



wwPDB EM Validation Summary Report ⓘ

Nov 30, 2022 – 01:14 AM JST

PDB ID : 7XL3
EMDB ID : EMD-33271
Title : Cryo-EM structure of *Pseudomonas aeruginosa* RNAP sigmaS holoenzyme complexes with transcription factor SutA (open lobe)
Authors : He, D.W.; You, L.L.; Zhang, Y.
Deposited on : 2022-04-21
Resolution : 3.13 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:

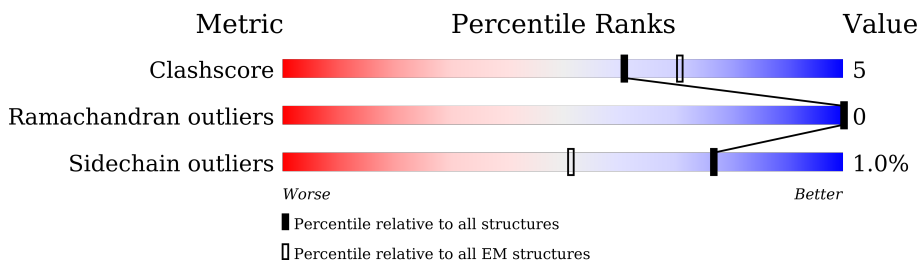
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.13 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

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	345	
1	B	345	
2	C	1359	
3	D	1412	
4	E	88	
5	G	109	
6	F	338	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25700 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	Total	C	N	O	S	0	0
			1617	1015	296	303	3		
1	B	216	Total	C	N	O	S	0	0
			1634	1019	299	313	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP O52760
A	-10	GLY	-	expression tag	UNP O52760
A	-9	HIS	-	expression tag	UNP O52760
A	-8	HIS	-	expression tag	UNP O52760
A	-7	HIS	-	expression tag	UNP O52760
A	-6	HIS	-	expression tag	UNP O52760
A	-5	HIS	-	expression tag	UNP O52760
A	-4	HIS	-	expression tag	UNP O52760
A	-3	HIS	-	expression tag	UNP O52760
A	-2	HIS	-	expression tag	UNP O52760
A	-1	HIS	-	expression tag	UNP O52760
A	0	HIS	-	expression tag	UNP O52760
B	-11	MET	-	initiating methionine	UNP O52760
B	-10	GLY	-	expression tag	UNP O52760
B	-9	HIS	-	expression tag	UNP O52760
B	-8	HIS	-	expression tag	UNP O52760
B	-7	HIS	-	expression tag	UNP O52760
B	-6	HIS	-	expression tag	UNP O52760
B	-5	HIS	-	expression tag	UNP O52760
B	-4	HIS	-	expression tag	UNP O52760
B	-3	HIS	-	expression tag	UNP O52760
B	-2	HIS	-	expression tag	UNP O52760
B	-1	HIS	-	expression tag	UNP O52760
B	0	HIS	-	expression tag	UNP O52760

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1324	9697	6060	1748	1850	39	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q51561
C	0	GLY	-	expression tag	UNP Q51561

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1338	10064	6292	1826	1904	42	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP Q9HWC9
D	1	LEU	-	expression tag	UNP Q9HWC9
D	1400	GLY	-	expression tag	UNP Q9HWC9
D	1401	SER	-	expression tag	UNP Q9HWC9
D	1402	GLY	-	expression tag	UNP Q9HWC9
D	1403	SER	-	expression tag	UNP Q9HWC9
D	1404	TRP	-	expression tag	UNP Q9HWC9
D	1405	SER	-	expression tag	UNP Q9HWC9
D	1406	HIS	-	expression tag	UNP Q9HWC9
D	1407	PRO	-	expression tag	UNP Q9HWC9
D	1408	GLN	-	expression tag	UNP Q9HWC9
D	1409	PHE	-	expression tag	UNP Q9HWC9
D	1410	GLU	-	expression tag	UNP Q9HWC9
D	1411	LYS	-	expression tag	UNP Q9HWC9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	71	511	320	96	94	1	0	0

- Molecule 5 is a protein called Transcriptional factor SutA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	37	Total	C	N	O	S	0	0
			276	170	50	55	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q9HTR9
G	-2	ALA	-	expression tag	UNP Q9HTR9
G	-1	MET	-	expression tag	UNP Q9HTR9
G	0	GLY	-	expression tag	UNP Q9HTR9

- Molecule 6 is a protein called RNA polymerase sigma factor RpoS.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	277	Total	C	N	O	S	0	0
			1898	1191	353	350	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P45684
F	-2	ALA	-	expression tag	UNP P45684
F	-1	MET	-	expression tag	UNP P45684
F	0	GLY	-	expression tag	UNP P45684

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

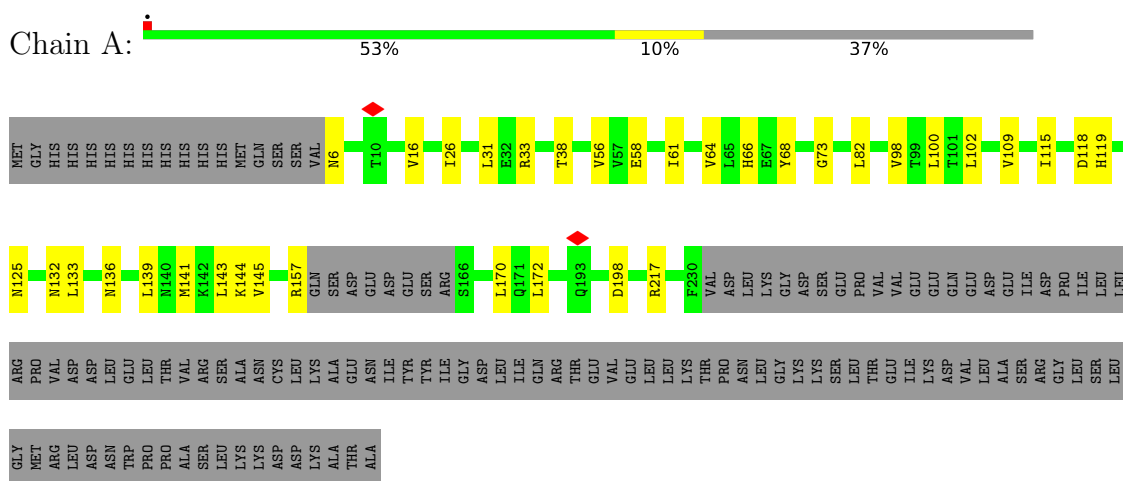
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

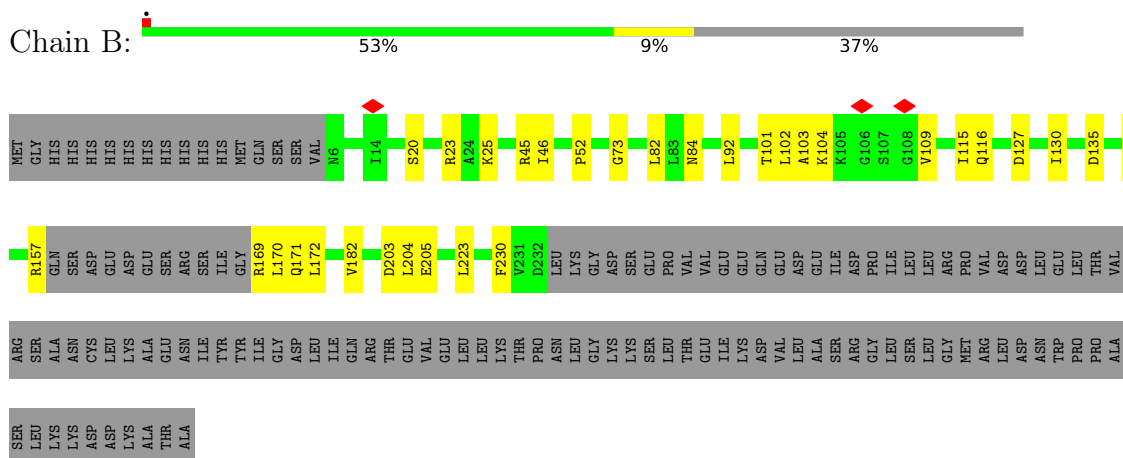
3 Residue-property plots

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.

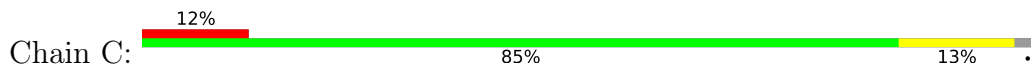
- Molecule 1: DNA-directed RNA polymerase subunit alpha

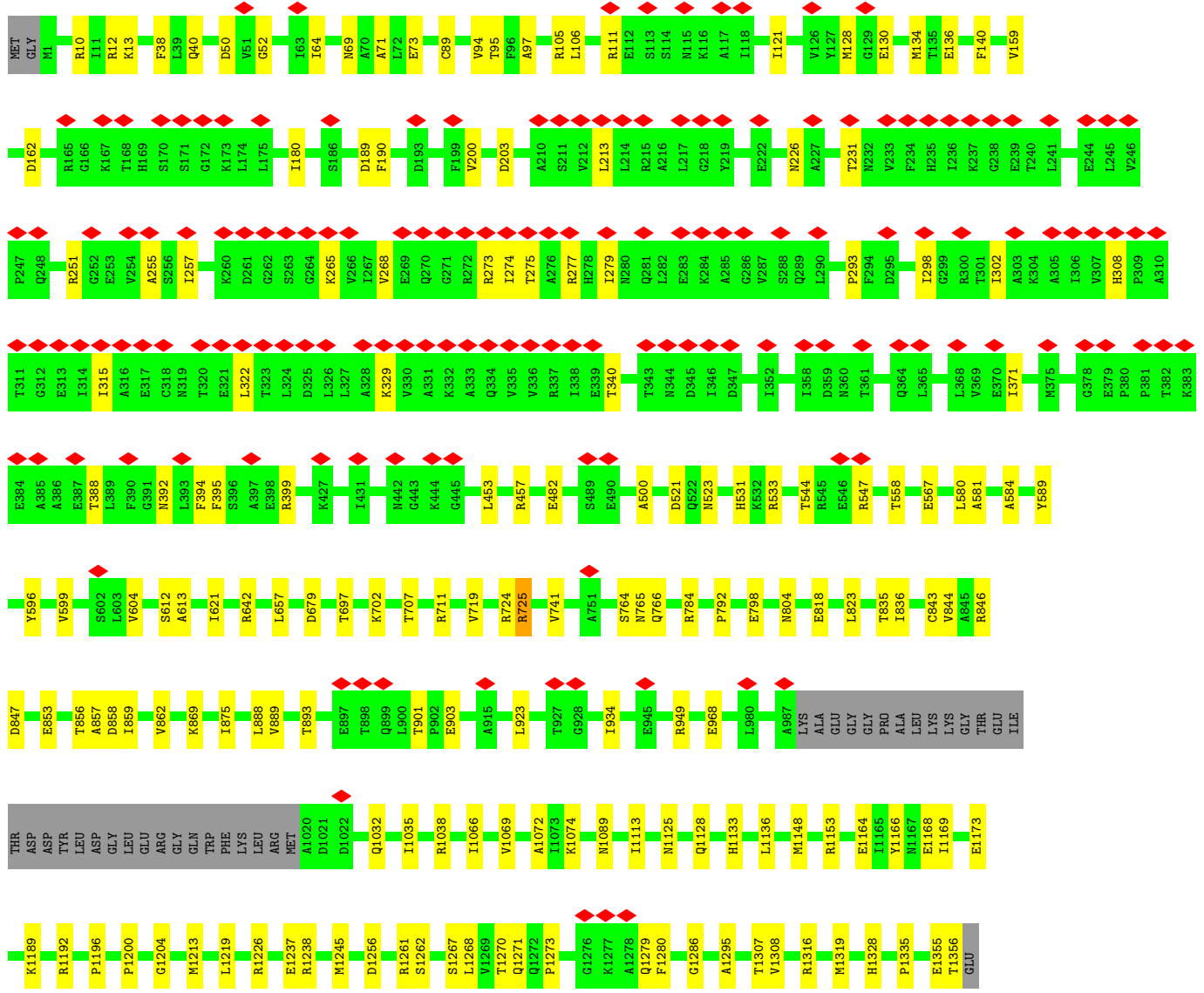


- Molecule 1: DNA-directed RNA polymerase subunit alpha

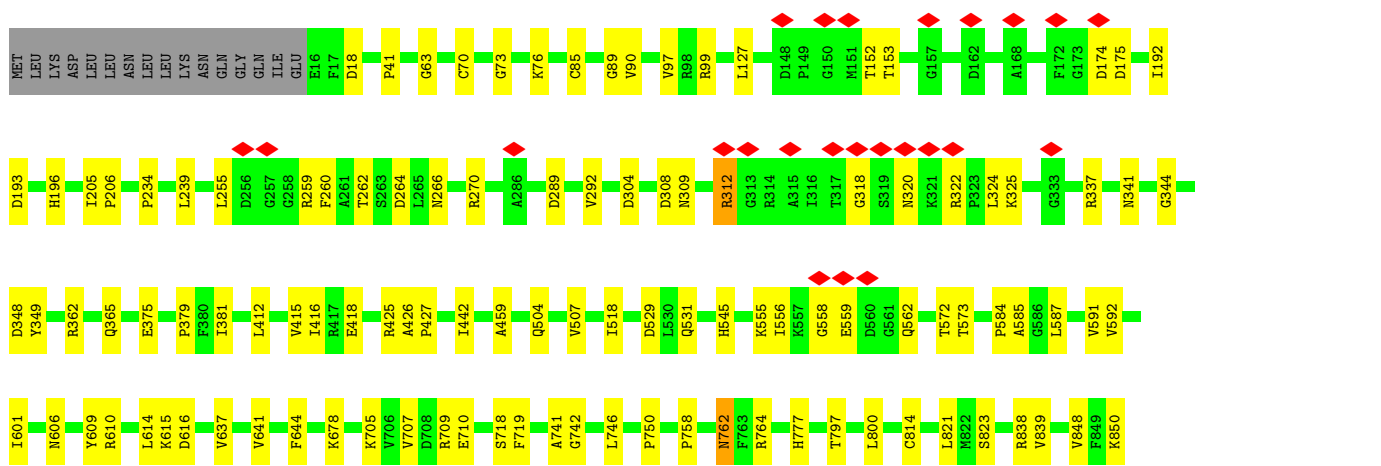
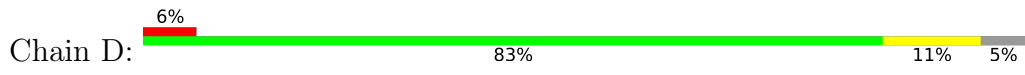


- Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138109	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.013	Depositor
Map size (\AA)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: 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	A	0.23	0/1633	0.42	0/2213
1	B	0.23	0/1651	0.42	0/2237
2	C	0.24	0/9831	0.40	0/13303
3	D	0.23	0/10214	0.40	0/13801
4	E	0.23	0/515	0.36	0/698
5	G	0.23	0/277	0.43	0/369
6	F	0.22	0/1917	0.38	0/2613
All	All	0.23	0/26038	0.40	0/35234

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	1617	0	1634	21	0
1	B	1634	0	1637	17	0
2	C	9697	0	9225	102	0
3	D	10064	0	9885	96	0
4	E	511	0	490	6	0
5	G	276	0	267	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1898	0	1653	10	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
All	All	25700	0	24791	233	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 5.

The worst 5 of 233 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)
2:C:1128:GLN:HG3	2:C:1245:MET:HE1	1.75	0.68
1:A:82:LEU:HD11	1:A:170:LEU:HD23	1.75	0.66
2:C:533:ARG:NH2	2:C:581:ALA:O	2.30	0.65
3:D:1025:HIS:HB2	3:D:1124:ILE:HB	1.81	0.63
2:C:453:LEU:H	2:C:558:THR:HG21	1.64	0.62

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	213/345 (62%)	207 (97%)	6 (3%)	0	100	100
1	B	212/345 (61%)	206 (97%)	6 (3%)	0	100	100
2	C	1320/1359 (97%)	1283 (97%)	37 (3%)	0	100	100
3	D	1332/1412 (94%)	1292 (97%)	40 (3%)	0	100	100
4	E	69/88 (78%)	66 (96%)	3 (4%)	0	100	100
5	G	35/109 (32%)	31 (89%)	4 (11%)	0	100	100
6	F	275/338 (81%)	271 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3456/3996 (86%)	3356 (97%)	100 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/295 (56%)	164 (100%)	0	100	100
1	B	169/295 (57%)	166 (98%)	3 (2%)	59	81
2	C	931/1144 (81%)	920 (99%)	11 (1%)	71	87
3	D	1013/1180 (86%)	1004 (99%)	9 (1%)	78	90
4	E	45/74 (61%)	45 (100%)	0	100	100
5	G	26/82 (32%)	25 (96%)	1 (4%)	33	64
6	F	145/300 (48%)	144 (99%)	1 (1%)	84	93
All	All	2493/3370 (74%)	2468 (99%)	25 (1%)	77	89

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	239	LEU
3	D	762	ASN
6	F	225	THR
3	D	545	HIS
3	D	839	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1328	HIS
6	F	192	HIS
3	D	519	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1326	GLN
3	D	477	GLN

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 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.

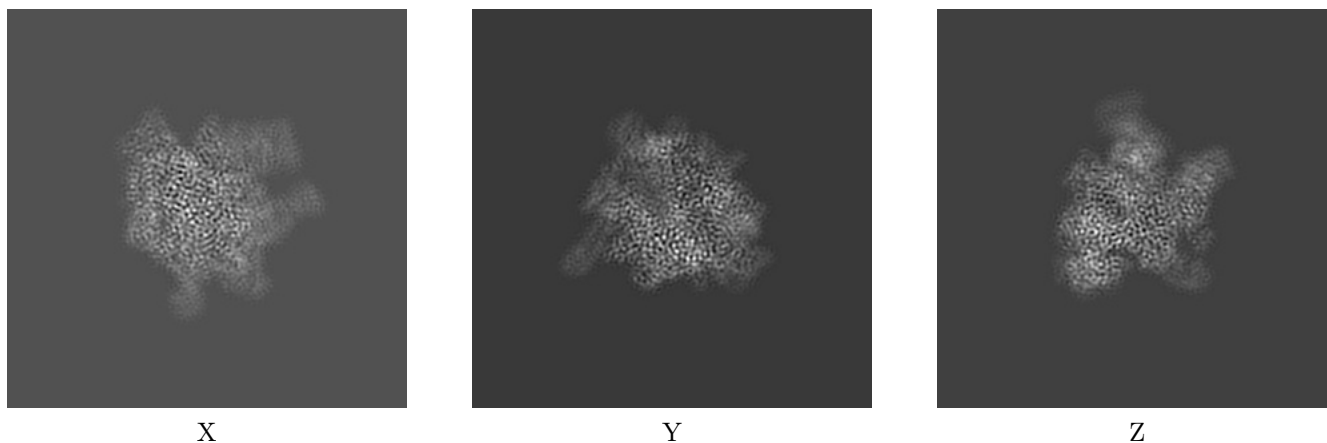
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33271. 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](#)

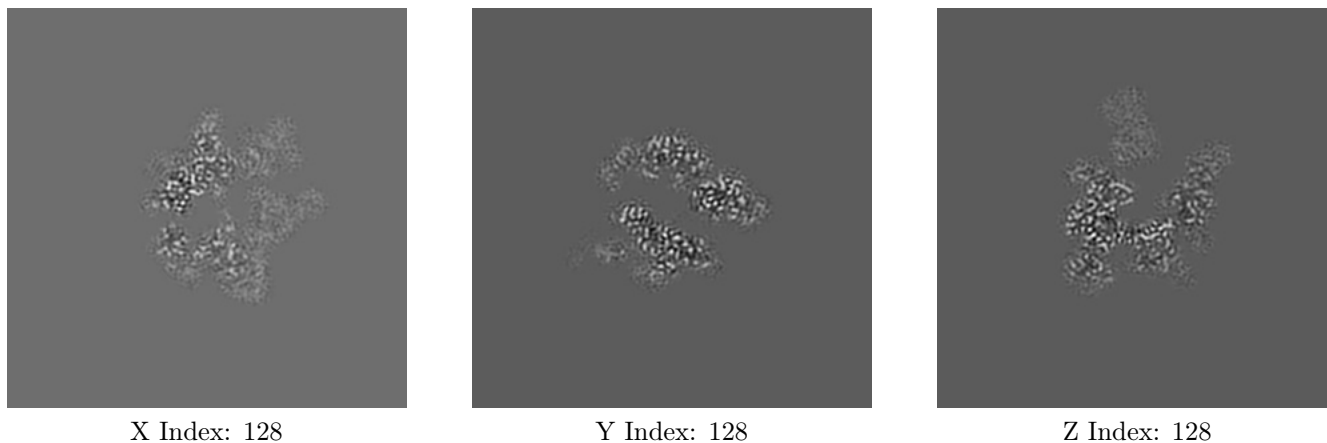
6.1.1 Primary map



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

6.2 Central slices [i](#)

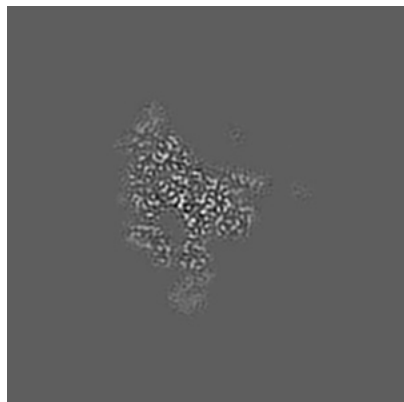
6.2.1 Primary map



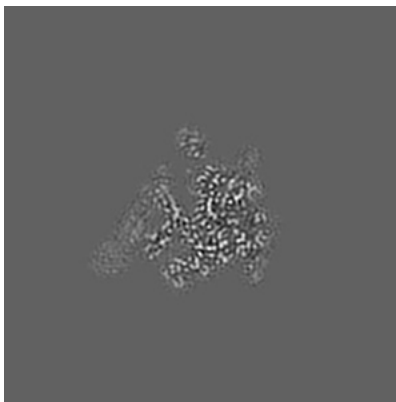
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

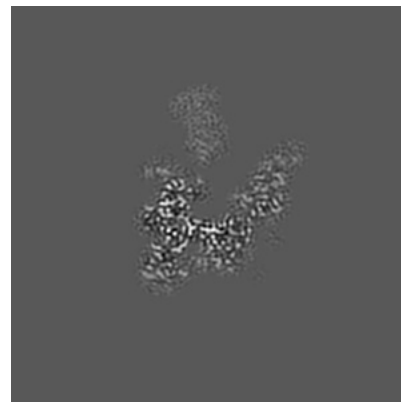
6.3.1 Primary map



X Index: 100



Y Index: 112



Z Index: 131

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

6.4 Orthogonal surface views [i](#)

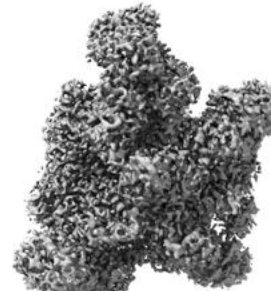
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

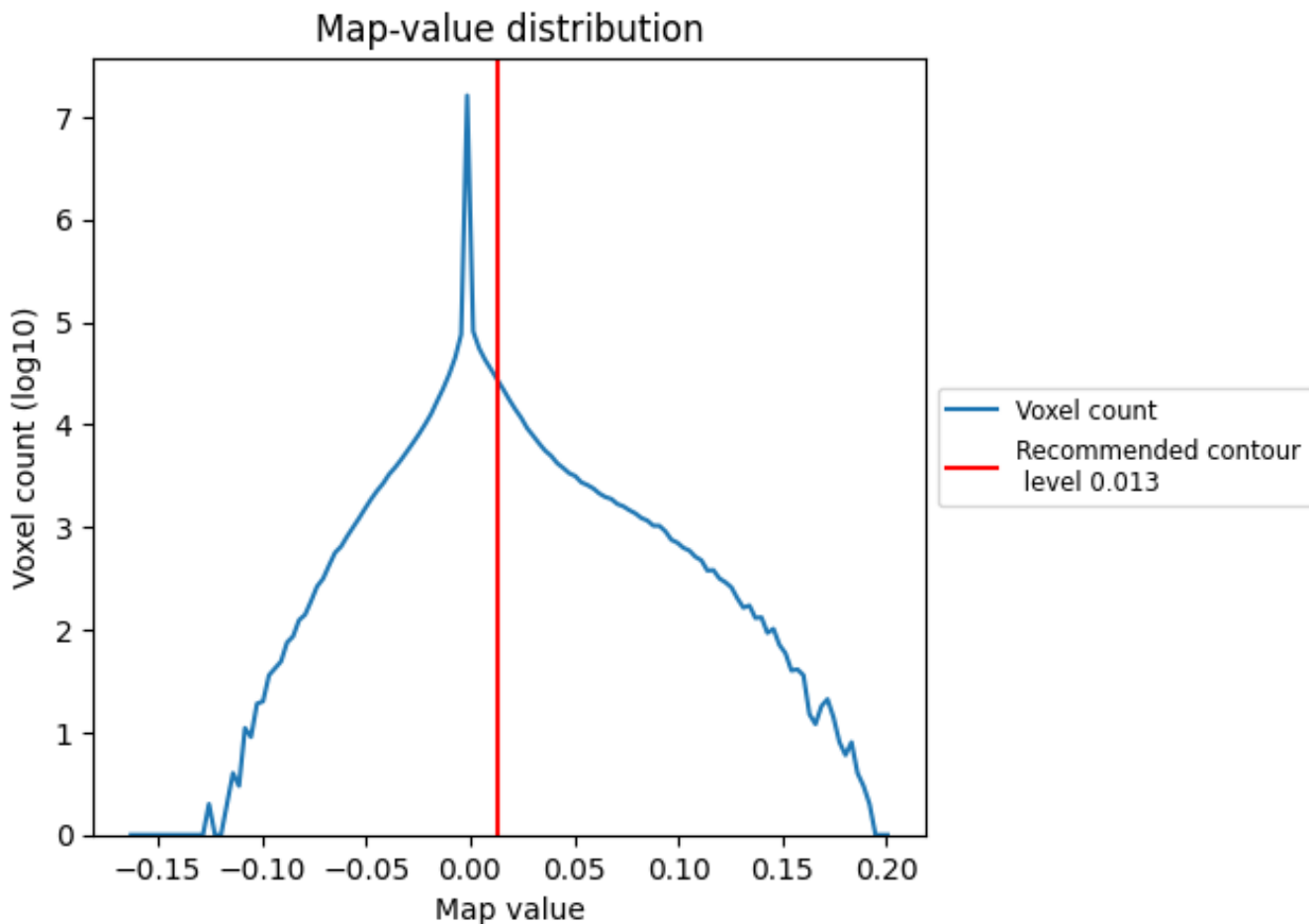
6.5 Mask visualisation

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

7 Map analysis [i](#)

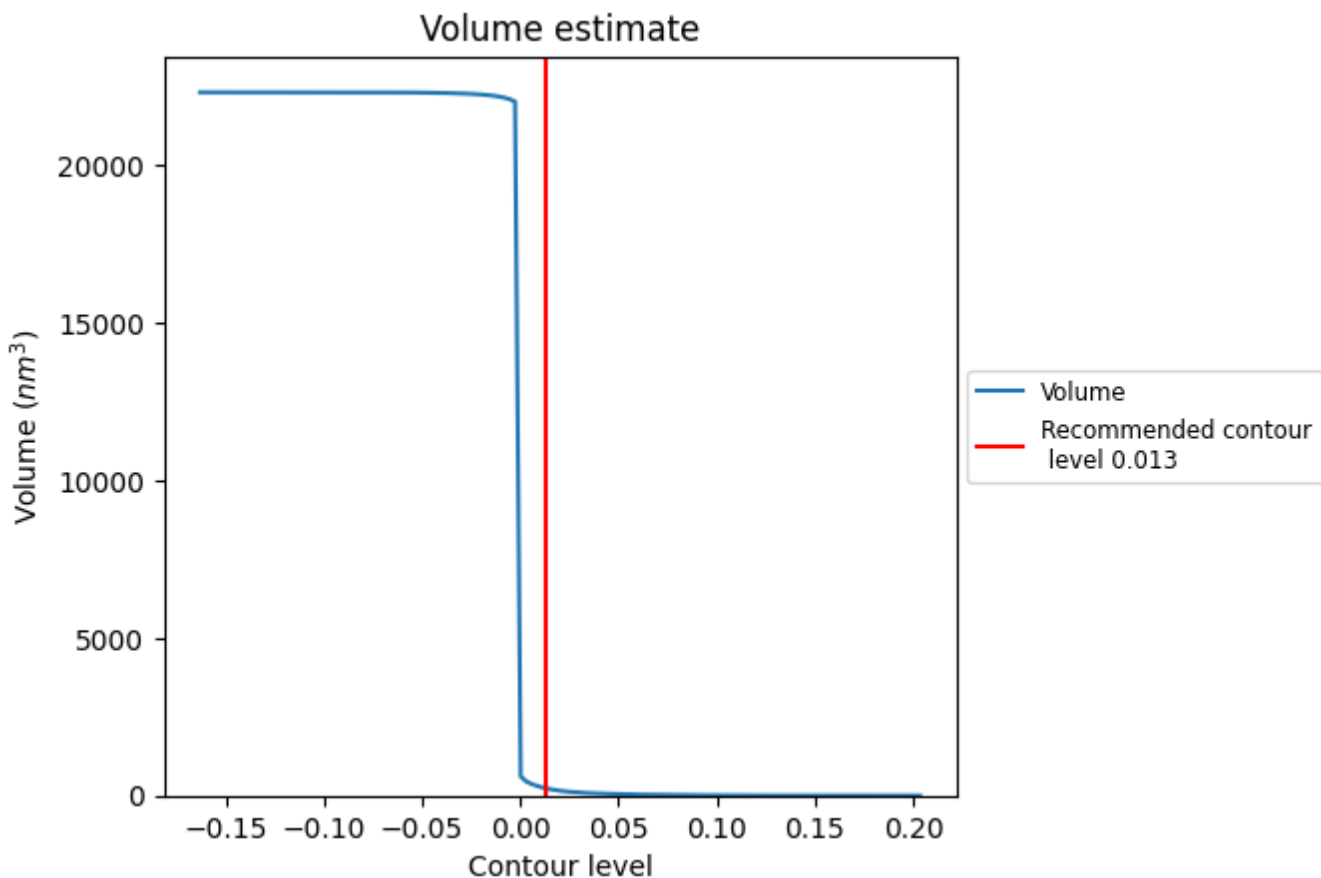
This section contains the results of statistical analysis of the map.

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.

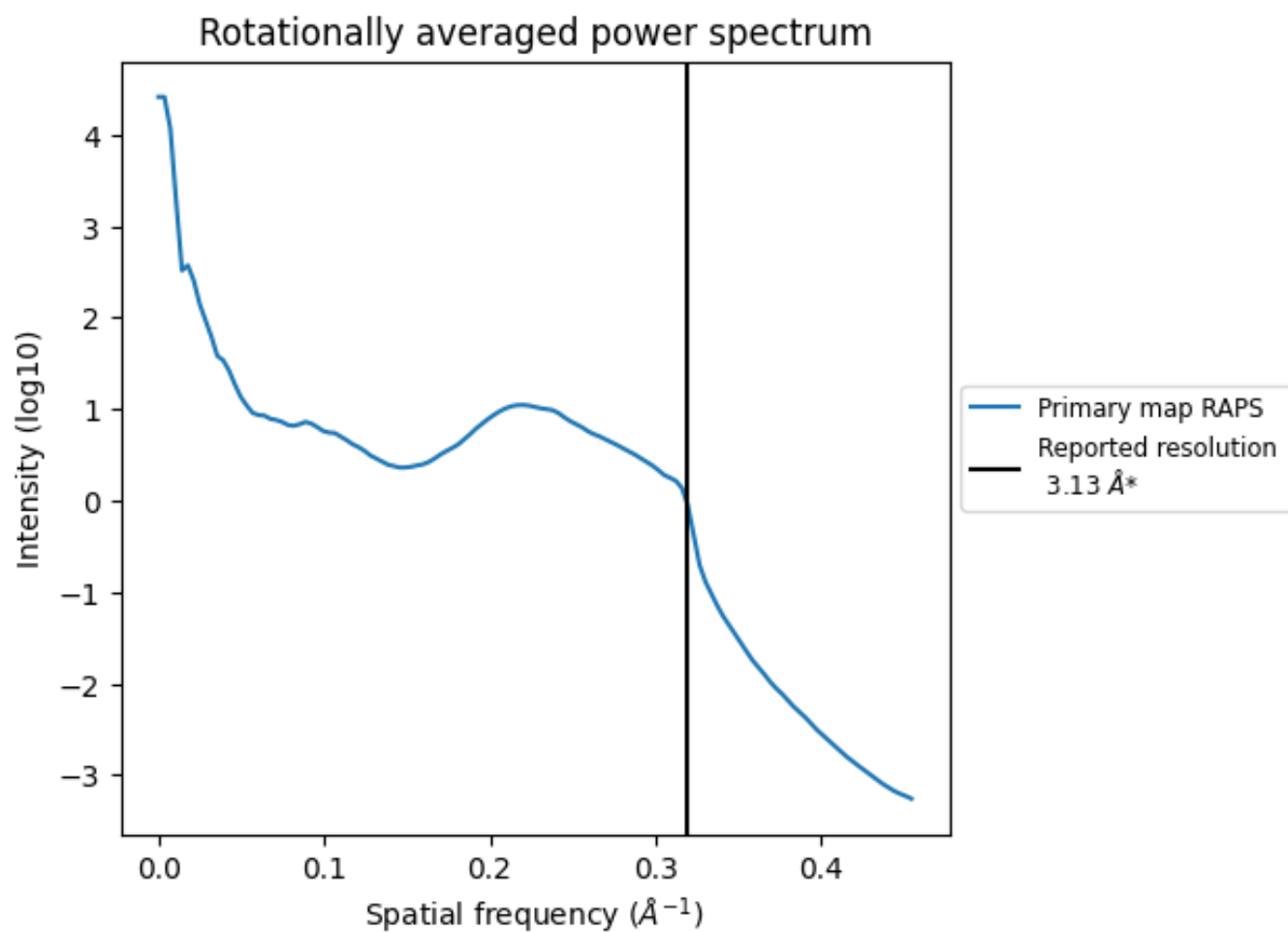
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 232 nm³; this corresponds to an approximate mass of 209 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](#)

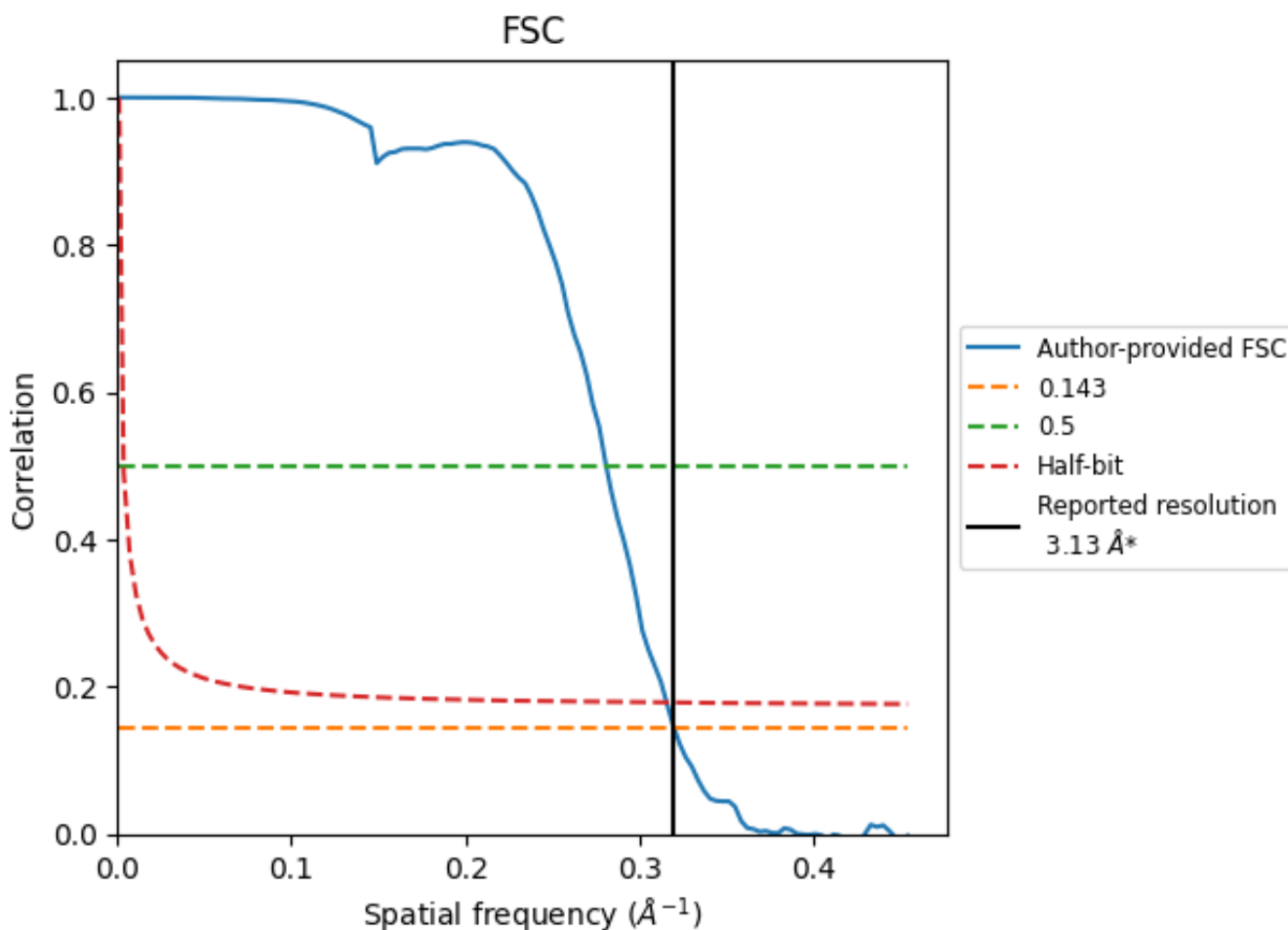


*Reported resolution corresponds to spatial frequency of 0.319\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8.2 Resolution estimates [i](#)

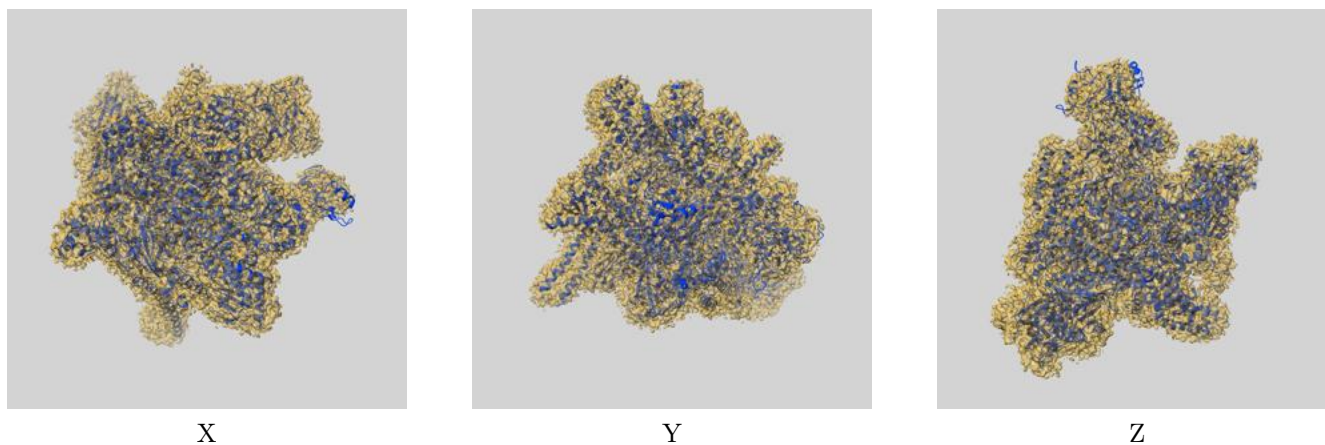
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.12	3.56	3.17
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

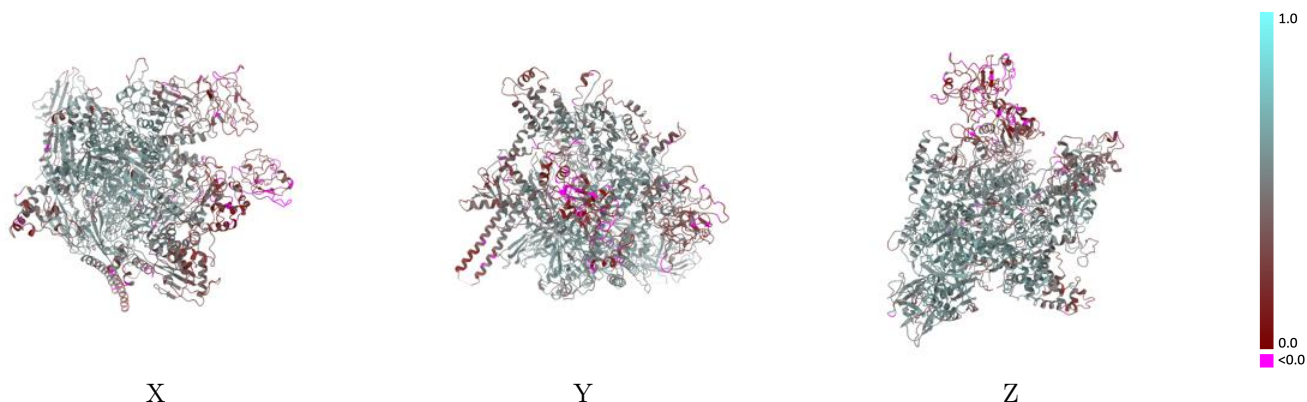
This section contains information regarding the fit between EMDB map EMD-33271 and PDB model 7XL3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



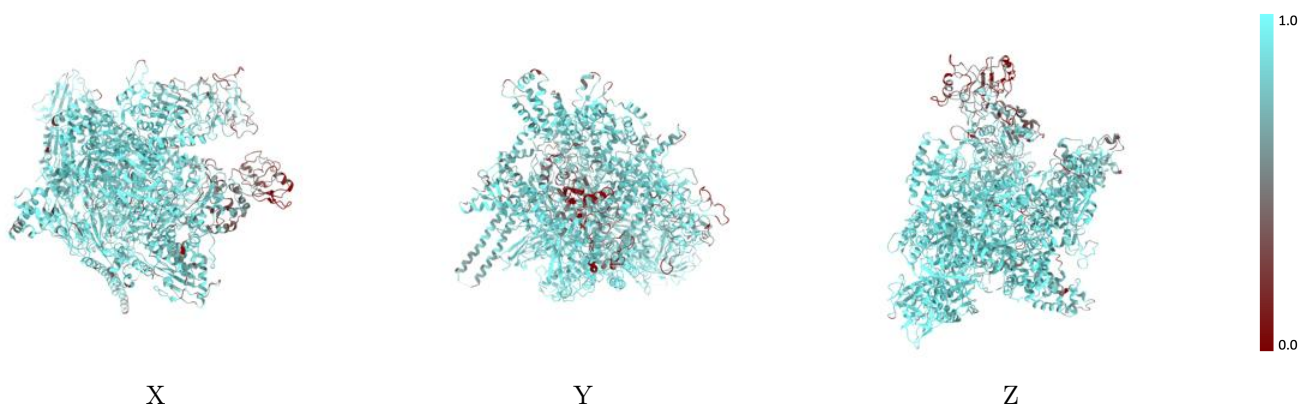
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



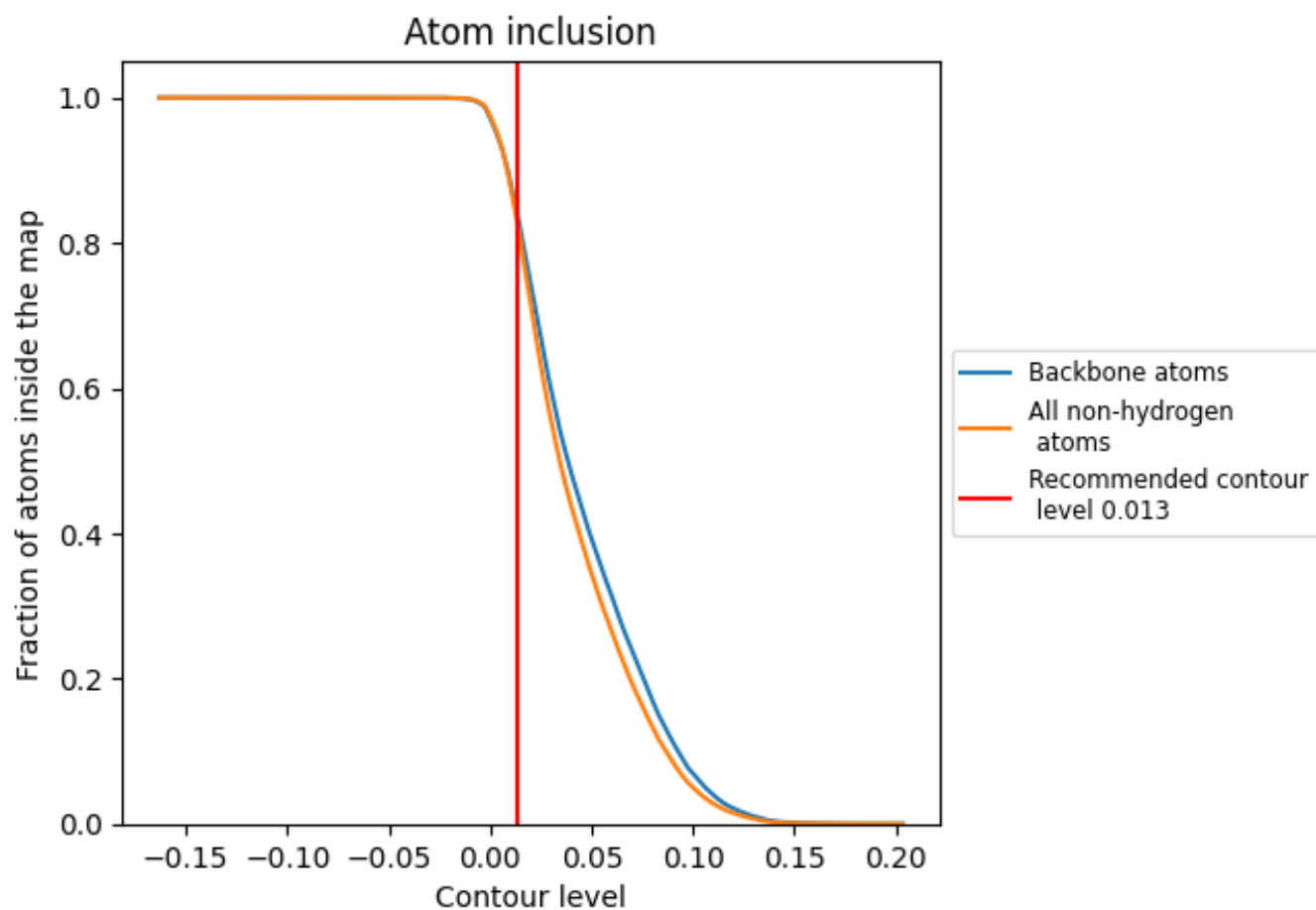
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

















9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.4680
A	 0.9148	 0.5360
B	 0.8894	 0.5030
C	 0.8146	 0.4570
D	 0.8459	 0.4800
E	 0.8500	 0.4940
F	 0.7592	 0.3800
G	 0.7684	 0.3840

