



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 10:30 am BST

PDB ID : 7PY6
EMDB ID : EMD-13714
Title : CryoEM structure of E.coli RNA polymerase elongation complex bound to NusA and NusG (NusA and NusG elongation complex in less-swiveled conformation)
Authors : Zhu, C.; Guo, X.; Weixlbaumer, A.
Deposited on : 2021-10-09
Resolution : 4.10 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

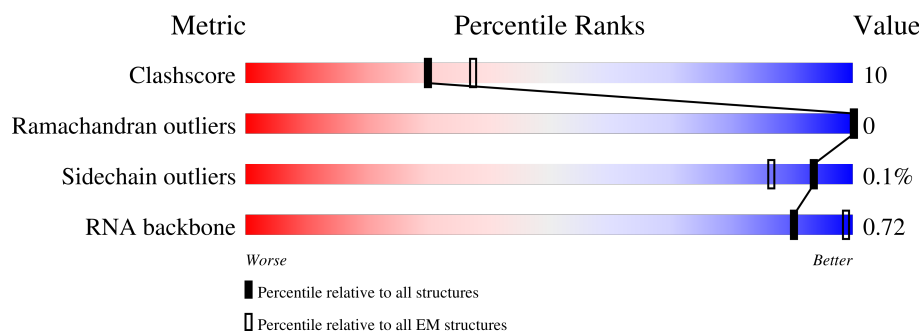
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



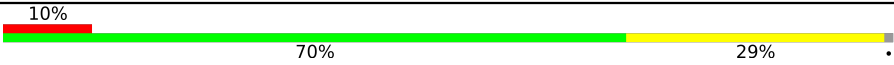

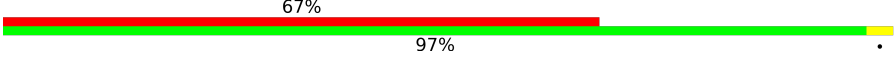
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	39	
2	T	39	
3	R	14	
4	A	329	
4	B	329	
5	C	1342	
6	D	1407	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	E	91	
8	G	181	
9	F	495	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 29959 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 DNA chain called ntDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	26	Total	C	N	O	P	0	0
			535	254	100	155	26		

- Molecule 2 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	30	Total	C	N	O	P	0	0
			611	289	110	182	30		

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	11	Total	C	N	O	P	0	0
			235	104	42	78	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	228	Total	C	N	O	S	0	0
			1768	1102	312	348	6		
4	B	220	Total	C	N	O	S	0	0
			1699	1061	299	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1341	Total	C	N	O	S	0	0
			10577	6636	1842	2056	43		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1335	Total	C	N	O	S	0	0
			10388	6526	1854	1958	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 8 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	123	Total	C	N	O	S	0	0
			987	622	182	176	7		

- Molecule 9 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	495	Total	C	N	O	S	0	0
			2447	1457	495	495			

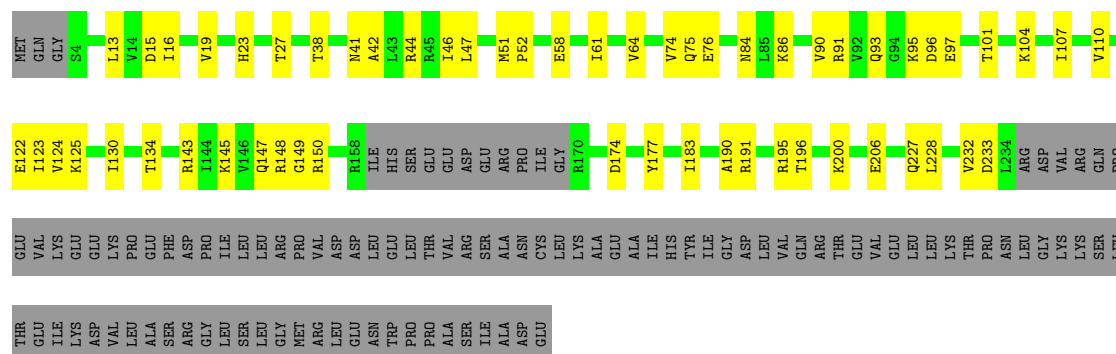
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

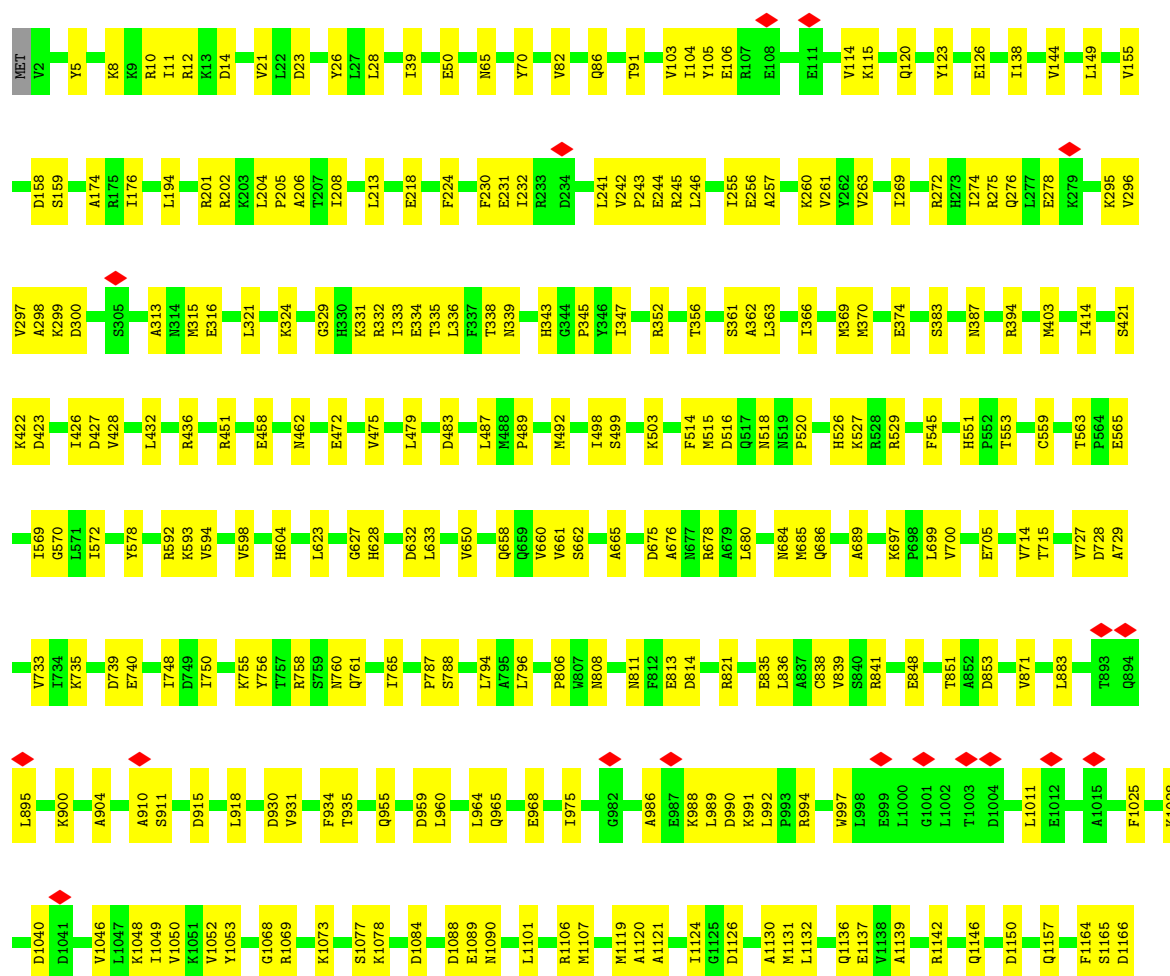
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

Chain B: 50% 17% 33%

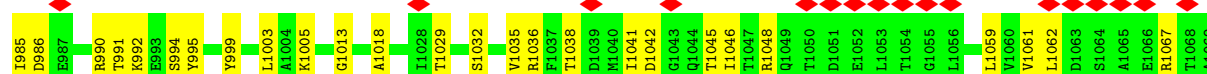
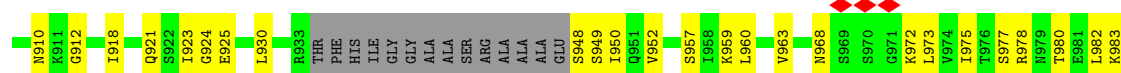
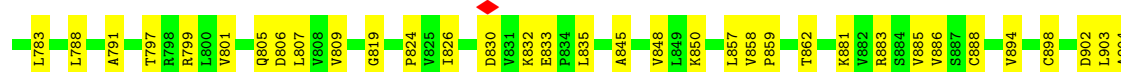
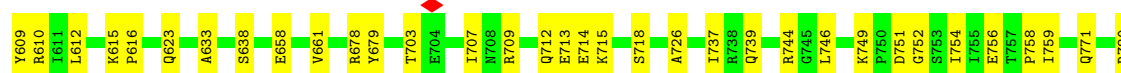
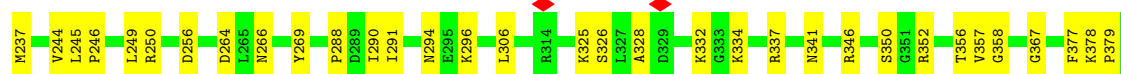
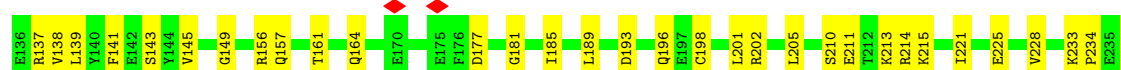


Chain C: 76% 24%



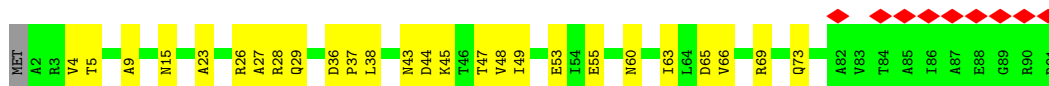


• Molecule 6: DNA-directed RNA polymerase subunit beta'

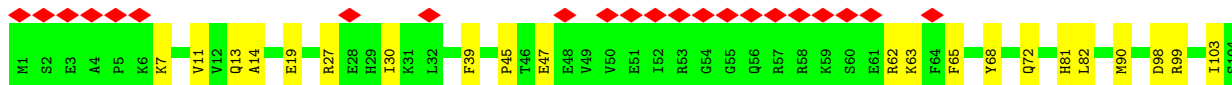




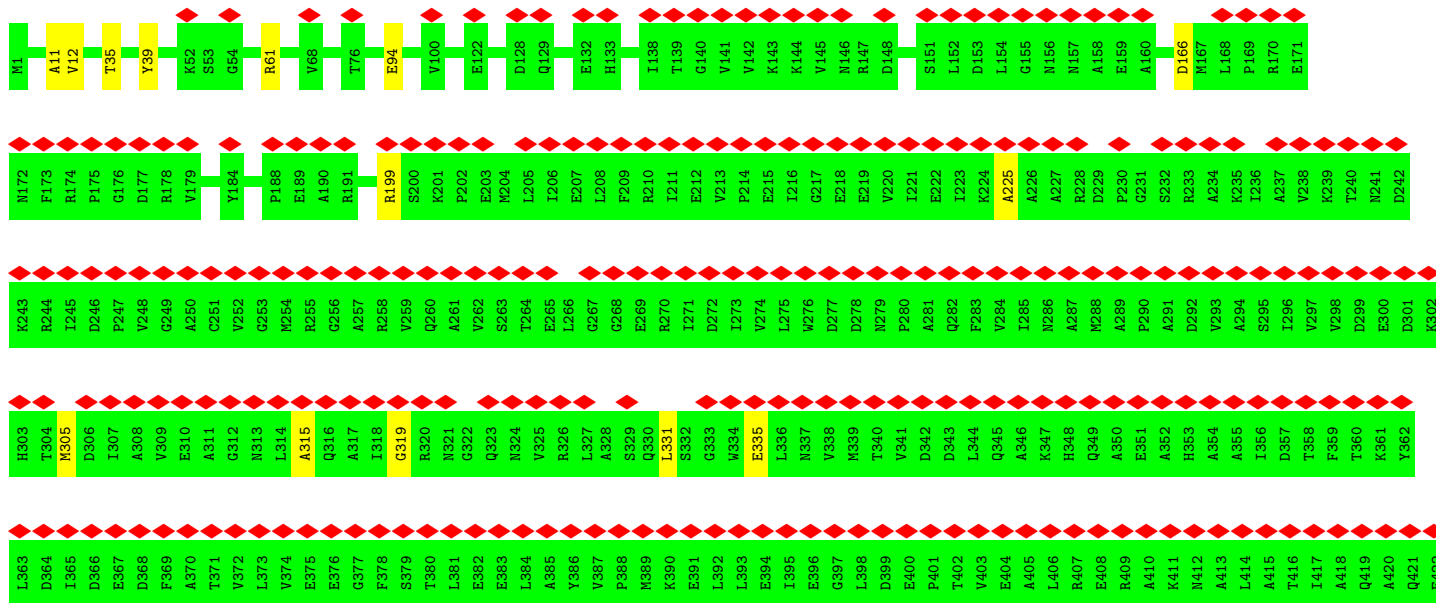
- Molecule 7: DNA-directed RNA polymerase subunit omega



- Molecule 8: Transcription termination/antitermination protein NusG



- Molecule 9: Transcription termination/antitermination protein NusA



M483	E423
A484	S424
A485	L425
R486	G426
N487	D427
I488	N428
C489	K429
W490	P430
F491	A431
G492	D432
D493	D433
E494	L434
A495	L435
	N436
	L437
	E438
	G439
	V440
	D441
	R442
	D443
	L444
	A445
	F446
	K447
	L448
	A449
	A450
	R451
	G452
	V453
	C454
	T455
	L456
	E457
	D458
	L459
	A460
	E461
	Q462
	G463
	T464
	D465
	D466
	L467
	A468
	D469
	T470
	E471
	G472
	L473
	T474
	D475
	E476
	K477
	A478
	G479
	A480
	L481
	T482

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94643	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.567	Depositor
Minimum map value	-0.739	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.282	Depositor
Map size (Å)	305.2, 305.2, 305.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.50	0/599	0.93	0/920
2	T	0.55	0/683	0.92	0/1051
3	R	0.20	0/261	0.81	0/405
4	A	0.25	0/1790	0.55	0/2426
4	B	0.24	0/1718	0.55	0/2328
5	C	0.25	0/10746	0.54	0/14499
6	D	0.25	0/10545	0.54	0/14236
7	E	0.26	0/711	0.63	1/956 (0.1%)
8	G	0.26	0/1008	0.58	0/1355
9	F	0.24	0/2446	0.44	0/3406
All	All	0.27	0/30507	0.57	1/41582 (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
4	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	36	ASP	CB-CG-OD2	5.53	123.28	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	29	GLU	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	535	0	294	10	0
2	T	611	0	337	17	0
3	R	235	0	120	6	0
4	A	1768	0	1793	44	0
4	B	1699	0	1734	38	0
5	C	10577	0	10591	217	0
6	D	10388	0	10613	255	0
7	E	709	0	719	18	0
8	G	987	0	993	17	0
9	F	2447	0	1180	7	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	29959	0	28374	582	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 10.

The worst 5 of 582 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)
6:D:72:CYS:HB2	6:D:88:CYS:SG	1.57	1.42
6:D:72:CYS:SG	6:D:87:LYS:HE3	2.05	0.95
6:D:72:CYS:CB	6:D:88:CYS:SG	2.53	0.95
6:D:582:ILE:HD12	6:D:623:GLN:HB3	1.57	0.85
6:D:72:CYS:SG	6:D:87:LYS:CE	2.68	0.81

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	
4	A	226/329 (69%)	217 (96%)	9 (4%)	0	100	100
4	B	216/329 (66%)	205 (95%)	11 (5%)	0	100	100
5	C	1339/1342 (100%)	1271 (95%)	68 (5%)	0	100	100
6	D	1329/1407 (94%)	1271 (96%)	58 (4%)	0	100	100
7	E	88/91 (97%)	85 (97%)	3 (3%)	0	100	100
8	G	121/181 (67%)	118 (98%)	3 (2%)	0	100	100
9	F	493/495 (100%)	474 (96%)	19 (4%)	0	100	100
All	All	3812/4174 (91%)	3641 (96%)	171 (4%)	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	
4	A	196/286 (68%)	196 (100%)	0	100	100
4	B	189/286 (66%)	187 (99%)	2 (1%)	73	84
5	C	1156/1157 (100%)	1155 (100%)	1 (0%)	93	97
6	D	1120/1168 (96%)	1119 (100%)	1 (0%)	93	97
7	E	74/75 (99%)	74 (100%)	0	100	100
8	G	107/158 (68%)	107 (100%)	0	100	100
All	All	2842/3130 (91%)	2838 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	41	ASN
4	B	195	ARG
5	C	1078	LYS
6	D	424	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	435	GLN
6	D	488	ASN
7	E	75	GLN
6	D	1049	GLN
5	C	761	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	10/14 (71%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	5	C

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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

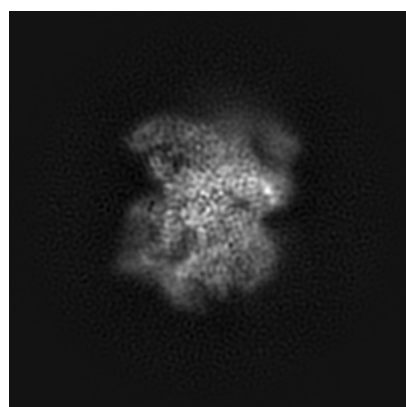
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13714. These allow visual inspection of the internal detail of the map and identification of artifacts.

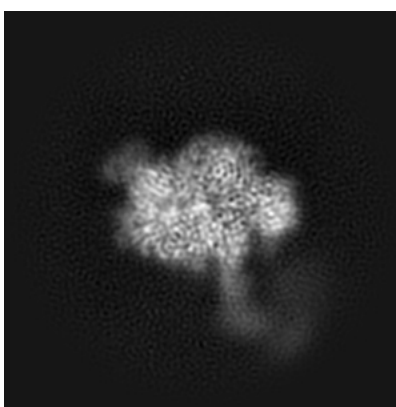
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

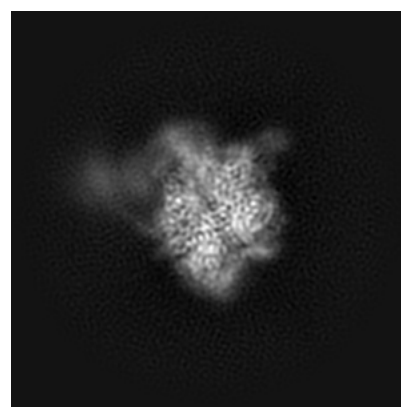
6.1.1 Primary map



X



Y

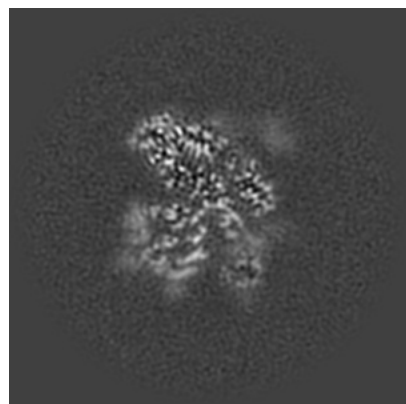


Z

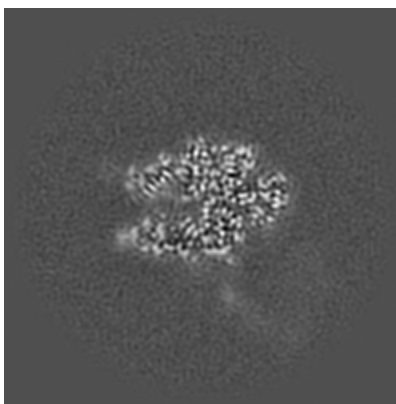
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

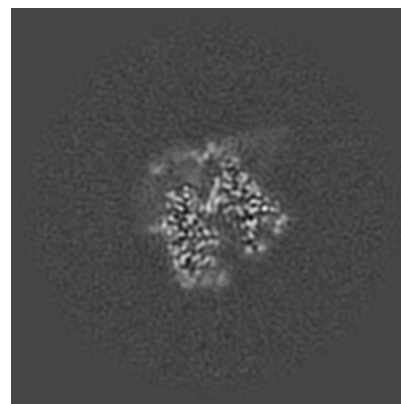
6.2.1 Primary map



X Index: 140



Y Index: 140

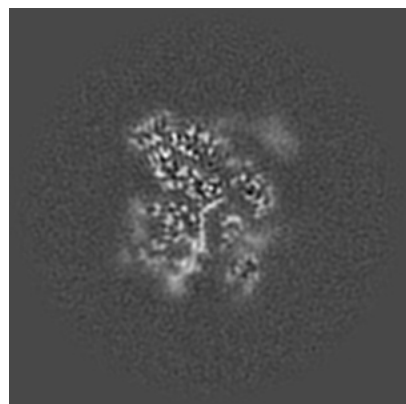


Z Index: 140

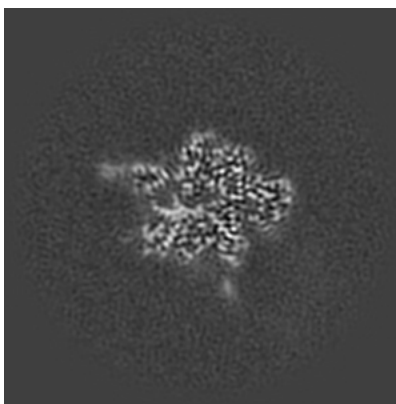
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

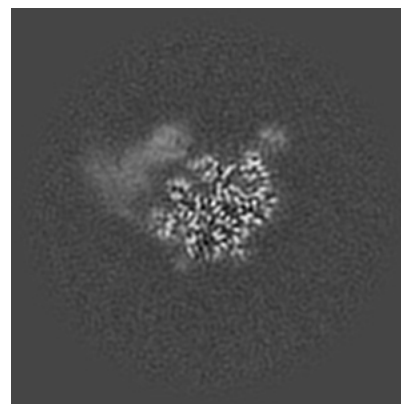
6.3.1 Primary map



X Index: 137



Y Index: 135

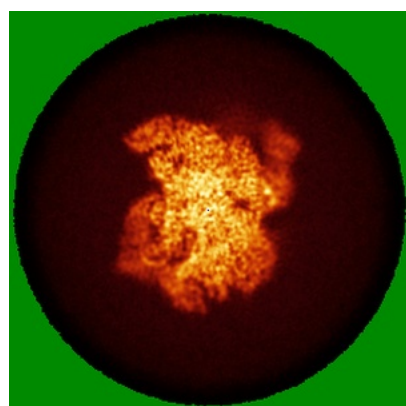


Z Index: 161

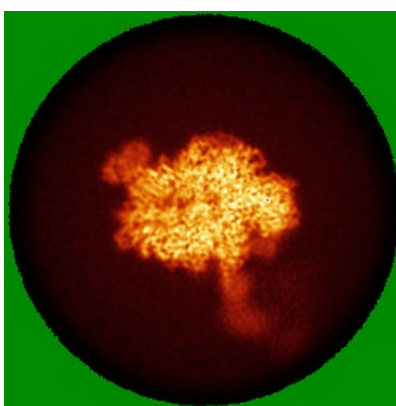
The images above show the largest variance slices of the map in three orthogonal directions.

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

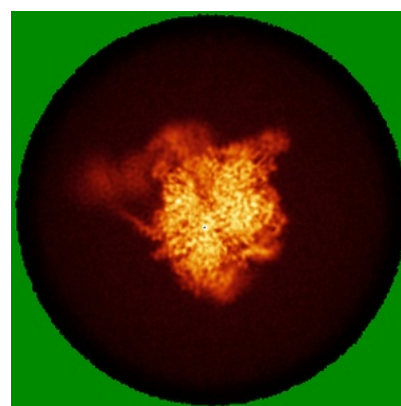
6.4.1 Primary map



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

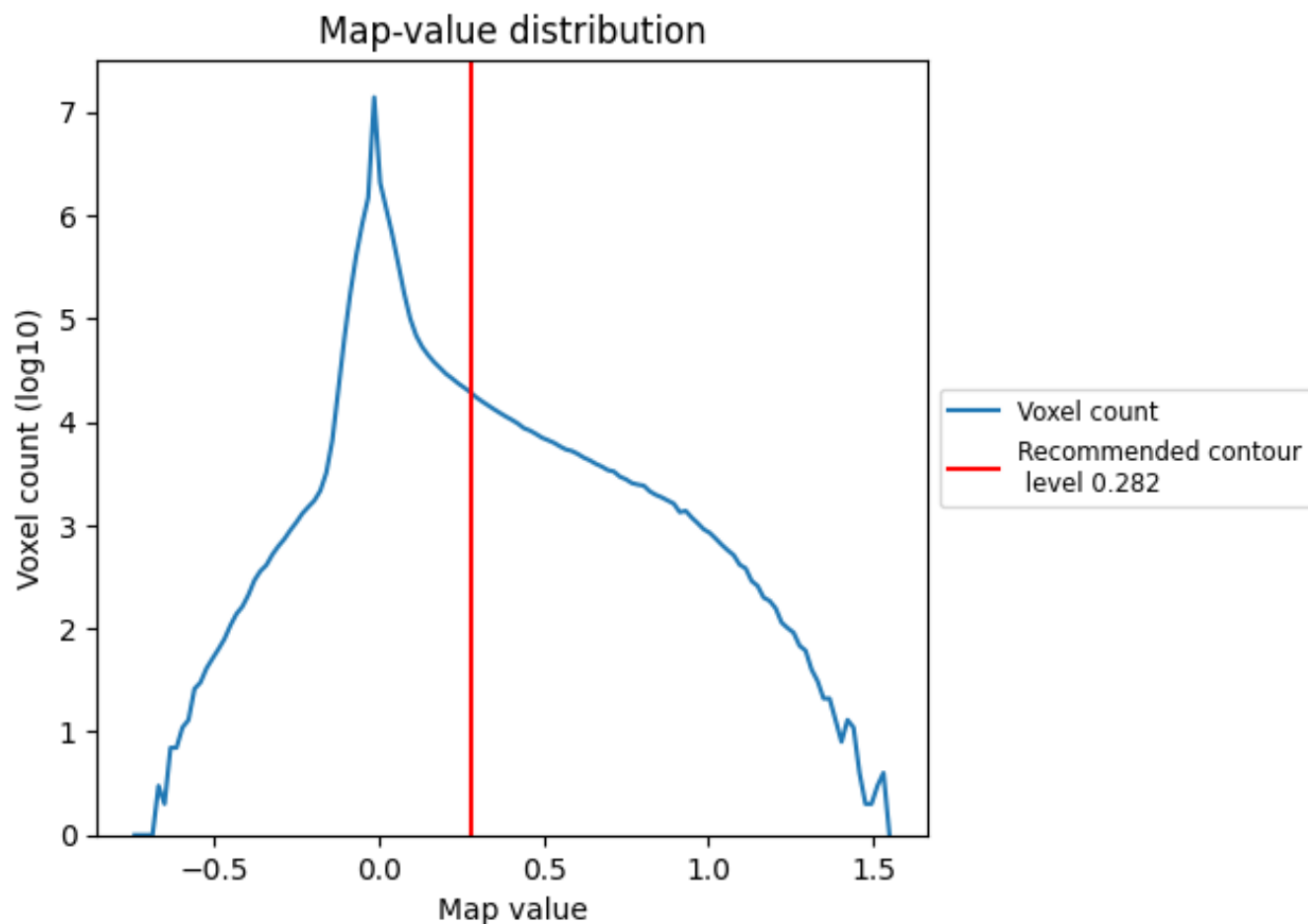
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

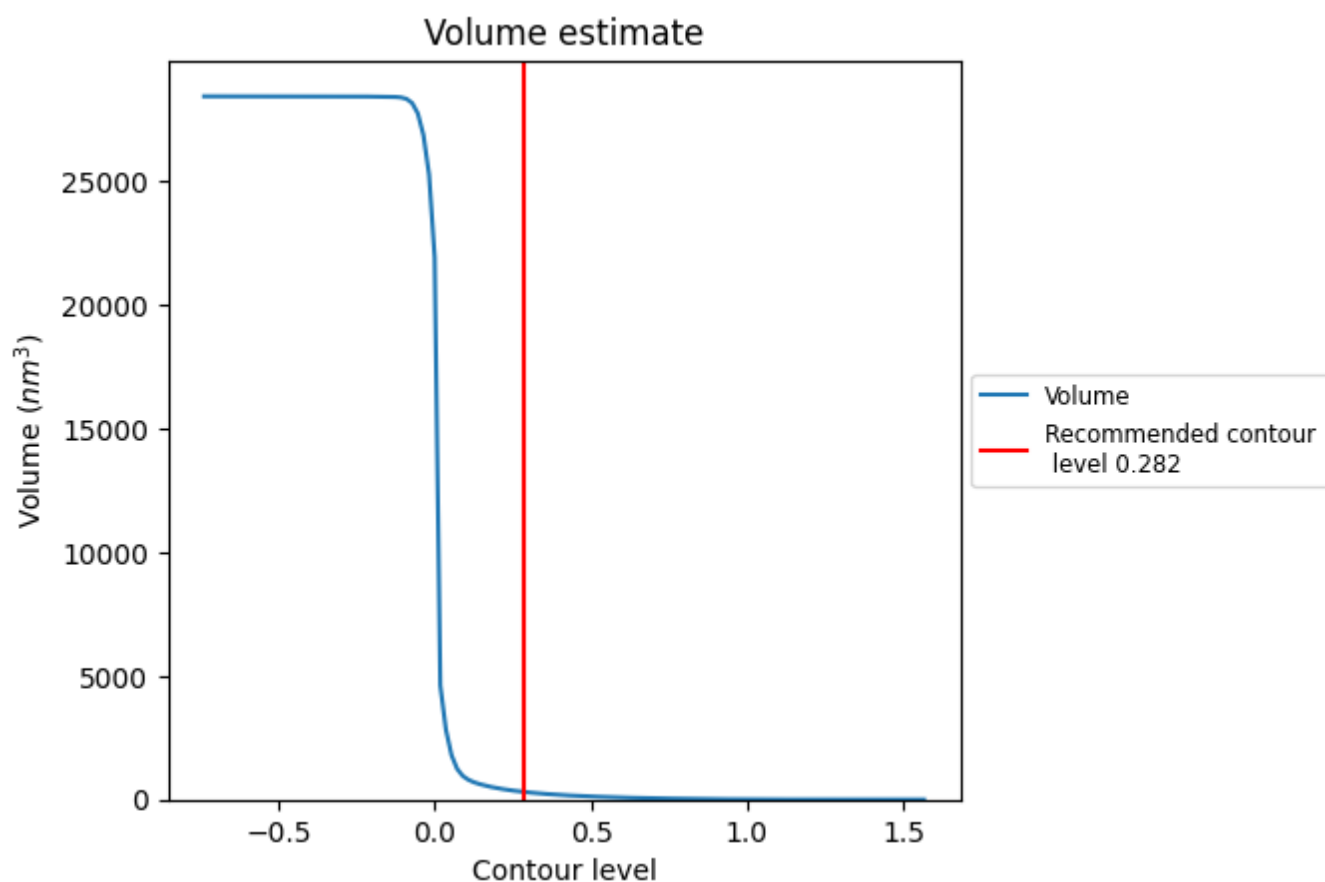
This section contains the results of statistical analysis of the map.

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.

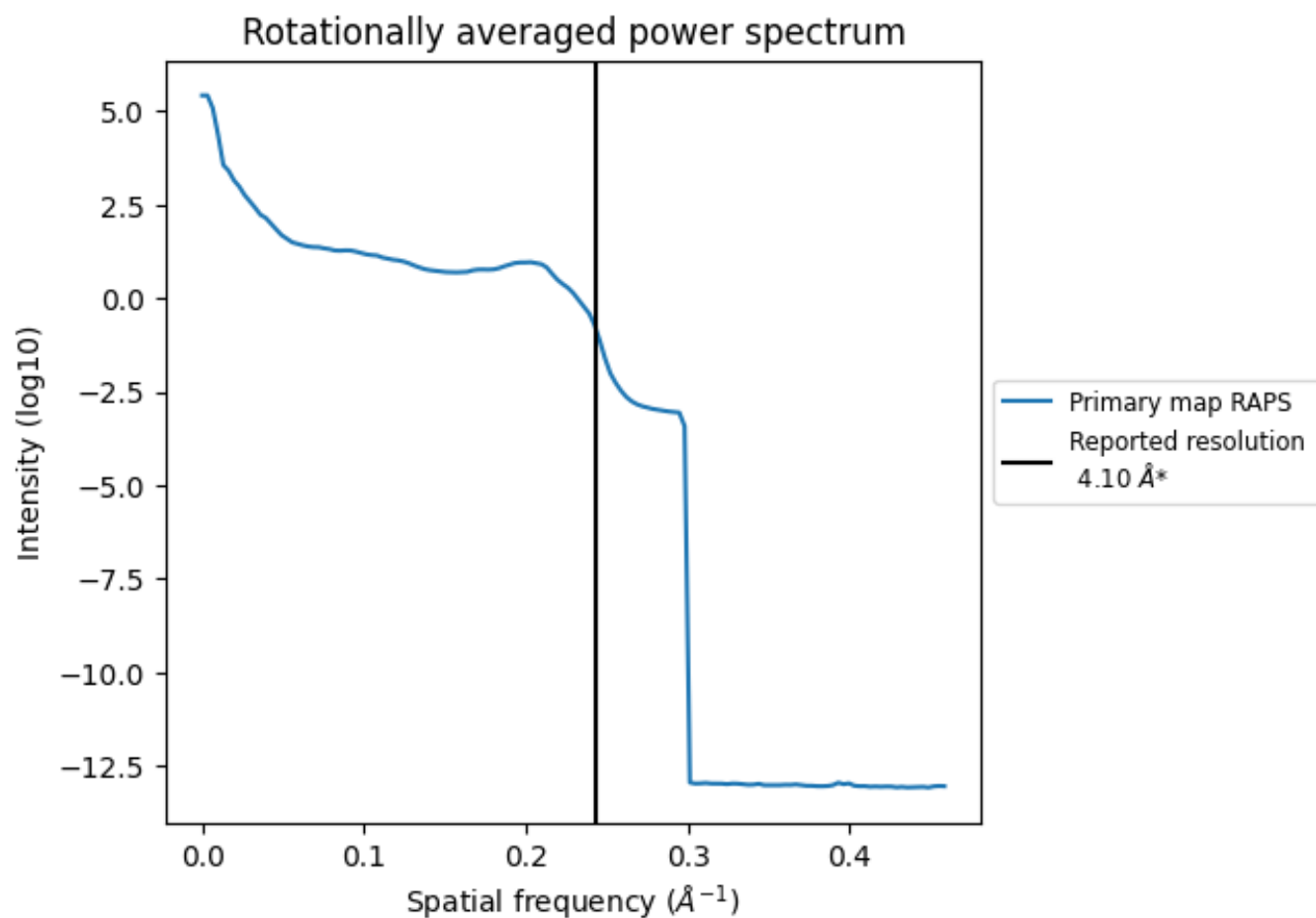
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 313 nm³; this corresponds to an approximate mass of 283 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 0.244 Å⁻¹

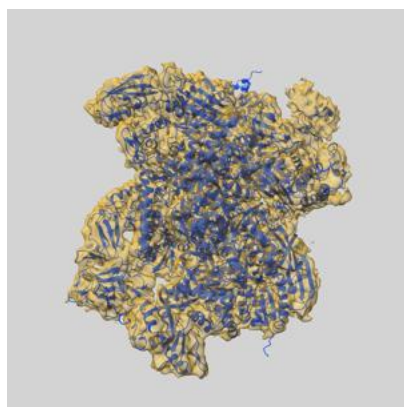
8 Fourier-Shell correlation

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

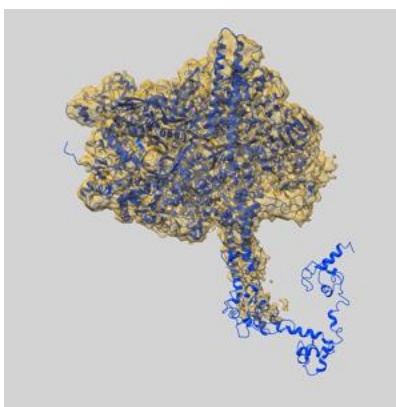
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13714 and PDB model 7PY6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

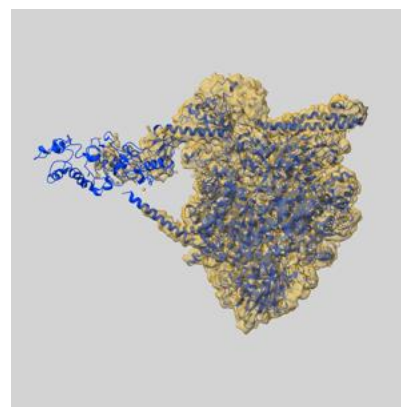
9.1 Map-model overlay [i](#)



X



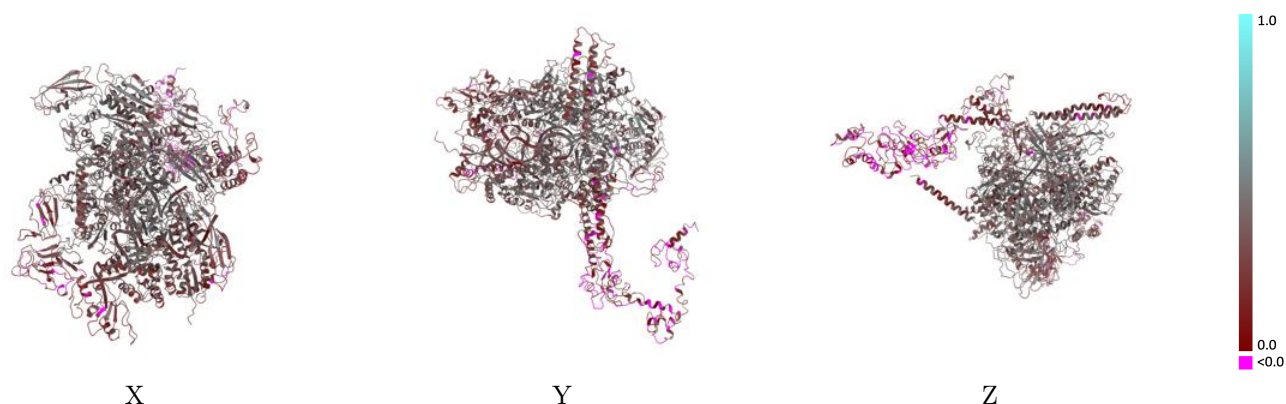
Y



Z

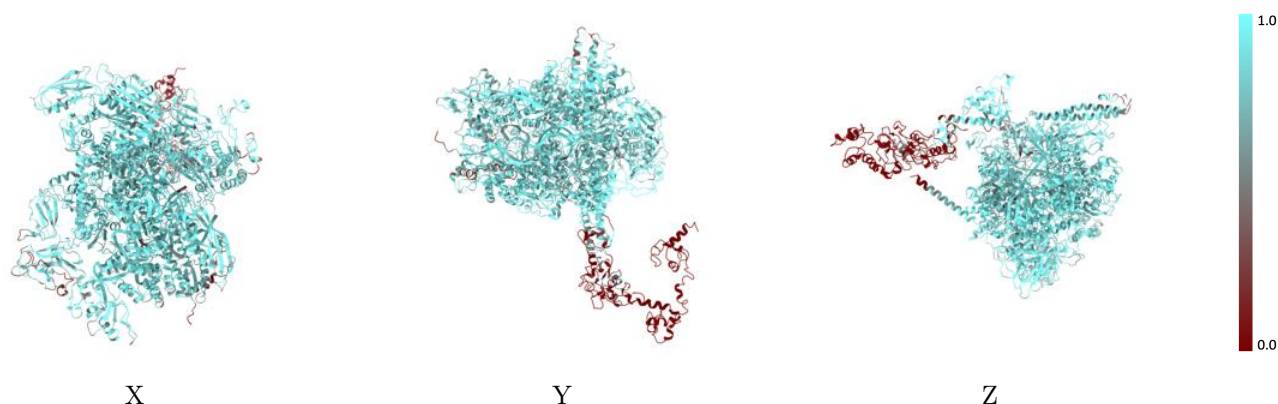
The images above show the 3D surface view of the map at the recommended contour level 0.282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



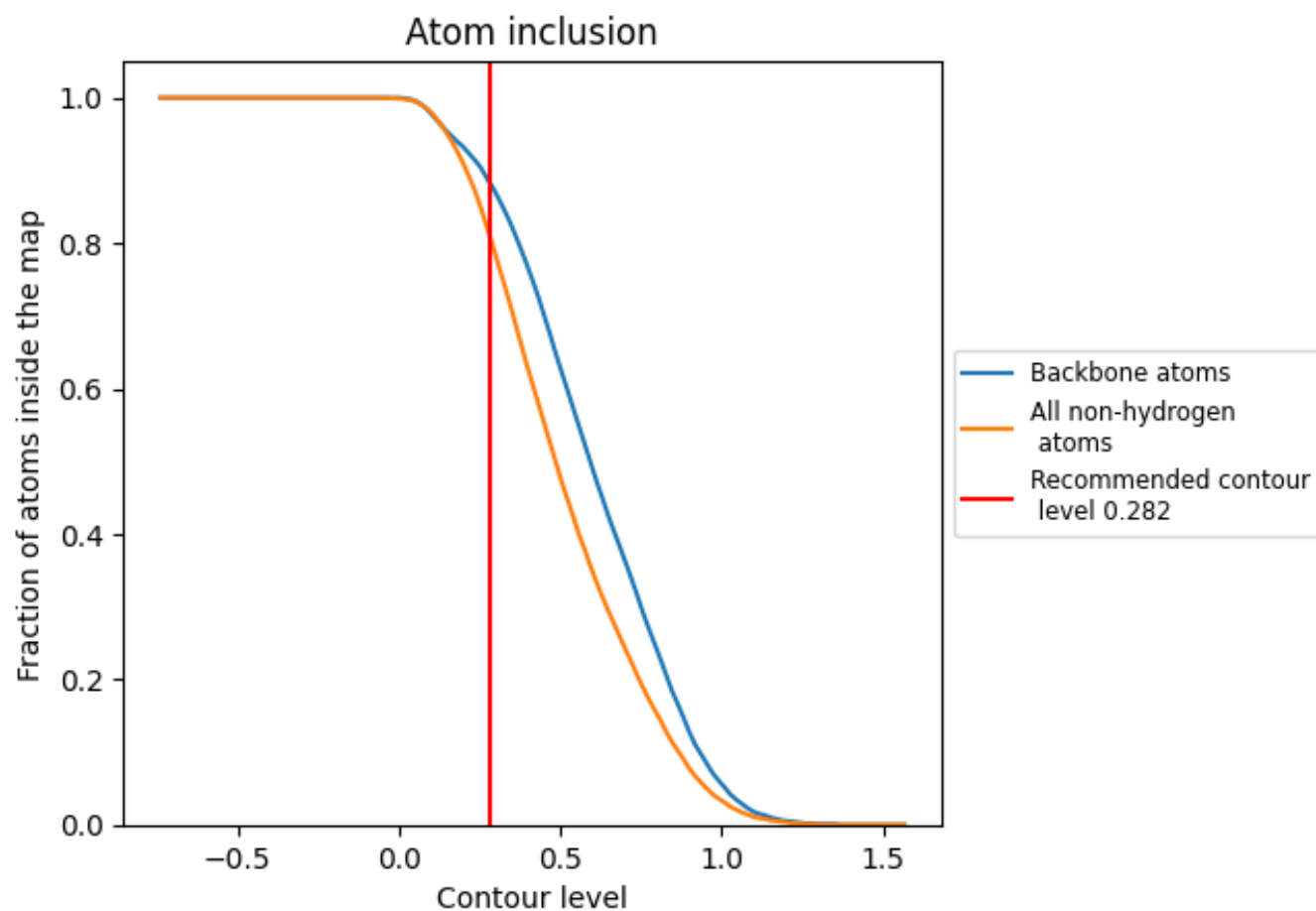
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.282).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8090	<div></div> 0.3480
A	<div></div> 0.8720	<div></div> 0.4090
B	<div></div> 0.8840	<div></div> 0.3910
C	<div></div> 0.8650	<div></div> 0.3730
D	<div></div> 0.8530	<div></div> 0.3630
E	<div></div> 0.7810	<div></div> 0.3450
F	<div></div> 0.3300	<div></div> 0.1470
G	<div></div> 0.6000	<div></div> 0.2690
N	<div></div> 0.8690	<div></div> 0.2830
R	<div></div> 0.8980	<div></div> 0.3720
T	<div></div> 0.9620	<div></div> 0.3410

1.0
0.0
<0.0