



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 08:34 am GMT

PDB ID : 7AMV
EMDB ID : EMD-11824
Title : Atomic structure of the poxvirus transcription pre-initiation complex in the initially melted state
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2020-10-09
Resolution : 2.80 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

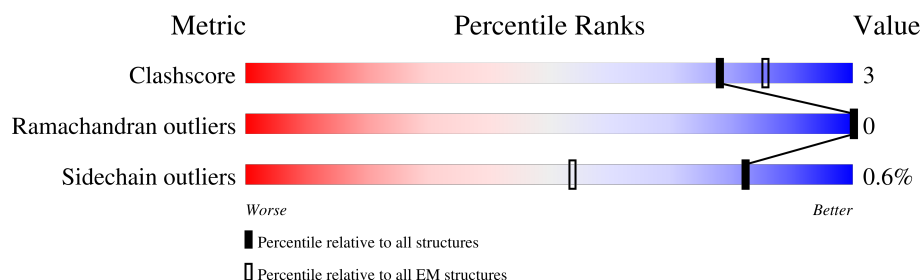
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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

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	1286	
2	B	1164	
3	C	305	
4	E	185	
5	F	164	
6	G	161	
7	I	795	
8	J	63	

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Mol	Chain	Length	Quality of chain
9	K	710	 89% 10%
10	N	60	 62% 8% 30%
11	S	259	 43% 5% 51%
12	T	60	 62% 8% 30%
13	W	637	 92% 8%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 45172 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1248	Total	C	N	O	S	0	0
			10017	6443	1651	1878	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1126	Total	C	N	O	S	0	0
			9060	5779	1543	1690	48		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	conflict	UNP Q49PH2

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	303	Total	C	N	O	S	0	0
			2475	1603	397	462	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	184	Total	C	N	O	S	0	0
			1495	966	248	276	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			849	545	148	153	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	158	Total	C	N	O	S	0	0
			1233	778	204	245	6		

- Molecule 7 is a protein called Protein H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	694	Total	C	N	O	S	0	0
			5807	3788	931	1067	21		

- Molecule 8 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	61	Total	C	N	O	S	0	0
			490	310	88	88	4		

- Molecule 9 is a protein called ETF large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	708	Total	C	N	O	S	0	0
			5776	3727	947	1071	31		

- Molecule 10 is a DNA chain called Synthetic promoter DNA oligomer, non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	42	Total	C	N	O	P	0	0
			861	412	161	246	42		

- Molecule 11 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	126	Total	C	N	O	S	0	0
			1036	659	169	204	4		

- Molecule 12 is a DNA chain called Synthetic promoter DNA oligomer, template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	42	Total	C	N	O	P	0	0
			861	414	147	258	42		

- Molecule 13 is a protein called ATP-dependent helicase VETFS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	637	Total	C	N	O	S	0	0
			5207	3360	854	970	23		

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

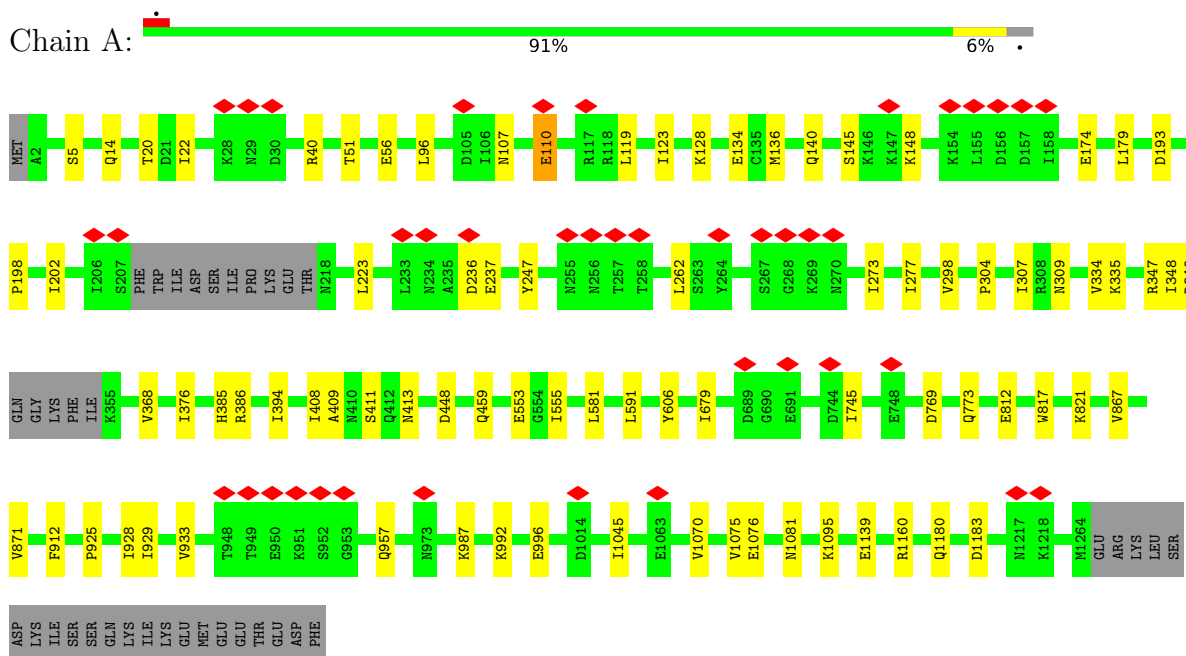
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

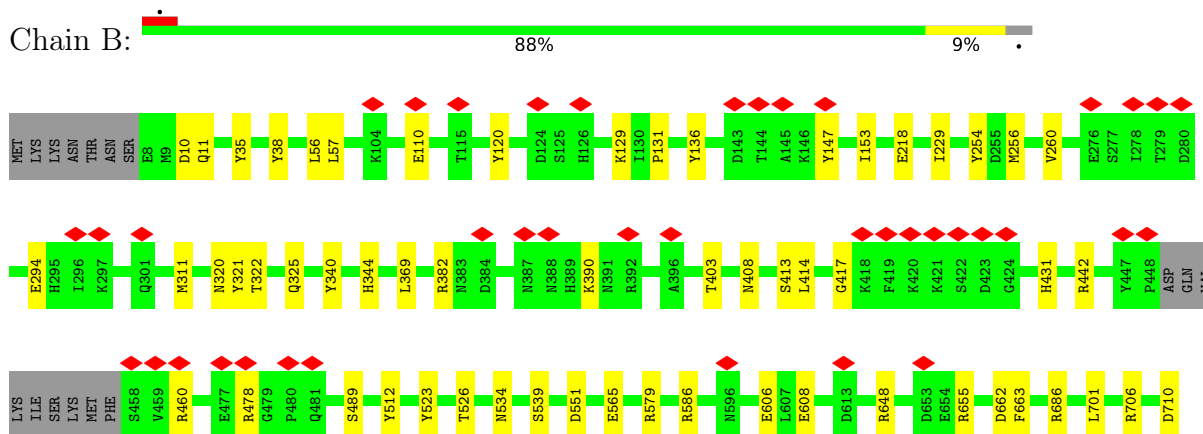
3 Residue-property plots

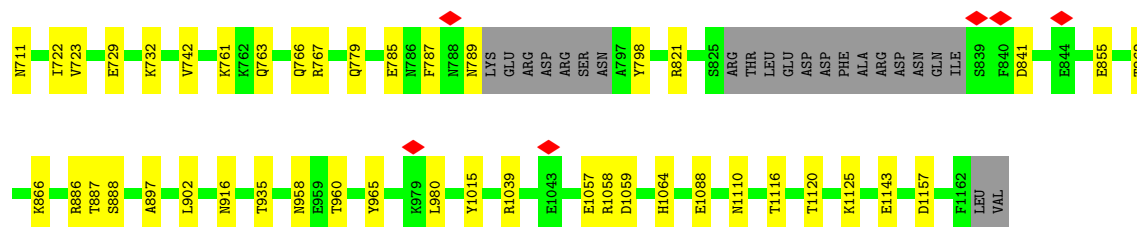
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 147 kDa polypeptide

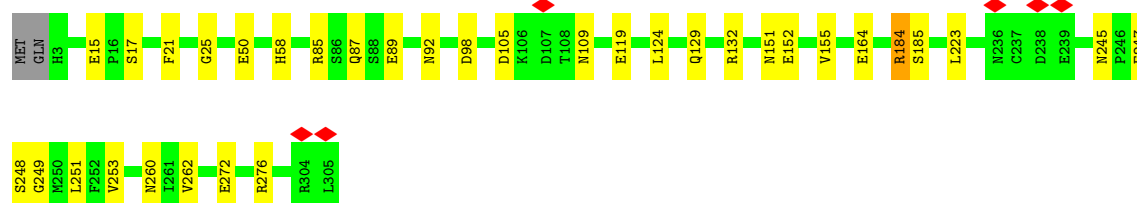
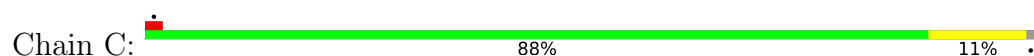


- Molecule 2: DNA-directed RNA polymerase





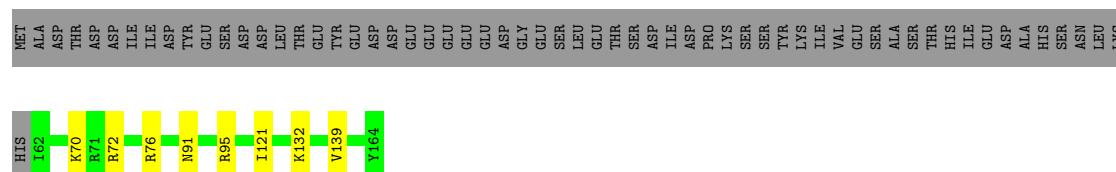
• Molecule 3: DNA-directed RNA polymerase 35 kDa subunit



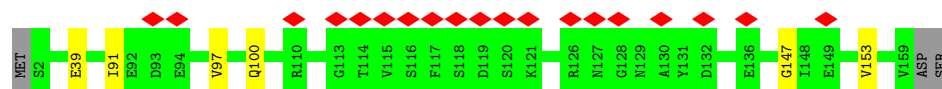
• Molecule 4: DNA-directed RNA polymerase subunit



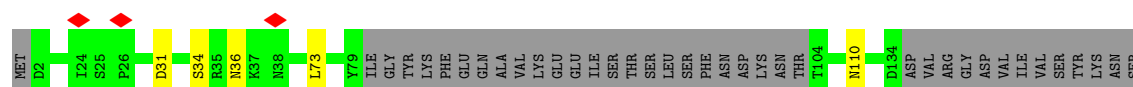
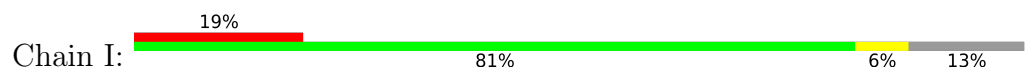
• Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

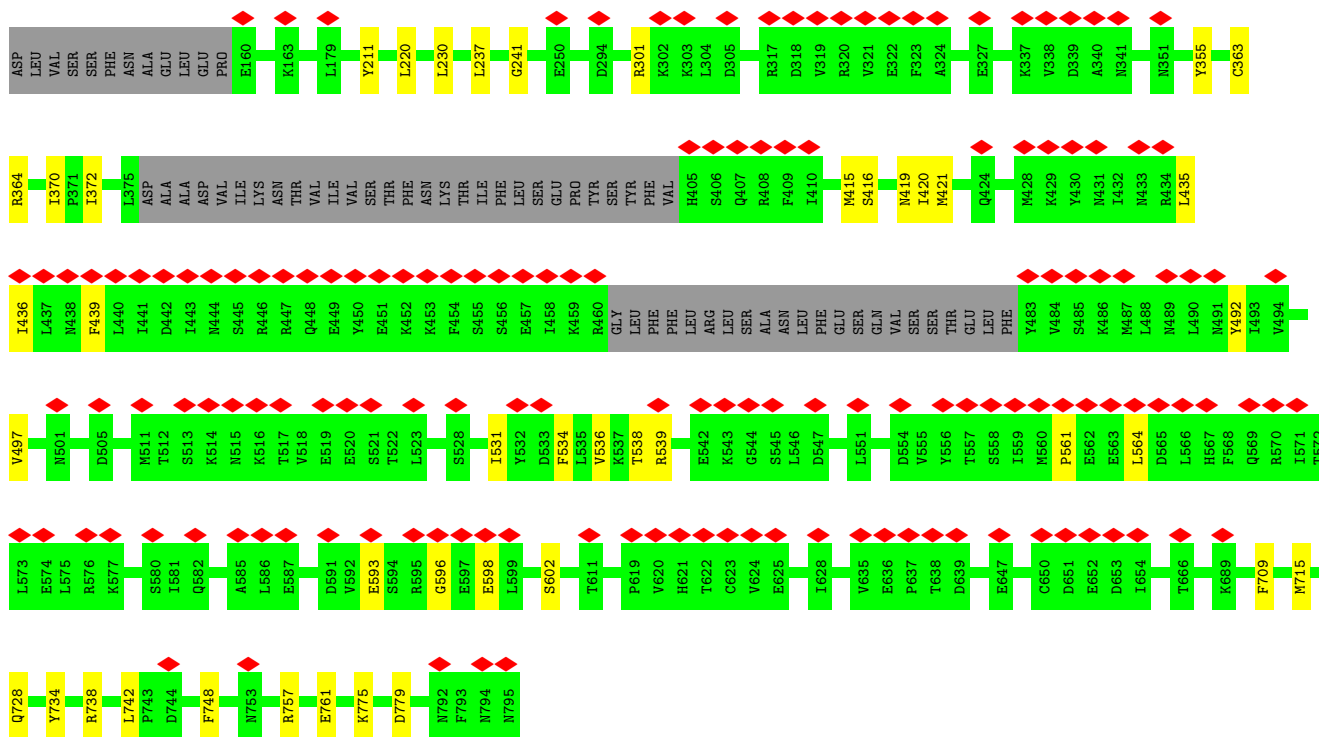


• Molecule 6: DNA-directed RNA polymerase 18 kDa subunit



• Molecule 7: Protein H4





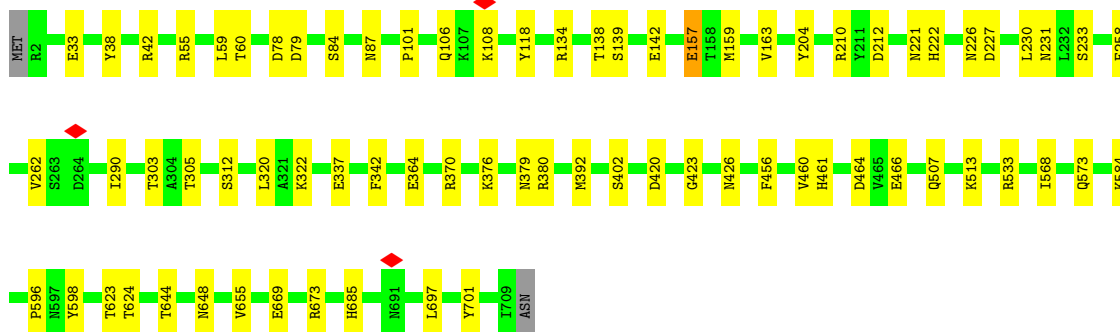
- Molecule 8: DNA-directed RNA polymerase 7 kDa subunit

Chain J: 83% 14%



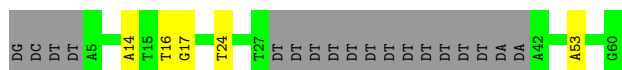
- Molecule 9: ETF large subunit

Chain K: 89% 10%



- Molecule 10: Synthetic promoter DNA oligomer, non-template strand

Chain N: 62% 8% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181788	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 ($e^-/\text{\AA}^2$)	78.90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	15.612	Depositor
Minimum map value	-7.424	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.009	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	163.70595, 180.58284, 199.14743	wwPDB
Map dimensions	214, 236, 194	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84384507, 0.84384507, 0.84384507	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: ZN, MG

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	0/10216	0.45	0/13810
2	B	0.25	0/9250	0.46	0/12496
3	C	0.25	0/2531	0.44	0/3428
4	E	0.25	0/1522	0.46	0/2069
5	F	0.24	0/863	0.43	0/1158
6	G	0.25	0/1252	0.48	0/1698
7	I	0.25	0/5935	0.44	0/8028
8	J	0.23	0/494	0.46	0/663
9	K	0.25	0/5898	0.47	0/7979
10	N	0.60	0/966	0.94	0/1485
11	S	0.25	0/1051	0.42	0/1407
12	T	0.60	0/962	1.03	0/1481
13	W	0.25	0/5321	0.45	0/7203
All	All	0.27	0/46261	0.49	0/62905

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	10017	0	10136	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9060	0	9108	60	0
3	C	2475	0	2462	23	0
4	E	1495	0	1548	5	0
5	F	849	0	874	5	0
6	G	1233	0	1218	2	0
7	I	5807	0	5868	31	0
8	J	490	0	528	7	0
9	K	5776	0	5824	45	0
10	N	861	0	475	5	0
11	S	1036	0	1037	9	0
12	T	861	0	481	5	0
13	W	5207	0	5210	30	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	J	1	0	0	0	0
All	All	45172	0	44769	245	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 3.

The worst 5 of 245 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:581:LEU:HD21	1:A:679:ILE:HG21	1.61	0.80
3:C:251:LEU:HD21	3:C:262:VAL:HG11	1.68	0.75
4:E:170:VAL:HG23	4:E:171:THR:HG23	1.71	0.71
4:E:129:GLN:O	5:F:70:LYS:NZ	2.23	0.71
7:I:715:MET:O	7:I:757:ARG:NH2	2.24	0.70

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	1242/1286 (97%)	1215 (98%)	27 (2%)	0	100	100
2	B	1118/1164 (96%)	1096 (98%)	22 (2%)	0	100	100
3	C	301/305 (99%)	294 (98%)	7 (2%)	0	100	100
4	E	182/185 (98%)	182 (100%)	0	0	100	100
5	F	101/164 (62%)	101 (100%)	0	0	100	100
6	G	156/161 (97%)	149 (96%)	7 (4%)	0	100	100
7	I	684/795 (86%)	652 (95%)	32 (5%)	0	100	100
8	J	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
9	K	706/710 (99%)	681 (96%)	25 (4%)	0	100	100
11	S	122/259 (47%)	115 (94%)	7 (6%)	0	100	100
13	W	635/637 (100%)	613 (96%)	22 (4%)	0	100	100
All	All	5306/5729 (93%)	5156 (97%)	150 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1120/1157 (97%)	1114 (100%)	6 (0%)	86	95
2	B	1027/1064 (96%)	1019 (99%)	8 (1%)	79	93
3	C	285/287 (99%)	284 (100%)	1 (0%)	89	96
4	E	174/175 (99%)	174 (100%)	0	100	100
5	F	94/151 (62%)	94 (100%)	0	100	100
6	G	141/144 (98%)	139 (99%)	2 (1%)	62	87
7	I	662/755 (88%)	658 (99%)	4 (1%)	84	95
8	J	60/62 (97%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	663/665 (100%)	660 (100%)	3 (0%)	86	95
11	S	117/240 (49%)	115 (98%)	2 (2%)	56	84
13	W	595/595 (100%)	593 (100%)	2 (0%)	91	97
All	All	4938/5295 (93%)	4910 (99%)	28 (1%)	82	95

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	184	ARG
13	W	449	ASN
7	I	73	LEU
11	S	108	LYS
6	G	100	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

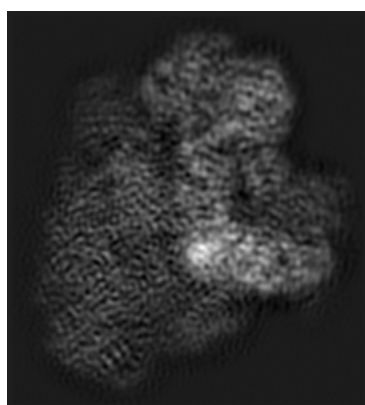
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11824. These allow visual inspection of the internal detail of the map and identification of artifacts.

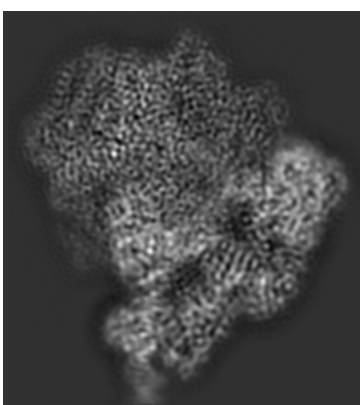
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

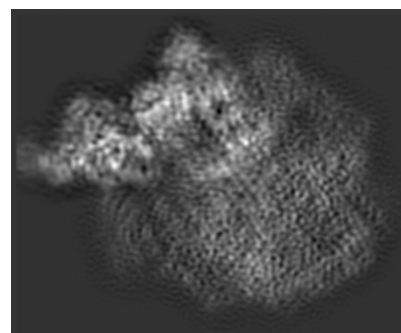
6.1.1 Primary map



X



Y

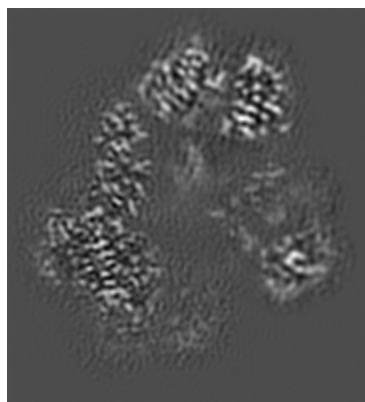


Z

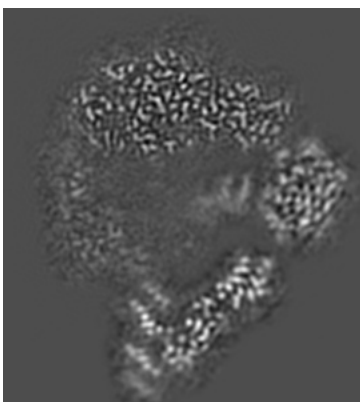
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

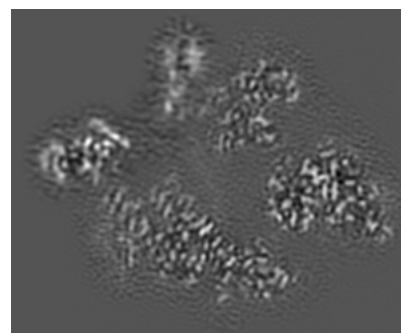
6.2.1 Primary map



X Index: 118



Y Index: 97

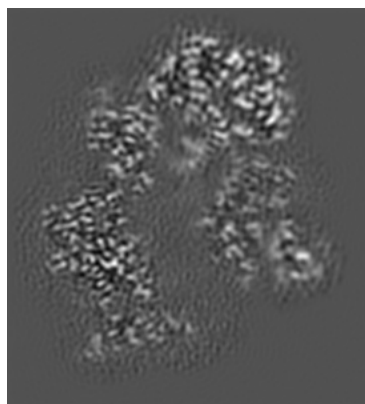


Z Index: 107

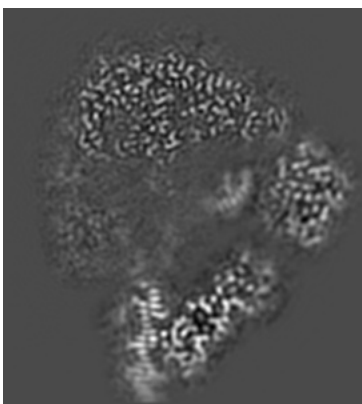
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

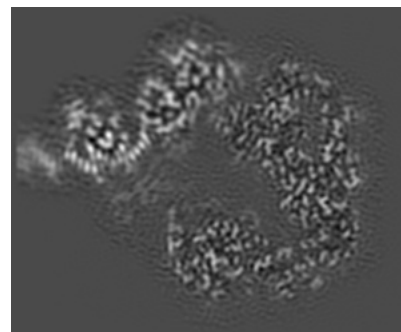
6.3.1 Primary map



X Index: 126



Y Index: 102

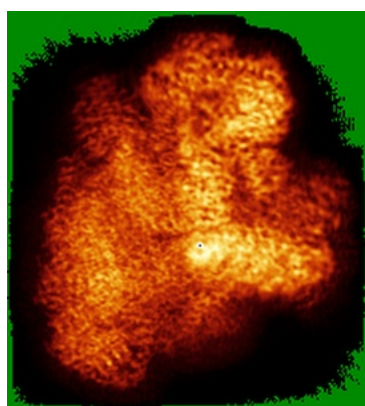


Z Index: 86

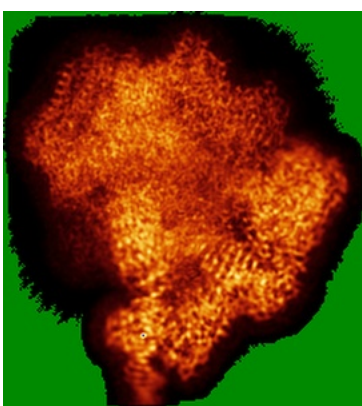
The images above show the largest variance slices of the map in three orthogonal directions.

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

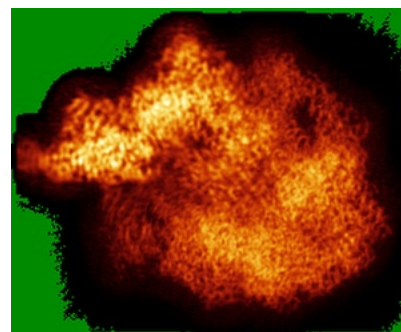
6.4.1 Primary map



X



Y

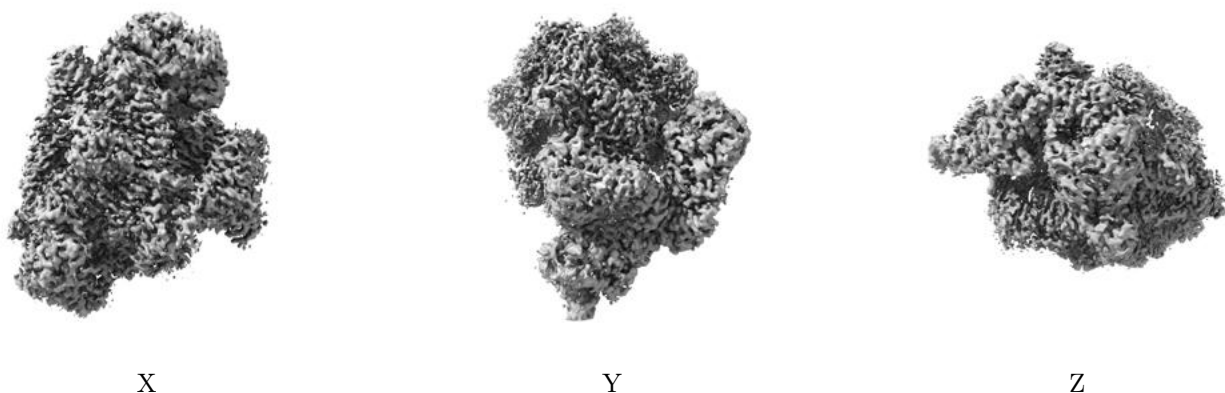


Z

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

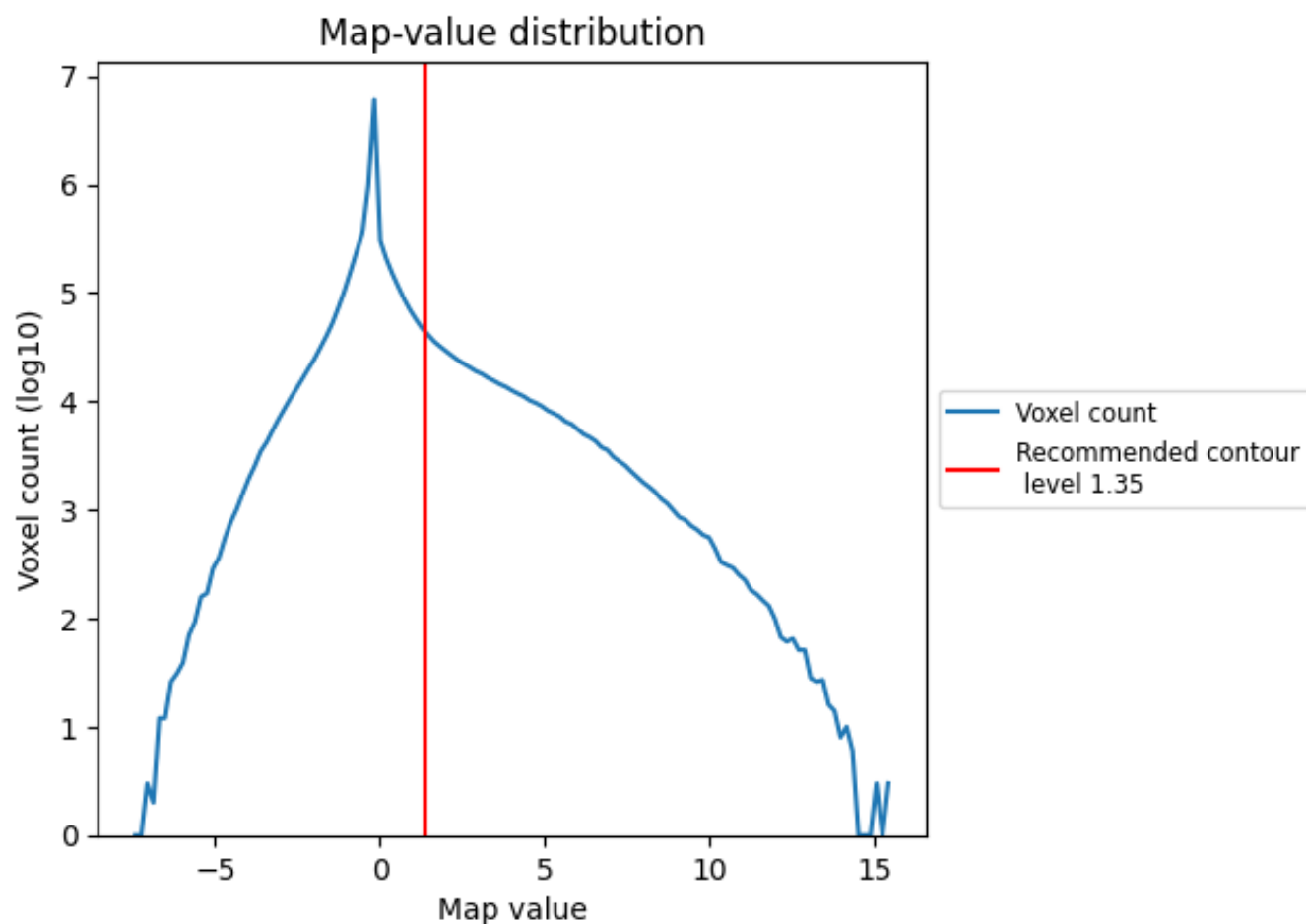
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

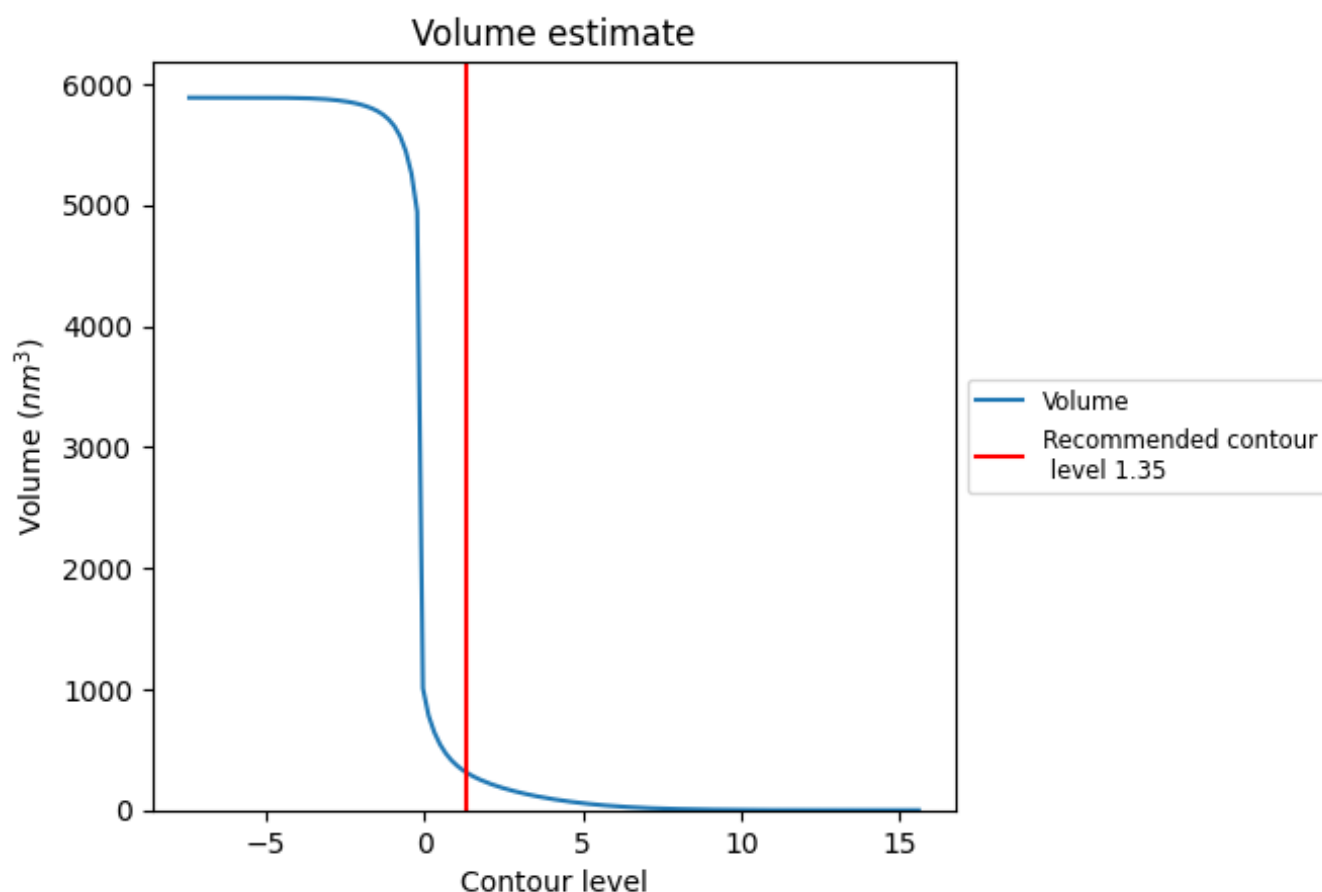
This section contains the results of statistical analysis of the map.

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 308 nm³; this corresponds to an approximate mass of 278 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

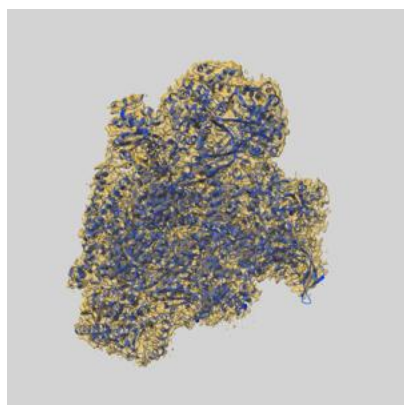
8 Fourier-Shell correlation

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

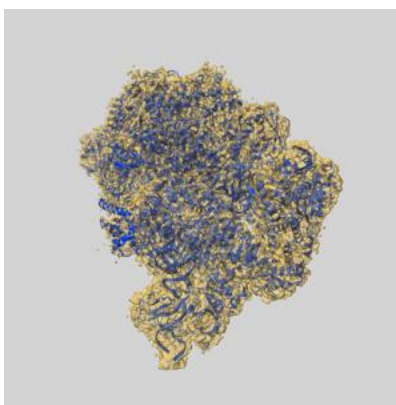
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11824 and PDB model 7AMV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

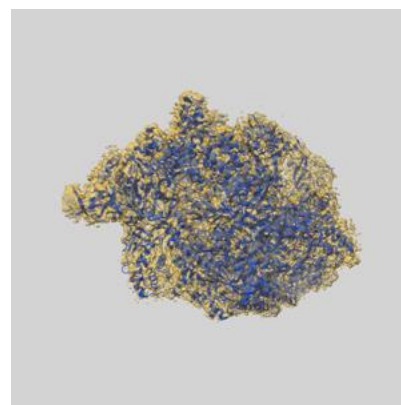
9.1 Map-model overlay [i](#)



X



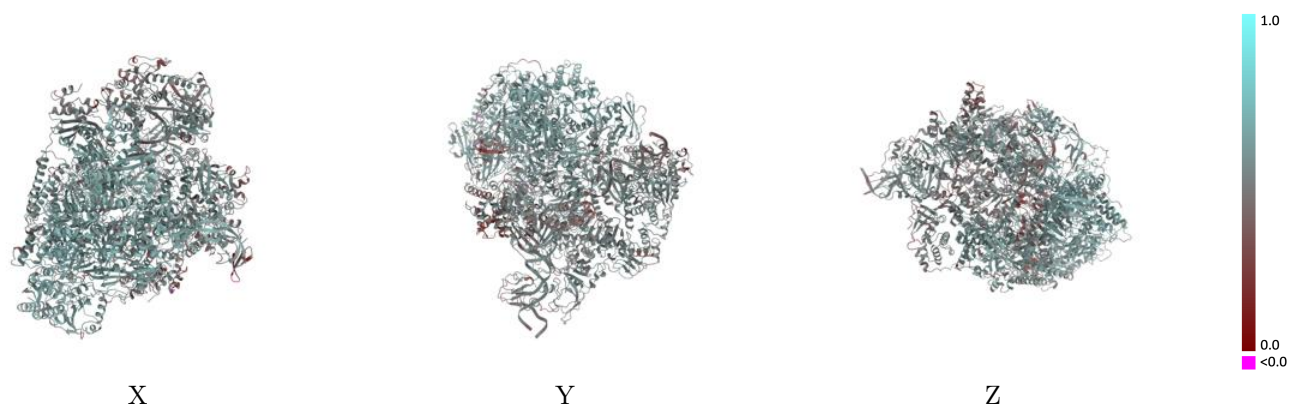
Y



Z

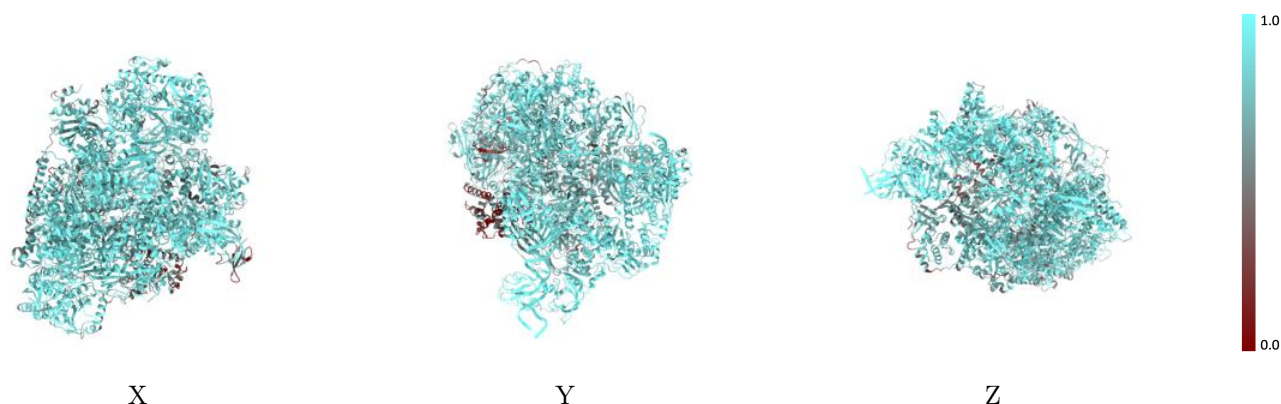
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



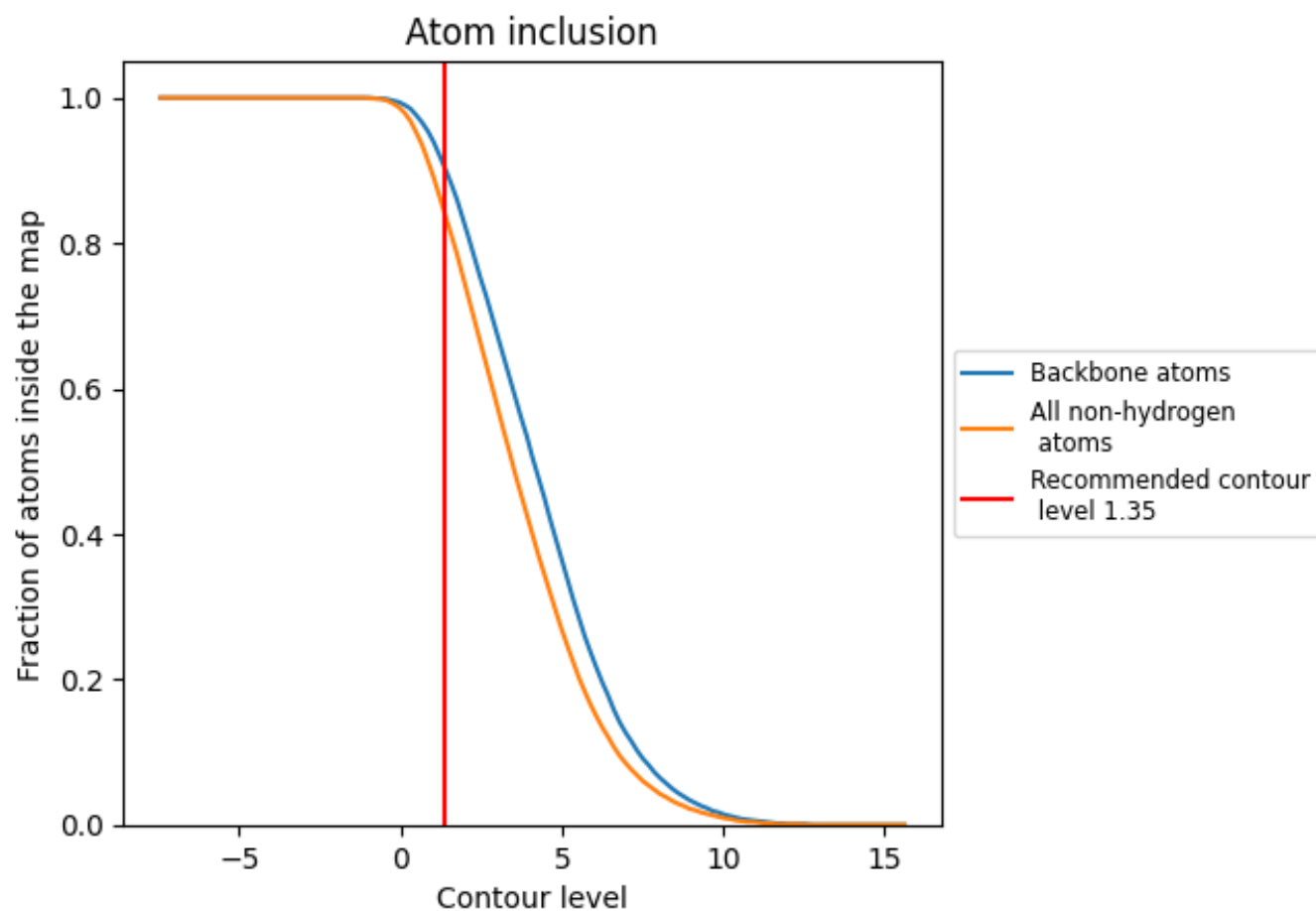
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.5370
A	 0.8560	 0.5830
B	 0.8380	 0.5700
C	 0.8880	 0.5760
E	 0.8890	 0.5920
F	 0.9170	 0.6040
G	 0.7600	 0.5260
I	 0.6500	 0.4760
J	 0.8960	 0.5890
K	 0.9290	 0.4920
N	 0.9540	 0.4680
S	 0.7530	 0.4960
T	 0.9730	 0.4970
W	 0.9070	 0.4910

