



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 02:51 AM UTC

PDB ID : 9JI5 / pdb_00009ji5
EMDB ID : EMD-61497
Title : Cryo-EM structure of Mycobacterium tuberculosis transcription activation complex with six PhoP molecules
Authors : Lin, W.; Feng, Y.
Deposited on : 2024-09-11
Resolution : 3.20 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:

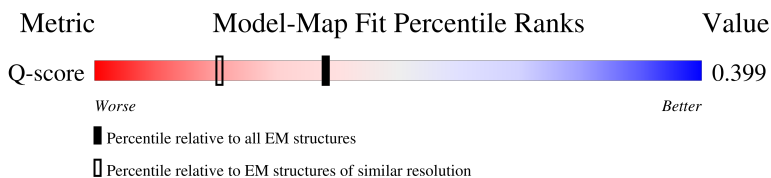
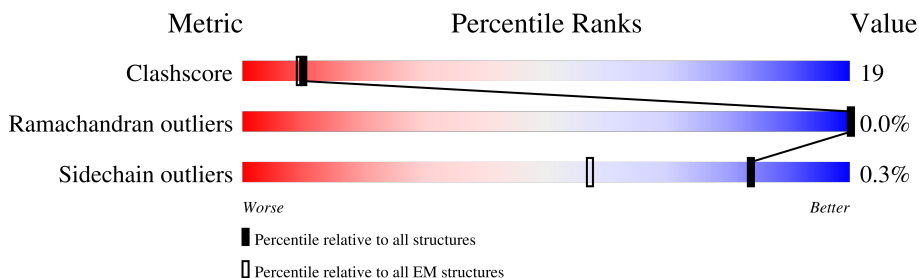
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

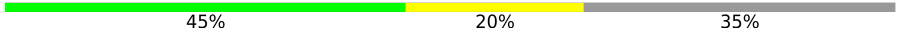
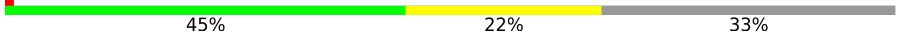
The reported resolution of this entry is 3.20 Å.

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.



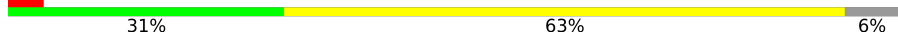
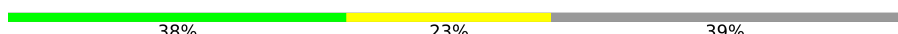
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	347	 45% 20% 35%
1	B	347	 45% 22% 33%
1	I	347	 5% 9% 8% 84%
2	C	1178	 66% 28% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1316	
4	E	110	
5	H	108	
6	G	108	
7	F	528	
8	J	247	
8	K	247	
8	L	247	
8	M	247	
8	N	247	
8	O	247	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 34369 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1710	1077	293	338	2		
1	B	234	Total	C	N	O	S	0	0
			1748	1105	298	342	3		
1	I	57	Total	C	N	O	S	0	0
			433	273	78	81	1		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8554	5360	1500	1655	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1263	Total	C	N	O	S	0	0
			9838	6162	1784	1851	41		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	102	Total	C	N	O	P	0	0
			2105	994	401	608	102		

- Molecule 6 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	100	Total	C	N	O	P	0	0
			2047	970	374	603	100		

- Molecule 7 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	322	Total	C	N	O	S	0	0
			2529	1577	454	489	9		

- Molecule 8 is a protein called DNA-binding response regulator.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	96	Total	C	N	O	0	0
			776	503	133	140		
8	M	98	Total	C	N	O	0	0
			792	513	135	144		
8	O	98	Total	C	N	O	0	0
			792	513	135	144		
8	K	97	Total	C	N	O	0	0
			795	513	137	145		
8	L	98	Total	C	N	O	0	0
			796	512	138	146		
8	N	98	Total	C	N	O	0	0
			802	518	138	146		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

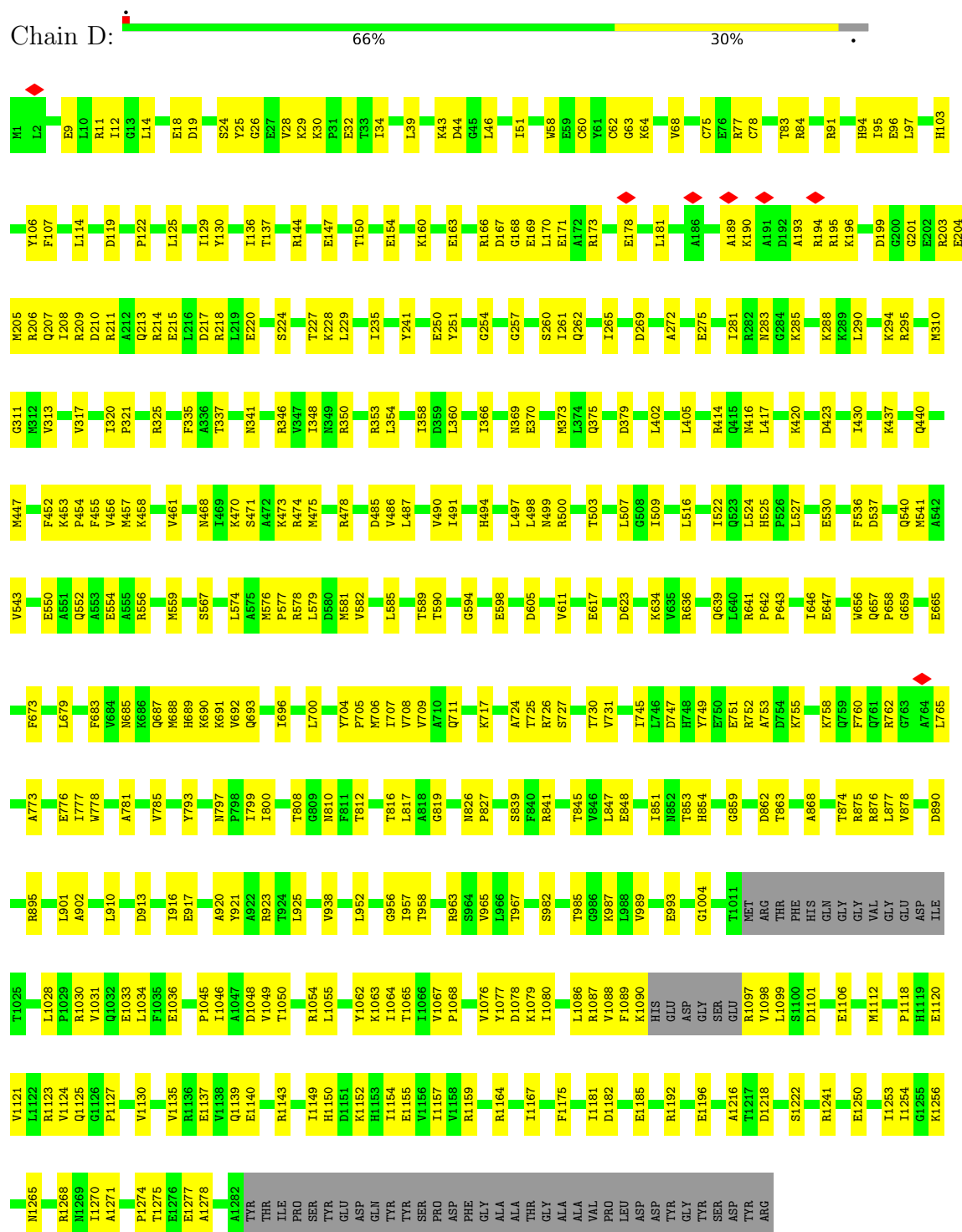
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

SER
ARG
ASN
GLU
SER
SER
ALA
SER
VAL
GLU
ASP
LEU
ALA

• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



• Molecule 4: DNA-directed RNA polymerase subunit omega

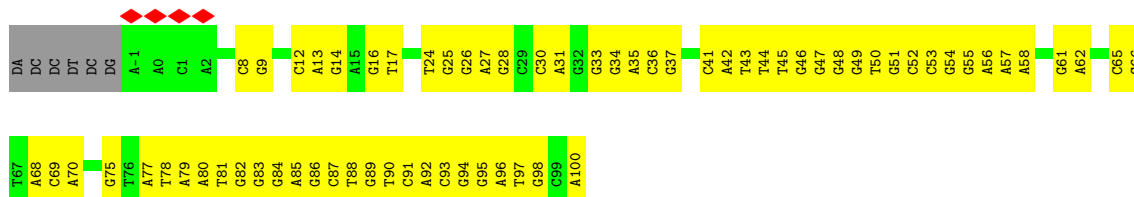
Chain E:

51%

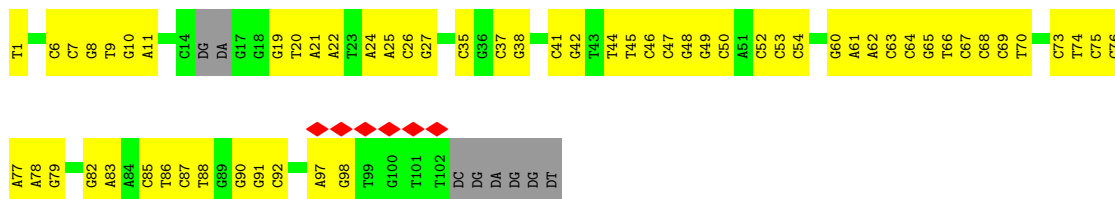
25%

25%

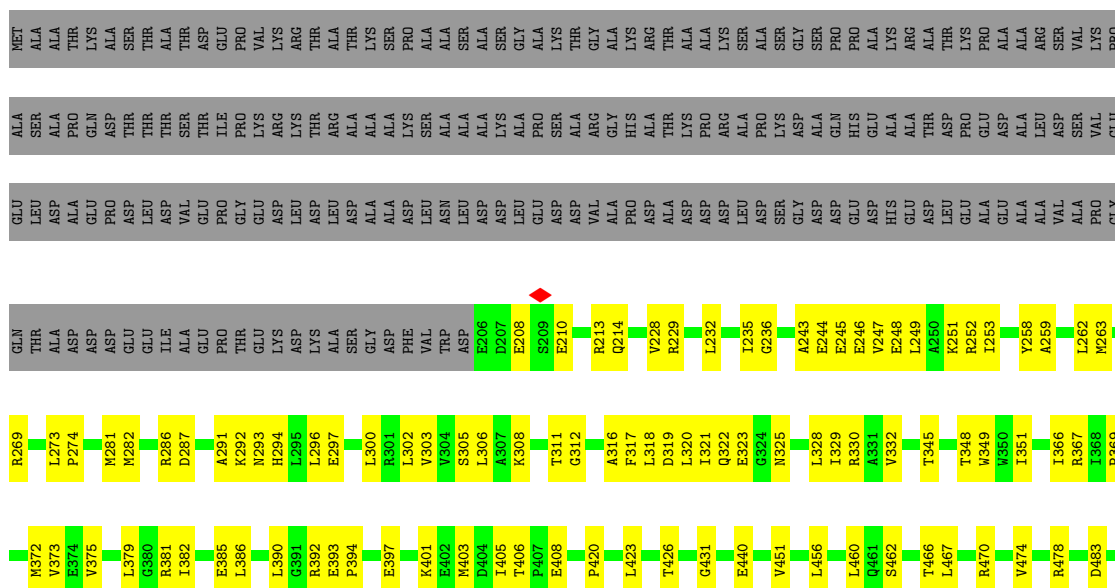
- Molecule 5: Non-template strand DNA

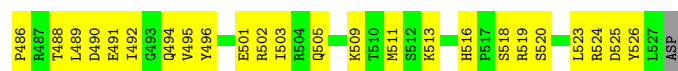


- Molecule 6: Template strand DNA

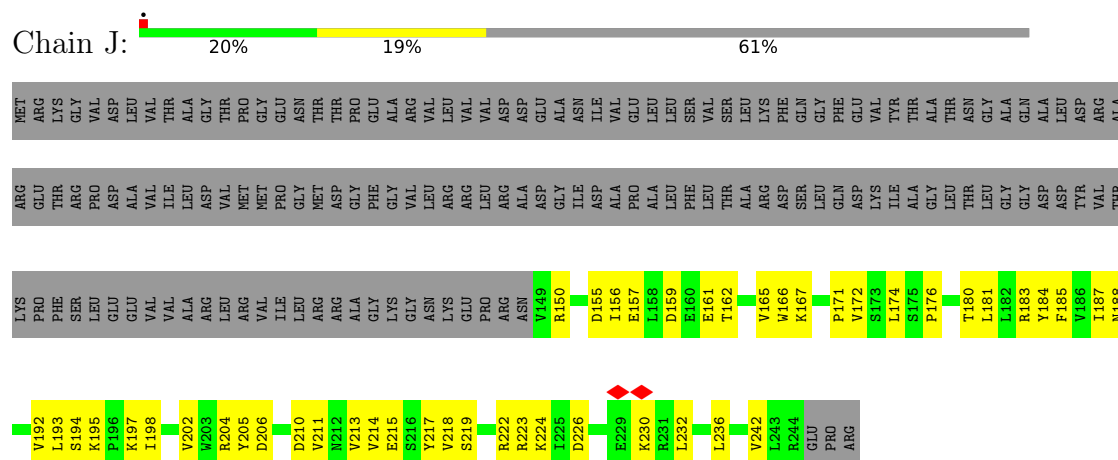


- Molecule 7: RNA polymerase sigma factor SigA

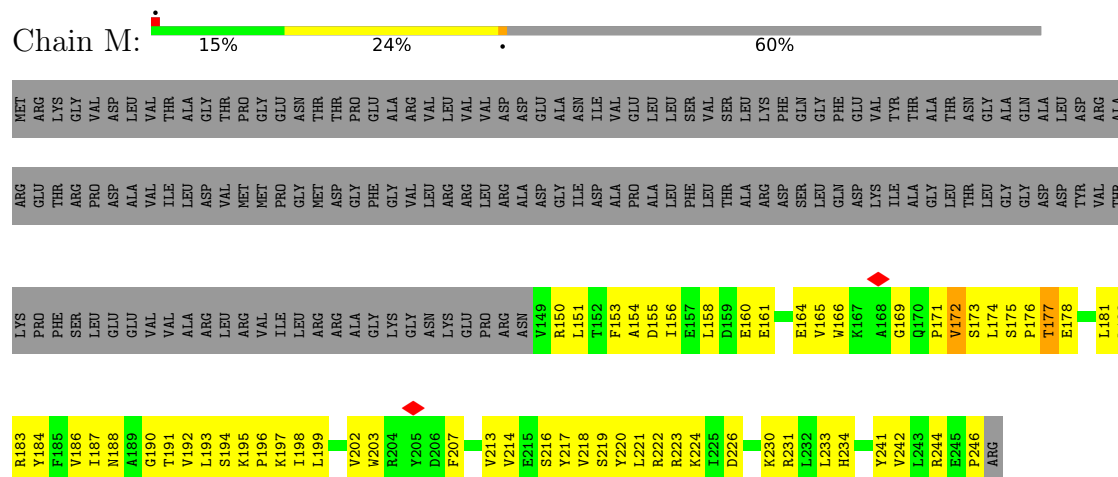




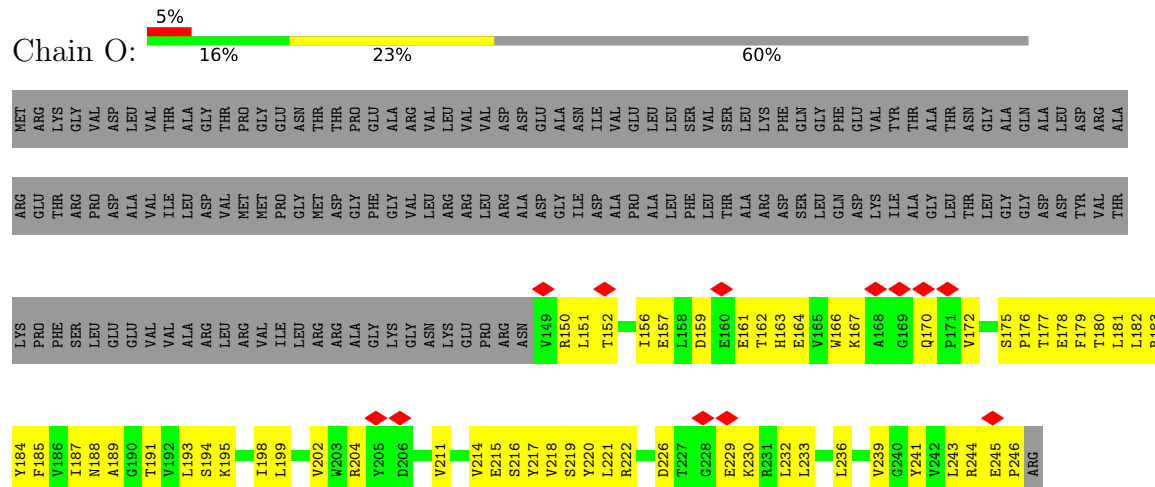
• Molecule 8: DNA-binding response regulator



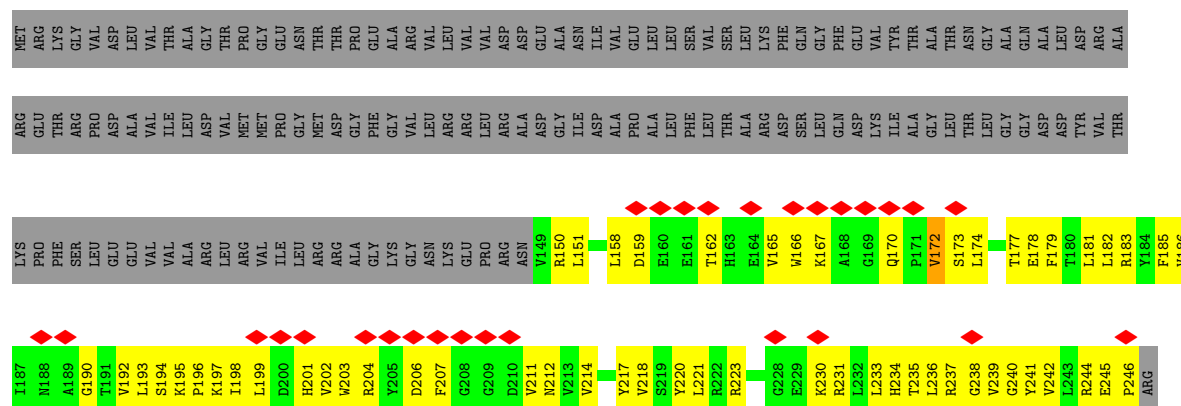
• Molecule 8: DNA-binding response regulator



• Molecule 8: DNA-binding response regulator



Chain K: 19% 20% 61%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227755	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.112	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	360.0, 360.0, 360.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.6, 0.6, 0.6	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.18	0/1736	0.39	0/2363
1	B	0.19	0/1774	0.41	0/2417
1	I	0.22	0/436	0.50	0/588
2	C	0.16	0/8709	0.37	0/11811
3	D	0.20	0/10002	0.41	0/13526
4	E	0.17	0/662	0.38	0/901
5	H	0.25	0/2365	0.48	0/3651
6	G	0.21	0/2293	0.42	0/3534
7	F	0.19	0/2559	0.38	0/3453
8	J	0.28	0/794	0.52	0/1079
8	K	0.36	0/813	0.53	0/1103
8	L	0.35	0/814	0.58	0/1106
8	M	0.52	0/811	0.77	0/1103
8	N	0.40	0/821	0.55	0/1115
8	O	0.27	0/811	0.47	0/1103
All	All	0.23	0/35400	0.43	0/48853

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

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	1710	0	1745	64	0
1	B	1748	0	1779	74	0
1	I	433	0	440	29	0
2	C	8554	0	8457	289	0
3	D	9838	0	9880	321	0
4	E	649	0	645	27	0
5	H	2105	0	1142	73	0
6	G	2047	0	1124	69	0
7	F	2529	0	2536	108	0
8	J	776	0	776	48	0
8	K	795	0	797	64	0
8	L	796	0	797	70	0
8	M	792	0	789	74	0
8	N	802	0	804	59	0
8	O	792	0	789	47	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	34369	0	32500	1289	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 19.

The worst 5 of 1289 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:I:265:LYS:HB3	1:I:266:ARG:NH2	1.61	1.16
2:C:222:VAL:HG23	2:C:234:VAL:HG23	1.39	1.04
1:B:59:VAL:HG11	1:B:66:VAL:HG12	1.40	1.04
2:C:445:PRO:HB2	2:C:713:MET:HE1	1.41	1.02
2:C:222:VAL:CG2	2:C:234:VAL:HG23	1.90	1.01

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	223/347 (64%)	220 (99%)	3 (1%)	0	100	100
1	B	232/347 (67%)	214 (92%)	18 (8%)	0	100	100
1	I	55/347 (16%)	52 (94%)	3 (6%)	0	100	100
2	C	1109/1178 (94%)	1041 (94%)	68 (6%)	0	100	100
3	D	1257/1316 (96%)	1211 (96%)	46 (4%)	0	100	100
4	E	81/110 (74%)	77 (95%)	4 (5%)	0	100	100
7	F	320/528 (61%)	313 (98%)	7 (2%)	0	100	100
8	J	94/247 (38%)	86 (92%)	8 (8%)	0	100	100
8	K	95/247 (38%)	90 (95%)	5 (5%)	0	100	100
8	L	96/247 (39%)	85 (88%)	11 (12%)	0	100	100
8	M	96/247 (39%)	85 (88%)	10 (10%)	1 (1%)	12	45
8	N	96/247 (39%)	90 (94%)	6 (6%)	0	100	100
8	O	96/247 (39%)	93 (97%)	3 (3%)	0	100	100
All	All	3850/5655 (68%)	3657 (95%)	192 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	154	ALA

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	A	193/297 (65%)	193 (100%)	0	100	100
1	B	193/297 (65%)	190 (98%)	3 (2%)	55	75
1	I	46/297 (16%)	46 (100%)	0	100	100
2	C	924/998 (93%)	922 (100%)	2 (0%)	87	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1037/1095 (95%)	1037 (100%)	0	100	100
4	E	69/90 (77%)	69 (100%)	0	100	100
7	F	264/427 (62%)	264 (100%)	0	100	100
8	J	84/208 (40%)	84 (100%)	0	100	100
8	K	87/208 (42%)	85 (98%)	2 (2%)	44	70
8	L	87/208 (42%)	87 (100%)	0	100	100
8	M	86/208 (41%)	83 (96%)	3 (4%)	32	64
8	N	88/208 (42%)	87 (99%)	1 (1%)	65	79
8	O	86/208 (41%)	86 (100%)	0	100	100
All	All	3244/4749 (68%)	3233 (100%)	11 (0%)	84	88

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	177	THR
8	K	151	LEU
8	N	172	VAL
8	K	234	HIS
2	C	841	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	70	GLN
8	O	170	GLN
8	N	170	GLN
8	O	188	ASN
2	C	442	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

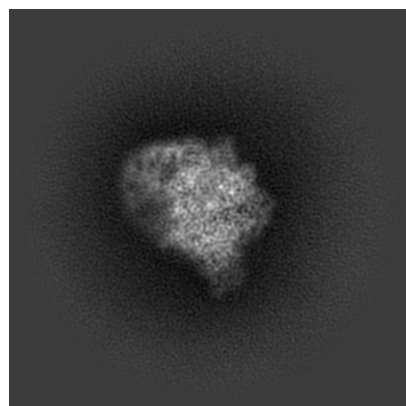
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61497. These allow visual inspection of the internal detail of the map and identification of artifacts.

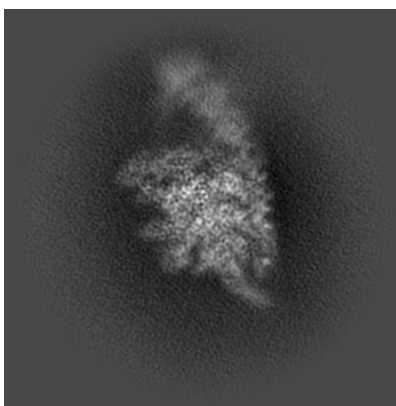
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

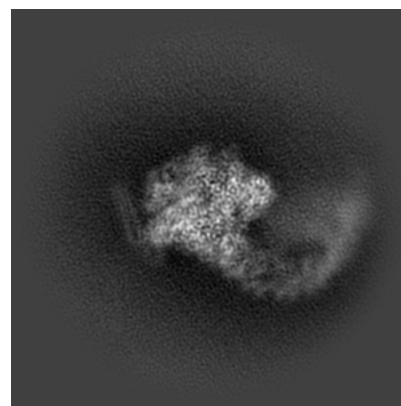
6.1.1 Primary map



X

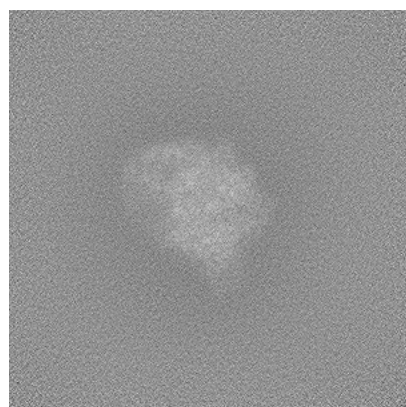


Y

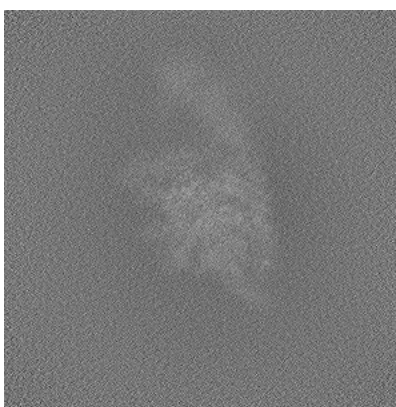


Z

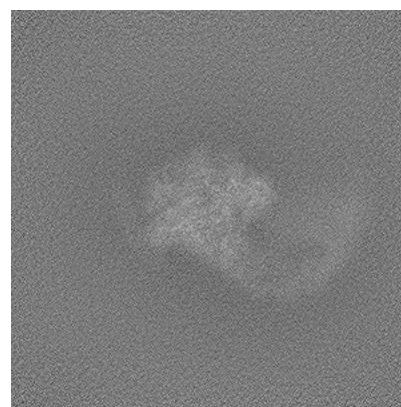
6.1.2 Raw map



X



Y

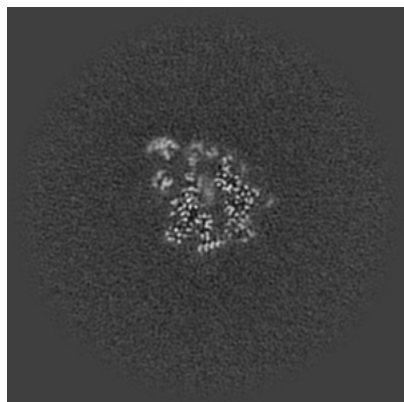


Z

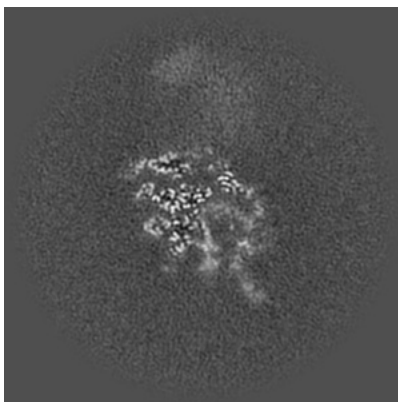
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

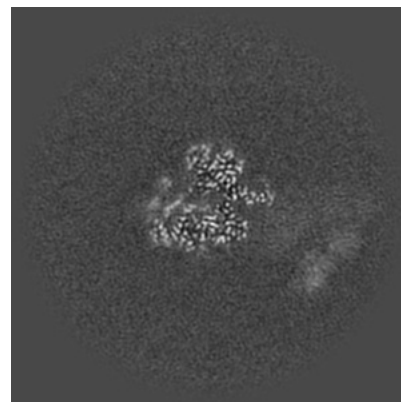
6.2.1 Primary map



X Index: 300

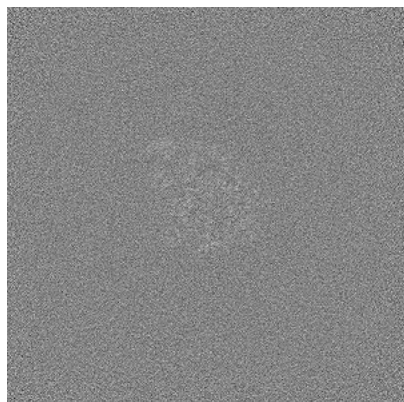


Y Index: 300

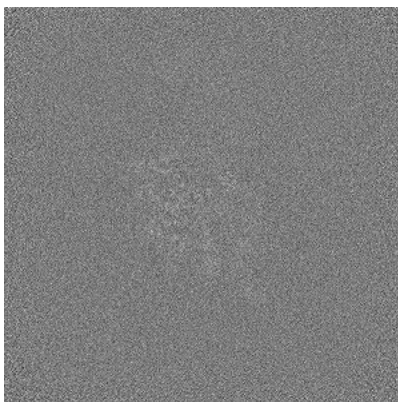


Z Index: 300

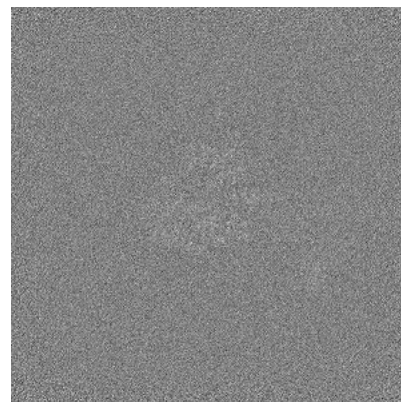
6.2.2 Raw map



X Index: 300



Y Index: 300

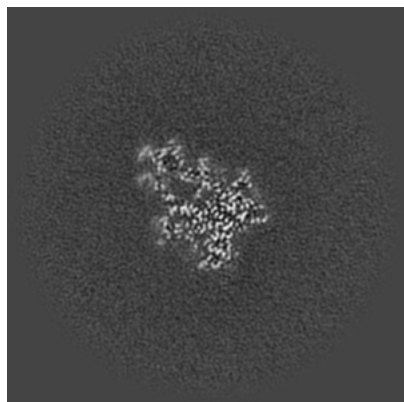


Z Index: 300

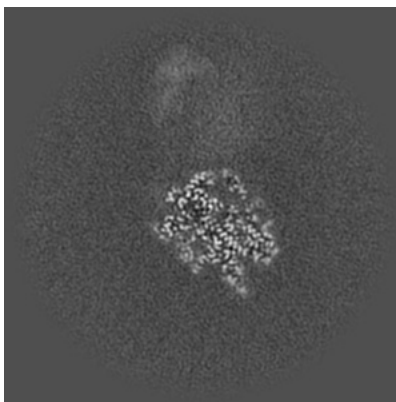
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

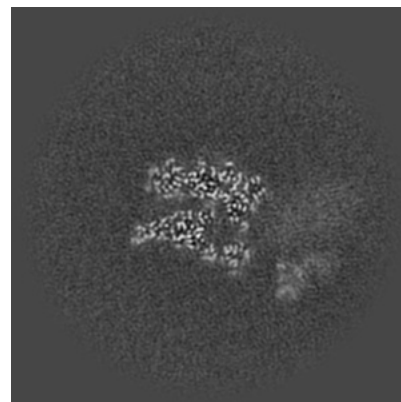
6.3.1 Primary map



X Index: 326

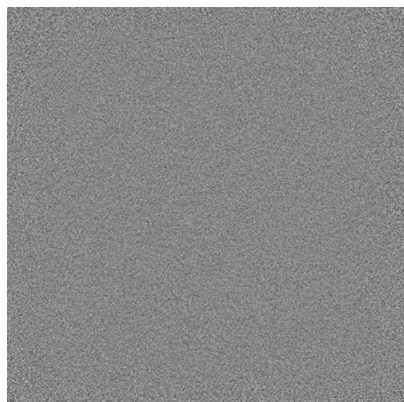


Y Index: 272

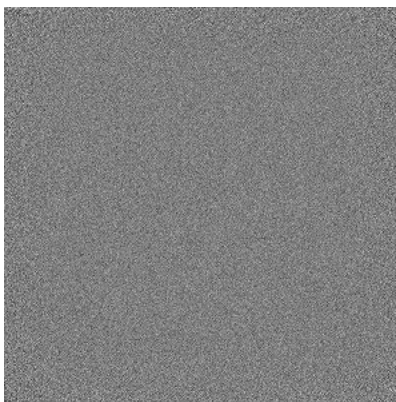


Z Index: 332

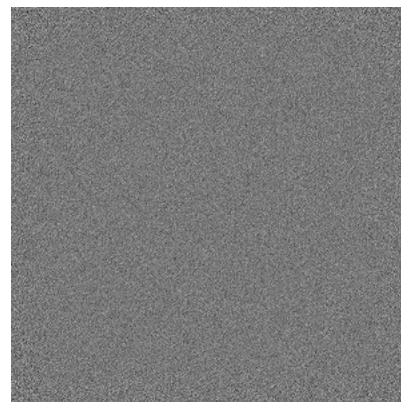
6.3.2 Raw map



X Index: 0



Y Index: 0

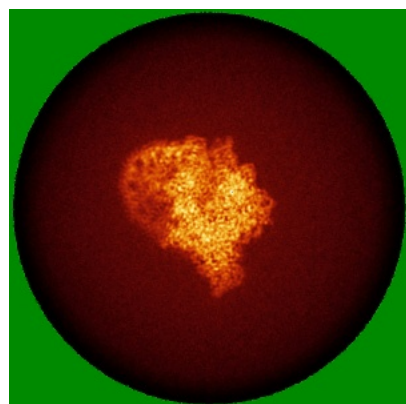


Z Index: 0

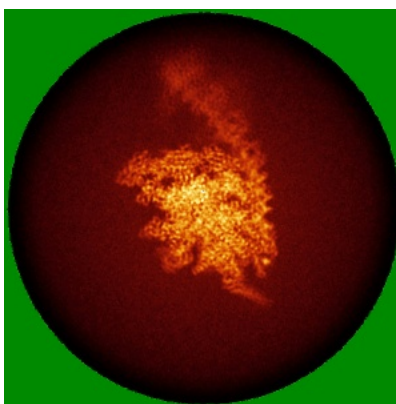
The images above show the largest variance slices of the map in three orthogonal directions.

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

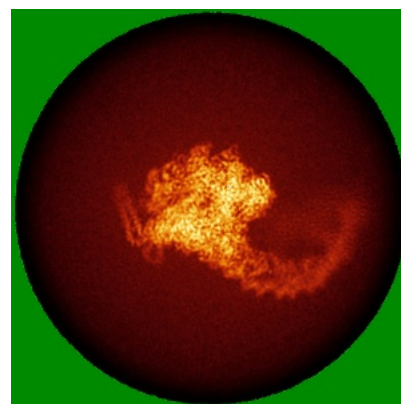
6.4.1 Primary map



X

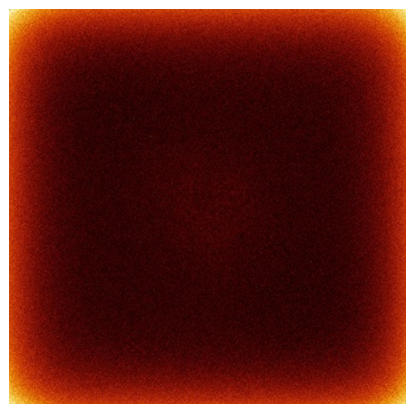


Y

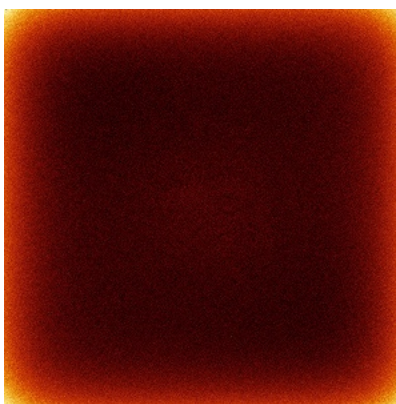


Z

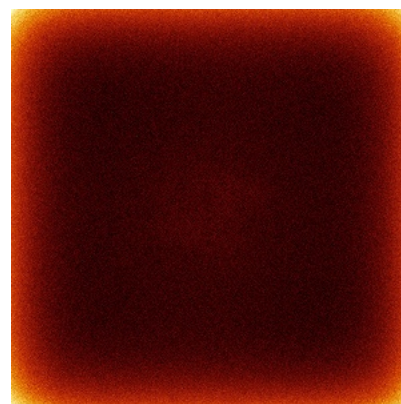
6.4.2 Raw map



X



Y

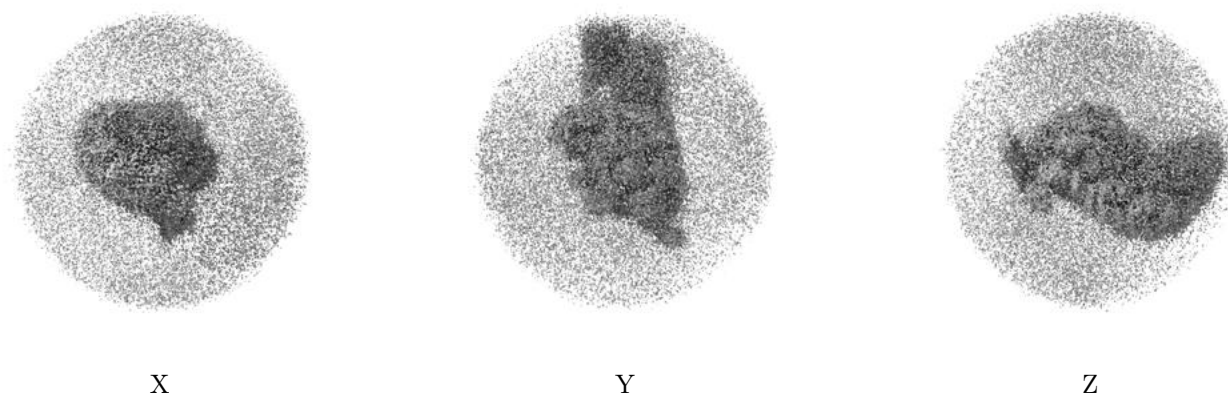


Z

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.

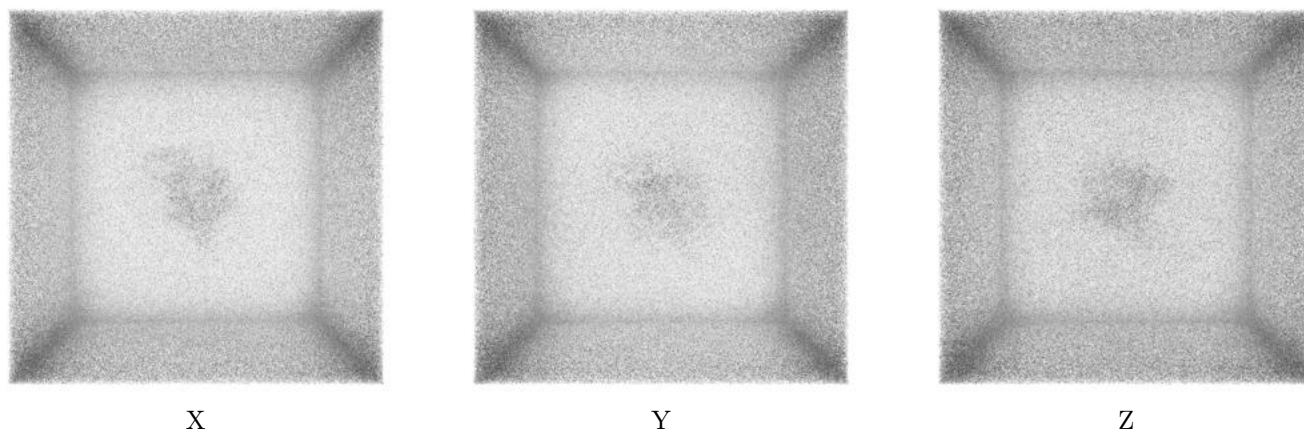
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

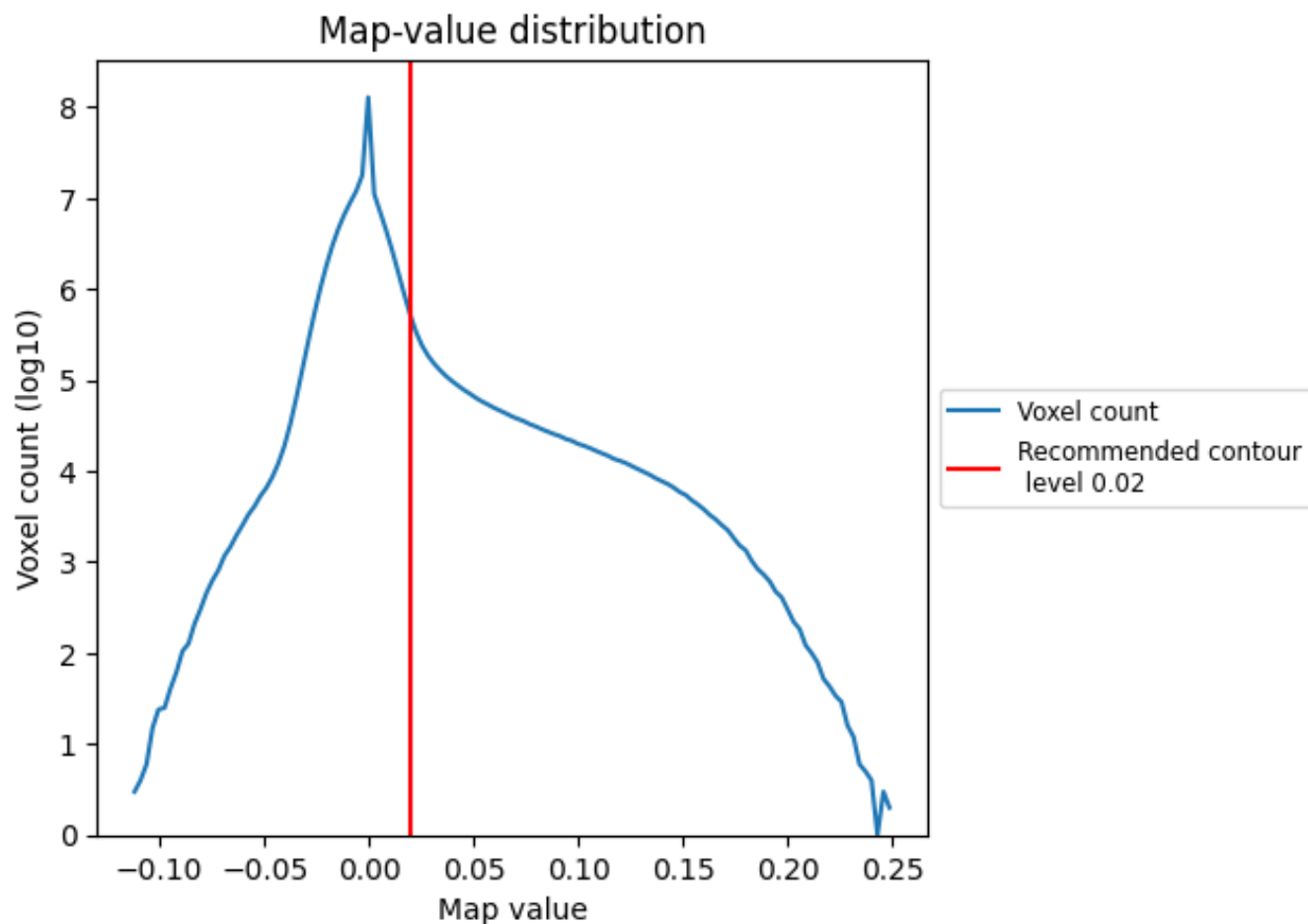
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

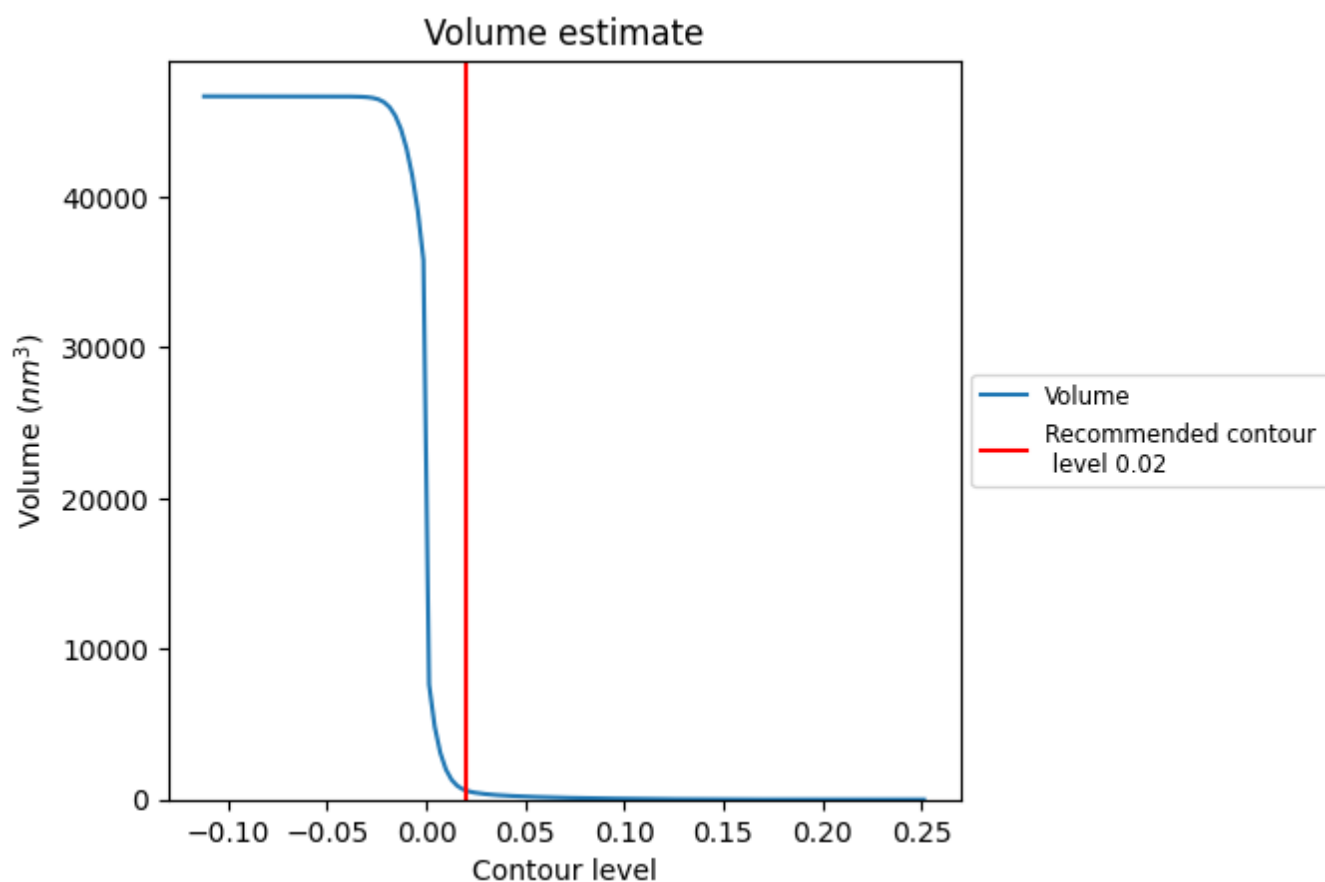
This section contains the results of statistical analysis of the map.

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.

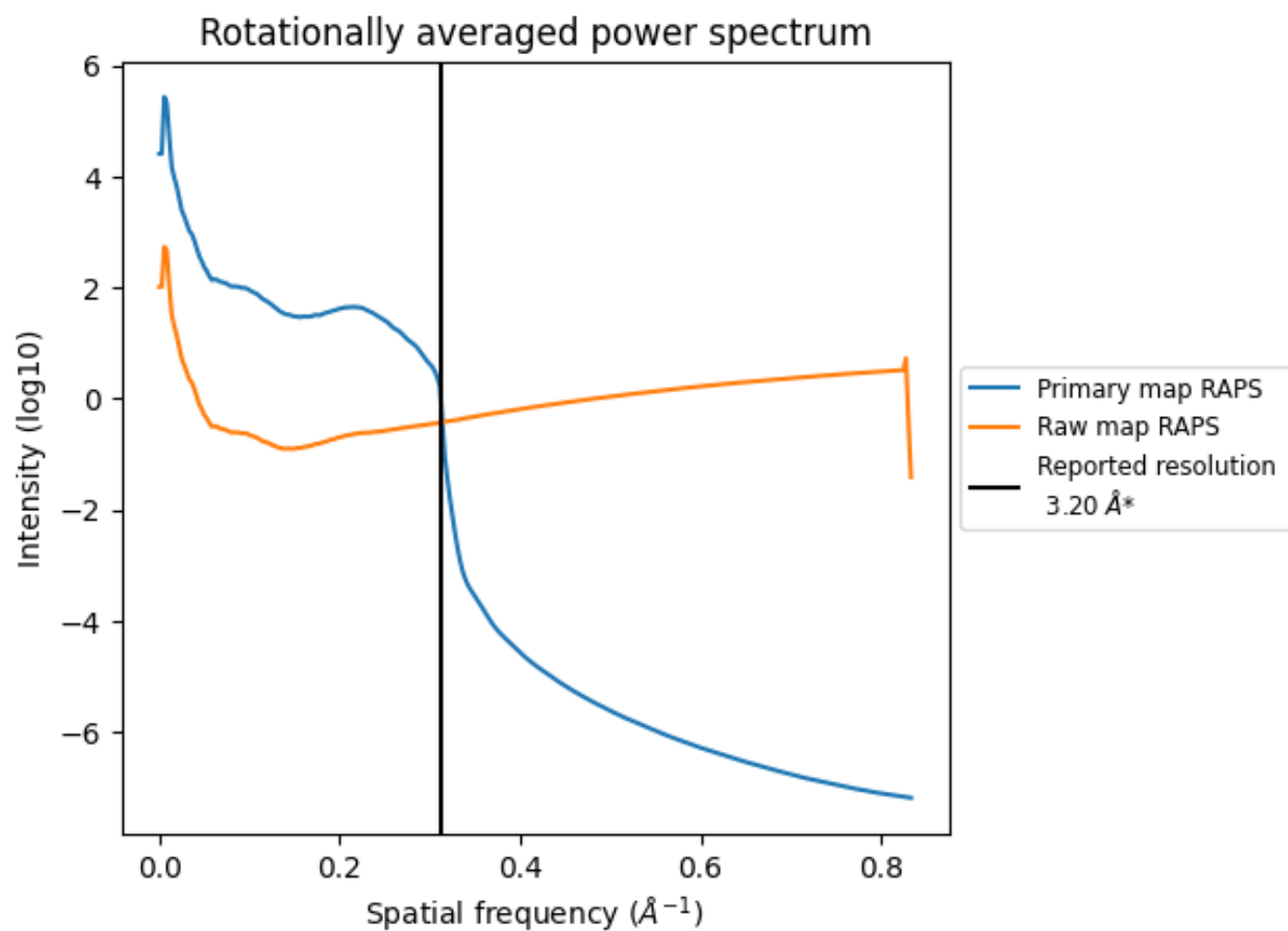
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 ⓘ

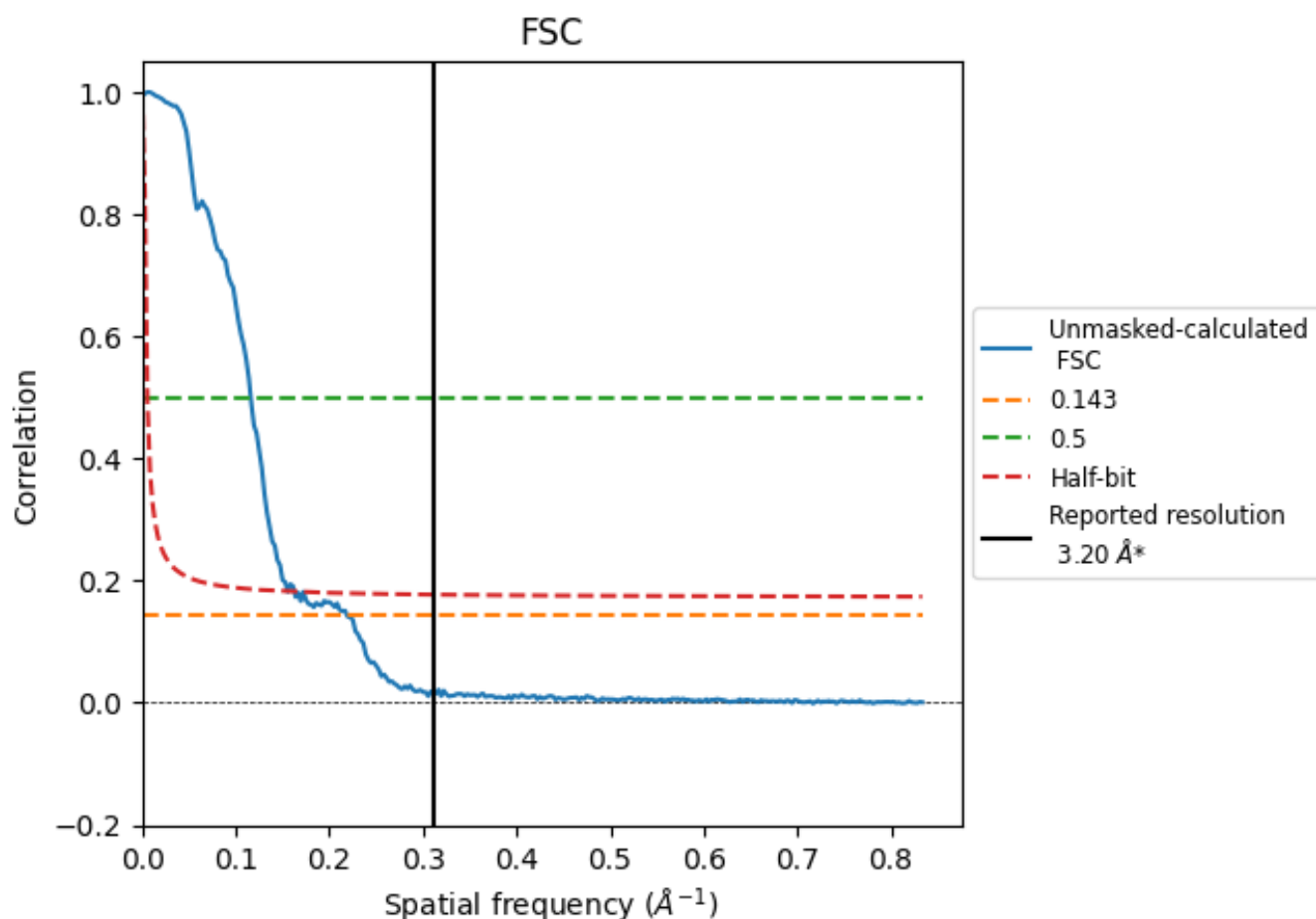


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

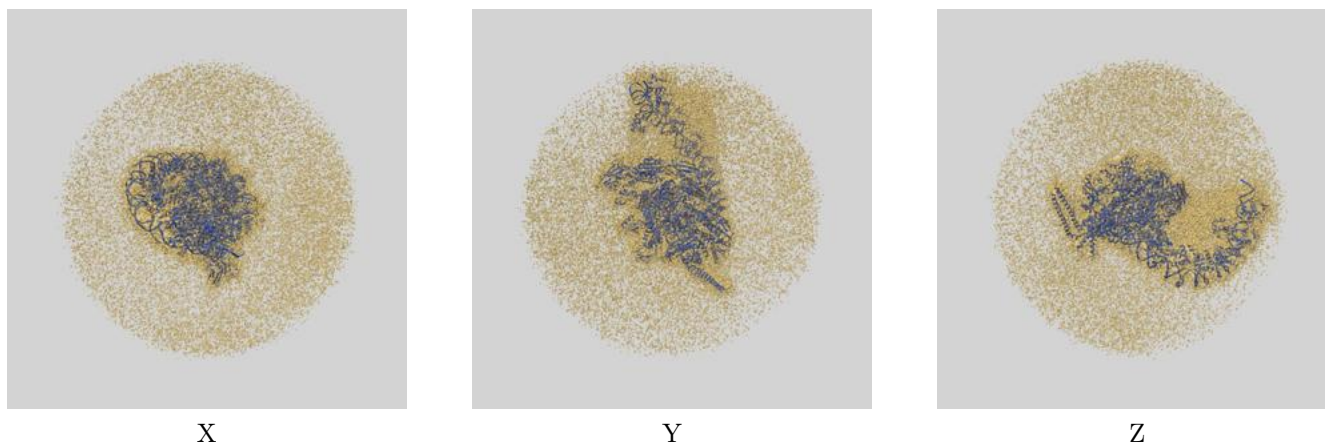
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.57	8.63	6.43

*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 4.57 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

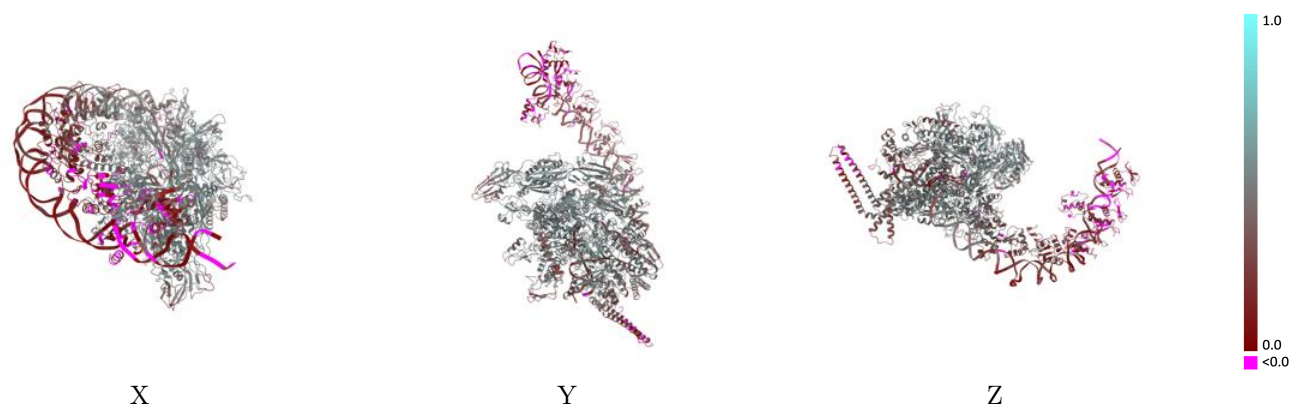
This section contains information regarding the fit between EMDB map EMD-61497 and PDB model 9JI5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



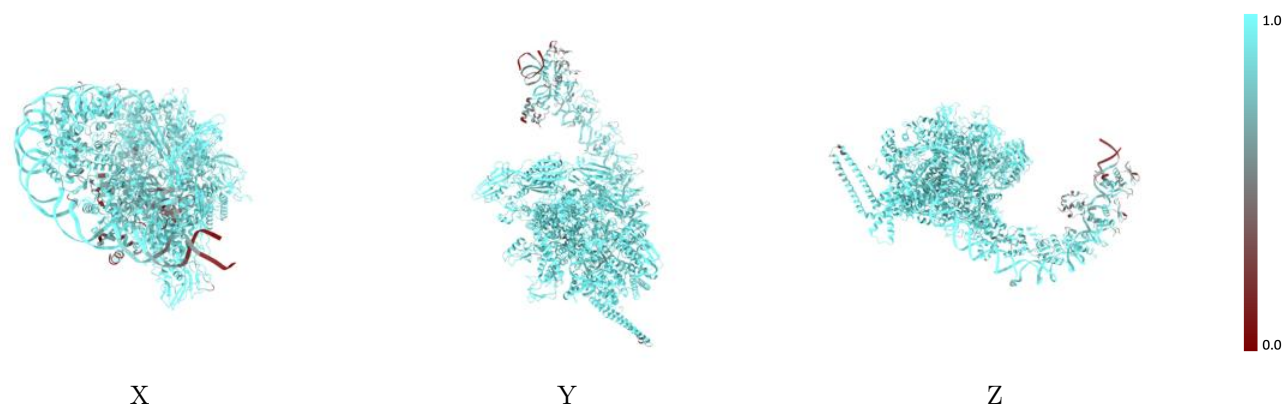
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



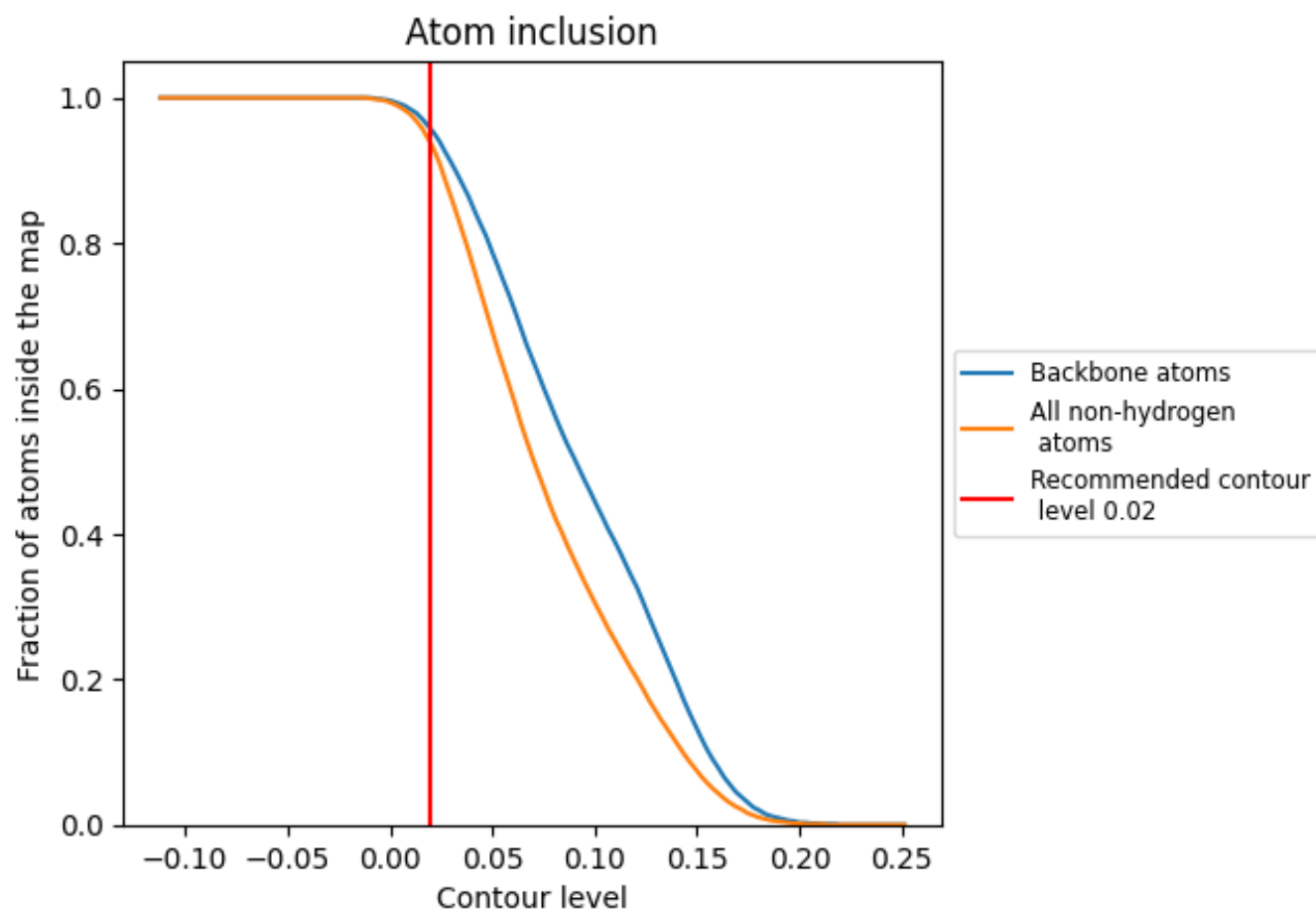
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9370	0.3990
A	0.9840	0.4970
B	0.9650	0.4440
C	0.9790	0.4900
D	0.9750	0.4680
E	0.9920	0.5040
F	0.9760	0.4170
G	0.8680	0.1730
H	0.8930	0.2350
I	0.6130	0.0920
J	0.9240	0.4220
K	0.8950	0.3260
L	0.8490	0.1740
M	0.8560	0.2220
N	0.6110	0.0770
O	0.7350	0.0740

1.0

0.0

<0.0