



wwPDB EM Validation Summary Report ⓘ

Feb 26, 2024 – 03:26 PM EST

PDB ID : 8G9S
EMDB ID : EMD-29877
Title : Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3
for Genome Editing Applications
Authors : Hu, C.; Nam, K.H.; Ke, A.
Deposited on : 2023-02-22
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:

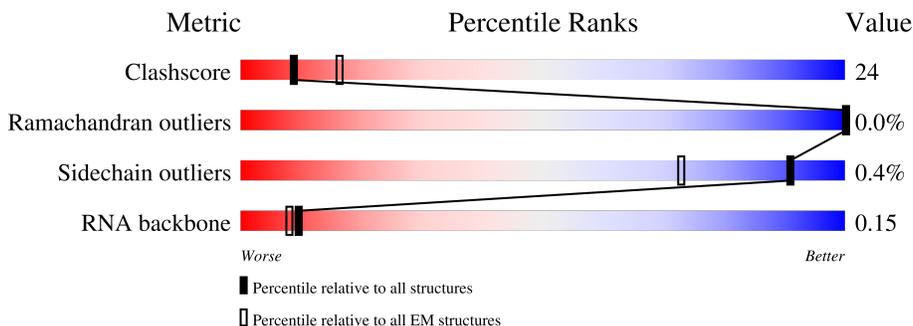
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.40 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.



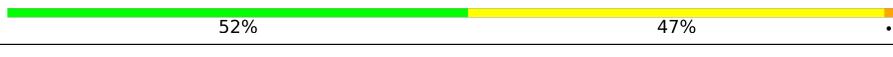
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	283	55% 45%
1	C	283	58% 42% .
1	D	283	60% 40%
1	E	283	53% 47%
1	F	283	46% 47% 6%
1	G	283	47% 49% .
1	M	283	53% 40% 7%

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Mol	Chain	Length	Quality of chain
2	H	124	 <p>49% 50%</p>
2	I	124	 <p>52% 47%</p>
2	J	124	 <p>52% 48%</p>
2	L	124	 <p>19% 60% 31% 8%</p>
3	N	205	 <p>49% 51%</p>
4	O	42	 <p>7% 40% 52%</p>
5	K	409	 <p>60% 40%</p>
6	A	70	 <p>50% 49%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25758 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 Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	283	2261	1408	406	436	11	0	0
1	C	283	2261	1408	406	436	11	0	0
1	D	283	2261	1408	406	436	11	0	0
1	E	283	2261	1408	406	436	11	0	0
1	F	265	2124	1331	379	404	10	0	0
1	G	271	2173	1360	391	411	11	0	0
1	M	264	2110	1318	379	402	11	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	284	GLY	-	expression tag	UNP A0A378VEU0
C	284	GLY	-	expression tag	UNP A0A378VEU0
D	284	GLY	-	expression tag	UNP A0A378VEU0
E	284	GLY	-	expression tag	UNP A0A378VEU0
F	284	GLY	-	expression tag	UNP A0A378VEU0
G	284	GLY	-	expression tag	UNP A0A378VEU0
M	284	GLY	-	expression tag	UNP A0A378VEU0

- Molecule 2 is a protein called Cas11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	124	1007	646	180	179	2	0	0
2	I	124	1007	646	180	179	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
2	L	114	Total	C	N	O	S	0	0
			917	588	163	165	1		

- Molecule 3 is a protein called Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	205	Total	C	N	O	S	0	0
			1673	1067	289	305	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	32	ALA	SER	conflict	UNP D0W8X4

- Molecule 4 is a RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	42	Total	C	N	O	P	0	0
			895	399	158	296	42		

- Molecule 5 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	409	Total	C	N	O	S	0	0
			3223	2056	569	586	12		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	initiating methionine	UNP A0A378VF47
K	2	ILE	-	expression tag	UNP A0A378VF47
K	3	LEU	-	expression tag	UNP A0A378VF47
K	4	HIS	-	expression tag	UNP A0A378VF47
K	5	ALA	-	expression tag	UNP A0A378VF47
K	6	LEU	VAL	conflict	UNP A0A378VF47
K	7	THR	SER	conflict	UNP A0A378VF47
K	9	TYR	ALA	conflict	UNP A0A378VF47
K	10	TYR	ASN	conflict	UNP A0A378VF47
K	12	ARG	THR	conflict	UNP A0A378VF47

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Chain	Residue	Modelled	Actual	Comment	Reference
K	13	LYS	GLN	conflict	UNP A0A378VF47
K	14	ALA	SER	conflict	UNP A0A378VF47
K	15	GLU	ASP	conflict	UNP A0A378VF47
K	16	SER	ASN	conflict	UNP A0A378VF47
K	190	ALA	VAL	conflict	UNP A0A378VF47
K	239	ALA	ILE	conflict	UNP A0A378VF47
K	242	ILE	VAL	conflict	UNP A0A378VF47
K	260	GLY	SER	conflict	UNP A0A378VF47
K	271	THR	ALA	conflict	UNP A0A378VF47

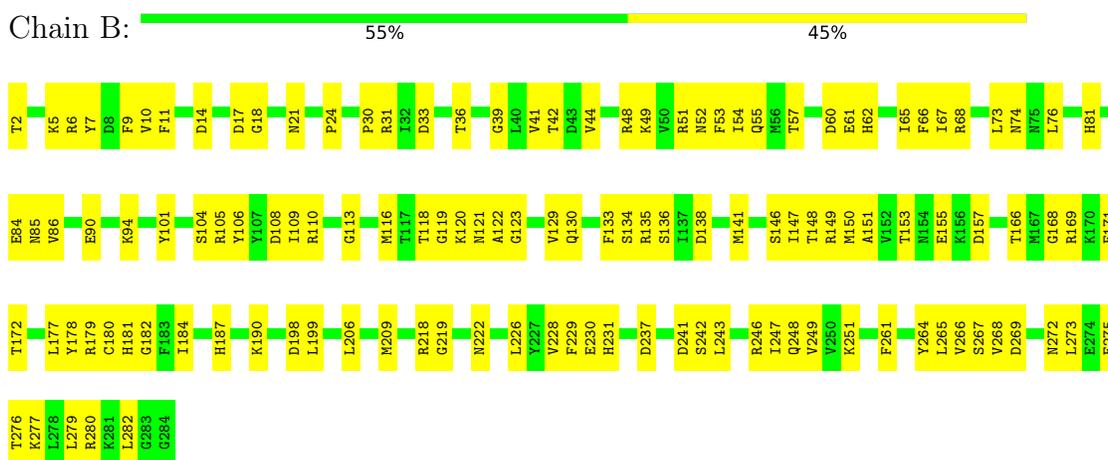
- Molecule 6 is a protein called AcrIC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	70	578	367	102	108	1	0	0

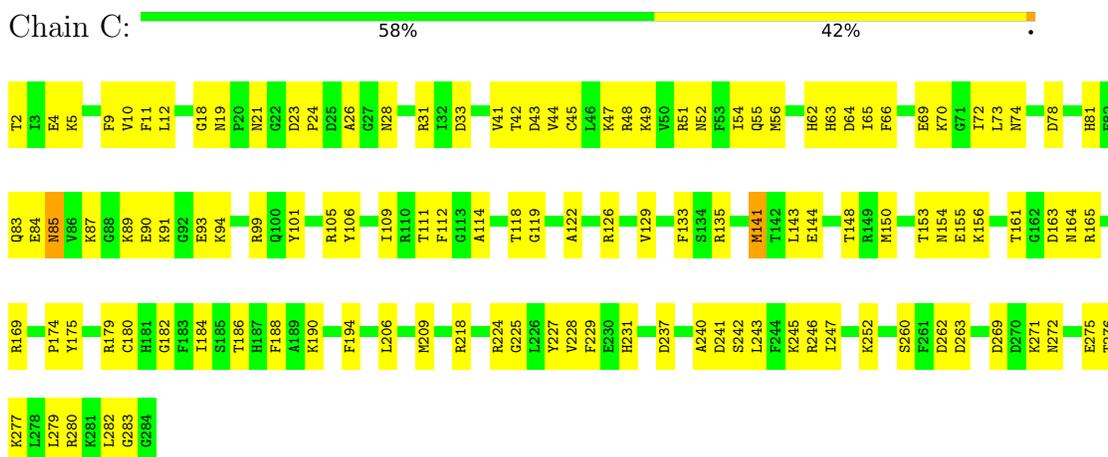
3 Residue-property plots [i](#)

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.

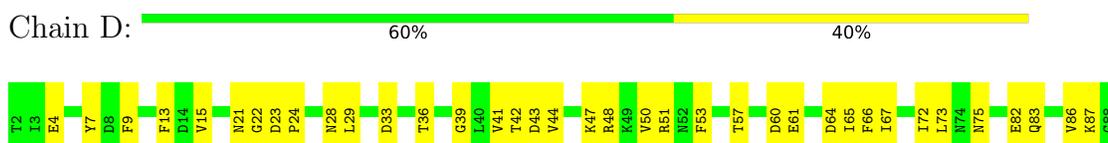
- Molecule 1: Cas7

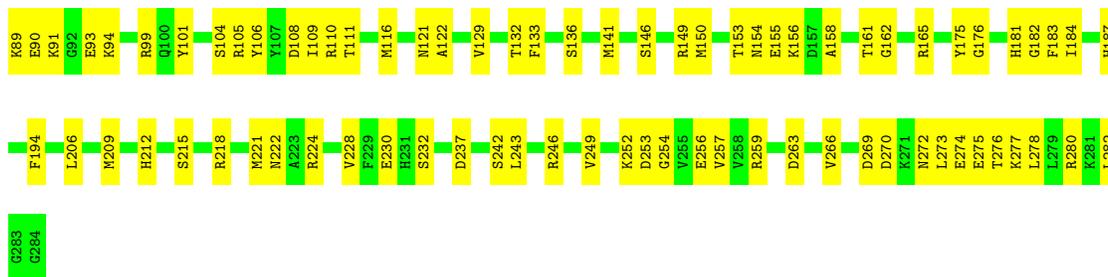


- Molecule 1: Cas7

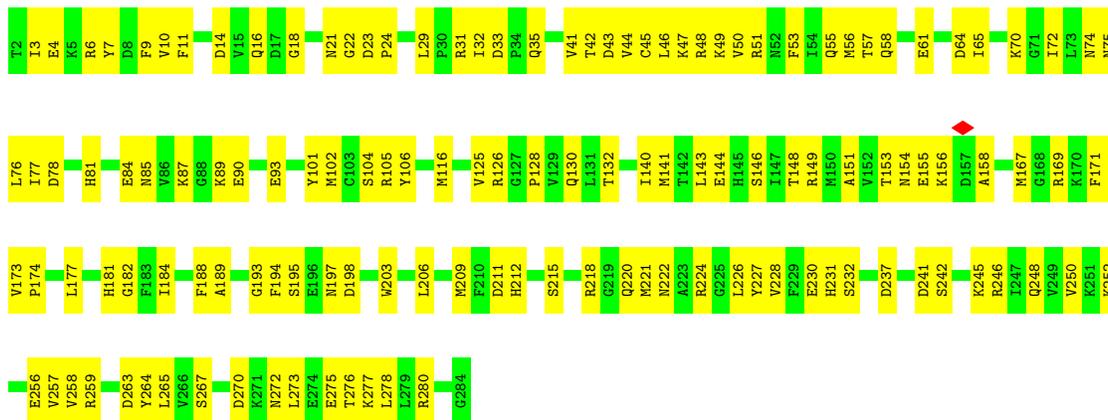


- Molecule 1: Cas7

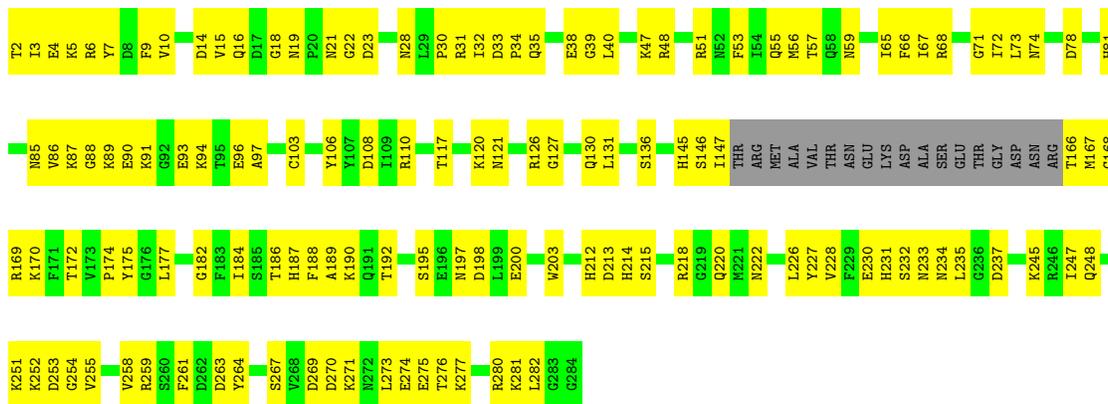




• Molecule 1: Cas7

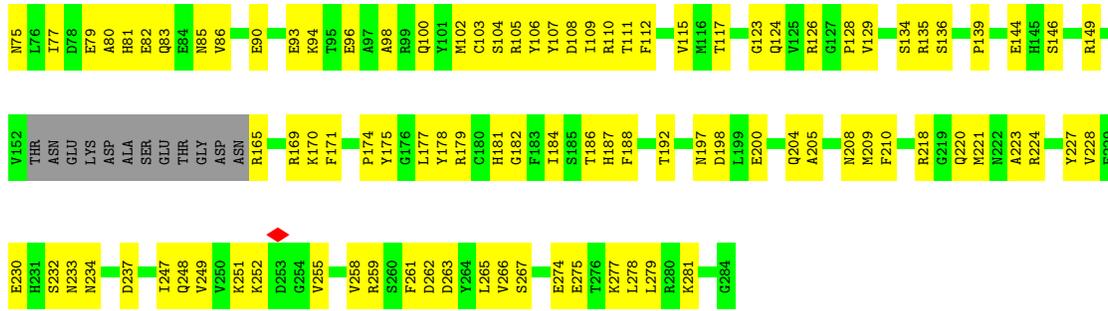


• Molecule 1: Cas7

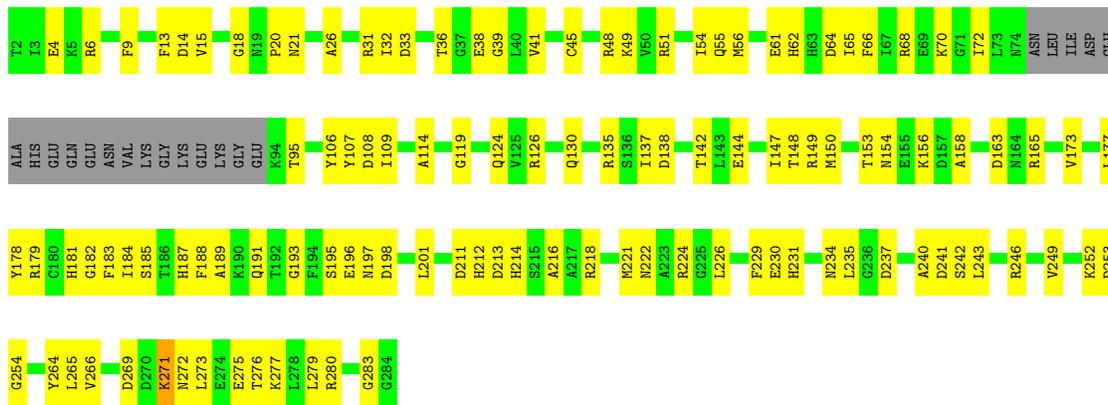


• Molecule 1: Cas7

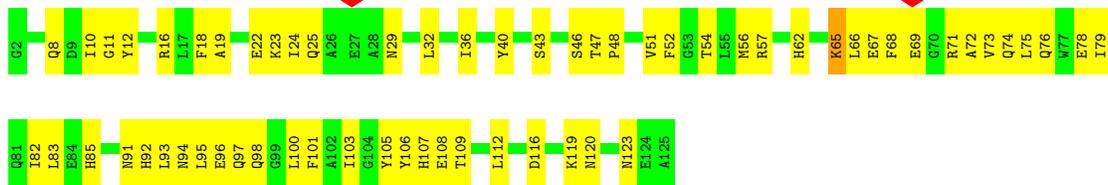




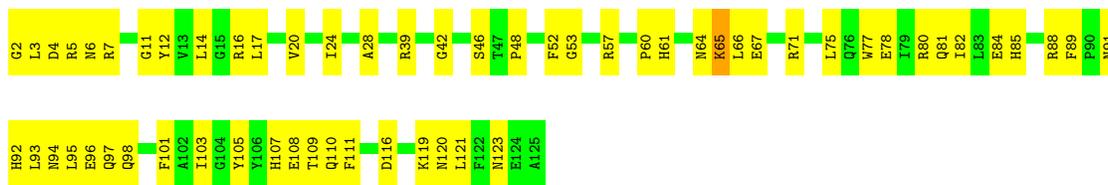
• Molecule 1: Cas7



• Molecule 2: Cas11



• Molecule 2: Cas11



• Molecule 2: Cas11

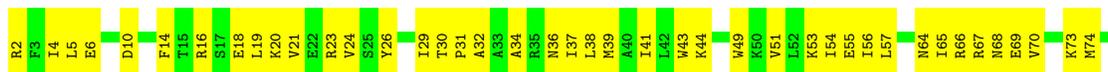




• Molecule 2: Cas11



• Molecule 3: Cas5



• Molecule 4: RNA (42-MER)



• Molecule 5: Cas8





• Molecule 6: AcrIC8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.085	Depositor
Minimum map value	-0.631	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.118	Depositor
Map size (Å)	353.1, 353.1, 353.1	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4124, 1.4124, 1.4124	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	B	0.49	0/2303	0.53	0/3101
1	C	0.52	0/2303	0.54	0/3101
1	D	0.48	0/2303	0.55	0/3101
1	E	0.44	0/2303	0.52	0/3101
1	F	0.36	0/2165	0.49	0/2914
1	G	0.29	0/2214	0.48	0/2979
1	M	0.43	0/2150	0.54	0/2896
2	H	0.34	0/1030	0.52	0/1392
2	I	0.37	0/1030	0.47	0/1392
2	J	0.36	0/1030	0.50	0/1392
2	L	0.29	0/934	0.46	0/1259
3	N	0.39	0/1711	0.52	0/2306
4	O	0.98	0/999	1.08	0/1555
5	K	0.38	0/3290	0.51	0/4450
6	A	0.35	0/591	0.52	0/792
All	All	0.45	0/26356	0.55	0/35731

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	B	2261	0	2193	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2261	0	2193	103	0
1	D	2261	0	2193	116	0
1	E	2261	0	2193	122	0
1	F	2124	0	2064	116	0
1	G	2173	0	2120	131	0
1	M	2110	0	2050	110	0
2	H	1007	0	992	59	0
2	I	1007	0	992	50	0
2	J	1007	0	992	51	0
2	L	917	0	909	35	0
3	N	1673	0	1663	110	0
4	O	895	0	453	76	0
5	K	3223	0	3241	126	0
6	A	578	0	557	36	0
All	All	25758	0	24805	1189	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 24.

The worst 5 of 1189 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)
6:A:11:LYS:HB3	6:A:23:SER:O	1.42	1.16
2:H:16:ARG:HG3	2:H:108:GLU:HG3	1.45	0.96
2:H:95:LEU:HD21	2:I:53:GLY:HA3	1.50	0.93
1:M:165:ARG:HD3	6:A:53:VAL:HG22	1.51	0.92
1:M:56:MET:SD	1:M:212:HIS:ND1	2.45	0.89

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	B	281/283 (99%)	256 (91%)	25 (9%)	0	100	100
1	C	281/283 (99%)	254 (90%)	27 (10%)	0	100	100
1	D	281/283 (99%)	250 (89%)	31 (11%)	0	100	100
1	E	281/283 (99%)	264 (94%)	17 (6%)	0	100	100
1	F	261/283 (92%)	248 (95%)	13 (5%)	0	100	100
1	G	267/283 (94%)	245 (92%)	22 (8%)	0	100	100
1	M	260/283 (92%)	227 (87%)	33 (13%)	0	100	100
2	H	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
2	I	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
2	J	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
2	L	108/124 (87%)	106 (98%)	2 (2%)	0	100	100
3	N	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
5	K	405/409 (99%)	368 (91%)	36 (9%)	1 (0%)	47	78
6	A	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
All	All	3062/3161 (97%)	2800 (91%)	261 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	314	GLY

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	B	245/245 (100%)	245 (100%)	0	100	100
1	C	245/245 (100%)	243 (99%)	2 (1%)	81	91
1	D	245/245 (100%)	245 (100%)	0	100	100
1	E	245/245 (100%)	245 (100%)	0	100	100
1	F	230/245 (94%)	229 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	235/245 (96%)	235 (100%)	0	100	100
1	M	229/245 (94%)	228 (100%)	1 (0%)	91	95
2	H	104/104 (100%)	103 (99%)	1 (1%)	76	88
2	I	104/104 (100%)	103 (99%)	1 (1%)	76	88
2	J	104/104 (100%)	104 (100%)	0	100	100
2	L	94/104 (90%)	93 (99%)	1 (1%)	73	86
3	N	181/181 (100%)	180 (99%)	1 (1%)	86	94
5	K	334/336 (99%)	333 (100%)	1 (0%)	92	97
6	A	57/57 (100%)	56 (98%)	1 (2%)	59	79
All	All	2652/2705 (98%)	2642 (100%)	10 (0%)	91	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	13	LYS
2	L	71	ARG
6	A	67	LYS
2	H	65	LYS
2	I	65	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	204	GLN
1	M	234	ASN
1	G	222	ASN
3	N	199	ASN
1	M	130	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	O	41/42 (97%)	25 (60%)	2 (4%)

5 of 25 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	O	3	U
4	O	4	G
4	O	6	A
4	O	9	A
4	O	13	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	O	24	U
4	O	39	U

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	16:SER	C	190:ALA	N	30.88

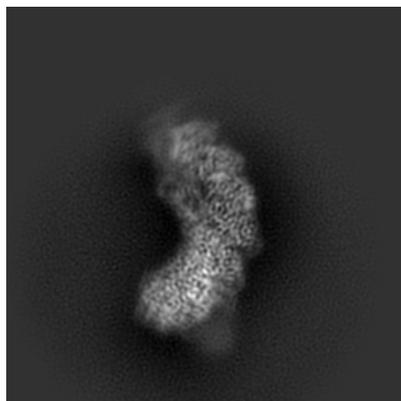
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29877. These allow visual inspection of the internal detail of the map and identification of artifacts.

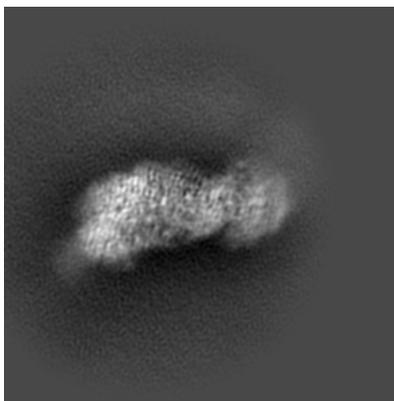
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

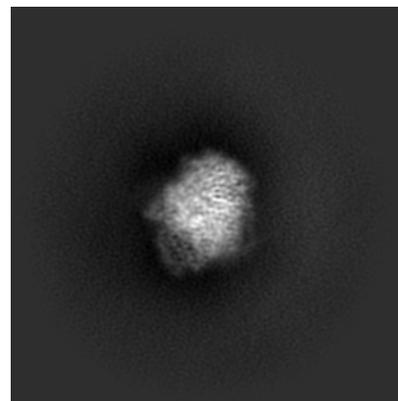
6.1.1 Primary map



X

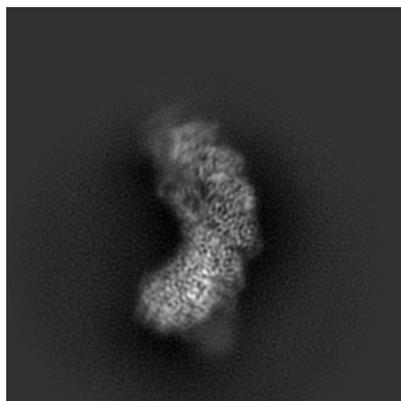


Y

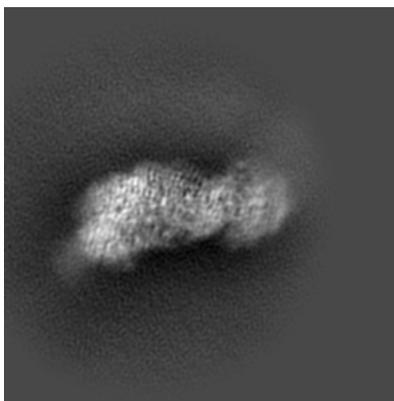


Z

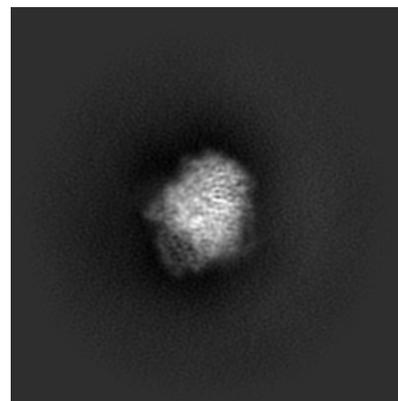
6.1.2 Raw map



X



Y

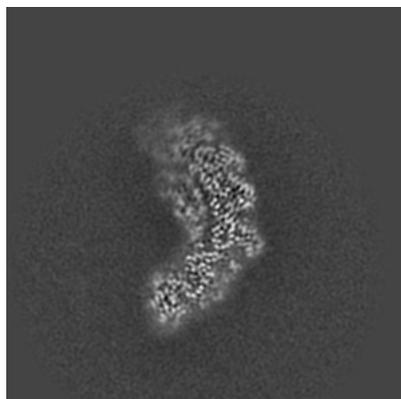


Z

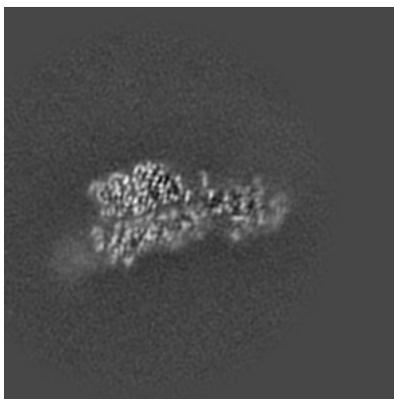
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

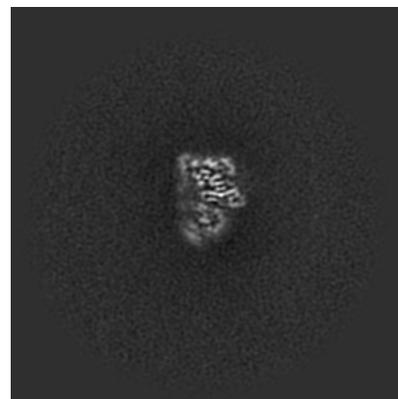
6.2.1 Primary map



X Index: 125

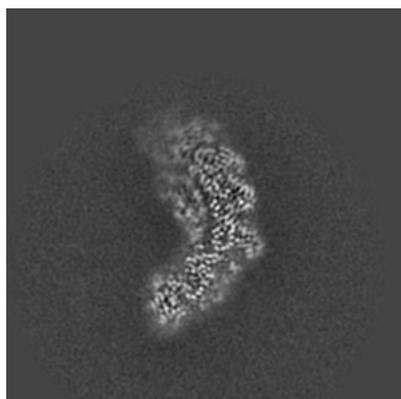


Y Index: 125

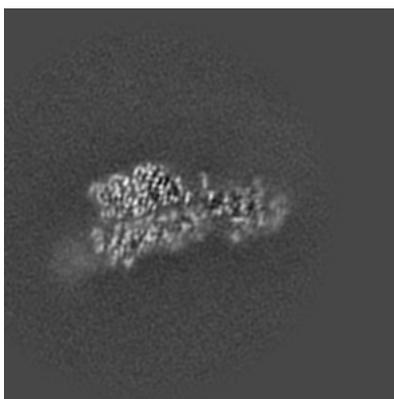


Z Index: 125

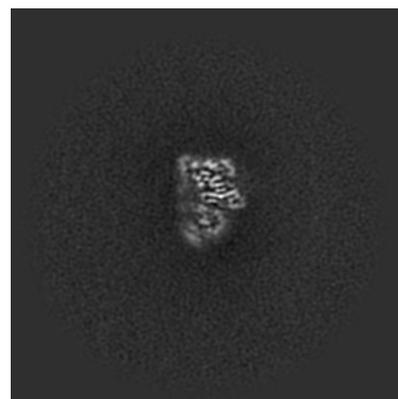
6.2.2 Raw map



X Index: 125



Y Index: 125

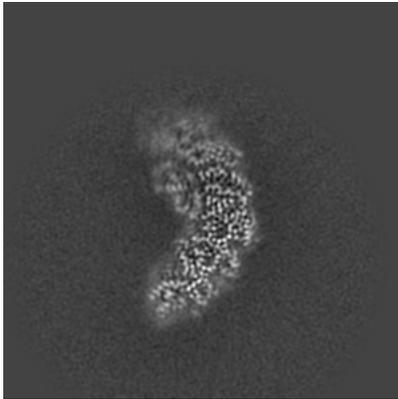


Z Index: 125

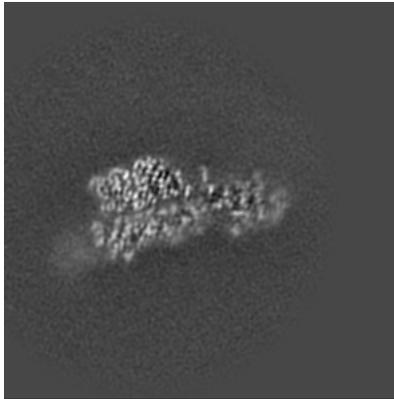
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

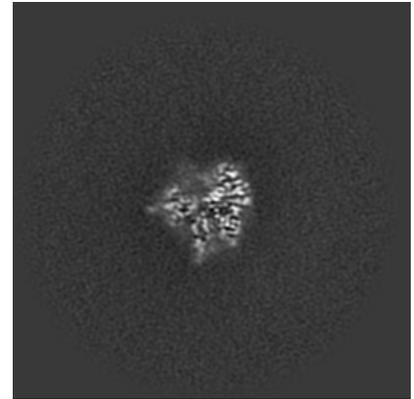
6.3.1 Primary map



X Index: 128

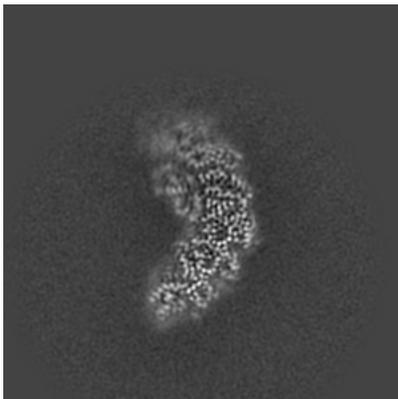


Y Index: 125

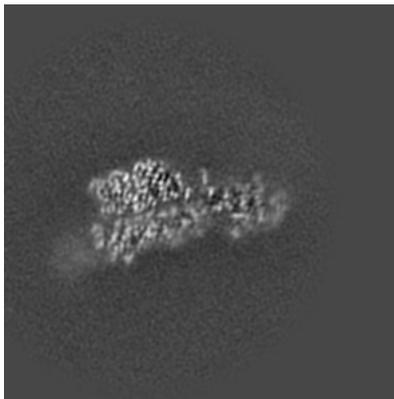


Z Index: 82

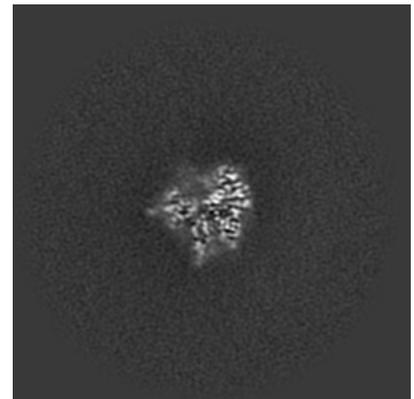
6.3.2 Raw map



X Index: 128



Y Index: 125

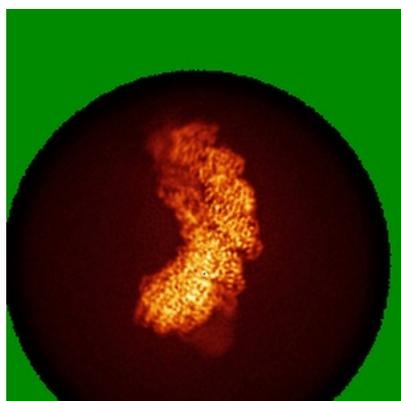


Z Index: 82

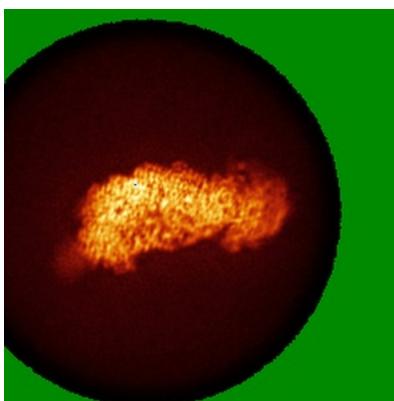
The images above show the largest variance slices of the map in three orthogonal directions.

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

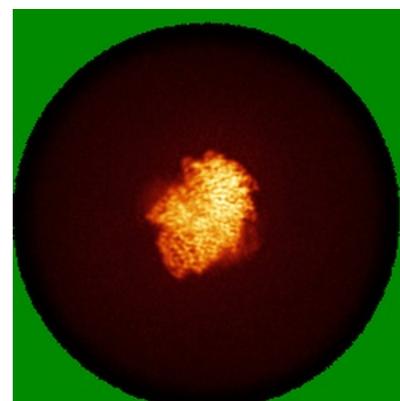
6.4.1 Primary map



X

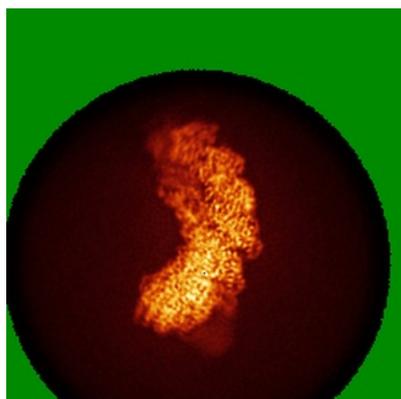


Y

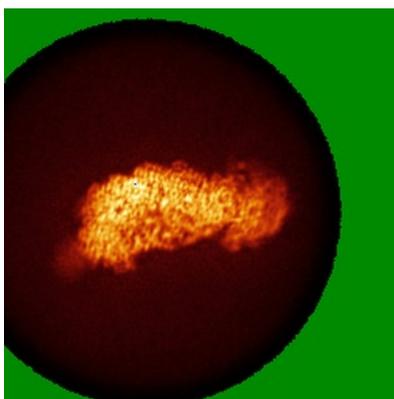


Z

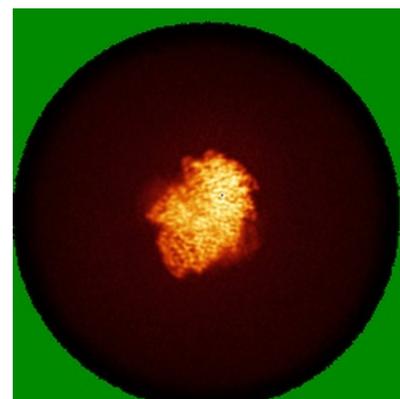
6.4.2 Raw map



X



Y

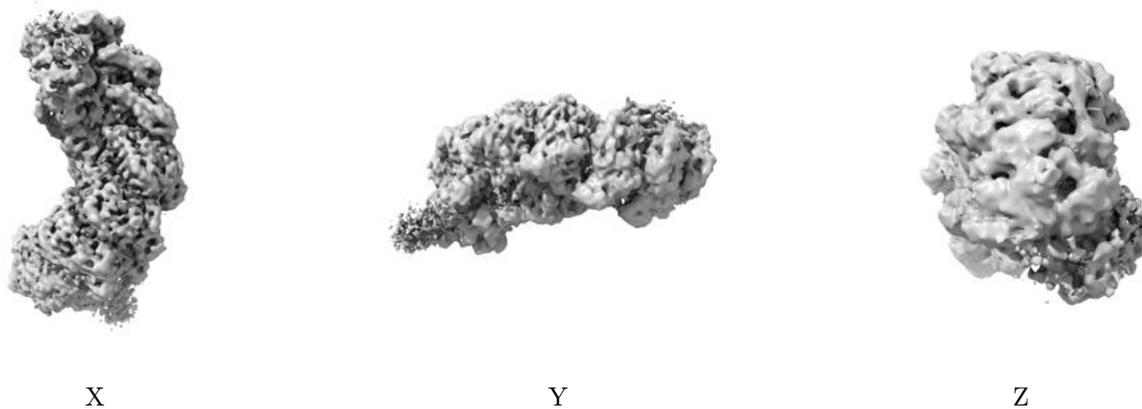


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

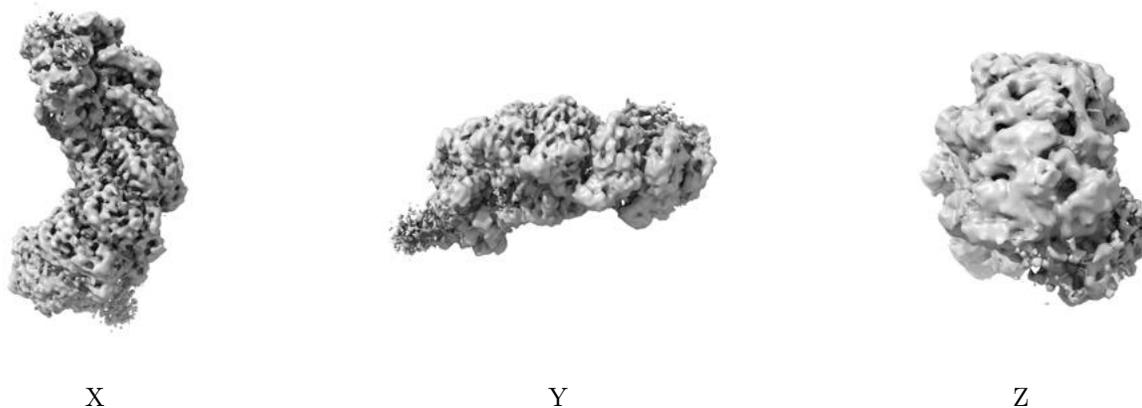
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

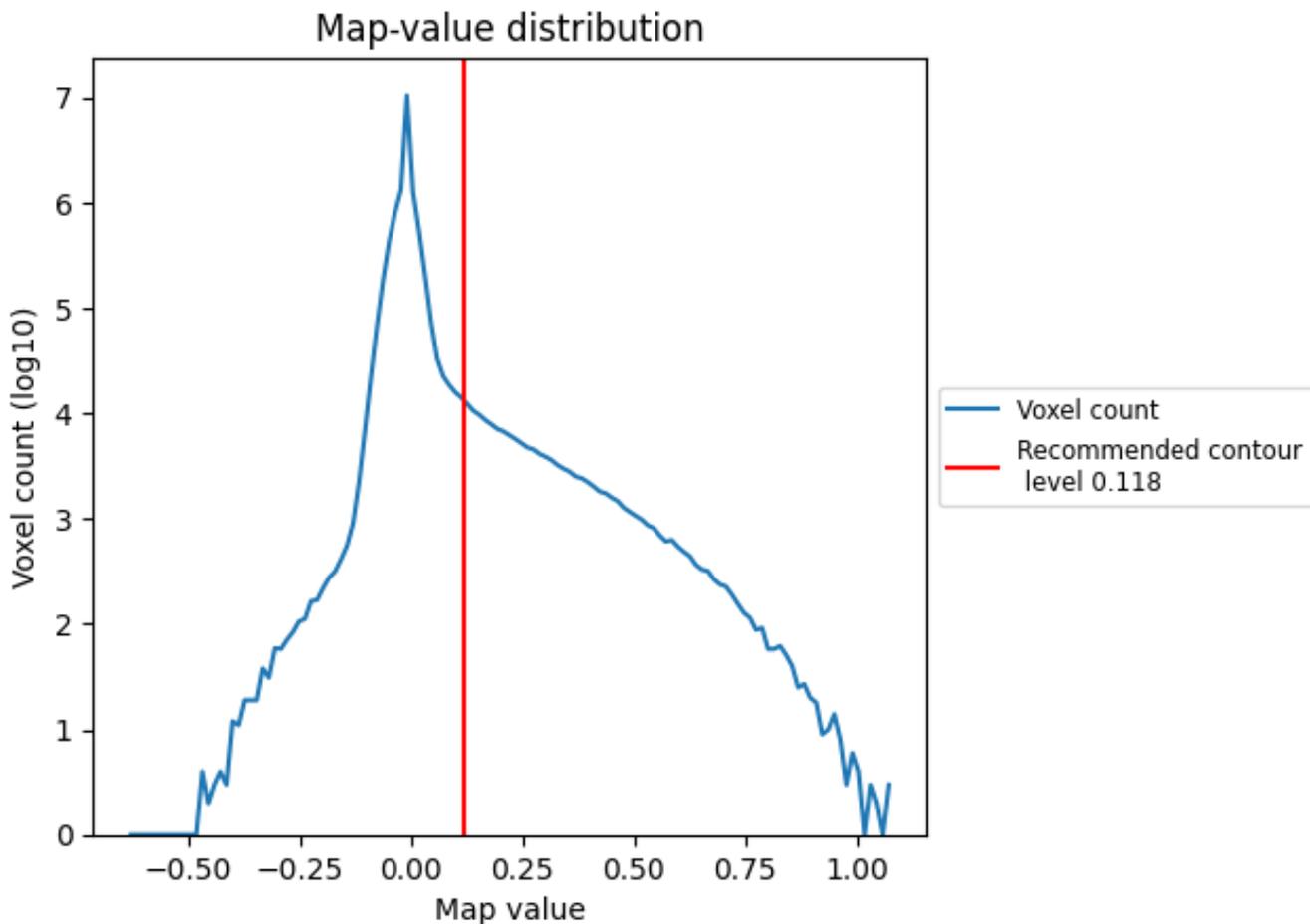
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

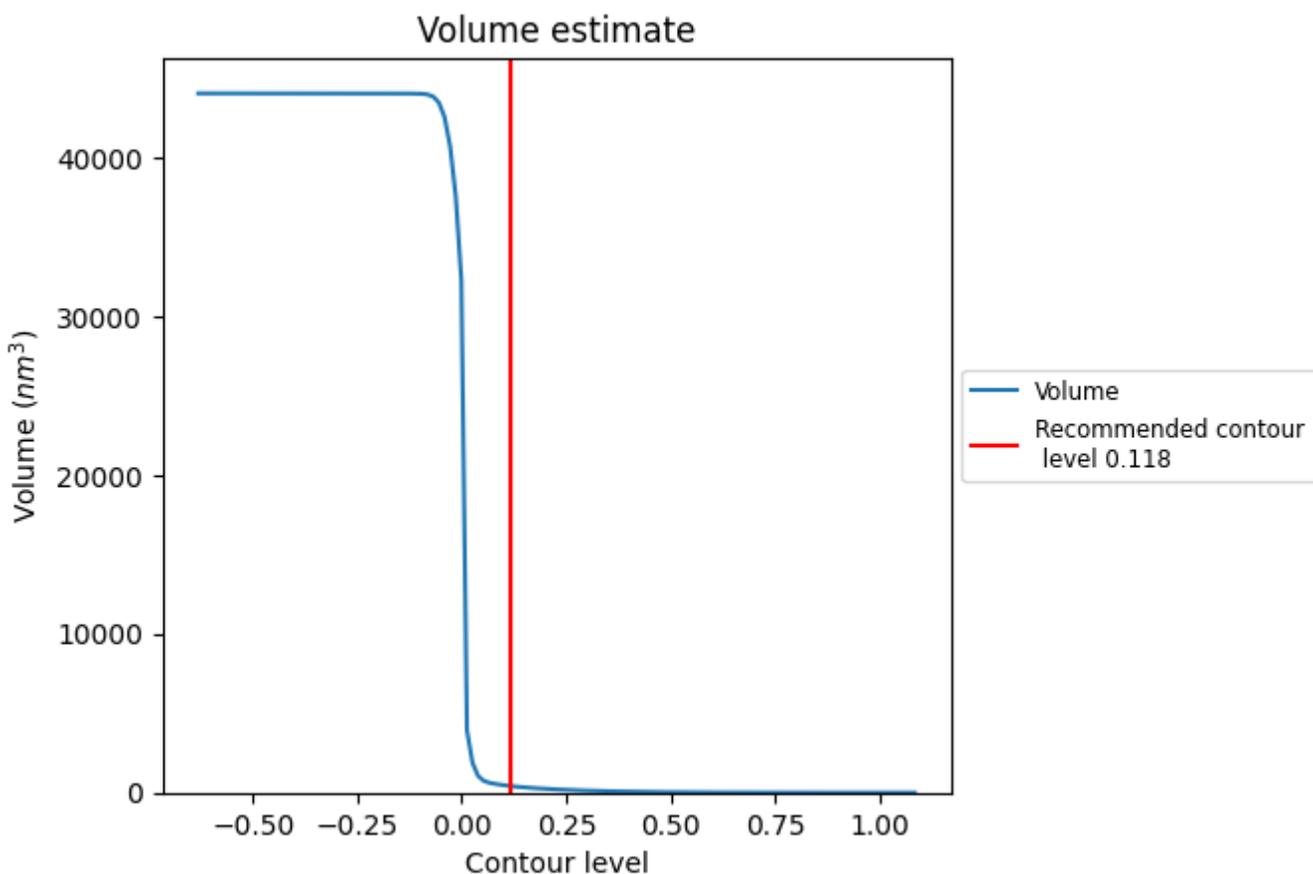
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

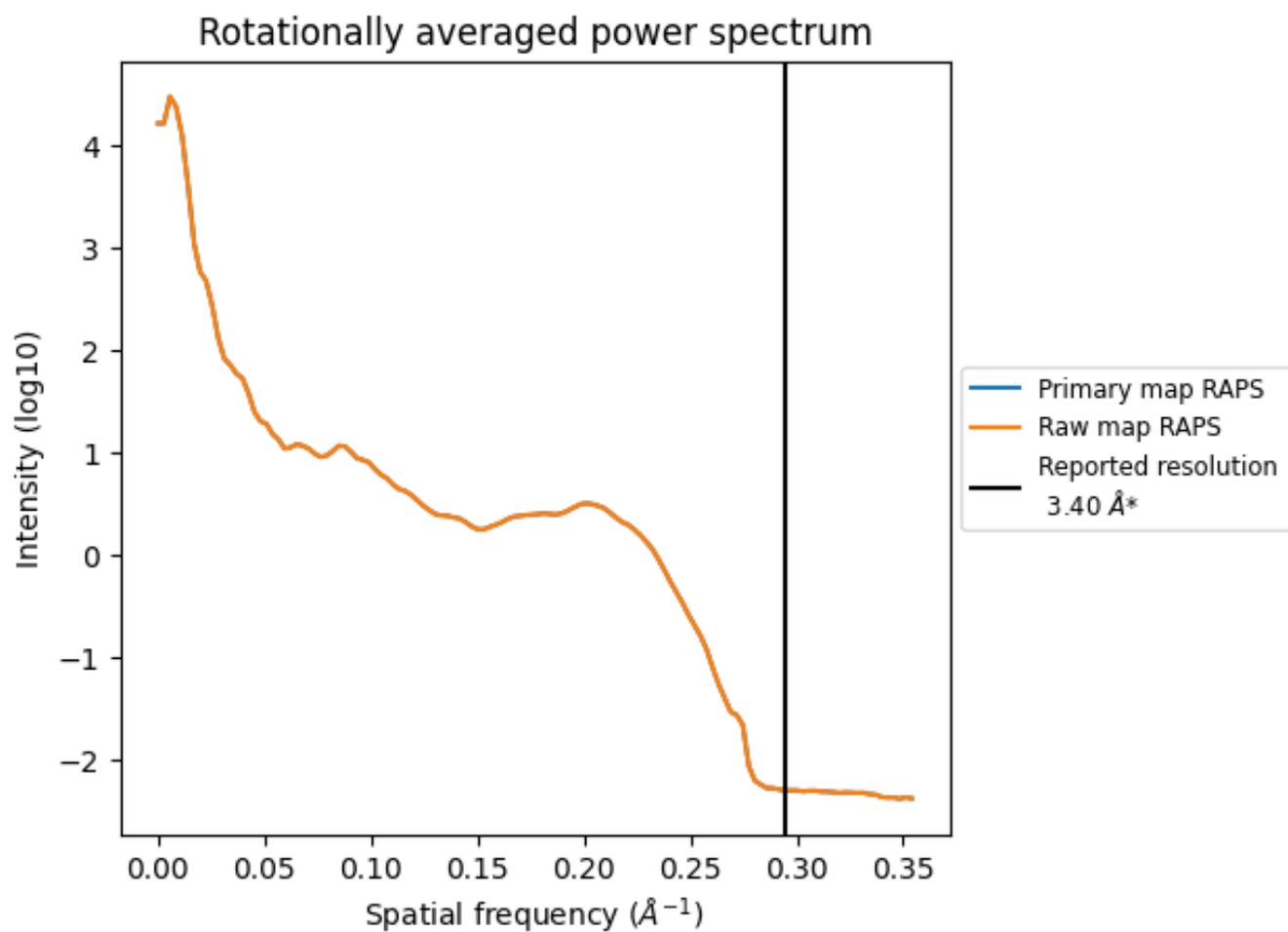
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 372 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](#)

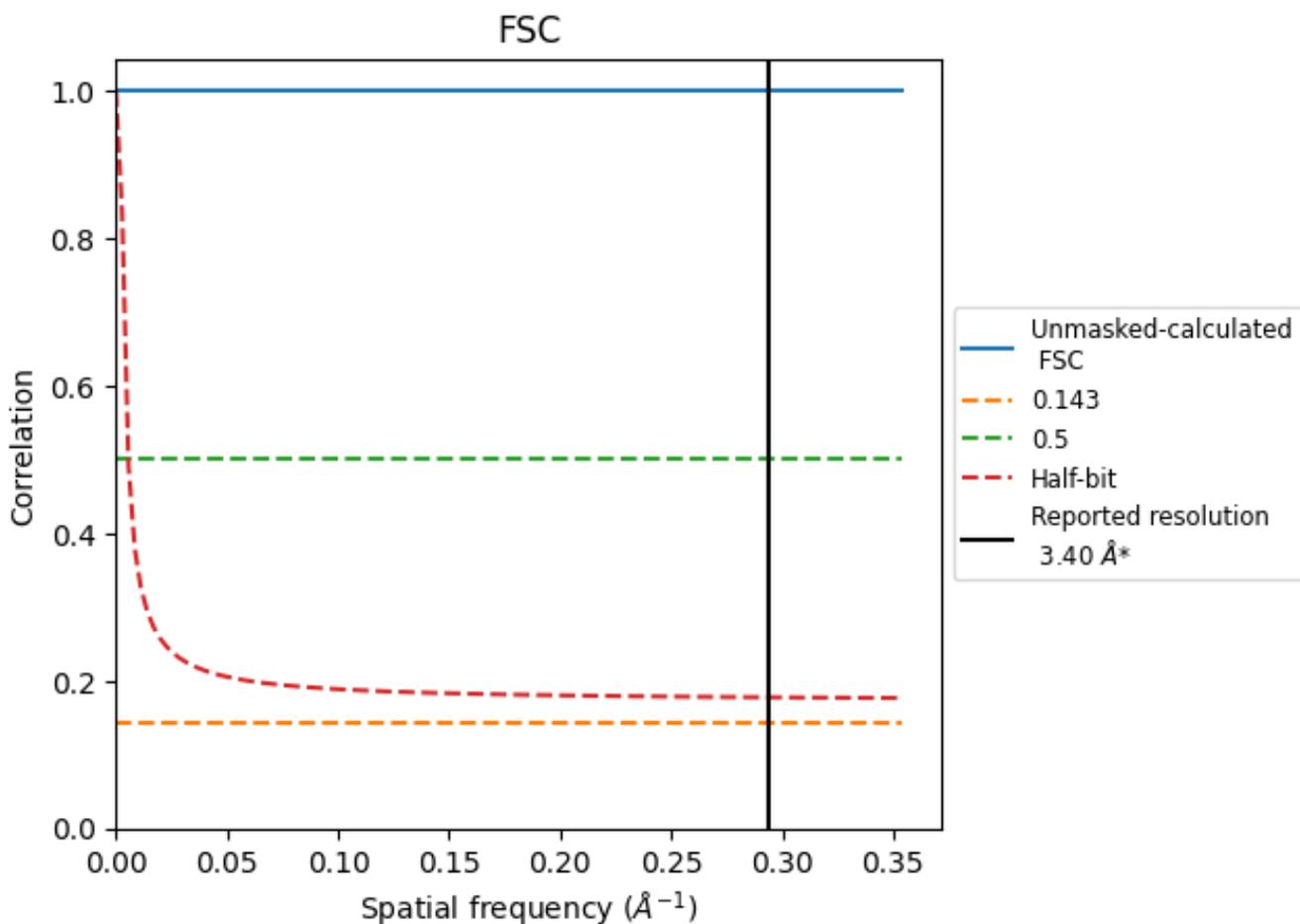


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

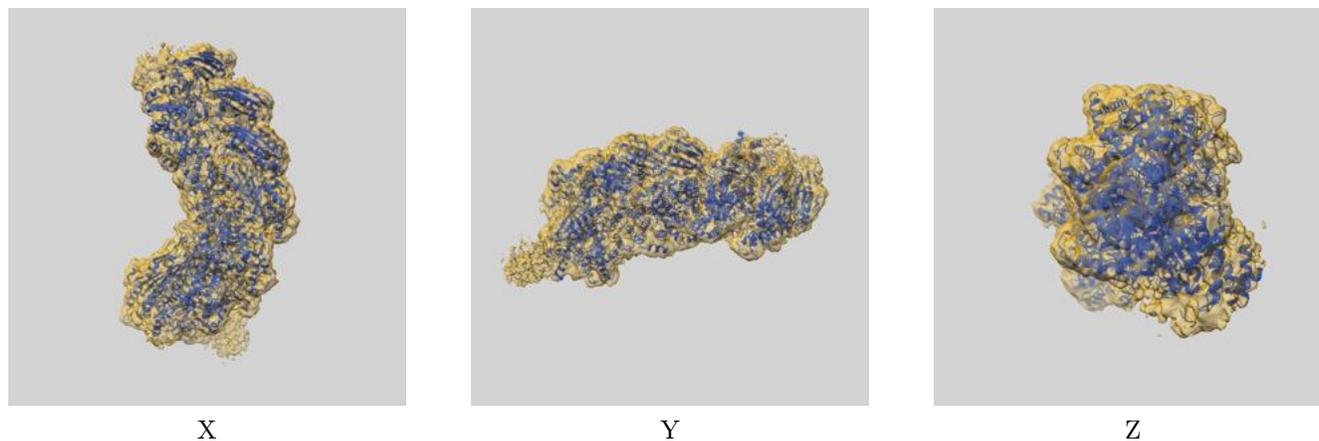
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

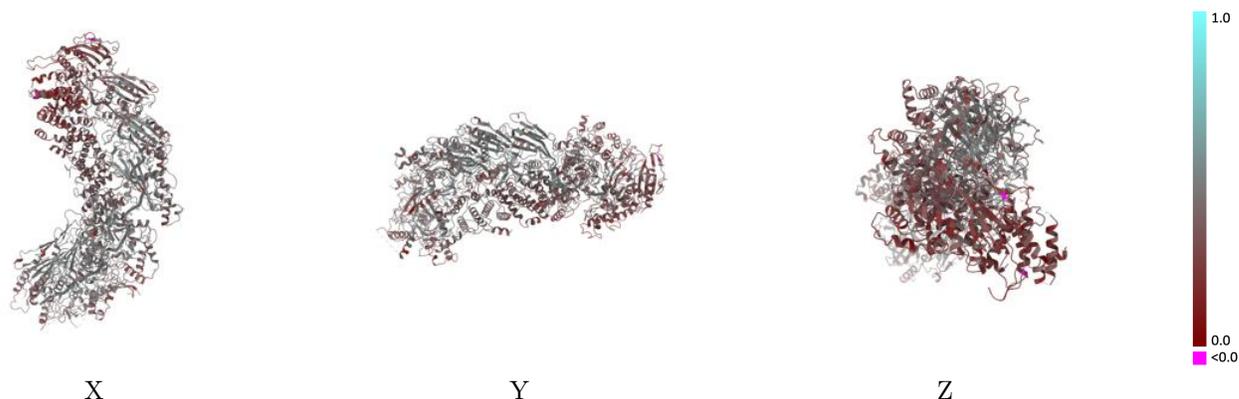
This section contains information regarding the fit between EMDB map EMD-29877 and PDB model 8G9S. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



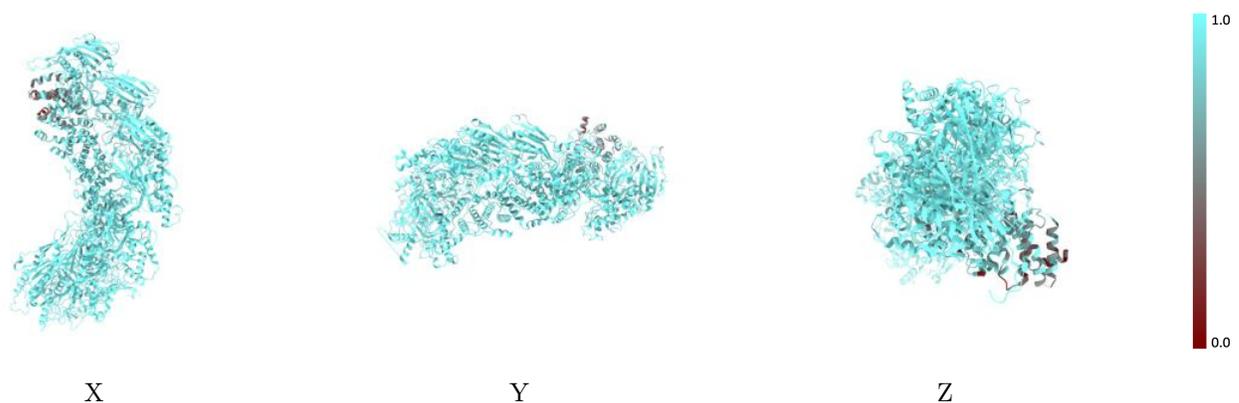
The images above show the 3D surface view of the map at the recommended contour level 0.118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



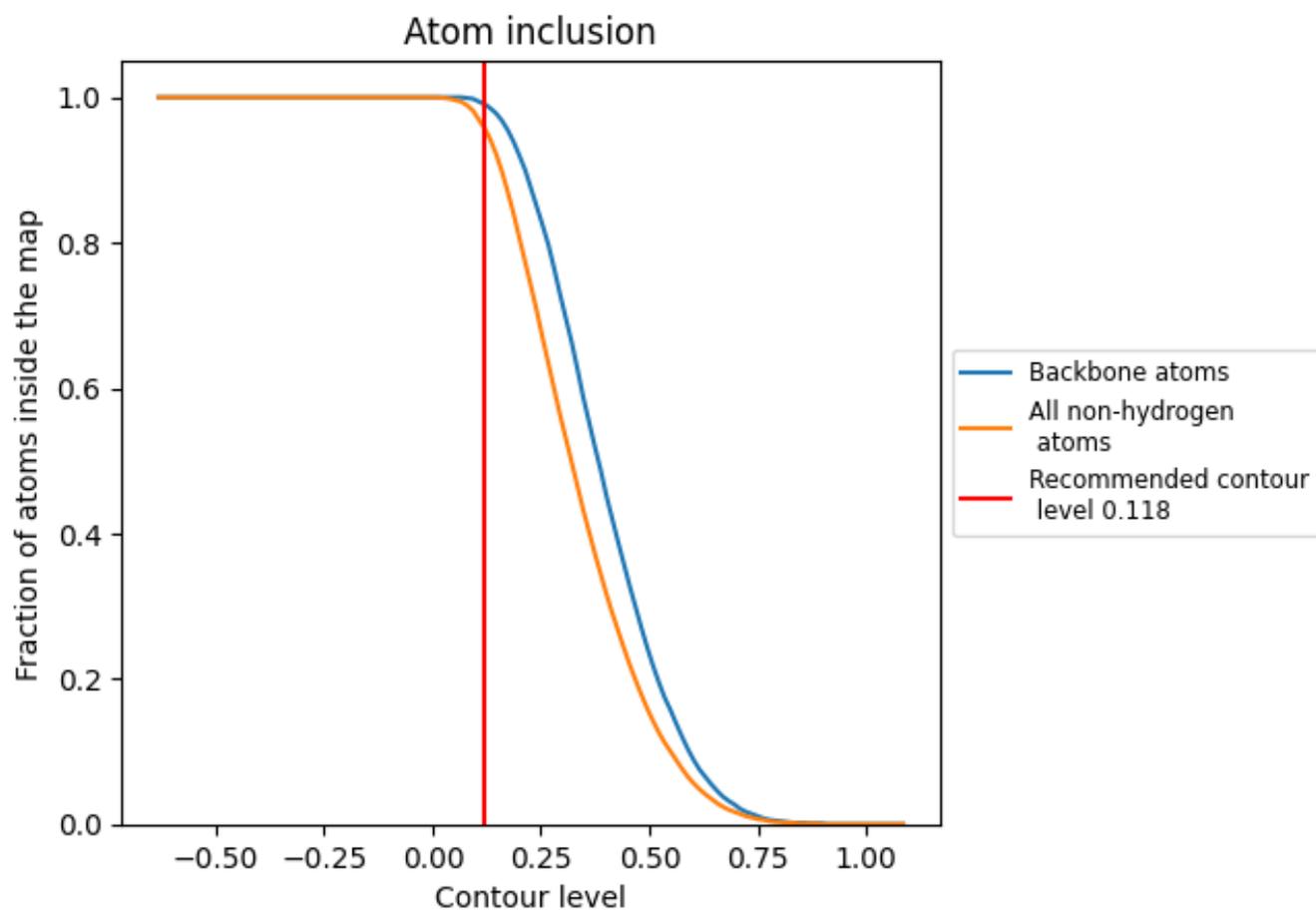
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.118).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.4010
A	 0.9790	 0.3730
B	 0.9930	 0.4580
C	 0.9840	 0.4570
D	 0.9790	 0.4550
E	 0.9630	 0.4190
F	 0.9660	 0.3680
G	 0.9400	 0.2840
H	 0.8500	 0.3180
I	 0.9480	 0.3630
J	 0.9860	 0.3680
K	 0.9850	 0.4050
L	 0.6140	 0.2610
M	 0.9950	 0.4460
N	 0.9880	 0.4170
O	 0.9970	 0.4780

