



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:13 PM UTC

PDB ID : 5FJ7 / pdb_00005fj7
EMDB ID : EMD-3187
Title : Structure of the P2 polymerase inside in vitro assembled bacteriophage phi6 polymerase complex, with P1 included
Authors : Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on : 2015-10-06
Resolution : 7.90 Å (reported)
Based on initial models : 4K7H, 1HHS

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

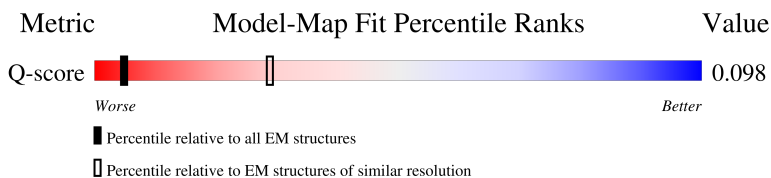
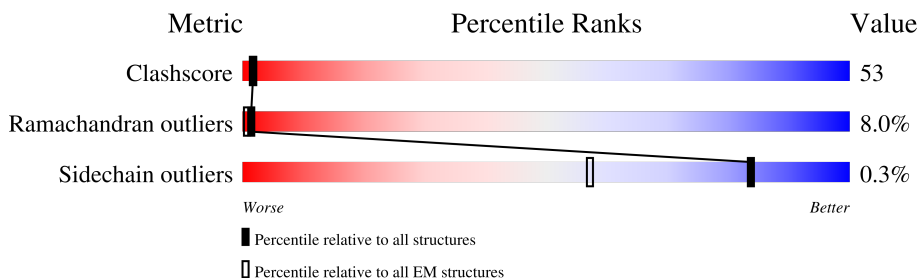
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 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	366 (7.40 - 8.40)

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	761	
1	B	761	
2	C	664	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17106 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 MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	664	Total	C	N	O	S	0	0
			5265	3342	914	977	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	456	MET	ILE	conflict	UNP P11124

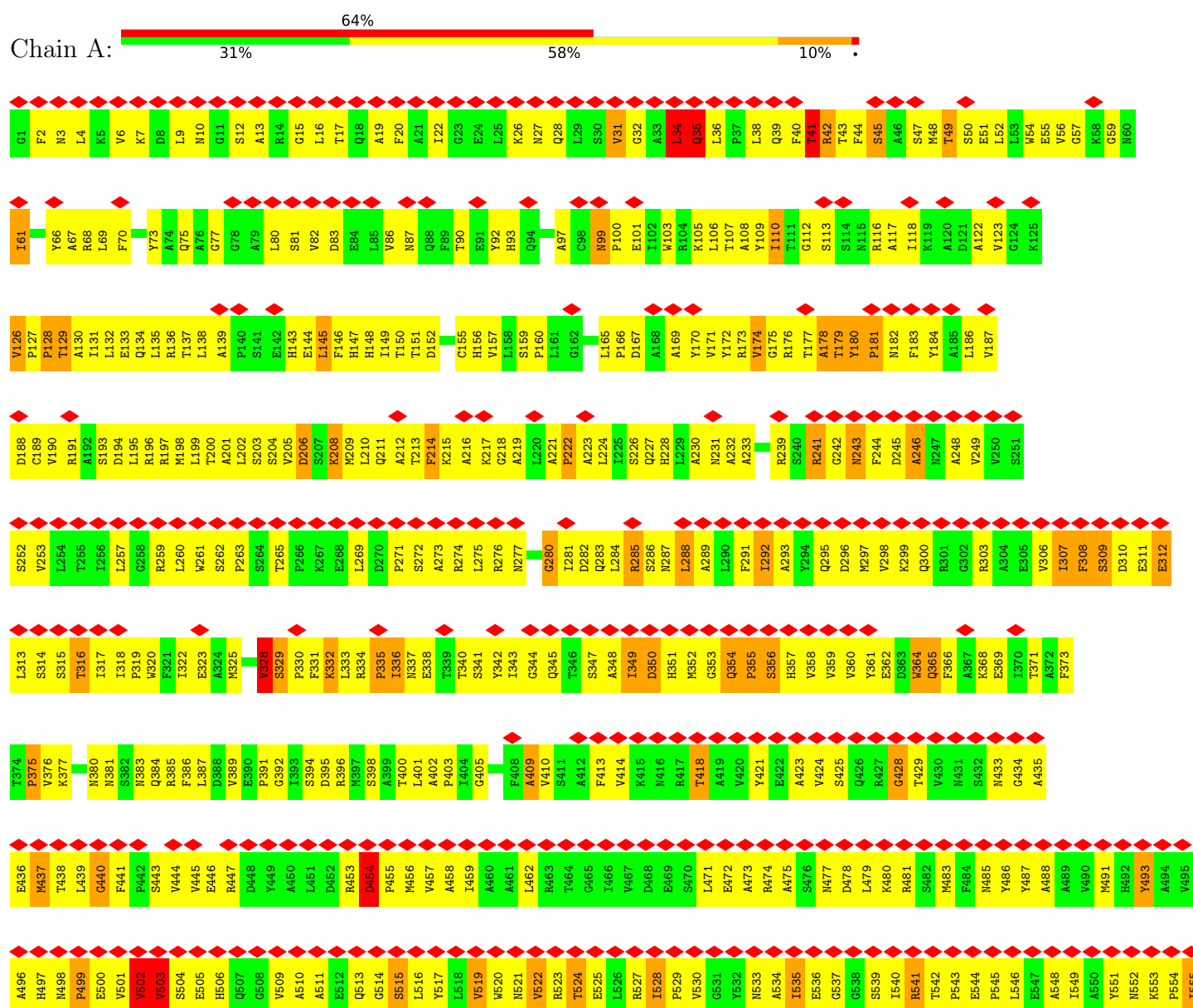
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

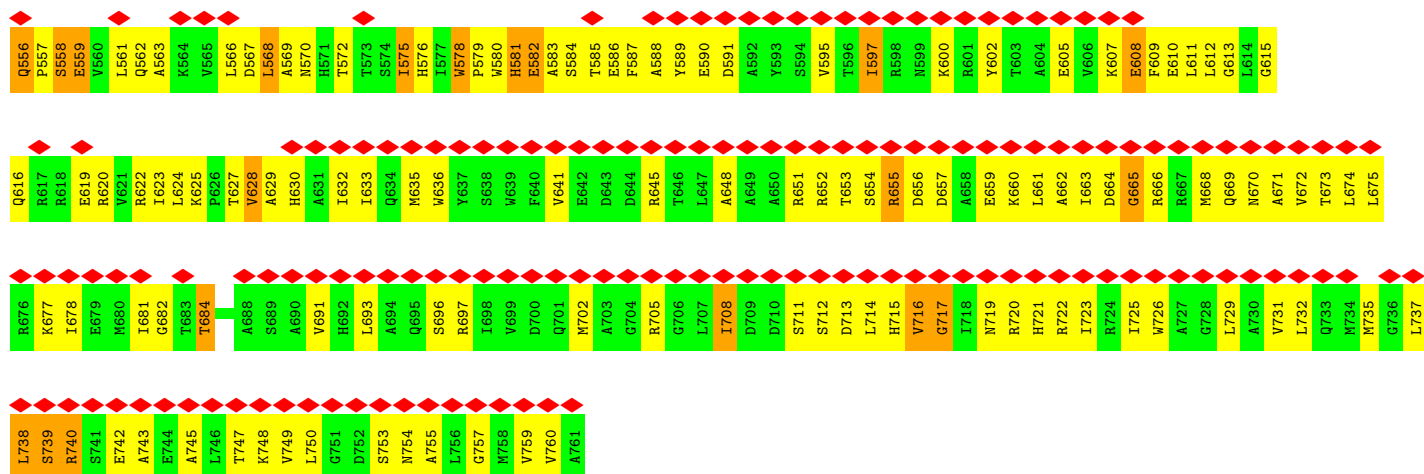
Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mn	0
			1	1	

3 Residue-property plots

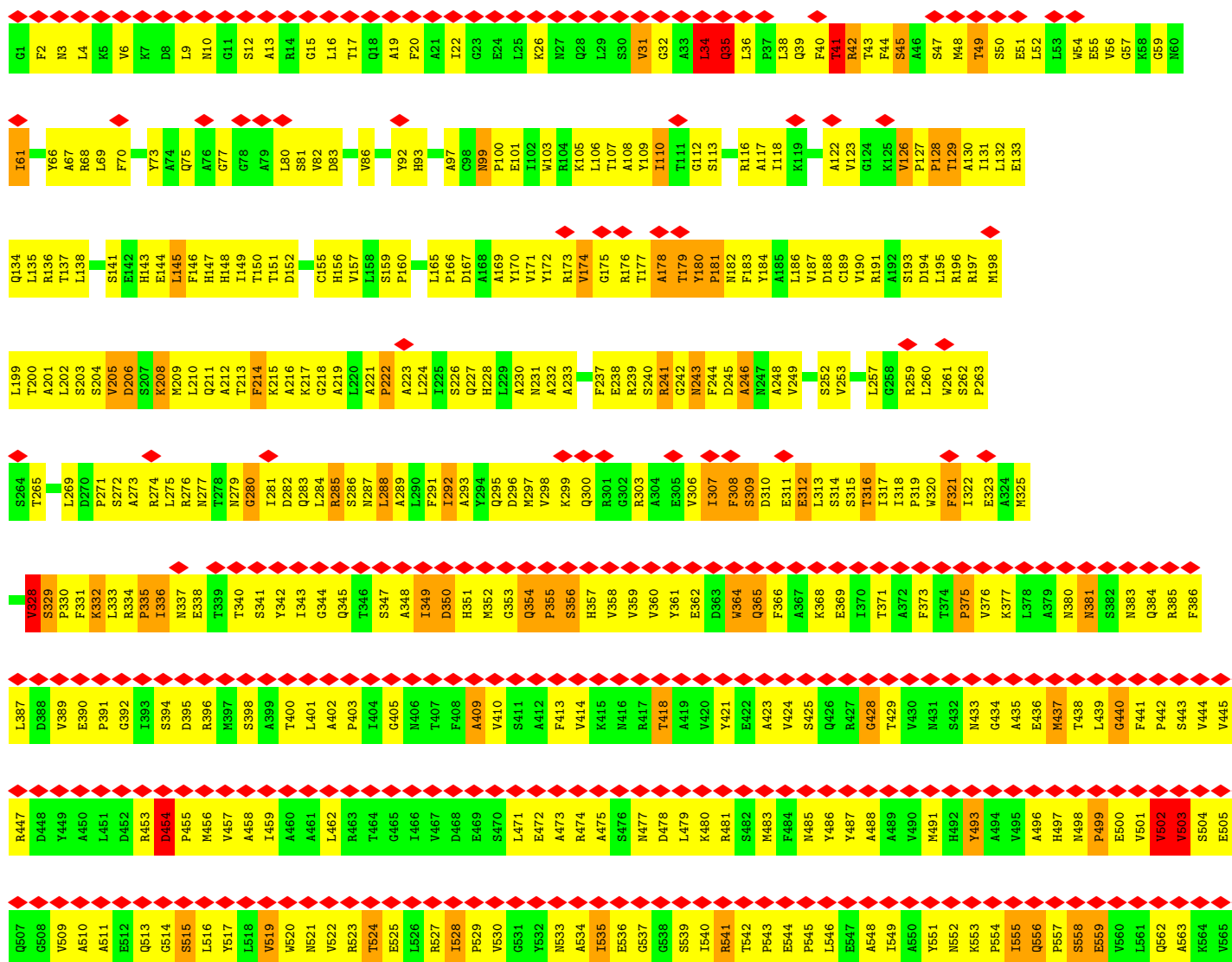
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

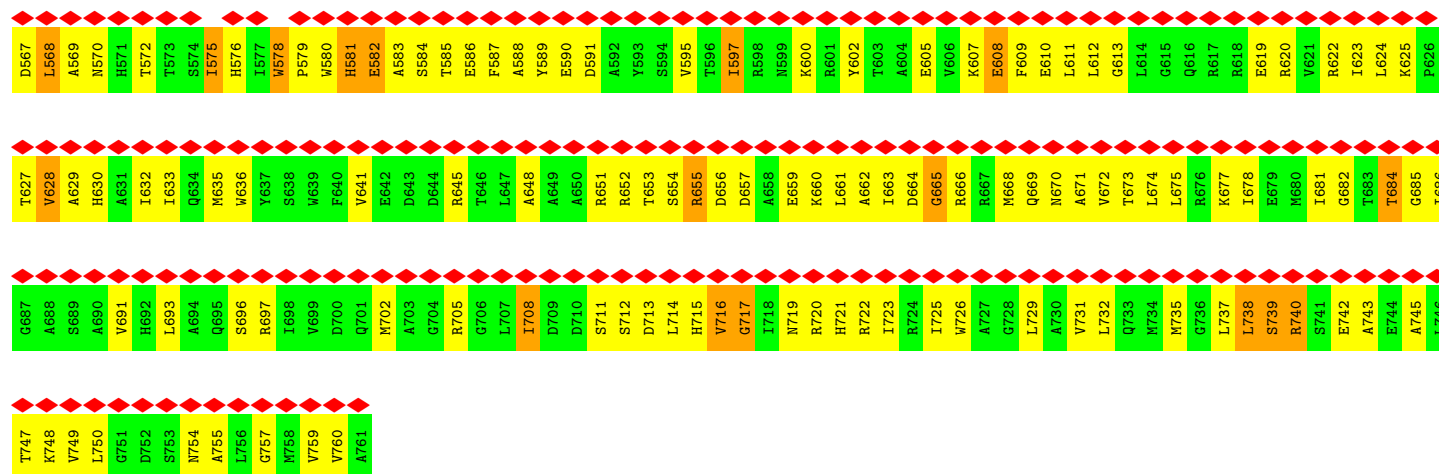
• Molecule 1: MAJOR INNER PROTEIN P1



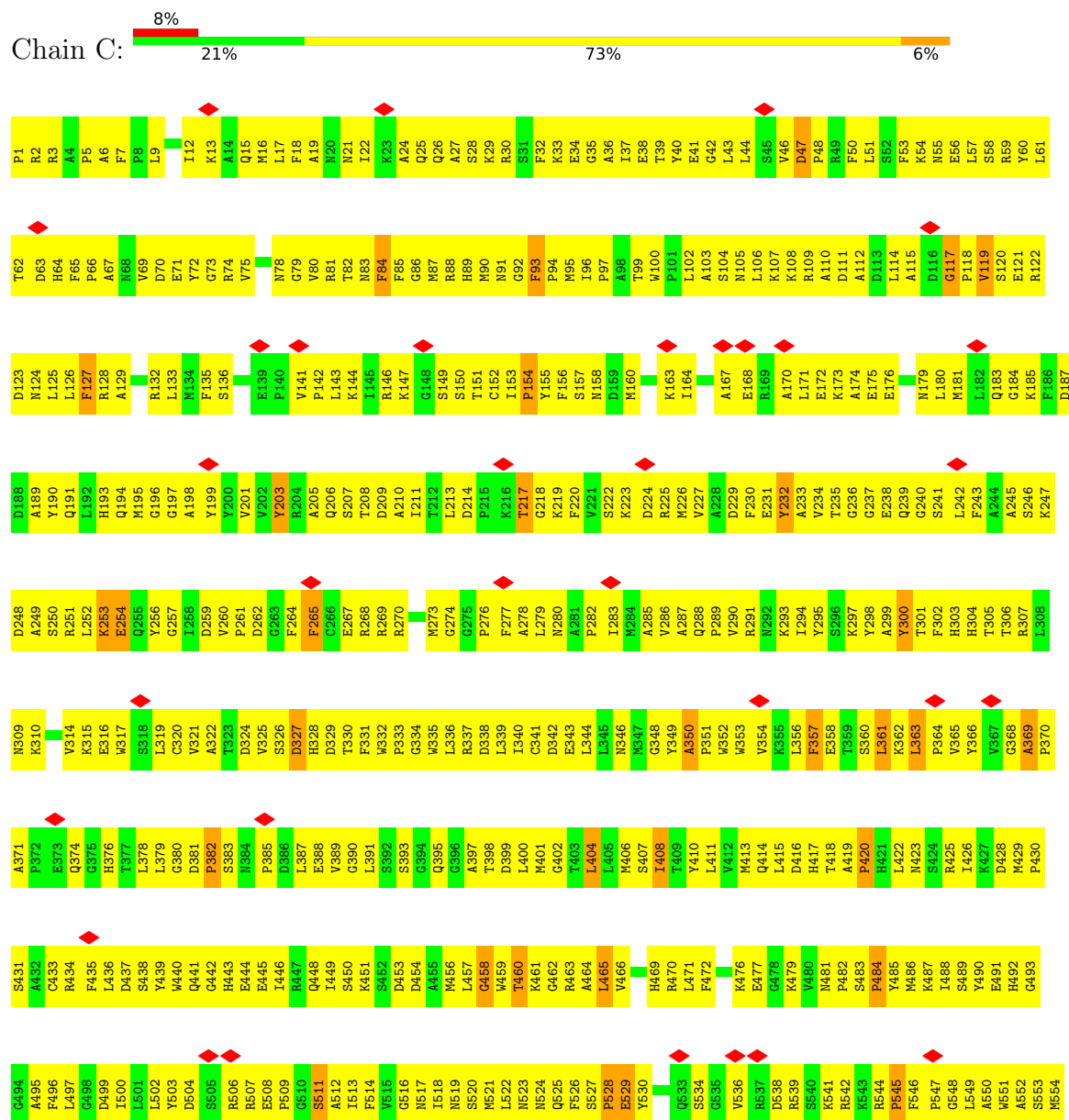


• Molecule 1: MAJOR INNER PROTEIN P1





• Molecule 2: RNA-DIRECTED RNA POLYMERASE



K555	D556	T557	Y558	G559	A560	C561	P562	I563	Y564	S565	D566	V567	L568	E569	A570	I571	E572	R573	C574	W575	W576	W577	A578	F579	G580	E581	S582	Y583	R584	A585	Y586	R587	E588	D589	M590	L591	K592	R593	L596	E597	L598	S599	R600	Y601	V602	A603	S604	M605	A606	R607	Q608	A609	G610	L611	A612	E613	L614	T615
P616	I617	D618	L619	E620	V621	L622	A623	D624	P625	N626	K627	L628	Q629	Y630	K631	W632	T633	E634	A635	D636	V637	S638	A639	M640	I641	H642	E643	V644	L645	M646	H647	G648	V649	S650	V651	E652	E655	R656	F657	L658	R659	S660	V661	M662	P663	R664												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43216	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	135.0, 135.0, 135.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.59	0/6040	1.12	44/8206 (0.5%)
1	B	0.59	0/6040	1.12	45/8206 (0.5%)
2	C	1.16	7/5396 (0.1%)	1.06	29/7297 (0.4%)
All	All	0.81	7/17476 (0.0%)	1.10	118/23709 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
2	C	0	1
All	All	0	11

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	361	LEU	CG-CD1	59.08	3.47	1.52
2	C	357	PHE	CD1-CE1	18.12	1.93	1.38
2	C	357	PHE	CD2-CE2	17.88	1.92	1.38
2	C	357	PHE	CE2-CZ	16.03	1.86	1.38
2	C	357	PHE	CE1-CZ	15.80	1.86	1.38

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	THR	N-CA-C	10.17	122.36	111.28
1	A	179	THR	N-CA-C	10.15	122.34	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	PRO	N-CA-C	9.12	125.96	113.65
1	A	128	PRO	N-CA-C	9.11	125.94	113.65
1	B	128	PRO	CA-C-N	8.46	136.93	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide
1	A	365	GLN	Peptide
1	A	437	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5920	0	5913	537	0
1	B	5920	0	5907	664	0
2	C	5265	0	5154	741	0
3	C	1	0	0	0	0
All	All	17106	0	16974	1812	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 53.

The worst 5 of 1812 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:PHE:CE1	2:C:357:PHE:CZ	1.86	1.58
2:C:357:PHE:CD2	2:C:357:PHE:CE2	1.92	1.58
2:C:357:PHE:CZ	2:C:357:PHE:CE2	1.86	1.56
2:C:357:PHE:CE1	2:C:357:PHE:CD1	1.93	1.53
1:B:237:PHE:O	2:C:425:ARG:NH2	1.58	1.36

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	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	0	7
1	B	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	0	7
2	C	662/664 (100%)	575 (87%)	61 (9%)	26 (4%)	2	19
All	All	2180/2186 (100%)	1763 (81%)	243 (11%)	174 (8%)	1	9

5 of 174 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL

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	629/629 (100%)	626 (100%)	3 (0%)	81	83
1	B	629/629 (100%)	626 (100%)	3 (0%)	81	83
2	C	557/557 (100%)	557 (100%)	0	100	100
All	All	1815/1815 (100%)	1809 (100%)	6 (0%)	84	86

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	503	VAL
1	B	519	VAL
1	B	528	ILE
1	A	519	VAL
1	A	503	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	158	ASN
2	C	448	GLN
2	C	191	GLN
2	C	309	ASN
2	C	481	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

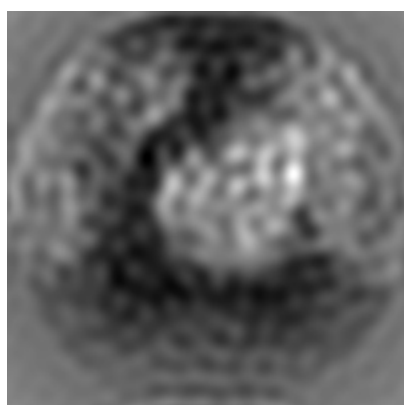
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3187. These allow visual inspection of the internal detail of the map and identification of artifacts.

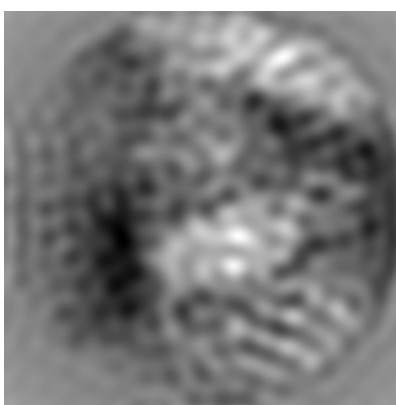
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

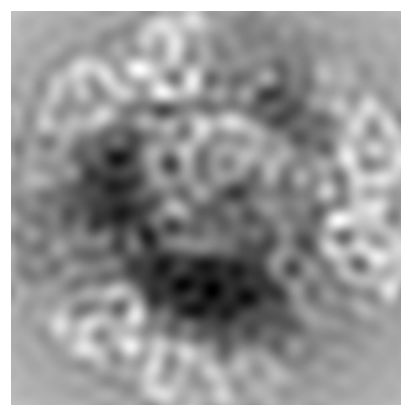
6.1.1 Primary map



X



Y

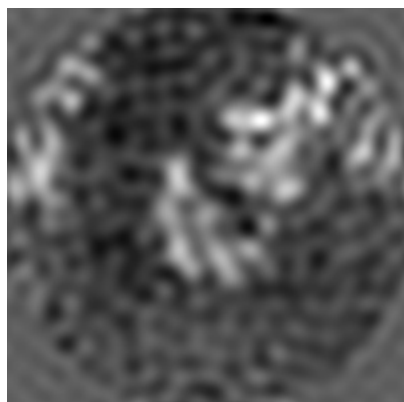


Z

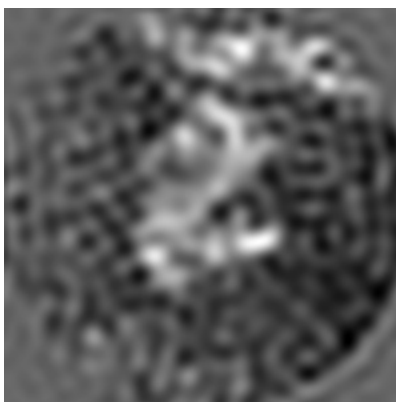
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

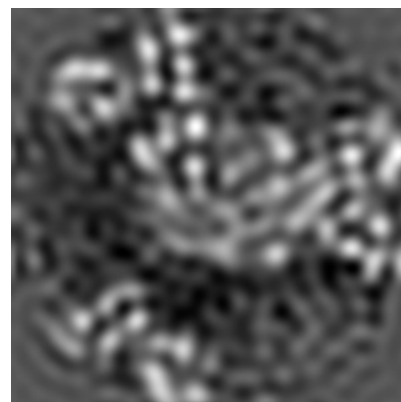
6.2.1 Primary map



X Index: 50



Y Index: 50

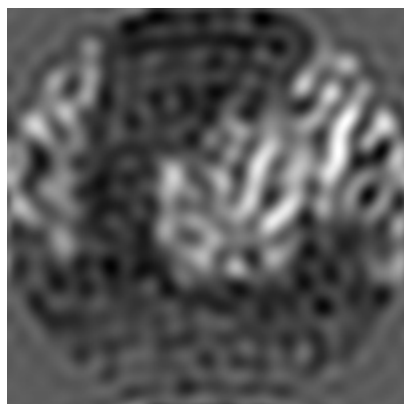


Z Index: 50

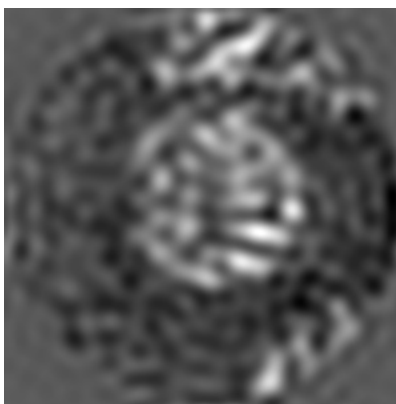
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

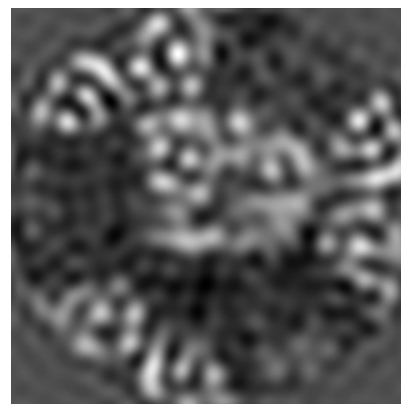
6.3.1 Primary map



X Index: 45



Y Index: 64

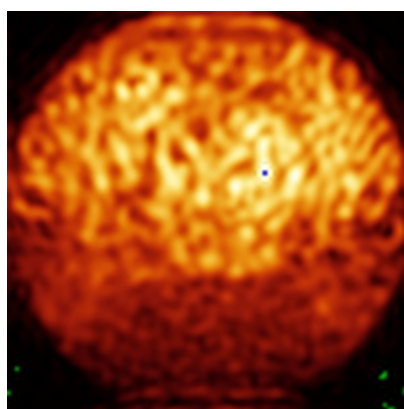


Z Index: 57

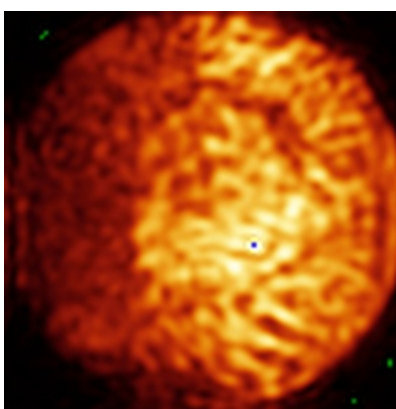
The images above show the largest variance slices of the map in three orthogonal directions.

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

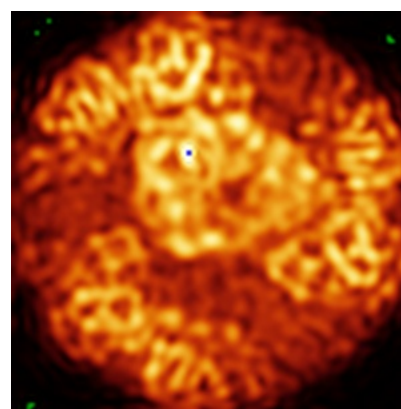
6.4.1 Primary map



X



Y

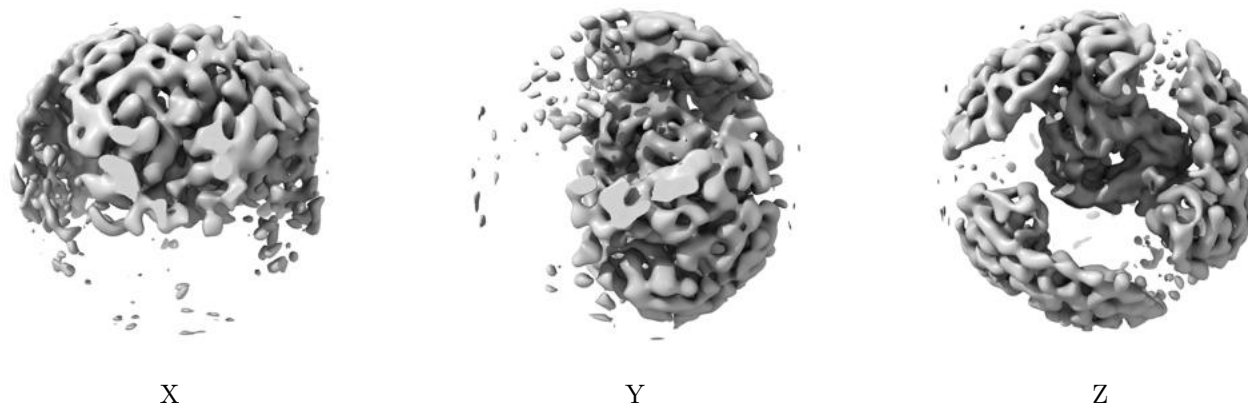


Z

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

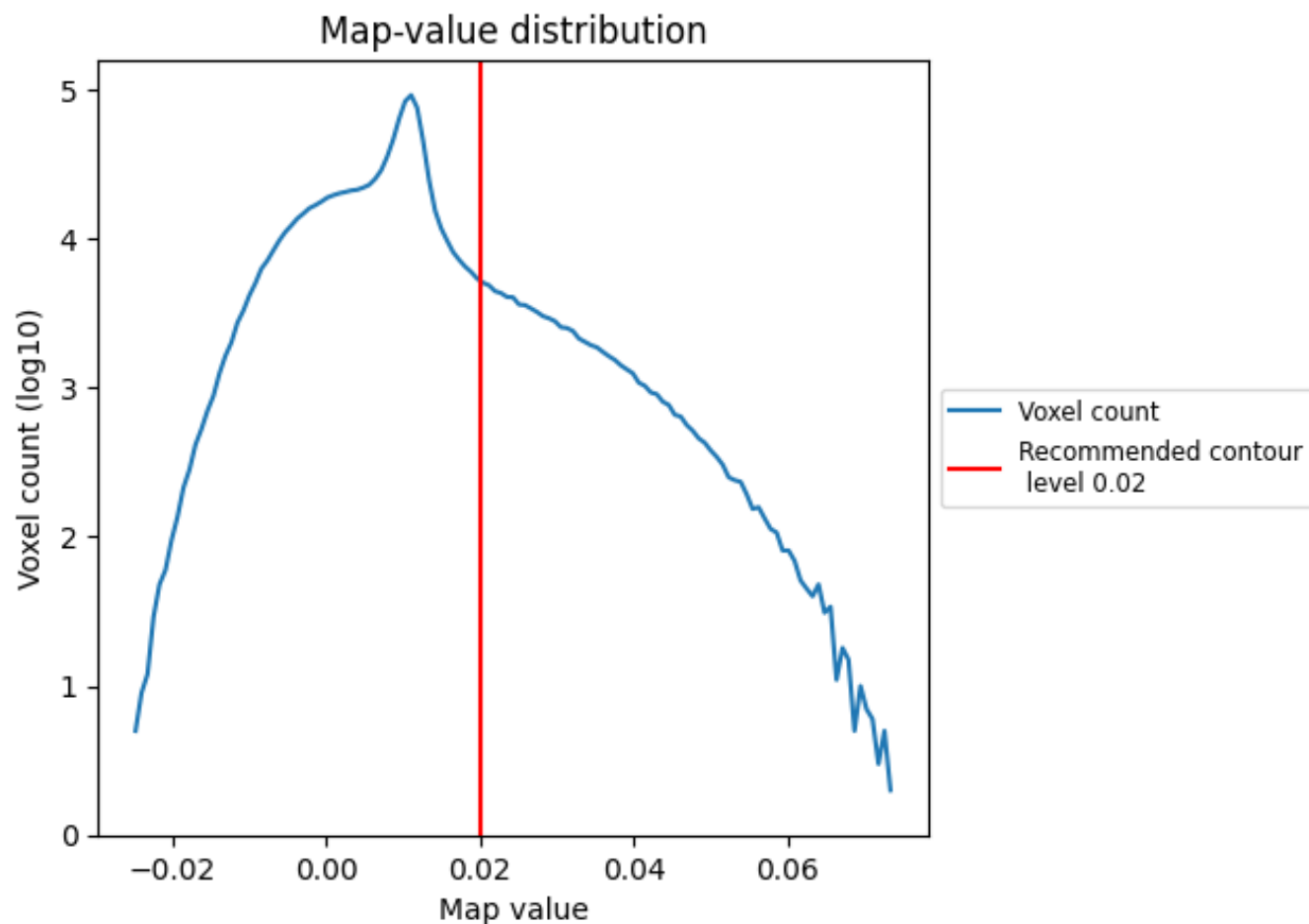
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

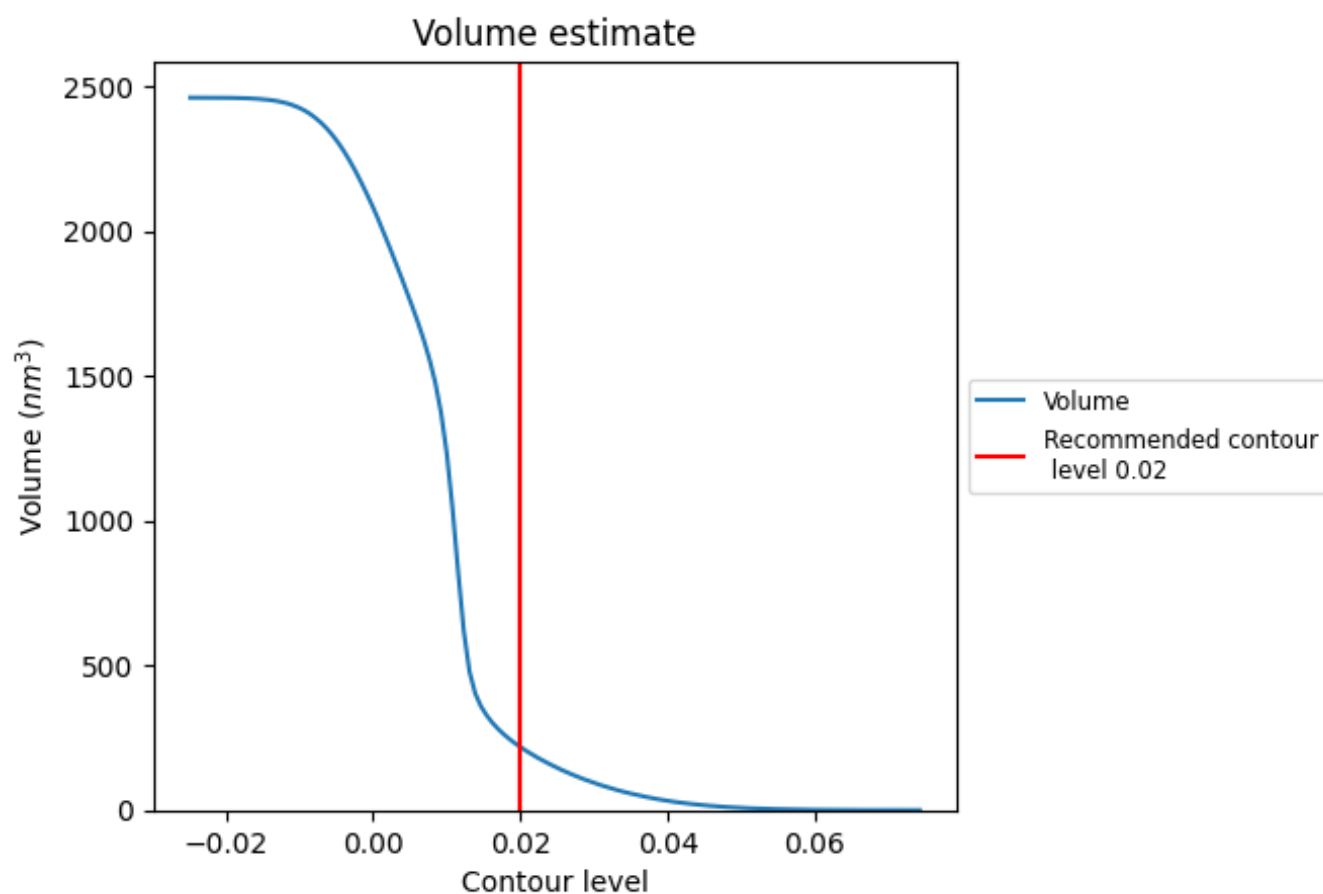
This section contains the results of statistical analysis of the map.

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.

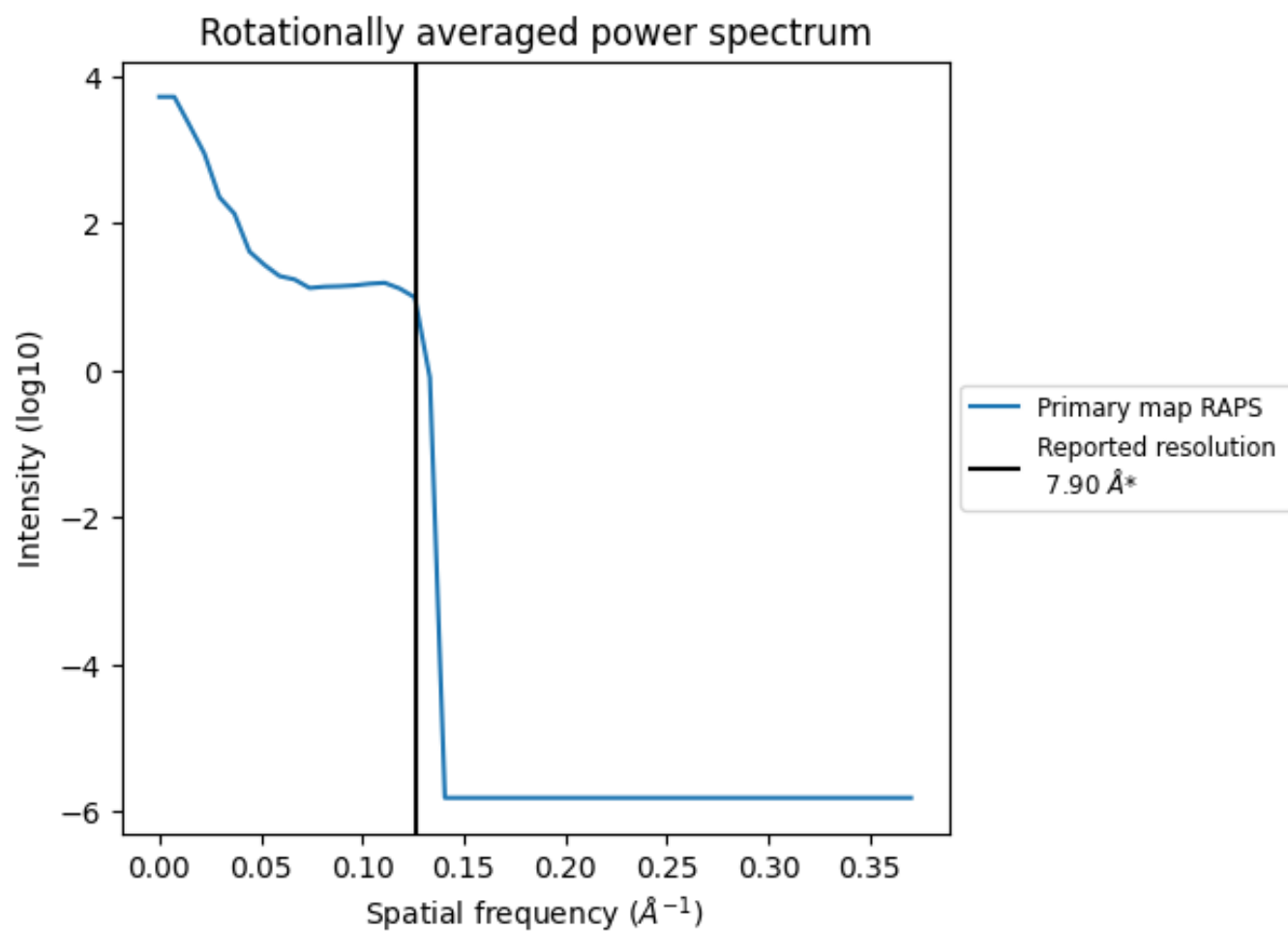
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm³; this corresponds to an approximate mass of 197 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 0.127 Å⁻¹

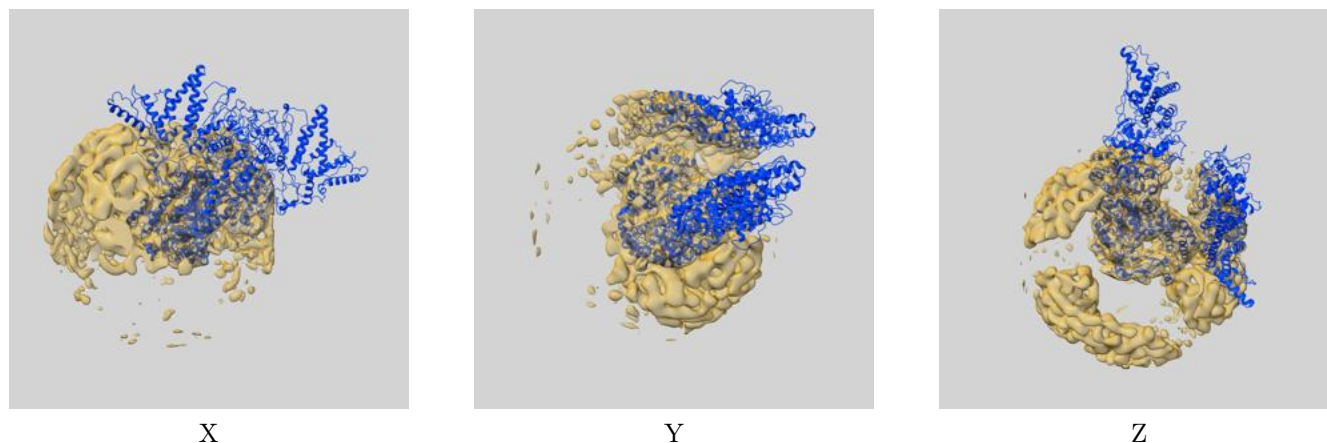
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

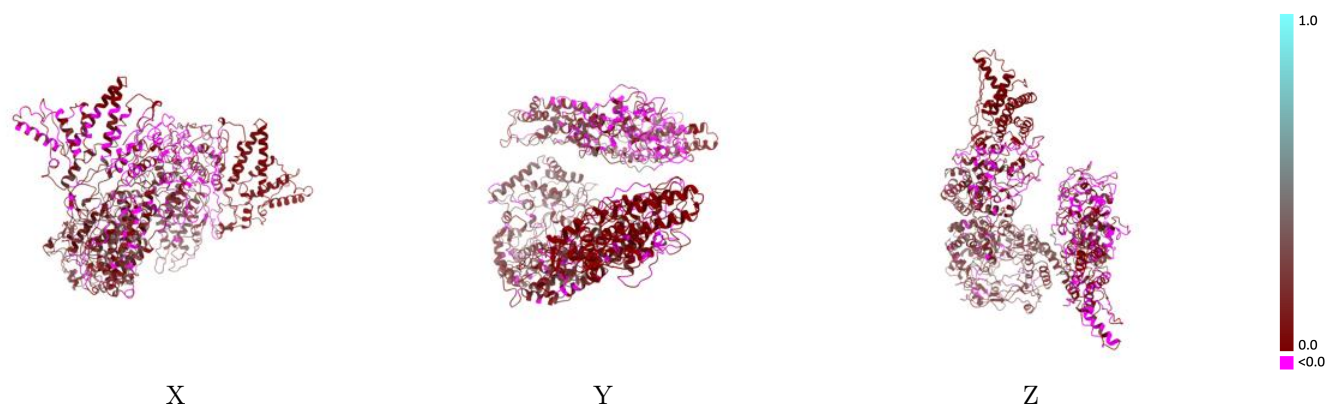
This section contains information regarding the fit between EMDB map EMD-3187 and PDB model 5FJ7. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



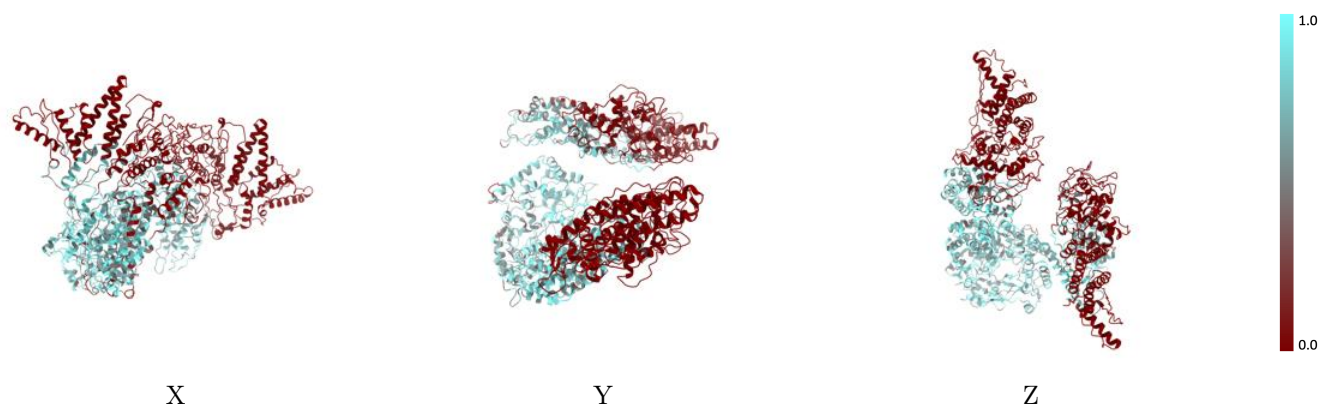
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



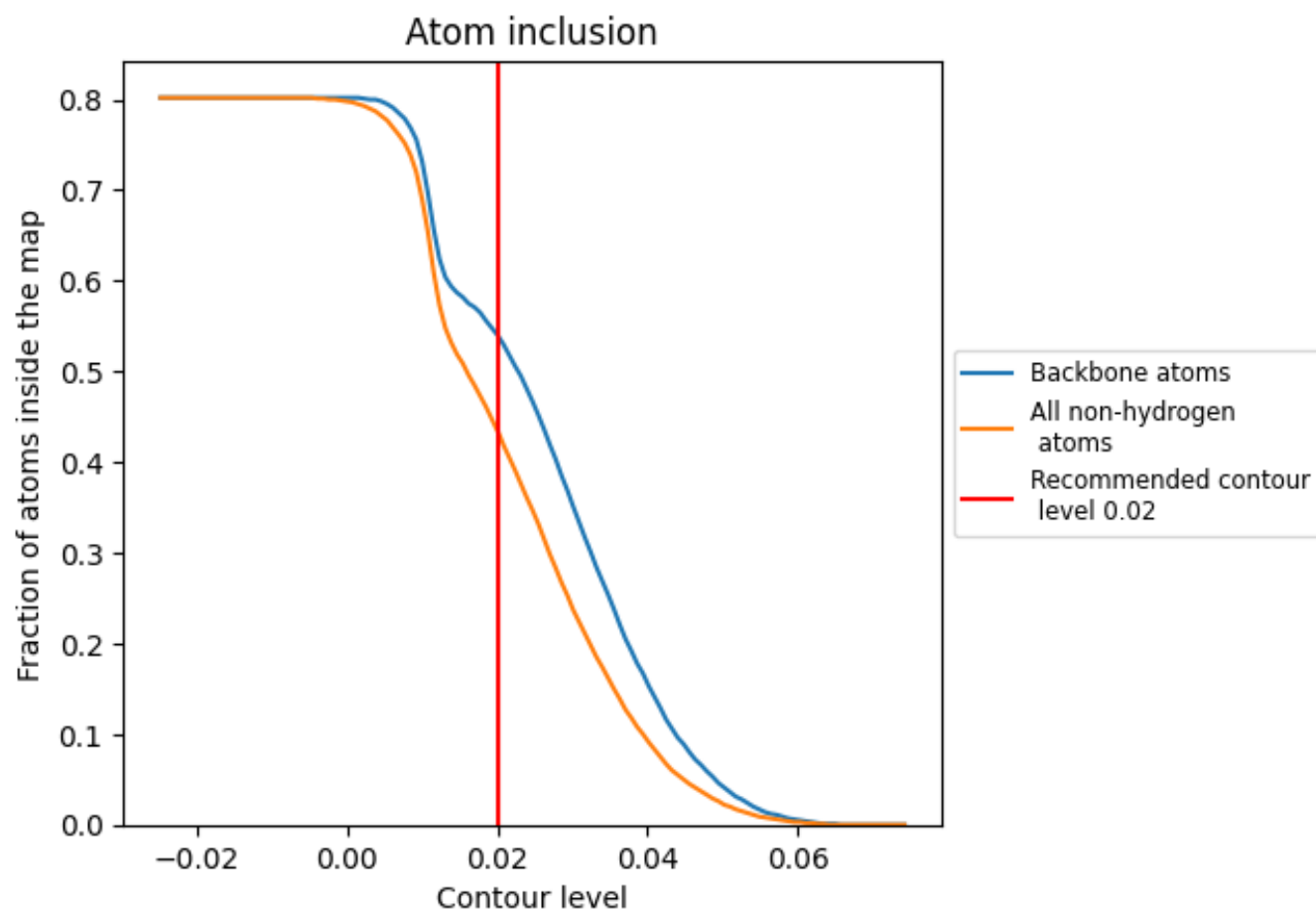
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 54% of all backbone atoms, 44% 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	0.4350	0.0980
A	0.2920	0.0640
B	0.2760	0.0630
C	0.7760	0.1760

