wwPDB EM Validation Summary Report ⓘ

Nov 6, 2024 – 03:23 pm GMT

PDB ID	:	5M5Y
EMDB ID	:	EMD-3448
Title	:	RNA Polymerase I elongation complex 2
Authors	:	Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzel, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.
Deposited on	:	2016-10-23
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:

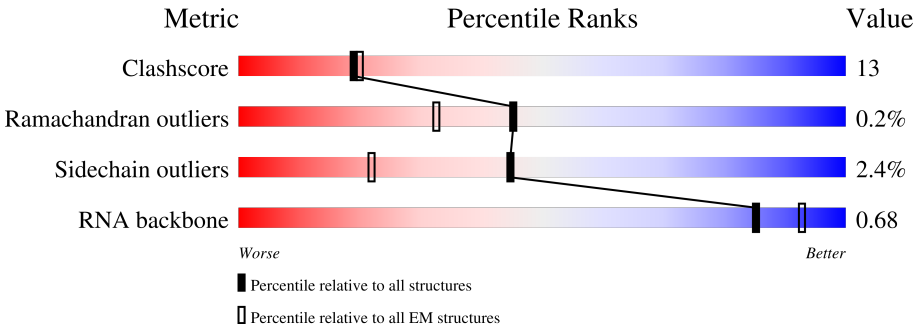
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	62% 25% 12%
2	B	1203	64% 32%
3	C	335	68% 22% 9%
4	D	137	15% 33% 9% 57%
5	E	215	74% 25%
6	F	155	49% 15% 35%
7	G	326	25% 45% 16% 38%

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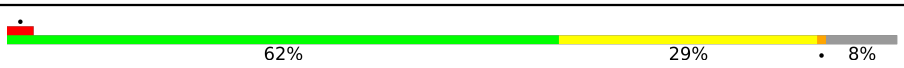
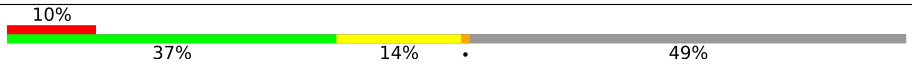
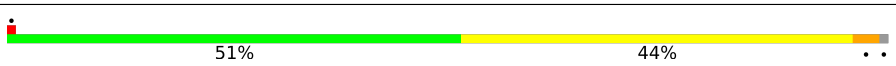
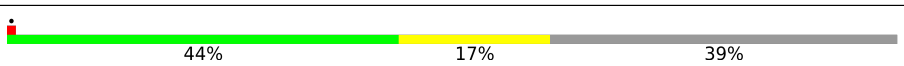
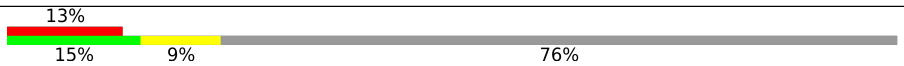
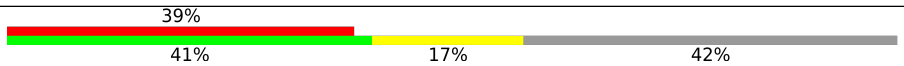
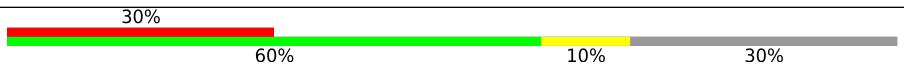
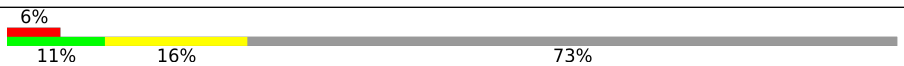
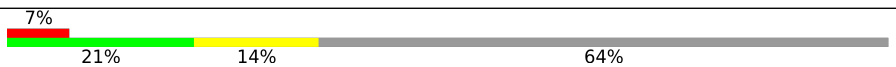
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	10	
16	S	70	
17	T	70	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 34104 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
			Total	C	N	O	S		
1	A	1466	11571	7309	2012	2188	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1170	9301	5888	1625	1737	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	304	2418	1536	414	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1751	1111	309	320	11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	202	Total	C	N	O	S	0	0
			1600	1026	276	293	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	134	Total	C	N	O	S	0	0
			1075	677	182	212	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	64	Total	C	N	O	S	0	0
			472	295	78	95	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			784	491	128	160	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	101	Total	C	N	O	0	0
			802	508	132	162		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	135	Total	C	N	O	S	0	0
			1070	685	175	206	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	7	Total	C	N	O	P	0	0
			145	65	22	51	7		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	19	Total	C	N	O	P	0	0
			397	188	82	108	19		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

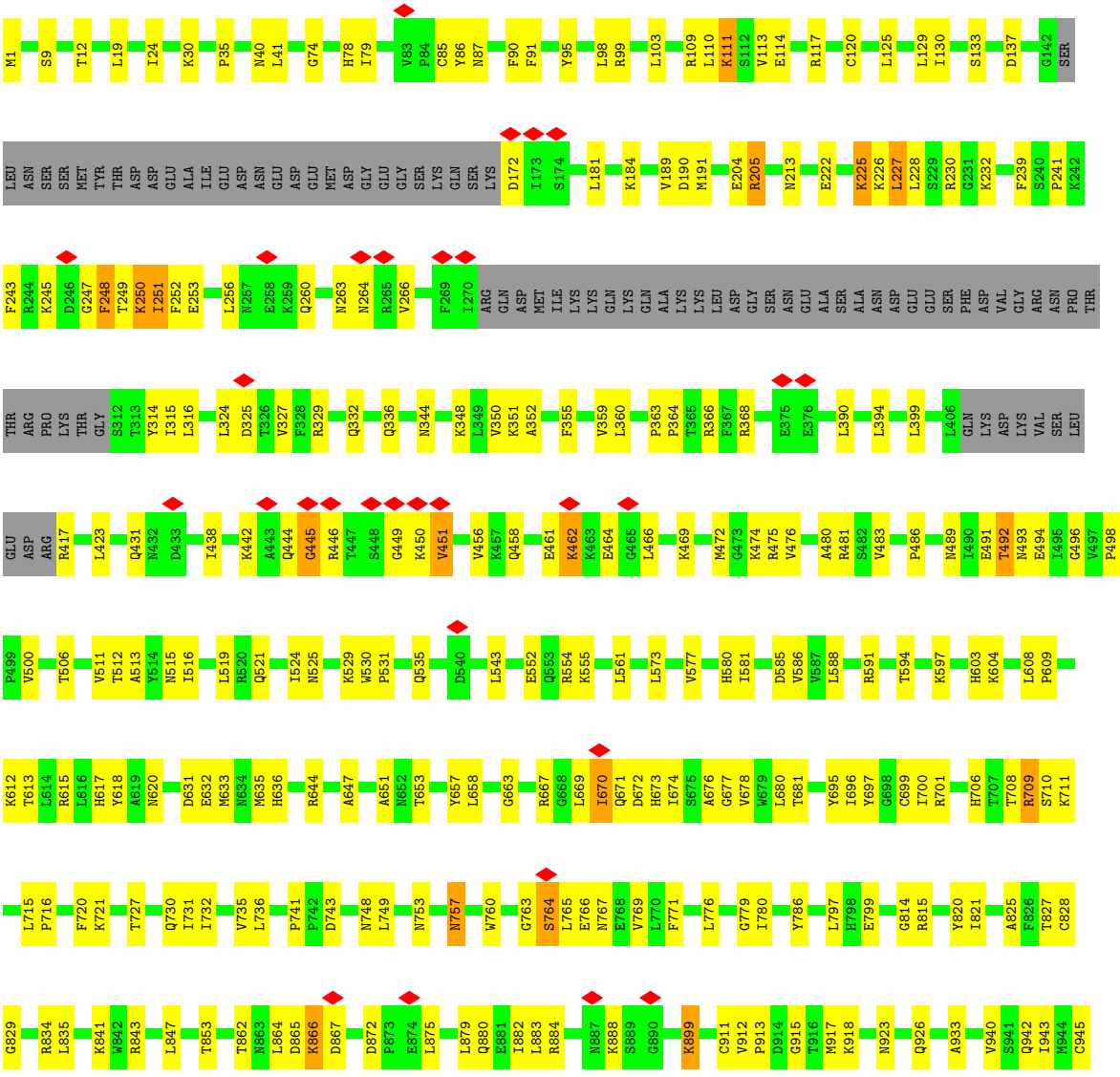
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

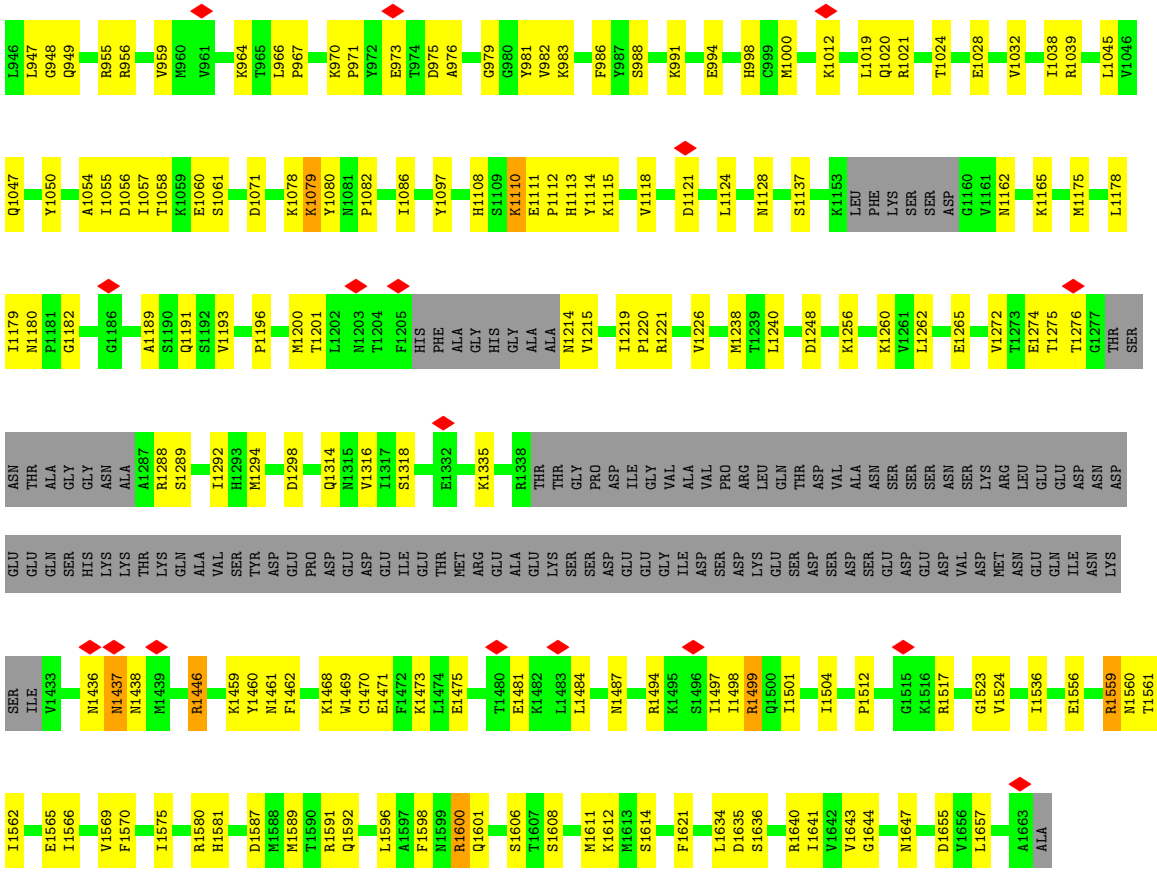
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

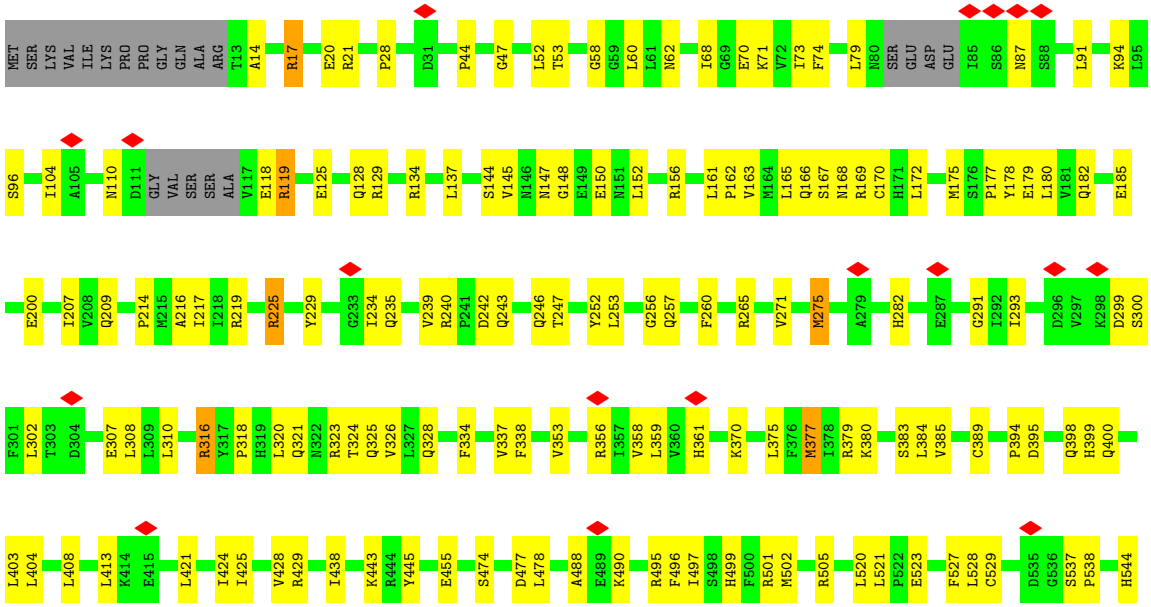
Chain A:

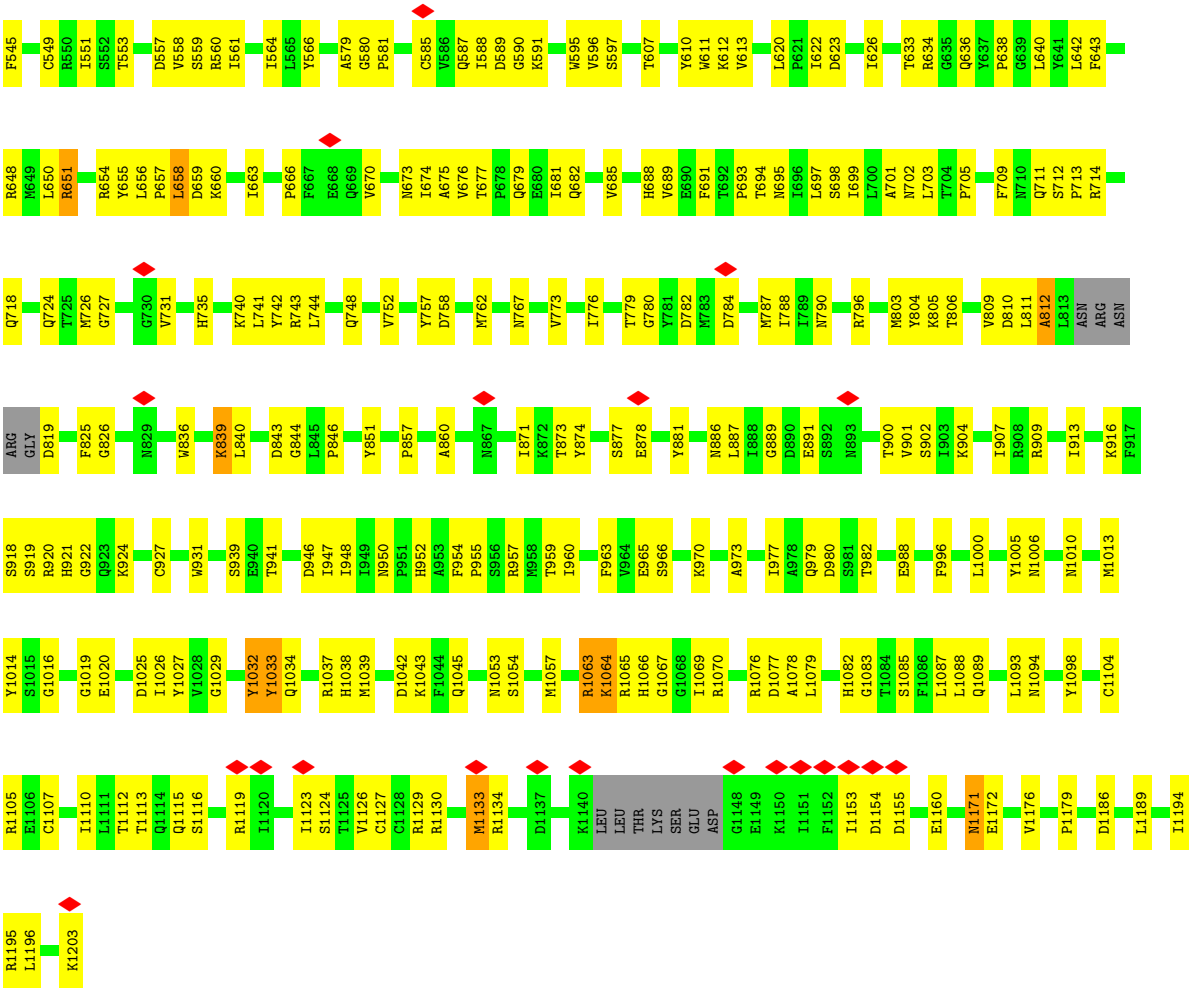




• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

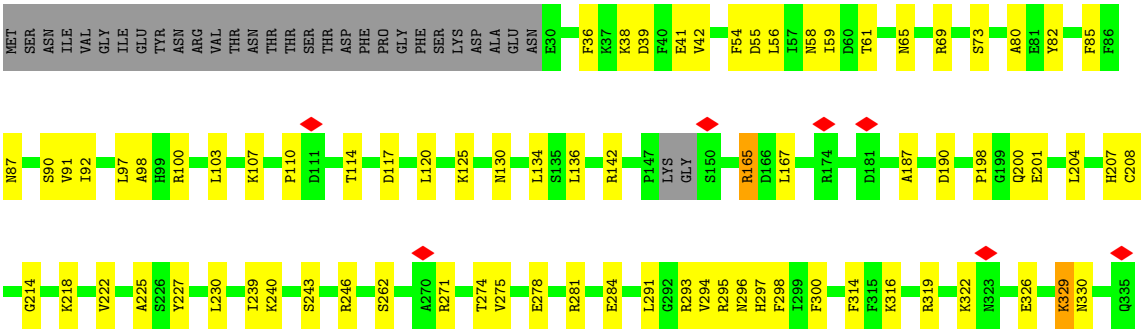
Chain B:





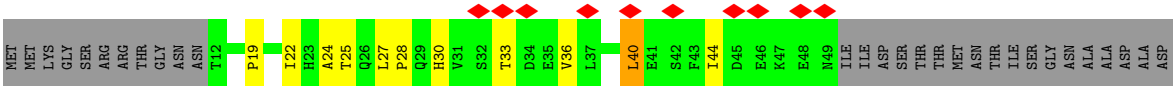
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

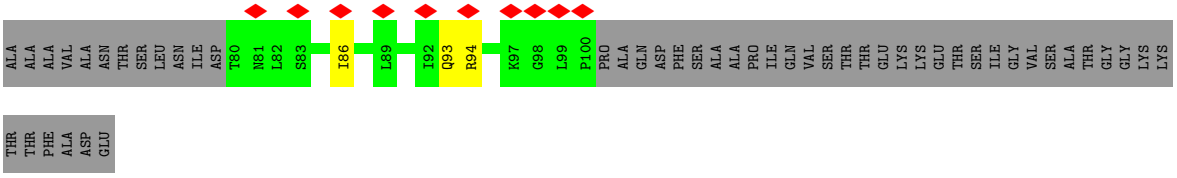
Chain C:



• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

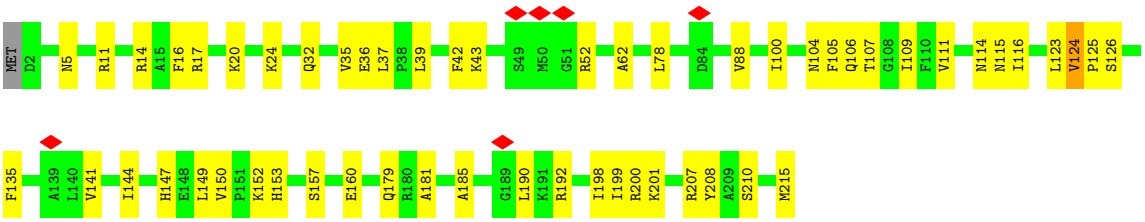
Chain D:





• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

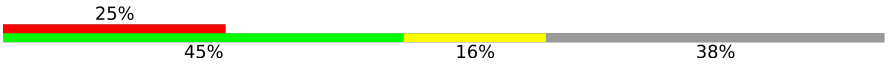


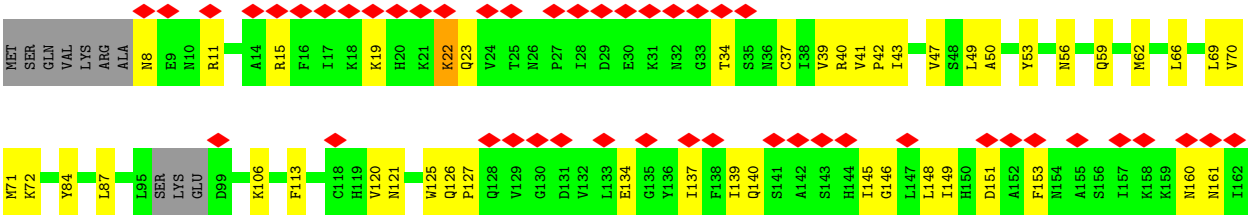
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

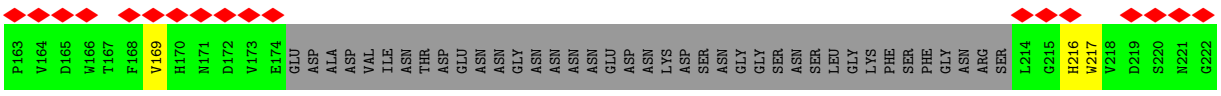
Chain F:

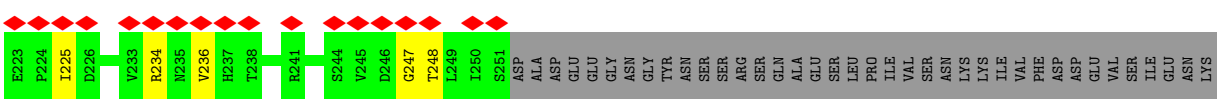
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

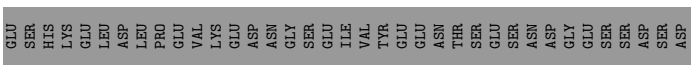
Chain G:





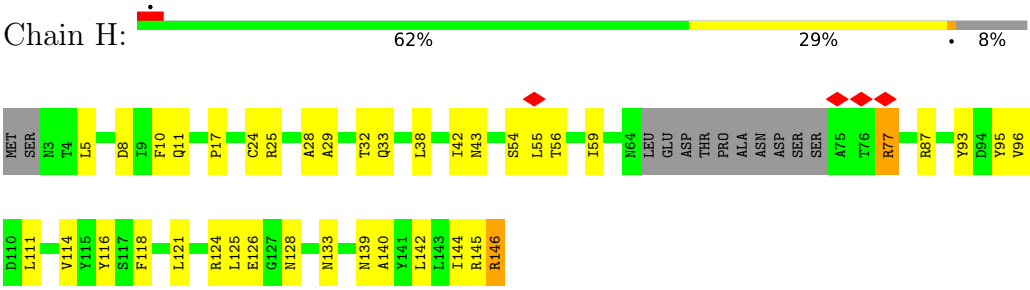






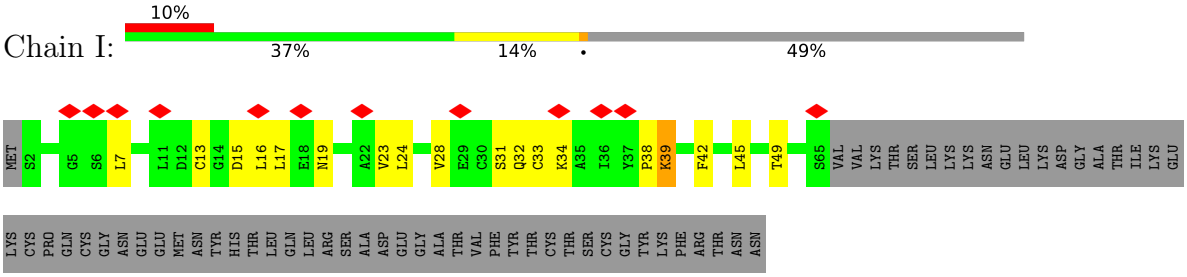
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



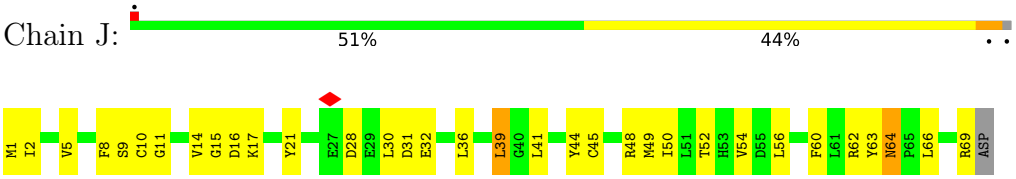
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:



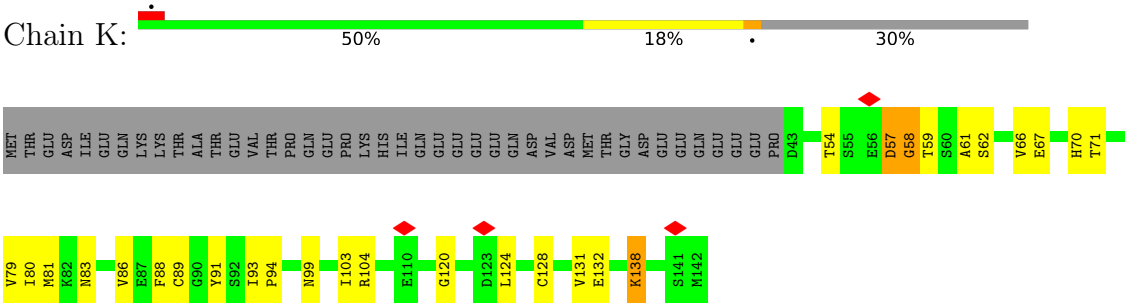
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



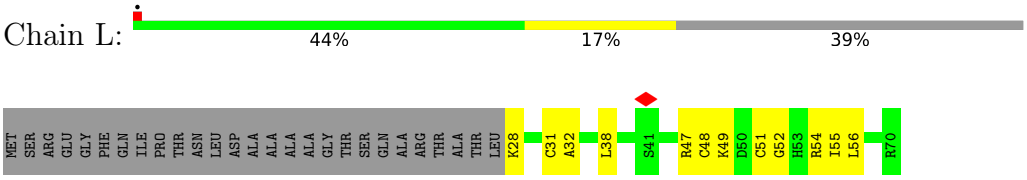
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



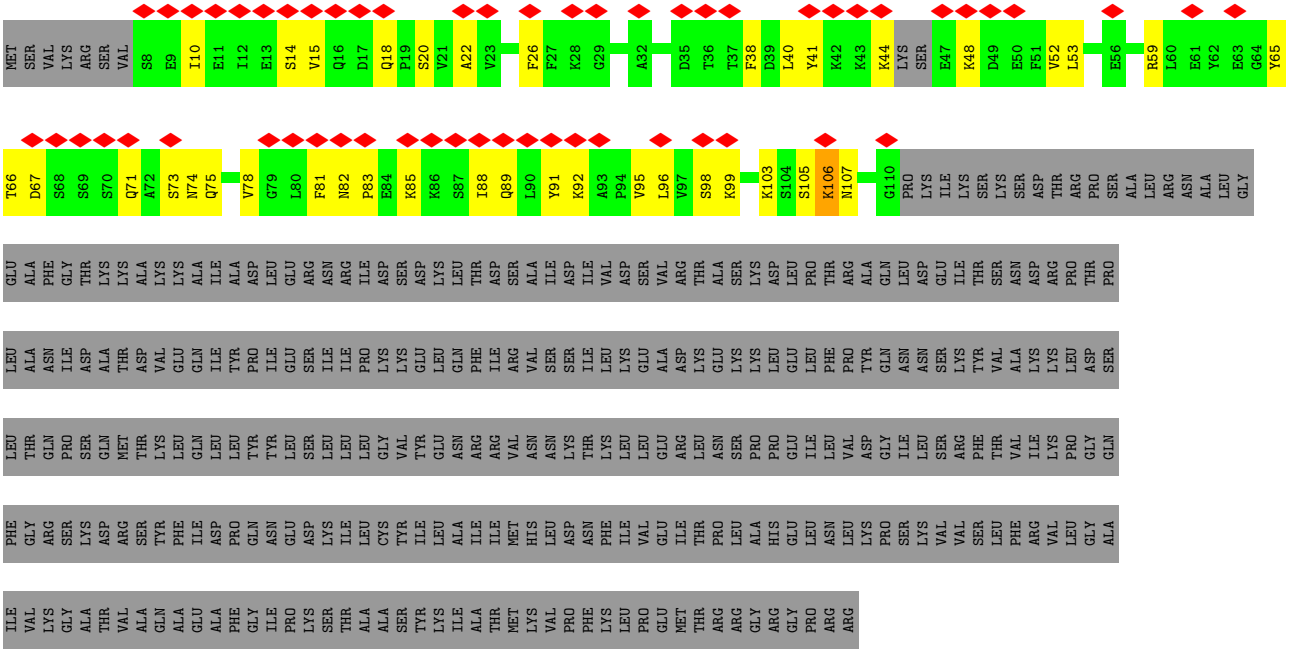
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



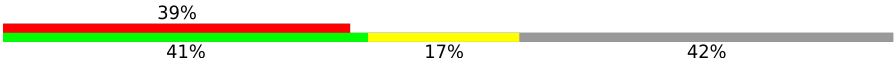
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

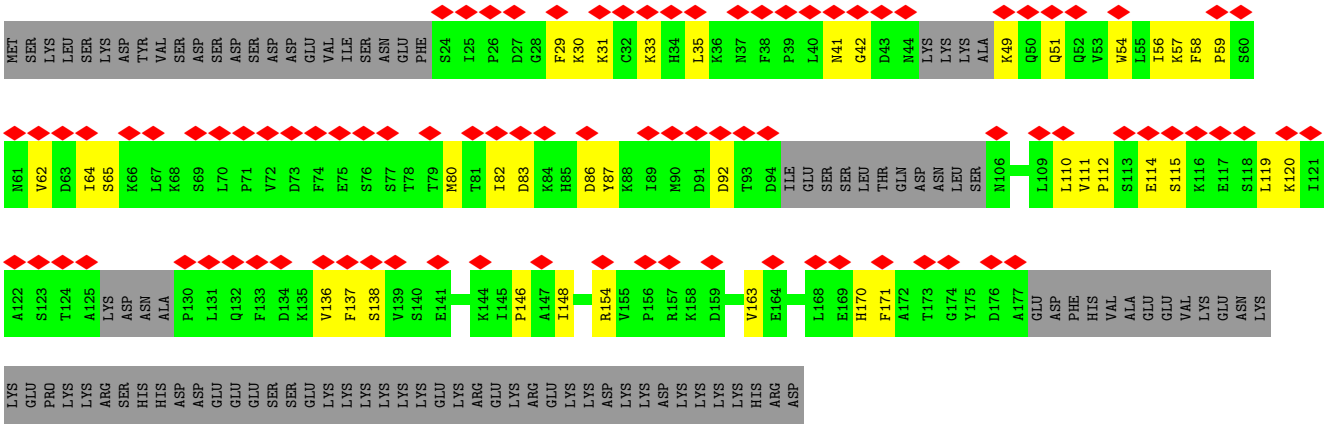
Chain M:



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

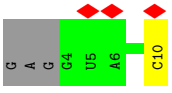
Chain N:





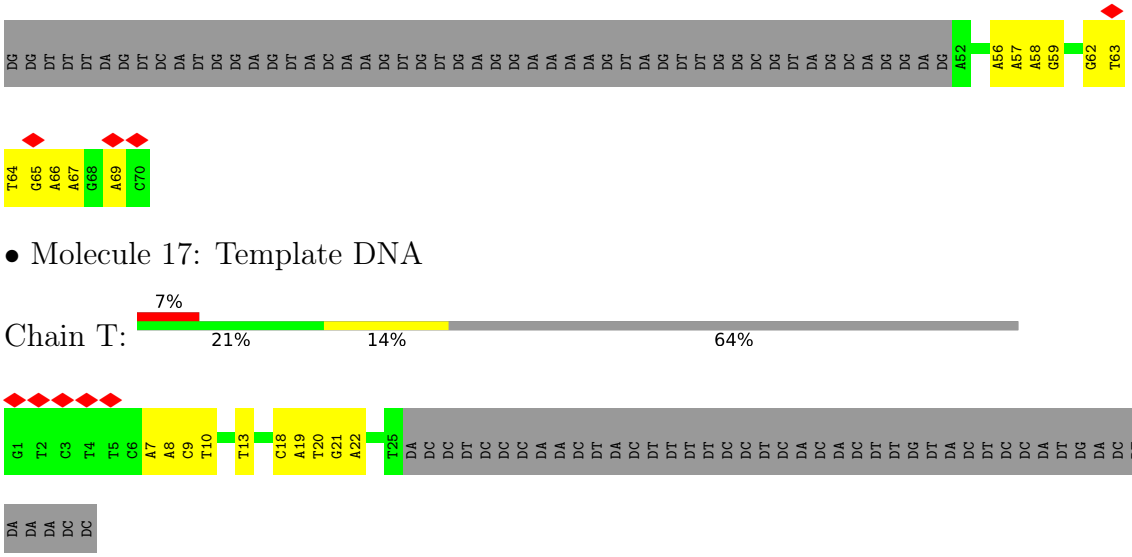
• Molecule 15: RNA

Chain R:



• Molecule 16: Non-template DNA

Chain S:



• Molecule 17: Template DNA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50784	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 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	0.25	1/11782 (0.0%)	0.47	6/15913 (0.0%)
2	B	0.24	1/9506 (0.0%)	0.46	3/12847 (0.0%)
3	C	0.24	0/2469	0.43	0/3347
4	D	0.23	0/473	0.44	0/641
5	E	0.24	0/1787	0.40	0/2406
6	F	0.23	0/838	0.39	0/1129
7	G	0.23	0/1637	0.44	0/2226
8	H	0.24	0/1093	0.47	0/1480
9	I	0.24	0/478	0.46	0/647
10	J	0.22	0/578	0.44	0/775
11	K	0.48	2/794 (0.3%)	0.81	4/1070 (0.4%)
12	L	0.23	0/346	0.44	0/457
13	M	0.26	0/816	0.48	0/1095
14	N	0.25	0/1090	0.49	0/1466
15	R	0.10	0/160	0.69	0/246
16	S	0.48	0/448	0.83	0/690
17	T	0.49	0/568	0.96	0/874
All	All	0.26	4/34863 (0.0%)	0.49	13/47309 (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
2	B	0	1
11	K	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	N-CA	10.21	1.66	1.46
1	A	763	GLY	N-CA	6.49	1.55	1.46
2	B	1064	LYS	N-CA	5.14	1.56	1.46
11	K	57	ASP	CA-CB	5.07	1.65	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	GLY	N-CA-C	-14.36	77.20	113.10
11	K	57	ASP	N-CA-C	-14.09	72.96	111.00
2	B	1064	LYS	N-CA-C	-12.01	78.58	111.00
11	K	57	ASP	CB-CA-C	-11.69	87.02	110.40
1	A	763	GLY	N-CA-C	-9.02	90.55	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	445	GLY	Mainchain
2	B	877	SER	Peptide
11	K	58	GLY	Mainchain

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	11571	0	11649	340	0
2	B	9301	0	9194	283	0
3	C	2418	0	2401	51	0
4	D	467	0	468	11	0
5	E	1751	0	1776	36	0
6	F	823	0	841	19	0
7	G	1600	0	1600	33	0
8	H	1075	0	1046	28	0
9	I	472	0	473	15	0
10	J	569	0	585	25	0
11	K	784	0	781	20	0
12	L	344	0	363	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	802	0	787	34	0
14	N	1070	0	1085	33	0
15	R	145	0	75	1	0
16	S	397	0	213	8	0
17	T	509	0	285	9	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	34104	0	33622	846	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 13.

The worst 5 of 846 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:A:450:LYS:O	1:A:451:VAL:HG22	1.31	1.26
1:A:865:ASP:C	1:A:866:LYS:HD2	1.63	1.18
1:A:865:ASP:HB3	1:A:866:LYS:NZ	1.59	1.16
1:A:450:LYS:O	1:A:451:VAL:CG2	2.04	1.05
1:A:865:ASP:CB	1:A:866:LYS:NZ	2.29	0.96

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	1450/1664 (87%)	1364 (94%)	80 (6%)	6 (0%)	30 66
2	B	1160/1203 (96%)	1094 (94%)	64 (6%)	2 (0%)	44 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
4	D	55/137 (40%)	54 (98%)	1 (2%)	0	100	100
5	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	196/326 (60%)	184 (94%)	12 (6%)	0	100	100
8	H	130/146 (89%)	125 (96%)	5 (4%)	0	100	100
9	I	62/125 (50%)	59 (95%)	3 (5%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	97/415 (23%)	90 (93%)	7 (7%)	0	100	100
14	N	127/233 (54%)	105 (83%)	22 (17%)	0	100	100
All	All	4093/5236 (78%)	3860 (94%)	225 (6%)	8 (0%)	45	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	VAL
2	B	812	ALA
1	A	227	LEU
1	A	248	PHE
1	A	765	LEU

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	1293/1465 (88%)	1264 (98%)	29 (2%)	47	65
2	B	1025/1053 (97%)	999 (98%)	26 (2%)	42	62
3	C	269/296 (91%)	266 (99%)	3 (1%)	70	80
4	D	56/116 (48%)	54 (96%)	2 (4%)	30	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	196/197 (100%)	193 (98%)	3 (2%)	60 75
6	F	90/137 (66%)	88 (98%)	2 (2%)	47 65
7	G	180/291 (62%)	174 (97%)	6 (3%)	33 55
8	H	117/128 (91%)	110 (94%)	7 (6%)	16 39
9	I	56/110 (51%)	54 (96%)	2 (4%)	30 52
10	J	64/65 (98%)	61 (95%)	3 (5%)	22 45
11	K	89/130 (68%)	88 (99%)	1 (1%)	70 80
12	L	38/57 (67%)	37 (97%)	1 (3%)	41 61
13	M	91/371 (24%)	90 (99%)	1 (1%)	70 80
14	N	125/220 (57%)	124 (99%)	1 (1%)	79 84
All	All	3689/4636 (80%)	3602 (98%)	87 (2%)	45 63

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	329	LYS
8	H	25	ARG
4	D	94	ARG
7	G	8	ASN
8	H	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	770	ASN
3	C	130	ASN
13	M	75	GLN
2	B	893	ASN
2	B	1171	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	6/10 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 6 ligands modelled in this entry, 6 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.

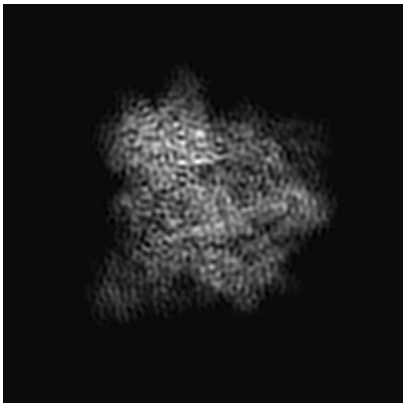
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3448. These allow visual inspection of the internal detail of the map and identification of artifacts.

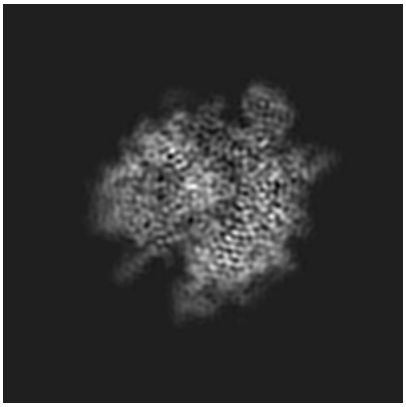
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

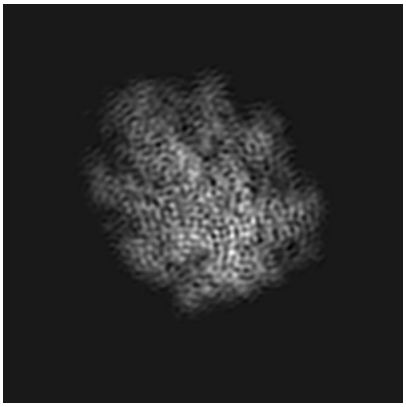
6.1.1 Primary map



X



Y

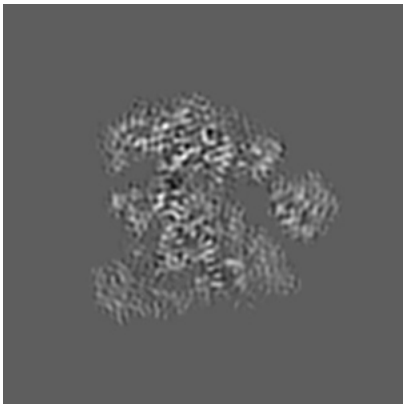


Z

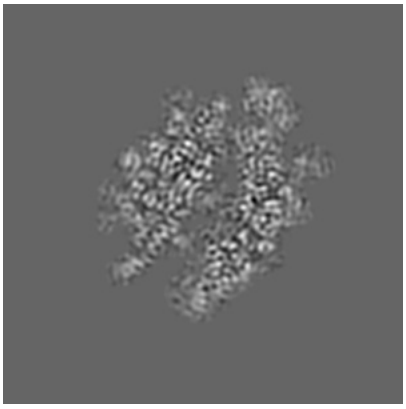
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 88



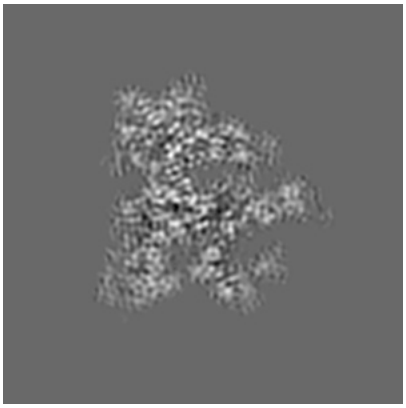
Y Index: 88

Z Index: 88

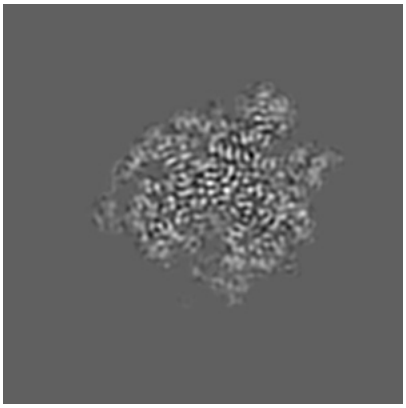
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

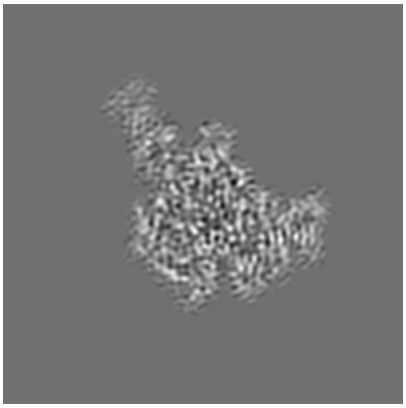
6.3.1 Primary map



X Index: 100



Y Index: 75

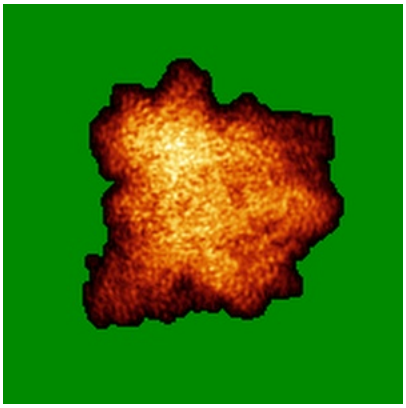


Z Index: 113

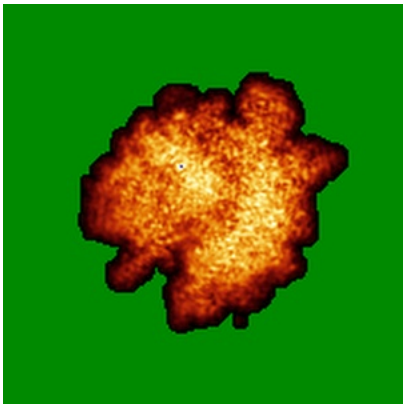
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

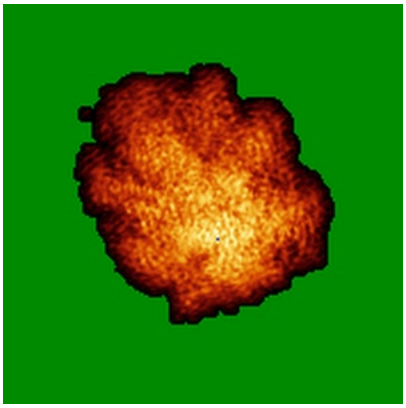
6.4.1 Primary map



X



Y

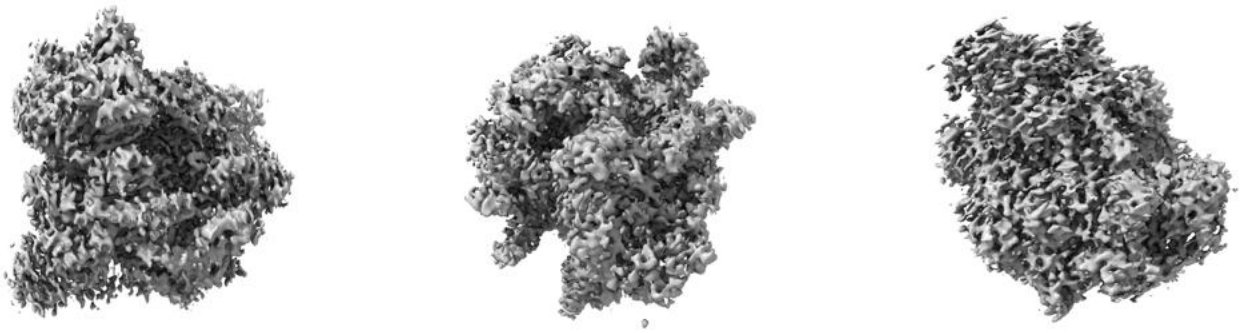


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

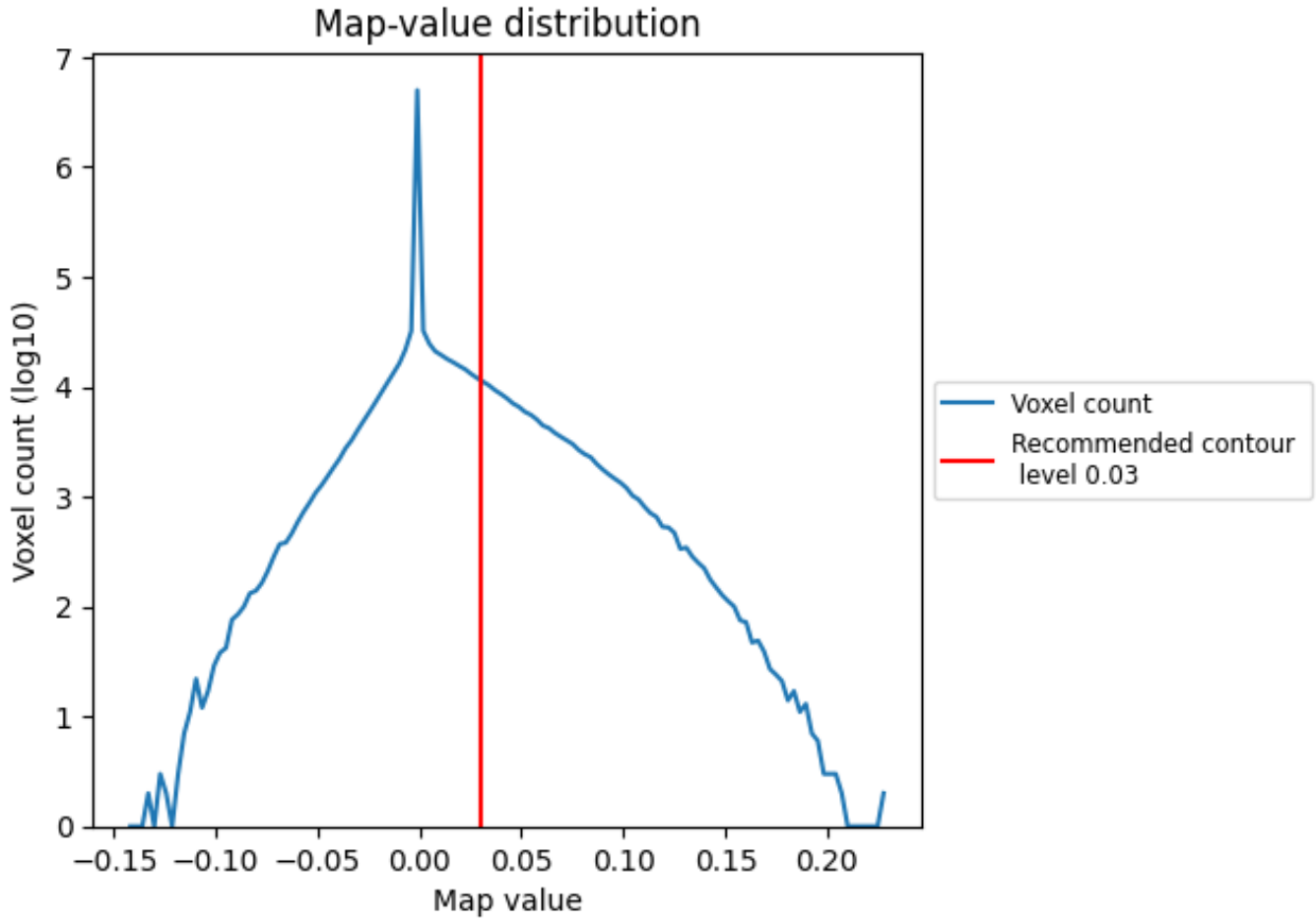
6.6 Mask visualisation (i)

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

7 Map analysis

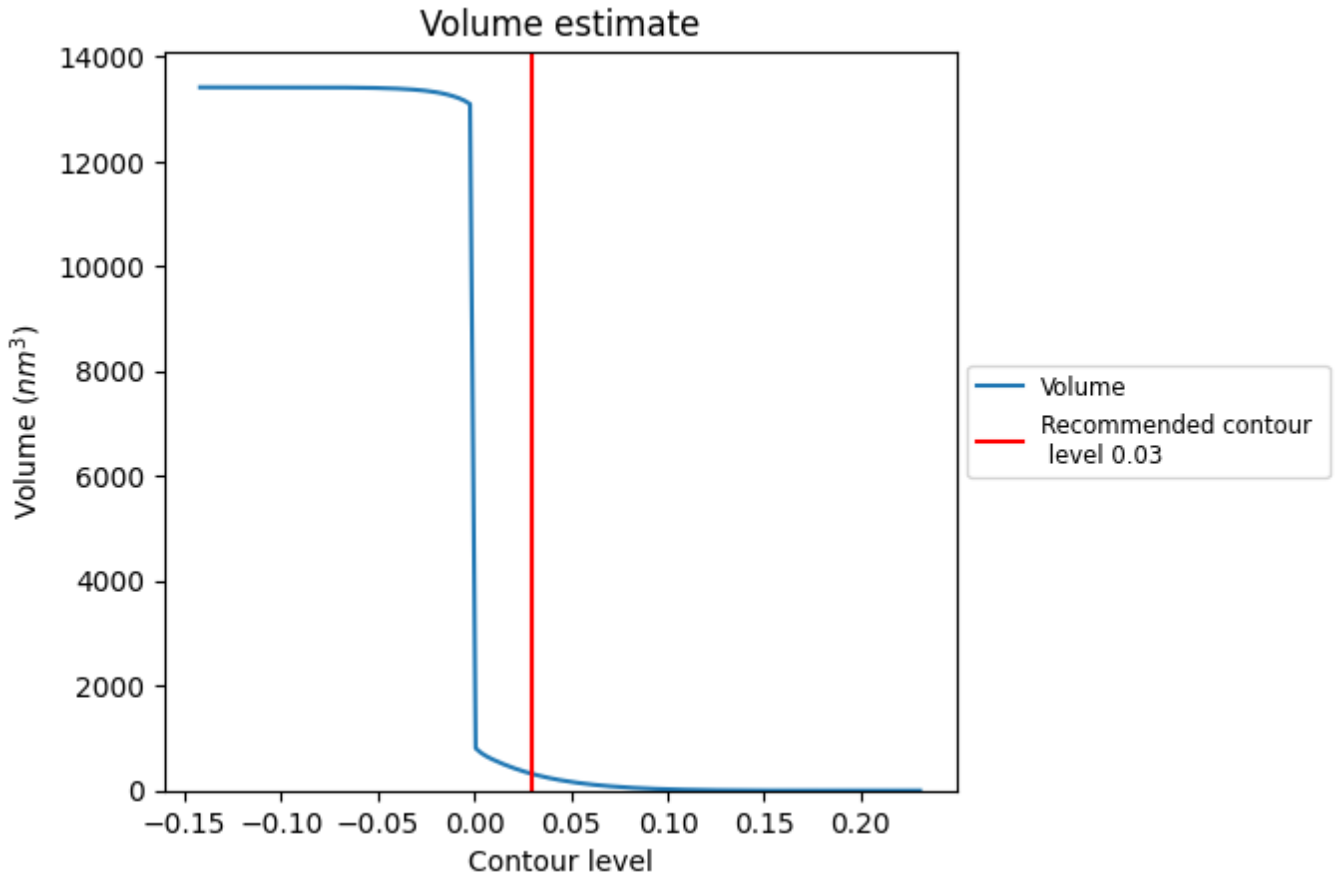
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

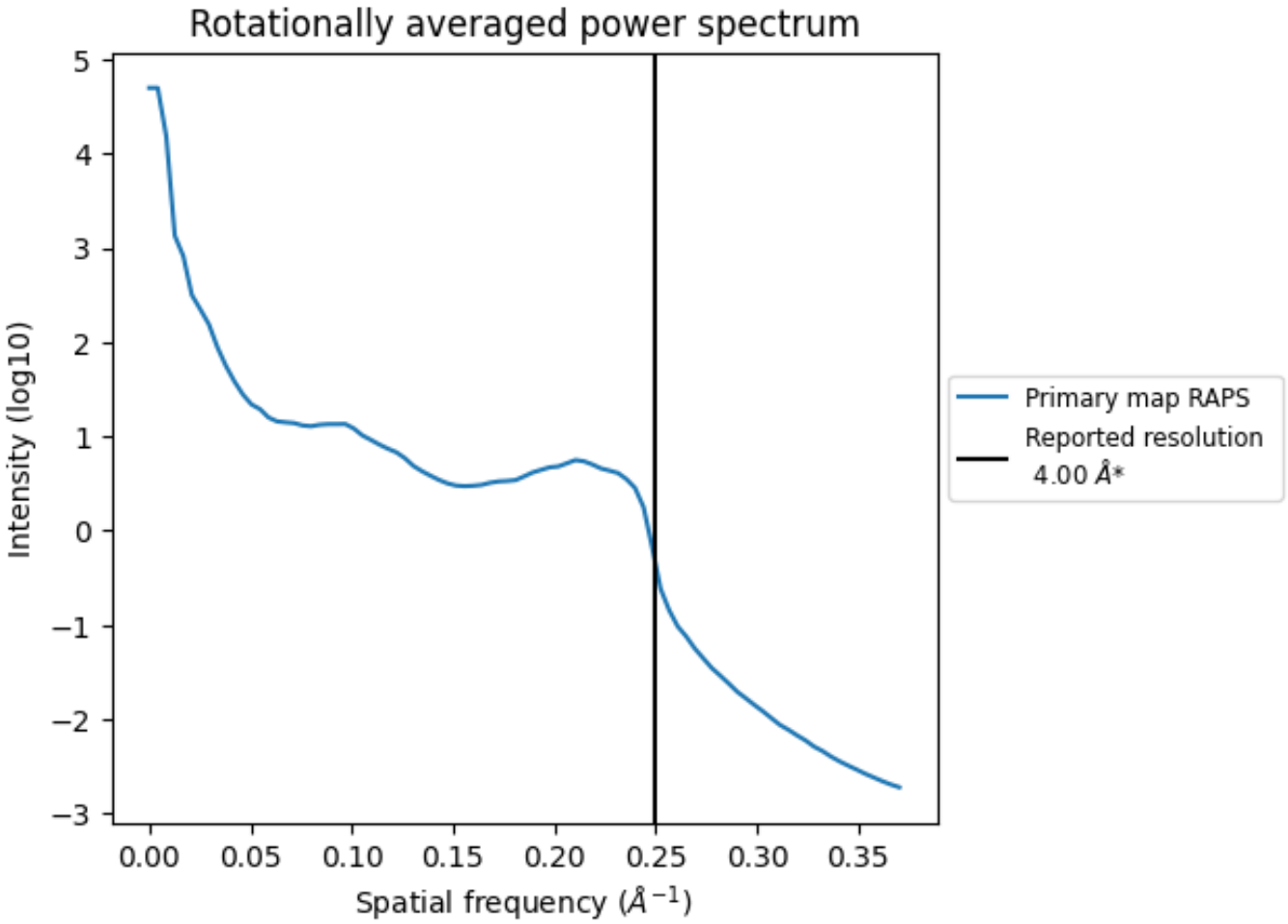
7.2 Volume estimate (i)



The volume at the recommended contour level is 317 nm^3; this corresponds to an approximate mass of 287 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

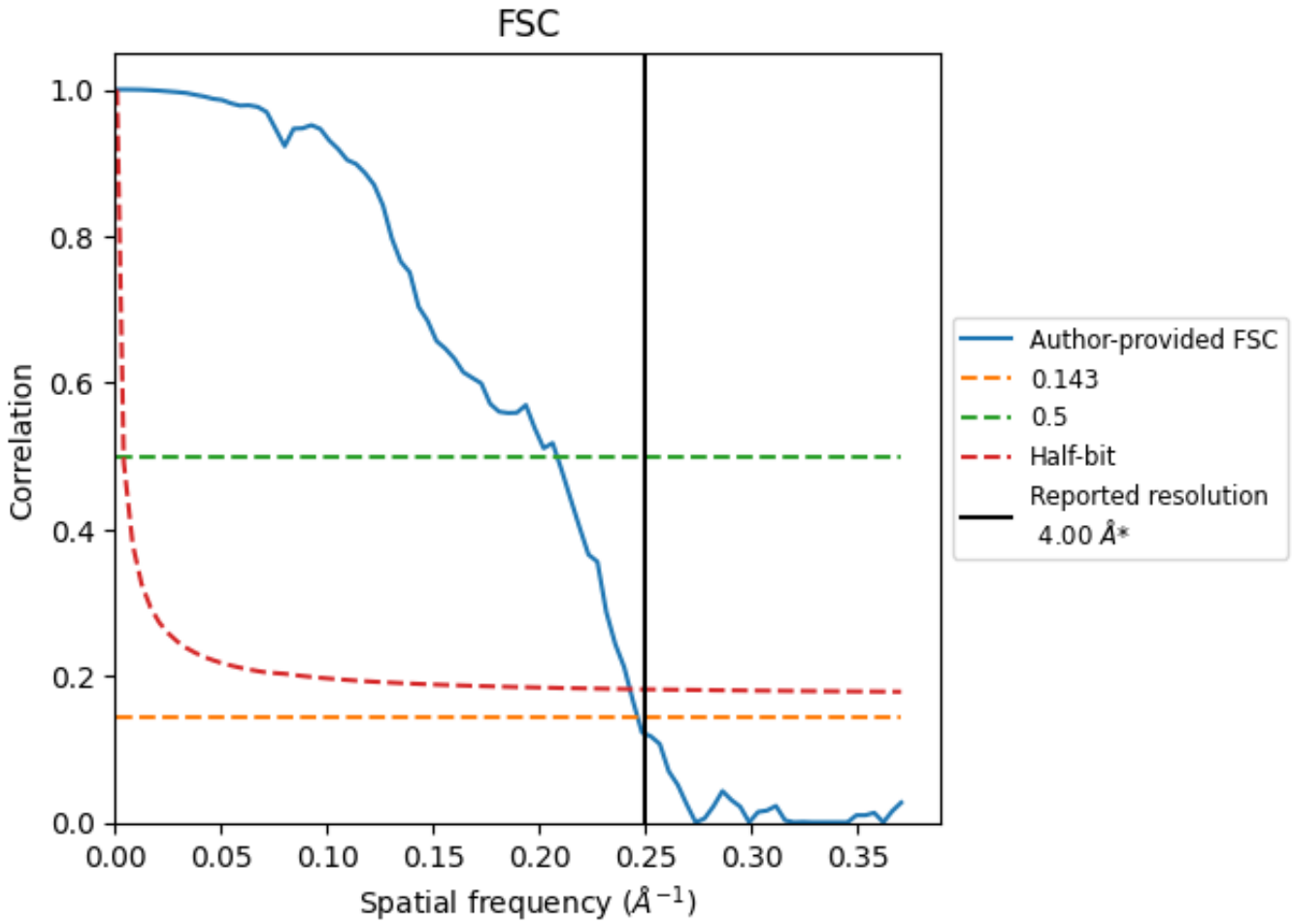


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

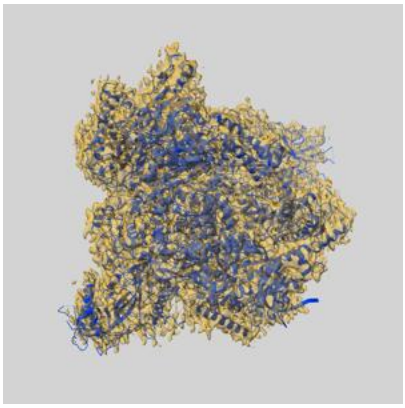
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.06	4.80	4.12
Unmasked-calculated*	-	-	-

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

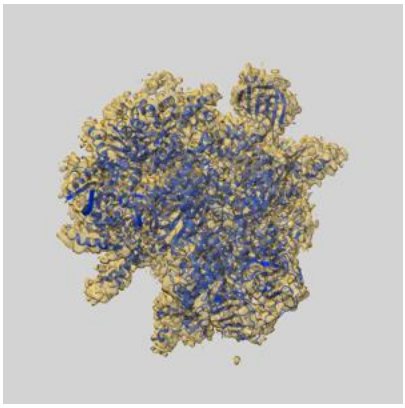
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3448 and PDB model 5M5Y. Per-residue inclusion information can be found in section 3 on page 7.

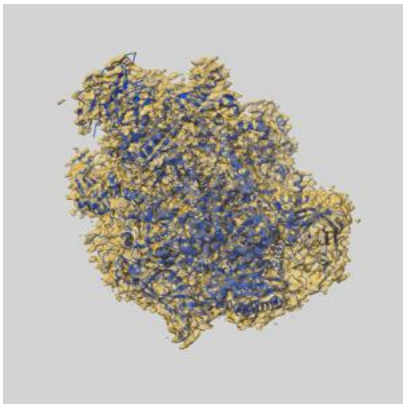
9.1 Map-model overlay



X



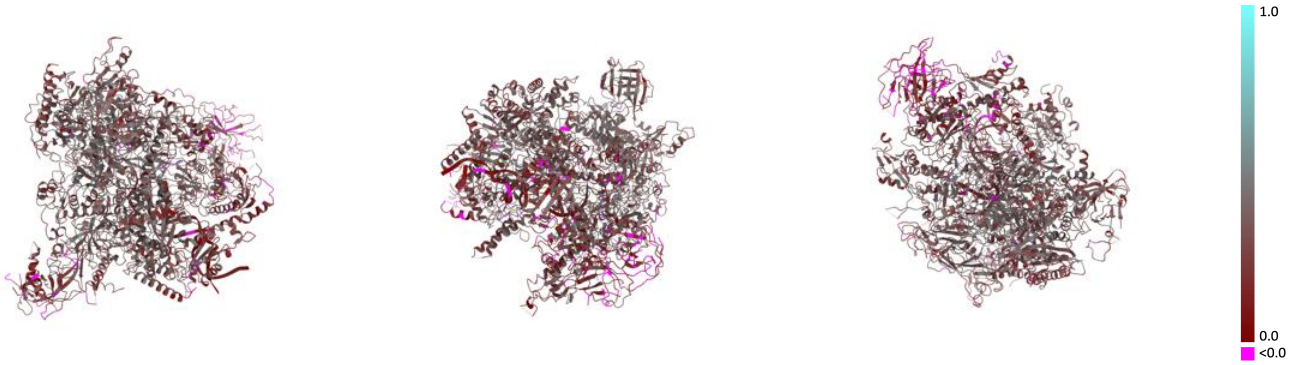
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

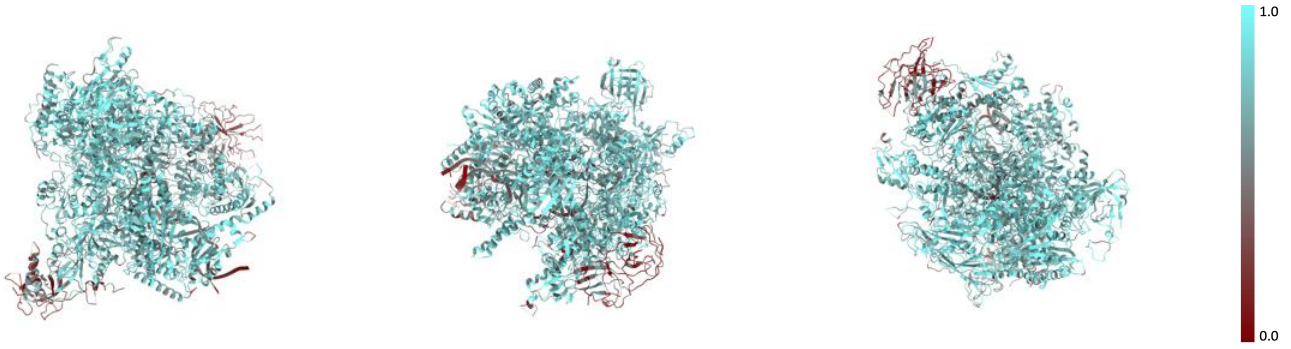
9.2 Q-score mapped to coordinate model



X Y Z

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

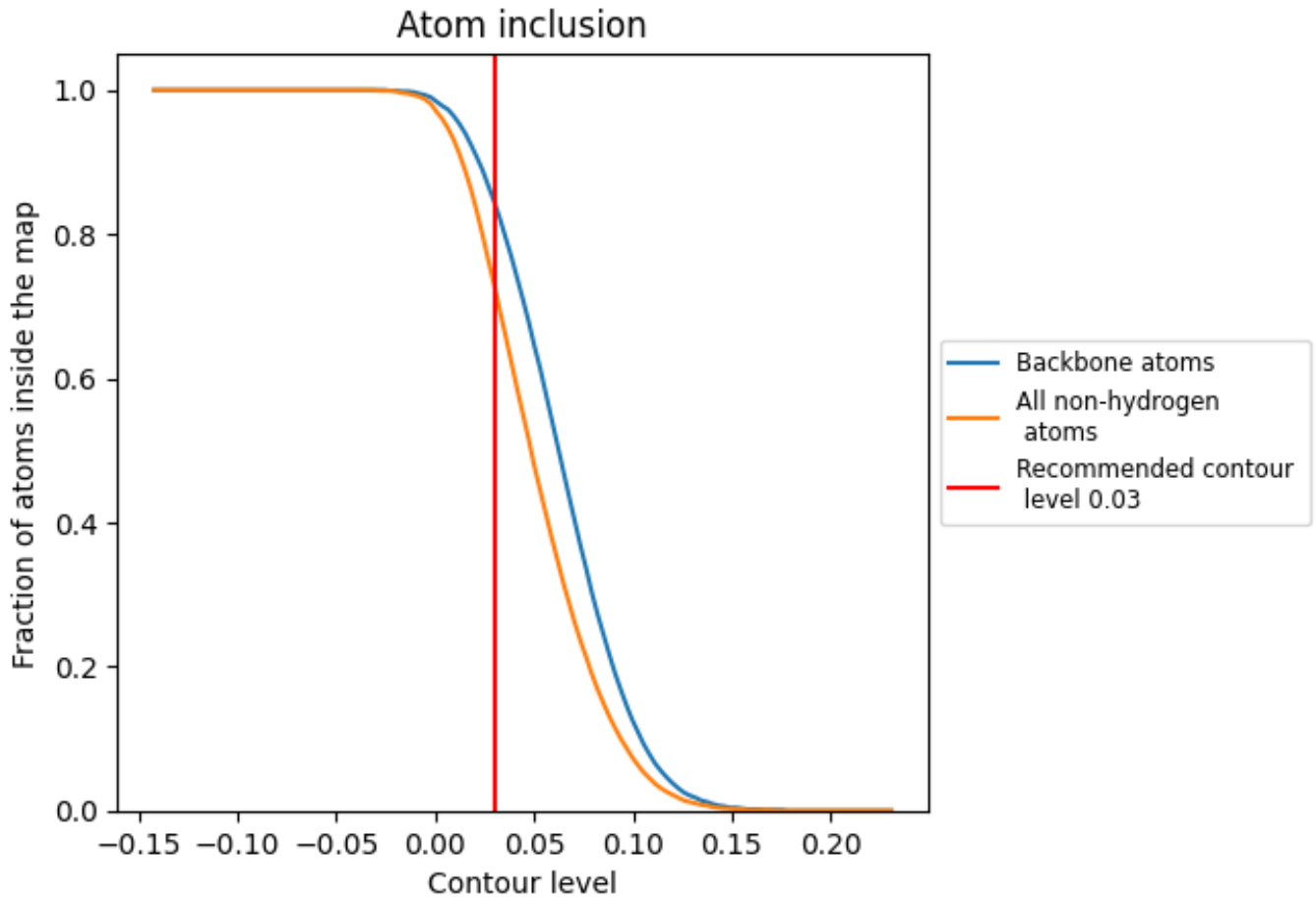
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.3080
A	0.7780	0.3290
B	0.7770	0.3320
C	0.7980	0.3360
D	0.4900	0.2350
E	0.7840	0.3240
F	0.7900	0.3400
G	0.4910	0.2520
H	0.7830	0.3260
I	0.6490	0.1970
J	0.8480	0.3980
K	0.7680	0.3310
L	0.7380	0.3060
M	0.3670	0.1350
N	0.3100	0.1440
R	0.3720	0.1200
S	0.5390	0.1180
T	0.5030	0.1660