



wwPDB EM Validation Summary Report ⓘ

Sep 12, 2026 – 07:47 am BST

PDB ID : 9TMS / pdb_00009tms
EMDB ID : EMD-56074
Title : Human sperm 20S-PA200 proteasome complex isolated from native source
Authors : Kolata, P.; Allegretti, M.
Deposited on : 2025-12-15
Resolution : 2.90 Å(reported)
Based on initial model : 6KWY

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:

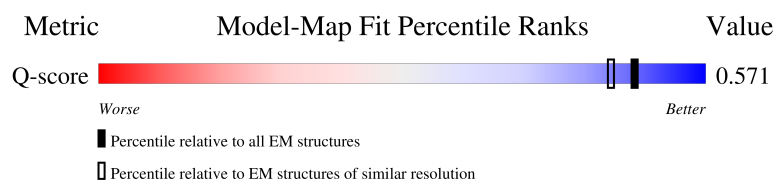
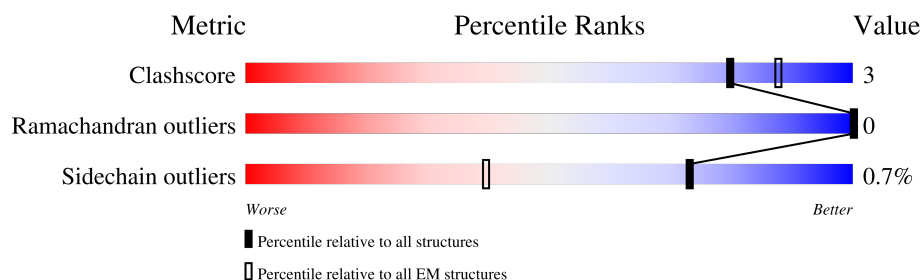
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 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.



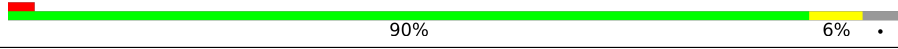
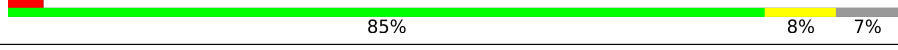
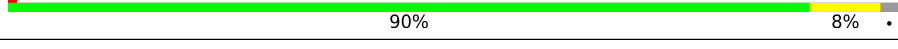
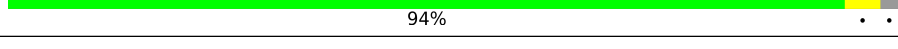
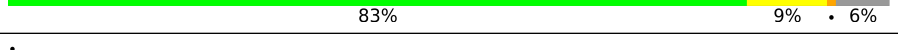
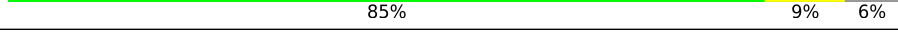
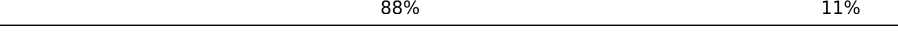
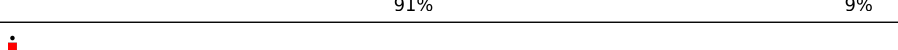
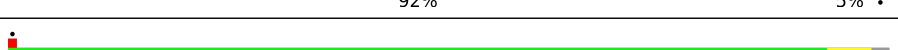
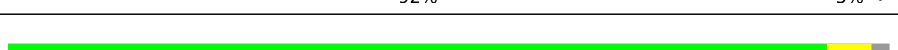
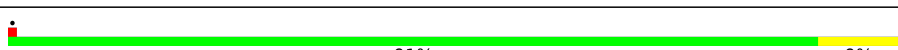
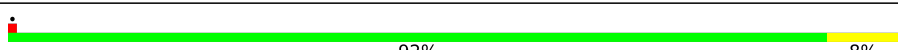
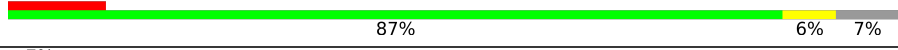
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	246	 87% 8% 5%
1	O	246	 89% 9% .
2	B	234	 86% 6% 8%
2	P	234	 5% 90% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	263	
3	T	263	
4	G	255	
4	U	255	
5	H	205	
5	V	205	
6	I	234	
6	W	234	
7	J	205	
7	X	205	
8	K	201	
8	Y	201	
9	L	204	
9	Z	204	
10	M	213	
10	a	213	
11	N	219	
11	b	219	
12	C	261	
12	Q	261	
13	D	250	
13	R	250	
14	E	241	
14	S	241	
15	c	1843	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 62124 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	234	Total	C	N	O	S	0	0
			1830	1164	304	349	13		
1	O	240	Total	C	N	O	S	0	0
			1872	1189	313	357	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	216	Total	C	N	O	S	0	0
			1692	1082	288	316	6		
2	P	229	Total	C	N	O	S	0	0
			1790	1144	304	336	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	237	Total	C	N	O	S	0	0
			1867	1171	335	349	12		
3	T	233	Total	C	N	O	S	0	0
			1828	1146	328	343	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	244	Total	C	N	O	S	0	0
			1905	1207	325	362	11		
4	U	238	Total	C	N	O	S	0	0
			1865	1183	318	353	11		

- Molecule 5 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	200	Total	C	N	O	S	0	0
			1499	939	256	292	12		
5	V	201	Total	C	N	O	S	0	0
			1506	943	257	294	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
6	W	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
7	X	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		
8	Y	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
9	Z	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

- Molecule 10 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	214	Total	C	N	O	S	0	0
			1673	1055	289	317	12		
11	b	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	242	Total	C	N	O	S	0	0
			1905	1206	326	363	10		
12	C	213	Total	C	N	O	S	0	0
			1664	1054	281	320	9		

- Molecule 13 is a protein called Isoform 3 of Proteasome subunit alpha-type 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	233	Total	C	N	O	S	0	0
			1824	1150	324	345	5		
13	D	217	Total	C	N	O	S	0	0
			1694	1069	296	324	5		

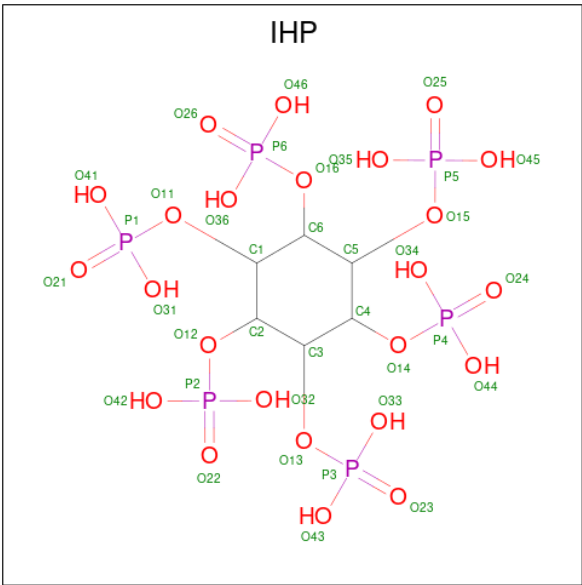
- Molecule 14 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	233	Total	C	N	O	S	0	0
			1777	1116	294	356	11		
14	E	229	Total	C	N	O	S	0	0
			1765	1113	293	348	11		

- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1784	Total	C	N	O	S	0	0
			14431	9280	2459	2611	81		

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
16	c	1	Total	C	O	P	0
			36	6	24	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.

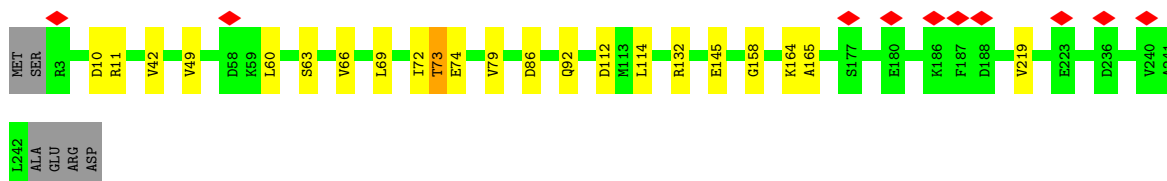
- Molecule 1: Proteasome subunit alpha type-6

Chain A: 



- Molecule 1: Proteasome subunit alpha type-6

Chain O: 



- Molecule 2: Proteasome subunit alpha type-2

Chain B: 



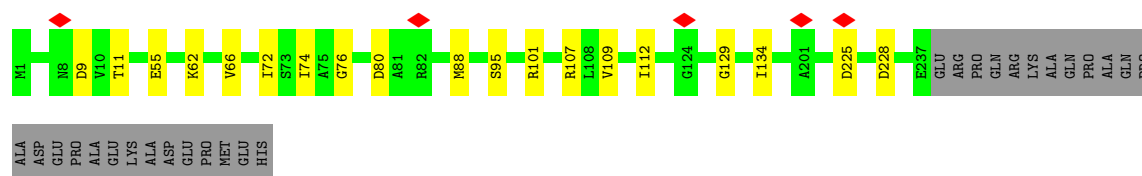
- Molecule 2: Proteasome subunit alpha type-2

Chain P: 

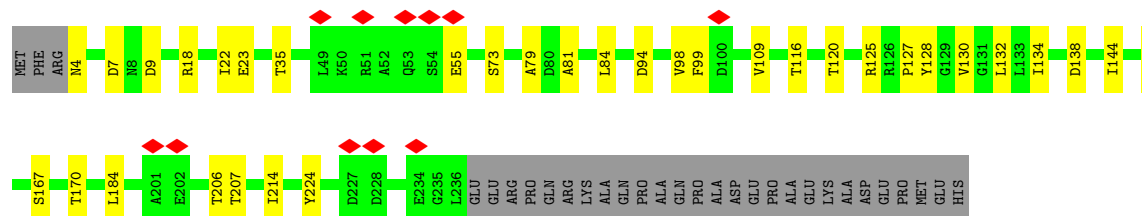
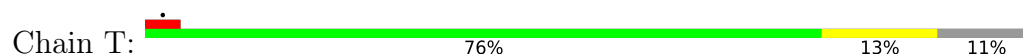


- Molecule 3: Proteasome subunit alpha type-1

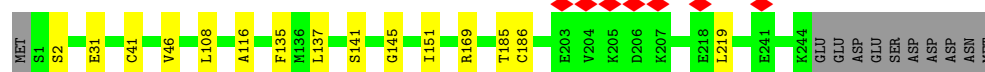
Chain F: 



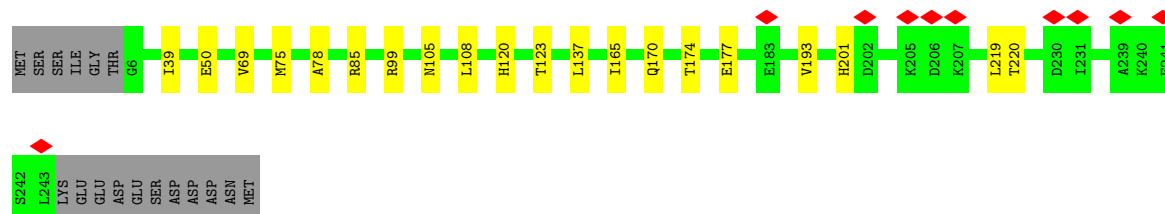
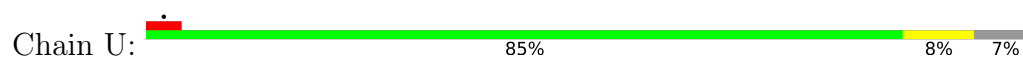
- Molecule 3: Proteasome subunit alpha type-1



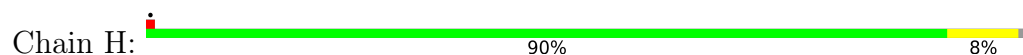
- Molecule 4: Proteasome subunit alpha type-3



- Molecule 4: Proteasome subunit alpha type-3



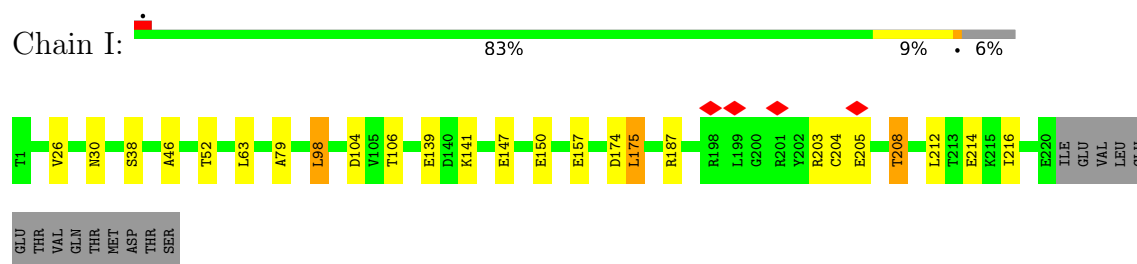
- Molecule 5: Proteasome subunit beta type-6



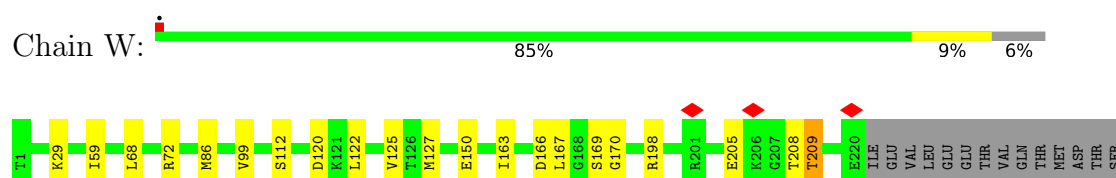
- Molecule 5: Proteasome subunit beta type-6



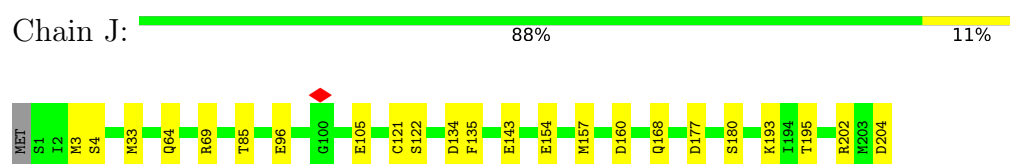
- Molecule 6: Proteasome subunit beta type-7



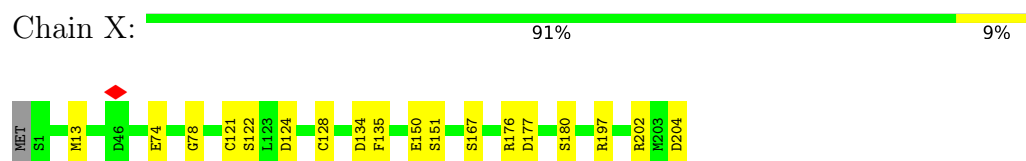
- Molecule 6: Proteasome subunit beta type-7



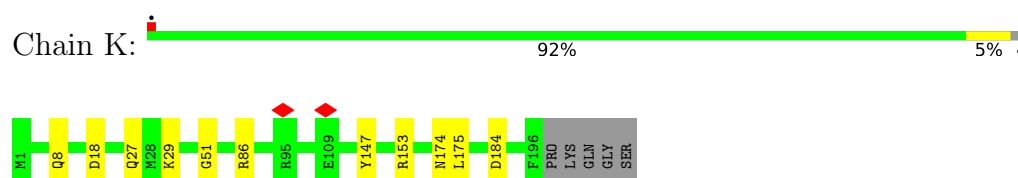
- Molecule 7: Proteasome subunit beta type-3



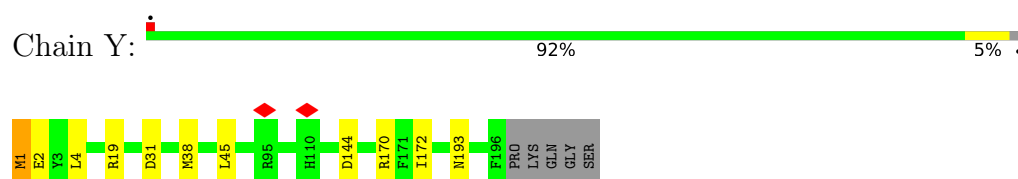
- Molecule 7: Proteasome subunit beta type-3



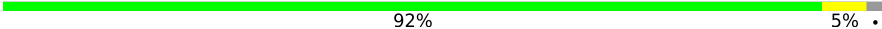
- Molecule 8: Proteasome subunit beta type-2

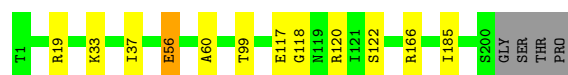


- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-5

Chain L:  92% 5%



- Molecule 9: Proteasome subunit beta type-5

Chain Z:  90% 8%

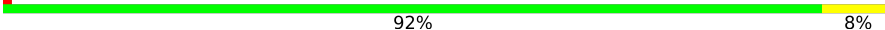


- Molecule 10: Proteasome subunit beta type-1

Chain M:  91% 9%

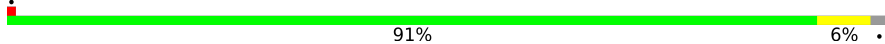


- Molecule 10: Proteasome subunit beta type-1

Chain a:  92% 8%



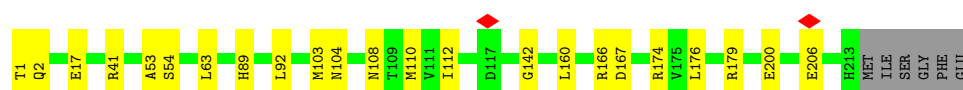
- Molecule 11: Proteasome subunit beta type-4

Chain N:  91% 6%

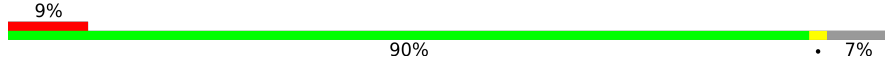


- Molecule 11: Proteasome subunit beta type-4

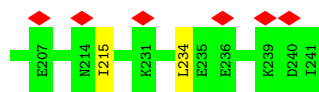
Chain b:  87% 11%



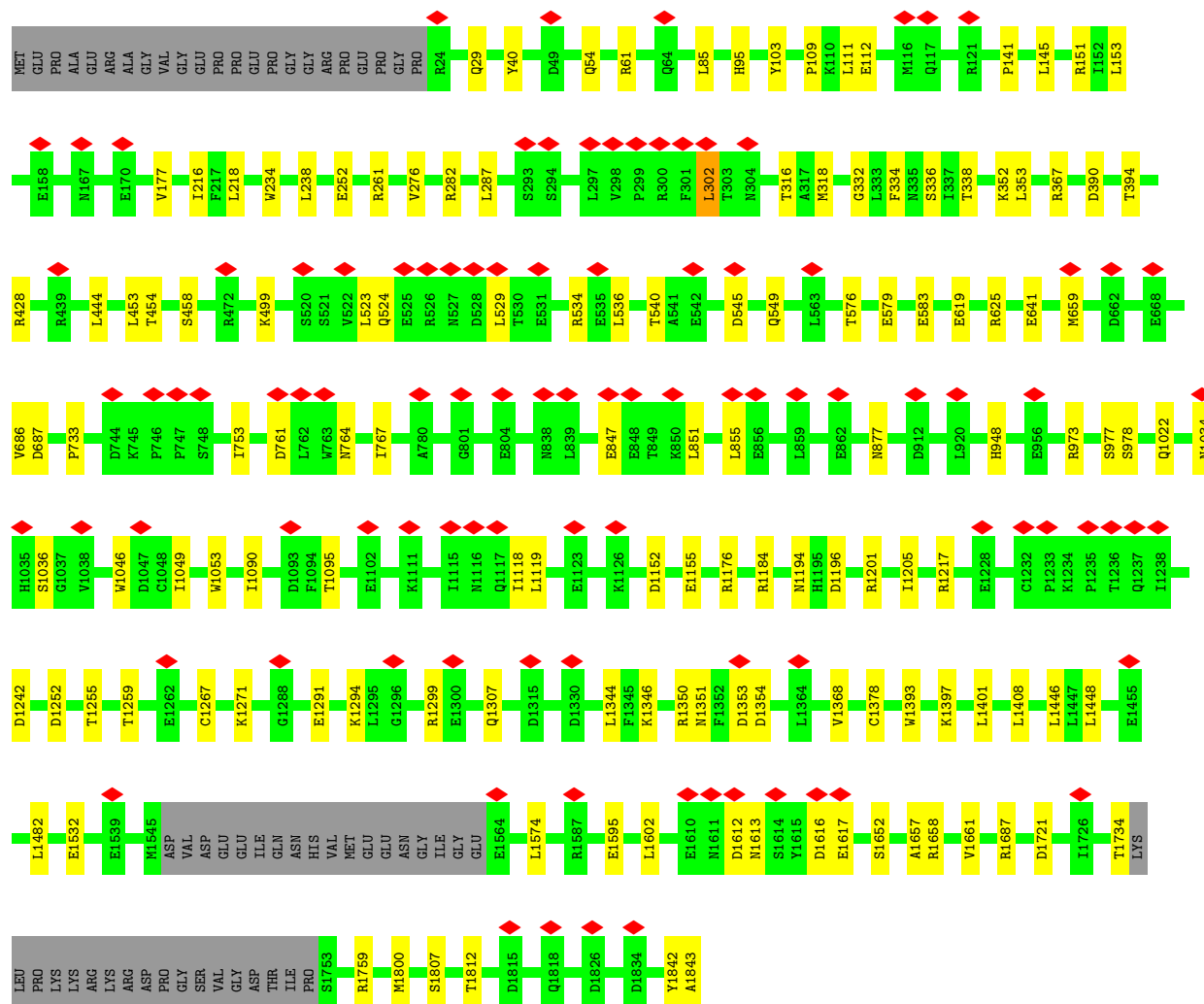
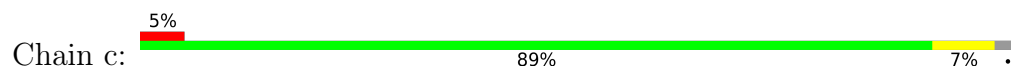
- Molecule 12: Proteasome subunit alpha type-4

Chain Q:  90% 7%





• Molecule 15: Proteasome activator complex subunit 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.947	Depositor
Minimum map value	-1.118	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	388.92, 388.92, 388.92	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92600006, 0.92600006, 0.92600006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	0.14	0/1863	0.27	0/2520
1	O	0.14	0/1906	0.33	0/2576
2	B	0.12	0/1727	0.28	0/2339
2	P	0.14	0/1829	0.33	0/2477
3	F	0.15	0/1902	0.34	0/2569
3	T	0.13	0/1862	0.29	0/2517
4	G	0.25	0/1940	0.40	0/2612
4	U	0.17	0/1900	0.32	0/2559
5	H	0.14	0/1525	0.30	0/2064
5	V	0.14	0/1532	0.30	0/2074
6	I	0.14	0/1686	0.33	0/2282
6	W	0.15	0/1686	0.35	0/2282
7	J	0.17	0/1620	0.31	0/2184
7	X	0.14	0/1620	0.34	0/2184
8	K	0.14	0/1603	0.32	0/2168
8	Y	0.13	0/1603	0.29	0/2168
9	L	0.13	0/1586	0.29	0/2142
9	Z	0.12	0/1586	0.29	0/2142
10	M	0.26	0/1672	0.43	0/2254
10	a	0.13	0/1672	0.31	0/2254
11	N	0.15	0/1706	0.35	0/2309
11	b	0.14	0/1698	0.33	0/2299
12	C	0.13	0/1686	0.31	0/2271
12	Q	0.13	0/1935	0.33	0/2608
13	D	0.14	0/1714	0.33	0/2307
13	R	0.13	0/1850	0.31	0/2496
14	E	0.14	0/1791	0.31	0/2417
14	S	0.18	0/1804	0.36	0/2437
15	c	0.14	0/14768	0.31	0/20030
All	All	0.15	0/63272	0.32	0/85541

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

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	1830	0	1844	13	0
1	O	1872	0	1882	16	0
2	B	1692	0	1697	11	0
2	P	1790	0	1784	10	0
3	F	1867	0	1860	13	0
3	T	1828	0	1820	22	0
4	G	1905	0	1895	9	0
4	U	1865	0	1848	12	0
5	H	1499	0	1469	8	0
5	V	1506	0	1476	6	0
6	I	1659	0	1681	14	0
6	W	1659	0	1681	15	0
7	J	1591	0	1612	17	0
7	X	1591	0	1612	10	0
8	K	1571	0	1573	9	0
8	Y	1571	0	1573	8	0
9	L	1555	0	1520	8	0
9	Z	1555	0	1520	8	0
10	M	1642	0	1640	11	0
10	a	1642	0	1640	9	0
11	N	1673	0	1650	9	0
11	b	1665	0	1641	13	0
12	C	1664	0	1696	7	0
12	Q	1905	0	1925	6	0
13	D	1694	0	1741	9	0
13	R	1824	0	1863	9	0
14	E	1765	0	1769	14	0
14	S	1777	0	1764	12	0
15	c	14431	0	14619	80	0
16	c	36	0	6	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	62124	0	62301	339	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 3.

The worst 5 of 339 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:205:GLU:O	6:W:208:THR:OG1	2.04	0.74
14:E:4:THR:HG22	15:c:1812:THR:HG21	1.70	0.73
11:b:63:LEU:HD13	11:b:110:MET:HE2	1.71	0.73
7:J:69:ARG:NH2	7:J:96:GLU:OE2	2.22	0.73
3:F:107:ARG:NH2	11:N:74:GLU:OE1	2.23	0.72

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	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
1	O	238/246 (97%)	230 (97%)	8 (3%)	0	100	100
2	B	214/234 (92%)	212 (99%)	2 (1%)	0	100	100
2	P	227/234 (97%)	223 (98%)	4 (2%)	0	100	100
3	F	235/263 (89%)	227 (97%)	8 (3%)	0	100	100
3	T	231/263 (88%)	224 (97%)	7 (3%)	0	100	100
4	G	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
4	U	236/255 (92%)	229 (97%)	7 (3%)	0	100	100
5	H	198/205 (97%)	193 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	V	199/205 (97%)	191 (96%)	8 (4%)	0	100	100
6	I	218/234 (93%)	214 (98%)	4 (2%)	0	100	100
6	W	218/234 (93%)	211 (97%)	7 (3%)	0	100	100
7	J	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
7	X	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
8	K	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
8	Y	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
9	L	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
9	Z	198/204 (97%)	193 (98%)	5 (2%)	0	100	100
10	M	210/213 (99%)	202 (96%)	8 (4%)	0	100	100
10	a	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
11	N	212/219 (97%)	203 (96%)	9 (4%)	0	100	100
11	b	211/219 (96%)	203 (96%)	8 (4%)	0	100	100
12	C	209/261 (80%)	207 (99%)	2 (1%)	0	100	100
12	Q	240/261 (92%)	231 (96%)	9 (4%)	0	100	100
13	D	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
13	R	231/250 (92%)	225 (97%)	6 (3%)	0	100	100
14	E	225/241 (93%)	221 (98%)	4 (2%)	0	100	100
14	S	231/241 (96%)	221 (96%)	10 (4%)	0	100	100
15	c	1778/1843 (96%)	1742 (98%)	36 (2%)	0	100	100
All	All	7846/8305 (94%)	7645 (97%)	201 (3%)	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	201/210 (96%)	201 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	205/210 (98%)	204 (100%)	1 (0%)	81	93
2	B	177/191 (93%)	177 (100%)	0	100	100
2	P	188/191 (98%)	187 (100%)	1 (0%)	81	93
3	F	203/224 (91%)	203 (100%)	0	100	100
3	T	199/224 (89%)	199 (100%)	0	100	100
4	G	201/212 (95%)	200 (100%)	1 (0%)	81	93
4	U	196/212 (92%)	196 (100%)	0	100	100
5	H	155/159 (98%)	153 (99%)	2 (1%)	61	86
5	V	156/159 (98%)	155 (99%)	1 (1%)	78	93
6	I	181/195 (93%)	174 (96%)	7 (4%)	28	63
6	W	181/195 (93%)	178 (98%)	3 (2%)	53	82
7	J	173/174 (99%)	173 (100%)	0	100	100
7	X	173/174 (99%)	171 (99%)	2 (1%)	63	86
8	K	167/171 (98%)	167 (100%)	0	100	100
8	Y	167/171 (98%)	166 (99%)	1 (1%)	78	93
9	L	156/159 (98%)	154 (99%)	2 (1%)	61	86
9	Z	156/159 (98%)	154 (99%)	2 (1%)	61	86
10	M	177/178 (99%)	175 (99%)	2 (1%)	65	88
10	a	177/178 (99%)	176 (99%)	1 (1%)	78	93
11	N	177/181 (98%)	177 (100%)	0	100	100
11	b	176/181 (97%)	175 (99%)	1 (1%)	78	93
12	C	179/221 (81%)	174 (97%)	5 (3%)	38	72
12	Q	204/221 (92%)	203 (100%)	1 (0%)	81	93
13	D	181/210 (86%)	181 (100%)	0	100	100
13	R	195/210 (93%)	192 (98%)	3 (2%)	57	84
14	E	195/203 (96%)	194 (100%)	1 (0%)	81	93
14	S	195/203 (96%)	195 (100%)	0	100	100
15	c	1625/1673 (97%)	1615 (99%)	10 (1%)	78	93
All	All	6716/7049 (95%)	6669 (99%)	47 (1%)	73	92

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Z	102	CYS
12	C	206	LEU
10	a	30	SER
12	C	41	ASP
15	c	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
9	Z	70	ASN
15	c	812	GLN
9	Z	175	ASN
13	D	202	GLN
15	c	930	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	IHP	c	1901	-	36,36,36	1.52	6 (16%)	54,60,60	0.76	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	IHP	c	1901	-	-	11/30/54/54	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	IHP	P5-O15	3.64	1.66	1.59
16	c	1901	IHP	P1-O11	3.26	1.65	1.59
16	c	1901	IHP	P4-O14	3.19	1.65	1.59
16	c	1901	IHP	P2-O12	3.18	1.65	1.59
16	c	1901	IHP	P6-O16	3.18	1.65	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	c	1901	IHP	O15-C5-C4	2.20	113.88	108.69

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

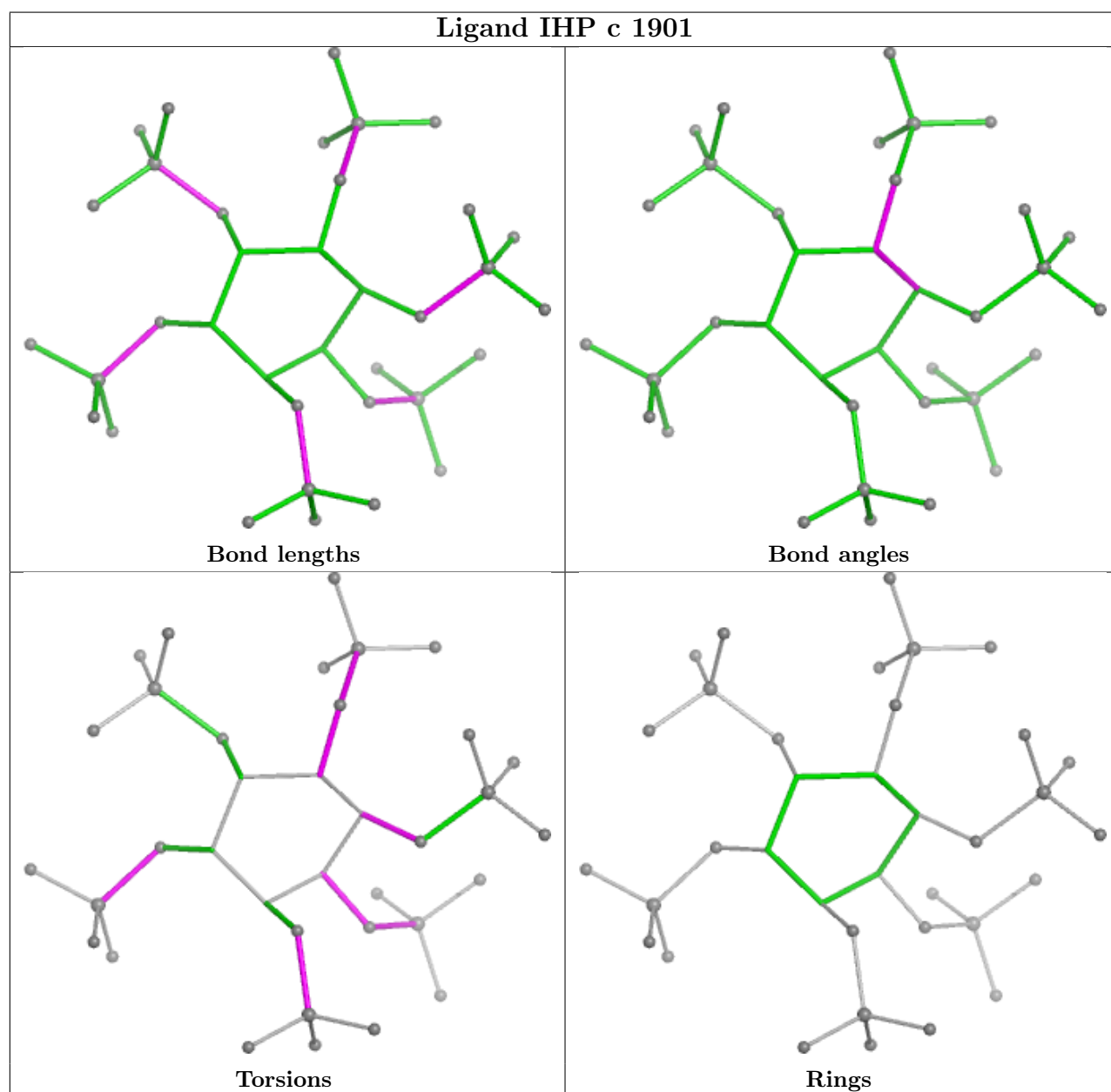
Mol	Chain	Res	Type	Atoms
16	c	1901	IHP	C4-C5-O15-P5
16	c	1901	IHP	C3-O13-P3-O23
16	c	1901	IHP	C1-O11-P1-O21
16	c	1901	IHP	C3-O13-P3-O43
16	c	1901	IHP	C5-O15-P5-O35

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	c	1901	IHP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

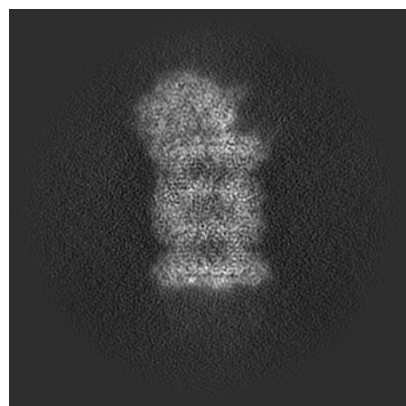
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56074. These allow visual inspection of the internal detail of the map and identification of artifacts.

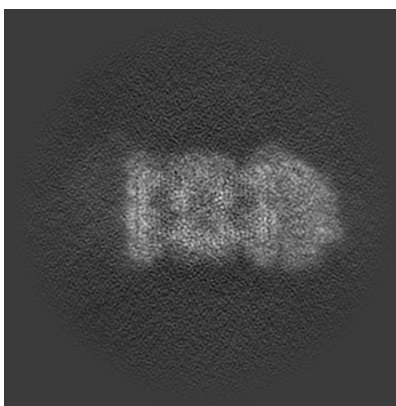
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

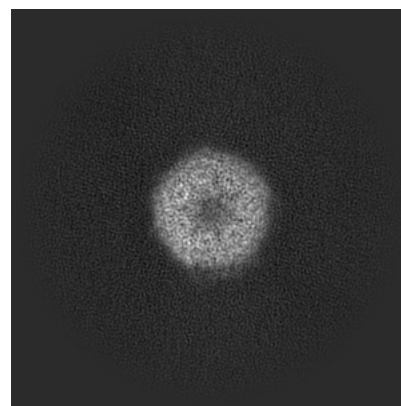
6.1.1 Primary map



X

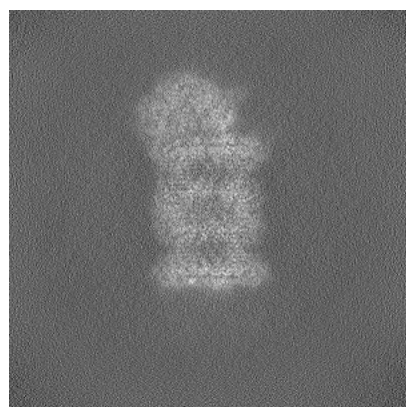


Y

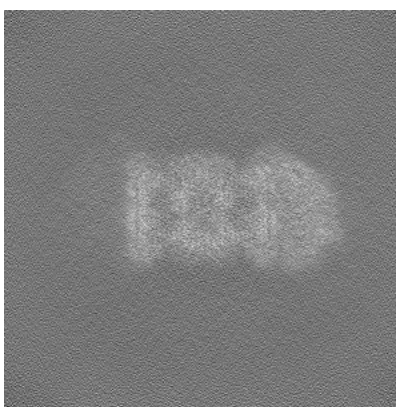


Z

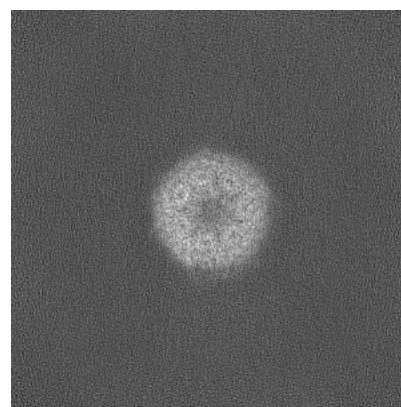
6.1.2 Raw map



X



Y

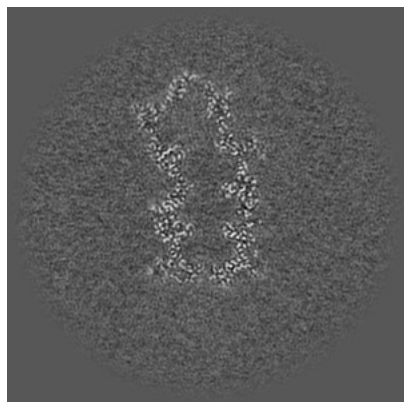


Z

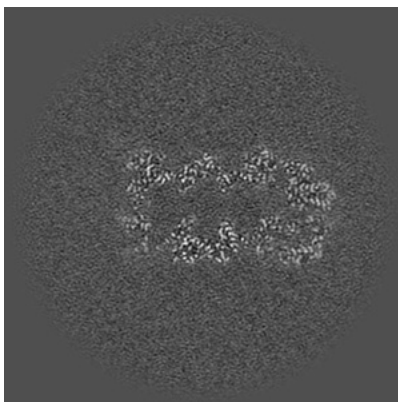
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

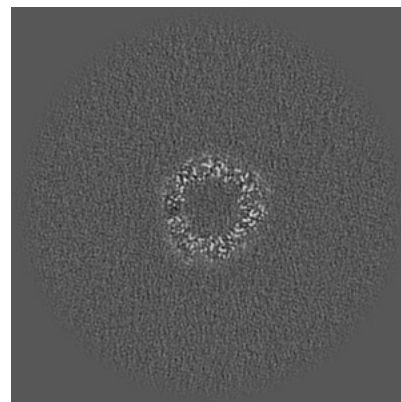
6.2.1 Primary map



X Index: 210

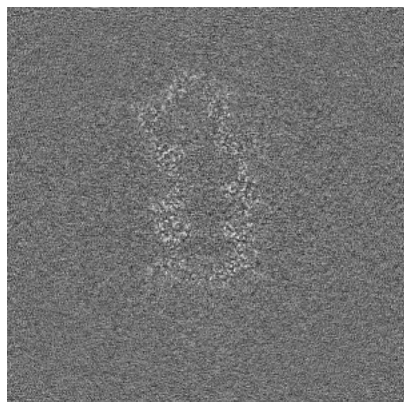


Y Index: 210

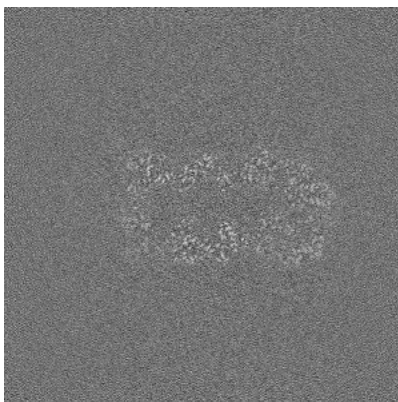


Z Index: 210

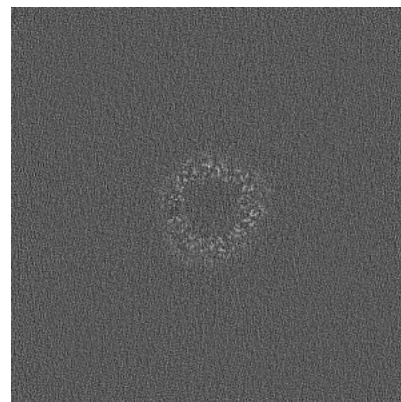
6.2.2 Raw map



X Index: 210



Y Index: 210

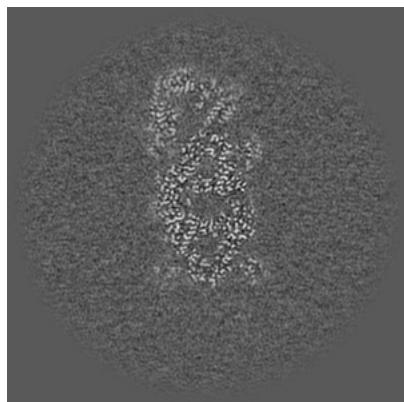


Z Index: 210

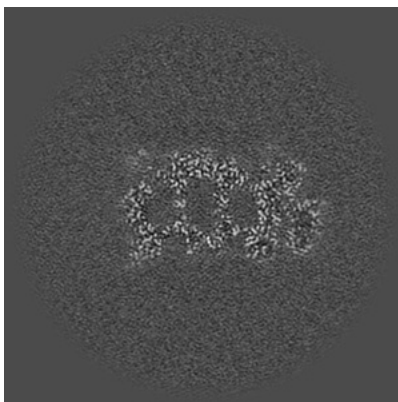
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

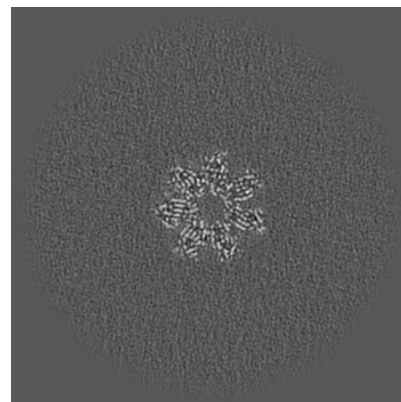
6.3.1 Primary map



X Index: 186

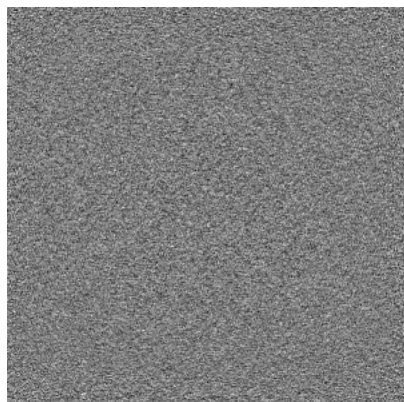


Y Index: 228

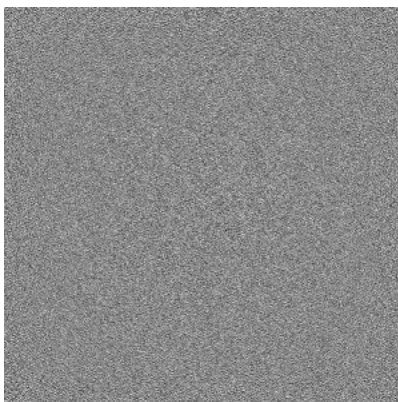


Z Index: 229

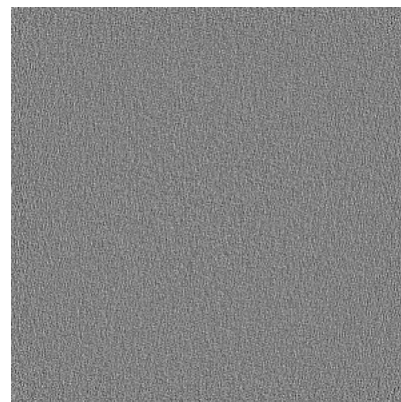
6.3.2 Raw map



X Index: 0



Y Index: 0

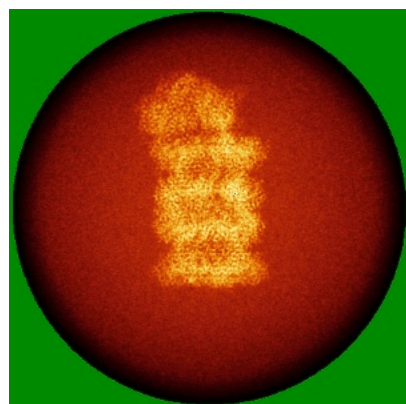


Z Index: 0

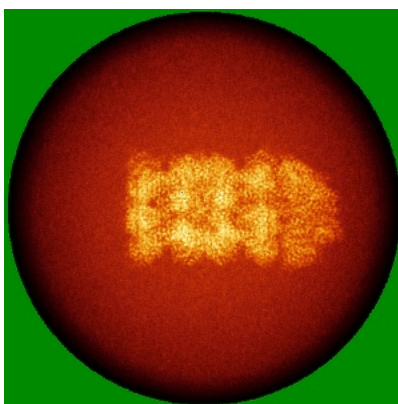
The images above show the largest variance slices of the map in three orthogonal directions.

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

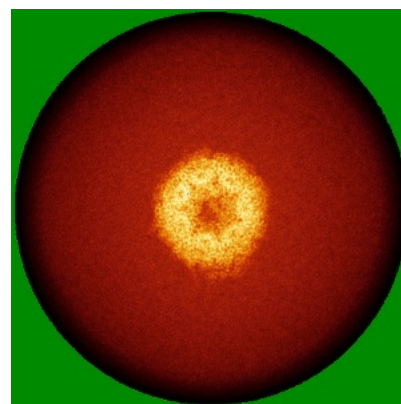
6.4.1 Primary map



X

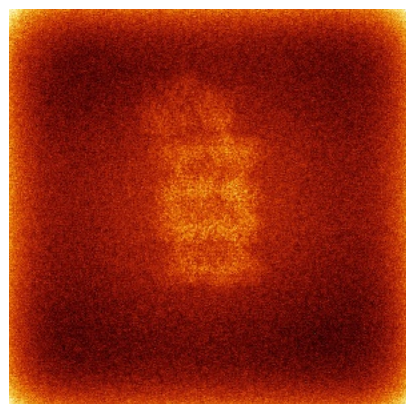


Y

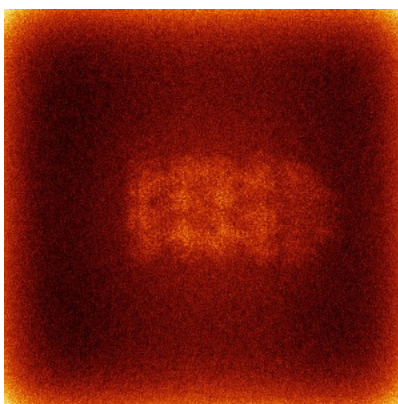


Z

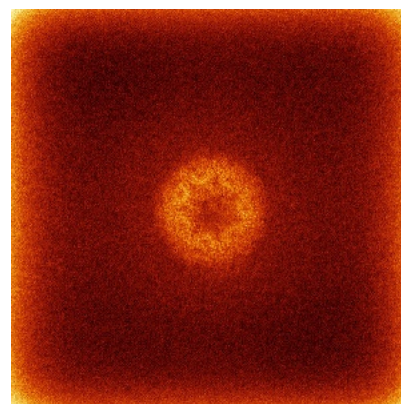
6.4.2 Raw map



X



Y

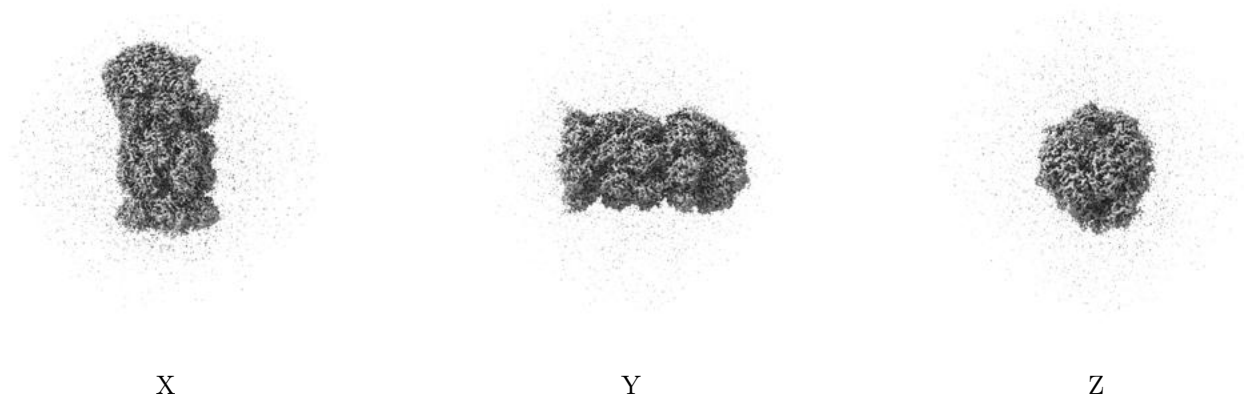


Z

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.

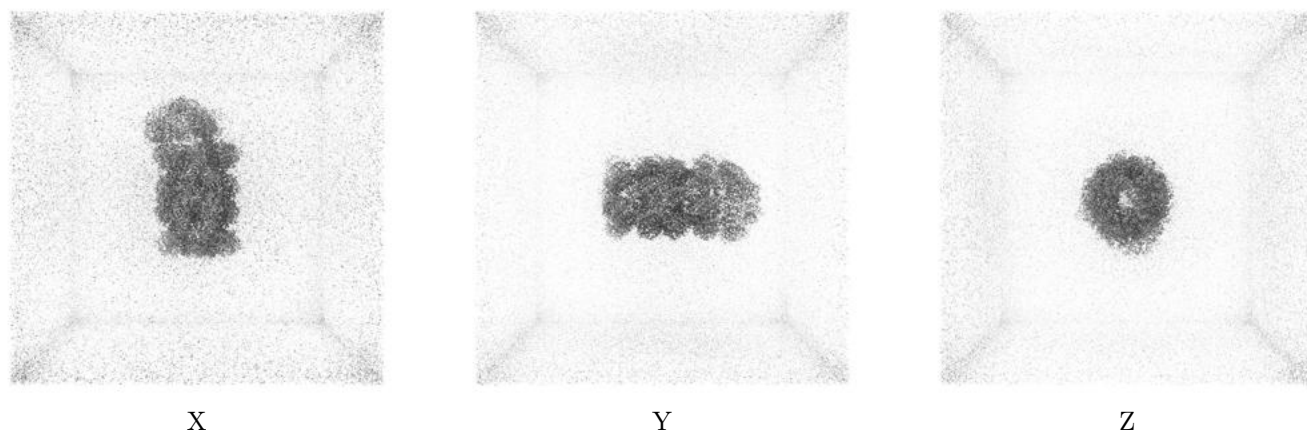
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

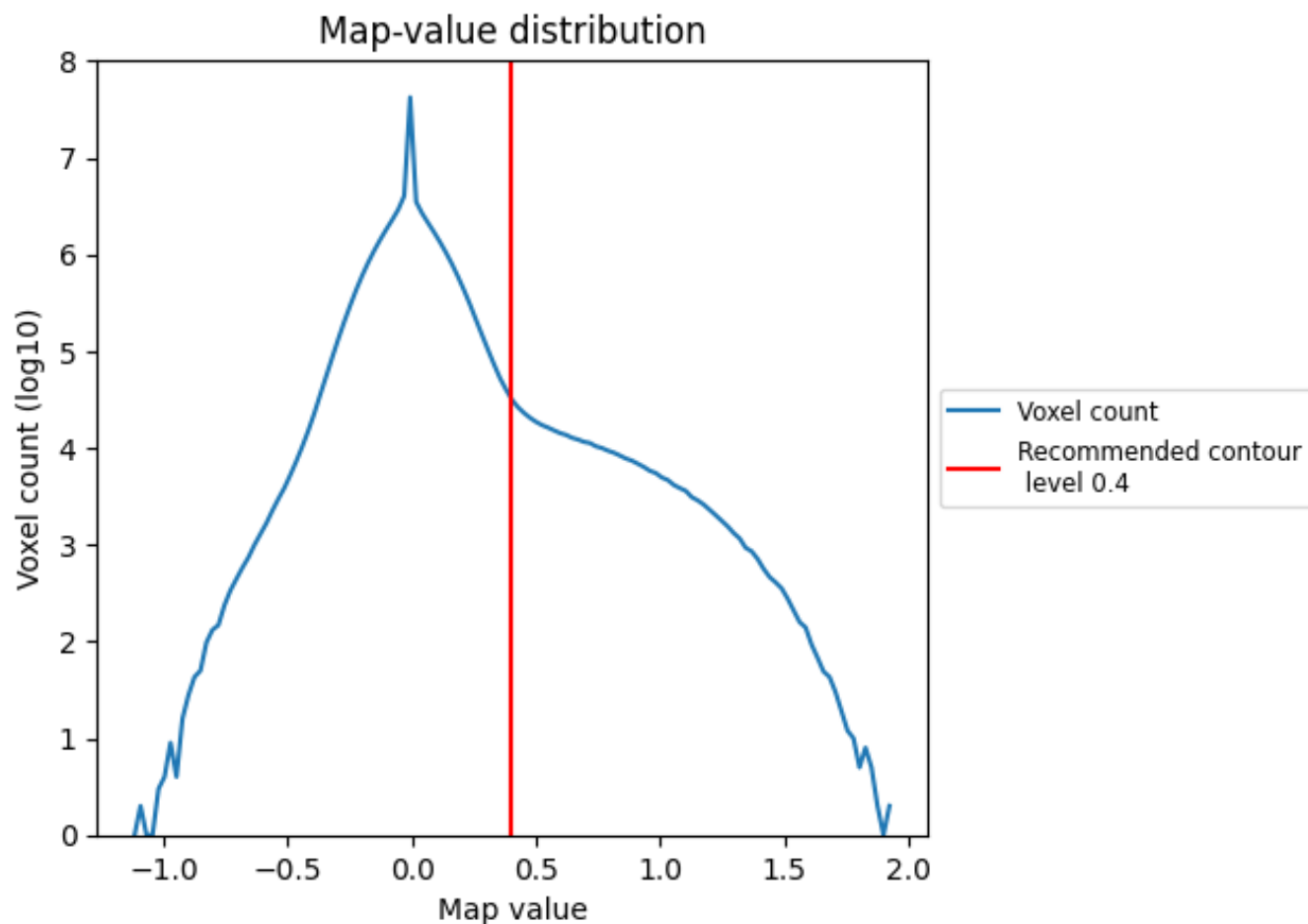
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

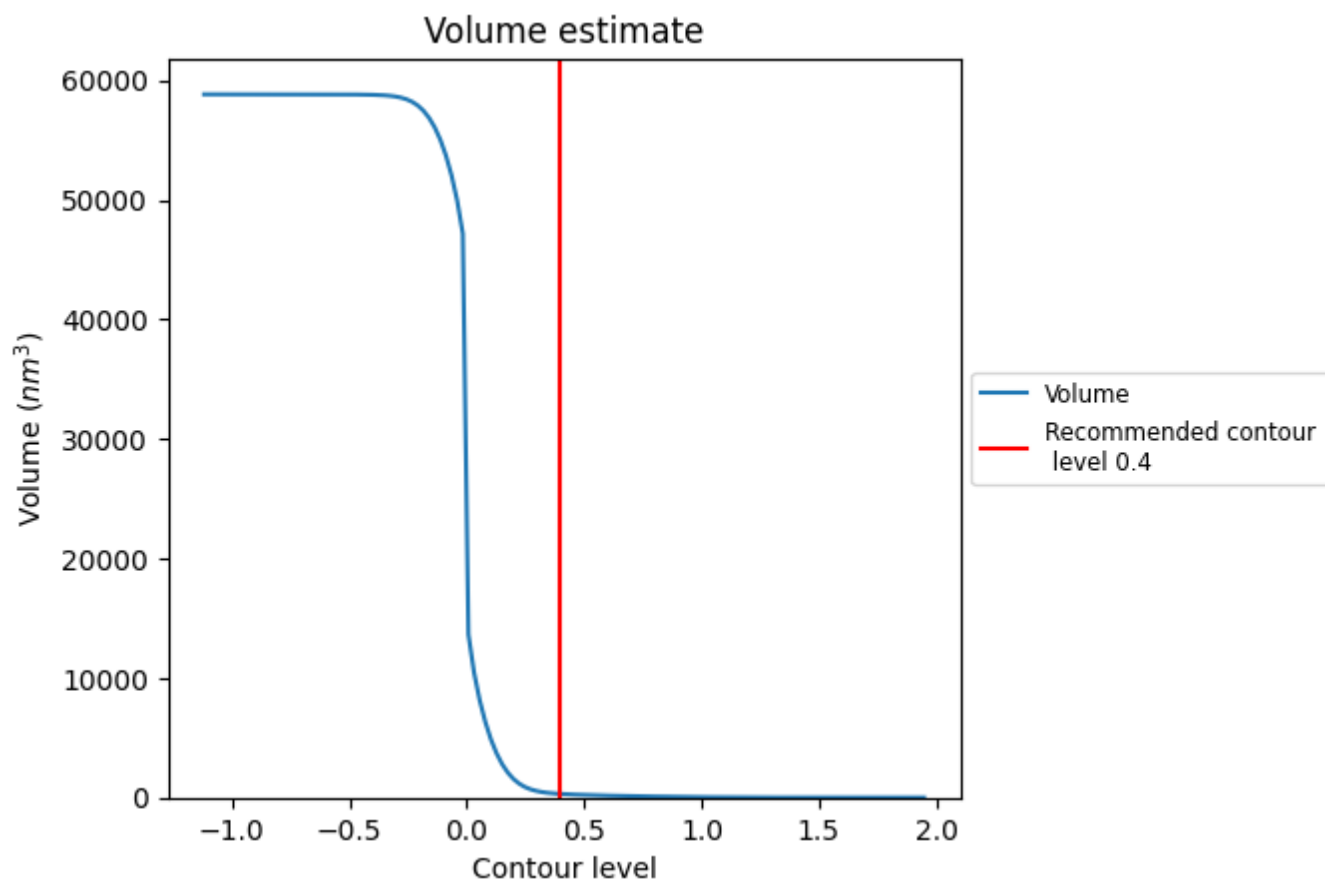
This section contains the results of statistical analysis of the map.

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.

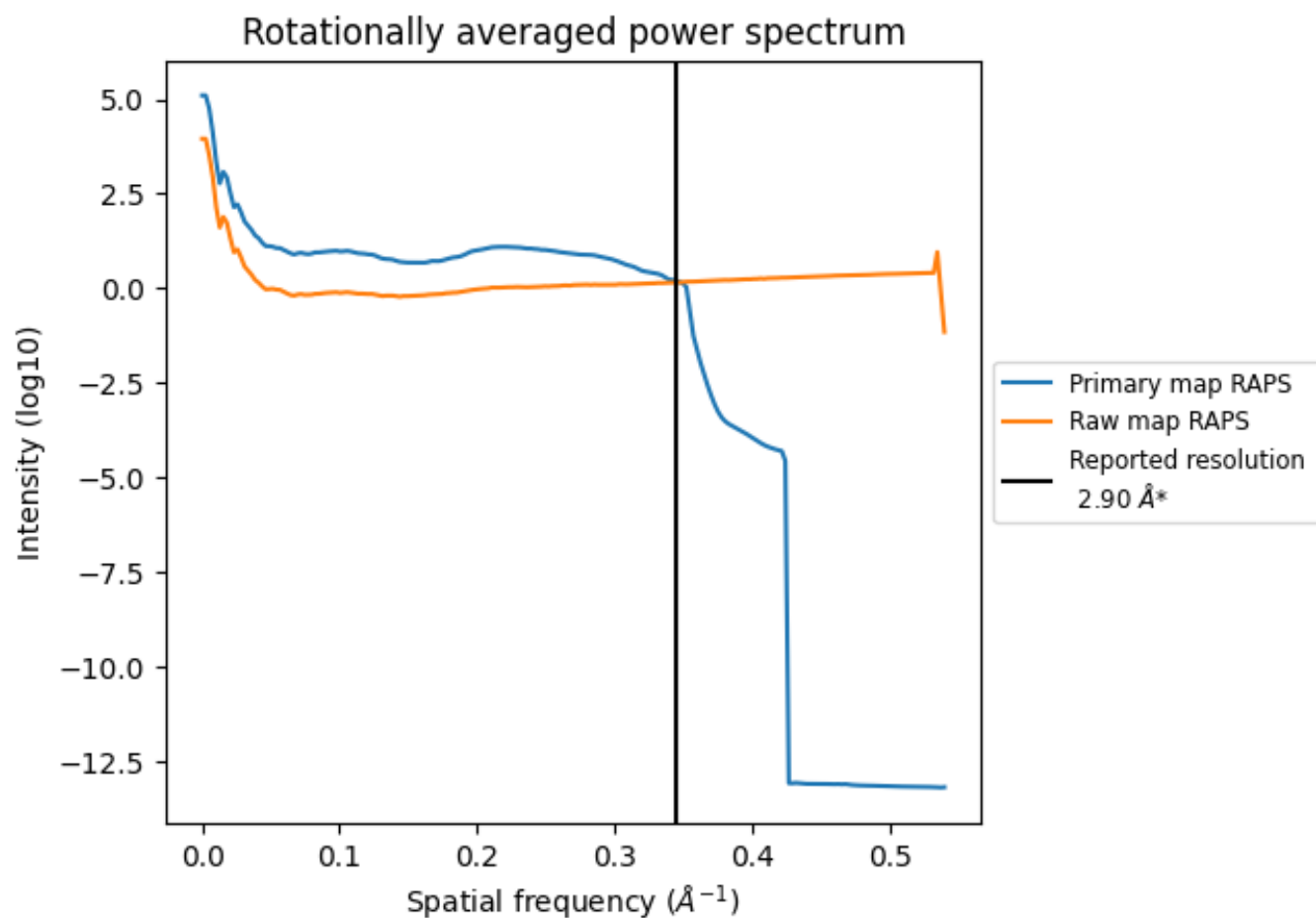
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 274 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 ⓘ

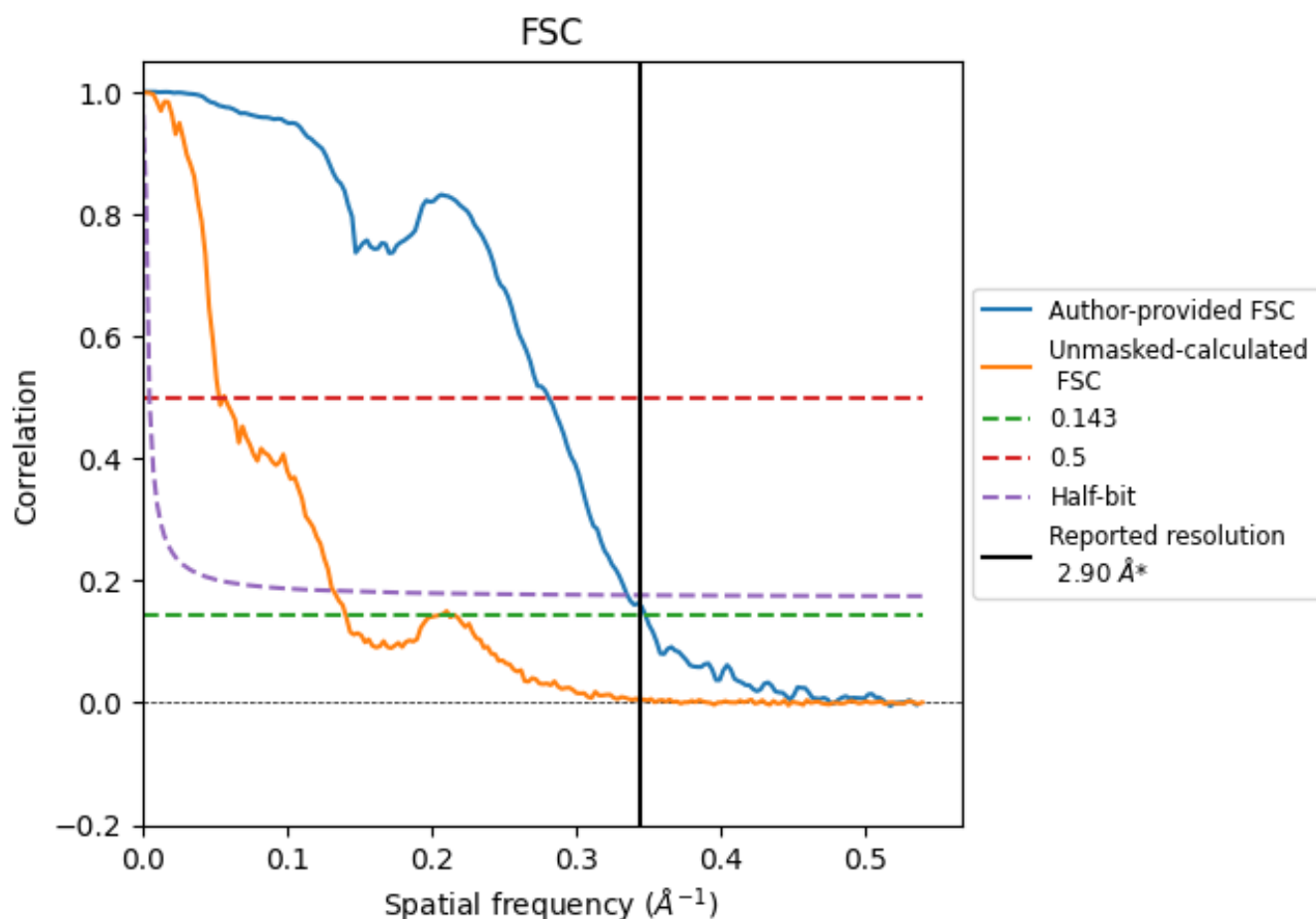


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

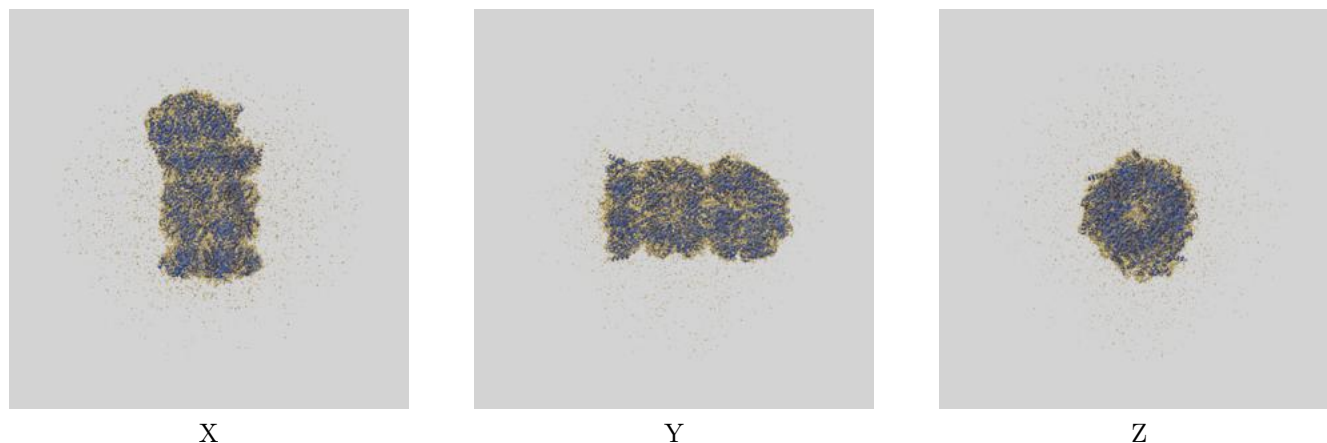
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.55	2.98
Unmasked-calculated*	7.09	18.80	7.55

*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 7.09 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

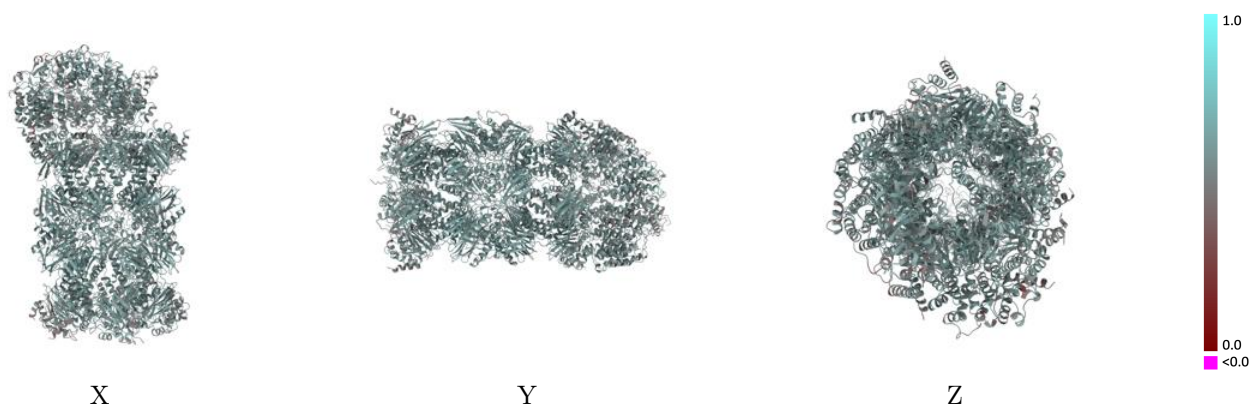
This section contains information regarding the fit between EMDB map EMD-56074 and PDB model 9TMS. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



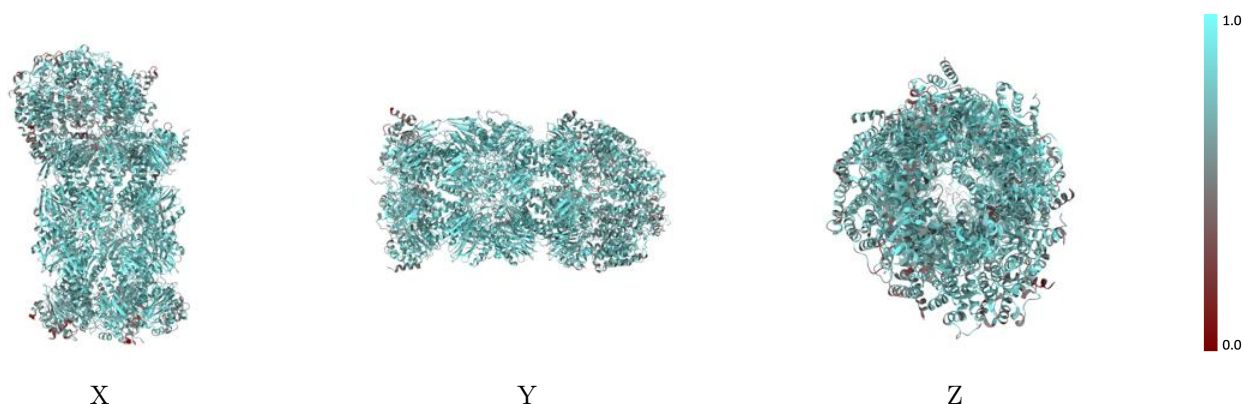
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



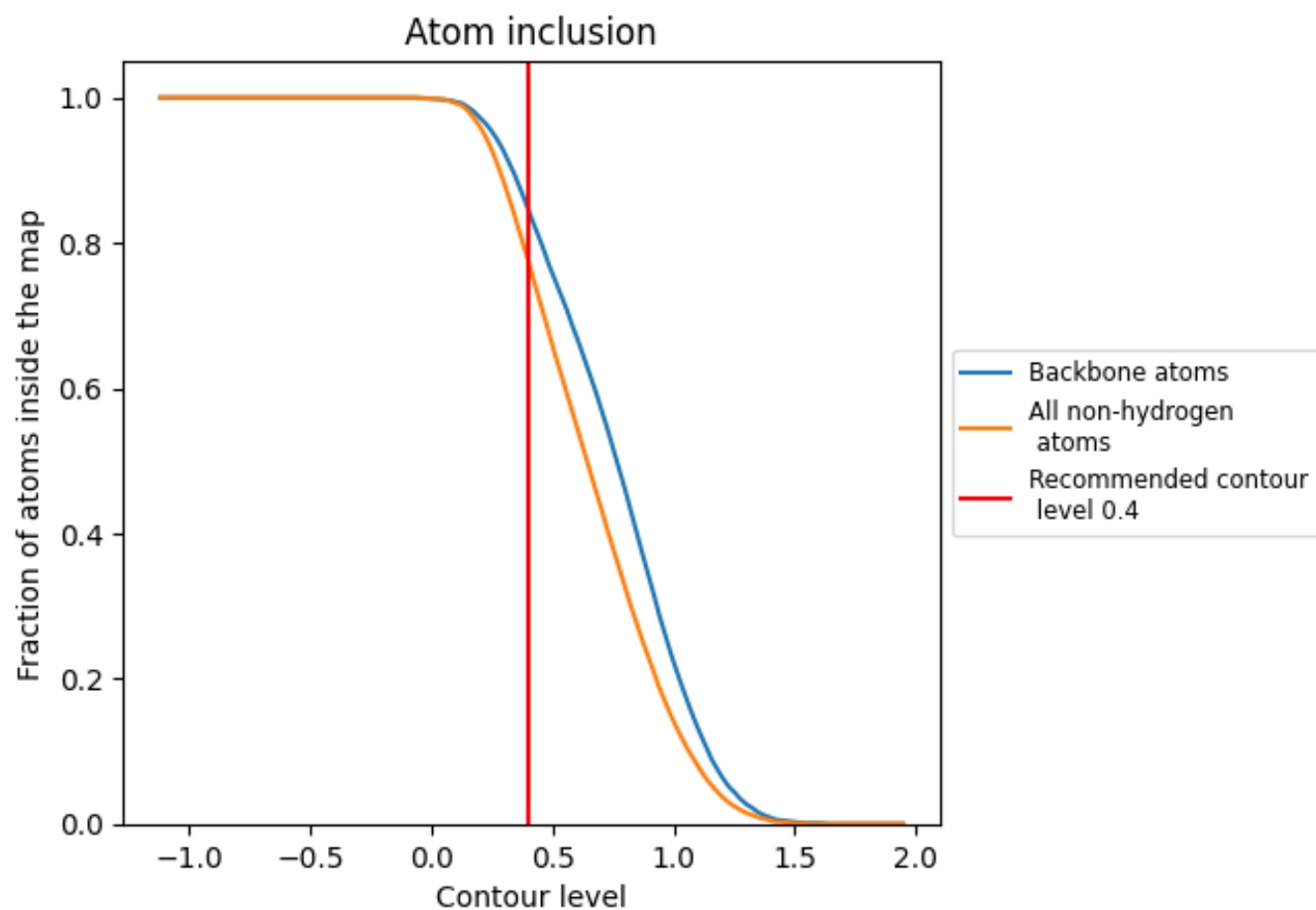
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.5710
A	 0.7750	 0.5740
B	 0.7950	 0.5790
C	 0.7160	 0.5620
D	 0.6980	 0.5520
E	 0.7170	 0.5580
F	 0.8140	 0.5790
G	 0.7830	 0.5720
H	 0.8560	 0.6030
I	 0.8310	 0.5890
J	 0.8360	 0.5900
K	 0.8490	 0.5960
L	 0.8480	 0.5970
M	 0.8200	 0.5860
N	 0.8410	 0.5960
O	 0.7560	 0.5660
P	 0.7780	 0.5690
Q	 0.7200	 0.5600
R	 0.6860	 0.5480
S	 0.7180	 0.5550
T	 0.7670	 0.5660
U	 0.7660	 0.5710
V	 0.8310	 0.5960
W	 0.8260	 0.5840
X	 0.8430	 0.5910
Y	 0.8450	 0.5990
Z	 0.8520	 0.5950
a	 0.8220	 0.5860
b	 0.8570	 0.5980
c	 0.7220	 0.5480

