



wwPDB EM Validation Summary Report ⓘ

Sep 21, 2026 – 12:42 PM JST

PDB ID : 9WWL / pdb_00009wwl
EMDB ID : EMD-66314
Title : Cryo-EM structure of transcription activation complex with DevR from Mycobacterium tuberculosis
Authors : Lin, W.; Shi, J.
Deposited on : 2025-09-24
Resolution : 4.00 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.dev133
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) : 2.50

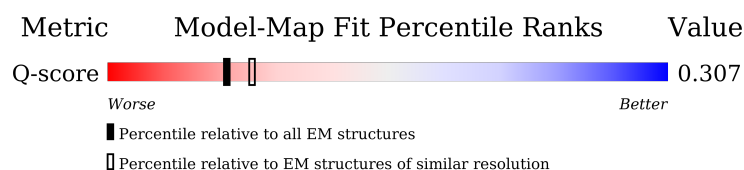
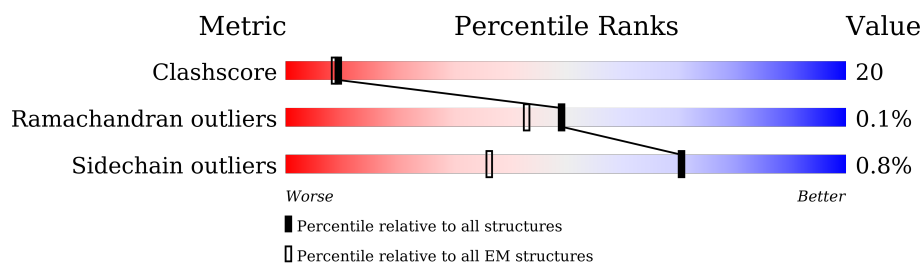
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



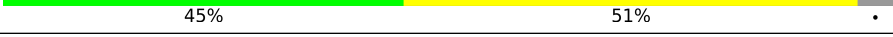
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	
1	B	347	
1	G	347	
2	C	1178	

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Mol	Chain	Length	Quality of chain
3	D	1316	
4	F	528	
5	O	124	
6	P	124	
7	E	110	
8	I	217	
8	J	217	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 31475 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
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		
1	G	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
			8577	5374	1502	1662	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1268	Total	C	N	O	S	0	0
			9862	6173	1791	1856	42		

- Molecule 4 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	322	Total	C	N	O	S	0	0
			2540	1583	459	489	9		

- Molecule 5 is a DNA chain called DNA (124-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	68	Total	C	N	O	P	0	0
			1399	662	256	413	68		

- Molecule 6 is a DNA chain called DNA (124-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	68	Total	C	N	O	P	0	0
			1402	661	272	401	68		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	83	Total	C	N	O	0	0
			644	409	108	127		

- Molecule 8 is a protein called DNA-binding transcriptional activator DevR/DosR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	209	Total	C	N	O	S	0	0
			1567	977	281	299	10		
8	J	209	Total	C	N	O	S	0	0
			1567	977	281	299	10		

- 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	

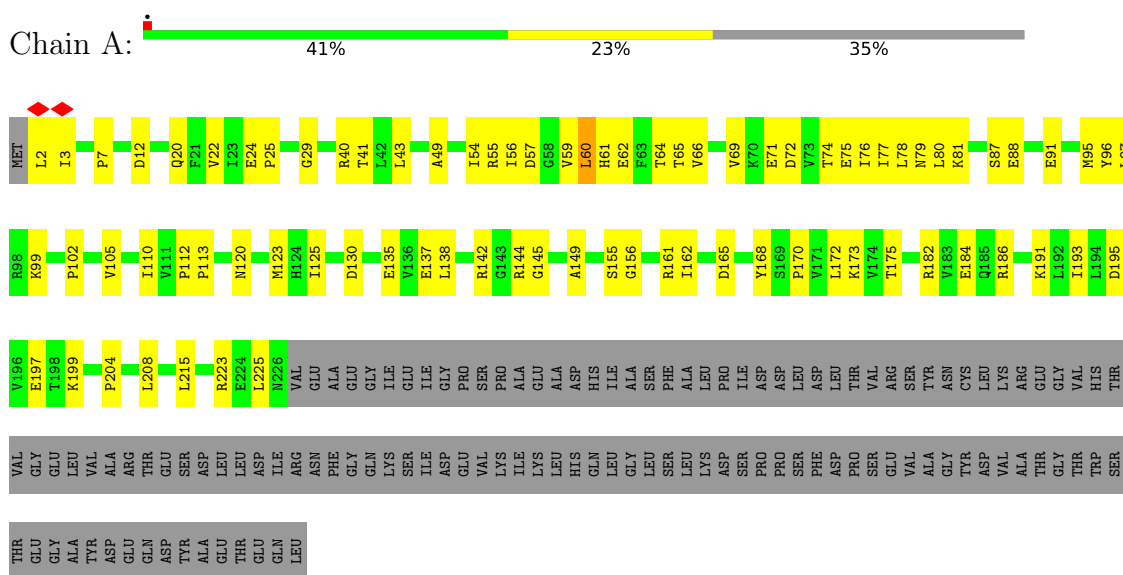
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

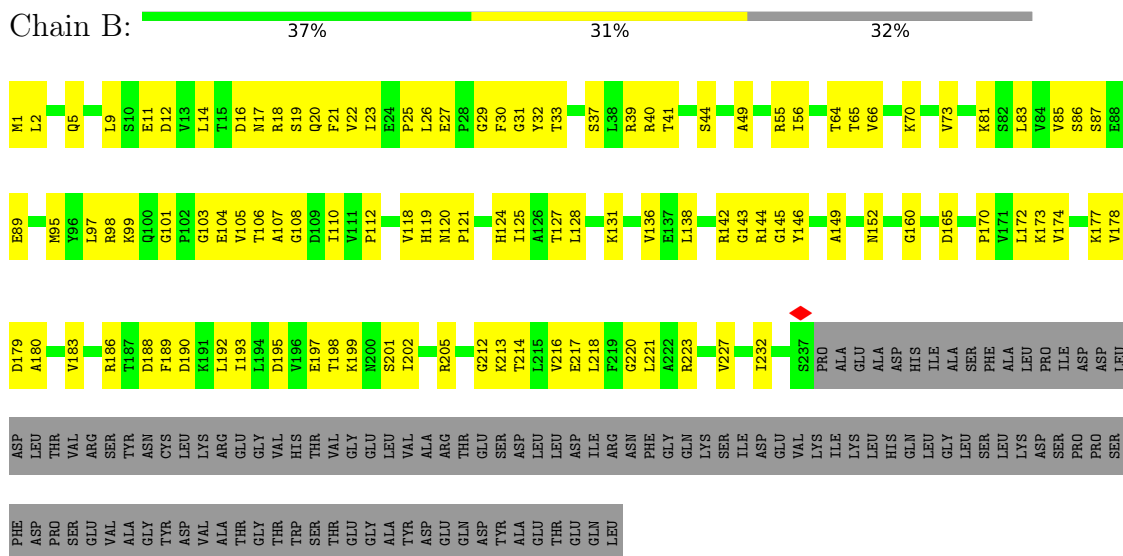
3 Residue-property plots

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.

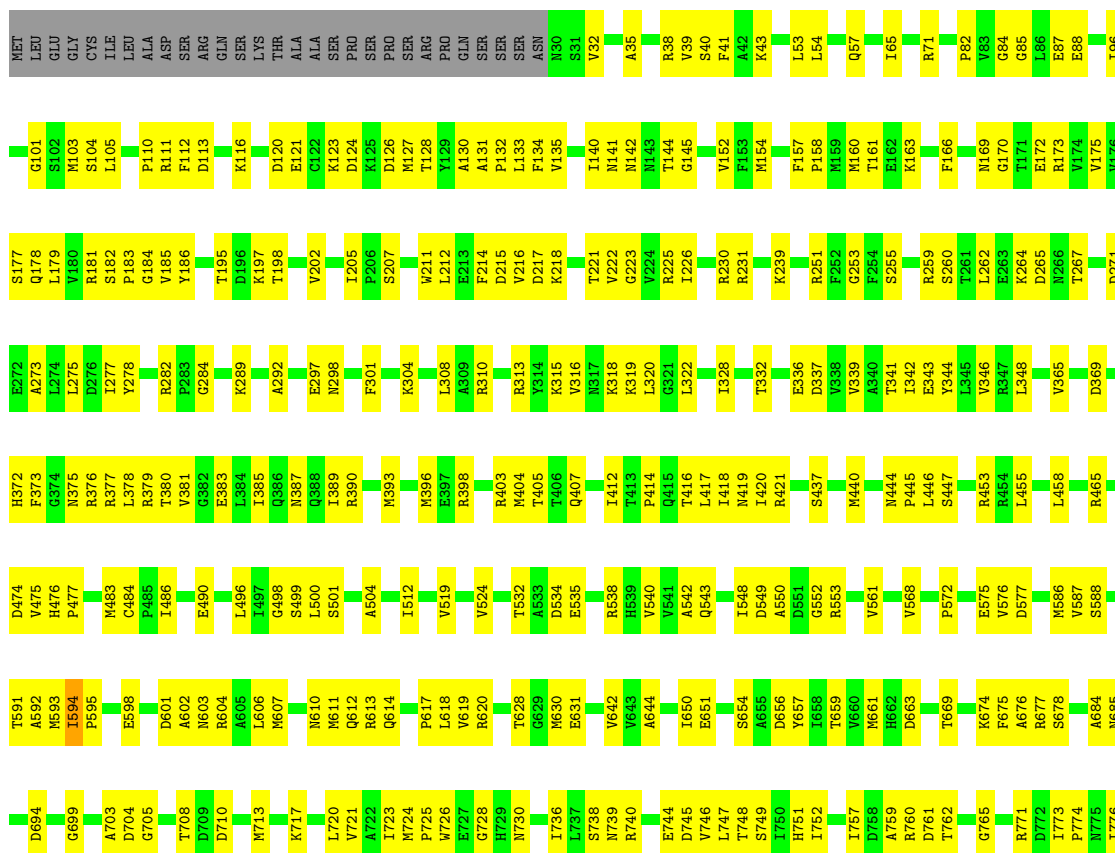
• Molecule 1: DNA-directed RNA polymerase subunit alpha



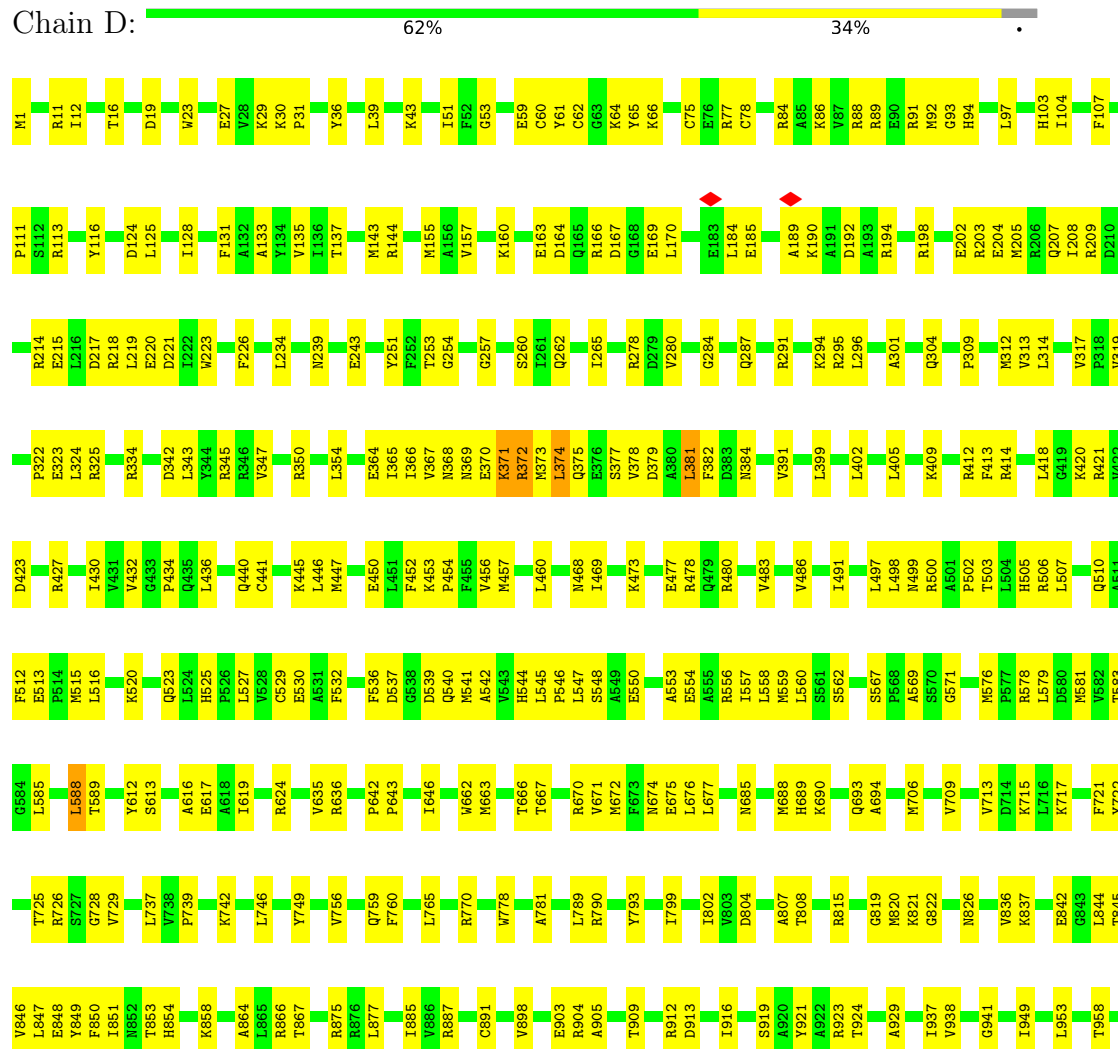
• Molecule 1: DNA-directed RNA polymerase subunit alpha



Chain G: 10% 7% 84%

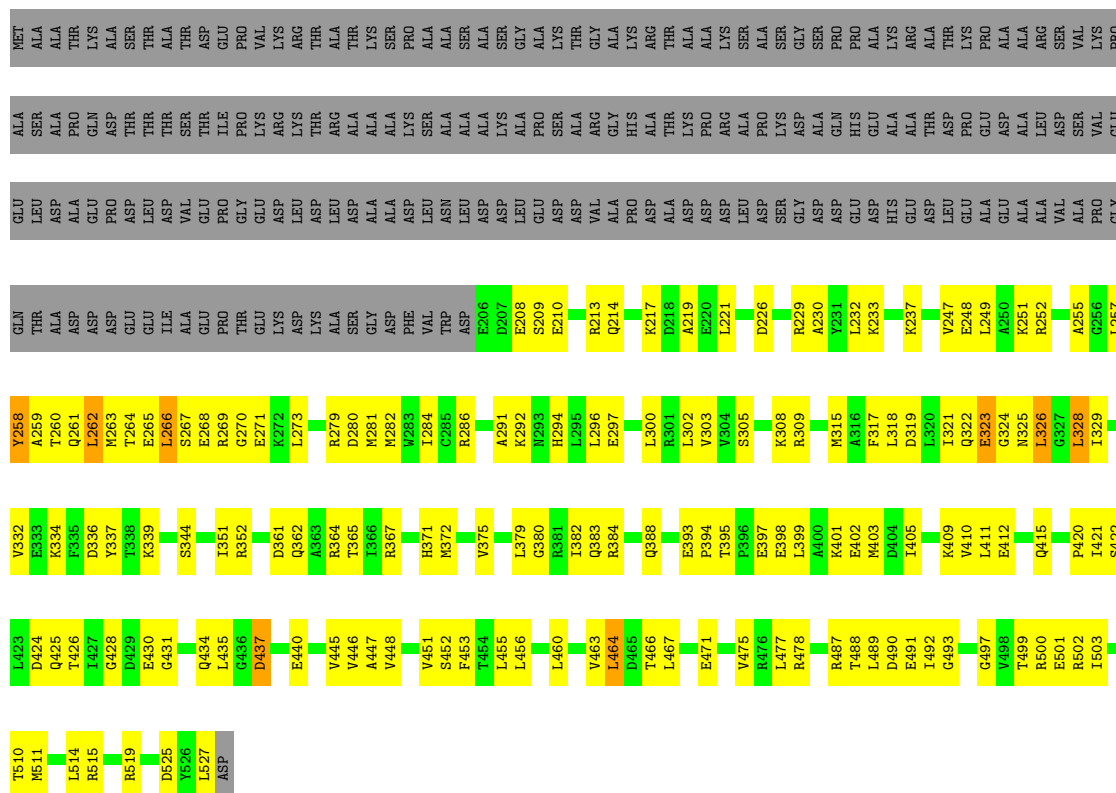


- Molecule 3: DNA-directed RNA polymerase subunit beta'

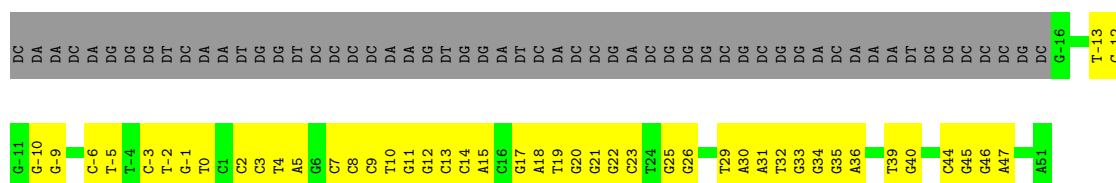




• Molecule 4: RNA polymerase sigma factor SigA



• Molecule 5: DNA (124-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	893467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS 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	0.407	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.13	0/1742	0.34	0/2370
1	B	0.13	0/1792	0.38	0/2442
1	G	0.10	0/436	0.31	0/588
2	C	0.12	0/8734	0.35	0/11845
3	D	0.12	0/10020	0.33	0/13544
4	F	0.16	0/2571	0.41	0/3468
5	O	0.20	0/1568	0.43	0/2420
6	P	0.21	0/1576	0.41	0/2431
7	E	0.14	0/656	0.38	0/892
8	I	0.10	0/1579	0.31	0/2129
8	J	0.13	0/1579	0.36	0/2129
All	All	0.13	0/32253	0.36	0/44258

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	1716	0	1756	73	0
1	B	1765	0	1794	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	433	0	440	16	0
2	C	8577	0	8486	343	0
3	D	9862	0	9902	385	0
4	F	2540	0	2552	208	0
5	O	1399	0	765	45	0
6	P	1402	0	759	35	0
7	E	644	0	630	31	0
8	I	1567	0	1635	82	0
8	J	1567	0	1635	91	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	31475	0	30354	1241	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 20.

The worst 5 of 1241 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)
3:D:373:MET:CE	4:F:318:LEU:HB3	1.36	1.51
3:D:373:MET:SD	4:F:318:LEU:HD13	1.67	1.33
3:D:373:MET:HE3	4:F:318:LEU:CB	1.67	1.22
3:D:367:VAL:O	3:D:371:LYS:HG3	1.41	1.21
3:D:373:MET:CG	4:F:318:LEU:HD13	1.79	1.12

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%)	216 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	235/347 (68%)	213 (91%)	22 (9%)	0	100	100
1	G	55/347 (16%)	54 (98%)	1 (2%)	0	100	100
2	C	1109/1178 (94%)	1049 (95%)	60 (5%)	0	100	100
3	D	1262/1316 (96%)	1219 (97%)	43 (3%)	0	100	100
4	F	320/528 (61%)	308 (96%)	12 (4%)	0	100	100
7	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
8	I	207/217 (95%)	196 (95%)	11 (5%)	0	100	100
8	J	207/217 (95%)	199 (96%)	6 (3%)	2 (1%)	12	45
All	All	3699/4607 (80%)	3530 (95%)	167 (4%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	145	ASP
8	J	144	GLN

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	194/297 (65%)	192 (99%)	2 (1%)	68	76
1	B	195/297 (66%)	195 (100%)	0	100	100
1	G	46/297 (16%)	46 (100%)	0	100	100
2	C	930/998 (93%)	926 (100%)	4 (0%)	84	84
3	D	1037/1095 (95%)	1030 (99%)	7 (1%)	76	79
4	F	266/427 (62%)	258 (97%)	8 (3%)	36	57
7	E	67/90 (74%)	66 (98%)	1 (2%)	57	70
8	I	164/171 (96%)	162 (99%)	2 (1%)	63	73
8	J	164/171 (96%)	164 (100%)	0	100	100
All	All	3063/3843 (80%)	3039 (99%)	24 (1%)	70	77

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	262	LEU
4	F	326	LEU
4	F	323	GLU
4	F	328	LEU
3	D	371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	377	ASN
7	E	69	ASN
4	F	388	GLN
7	E	70	GLN
3	D	351	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 ⓘ

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.

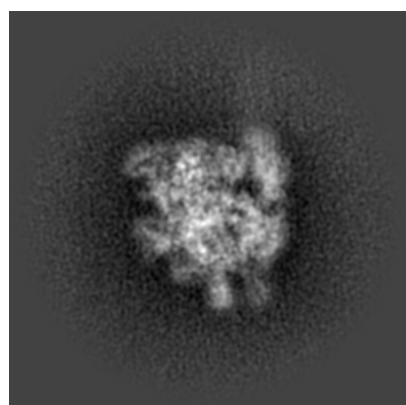
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66314. These allow visual inspection of the internal detail of the map and identification of artifacts.

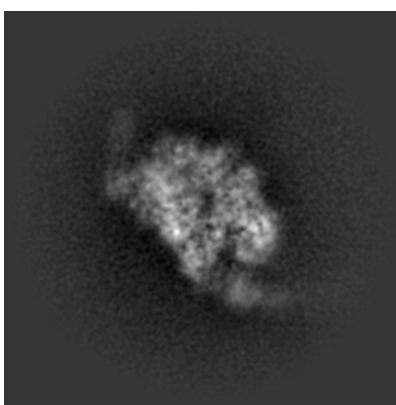
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

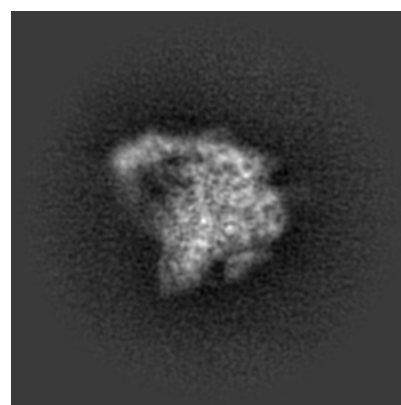
6.1.1 Primary map



X



Y

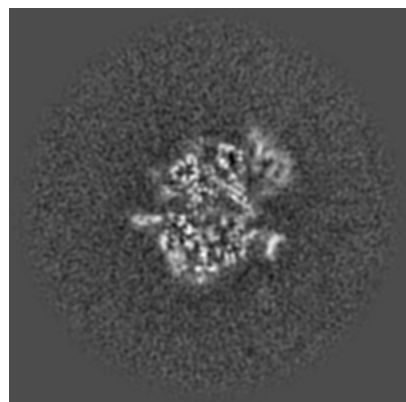


Z

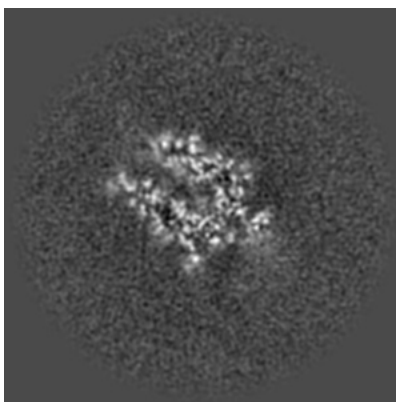
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

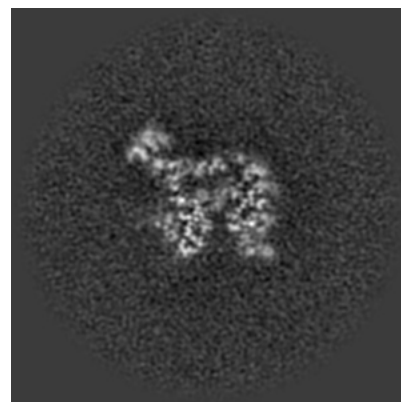
6.2.1 Primary map



X Index: 150



Y Index: 150

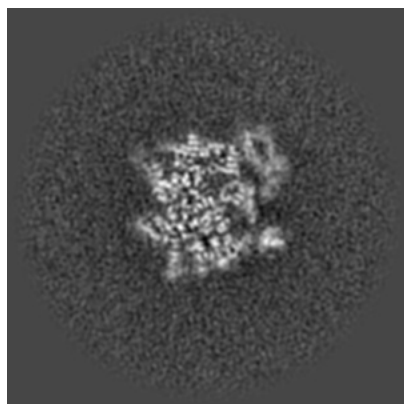


Z Index: 150

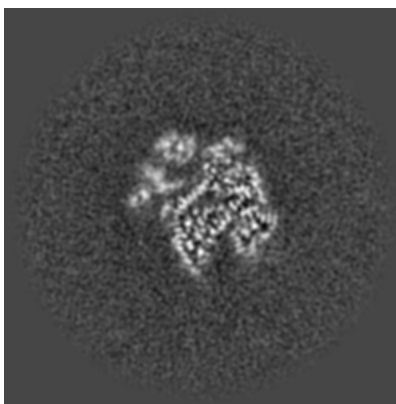
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

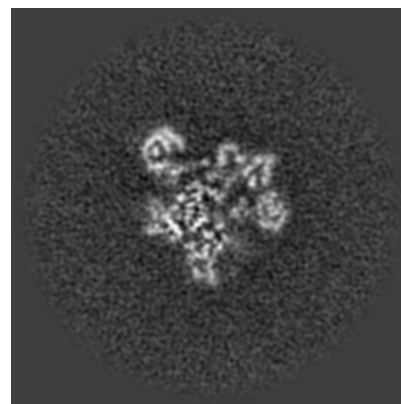
6.3.1 Primary map



X Index: 143



Y Index: 136

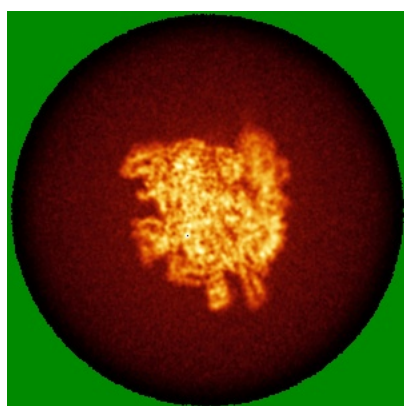


Z Index: 139

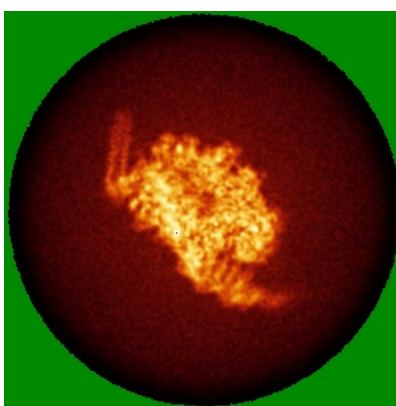
The images above show the largest variance slices of the map in three orthogonal directions.

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

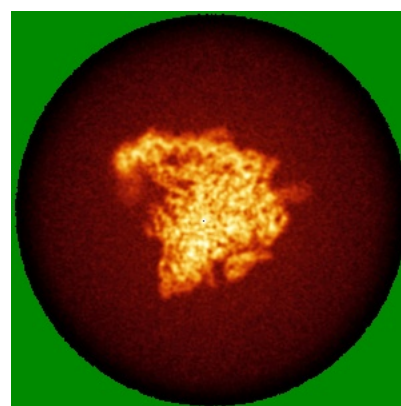
6.4.1 Primary map



X



Y

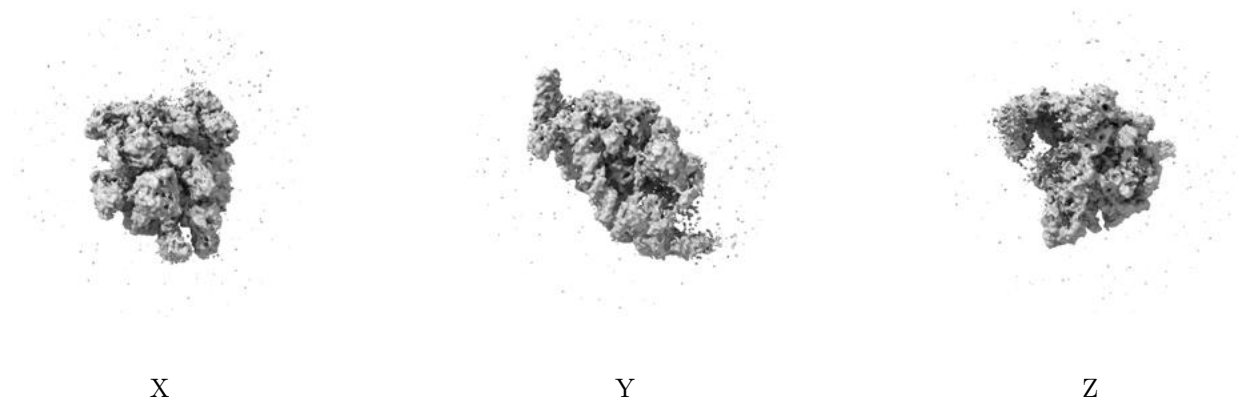


Z

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

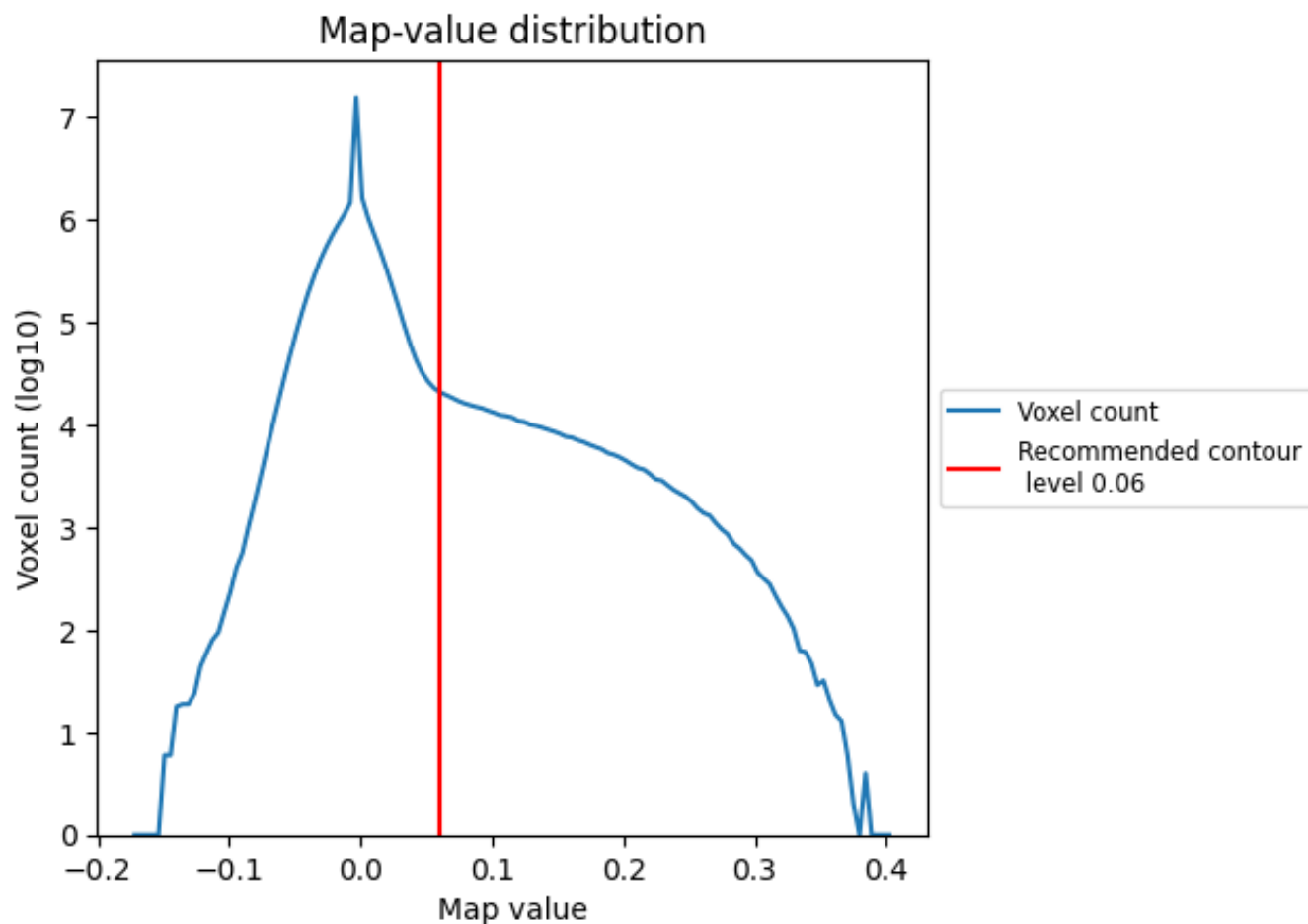
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

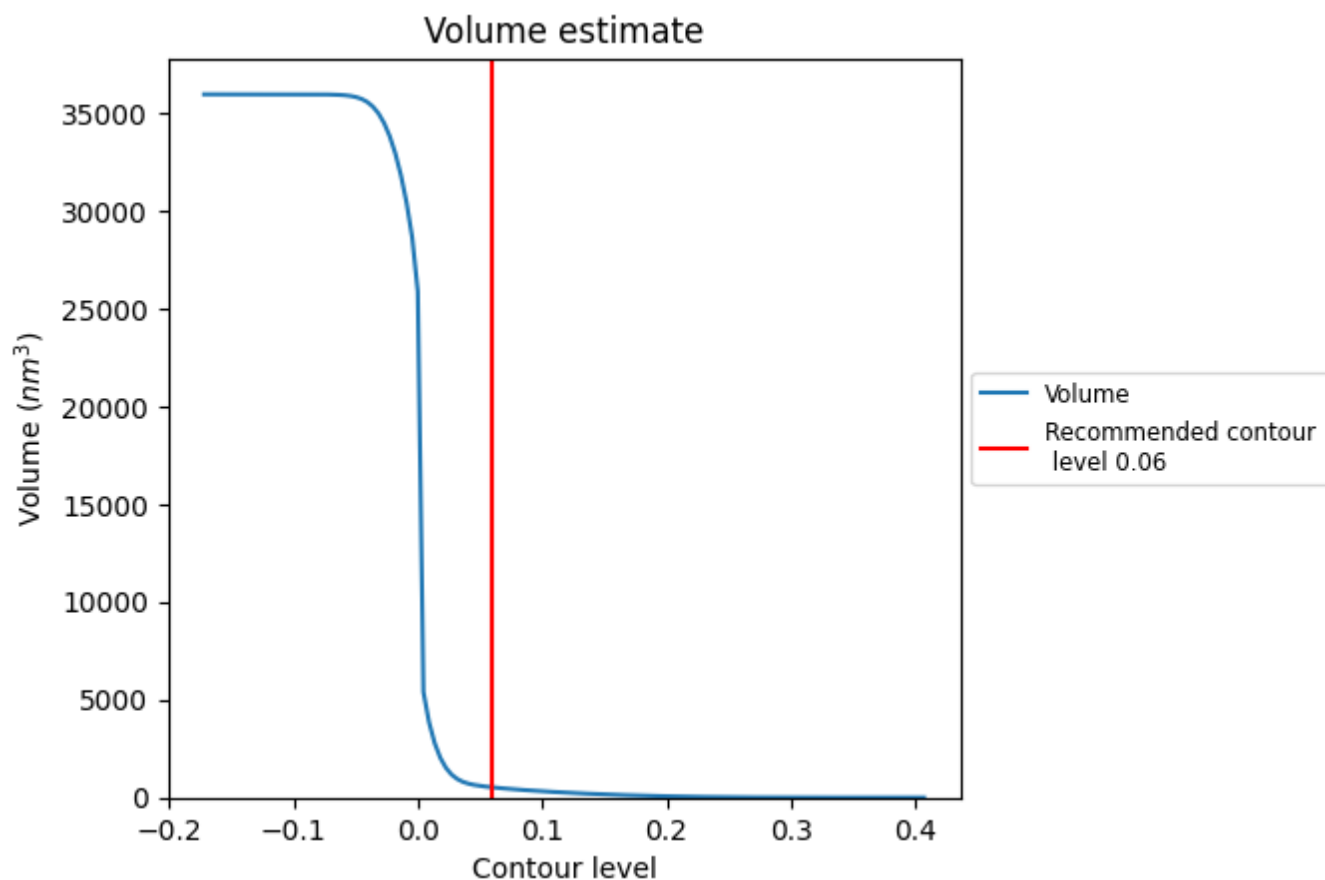
This section contains the results of statistical analysis of the map.

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.

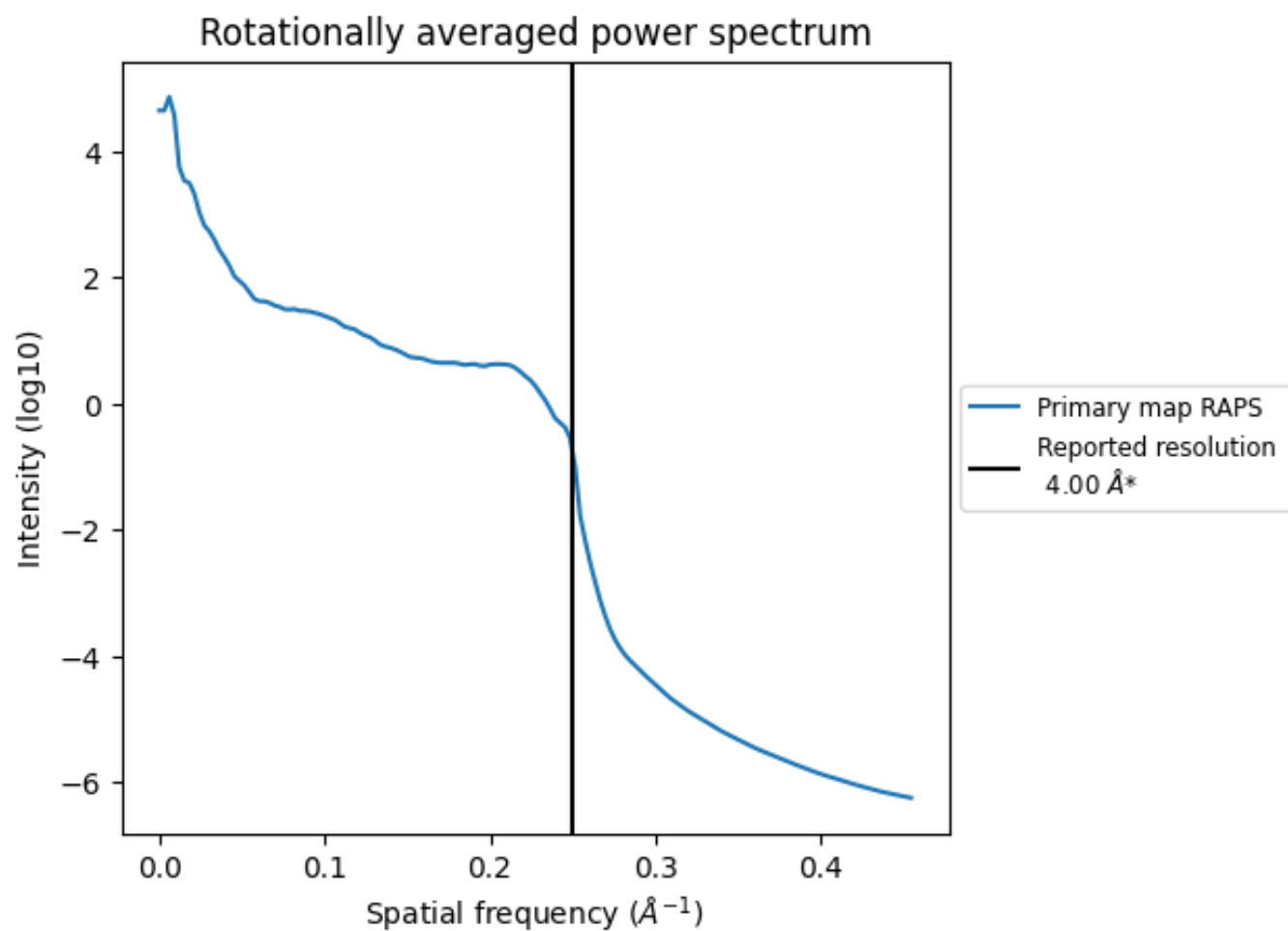
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 521 nm³; this corresponds to an approximate mass of 471 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 0.250 Å⁻¹

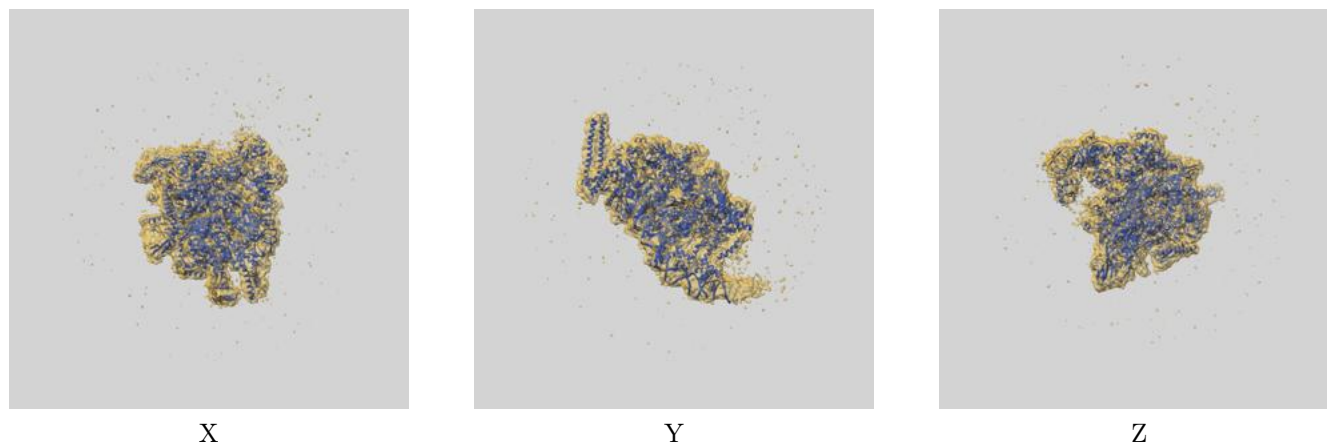
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

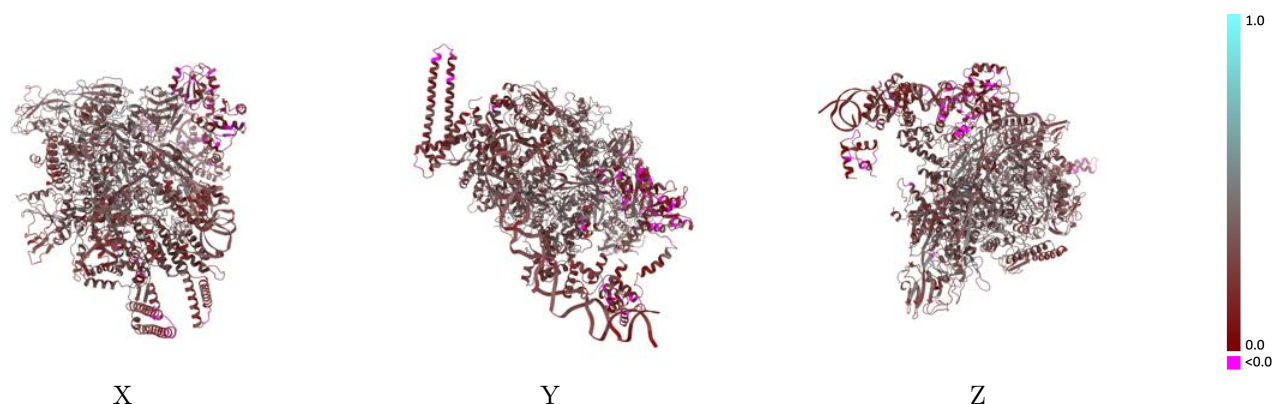
This section contains information regarding the fit between EMDB map EMD-66314 and PDB model 9WWL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



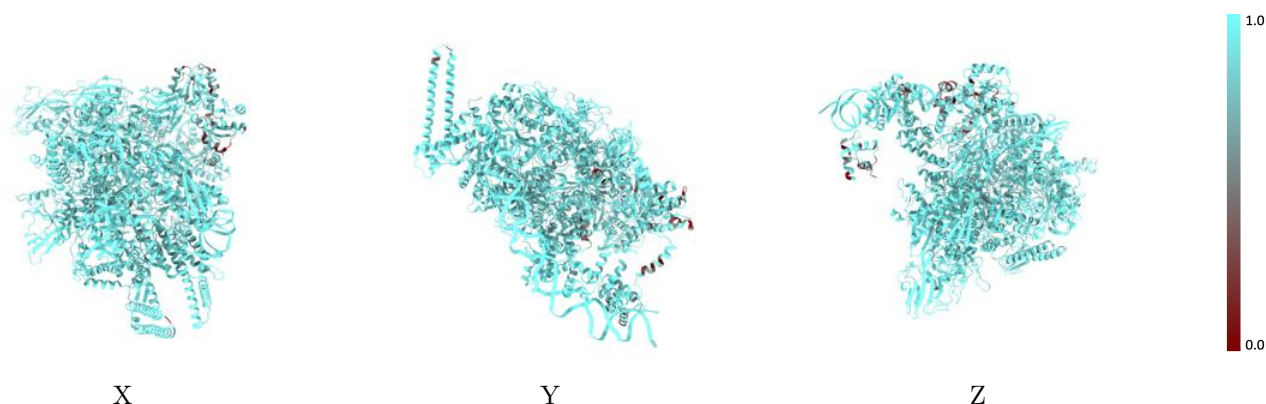
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



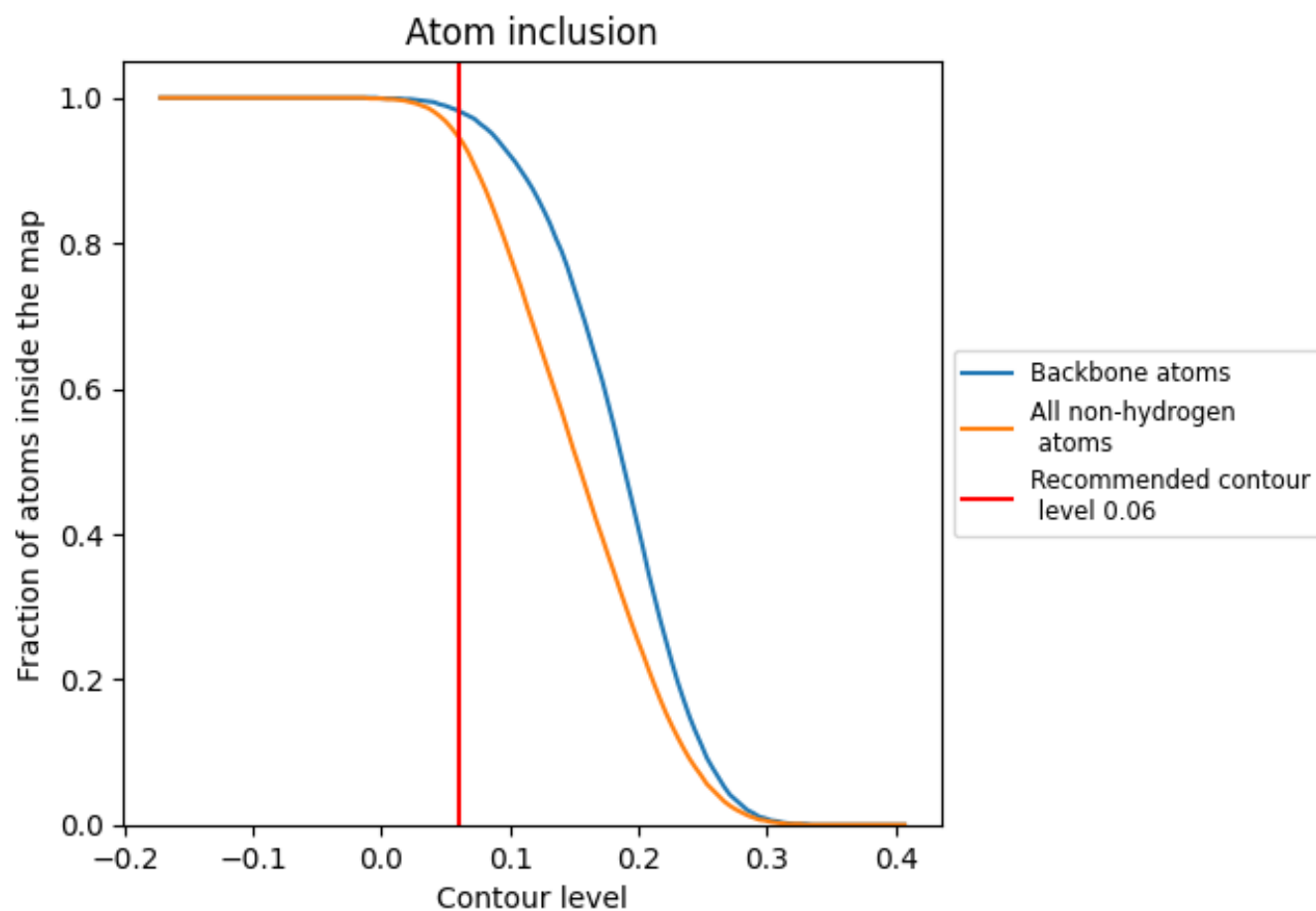
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.3070
A	 0.9550	 0.3580
B	 0.9670	 0.3230
C	 0.9560	 0.3450
D	 0.9600	 0.3310
E	 0.9810	 0.3350
F	 0.9490	 0.2810
G	 0.7170	 0.1030
I	 0.8650	 0.1740
J	 0.8390	 0.1540
O	 0.9860	 0.2750
P	 0.9670	 0.2610

