



# wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 08:02 PM JST

PDB ID : 9K58 / pdb\_00009k58  
EMDB ID : EMD-62084  
Title : Structure of substrate-engaged single-cap human proteasome in state EB  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 4.50 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](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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the 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

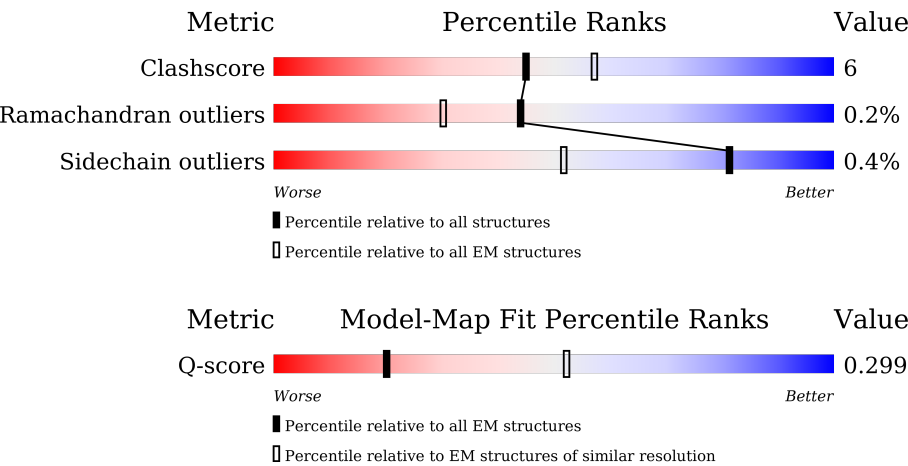


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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	A	433	<div><div>22%</div><div>78%</div><div>15%</div><div>6%</div></div>
2	B	440	<div><div>26%</div><div>71%</div><div>18%</div><div>10%</div></div>
3	C	398	<div><div>38%</div><div>72%</div><div>22%</div><div>• •</div></div>
4	D	418	<div><div>20%</div><div>72%</div><div>17%</div><div>• 9%</div></div>

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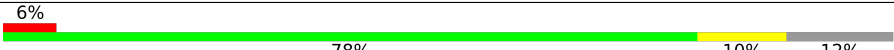
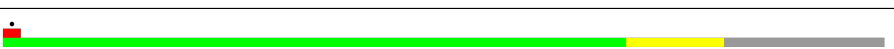

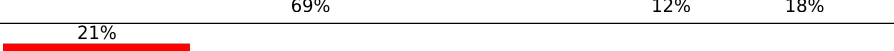
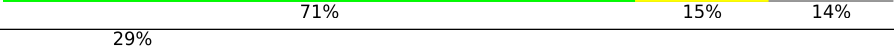





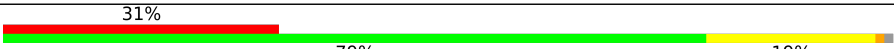

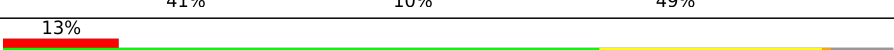
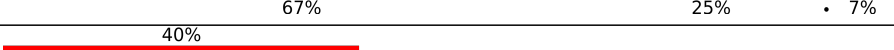



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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
34	v	28	



## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106247 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total	C	N	O	S	0	0
			3164	1992	555	600	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			3099	1953	525	606	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total	C	N	O	S	0	0
			2978	1872	536	554	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

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

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.



Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

- Molecule 33 is a protein called Ubiquitin.

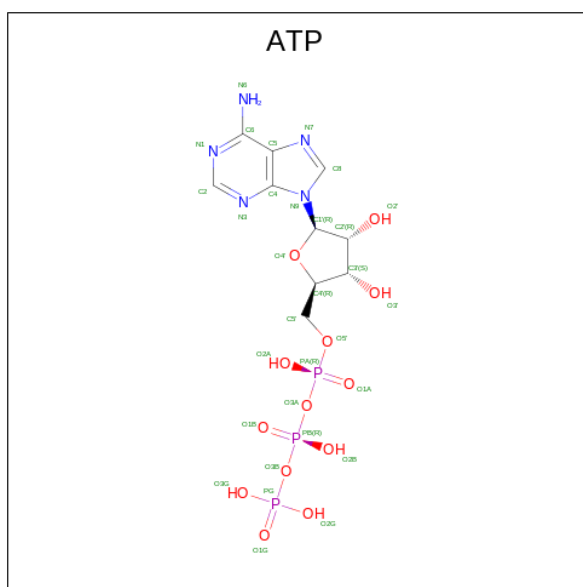
Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	28	Total	C	N	O	0	0
			143	86	29	28		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





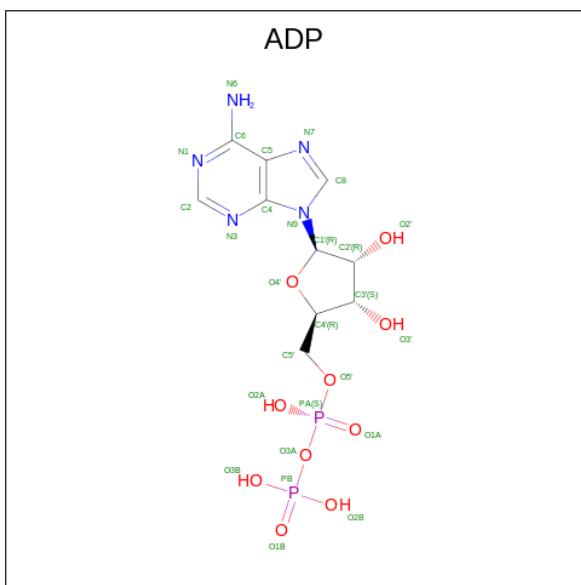
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





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

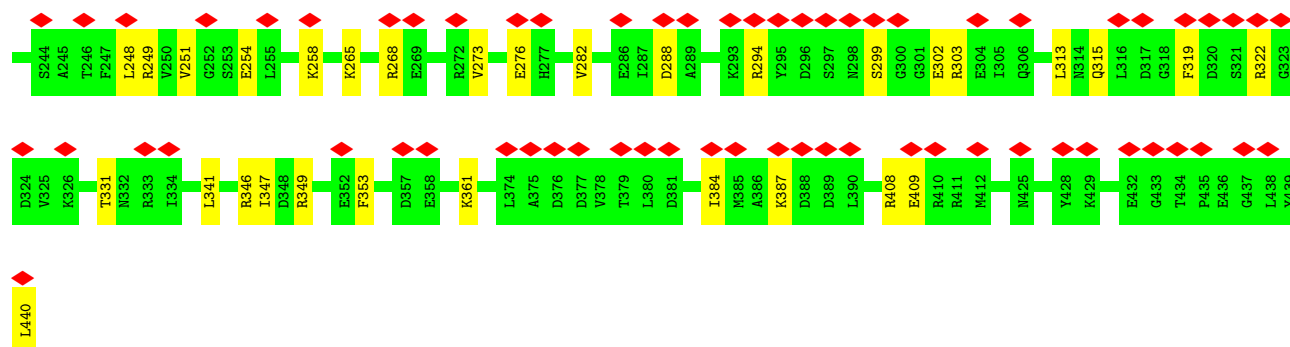
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

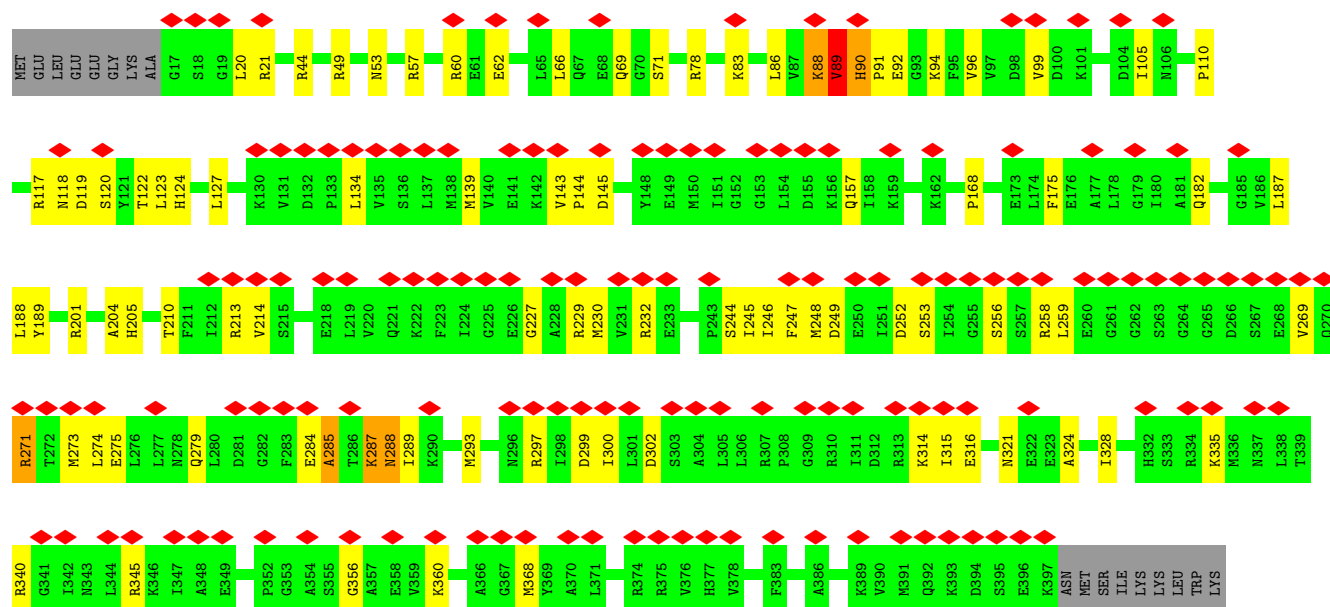




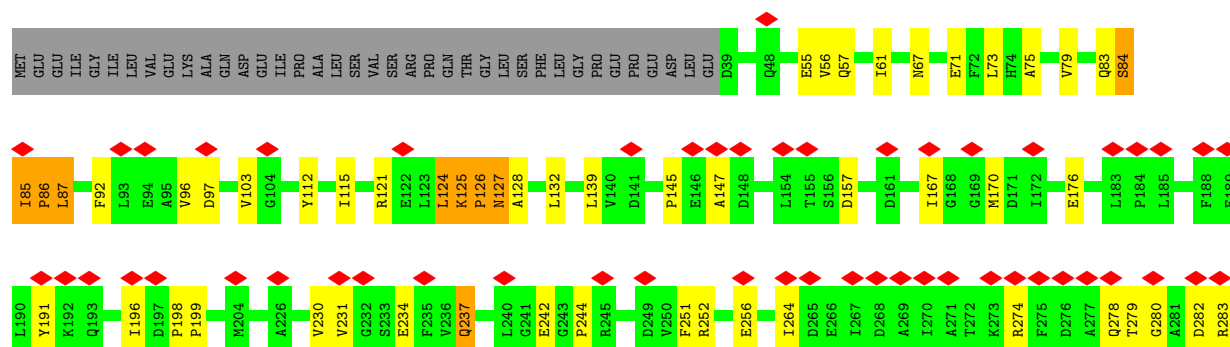
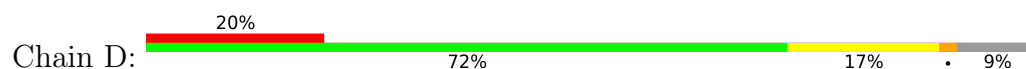




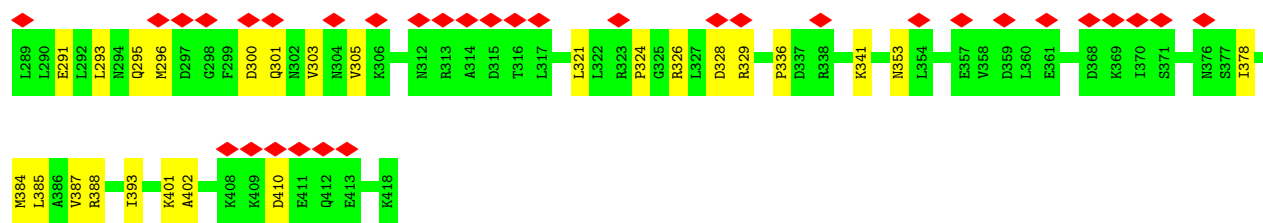
• Molecule 3: 26S proteasome regulatory subunit 8



• Molecule 4: 26S proteasome regulatory subunit 6B

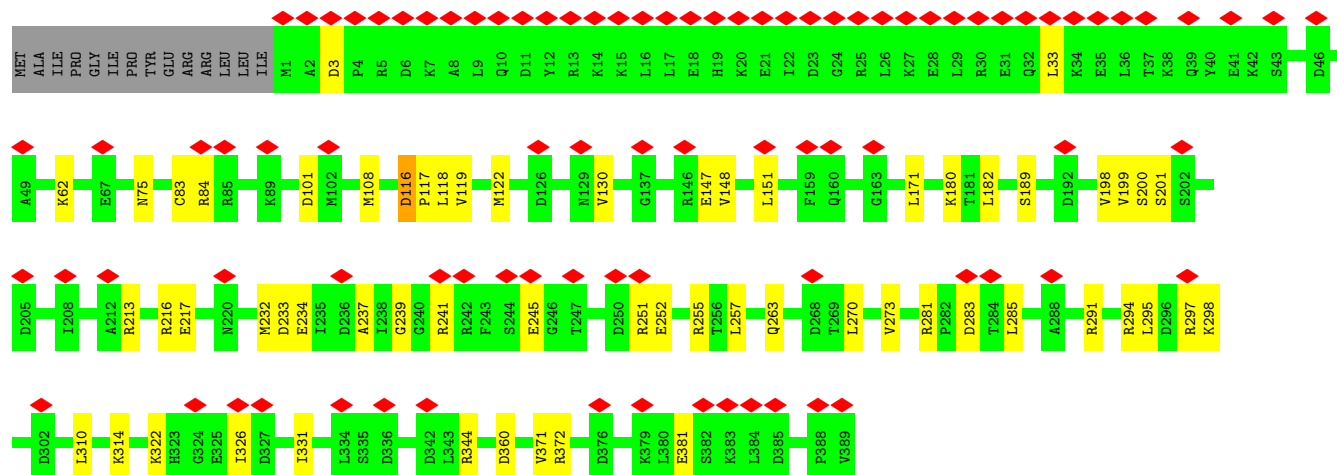






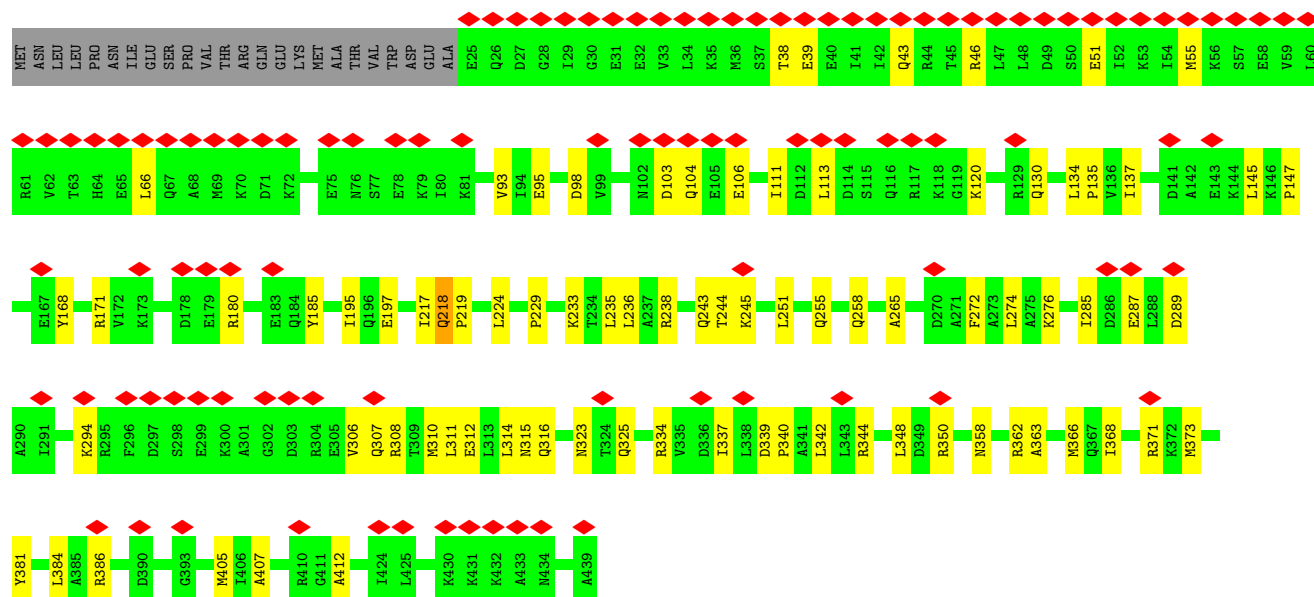
• Molecule 5: Proteasome 26S subunit, ATPase 6

Chain E: 22% 82% 15%



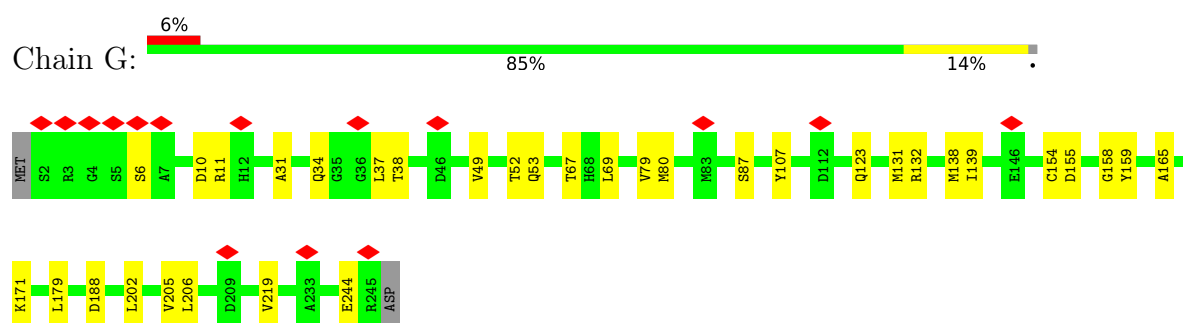
• Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 25% 76% 19% 5%

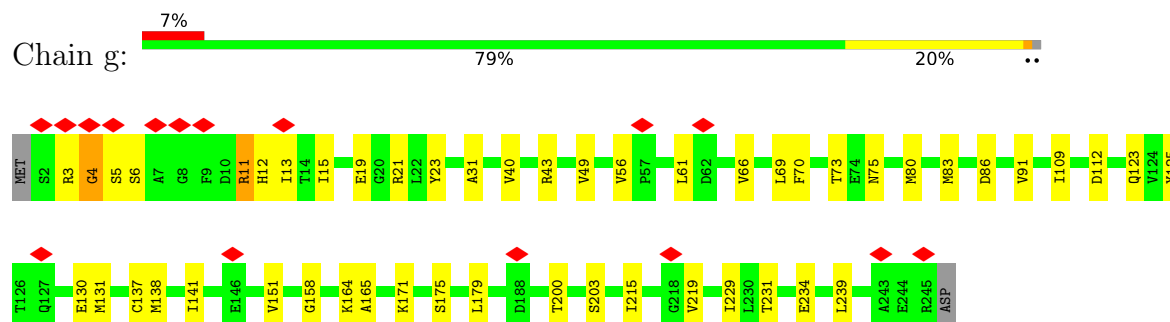


• Molecule 7: Proteasome subunit alpha type-6

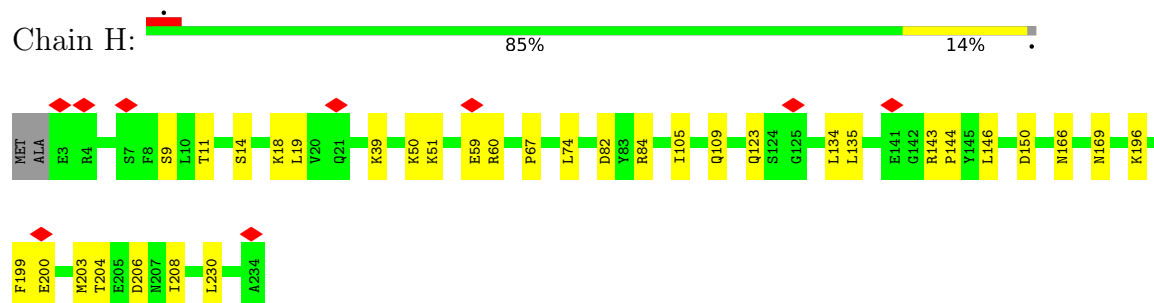




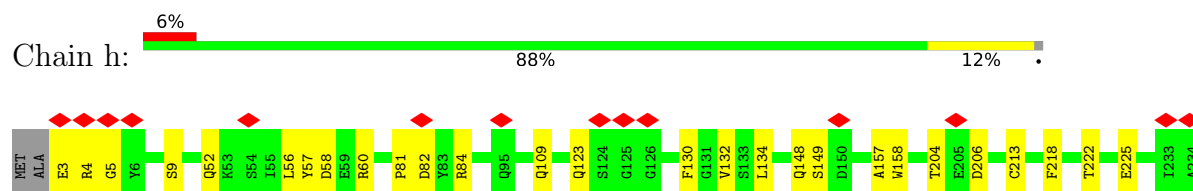
- Molecule 7: Proteasome subunit alpha type-6



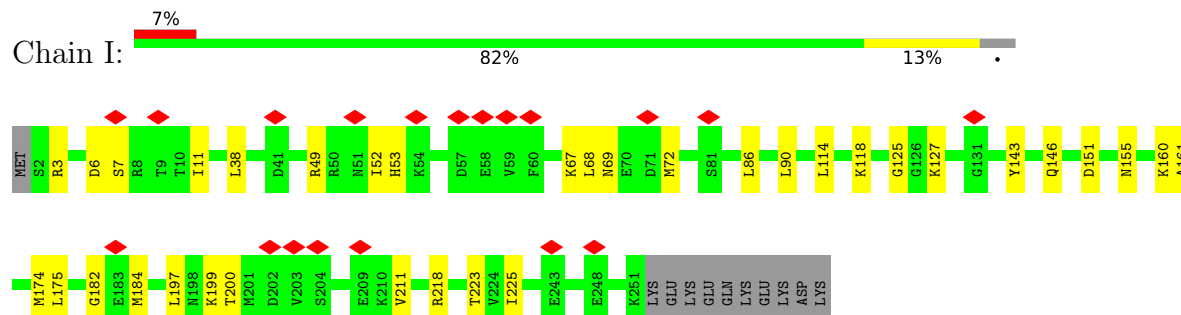
- Molecule 8: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-2

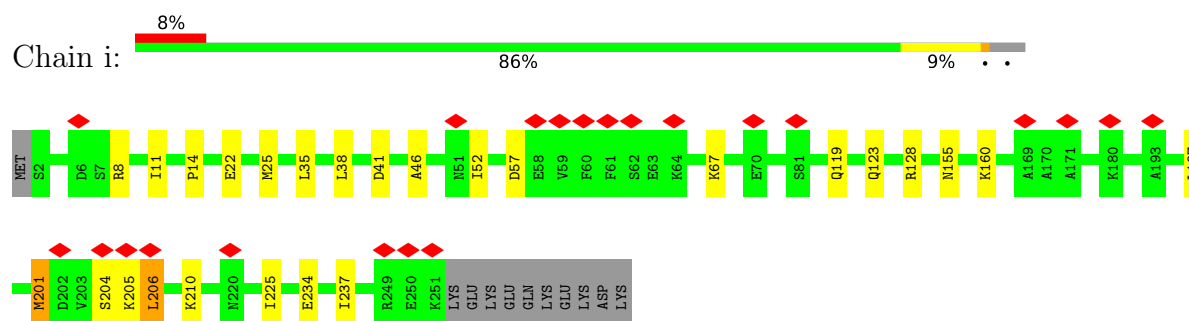


- Molecule 9: Proteasome subunit alpha type-4

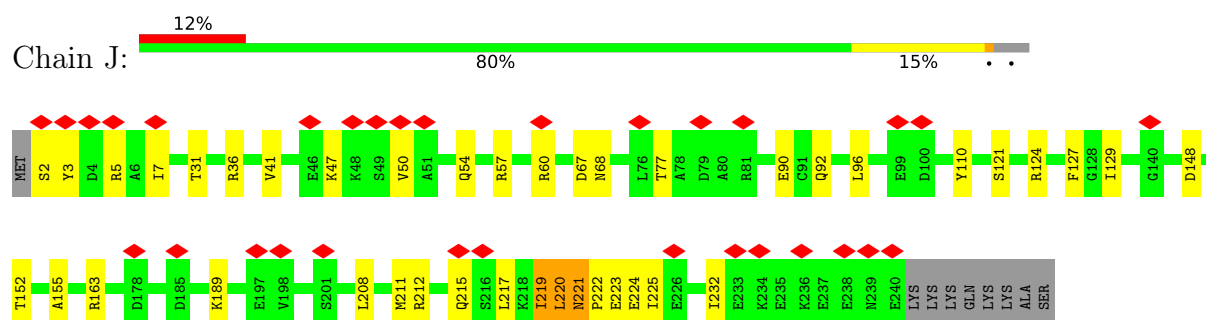




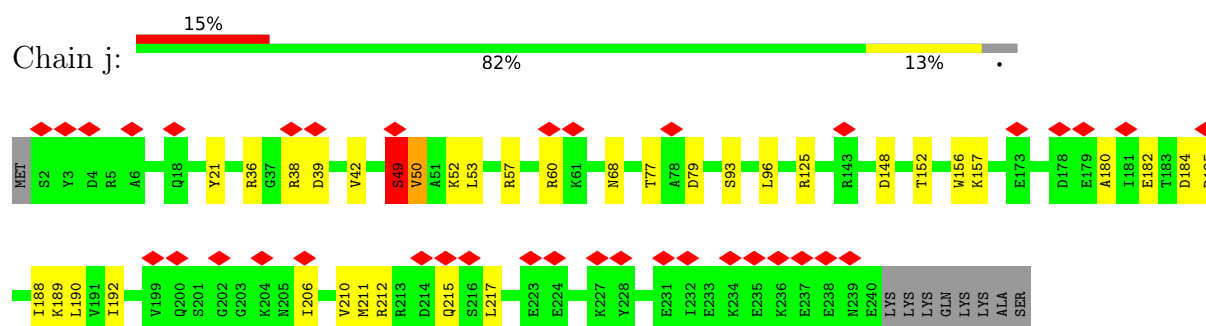
- Molecule 9: Proteasome subunit alpha type-4



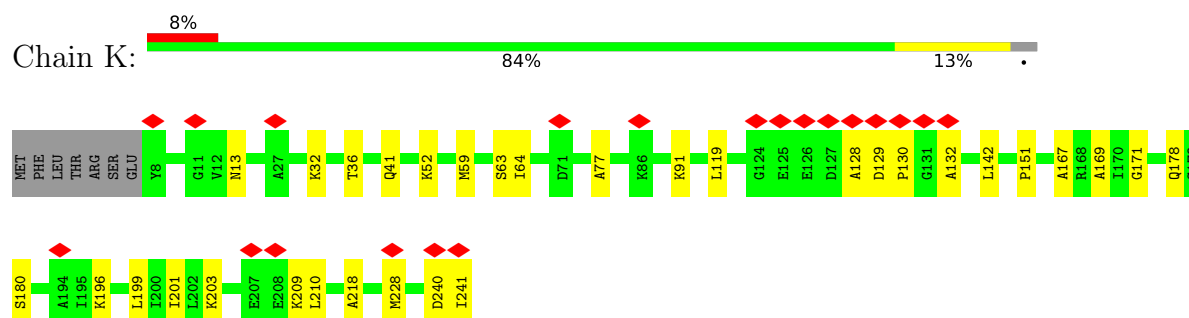
- Molecule 10: Proteasome subunit alpha type-7



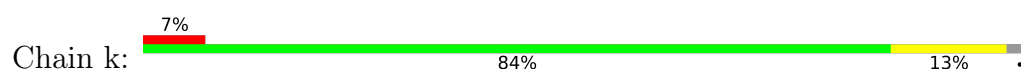
- Molecule 10: Proteasome subunit alpha type-7



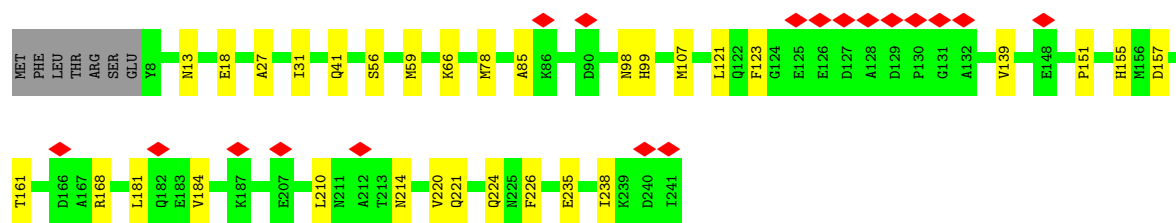
- Molecule 11: Proteasome subunit alpha type-5



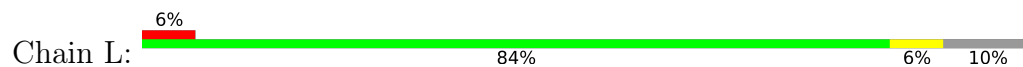
- Molecule 11: Proteasome subunit alpha type-5



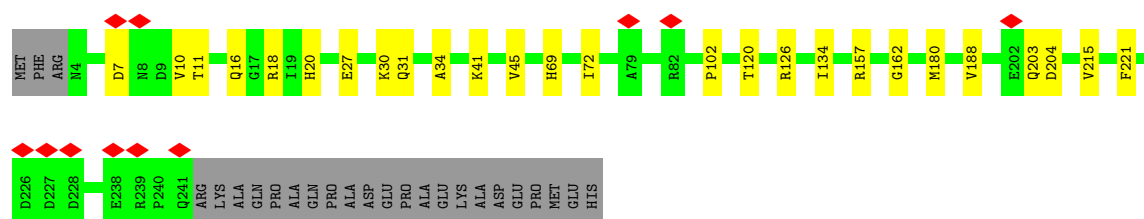
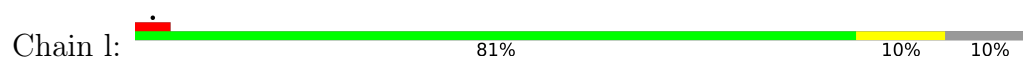




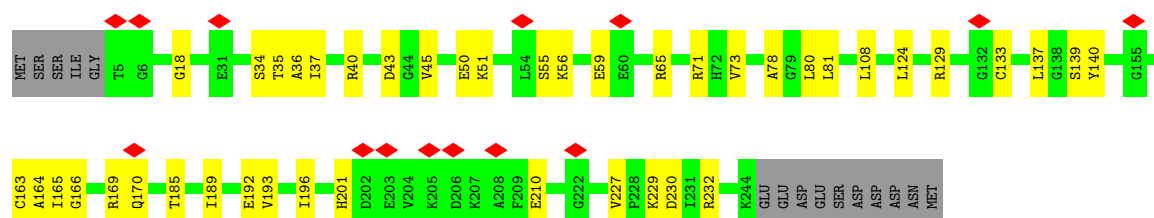
• Molecule 12: Proteasome subunit alpha type-1



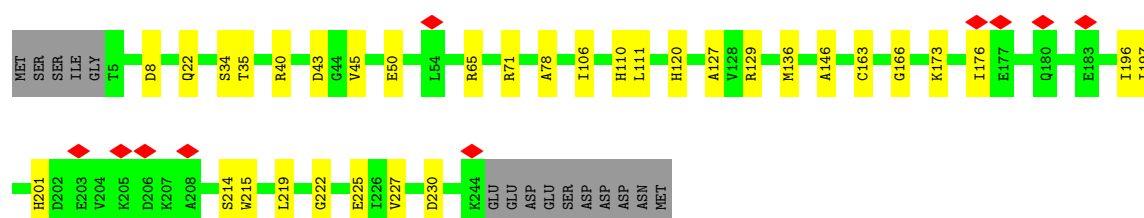
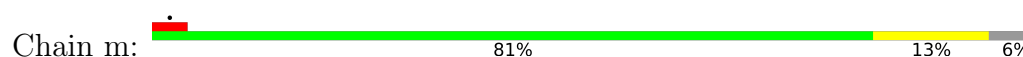
• Molecule 12: Proteasome subunit alpha type-1



• Molecule 13: Proteasome subunit alpha type-3

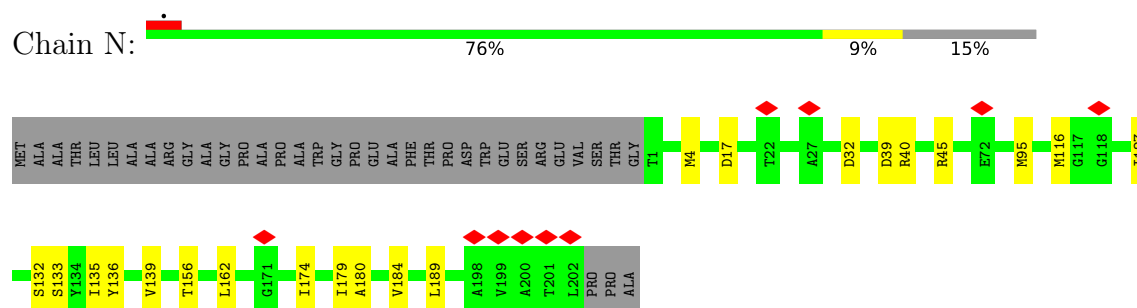


• Molecule 13: Proteasome subunit alpha type-3

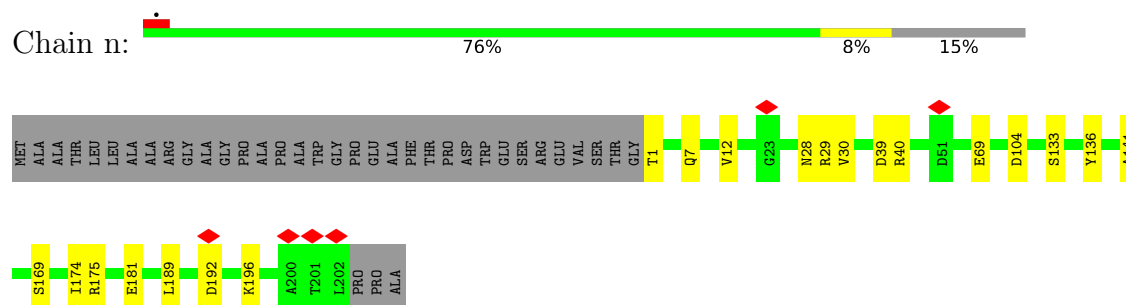




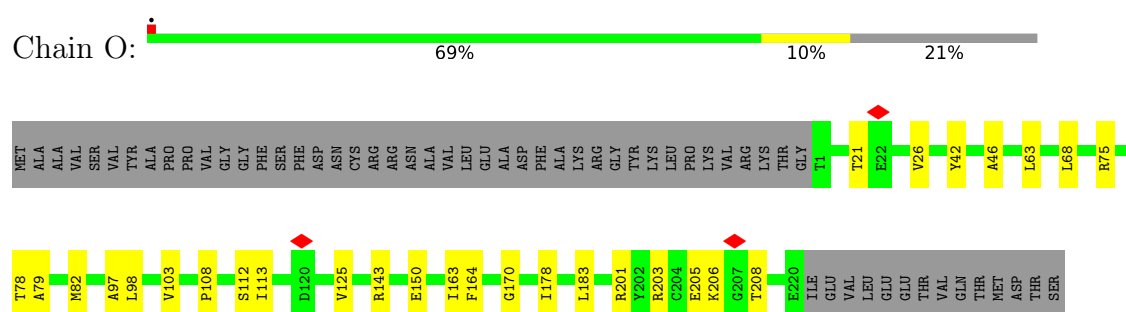
- Molecule 14: Proteasome subunit beta type-6



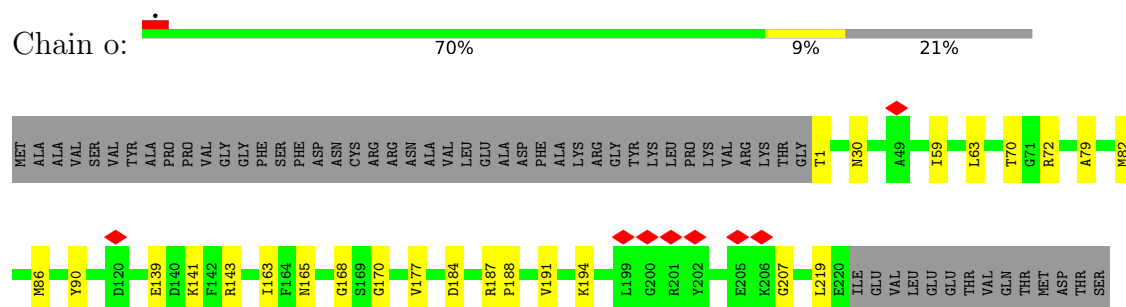
- Molecule 14: Proteasome subunit beta type-6



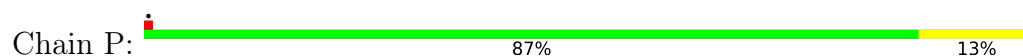
- Molecule 15: Proteasome subunit beta type-7



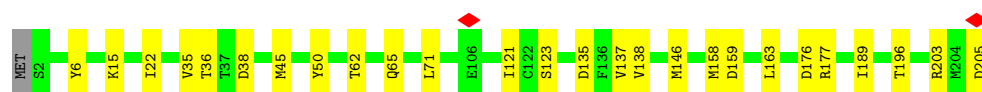
- Molecule 15: Proteasome subunit beta type-7



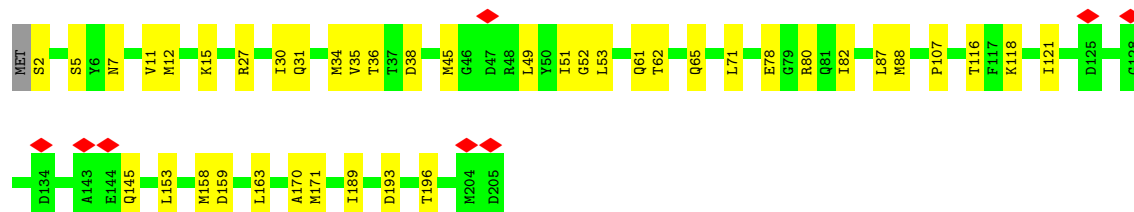
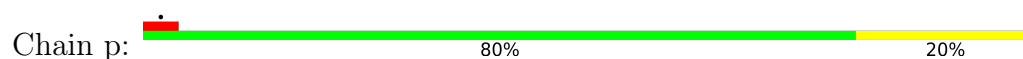
- Molecule 16: Proteasome subunit beta type-3



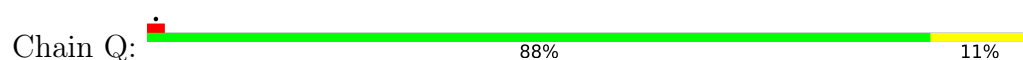




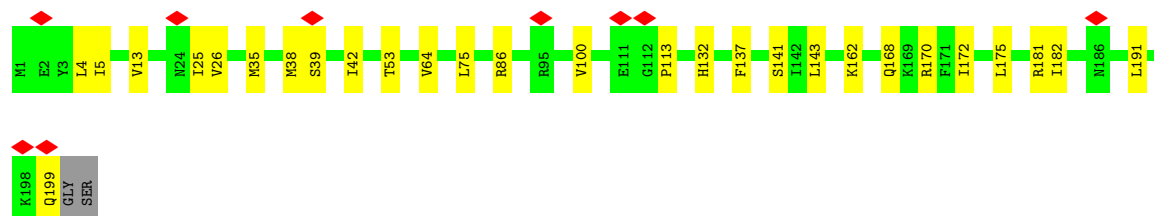
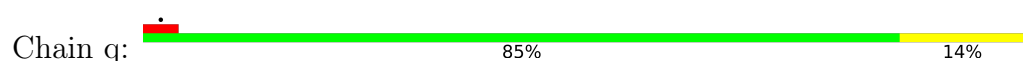
- Molecule 16: Proteasome subunit beta type-3



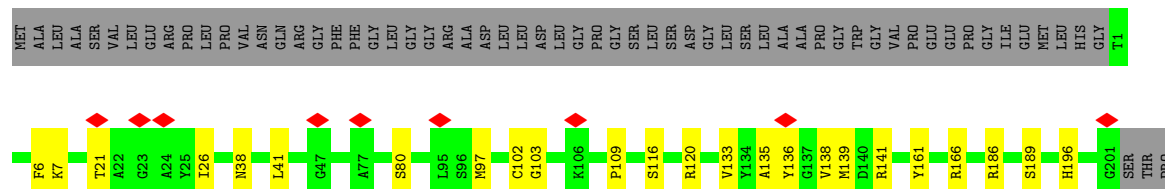
- Molecule 17: Proteasome subunit beta type-2



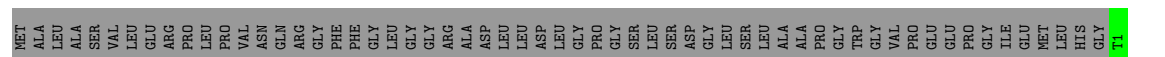
- Molecule 17: Proteasome subunit beta type-2



- Molecule 18: Proteasome subunit beta type-5



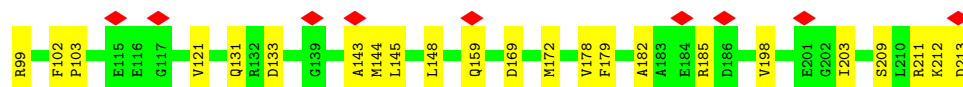
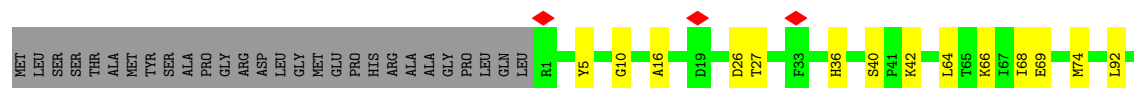
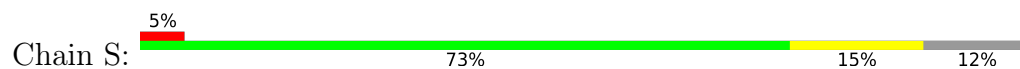
- Molecule 18: Proteasome subunit beta type-5



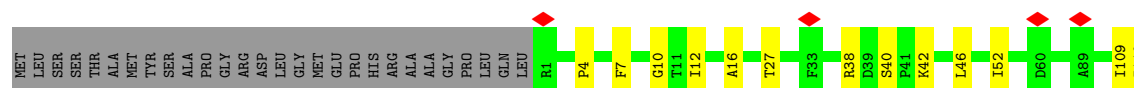
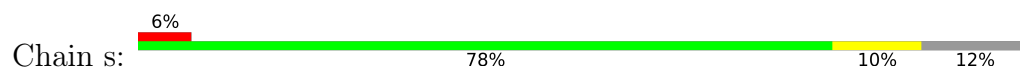




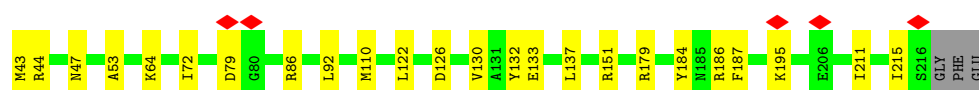
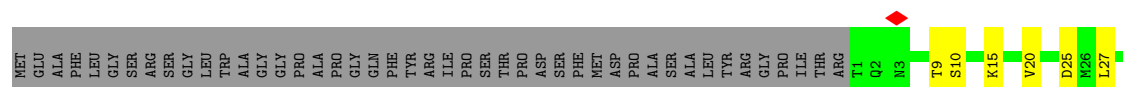
- Molecule 19: Proteasome subunit beta type-1



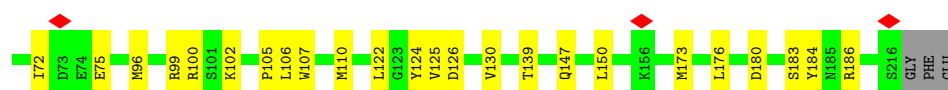
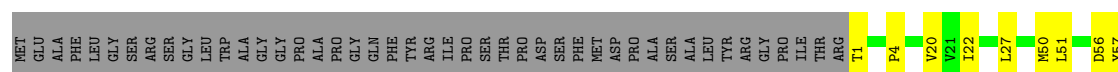
- Molecule 19: Proteasome subunit beta type-1



- Molecule 20: Proteasome subunit beta type-4

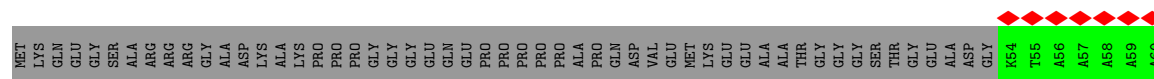


- Molecule 20: Proteasome subunit beta type-4

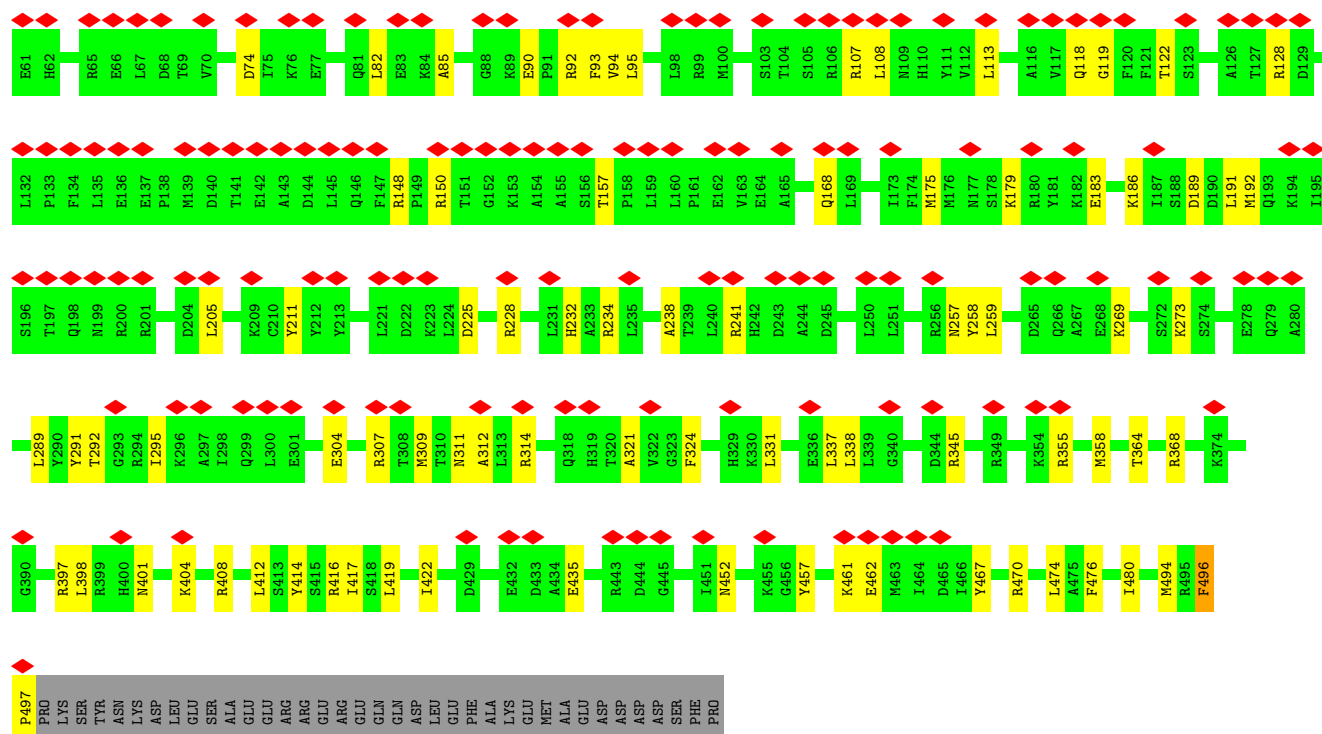


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

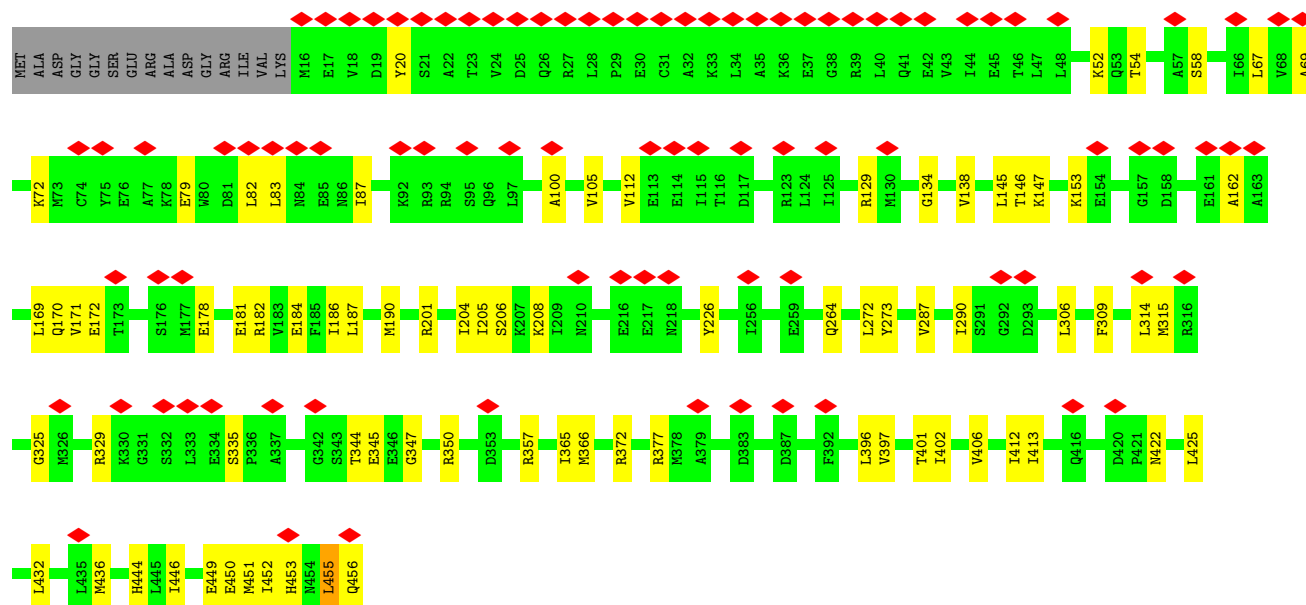
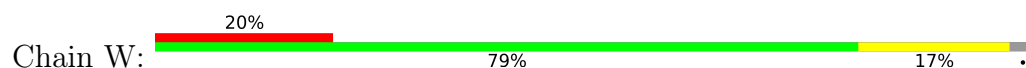




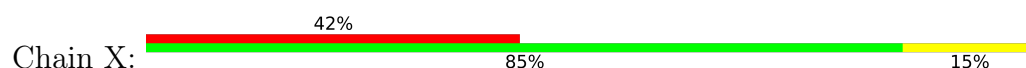




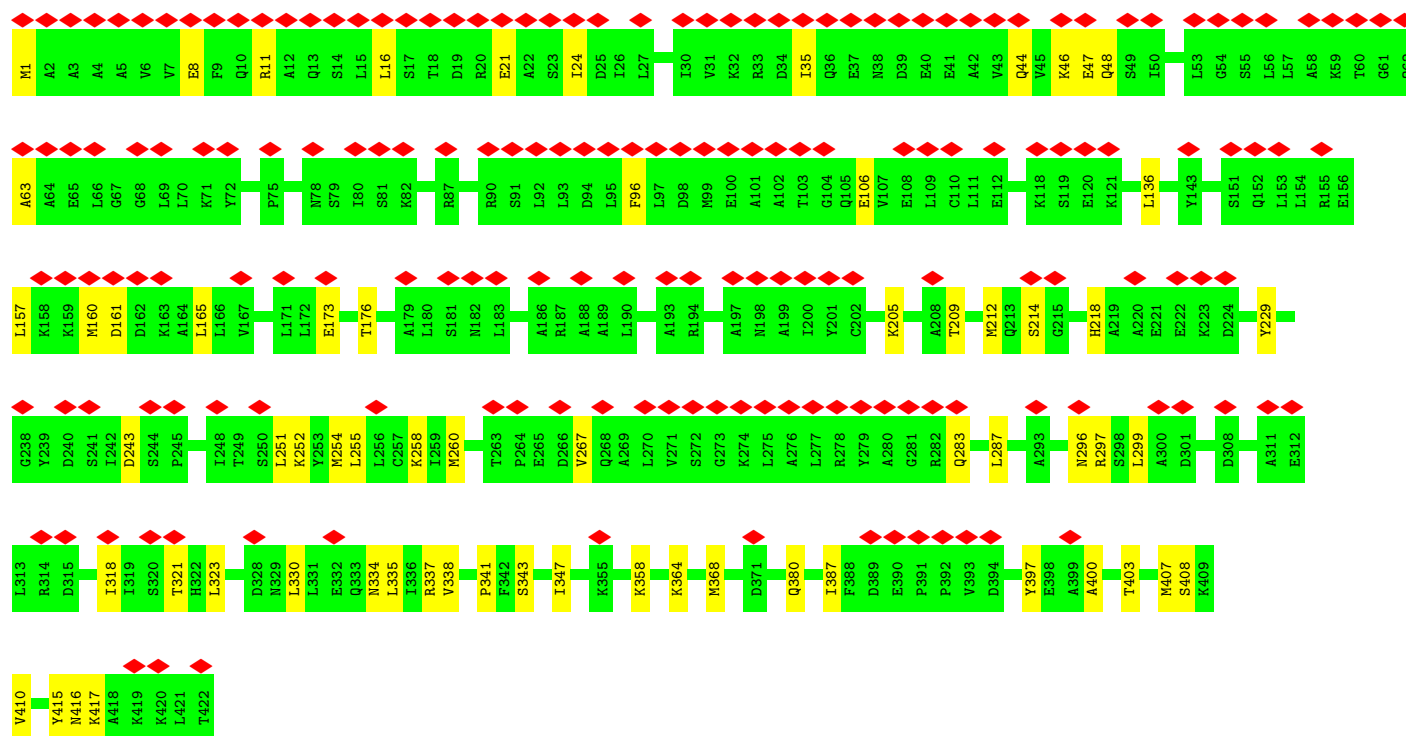
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



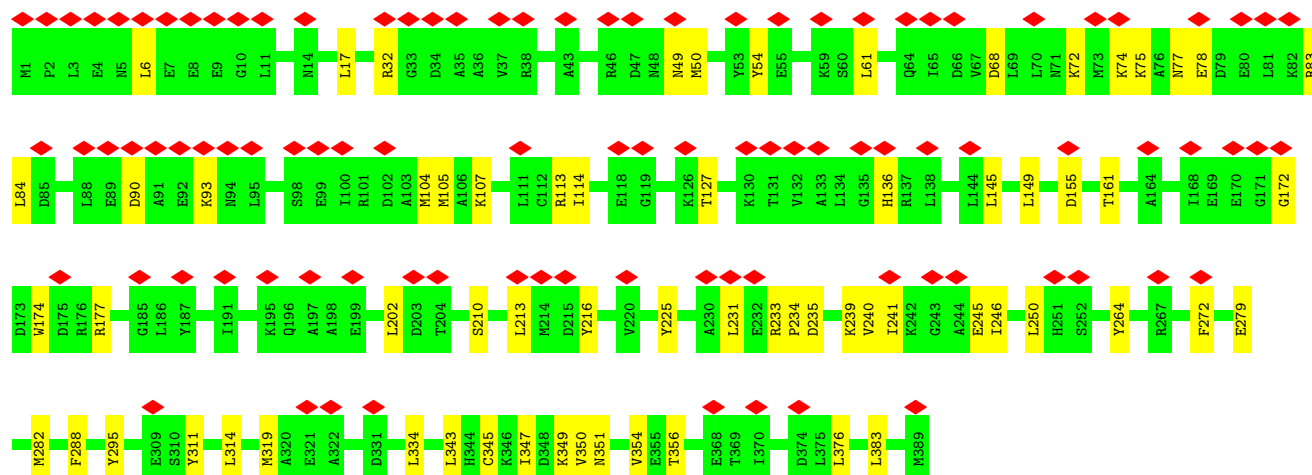
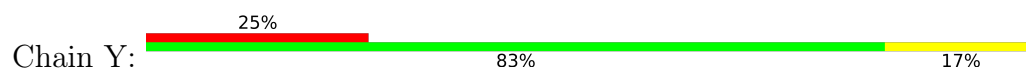
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



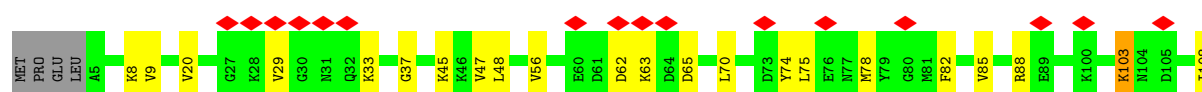




• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



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

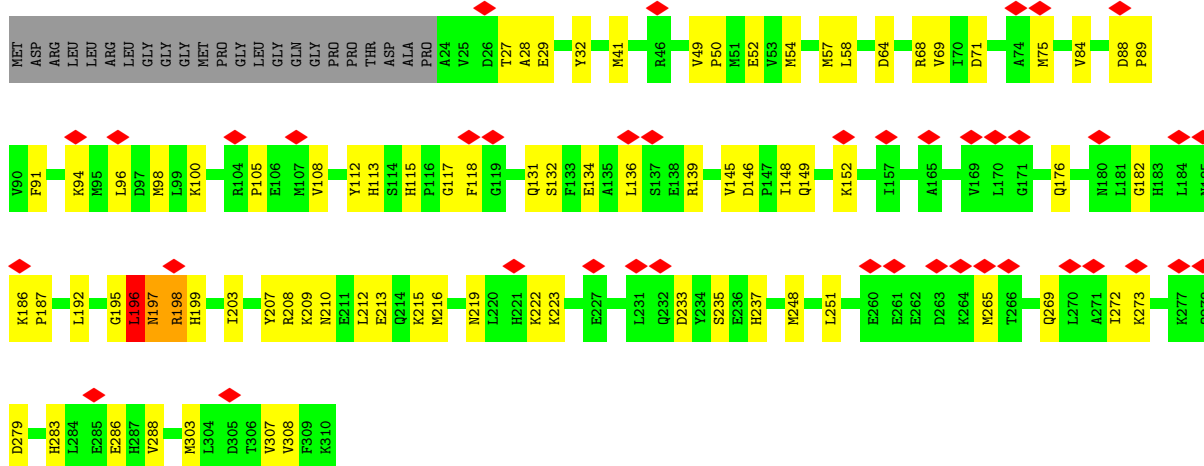




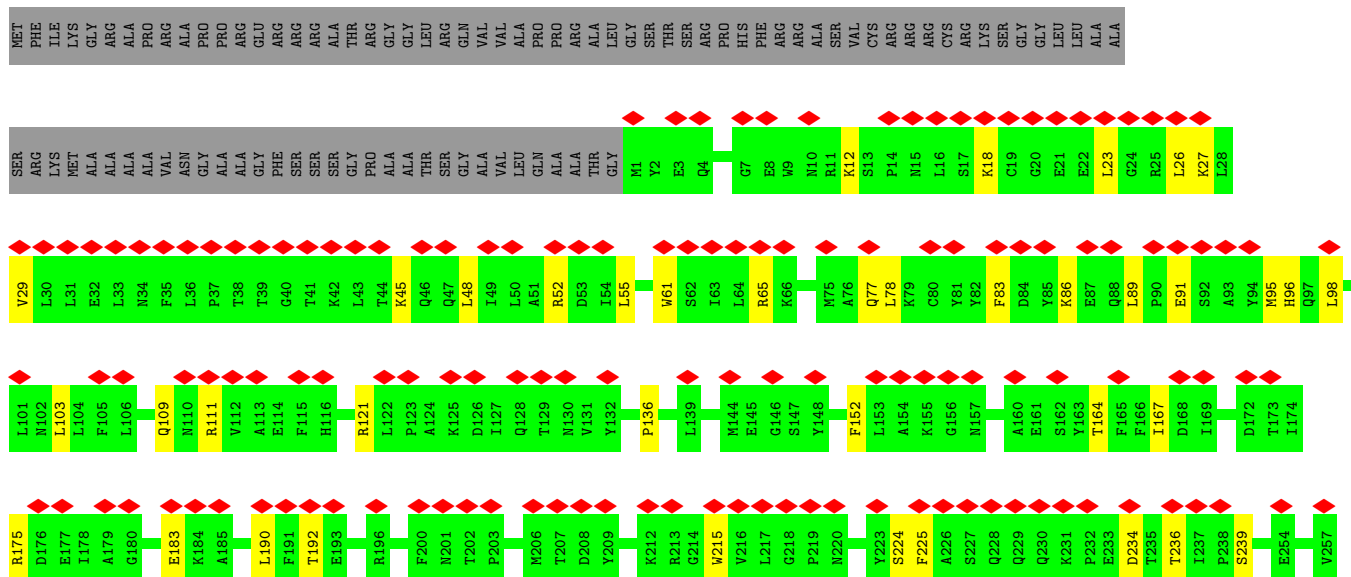




- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 31: 26S proteasome complex subunit SEM1

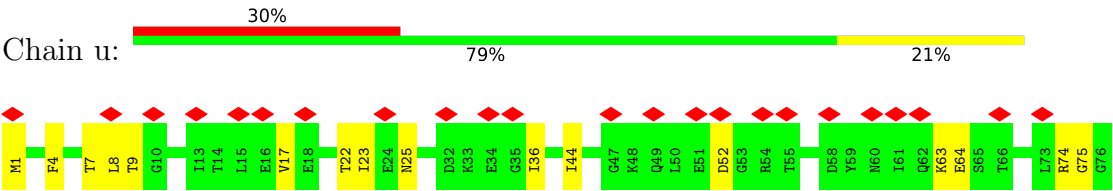




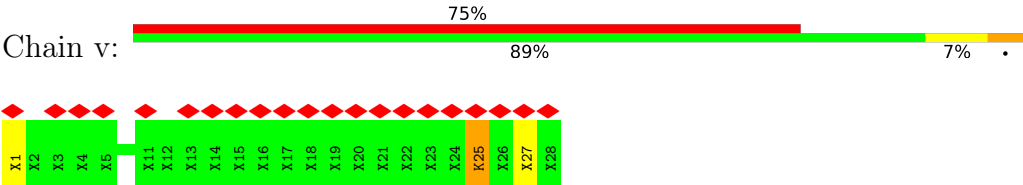




● Molecule 33: Ubiquitin



● Molecule 34: Substrate





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00588	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/3215	0.59	1/4340 (0.0%)
2	B	0.23	0/3144	0.55	0/4245
3	C	0.23	0/3017	0.57	4/4058 (0.1%)
4	D	0.27	0/3089	0.58	1/4168 (0.0%)
5	E	0.20	0/3145	0.51	0/4233
6	F	0.20	0/3292	0.52	0/4435
7	G	0.24	1/1923 (0.1%)	0.48	0/2601
7	g	0.24	0/1914	0.52	1/2590 (0.0%)
8	H	0.20	0/1844	0.49	0/2499
8	h	0.21	0/1844	0.48	0/2497
9	I	0.23	0/1985	0.53	0/2677
9	i	0.23	0/1985	0.52	1/2677 (0.0%)
10	J	0.21	0/1906	0.48	0/2573
10	j	0.21	0/1887	0.48	0/2549
11	K	0.21	0/1804	0.45	0/2436
11	k	0.19	0/1809	0.46	0/2444
12	L	0.20	0/1901	0.45	0/2570
12	l	0.18	0/1896	0.45	0/2565
13	M	0.19	0/1911	0.47	0/2573
13	m	0.20	0/1916	0.44	0/2580
14	N	0.19	0/1540	0.46	0/2085
14	n	0.19	0/1536	0.42	0/2080
15	O	0.19	0/1676	0.42	0/2271
15	o	0.17	0/1686	0.42	0/2282
16	P	0.19	0/1616	0.48	0/2180
16	p	0.21	0/1620	0.50	0/2184
17	Q	0.19	0/1621	0.42	0/2194
17	q	0.17	0/1621	0.41	0/2194
18	R	0.19	0/1590	0.44	0/2147
18	r	0.18	0/1590	0.43	0/2147
19	S	0.19	0/1671	0.47	0/2252
19	s	0.20	0/1684	0.47	0/2268



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.21	0/1716	0.47	0/2323
20	t	0.20	0/1720	0.46	0/2328
21	U	0.19	0/6488	0.50	0/8782
22	V	0.19	0/3681	0.43	0/4969
23	W	0.17	0/3644	0.45	0/4901
24	X	0.19	0/3381	0.48	0/4558
25	Y	0.19	0/3261	0.50	0/4393
26	Z	0.21	0/2324	0.59	0/3150
27	a	0.24	0/3053	0.57	0/4133
28	b	0.24	0/1478	0.59	0/2001
29	c	0.25	0/2302	0.60	0/3110
30	d	0.21	0/2162	0.57	0/2919
31	e	0.17	0/437	0.49	0/595
32	f	0.23	0/6640	0.55	4/8988 (0.0%)
33	u	0.25	0/607	0.44	0/816
34	v	0.01	0/8	0.05	0/8
All	All	0.21	1/107780 (0.0%)	0.50	12/145568 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	131	MET	C-N	6.38	1.42	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	N-CA-C	-10.29	100.03	111.14
4	D	86	PRO	N-CA-C	-9.00	103.16	114.68
3	C	288	ASN	CA-C-N	-6.08	114.34	122.98
3	C	288	ASN	C-N-CA	-6.08	114.34	122.98
32	f	89	MET	CA-C-N	5.88	136.85	126.45

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3164	0	3201	44	0
2	B	3099	0	3143	59	0
3	C	2978	0	3075	68	0
4	D	3039	0	3075	67	0
5	E	3097	0	3174	41	0
6	F	3251	0	3319	60	0
7	G	1889	0	1885	22	0
7	g	1880	0	1875	32	0
8	H	1805	0	1784	20	0
8	h	1805	0	1798	19	0
9	I	1955	0	1955	19	0
9	i	1955	0	1955	18	0
10	J	1880	0	1892	31	0
10	j	1861	0	1865	24	0
11	K	1777	0	1762	23	0
11	k	1782	0	1766	18	0
12	L	1866	0	1852	12	0
12	l	1861	0	1839	15	0
13	M	1876	0	1861	27	0
13	m	1881	0	1868	22	0
14	N	1514	0	1487	12	0
14	n	1510	0	1483	14	0
15	O	1649	0	1659	17	0
15	o	1659	0	1681	15	0
16	P	1587	0	1598	20	0
16	p	1591	0	1609	29	0
17	Q	1588	0	1584	24	0
17	q	1588	0	1584	19	0
18	R	1559	0	1523	16	0
18	r	1559	0	1523	12	0
19	S	1641	0	1639	25	0
19	s	1654	0	1656	15	0
20	T	1683	0	1662	22	0
20	t	1687	0	1666	20	0
21	U	6373	0	6409	87	0
22	V	3612	0	3682	58	0
23	W	3596	0	3713	52	0
24	X	3335	0	3435	38	0
25	Y	3202	0	3204	43	0
26	Z	2281	0	2312	41	0
27	a	2995	0	3012	52	0
28	b	1458	0	1505	26	0
29	c	2260	0	2276	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	24	0
31	e	425	0	328	7	0
32	f	6529	0	6541	112	0
33	u	601	0	629	16	0
34	v	143	0	46	2	0
35	A	31	0	12	1	0
35	D	31	0	12	0	0
35	F	31	0	12	1	0
36	A	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	B	27	0	12	3	0
37	E	27	0	12	3	0
38	c	1	0	0	0	0
All	All	106247	0	106596	1341	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 6.

The worst 5 of 1341 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)
32:f:585:GLU:HB2	32:f:586:PRO:HD2	1.49	0.93
3:C:44:ARG:HG3	22:V:496:PHE:HE2	1.38	0.88
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.59	0.83
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.63	0.80
7:g:130:GLU:HG2	8:h:5:GLY:HA2	1.63	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/433 (93%)	361 (89%)	41 (10%)	2 (0%)	24	63
2	B	395/440 (90%)	349 (88%)	43 (11%)	3 (1%)	16	53
3	C	379/398 (95%)	330 (87%)	47 (12%)	2 (0%)	24	63
4	D	378/418 (90%)	324 (86%)	51 (14%)	3 (1%)	16	53
5	E	387/403 (96%)	351 (91%)	35 (9%)	1 (0%)	36	71
6	F	413/439 (94%)	378 (92%)	35 (8%)	0	100	100
7	G	242/246 (98%)	233 (96%)	9 (4%)	0	100	100
7	g	242/246 (98%)	222 (92%)	19 (8%)	1 (0%)	30	67
8	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	248/261 (95%)	240 (97%)	7 (3%)	1 (0%)	30	67
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	223 (94%)	12 (5%)	2 (1%)	16	53
10	j	237/248 (96%)	226 (95%)	9 (4%)	2 (1%)	16	53
11	K	232/241 (96%)	221 (95%)	10 (4%)	1 (0%)	30	67
11	k	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
12	L	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
12	l	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
13	m	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
14	N	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
16	p	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	188 (95%)	9 (5%)	0	100	100
18	R	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
20	t	214/264 (81%)	204 (95%)	10 (5%)	0	100	100
21	U	812/953 (85%)	767 (94%)	45 (6%)	0	100	100
22	V	442/534 (83%)	434 (98%)	7 (2%)	1 (0%)	43	77
23	W	439/456 (96%)	433 (99%)	6 (1%)	0	100	100
24	X	420/422 (100%)	401 (96%)	19 (4%)	0	100	100
25	Y	387/389 (100%)	361 (93%)	25 (6%)	1 (0%)	36	71
26	Z	284/324 (88%)	255 (90%)	29 (10%)	0	100	100
27	a	371/376 (99%)	339 (91%)	31 (8%)	1 (0%)	36	71
28	b	189/377 (50%)	167 (88%)	22 (12%)	0	100	100
29	c	285/310 (92%)	259 (91%)	24 (8%)	2 (1%)	18	55
30	d	255/350 (73%)	213 (84%)	42 (16%)	0	100	100
31	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
32	f	840/908 (92%)	796 (95%)	39 (5%)	5 (1%)	21	58
33	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
34	v	1/28 (4%)	1 (100%)	0	0	100	100
All	All	13411/14980 (90%)	12599 (94%)	784 (6%)	28 (0%)	44	77

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	PRO
4	D	85	ILE
9	I	53	HIS
29	c	196	LEU
32	f	349	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	A	342/372 (92%)	338 (99%)	4 (1%)	63	73
2	B	345/385 (90%)	344 (100%)	1 (0%)	86	84
3	C	326/346 (94%)	320 (98%)	6 (2%)	51	67
4	D	333/366 (91%)	326 (98%)	7 (2%)	47	65
5	E	341/353 (97%)	339 (99%)	2 (1%)	78	80
6	F	357/379 (94%)	356 (100%)	1 (0%)	86	84
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	200 (99%)	2 (1%)	68	76
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	187 (100%)	1 (0%)	81	81
9	I	206/221 (93%)	205 (100%)	1 (0%)	81	81
9	i	206/221 (93%)	205 (100%)	1 (0%)	81	81
10	J	201/211 (95%)	198 (98%)	3 (2%)	57	70
10	j	196/211 (93%)	195 (100%)	1 (0%)	81	81
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	201 (100%)	1 (0%)	81	81
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	195 (100%)	1 (0%)	81	81
13	m	198/212 (93%)	197 (100%)	1 (0%)	81	81
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	167 (99%)	1 (1%)	78	80
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	695 (100%)	1 (0%)	88	88
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	81
24	X	362/362 (100%)	361 (100%)	1 (0%)	86	84
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	82
27	a	333/336 (99%)	331 (99%)	2 (1%)	78	80
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	250 (99%)	2 (1%)	73	77
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	706 (99%)	5 (1%)	76	79
33	u	68/68 (100%)	68 (100%)	0	100	100
34	v	1/1 (100%)	0	1 (100%)	0	0
All	All	11459/12683 (90%)	11410 (100%)	49 (0%)	81	82

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

Mol	Chain	Res	Type
21	U	527	GLN
29	c	196	LEU
23	W	345	GLU
26	Z	103	LYS
32	f	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	167	GLN
15	o	116	HIS
26	Z	189	GLN
14	n	106	GLN
9	i	142	HIS



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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
37	ADP	E	401	-	27,29,29	1.36	4 (14%)	42,45,45	2.02	9 (21%)
35	ATP	A	501	36	29,33,33	0.30	0	44,52,52	0.47	1 (2%)
37	ADP	B	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.02	10 (23%)
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.47	0
35	ATP	F	501	36	29,33,33	0.30	0	44,52,52	0.51	1 (2%)

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
37	ADP	E	401	-	-	3/16/32/32	0/3/3/3
35	ATP	A	501	36	-	2/22/38/38	0/3/3/3
37	ADP	B	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	D	501	36	-	5/22/38/38	0/3/3/3
35	ATP	F	501	36	-	2/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	401	ADP	C5-C4	4.59	1.47	1.39
37	B	501	ADP	C5-C4	4.57	1.47	1.39
37	B	501	ADP	C5-C6	2.59	1.48	1.41
37	E	401	ADP	C5-C6	2.56	1.48	1.41
37	E	401	ADP	C5-N7	-2.36	1.34	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	401	ADP	C5-C4-N3	-6.63	118.10	126.75
37	B	501	ADP	C5-C4-N3	-6.53	118.23	126.75
37	E	401	ADP	N3-C4-N9	5.30	135.82	127.08
37	B	501	ADP	N3-C4-N9	5.16	135.59	127.08
37	E	401	ADP	C2-N3-C4	3.90	120.97	111.75

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

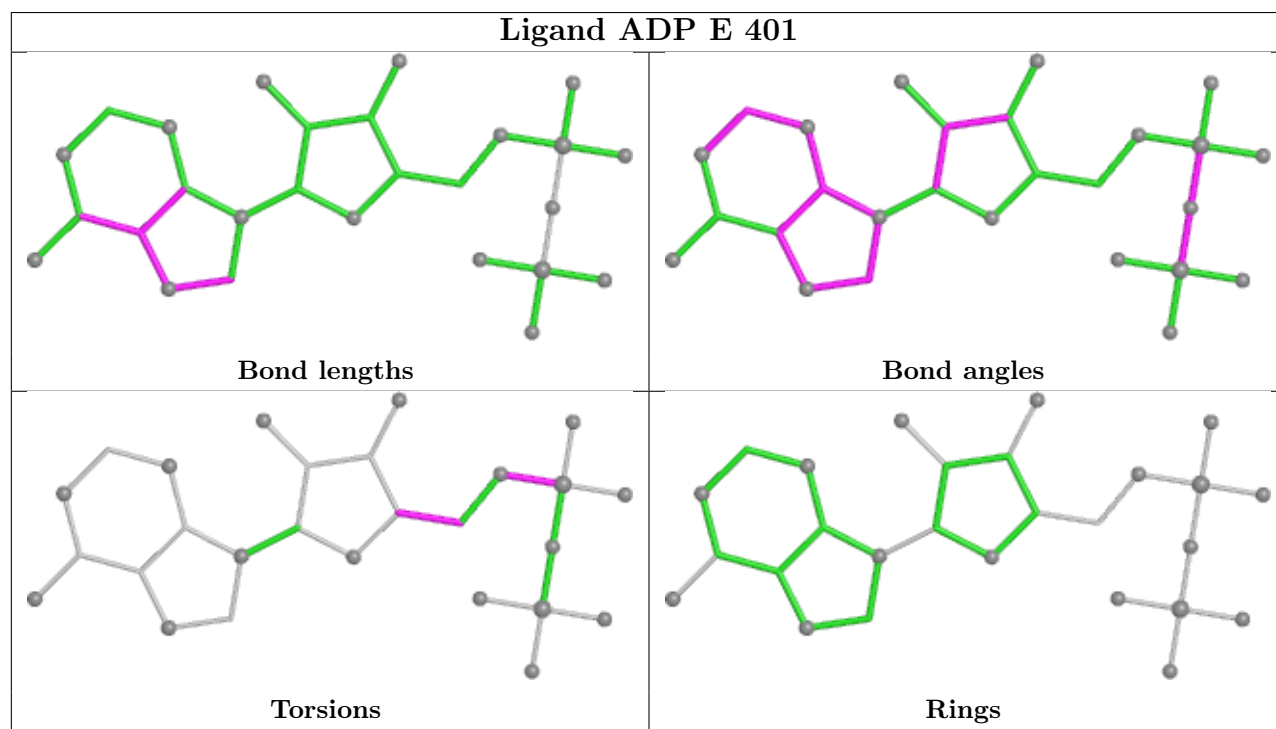
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	3	0
35	A	501	ATP	1	0
37	B	501	ADP	3	0
35	F	501	ATP	1	0

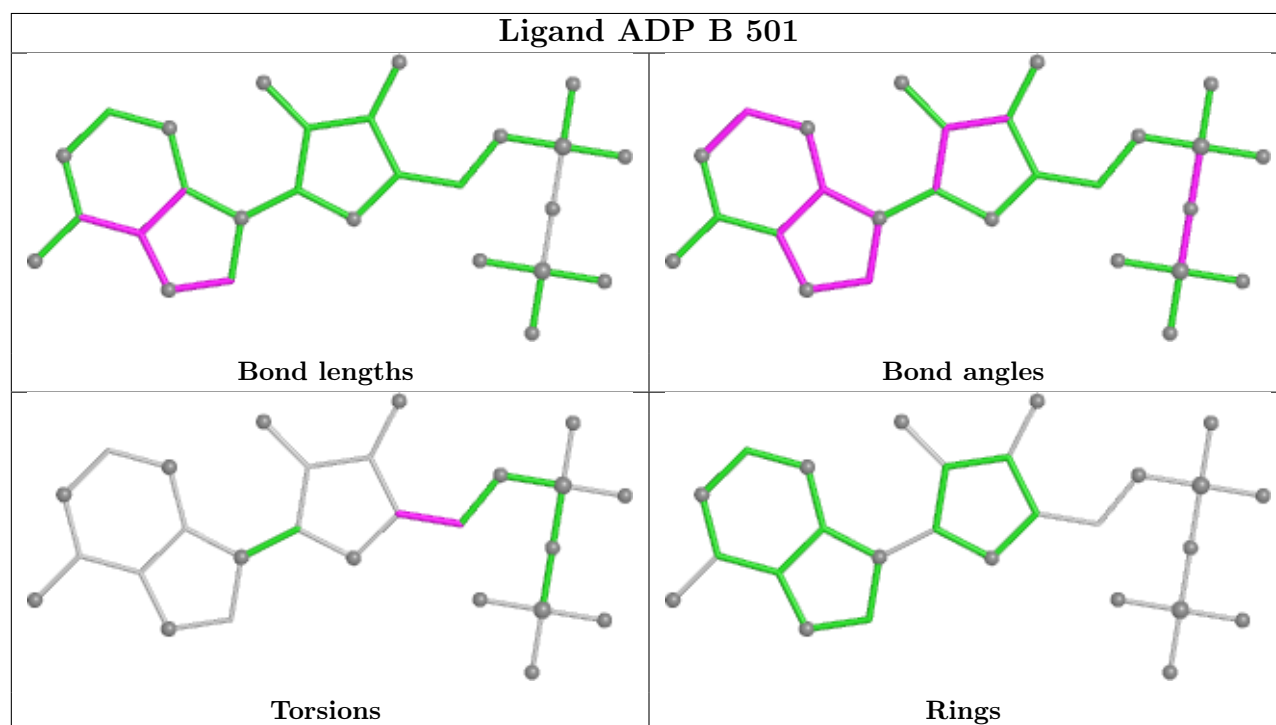
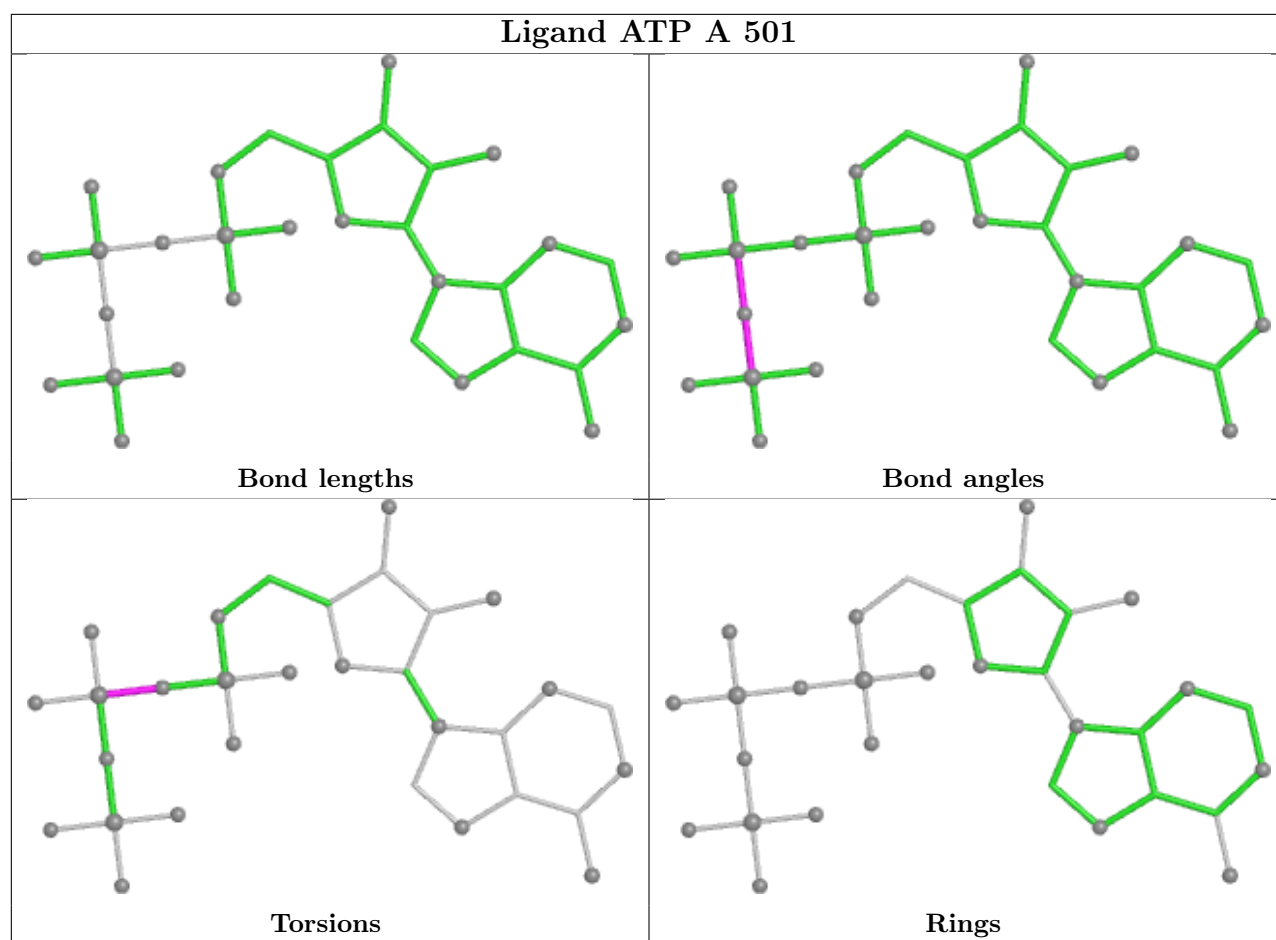
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



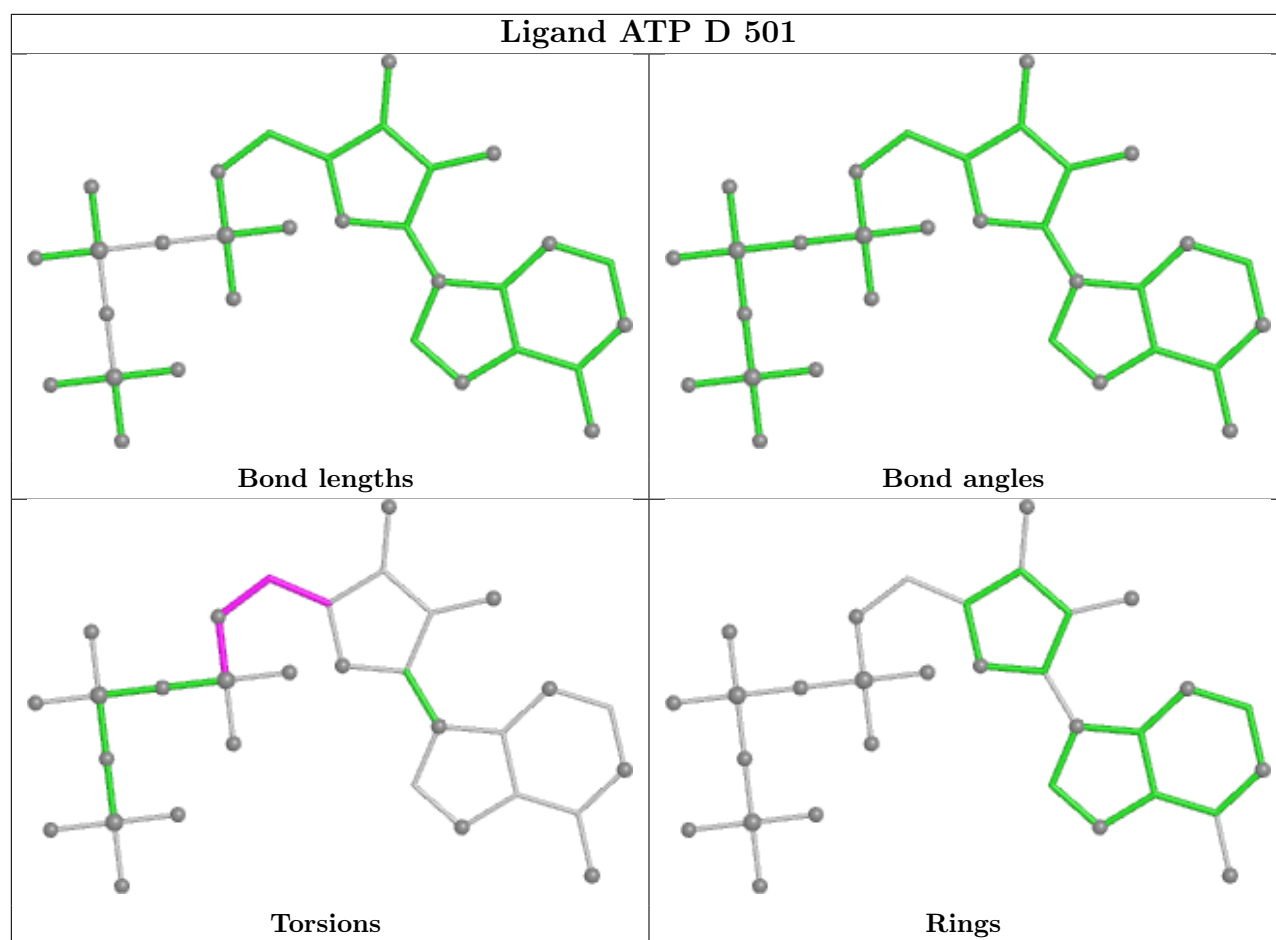
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



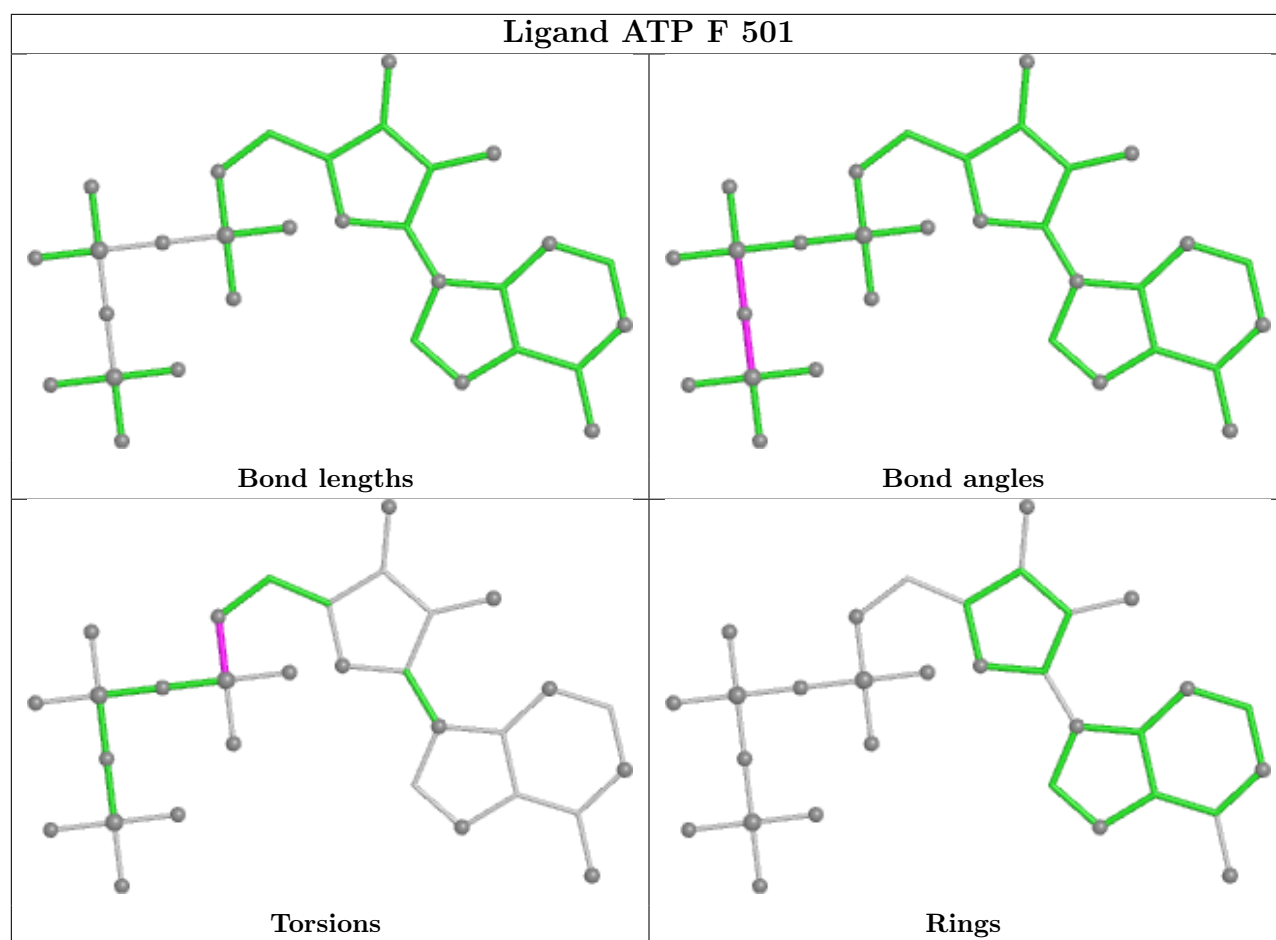












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



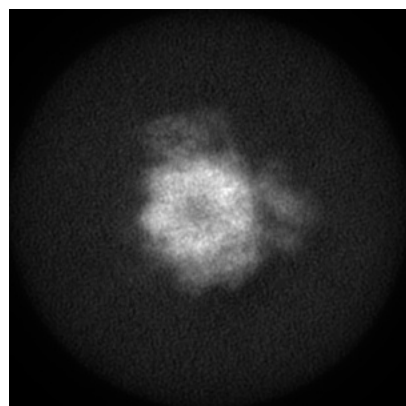
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62084. These allow visual inspection of the internal detail of the map and identification of artifacts.

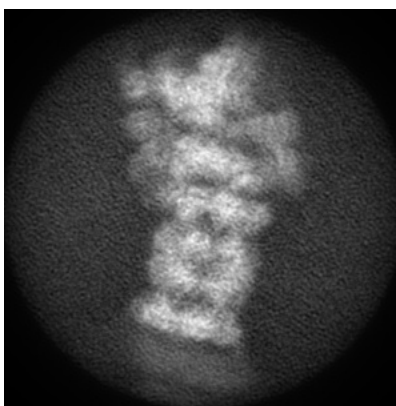
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

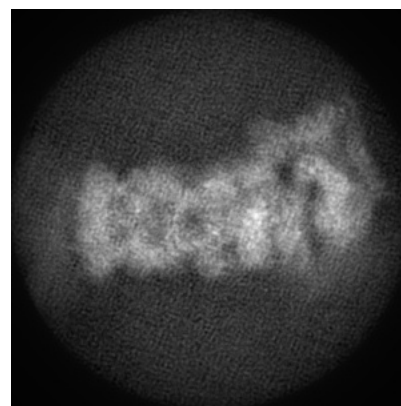
#### 6.1.1 Primary map



X

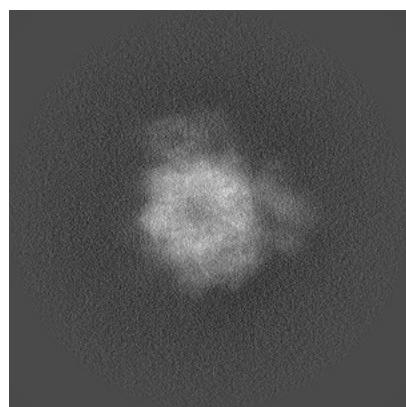


Y

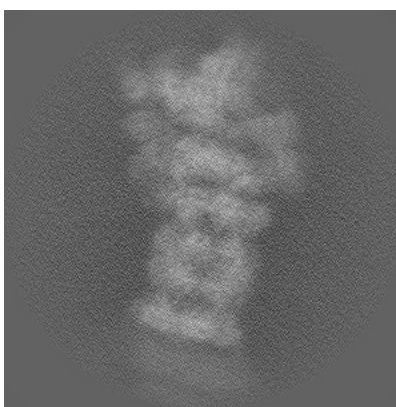


Z

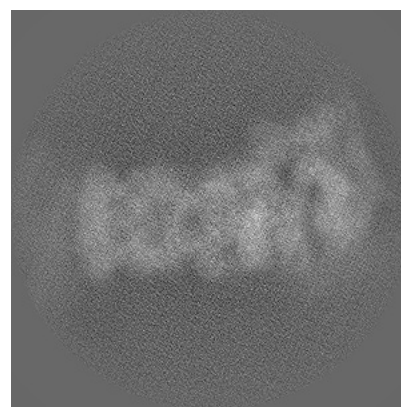
#### 6.1.2 Raw map



X



Y



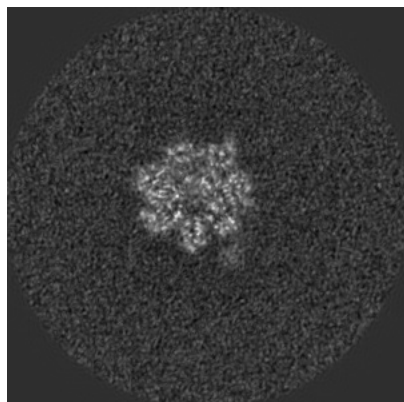
Z

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

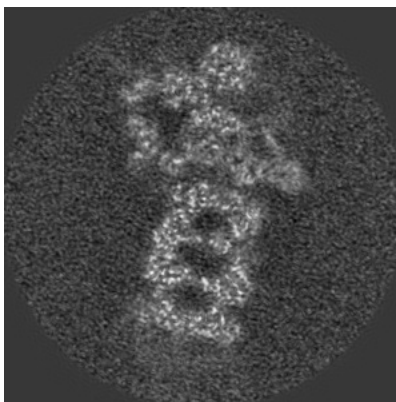


## 6.2 Central slices [i](#)

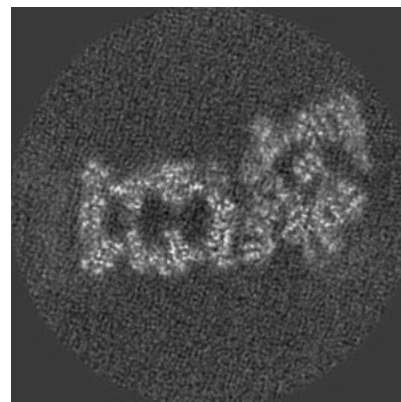
### 6.2.1 Primary map



X Index: 300

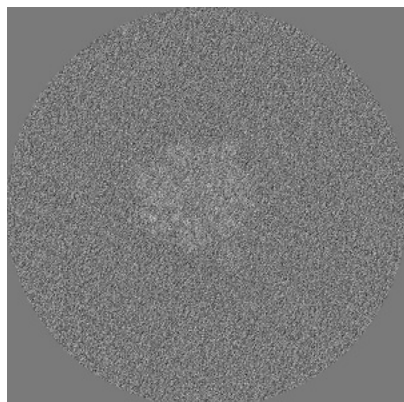


Y Index: 300

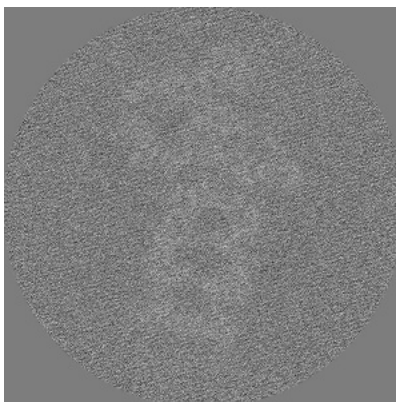


Z Index: 300

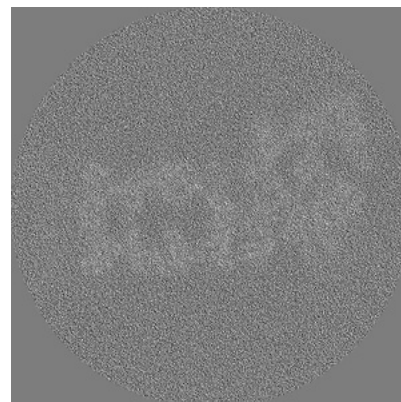
### 6.2.2 Raw map



X Index: 300



Y Index: 300



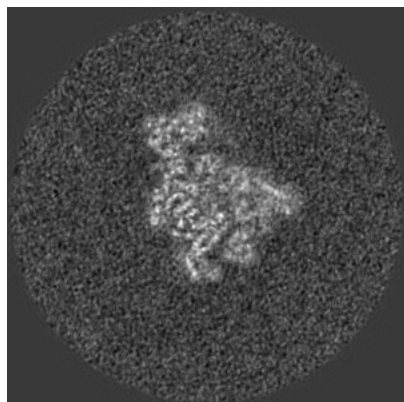
Z Index: 300

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

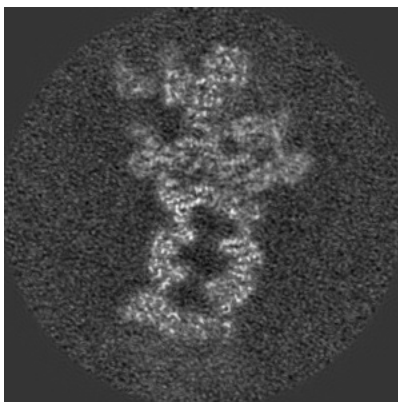


## 6.3 Largest variance slices [i](#)

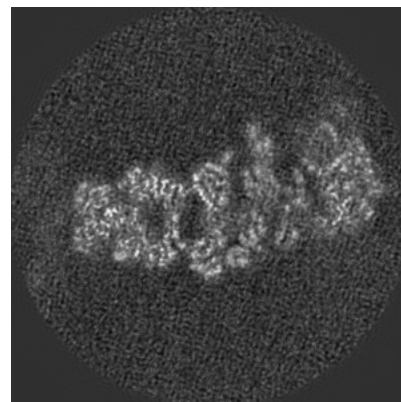
### 6.3.1 Primary map



X Index: 372

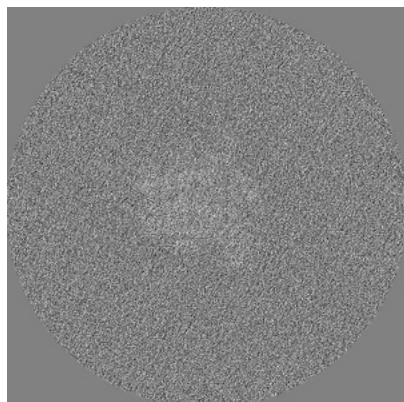


Y Index: 286

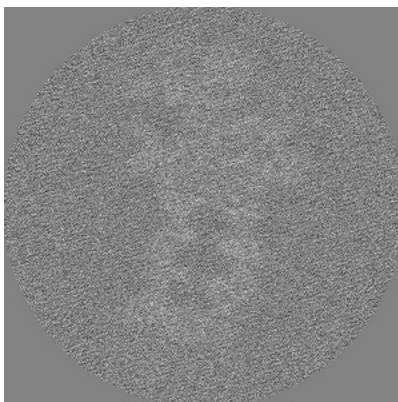


Z Index: 329

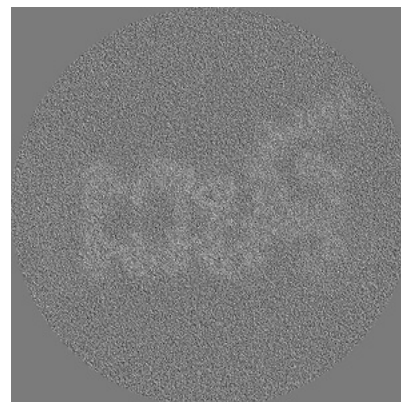
### 6.3.2 Raw map



X Index: 311



Y Index: 288



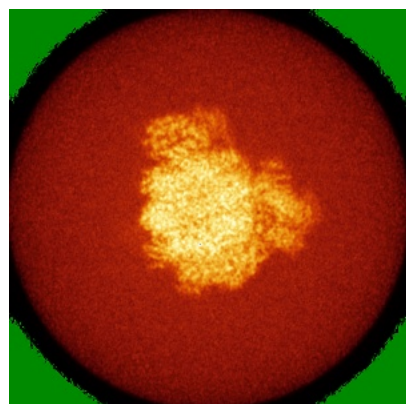
Z Index: 284

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

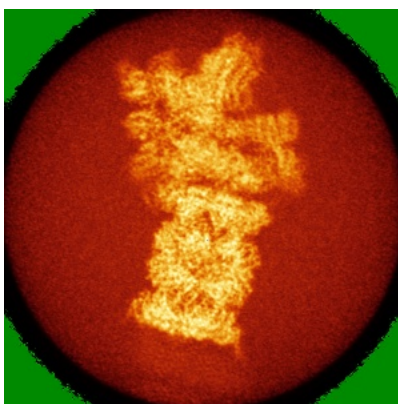


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

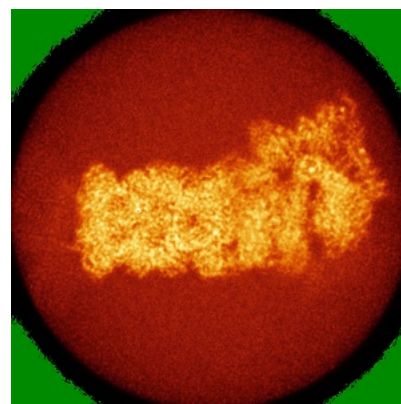
### 6.4.1 Primary map



X

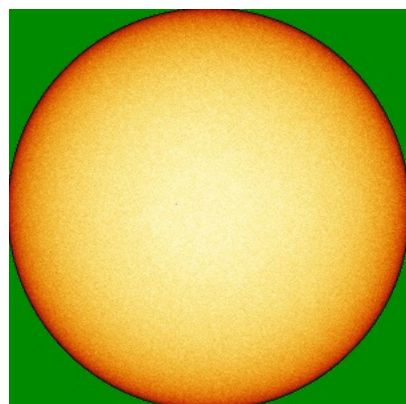


Y

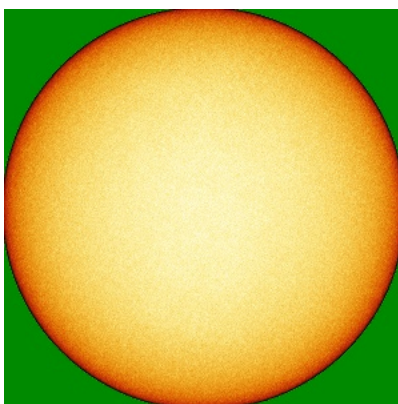


Z

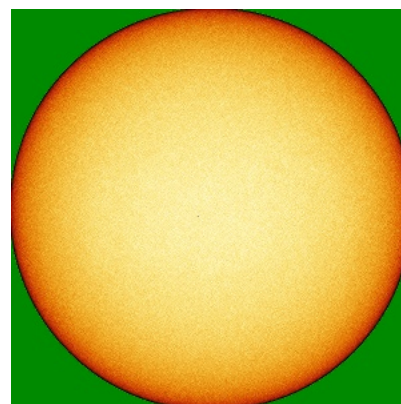
### 6.4.2 Raw map



X



Y



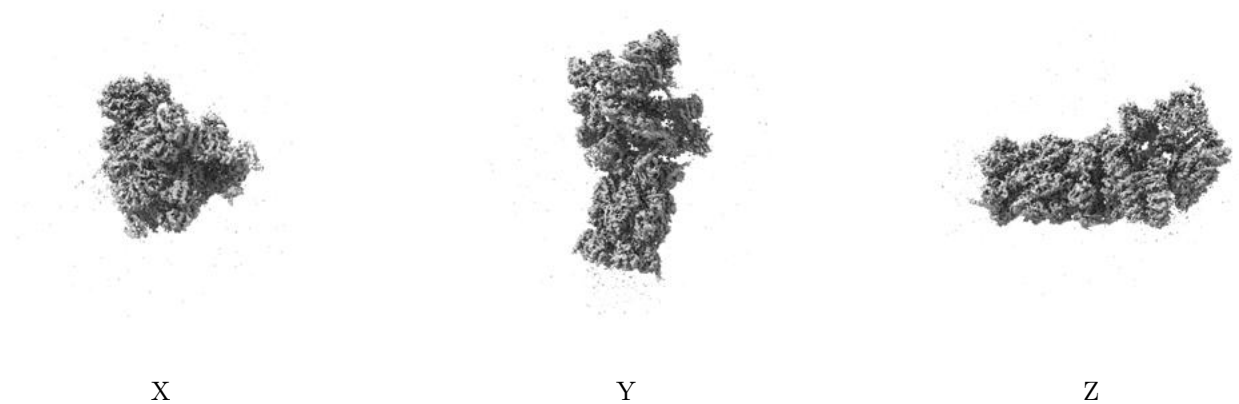
Z

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.



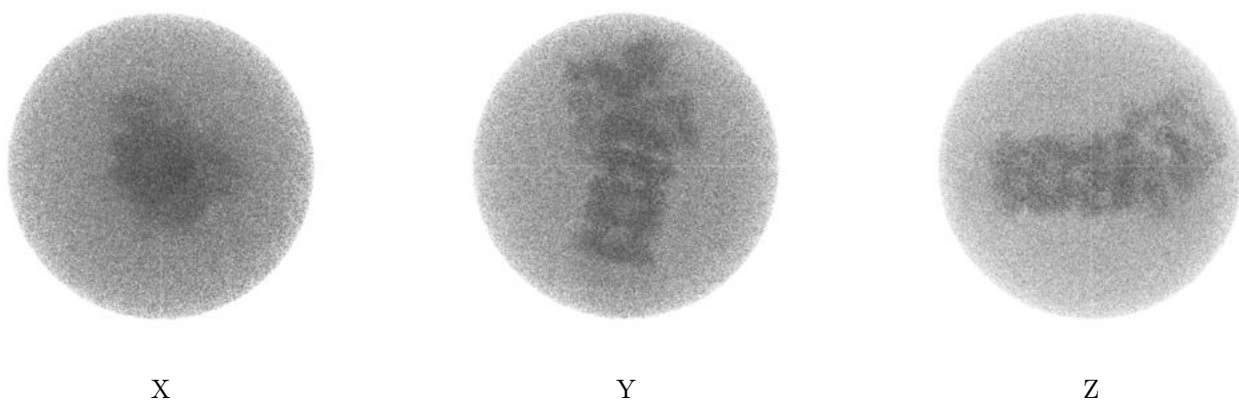
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00588. 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](#)

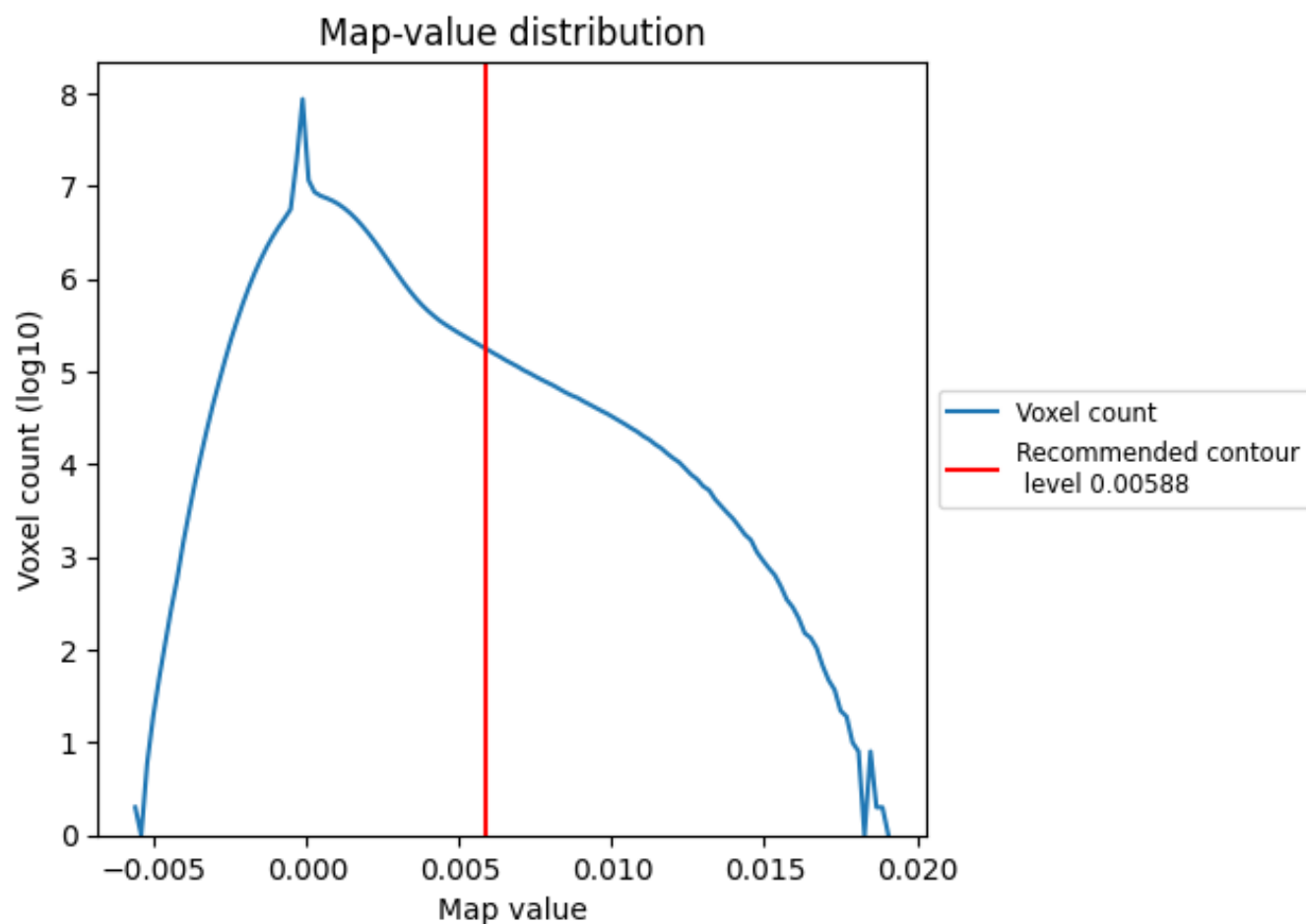
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

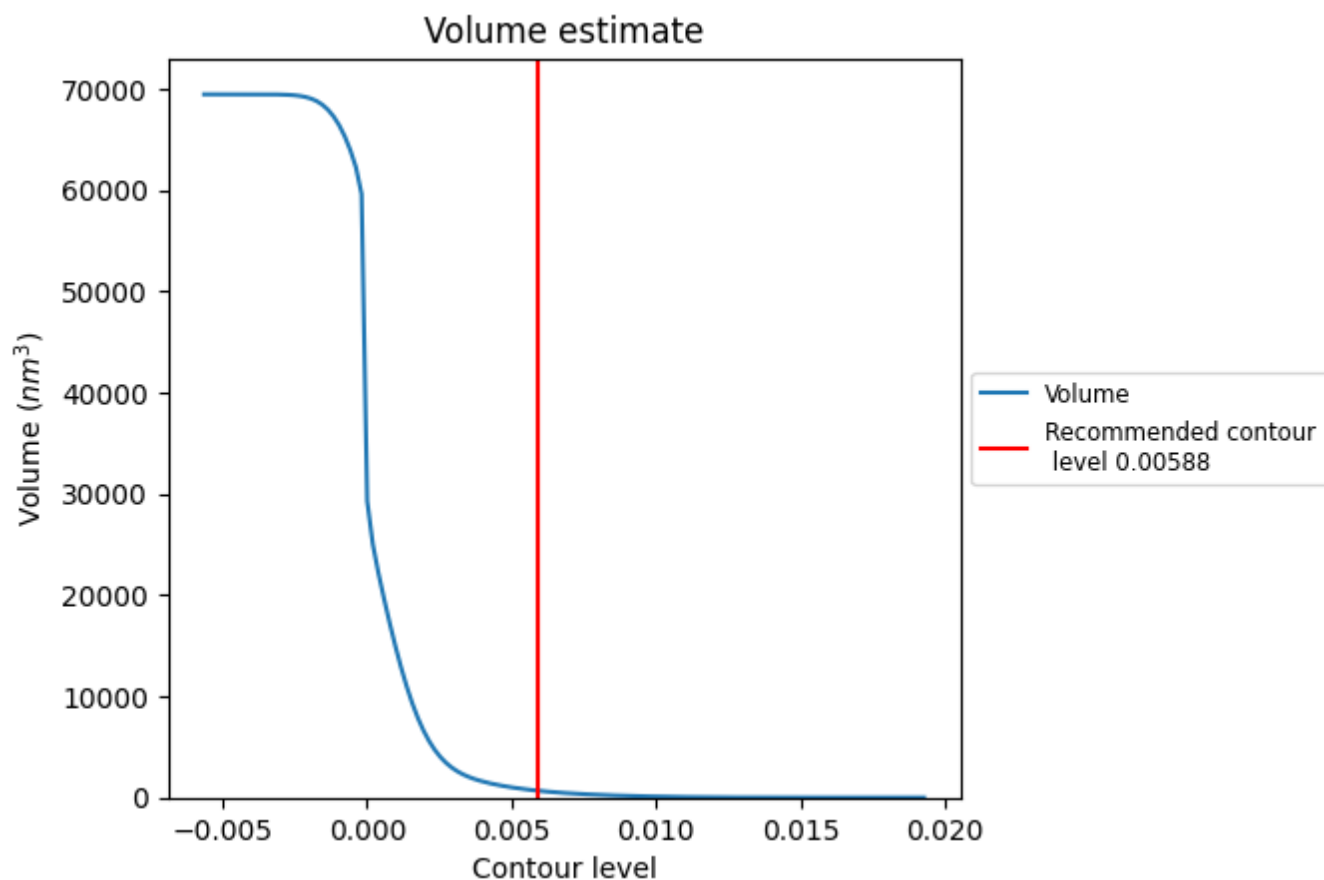
### 7.1 Map-value distribution [i](#)



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](#)

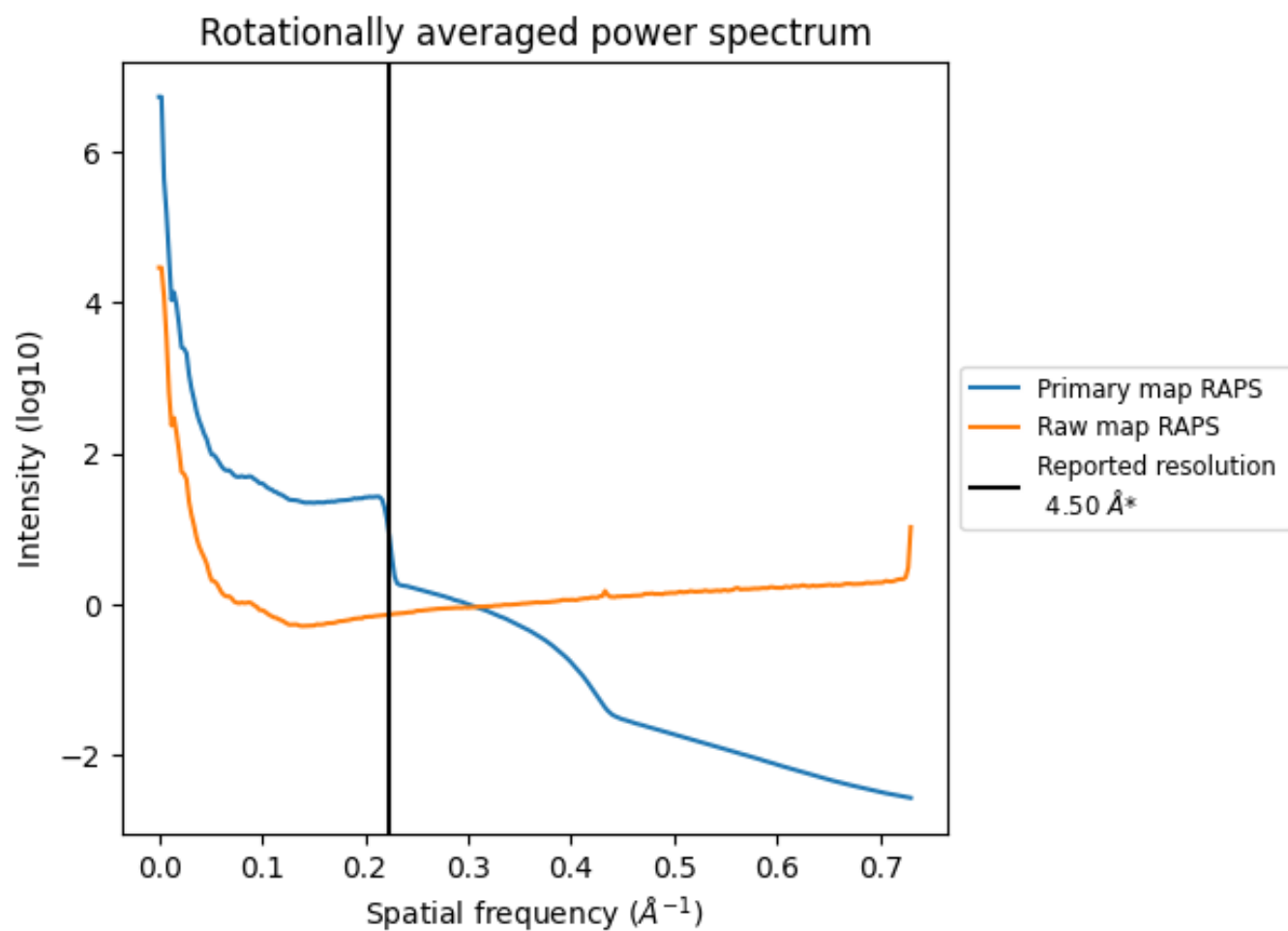


The volume at the recommended contour level is 688 nm<sup>3</sup>; this corresponds to an approximate mass of 621 kDa.

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 ⓘ



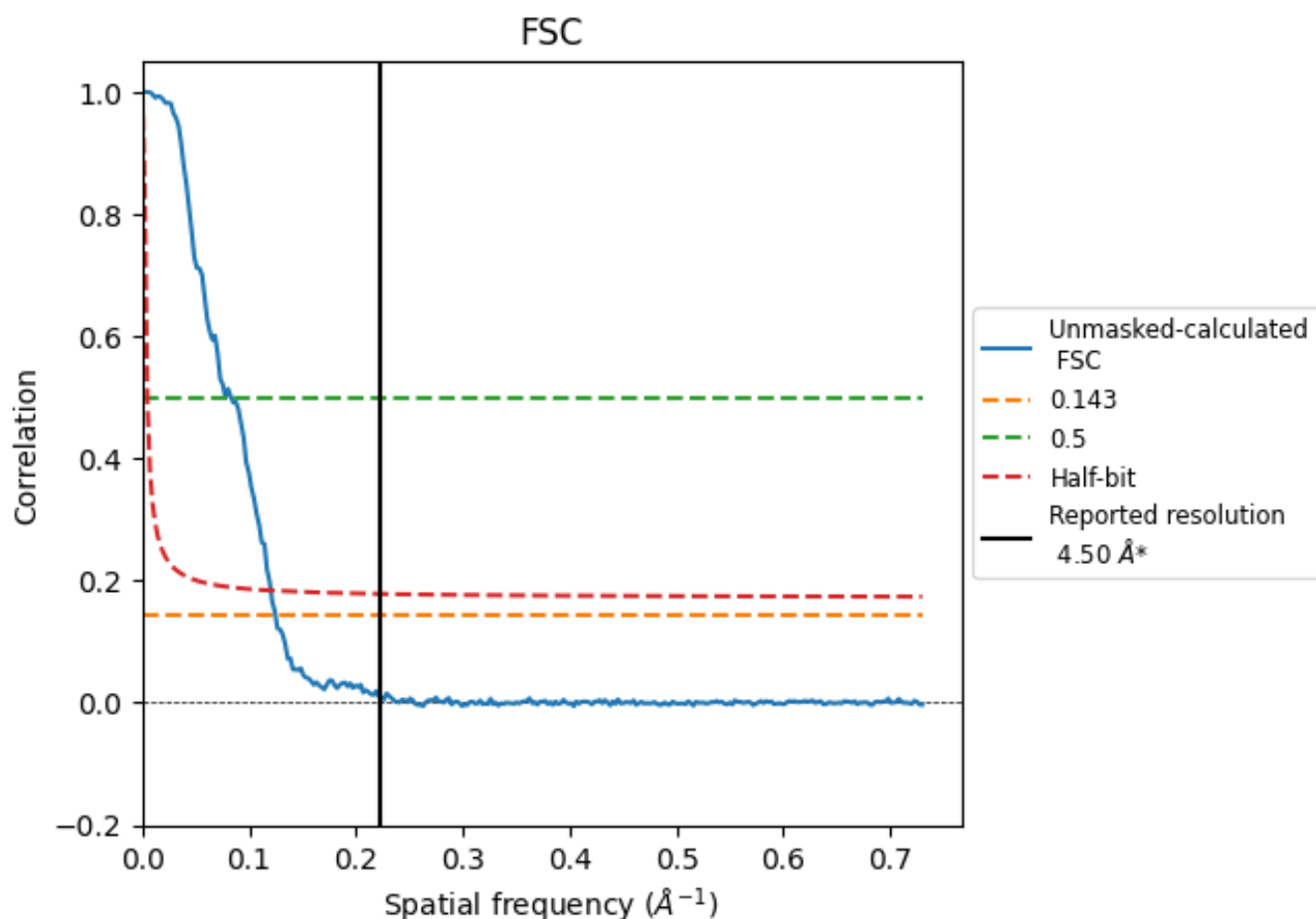
\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.222 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	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.02	12.87	8.31

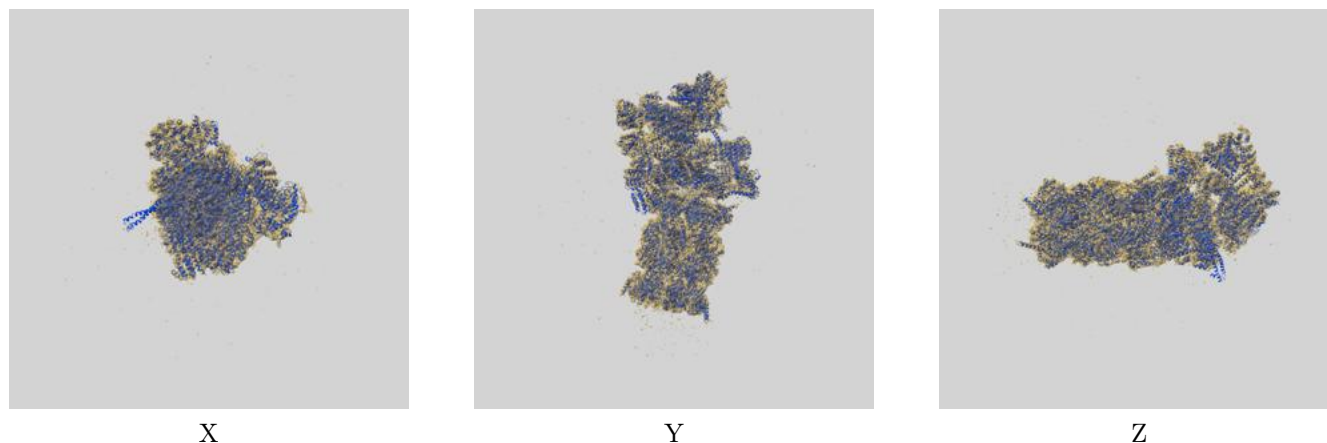
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.02 differs from the reported value 4.5 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-62084 and PDB model 9K58. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

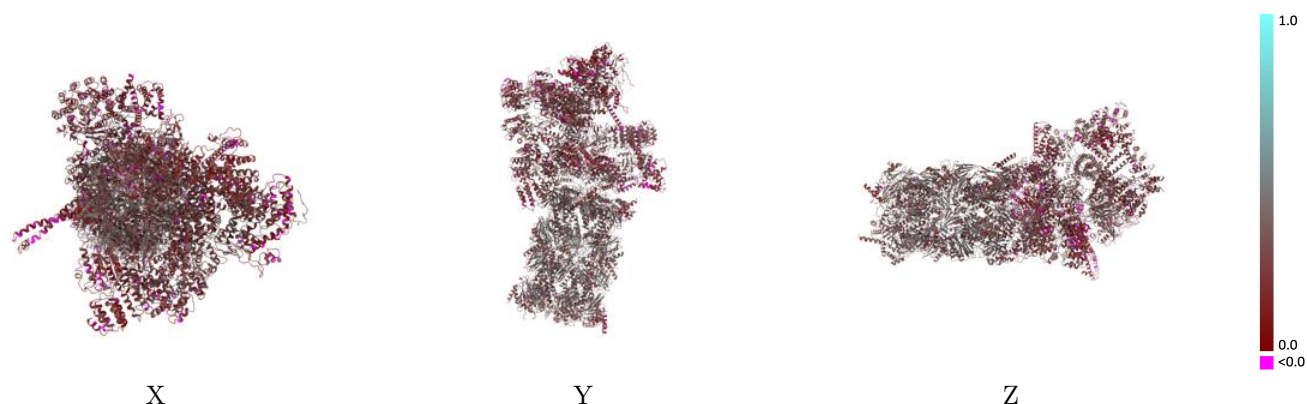
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.00588 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.

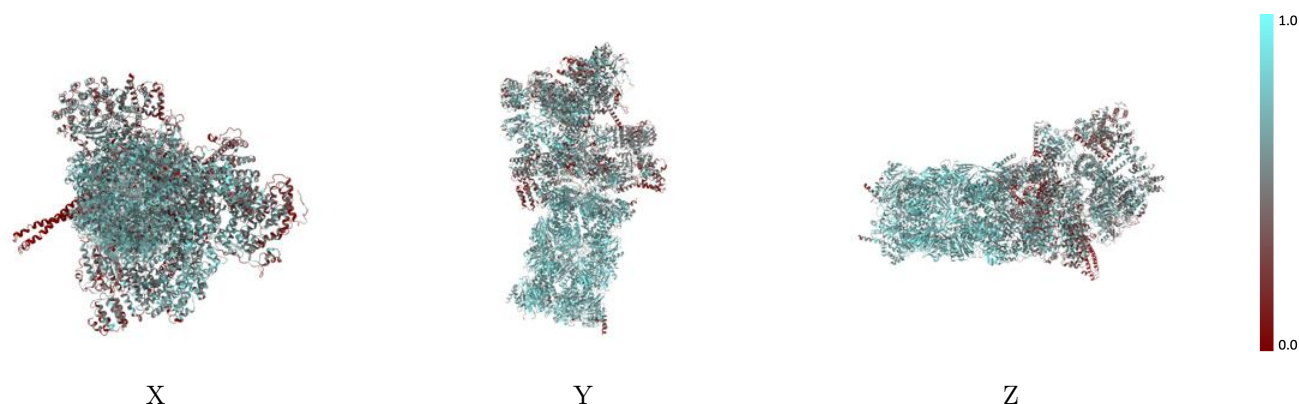


## 9.2 Q-score mapped to coordinate model [i](#)



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.

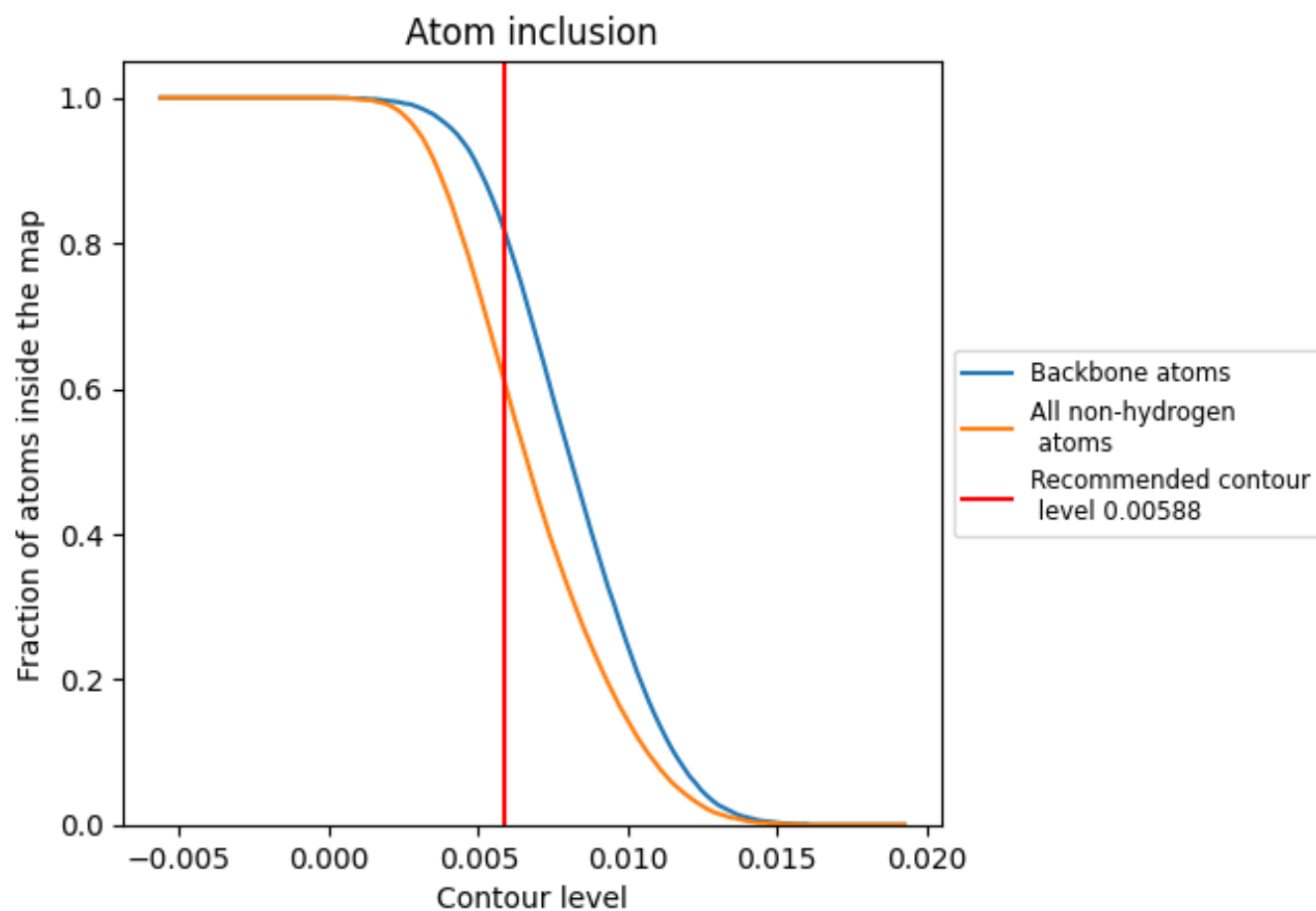
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.00588).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 82% of all backbone atoms, 61% 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 (0.00588) and Q-score for the entire model and for each chain.





























Chain	Atom inclusion	Q-score
All	 0.6100	 0.2990
A	 0.5490	 0.2770
B	 0.5110	 0.2630
C	 0.4650	 0.2390
D	 0.5650	 0.2890
E	 0.5620	 0.2890
F	 0.5300	 0.2890
G	 0.6970	 0.3580
H	 0.7220	 0.3630
I	 0.6820	 0.3340
J	 0.6450	 0.3100
K	 0.6740	 0.3470
L	 0.7270	 0.3620
M	 0.7080	 0.3400
N	 0.7540	 0.3660
O	 0.7610	 0.3640
P	 0.7640	 0.3780
Q	 0.7660	 0.3620
R	 0.7720	 0.3560
S	 0.7440	 0.3650
T	 0.7610	 0.3700
U	 0.5520	 0.2590
V	 0.4900	 0.2460
W	 0.5600	 0.2640
X	 0.4610	 0.2560
Y	 0.5660	 0.2360
Z	 0.6080	 0.3000
a	 0.5160	 0.2300
b	 0.4330	 0.2630
c	 0.6210	 0.3180
d	 0.3720	 0.1890
e	 0.4080	 0.2260
f	 0.4310	 0.2110
g	 0.7100	 0.3460
h	 0.7130	 0.3390



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Chain	Atom inclusion	Q-score
i	 0.6820	 0.3420
j	 0.6350	 0.3120
k	 0.6780	 0.3420
l	 0.7280	 0.3440
m	 0.7260	 0.3450
n	 0.7490	 0.3680
o	 0.7540	 0.3680
p	 0.7480	 0.3520
q	 0.7520	 0.3490
r	 0.7680	 0.3570
s	 0.7210	 0.3530
t	 0.7710	 0.3540
u	 0.5240	 0.2470
v	 0.2940	 0.1980