



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 08:57 AM EST

PDB ID : 6XRE
EMDB ID : EMD-22294
Title : Structure of the p53/RNA polymerase II assembly
Authors : Liou, S.-H.; Singh, S.; Singer, R.H.; Coleman, R.A.; Liu, W.
Deposited on : 2020-07-12
Resolution : 4.60 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) : 2.31.2

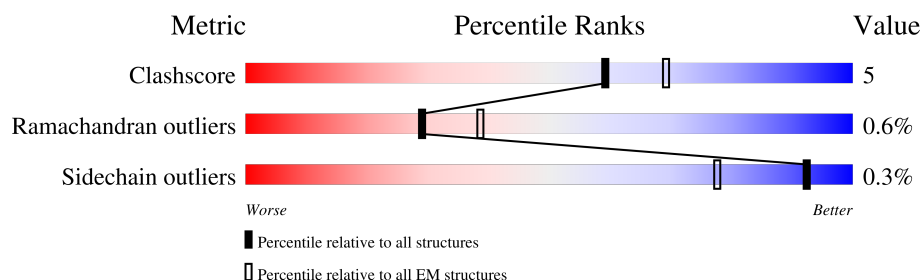
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	 85% 10% 6%
10	J	67	 88% 10% .
11	K	117	 89% 11%
12	L	58	 74% 5% 21%
13	M	393	 19% 67% 9% . . 20%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 68542 atoms, of which 34248 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 II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1467	Total	C	H	N	O	S	0	0
			23335	7301	11709	2073	2179	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1150	Total	C	H	N	O	S	0	0
			18407	5807	9209	1619	1710	62		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	275	Total	C	H	N	O	S	0	0
			4368	1386	2155	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	129	Total	C	H	N	O	S	0	0
			2105	665	1043	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	207	Total	C	H	N	O	S	0	0
			3425	1075	1726	298	318	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	78	Total	C	H	N	O	S	0	0
			1287	402	660	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2707	875	1356	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	150	Total	C	H	N	O	S	0	0
			2371	764	1166	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	118	Total	C	H	N	O	S	0	0
			1851	592	893	170	185	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	67	Total	C	H	N	O	S	0	0
			1088	345	555	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	117	Total	C	H	N	O	S	0	0
			1894	604	957	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			786	241	398	75	66	6		

- Molecule 13 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	314	Total	C	H	N	O	S	0	0
			4909	1550	2421	444	475	19		

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

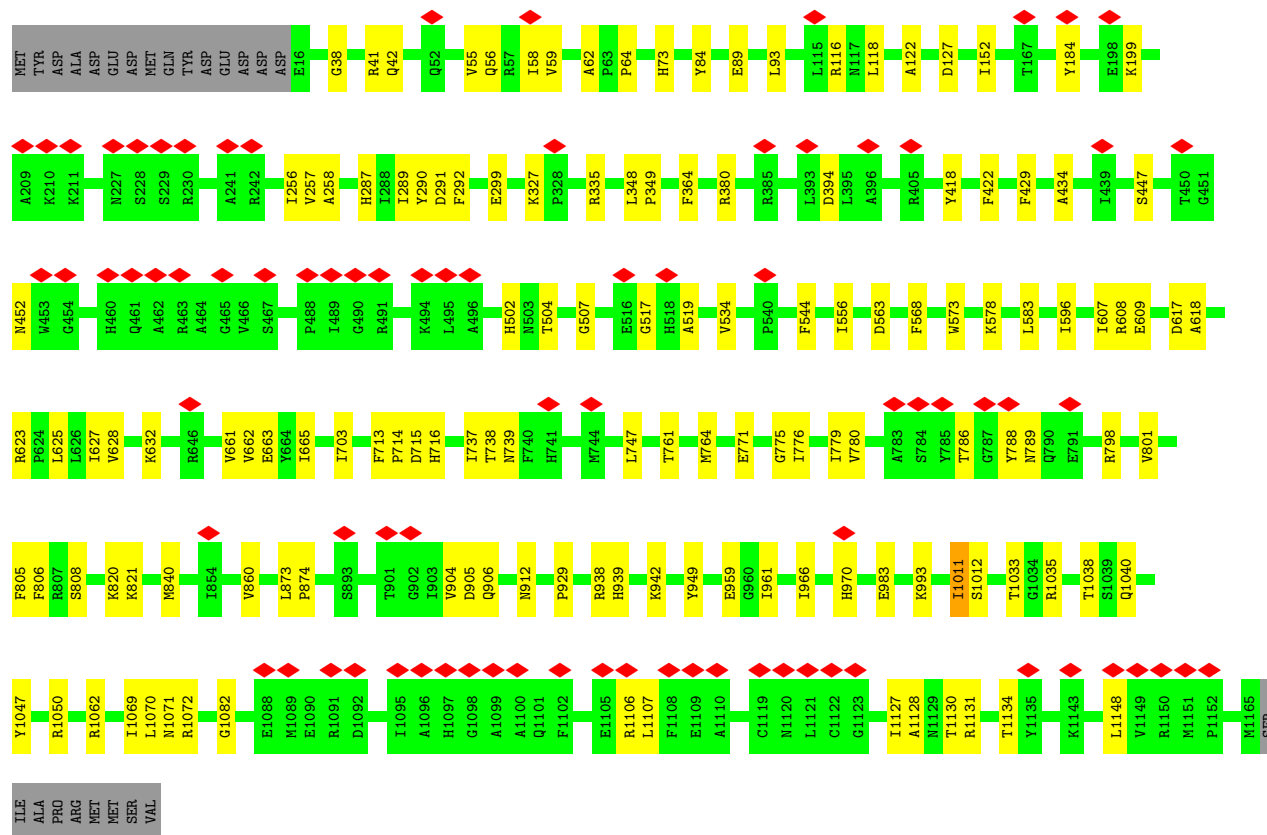
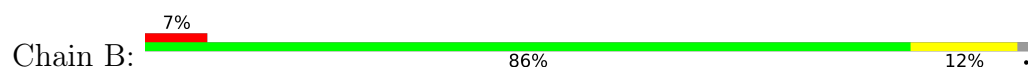
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

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

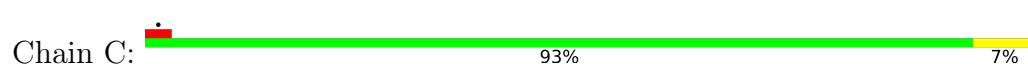
Mol	Chain	Residues	Atoms		AltConf
15	A	3	Total	Zn	0
			3	3	
15	B	1	Total	Zn	0
			1	1	
15	C	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	
15	L	1	Total	Zn	0
			1	1	

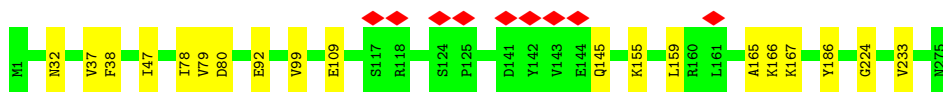
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- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

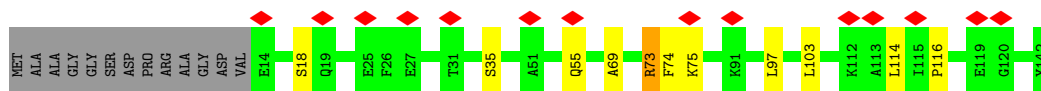
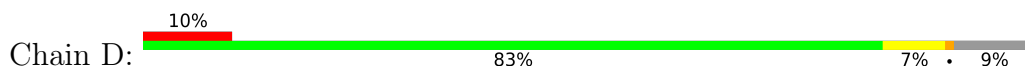


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

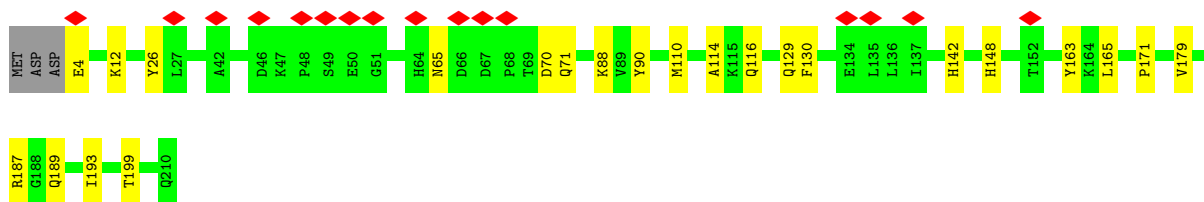
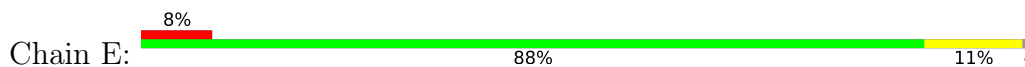




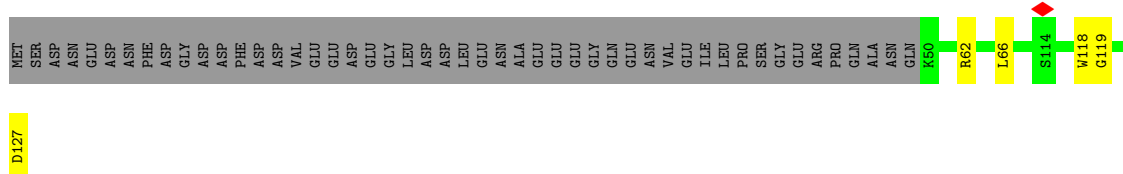
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



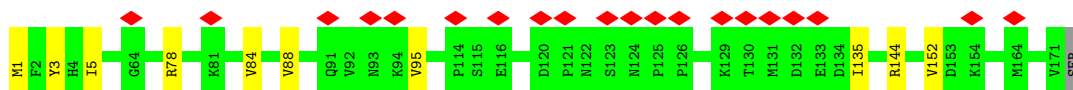
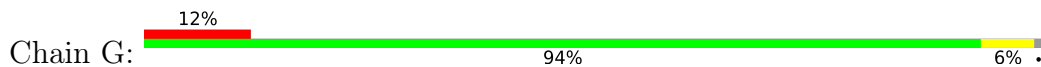
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



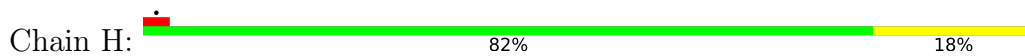
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



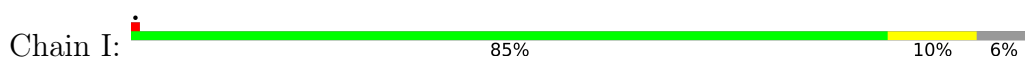
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

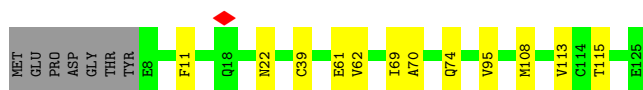


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

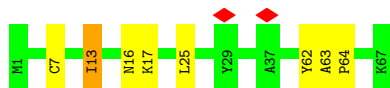
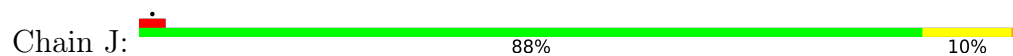


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

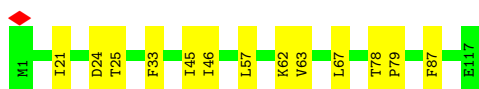




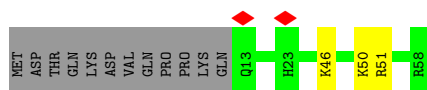
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



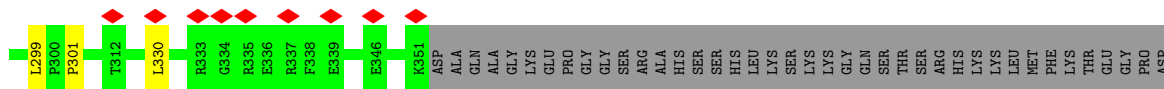
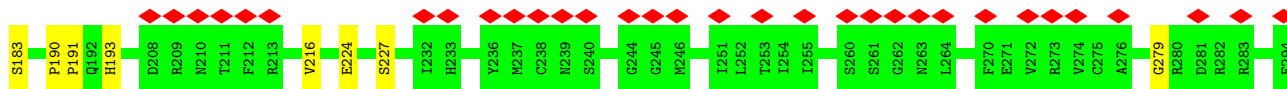
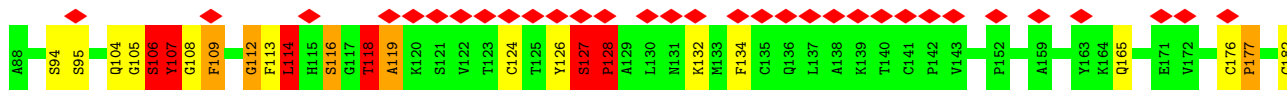
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: Cellular tumor antigen p53



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92522	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 ($e^-/\text{\AA}^2$)	1.16	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	0.047	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	0.77	13/11840 (0.1%)	0.56	6/15983 (0.0%)
2	B	0.69	0/9382	0.55	1/12667 (0.0%)
3	C	0.75	0/2259	0.51	0/3073
4	D	0.88	0/1077	0.44	0/1446
5	E	0.76	0/1729	0.55	0/2336
6	F	0.76	0/637	0.55	0/861
7	G	0.64	0/1382	0.52	0/1874
8	H	0.71	0/1227	0.55	0/1654
9	I	0.73	0/981	0.53	0/1329
10	J	0.68	0/542	0.57	0/730
11	K	0.75	0/956	0.47	0/1294
12	L	0.72	0/394	0.58	0/524
13	M	0.98	9/2553 (0.4%)	1.25	21/3466 (0.6%)
All	All	0.76	22/34959 (0.1%)	0.62	28/47237 (0.1%)

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	A	0	1
13	M	0	7
All	All	0	8

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	PRO	N-CA	13.61	1.70	1.47
1	A	623	PRO	N-CA	13.44	1.70	1.47
13	M	47	PRO	N-CA	13.28	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	PRO	N-CA	13.19	1.69	1.47
13	M	177	PRO	N-CA	13.17	1.69	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	127	SER	C-N-CD	-48.09	14.80	120.60
13	M	53	TRP	C-N-CA	13.00	154.20	121.70
1	A	582	PRO	CA-N-CD	-9.75	97.85	111.50
13	M	177	PRO	CA-N-CD	-9.42	98.31	111.50
13	M	116	SER	O-C-N	-9.40	107.23	123.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	LYS	Mainchain
13	M	106	SER	Mainchain
13	M	107	TYR	Mainchain
13	M	112	GLY	Mainchain
13	M	114	LEU	Mainchain

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	11626	11709	11706	130	0
2	B	9198	9209	9208	99	0
3	C	2213	2155	2157	14	0
4	D	1062	1043	1042	8	0
5	E	1699	1726	1725	19	0
6	F	627	660	659	3	0
7	G	1351	1356	1358	8	0
8	H	1205	1166	1168	22	0
9	I	958	893	892	8	0
10	J	533	555	557	7	0
11	K	937	957	959	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	388	398	397	2	0
13	M	2488	2421	2419	32	0
14	A	1	0	0	0	0
15	A	3	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	L	1	0	0	0	0
All	All	34294	34248	34247	330	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 330 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)
13:M:47:PRO:N	13:M:47:PRO:CA	1.69	1.48
13:M:177:PRO:N	13:M:177:PRO:CA	1.69	1.48
1:A:245:PRO:N	1:A:245:PRO:CA	1.68	1.44
1:A:623:PRO:N	1:A:623:PRO:CA	1.70	1.41
1:A:335:PRO:N	1:A:335:PRO:CA	1.70	1.40

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	1465/1970 (74%)	1348 (92%)	105 (7%)	12 (1%)	19	60
2	B	1148/1174 (98%)	1027 (90%)	119 (10%)	2 (0%)	47	81
3	C	273/275 (99%)	253 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	127/142 (89%)	125 (98%)	2 (2%)	0	100	100
5	E	205/210 (98%)	200 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100	100
7	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
8	H	148/150 (99%)	128 (86%)	20 (14%)	0	100	100
9	I	116/125 (93%)	109 (94%)	7 (6%)	0	100	100
10	J	65/67 (97%)	60 (92%)	4 (6%)	1 (2%)	10	46
11	K	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	M	310/393 (79%)	259 (84%)	41 (13%)	10 (3%)	4	30
All	All	4261/4980 (86%)	3900 (92%)	336 (8%)	25 (1%)	29	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	A	582	PRO
1	A	623	PRO
13	M	54	PHE
13	M	118	THR

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	1290/1748 (74%)	1283 (100%)	7 (0%)	88	93
2	B	1006/1028 (98%)	1005 (100%)	1 (0%)	93	96
3	C	252/252 (100%)	252 (100%)	0	100	100
4	D	119/126 (94%)	118 (99%)	1 (1%)	81	89
5	E	189/192 (98%)	188 (100%)	1 (0%)	88	93
6	F	68/111 (61%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	152/153 (99%)	151 (99%)	1 (1%)	84	90
8	H	131/131 (100%)	131 (100%)	0	100	100
9	I	106/112 (95%)	106 (100%)	0	100	100
10	J	56/56 (100%)	55 (98%)	1 (2%)	59	77
11	K	106/106 (100%)	106 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	285/346 (82%)	284 (100%)	1 (0%)	91	94
All	All	3803/4416 (86%)	3790 (100%)	13 (0%)	92	95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1011	ILE
4	D	73	ARG
13	M	132	LYS
7	G	78	ARG
10	J	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	525	ASN
2	B	716	HIS
11	K	65	HIS
4	D	38	HIS
5	E	129	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

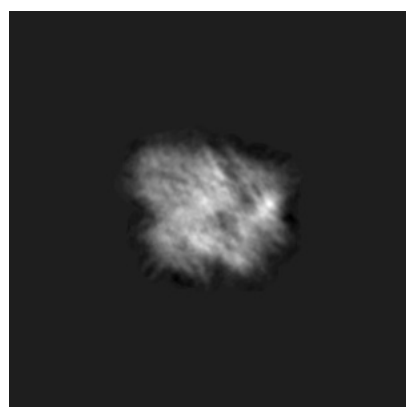
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22294. These allow visual inspection of the internal detail of the map and identification of artifacts.

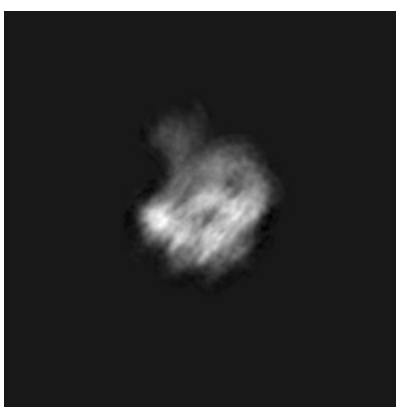
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

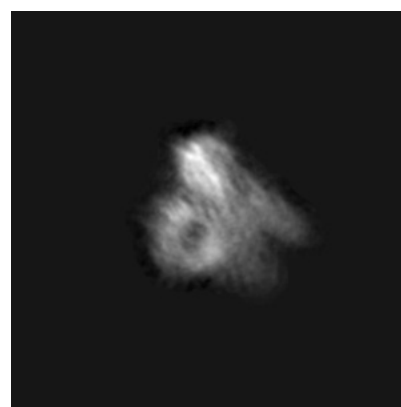
6.1.1 Primary map



X



Y

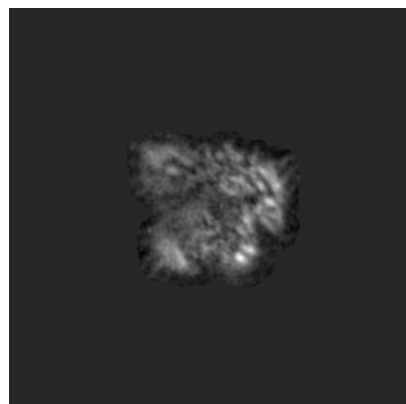


Z

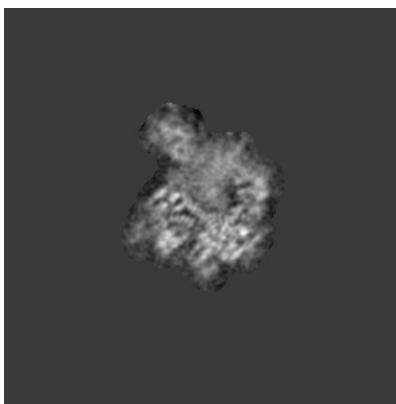
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

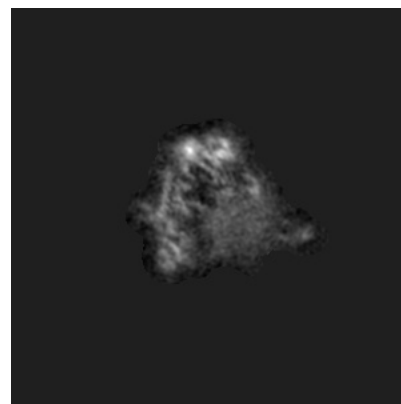
6.2.1 Primary map



X Index: 150



Y Index: 150

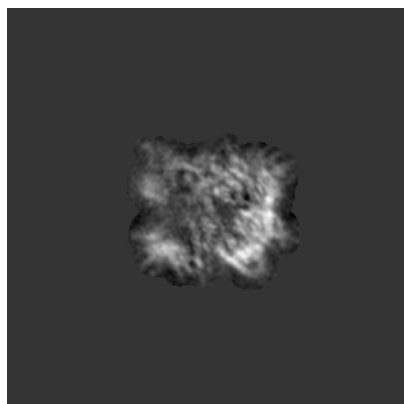


Z Index: 150

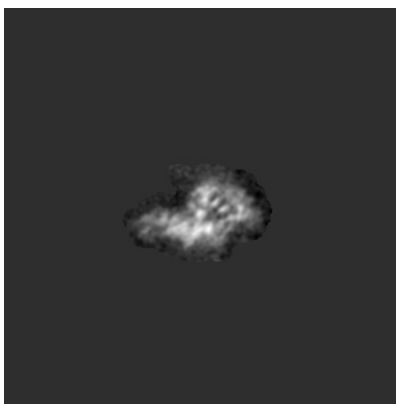
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

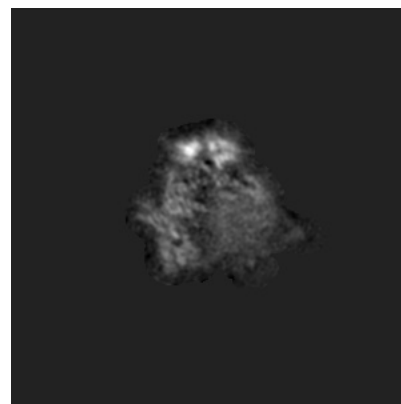
6.3.1 Primary map



X Index: 140



Y Index: 190

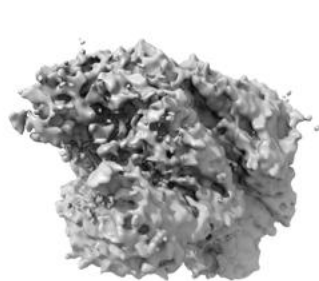


Z Index: 153

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

6.4 Orthogonal surface views [i](#)

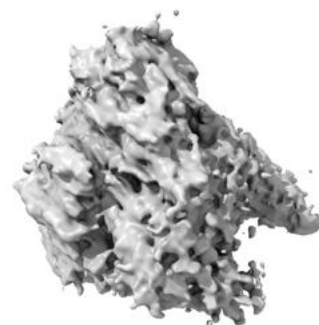
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

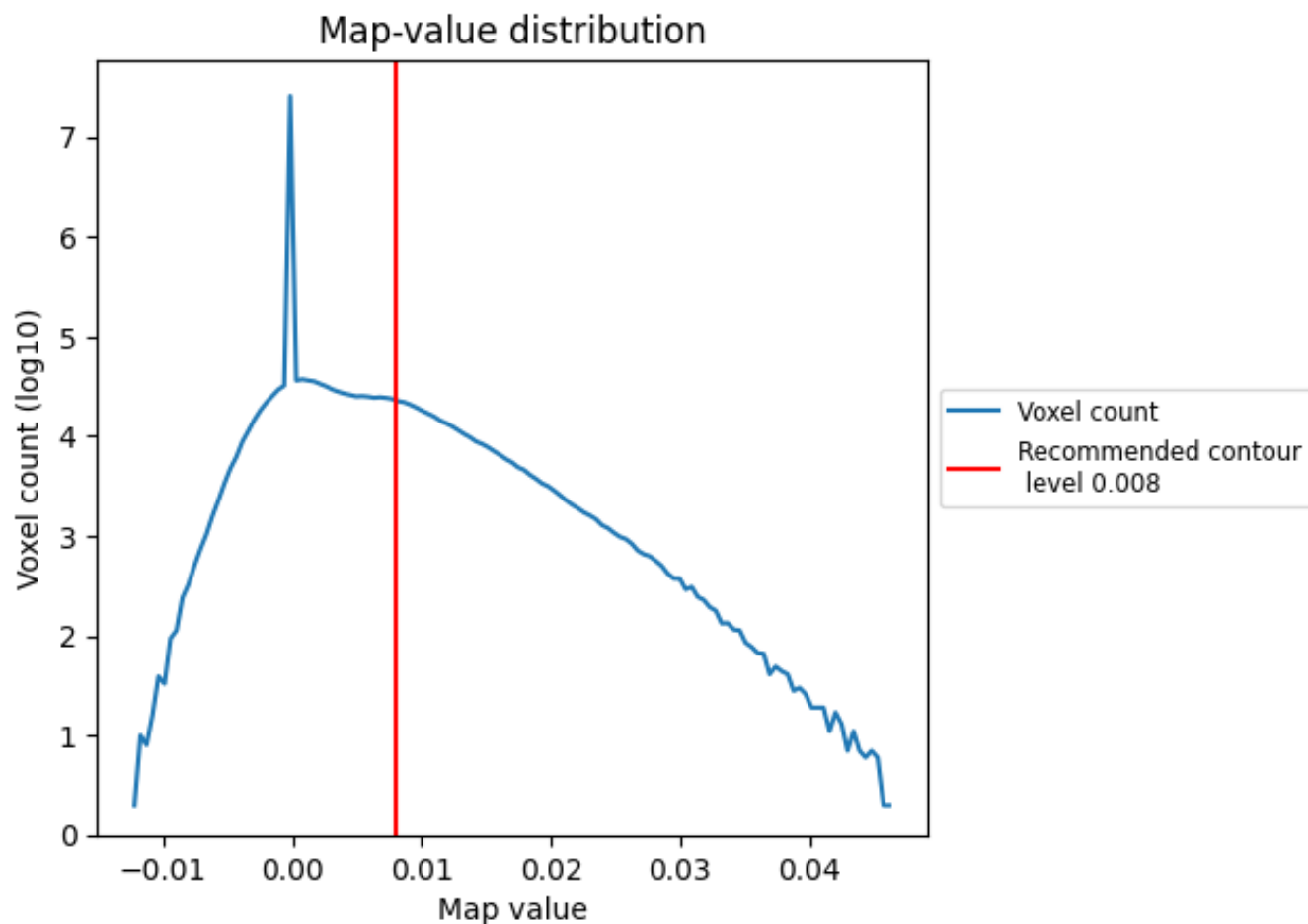
6.5 Mask visualisation

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

7 Map analysis [i](#)

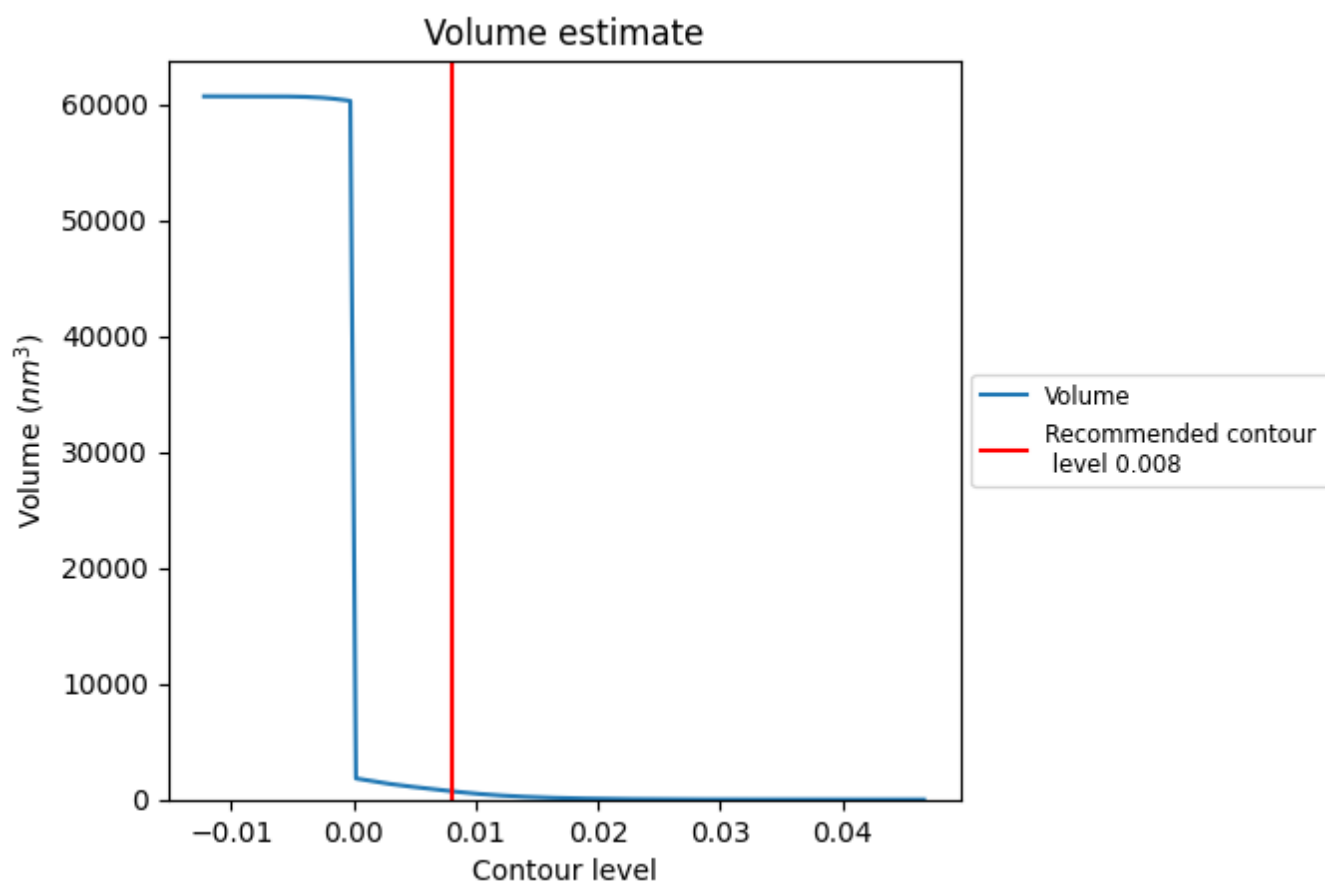
This section contains the results of statistical analysis of the map.

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.

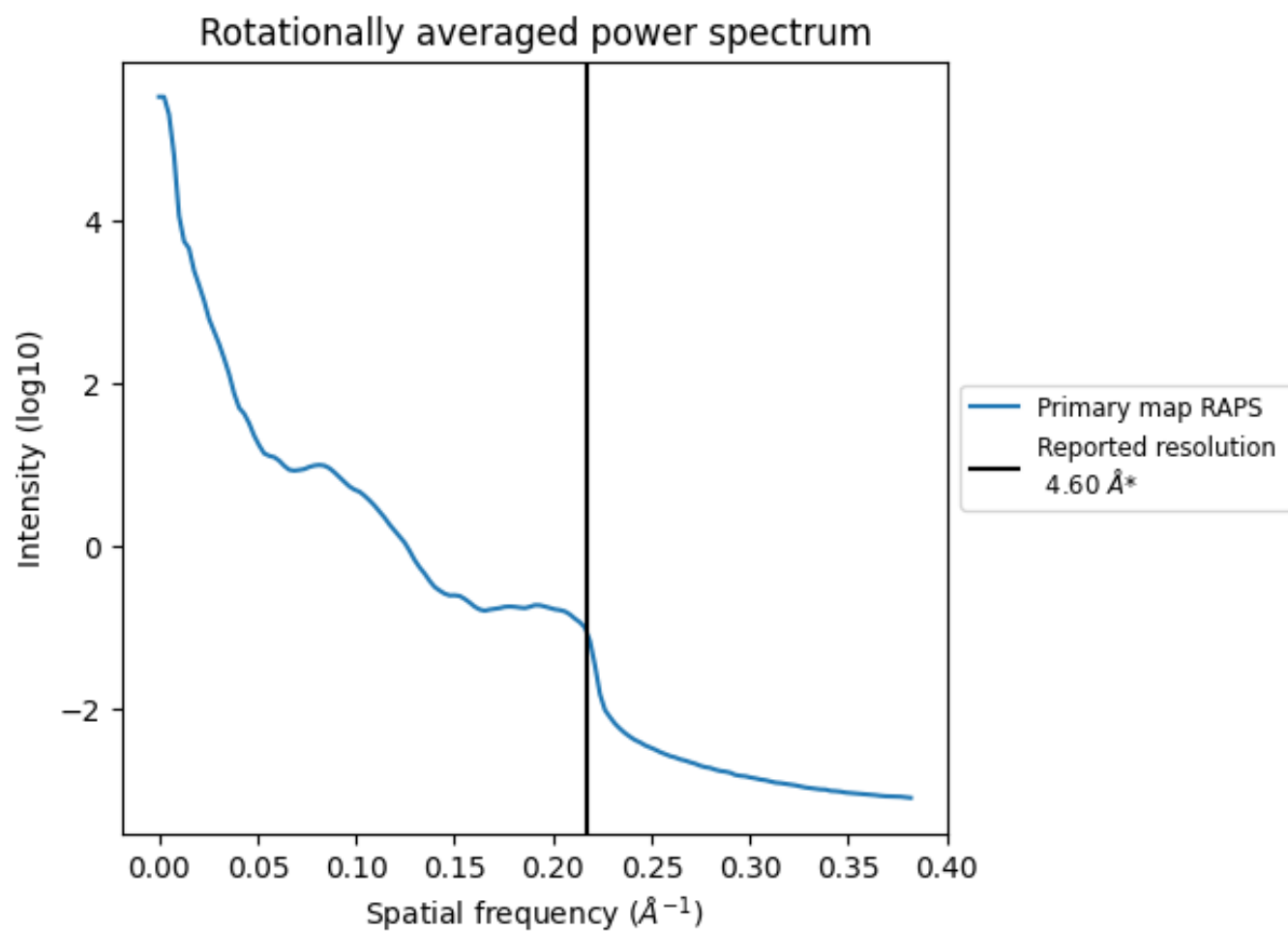
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 721 nm³; this corresponds to an approximate mass of 652 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 ⓘ

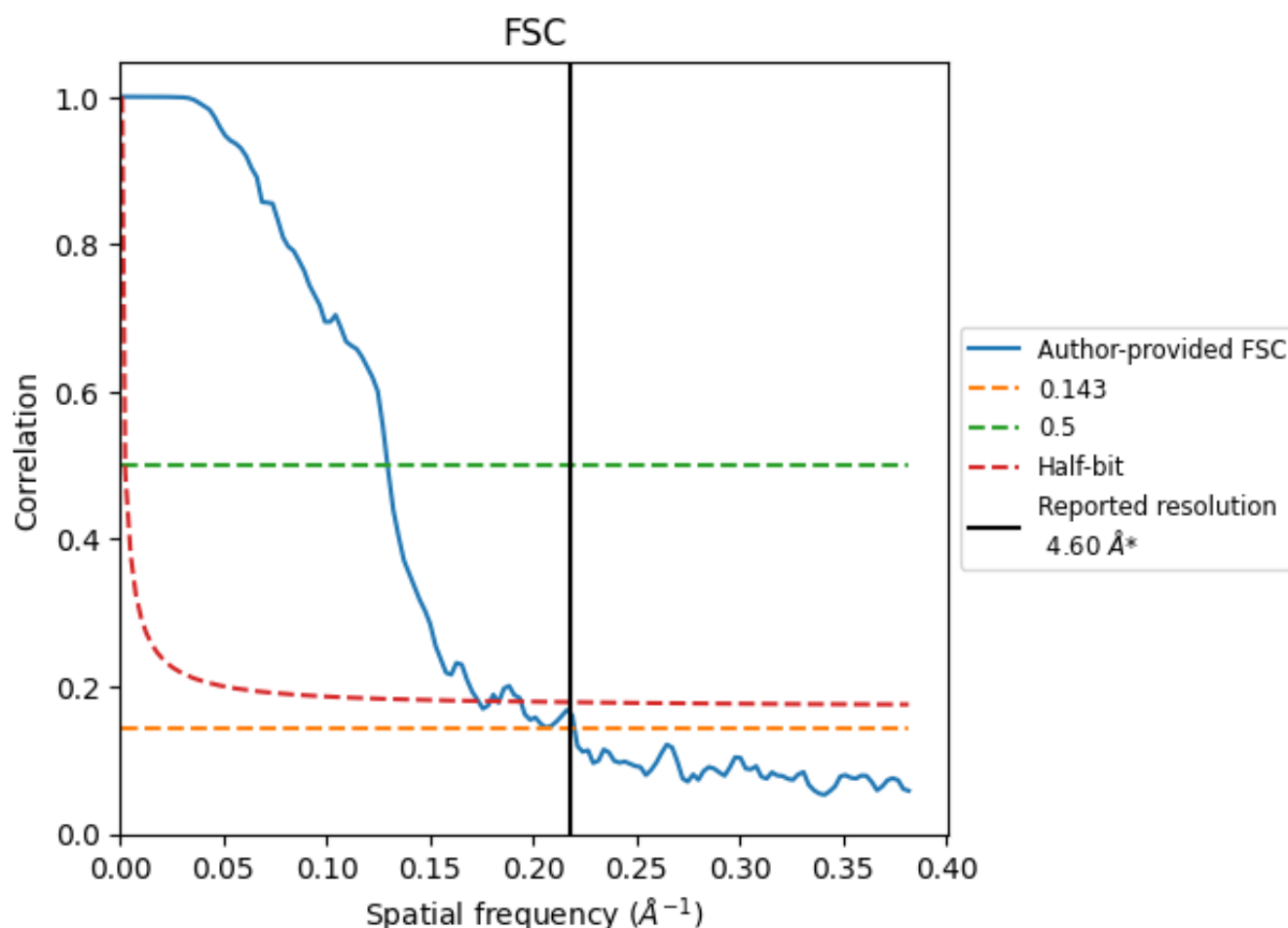


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

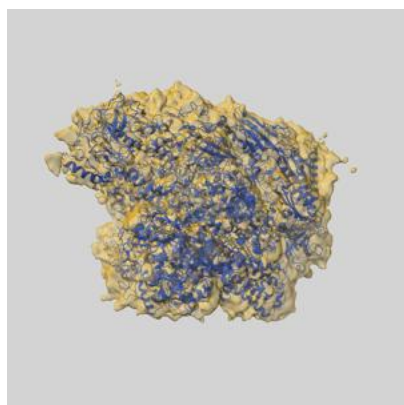
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.55	7.73	5.77
Unmasked-calculated*	-	-	-

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

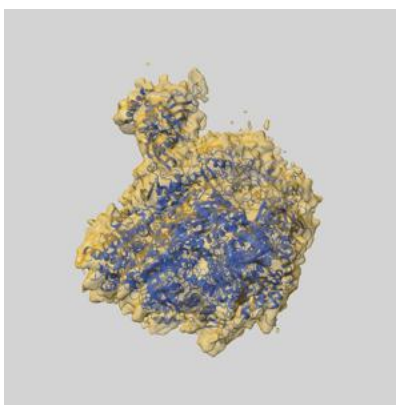
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22294 and PDB model 6XRE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

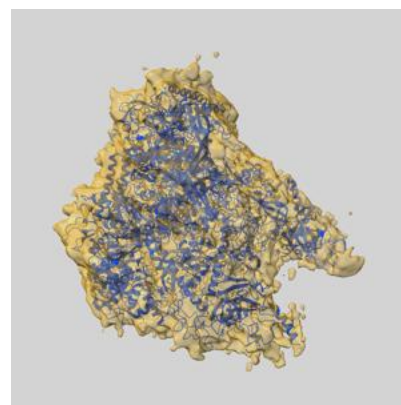
9.1 Map-model overlay [i](#)



X



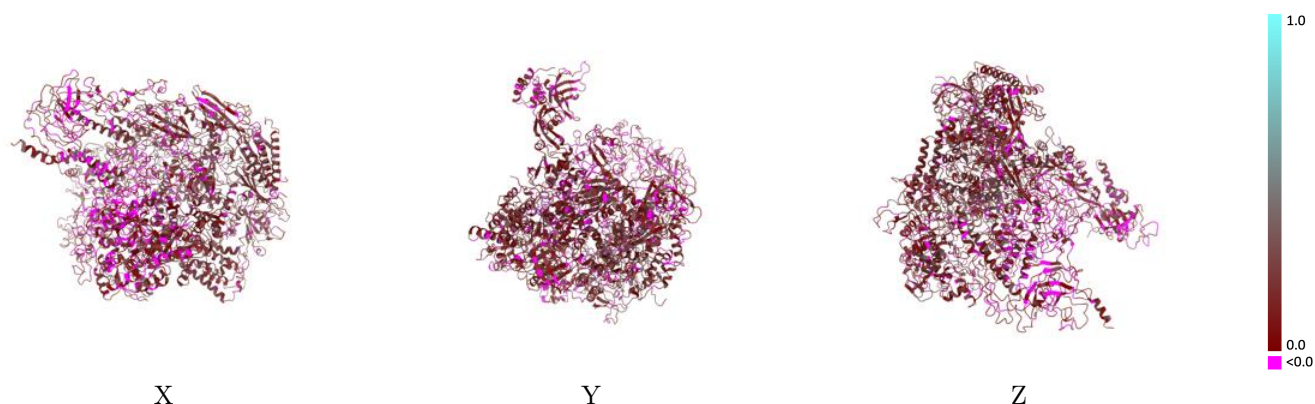
Y



Z

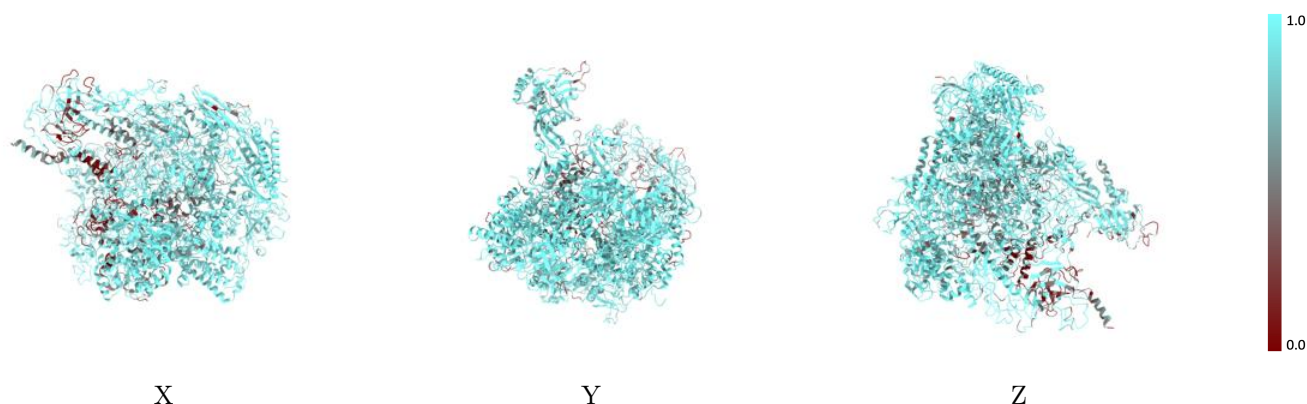
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



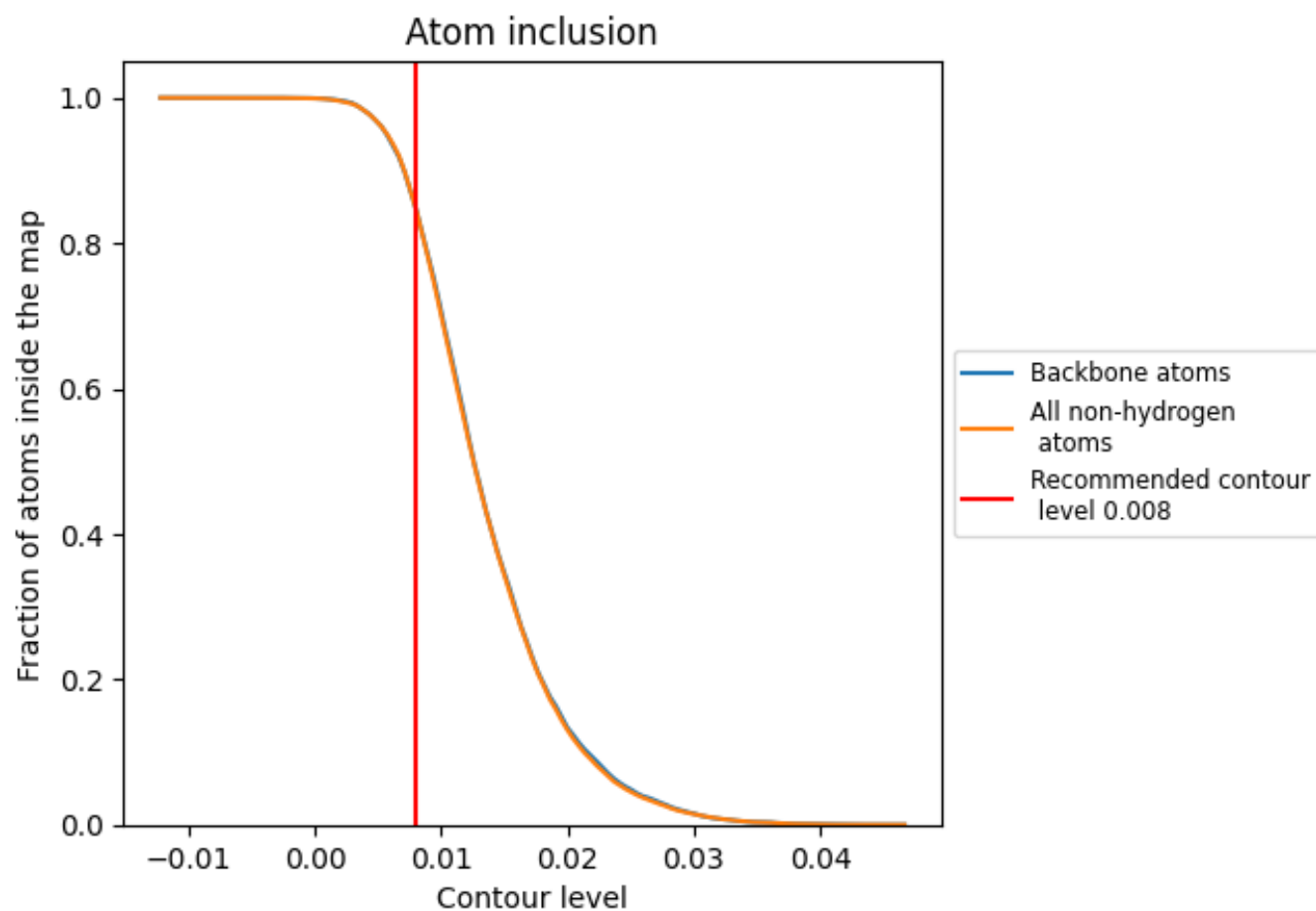
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8473	 0.1340
A	 0.8382	 0.1220
B	 0.8571	 0.1540
C	 0.9156	 0.1400
D	 0.7811	 0.0900
E	 0.8450	 0.1540
F	 0.9062	 0.1770
G	 0.8056	 0.0950
H	 0.9177	 0.1290
I	 0.9361	 0.1400
J	 0.9154	 0.1500
K	 0.9774	 0.1900
L	 0.9086	 0.1210
M	 0.7032	 0.0980

