



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 12:44 AM UTC

PDB ID : 5MS0 / pdb_00005ms0
EMDB ID : EMD-3561
Title : pseudo-atomic model of the RNA polymerase lambda-based antitermination complex solved by cryo-EM
Authors : Said, N.; Krupp, F.
Deposited on : 2016-12-29
Resolution : 9.80 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:

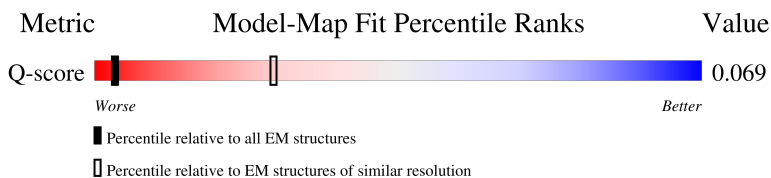
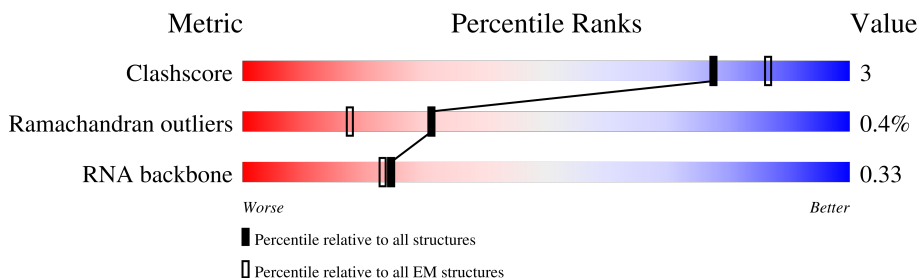
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 9.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
RNA backbone	8273	3508	-
Q-score	-	25397	157 (9.30 - 10.30)

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	N	85	20% (red), 85% (green), 14% (yellow), . (grey)
2	R	29	28% (red), 38% (green), 52% (yellow), 10% (orange)
3	A	329	8% (red), 67% (green), 5% (yellow), 29% (grey)
3	B	329	25% (red), 67% (green), 5% (yellow), 29% (grey)

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Mol	Chain	Length	Quality of chain
4	C	1342	
5	D	1416	
6	E	100	
7	F	183	
8	H	14	
9	I	27	
10	J	39	
11	L	139	
12	M	497	
13	O	91	

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 22698 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 Antitermination protein N.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	N	85	424	254	85	85	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	2	ALA	-	expression tag	UNP P03045
N	56	ALA	ASP	conflict	UNP P03045
N	57	ASP	LEU	conflict	UNP P03045
N	58	LEU	THR	conflict	UNP P03045
N	59	THR	VAL	conflict	UNP P03045
N	60	VAL	LEU	conflict	UNP P03045

- Molecule 2 is a RNA chain called nascent RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	R	29	623	279	117	198	29	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	A	235	1159	689	235	235	0	0
3	B	235	1159	689	235	235	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	1291	6355	3773	1291	1291	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	conflict	UNP P0A8V2

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
5	D	1364	6709	3981	1364	1364	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	VAL	-	expression tag	UNP P0A8T7
D	1411	HIS	-	expression tag	UNP P0A8T7
D	1412	HIS	-	expression tag	UNP P0A8T7
D	1413	HIS	-	expression tag	UNP P0A8T7
D	1414	HIS	-	expression tag	UNP P0A8T7
D	1415	HIS	-	expression tag	UNP P0A8T7
D	1416	HIS	-	expression tag	UNP P0A8T7

- Molecule 6 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
6	E	100	496	296	100	100	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	46	SER	LYS	conflict	UNP P0A7R5

- Molecule 7 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
7	F	181	891	529	181	181	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P0AFG0
F	0	ALA	-	expression tag	UNP P0AFG0

- Molecule 8 is a RNA chain called RNA transcription bubble.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	14	301	135	59	93	14	0	0

- Molecule 9 is a DNA chain called DNAI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	I	27	552	266	103	158	25	0	0

- Molecule 10 is a DNA chain called DNAII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	J	39	792	380	142	232	38	0	0

- Molecule 11 is a protein called Transcription antitermination protein NusB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	L	139	690	412	139	139	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	GLU	LYS	conflict	UNP P0A780

- Molecule 12 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	M	425	2104	1254	425	425	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLY	-	expression tag	UNP P0AFF6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ALA	-	expression tag	UNP P0AFF6
M	462	GLN	GLU	conflict	UNP P0AFF6

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

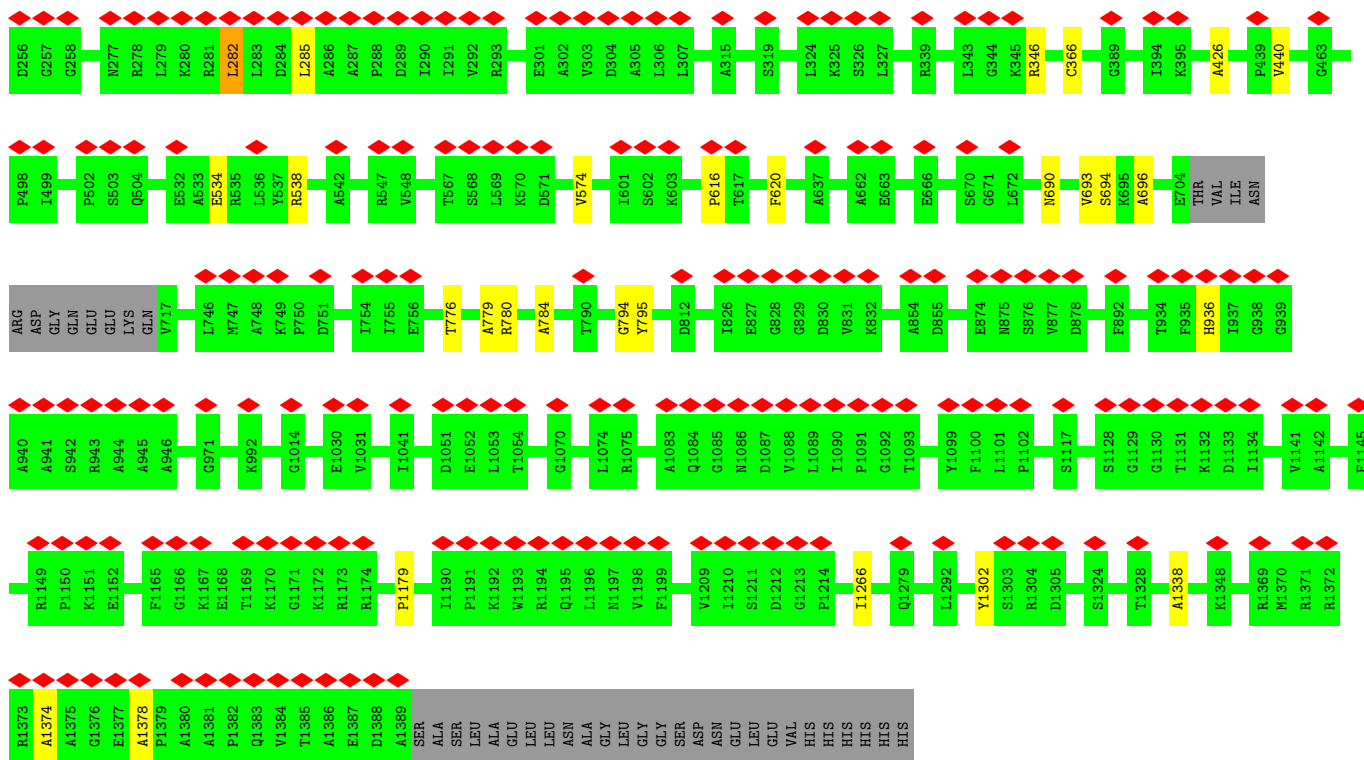
Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	89	Total	C	N	O	0	0
			440	262	89	89		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

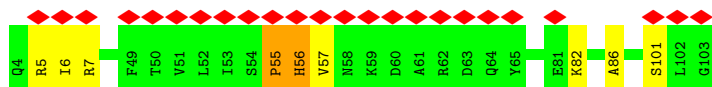
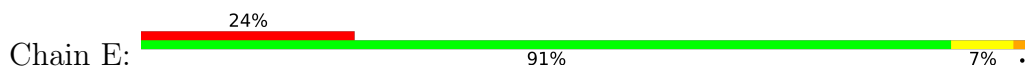
Mol	Chain	Residues	Atoms		AltConf
14	D	1	Total	Mg	0
			1	1	

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

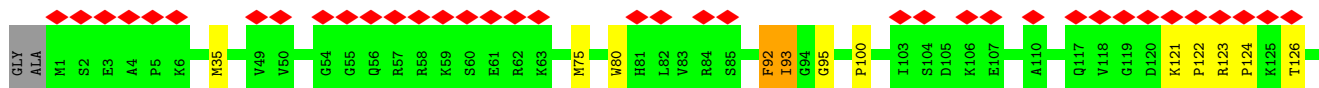
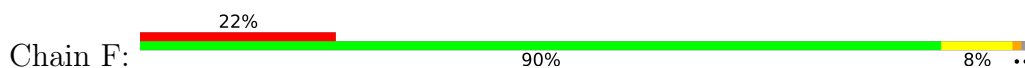
Mol	Chain	Residues	Atoms		AltConf
15	D	2	Total	Zn	0
			2	2	



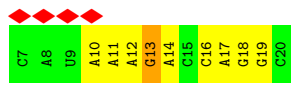
• Molecule 6: 30S ribosomal protein S10



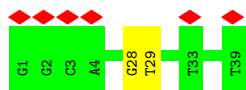
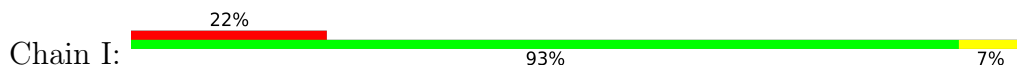
• Molecule 7: Transcription termination/antitermination protein NusG



• Molecule 8: RNA transcription bubble



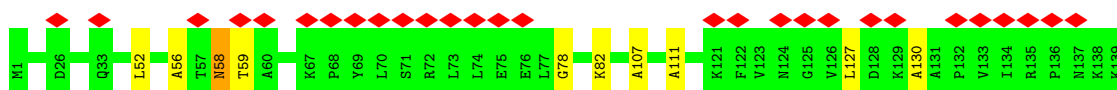
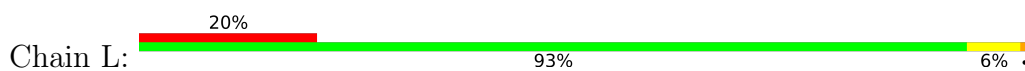
• Molecule 9: DNAI



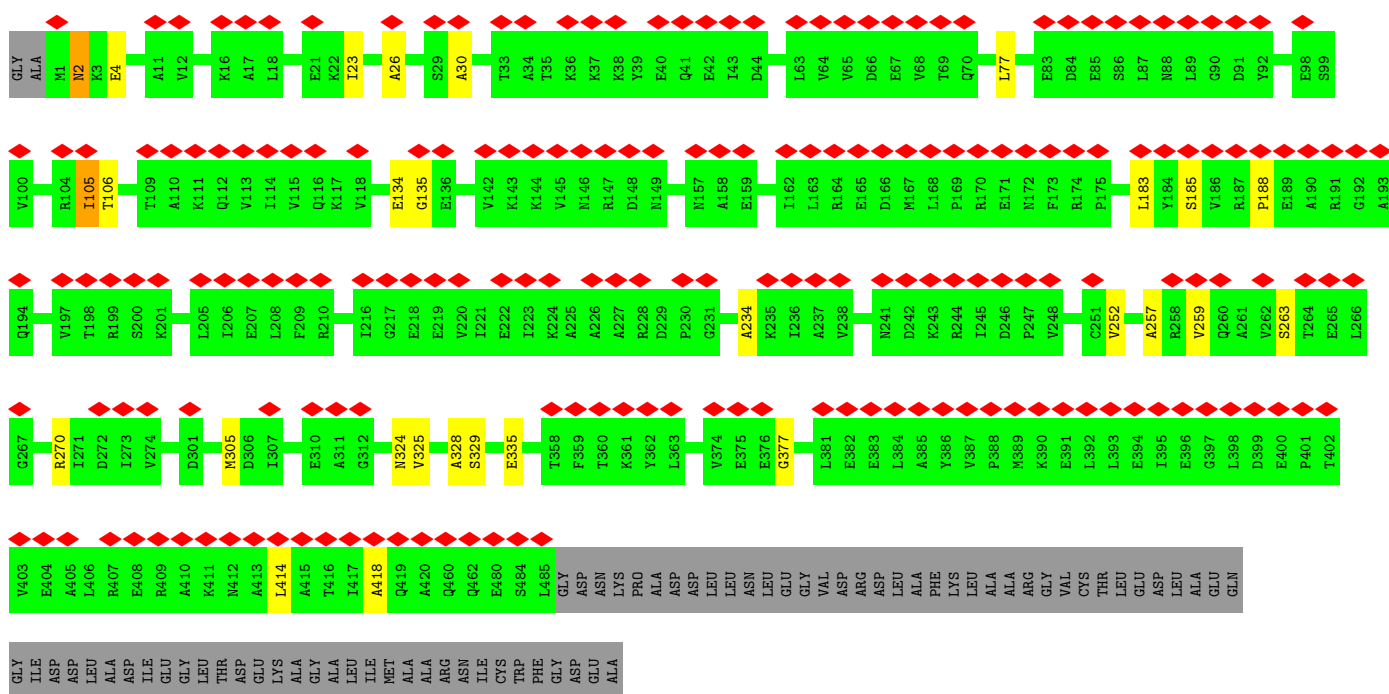
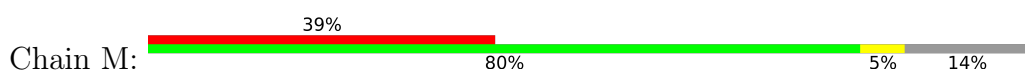
• Molecule 10: DNAII



• Molecule 11: Transcription antitermination protein NusB

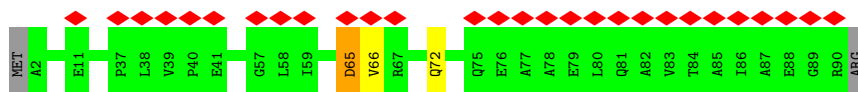


• Molecule 12: Transcription termination/antitermination protein NusA



• Molecule 13: DNA-directed RNA polymerase subunit omega





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	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	0.028	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.28, 1.28, 1.28	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	N	0.39	0/422	1.16	4/587 (0.7%)
2	R	0.20	0/698	0.82	5/1084 (0.5%)
3	A	0.30	0/1153	0.78	4/1595 (0.3%)
3	B	0.30	0/1153	0.77	4/1595 (0.3%)
4	C	0.27	1/6348 (0.0%)	0.70	9/8816 (0.1%)
5	D	0.28	0/6701	0.74	25/9302 (0.3%)
6	E	0.33	0/495	0.89	2/689 (0.3%)
7	F	1.76	3/890 (0.3%)	1.60	18/1236 (1.5%)
8	H	0.17	0/337	0.39	0/523
9	I	0.22	0/619	0.50	0/953
10	J	0.31	0/887	0.62	1/1366 (0.1%)
11	L	0.29	0/689	0.88	3/960 (0.3%)
12	M	0.34	0/2103	0.96	9/2930 (0.3%)
13	O	0.40	0/438	1.08	3/607 (0.5%)
All	All	0.45	4/22933 (0.0%)	0.82	87/32243 (0.3%)

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	N	0	2
3	A	0	2
3	B	0	2
4	C	0	6
5	D	0	6
6	E	0	3
7	F	0	2
11	L	0	1
12	M	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	92	PHE	C-N	40.46	1.73	1.33
7	F	93	ILE	N-CA	30.52	1.79	1.46
7	F	123	ARG	C-N	6.45	1.49	1.33
4	C	1043	ALA	C-N	5.67	1.41	1.34

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	92	PHE	CA-C-N	25.41	164.58	121.63
7	F	92	PHE	C-N-CA	25.41	164.58	121.63
7	F	92	PHE	CA-C-O	-17.38	101.86	120.46
2	R	11	U	OP1-P-O3'	-11.90	72.28	108.00
2	R	11	U	OP2-P-O3'	-10.53	76.41	108.00

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	158	ARG	Peptide
3	A	19	VAL	Peptide
3	B	19	VAL	Peptide
1	N	42	ARG	Peptide
1	N	82	TRP	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	N	424	0	194	7	0
2	R	623	0	314	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1159	0	525	6	0
3	B	1159	0	525	6	0
4	C	6355	0	2858	15	0
5	D	6709	0	3134	24	0
6	E	496	0	225	3	0
7	F	891	0	393	6	0
8	H	301	0	154	7	0
9	I	552	0	309	1	0
10	J	792	0	442	11	0
11	L	690	0	334	5	0
12	M	2104	0	1001	13	0
13	O	440	0	212	0	0
14	D	1	0	0	0	0
15	D	2	0	0	0	0
All	All	22698	0	10620	97	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 97 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:F:92:PHE:C	7:F:93:ILE:N	1.73	1.44
7:F:93:ILE:N	7:F:93:ILE:CA	1.79	1.44
3:B:169:GLY:C	3:B:170:ARG:N	2.08	1.12
3:A:169:GLY:C	3:A:170:ARG:N	2.08	1.11
3:B:187:VAL:C	3:B:188:GLU:N	2.09	1.10

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	N	82/85 (96%)	68 (83%)	11 (13%)	3 (4%)	2	20
3	A	224/329 (68%)	192 (86%)	31 (14%)	1 (0%)	30	67
3	B	224/329 (68%)	192 (86%)	31 (14%)	1 (0%)	30	67
4	C	1277/1342 (95%)	1132 (89%)	142 (11%)	3 (0%)	43	78
5	D	1348/1416 (95%)	1218 (90%)	125 (9%)	5 (0%)	30	67
6	E	98/100 (98%)	89 (91%)	7 (7%)	2 (2%)	6	31
7	F	179/183 (98%)	160 (89%)	18 (10%)	1 (1%)	21	59
11	L	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
12	M	423/497 (85%)	370 (88%)	52 (12%)	1 (0%)	43	78
13	O	85/91 (93%)	70 (82%)	14 (16%)	1 (1%)	10	44
All	All	4077/4511 (90%)	3615 (89%)	444 (11%)	18 (0%)	31	67

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	33	VAL
4	C	1048	LYS
5	D	148	GLU
5	D	170	GLU
5	D	171	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	29/29 (100%)	15 (51%)	4 (13%)
8	H	13/14 (92%)	2 (15%)	1 (7%)
All	All	42/43 (97%)	17 (40%)	5 (11%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	8	U
2	R	11	U
2	R	12	U

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Mol	Chain	Res	Type
2	R	13	A
2	R	14	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	7	A
2	R	10	U
2	R	11	U
2	R	34	G
8	H	12	A

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 3 ligands modelled in this entry, 3 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	D	6
3	A	5
3	B	5
4	C	3
13	O	1
1	N	1
7	F	1

The worst 5 of 22 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	146:VAL	C	147:ILE	N	9.08
1	O	76:GLU	C	77:ALA	N	9.08
1	D	175:GLU	C	176:PHE	N	8.86
1	C	1170:MET	C	1171:ARG	N	7.38
1	D	191:SER	C	192:MET	N	5.59

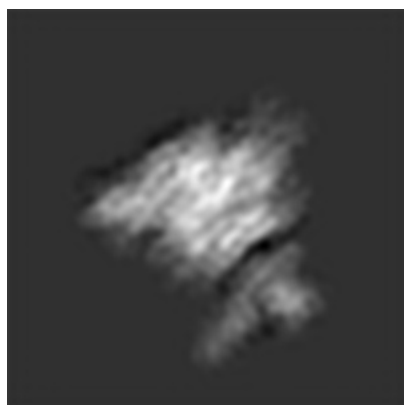
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3561. These allow visual inspection of the internal detail of the map and identification of artifacts.

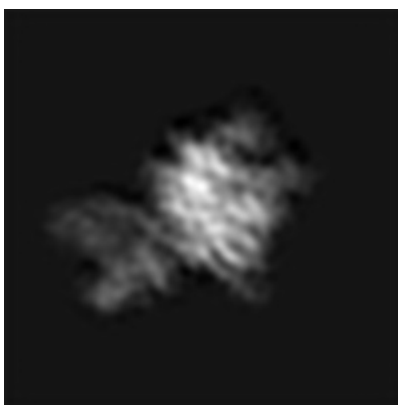
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

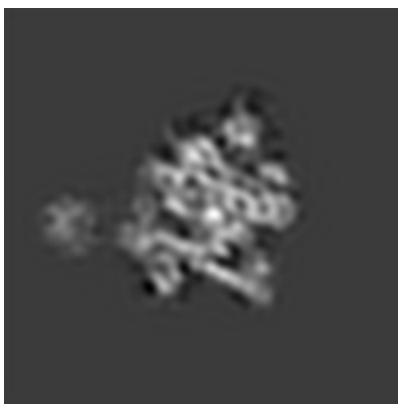
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

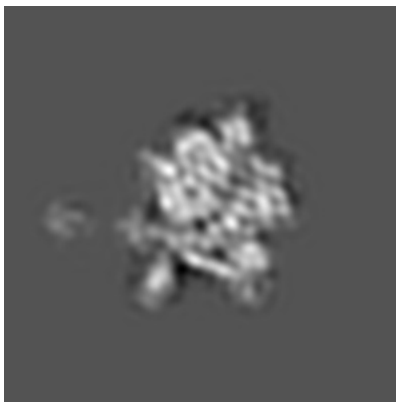
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

6.3.1 Primary map



X Index: 117



Y Index: 113



Z Index: 127

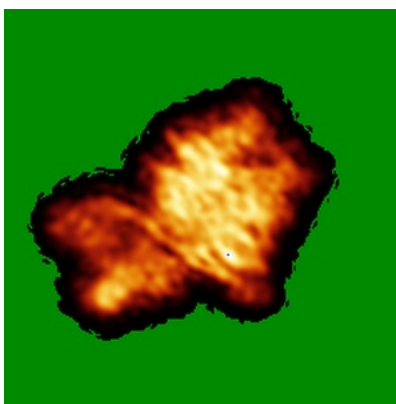
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

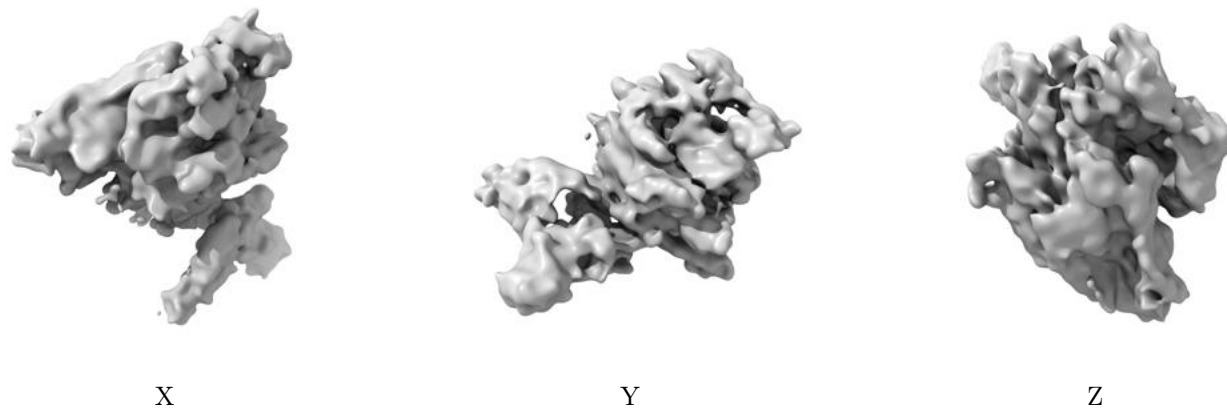


Z

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

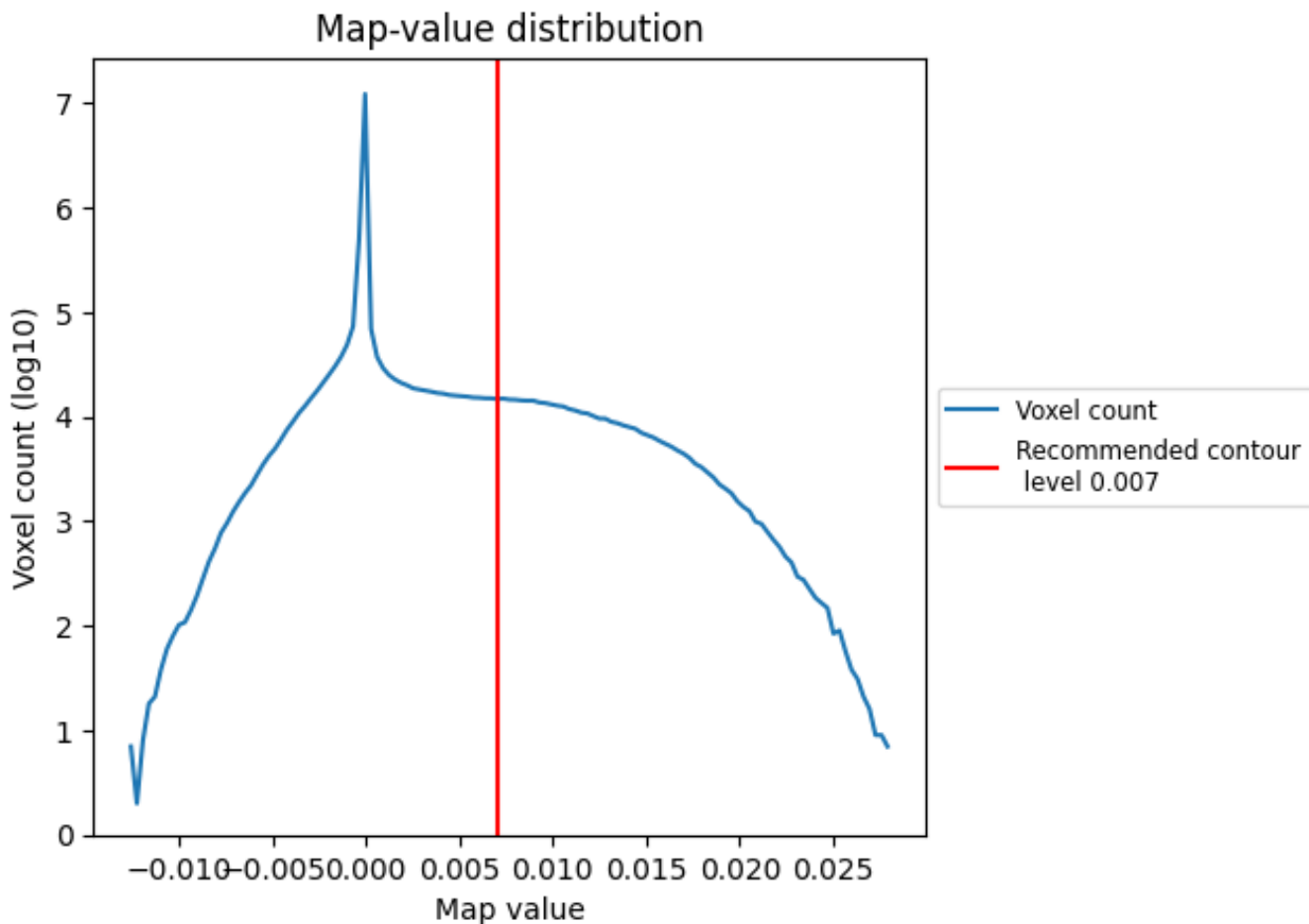
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

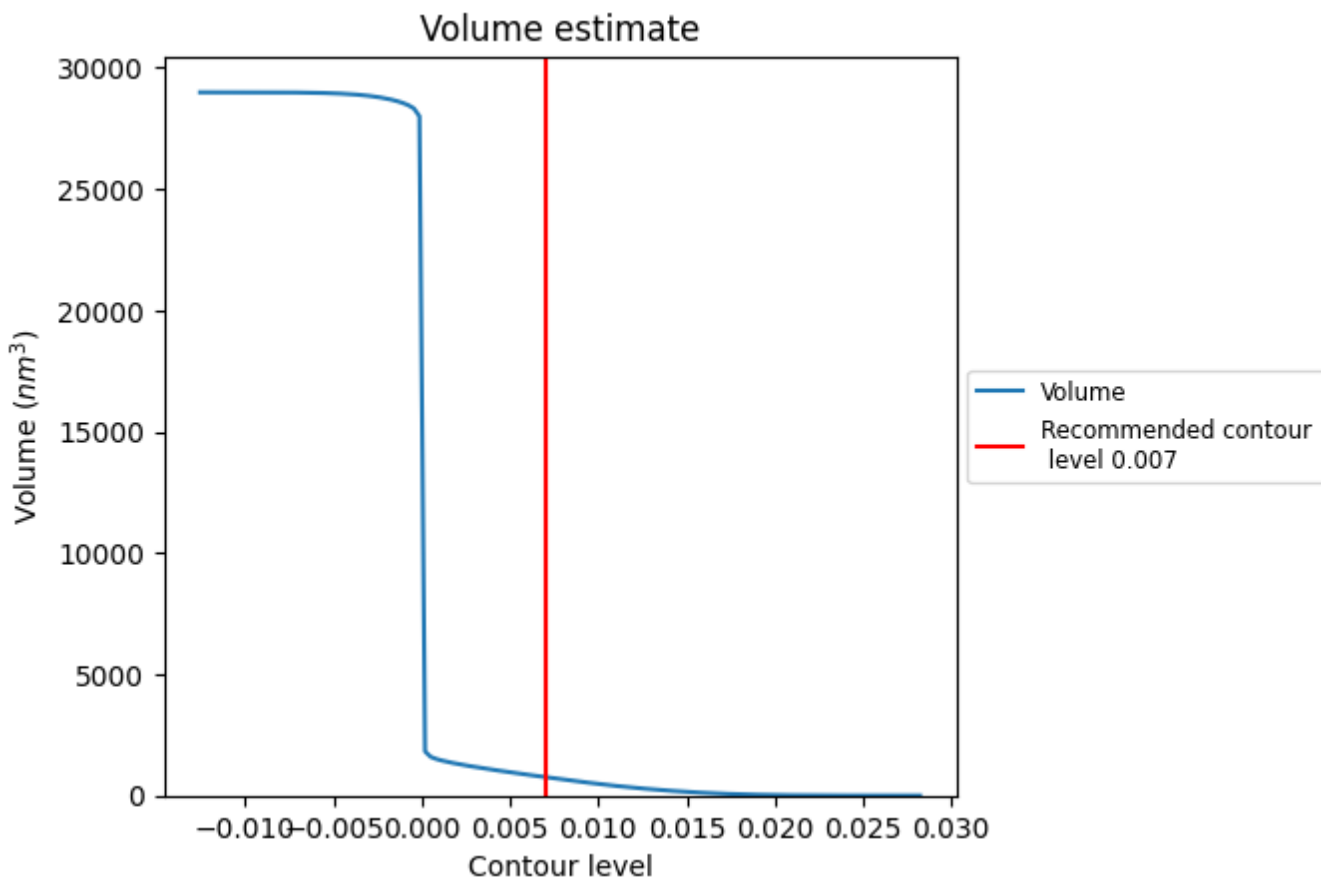
This section contains the results of statistical analysis of the map.

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.

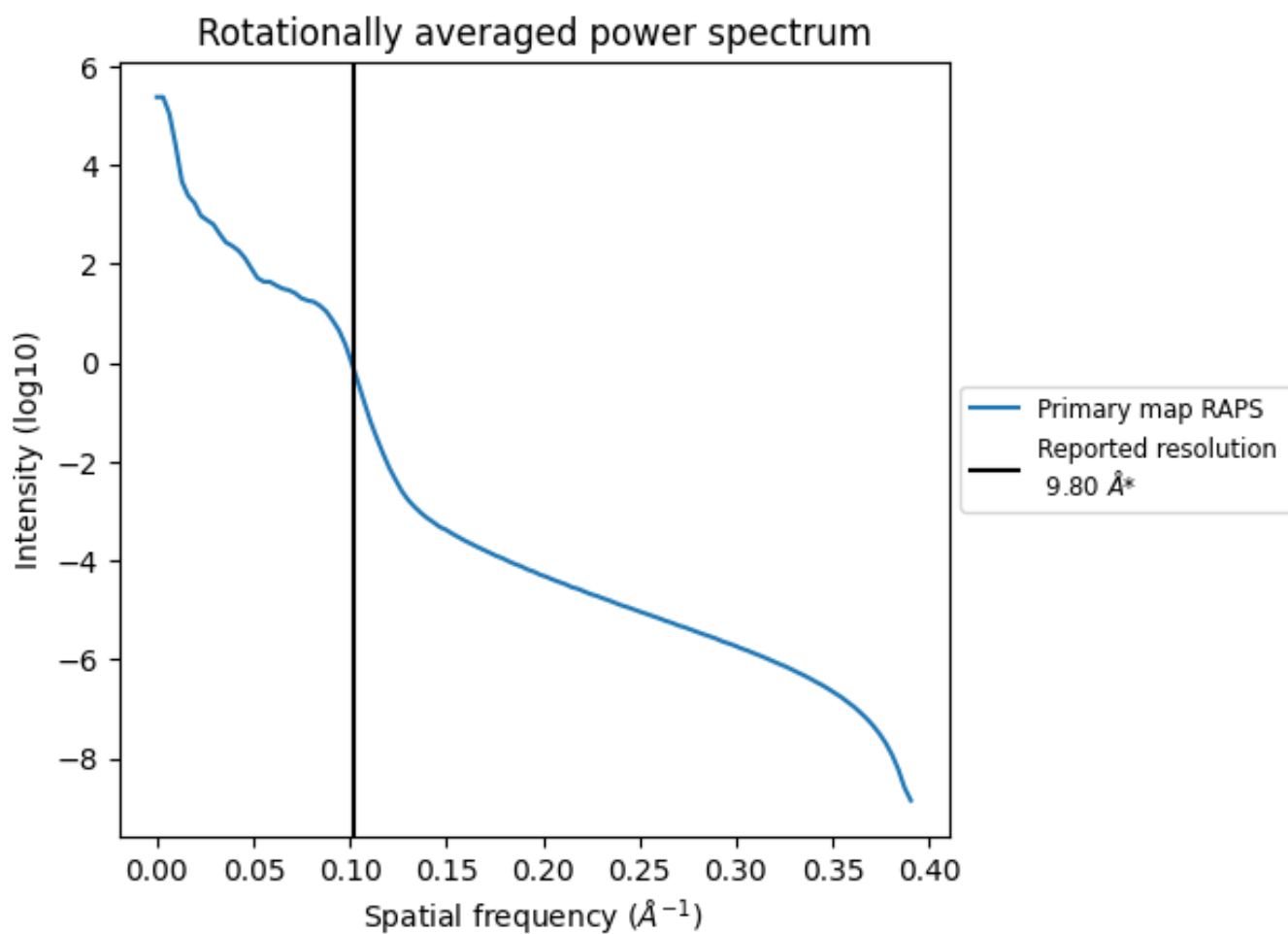
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 762 nm³; this corresponds to an approximate mass of 688 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 0.102 Å⁻¹

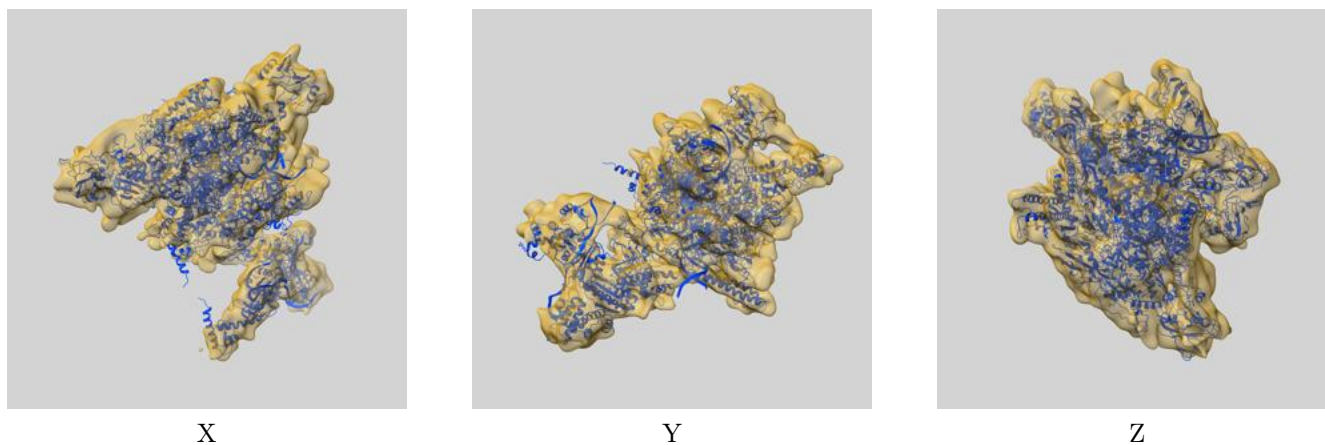
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

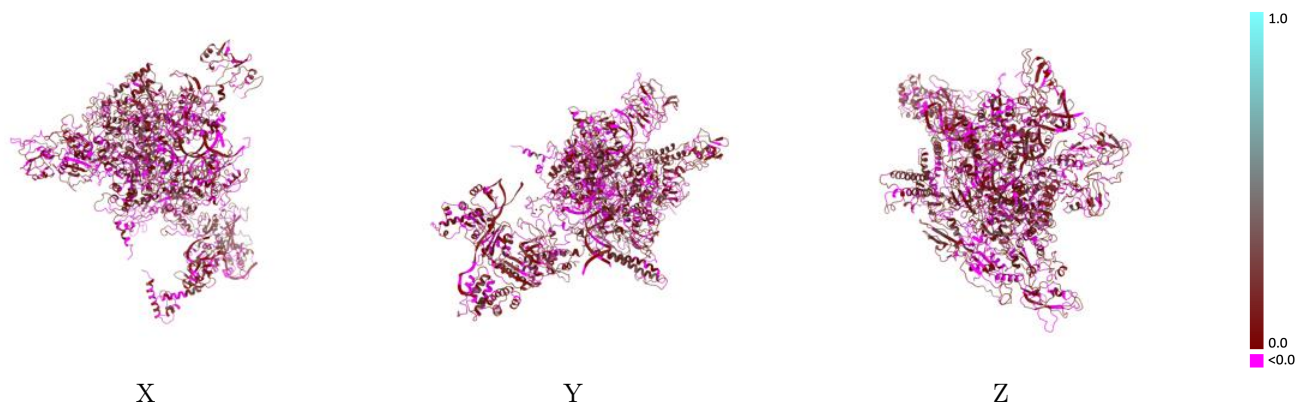
This section contains information regarding the fit between EMDB map EMD-3561 and PDB model 5MS0. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



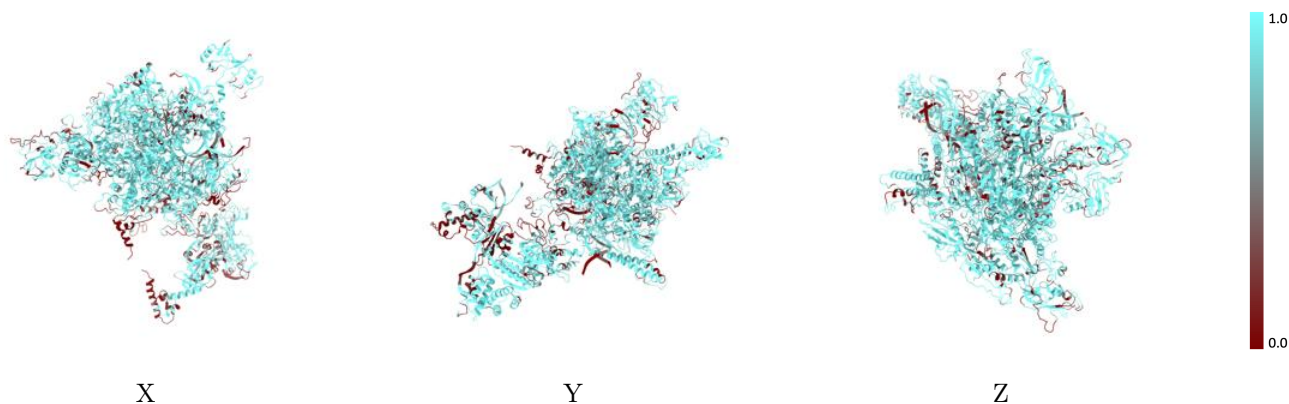
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



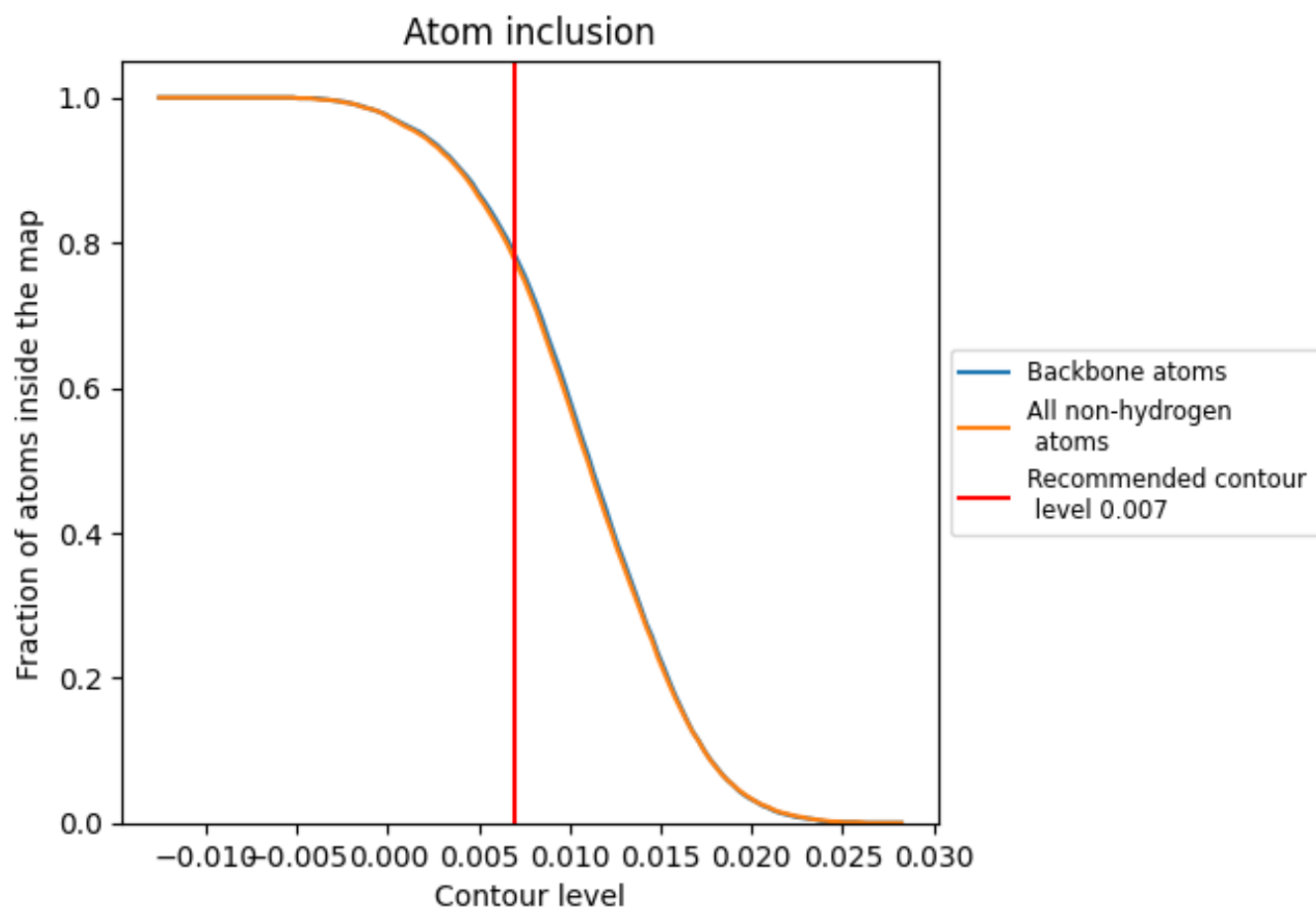
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.0690
A	 0.8790	 0.0750
B	 0.6620	 0.0140
C	 0.8570	 0.0880
D	 0.8000	 0.0610
E	 0.7480	 0.0930
F	 0.7590	 0.0390
H	 0.6740	 0.0320
I	 0.6300	 0.0400
J	 0.8130	 0.0850
L	 0.7970	 0.0700
M	 0.5430	 0.0700
N	 0.7830	 0.1130
O	 0.6840	 0.0420
R	 0.6740	 0.0830

