



wwPDB EM Validation Summary Report ⓘ

Jul 21, 2026 – 05:02 PM EDT

PDB ID : 9PMO / pdb_00009pmo
EMDB ID : EMD-71740
Title : Human 26S proteasome bound to TXNL1 with opened gate of core particle
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-18
Resolution : 3.82 Å (reported)
Based on initial models : 1WWY, 7WSI, 1GH2

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:

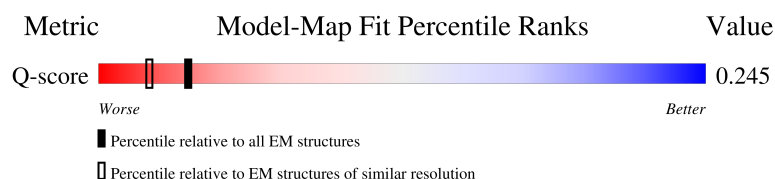
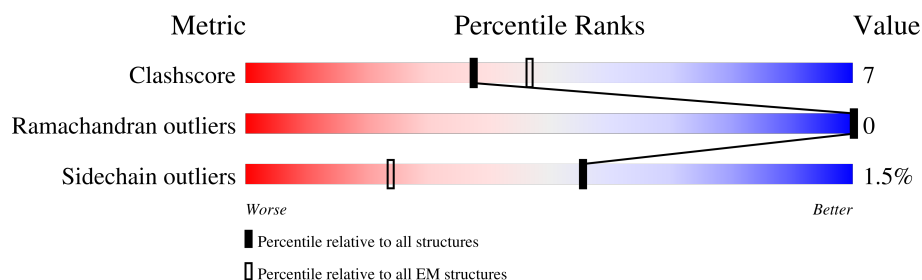
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB 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 i

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

The reported resolution of this entry is 3.82 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.



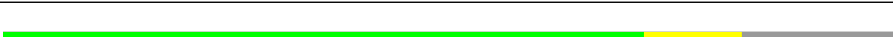
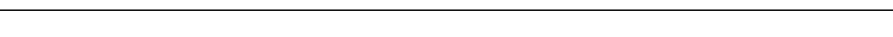
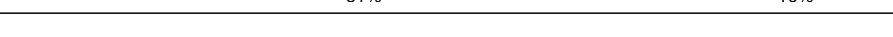
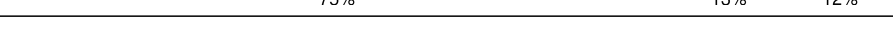
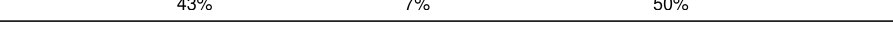
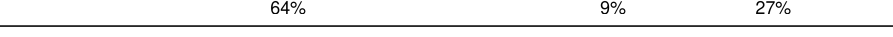
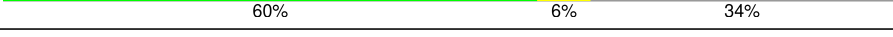
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9152 (3.32 - 4.32)

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	433	 72% 19% • 8%
2	B	440	 73% 16% 11%
3	C	406	 73% 21% • 5%
4	D	418	 65% 18% • 14%

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	269	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	a	376	
21	b	377	
22	c	310	
23	d	350	
24	e	70	
25	f	908	
26	g	289	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 71052 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3137	1974	552	594	17		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	390	Total	C	N	O	S	0	0
			3058	1922	522	599	15		

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	384	Total	C	N	O	S	0	0
			3033	1910	544	561	18		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	360	Total	C	N	O	S	0	0
			2876	1820	496	547	13		

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	360	Total	C	N	O	S	0	0
			2875	1810	513	536	16		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	379	Total	C	N	O	S	0	0
			2961	1867	509	567	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1876	1192	313	358	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	224	Total	C	N	O	S	0	0
			1742	1112	295	329	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	244	Total	C	N	O	S	0	0
			1917	1214	327	366	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	235	Total	C	N	O	S	0	0
			1846	1158	326	357	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1749	1102	289	347	11		

- Molecule 12 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	861	Total	C	N	O	S	0	0
			6717	4262	1143	1268	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	445	Total	C	N	O	S	0	0
			3619	2306	646	654	13		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	420	Total	C	N	O	S	0	0
			3422	2172	579	648	23		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	368	Total	C	N	O	S	0	0
			2909	1859	492	547	11		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	187	Total	C	N	O	S	0	0
			1433	893	257	275	8		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	256	Total	C	N	O	S	0	0
			2108	1366	345	388	9		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	46	Total	C	N	O	0	0
			389	238	61	90		

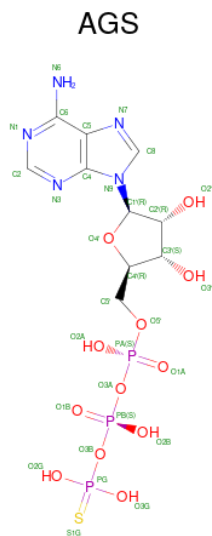
- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	847	Total	C	N	O	S	0	0
			6542	4113	1113	1270	46		

- Molecule 26 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	289	Total	C	N	O	S	0	0
			2263	1419	381	448	15		

- Molecule 27 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

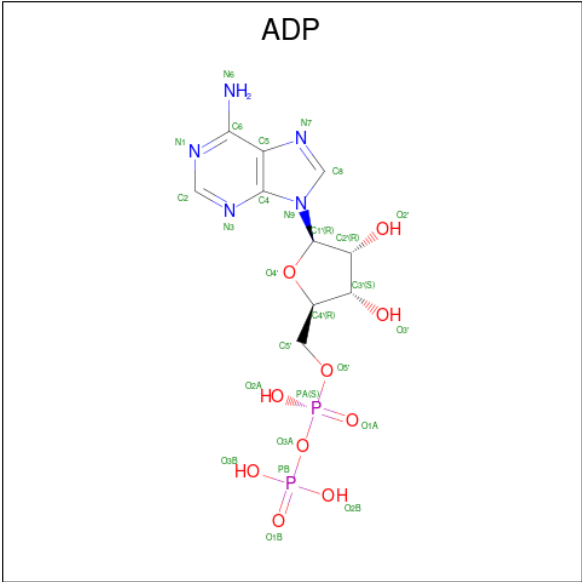


Mol	Chain	Residues	Atoms					AltConf	
27	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
27	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
27	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
27	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total Mg 1 1	0
28	B	1	Total Mg 1 1	0
28	F	1	Total Mg 1 1	0

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

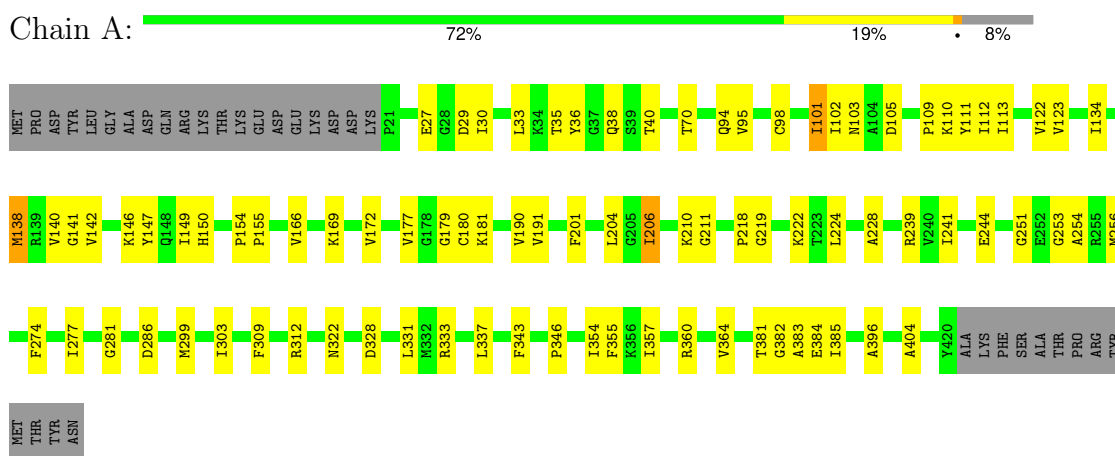
- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	c	1	Total	Zn	0
			1	1	

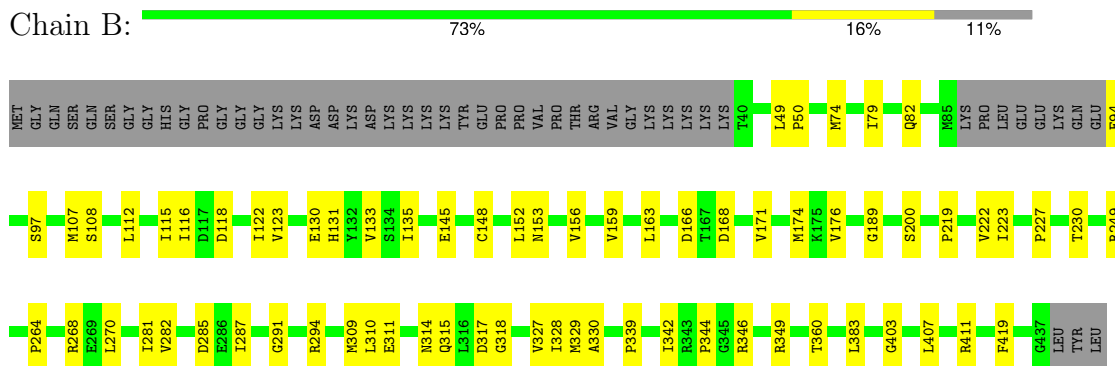
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

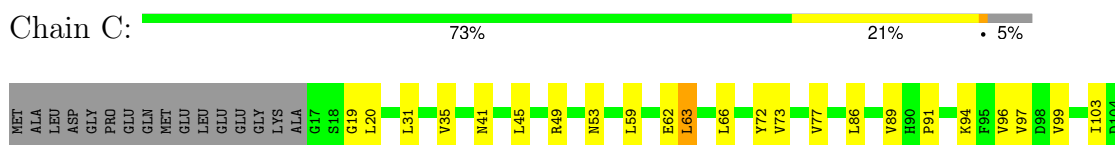
- Molecule 1: 26S proteasome regulatory subunit 7

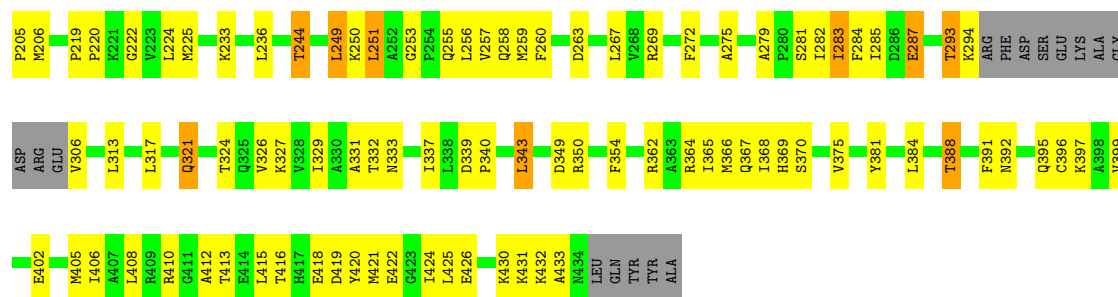


- Molecule 2: 26S proteasome regulatory subunit 4

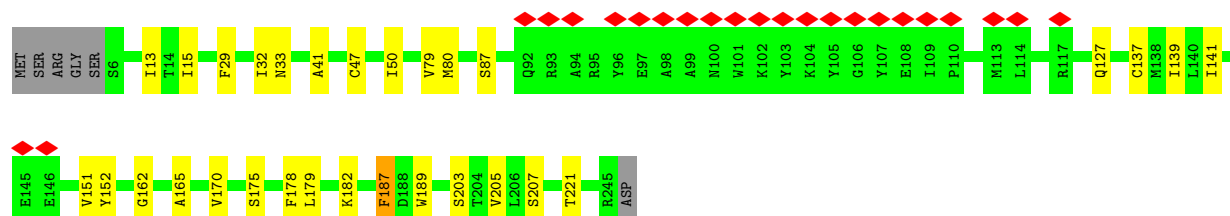
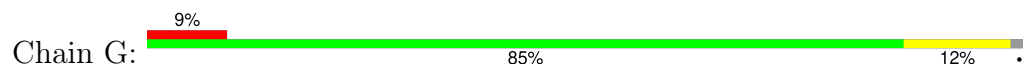


- Molecule 3: 26S protease regulatory subunit 8

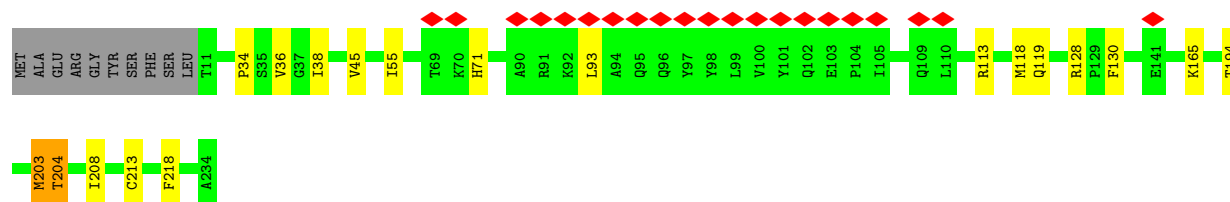




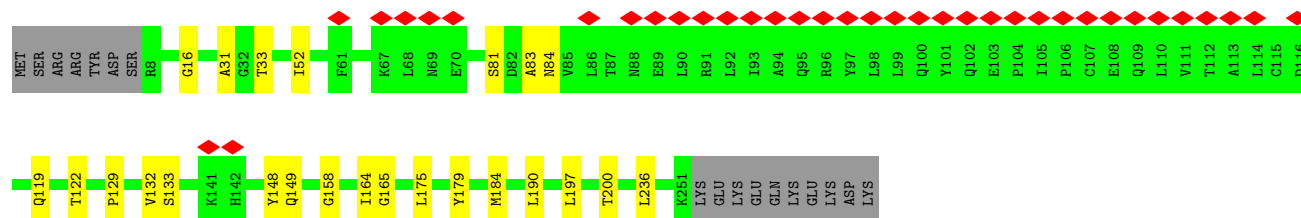
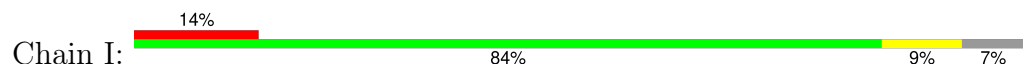
• Molecule 7: Proteasome subunit alpha type-6



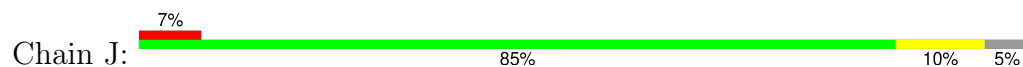
• Molecule 8: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-4

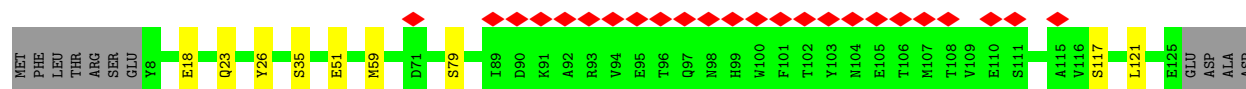
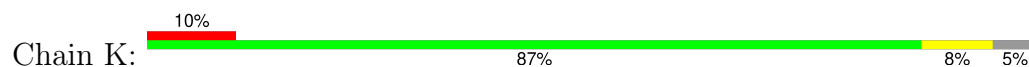


• Molecule 10: Proteasome subunit alpha type-7

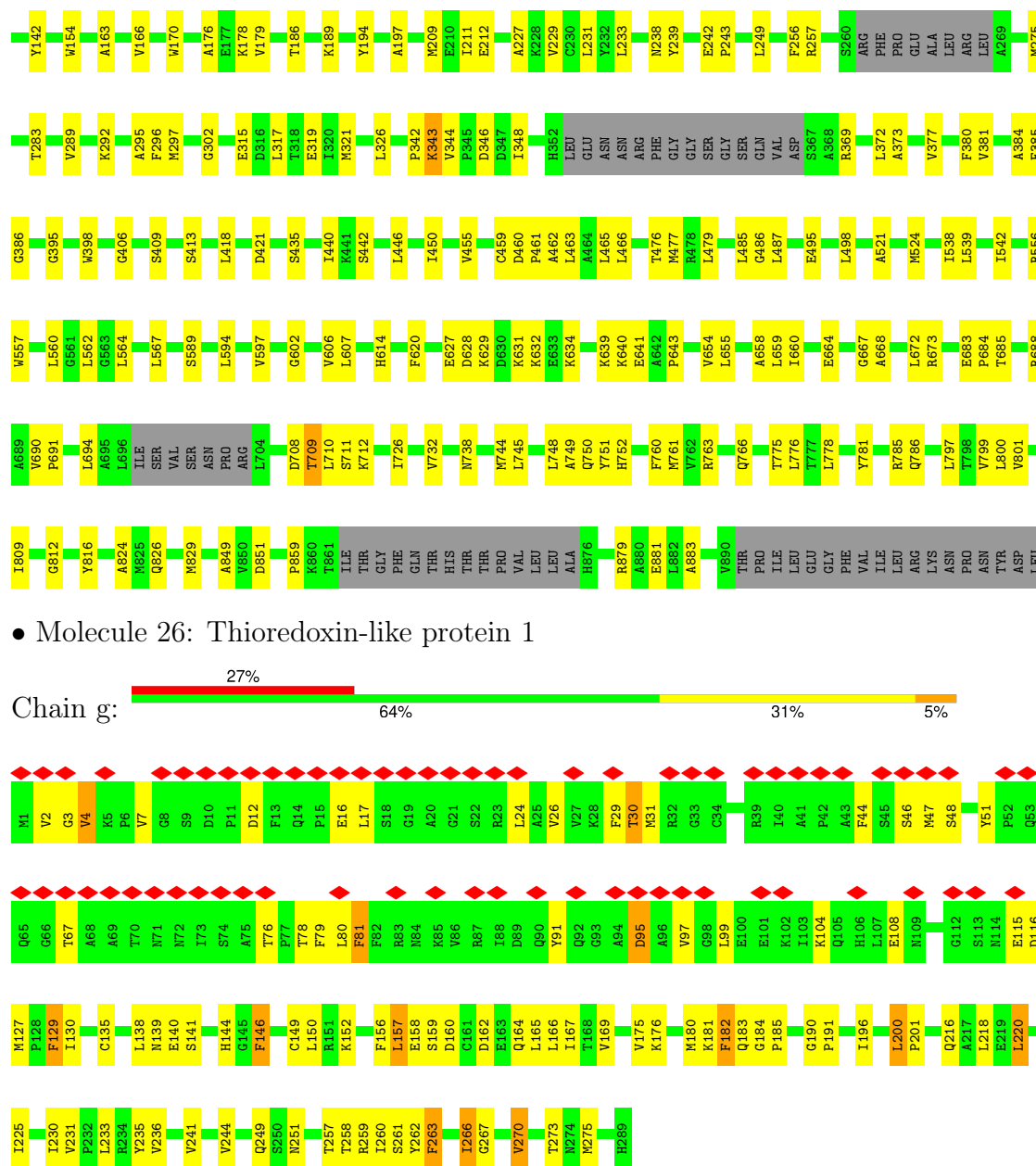




• Molecule 11: Proteasome subunit alpha type-5







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ADP, AGS

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	0.60	0/3187	0.90	0/4302
2	B	0.37	0/3102	0.74	0/4185
3	C	0.56	0/3073	0.94	0/4130
4	D	0.64	0/2918	0.95	0/3933
5	E	0.56	0/2916	0.91	0/3920
6	F	0.82	0/2996	1.11	0/4035
7	G	0.32	0/1910	0.66	0/2582
8	H	0.45	0/1779	0.72	0/2411
9	I	0.26	0/1946	0.64	0/2621
10	J	0.27	0/1871	0.67	0/2526
11	K	0.28	0/1775	0.64	0/2394
12	L	0.29	0/1908	0.62	0/2579
13	M	0.27	0/1916	0.67	0/2580
14	U	0.43	0/6834	0.84	0/9239
15	V	0.34	0/3689	0.74	0/4981
16	W	0.31	0/3468	0.71	0/4665
17	X	0.53	0/2951	0.81	0/3974
18	Y	0.34	0/3173	0.75	0/4273
19	Z	0.37	0/2324	0.69	0/3150
20	a	0.37	0/3061	0.75	0/4144
21	b	0.23	0/1453	0.63	0/1967
22	c	0.81	0/2315	1.14	0/3129
23	d	0.36	0/2154	0.72	0/2909
24	e	0.30	0/400	0.73	0/545
25	f	0.40	0/6645	0.81	0/8971
26	g	1.01	0/2309	1.29	0/3120
All	All	0.49	0/72073	0.83	0/97265

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	3137	0	3199	70	0
2	B	3058	0	3117	45	0
3	C	3033	0	3154	74	0
4	D	2876	0	2927	77	0
5	E	2875	0	2959	84	0
6	F	2961	0	3067	116	0
7	G	1876	0	1885	16	0
8	H	1742	0	1734	13	0
9	I	1917	0	1943	17	0
10	J	1846	0	1863	14	0
11	K	1749	0	1743	12	0
12	L	1873	0	1860	14	0
13	M	1881	0	1868	12	0
14	U	6717	0	6780	91	0
15	V	3619	0	3689	44	0
16	W	3422	0	3532	38	0
17	X	2909	0	3018	34	0
18	Y	3115	0	3120	37	0
19	Z	2281	0	2312	41	0
20	a	3003	0	3016	29	0
21	b	1433	0	1475	13	0
22	c	2272	0	2288	74	0
23	d	2108	0	2134	19	0
24	e	389	0	305	4	0
25	f	6542	0	6540	136	0
26	g	2263	0	2192	76	0
27	A	31	0	12	3	0
27	B	31	0	12	0	0
27	C	31	0	12	4	0
27	F	31	0	12	1	0
28	A	1	0	0	0	0
28	B	1	0	0	0	0
28	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	D	27	0	12	1	0
30	c	1	0	0	0	0
All	All	71052	0	71780	1065	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 7.

The worst 5 of 1065 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:F:224:LEU:HB2	6:F:331:ALA:HB2	1.64	0.78
25:f:691:PRO:HA	25:f:694:LEU:HB3	1.65	0.78
19:Z:13:PRO:HG2	22:c:220:LEU:HD22	1.65	0.78
5:E:137:GLY:HA3	5:E:312:ILE:HD11	1.66	0.78
1:A:354:ILE:HG21	1:A:382:GLY:HA2	1.66	0.77

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	398/433 (92%)	361 (91%)	37 (9%)	0	100	100
2	B	386/440 (88%)	358 (93%)	28 (7%)	0	100	100
3	C	380/406 (94%)	356 (94%)	24 (6%)	0	100	100
4	D	354/418 (85%)	315 (89%)	39 (11%)	0	100	100
5	E	354/389 (91%)	311 (88%)	43 (12%)	0	100	100
6	F	373/439 (85%)	324 (87%)	49 (13%)	0	100	100
7	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
8	H	222/234 (95%)	212 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	242/261 (93%)	234 (97%)	8 (3%)	0	100	100
10	J	233/248 (94%)	221 (95%)	12 (5%)	0	100	100
11	K	224/241 (93%)	215 (96%)	9 (4%)	0	100	100
12	L	236/269 (88%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
14	U	855/953 (90%)	797 (93%)	58 (7%)	0	100	100
15	V	443/534 (83%)	409 (92%)	34 (8%)	0	100	100
16	W	416/456 (91%)	397 (95%)	19 (5%)	0	100	100
17	X	362/422 (86%)	356 (98%)	6 (2%)	0	100	100
18	Y	376/389 (97%)	354 (94%)	22 (6%)	0	100	100
19	Z	284/324 (88%)	273 (96%)	11 (4%)	0	100	100
20	a	372/376 (99%)	354 (95%)	18 (5%)	0	100	100
21	b	185/377 (49%)	171 (92%)	14 (8%)	0	100	100
22	c	287/310 (93%)	262 (91%)	25 (9%)	0	100	100
23	d	254/350 (73%)	240 (94%)	14 (6%)	0	100	100
24	e	44/70 (63%)	37 (84%)	7 (16%)	0	100	100
25	f	837/908 (92%)	738 (88%)	99 (12%)	0	100	100
26	g	287/289 (99%)	263 (92%)	24 (8%)	0	100	100
All	All	8880/10037 (88%)	8243 (93%)	637 (7%)	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	343/372 (92%)	336 (98%)	7 (2%)	48	64
2	B	343/385 (89%)	343 (100%)	0	100	100
3	C	335/352 (95%)	325 (97%)	10 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	317/366 (87%)	299 (94%)	18 (6%)	18	44
5	E	318/341 (93%)	310 (98%)	8 (2%)	42	61
6	F	327/379 (86%)	307 (94%)	20 (6%)	17	43
7	G	205/210 (98%)	204 (100%)	1 (0%)	81	81
8	H	182/191 (95%)	179 (98%)	3 (2%)	55	68
9	I	204/221 (92%)	204 (100%)	0	100	100
10	J	198/211 (94%)	198 (100%)	0	100	100
11	K	192/203 (95%)	192 (100%)	0	100	100
12	L	204/230 (89%)	204 (100%)	0	100	100
13	M	198/212 (93%)	198 (100%)	0	100	100
14	U	734/816 (90%)	726 (99%)	8 (1%)	65	73
15	V	391/460 (85%)	391 (100%)	0	100	100
16	W	386/416 (93%)	383 (99%)	3 (1%)	73	75
17	X	315/362 (87%)	312 (99%)	3 (1%)	68	74
18	Y	334/344 (97%)	333 (100%)	1 (0%)	86	85
19	Z	257/295 (87%)	255 (99%)	2 (1%)	73	75
20	a	334/336 (99%)	333 (100%)	1 (0%)	86	85
21	b	165/312 (53%)	165 (100%)	0	100	100
22	c	253/268 (94%)	250 (99%)	3 (1%)	63	71
23	d	230/294 (78%)	228 (99%)	2 (1%)	70	74
24	e	40/63 (64%)	40 (100%)	0	100	100
25	f	709/763 (93%)	706 (100%)	3 (0%)	84	83
26	g	253/253 (100%)	229 (90%)	24 (10%)	8	30
All	All	7767/8655 (90%)	7650 (98%)	117 (2%)	55	69

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	333	ASN
26	g	220	LEU
14	U	559	ARG
26	g	218	LEU
26	g	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
20	a	62	ASN
25	f	724	ASN
20	a	258	GLN
22	c	269	GLN
6	F	417	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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
27	AGS	A	501	28	32,33,33	0.64	0	45,52,52	0.56	0
27	AGS	F	501	28	32,33,33	0.67	1 (3%)	45,52,52	0.46	0
27	AGS	B	501	28	32,33,33	0.67	1 (3%)	45,52,52	0.55	0
29	ADP	D	501	-	28,29,29	0.45	0	43,45,45	0.50	0
27	AGS	C	501	-	32,33,33	0.65	0	45,52,52	0.53	0

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
27	AGS	A	501	28	-	6/21/38/38	0/3/3/3
27	AGS	F	501	28	-	3/21/38/38	0/3/3/3
27	AGS	B	501	28	-	3/21/38/38	0/3/3/3
29	ADP	D	501	-	-	2/16/32/32	0/3/3/3
27	AGS	C	501	-	-	5/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	501	AGS	PG-S1G	2.18	1.95	1.90
27	F	501	AGS	PG-S1G	2.13	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	501	AGS	PB-O3B-PG-O2G
27	A	501	AGS	PB-O3B-PG-O3G
27	A	501	AGS	O4'-C4'-C5'-O5'
27	C	501	AGS	C5'-O5'-PA-O1A
27	C	501	AGS	C5'-O5'-PA-O3A

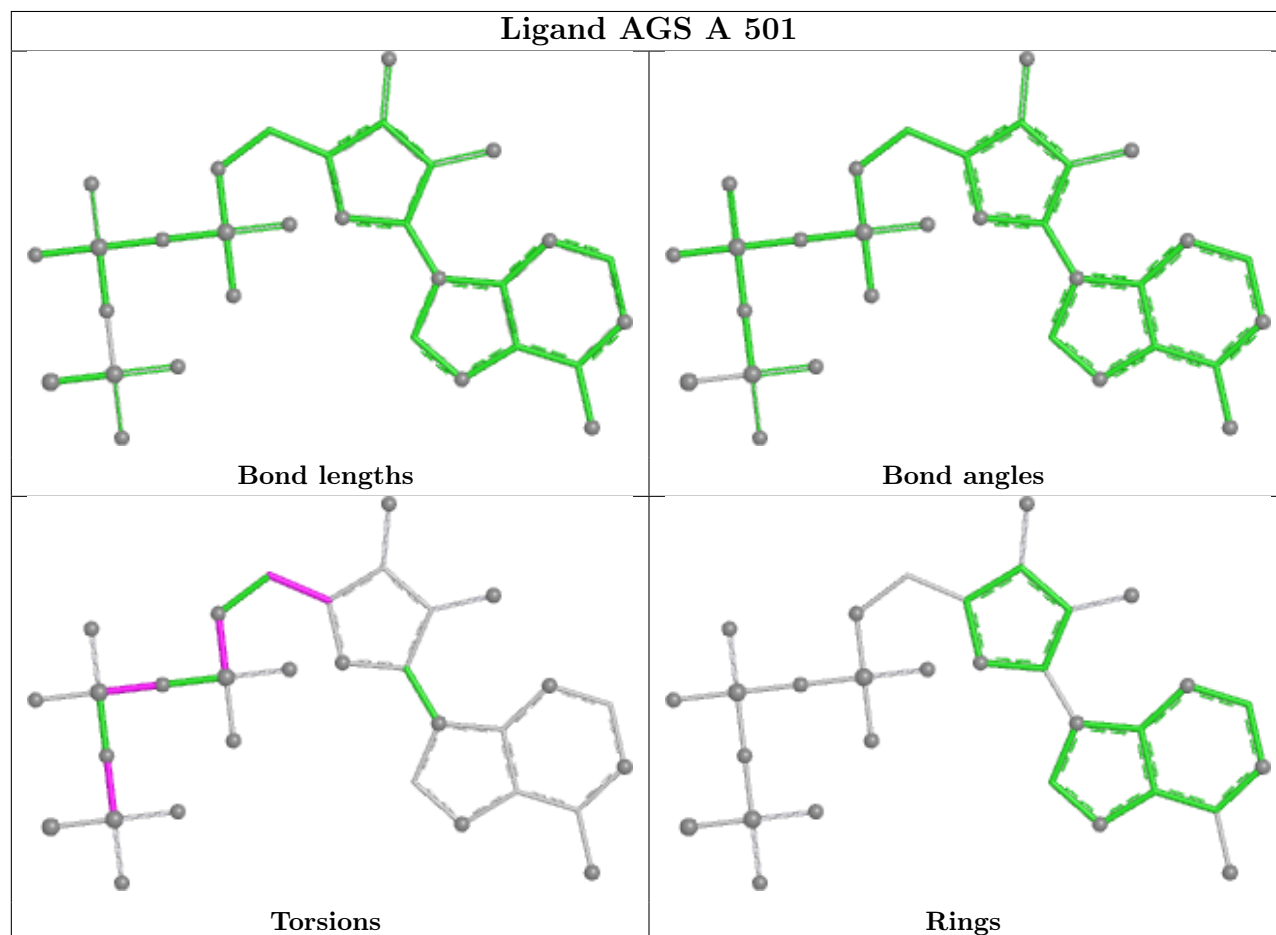
There are no ring outliers.

4 monomers are involved in 9 short contacts:

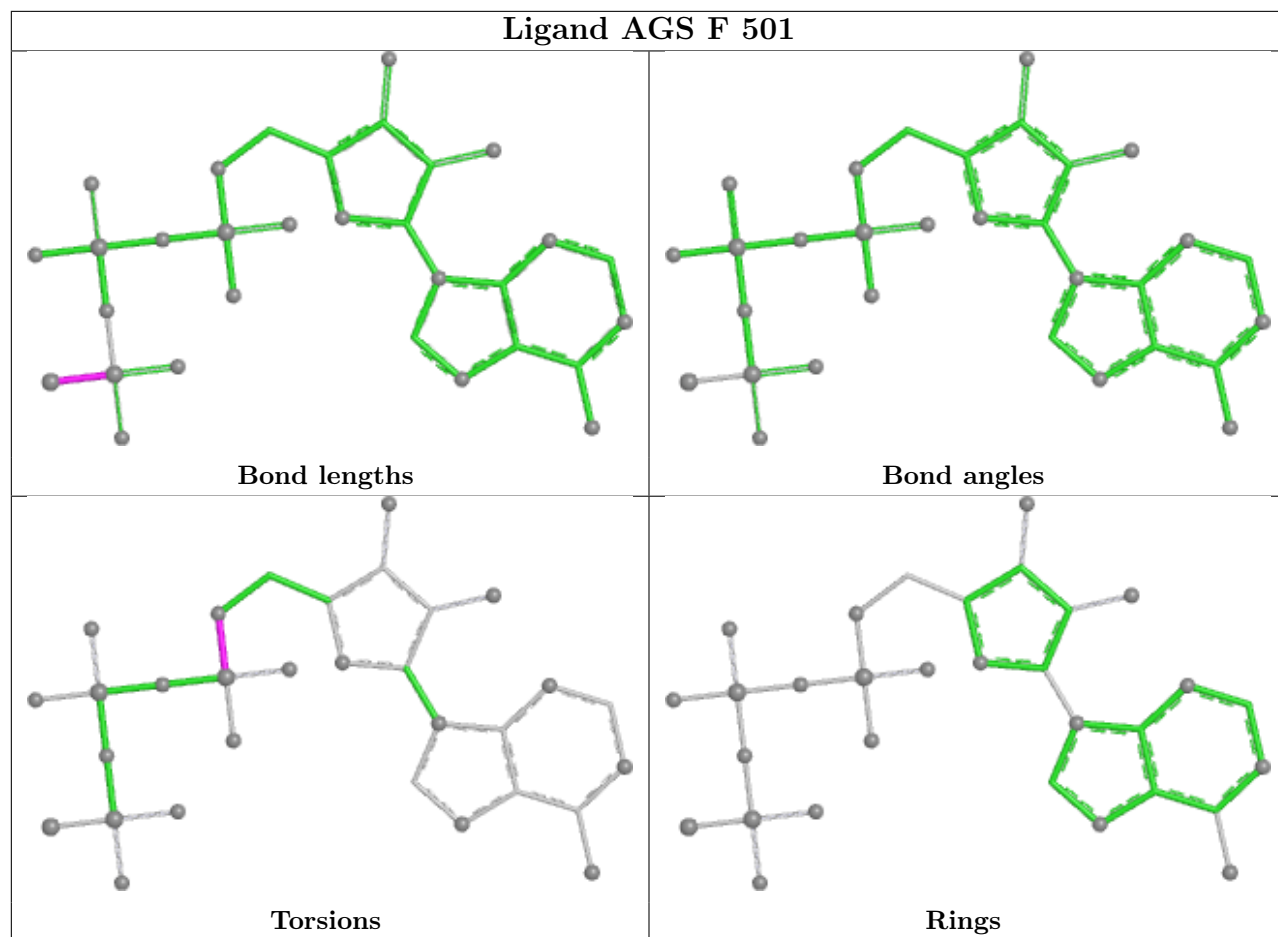
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	501	AGS	3	0
27	F	501	AGS	1	0
29	D	501	ADP	1	0
27	C	501	AGS	4	0

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.

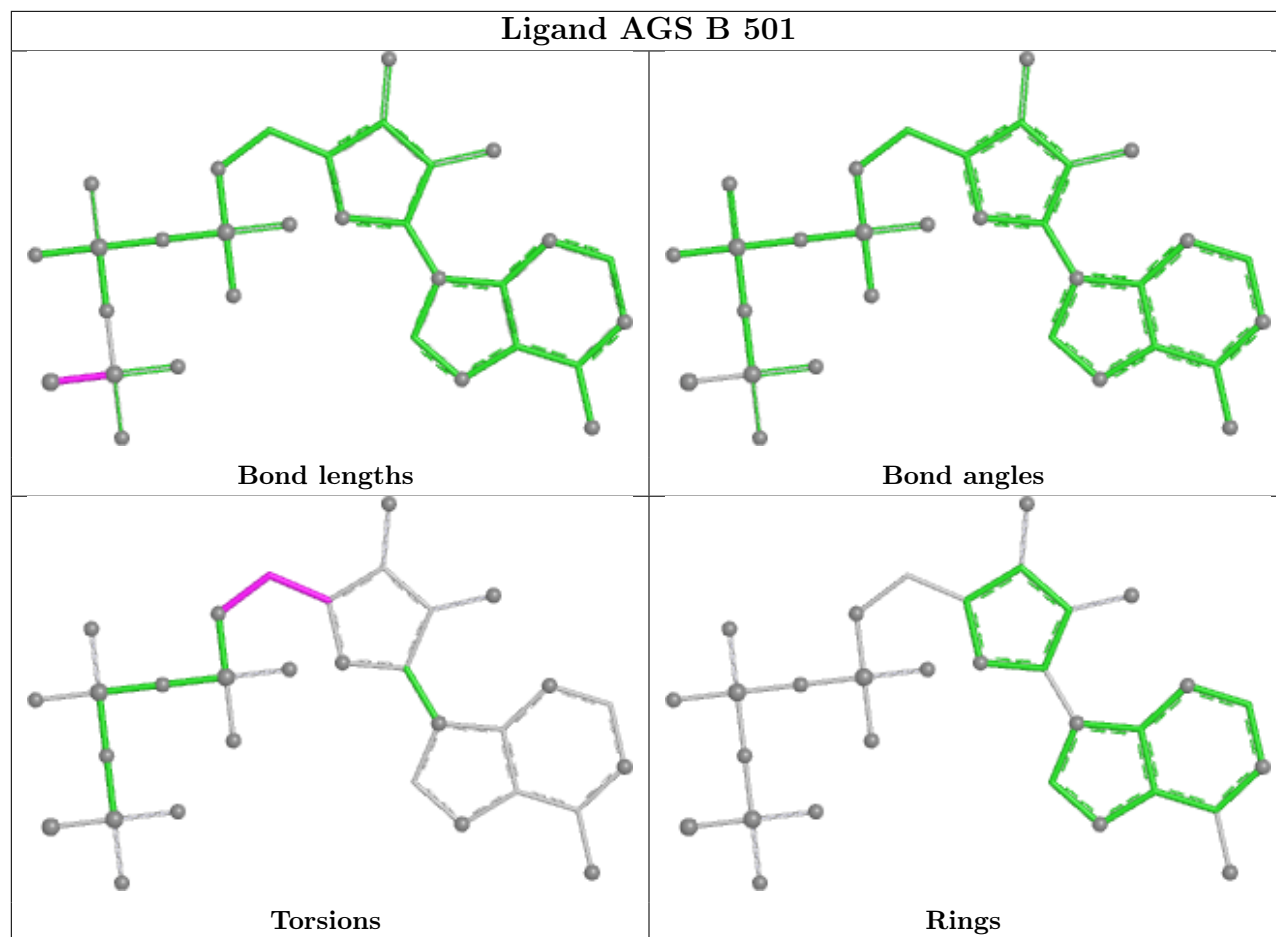
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



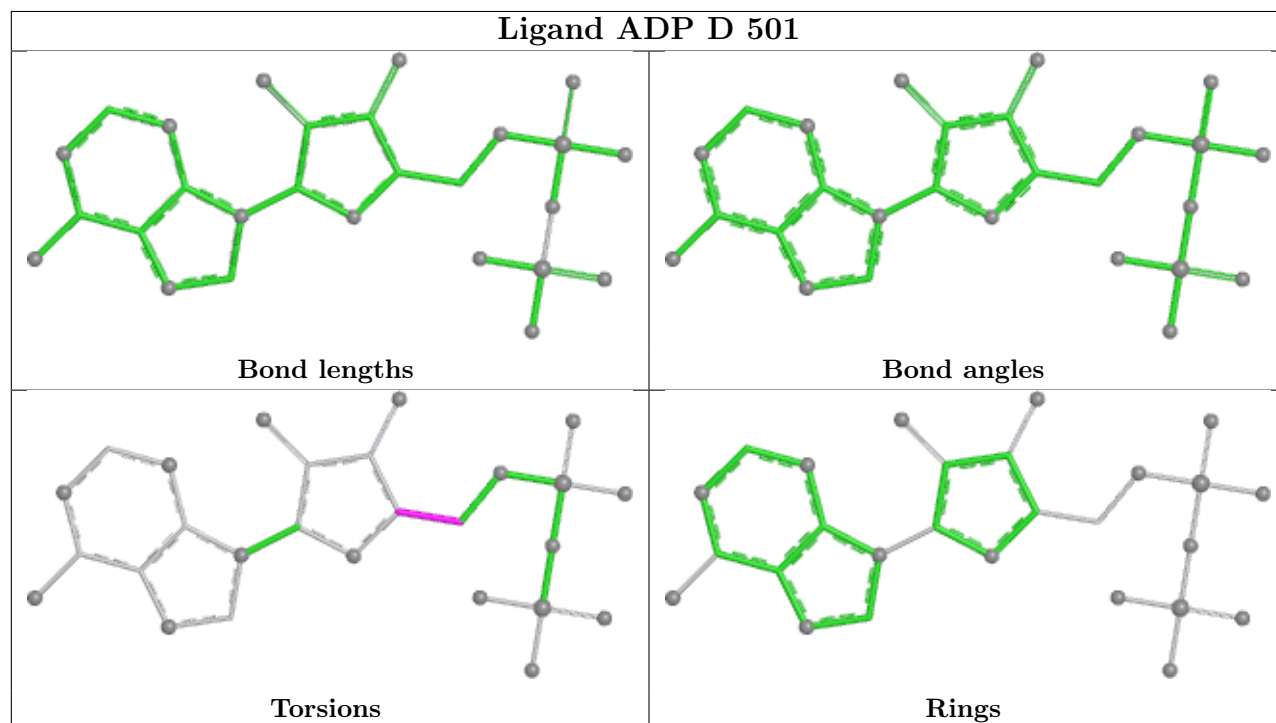
Ligand AGS F 501

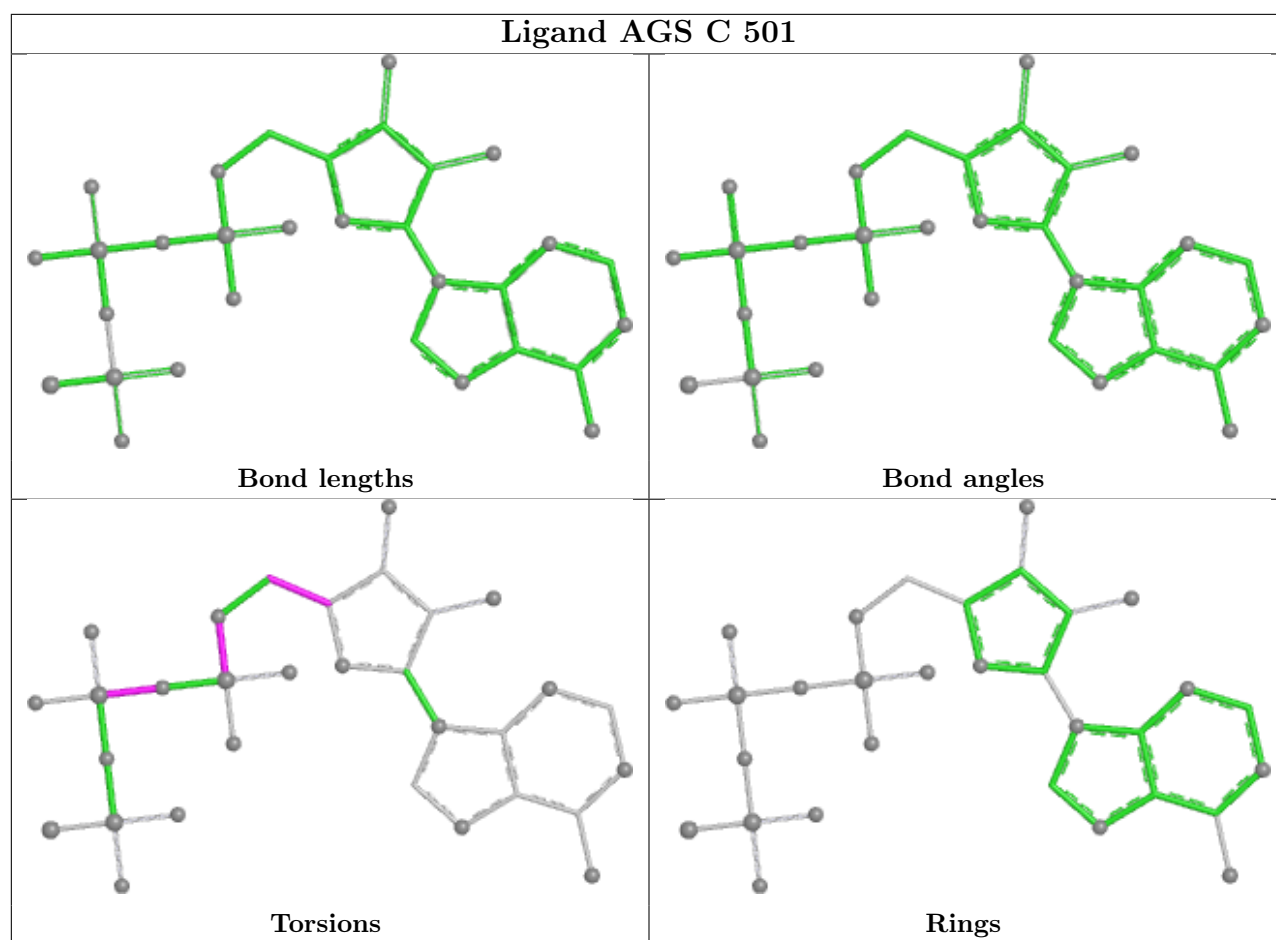


Ligand AGS B 501



Ligand ADP D 501





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.

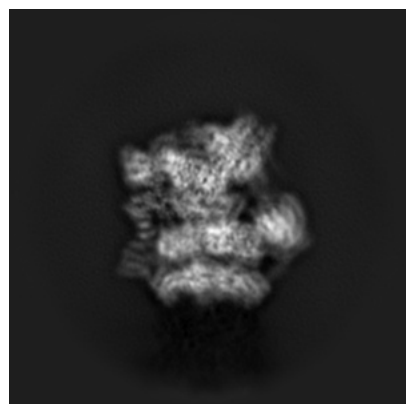
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71740. These allow visual inspection of the internal detail of the map and identification of artifacts.

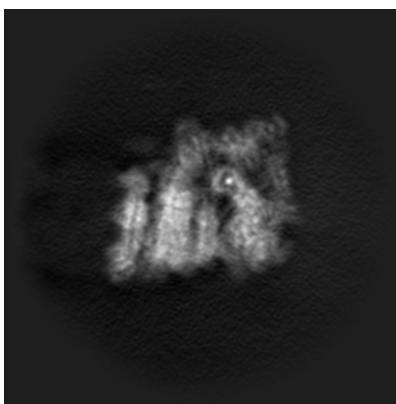
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

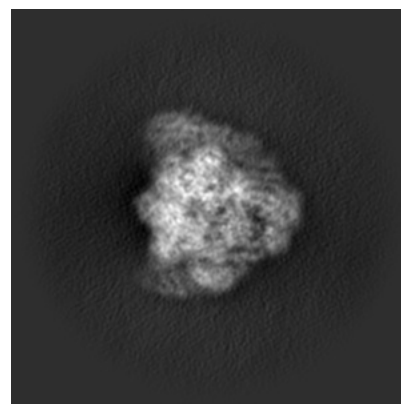
6.1.1 Primary map



X

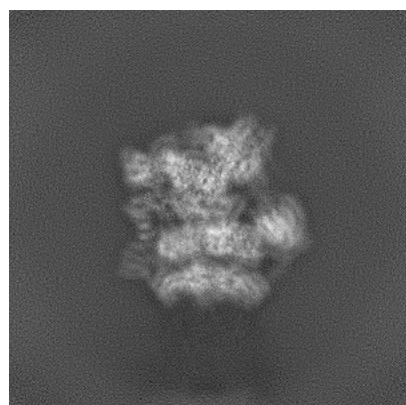


Y

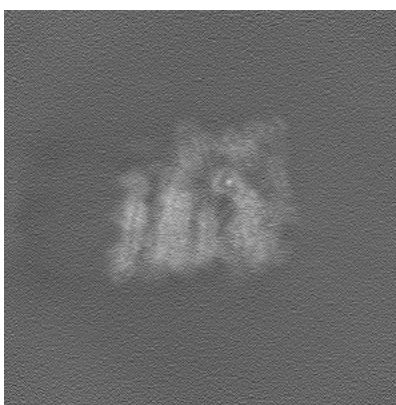


Z

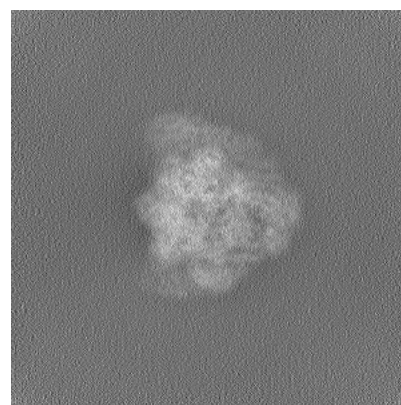
6.1.2 Raw map



X



Y

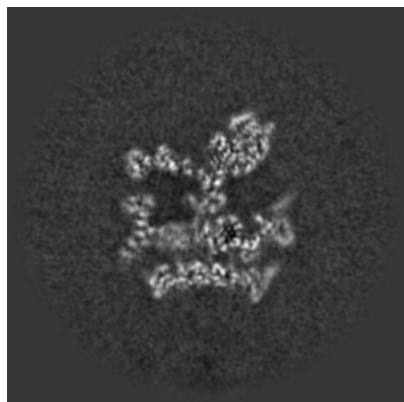


Z

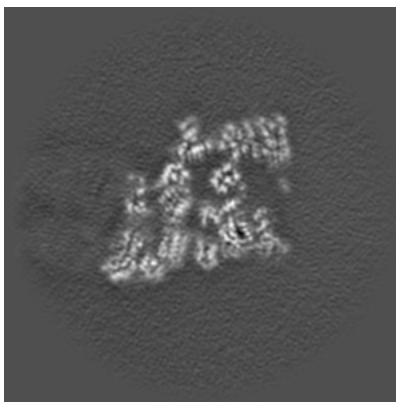
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

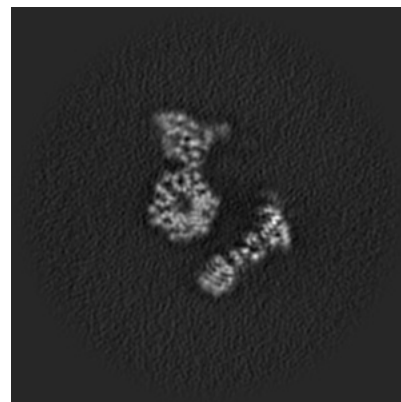
6.2.1 Primary map



X Index: 240

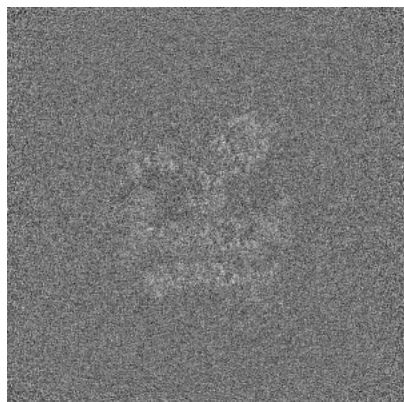


Y Index: 240

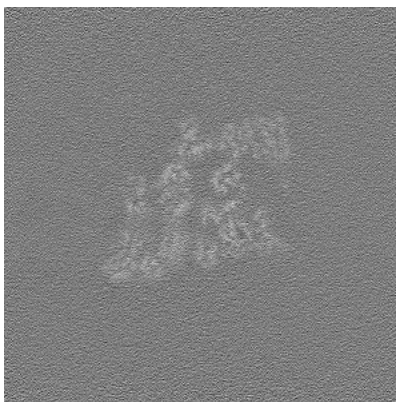


Z Index: 240

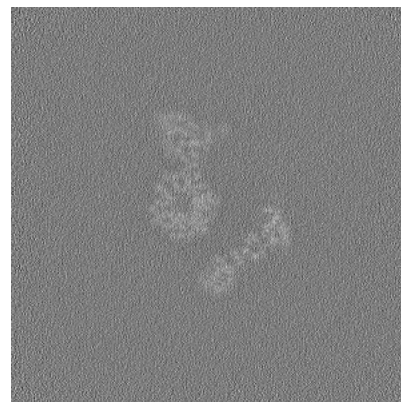
6.2.2 Raw map



X Index: 240



Y Index: 240

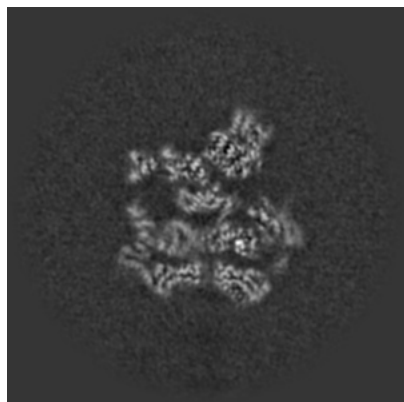


Z Index: 240

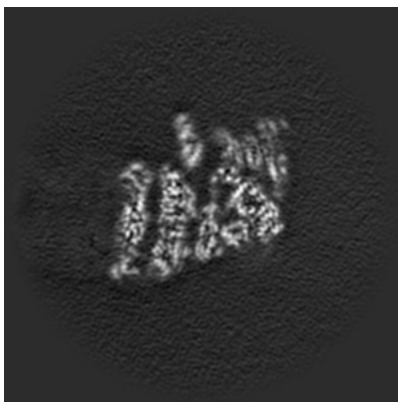
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

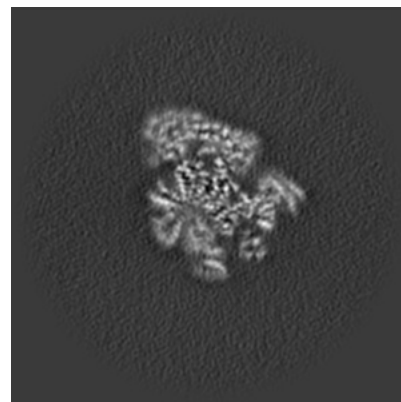
6.3.1 Primary map



X Index: 228

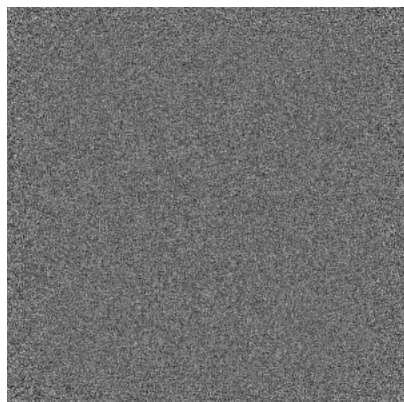


Y Index: 257

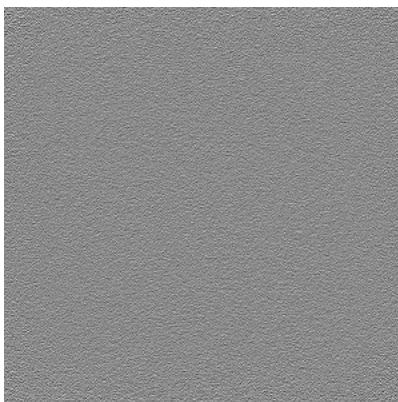


Z Index: 212

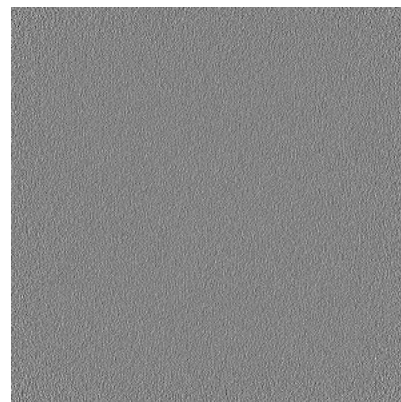
6.3.2 Raw map



X Index: 0



Y Index: 0

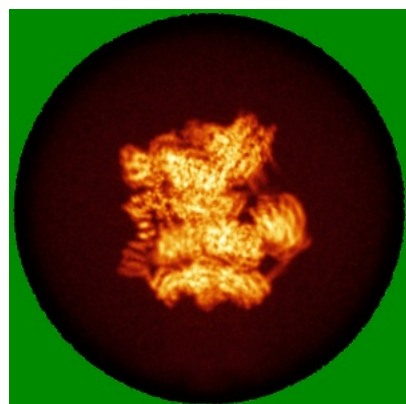


Z Index: 0

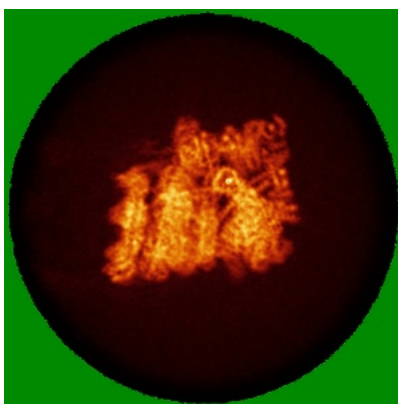
The images above show the largest variance slices of the map in three orthogonal directions.

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

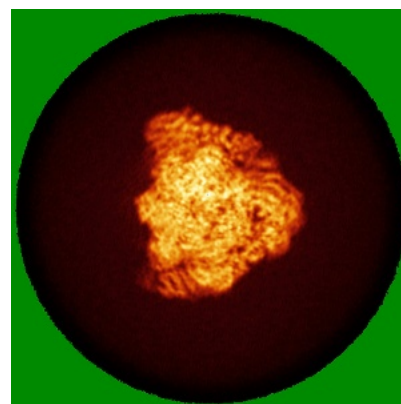
6.4.1 Primary map



X

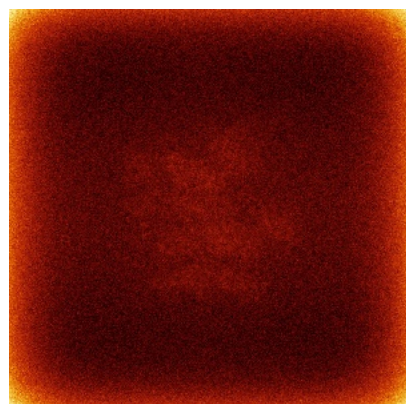


Y

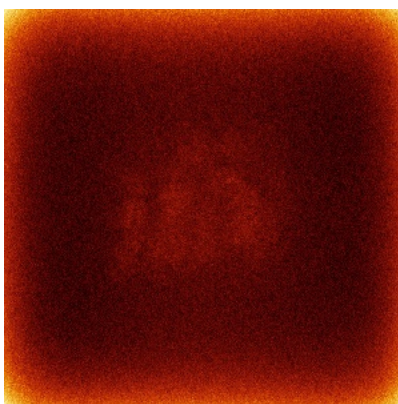


Z

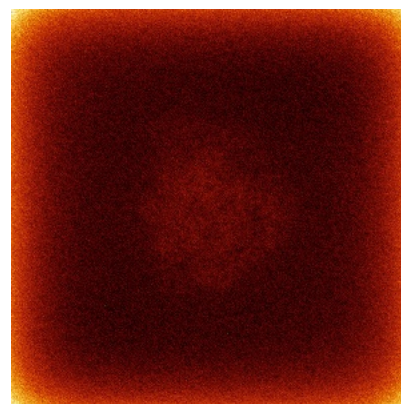
6.4.2 Raw map



X



Y

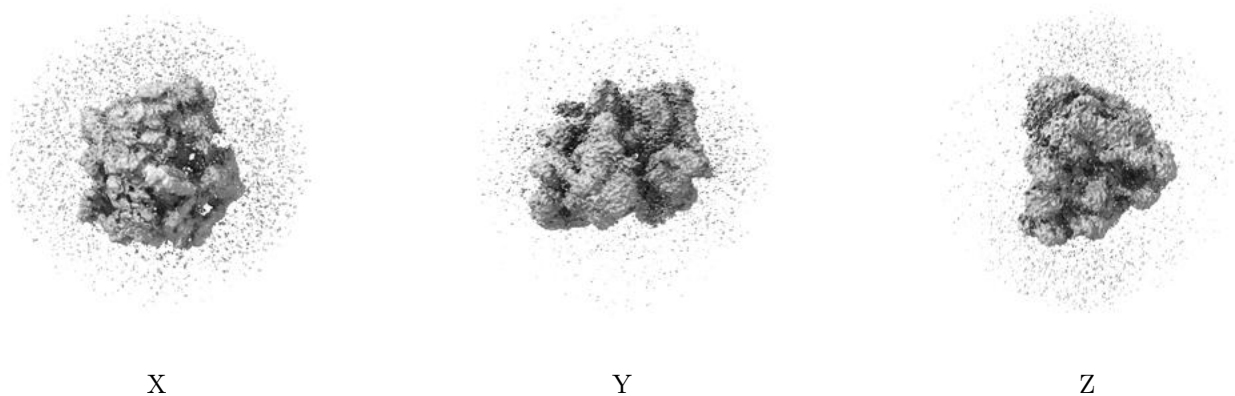


Z

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.

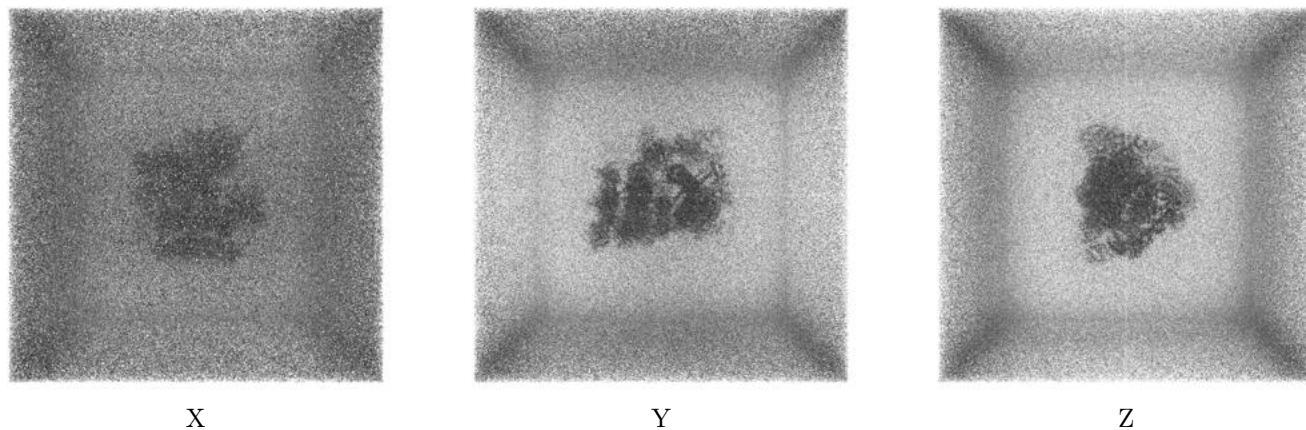
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

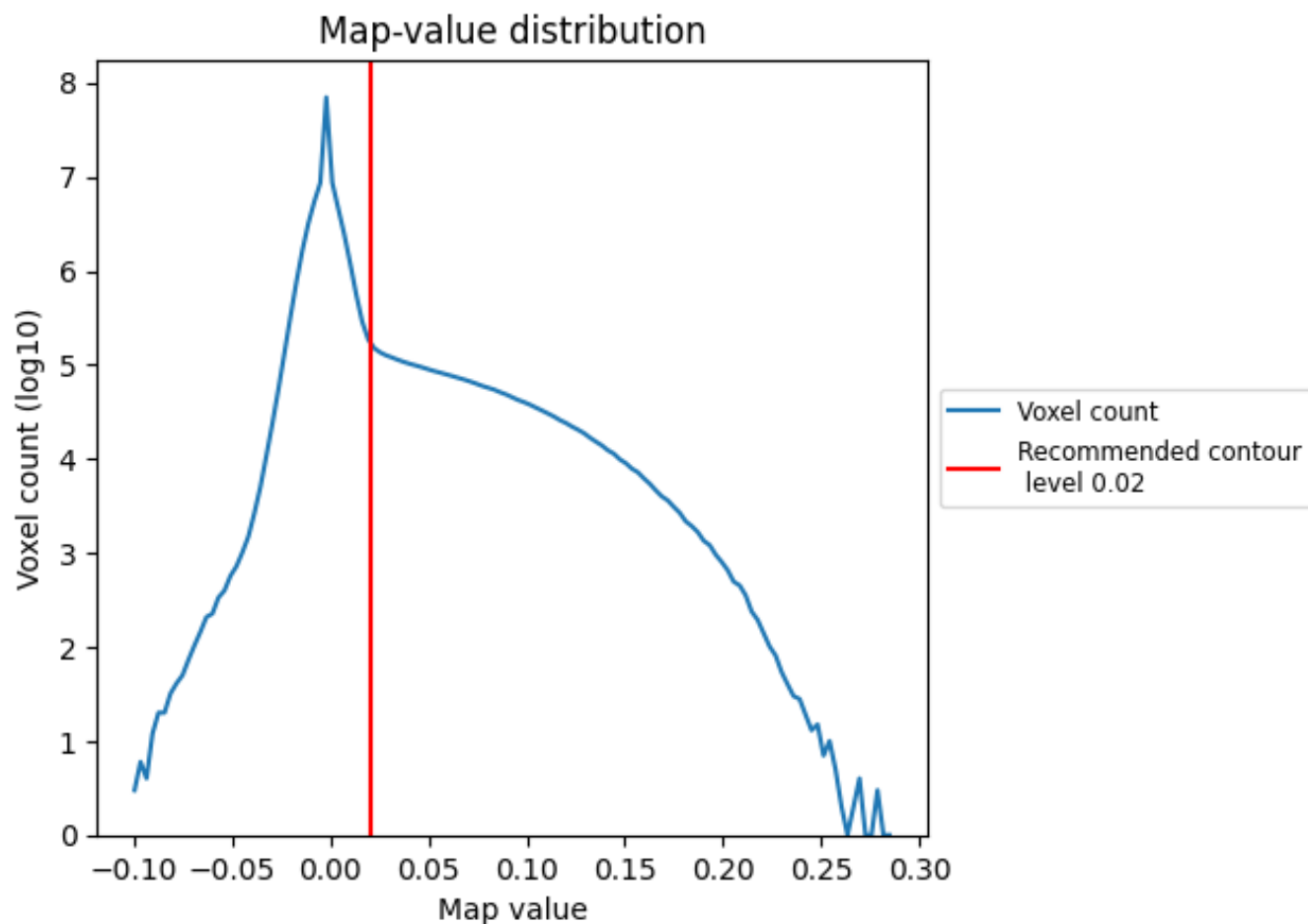
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

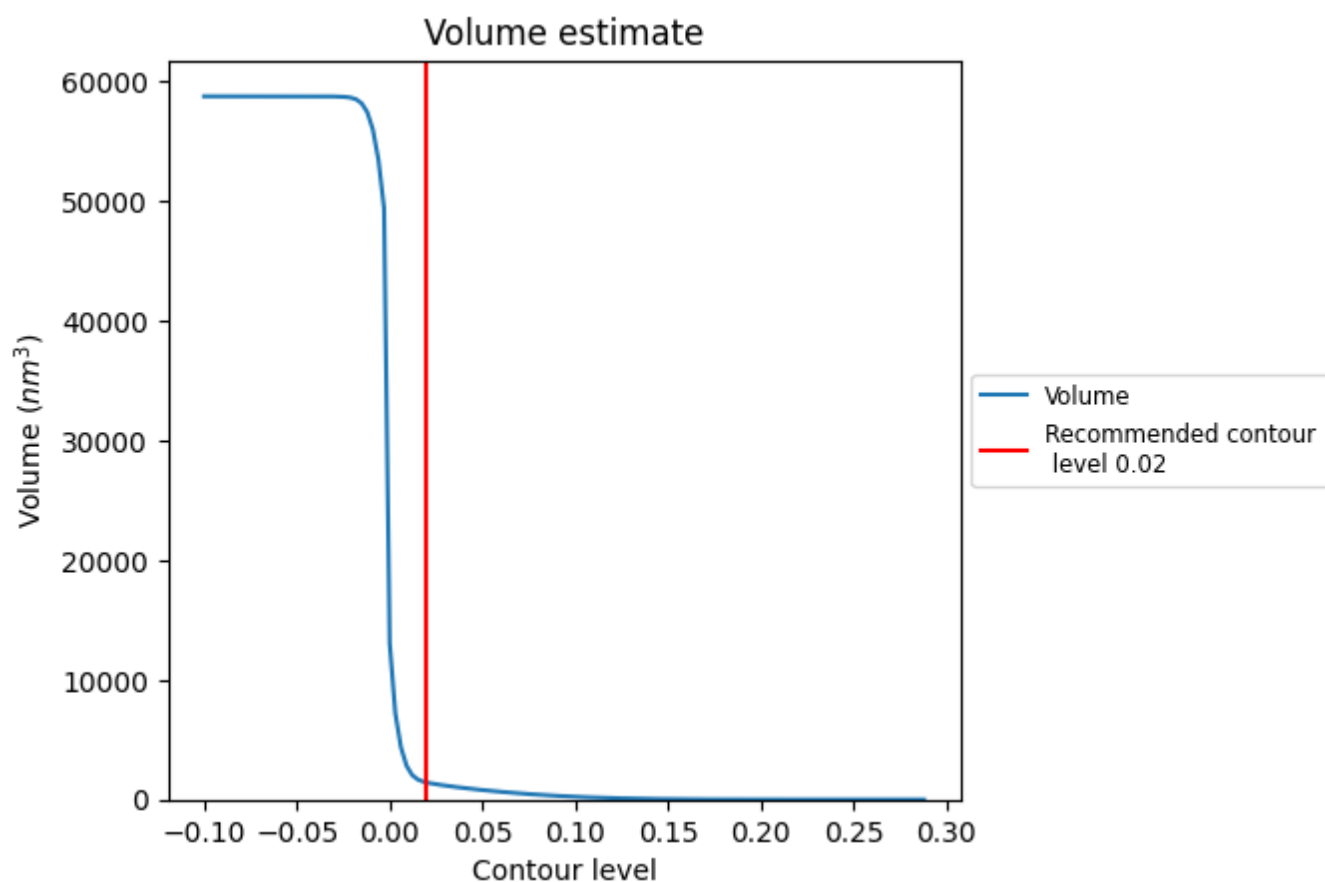
This section contains the results of statistical analysis of the map.

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.

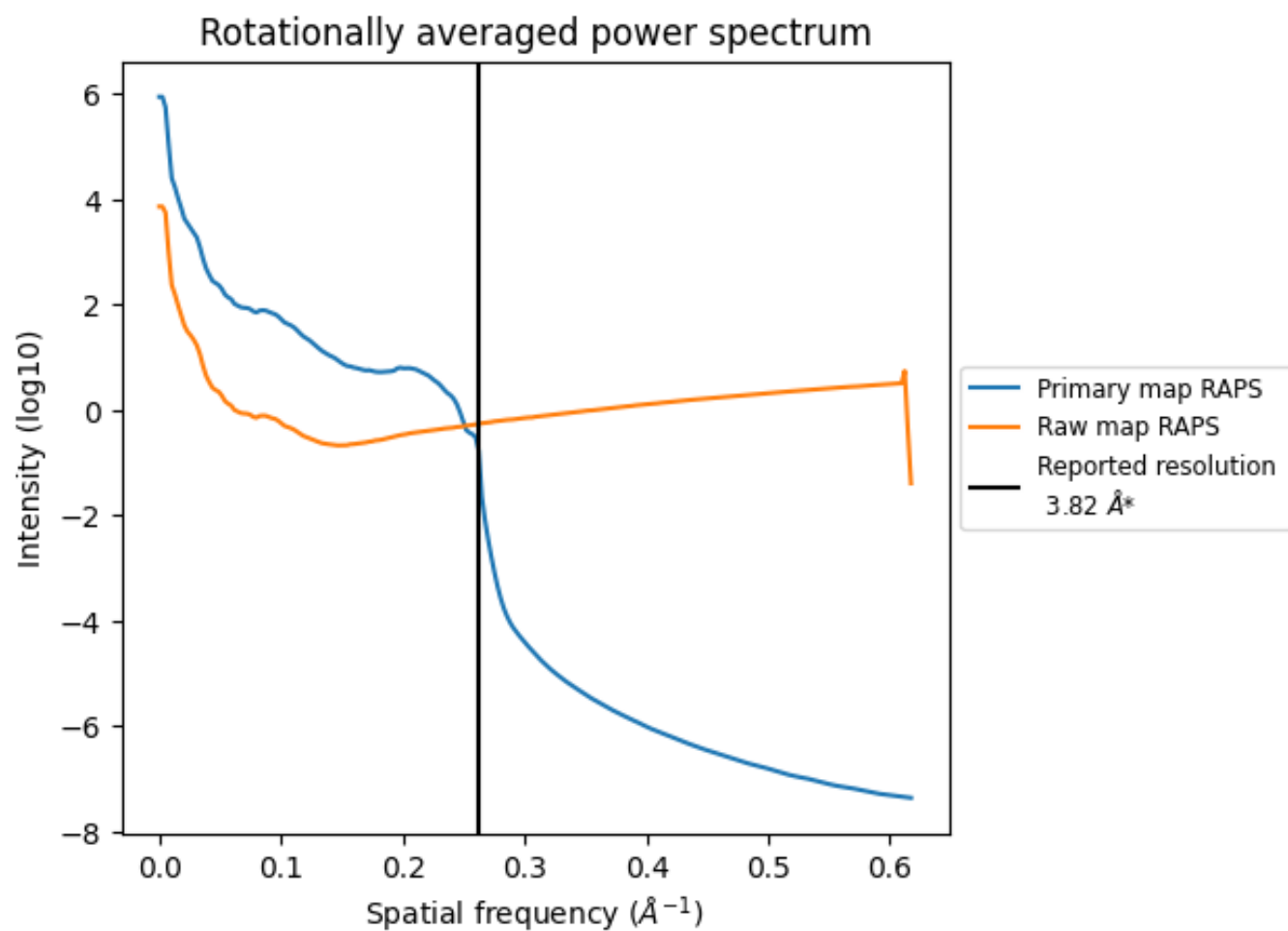
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1431 nm^3 ; this corresponds to an approximate mass of 1293 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 ⓘ

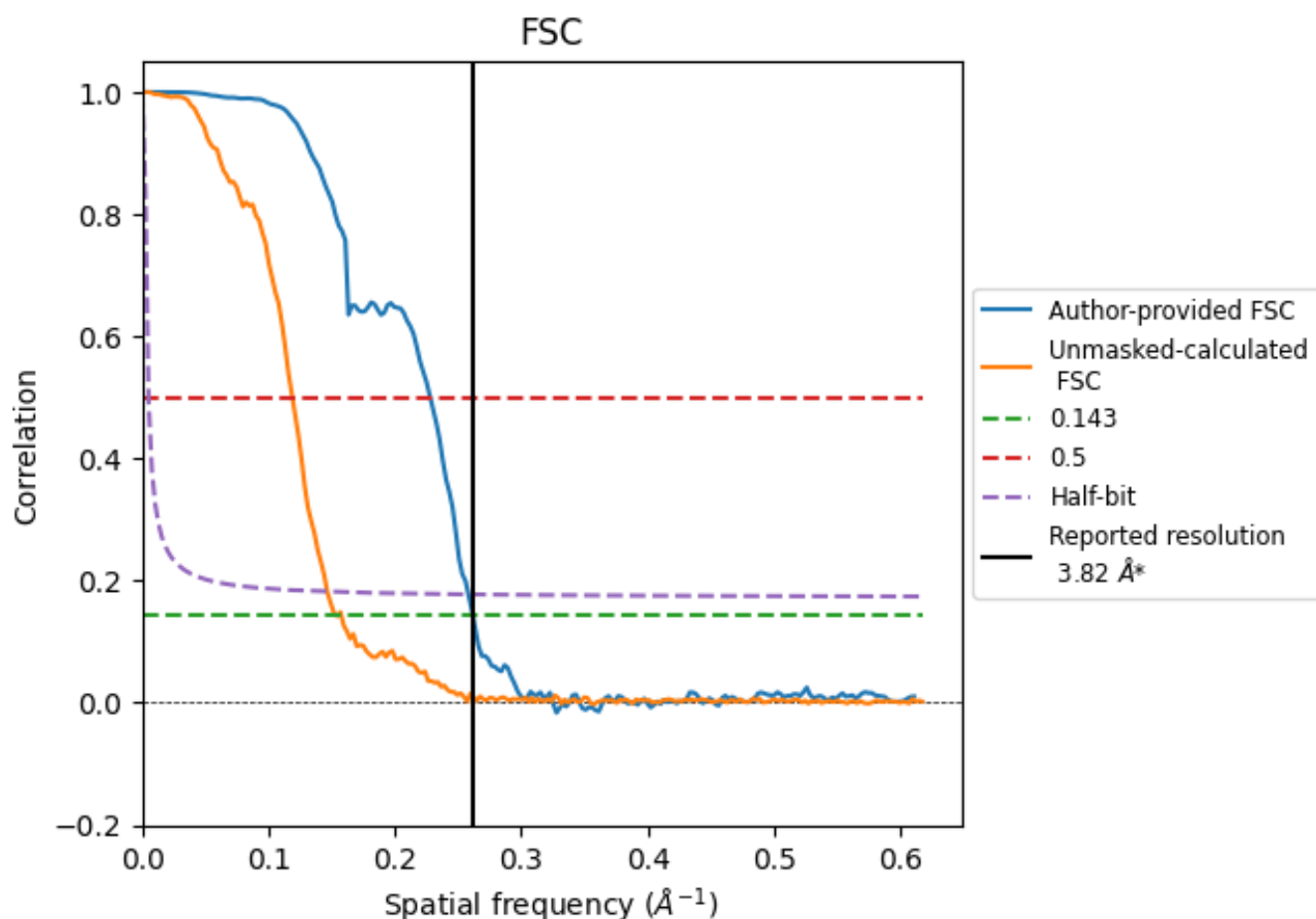


*Reported resolution corresponds to spatial frequency of 0.262 $\text{\AA}^{-1}$

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 $0.262 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

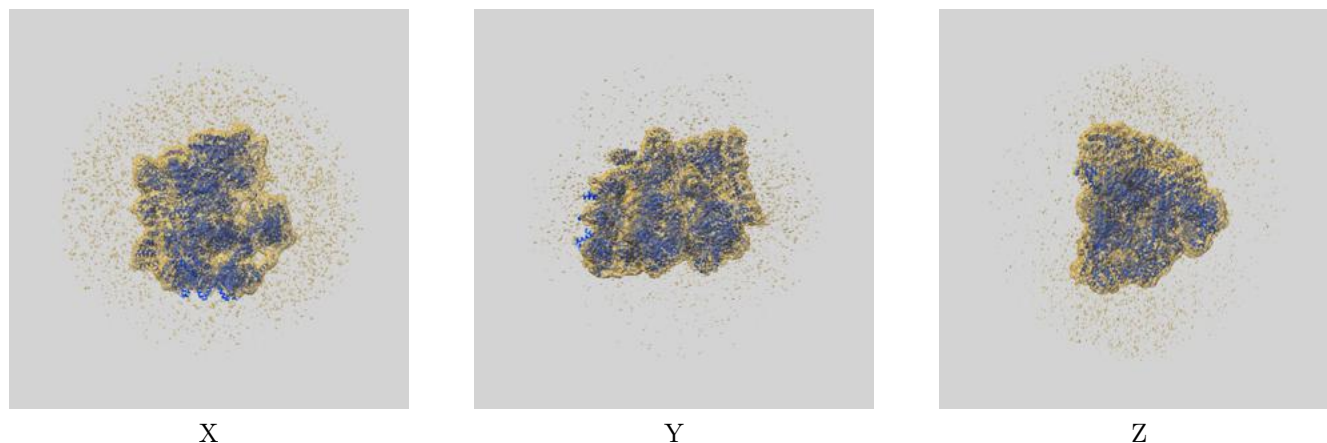
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.82	4.39	3.87
Unmasked-calculated*	6.51	8.42	6.83

*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 6.51 differs from the reported value 3.82 by more than 10 %

9 Map-model fit [i](#)

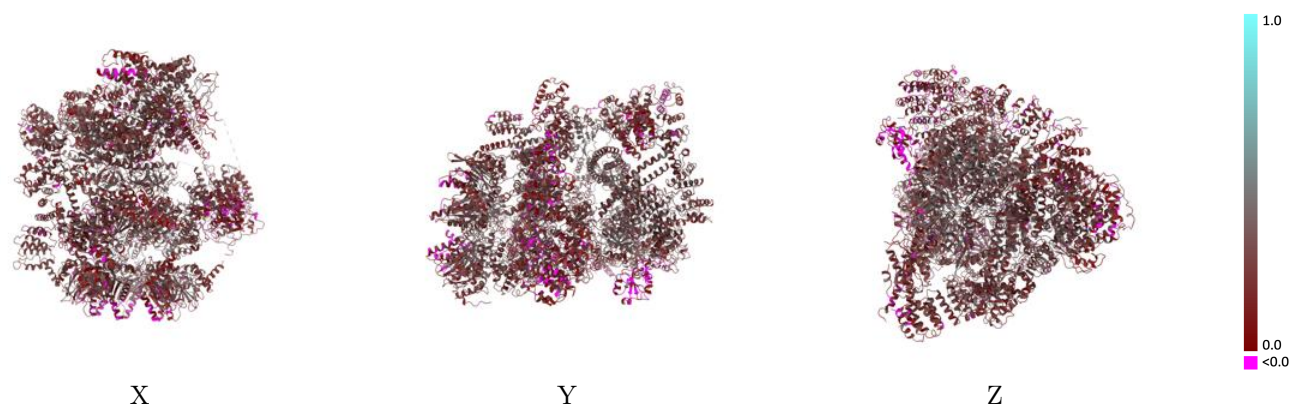
This section contains information regarding the fit between EMDB map EMD-71740 and PDB model 9PMO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



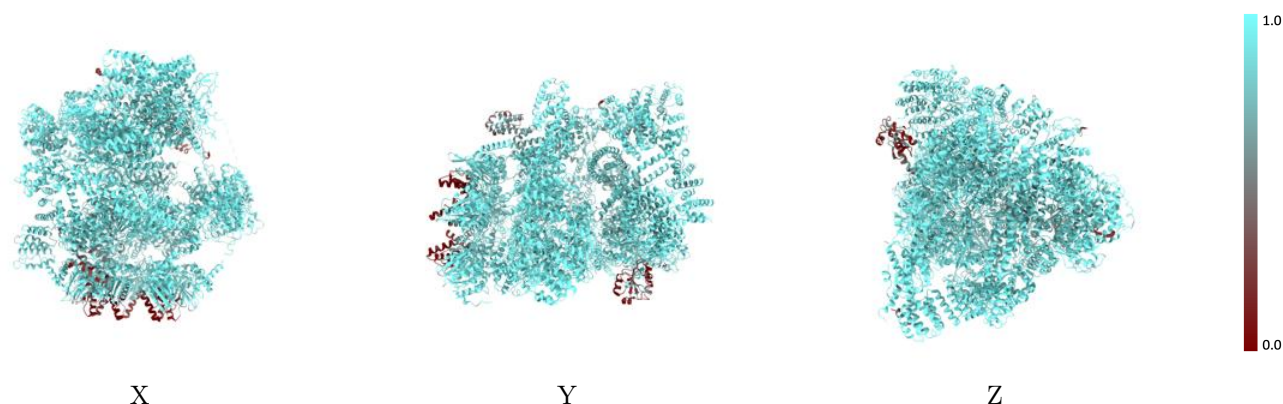
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



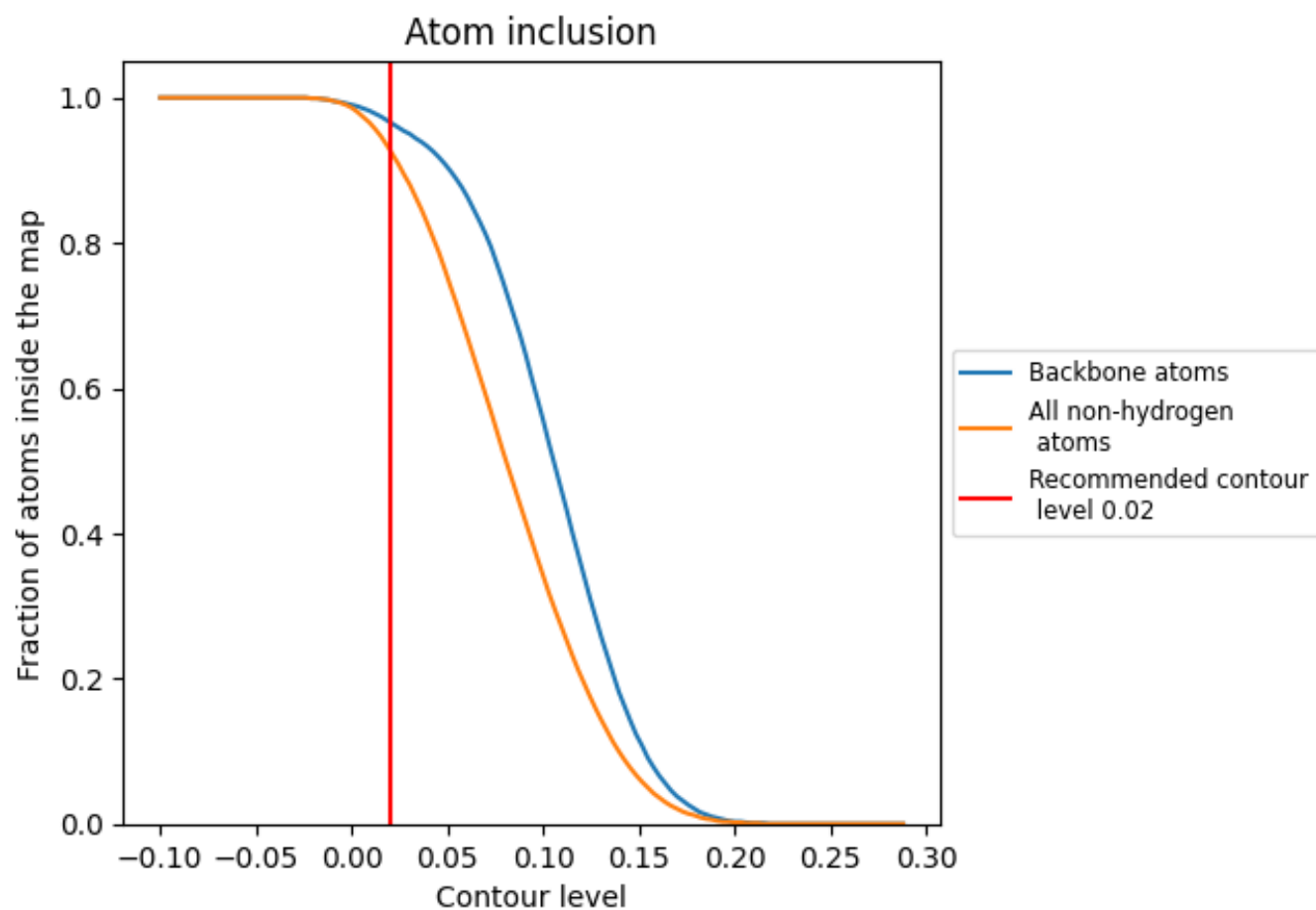
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.2450
A	 0.9700	 0.2810
B	 0.9650	 0.3040
C	 0.9690	 0.3190
D	 0.9590	 0.2870
E	 0.9740	 0.1800
F	 0.9500	 0.2270
G	 0.8740	 0.2540
H	 0.8650	 0.2430
I	 0.8080	 0.2190
J	 0.8950	 0.2710
K	 0.8350	 0.2500
L	 0.8590	 0.2350
M	 0.8110	 0.2300
U	 0.9700	 0.2990
V	 0.9420	 0.2300
W	 0.9610	 0.2290
X	 0.8140	 0.2330
Y	 0.9690	 0.2420
Z	 0.9680	 0.3130
a	 0.9730	 0.2520
b	 0.9750	 0.2320
c	 0.9610	 0.3210
d	 0.9240	 0.1930
e	 0.9610	 0.2050
f	 0.9690	 0.1480
g	 0.6880	 0.1840

