



wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 10:57 am BST

PDB ID : 9G09 / pdb_00009g09
EMDB ID : EMD-50914
Title : Structure of human RNF213 bound to the secreted effector IpaH2.5 from
Shigella flexneri
Authors : Naydenova, K.; Randow, F.
Deposited on : 2024-07-07
Resolution : 3.40 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.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

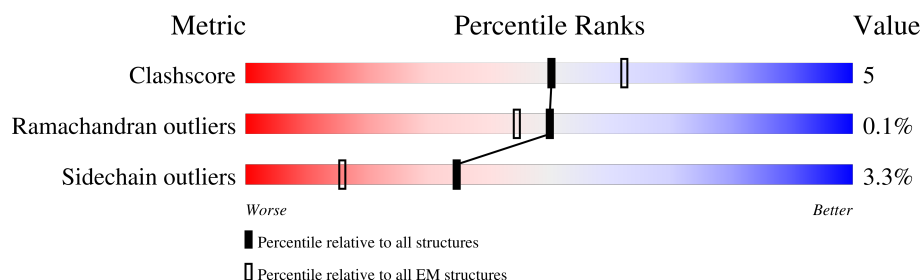
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	B	563	
2	A	5247	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38435 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 E3 ubiquitin-protein ligase IpaH2.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	237	Total	C	N	O	S	0	0
			1886	1206	324	349	7		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4529	Total	C	N	O	S	0	0
			36514	23323	6289	6682	220		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP Q63HN8
A	-38	ALA	-	expression tag	UNP Q63HN8
A	-37	SER	-	expression tag	UNP Q63HN8
A	-36	TRP	-	expression tag	UNP Q63HN8
A	-35	SER	-	expression tag	UNP Q63HN8
A	-34	HIS	-	expression tag	UNP Q63HN8
A	-33	PRO	-	expression tag	UNP Q63HN8
A	-32	GLN	-	expression tag	UNP Q63HN8
A	-31	PHE	-	expression tag	UNP Q63HN8
A	-30	GLU	-	expression tag	UNP Q63HN8
A	-29	LYS	-	expression tag	UNP Q63HN8
A	-28	GLY	-	expression tag	UNP Q63HN8
A	-27	SER	-	expression tag	UNP Q63HN8
A	-26	ALA	-	expression tag	UNP Q63HN8
A	-25	GLY	-	expression tag	UNP Q63HN8
A	-24	SER	-	expression tag	UNP Q63HN8
A	-23	ALA	-	expression tag	UNP Q63HN8
A	-22	ALA	-	expression tag	UNP Q63HN8
A	-21	GLY	-	expression tag	UNP Q63HN8
A	-20	SER	-	expression tag	UNP Q63HN8
A	-19	GLY	-	expression tag	UNP Q63HN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	ALA	-	expression tag	UNP Q63HN8
A	-17	GLY	-	expression tag	UNP Q63HN8
A	-16	TRP	-	expression tag	UNP Q63HN8
A	-15	SER	-	expression tag	UNP Q63HN8
A	-14	HIS	-	expression tag	UNP Q63HN8
A	-13	PRO	-	expression tag	UNP Q63HN8
A	-12	GLN	-	expression tag	UNP Q63HN8
A	-11	PHE	-	expression tag	UNP Q63HN8
A	-10	GLU	-	expression tag	UNP Q63HN8
A	-9	LYS	-	expression tag	UNP Q63HN8
A	-8	GLU	-	expression tag	UNP Q63HN8
A	-7	ASN	-	expression tag	UNP Q63HN8
A	-6	LEU	-	expression tag	UNP Q63HN8
A	-5	TYR	-	expression tag	UNP Q63HN8
A	-4	PHE	-	expression tag	UNP Q63HN8
A	-3	GLN	-	expression tag	UNP Q63HN8
A	-2	ALA	-	expression tag	UNP Q63HN8
A	-1	MET	-	expression tag	UNP Q63HN8
A	0	SER	-	expression tag	UNP Q63HN8

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total 3	Zn 3	0







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213053	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.391	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	494.99997, 494.99997, 494.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	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: MG, ZN, ATP

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	B	0.28	0/1930	0.59	6/2634 (0.2%)
2	A	0.31	0/37286	0.47	17/50439 (0.0%)
All	All	0.31	0/39216	0.48	23/53073 (0.0%)

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
2	A	0	2

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1874	VAL	CG1-CB-CG2	8.46	124.43	110.90
2	A	1989	VAL	CG1-CB-CG2	8.15	123.95	110.90
2	A	4971	LEU	CD1-CG-CD2	8.11	134.81	110.50
2	A	4918	LEU	CD1-CG-CD2	7.85	134.05	110.50
2	A	3165	LEU	CB-CG-CD1	5.86	120.96	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2237	PRO	Peptide
2	A	4981	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1886	0	1912	50	0
2	A	36514	0	36697	371	0
3	A	31	0	12	2	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	38435	0	38621	418	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 5.

The worst 5 of 418 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)
2:A:4817:SER:O	2:A:4822:ARG:NH2	1.97	0.96
2:A:1511:ASP:OD1	2:A:1514:ARG:NH1	2.02	0.92
2:A:4973:LEU:HD22	2:A:4974:LYS:H	1.36	0.89
2:A:4005:LYS:NZ	2:A:4017:CYS:SG	2.45	0.89
2:A:1595:MET:O	2:A:1598:LYS:NZ	2.08	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	235/563 (42%)	209 (89%)	26 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	4479/5247 (85%)	4268 (95%)	206 (5%)	5 (0%)	48 78
All	All	4714/5810 (81%)	4477 (95%)	232 (5%)	5 (0%)	50 78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1236	PHE
2	A	1235	LEU
2	A	3104	ASN
2	A	4981	TYR
2	A	1396	ILE

5.3.2 Protein sidechains ⓘ

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	B	216/492 (44%)	200 (93%)	16 (7%)	11 35
2	A	4076/4653 (88%)	3950 (97%)	126 (3%)	35 60
All	All	4292/5145 (83%)	4150 (97%)	142 (3%)	35 58

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4225	TYR
2	A	4300	ARG
2	A	4737	CYS
2	A	1331	ASP
2	A	1288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4262	GLN

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Mol	Chain	Res	Type
2	A	4906	ASN
2	A	4293	GLN
2	A	4654	HIS
2	A	5134	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 [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
3	ATP	A	5301	4	26,33,33	0.87	1 (3%)	31,52,52	1.59	5 (16%)

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
3	ATP	A	5301	4	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5301	ATP	C5-C4	2.16	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5301	ATP	PA-O3A-PB	-3.80	119.78	132.83
3	A	5301	ATP	PB-O3B-PG	-3.58	120.54	132.83
3	A	5301	ATP	N3-C2-N1	-3.30	123.51	128.68
3	A	5301	ATP	C3'-C2'-C1'	2.90	105.34	100.98
3	A	5301	ATP	C4-C5-N7	-2.23	107.08	109.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

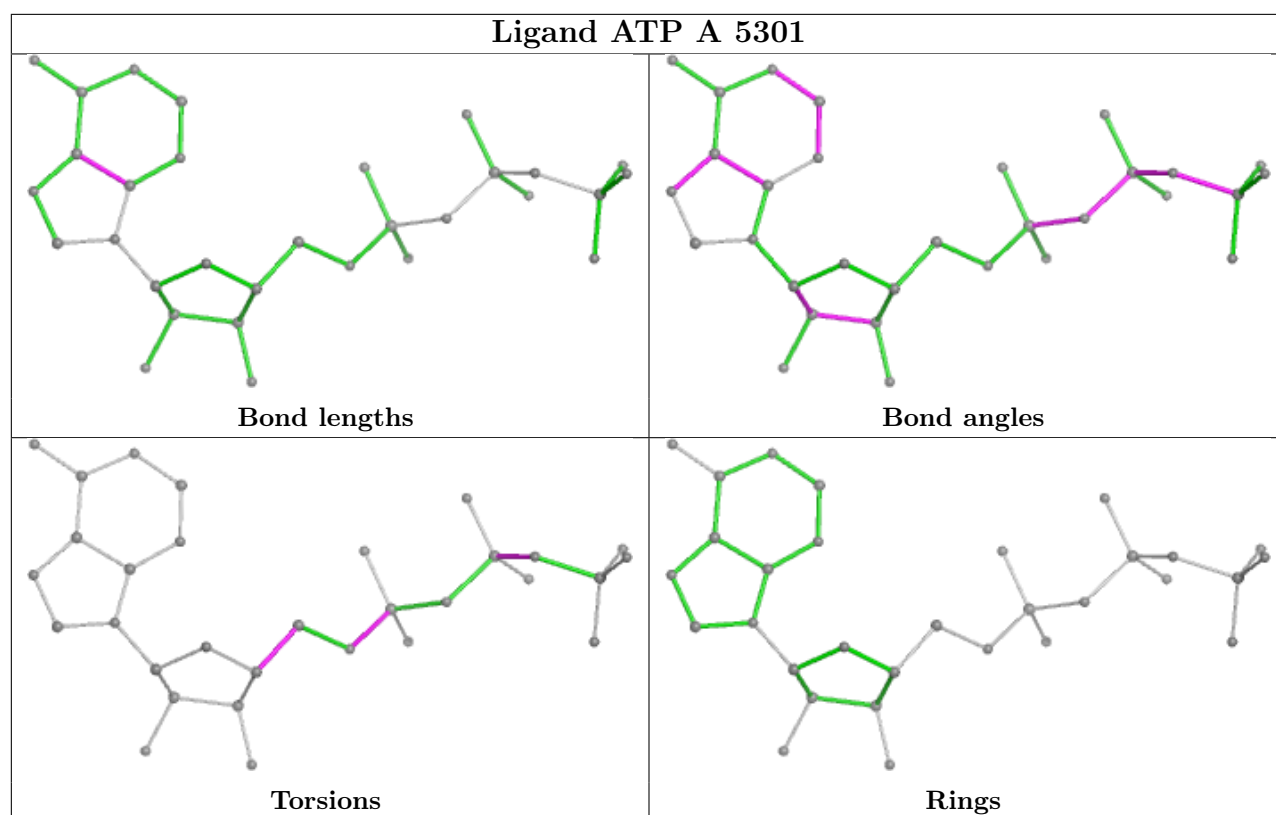
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	PG-O3B-PB-O2B
3	A	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	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.

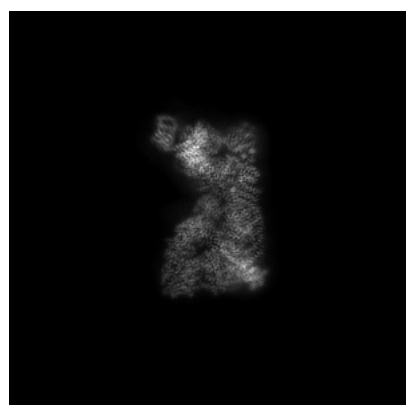
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50914. These allow visual inspection of the internal detail of the map and identification of artifacts.

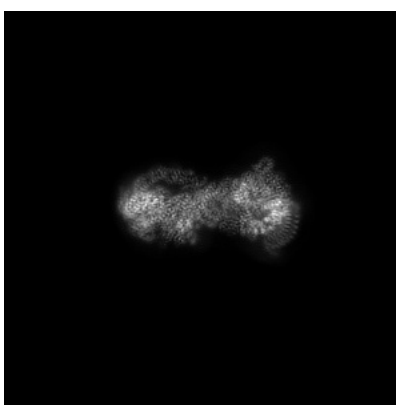
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

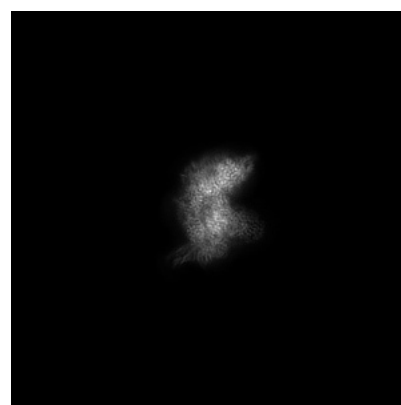
6.1.1 Primary map



X



Y

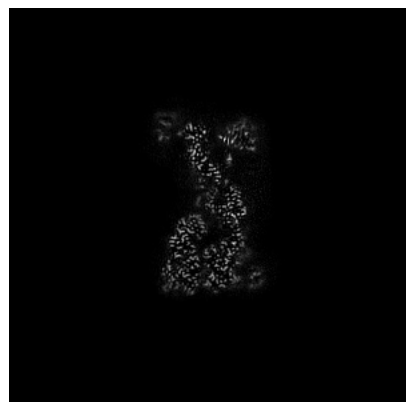


Z

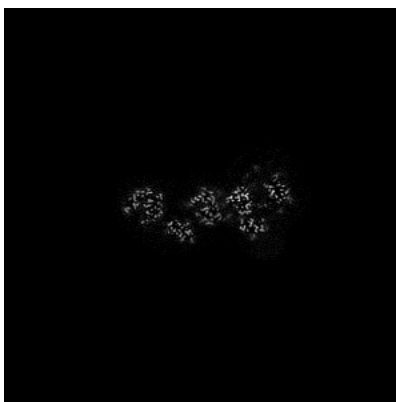
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

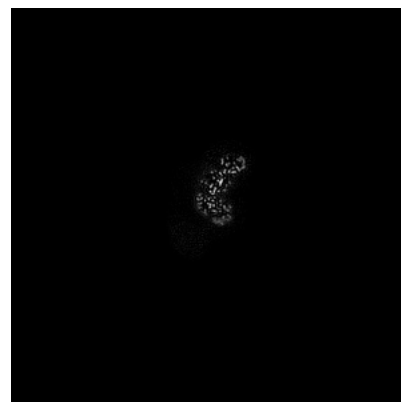
6.2.1 Primary map



X Index: 200



Y Index: 200

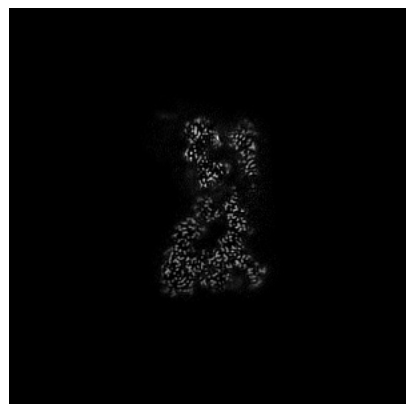


Z Index: 200

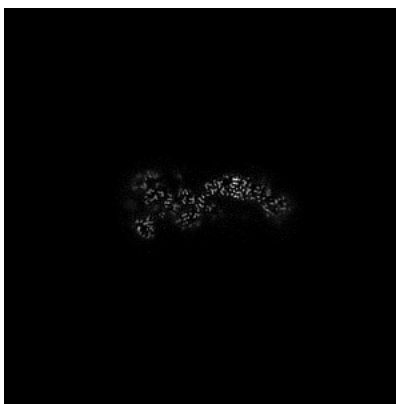
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

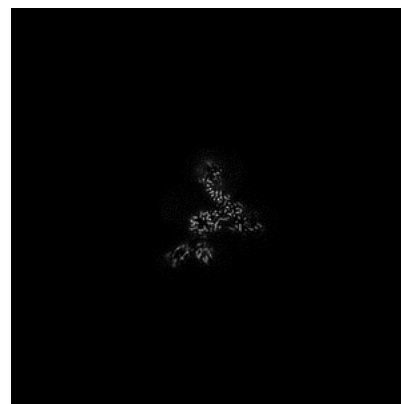
6.3.1 Primary map



X Index: 207



Y Index: 232

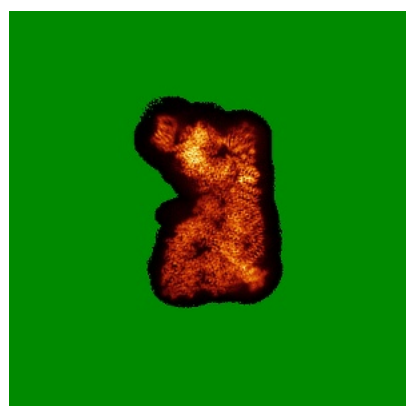


Z Index: 269

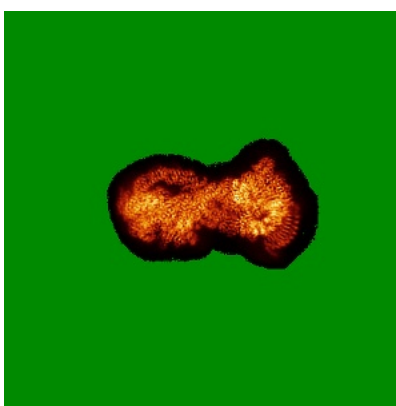
The images above show the largest variance slices of the map in three orthogonal directions.

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

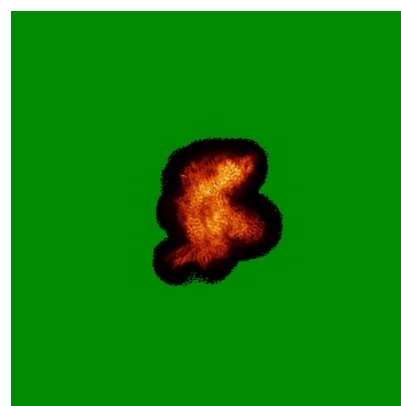
6.4.1 Primary map



X



Y

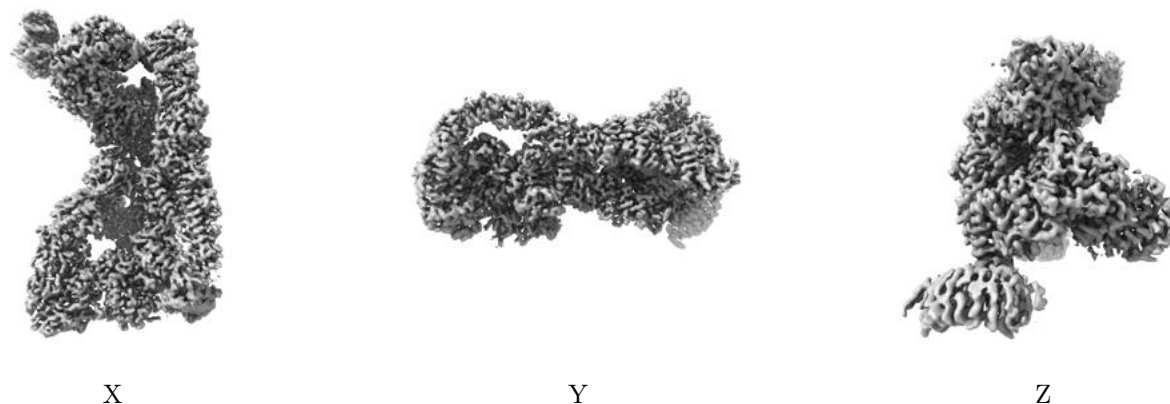


Z

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

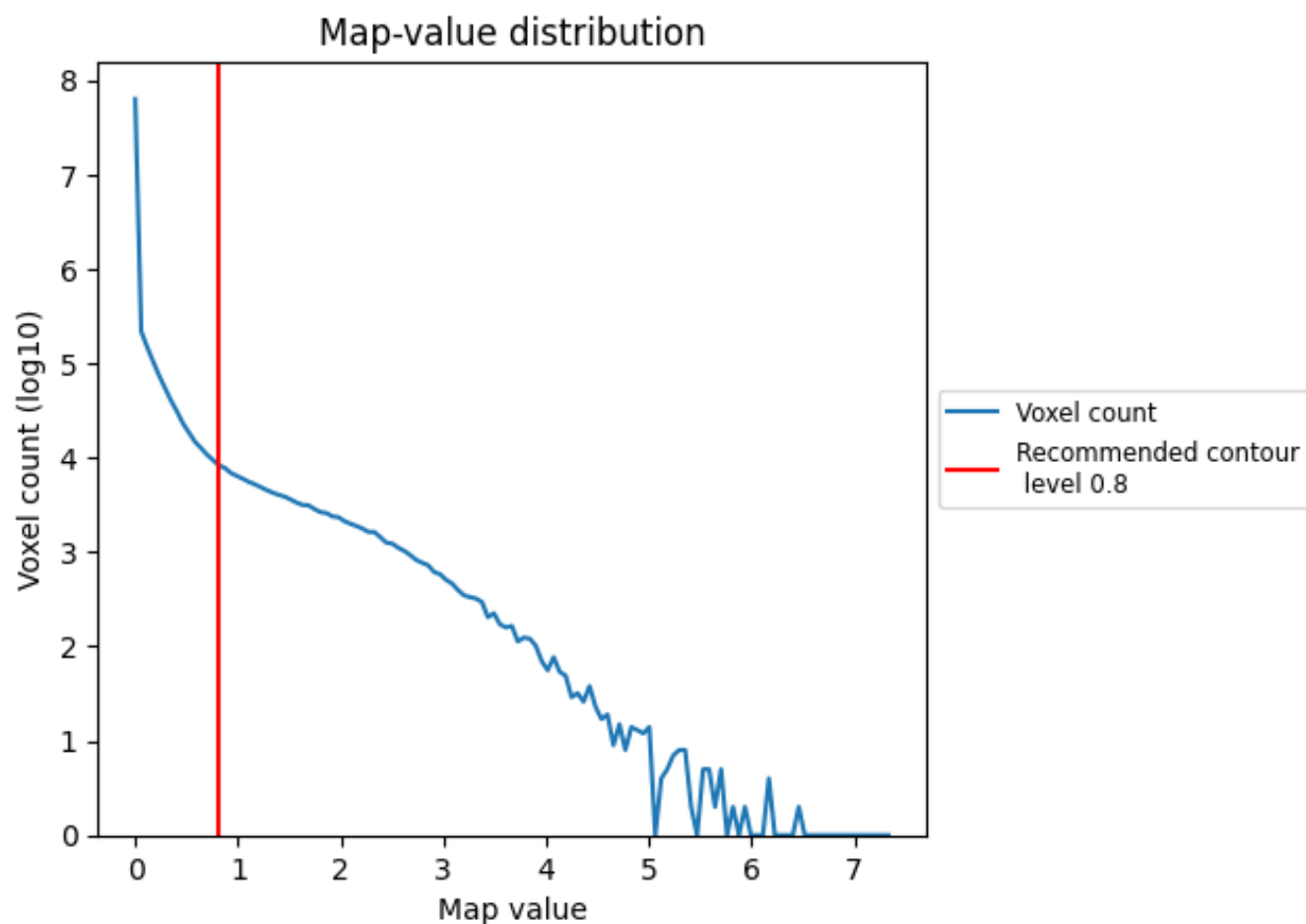
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

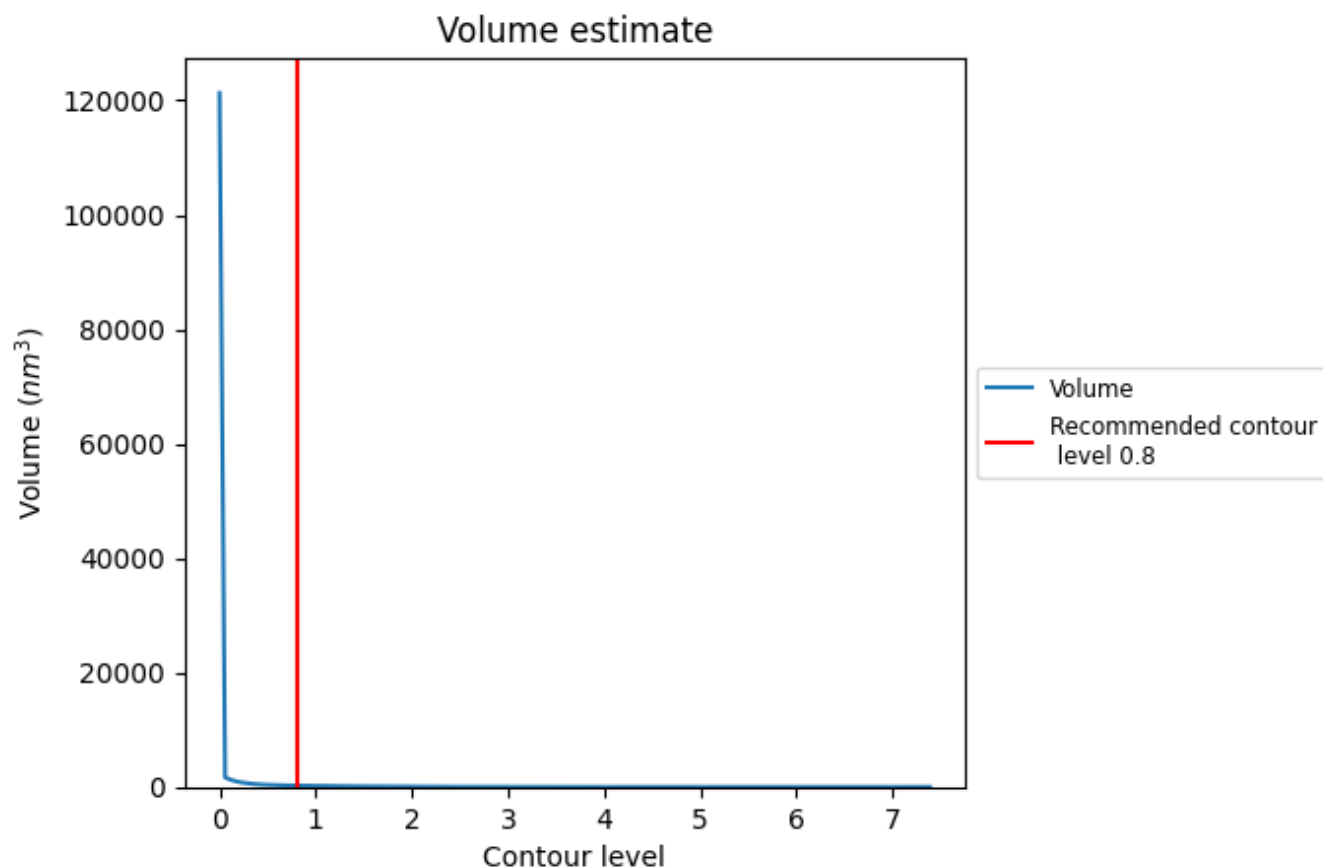
This section contains the results of statistical analysis of the map.

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.

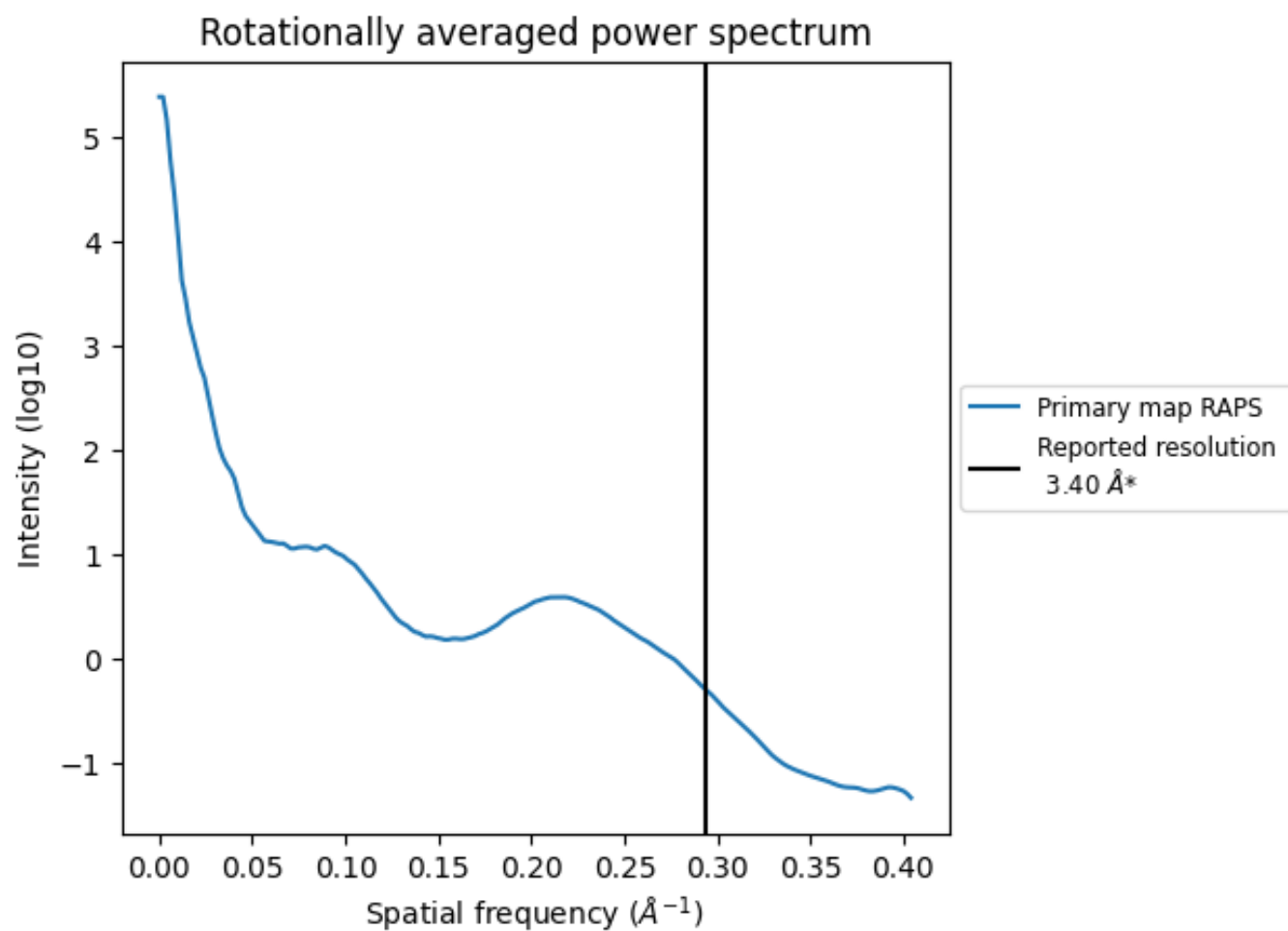
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 232 nm³; this corresponds to an approximate mass of 210 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 0.294 Å⁻¹

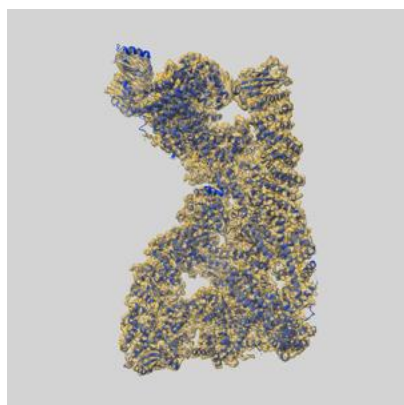
8 Fourier-Shell correlation

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

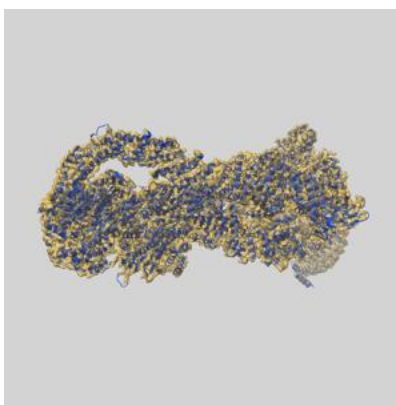
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50914 and PDB model 9G09. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

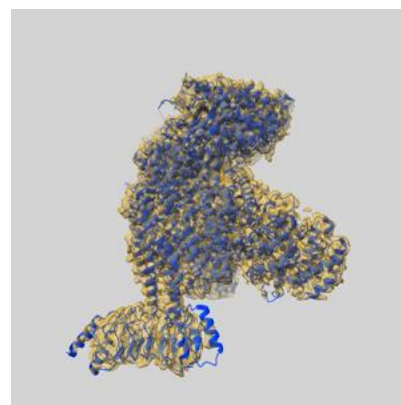
9.1 Map-model overlay [i](#)



X



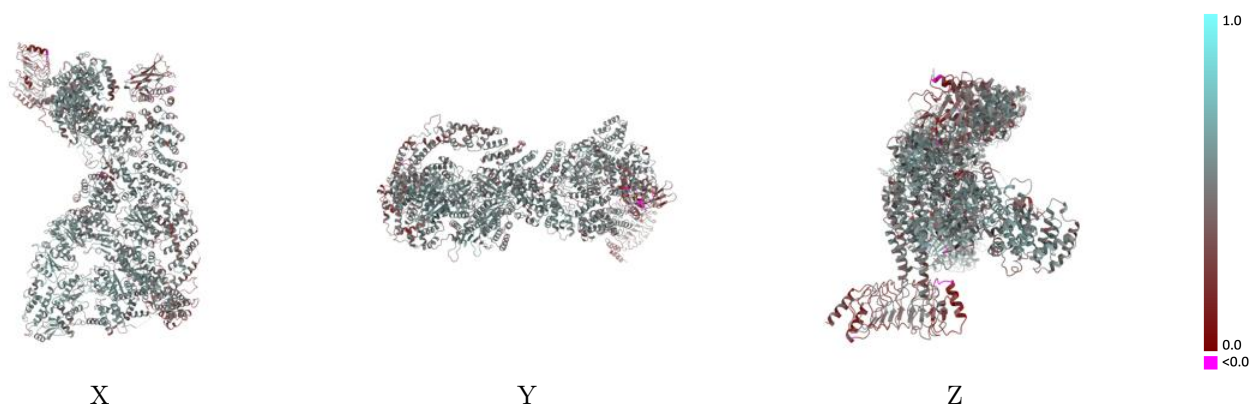
Y



Z

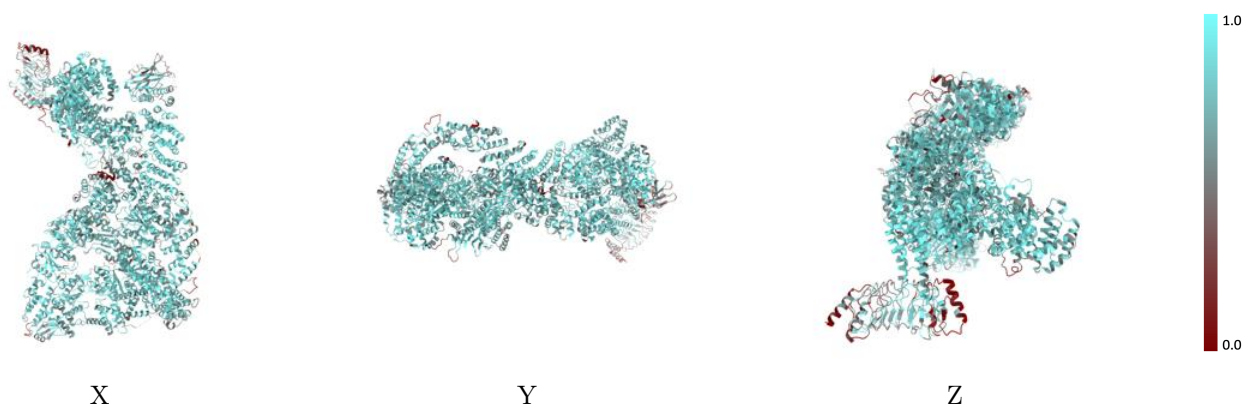
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



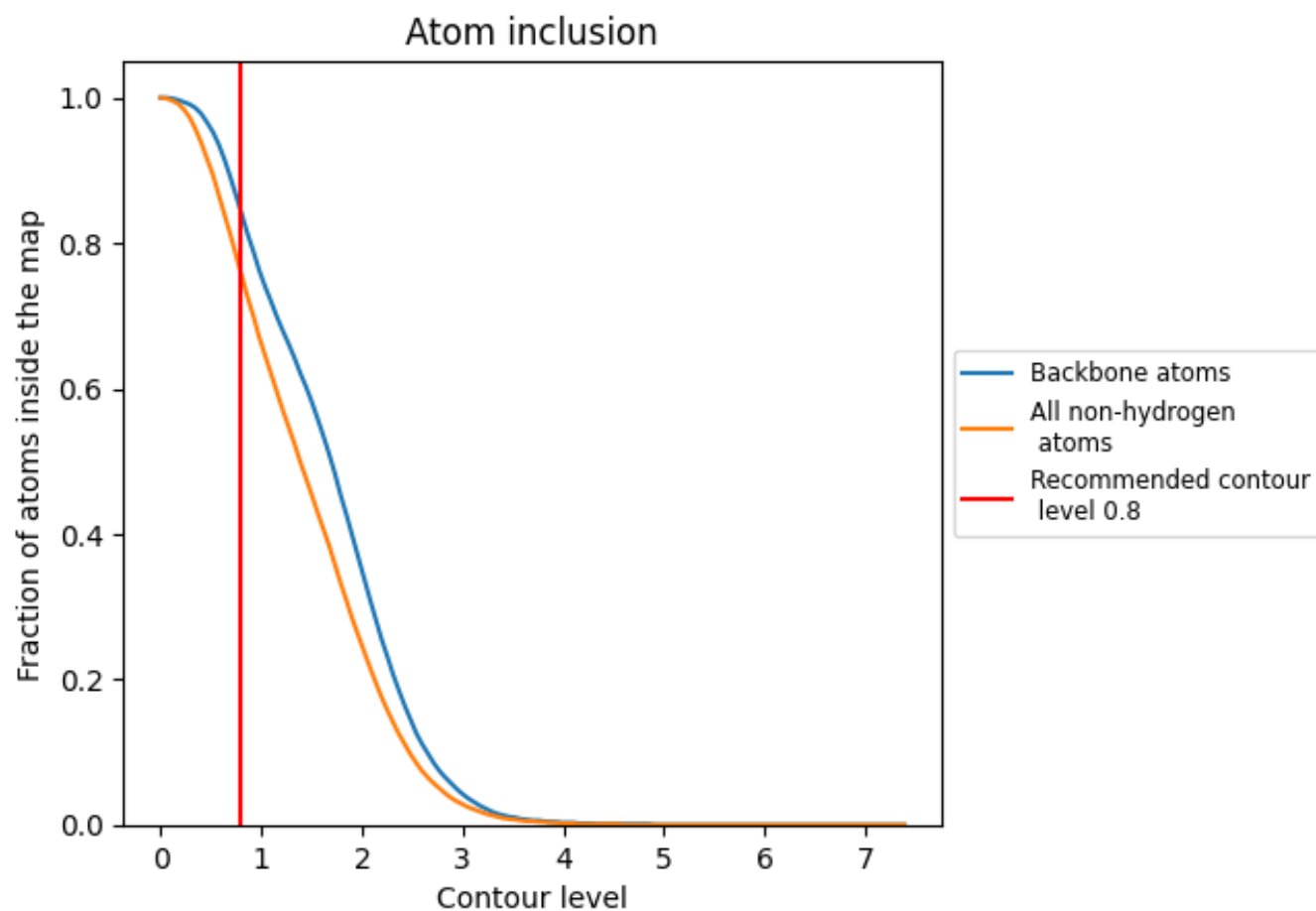
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7580	<div></div> 0.4850
A	<div></div> 0.7750	<div></div> 0.4950
B	<div></div> 0.4390	<div></div> 0.2860

