



## wwPDB EM Validation Summary Report ⓘ

Apr 11, 2024 – 04:35 pm BST

PDB ID : 8QYS  
EMDB ID : EMD-18761  
Title : Human preholo proteasome 20S core particle  
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;  
Walsh Jr, R.M.; Goodall, E.A.  
Deposited on : 2023-10-26  
Resolution : 3.89 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

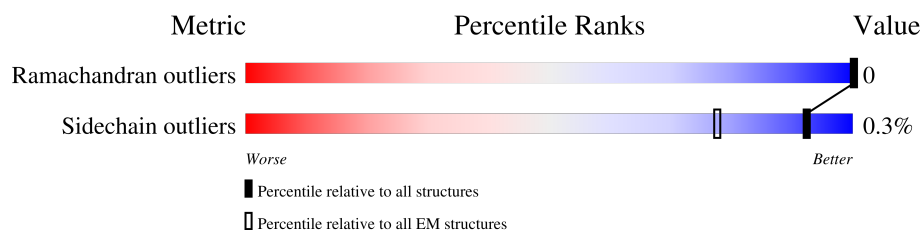
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 3.89 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.



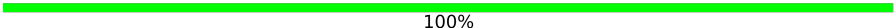
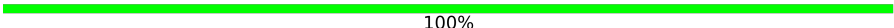

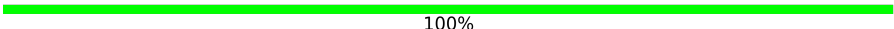
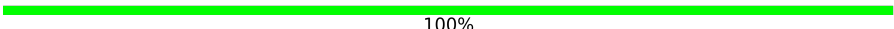




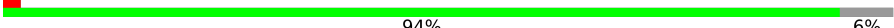

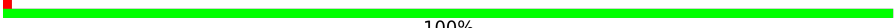
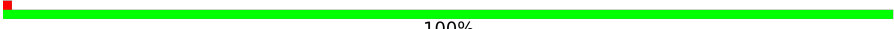
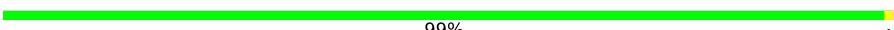
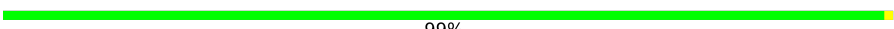
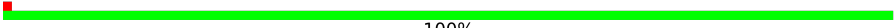
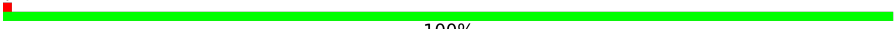
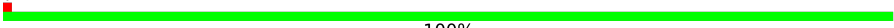
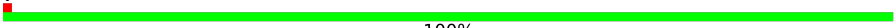
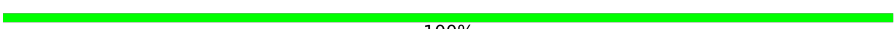
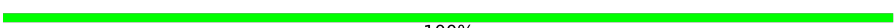
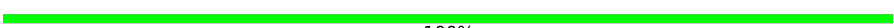
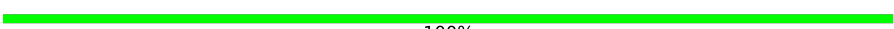


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	234	98% .
1	R	234	98% .
2	B	248	100%
2	S	248	100%
3	C	234	100%
3	T	234	100%
4	D	240	98% .
4	U	240	98% .
5	E	241	100%

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Mol	Chain	Length	Quality of chain
5	V	241	 100%
6	F	241	 100%
6	W	241	 100%
7	G	244	 100%
7	X	244	 100%
8	H	141	 83% 16%
8	Y	141	 83% 16%
9	I	288	 93% 7%
9	Z	288	 93% 7%
10	J	264	 94% 6%
10	a	264	 94% 6%
11	K	262	 100%
11	b	262	 100%
12	L	203	 99%
12	c	203	 99%
13	M	197	 100%
13	d	197	 100%
14	N	208	 100%
14	e	208	 100%
15	O	212	 100%
15	f	212	 100%
16	P	208	 100%
16	g	208	 100%
17	Q	197	 100%
17	h	197	 100%

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 57862 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1720	1106	293	315	6		
1	R	229	Total	C	N	O	S	0	0
			1720	1106	293	315	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			1808	1149	311	338	10		
2	S	248	Total	C	N	O	S	0	0
			1808	1149	311	338	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1744	1095	315	329	5		
3	T	234	Total	C	N	O	S	0	0
			1744	1095	315	329	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1760	1110	294	344	12		
4	U	236	Total	C	N	O	S	0	0
			1760	1110	294	344	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	241	Total	C	N	O	S	0	0
			1863	1170	337	345	11		
5	V	241	Total	C	N	O	S	0	0
			1863	1170	337	345	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	241	Total	C	N	O	S	0	0
			1847	1172	315	349	11		
6	W	241	Total	C	N	O	S	0	0
			1847	1172	315	349	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1846	1172	314	348	12		
7	X	244	Total	C	N	O	S	0	0
			1846	1172	314	348	12		

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	118	Total	C	N	O	S	0	0
			937	595	157	180	5		
8	Y	118	Total	C	N	O	S	0	0
			937	595	157	180	5		

- Molecule 9 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	268	Total	C	N	O	S	0	0
			2040	1312	335	378	15		
9	Z	268	Total	C	N	O	S	0	0
			2040	1312	335	378	15		

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	248	Total	C	N	O	S	0	0
			1885	1216	307	348	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	248	Total	C	N	O	S	0	0
			1885	1216	307	348	14		

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	262	Total	C	N	O	S	0	0
			1980	1249	343	375	13		
11	b	262	Total	C	N	O	S	0	0
			1980	1249	343	375	13		

- Molecule 12 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	203	Total	C	N	O	S	0	0
			1585	1010	264	292	19		
12	c	203	Total	C	N	O	S	0	0
			1585	1010	264	292	19		

- Molecule 13 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	197	Total	C	N	O	S	0	0
			1568	1006	265	288	9		
13	d	197	Total	C	N	O	S	0	0
			1568	1006	265	288	9		

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	208	Total	C	N	O	S	0	0
			1607	1014	280	303	10		
14	e	208	Total	C	N	O	S	0	0
			1607	1014	280	303	10		

- Molecule 15 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
15	f	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	208	Total	C	N	O	S	0	0
			1623	1024	279	309	11		
16	g	208	Total	C	N	O	S	0	0
			1623	1024	279	309	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	234	THR	ILE	variant	UNP P28070
g	234	THR	ILE	variant	UNP P28070

- Molecule 17 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	197	Total	C	N	O	S	0	0
			1475	923	253	287	12		
17	h	197	Total	C	N	O	S	0	0
			1475	923	253	287	12		

There are 2 discrepancies between the modelled and reference sequences:

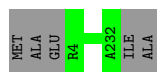
Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	GLY	VAL	variant	UNP P28072
h	145	GLY	VAL	variant	UNP P28072

### 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.

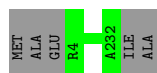
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98%



- Molecule 1: Proteasome subunit alpha type-2

Chain R:  98%



- Molecule 2: Proteasome subunit alpha type-4

Chain B:  100%



- Molecule 2: Proteasome subunit alpha type-4

Chain S:  100%




- Molecule 3: Proteasome subunit alpha type-7

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Proteasome subunit alpha type-7

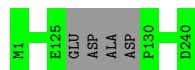


Chain T:  100%

There are no outlier residues recorded for this chain.

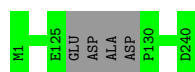
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  98%



- Molecule 4: Proteasome subunit alpha type-5

Chain U:  98%



- Molecule 5: Proteasome subunit alpha type-1

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Proteasome subunit alpha type-1

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Proteasome subunit alpha type-3

Chain F:  100%



- Molecule 6: Proteasome subunit alpha type-3

Chain W:  100%

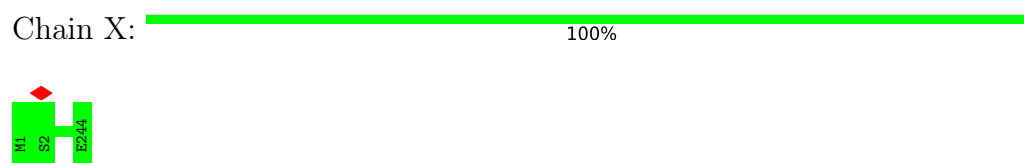


- Molecule 7: Proteasome subunit alpha type-6

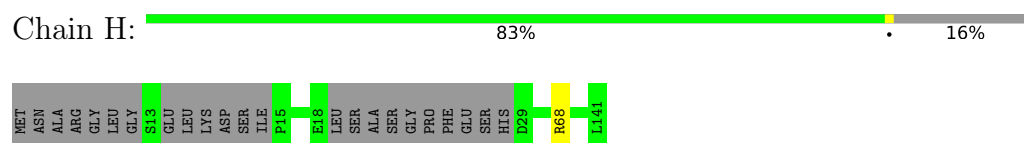
Chain G:  100%



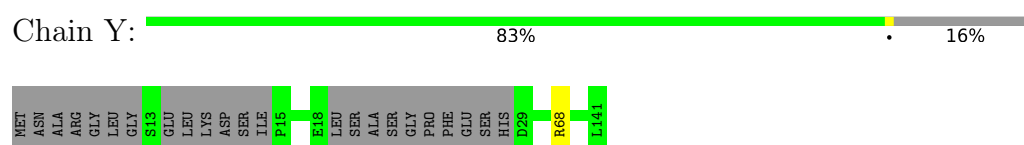
- Molecule 7: Proteasome subunit alpha type-6



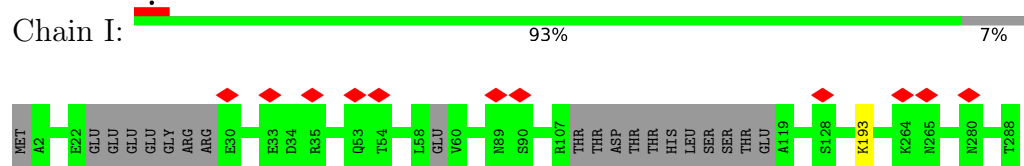
- Molecule 8: Proteasome maturation protein



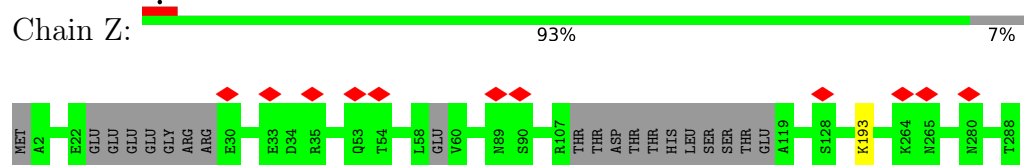
- Molecule 8: Proteasome maturation protein



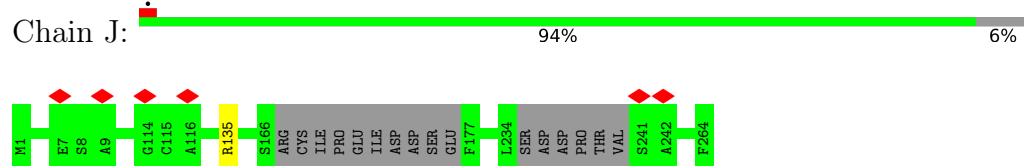
- Molecule 9: Proteasome assembly chaperone 1



- Molecule 9: Proteasome assembly chaperone 1

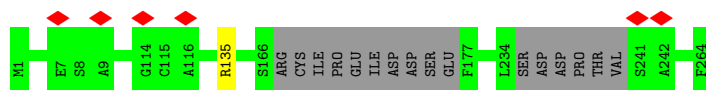


- Molecule 10: Proteasome assembly chaperone 2



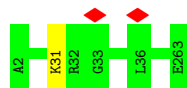
- Molecule 10: Proteasome assembly chaperone 2





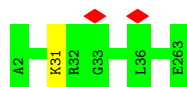
- Molecule 11: Proteasome subunit beta type-7

Chain K: 100%



- Molecule 11: Proteasome subunit beta type-7

Chain b: 100%



- Molecule 12: Proteasome subunit beta type-3

Chain L: 99%



- Molecule 12: Proteasome subunit beta type-3

Chain c: 99%



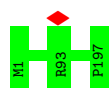
- Molecule 13: Proteasome subunit beta type-2

Chain M: 100%



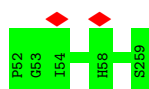
- Molecule 13: Proteasome subunit beta type-2

Chain d: 100%



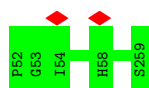
- Molecule 14: Proteasome subunit beta type-5

Chain N:  100%



- Molecule 14: Proteasome subunit beta type-5

Chain e:  100%



- Molecule 15: Proteasome subunit beta type-1

Chain O:  100%



- Molecule 15: Proteasome subunit beta type-1

Chain f:  100%



- Molecule 16: Proteasome subunit beta type-4

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: Proteasome subunit beta type-4

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Proteasome subunit beta type-6

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Proteasome subunit beta type-6

Chain h:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.688	Depositor
Minimum map value	-1.302	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.37	Depositor
Map size ( $\text{\AA}$ )	316.68, 316.68, 316.68	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.885, 1.885, 1.885	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/1759	0.48	0/2394
1	R	0.27	0/1759	0.48	0/2394
2	B	0.26	0/1837	0.49	0/2499
2	S	0.25	0/1837	0.48	0/2499
3	C	0.25	0/1767	0.50	0/2399
3	T	0.25	0/1767	0.50	0/2399
4	D	0.27	0/1788	0.50	0/2422
4	U	0.27	0/1788	0.50	0/2422
5	E	0.25	0/1899	0.53	0/2572
5	V	0.25	0/1899	0.53	0/2572
6	F	0.26	0/1882	0.49	0/2542
6	W	0.26	0/1882	0.49	0/2542
7	G	0.25	0/1879	0.49	0/2547
7	X	0.25	0/1879	0.49	0/2547
8	H	0.26	0/951	0.49	0/1277
8	Y	0.26	0/951	0.50	0/1277
9	I	0.24	0/2083	0.47	0/2839
9	Z	0.24	0/2083	0.47	0/2839
10	J	0.25	0/1925	0.47	0/2615
10	a	0.25	0/1925	0.47	0/2615
11	K	0.26	0/2015	0.49	0/2726
11	b	0.25	0/2015	0.49	0/2726
12	L	0.27	0/1614	0.53	0/2176
12	c	0.27	0/1614	0.53	0/2176
13	M	0.32	0/1601	0.51	0/2168
13	d	0.32	0/1601	0.51	0/2168
14	N	0.27	0/1640	0.53	0/2215
14	e	0.27	0/1640	0.53	0/2215
15	O	0.27	0/1673	0.51	0/2254
15	f	0.26	0/1673	0.50	0/2254
16	P	0.27	0/1654	0.52	0/2238
16	g	0.27	0/1654	0.52	0/2238
17	Q	0.27	0/1501	0.51	0/2030
17	h	0.27	0/1501	0.51	0/2030

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.26	0/58936	0.50	0/79826

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	227/234 (97%)	199 (88%)	28 (12%)	0	100	100
1	R	227/234 (97%)	199 (88%)	28 (12%)	0	100	100
2	B	246/248 (99%)	211 (86%)	35 (14%)	0	100	100
2	S	246/248 (99%)	210 (85%)	36 (15%)	0	100	100
3	C	232/234 (99%)	206 (89%)	26 (11%)	0	100	100
3	T	232/234 (99%)	206 (89%)	26 (11%)	0	100	100
4	D	232/240 (97%)	215 (93%)	17 (7%)	0	100	100
4	U	232/240 (97%)	215 (93%)	17 (7%)	0	100	100
5	E	239/241 (99%)	210 (88%)	29 (12%)	0	100	100
5	V	239/241 (99%)	211 (88%)	28 (12%)	0	100	100
6	F	239/241 (99%)	215 (90%)	24 (10%)	0	100	100
6	W	239/241 (99%)	215 (90%)	24 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	242/244 (99%)	226 (93%)	16 (7%)	0	100	100
7	X	242/244 (99%)	227 (94%)	15 (6%)	0	100	100
8	H	113/141 (80%)	100 (88%)	13 (12%)	0	100	100
8	Y	113/141 (80%)	100 (88%)	13 (12%)	0	100	100
9	I	260/288 (90%)	234 (90%)	26 (10%)	0	100	100
9	Z	260/288 (90%)	234 (90%)	26 (10%)	0	100	100
10	J	242/264 (92%)	229 (95%)	13 (5%)	0	100	100
10	a	242/264 (92%)	229 (95%)	13 (5%)	0	100	100
11	K	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
11	b	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
12	L	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
12	c	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
13	M	195/197 (99%)	167 (86%)	28 (14%)	0	100	100
13	d	195/197 (99%)	167 (86%)	28 (14%)	0	100	100
14	N	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
14	e	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
15	O	210/212 (99%)	186 (89%)	24 (11%)	0	100	100
15	f	210/212 (99%)	185 (88%)	25 (12%)	0	100	100
16	P	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
16	g	206/208 (99%)	188 (91%)	18 (9%)	0	100	100
17	Q	195/197 (99%)	175 (90%)	20 (10%)	0	100	100
17	h	195/197 (99%)	175 (90%)	20 (10%)	0	100	100
All	All	7490/7724 (97%)	6737 (90%)	753 (10%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/191 (90%)	171 (100%)	0	100	100
1	R	171/191 (90%)	171 (100%)	0	100	100
2	B	173/208 (83%)	173 (100%)	0	100	100
2	S	173/208 (83%)	173 (100%)	0	100	100
3	C	173/198 (87%)	173 (100%)	0	100	100
3	T	173/198 (87%)	173 (100%)	0	100	100
4	D	186/202 (92%)	186 (100%)	0	100	100
4	U	186/202 (92%)	186 (100%)	0	100	100
5	E	197/207 (95%)	197 (100%)	0	100	100
5	V	197/207 (95%)	197 (100%)	0	100	100
6	F	189/198 (96%)	188 (100%)	1 (0%)	88	93
6	W	189/198 (96%)	188 (100%)	1 (0%)	88	93
7	G	193/208 (93%)	193 (100%)	0	100	100
7	X	193/208 (93%)	193 (100%)	0	100	100
8	H	109/128 (85%)	108 (99%)	1 (1%)	78	87
8	Y	109/128 (85%)	108 (99%)	1 (1%)	78	87
9	I	217/262 (83%)	216 (100%)	1 (0%)	88	93
9	Z	217/262 (83%)	216 (100%)	1 (0%)	88	93
10	J	208/237 (88%)	207 (100%)	1 (0%)	88	93
10	a	208/237 (88%)	207 (100%)	1 (0%)	88	93
11	K	213/213 (100%)	212 (100%)	1 (0%)	88	93
11	b	213/213 (100%)	212 (100%)	1 (0%)	88	93
12	L	172/172 (100%)	170 (99%)	2 (1%)	71	83
12	c	172/172 (100%)	170 (99%)	2 (1%)	71	83
13	M	166/168 (99%)	166 (100%)	0	100	100
13	d	166/168 (99%)	166 (100%)	0	100	100
14	N	161/162 (99%)	161 (100%)	0	100	100
14	e	161/162 (99%)	161 (100%)	0	100	100
15	O	177/177 (100%)	176 (99%)	1 (1%)	86	91
15	f	177/177 (100%)	176 (99%)	1 (1%)	86	91
16	P	171/171 (100%)	171 (100%)	0	100	100
16	g	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	152/153 (99%)	152 (100%)	0	100	100
17	h	152/153 (99%)	152 (100%)	0	100	100
All	All	6056/6510 (93%)	6040 (100%)	16 (0%)	92	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	c	145	GLN
12	c	80	ARG
6	W	98	ASN
11	b	31	LYS
15	O	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
7	X	12	HIS
9	Z	208	GLN
15	f	180	GLN
10	a	58	ASN
10	J	58	ASN

### 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](#)

There are no ligands in this entry.

## 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.

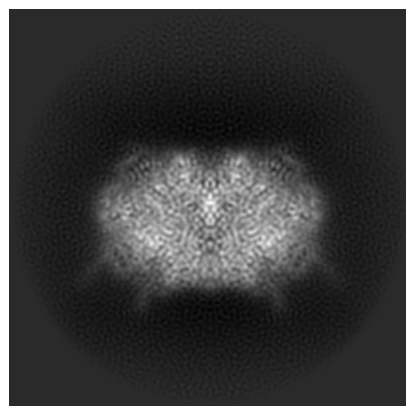
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18761. These allow visual inspection of the internal detail of the map and identification of artifacts.

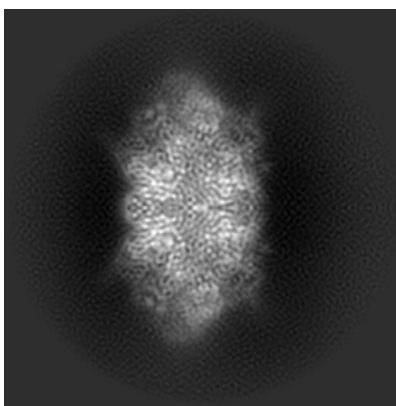
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

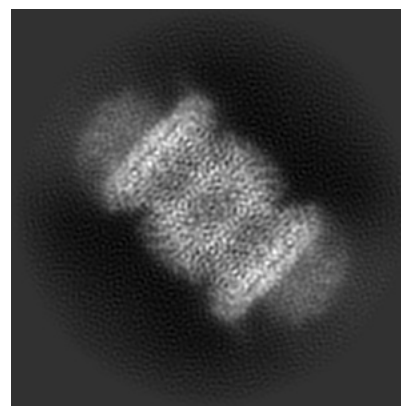
#### 6.1.1 Primary map



X

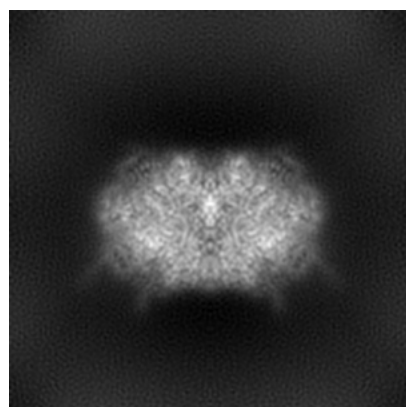


Y

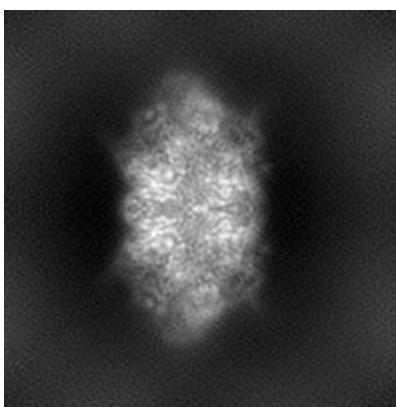


Z

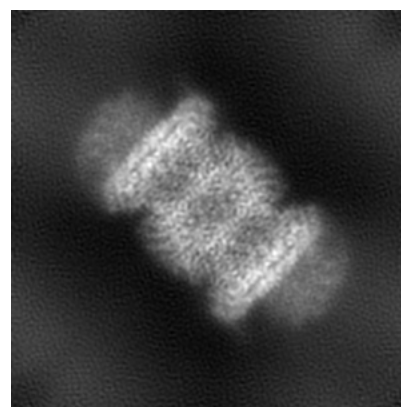
#### 6.1.2 Raw map



X



Y

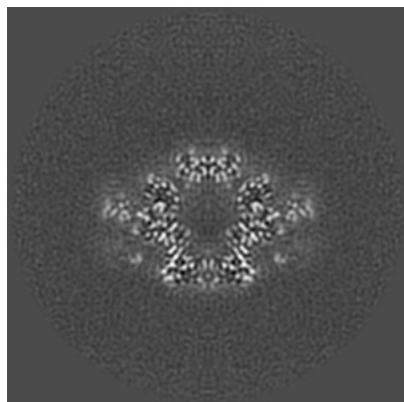


Z

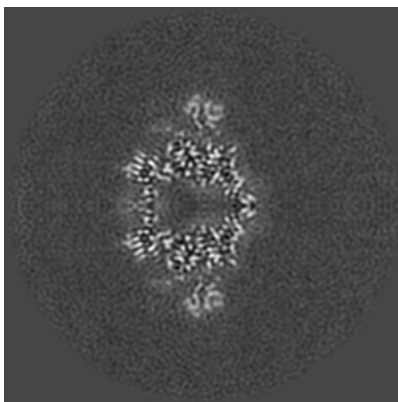
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

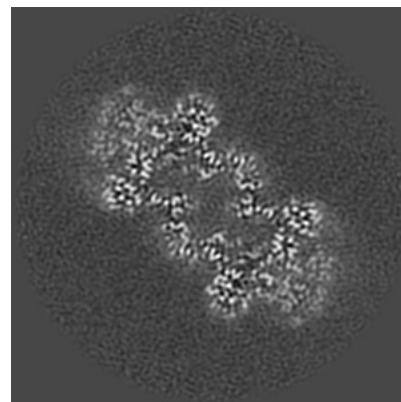
### 6.2.1 Primary map



X Index: 84

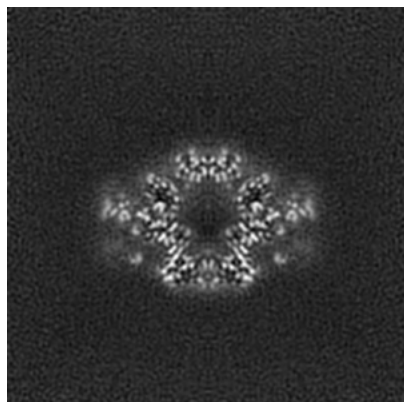


Y Index: 84

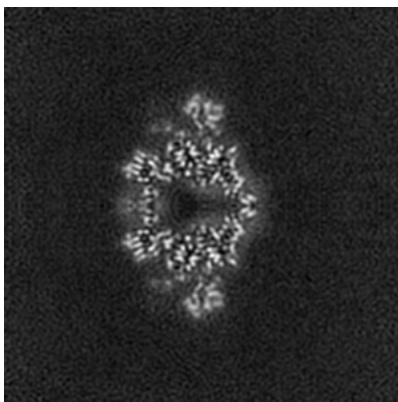


Z Index: 84

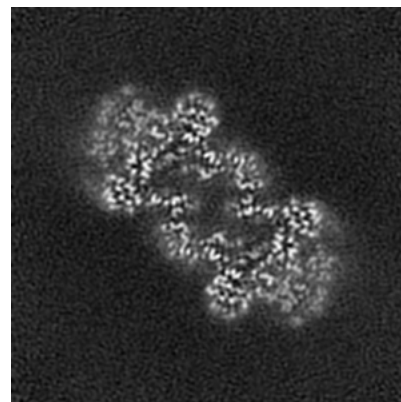
### 6.2.2 Raw map



X Index: 84



Y Index: 84

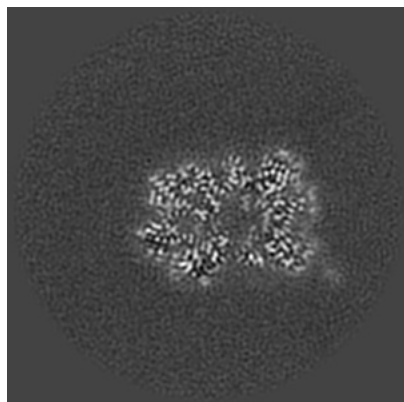


Z Index: 84

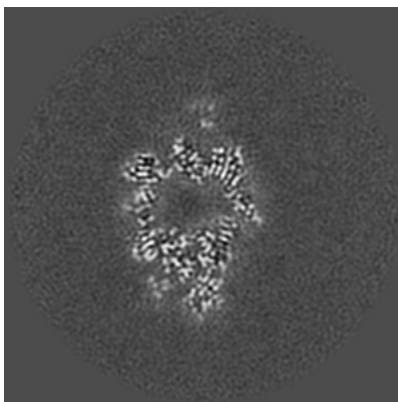
The images above show central slices of the map in three orthogonal directions.

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

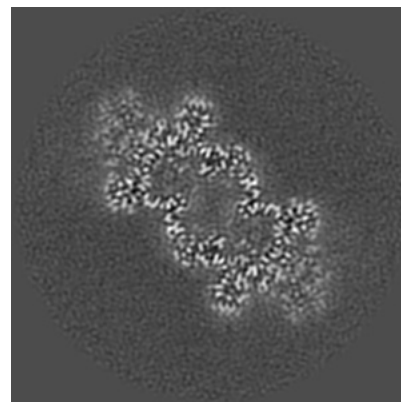
### 6.3.1 Primary map



X Index: 72

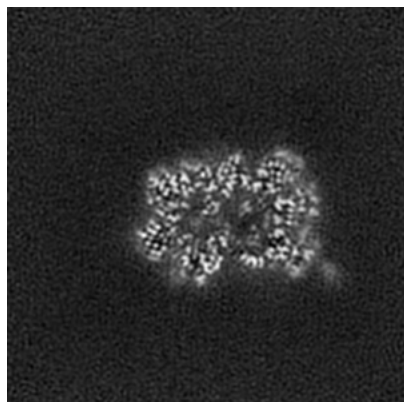


Y Index: 86

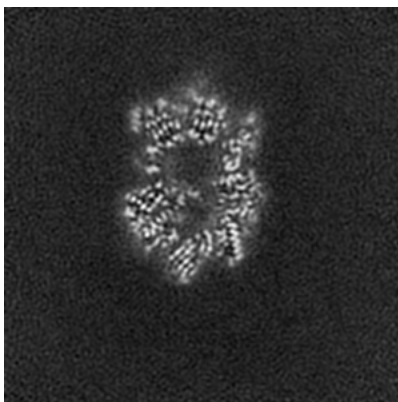


Z Index: 86

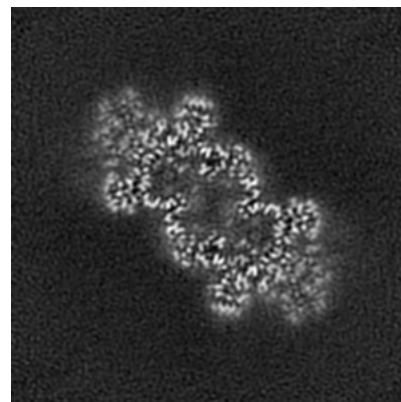
### 6.3.2 Raw map



X Index: 73



Y Index: 74



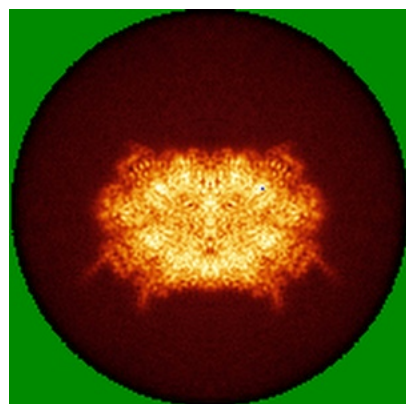
Z Index: 86

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

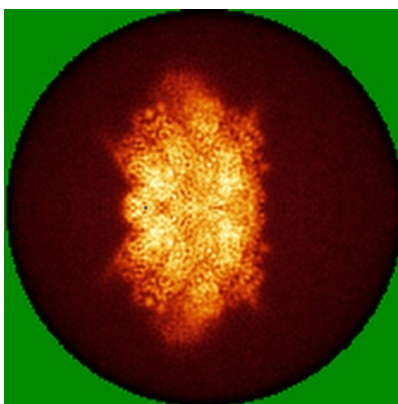


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

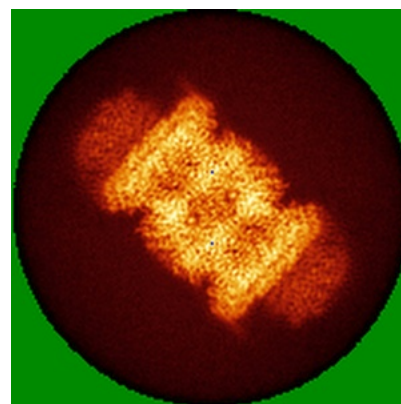
### 6.4.1 Primary map



X

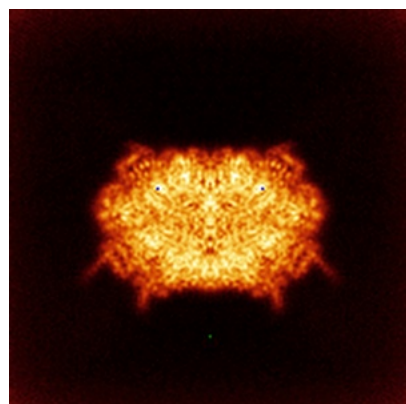


Y

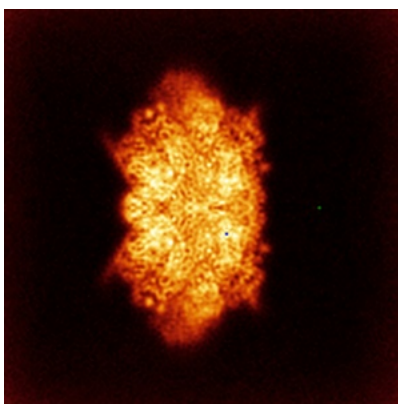


Z

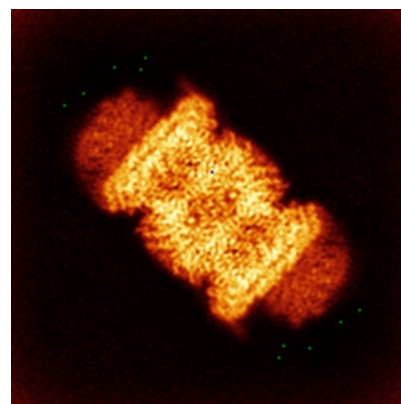
### 6.4.2 Raw map



X



Y

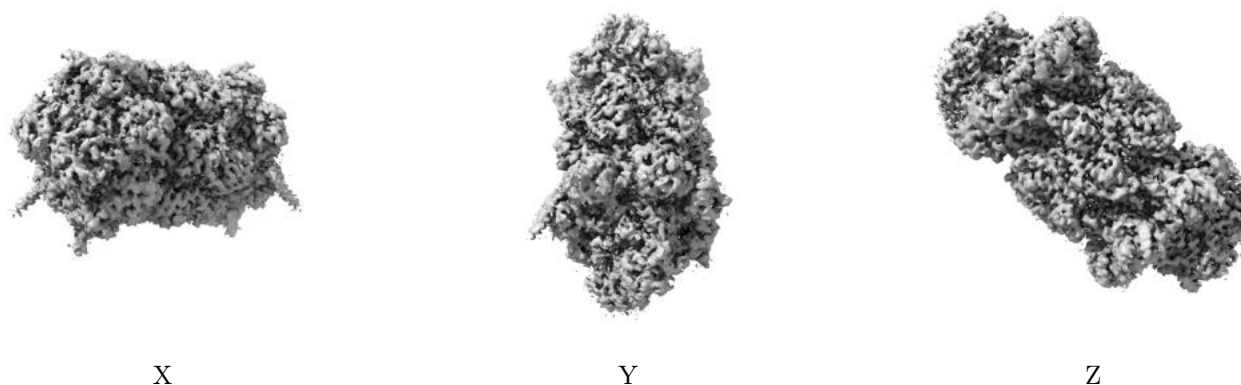


Z

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.

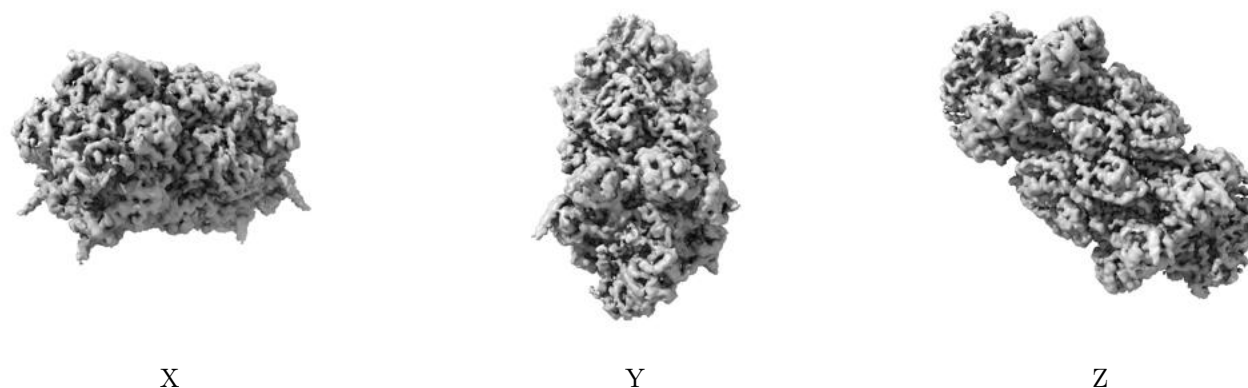
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



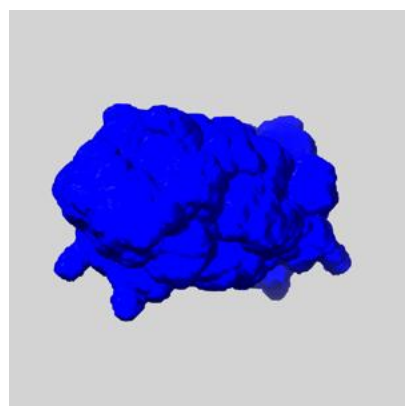
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

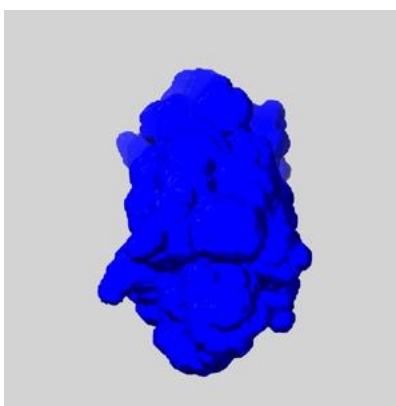
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

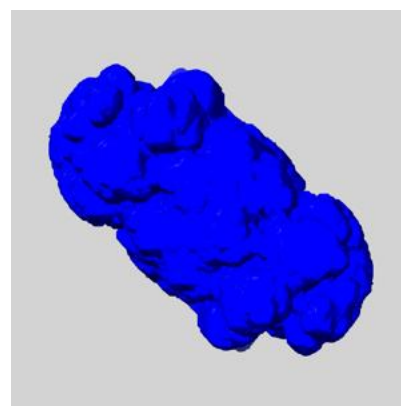
### 6.6.1 emd\_18761\_msk\_1.map [i](#)



X



Y

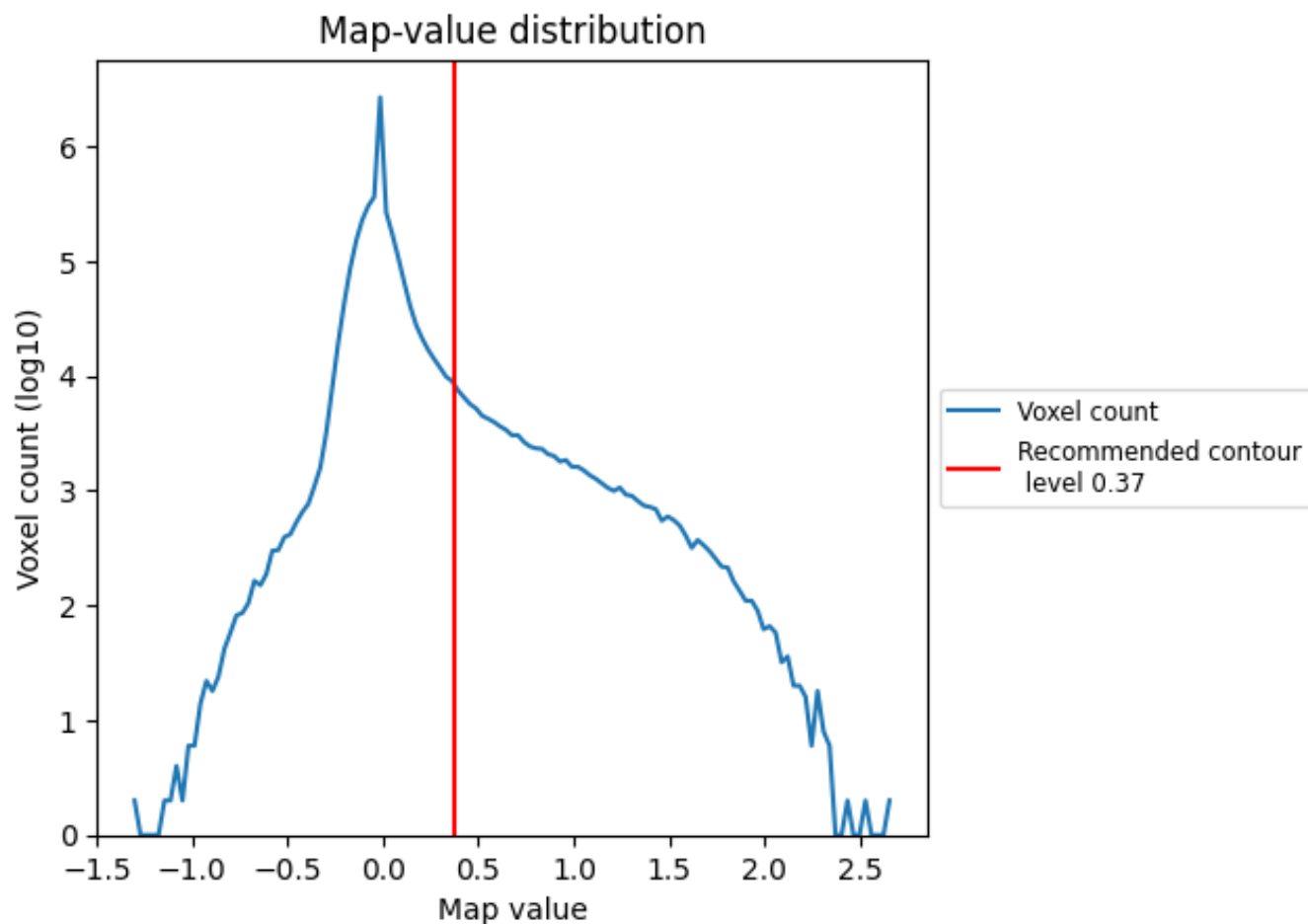


Z

## 7 Map analysis [i](#)

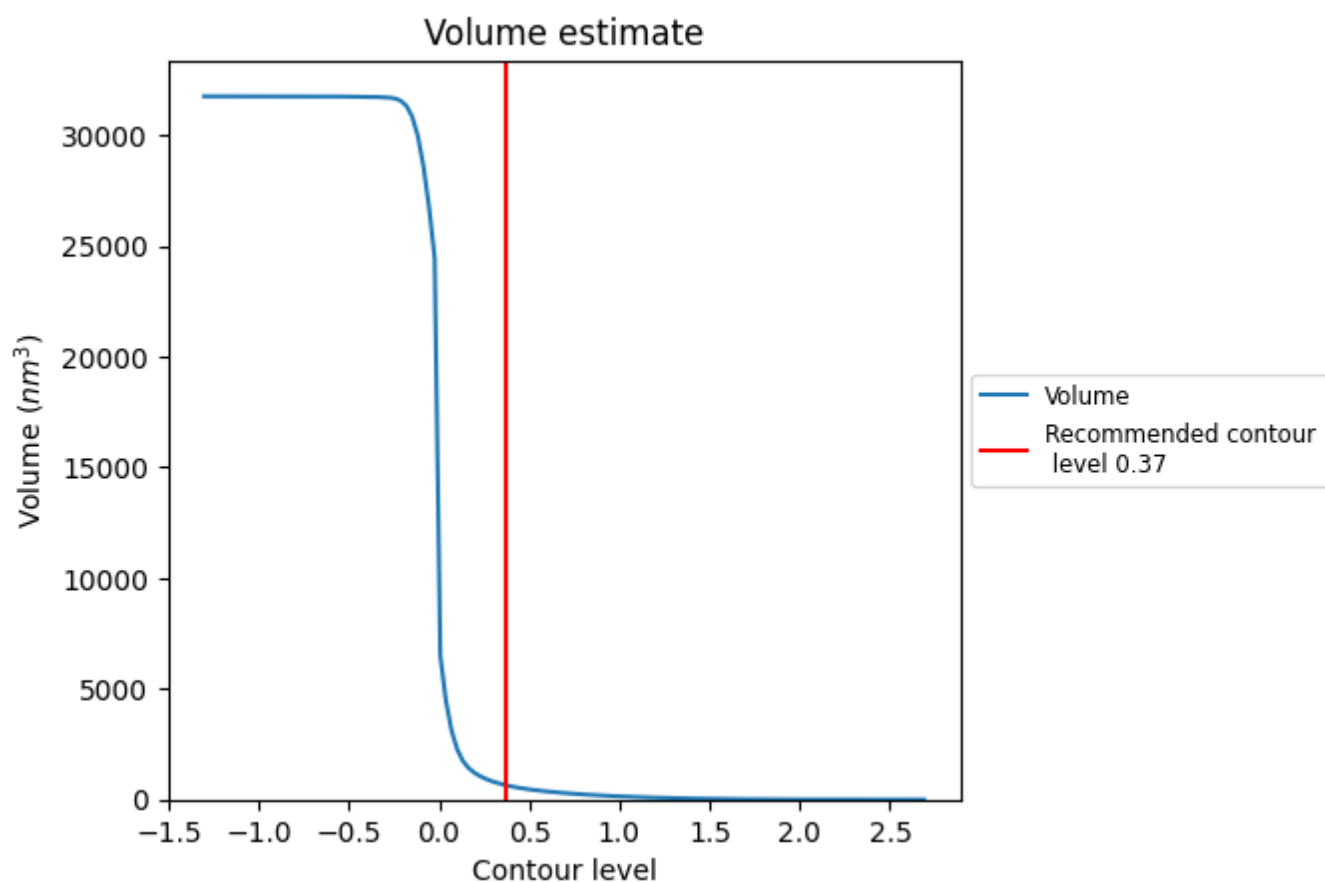
This section contains the results of statistical analysis of the map.

### 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.

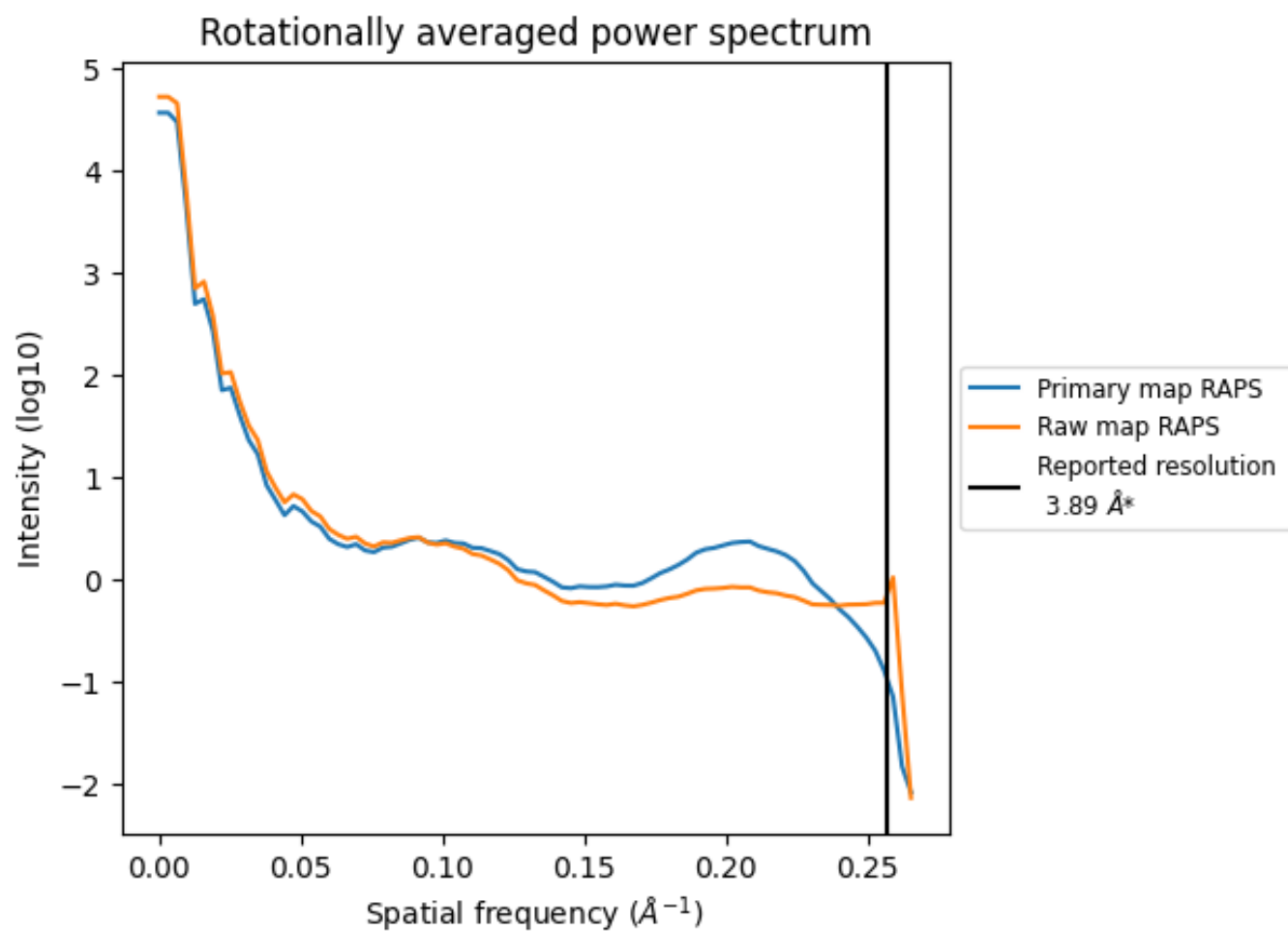
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm<sup>3</sup>; this corresponds to an approximate mass of 587 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 ⓘ

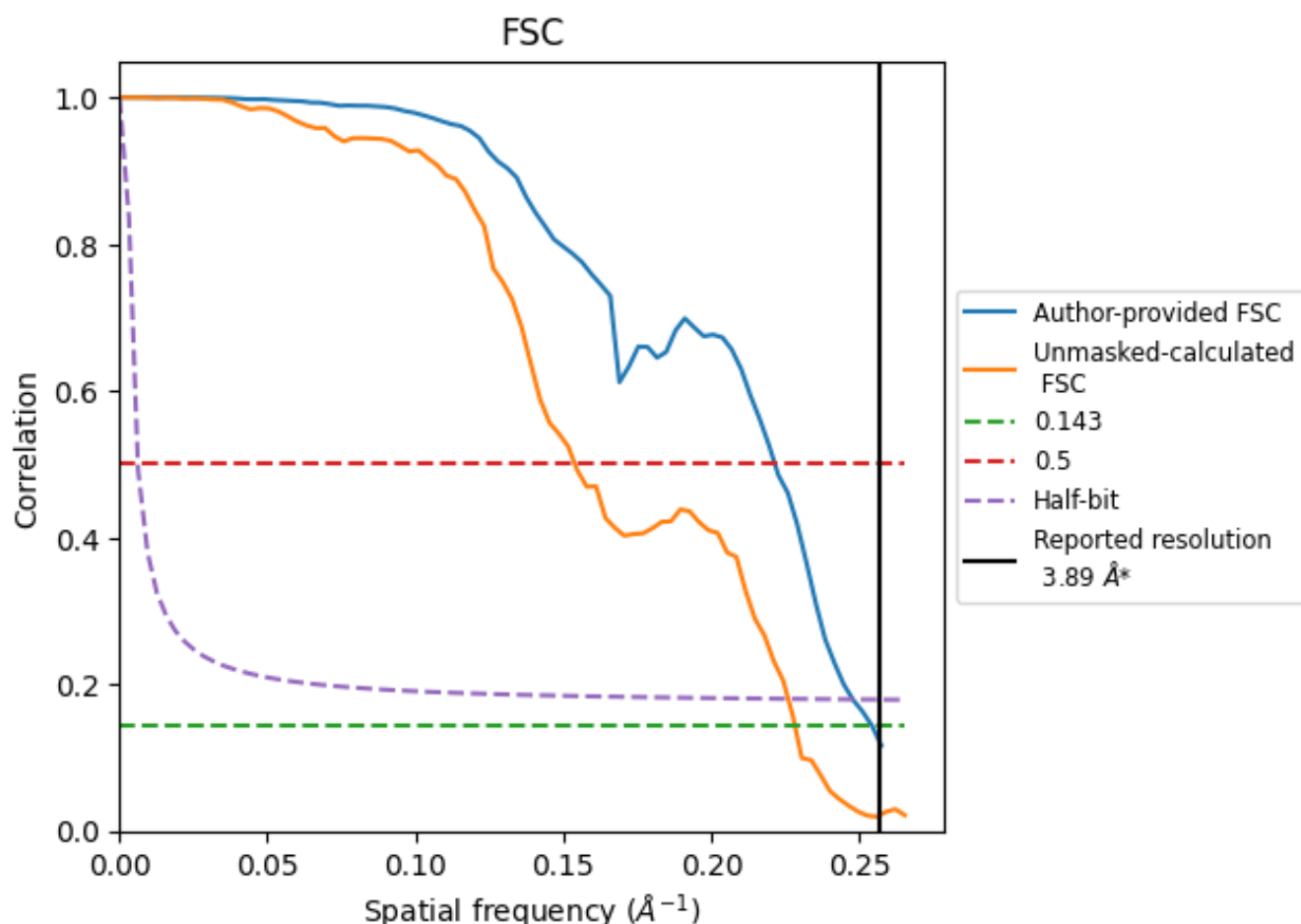


\*Reported resolution corresponds to spatial frequency of 0.257 Å<sup>-1</sup>

## 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 0.257 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

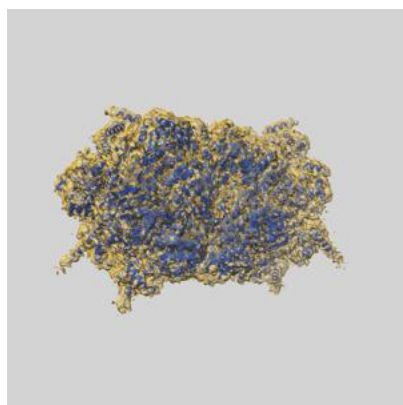
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.93	4.52	4.04
Unmasked-calculated*	4.38	6.50	4.43

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 3.89 by more than 10 %

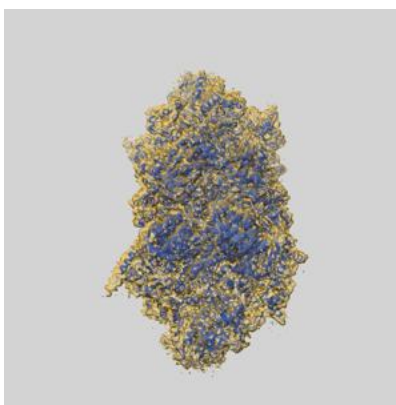
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18761 and PDB model 8QYS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

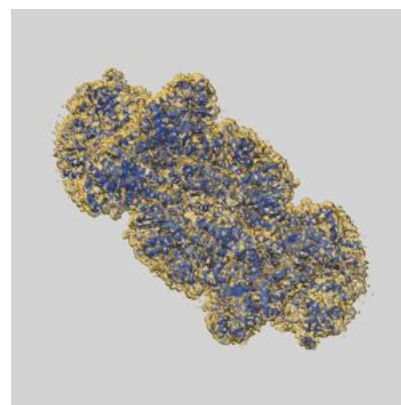
### 9.1 Map-model overlay [i](#)



X



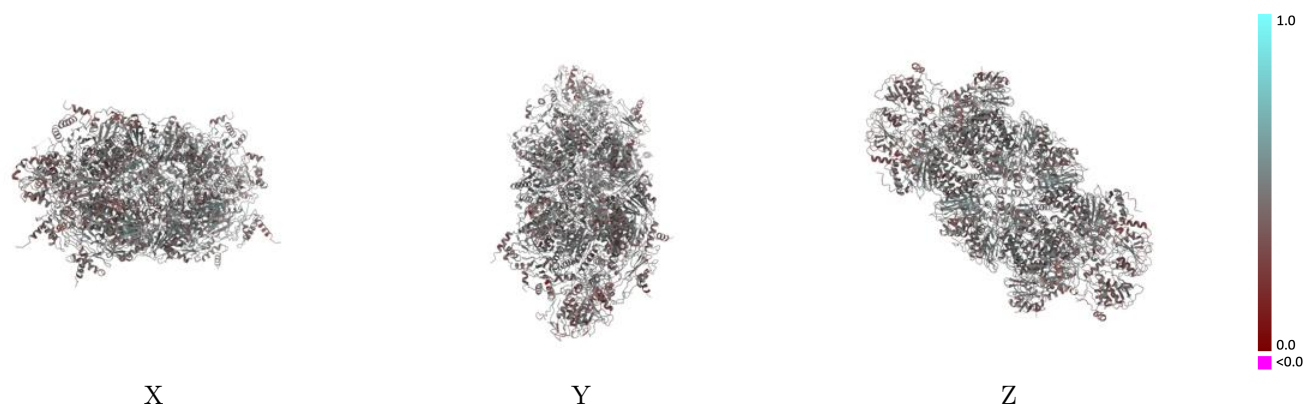
Y



Z

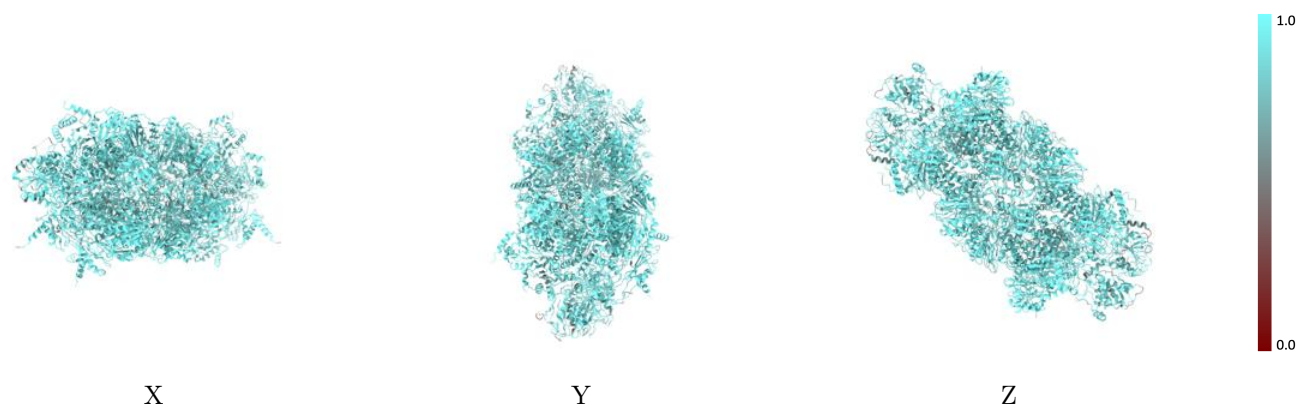
The images above show the 3D surface view of the map at the recommended contour level 0.37 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

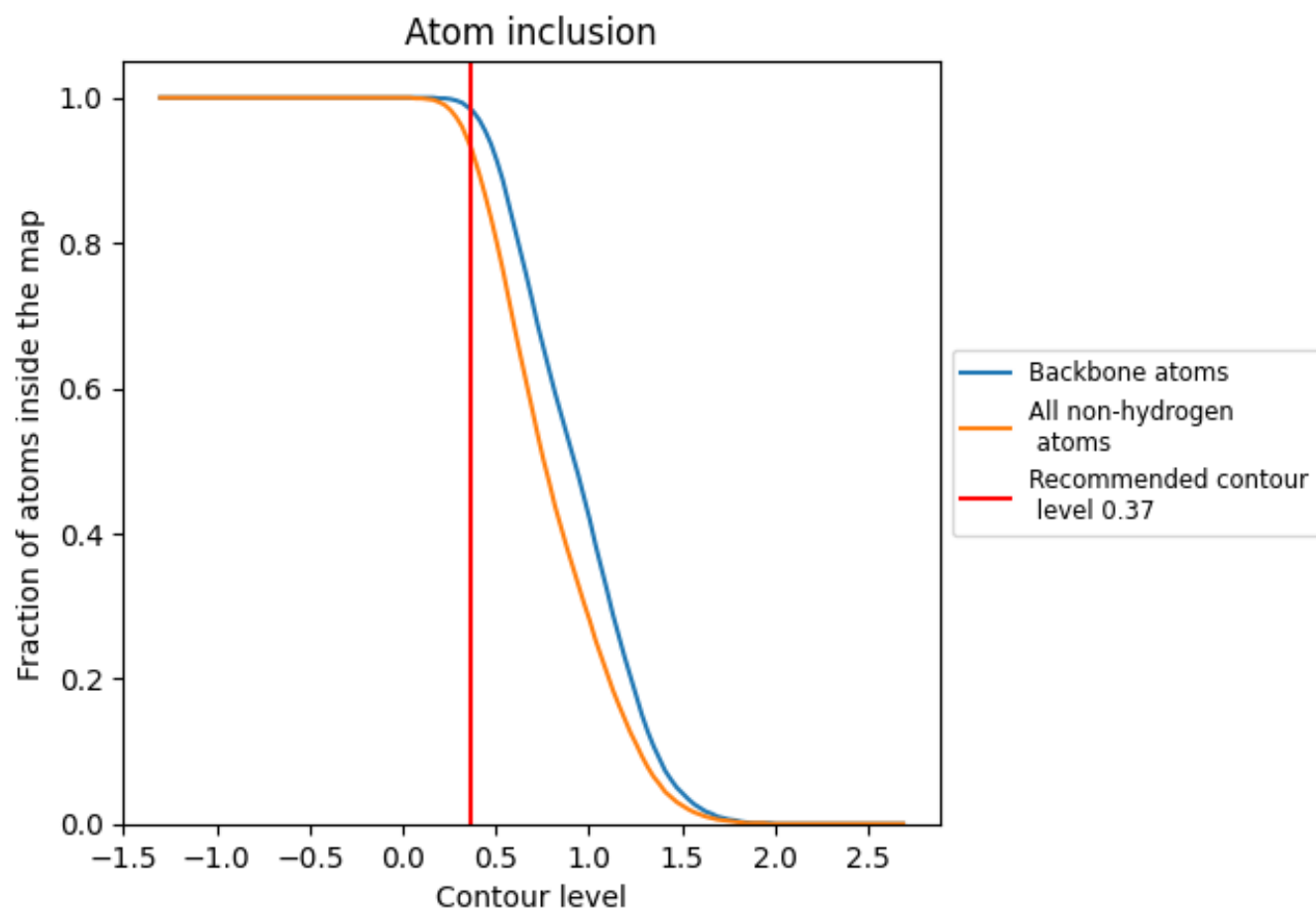
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.37).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.4560
A	 0.9590	 0.4560
B	 0.9630	 0.4660
C	 0.9560	 0.4600
D	 0.9400	 0.4510
E	 0.9500	 0.4670
F	 0.9540	 0.4530
G	 0.9430	 0.4530
H	 0.8120	 0.4430
I	 0.8260	 0.4180
J	 0.8730	 0.4270
K	 0.9190	 0.4620
L	 0.9450	 0.4760
M	 0.9450	 0.4690
N	 0.9440	 0.4610
O	 0.9390	 0.4720
P	 0.9540	 0.4650
Q	 0.9480	 0.4630
R	 0.9590	 0.4560
S	 0.9630	 0.4690
T	 0.9570	 0.4620
U	 0.9400	 0.4520
V	 0.9500	 0.4670
W	 0.9540	 0.4530
X	 0.9430	 0.4500
Y	 0.8110	 0.4420
Z	 0.8260	 0.4160
a	 0.8730	 0.4260
b	 0.9190	 0.4640
c	 0.9450	 0.4740
d	 0.9440	 0.4660
e	 0.9440	 0.4610
f	 0.9400	 0.4720
g	 0.9540	 0.4660
h	 0.9480	 0.4650

