



wwPDB EM Validation Summary Report ⓘ

Sep 4, 2025 – 06:26 PM JST

PDB ID : 9UG9 / pdb_00009ug9
EMDB ID : EMD-64133
Title : The cryo-EM structure of 26S proteasome-Midnolin complex MB state
Authors : Wang, H.Y.; Xu, W.Q.
Deposited on : 2025-04-11
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

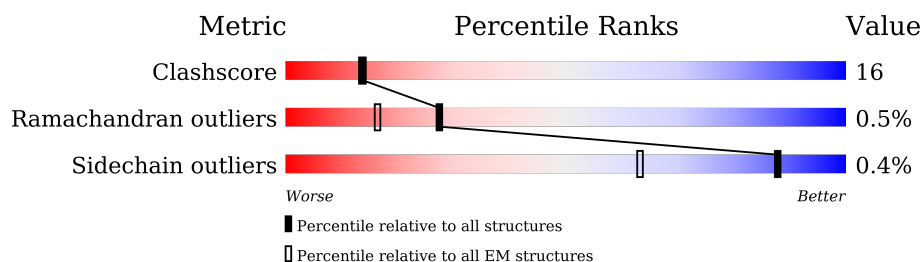
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	u	491	 17% 5% 77%
2	d	350	 47% 27% 26%
3	M	255	 76% 17% 6%
3	m	255	 79% 15% 6%
4	R	263	 63% 13% 22%
4	r	263	 67% 10% 24%
5	N	239	 72% 11% 17%
5	n	239	 67% 17% 16%

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Mol	Chain	Length	Quality of chain
6	E	389	
7	B	440	
8	e	70	
9	O	277	
9	o	277	
10	S	241	
10	s	241	
11	D	418	
12	F	439	
13	P	205	
13	p	205	
14	U	953	
15	C	406	
16	G	246	
16	g	246	
17	Q	201	
17	q	201	
18	A	433	
19	V	534	
20	T	264	
20	t	264	
21	v	15	
22	W	456	
23	H	234	
23	h	234	

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Mol	Chain	Length	Quality of chain
24	f	908	
25	X	422	
26	I	261	
26	i	261	
27	Y	389	
28	J	248	
28	j	248	
29	Z	324	
30	K	241	
30	k	241	
31	a	376	
32	L	263	
32	l	263	
33	b	377	
34	c	310	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	ADP	B	501	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 103692 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 Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	114	Total	C	N	O	S	0	0
			908	558	185	163	2		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	MET	-	initiating methionine	UNP Q504T8
u	469	GLY	-	expression tag	UNP Q504T8
u	470	SER	-	expression tag	UNP Q504T8
u	471	ASP	-	expression tag	UNP Q504T8
u	472	TYR	-	expression tag	UNP Q504T8
u	473	LYS	-	expression tag	UNP Q504T8
u	474	ASP	-	expression tag	UNP Q504T8
u	475	ASP	-	expression tag	UNP Q504T8
u	476	ASP	-	expression tag	UNP Q504T8
u	477	ASP	-	expression tag	UNP Q504T8
u	478	LYS	-	expression tag	UNP Q504T8
u	479	GLY	-	expression tag	UNP Q504T8
u	480	SER	-	expression tag	UNP Q504T8
u	481	HIS	-	expression tag	UNP Q504T8
u	482	HIS	-	expression tag	UNP Q504T8
u	483	HIS	-	expression tag	UNP Q504T8
u	484	HIS	-	expression tag	UNP Q504T8
u	485	HIS	-	expression tag	UNP Q504T8
u	486	HIS	-	expression tag	UNP Q504T8
u	487	HIS	-	expression tag	UNP Q504T8
u	488	HIS	-	expression tag	UNP Q504T8
u	489	HIS	-	expression tag	UNP Q504T8
u	490	HIS	-	expression tag	UNP Q504T8

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	260	Total	C	N	O	S	0	0
			2091	1345	348	389	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	239	Total	C	N	O	S	0	0
			1849	1174	313	351	11		
3	M	240	Total	C	N	O	S	0	0
			1839	1163	313	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	206	Total	C	N	O	S	0	0
			1571	987	280	295	9		
4	r	201	Total	C	N	O	S	0	0
			1541	968	273	291	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	n	201	Total	C	N	O	S	0	0
			1492	932	255	293	12		
5	N	199	Total	C	N	O	S	0	0
			1488	930	255	291	12		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	354	Total	C	N	O	S	0	0
			2782	1751	493	522	16		

- Molecule 7 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	395	Total	C	N	O	S	0	0
			3034	1916	506	597	15		

- Molecule 8 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	e	31	Total	C	N	O	0	0
			180	105	32	43		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
9	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
10	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	380	Total	C	N	O	S	0	0
			2997	1894	514	577	12		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	369	Total	C	N	O	S	0	0
			2867	1802	494	556	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
13	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	814	Total	C	N	O	S	0	0
			6298	3995	1069	1190	44		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	374	Total	C	N	O	S	0	0
			2877	1810	518	535	14		

- Molecule 16 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	240	Total	C	N	O	S	0	0
			1820	1154	305	348	13		
16	g	239	Total	C	N	O	S	0	0
			1798	1142	300	344	12		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	198	Total	C	N	O	S	0	0
			1565	1003	264	289	9		
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	393	Total	C	N	O	S	0	0
			3059	1925	537	580	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	472	Total	C	N	O	S	0	0
			3761	2385	668	694	14		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1662	1049	284	317	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	215	Total	C	N	O	S	0	0
			1662	1049	284	317	12		

- Molecule 21 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	v	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	456	Total	C	N	O	S	0	0
			3663	2309	631	700	23		

- Molecule 23 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	231	Total	C	N	O	S	0	0
			1702	1078	288	331	5		
23	h	229	Total	C	N	O	S	0	0
			1671	1058	282	326	5		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	f	889	Total	C	N	O	S	0	0
			6636	4146	1135	1313	42		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	380	Total	C	N	O	S	0	0
			3004	1915	507	570	12		

- Molecule 26 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	256	Total	C	N	O	S	0	0
			1966	1237	339	382	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	250	Total	C	N	O	S	0	0
			1900	1192	329	371	8		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	378	Total	C	N	O	S	0	0
			2995	1901	514	564	16		

- Molecule 28 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	239	Total	C	N	O	S	0	0
			1700	1054	307	334	5		
28	j	238	Total	C	N	O	S	0	0
			1684	1040	306	333	5		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	286	Total	C	N	O	S	0	0
			2260	1441	389	425	5		

- Molecule 30 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	234	Total	C	N	O	S	0	0
			1742	1087	288	356	11		
30	k	234	Total	C	N	O	S	0	0
			1743	1092	288	352	11		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	373	Total	C	N	O	S	0	0
			2989	1907	510	557	15		

- Molecule 32 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L	239	Total	C	N	O	S	0	0
			1844	1156	330	347	11		
32	l	237	Total	C	N	O	S	0	0
			1838	1150	333	344	11		

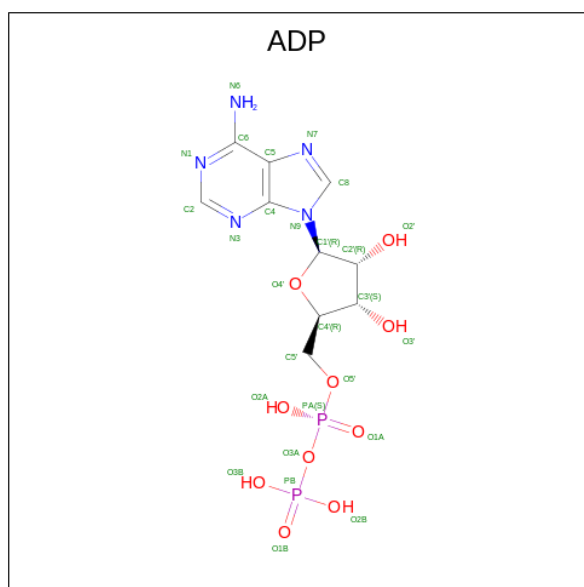
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	190	Total	C	N	O	S	0	0
			1444	901	259	277	7		

- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	287	Total	C	N	O	S	0	0
			2239	1411	388	422	18		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



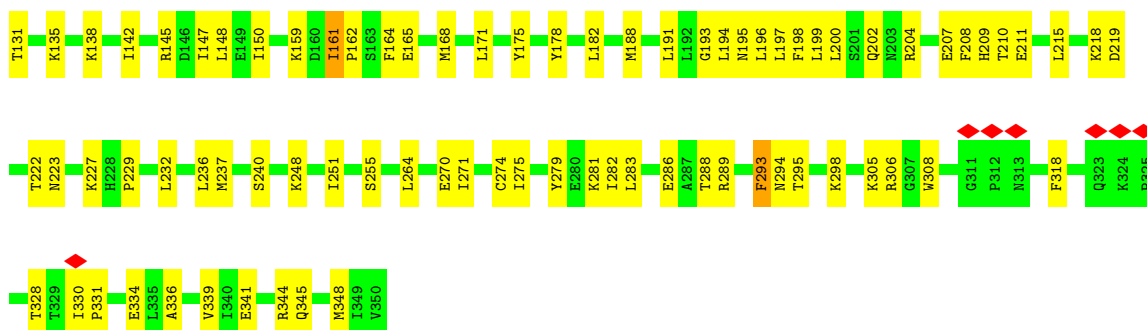
Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$)

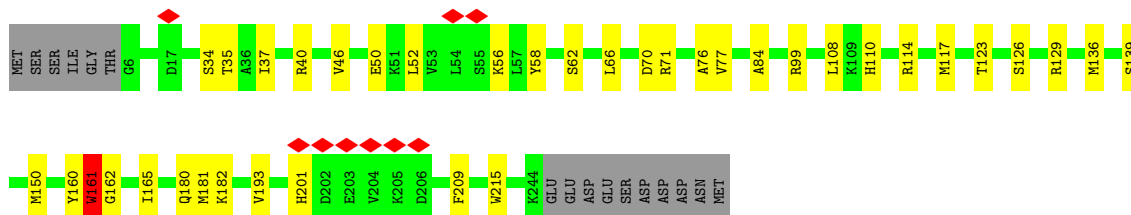
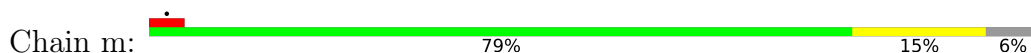
ATP

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

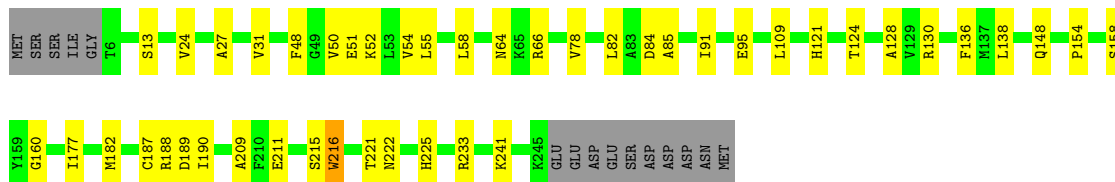
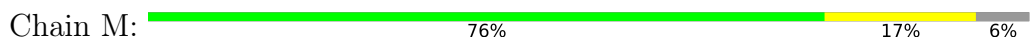




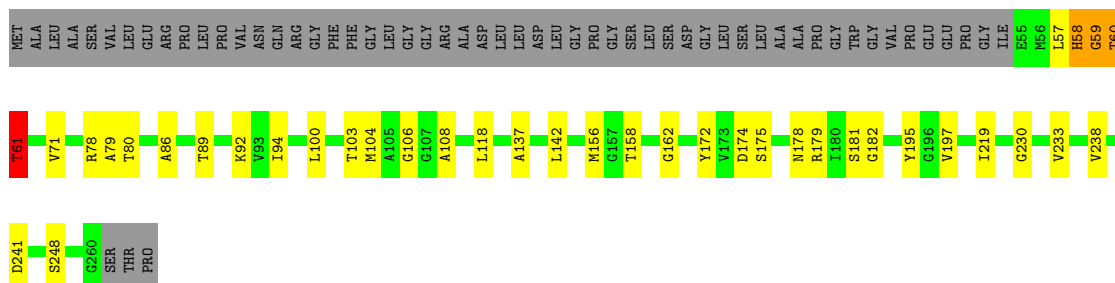
• Molecule 3: Proteasome subunit alpha type-3



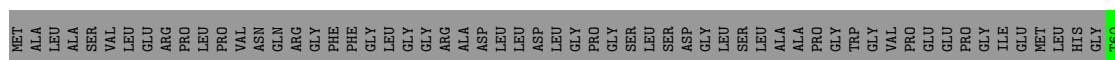
• Molecule 3: Proteasome subunit alpha type-3

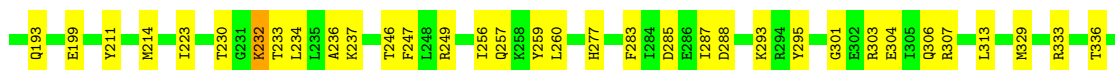


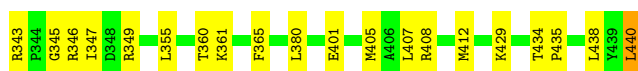
• Molecule 4: Proteasome subunit beta type-5



• Molecule 4: Proteasome subunit beta type-5

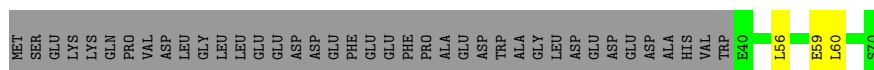






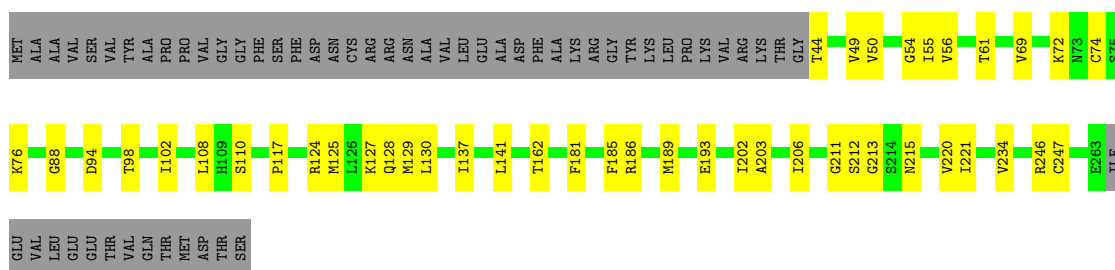
- Molecule 8: 26S proteasome complex subunit SEM1

Chain e: 40% 56%



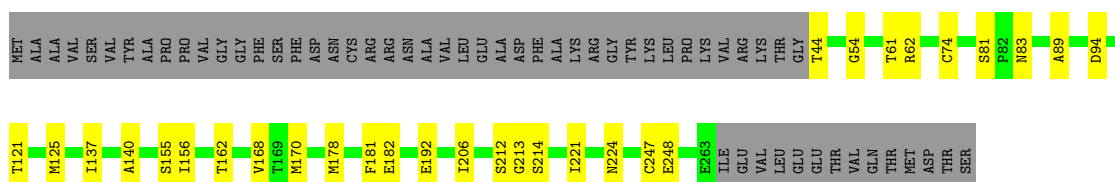
- Molecule 9: Proteasome subunit beta type-7

Chain o: 64% 16% 21%



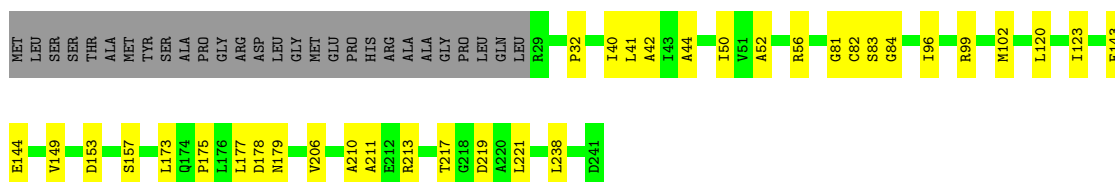
- Molecule 9: Proteasome subunit beta type-7

Chain O: 69% 11% 21%



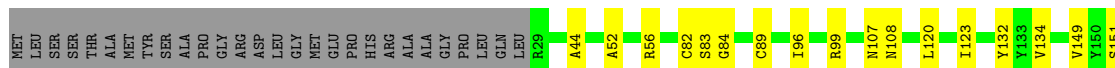
- Molecule 10: Proteasome subunit beta type-1

Chain S: 74% 15% 12%



- Molecule 10: Proteasome subunit beta type-1

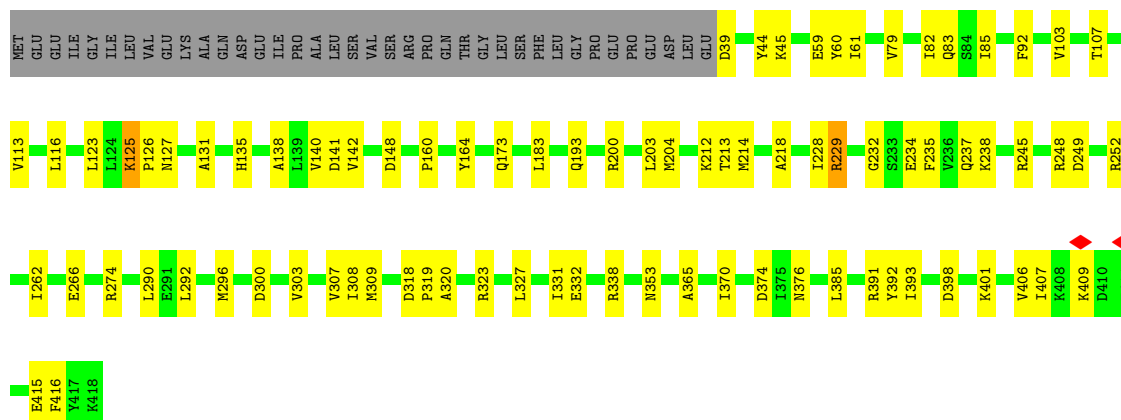
Chain s: 74% 15% 12%





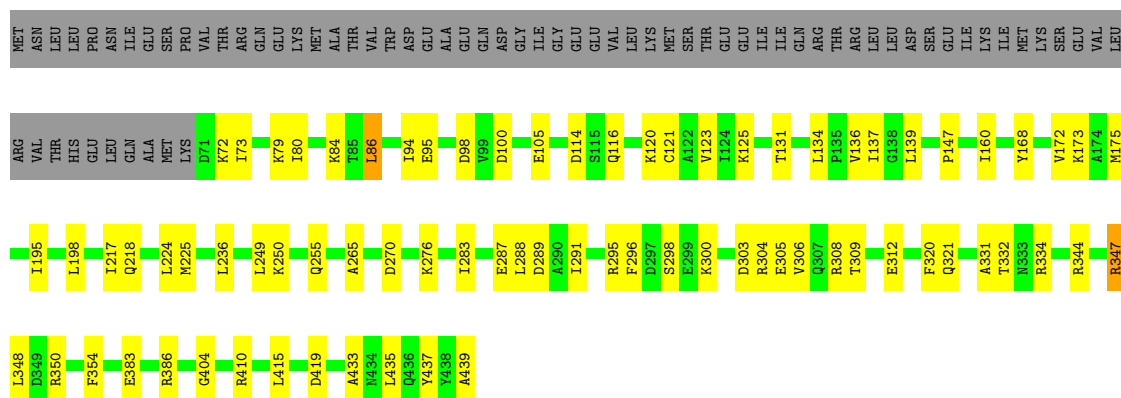
- Molecule 11: 26S proteasome regulatory subunit 6B

Chain D: 71% 20% 9%



- Molecule 12: 26S proteasome regulatory subunit 6A

Chain F: 67% 17% 16%



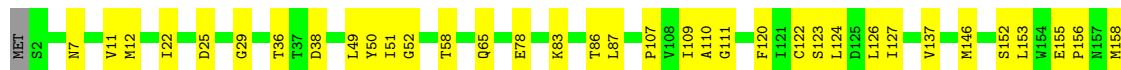
- Molecule 13: Proteasome subunit beta type-3

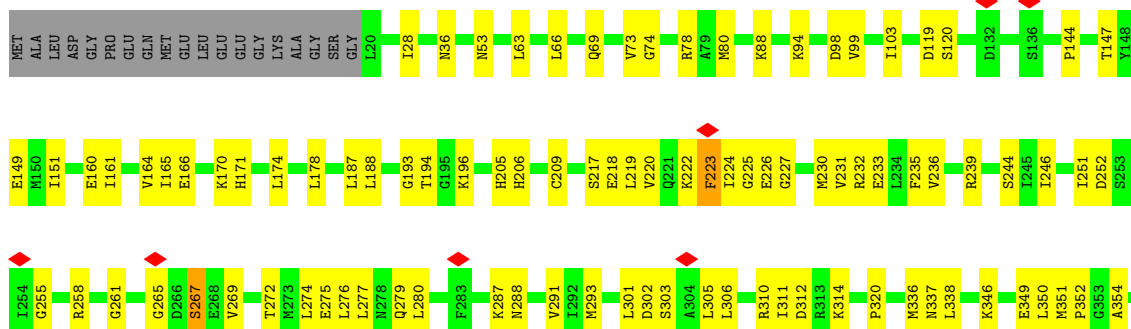
Chain p: 87% 13%

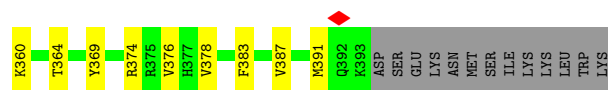


- Molecule 13: Proteasome subunit beta type-3

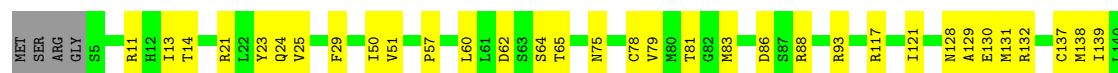
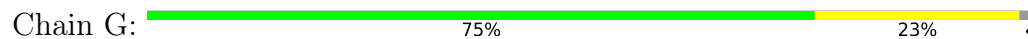
Chain P: 78% 22%



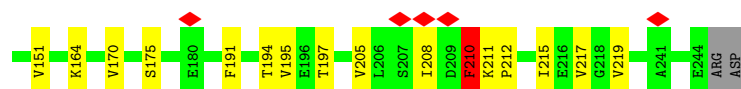
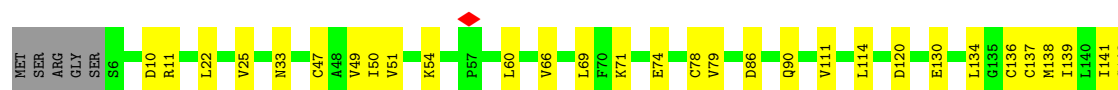
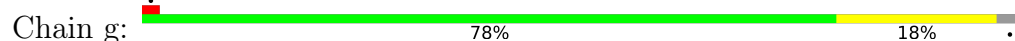




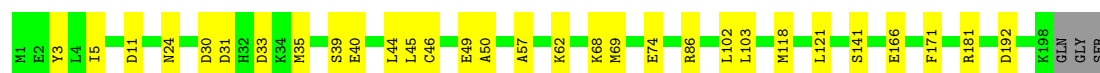
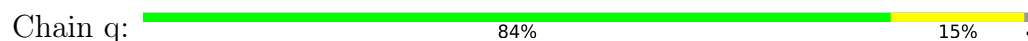
- Molecule 16: Proteasome subunit alpha type-6



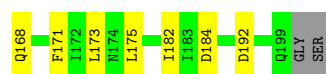
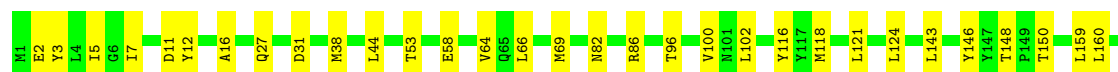
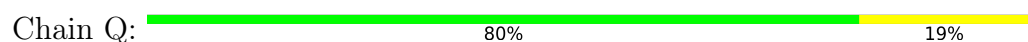
- Molecule 16: Proteasome subunit alpha type-6



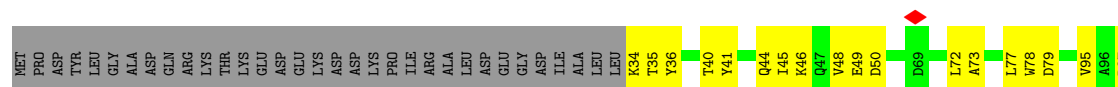
- Molecule 17: Proteasome subunit beta type-2

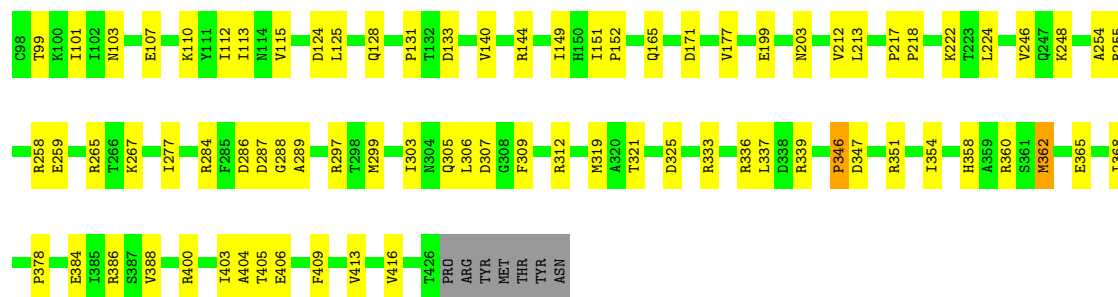


- Molecule 17: Proteasome subunit beta type-2

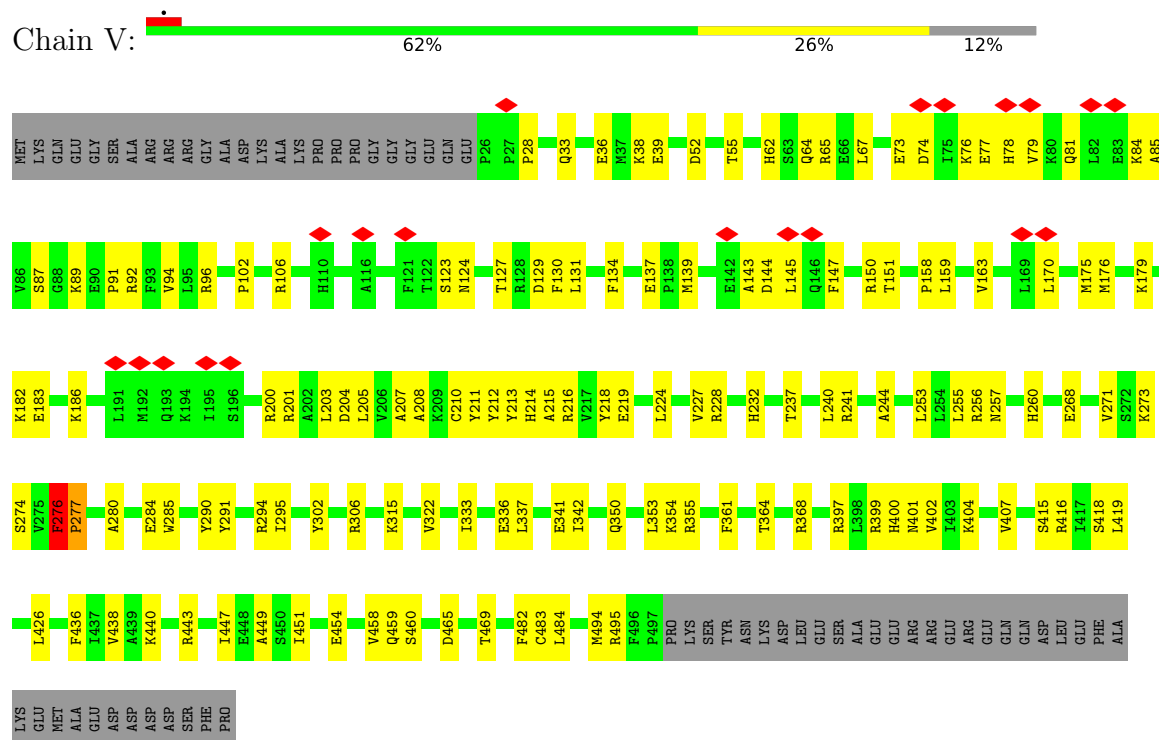


- Molecule 18: 26S proteasome regulatory subunit 7

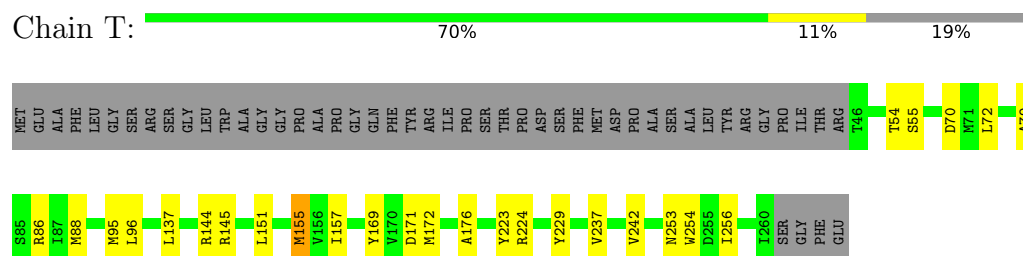




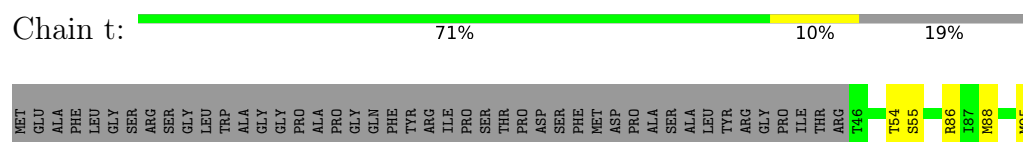
• Molecule 19: 26S proteasome non-ATPase regulatory subunit 3



• Molecule 20: Proteasome subunit beta type-4

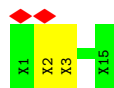
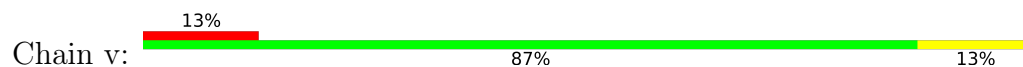


• Molecule 20: Proteasome subunit beta type-4

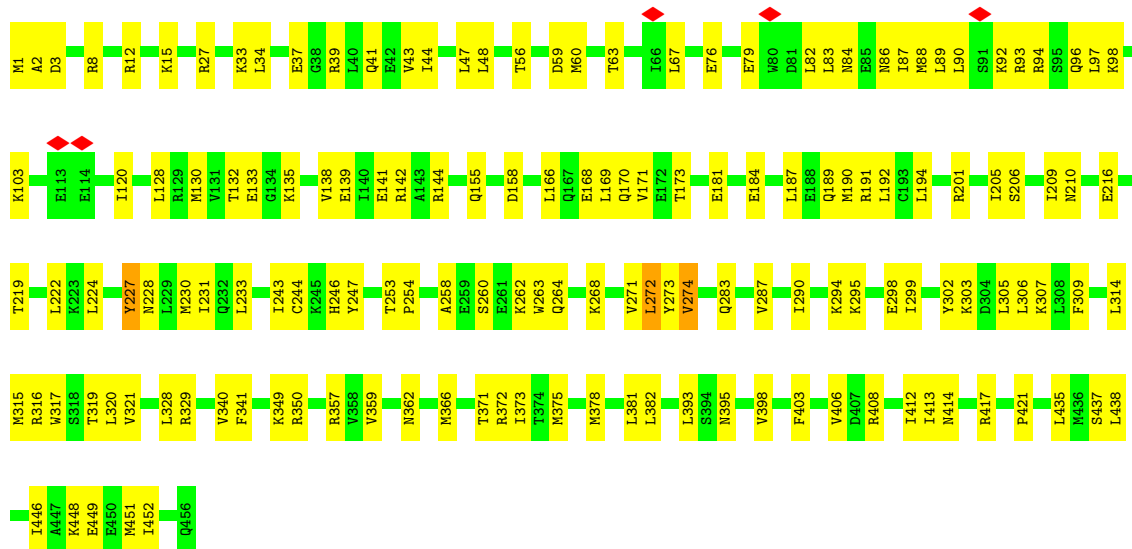




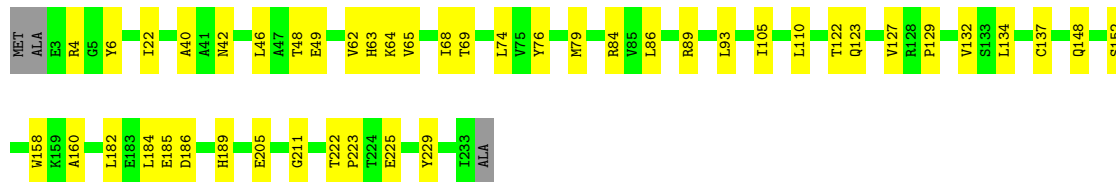
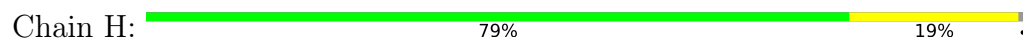
• Molecule 21: Substrate



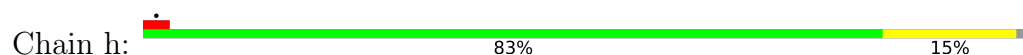
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12

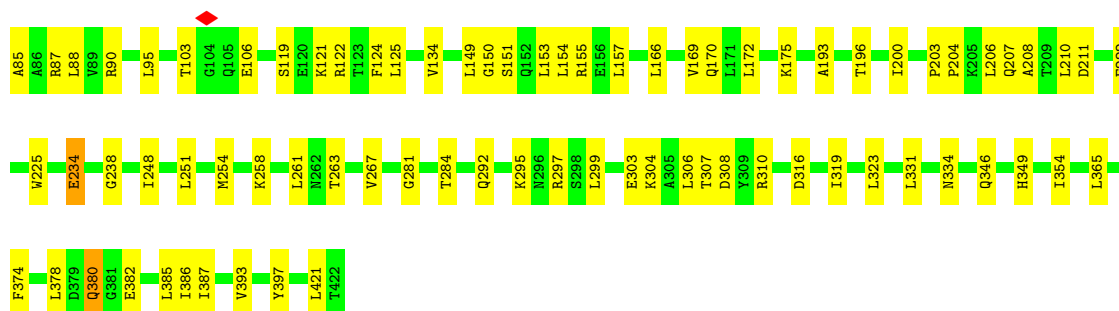


• Molecule 23: Proteasome subunit alpha type-2



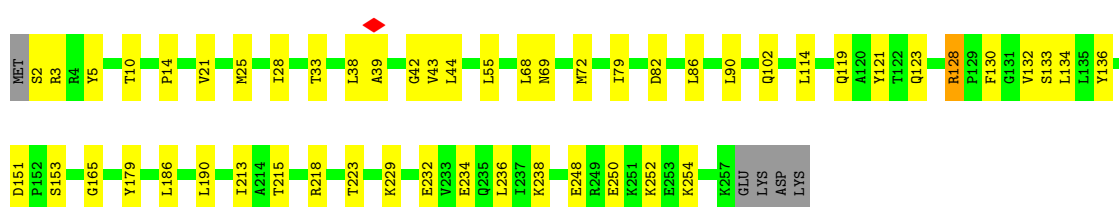
• Molecule 23: Proteasome subunit alpha type-2





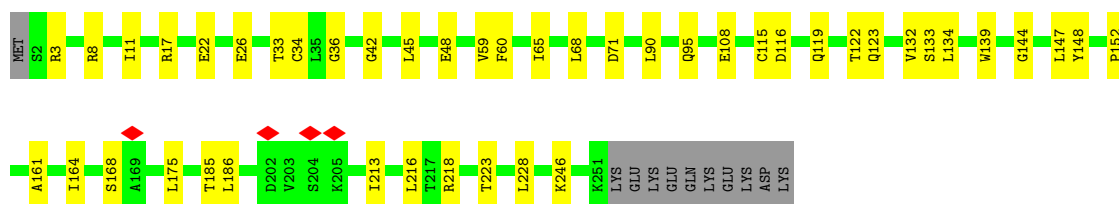
• Molecule 26: Proteasome subunit alpha type-4

Chain I: 78% 20% .



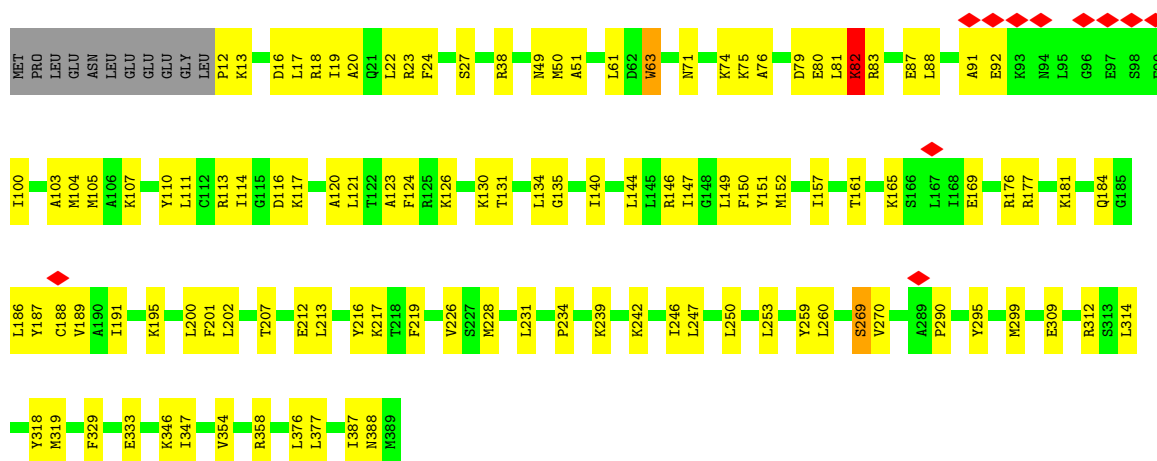
• Molecule 26: Proteasome subunit alpha type-4

Chain i: 79% 17% .



• Molecule 27: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 68% 28% . .



• Molecule 28: Proteasome subunit alpha type-7

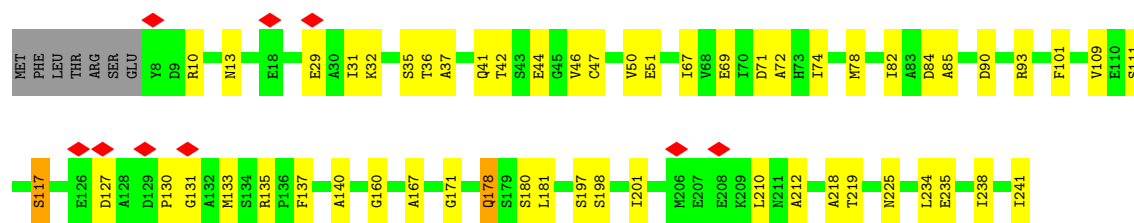
- Molecule 28: Proteasome subunit alpha type-7

- Molecule 29: 26S proteasome non-ATPase regulatory subunit 7

- Molecule 30: Proteasome subunit alpha type-5

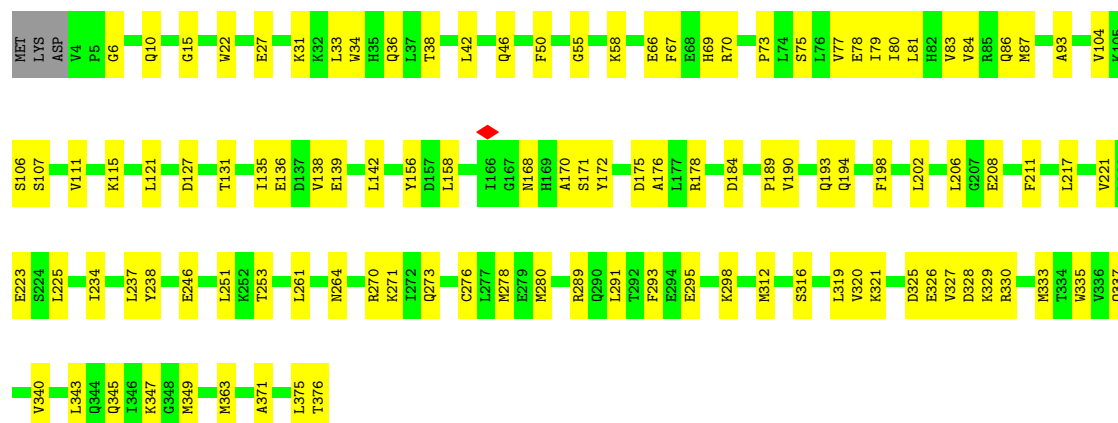
- Molecule 30: Proteasome subunit alpha type-5

WORLDWIDE
PDB
PROTEIN DATA BANK



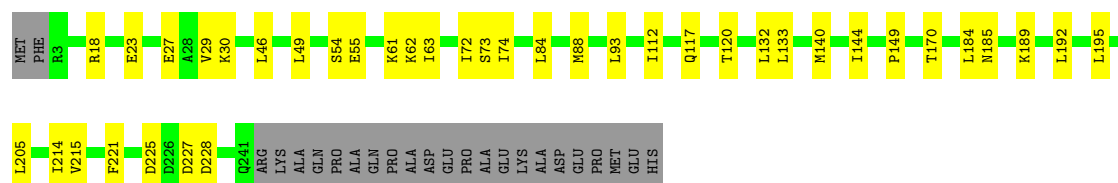
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 70% 29%



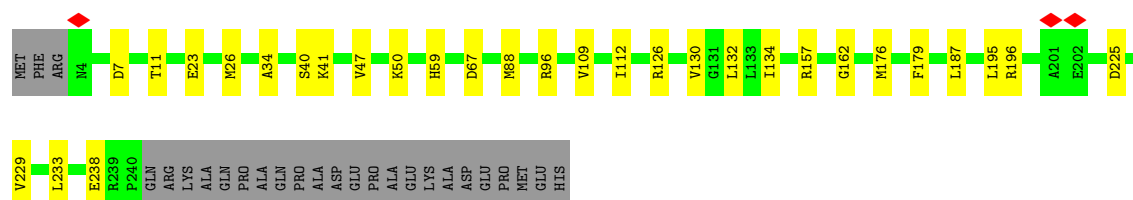
• Molecule 32: Proteasome subunit alpha type-1

Chain L: 76% 15% 9%



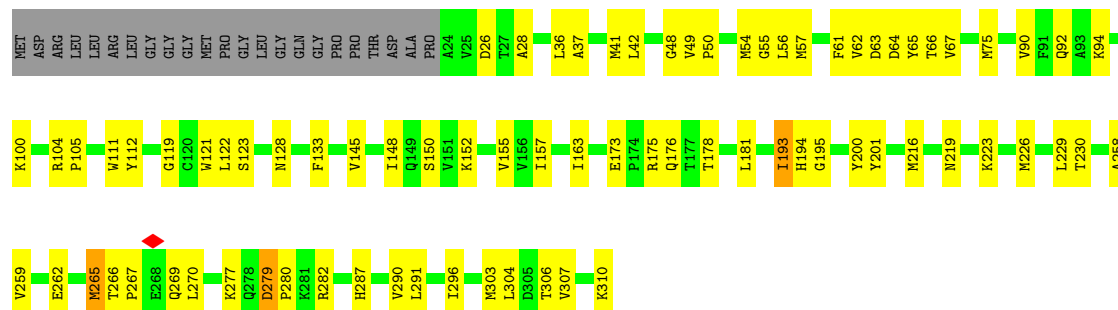
• Molecule 32: Proteasome subunit alpha type-1

Chain I: 79% 11% 10%



• Molecule 33: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 35% 15% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108120	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.946	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.09	Depositor
Map size (\AA)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	u	0.54	0/915	1.03	0/1222
2	d	0.37	1/2133 (0.0%)	0.81	3/2882 (0.1%)
3	M	0.25	0/1872	0.55	0/2528
3	m	0.24	0/1884	0.55	2/2542 (0.1%)
4	R	0.31	0/1602	0.63	5/2165 (0.2%)
4	r	0.23	0/1571	0.47	0/2123
5	N	0.34	0/1513	0.55	2/2048 (0.1%)
5	n	0.33	0/1517	0.60	1/2056 (0.0%)
6	E	0.25	0/2827	0.58	0/3814
7	B	0.27	0/3078	0.65	2/4163 (0.0%)
8	e	0.23	0/179	0.72	0/246
9	O	0.22	0/1670	0.45	0/2265
9	o	0.23	0/1670	0.50	0/2265
10	S	0.24	0/1671	0.50	0/2253
10	s	0.24	0/1671	0.44	0/2253
11	D	0.28	0/3045	0.59	1/4116 (0.0%)
12	F	0.28	0/2907	0.59	0/3923
13	P	0.22	0/1614	0.48	0/2177
13	p	0.26	0/1614	0.54	0/2177
14	U	0.25	0/6406	0.64	0/8672
15	C	0.27	0/2914	0.66	2/3927 (0.1%)
16	G	0.26	0/1852	0.54	1/2514 (0.0%)
16	g	0.24	0/1831	0.51	1/2492 (0.0%)
17	Q	0.23	0/1603	0.46	0/2174
17	q	0.28	0/1598	0.53	0/2167
18	A	0.29	0/3109	0.65	3/4198 (0.1%)
19	V	0.28	0/3835	0.70	4/5185 (0.1%)
20	T	0.23	0/1695	0.50	0/2298
20	t	0.25	0/1695	0.52	0/2298
22	W	0.29	0/3709	0.73	1/4990 (0.0%)
23	H	0.21	0/1737	0.49	0/2365
23	h	0.21	0/1705	0.50	0/2324

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	f	0.42	0/6737	0.86	0/9132
25	X	0.26	0/3047	0.60	0/4107
26	I	0.25	0/1996	0.54	0/2697
26	i	0.24	0/1928	0.59	2/2610 (0.1%)
27	Y	0.27	0/3045	0.70	1/4108 (0.0%)
28	J	0.20	0/1724	0.52	0/2353
28	j	0.18	0/1706	0.52	1/2329 (0.0%)
29	Z	0.26	0/2303	0.58	1/3123 (0.0%)
30	K	0.27	0/1766	0.52	0/2393
30	k	0.27	0/1769	0.62	1/2397 (0.0%)
31	a	0.26	0/3047	0.66	3/4125 (0.1%)
32	L	0.24	0/1878	0.56	0/2544
32	l	0.19	0/1872	0.47	0/2534
33	b	0.22	0/1464	0.62	0/1984
34	c	0.32	0/2280	0.65	2/3083 (0.1%)
All	All	0.28	1/105204 (0.0%)	0.62	39/142341 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	161	ILE	C-N	5.27	1.40	1.34

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	j	59	VAL	N-CA-C	-8.67	105.48	113.71
27	Y	82	LYS	N-CA-C	-7.86	102.65	111.14
18	A	346	PRO	CA-C-N	6.72	134.38	121.54
18	A	346	PRO	C-N-CA	6.72	134.38	121.54
4	R	60	THR	CA-C-N	6.57	134.09	121.54

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	u	908	0	973	66	0
2	d	2091	0	2097	126	0
3	M	1839	0	1791	42	0
3	m	1849	0	1809	38	0
4	R	1571	0	1509	47	0
4	r	1541	0	1489	15	0
5	N	1488	0	1454	34	0
5	n	1492	0	1449	55	0
6	E	2782	0	2827	82	0
7	B	3034	0	3037	120	0
8	e	180	0	108	10	0
9	O	1643	0	1641	18	0
9	o	1643	0	1641	37	0
10	S	1641	0	1615	25	0
10	s	1641	0	1615	24	0
11	D	2997	0	3001	102	0
12	F	2867	0	2905	93	0
13	P	1585	0	1598	46	0
13	p	1585	0	1598	30	0
14	U	6298	0	6309	223	0
15	C	2877	0	2937	117	0
16	G	1820	0	1789	68	0
16	g	1798	0	1738	56	0
17	Q	1570	0	1547	32	0
17	q	1565	0	1545	38	0
18	A	3059	0	3083	107	0
19	V	3761	0	3772	148	0
20	T	1662	0	1614	35	0
20	t	1662	0	1614	29	0
21	v	75	0	22	3	0
22	W	3663	0	3750	215	0
23	H	1702	0	1589	41	0
23	h	1671	0	1552	33	0
24	f	6636	0	6461	514	0
25	X	3004	0	3108	87	0
26	I	1966	0	1910	59	0
26	i	1900	0	1837	44	0
27	Y	2995	0	2927	157	0
28	J	1700	0	1511	29	0
28	j	1684	0	1497	34	0
29	Z	2260	0	2263	87	0
30	K	1742	0	1688	49	0
30	k	1743	0	1692	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	2989	0	3001	107	0
32	L	1844	0	1808	40	0
32	l	1838	0	1813	24	0
33	b	1444	0	1477	54	0
34	c	2239	0	2226	96	0
35	B	27	0	12	10	0
35	E	27	0	12	2	0
36	A	31	0	12	2	0
36	D	31	0	12	4	0
36	F	31	0	12	0	0
37	c	1	0	0	0	0
All	All	103692	0	102297	3237	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 16.

The worst 5 of 3237 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)
12:F:435:LEU:HD13	30:K:20:ARG:CD	1.28	1.53
12:F:435:LEU:CD1	30:K:20:ARG:HD3	1.28	1.53
14:U:695:MET:HE1	14:U:709:PHE:CD2	1.44	1.51
30:k:133:MET:HE1	30:k:137:PHE:CE2	1.56	1.40
30:K:21:LEU:CD2	30:K:24:VAL:HG23	1.51	1.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	u	110/491 (22%)	101 (92%)	8 (7%)	1 (1%)	14 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	258/350 (74%)	215 (83%)	40 (16%)	3 (1%)	11	43
3	M	238/255 (93%)	218 (92%)	19 (8%)	1 (0%)	30	64
3	m	237/255 (93%)	222 (94%)	15 (6%)	0	100	100
4	R	204/263 (78%)	188 (92%)	14 (7%)	2 (1%)	13	46
4	r	199/263 (76%)	190 (96%)	9 (4%)	0	100	100
5	N	197/239 (82%)	184 (93%)	11 (6%)	2 (1%)	13	46
5	n	199/239 (83%)	185 (93%)	12 (6%)	2 (1%)	13	46
6	E	352/389 (90%)	317 (90%)	34 (10%)	1 (0%)	37	68
7	B	393/440 (89%)	344 (88%)	48 (12%)	1 (0%)	37	68
8	e	29/70 (41%)	21 (72%)	8 (28%)	0	100	100
9	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
9	o	218/277 (79%)	205 (94%)	13 (6%)	0	100	100
10	S	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
10	s	211/241 (88%)	203 (96%)	7 (3%)	1 (0%)	25	59
11	D	378/418 (90%)	332 (88%)	44 (12%)	2 (0%)	25	59
12	F	367/439 (84%)	326 (89%)	40 (11%)	1 (0%)	37	68
13	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
13	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
14	U	808/953 (85%)	719 (89%)	83 (10%)	6 (1%)	19	53
15	C	372/406 (92%)	338 (91%)	32 (9%)	2 (0%)	25	59
16	G	238/246 (97%)	231 (97%)	7 (3%)	0	100	100
16	g	237/246 (96%)	224 (94%)	13 (6%)	0	100	100
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
17	q	196/201 (98%)	175 (89%)	21 (11%)	0	100	100
18	A	391/433 (90%)	340 (87%)	48 (12%)	3 (1%)	16	51
19	V	470/534 (88%)	413 (88%)	56 (12%)	1 (0%)	44	75
20	T	213/264 (81%)	201 (94%)	12 (6%)	0	100	100
20	t	213/264 (81%)	203 (95%)	10 (5%)	0	100	100
22	W	454/456 (100%)	412 (91%)	40 (9%)	2 (0%)	30	64
23	H	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
23	h	227/234 (97%)	214 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	f	887/908 (98%)	717 (81%)	156 (18%)	14 (2%)	8	38
25	X	378/422 (90%)	345 (91%)	31 (8%)	2 (0%)	25	59
26	I	254/261 (97%)	232 (91%)	22 (9%)	0	100	100
26	i	248/261 (95%)	225 (91%)	22 (9%)	1 (0%)	30	64
27	Y	376/389 (97%)	319 (85%)	54 (14%)	3 (1%)	16	51
28	J	237/248 (96%)	216 (91%)	20 (8%)	1 (0%)	30	64
28	j	236/248 (95%)	211 (89%)	23 (10%)	2 (1%)	16	51
29	Z	284/324 (88%)	261 (92%)	22 (8%)	1 (0%)	30	64
30	K	232/241 (96%)	211 (91%)	20 (9%)	1 (0%)	30	64
30	k	232/241 (96%)	207 (89%)	22 (10%)	3 (1%)	10	41
31	a	371/376 (99%)	329 (89%)	41 (11%)	1 (0%)	37	68
32	L	237/263 (90%)	220 (93%)	17 (7%)	0	100	100
32	l	235/263 (89%)	216 (92%)	19 (8%)	0	100	100
33	b	188/377 (50%)	172 (92%)	15 (8%)	1 (0%)	25	59
34	c	285/310 (92%)	259 (91%)	24 (8%)	2 (1%)	19	53
All	All	13348/15361 (87%)	12062 (90%)	1223 (9%)	63 (0%)	27	59

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	u	90	VAL
4	R	61	THR
5	n	229	PRO
7	B	232	LYS
11	D	125	LYS

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	u	99/398 (25%)	96 (97%)	3 (3%)	36	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	224/294 (76%)	224 (100%)	0	100	100
3	M	189/212 (89%)	188 (100%)	1 (0%)	86	93
3	m	191/212 (90%)	190 (100%)	1 (0%)	86	93
4	R	153/202 (76%)	151 (99%)	2 (1%)	65	81
4	r	152/202 (75%)	151 (99%)	1 (1%)	81	89
5	N	154/181 (85%)	154 (100%)	0	100	100
5	n	153/181 (84%)	153 (100%)	0	100	100
6	E	305/341 (89%)	305 (100%)	0	100	100
7	B	332/385 (86%)	331 (100%)	1 (0%)	91	96
8	e	10/63 (16%)	10 (100%)	0	100	100
9	O	177/228 (78%)	177 (100%)	0	100	100
9	o	177/228 (78%)	177 (100%)	0	100	100
10	S	174/199 (87%)	174 (100%)	0	100	100
10	s	174/199 (87%)	174 (100%)	0	100	100
11	D	324/366 (88%)	320 (99%)	4 (1%)	67	82
12	F	310/379 (82%)	308 (99%)	2 (1%)	84	91
13	P	172/174 (99%)	172 (100%)	0	100	100
13	p	172/174 (99%)	172 (100%)	0	100	100
14	U	683/816 (84%)	683 (100%)	0	100	100
15	C	308/352 (88%)	307 (100%)	1 (0%)	91	96
16	G	192/210 (91%)	192 (100%)	0	100	100
16	g	186/210 (89%)	185 (100%)	1 (0%)	86	93
17	Q	164/171 (96%)	164 (100%)	0	100	100
17	q	164/171 (96%)	164 (100%)	0	100	100
18	A	330/372 (89%)	329 (100%)	1 (0%)	91	96
19	V	400/460 (87%)	398 (100%)	2 (0%)	86	93
20	T	173/215 (80%)	172 (99%)	1 (1%)	84	91
20	t	173/215 (80%)	173 (100%)	0	100	100
22	W	407/416 (98%)	403 (99%)	4 (1%)	73	84
23	H	164/191 (86%)	164 (100%)	0	100	100
23	h	160/191 (84%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	f	695/763 (91%)	686 (99%)	9 (1%)	65	81
25	X	326/362 (90%)	324 (99%)	2 (1%)	84	91
26	I	199/221 (90%)	198 (100%)	1 (0%)	86	93
26	i	191/221 (86%)	191 (100%)	0	100	100
27	Y	308/344 (90%)	307 (100%)	1 (0%)	91	96
28	J	151/211 (72%)	150 (99%)	1 (1%)	81	89
28	j	149/211 (71%)	149 (100%)	0	100	100
29	Z	251/295 (85%)	249 (99%)	2 (1%)	79	88
30	K	186/203 (92%)	184 (99%)	2 (1%)	70	83
30	k	186/203 (92%)	185 (100%)	1 (0%)	86	93
31	a	331/336 (98%)	331 (100%)	0	100	100
32	L	196/224 (88%)	196 (100%)	0	100	100
32	l	197/224 (88%)	196 (100%)	1 (0%)	86	93
33	b	164/312 (53%)	164 (100%)	0	100	100
34	c	246/268 (92%)	242 (98%)	4 (2%)	58	76
All	All	10922/13006 (84%)	10873 (100%)	49 (0%)	88	95

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	f	473	ASN
26	I	128	ARG
24	f	474	SER
25	X	87	ARG
3	M	216	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
26	i	102	GLN
17	Q	32	HIS
29	Z	223	ASN
31	a	231	GLN
34	c	176	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is 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$
36	ATP	D	501	-	26,33,33	0.64	0	31,52,52	0.80	1 (3%)
36	ATP	A	501	-	26,33,33	0.63	0	31,52,52	0.84	2 (6%)
35	ADP	B	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.42	4 (13%)
36	ATP	F	501	-	26,33,33	0.65	0	31,52,52	0.81	1 (3%)
35	ADP	E	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.61	4 (13%)

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
36	ATP	D	501	-	-	6/18/38/38	0/3/3/3
36	ATP	A	501	-	-	7/18/38/38	0/3/3/3
35	ADP	B	501	-	-	4/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	F	501	-	-	3/18/38/38	0/3/3/3
35	ADP	E	401	-	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	401	ADP	C5-C4	2.38	1.47	1.40
35	B	501	ADP	C5-C4	2.36	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	401	ADP	PA-O3A-PB	-4.41	117.70	132.83
35	E	401	ADP	C3'-C2'-C1'	3.81	106.72	100.98
35	B	501	ADP	C3'-C2'-C1'	3.74	106.61	100.98
35	E	401	ADP	N3-C2-N1	-3.23	123.63	128.68
35	B	501	ADP	N3-C2-N1	-2.99	124.00	128.68

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	E	401	ADP	C5'-O5'-PA-O2A
36	D	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C4'-C5'-O5'-PA
36	F	501	ATP	C5'-O5'-PA-O3A
36	A	501	ATP	C5'-O5'-PA-O1A

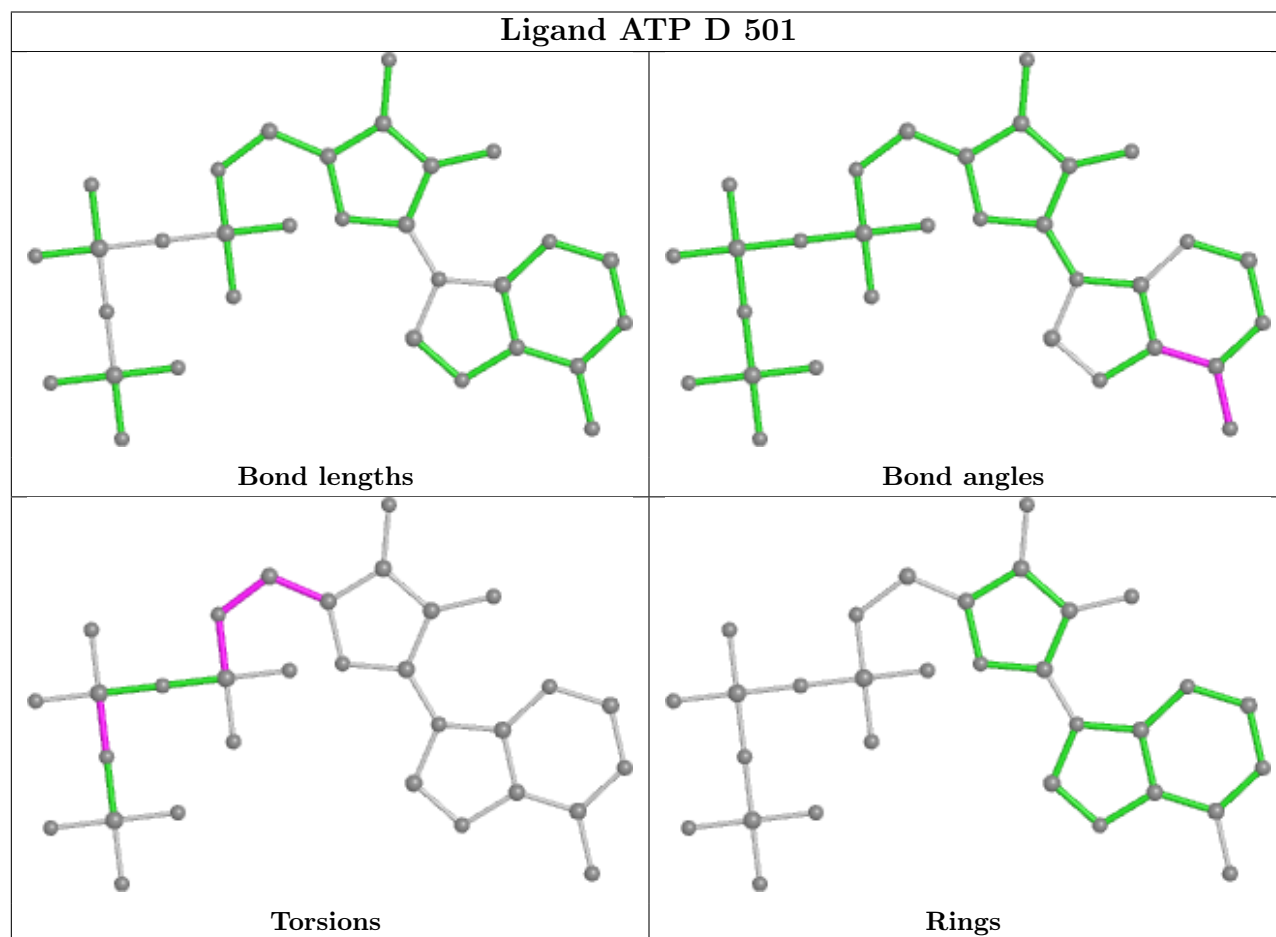
There are no ring outliers.

4 monomers are involved in 18 short contacts:

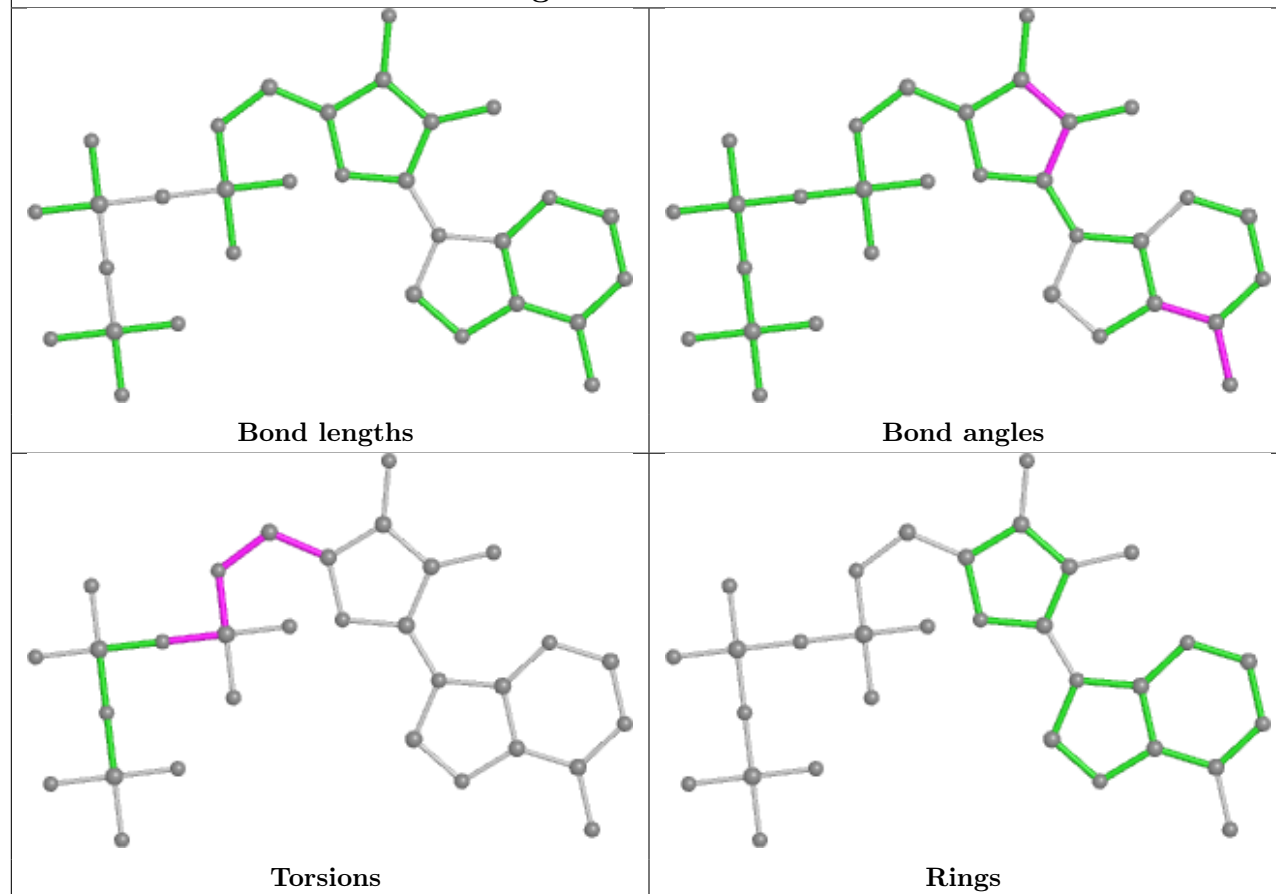
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	D	501	ATP	4	0
36	A	501	ATP	2	0
35	B	501	ADP	10	0
35	E	401	ADP	2	0

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

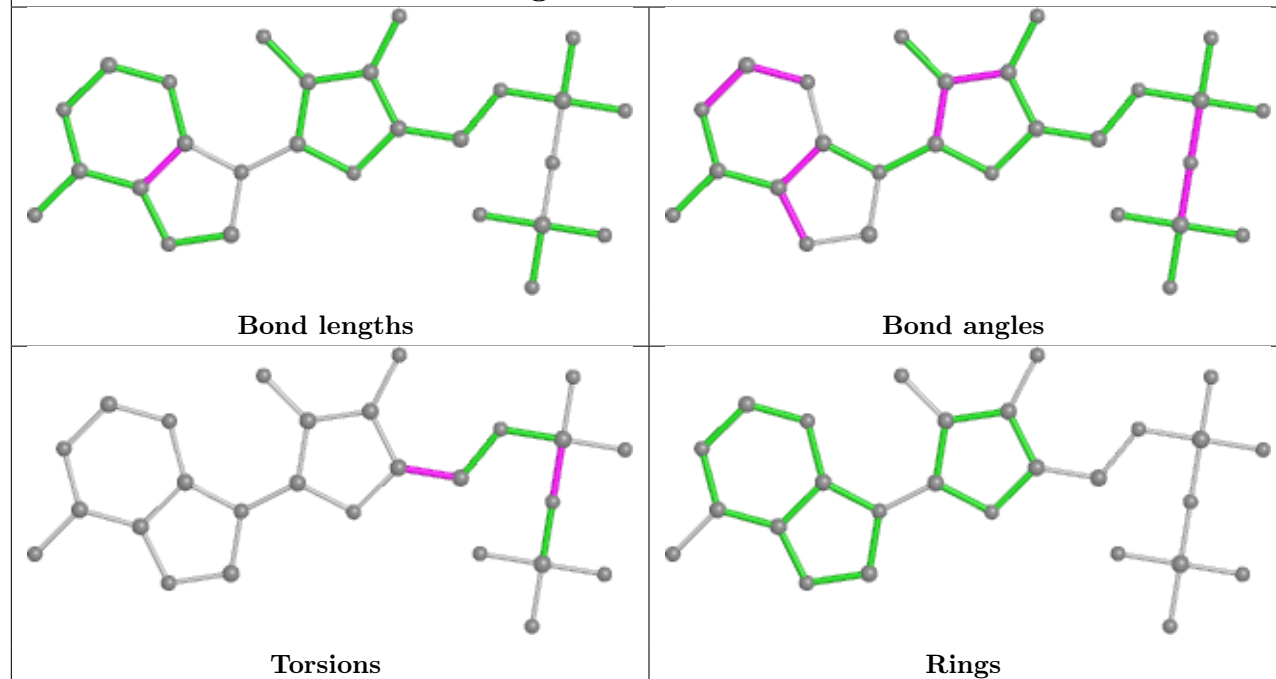
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



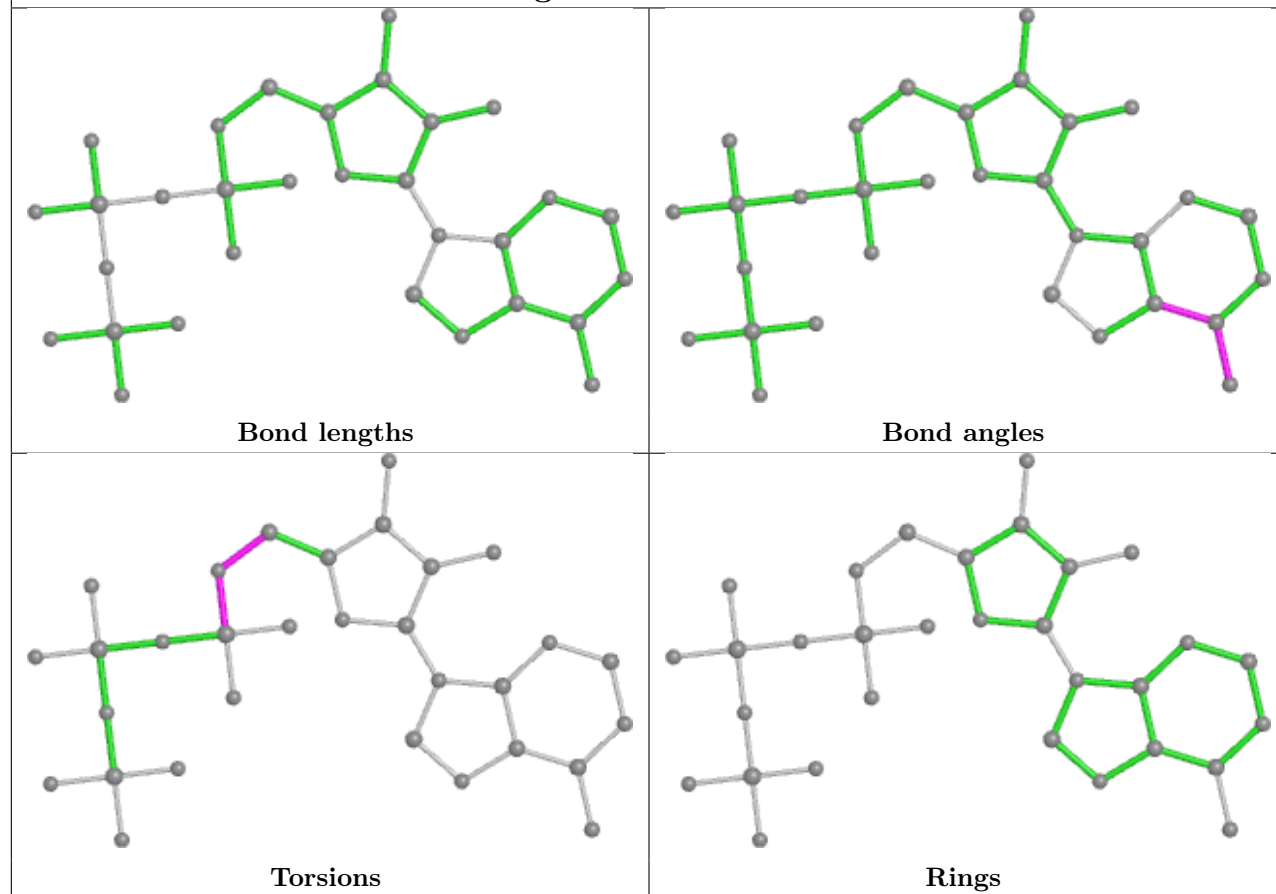
Ligand ATP A 501



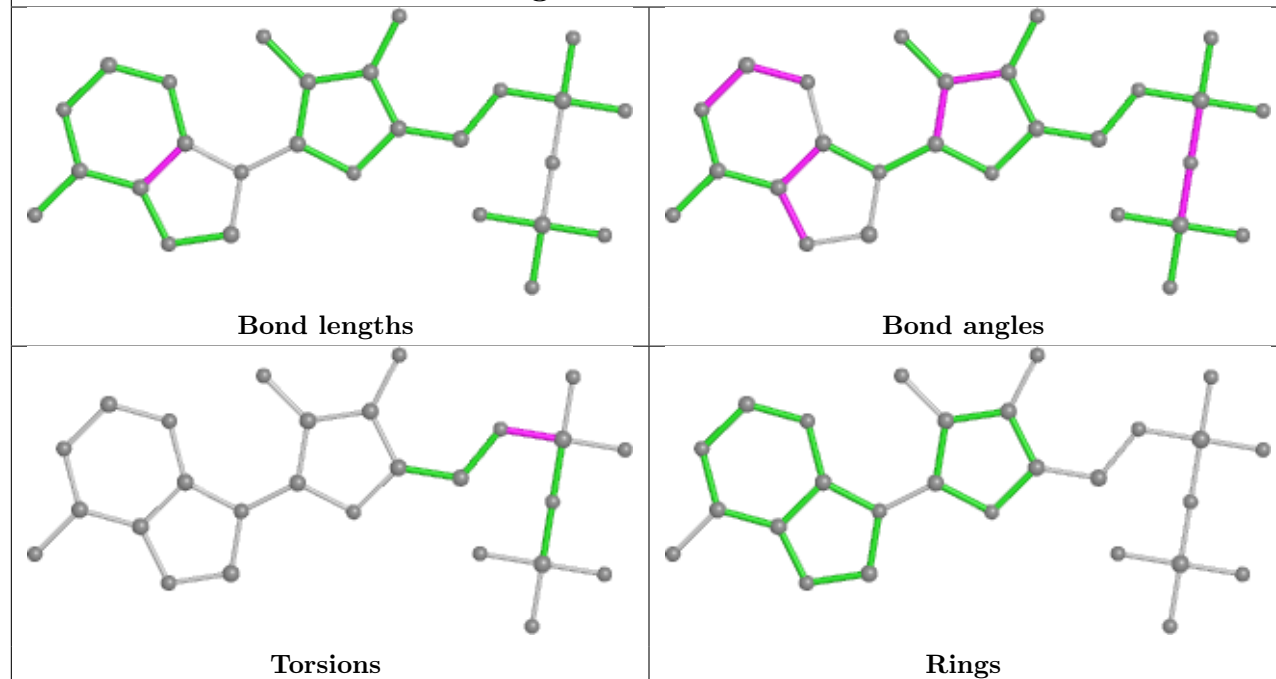
Ligand ADP B 501



Ligand ATP F 501



Ligand ADP E 401



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.

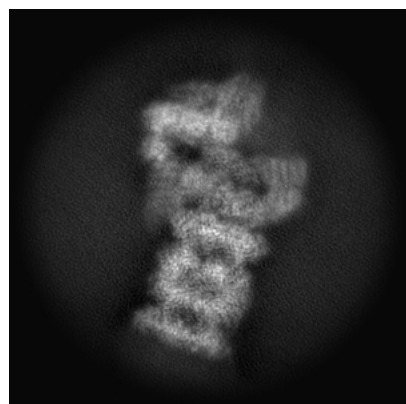
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64133. These allow visual inspection of the internal detail of the map and identification of artifacts.

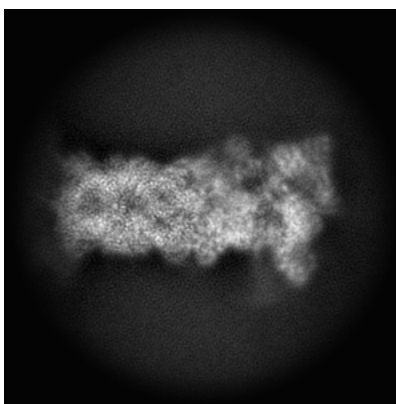
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

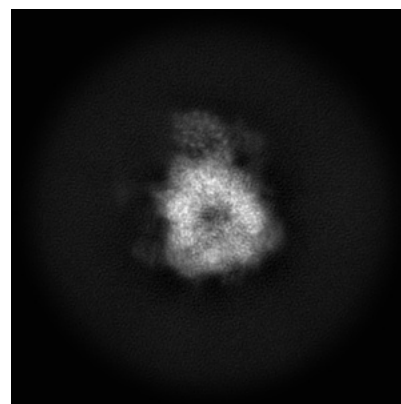
6.1.1 Primary map



X

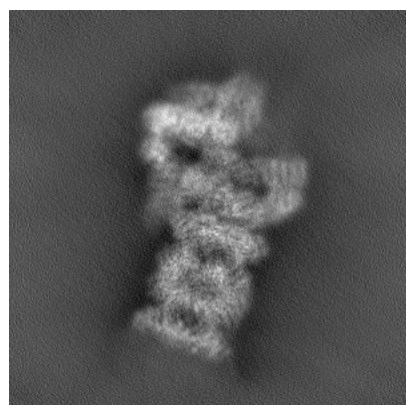


Y

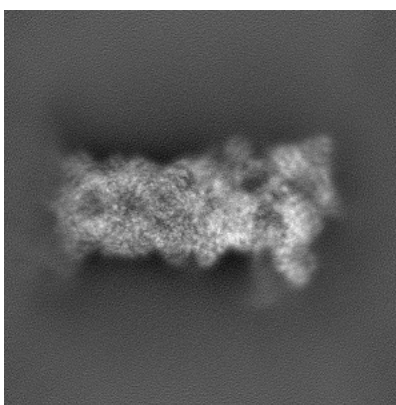


Z

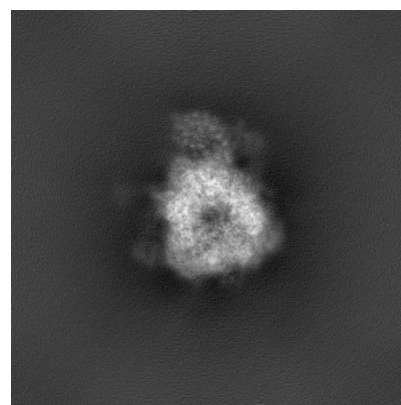
6.1.2 Raw map



X



Y

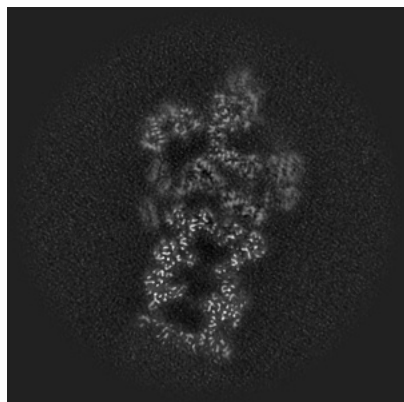


Z

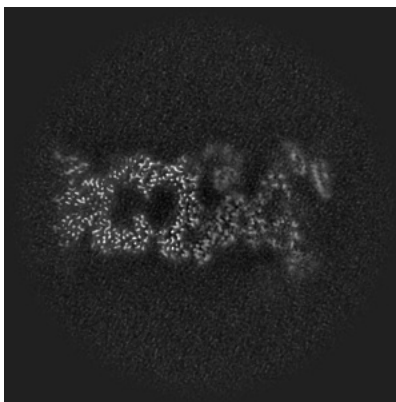
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

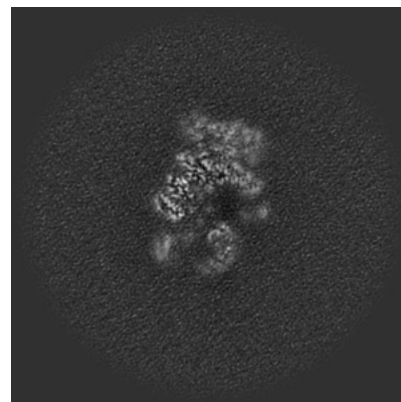
6.2.1 Primary map



X Index: 210

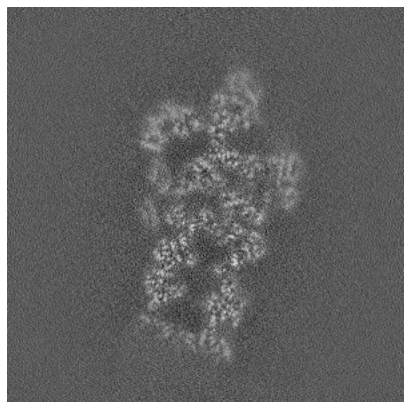


Y Index: 210

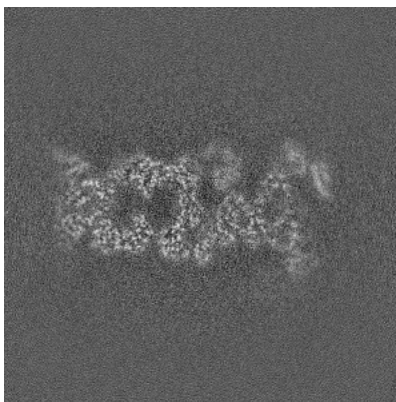


Z Index: 210

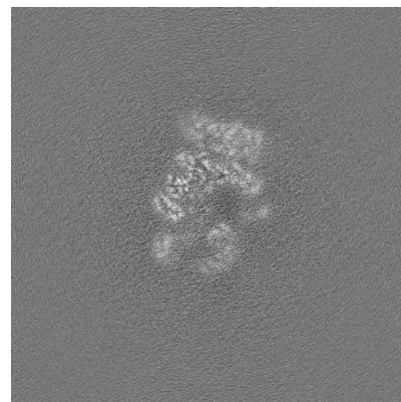
6.2.2 Raw map



X Index: 210



Y Index: 210

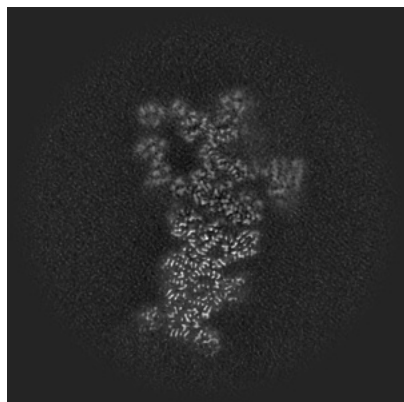


Z Index: 210

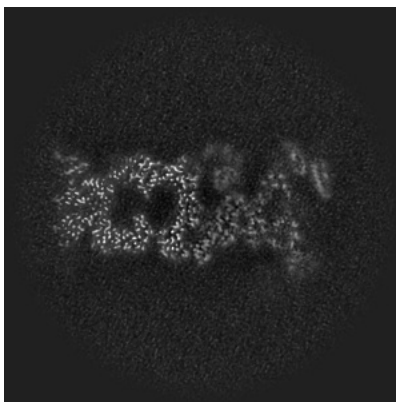
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

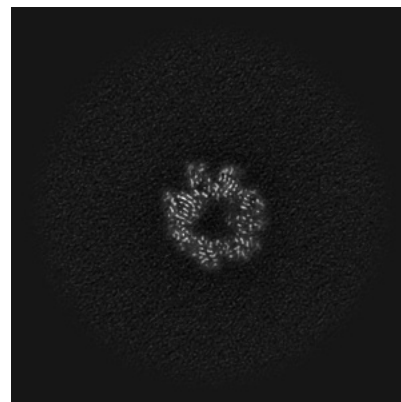
6.3.1 Primary map



X Index: 184

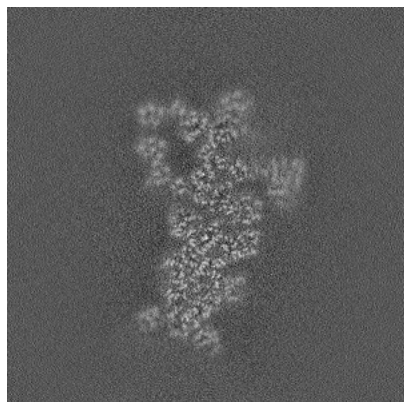


Y Index: 210

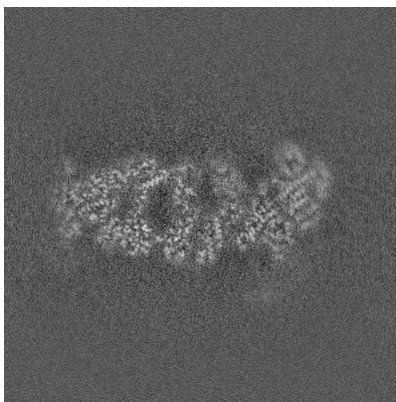


Z Index: 139

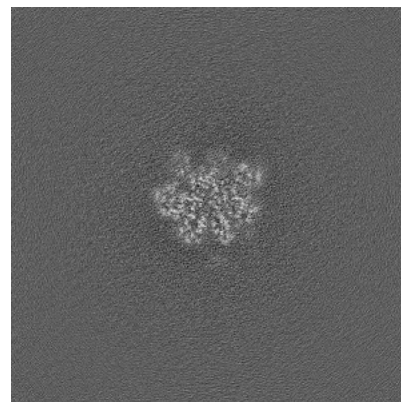
6.3.2 Raw map



X Index: 184



Y Index: 219

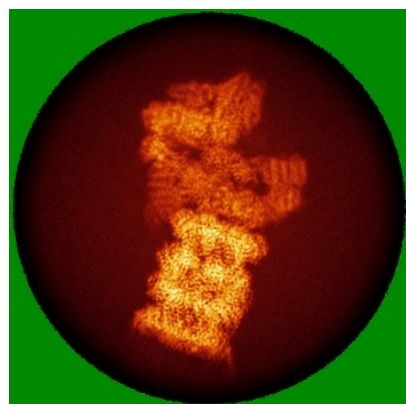


Z Index: 184

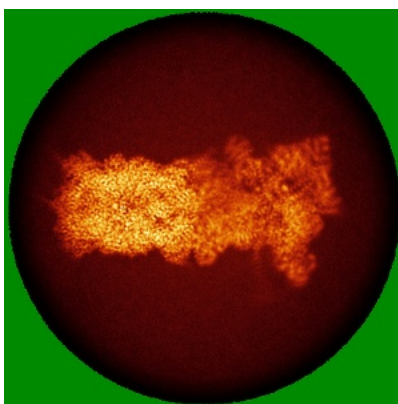
The images above show the largest variance slices of the map in three orthogonal directions.

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

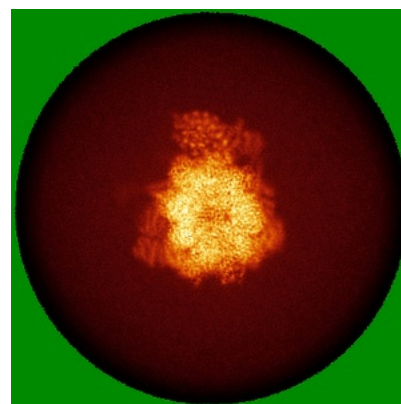
6.4.1 Primary map



X

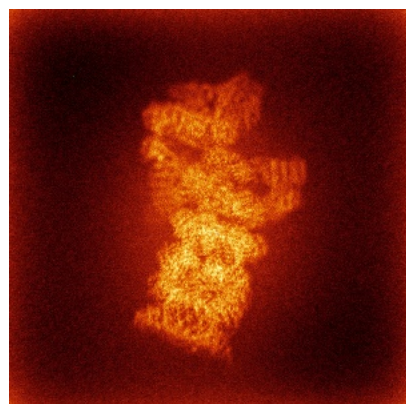


Y

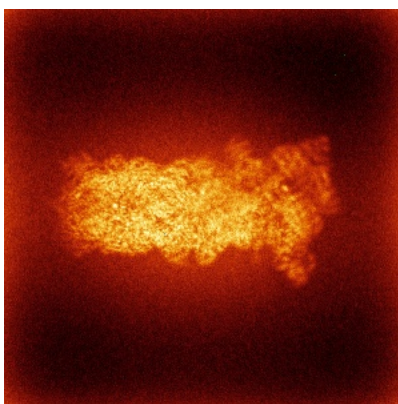


Z

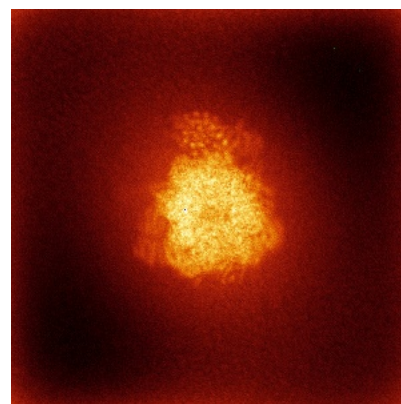
6.4.2 Raw map



X



Y

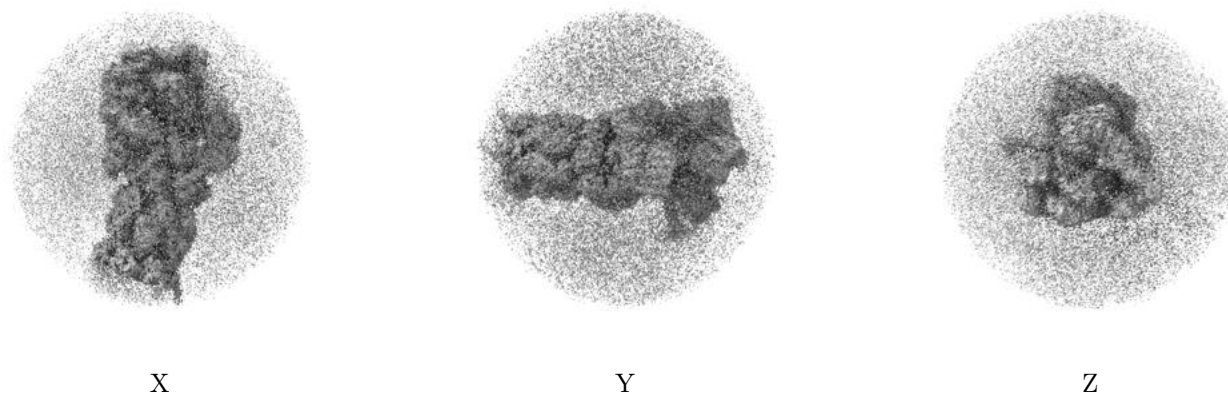


Z

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.

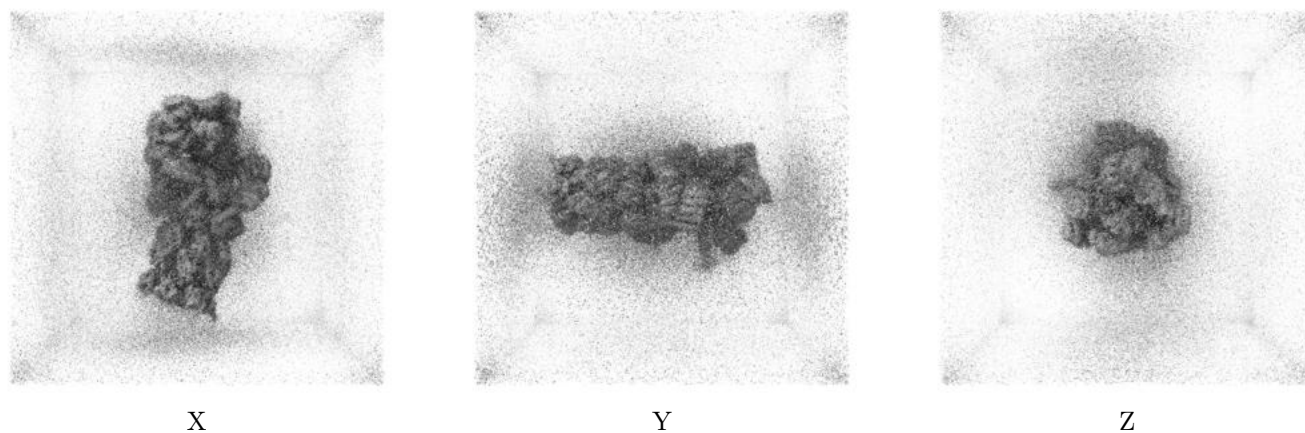
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

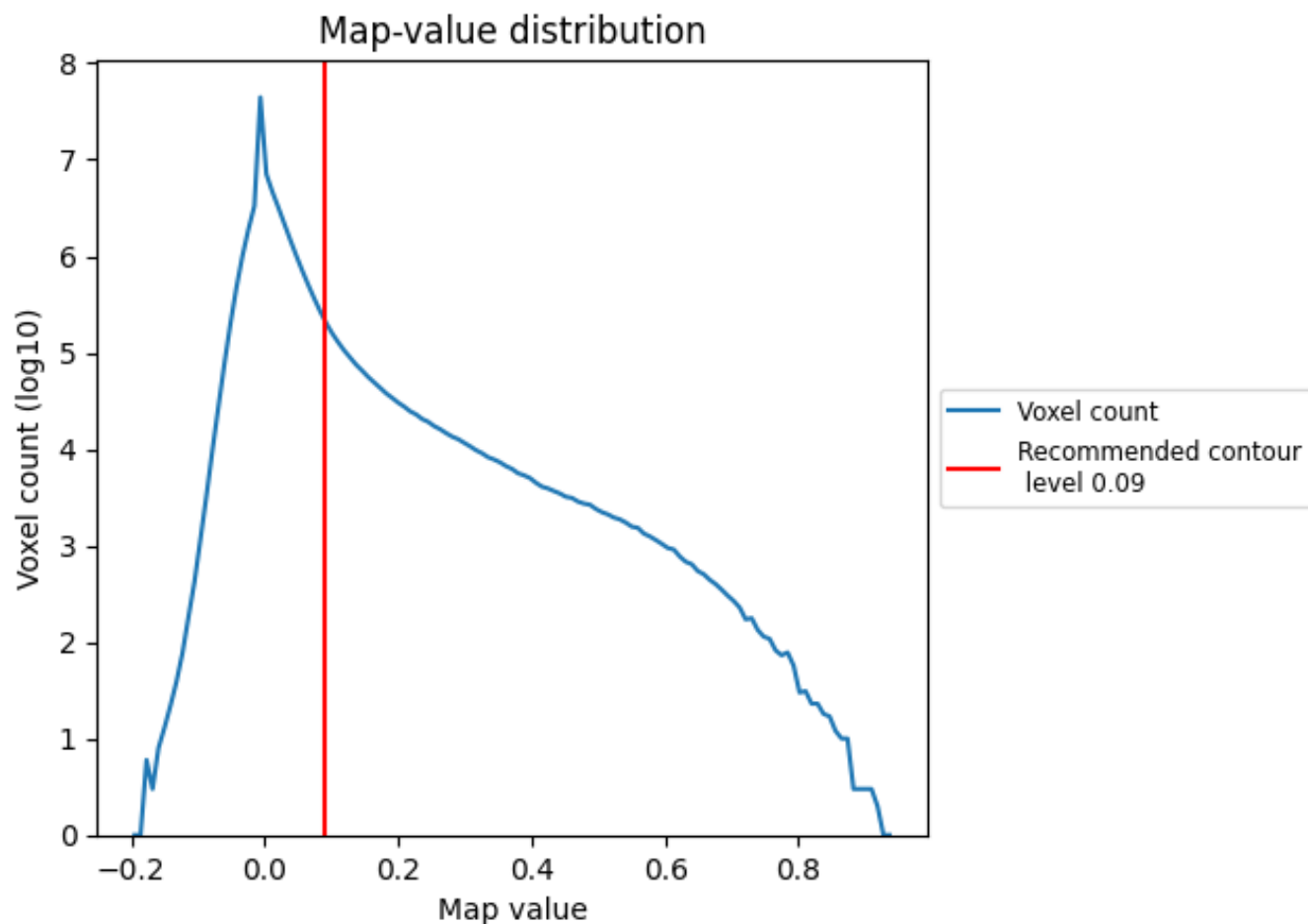
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

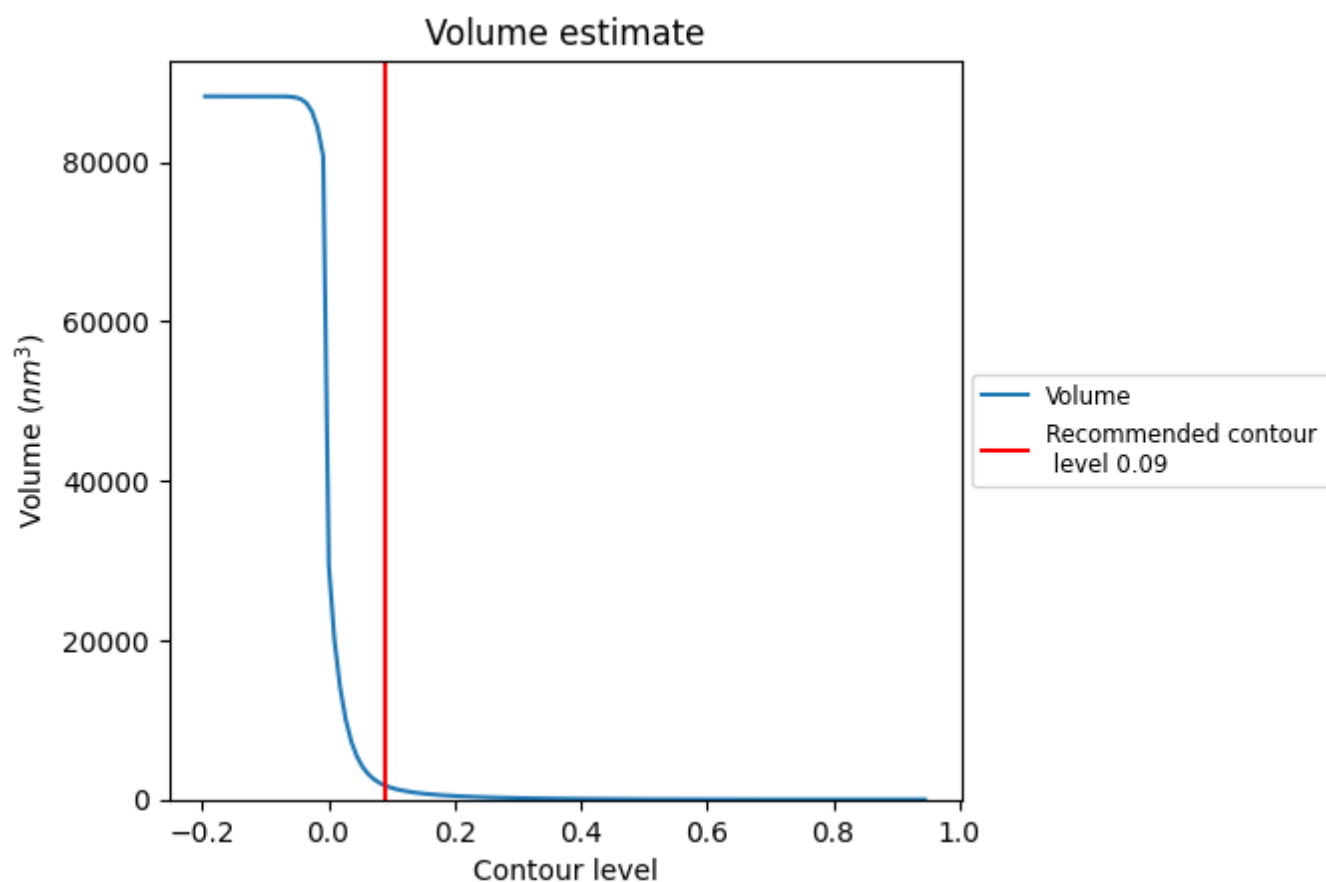
This section contains the results of statistical analysis of the map.

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.

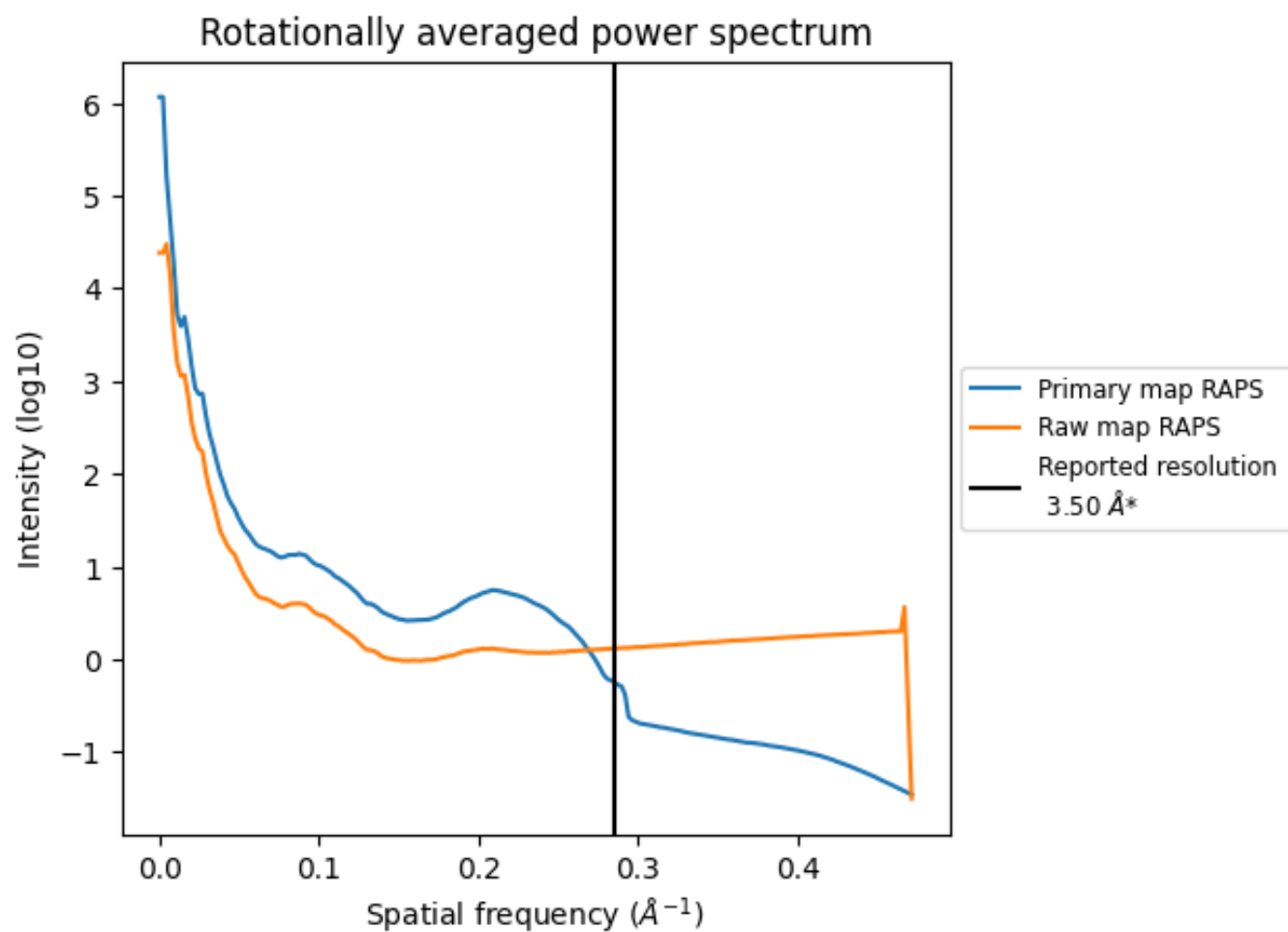
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1756 nm³; this corresponds to an approximate mass of 1586 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 ⓘ

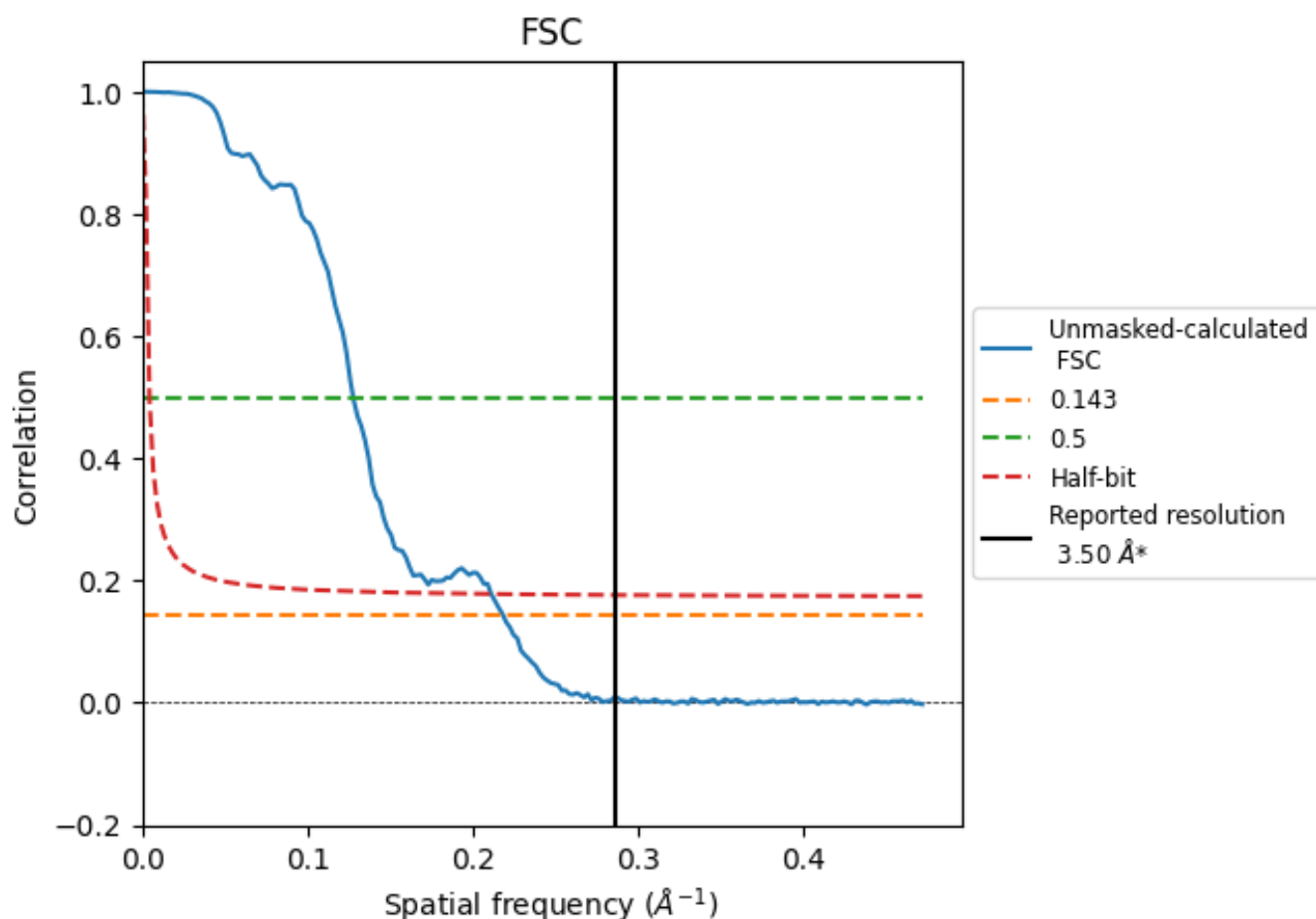


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

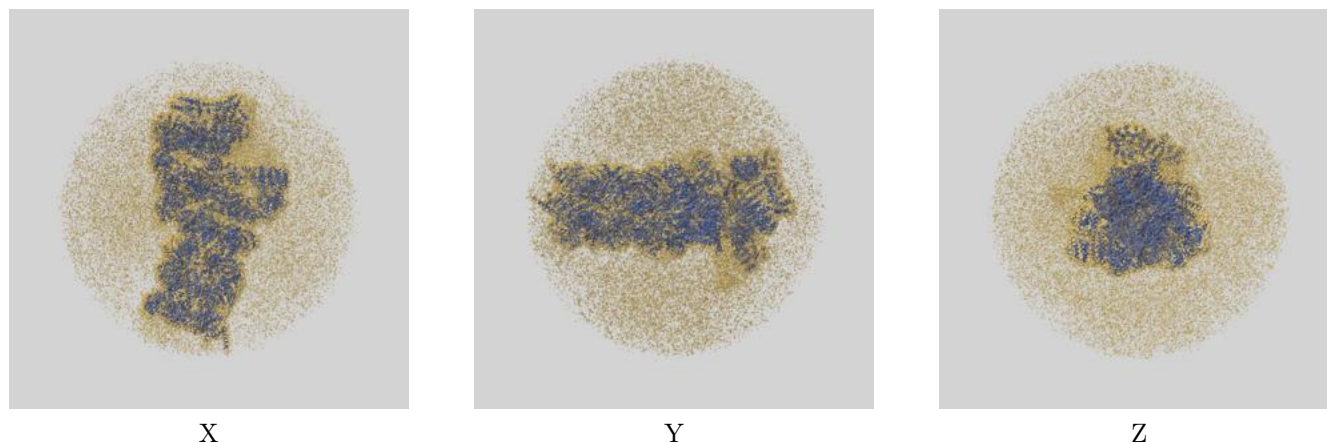
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.58	7.84	4.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.58 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

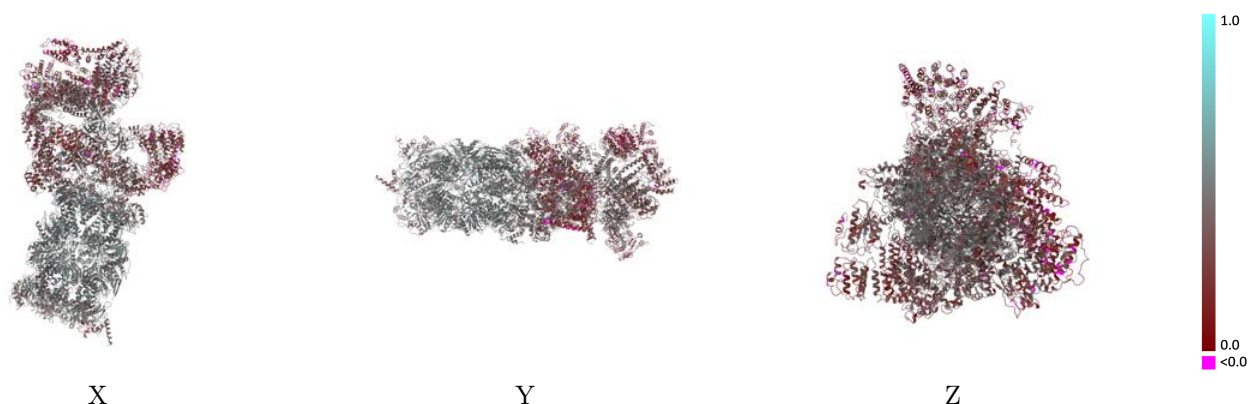
This section contains information regarding the fit between EMDB map EMD-64133 and PDB model 9UG9. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



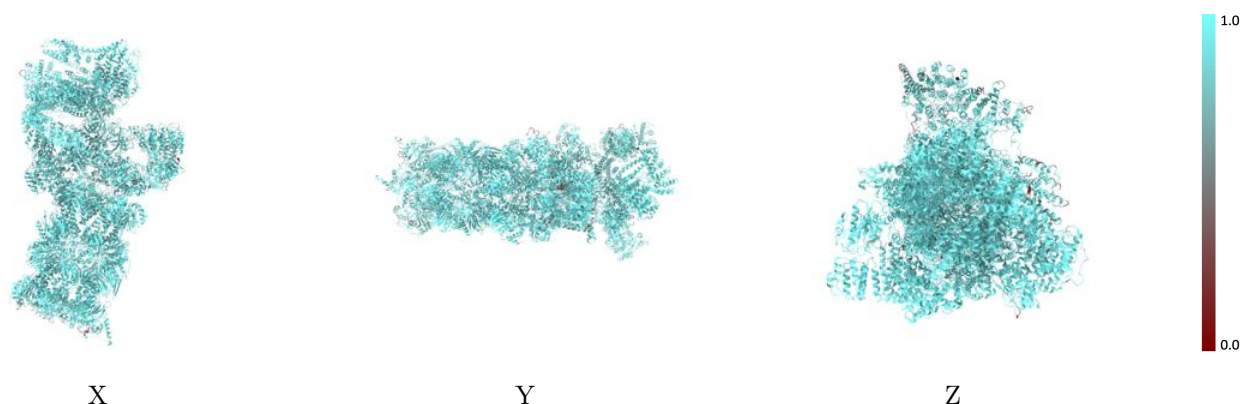
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



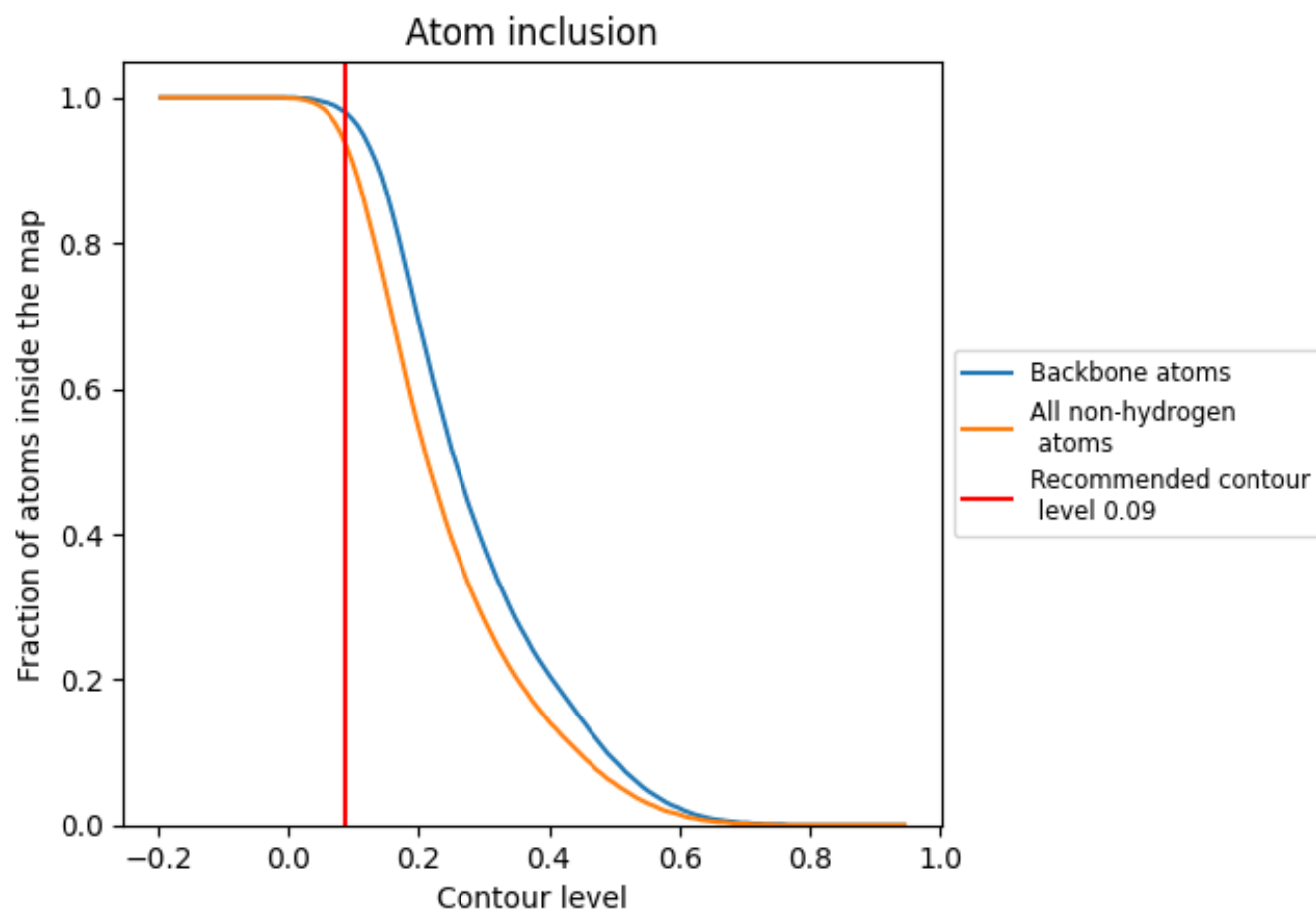
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





























The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.3990
A	 0.9250	 0.3800
B	 0.9190	 0.3780
C	 0.8750	 0.3450
D	 0.9160	 0.4090
E	 0.9400	 0.4240
F	 0.9420	 0.4290
G	 0.9650	 0.4670
H	 0.9710	 0.4780
I	 0.9610	 0.4480
J	 0.9840	 0.4710
K	 0.9760	 0.4730
L	 0.9740	 0.4760
M	 0.9710	 0.4760
N	 0.9800	 0.4960
O	 0.9900	 0.5020
P	 0.9840	 0.4940
Q	 0.9880	 0.5090
R	 0.9920	 0.4990
S	 0.9830	 0.4950
T	 0.9860	 0.5030
U	 0.9530	 0.3290
V	 0.8690	 0.2550
W	 0.9150	 0.3040
X	 0.8860	 0.3330
Y	 0.9190	 0.3070
Z	 0.9390	 0.4000
a	 0.9520	 0.3010
b	 0.9370	 0.3410
c	 0.9420	 0.3960
d	 0.8920	 0.2400
e	 0.9780	 0.3130
f	 0.8700	 0.2480
g	 0.8770	 0.4470
h	 0.9160	 0.4600



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Chain	Atom inclusion	Q-score
i	 0.9150	 0.4420
j	 0.8900	 0.4240
k	 0.8930	 0.4420
l	 0.9200	 0.4670
m	 0.8750	 0.4500
n	 0.9900	 0.4870
o	 0.9920	 0.4870
p	 0.9880	 0.4940
q	 0.9870	 0.4900
r	 0.9910	 0.5030
s	 0.9840	 0.4970
t	 0.9850	 0.5030
u	 0.8250	 0.2830
v	 0.8530	 0.4750