



## wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 11:38 PM UTC

PDB ID : 9HEU / pdb\_00009heu  
EMDB ID : EMD-52097  
Title : Co-chaperone Bag1-bound human 26S proteasome in SBAG1 state  
Authors : Cheng, T.C.; Sakata, E.; Muntaner, J.; Maestro-Lopez, M.; Cuellar, J.; Valpuesta, J.M.  
Deposited on : 2024-11-14  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

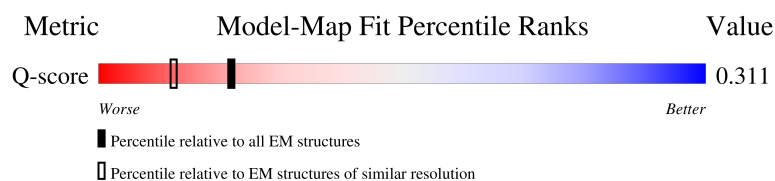
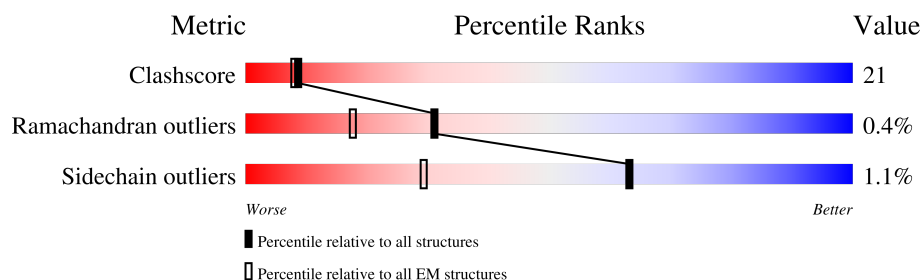
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



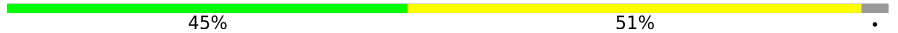

The reported resolution of this entry is 3.60 Å.

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	12797 ( 3.10 - 4.10 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	246	
1	g	246	
2	H	234	
2	h	234	



















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Mol	Chain	Length	Quality of chain
3	I	261	
3	i	261	
4	J	248	
4	j	248	
5	L	269	
5	l	269	
6	M	255	
6	m	255	
7	A	433	
8	B	440	
9	C	398	
10	D	418	
11	E	403	
12	F	439	
13	K	241	
13	k	241	
14	f	908	
15	a	376	
16	b	377	
17	c	310	
18	d	350	
19	e	70	
20	N	239	
20	n	239	
21	O	277	

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Mol	Chain	Length	Quality of chain
21	o	277	
22	P	205	
22	p	205	
23	Q	201	
23	q	201	
24	R	263	
24	r	263	
25	S	241	
25	s	241	
26	T	264	
26	t	264	
27	U	953	
28	V	534	
29	X	422	
30	Y	389	
31	Z	324	
32	W	456	
33	x	230	

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 104160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	237	Total	C	N	O	S	0	0
			1841	1168	307	353	13		
1	g	243	Total	C	N	O	S	0	0
			1885	1194	316	362	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	226	Total	C	N	O	S	0	0
			1749	1116	297	330	6		
2	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	248	Total	C	N	O	S	9	0
			2025	1279	349	388	9		
3	i	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	237	Total	C	N	O	S	0	0
			1869	1171	332	361	5		
4	j	238	Total	C	N	O	S	0	0
			1878	1178	333	362	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		
5	l	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	238	Total	C	N	O	S	0	0
			1862	1180	318	353	11		
6	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	403	Total	C	N	O	S	0	0
			3119	1958	548	596	17		

- Molecule 8 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	400	Total	C	N	O	S	0	0
			3060	1918	527	601	14		

- Molecule 9 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	368	Total	C	N	O	S	0	0
			2839	1766	518	537	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	372	Total	C	N	O	S	0	0
			2904	1827	506	560	11		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	361	Total	C	N	O	S	0	0
			2775	1733	500	526	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	355	Total	C	N	O	S	0	0
			2709	1705	468	519	17		

- Molecule 13 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	222	Total	C	N	O	S	0	0
			1694	1066	280	338	10		
13	k	234	Total	C	N	O	S	0	0
			1789	1125	295	358	11		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	823	Total	C	N	O	S	0	0
			6292	3963	1077	1208	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	373	Total	C	N	O	S	0	0
			2969	1887	510	557	15		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	287	Total	C	N	O	S	0	0
			2224	1398	388	419	19		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	252	Total	C	N	O	S	0	0
			2063	1338	335	382	8		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	e	50	Total	C	N	O	0	0
			407	244	63	100		

- Molecule 20 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	n	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
20	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		

- Molecule 21 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
21	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 22 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
22	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		
23	Q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 24 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 25 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
25	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
26	T	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	859	Total	C	N	O	S	0	0
			6648	4199	1136	1269	44		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	444	Total	C	N	O	S	0	0
			3600	2289	645	653	13		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	380	Total	C	N	O	S	0	0
			3002	1912	509	569	12		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	380	Total	C	N	O	S	0	0
			3021	1904	530	570	17		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	286	Total	C	N	O	S	0	0
			2248	1427	392	424	5		

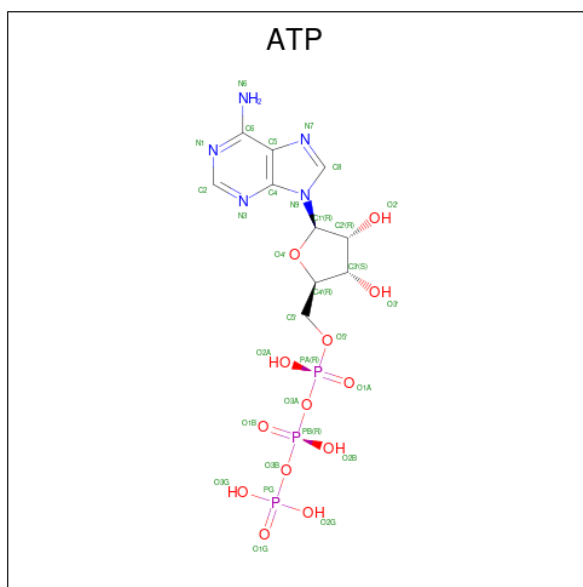
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	444	Total	C	N	O	S	0	0
			3570	2250	616	680	24		

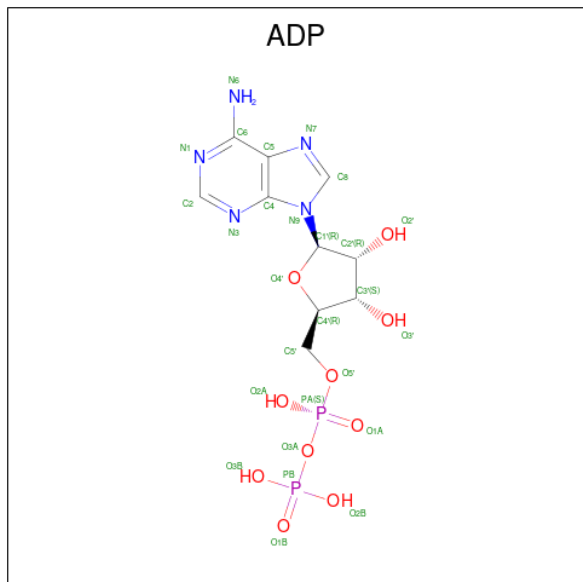
- Molecule 33 is a protein called BAG family molecular chaperone regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	85	Total	C	N	O	S	0	0
			635	397	110	125	3		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



- 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	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

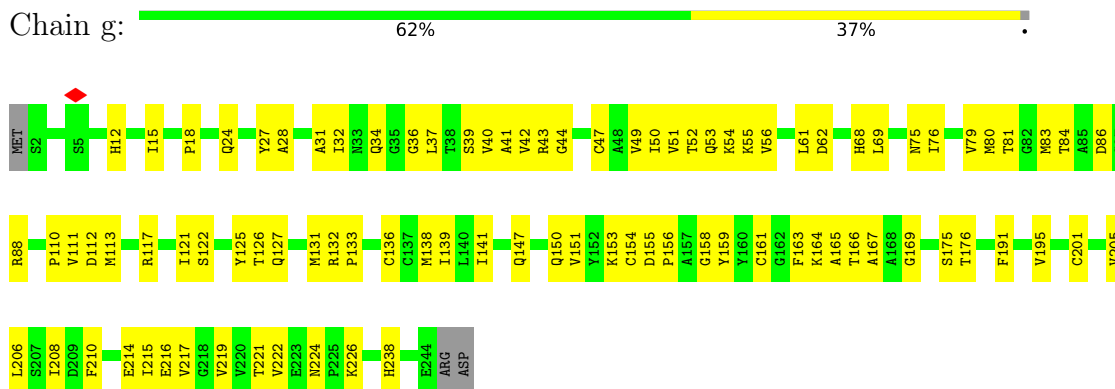
### 3 Residue-property plots

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

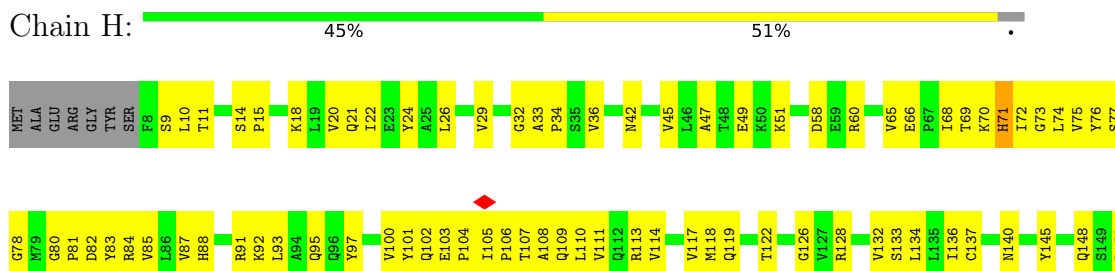
#### • Molecule 1: Proteasome subunit alpha type-6



#### • Molecule 1: Proteasome subunit alpha type-6



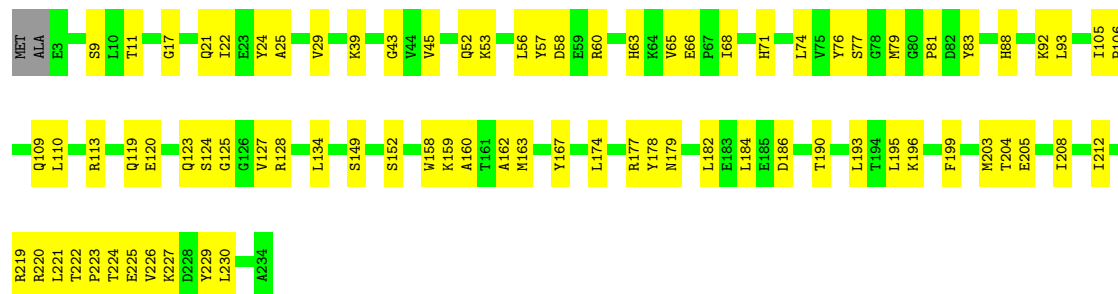
#### • Molecule 2: Proteasome subunit alpha type-2





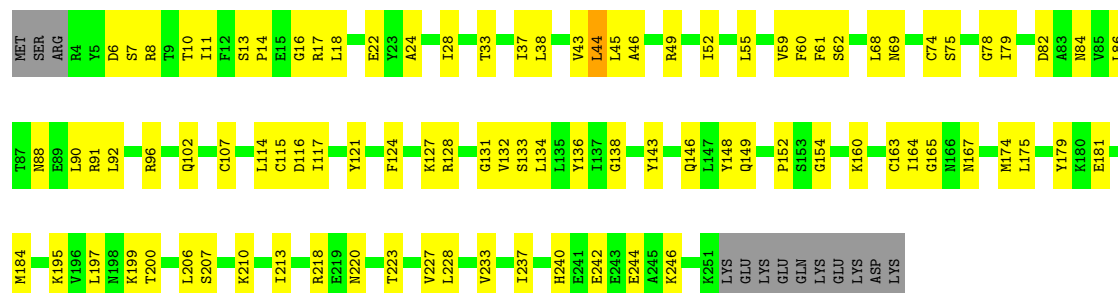
• Molecule 2: Proteasome subunit alpha type-2

Chain h: 65% 34%



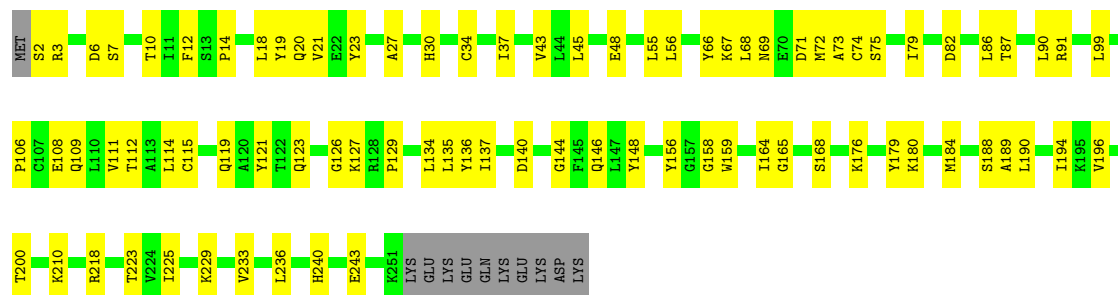
• Molecule 3: Proteasome subunit alpha type-4

Chain I: 60% 35% 5%



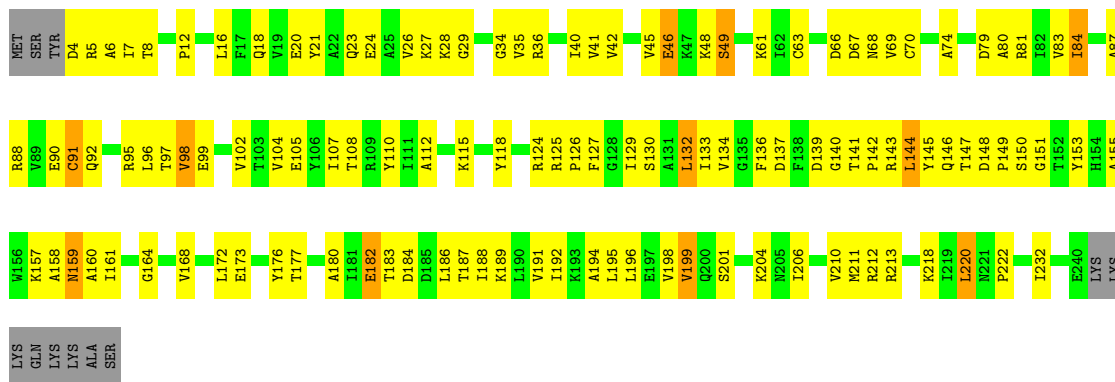
• Molecule 3: Proteasome subunit alpha type-4

Chain i: 64% 32%

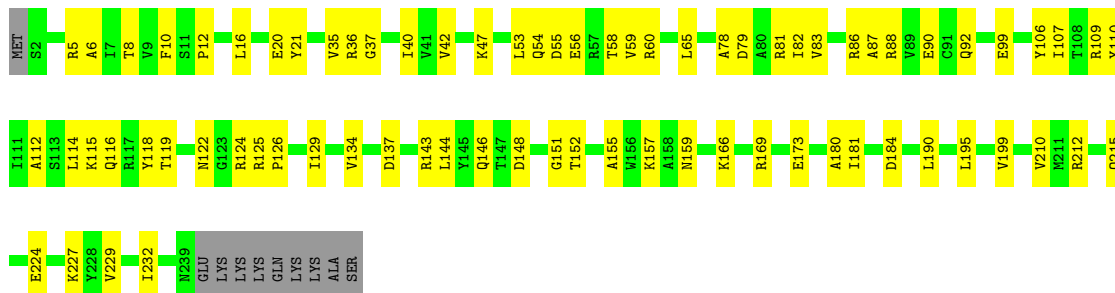


• Molecule 4: Proteasome subunit alpha type-7

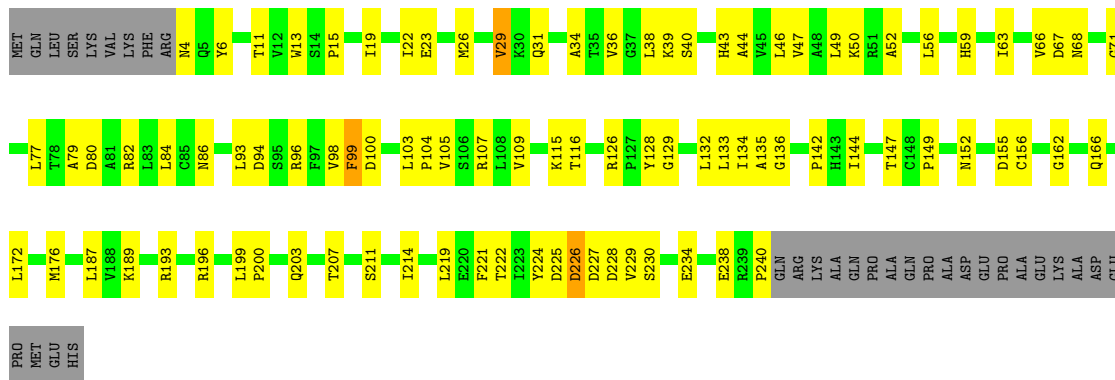
Chain J: 47% 44%



- Molecule 4: Proteasome subunit alpha type-7

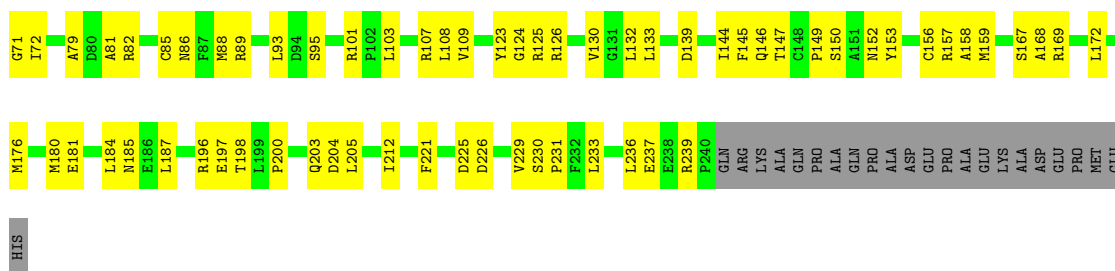


- Molecule 5: Isoform Long of Proteasome subunit alpha type-1

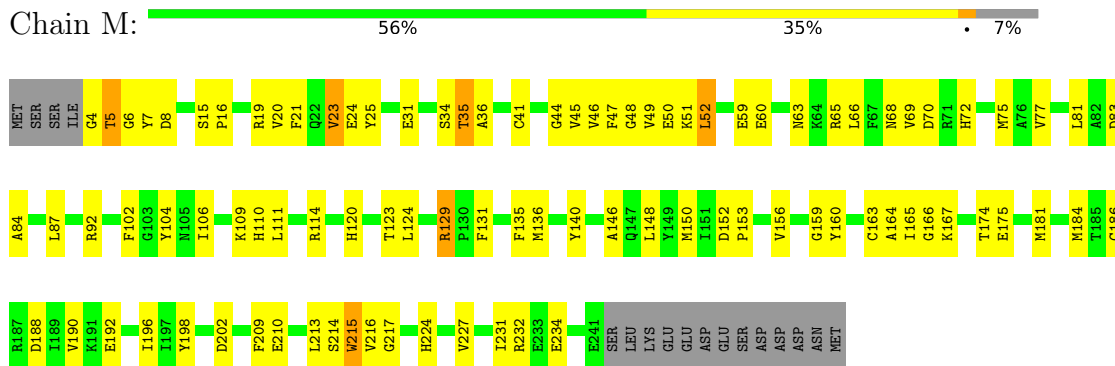


- Molecule 5: Isoform Long of Proteasome subunit alpha type-1





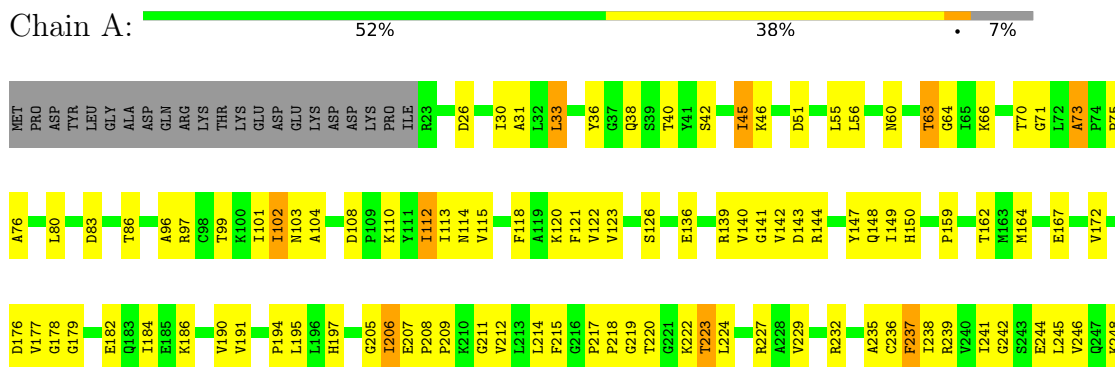
• Molecule 6: Proteasome subunit alpha type-3

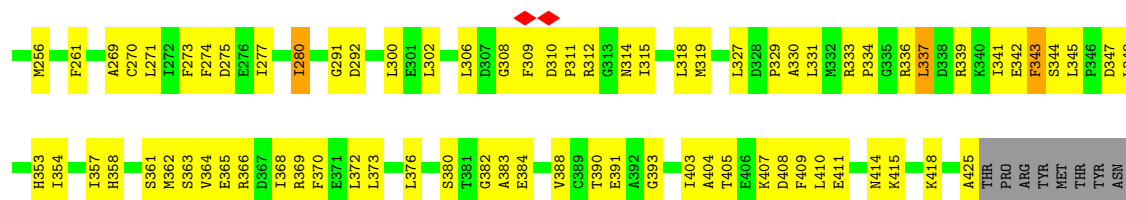


• Molecule 6: Proteasome subunit alpha type-3

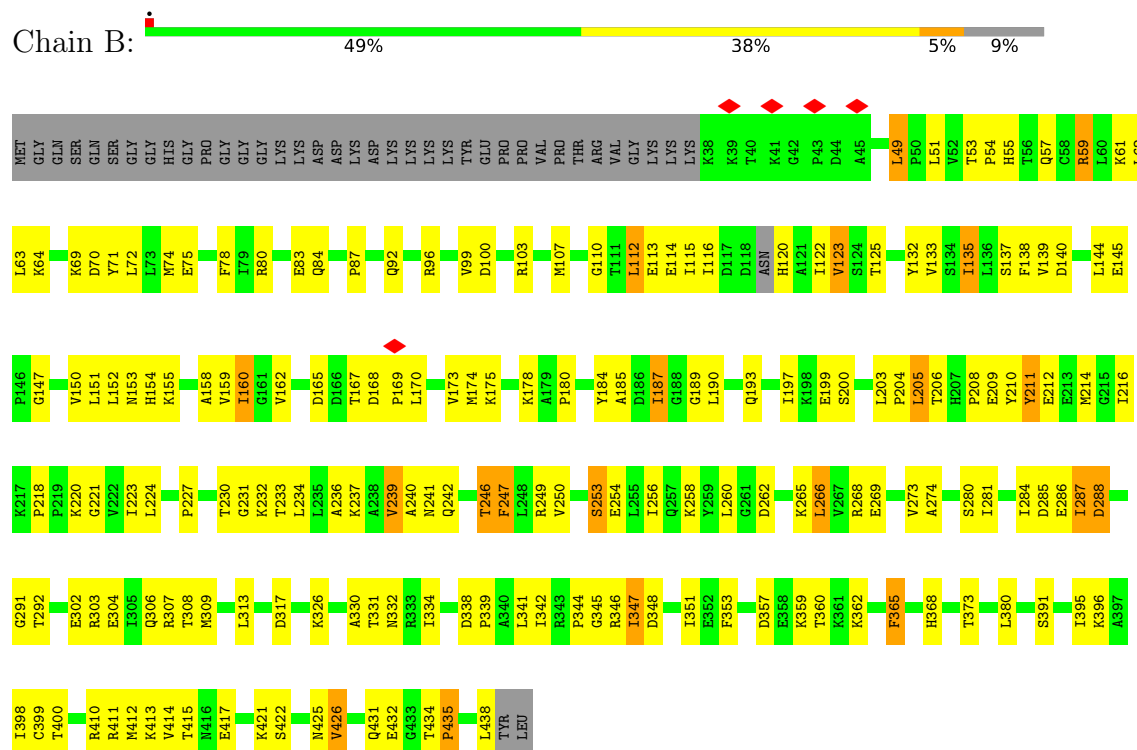


• Molecule 7: 26S protease regulatory subunit 7

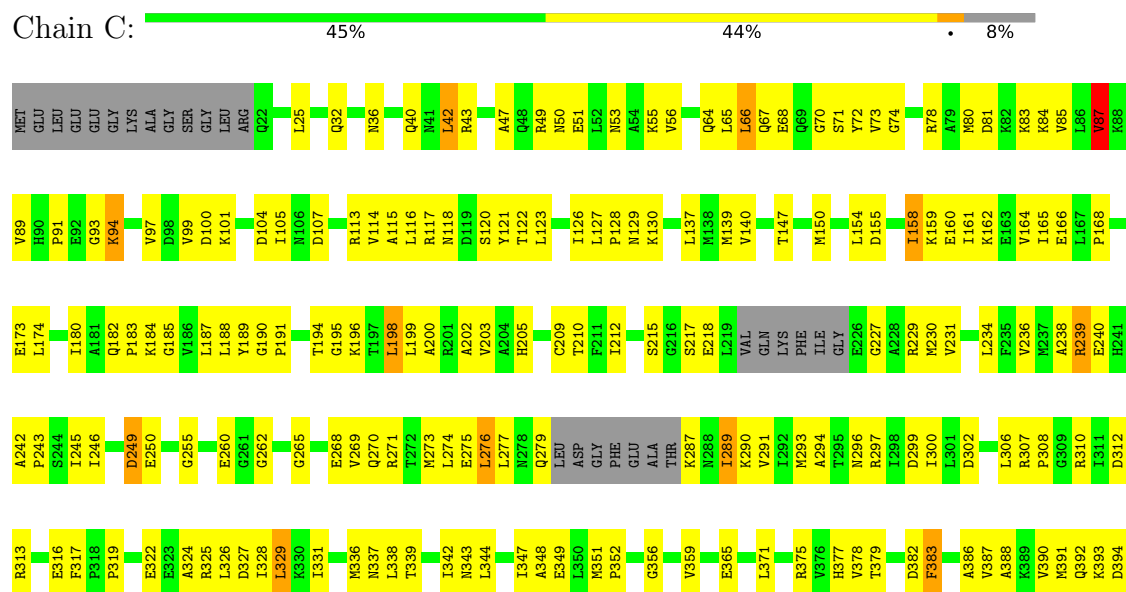




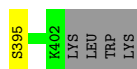
• Molecule 8: 26S protease regulatory subunit 4



• Molecule 9: Isoform 2 of 26S proteasome regulatory subunit 8

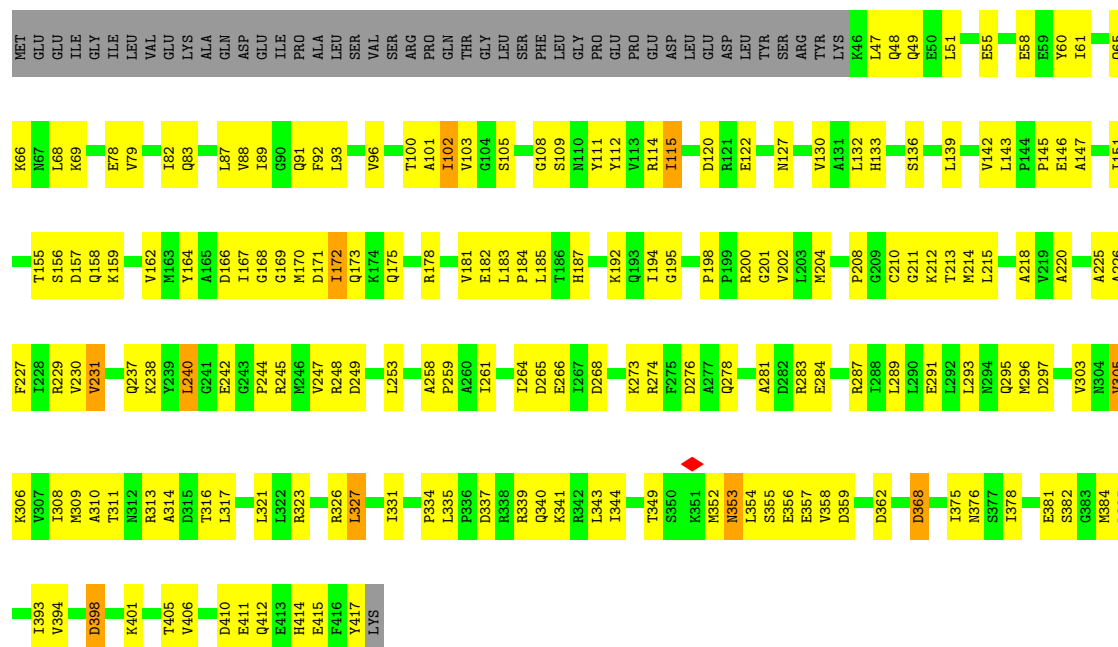






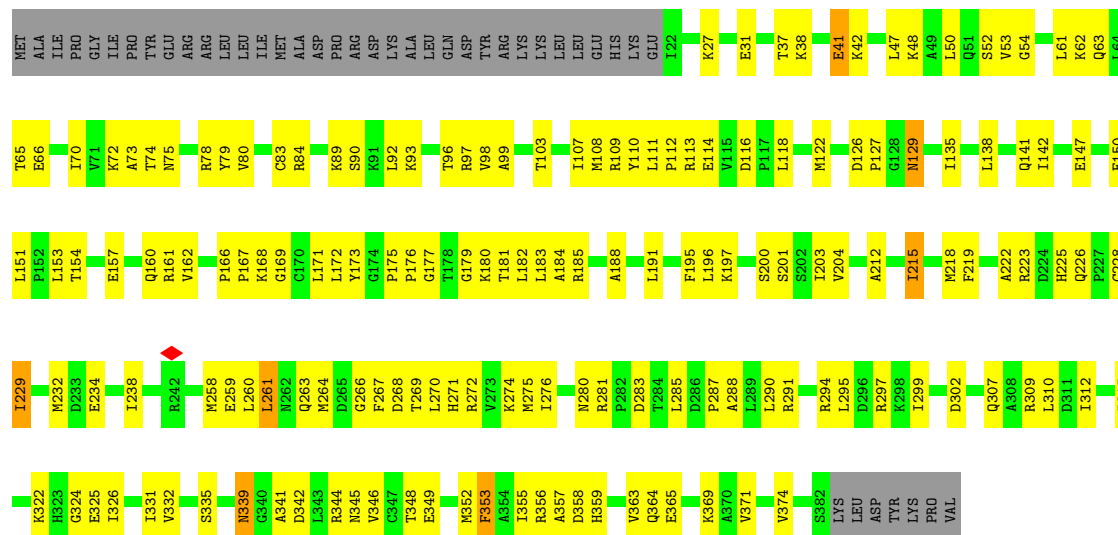
• Molecule 10: 26S protease regulatory subunit 6B

Chain D: 46% 40% 11%



• Molecule 11: 26S proteasome regulatory subunit 10B

Chain E: 49% 39% 10%



• Molecule 12: 26S protease regulatory subunit 6A

Chain F: 40% 38% 19%



M189	M190	L191	L199	L200	L201	L202	V205	M206	L210	I215	E216	L217	A218	T219	V220	Q221	P222	G223	Q224	N225	F226	H227	M228	F229	T230	K231	E232	E233	L234	E235	E236	V237	L238	L241	M153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137	E137	V146	L153	M156	D157	P158	S159	F162	C165	D166	A167	A169	I170	L181	Q182	F183	M184	A83	D84	A85	R83	Q97	F101	M104	E105	T106	T108	V112	S117	L121	Q122	PHE	GLY	GLU	GLU	ASP	ALA	ASP	PRO	GLY	ALA	MET	S134	R135	P136	F137</
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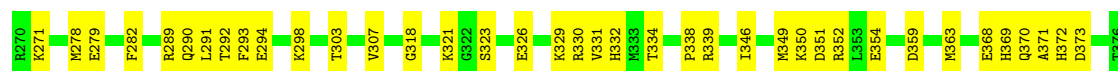
- Molecule 13: Proteasome subunit alpha type-5

[illegible]

- Molecule 14: 26S proteasome non-ATPase regulatory subunit 2

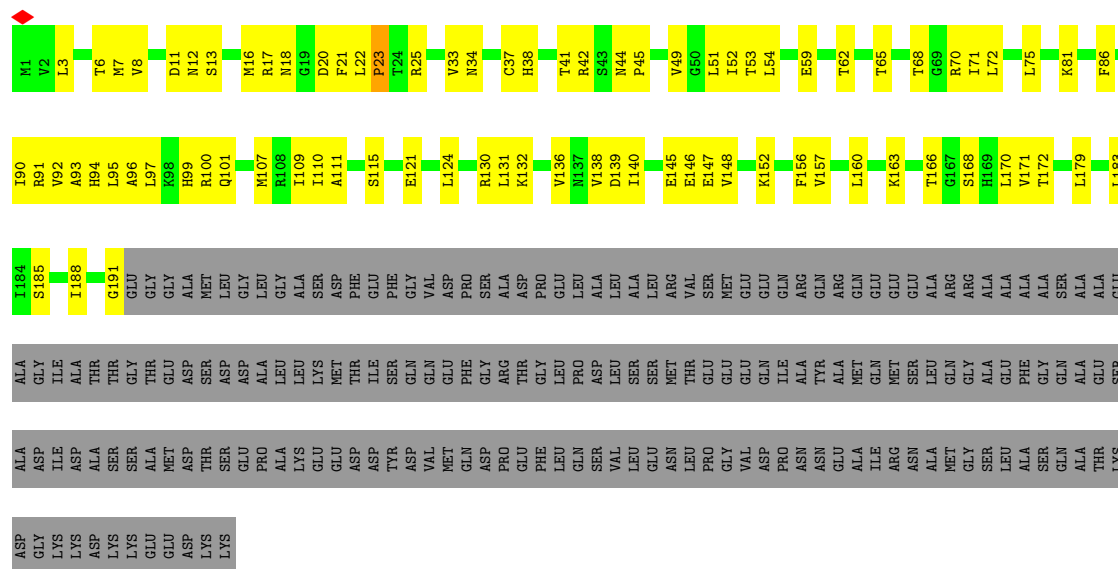


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E149	E150	L151	W154	Q155	H156	E157	Y158	V159	H161	L162	A163	G164
E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177
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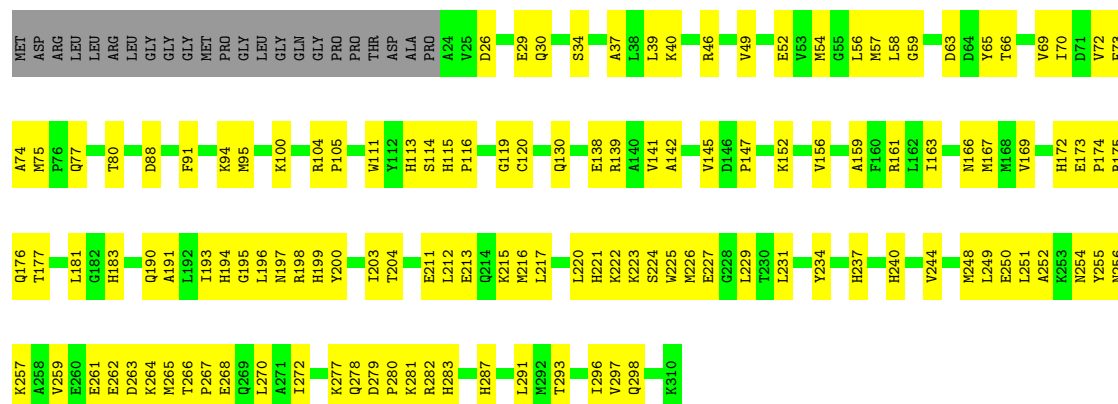
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 29% 21% 49%



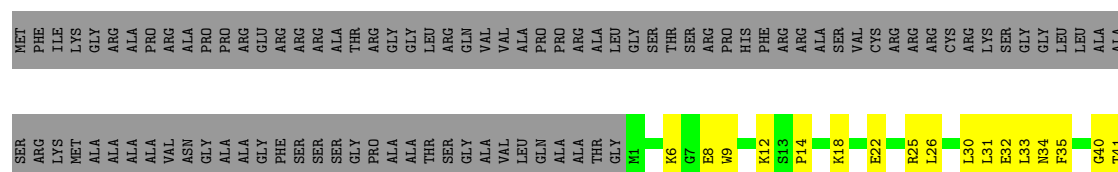
• Molecule 17: 26S proteasome non-ATPase regulatory subunit 14

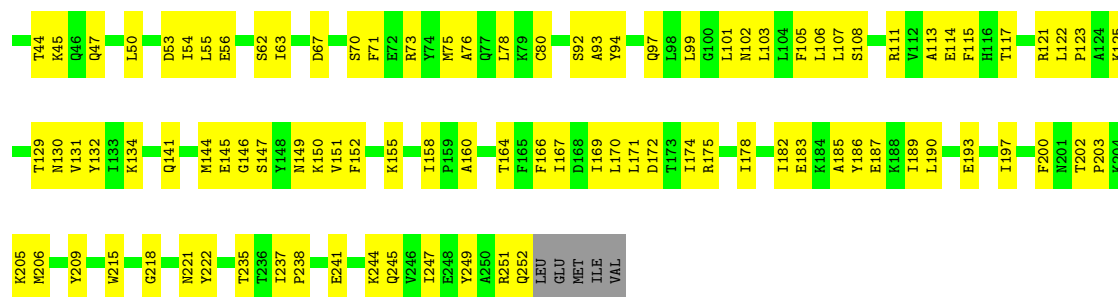
Chain c: 51% 41% 7%



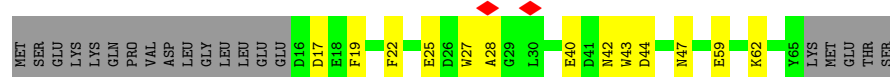
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 40% 32% 28%

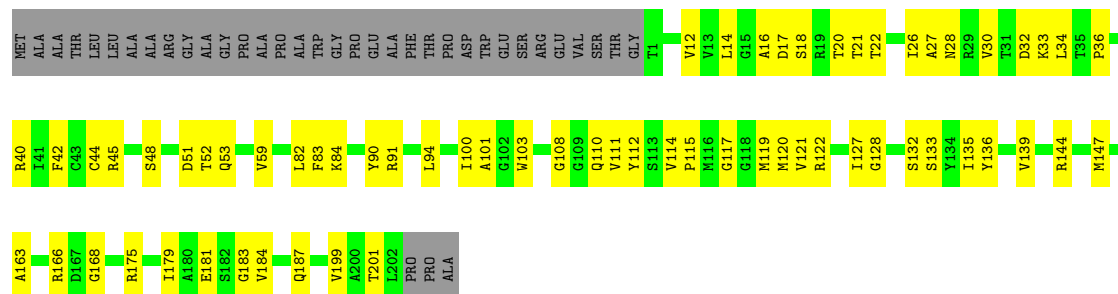




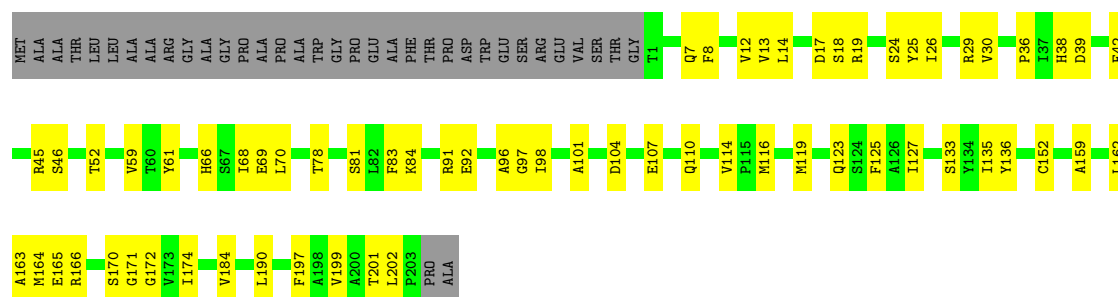
• Molecule 19: 26S proteasome complex subunit SEM1



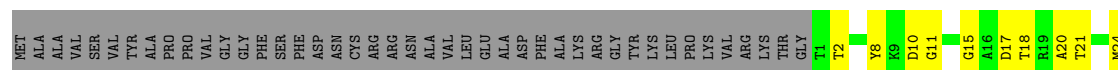
• Molecule 20: Proteasome subunit beta type-6



• Molecule 20: Proteasome subunit beta type-6



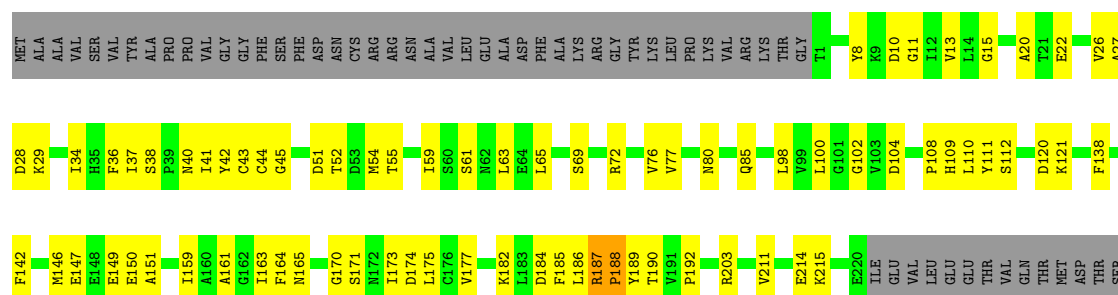
• Molecule 21: Proteasome subunit beta type-7





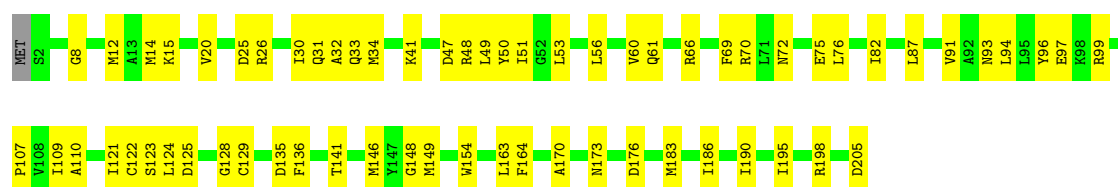
- Molecule 21: Proteasome subunit beta type-7

Chain O: 52% 27% 21%



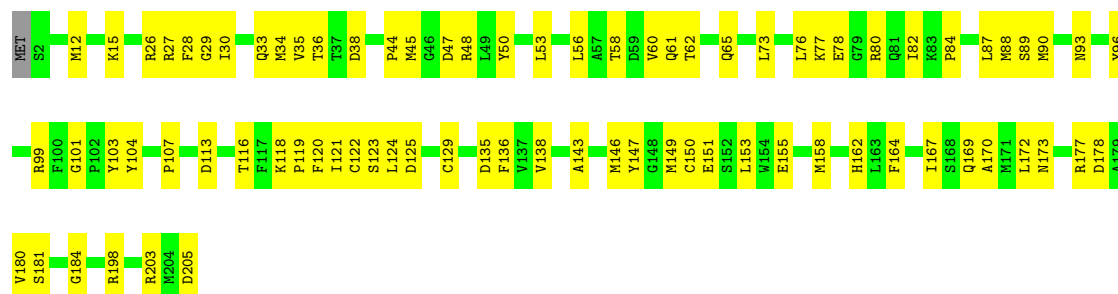
- Molecule 22: Proteasome subunit beta type-3

Chain p: 68% 31%



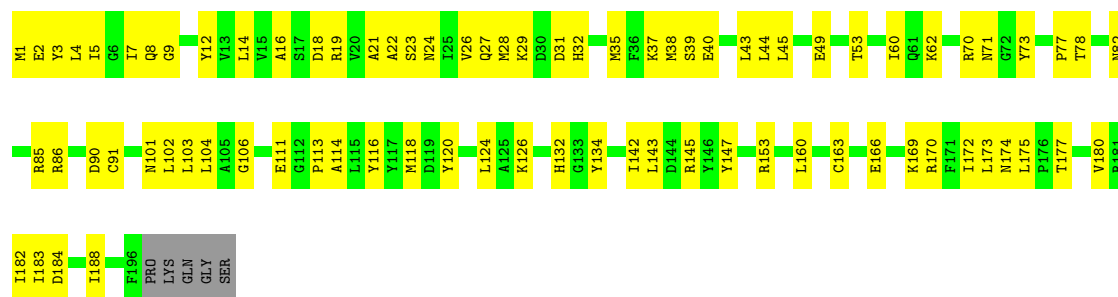
- Molecule 22: Proteasome subunit beta type-3

Chain P: 60% 39%

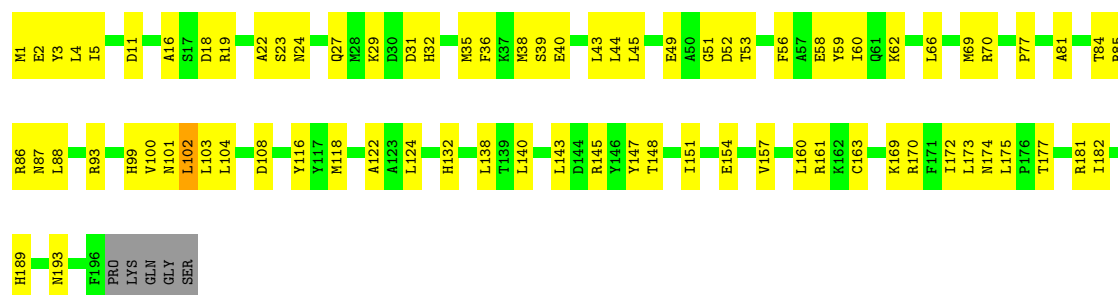


- Molecule 23: Proteasome subunit beta type-2

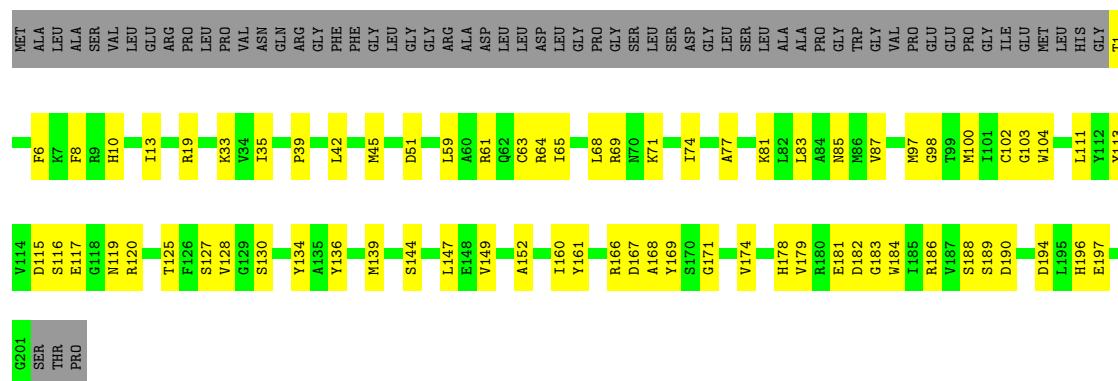
Chain q: 58% 40%



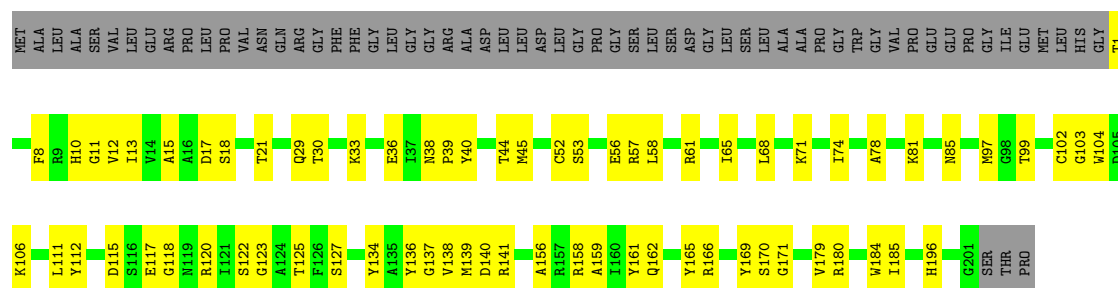
• Molecule 23: Proteasome subunit beta type-2



• Molecule 24: Proteasome subunit beta type-5

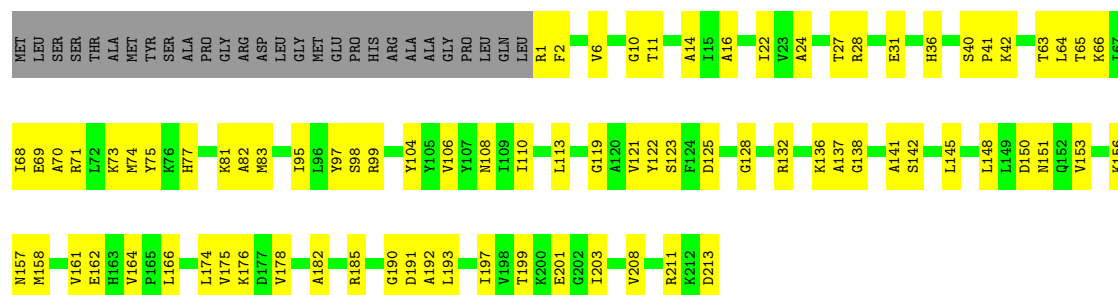


• Molecule 24: Proteasome subunit beta type-5



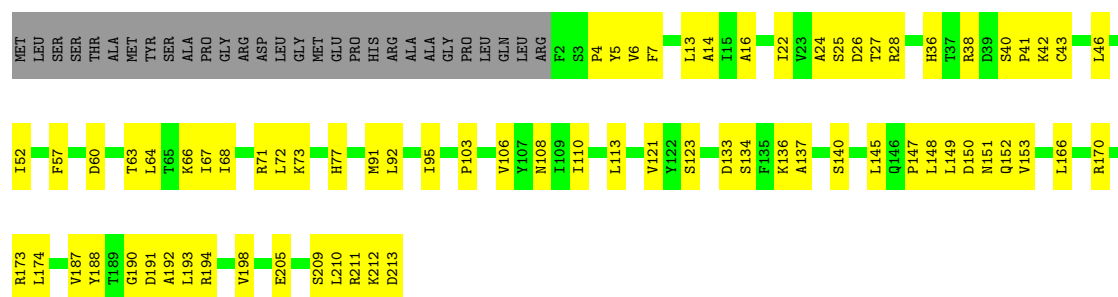
- Molecule 25: Proteasome subunit beta type-1

Chain s: 



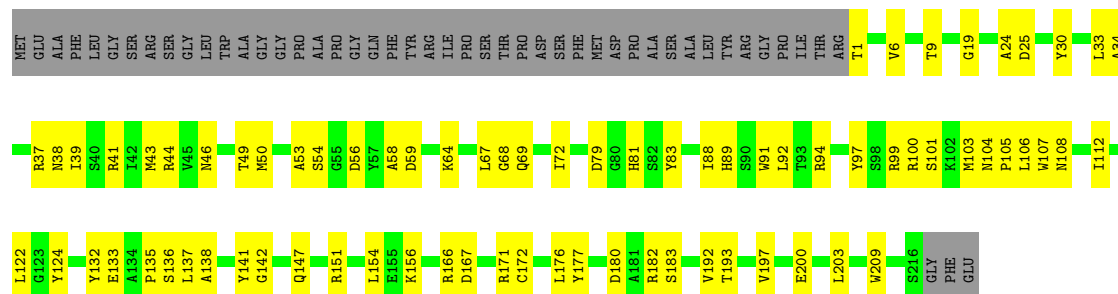
- Molecule 25: Proteasome subunit beta type-1

Chain S: 



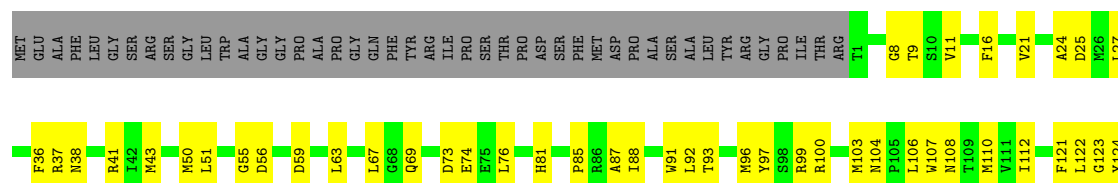
- Molecule 26: Proteasome subunit beta type-4

Chain t: 



- Molecule 26: Proteasome subunit beta type-4

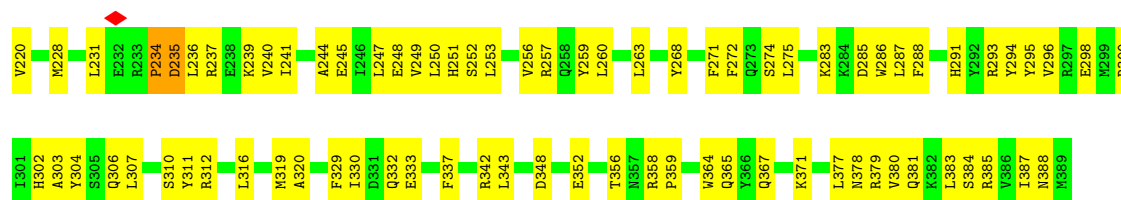
Chain T: 





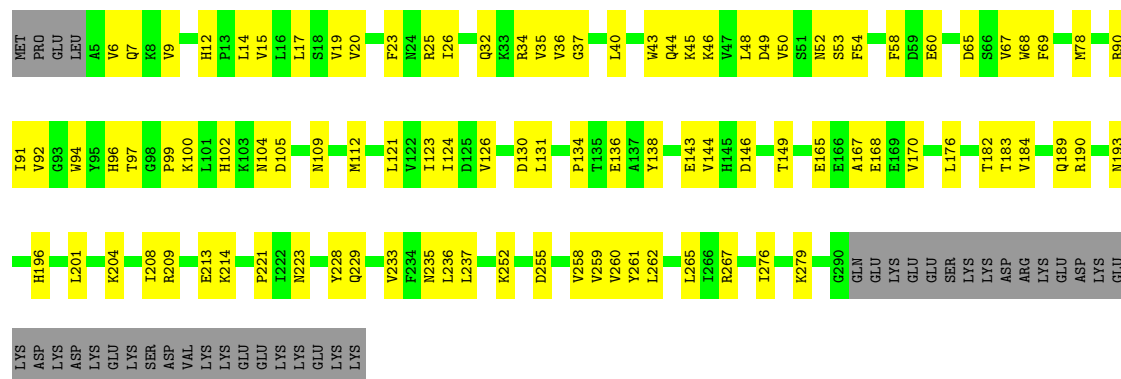






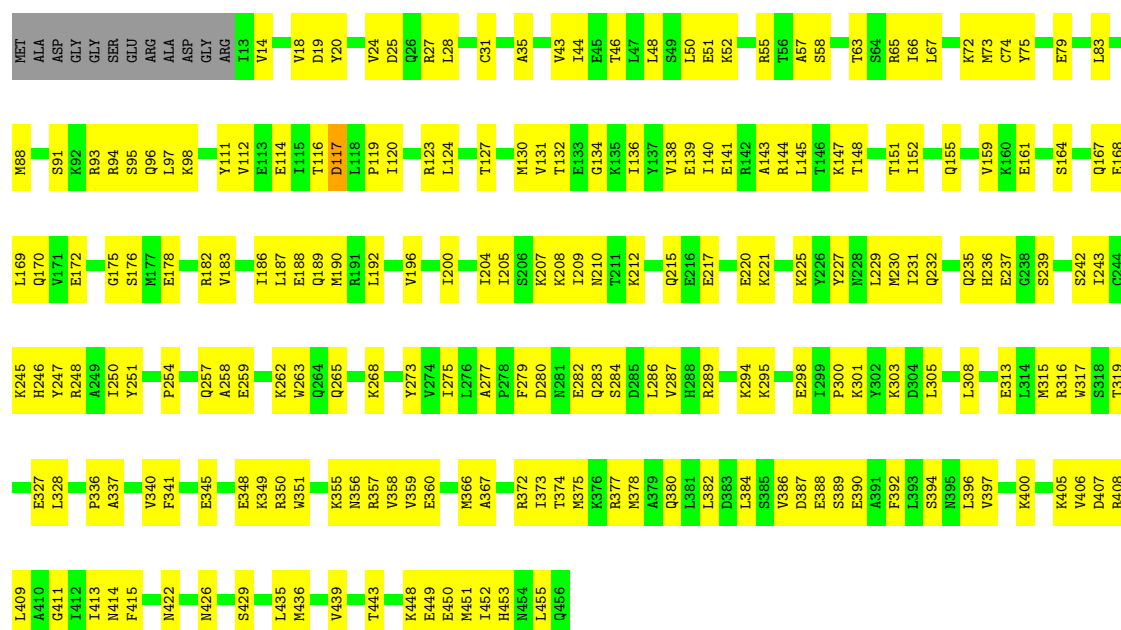
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 58% 30% 12%



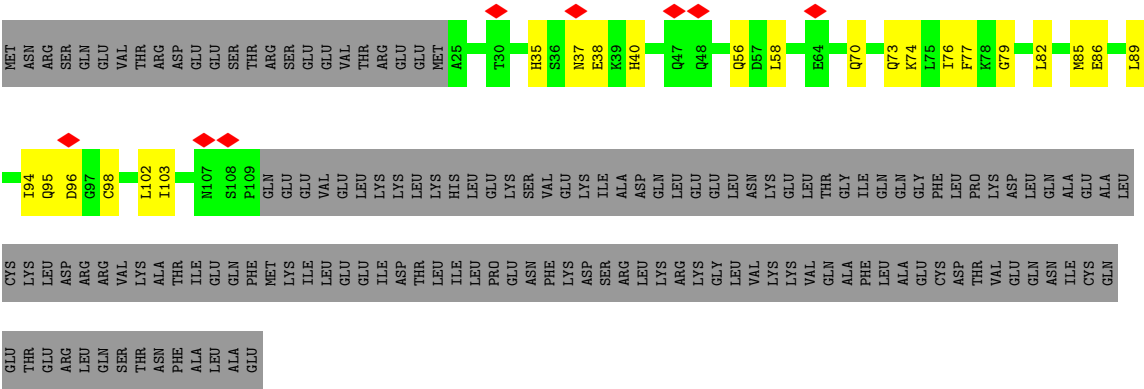
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 52% 45% .



• Molecule 33: BAG family molecular chaperone regulator 1

Chain x: 27% 10% 63%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	37	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.227	Depositor
Minimum map value	-1.015	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	423.9999, 423.9999, 423.9999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.413333, 1.413333, 1.413333	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	G	0.27	0/1873	0.40	0/2533
1	g	0.13	0/1918	0.38	0/2592
2	H	0.32	0/1784	0.48	0/2416
2	h	0.13	0/1852	0.38	0/2507
3	I	0.28	0/2056	0.42	0/2770
3	i	0.14	0/2001	0.36	0/2694
4	J	0.23	0/1894	0.46	0/2555
4	j	0.13	0/1904	0.33	0/2569
5	L	0.25	0/1899	0.41	0/2567
5	l	0.13	0/1899	0.35	0/2567
6	M	0.26	0/1897	0.41	0/2555
6	m	0.16	0/1916	0.42	0/2580
7	A	0.18	0/3165	0.45	0/4273
8	B	0.21	0/3100	0.50	0/4189
9	C	0.19	0/2865	0.46	0/3851
10	D	0.20	0/2945	0.46	0/3979
11	E	0.17	0/2810	0.41	0/3789
12	F	0.17	0/2741	0.40	0/3700
13	K	0.24	0/1718	0.42	0/2319
13	k	0.12	0/1817	0.30	0/2455
14	f	0.16	0/6385	0.39	0/8637
15	a	0.14	0/3023	0.40	0/4093
16	b	0.14	0/1478	0.44	0/2001
17	c	0.16	0/2260	0.43	0/3052
18	d	0.15	0/2109	0.42	0/2851
19	e	0.13	0/415	0.37	0/563
20	N	0.18	0/1548	0.33	0/2097
20	n	0.15	0/1540	0.37	0/2085
21	O	0.20	0/1686	0.38	0/2282
21	o	0.16	0/1686	0.37	0/2282
22	P	0.21	0/1620	0.37	0/2184
22	p	0.16	0/1620	0.34	0/2184

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
23	Q	0.27	0/1603	0.46	1/2168 (0.0%)
23	q	0.16	0/1603	0.37	0/2168
24	R	0.17	0/1590	0.32	0/2147
24	r	0.16	0/1590	0.30	0/2147
25	S	0.21	0/1673	0.42	0/2254
25	s	0.17	0/1684	0.36	0/2268
26	T	0.16	0/1720	0.30	0/2328
26	t	0.18	0/1720	0.35	0/2328
27	U	0.15	0/6750	0.41	0/9116
28	V	0.15	0/3667	0.37	0/4951
29	X	0.14	0/3045	0.34	0/4104
30	Y	0.16	0/3063	0.42	0/4123
31	Z	0.15	0/2286	0.42	0/3099
32	W	0.16	0/3610	0.43	0/4853
33	x	0.11	0/643	0.31	0/868
All	All	0.18	0/105671	0.40	1/142693 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	102	LEU	N-CA-C	5.83	118.55	109.52

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	G	1841	0	1848	107	0
1	g	1885	0	1891	77	0
2	H	1749	0	1750	143	0
2	h	1813	0	1806	66	0
3	I	2025	0	2036	99	0
3	i	1971	0	1992	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	1869	0	1891	120	0
4	j	1878	0	1899	66	0
5	L	1864	0	1852	97	0
5	l	1864	0	1852	84	0
6	M	1862	0	1840	92	0
6	m	1881	0	1868	94	0
7	A	3119	0	3162	185	0
8	B	3060	0	3090	189	0
9	C	2839	0	2942	189	0
10	D	2904	0	2925	178	0
11	E	2775	0	2814	168	0
12	F	2709	0	2760	168	0
13	K	1694	0	1691	80	0
13	k	1789	0	1773	68	0
14	f	6292	0	6314	297	0
15	a	2969	0	2984	109	0
16	b	1458	0	1505	71	0
17	c	2224	0	2240	117	0
18	d	2063	0	2078	101	0
19	e	407	0	312	15	0
20	N	1521	0	1494	59	0
20	n	1514	0	1487	64	0
21	O	1659	0	1681	63	0
21	o	1659	0	1681	62	0
22	P	1591	0	1609	78	0
22	p	1591	0	1609	51	0
23	Q	1571	0	1573	81	0
23	q	1571	0	1573	71	0
24	R	1559	0	1523	55	0
24	r	1559	0	1523	58	0
25	S	1643	0	1640	61	0
25	s	1654	0	1656	66	0
26	T	1687	0	1666	54	0
26	t	1687	0	1666	67	0
27	U	6648	0	6713	289	0
28	V	3600	0	3668	182	0
29	X	3002	0	3106	117	0
30	Y	3021	0	3022	130	0
31	Z	2248	0	2277	97	0
32	W	3570	0	3696	179	0
33	x	635	0	652	16	0
34	A	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	27	0	12	5	0
35	C	27	0	12	6	0
35	D	27	0	12	4	0
35	E	27	0	12	3	0
35	F	27	0	12	5	0
All	All	104160	0	104702	4424	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 21.

The worst 5 of 4424 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:M:36:ALA:HB1	6:M:49:VAL:HG22	1.32	1.11
5:L:49:LEU:HD21	5:L:199:LEU:HD11	1.31	1.09
2:H:68:ILE:HD11	2:H:74:LEU:HD22	1.35	1.07
9:C:140:VAL:HG11	9:C:234:LEU:CD2	1.84	1.07
10:D:83:GLN:HG2	17:c:152:LYS:HG3	1.36	1.07

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	G	235/246 (96%)	212 (90%)	20 (8%)	3 (1%)	9	39
1	g	241/246 (98%)	229 (95%)	12 (5%)	0	100	100
2	H	224/234 (96%)	184 (82%)	40 (18%)	0	100	100
2	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
3	I	254/261 (97%)	231 (91%)	23 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	i	248/261 (95%)	237 (96%)	11 (4%)	0	100	100
4	J	235/248 (95%)	203 (86%)	27 (12%)	5 (2%)	5	31
4	j	236/248 (95%)	226 (96%)	10 (4%)	0	100	100
5	L	235/269 (87%)	218 (93%)	15 (6%)	2 (1%)	14	46
5	l	160/269 (60%)	153 (96%)	7 (4%)	0	100	100
6	M	236/255 (92%)	218 (92%)	16 (7%)	2 (1%)	16	49
6	m	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
7	A	401/433 (93%)	350 (87%)	44 (11%)	7 (2%)	7	35
8	B	398/440 (90%)	341 (86%)	51 (13%)	6 (2%)	8	37
9	C	362/398 (91%)	311 (86%)	47 (13%)	4 (1%)	11	43
10	D	370/418 (88%)	306 (83%)	57 (15%)	7 (2%)	6	33
11	E	359/403 (89%)	315 (88%)	43 (12%)	1 (0%)	36	65
12	F	348/439 (79%)	311 (89%)	31 (9%)	6 (2%)	7	35
13	K	178/241 (74%)	169 (95%)	7 (4%)	2 (1%)	11	43
13	k	232/241 (96%)	221 (95%)	10 (4%)	1 (0%)	30	61
14	f	757/908 (83%)	716 (95%)	41 (5%)	0	100	100
15	a	371/376 (99%)	343 (92%)	28 (8%)	0	100	100
16	b	189/377 (50%)	176 (93%)	12 (6%)	1 (0%)	24	57
17	c	285/310 (92%)	248 (87%)	37 (13%)	0	100	100
18	d	50/350 (14%)	39 (78%)	11 (22%)	0	100	100
20	N	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
20	n	200/239 (84%)	193 (96%)	7 (4%)	0	100	100
21	O	218/277 (79%)	211 (97%)	5 (2%)	2 (1%)	14	46
21	o	218/277 (79%)	208 (95%)	10 (5%)	0	100	100
22	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
22	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
23	Q	194/201 (96%)	188 (97%)	6 (3%)	0	100	100
23	q	168/201 (84%)	164 (98%)	4 (2%)	0	100	100
24	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
24	r	199/263 (76%)	197 (99%)	2 (1%)	0	100	100
25	S	210/241 (87%)	206 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	s	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	24	57
26	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
26	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
27	U	853/953 (90%)	794 (93%)	59 (7%)	0	100	100
28	V	442/534 (83%)	421 (95%)	21 (5%)	0	100	100
29	X	378/422 (90%)	362 (96%)	15 (4%)	1 (0%)	36	65
30	Y	378/389 (97%)	339 (90%)	36 (10%)	3 (1%)	16	49
31	Z	284/324 (88%)	258 (91%)	25 (9%)	1 (0%)	30	61
32	W	442/456 (97%)	412 (93%)	28 (6%)	2 (0%)	24	57
33	x	83/230 (36%)	81 (98%)	2 (2%)	0	100	100
All	All	12782/15048 (85%)	11835 (93%)	890 (7%)	57 (0%)	31	61

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	164	LYS
4	J	49	SER
4	J	199	VAL
5	L	226	ASP
6	M	104	TYR

### 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	G	201/210 (96%)	200 (100%)	1 (0%)	81	80
1	g	206/210 (98%)	206 (100%)	0	100	100
2	H	184/191 (96%)	183 (100%)	1 (0%)	81	80
2	h	190/191 (100%)	189 (100%)	1 (0%)	81	80
3	I	215/221 (97%)	211 (98%)	4 (2%)	50	67
3	i	210/221 (95%)	210 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	201/211 (95%)	194 (96%)	7 (4%)	32	57
4	j	202/211 (96%)	202 (100%)	0	100	100
5	L	203/230 (88%)	199 (98%)	4 (2%)	48	66
5	l	203/230 (88%)	203 (100%)	0	100	100
6	M	195/212 (92%)	188 (96%)	7 (4%)	31	56
6	m	198/212 (93%)	198 (100%)	0	100	100
7	A	338/372 (91%)	325 (96%)	13 (4%)	29	55
8	B	333/385 (86%)	311 (93%)	22 (7%)	15	43
9	C	313/346 (90%)	296 (95%)	17 (5%)	20	47
10	D	314/366 (86%)	302 (96%)	12 (4%)	29	55
11	E	299/353 (85%)	290 (97%)	9 (3%)	36	59
12	F	292/379 (77%)	276 (94%)	16 (6%)	19	47
13	K	187/203 (92%)	177 (95%)	10 (5%)	20	48
13	k	196/203 (97%)	196 (100%)	0	100	100
14	f	682/763 (89%)	680 (100%)	2 (0%)	86	83
15	a	329/336 (98%)	329 (100%)	0	100	100
16	b	167/312 (54%)	167 (100%)	0	100	100
17	c	247/268 (92%)	247 (100%)	0	100	100
18	d	224/294 (76%)	224 (100%)	0	100	100
19	e	42/63 (67%)	42 (100%)	0	100	100
20	N	158/181 (87%)	158 (100%)	0	100	100
20	n	157/181 (87%)	157 (100%)	0	100	100
21	O	181/228 (79%)	181 (100%)	0	100	100
21	o	181/228 (79%)	181 (100%)	0	100	100
22	P	173/174 (99%)	173 (100%)	0	100	100
22	p	173/174 (99%)	173 (100%)	0	100	100
23	Q	167/171 (98%)	167 (100%)	0	100	100
23	q	167/171 (98%)	167 (100%)	0	100	100
24	R	156/202 (77%)	156 (100%)	0	100	100
24	r	156/202 (77%)	156 (100%)	0	100	100
25	S	177/199 (89%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	s	178/199 (89%)	178 (100%)	0	100	100
26	T	179/215 (83%)	179 (100%)	0	100	100
26	t	179/215 (83%)	179 (100%)	0	100	100
27	U	727/816 (89%)	726 (100%)	1 (0%)	88	87
28	V	388/460 (84%)	388 (100%)	0	100	100
29	X	326/362 (90%)	326 (100%)	0	100	100
30	Y	320/344 (93%)	320 (100%)	0	100	100
31	Z	252/295 (85%)	252 (100%)	0	100	100
32	W	402/416 (97%)	402 (100%)	0	100	100
33	x	73/207 (35%)	73 (100%)	0	100	100
All	All	11241/12833 (88%)	11114 (99%)	127 (1%)	63	74

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B	365	PHE
12	F	384	LEU
9	C	289	ILE
12	F	369	HIS
13	K	156	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
21	O	85	GLN
28	V	365	GLN
22	P	93	ASN
27	U	373	ASN
29	X	405	GLN

### 5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
35	ADP	F	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.86	9 (20%)
35	ADP	B	501	-	28,29,29	1.39	5 (17%)	43,45,45	1.80	11 (25%)
35	ADP	C	501	-	28,29,29	1.45	5 (17%)	43,45,45	1.83	9 (20%)
35	ADP	D	501	-	28,29,29	1.36	4 (14%)	43,45,45	1.92	9 (20%)
34	ATP	A	501	-	32,33,33	0.44	0	48,52,52	0.33	0
35	ADP	E	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.84	11 (25%)

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
35	ADP	F	501	-	-	3/16/32/32	0/3/3/3
35	ADP	B	501	-	-	2/16/32/32	0/3/3/3
35	ADP	C	501	-	-	6/16/32/32	0/3/3/3
35	ADP	D	501	-	-	8/16/32/32	0/3/3/3
34	ATP	A	501	-	-	5/22/38/38	0/3/3/3
35	ADP	E	501	-	-	4/16/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	501	ADP	C5-C4	4.59	1.47	1.39
35	F	501	ADP	C5-C4	4.51	1.47	1.39
35	E	501	ADP	C5-C4	4.46	1.47	1.39
35	D	501	ADP	C5-C4	4.40	1.46	1.39
35	B	501	ADP	C5-C4	4.39	1.46	1.39

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	501	ADP	C5-C4-N3	-6.11	118.31	126.72
35	C	501	ADP	C5-C4-N3	-5.97	118.49	126.72
35	F	501	ADP	C5-C4-N3	-5.88	118.62	126.72
35	E	501	ADP	C5-C4-N3	-5.58	119.04	126.72
35	B	501	ADP	C5-C4-N3	-5.25	119.49	126.72

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ADP	C5'-O5'-PA-O3A
35	C	501	ADP	C5'-O5'-PA-O2A
35	D	501	ADP	C5'-O5'-PA-O1A
35	D	501	ADP	C5'-O5'-PA-O2A
35	D	501	ADP	C5'-O5'-PA-O3A

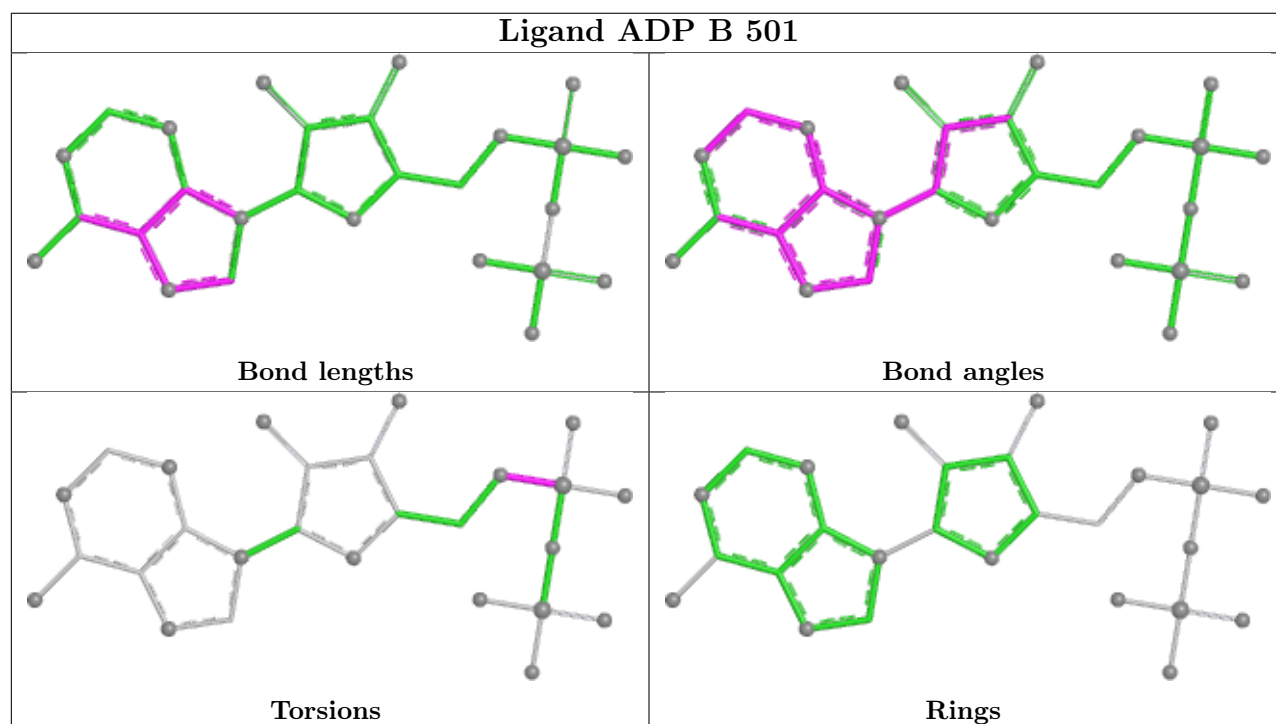
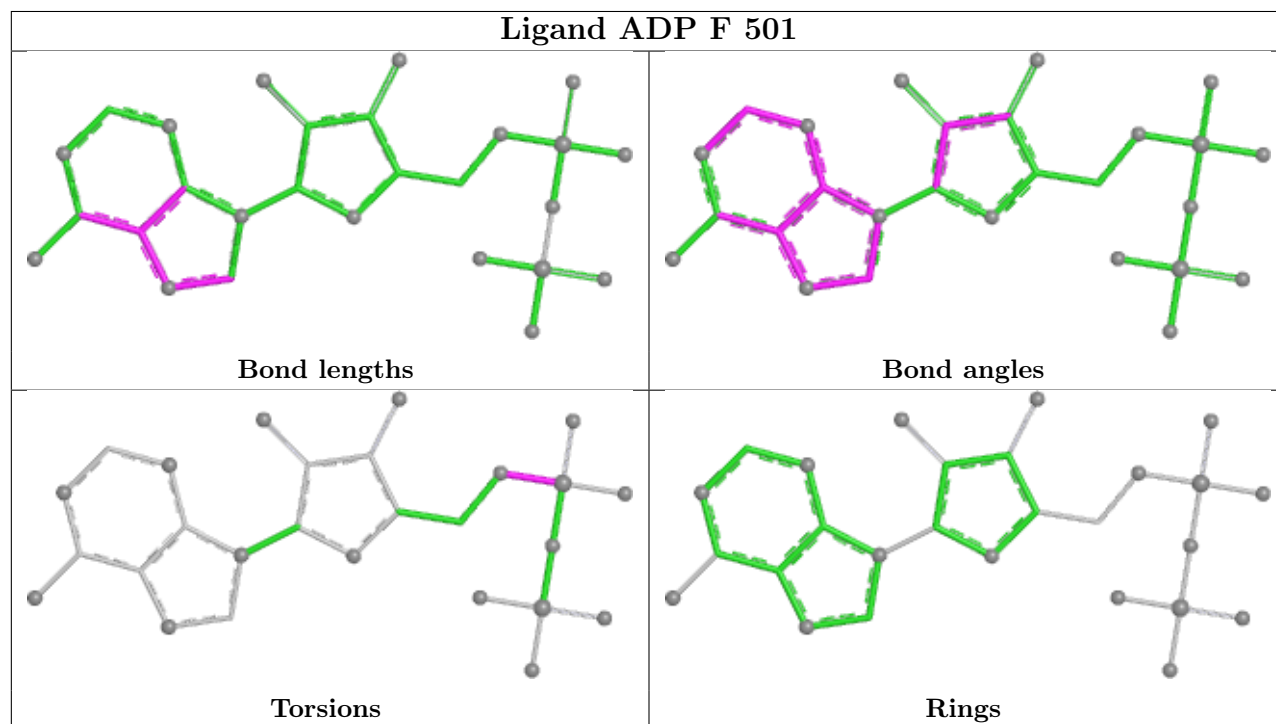
There are no ring outliers.

6 monomers are involved in 28 short contacts:

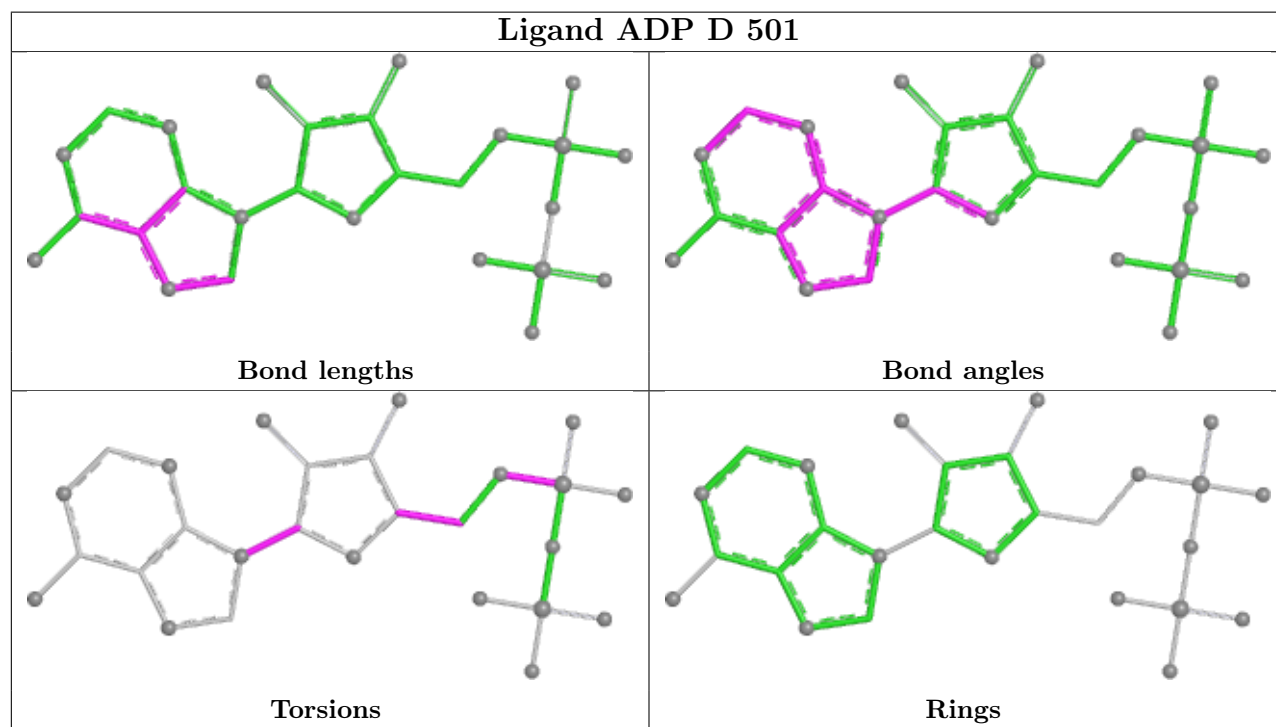
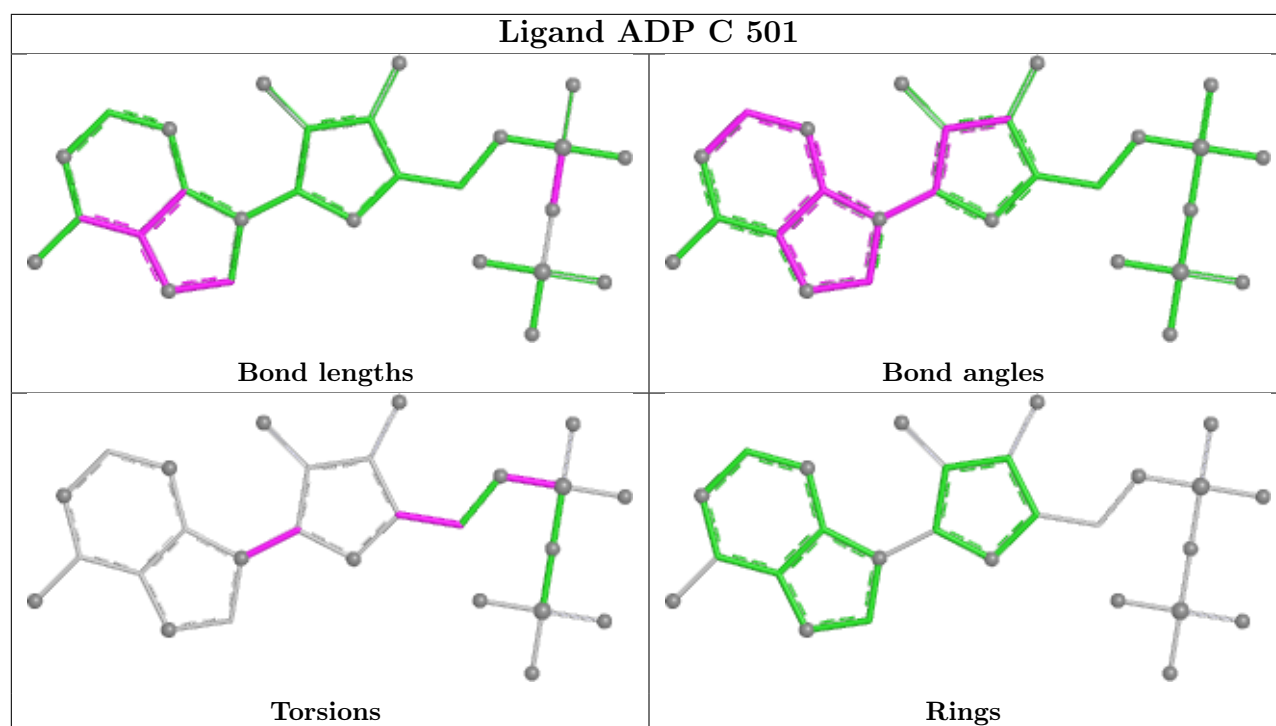
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	F	501	ADP	5	0
35	B	501	ADP	5	0
35	C	501	ADP	6	0
35	D	501	ADP	4	0
34	A	501	ATP	5	0
35	E	501	ADP	3	0

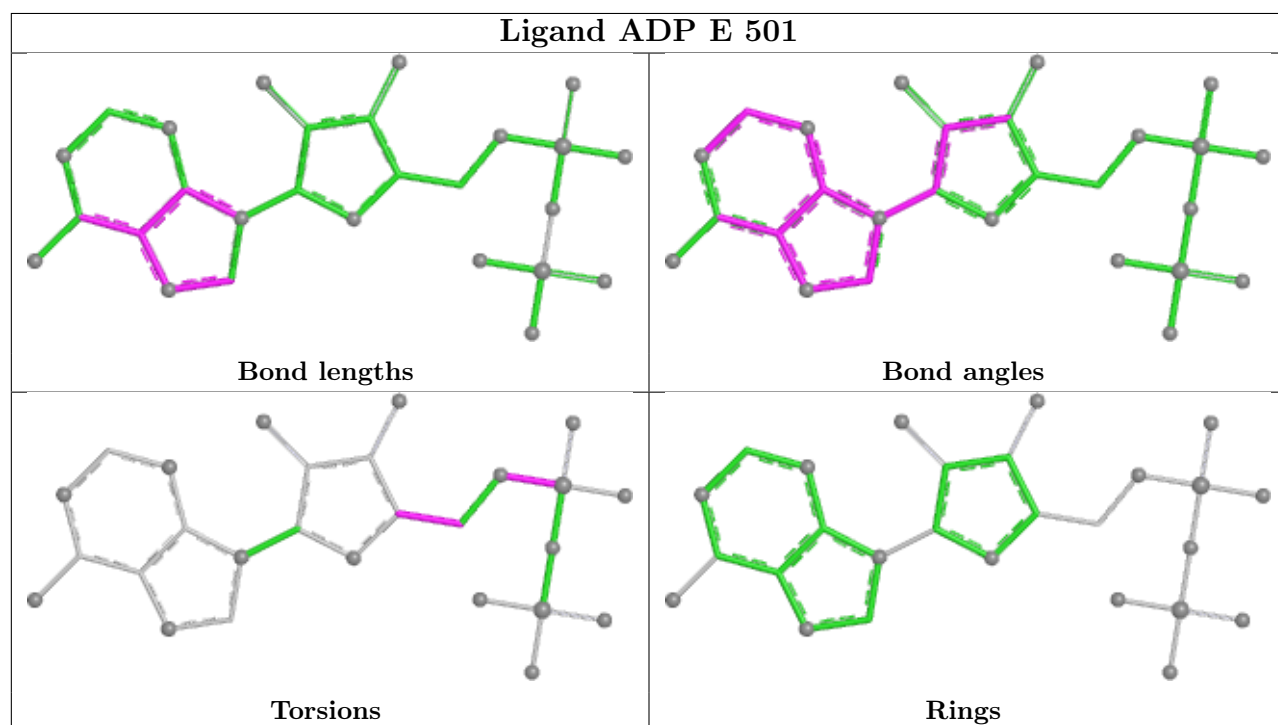
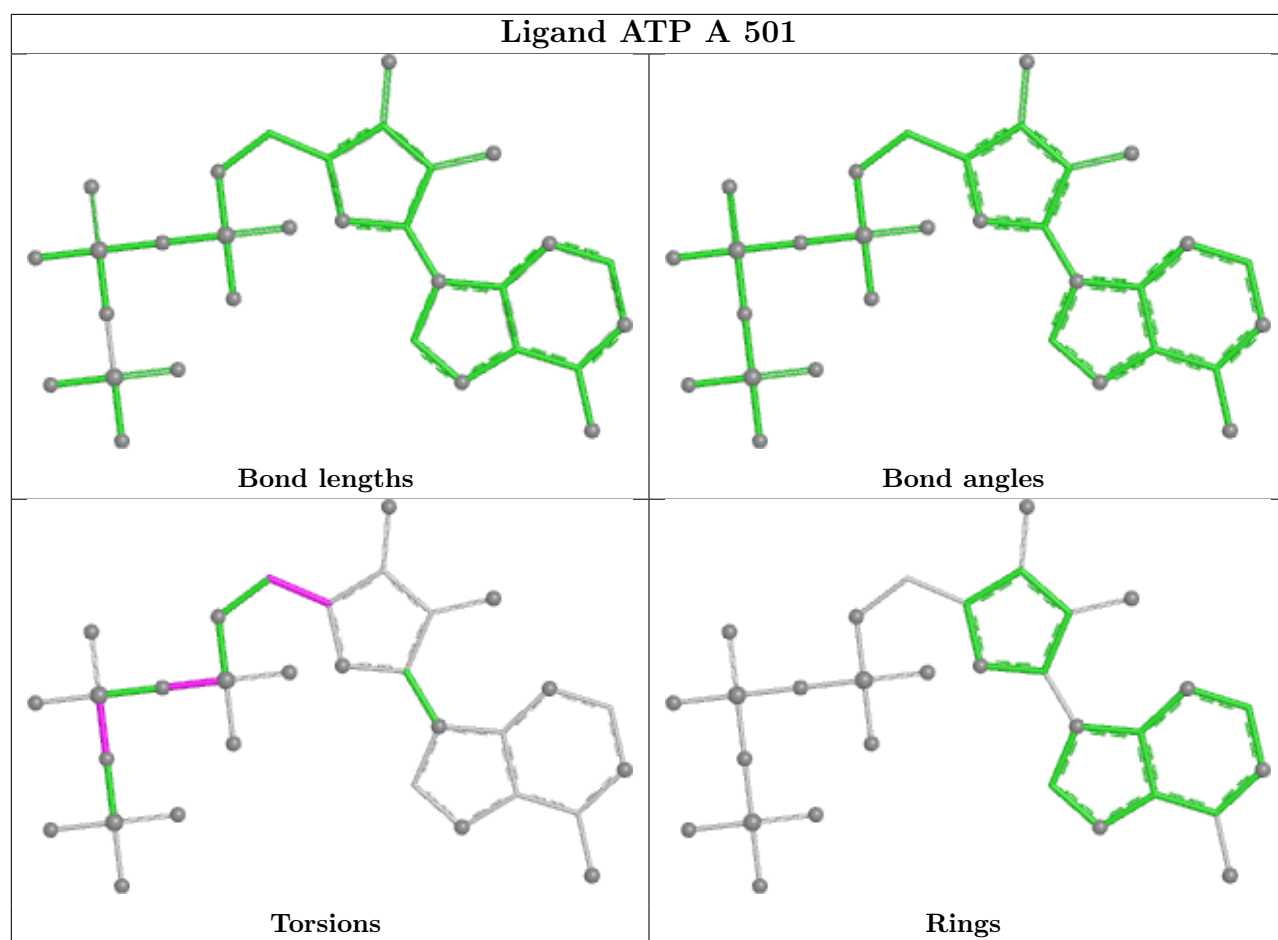
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

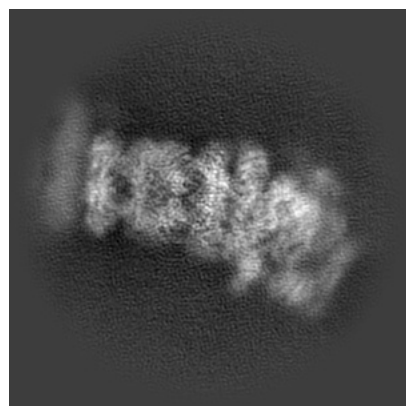
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52097. These allow visual inspection of the internal detail of the map and identification of artifacts.

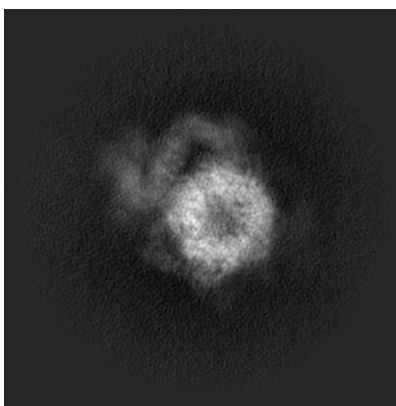
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

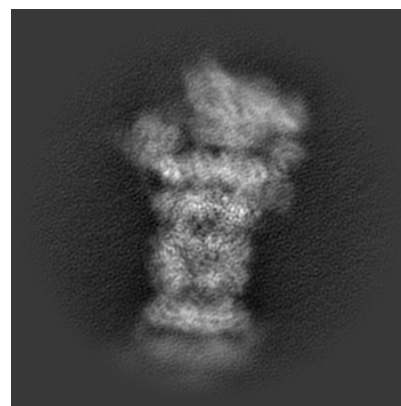
#### 6.1.1 Primary map



X

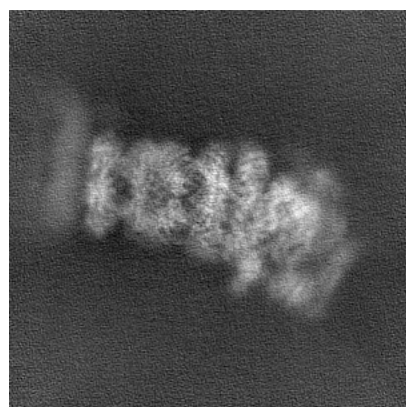


Y

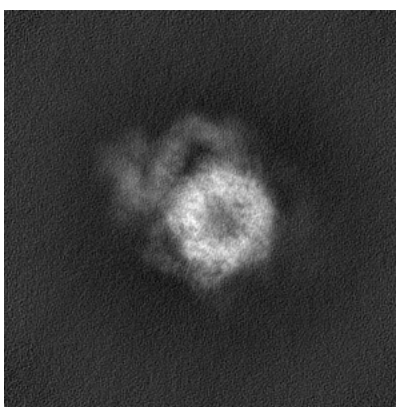


Z

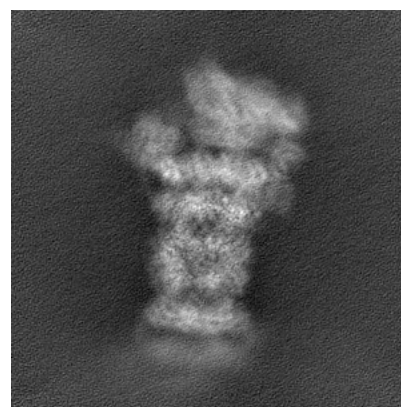
#### 6.1.2 Raw map



X



Y

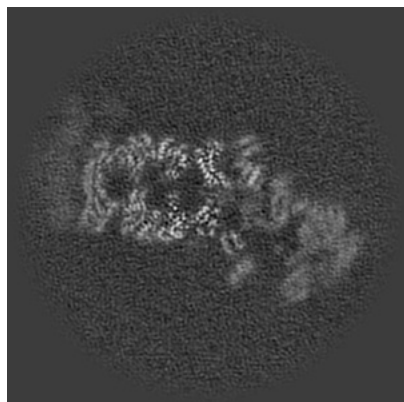


Z

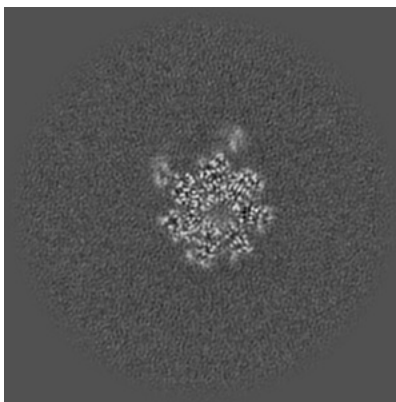
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

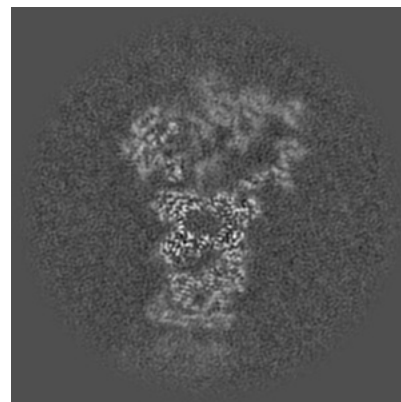
### 6.2.1 Primary map



X Index: 150

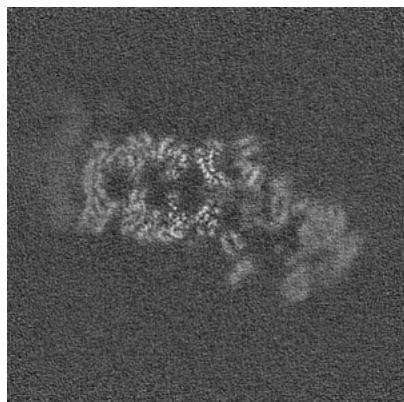


Y Index: 150

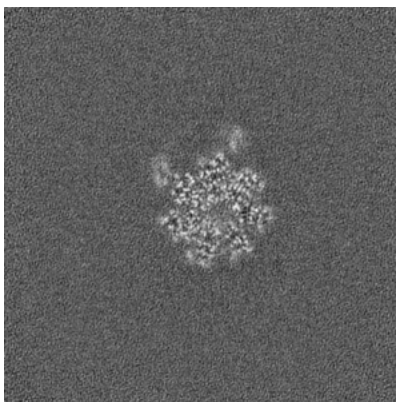


Z Index: 150

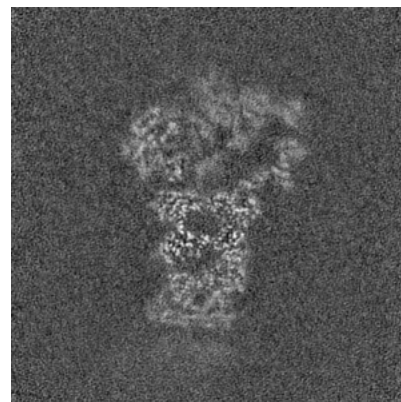
### 6.2.2 Raw map



X Index: 150



Y Index: 150



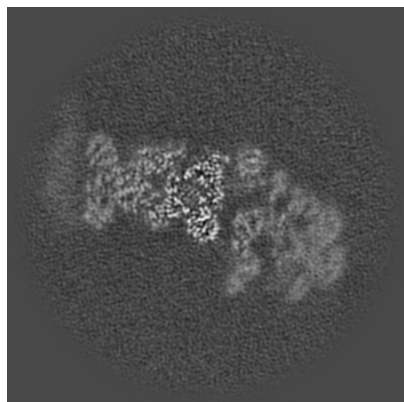
Z Index: 150

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

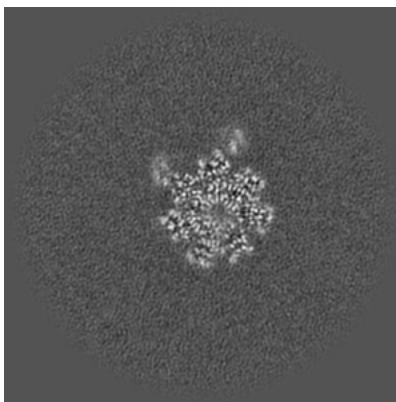


## 6.3 Largest variance slices [i](#)

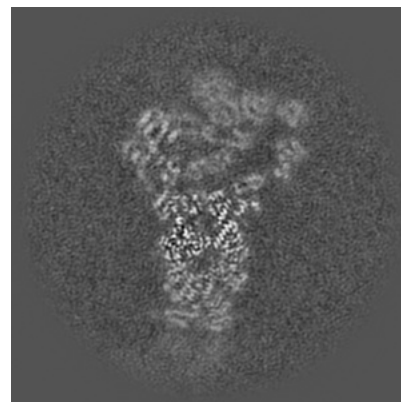
### 6.3.1 Primary map



X Index: 161

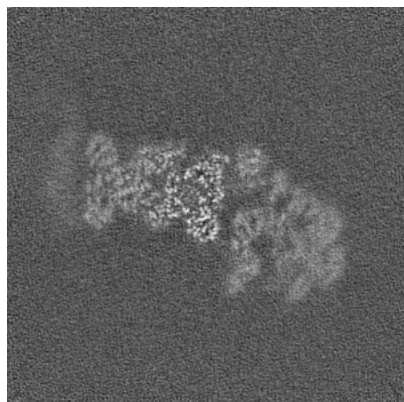


Y Index: 151

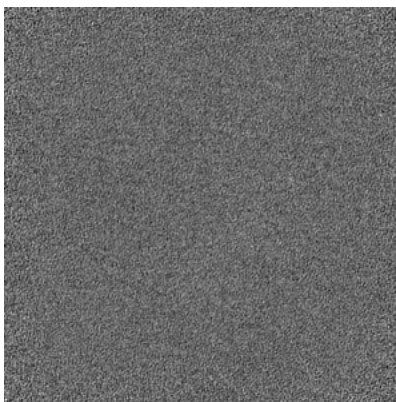


Z Index: 147

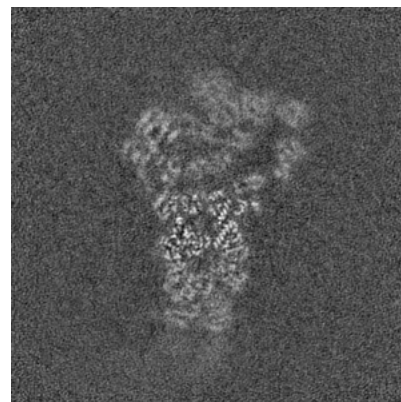
### 6.3.2 Raw map



X Index: 161



Y Index: 0

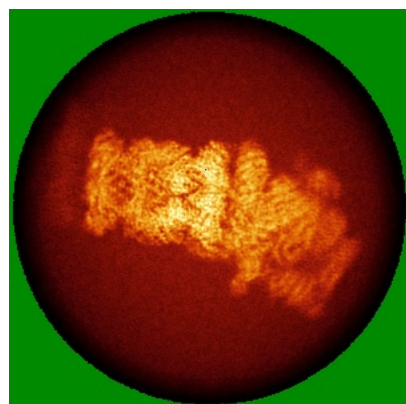


Z Index: 147

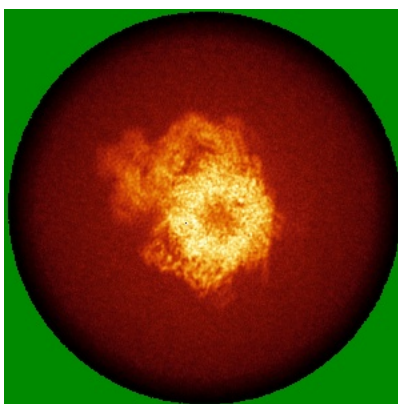
The images above show the largest variance slices of the map in three orthogonal directions.

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

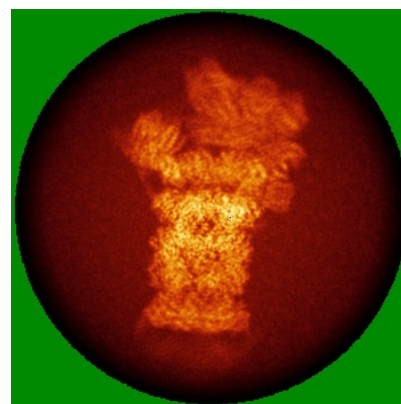
### 6.4.1 Primary map



X

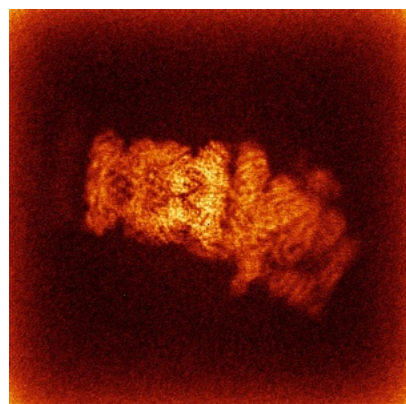


Y

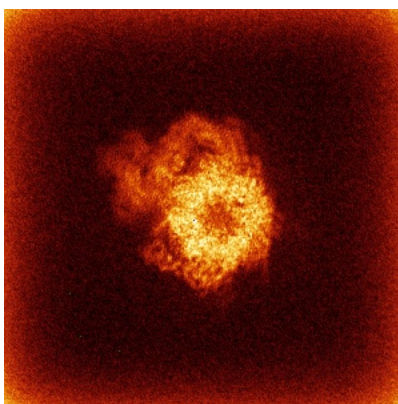


Z

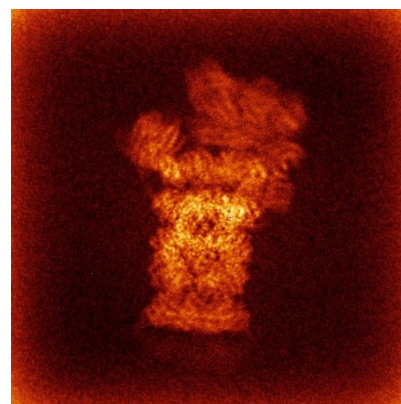
### 6.4.2 Raw map



X



Y

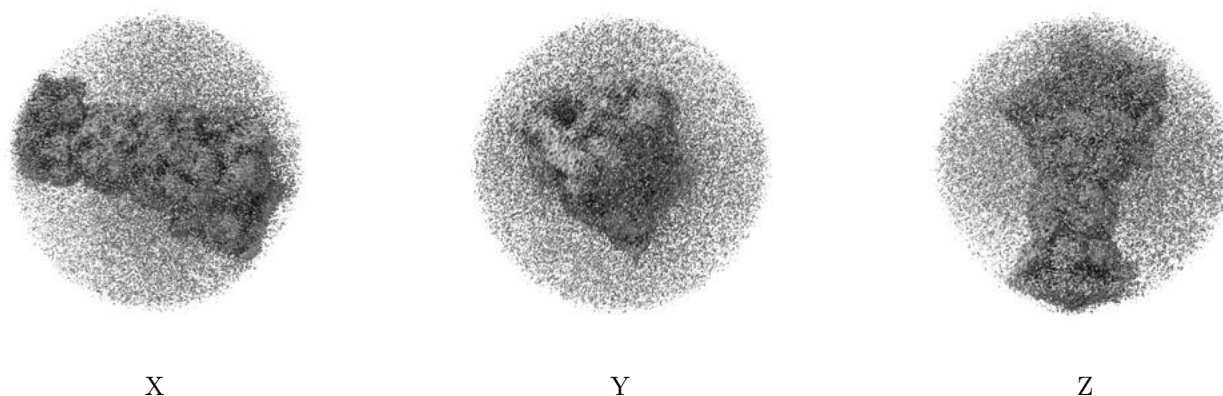


Z

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

## 6.6 Mask visualisation [i](#)

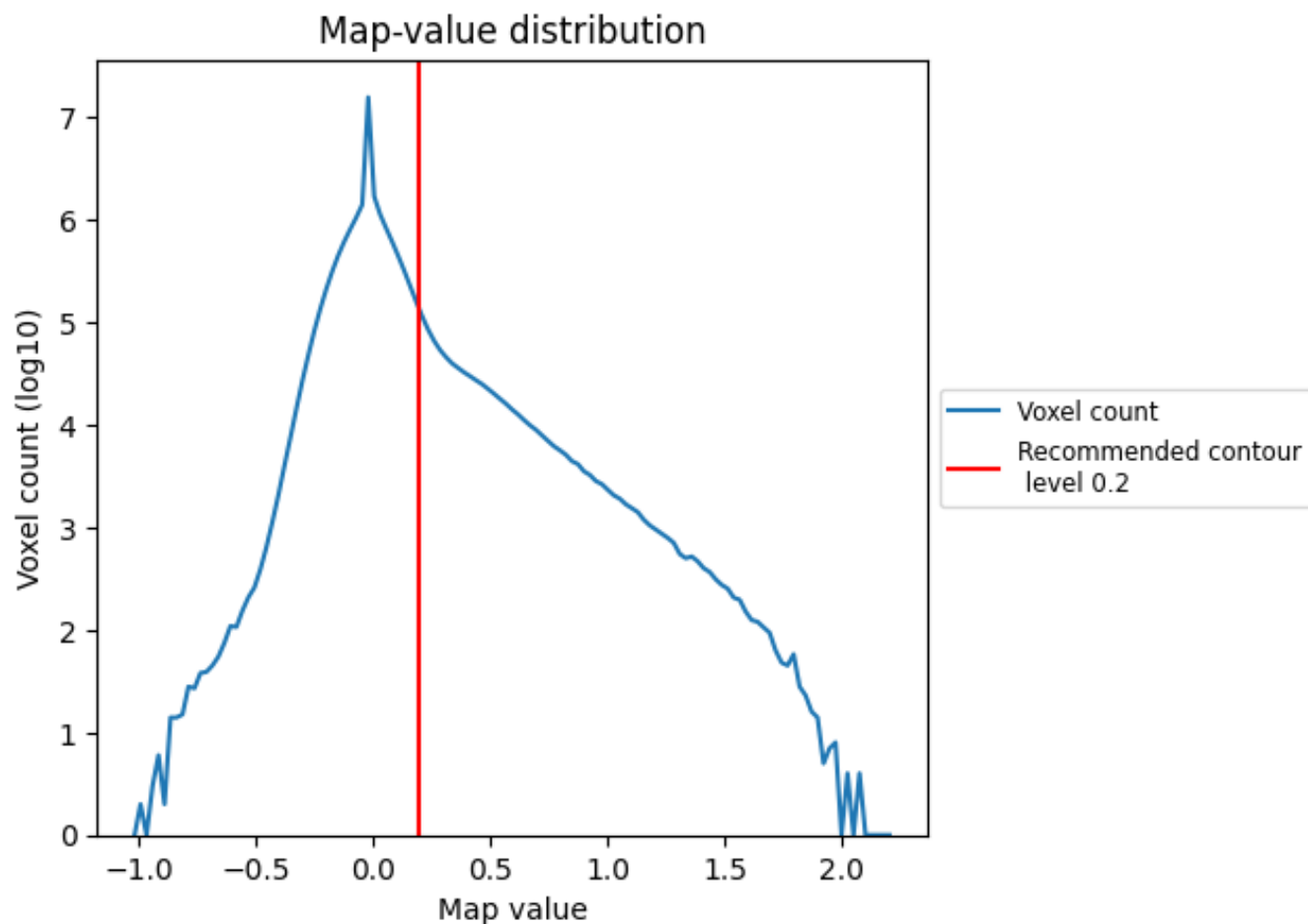
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

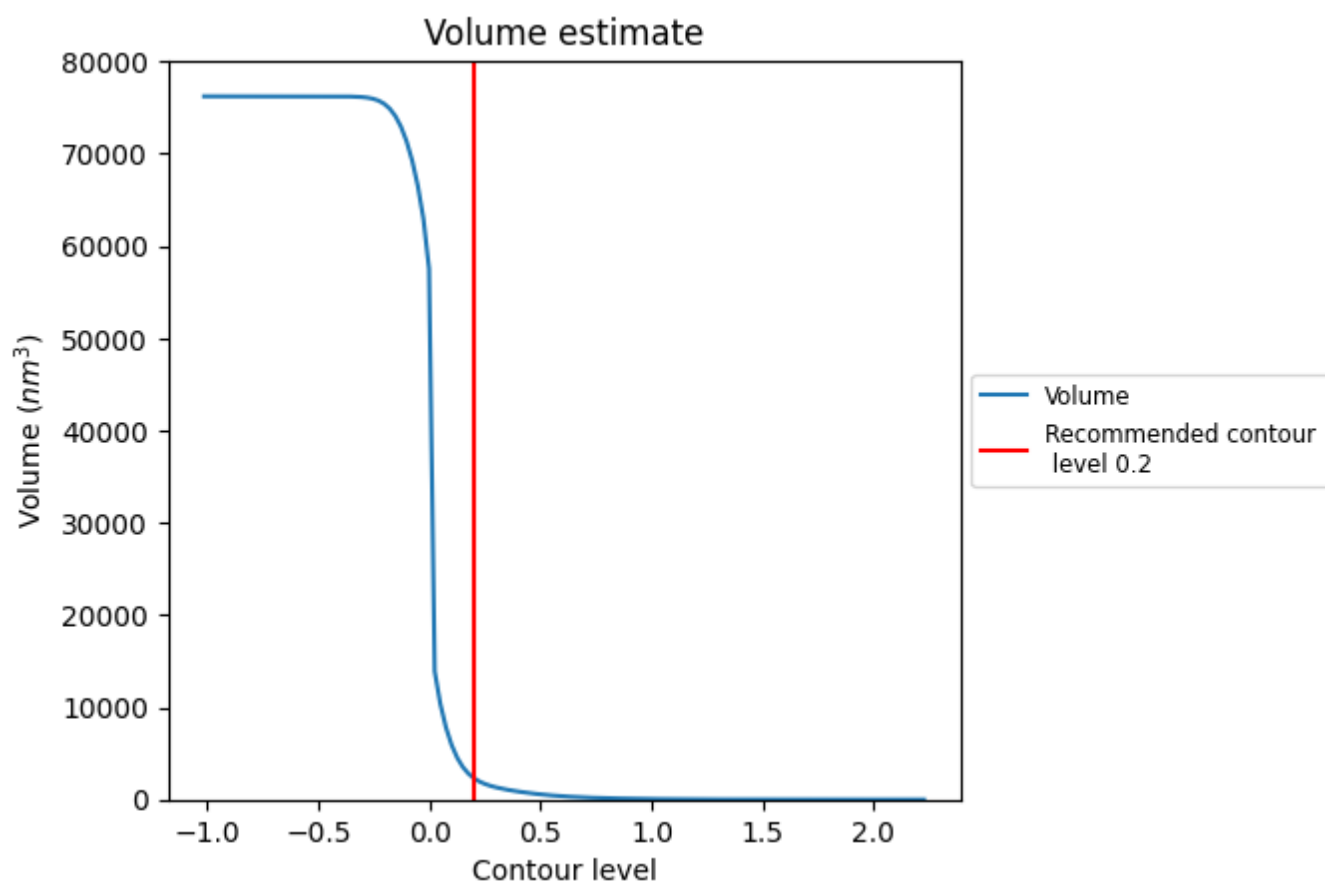
This section contains the results of statistical analysis of the map.

### 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.

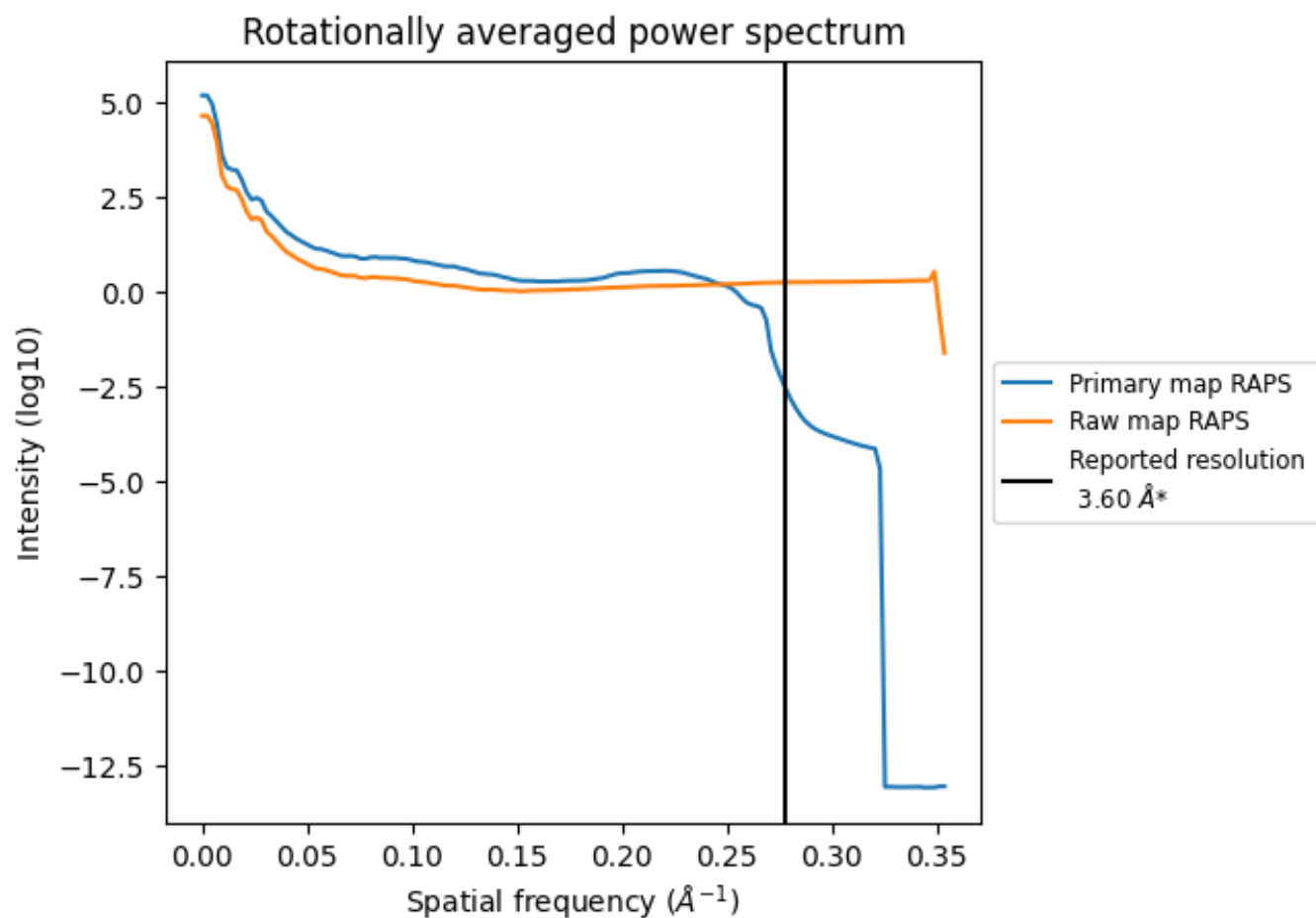
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2315 nm<sup>3</sup>; this corresponds to an approximate mass of 2091 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 ⓘ

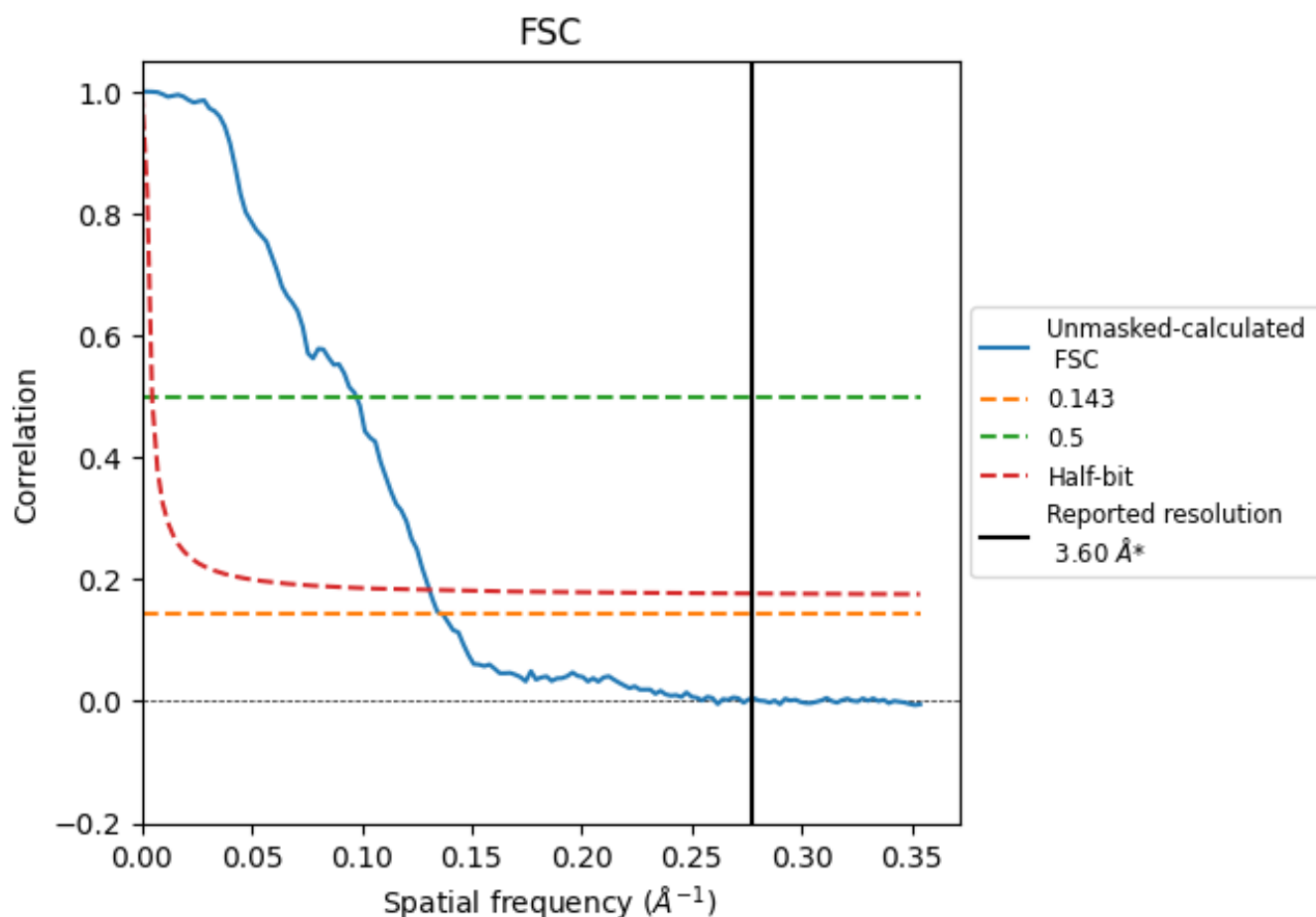


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

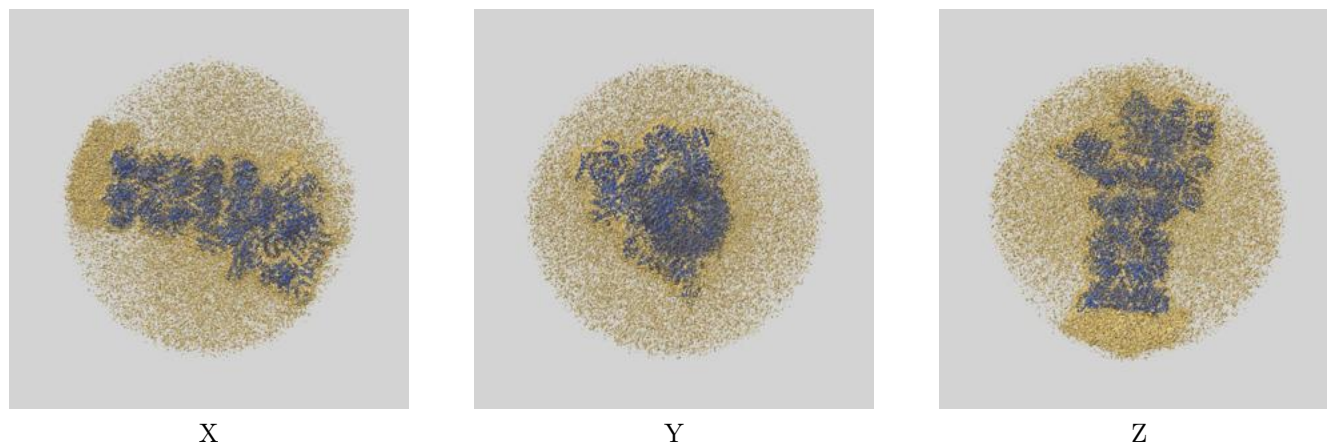
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.32	10.28	7.65

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.32 differs from the reported value 3.6 by more than 10 %

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

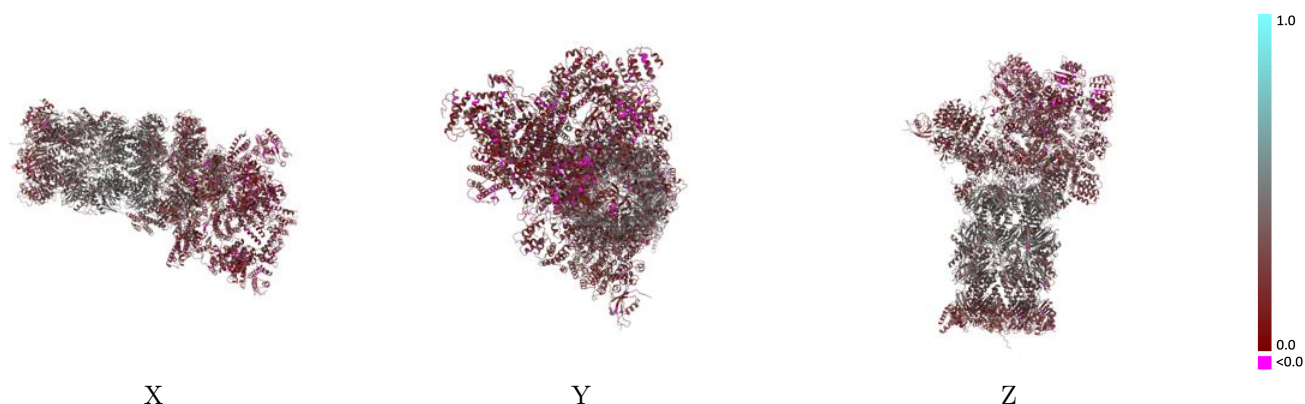
This section contains information regarding the fit between EMDB map EMD-52097 and PDB model 9HEU. Per-residue inclusion information can be found in section 3 on page 12.

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



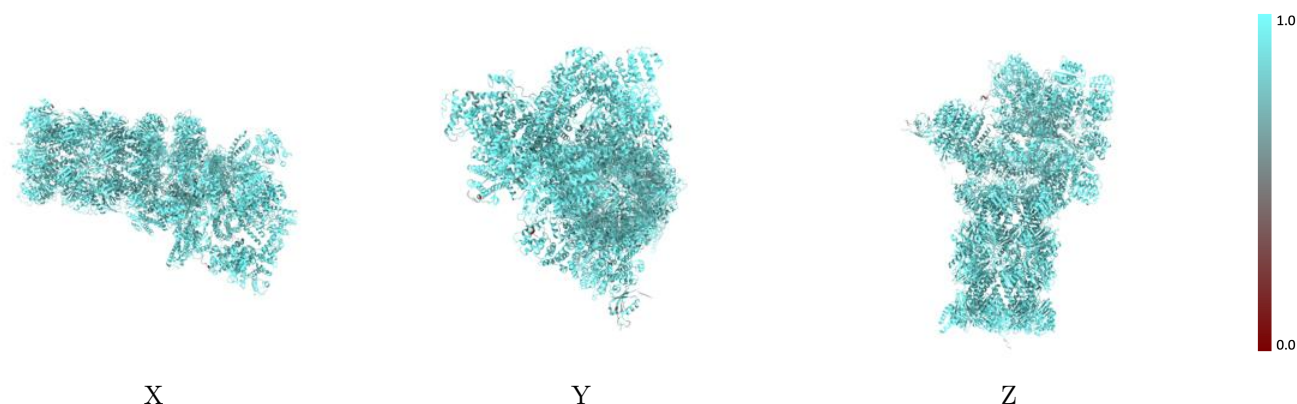
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



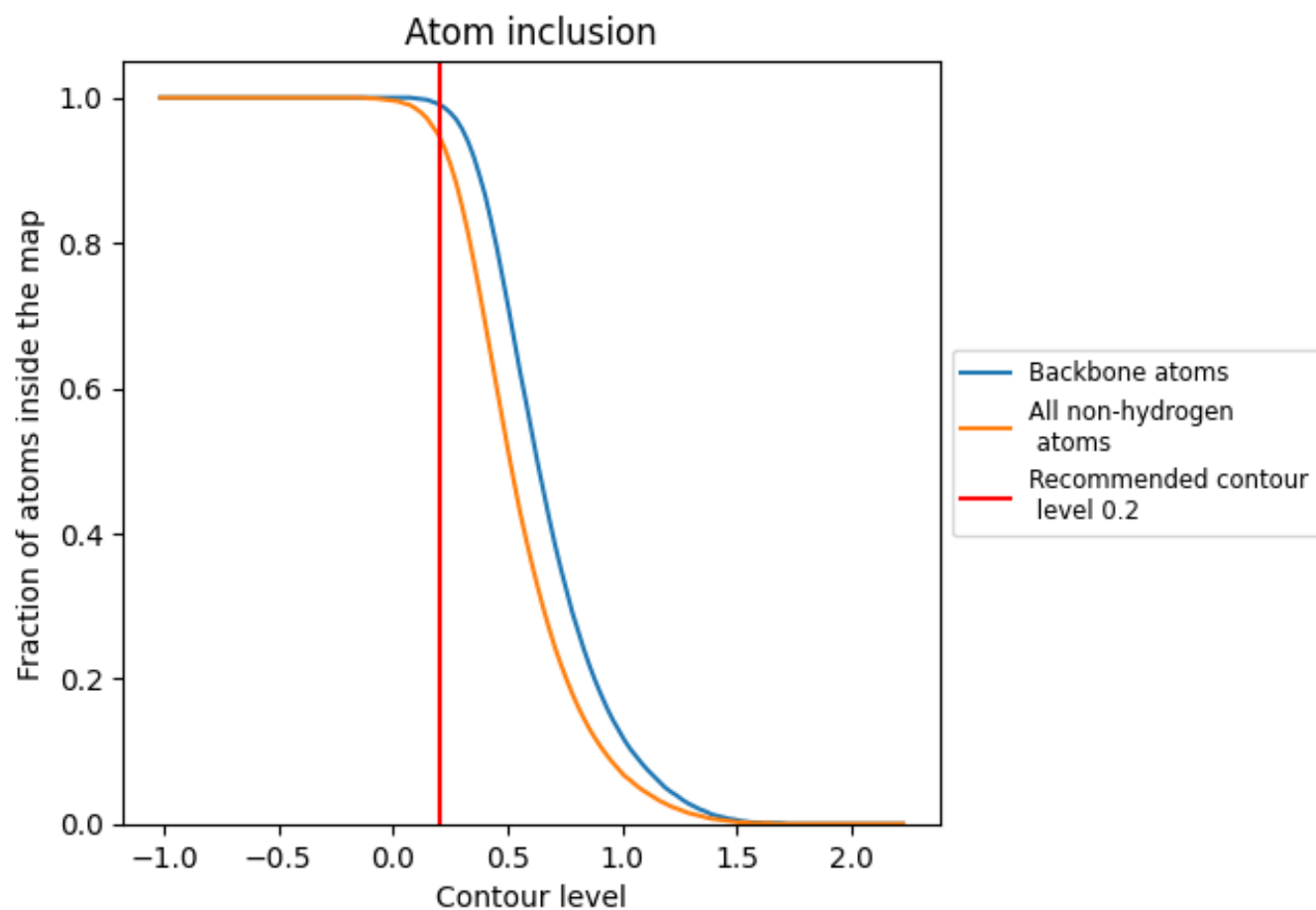
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.3110
A	 0.9160	 0.2720
B	 0.8930	 0.2900
C	 0.9070	 0.2750
D	 0.9100	 0.2840
E	 0.9260	 0.2960
F	 0.9320	 0.2660
G	 0.9660	 0.4330
H	 0.9440	 0.4220
I	 0.9470	 0.4200
J	 0.9380	 0.3850
K	 0.9410	 0.3910
L	 0.9540	 0.4200
M	 0.9570	 0.4240
N	 0.9700	 0.4270
O	 0.9800	 0.4360
P	 0.9800	 0.4450
Q	 0.9640	 0.4350
R	 0.9770	 0.4330
S	 0.9660	 0.4230
T	 0.9590	 0.4210
U	 0.9620	 0.2070
V	 0.9450	 0.2170
W	 0.9570	 0.2580
X	 0.9460	 0.2970
Y	 0.9530	 0.2350
Z	 0.9630	 0.2180
a	 0.9590	 0.2120
b	 0.9590	 0.1960
c	 0.9500	 0.2280
d	 0.9230	 0.2070
e	 0.9110	 0.2410
f	 0.9550	 0.2860
g	 0.9570	 0.3000
h	 0.9490	 0.2950



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.9470	 0.2920
j	 0.9570	 0.2960
k	 0.9380	 0.2860
l	 0.9520	 0.3010
m	 0.9440	 0.2820
n	 0.9760	 0.3840
o	 0.9690	 0.3780
p	 0.9800	 0.3930
q	 0.9690	 0.3890
r	 0.9780	 0.4040
s	 0.9620	 0.3960
t	 0.9700	 0.3910
x	 0.7280	 0.2200