

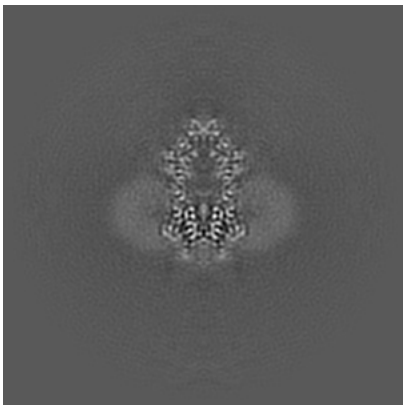

Y Index: 128

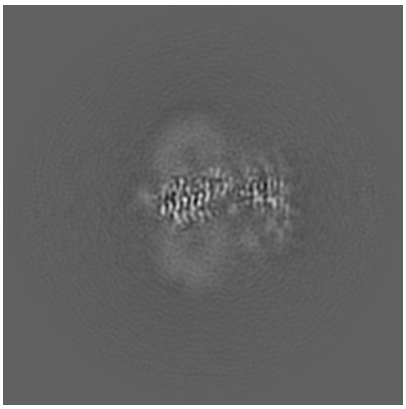

Z Index: 128

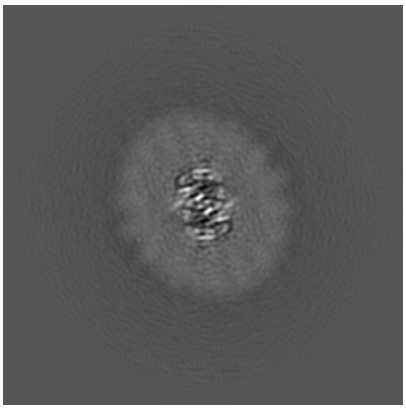
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

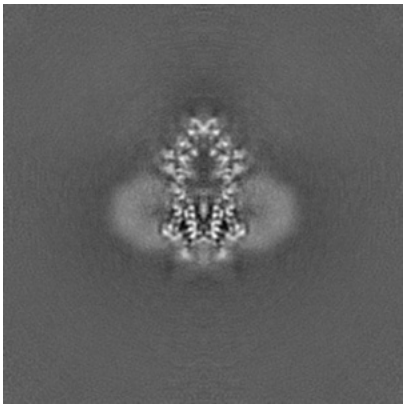
6.3.1 Primary map

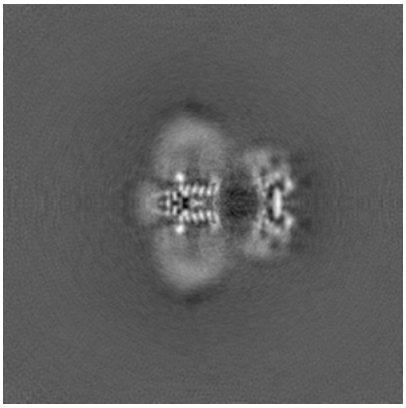

X Index: 128

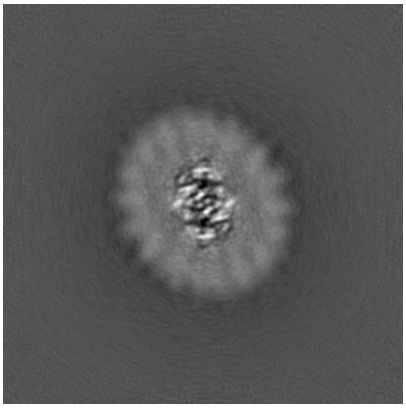

Y Index: 120


Z Index: 113

6.3.2 Raw map


X Index: 128

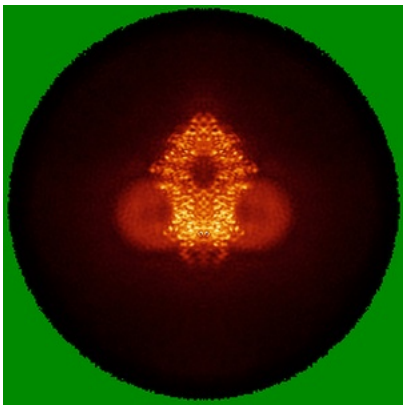

Y Index: 128

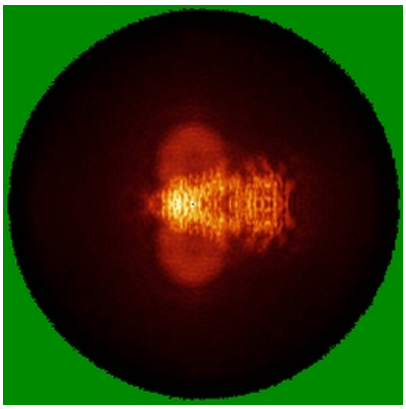

Z Index: 113

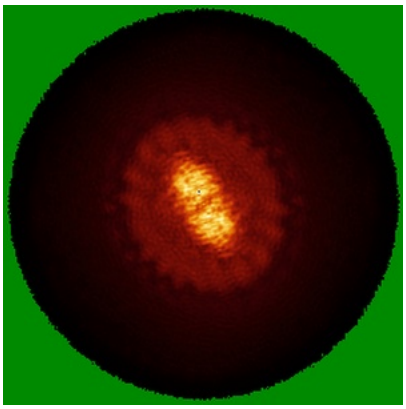
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

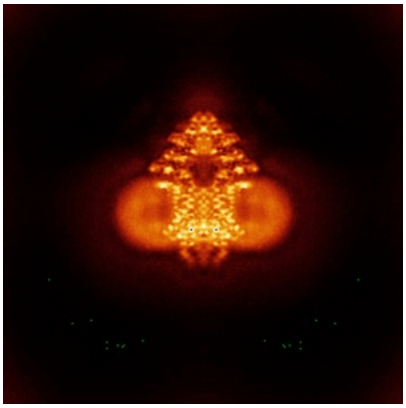
6.4.1 Primary map

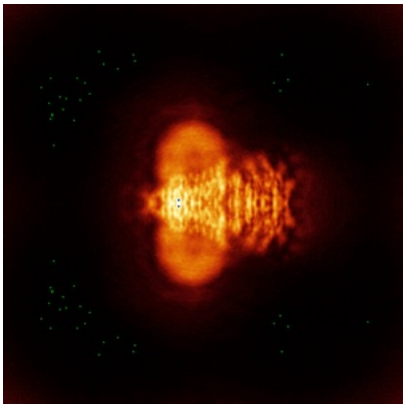

X

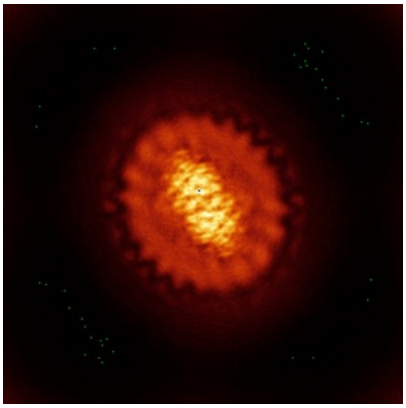

Y


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.

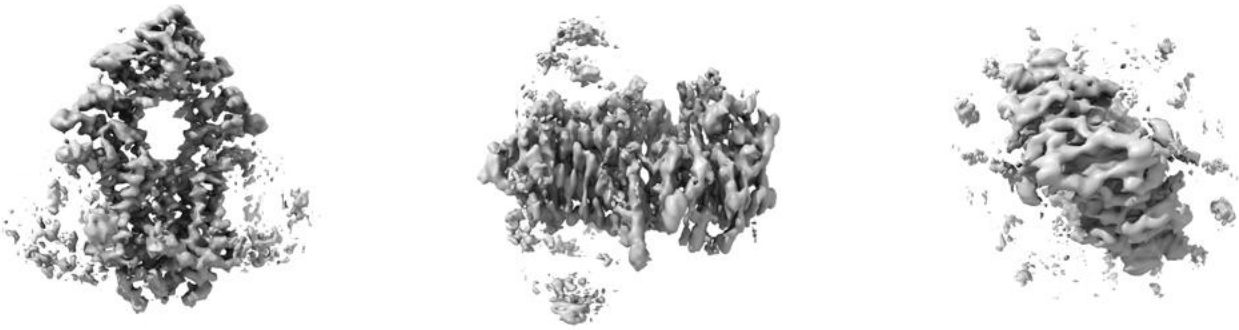
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

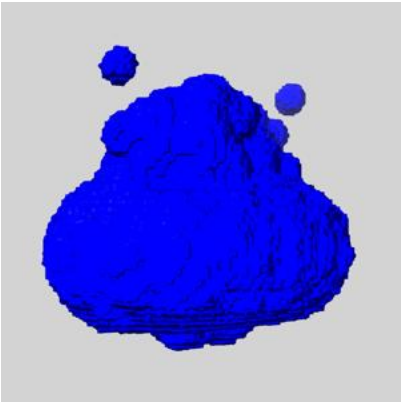
6.6 Mask visualisation (i)

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

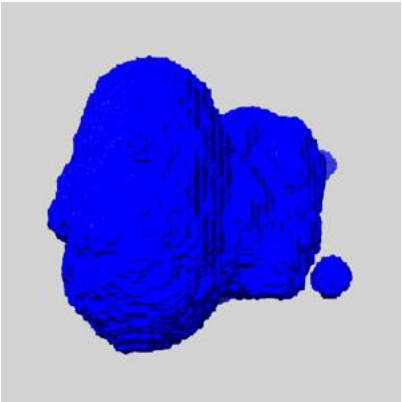
A mask typically either:

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

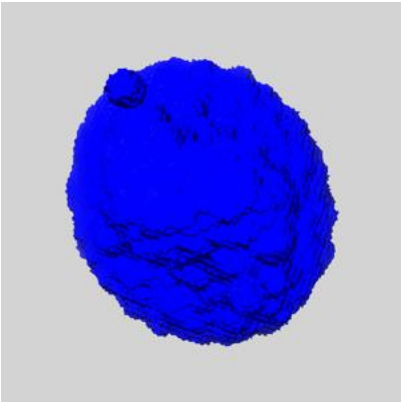
6.6.1 emd_37426_msk_1.map (i)



X



Y

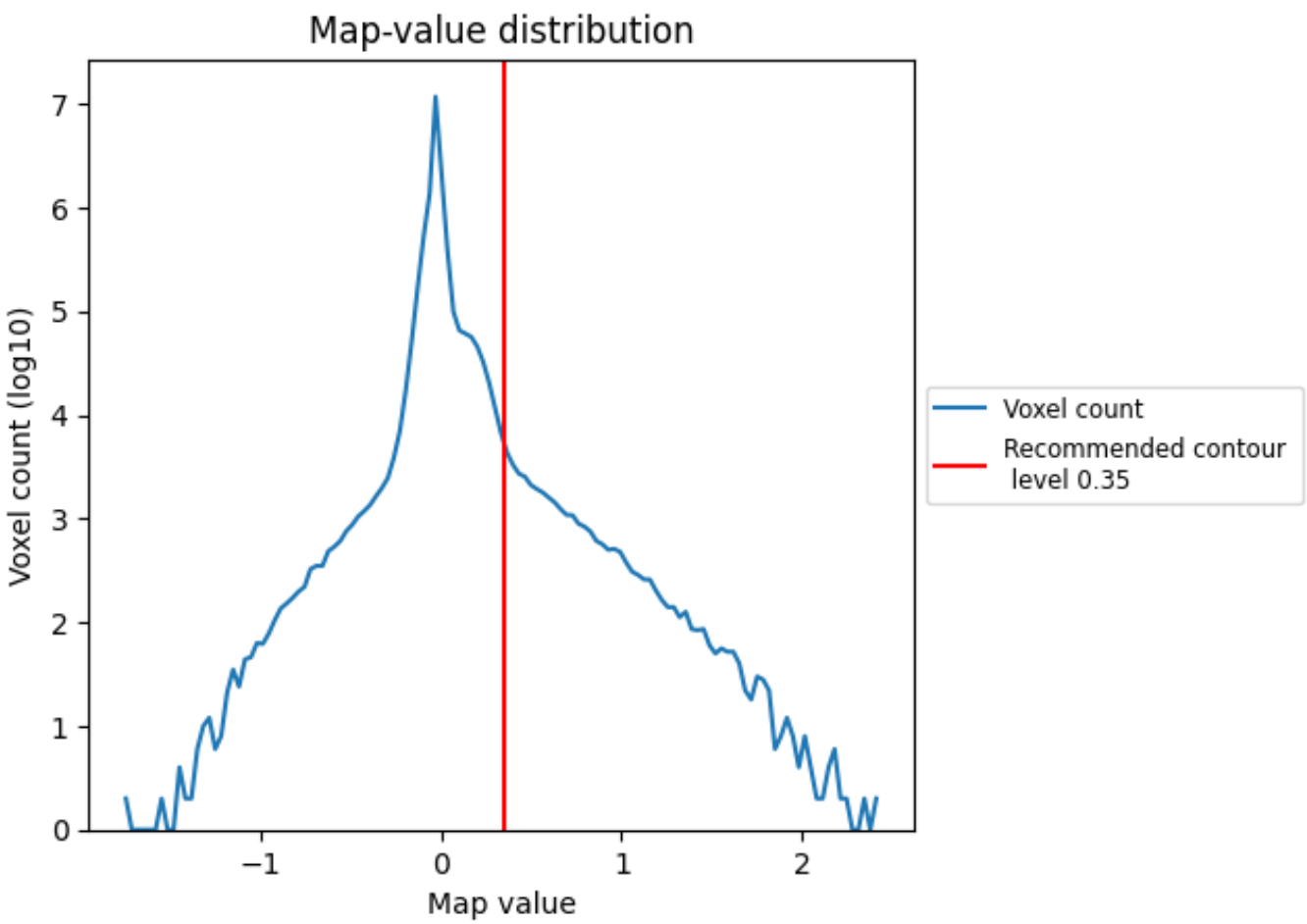


Z

7 Map analysis (i)

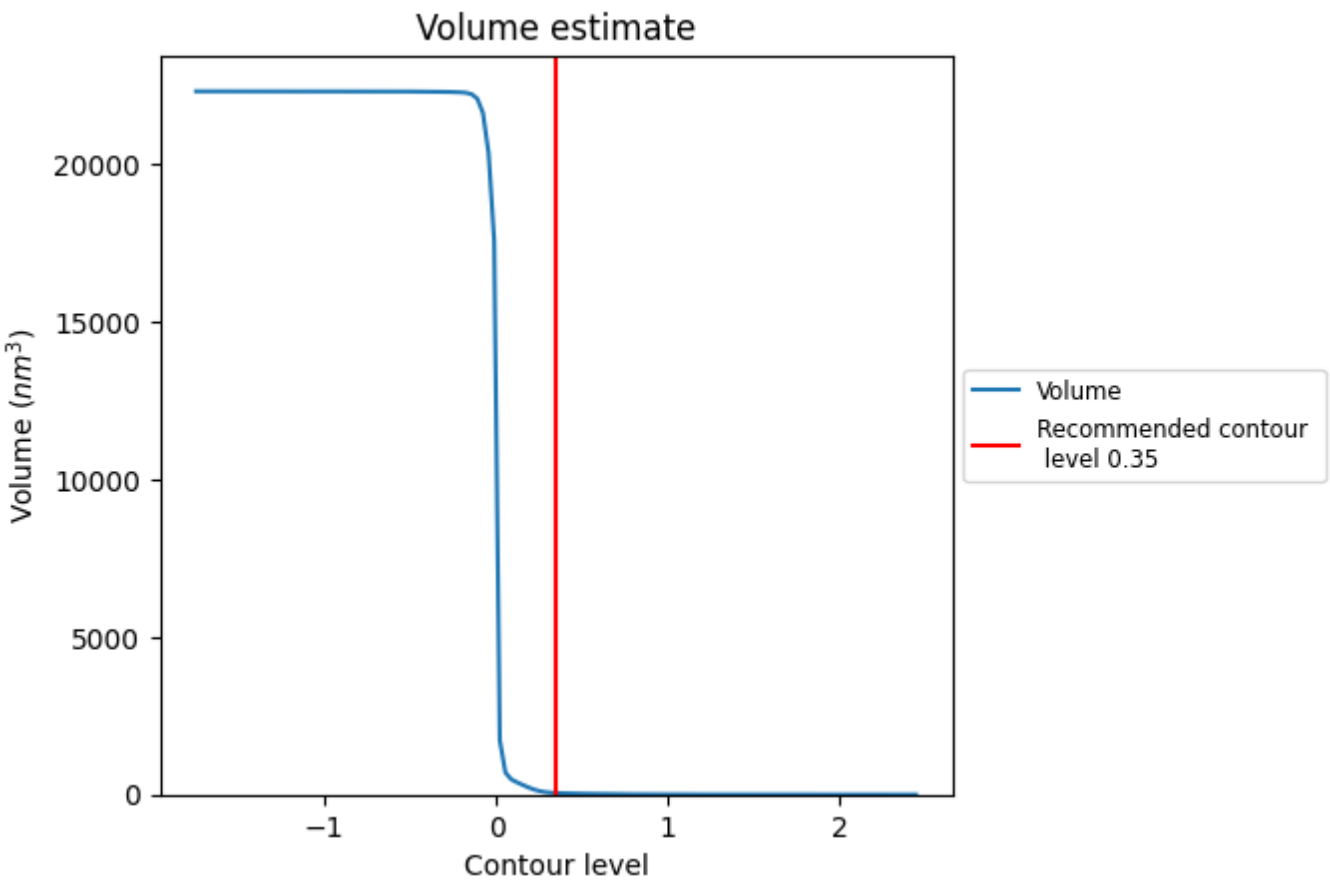
This section contains the results of statistical analysis of the map.

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.

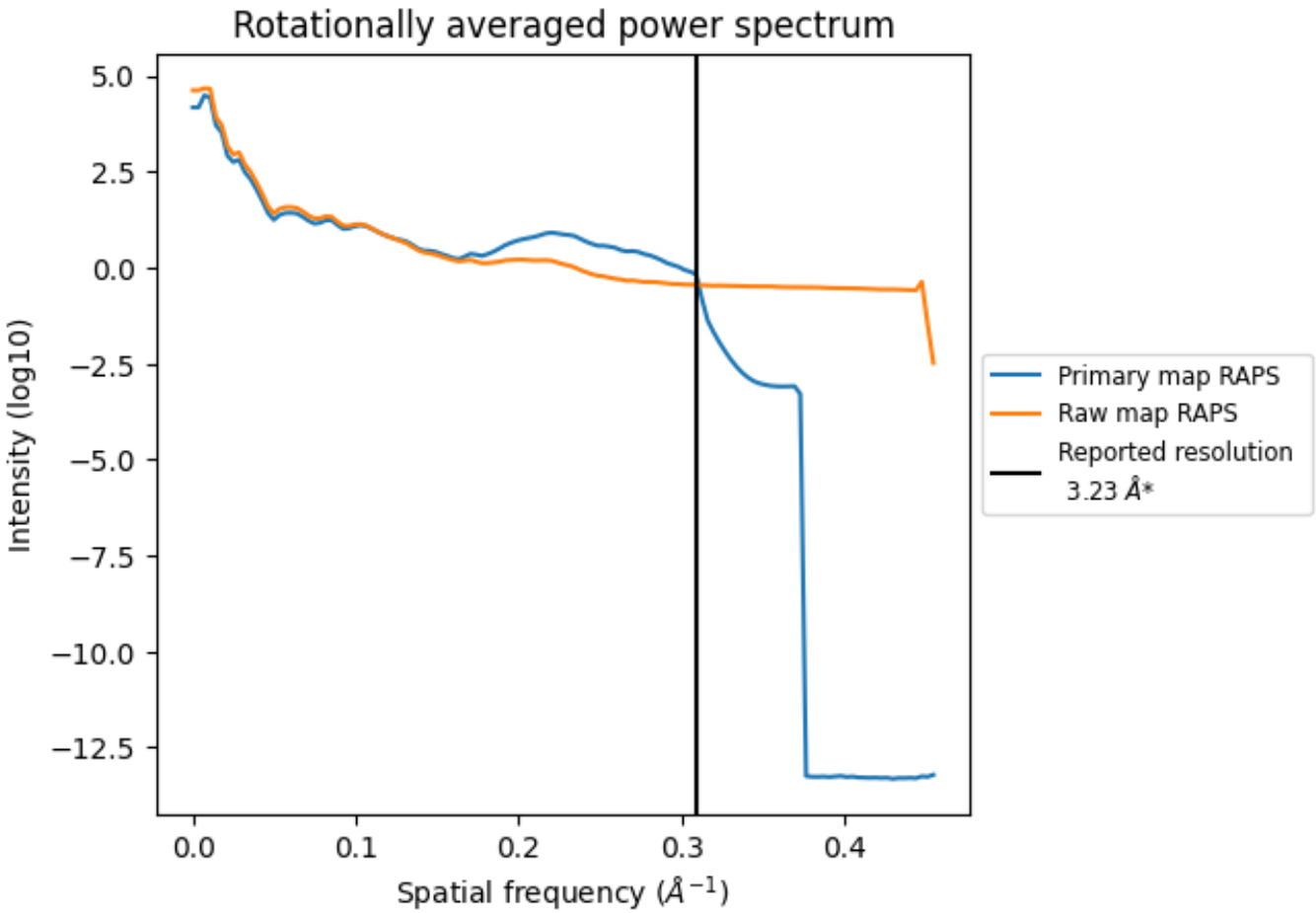
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 44 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)

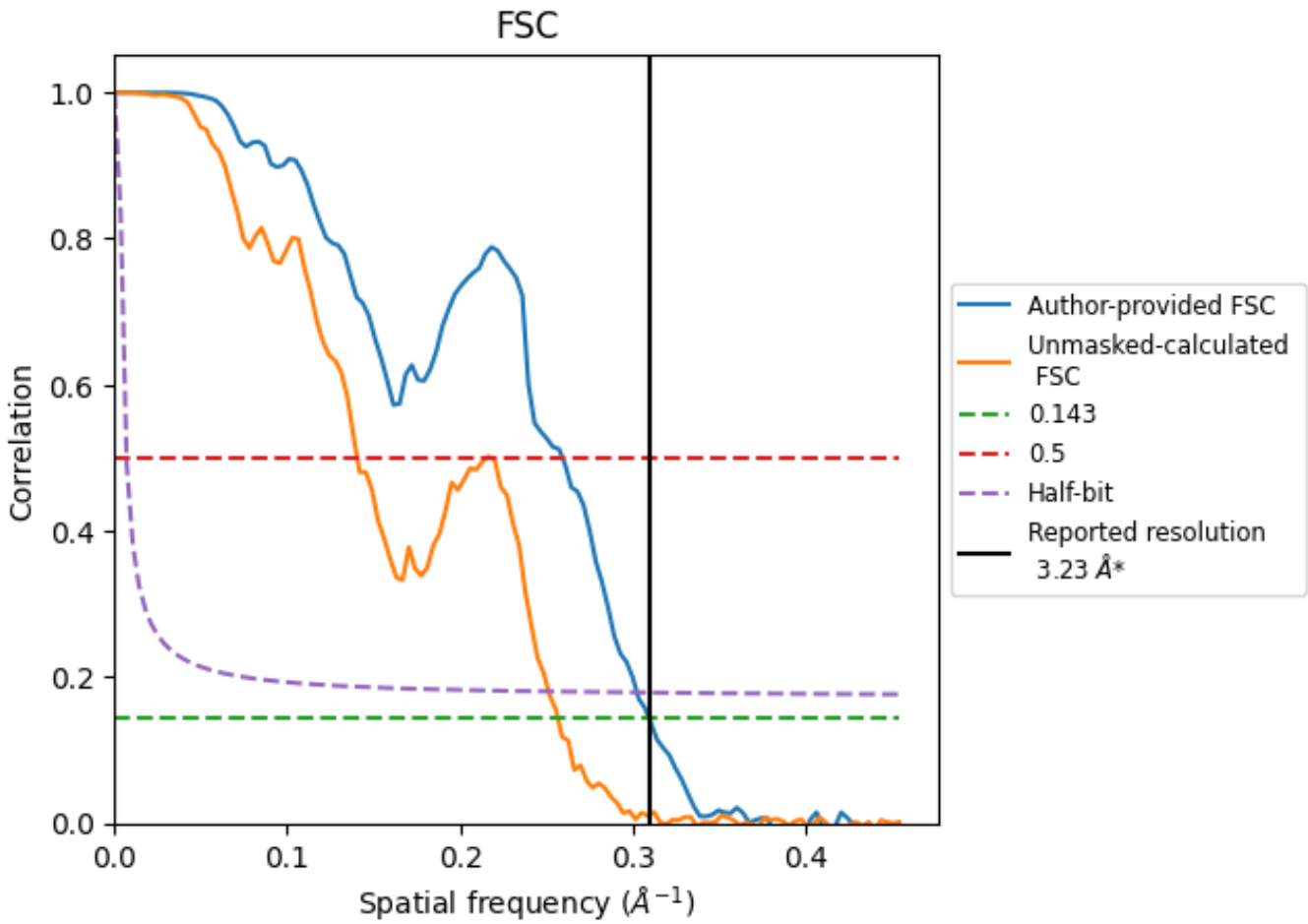


*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

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 0.310 Å^{-1}

8.2 Resolution estimates (i)

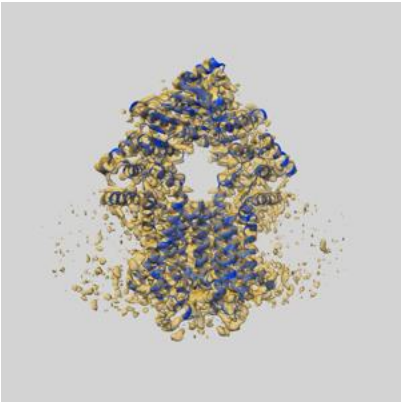
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.86	3.30
Unmasked-calculated*	3.89	7.11	3.98

*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 3.89 differs from the reported value 3.23 by more than 10 %

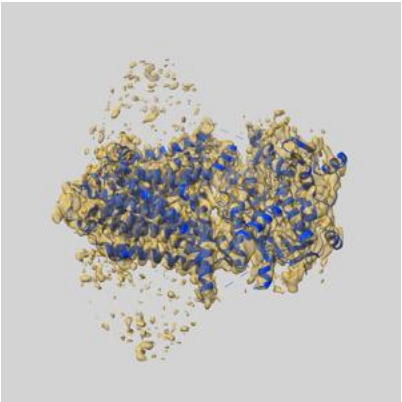
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37426 and PDB model 8WBX. Per-residue inclusion information can be found in section 3 on page 6.

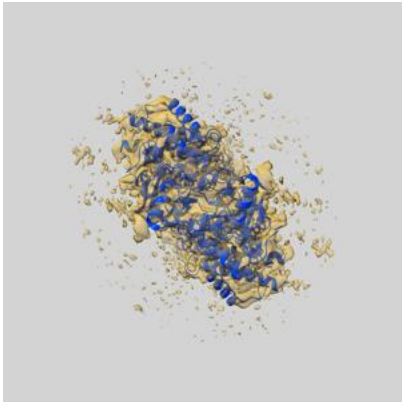
9.1 Map-model overlay (i)



X



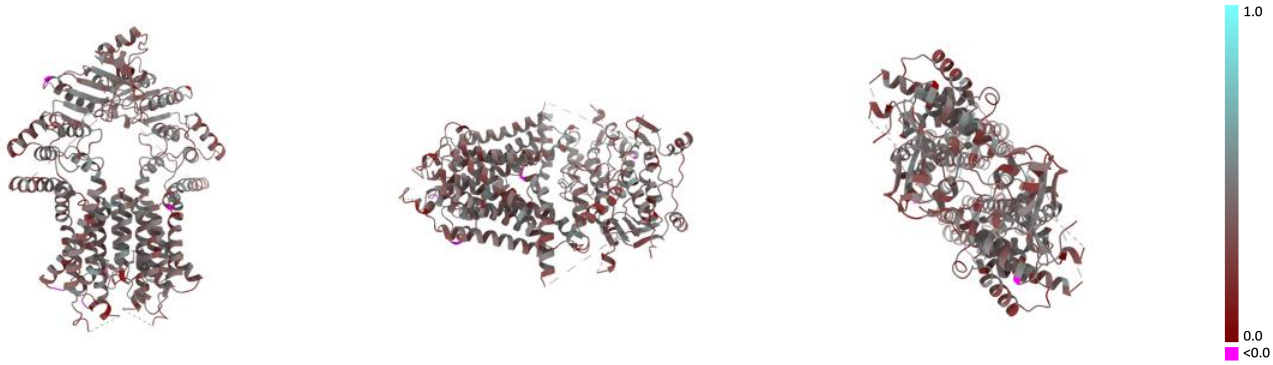
Y



Z

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

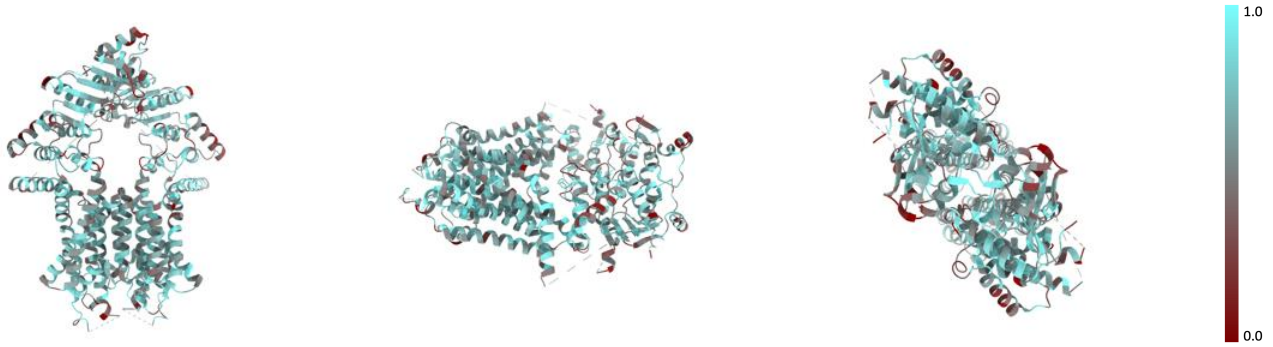
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

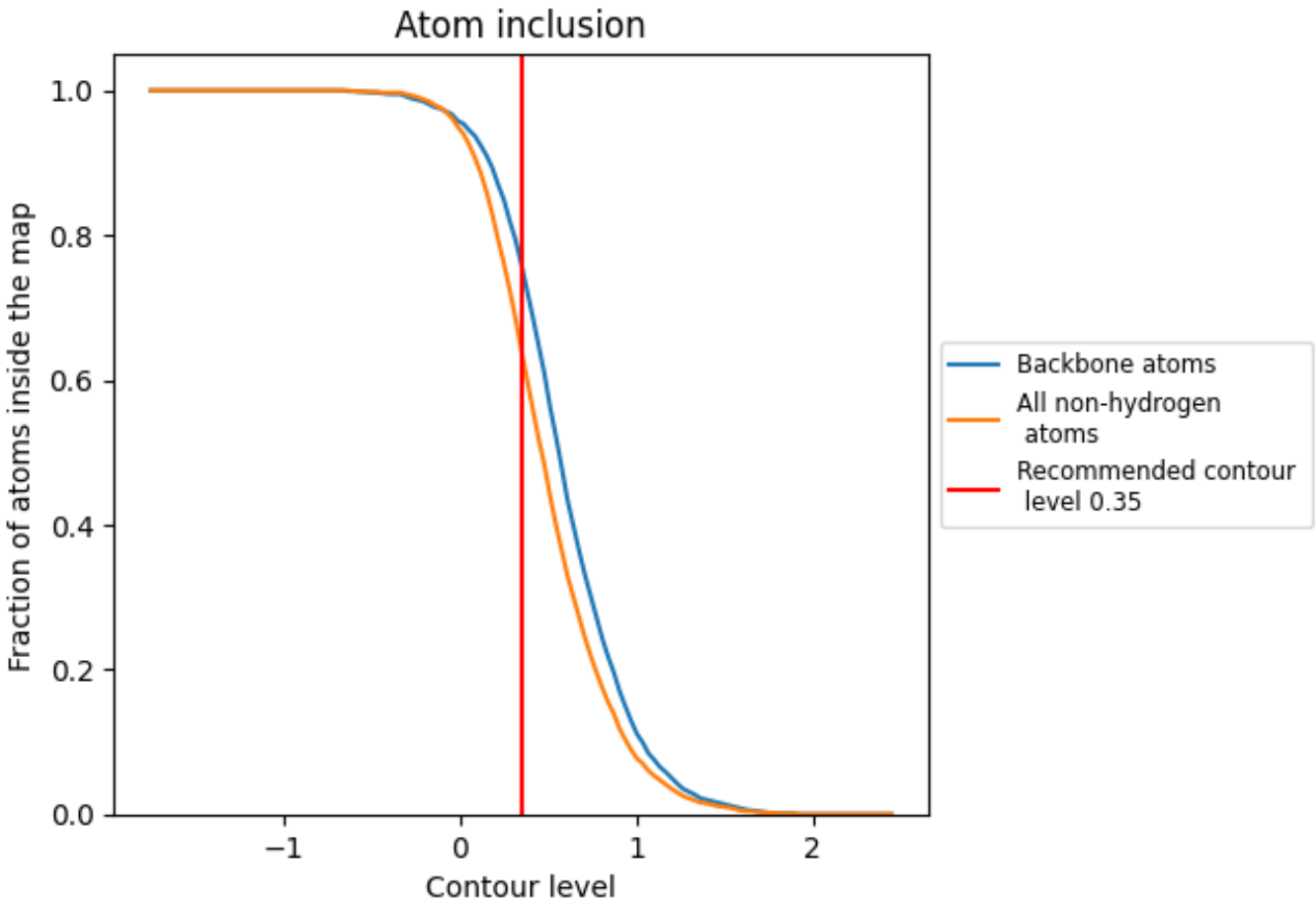
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.3740
A	0.6370	0.3710
B	0.6450	0.3770