



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:17 AM UTC

PDB ID : 7AP9 / pdb_00007ap9
EMDB ID : EMD-11851
Title : Atomic structure of the poxvirus initially transcribing complex in conformation 3
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2020-10-16
Resolution : 3.01 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:

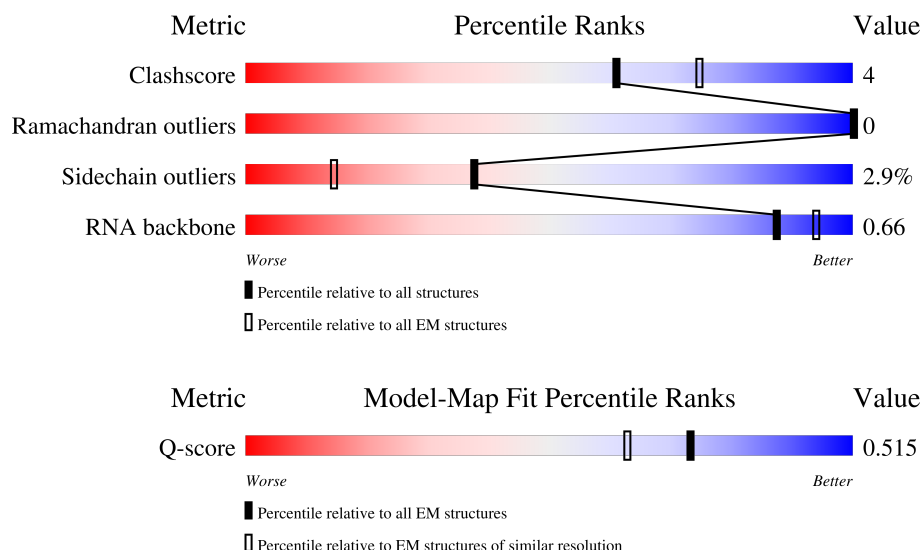
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.01 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13882 (2.51 - 3.51)

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	

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Mol	Chain	Length	Quality of chain
4	E	185	 90% 9%
5	F	164	 59% 37%
6	G	161	 79% 15% 5%
7	I	795	 49% 9% 42%
8	J	63	 78% 17%
9	P	5	 80% 20%
10	S	259	 36% 9% 55%
11	T	60	 10% 90%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 30881 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	1268	Total	C	N	O	S	0	0
			10188	6556	1679	1908	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1129	Total	C	N	O	S	0	0
			9091	5794	1554	1695	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	304	Total	C	N	O	S	0	0
			2484	1608	399	464	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	153	Total	C	N	O	S	0	0
			1192	753	198	235	6		

- Molecule 7 is a protein called Protein H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	464	Total	C	N	O	S	0	0
			3903	2552	627	710	14		

- 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 RNA chain called RNA (5'-R(P*AP*UP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	5	Total	C	N	O	P	0	0
			108	49	22	32	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	116	Total	C	N	O	S	0	0
			952	608	154	186	4		

- Molecule 11 is a DNA chain called Synthetic promoter DNA oligomer, template strand.

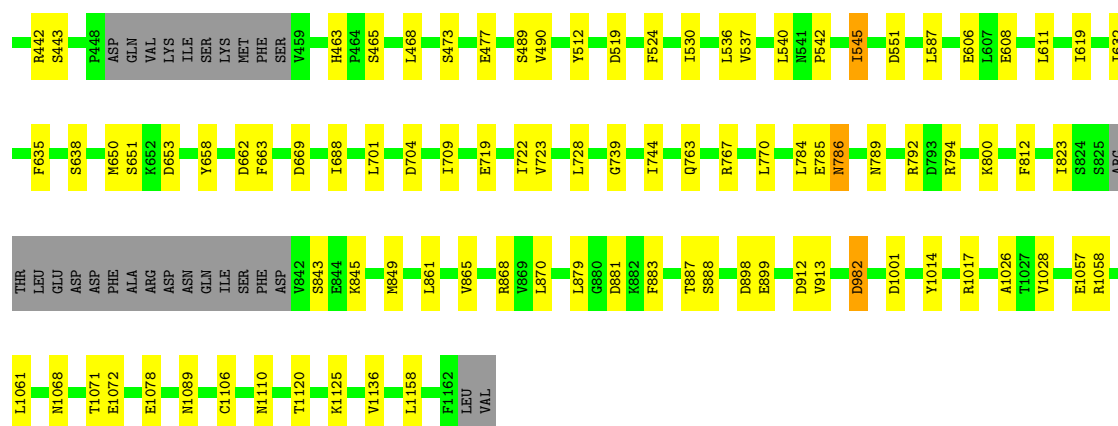
Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	6	Total	C	N	O	P	0	0
			124	60	21	37	6		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total 2	Zn 2	0
13	B	1	Total 1	Zn 1	0
13	I	1	Total 1	Zn 1	0



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

Chain C: 92% 8%



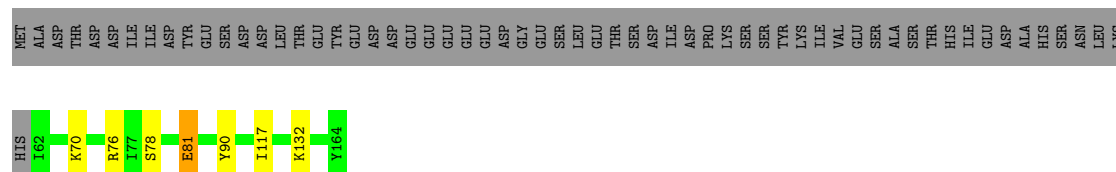
- Molecule 4: DNA-directed RNA polymerase subunit

Chain E: 90% 9%



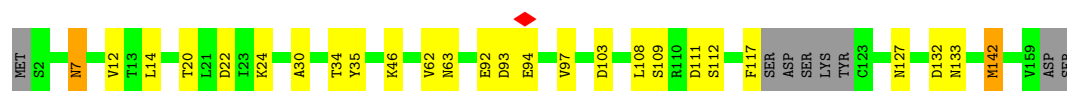
- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

Chain F: 59% 37%



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

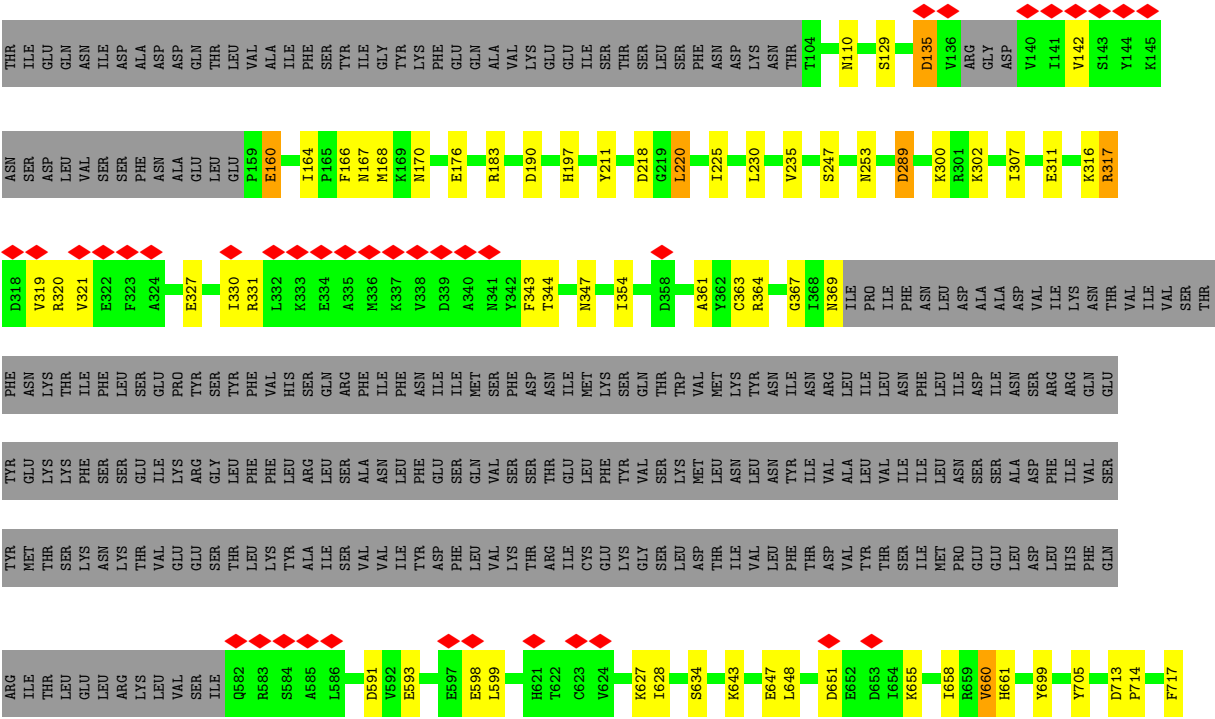
Chain G: 79% 15% 5%



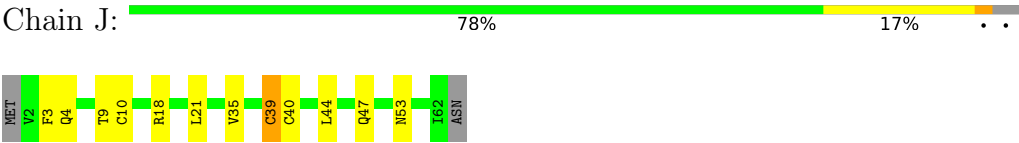
- Molecule 7: Protein H4

Chain I: 5% 49% 9% 42%

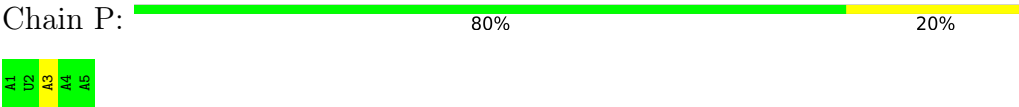




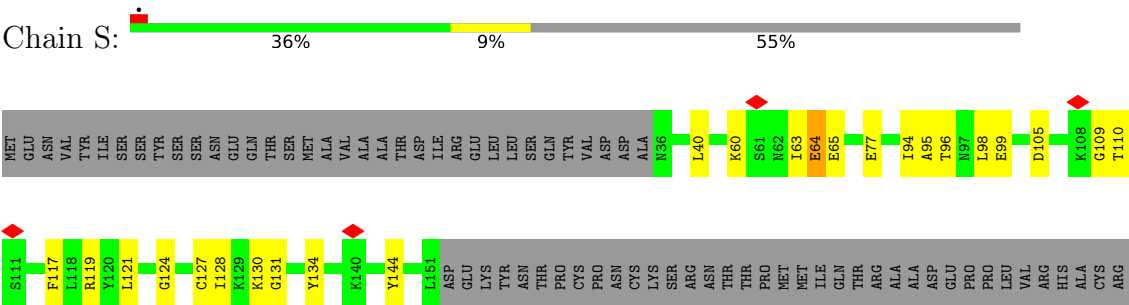
• Molecule 8: DNA-directed RNA polymerase 7 kDa subunit



• Molecule 9: RNA (5'-R(P*AP*UP*AP*AP*A)-3')



• Molecule 10: DNA-directed RNA polymerase 30 kDa polypeptide



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- Molecule 11: Synthetic promoter DNA oligomer, template strand

Chain T: 10% 90%

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96165	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	0.119	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	340.32, 340.32, 340.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	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, 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	0.40	0/10394	0.42	0/14052
2	B	0.41	0/9281	0.42	1/12537 (0.0%)
3	C	0.41	0/2540	0.41	0/3440
4	E	0.40	0/1522	0.41	0/2069
5	F	0.44	0/863	0.43	0/1158
6	G	0.32	0/1209	0.37	0/1639
7	I	0.27	0/4000	0.38	0/5411
8	J	0.44	0/494	0.46	0/663
9	P	0.17	0/121	0.31	0/186
10	S	0.25	0/967	0.44	0/1294
11	T	0.23	0/138	0.53	0/211
All	All	0.38	0/31529	0.41	1/42660 (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
7	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	VAL	N-CA-C	-5.94	106.70	111.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	I	660	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	10188	0	10312	108	0
2	B	9091	0	9146	92	0
3	C	2484	0	2470	15	0
4	E	1495	0	1548	9	0
5	F	849	0	874	5	0
6	G	1192	0	1181	14	0
7	I	3903	0	3905	47	0
8	J	490	0	530	6	0
9	P	108	0	55	1	0
10	S	952	0	957	16	0
11	T	124	0	70	0	0
12	A	1	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	1	0	0	0	0
All	All	30881	0	31048	273	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 4.

The worst 5 of 273 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)
7:I:735:ASN:ND2	7:I:747:VAL:O	2.16	0.79
2:B:477:GLU:N	2:B:477:GLU:OE1	2.17	0.78
7:I:627:LYS:NZ	7:I:628:ILE:O	2.18	0.77
2:B:303:THR:OG1	2:B:305:ASN:O	2.02	0.76
2:B:704:ASP:OD1	8:J:53:ASN:ND2	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1266/1286 (98%)	1189 (94%)	77 (6%)	0	100	100
2	B	1123/1164 (96%)	1047 (93%)	76 (7%)	0	100	100
3	C	302/305 (99%)	279 (92%)	23 (8%)	0	100	100
4	E	182/185 (98%)	169 (93%)	13 (7%)	0	100	100
5	F	101/164 (62%)	96 (95%)	5 (5%)	0	100	100
6	G	149/161 (92%)	138 (93%)	11 (7%)	0	100	100
7	I	456/795 (57%)	422 (92%)	34 (8%)	0	100	100
8	J	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
10	S	114/259 (44%)	97 (85%)	17 (15%)	0	100	100
All	All	3752/4382 (86%)	3492 (93%)	260 (7%)	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	1139/1157 (98%)	1104 (97%)	35 (3%)	35	67
2	B	1030/1064 (97%)	1002 (97%)	28 (3%)	39	70
3	C	286/287 (100%)	279 (98%)	7 (2%)	43	72
4	E	174/175 (99%)	173 (99%)	1 (1%)	78	87
5	F	94/151 (62%)	93 (99%)	1 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	136/144 (94%)	130 (96%)	6 (4%)	25	58
7	I	440/755 (58%)	425 (97%)	15 (3%)	32	64
8	J	60/62 (97%)	56 (93%)	4 (7%)	15	44
10	S	107/240 (45%)	103 (96%)	4 (4%)	30	63
All	All	3466/4035 (86%)	3365 (97%)	101 (3%)	38	68

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	879	LEU
5	F	81	GLU
10	S	98	LEU
2	B	1028	VAL
3	C	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	958	ASN
7	I	794	ASN
2	B	1020	HIS
10	S	62	ASN
7	I	621	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	P	4/5 (80%)	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 ⓘ

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

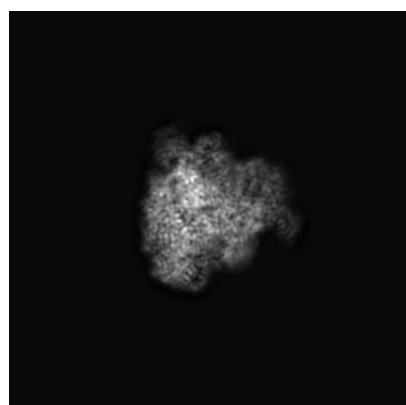
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11851. These allow visual inspection of the internal detail of the map and identification of artifacts.

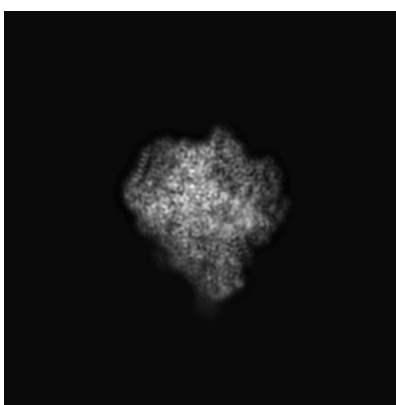
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

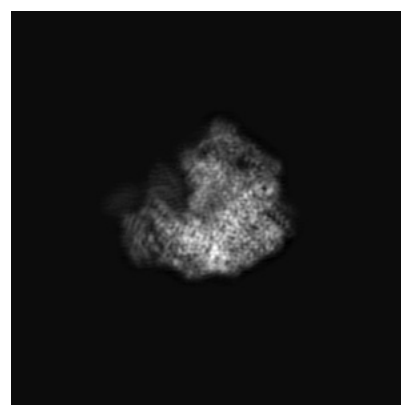
6.1.1 Primary map



X



Y

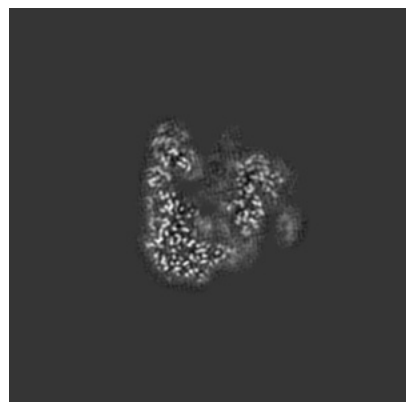


Z

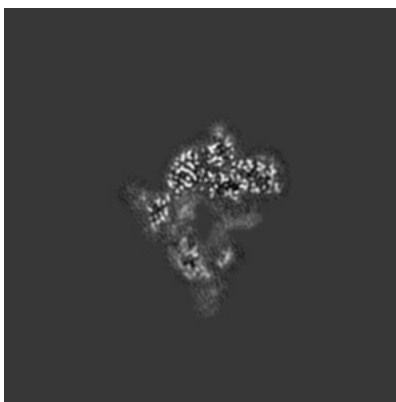
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

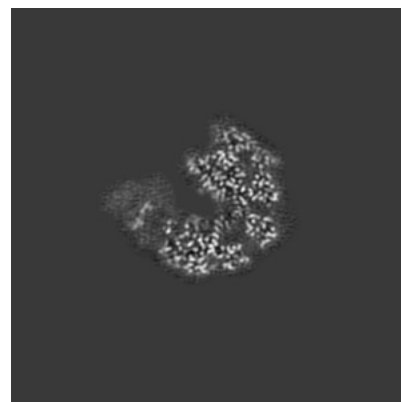
6.2.1 Primary map



X Index: 160



Y Index: 160

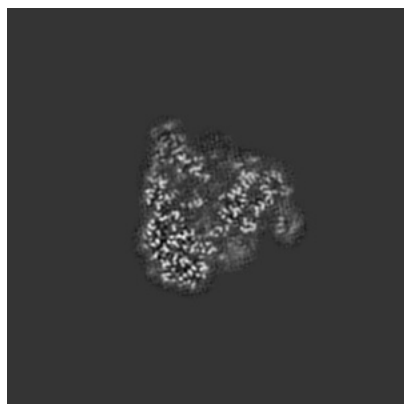


Z Index: 160

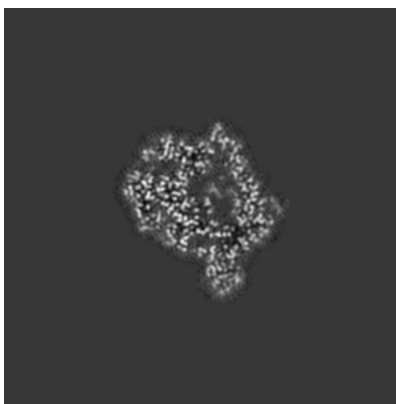
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

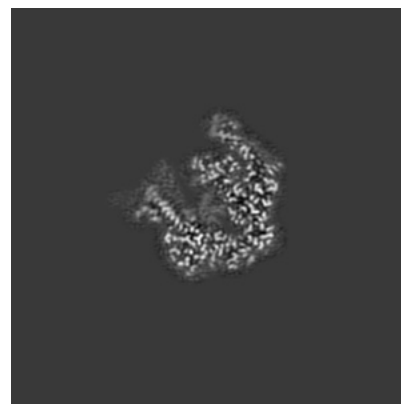
6.3.1 Primary map



X Index: 167



Y Index: 140

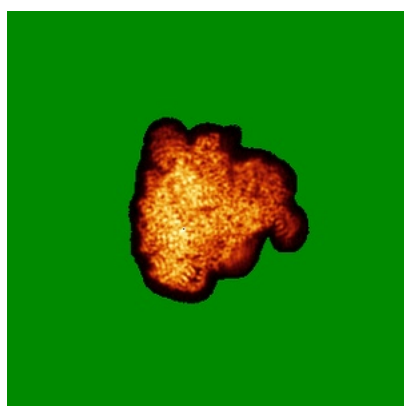


Z Index: 151

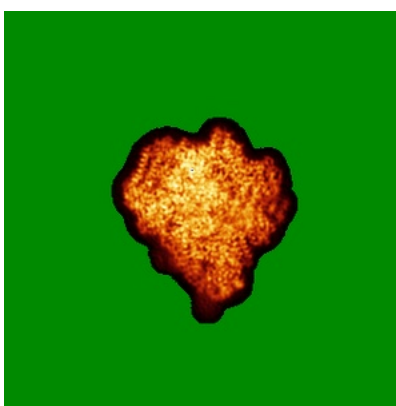
The images above show the largest variance slices of the map in three orthogonal directions.

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

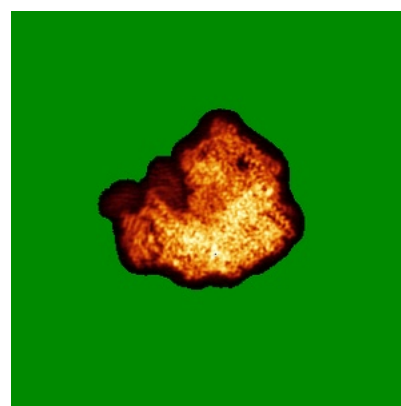
6.4.1 Primary map



X



Y

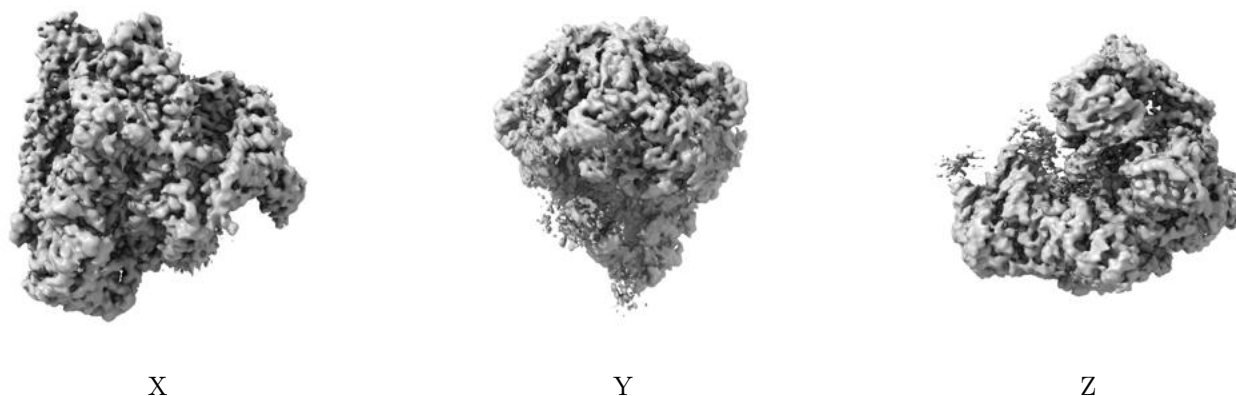


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

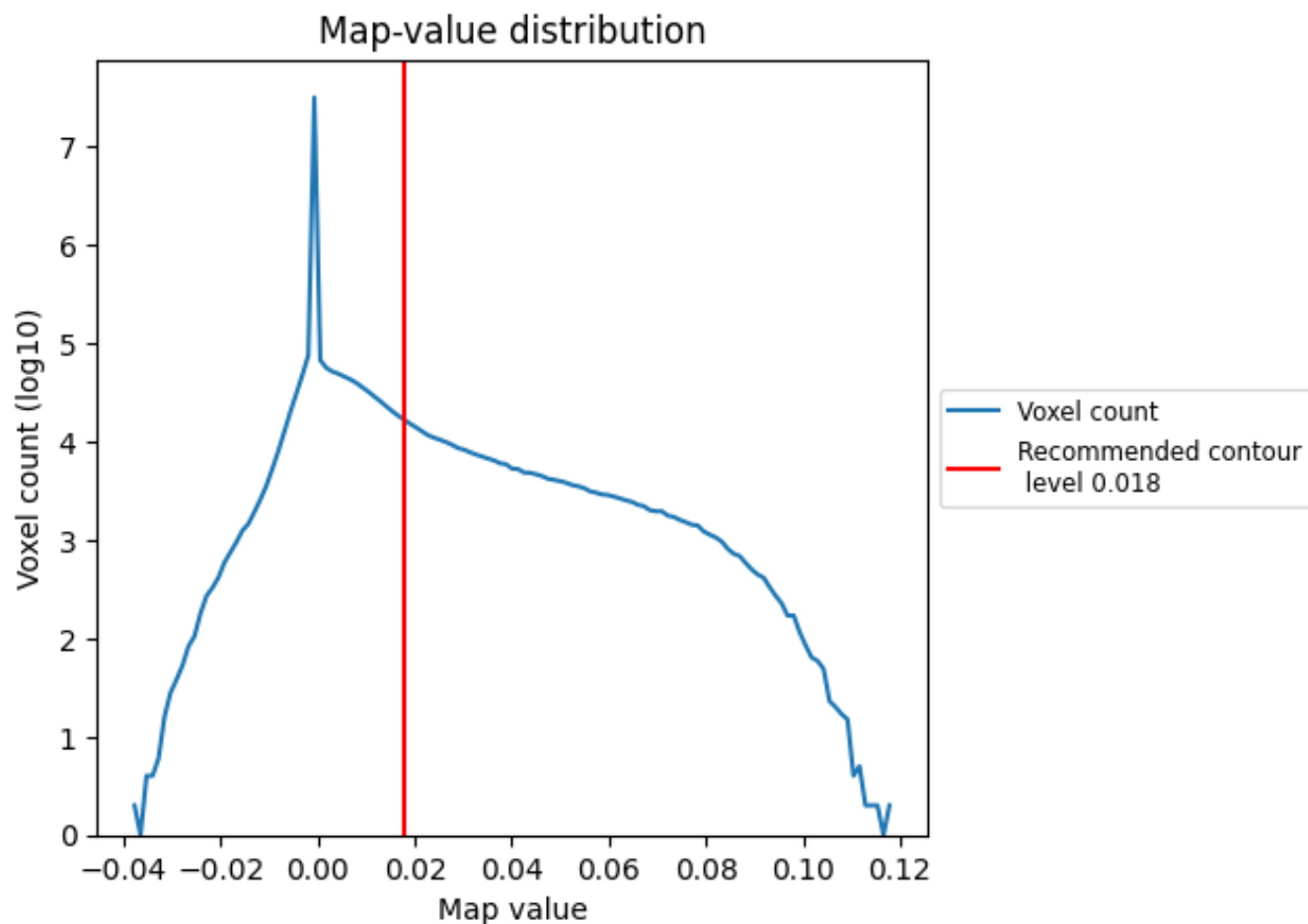
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

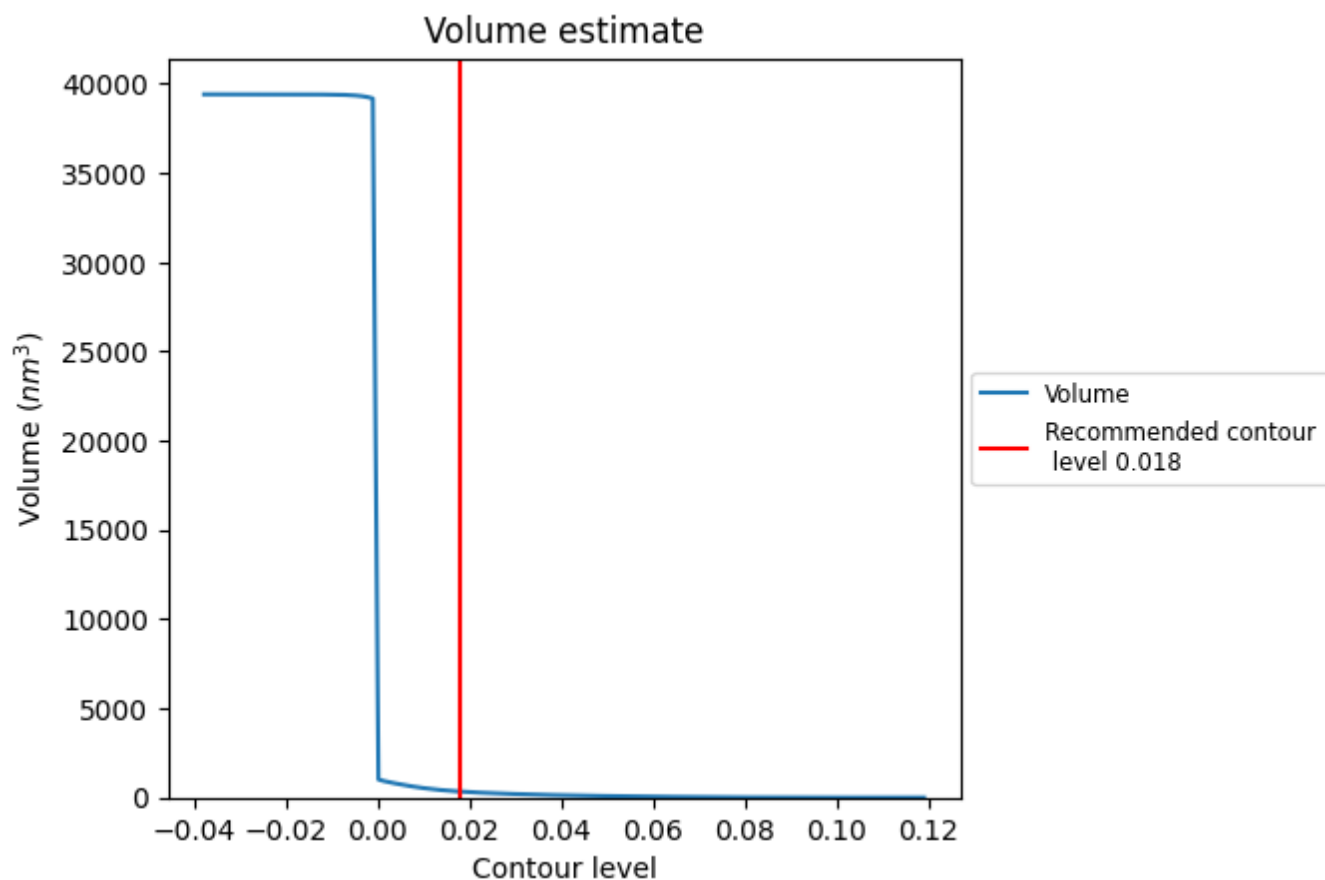
This section contains the results of statistical analysis of the map.

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.

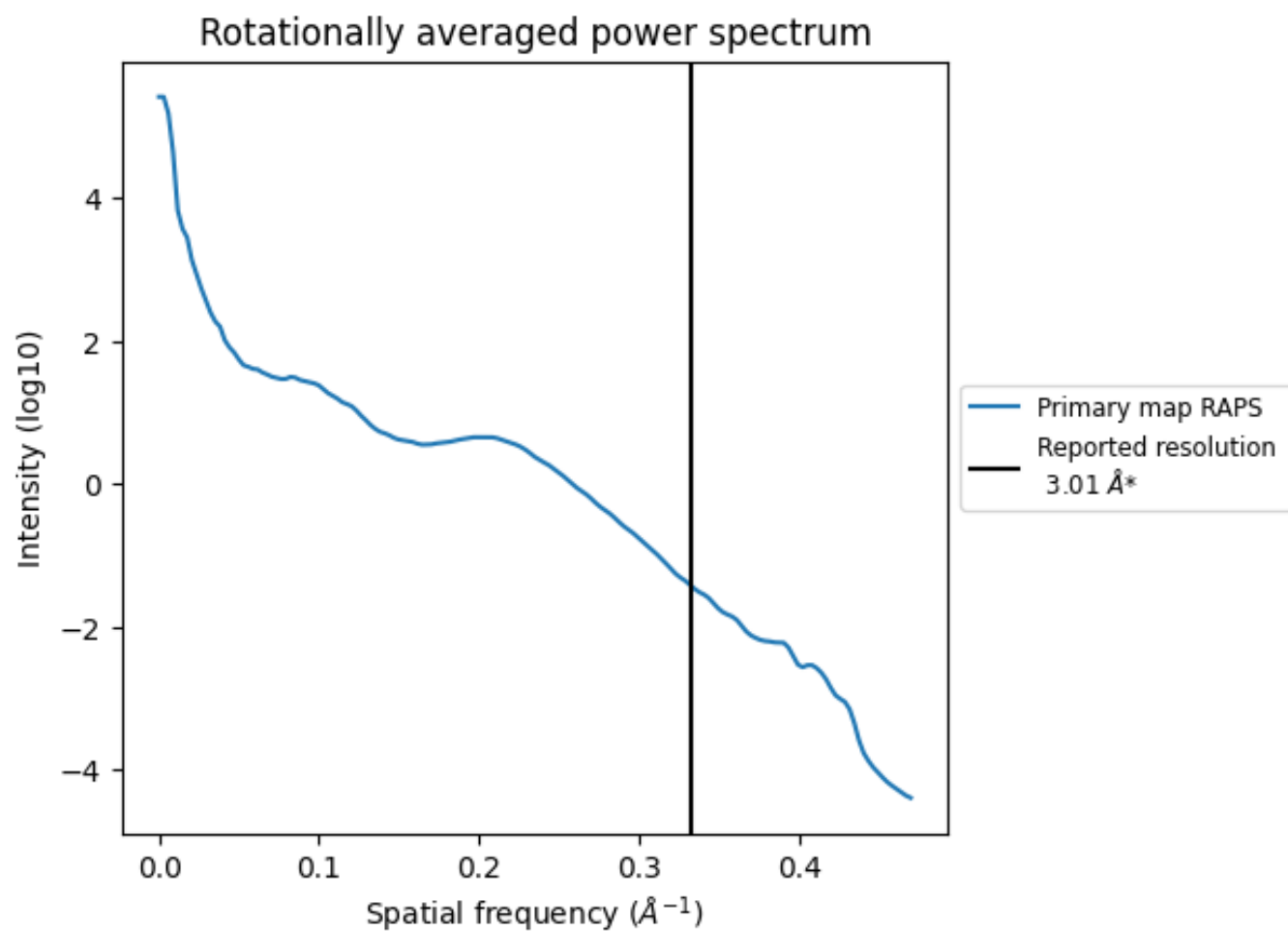
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 0.332 Å⁻¹

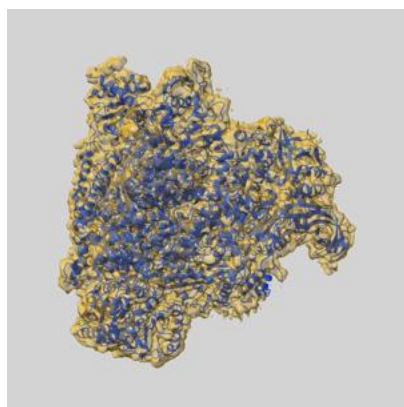
8 Fourier-Shell correlation

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

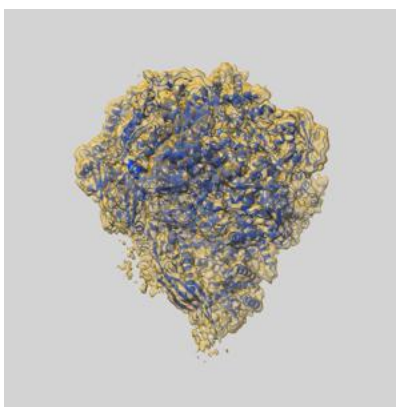
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11851 and PDB model 7AP9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

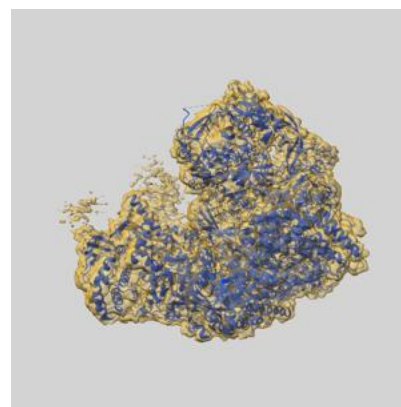
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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](#)

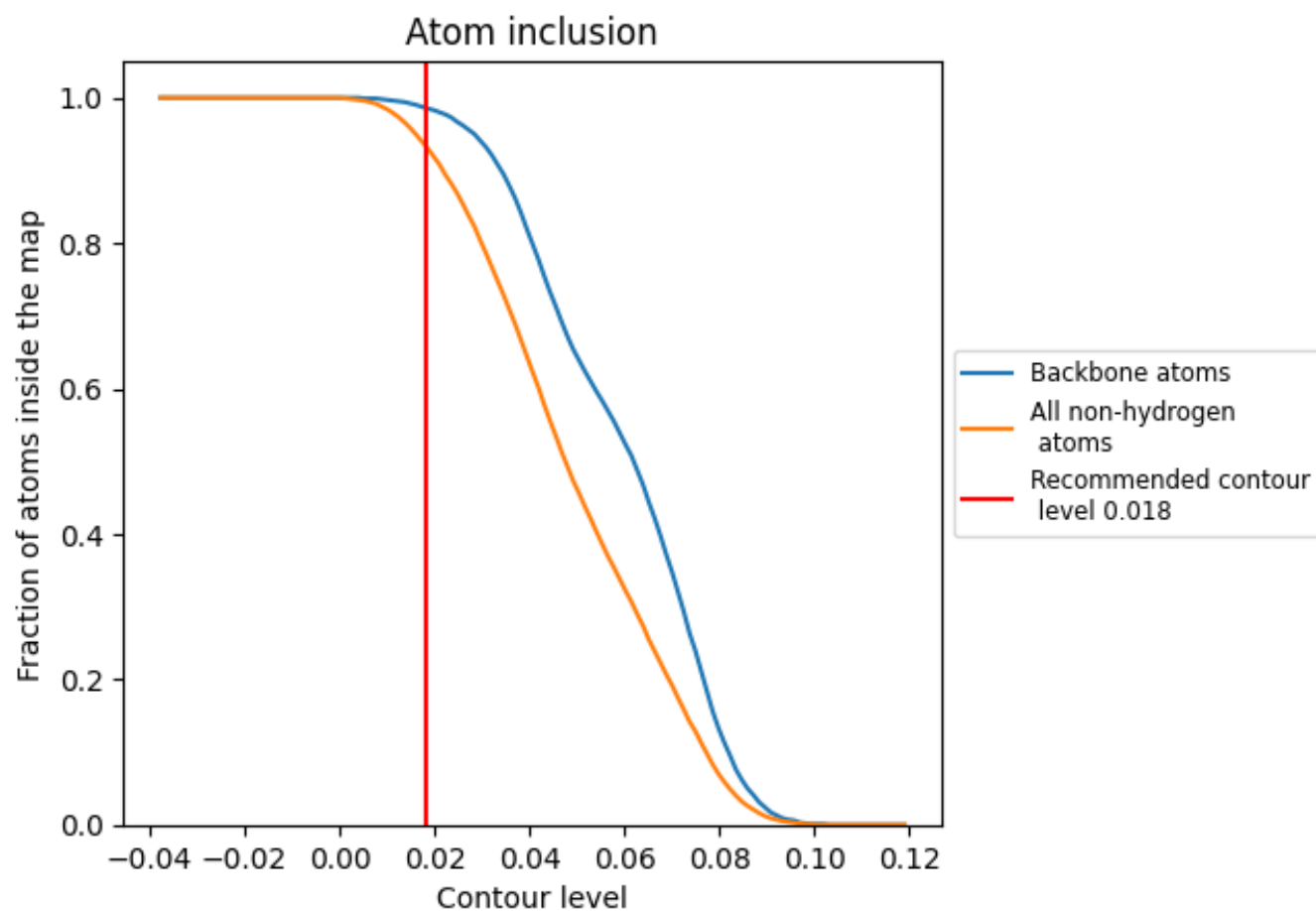


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.5150
A	 0.9480	 0.5240
B	 0.9580	 0.5300
C	 0.9670	 0.5340
E	 0.9680	 0.5450
F	 0.9740	 0.5510
G	 0.9270	 0.5080
I	 0.8360	 0.4490
J	 0.9790	 0.5420
P	 0.7590	 0.3120
S	 0.8230	 0.4460
T	 0.8550	 0.2920

