



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 07:37 AM JST

PDB ID : 7WUJ
EMDB ID : EMD-32837
Title : Tethered peptide activation mechanism of adhesion GPCRs ADGRG2 and ADGRG4
Authors : Guo, S.C.; Huang, S.M.; He, Q.T.; Xiao, P.; Sun, J.P.; Yu, X.
Deposited on : 2022-02-08
Resolution : 3.30 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.dev113
MolProbity : 4.02b-467
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) : 2.39

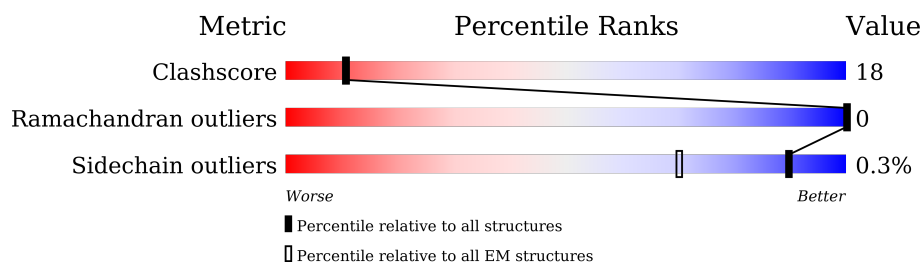
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	361	 55% 10% 35%
2	B	358	 59% 34% 7%
3	E	631	 30% 12% 58%
4	S	250	 65% 24% 11%
5	Y	71	 68% 11% 21%
6	N	128	 65% 11% 24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8600 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 mini-Gs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1655	1064	301	285	5		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	334	Total	C	N	O	S	0	0
			2318	1464	411	424	19		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Adhesion G-protein coupled receptor G4, Uncharacterized pro-

tein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	267	Total 1995	C 1341	N 310	O 326	S 18	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2704	MET	-	expression tag	UNP Q8IZF6
E	2705	LYS	-	expression tag	UNP Q8IZF6
E	2706	THR	-	expression tag	UNP Q8IZF6
E	2707	ILE	-	expression tag	UNP Q8IZF6
E	2708	ILE	-	expression tag	UNP Q8IZF6
E	2709	ALA	-	expression tag	UNP Q8IZF6
E	2710	LEU	-	expression tag	UNP Q8IZF6
E	2711	SER	-	expression tag	UNP Q8IZF6
E	2712	TYR	-	expression tag	UNP Q8IZF6
E	2713	ILE	-	expression tag	UNP Q8IZF6
E	2714	PHE	-	expression tag	UNP Q8IZF6
E	2715	CYS	-	expression tag	UNP Q8IZF6
E	2716	LEU	-	expression tag	UNP Q8IZF6
E	2717	VAL	-	expression tag	UNP Q8IZF6
E	2718	PHE	-	expression tag	UNP Q8IZF6
E	2719	ALA	-	expression tag	UNP Q8IZF6
E	3081	HIS	-	linker	UNP Q8IZF6
E	3082	HIS	-	linker	UNP Q8IZF6
E	3083	HIS	-	linker	UNP Q8IZF6
E	3084	HIS	-	linker	UNP Q8IZF6
E	3085	HIS	-	linker	UNP Q8IZF6
E	3086	HIS	-	linker	UNP Q8IZF6
E	3087	HIS	-	linker	UNP Q8IZF6
E	3088	HIS	-	linker	UNP Q8IZF6
E	3089	GLY	-	linker	UNP Q8IZF6
E	3090	SER	-	linker	UNP Q8IZF6
E	3091	ALA	-	linker	UNP Q8IZF6
E	3092	GLU	-	linker	UNP Q8IZF6
E	3093	ASN	-	linker	UNP Q8IZF6
E	3094	LEU	-	linker	UNP Q8IZF6
E	3095	TYR	-	linker	UNP Q8IZF6
E	3096	PHE	-	linker	UNP Q8IZF6
E	3097	GLN	-	linker	UNP Q8IZF6
E	3098	GLY	-	linker	UNP Q8IZF6

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	222	Total	C	N	O	S	0	0
			1574	1007	258	301	8		

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	56	Total	C	N	O	S	0	0
			363	234	62	65	2		

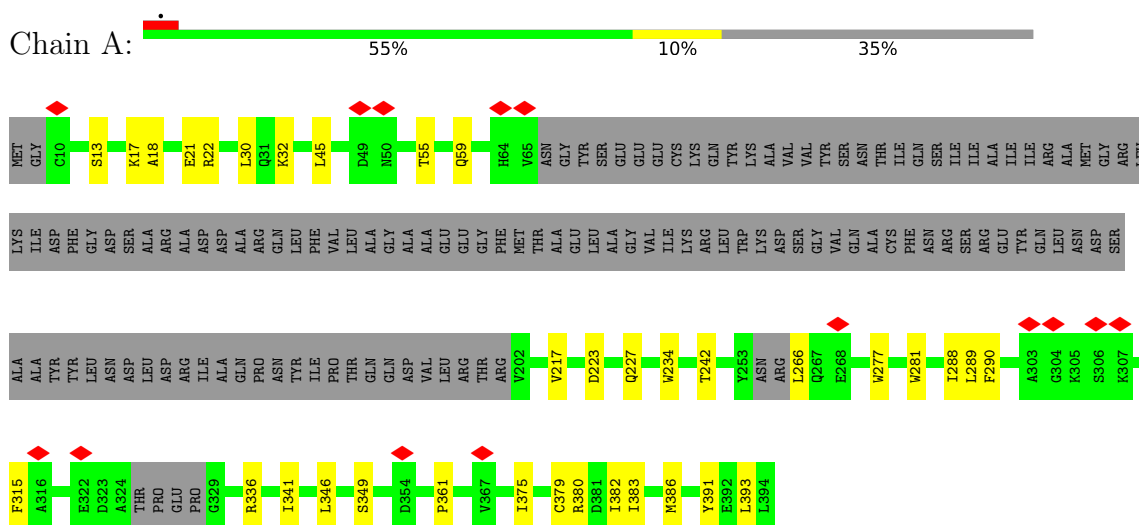
- Molecule 6 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	97	Total	C	N	O	S	0	0
			695	435	119	136	5		

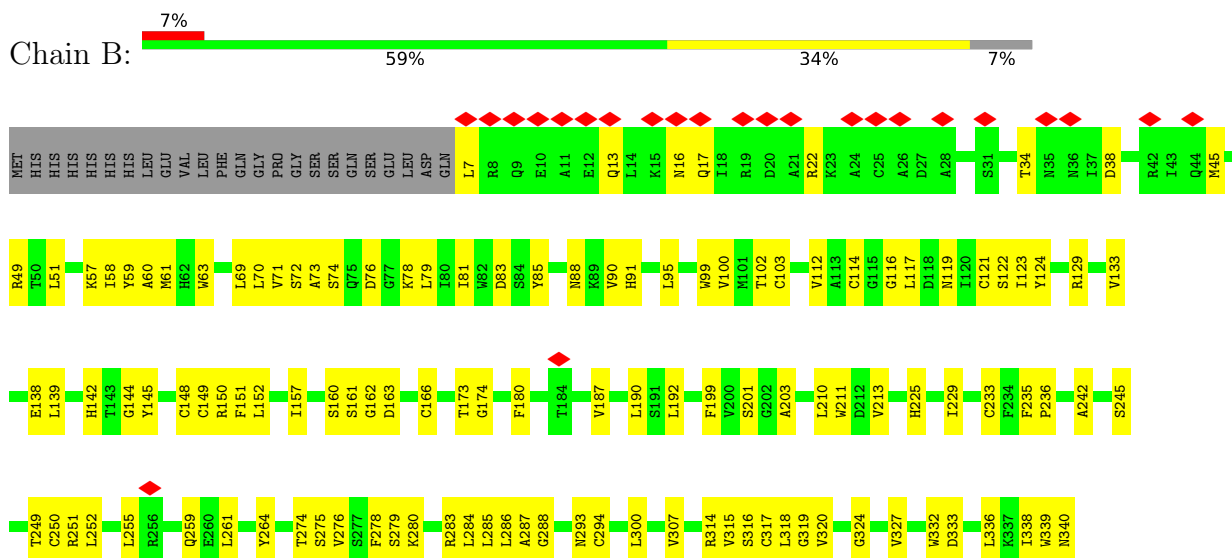
3 Residue-property plots

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: mini-Gs



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Adhesion G-protein coupled receptor G4, Uncharacterized protein

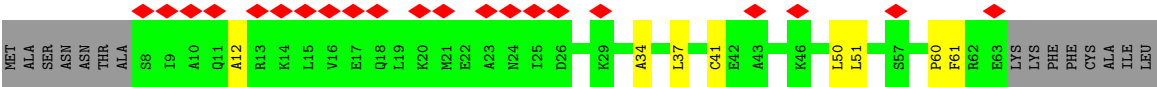
Frequency	Percentage
Daily	30%
Weekly	12%
Monthly	58%



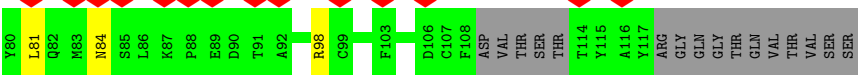
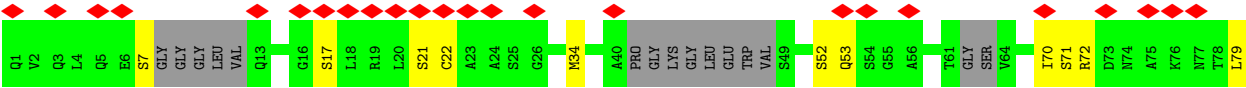
Frequency	Percentage
Daily	11%
Often	65%
Sometimes	24%
Never	11%



Frequency	Percentage
Very often	30%
Often	68%
Sometimes	11%
Never	21%



● Molecule 6: Nanobody-35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	619803	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	192.0, 192.0, 192.0	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/1685	0.52	0/2291
2	B	0.45	0/2363	0.64	0/3231
3	E	0.35	0/2048	0.56	0/2798
4	S	0.36	0/1614	0.59	0/2202
5	Y	0.28	0/369	0.52	0/510
6	N	0.34	0/706	0.57	0/959
All	All	0.38	0/8785	0.58	0/11991

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	1655	0	1443	39	0
2	B	2318	0	2118	110	0
3	E	1995	0	1899	88	0
4	S	1574	0	1391	68	0
5	Y	363	0	325	15	0
6	N	695	0	613	8	0
All	All	8600	0	7789	300	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 18.

The worst 5 of 300 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:288:ILE:HG22	1:A:290:PHE:CD1	1.61	1.34
3:E:2782:ASN:HB3	3:E:2826:TRP:CZ2	1.67	1.28
3:E:2913:PHE:CD1	3:E:2945:LEU:HD23	1.72	1.23
3:E:2948:LEU:HG	3:E:2986:HIS:HE1	1.09	1.15
1:A:288:ILE:CG2	1:A:290:PHE:CD1	2.30	1.14

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	225/361 (62%)	207 (92%)	18 (8%)	0	100	100
2	B	332/358 (93%)	308 (93%)	24 (7%)	0	100	100
3	E	259/631 (41%)	247 (95%)	12 (5%)	0	100	100
4	S	214/250 (86%)	195 (91%)	19 (9%)	0	100	100
5	Y	54/71 (76%)	50 (93%)	4 (7%)	0	100	100
6	N	87/128 (68%)	81 (93%)	6 (7%)	0	100	100
All	All	1171/1799 (65%)	1088 (93%)	83 (7%)	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	133/315 (42%)	133 (100%)	0	100	100
2	B	211/299 (71%)	211 (100%)	0	100	100
3	E	194/552 (35%)	192 (99%)	2 (1%)	73	84
4	S	149/202 (74%)	149 (100%)	0	100	100
5	Y	28/58 (48%)	28 (100%)	0	100	100
6	N	67/106 (63%)	67 (100%)	0	100	100
All	All	782/1532 (51%)	780 (100%)	2 (0%)	90	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	2809	CYS
3	E	2827	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	2919	GLN
3	E	2978	GLN
6	N	3	GLN
3	E	2986	HIS
2	B	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [i](#)

There are no ligands in this entry.

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.

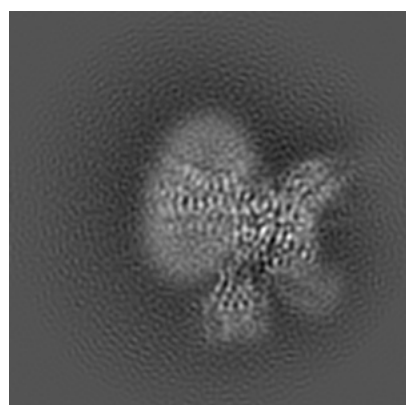
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32837. These allow visual inspection of the internal detail of the map and identification of artifacts.

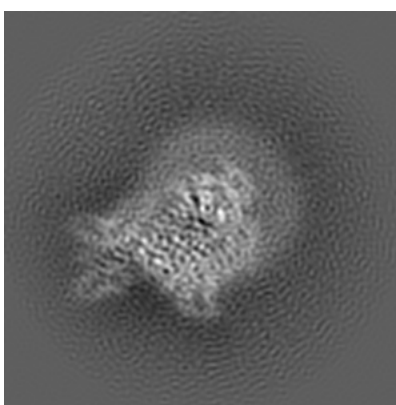
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

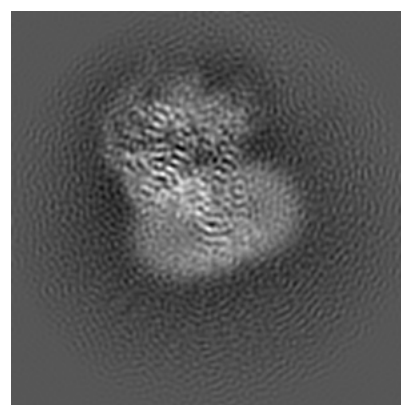
6.1.1 Primary map



X



Y

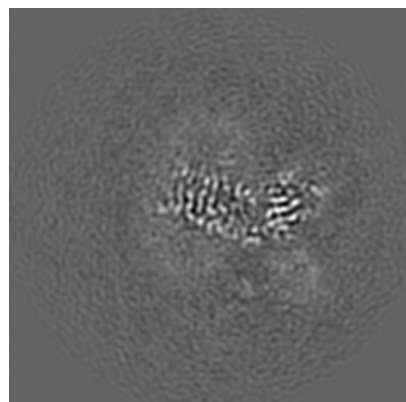


Z

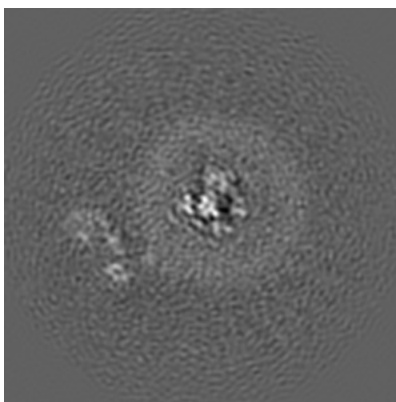
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

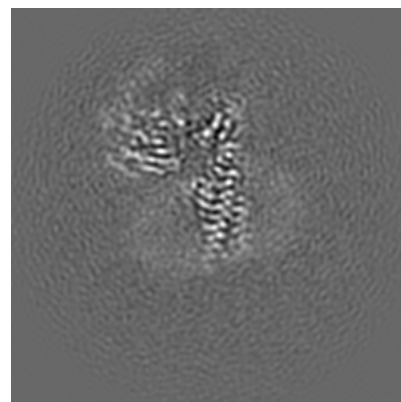
6.2.1 Primary map



X Index: 64



Y Index: 64

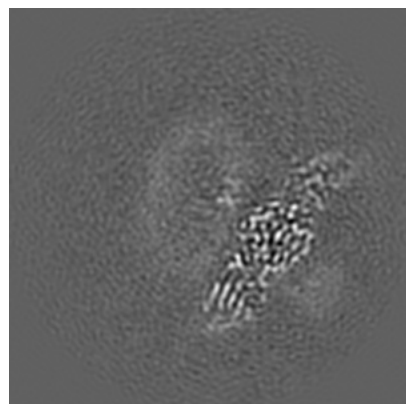


Z Index: 64

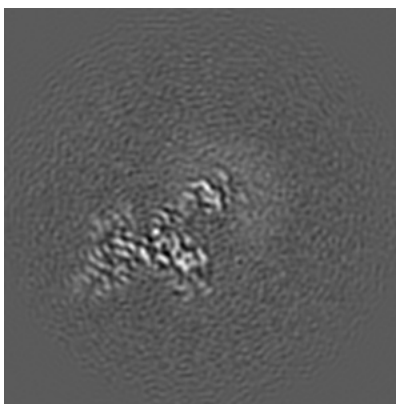
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

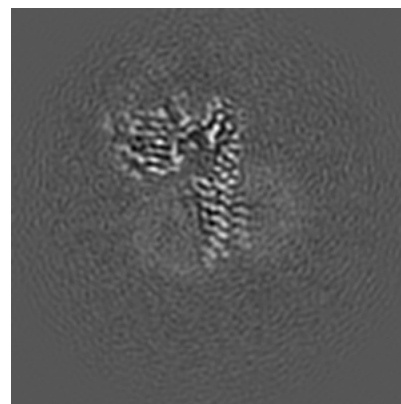
6.3.1 Primary map



X Index: 54



Y Index: 75

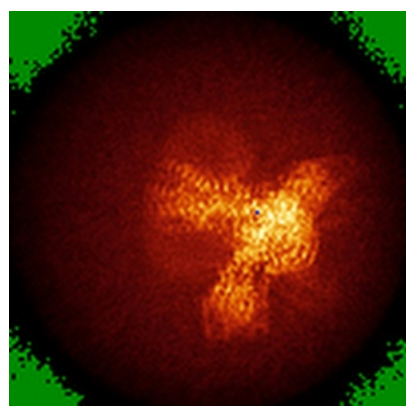


Z Index: 63

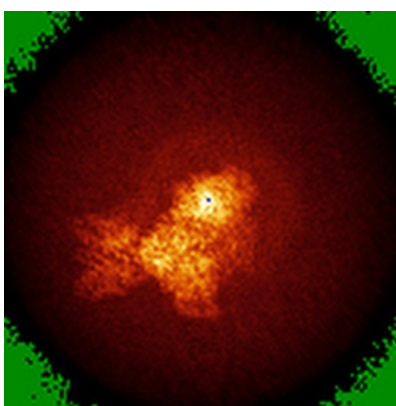
The images above show the largest variance slices of the map in three orthogonal directions.

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

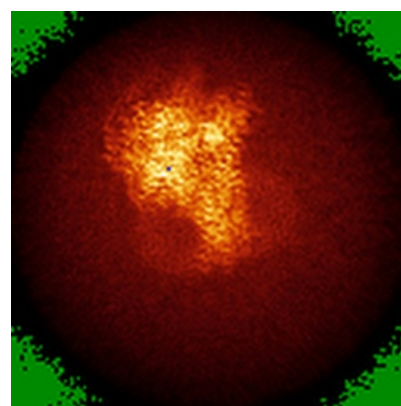
6.4.1 Primary map



X



Y

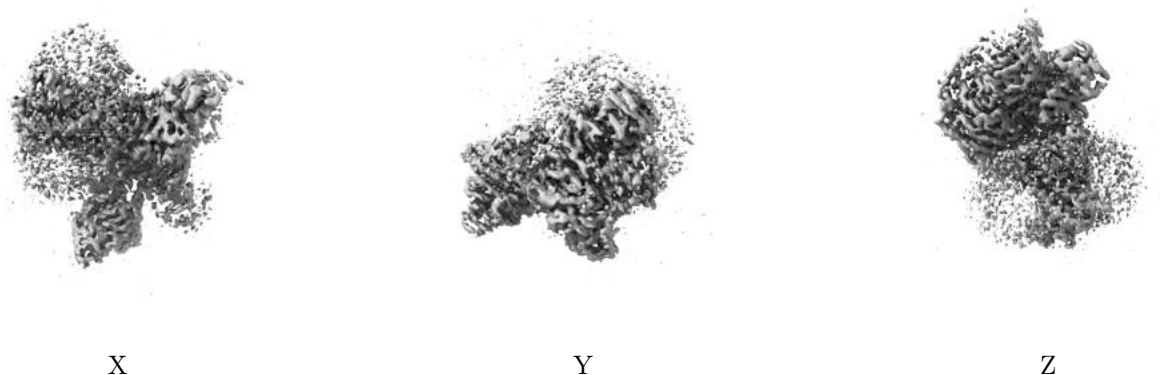


Z

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

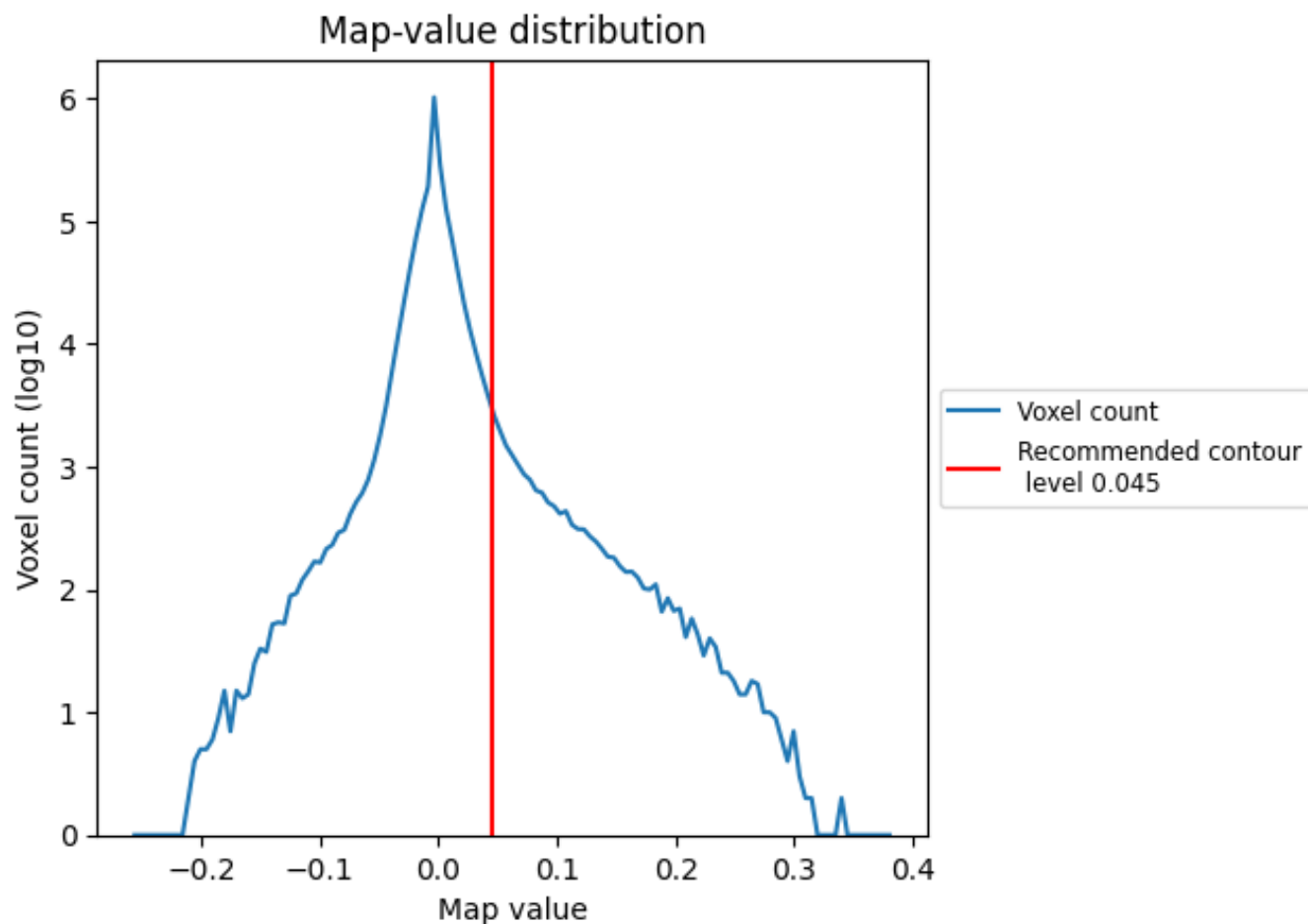
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

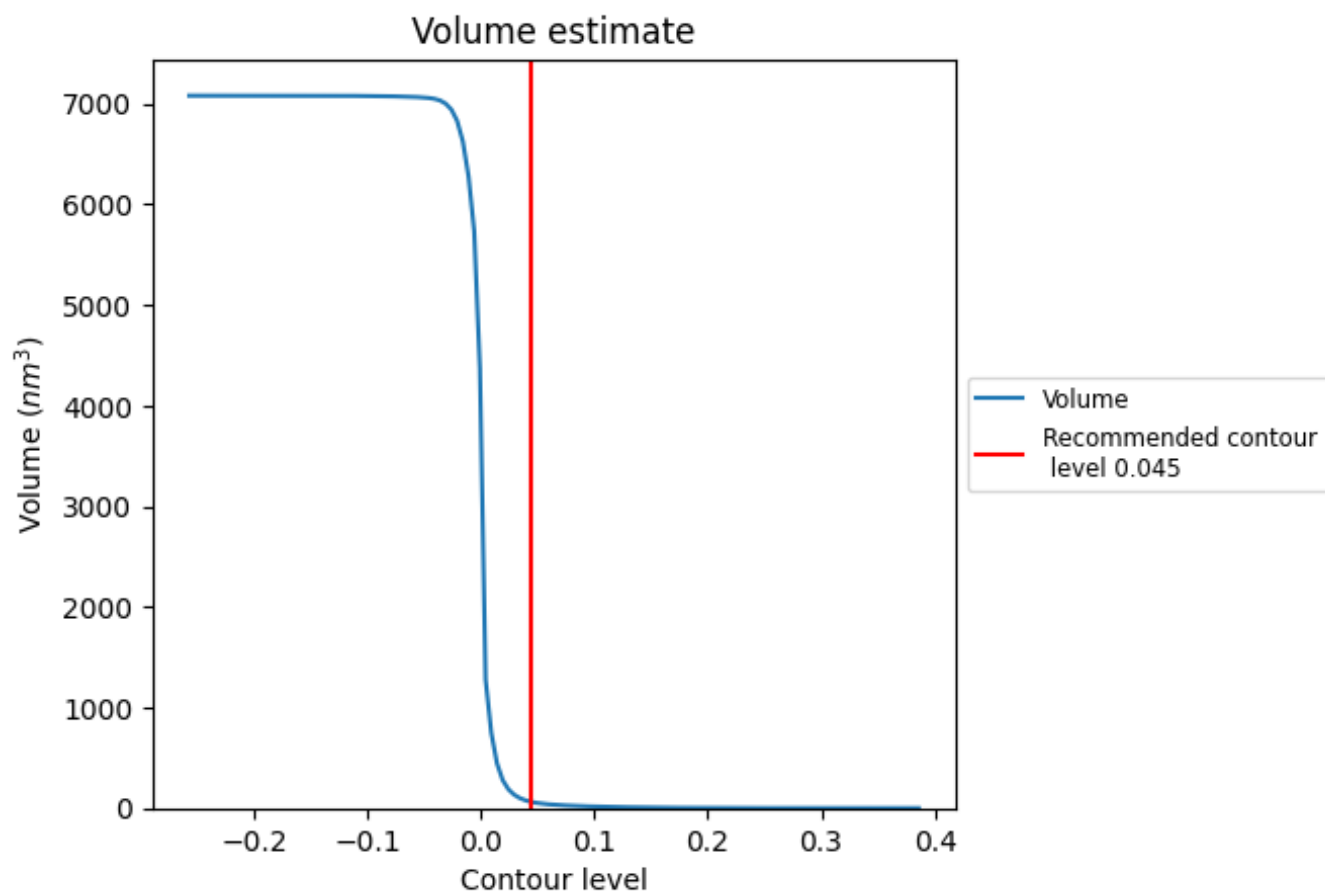
This section contains the results of statistical analysis of the map.

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.

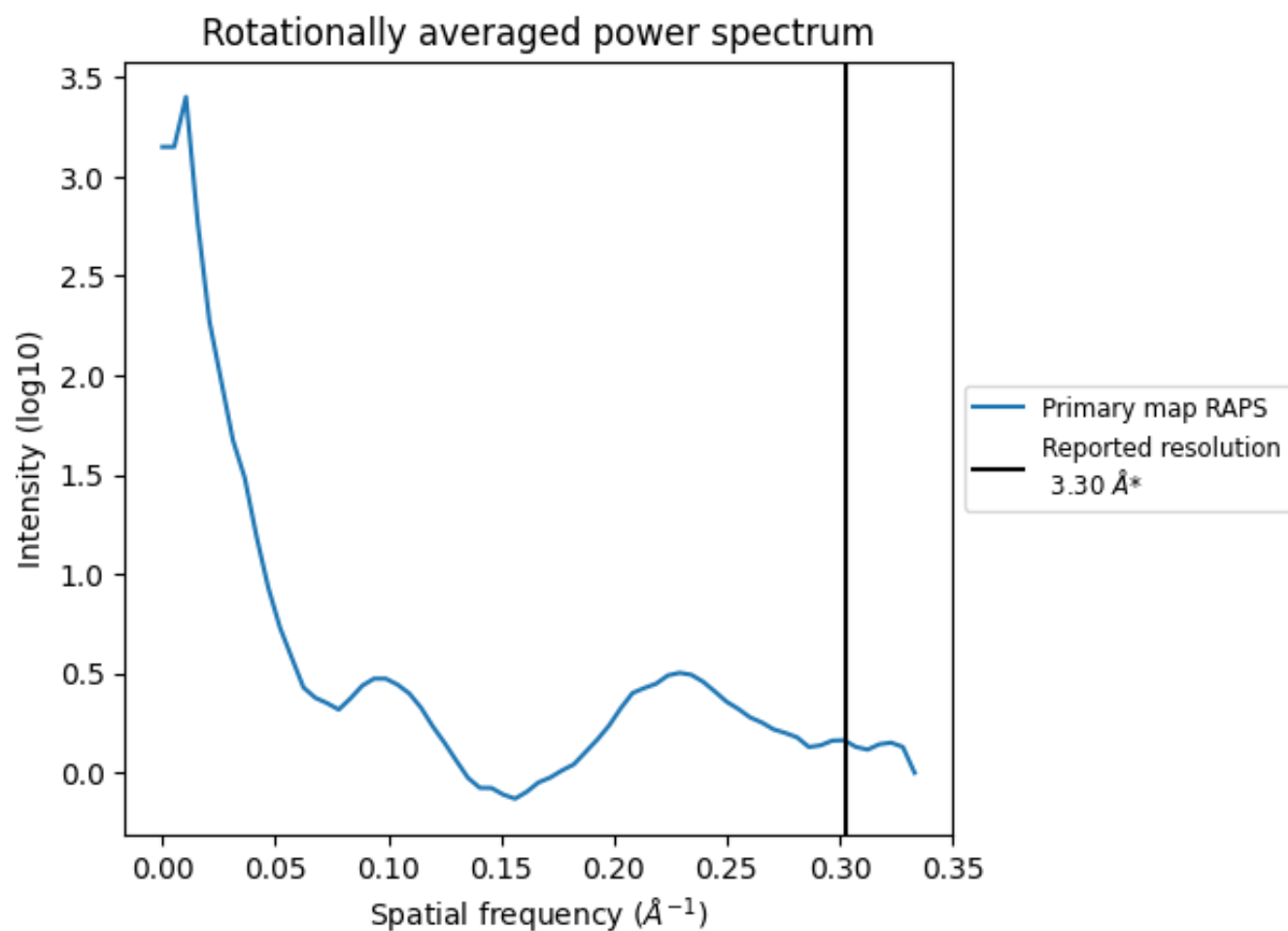
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm³; this corresponds to an approximate mass of 55 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 0.303 Å⁻¹

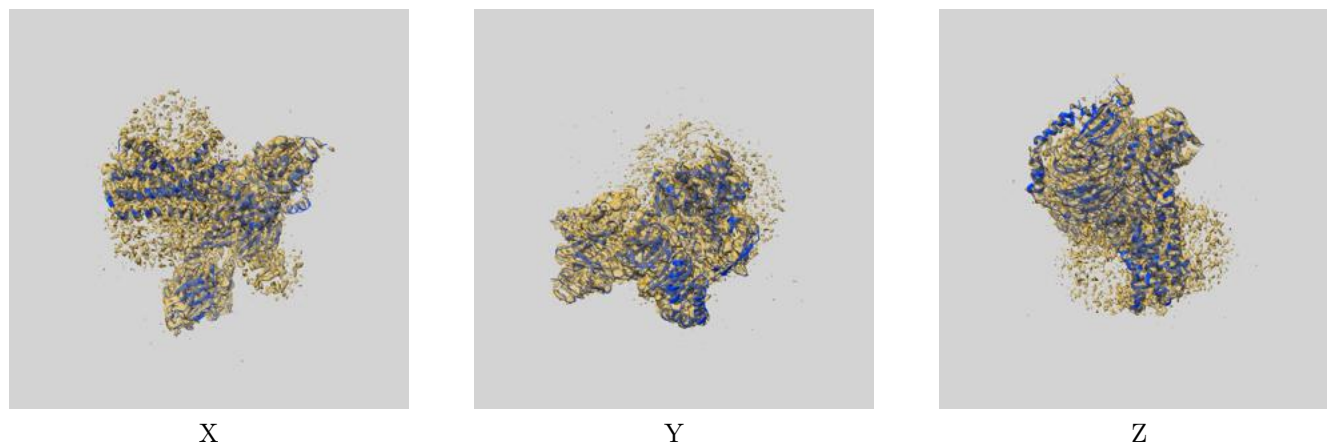
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

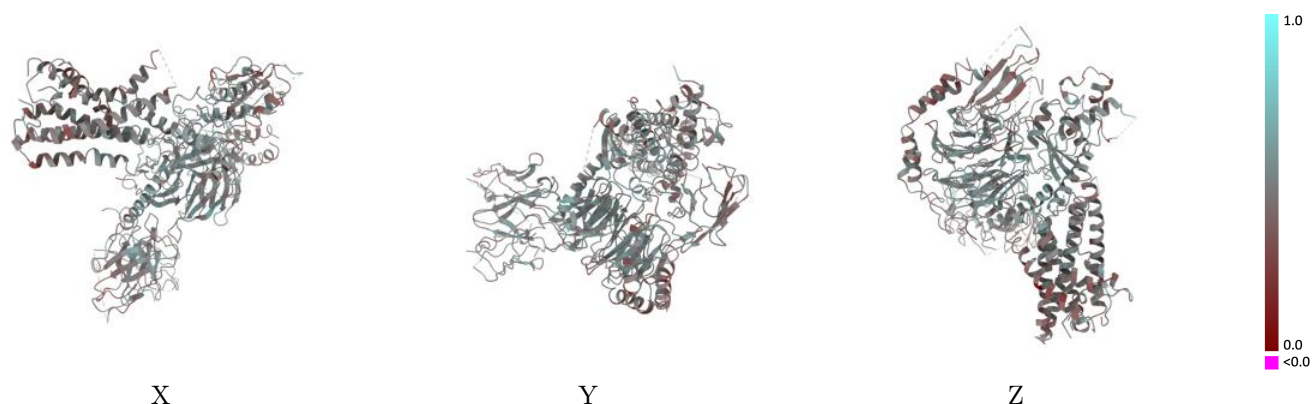
This section contains information regarding the fit between EMDB map EMD-32837 and PDB model 7WUJ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



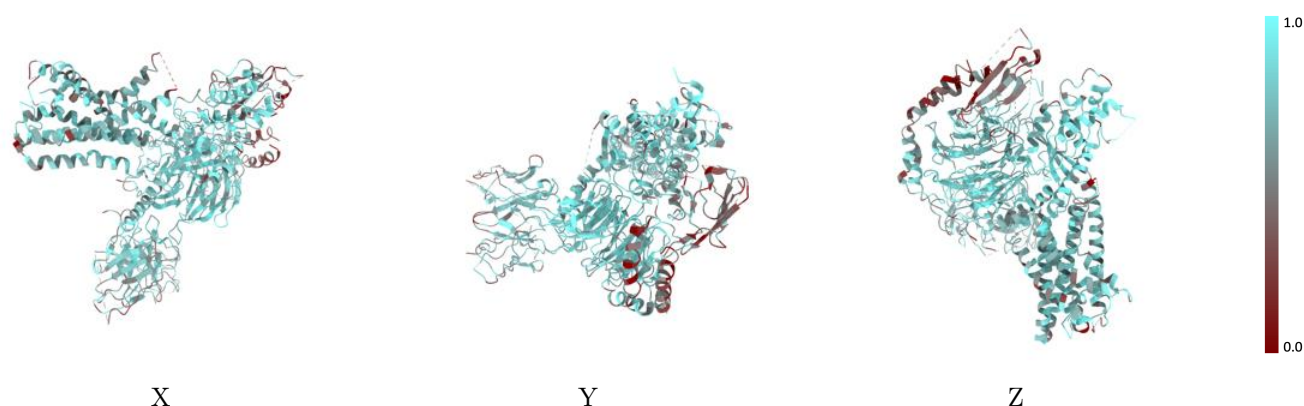
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



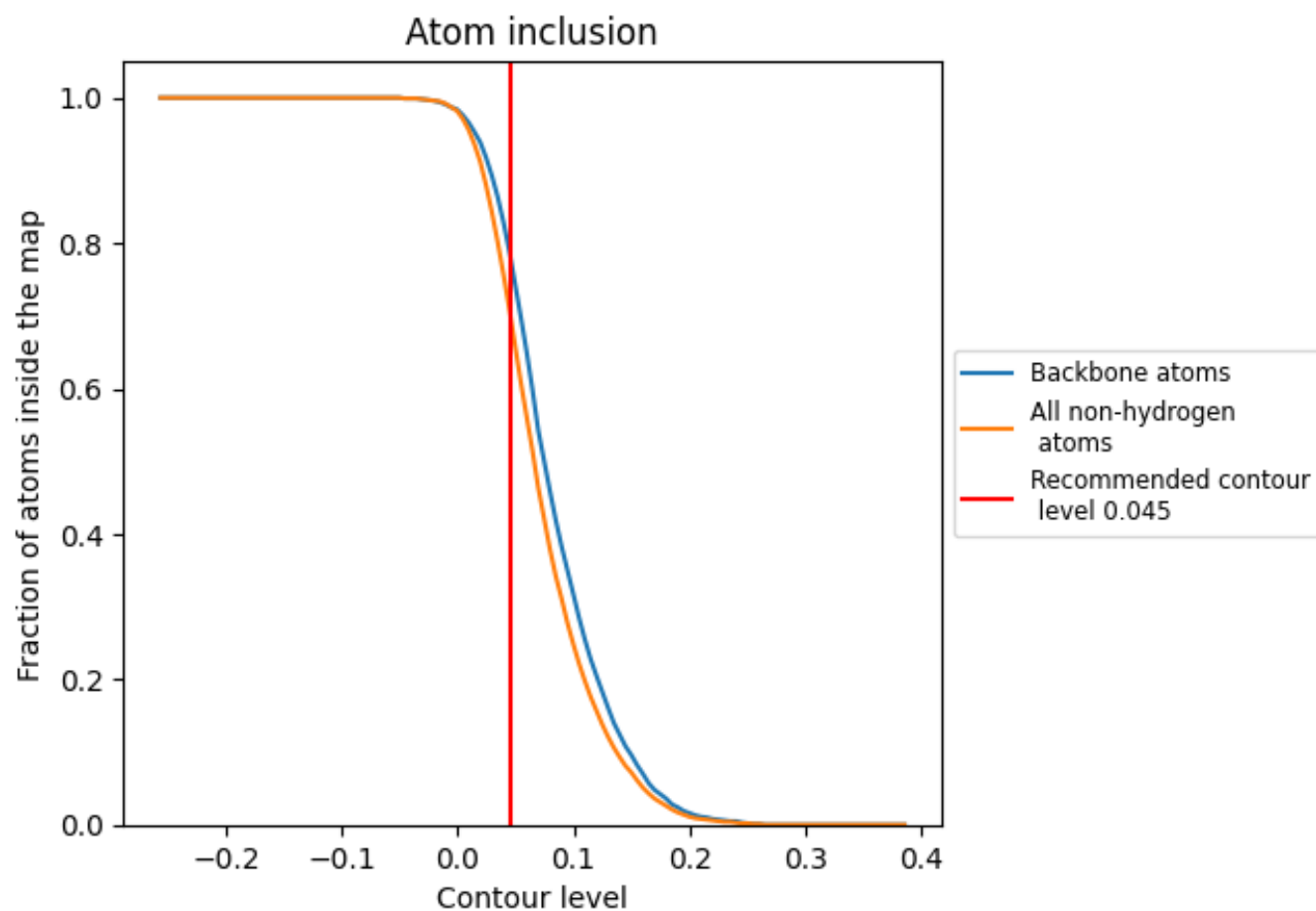
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.4740
A	<div></div> 0.7840	<div></div> 0.5050
B	<div></div> 0.7640	<div></div> 0.4940
E	<div></div> 0.7000	<div></div> 0.4470
N	<div></div> 0.5230	<div></div> 0.4550
S	<div></div> 0.6700	<div></div> 0.4680
Y	<div></div> 0.5140	<div></div> 0.4230

