Full wwPDB EM Validation Report ⓘ

Oct 24, 2022 – 06:56 PM EDT

PDB ID	:	7NAO
EMDB ID	:	EMD-24276
Title	:	Human PA28-20S proteasome complex
Authors	:	Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.
Deposited on	:	2021-06-22
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation 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:

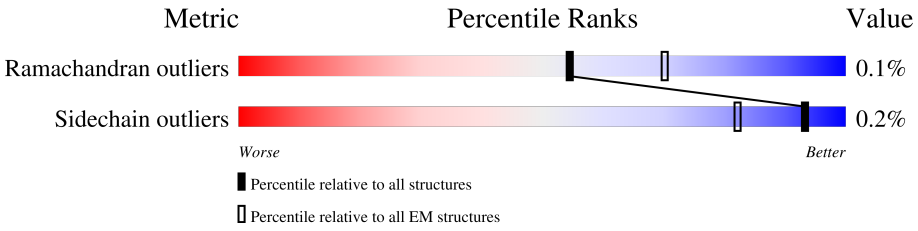
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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 >=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 <=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	O	234	98% .
2	B	261	95% 5%
2	P	261	96% .
3	C	248	95% 5%
3	Q	248	95% 5%
4	D	241	. 99% .
4	R	241	. 97% .
5	E	263	91% 9%

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Mol	Chain	Length	Quality of chain
5	S	263	90% 10%
6	F	255	94% 6%
6	T	255	94% 6%
7	G	246	97%
7	U	246	98%
8	H	277	79% 20%
8	V	277	80% 20%
9	I	205	99%
9	W	205	99%
10	J	201	98%
10	X	201	98%
11	K	263	76% 24%
11	Y	263	76% 24%
12	L	241	88% 12%
12	Z	241	88% 12%
13	M	264	81% 19%
13	a	264	81% 19%
14	N	239	85% 15%
14	b	239	85% 15%
15	d	239	91% 9%
15	f	239	88% 12%
15	h	239	90% 10%
15	i	239	90% 9%
16	c	249	85% 15%
16	e	249	85% 15%

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Mol	Chain	Length	Quality of chain
16	g	249	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 58083 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
			1696	1101	294	295	6		
1	O	229	Total	C	N	O	S	0	0
			1678	1089	290	293	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	249	Total	C	N	O	S	0	0
			1793	1146	318	319	10		
2	P	251	Total	C	N	O	S	0	0
			1843	1174	328	331	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1703	1082	314	302	5		
3	Q	236	Total	C	N	O	S	0	0
			1723	1095	320	303	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1751	1116	301	322	12		
4	R	235	Total	C	N	O	S	0	0
			1693	1076	292	314	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	239	Total	C	N	O	S	0	0
			1810	1144	331	324	11		
5	S	237	Total	C	N	O	S	0	0
			1759	1119	329	301	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	240	Total	C	N	O	S	0	0
			1785	1145	313	316	11		
6	T	239	Total	C	N	O	S	0	0
			1784	1143	314	317	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1769	1133	305	319	12		
7	U	242	Total	C	N	O	S	0	0
			1789	1146	307	323	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	222	Total	C	N	O	S	0	0
			1609	1023	276	299	11		
8	V	222	Total	C	N	O	S	0	0
			1612	1023	274	304	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1564	1003	264	278	19		
9	W	204	Total	C	N	O	S	0	0
			1559	1000	264	277	18		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	197	Total	C	N	O	S	0	0
			1544	998	265	272	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	0	0
			1535	990	264	273	8		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1525	968	273	275	9		
11	Y	200	Total	C	N	O	S	0	0
			1532	970	272	281	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1599	1022	279	288	10		
12	Z	213	Total	C	N	O	S	0	0
			1593	1022	281	280	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	215	Total	C	N	O	S	0	0
			1643	1043	289	299	12		
13	a	215	Total	C	N	O	S	0	0
			1624	1034	288	290	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1491	939	258	282	12		
14	b	202	Total	C	N	O	S	0	0
			1478	934	258	274	12		

- Molecule 15 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d	217	Total	C	N	O	S	0	0
			1686	1094	284	304	4		
15	f	211	Total	C	N	O	S	0	0
			1648	1069	279	297	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	216	Total	C	N	O	S	0	0
			1677	1087	285	301	4		
15	i	217	Total	C	N	O	S	0	0
			1695	1099	287	305	4		

- Molecule 16 is a protein called Proteasome activator complex subunit 1.

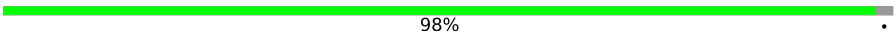
Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	212	Total	C	N	O	S	0	0
			1626	1049	282	291	4		
16	e	211	Total	C	N	O	S	0	0
			1641	1059	282	295	5		
16	g	211	Total	C	N	O	S	0	0
			1626	1050	281	289	6		

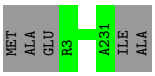
3 Residue-property plots (i)

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

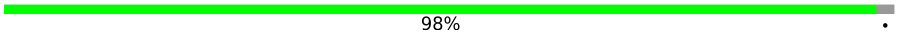
Chain A:

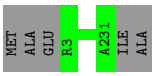




• Molecule 1: Proteasome subunit alpha type-2

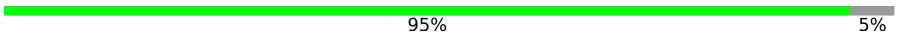
Chain O:

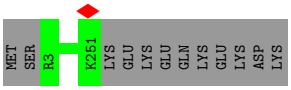




• Molecule 2: Proteasome subunit alpha type-4

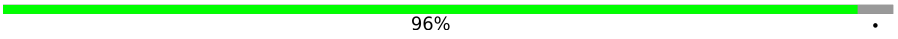
Chain B:

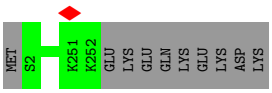




• Molecule 2: Proteasome subunit alpha type-4

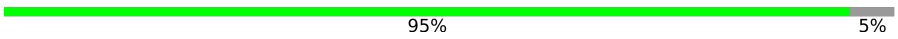
Chain P:





• Molecule 3: Proteasome subunit alpha type-7

Chain C:

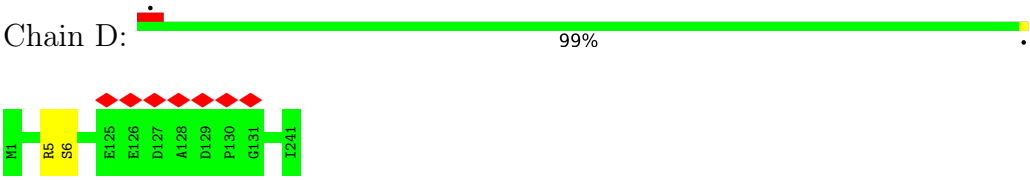


• Molecule 3: Proteasome subunit alpha type-7

Chain Q:

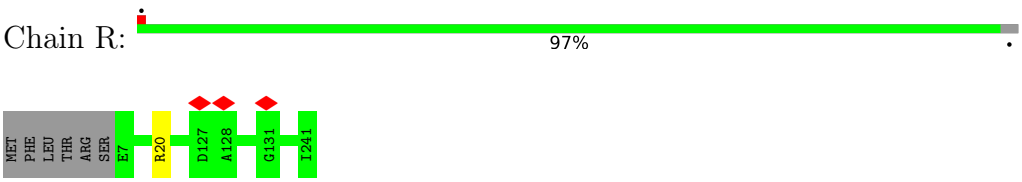
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



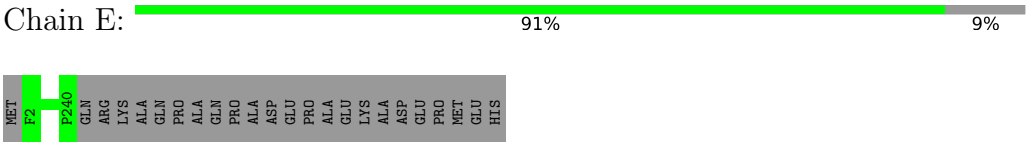
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



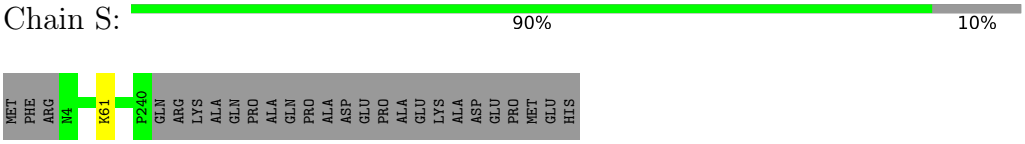
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



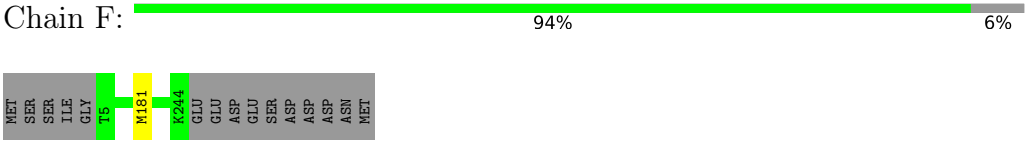
• Molecule 5: Proteasome subunit alpha type-1

Chain S:



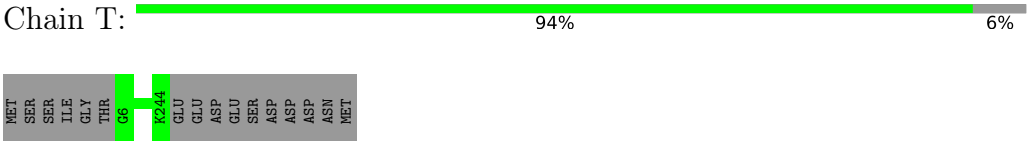
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



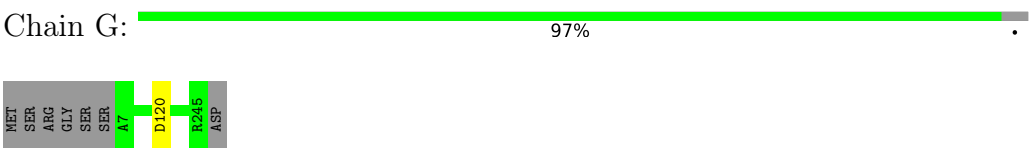
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



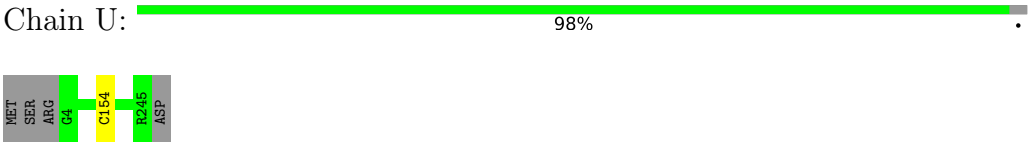
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



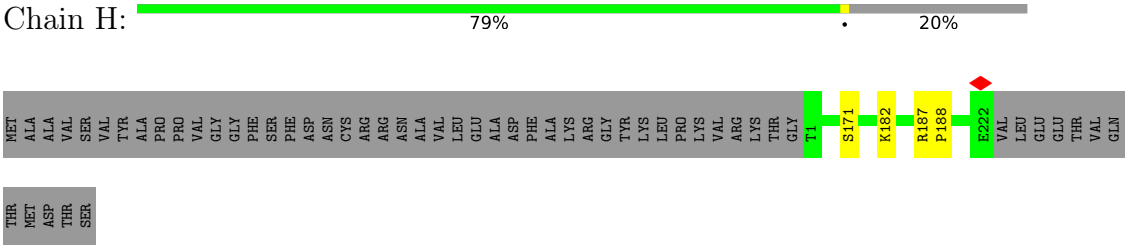
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



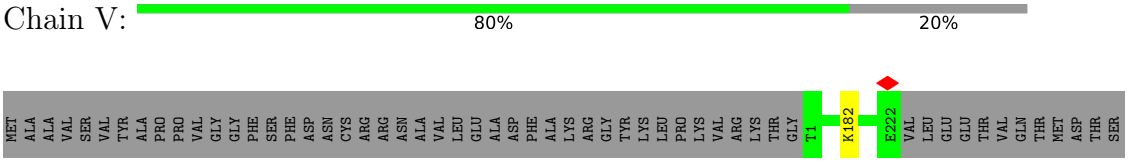
• Molecule 8: Proteasome subunit beta type-7

Chain H:



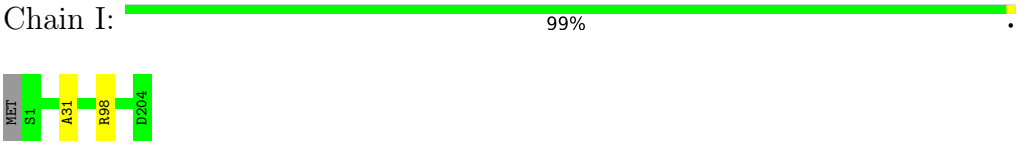
• Molecule 8: Proteasome subunit beta type-7

Chain V:



• Molecule 9: Proteasome subunit beta type-3

Chain I:

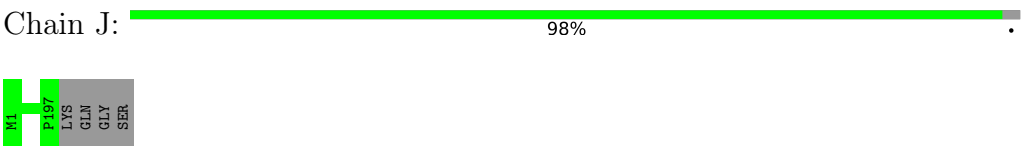


• Molecule 9: Proteasome subunit beta type-3

Chain W:

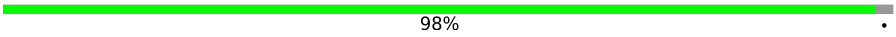
• Molecule 10: Proteasome subunit beta type-2

Chain J:



• Molecule 10: Proteasome subunit beta type-2

Chain X:



• Molecule 11: Proteasome subunit beta type-5

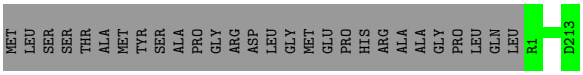
Chain K:

• Molecule 11: Proteasome subunit beta type-5

Chain Y:

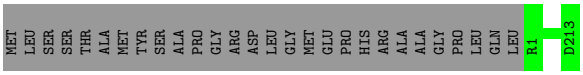
• Molecule 12: Proteasome subunit beta type-1

Chain L:



• Molecule 12: Proteasome subunit beta type-1

Chain Z:



• Molecule 13: Proteasome subunit beta type-4

Chain M:

• Molecule 13: Proteasome subunit beta type-4

Chain a:

• Molecule 14: Proteasome subunit beta type-6

Chain N:

• Molecule 14: Proteasome subunit beta type-6

Chain b:

• Molecule 15: Proteasome activator complex subunit 2

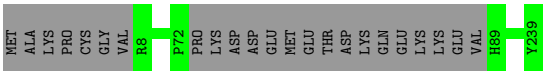
Chain d:

• Molecule 15: Proteasome activator complex subunit 2

Chain f:

• Molecule 15: Proteasome activator complex subunit 2

Chain h:

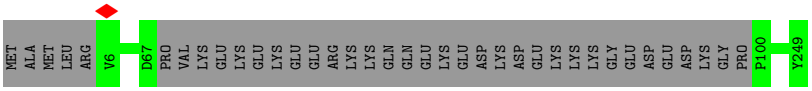


• Molecule 15: Proteasome activator complex subunit 2

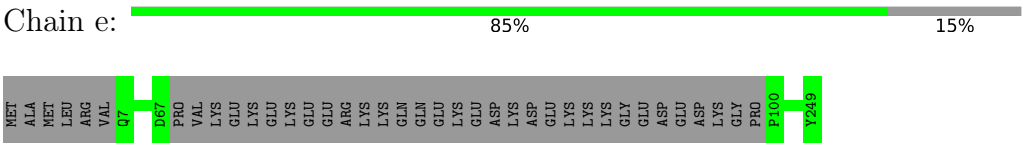
Chain i:

• Molecule 16: Proteasome activator complex subunit 1

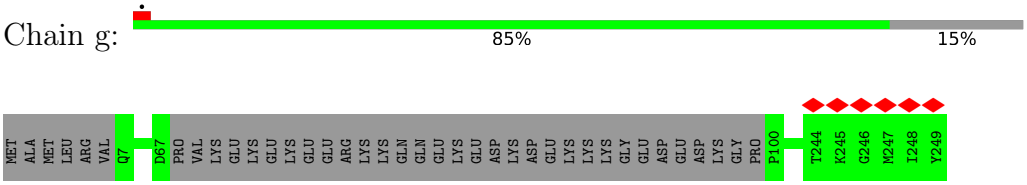
Chain c:



• Molecule 16: Proteasome activator complex subunit 1



• Molecule 16: Proteasome activator complex subunit 1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	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	26.106	Depositor
Minimum map value	-10.669	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	388.992, 388.992, 388.992	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality

5.1 Standard geometry

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	0.34	0/1735	0.55	0/2362
1	O	0.34	0/1717	0.51	0/2339
2	B	0.31	0/1821	0.52	0/2477
2	P	0.30	0/1872	0.54	0/2541
3	C	0.32	0/1729	0.57	0/2356
3	Q	0.31	0/1749	0.60	1/2380 (0.0%)
4	D	0.31	0/1780	0.54	0/2417
4	R	0.29	0/1720	0.49	0/2336
5	E	0.31	0/1845	0.58	0/2504
5	S	0.31	0/1794	0.58	0/2437
6	F	0.35	0/1820	0.54	0/2464
6	T	0.32	0/1819	0.53	0/2463
7	G	0.33	0/1802	0.54	1/2449 (0.0%)
7	U	0.33	0/1823	0.51	0/2478
8	H	0.32	0/1636	0.58	0/2223
8	V	0.32	0/1639	0.58	0/2228
9	I	0.33	0/1593	0.55	0/2149
9	W	0.33	0/1588	0.53	0/2144
10	J	0.34	0/1577	0.55	0/2138
10	X	0.34	0/1567	0.55	0/2124
11	K	0.33	0/1556	0.56	0/2104
11	Y	0.33	0/1563	0.59	0/2115
12	L	0.33	0/1629	0.56	0/2201
12	Z	0.33	0/1623	0.56	0/2192
13	M	0.33	0/1676	0.61	1/2272 (0.0%)
13	a	0.32	0/1657	0.59	0/2250
14	N	0.34	0/1517	0.55	0/2056
14	b	0.33	0/1504	0.54	0/2038
15	d	0.30	0/1720	0.51	0/2338
15	f	0.30	0/1680	0.50	0/2281
15	h	0.30	0/1710	0.51	0/2322
15	i	0.30	0/1729	0.52	0/2349
16	c	0.30	0/1657	0.49	0/2250
16	e	0.30	0/1672	0.52	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
16	g	0.30	0/1657	0.51	0/2247
All	All	0.32	0/59176	0.55	3/80289 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
8	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	50	VAL	CG1-CB-CG2	7.85	123.46	110.90
13	M	73	ASP	CB-CG-OD1	5.66	123.39	118.30
7	G	120	ASP	CB-CG-OD1	5.60	123.34	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	5	ARG	Peptide
8	H	187	ARG	Peptide

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%)	225 (99%)	2 (1%)	0	100	100
1	O	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
2	B	247/261 (95%)	244 (99%)	3 (1%)	0	100	100
2	P	249/261 (95%)	243 (98%)	6 (2%)	0	100	100
3	C	233/248 (94%)	228 (98%)	5 (2%)	0	100	100
3	Q	234/248 (94%)	234 (100%)	0	0	100	100
4	D	239/241 (99%)	232 (97%)	6 (2%)	1 (0%)	34	66
4	R	233/241 (97%)	229 (98%)	4 (2%)	0	100	100
5	E	237/263 (90%)	233 (98%)	4 (2%)	0	100	100
5	S	235/263 (89%)	230 (98%)	4 (2%)	1 (0%)	34	66
6	F	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
6	T	237/255 (93%)	235 (99%)	2 (1%)	0	100	100
7	G	237/246 (96%)	234 (99%)	3 (1%)	0	100	100
7	U	240/246 (98%)	238 (99%)	2 (1%)	0	100	100
8	H	220/277 (79%)	215 (98%)	3 (1%)	2 (1%)	17	48
8	V	220/277 (79%)	217 (99%)	3 (1%)	0	100	100
9	I	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	29	61
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
10	X	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
11	K	198/263 (75%)	197 (100%)	1 (0%)	0	100	100
11	Y	198/263 (75%)	194 (98%)	4 (2%)	0	100	100
12	L	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
12	Z	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
13	M	213/264 (81%)	210 (99%)	3 (1%)	0	100	100
13	a	213/264 (81%)	208 (98%)	5 (2%)	0	100	100
14	N	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
14	b	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
15	d	213/239 (89%)	211 (99%)	2 (1%)	0	100	100
15	f	207/239 (87%)	205 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	h	212/239 (89%)	210 (99%)	2 (1%)	0	100 100
15	i	213/239 (89%)	210 (99%)	3 (1%)	0	100 100
16	c	208/249 (84%)	207 (100%)	1 (0%)	0	100 100
16	e	207/249 (83%)	206 (100%)	1 (0%)	0	100 100
16	g	207/249 (83%)	206 (100%)	1 (0%)	0	100 100
All	All	7657/8579 (89%)	7552 (99%)	100 (1%)	5 (0%)	54 82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	31	ALA
5	S	61	LYS
4	D	6	SER
8	H	171	SER
8	H	188	PRO

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	158/191 (83%)	158 (100%)	0	100 100
1	O	155/191 (81%)	155 (100%)	0	100 100
2	B	159/221 (72%)	159 (100%)	0	100 100
2	P	171/221 (77%)	171 (100%)	0	100 100
3	C	152/211 (72%)	152 (100%)	0	100 100
3	Q	157/211 (74%)	157 (100%)	0	100 100
4	D	173/203 (85%)	173 (100%)	0	100 100
4	R	164/203 (81%)	163 (99%)	1 (1%)	86 96
5	E	181/224 (81%)	181 (100%)	0	100 100
5	S	169/224 (75%)	169 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	167/212 (79%)	166 (99%)	1 (1%)	86 96
6	T	168/212 (79%)	168 (100%)	0	100 100
7	G	175/210 (83%)	175 (100%)	0	100 100
7	U	177/210 (84%)	176 (99%)	1 (1%)	86 96
8	H	165/228 (72%)	164 (99%)	1 (1%)	86 96
8	V	166/228 (73%)	165 (99%)	1 (1%)	86 96
9	I	164/174 (94%)	163 (99%)	1 (1%)	86 96
9	W	162/174 (93%)	161 (99%)	1 (1%)	86 96
10	J	156/171 (91%)	156 (100%)	0	100 100
10	X	156/171 (91%)	156 (100%)	0	100 100
11	K	146/202 (72%)	146 (100%)	0	100 100
11	Y	147/202 (73%)	147 (100%)	0	100 100
12	L	161/199 (81%)	161 (100%)	0	100 100
12	Z	160/199 (80%)	160 (100%)	0	100 100
13	M	166/215 (77%)	166 (100%)	0	100 100
13	a	160/215 (74%)	159 (99%)	1 (1%)	86 96
14	N	149/181 (82%)	149 (100%)	0	100 100
14	b	145/181 (80%)	145 (100%)	0	100 100
15	d	174/212 (82%)	174 (100%)	0	100 100
15	f	172/212 (81%)	172 (100%)	0	100 100
15	h	173/212 (82%)	173 (100%)	0	100 100
15	i	175/212 (82%)	174 (99%)	1 (1%)	86 96
16	c	165/224 (74%)	165 (100%)	0	100 100
16	e	170/224 (76%)	170 (100%)	0	100 100
16	g	167/224 (75%)	167 (100%)	0	100 100
All	All	5725/7204 (80%)	5716 (100%)	9 (0%)	93 98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	181	MET
8	H	182	LYS
9	I	98	ARG

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Mol	Chain	Res	Type
4	R	20	ARG
7	U	154	CYS
8	V	182	LYS
9	W	98	ARG
13	a	100	ARG
15	i	118	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	109	GLN
3	C	15	HIS
3	C	146	GLN
4	D	122	GLN
10	J	63	ASN
12	L	157	ASN
14	N	77	HIS
14	N	110	GLN
2	P	109	GLN
5	S	68	ASN
5	S	146	GLN
7	U	128	ASN
9	W	6	ASN
9	W	172	ASN
10	X	63	ASN
10	X	71	ASN
12	Z	108	ASN
12	Z	157	ASN
15	d	183	HIS
16	e	147	ASN
16	g	27	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.

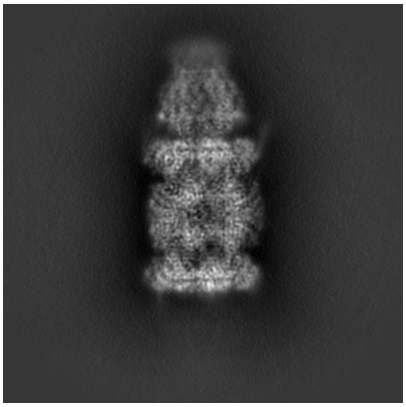
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24276. These allow visual inspection of the internal detail of the map and identification of artifacts.

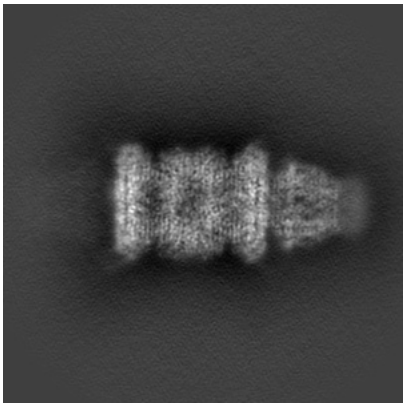
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

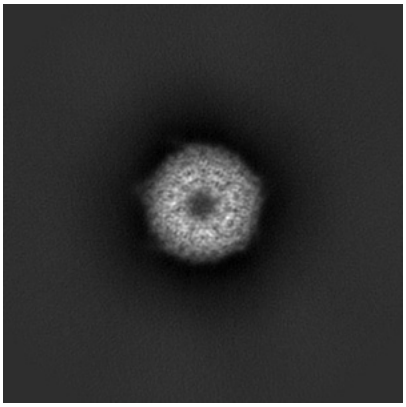
6.1.1 Primary map



X



Y

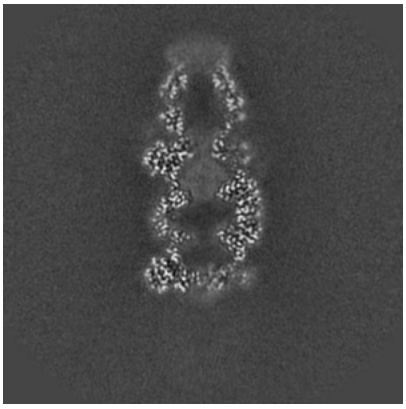


Z

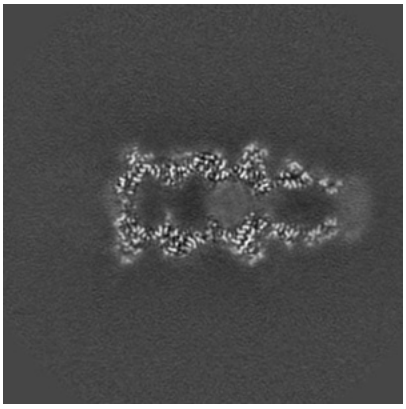
The images above show the map projected in three orthogonal directions.

6.2 Central slices

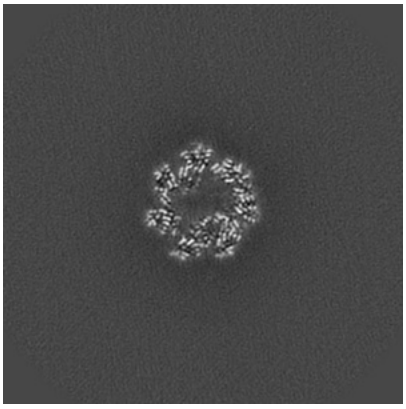
6.2.1 Primary map



X Index: 160



Y Index: 160

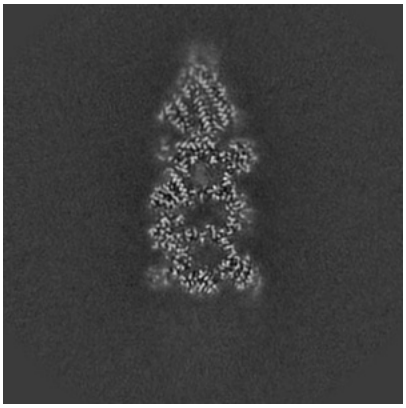


Z Index: 160

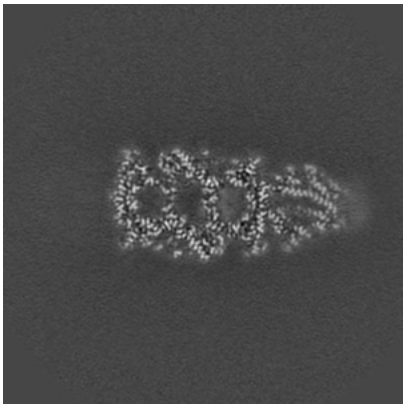
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

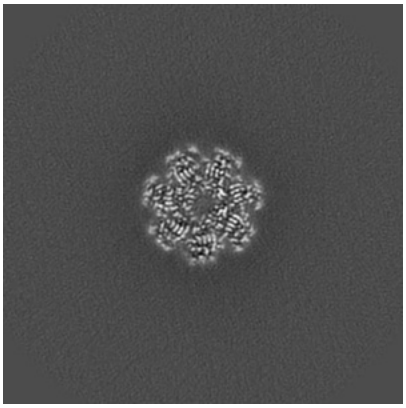
6.3.1 Primary map



X Index: 176



Y Index: 145



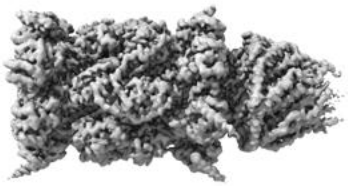
Z Index: 197

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

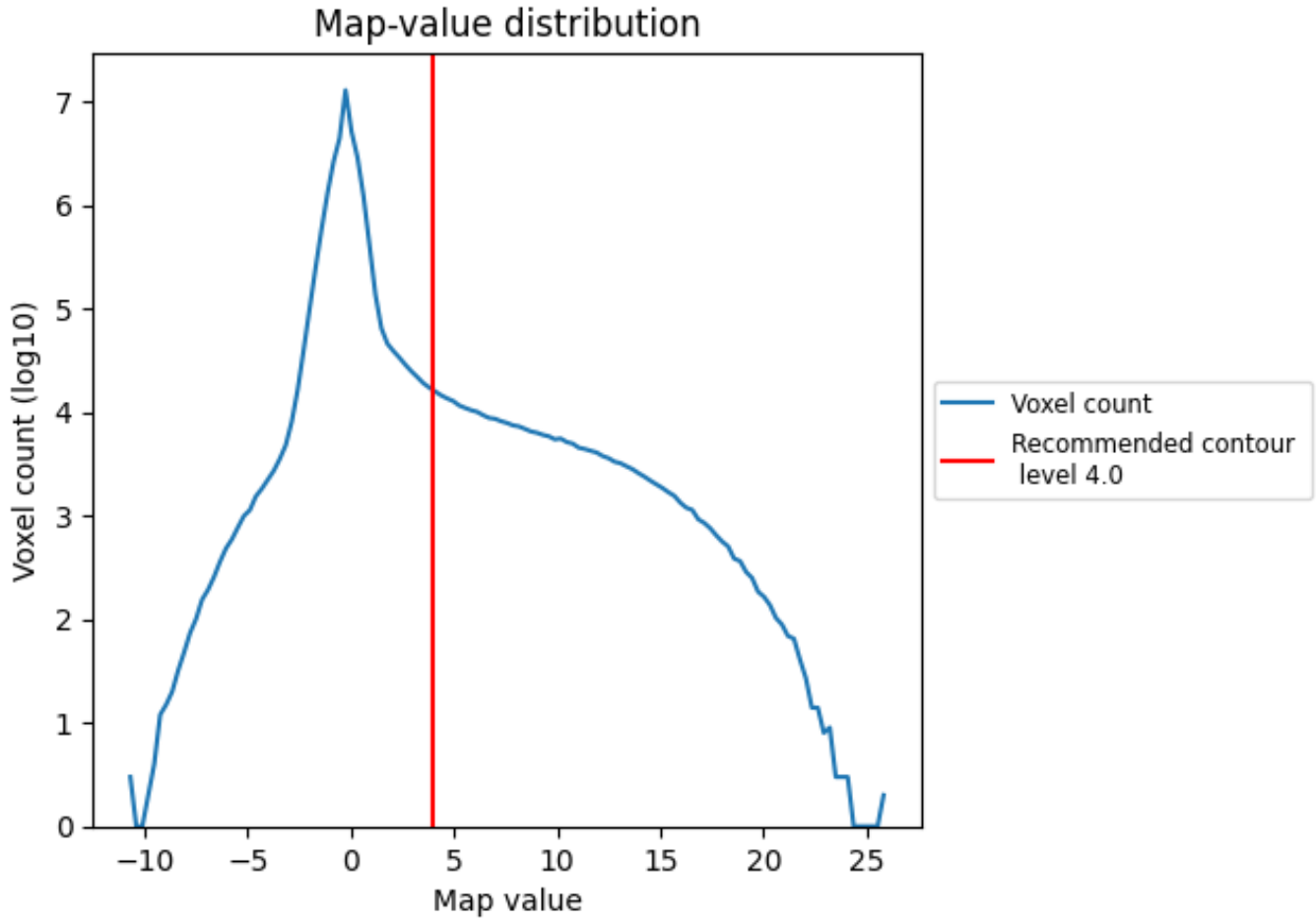
6.5 Mask visualisation (i)

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

7 Map analysis

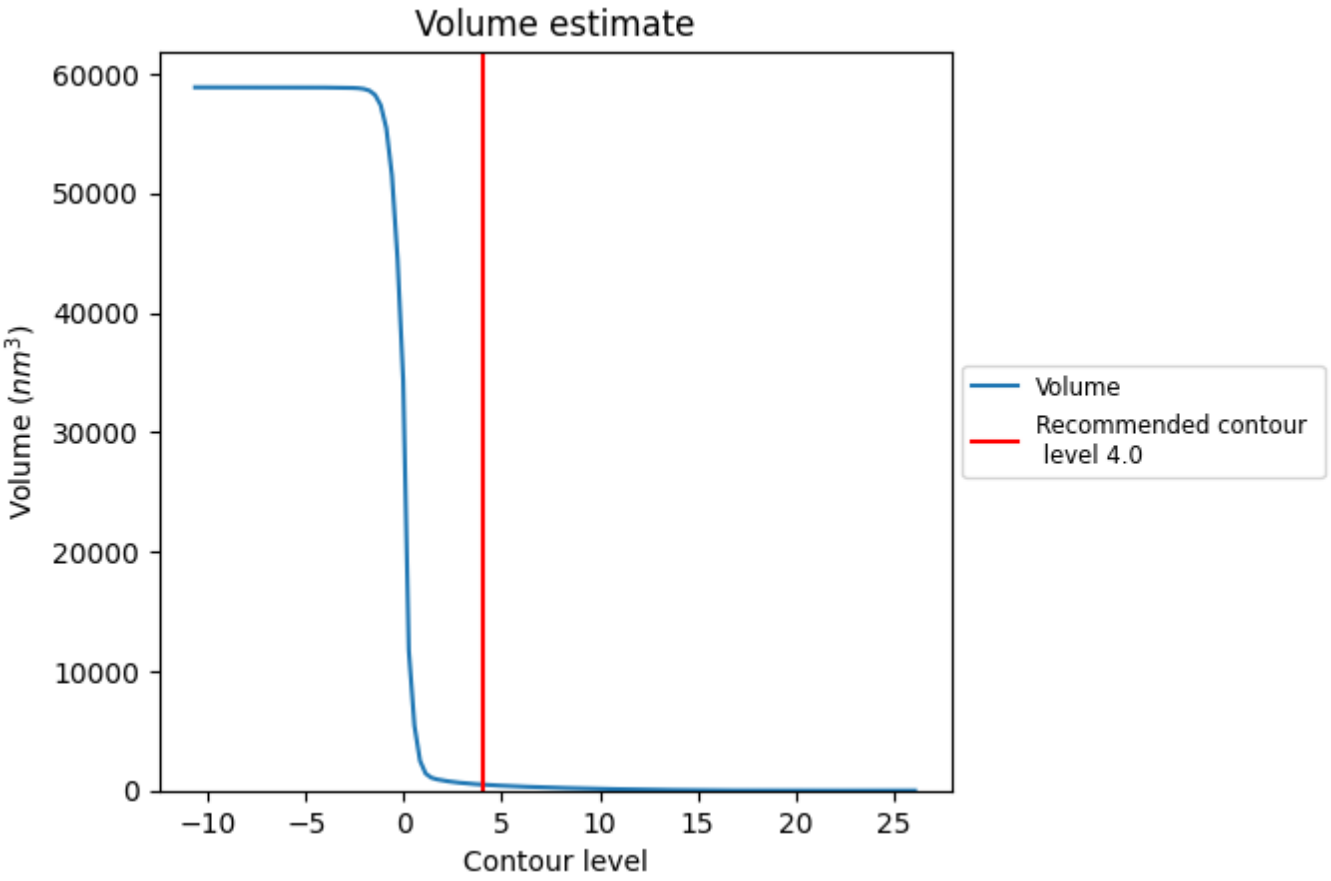
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

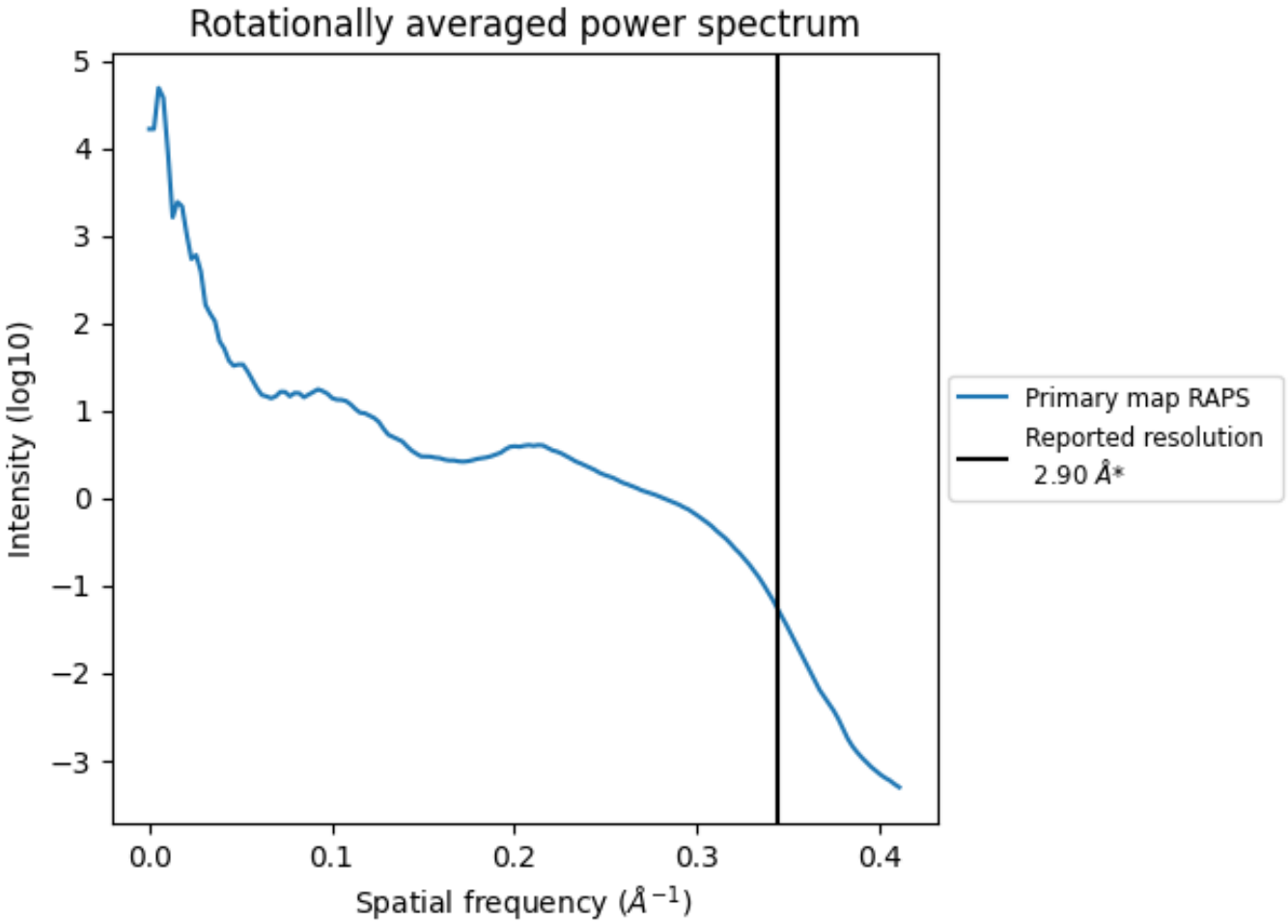
7.2 Volume estimate



The volume at the recommended contour level is 499 nm^3; this corresponds to an approximate mass of 451 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)

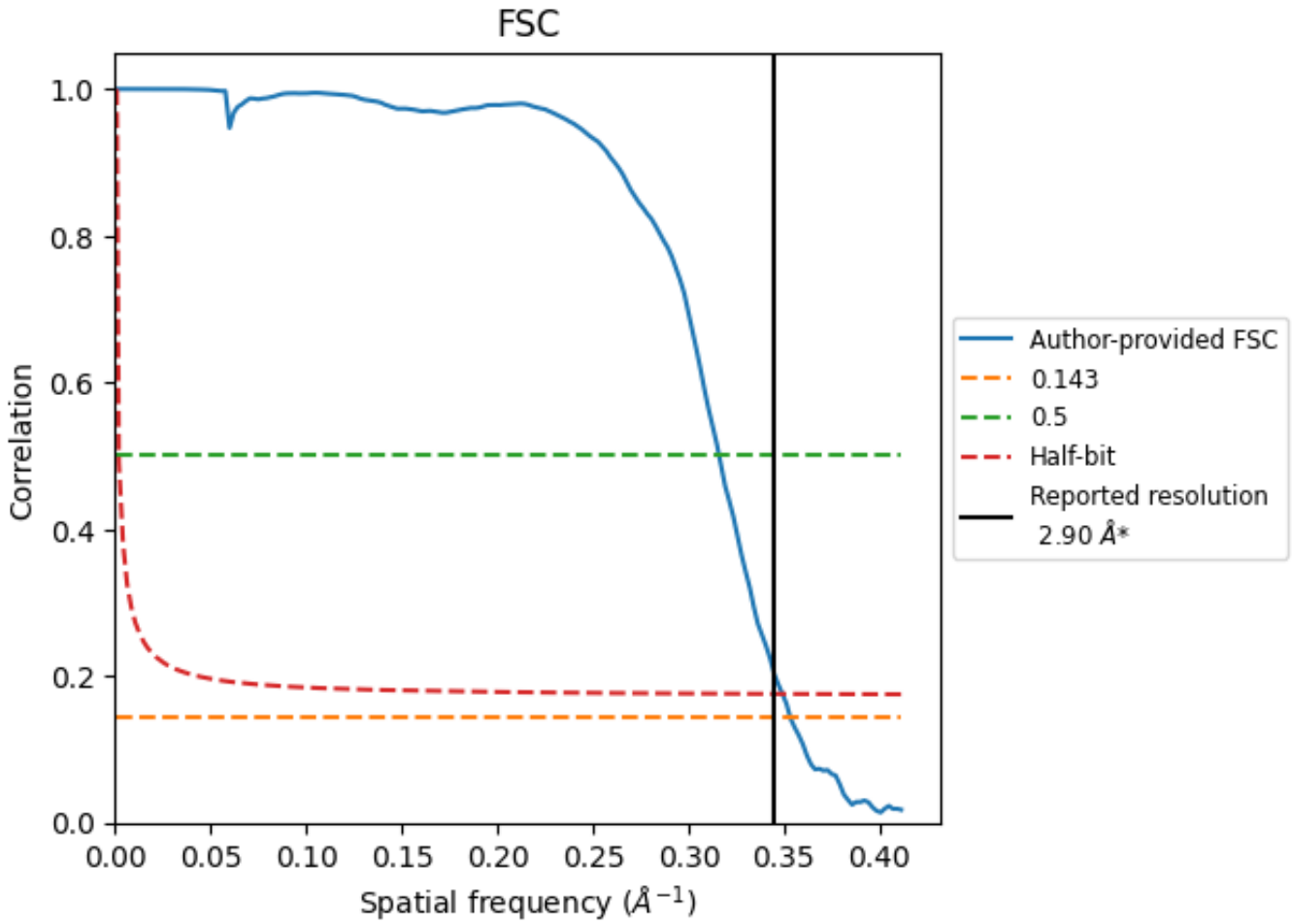


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

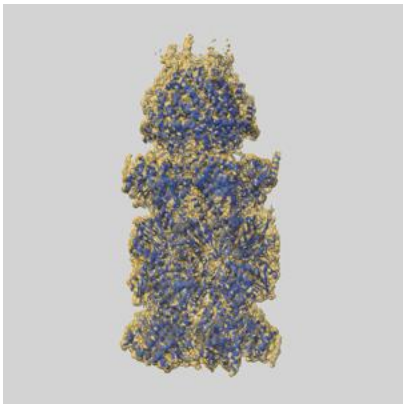
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.83	3.16	2.86
Unmasked-calculated*	-	-	-

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

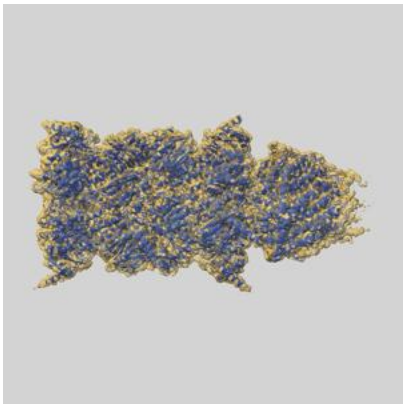
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24276 and PDB model 7NAO. Per-residue inclusion information can be found in section 3 on page 9.

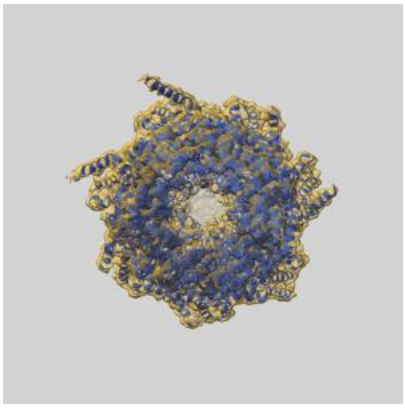
9.1 Map-model overlay



X



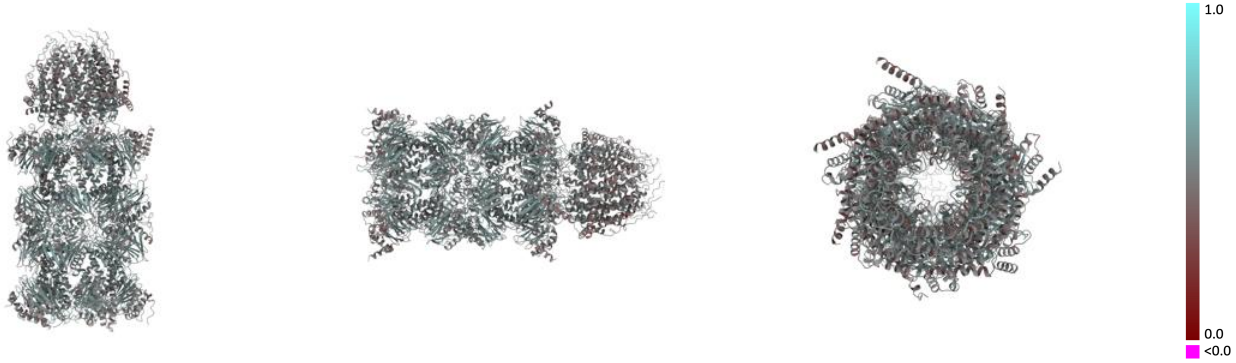
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

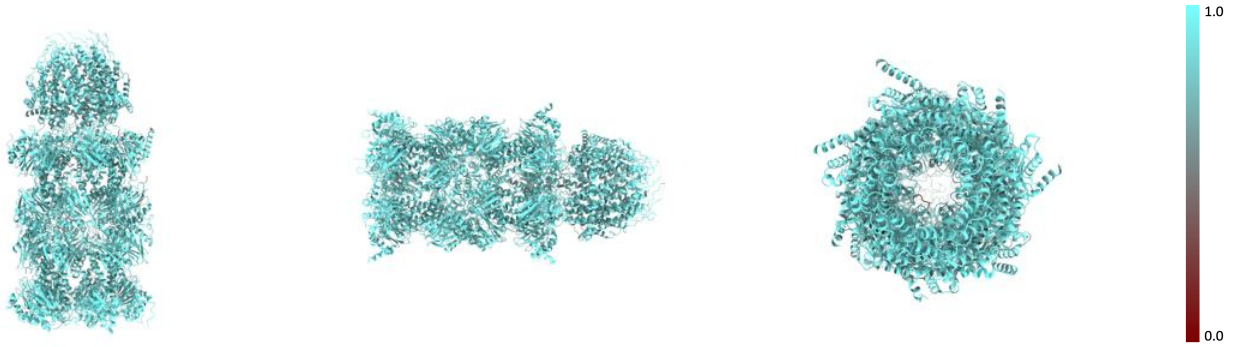
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

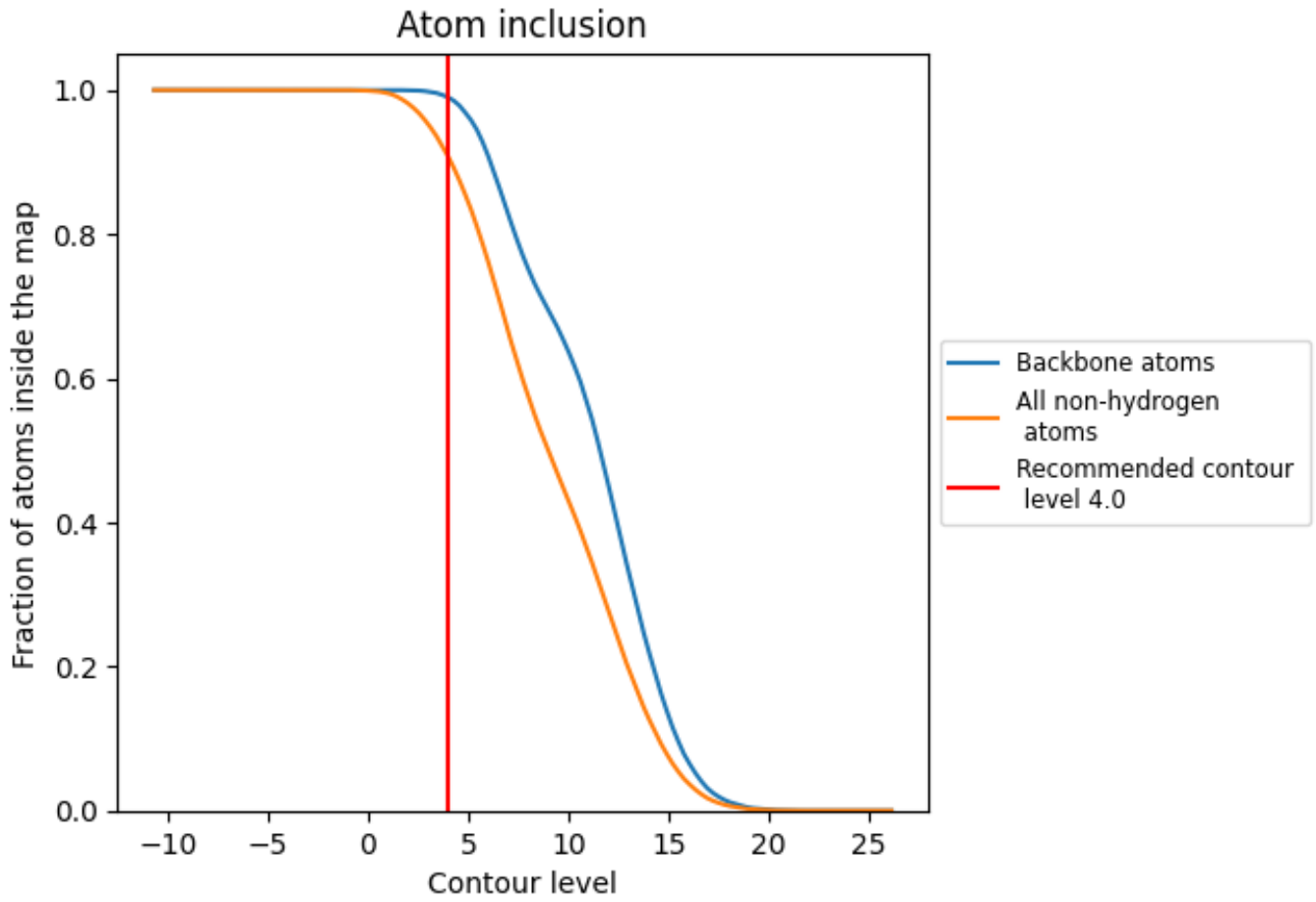
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9073	0.5120
A	0.9146	0.5150
B	0.8988	0.5130
C	0.9168	0.5120
D	0.8857	0.5080
E	0.9134	0.5170
F	0.9100	0.5230
G	0.9160	0.5170
H	0.9287	0.5290
I	0.8990	0.5290
J	0.9079	0.5340
K	0.9336	0.5330
L	0.9125	0.5320
M	0.9155	0.5230
N	0.9246	0.5400
O	0.9380	0.5230
P	0.9131	0.5070
Q	0.9135	0.4990
R	0.9028	0.5060
S	0.9277	0.5120
T	0.9334	0.5120
U	0.9250	0.5180
V	0.9212	0.5270
W	0.9196	0.5400
X	0.9173	0.5350
Y	0.9291	0.5220
Z	0.9243	0.5380
a	0.9354	0.5400
b	0.9267	0.5400
c	0.8575	0.4730
d	0.8878	0.4810
e	0.8793	0.4780
f	0.8779	0.4800
g	0.8544	0.4750
h	0.8526	0.4620
i	0.8505	0.4600