



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 07:52 PM UTC

PDB ID : 5M3M / pdb_00005m3m
EMDB ID : EMD-4148
Title : Free monomeric RNA polymerase I at 4.0A resolution
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : 2016-10-15
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

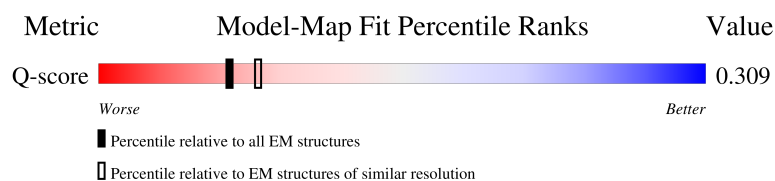
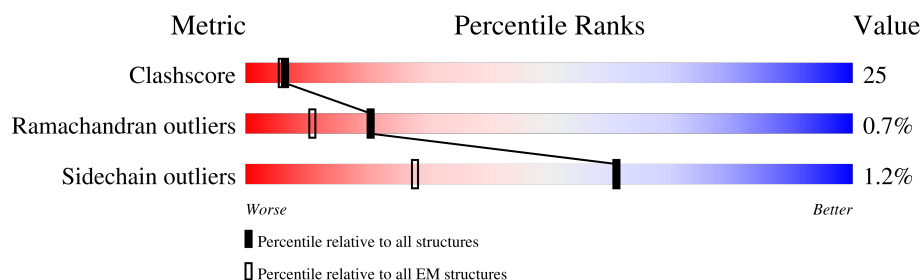
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	1664	61% 43% 45% 12%
2	B	1203	51% 48% 48%
3	C	335	52% 41% 50% 9%
4	E	215	87% 43% 55%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	125	
8	J	70	
9	K	142	
10	L	70	
11	M	415	
12	N	233	
13	D	137	
14	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33233 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11558	7304	2006	2187	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1166	Total	C	N	O	S	0	0
			9266	5864	1617	1734	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	98	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	97	Total	C	N	O		0	0
			771	490	124	157			

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	58	Total	C	N	O		0	0
			459	289	78	92			

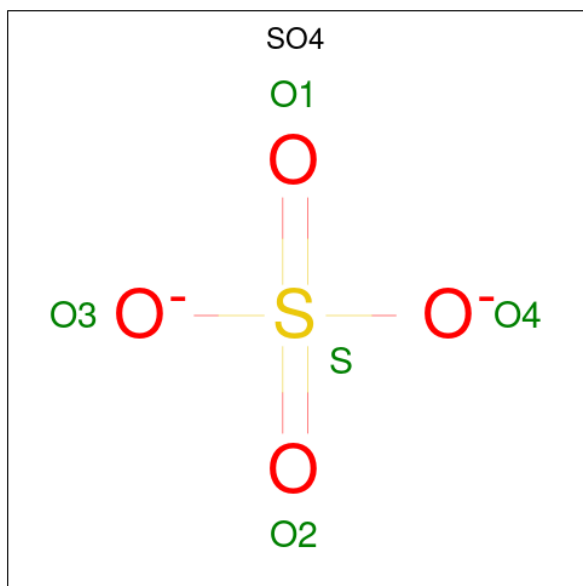
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

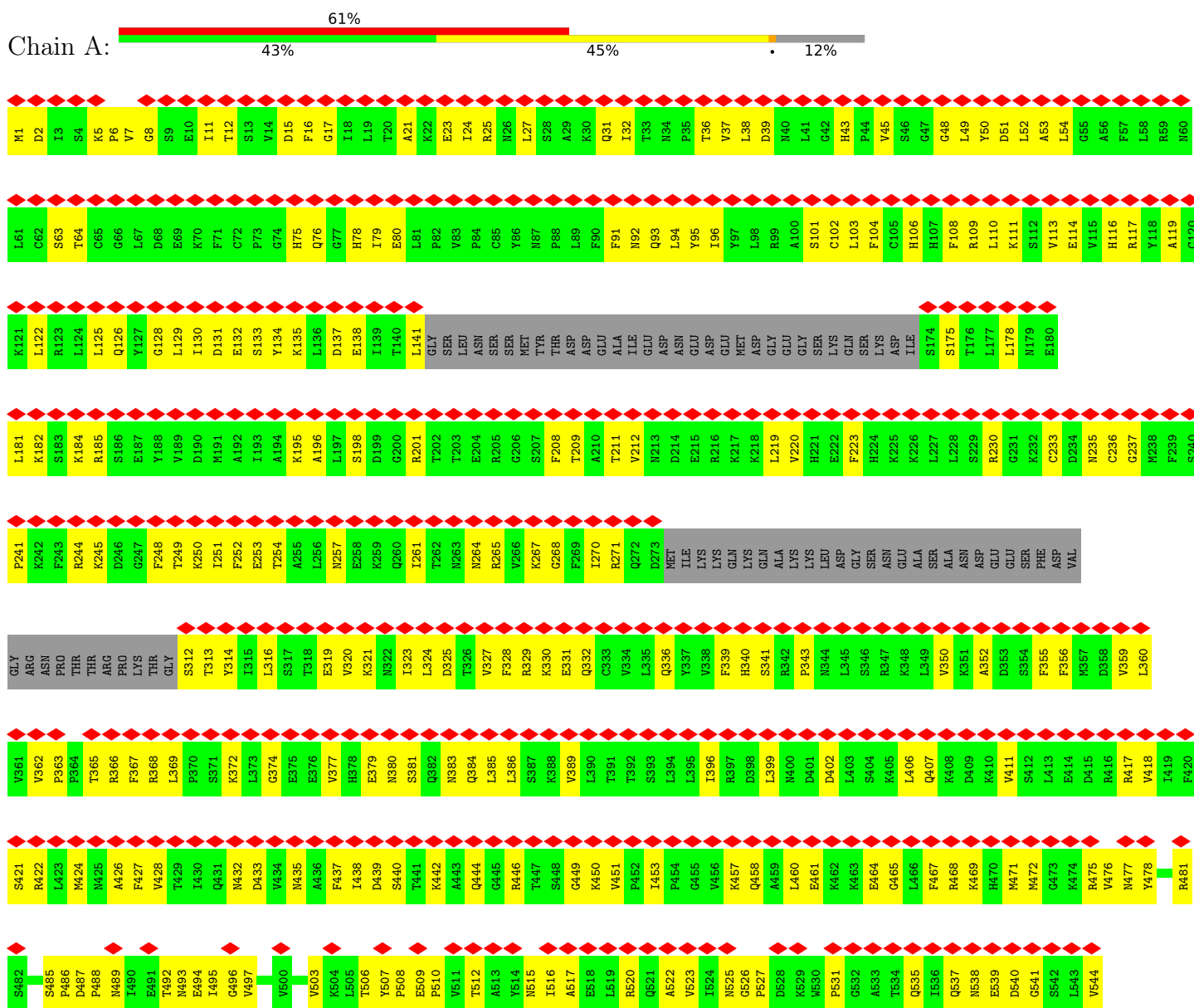


Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

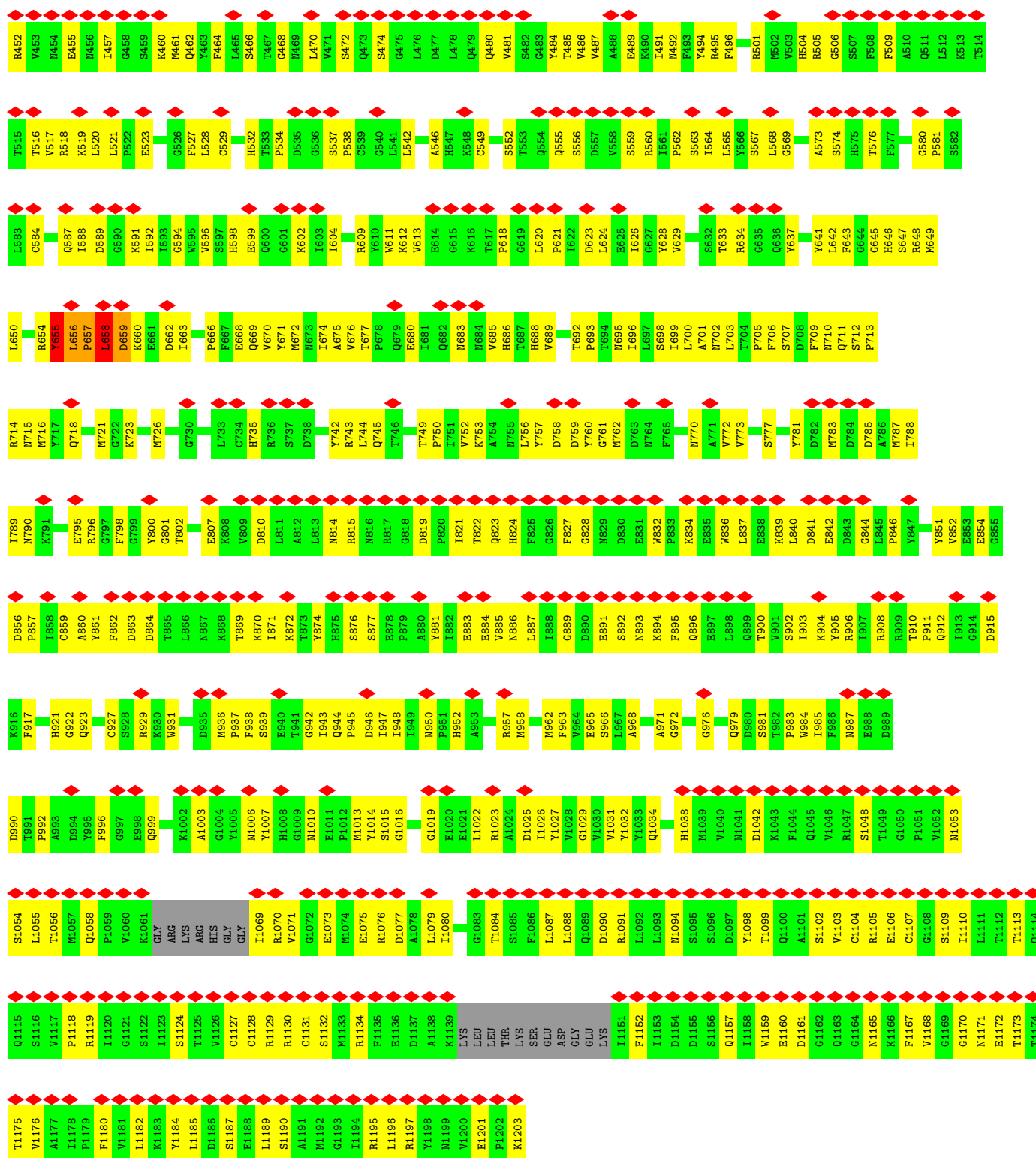
3 Residue-property plots

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 I subunit RPA190

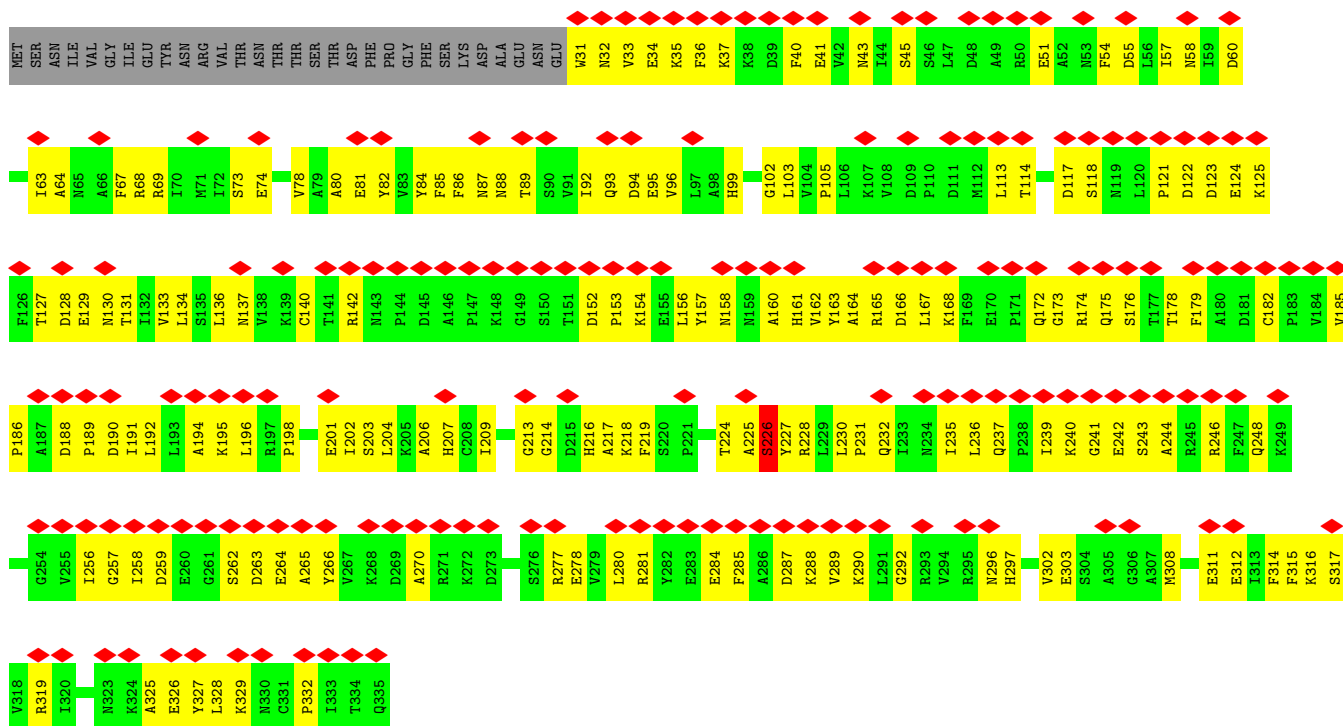




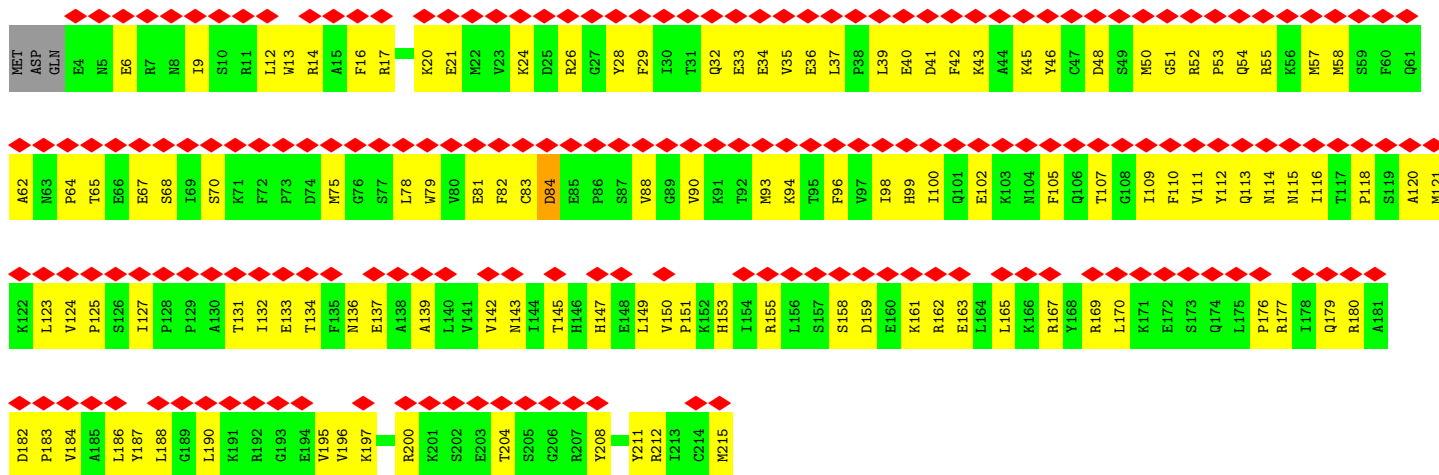
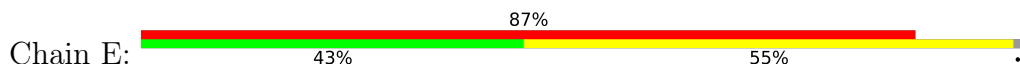


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

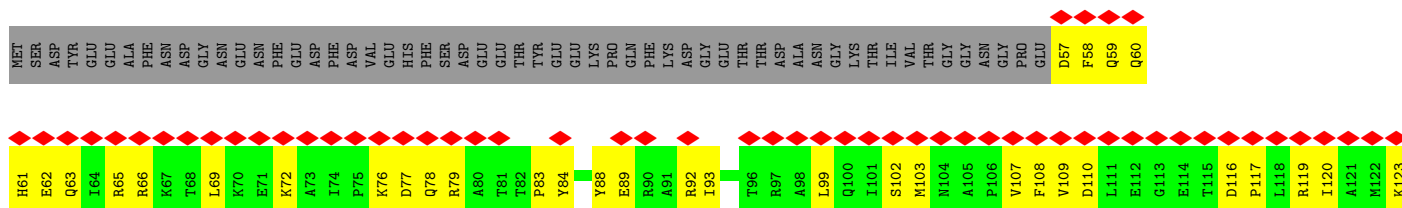


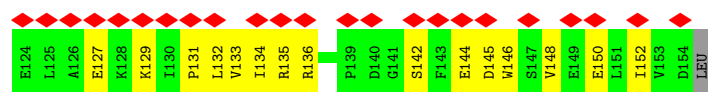


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

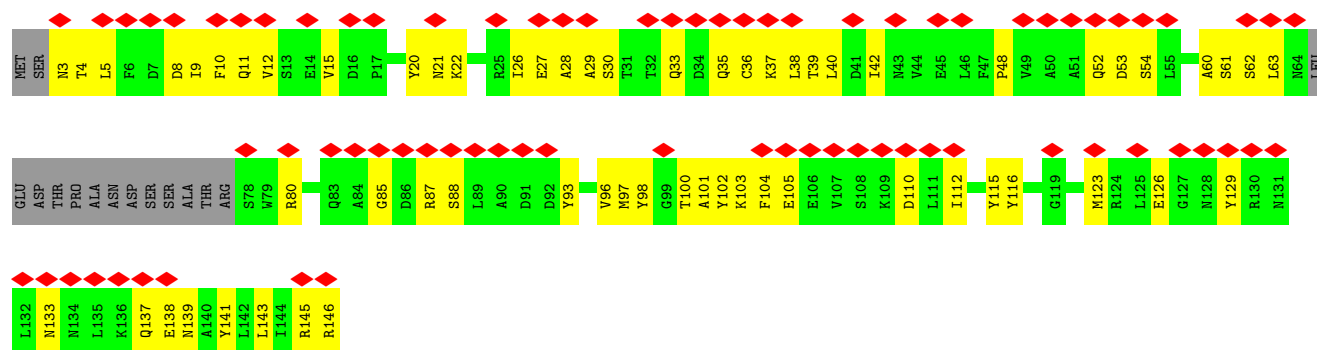


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

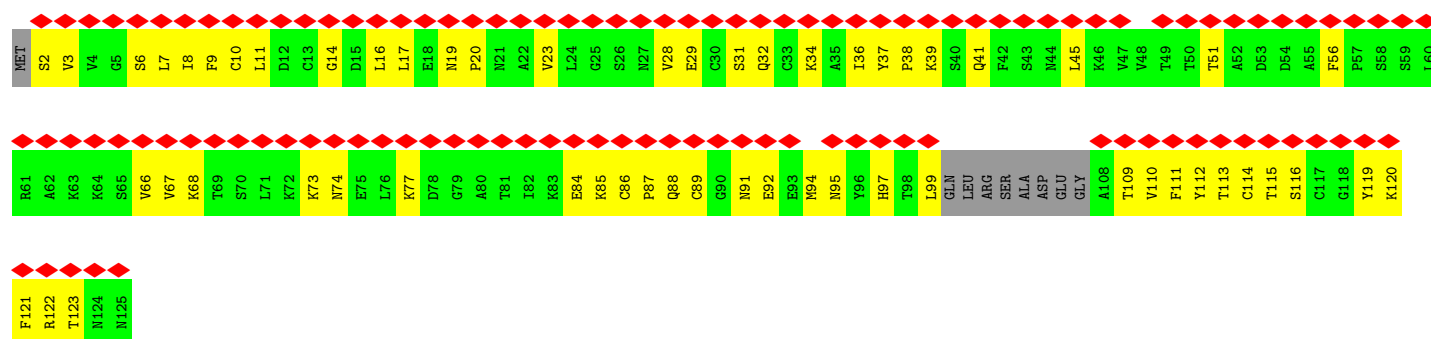
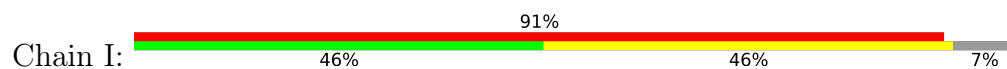




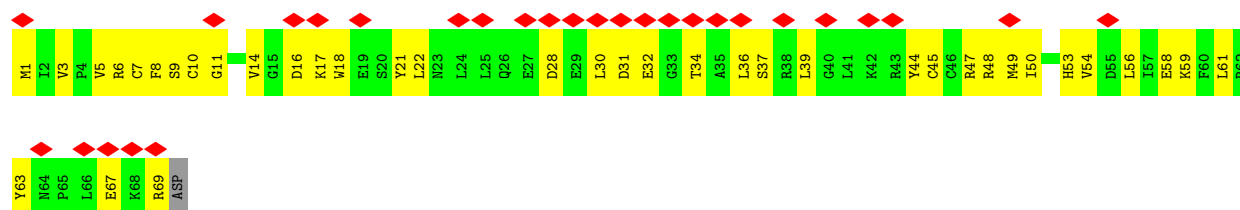
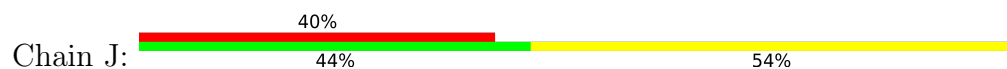
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 7: DNA-directed RNA polymerase I subunit RPA12

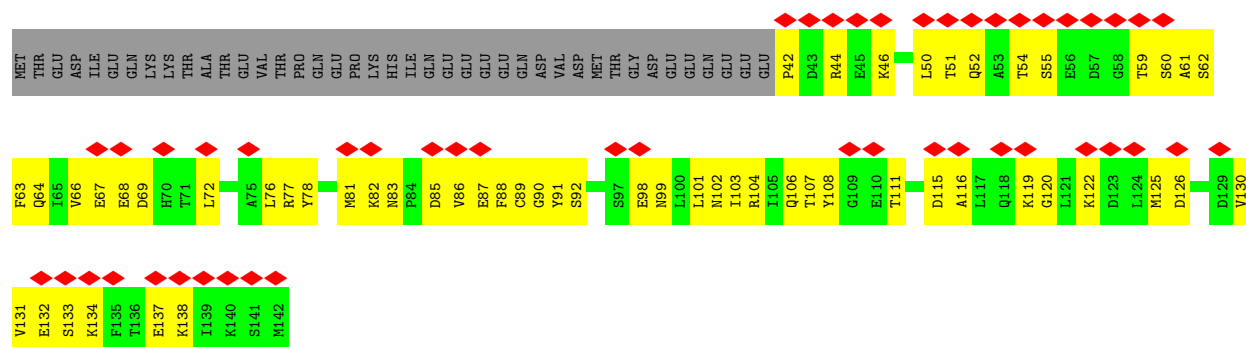


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

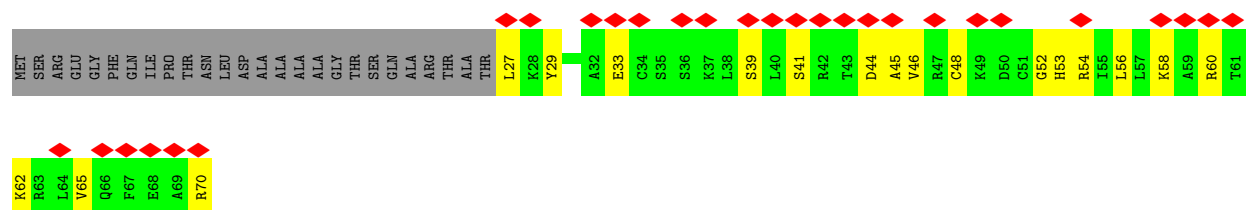


• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

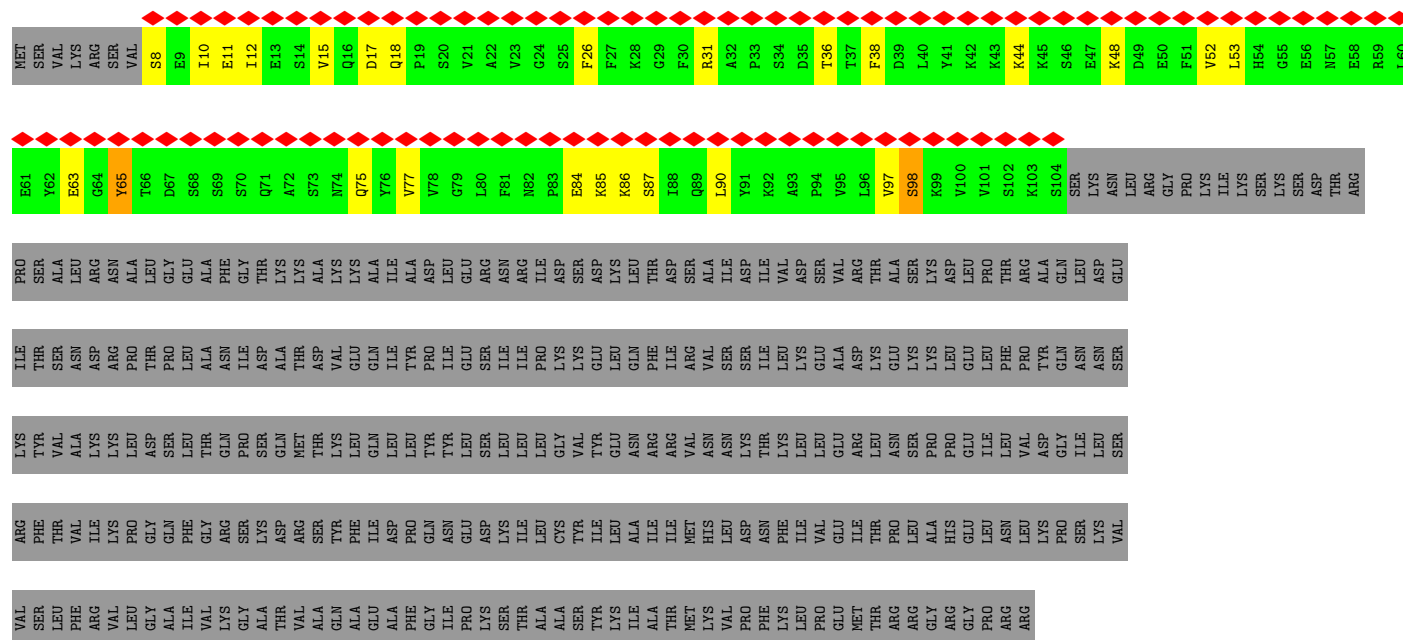




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

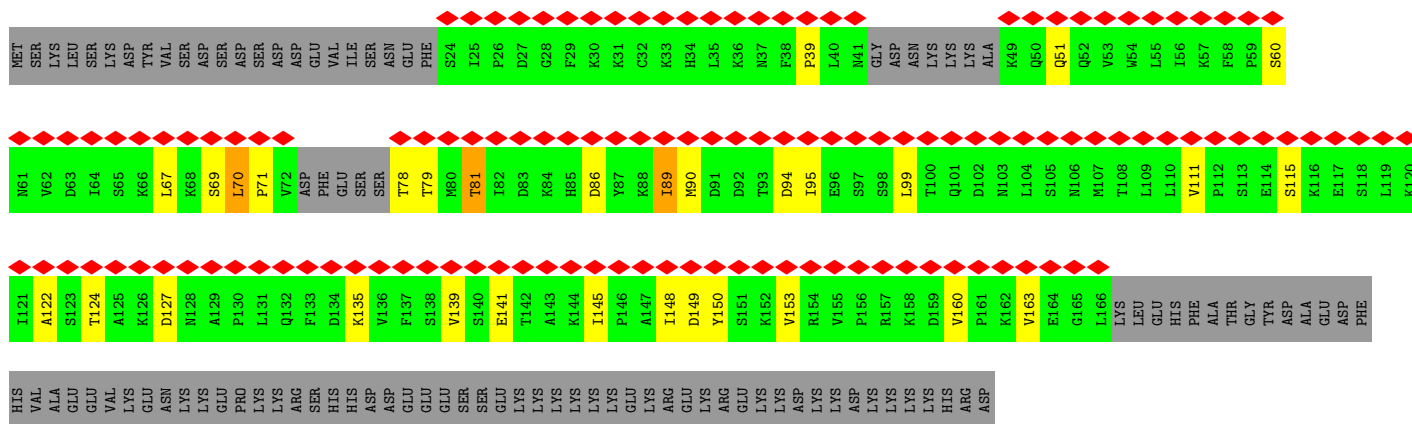


- Molecule 11: DNA-directed RNA polymerase I subunit RPA49

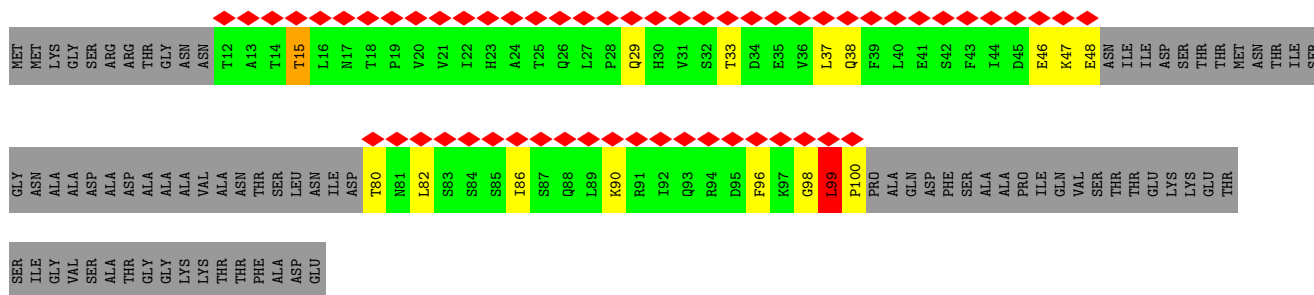
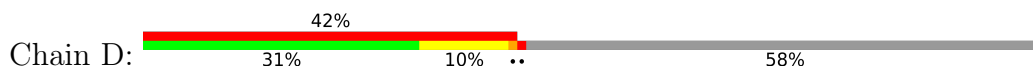


- Molecule 12: DNA-directed RNA polymerase I subunit RPA34

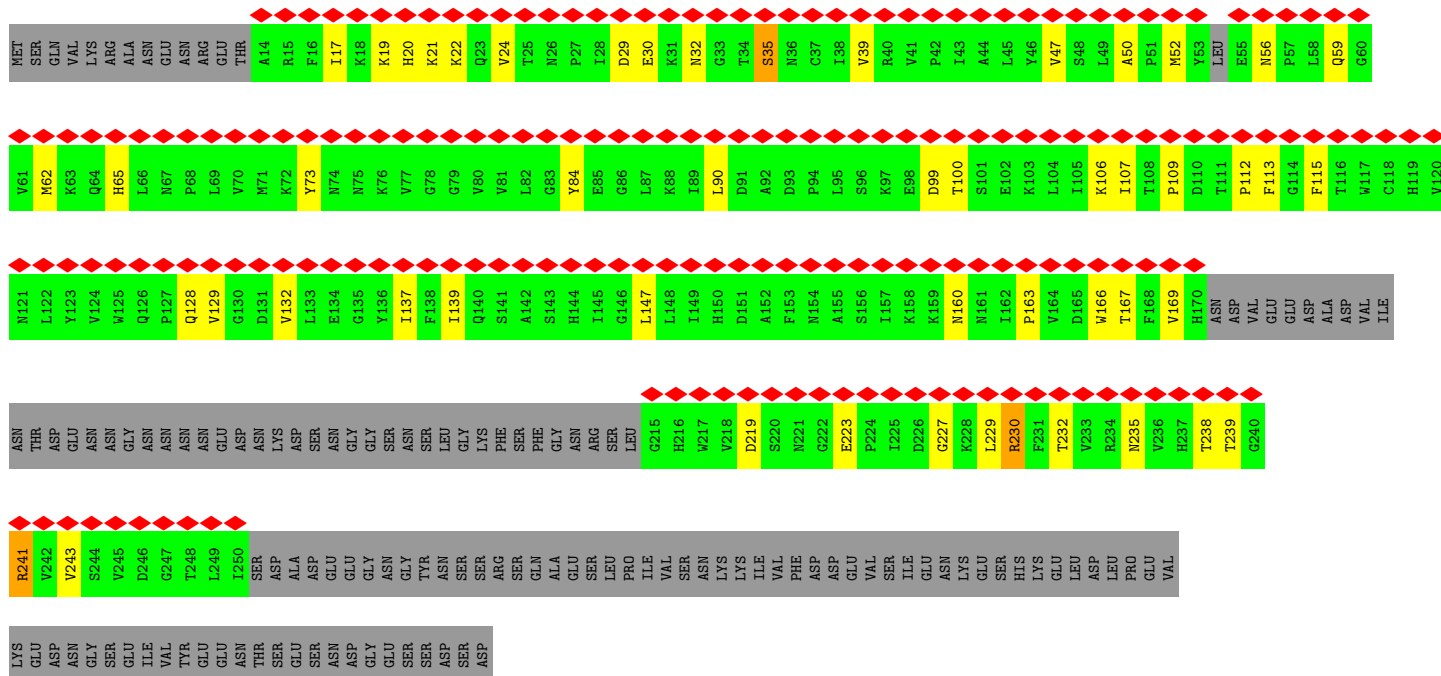
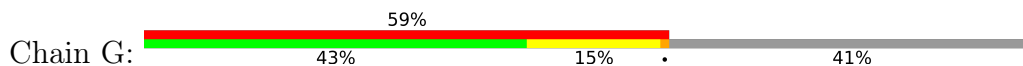




- Molecule 13: DNA-directed RNA polymerase I subunit RPA14



- Molecule 14: DNA-directed RNA polymerase I subunit RPA43



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.36	0/11770	0.58	3/15895 (0.0%)
2	B	0.42	0/9471	0.59	0/12805
3	C	0.41	0/2475	0.57	0/3354
4	E	0.36	0/1771	0.59	2/2383 (0.1%)
5	F	0.31	0/821	0.53	0/1106
6	H	0.38	0/1070	0.56	0/1449
7	I	0.28	0/895	0.50	0/1205
8	J	0.44	0/578	0.60	0/775
9	K	0.44	0/804	0.60	0/1083
10	L	0.37	0/354	0.58	0/468
11	M	0.48	0/786	0.87	0/1057
12	N	0.46	0/1052	0.88	1/1418 (0.1%)
13	D	0.51	0/465	0.81	0/630
14	G	0.50	0/1555	0.84	3/2113 (0.1%)
All	All	0.40	0/33867	0.62	9/45741 (0.0%)

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	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1648	ASN	N-CA-C	7.34	122.65	112.45
1	A	1648	ASN	CA-C-N	6.91	134.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1648	ASN	C-N-CA	6.91	134.13	121.70
14	G	241	ARG	CD-NE-CZ	5.51	132.12	124.40
12	N	127	ASP	N-CA-C	-5.37	106.21	114.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	11558	0	11642	688	0
2	B	9266	0	9151	568	0
3	C	2423	0	2412	160	0
4	E	1735	0	1764	103	0
5	F	807	0	827	45	0
6	H	1052	0	1021	48	0
7	I	883	0	879	61	0
8	J	569	0	585	37	0
9	K	793	0	790	62	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	28	0
13	D	459	0	462	8	0
14	G	1518	0	1528	34	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	5	0	0	8	0
All	All	33233	0	33259	1673	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 25.

The worst 5 of 1673 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:B:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93

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	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	21	57
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	21	57
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	36	70
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	5	32
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	3	25
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	11	44
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	20	54

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	SER

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	1292/1465 (88%)	1286 (100%)	6 (0%)	81	82
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	87	87
3	C	269/296 (91%)	268 (100%)	1 (0%)	84	84
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	88/137 (64%)	88 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	103/110 (94%)	103 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	M	88/371 (24%)	77 (88%)	11 (12%)	4	20
12	N	124/220 (56%)	117 (94%)	7 (6%)	19	43
13	D	55/116 (47%)	50 (91%)	5 (9%)	9	30
14	G	170/291 (58%)	157 (92%)	13 (8%)	12	36
All	All	3714/4636 (80%)	3669 (99%)	45 (1%)	61	73

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	D	29	GLN
14	G	39	VAL
13	D	38	GLN
14	G	21	LYS
14	G	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
9	K	70	HIS
11	M	82	ASN
2	B	243	GLN
2	B	45	HIS
12	N	61	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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	SO4	B	1301	-	4,4,4	0.22	0	6,6,6	0.36	0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.

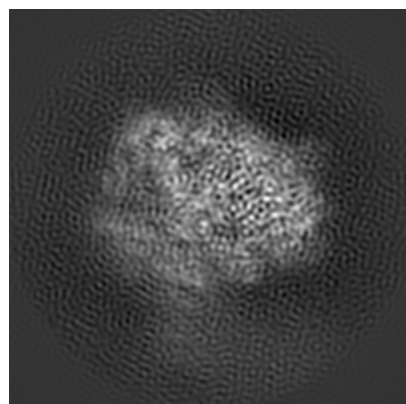
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4148. These allow visual inspection of the internal detail of the map and identification of artifacts.

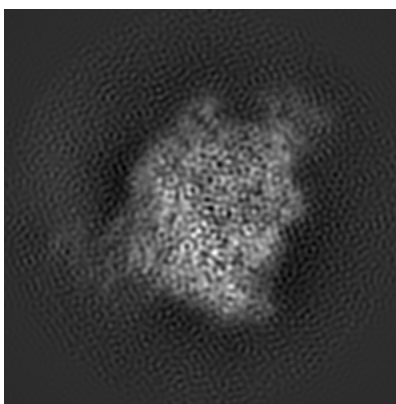
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

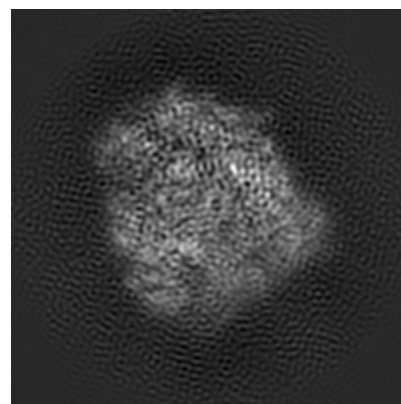
6.1.1 Primary map



X

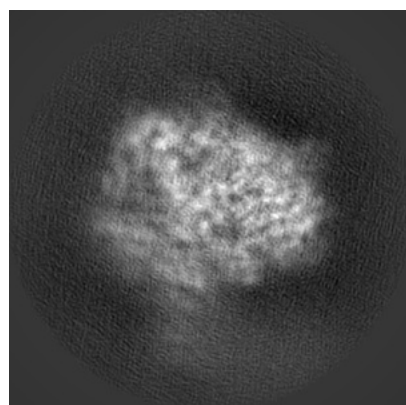


Y

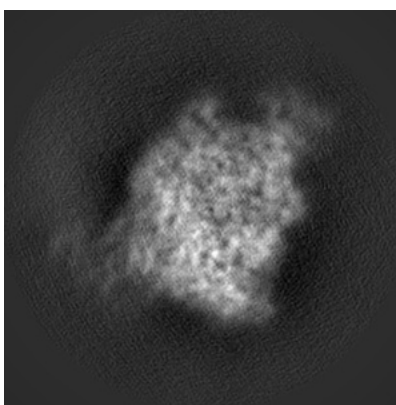


Z

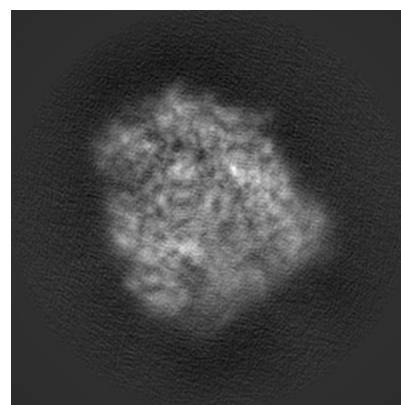
6.1.2 Raw map



X



Y

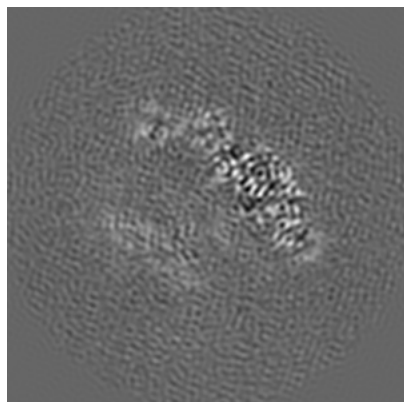


Z

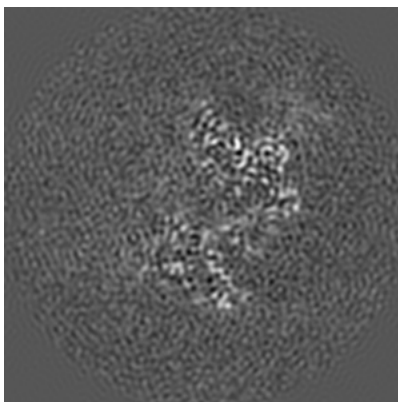
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

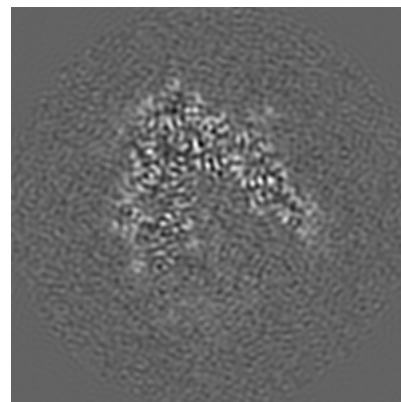
6.2.1 Primary map



X Index: 115

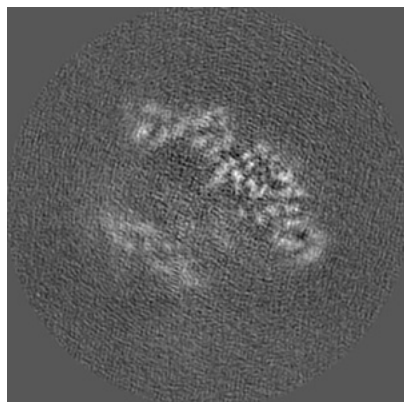


Y Index: 115

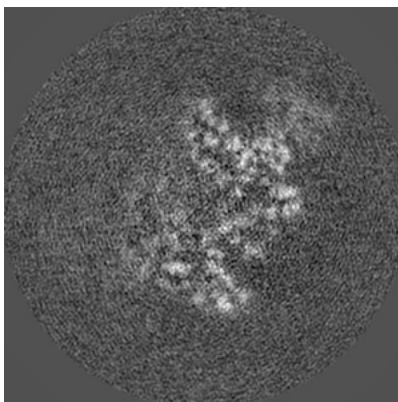


Z Index: 115

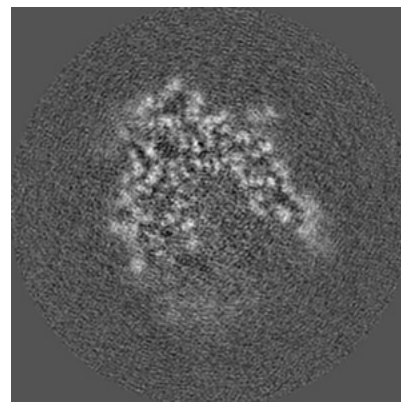
6.2.2 Raw map



X Index: 115



Y Index: 115

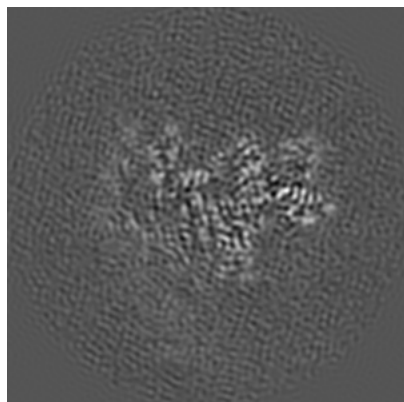


Z Index: 115

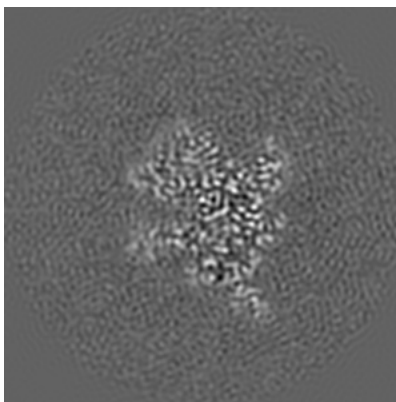
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

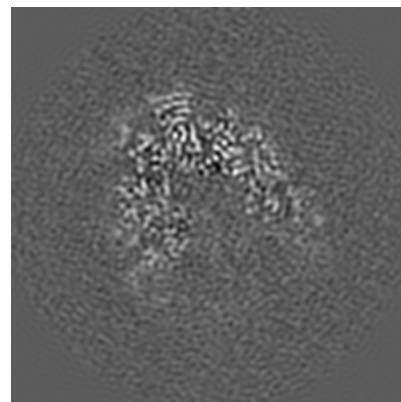
6.3.1 Primary map



X Index: 95

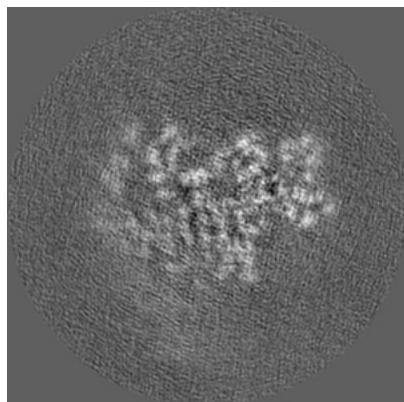


Y Index: 137

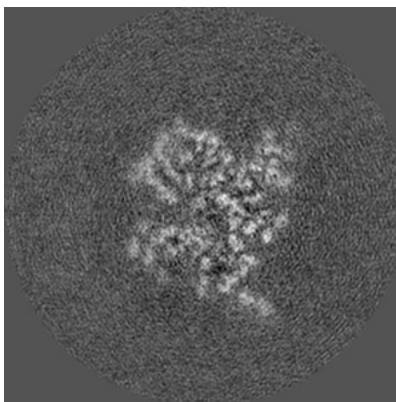


Z Index: 120

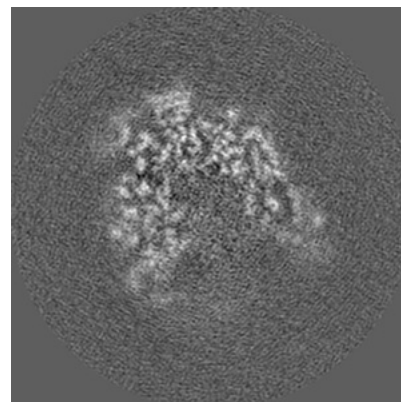
6.3.2 Raw map



X Index: 96



Y Index: 134

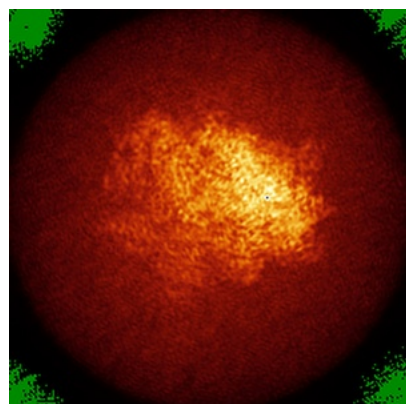


Z Index: 120

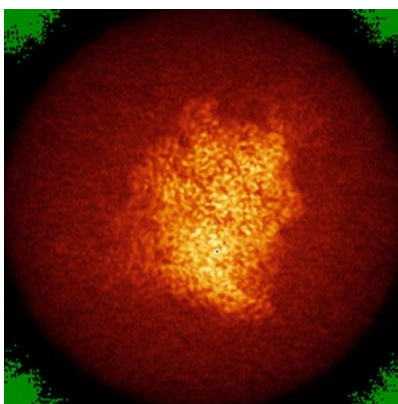
The images above show the largest variance slices of the map in three orthogonal directions.

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

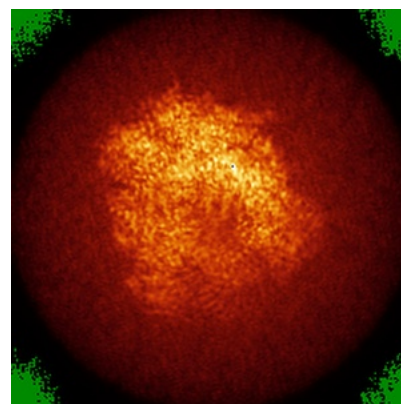
6.4.1 Primary map



X

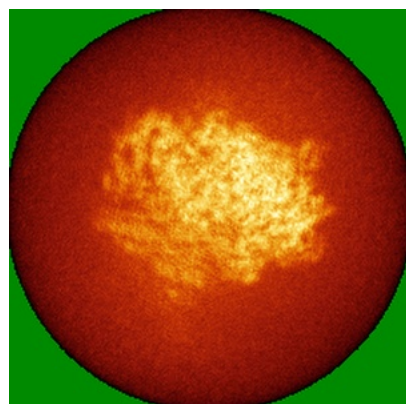


Y

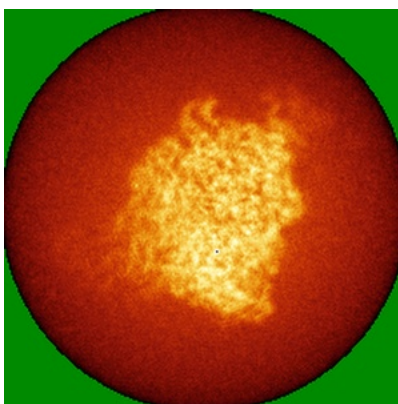


Z

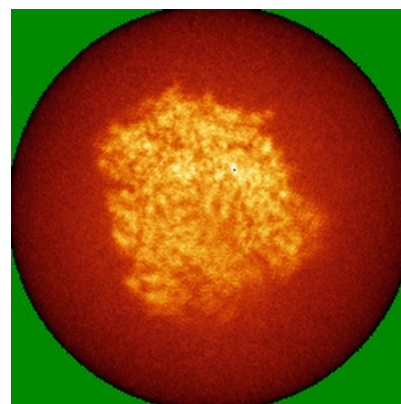
6.4.2 Raw map



X



Y

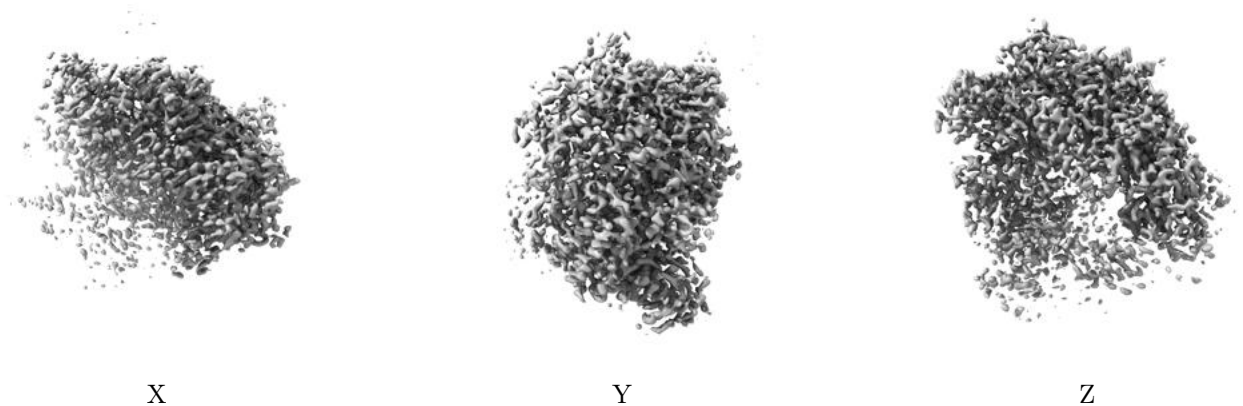


Z

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.

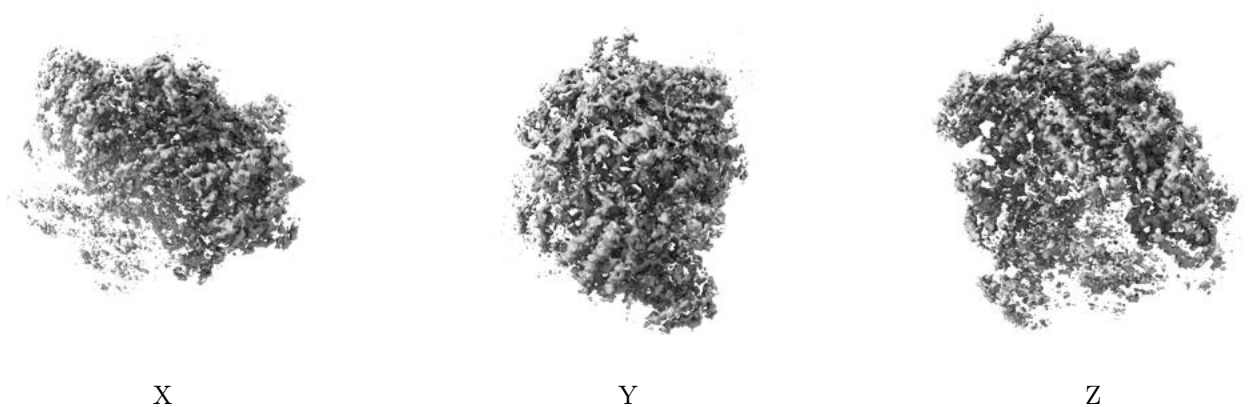
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

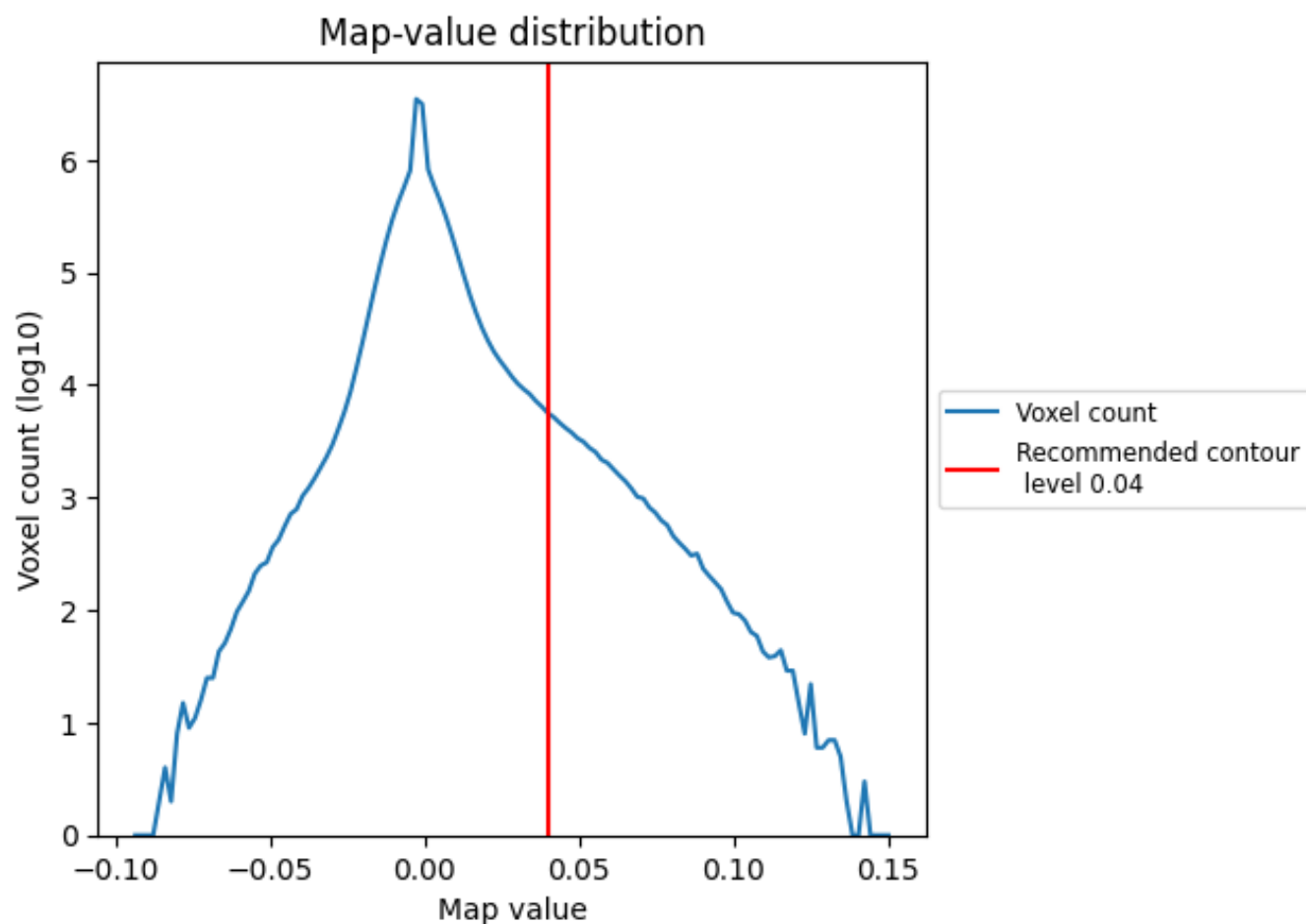
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

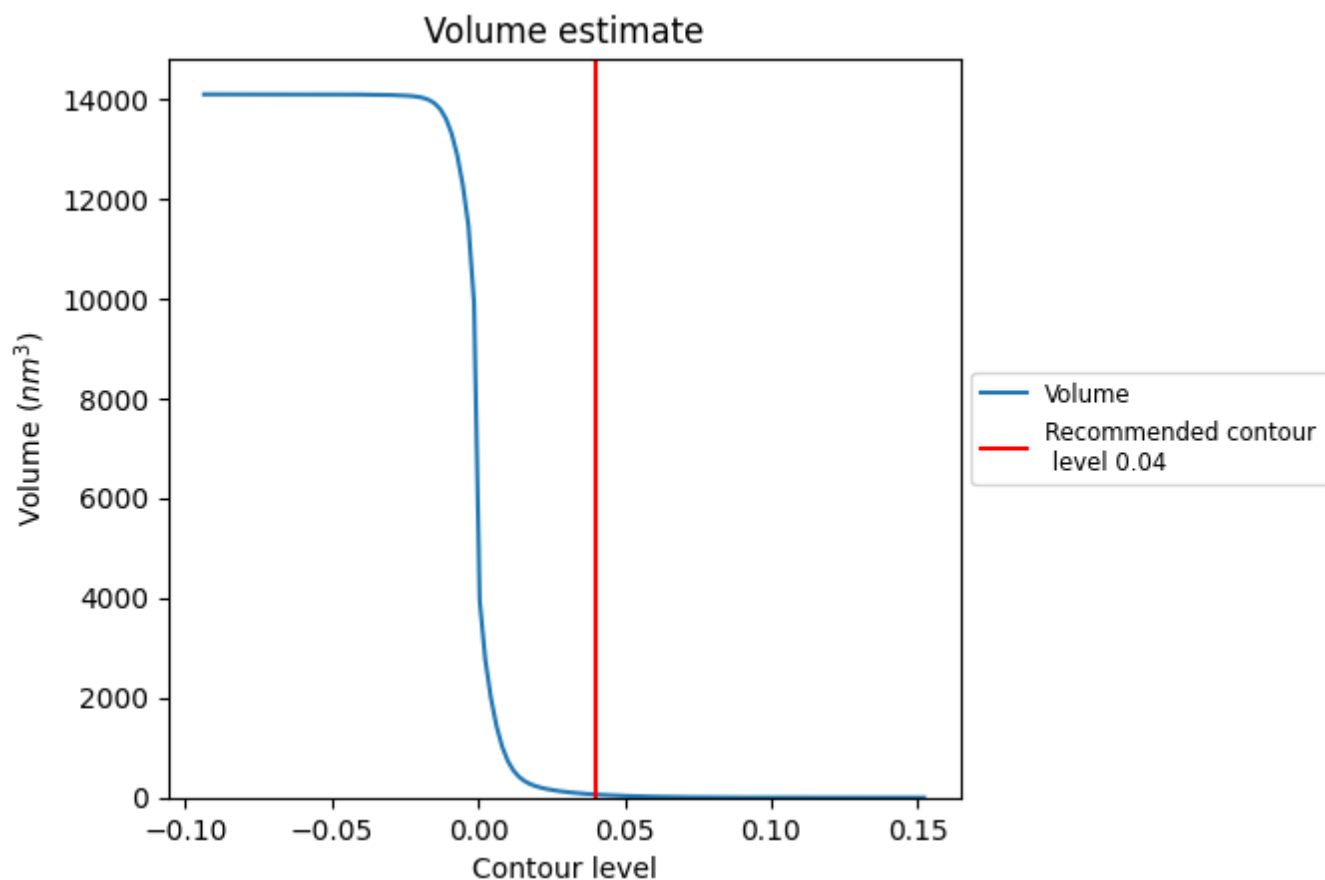
This section contains the results of statistical analysis of the map.

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.

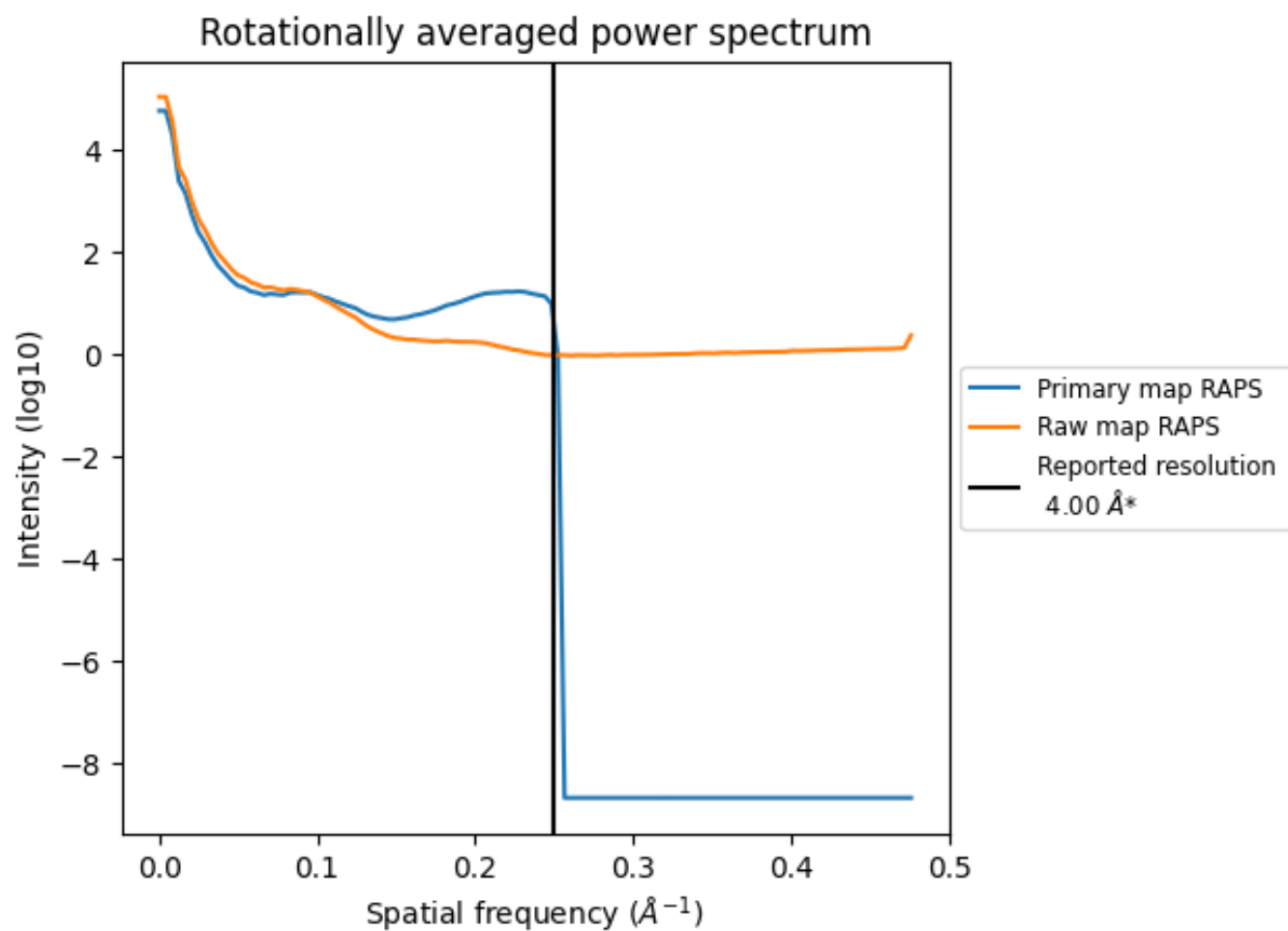
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 ⓘ

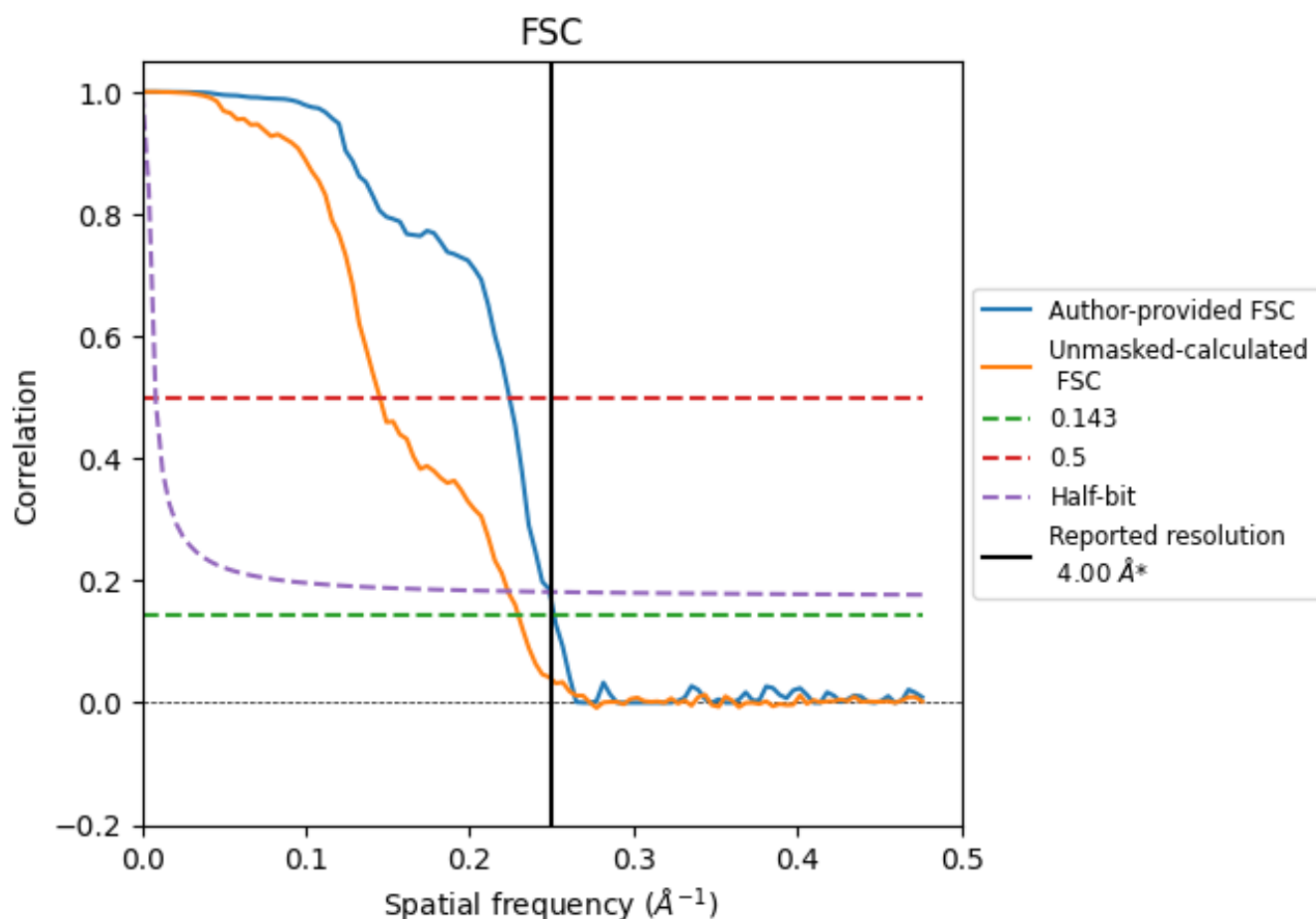


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

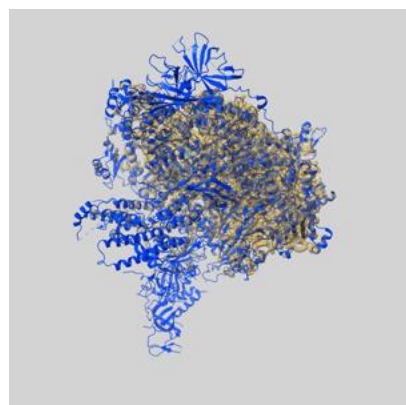
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.46	4.02
Unmasked-calculated*	4.35	6.89	4.48

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

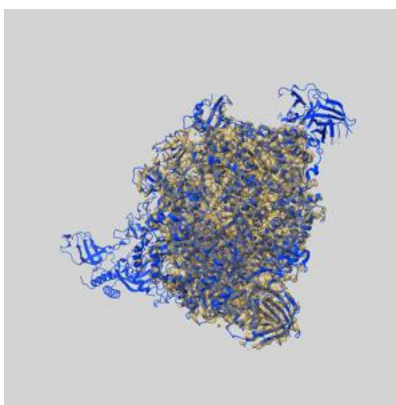
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4148 and PDB model 5M3M. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

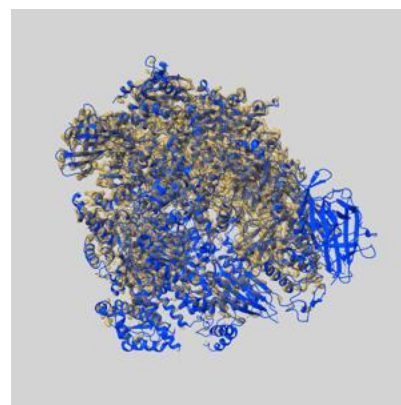
9.1 Map-model overlay [i](#)



X



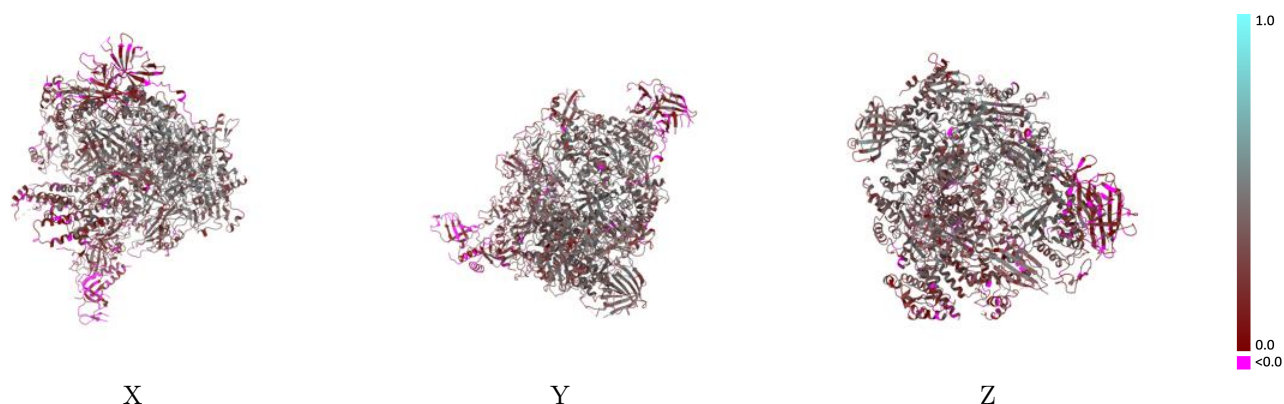
Y



Z

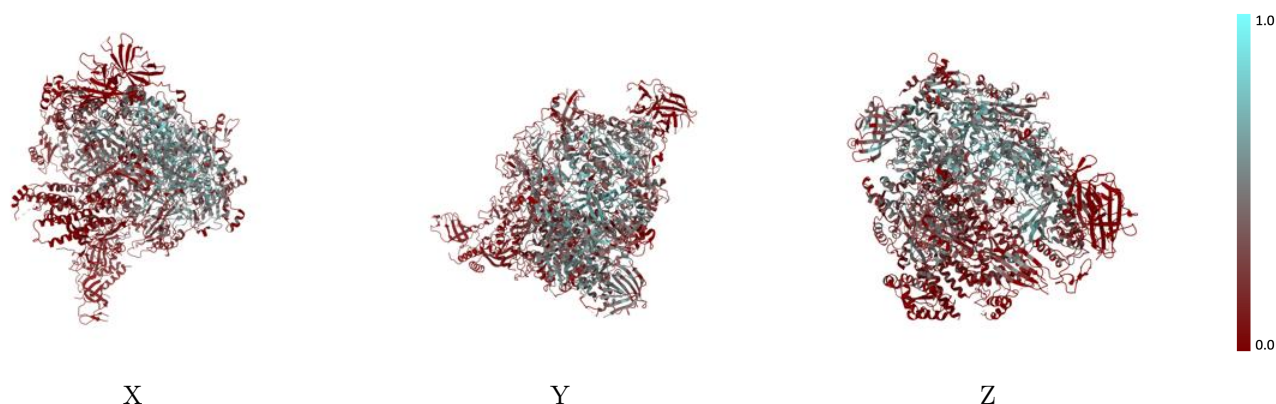
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



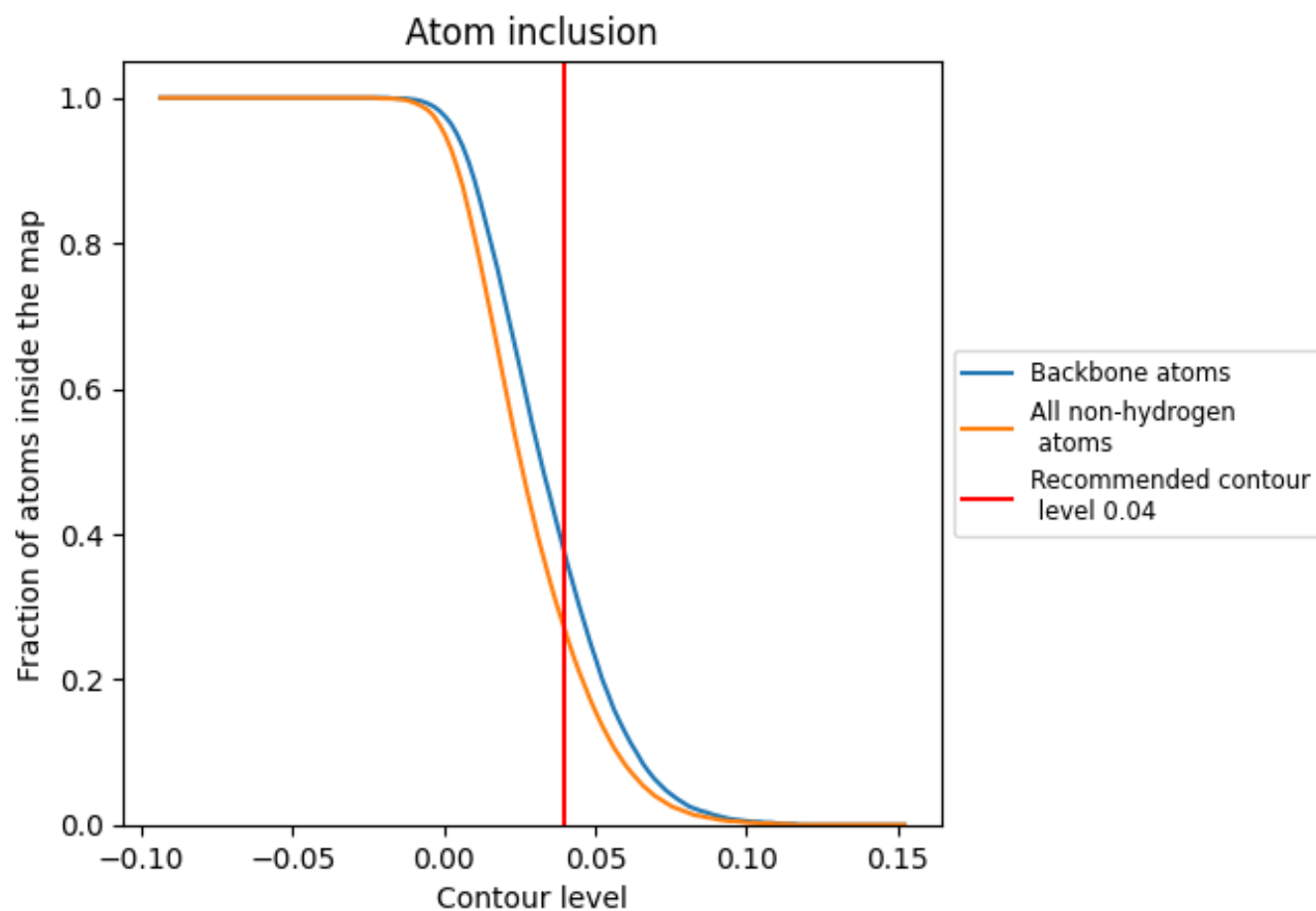
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 27% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2670	0.3090
A	0.2530	0.3180
B	0.3860	0.3650
C	0.3500	0.3600
D	0.0040	0.0810
E	0.1450	0.2700
F	0.1920	0.2950
G	0.0080	0.1250
H	0.3410	0.3680
I	0.0630	0.2470
J	0.4730	0.3920
K	0.3930	0.3660
L	0.3350	0.3610
M	0.0030	0.1250
N	0.0000	0.0710

1.0

0.0

<0.0