



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 08:28 PM JST

PDB ID : 9K5D / pdb_00009k5d
EMDB ID : EMD-62089
Title : Structure of substrate-engaged single-cap human proteasome in state ED2
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

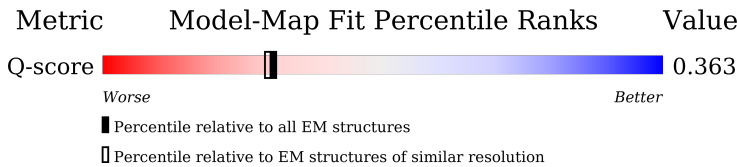
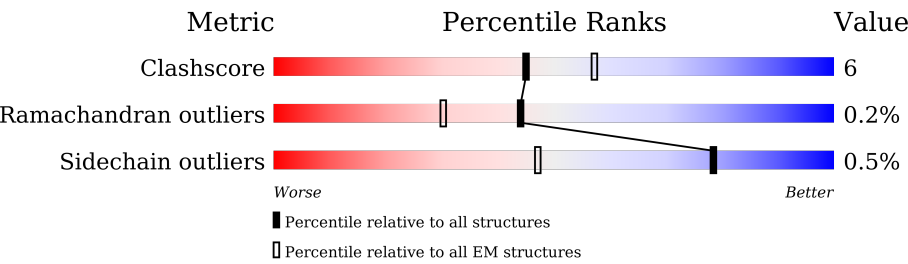
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	









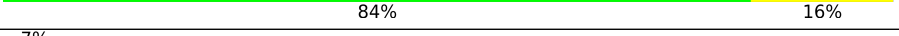
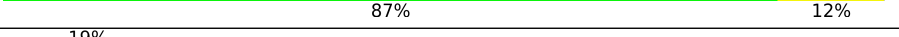
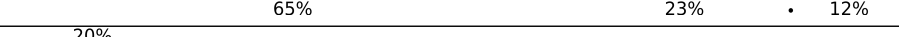

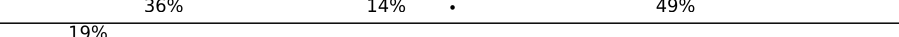
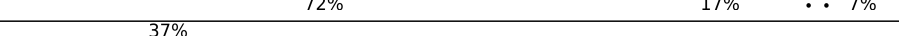



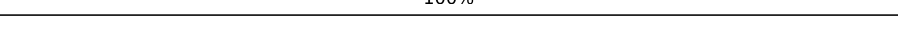
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	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	v	36	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106302 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	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- 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
			3040	1923	524	580	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	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	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
			1801	1149	304	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	248	Total	C	N	O	S	0	0
			1933	1222	330	371	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
			1861	1166	327	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	238	Total	C	N	O	S	0	0
			1813	1139	302	361	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	240	Total	C	N	O	S	0	0
			1876	1175	338	352	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	242	Total	C	N	O	S	0	0
			1890	1200	323	356	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	203	Total	C	N	O	S	0	0
			1521	954	259	296	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
			1645	1035	278	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
			1578	1012	267	290	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
			1549	977	270	293	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
			1650	1044	283	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	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- 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		

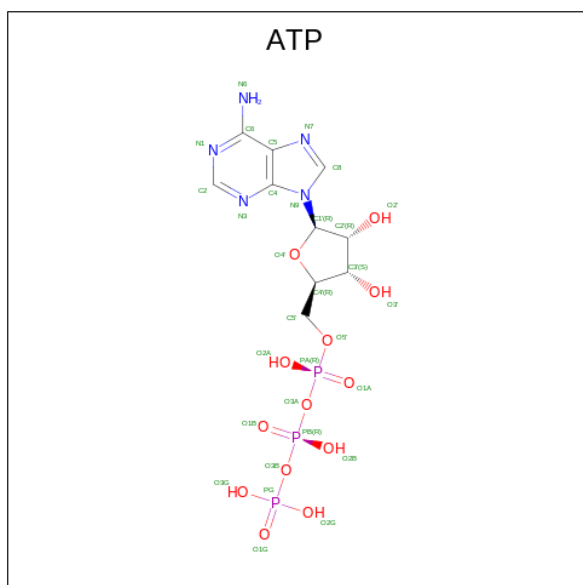
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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 Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	36	Total	C	N	O	0	0
			180	108	36	36		

- 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).



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

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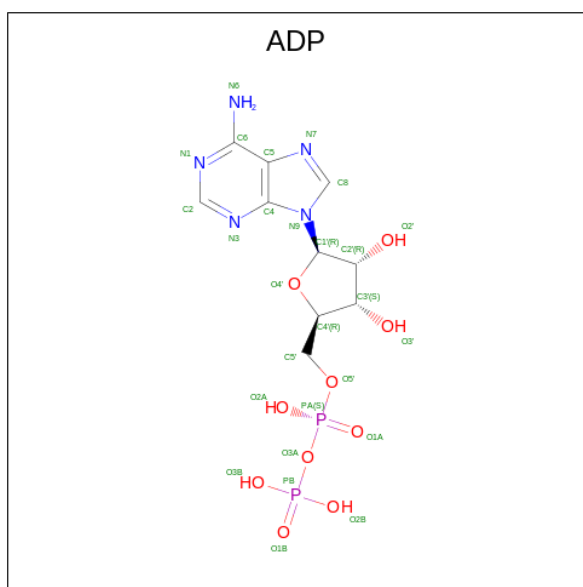
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Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

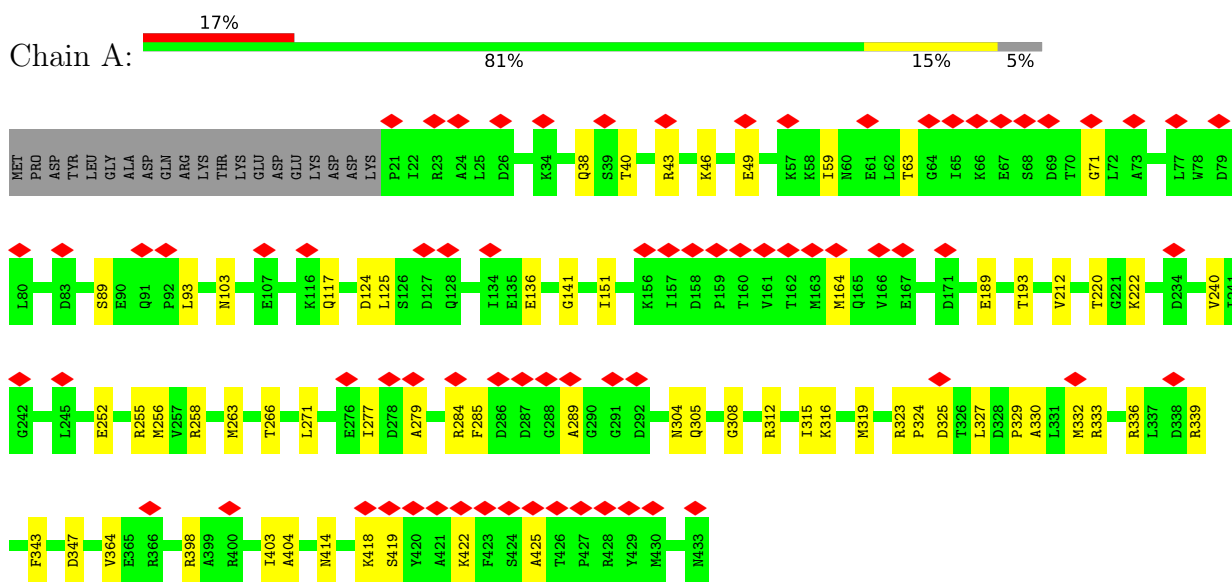
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

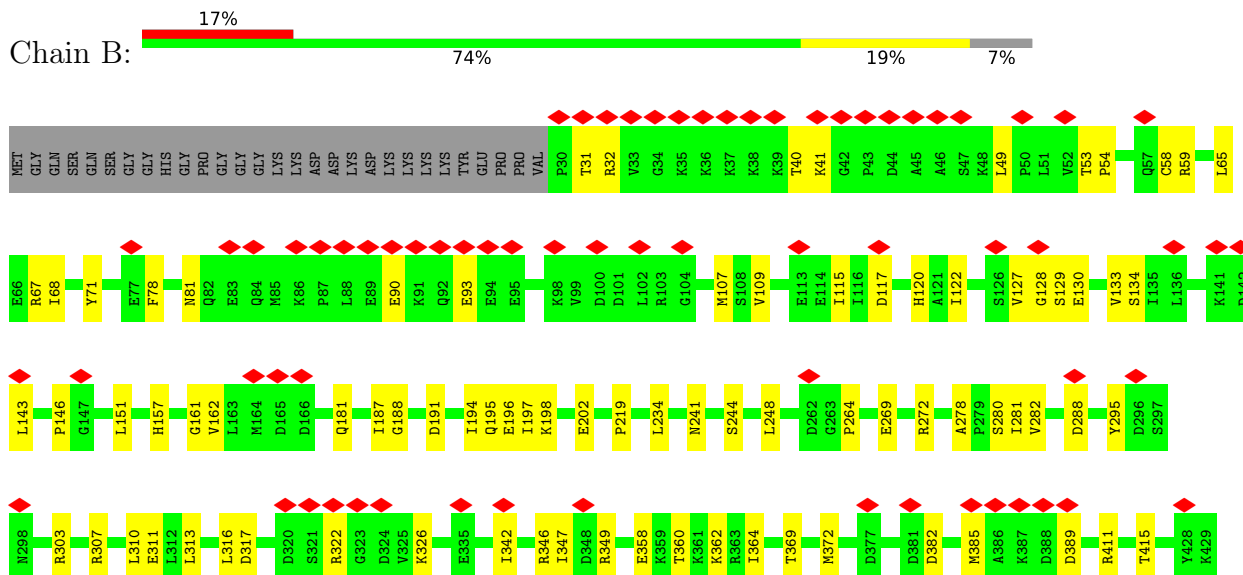
3 Residue-property plots

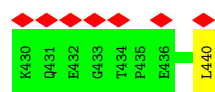
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome regulatory subunit 7

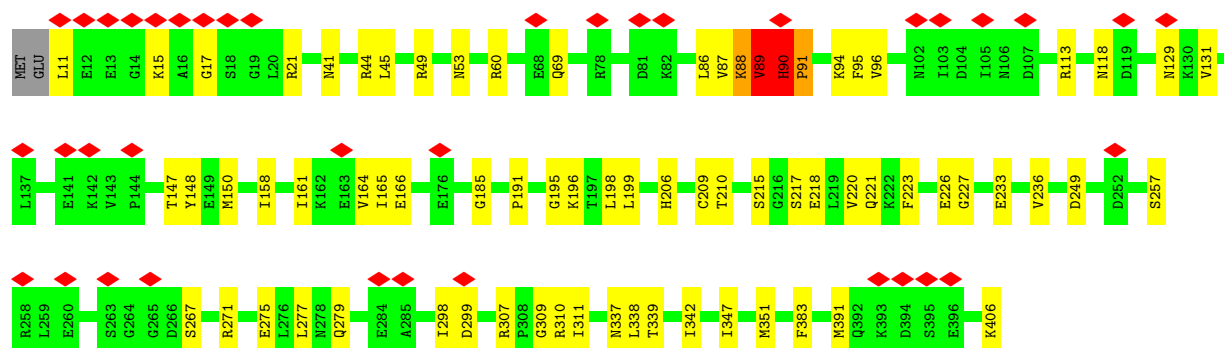
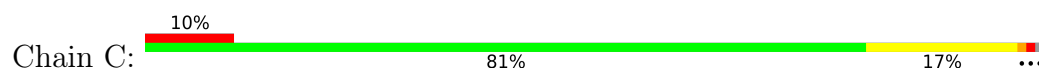


- Molecule 2: 26S proteasome regulatory subunit 4

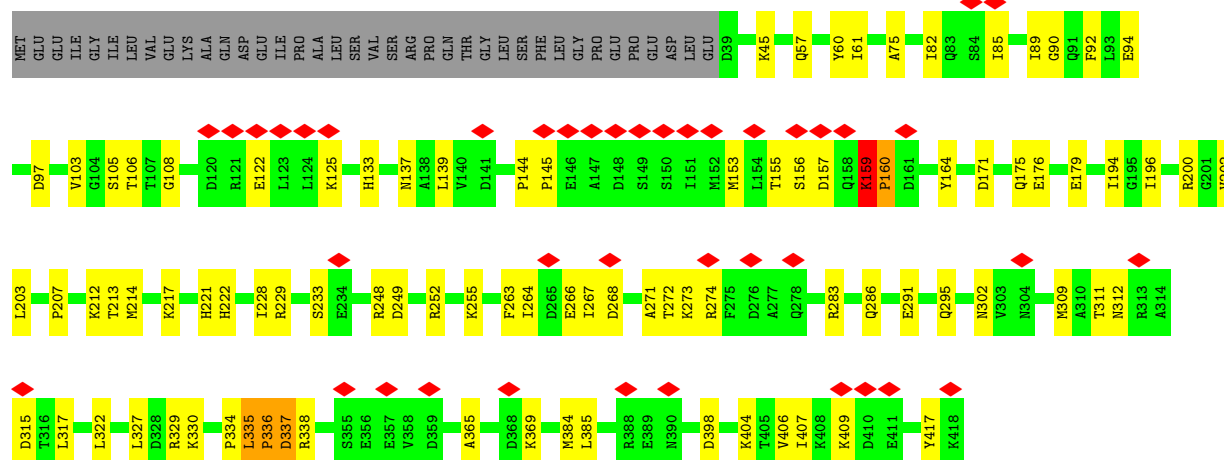




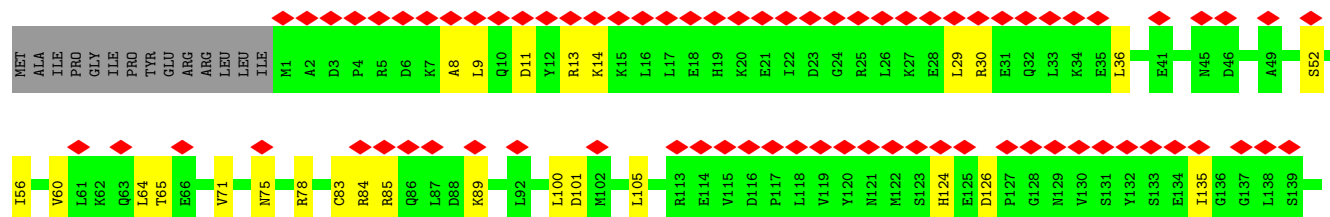
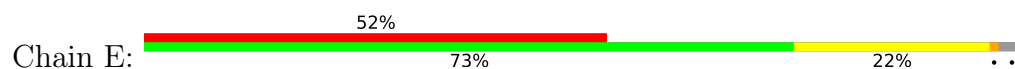
• Molecule 3: 26S proteasome regulatory subunit 8

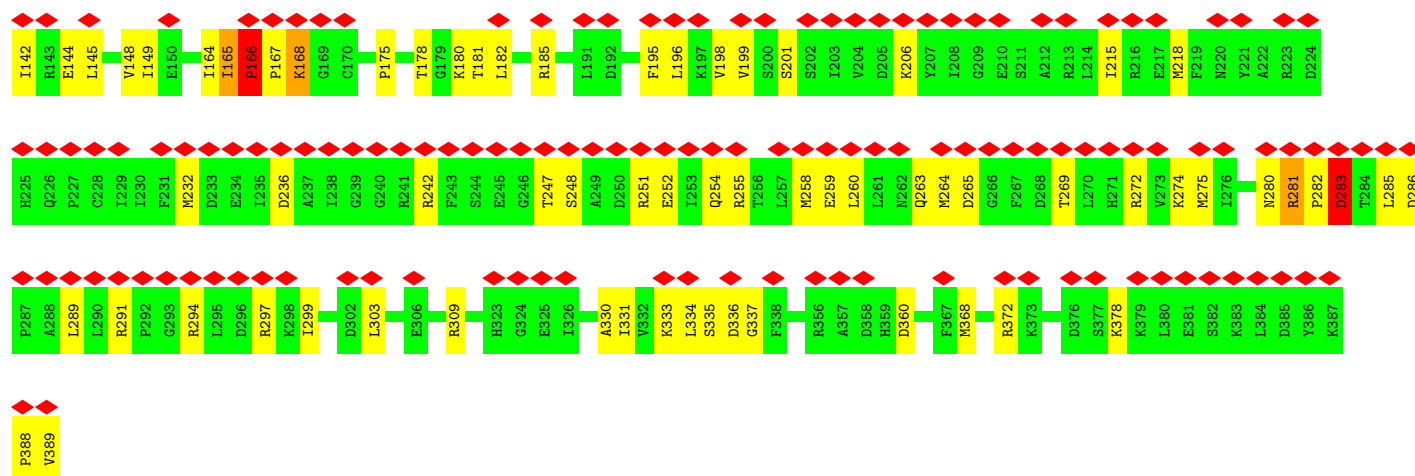


• Molecule 4: 26S proteasome regulatory subunit 6B



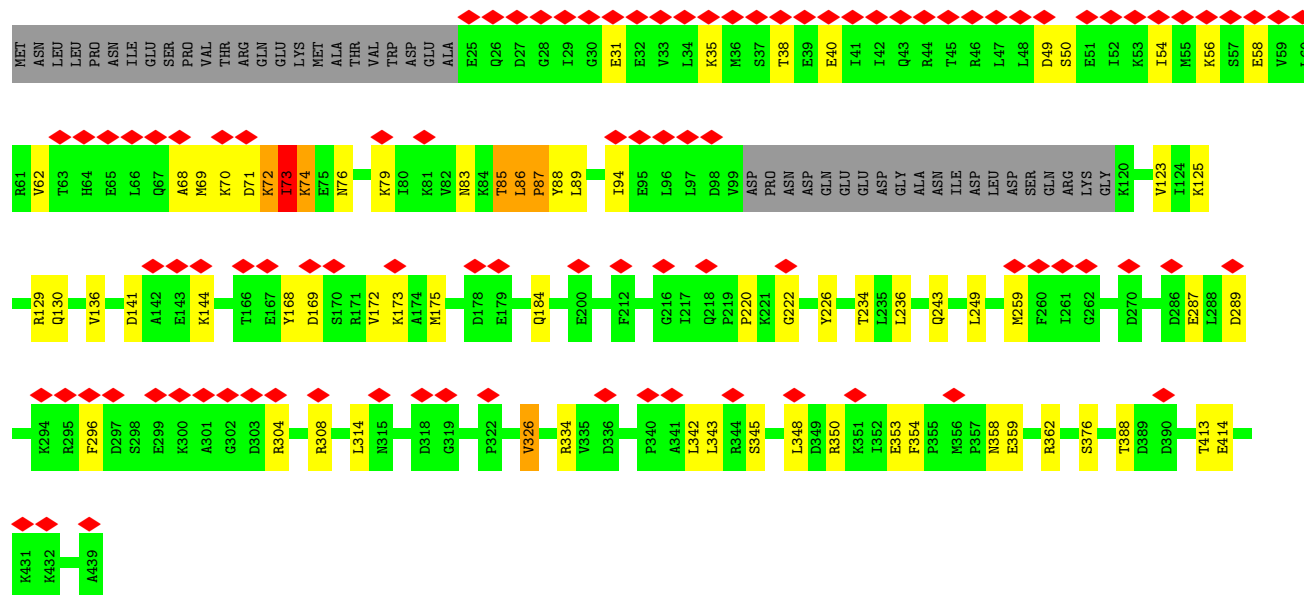
• Molecule 5: Proteasome 26S subunit, ATPase 6





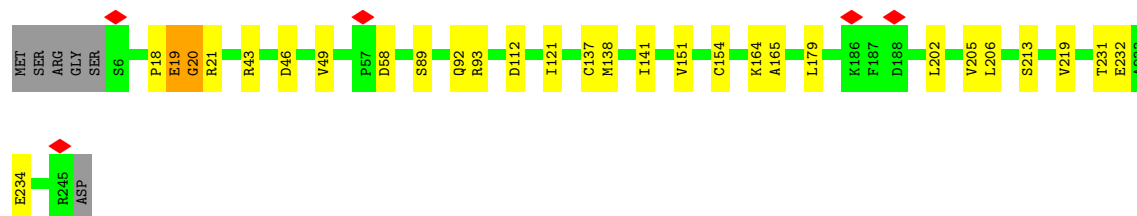
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 22% 74% 14% 10%




- Molecule 7: Proteasome subunit alpha type-6

Chain G: 86% 11%




- Molecule 7: Proteasome subunit alpha type-6

Chain g:  91% 9%




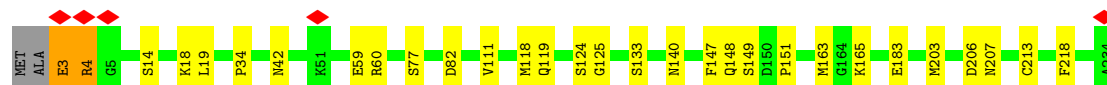
- Molecule 8: Proteasome subunit alpha type-2

Chain H:  88% 12%




- Molecule 8: Proteasome subunit alpha type-2

Chain h:  86% 12%




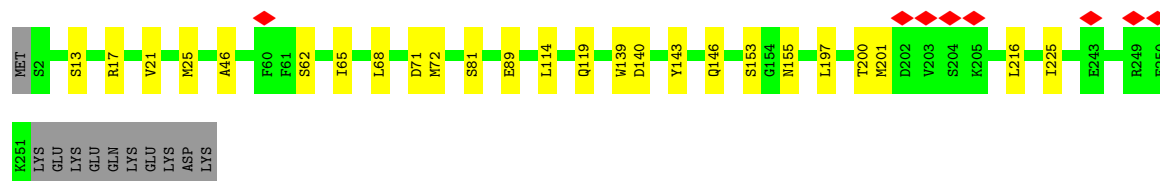
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  88% 7% 5%




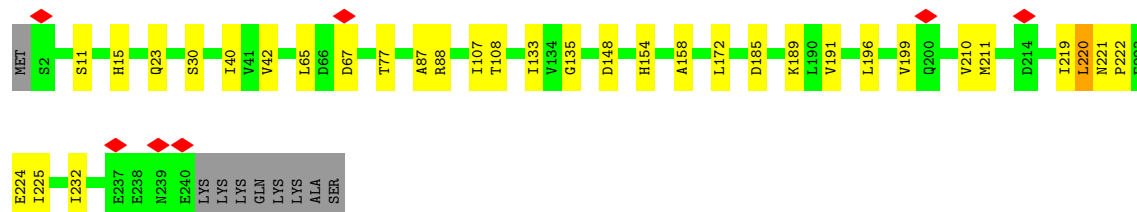
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  86% 10%

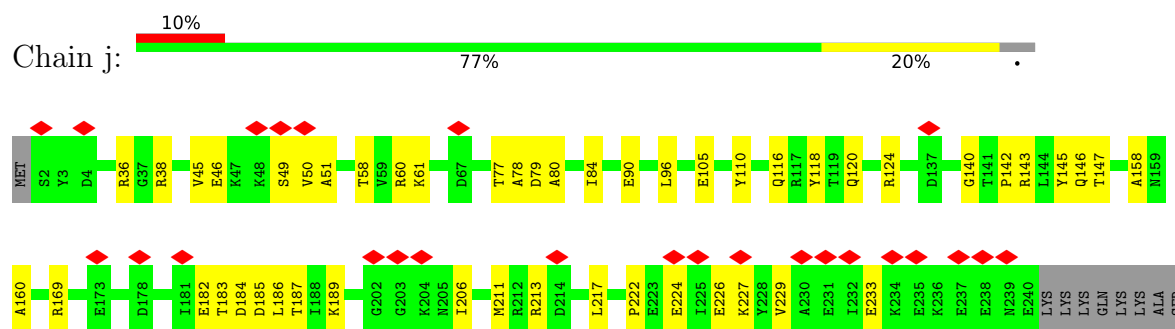


- Molecule 10: Proteasome subunit alpha type-7

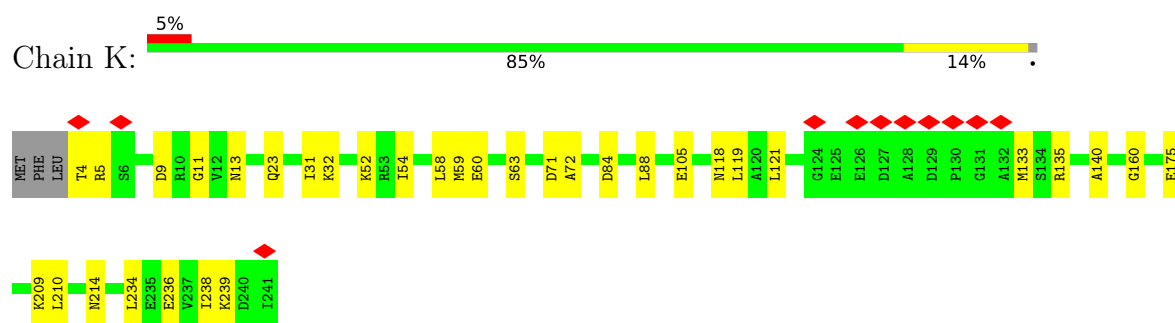
Chain J:  83% 13%



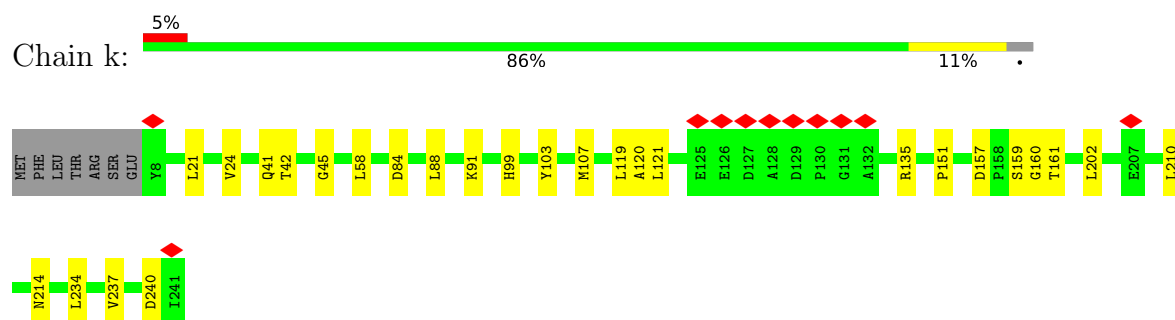
- Molecule 10: Proteasome subunit alpha type-7



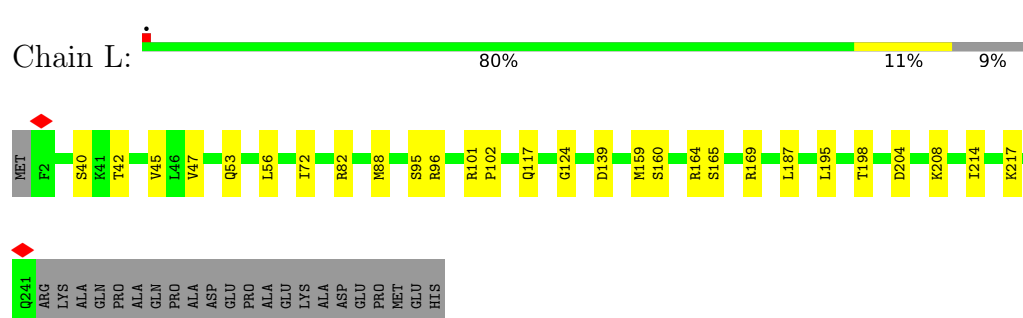
- Molecule 11: Proteasome subunit alpha type-5



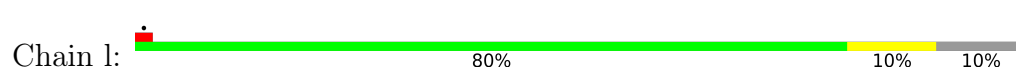
- Molecule 11: Proteasome subunit alpha type-5

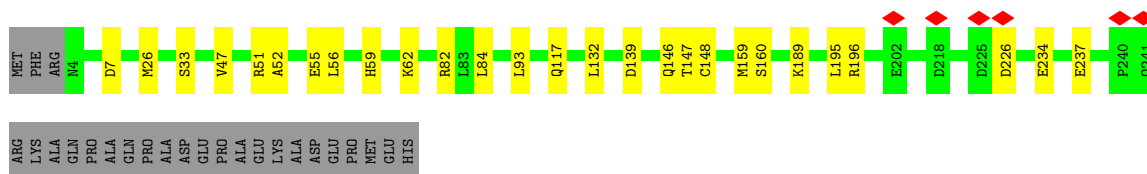


- Molecule 12: Proteasome subunit alpha type-1



- Molecule 12: Proteasome subunit alpha type-1





- Molecule 13: Proteasome subunit alpha type-3

Chain M: 87% 8% 5%



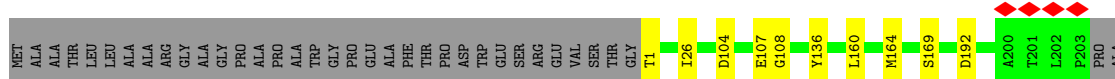
- Molecule 13: Proteasome subunit alpha type-3

Chain m: 81% 13% 6%



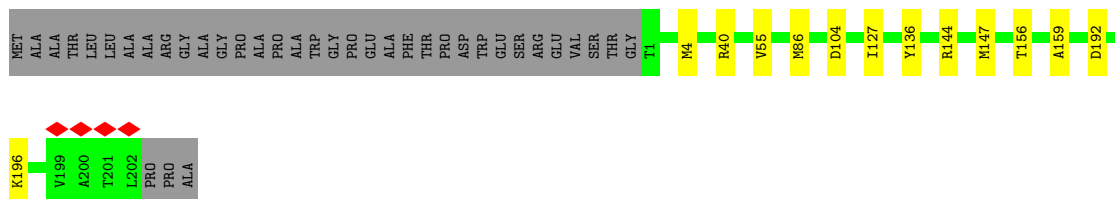
- Molecule 14: Proteasome subunit beta type-6

Chain N: 81% 15%



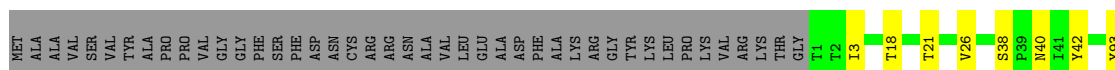
- Molecule 14: Proteasome subunit beta type-6

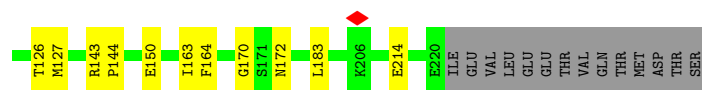
Chain n: 79% 5% 15%



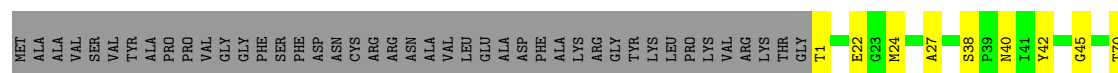
- Molecule 15: Proteasome subunit beta type-7

Chain O: 73% 7% 21%

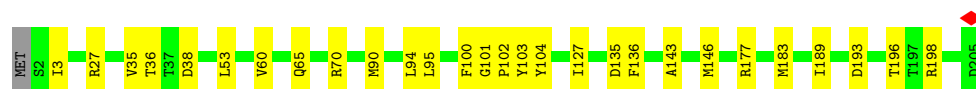
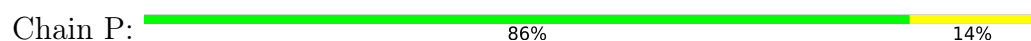




• Molecule 15: Proteasome subunit beta type-7



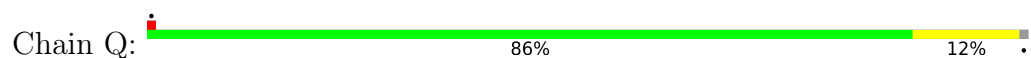
• Molecule 16: Proteasome subunit beta type-3



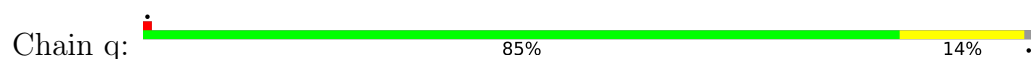
• Molecule 16: Proteasome subunit beta type-3



• Molecule 17: Proteasome subunit beta type-2

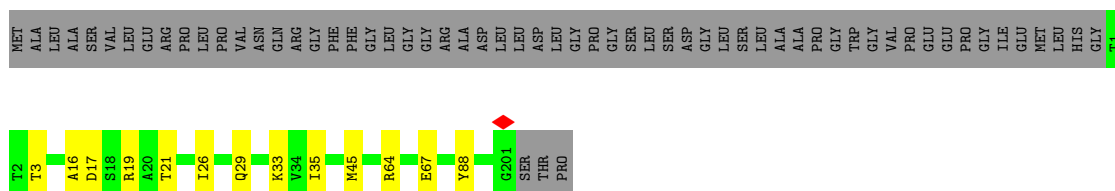


• Molecule 17: Proteasome subunit beta type-2



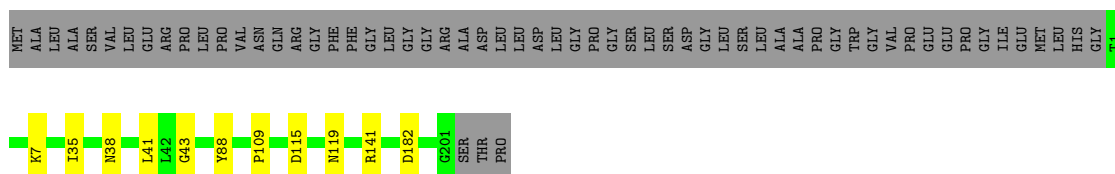
• Molecule 18: Proteasome subunit beta type-5





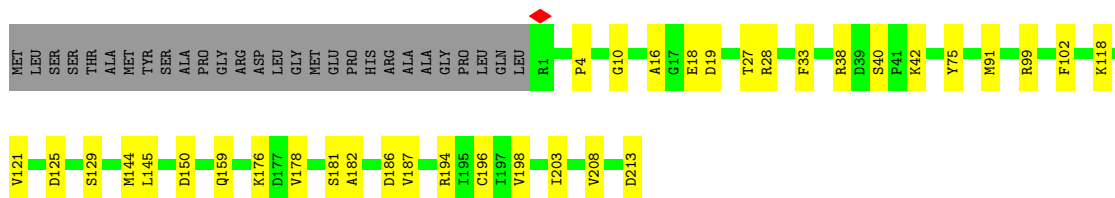
• Molecule 18: Proteasome subunit beta type-5

Chain r: 72% 24%



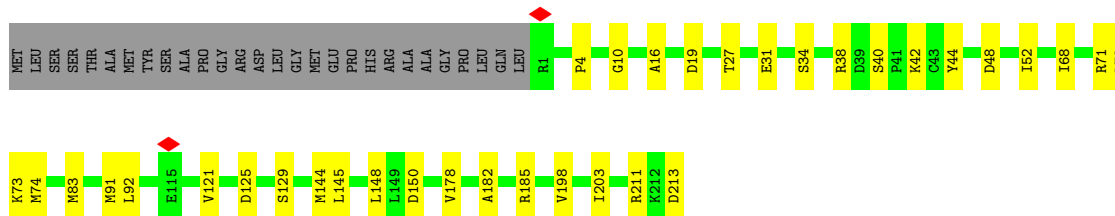
• Molecule 19: Proteasome subunit beta type-1

Chain S: 74% 15% 12%



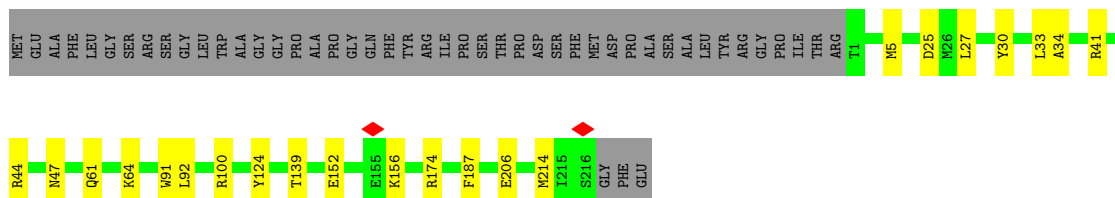
• Molecule 19: Proteasome subunit beta type-1

Chain s: 74% 15% 12%

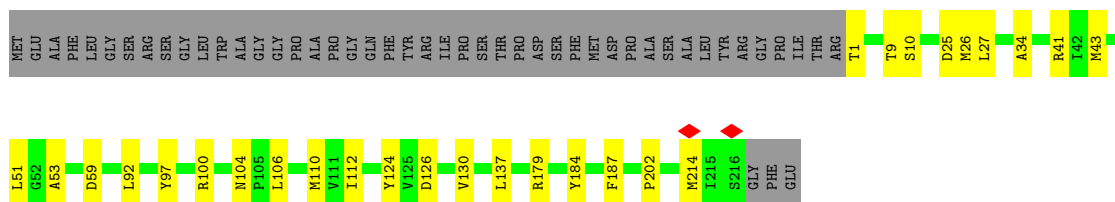


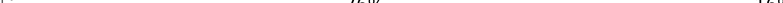
• Molecule 20: Proteasome subunit beta type-4

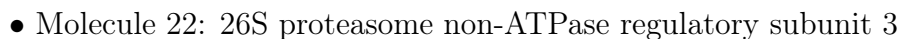
Chain T: 73% 8% 18%

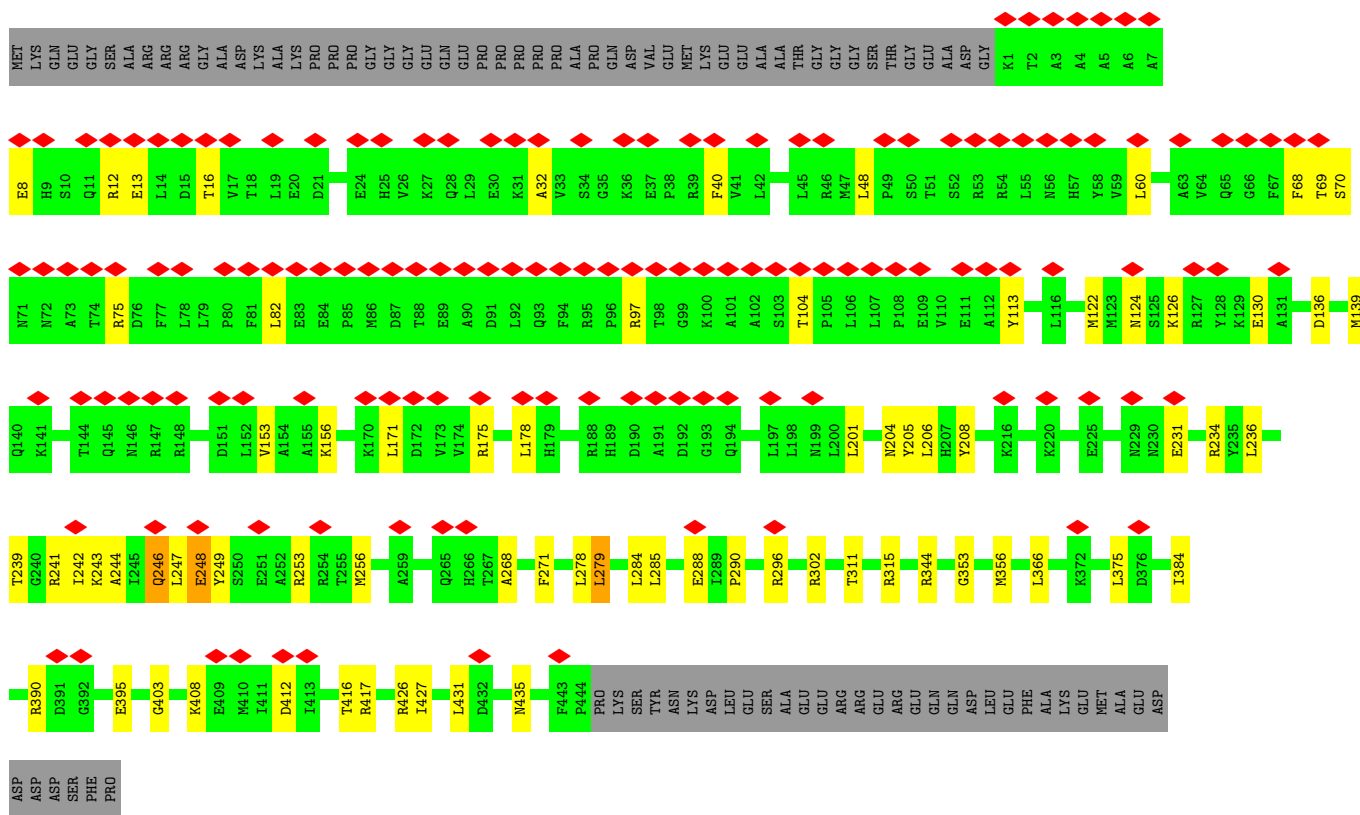


• Molecule 20: Proteasome subunit beta type-4

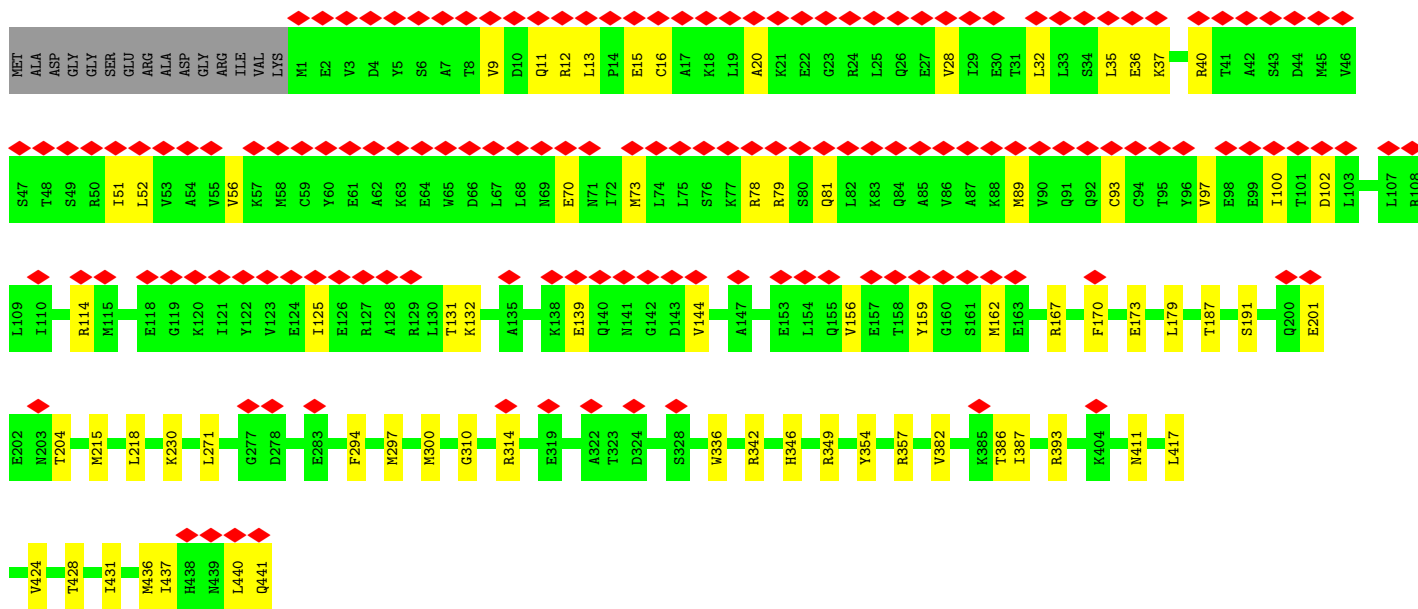
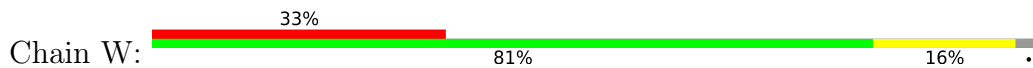


- Chain U:  22% 76% 16% 8%

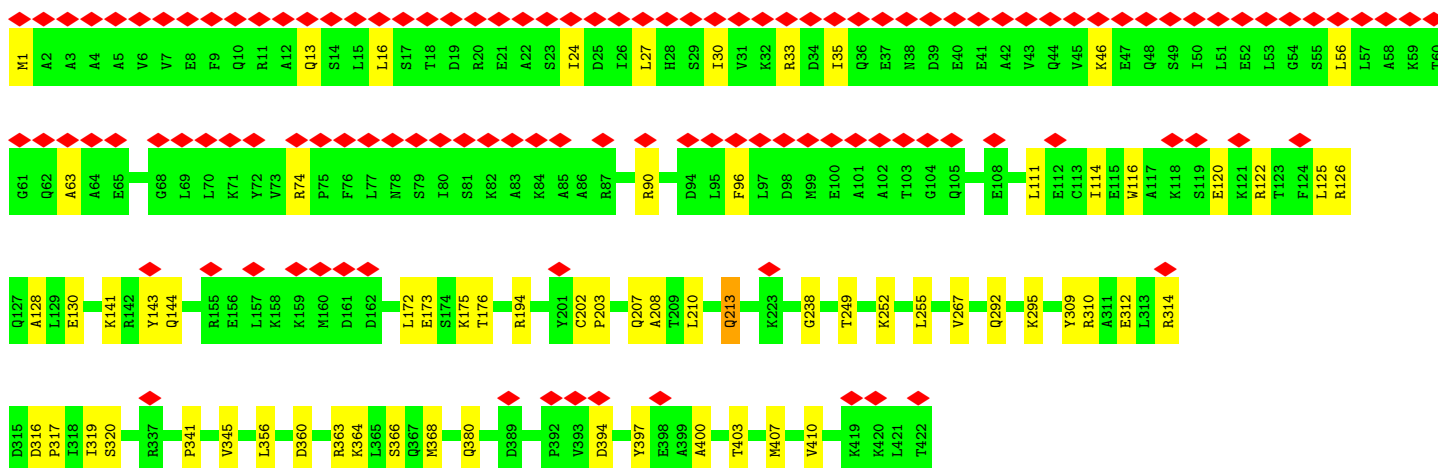
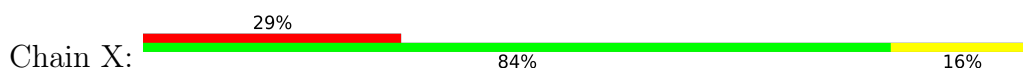




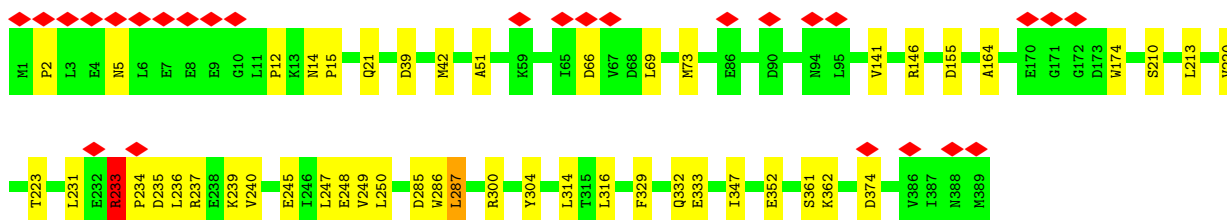
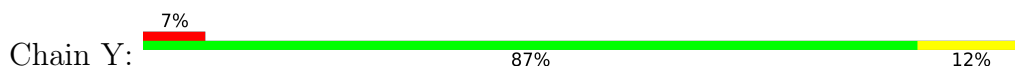
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



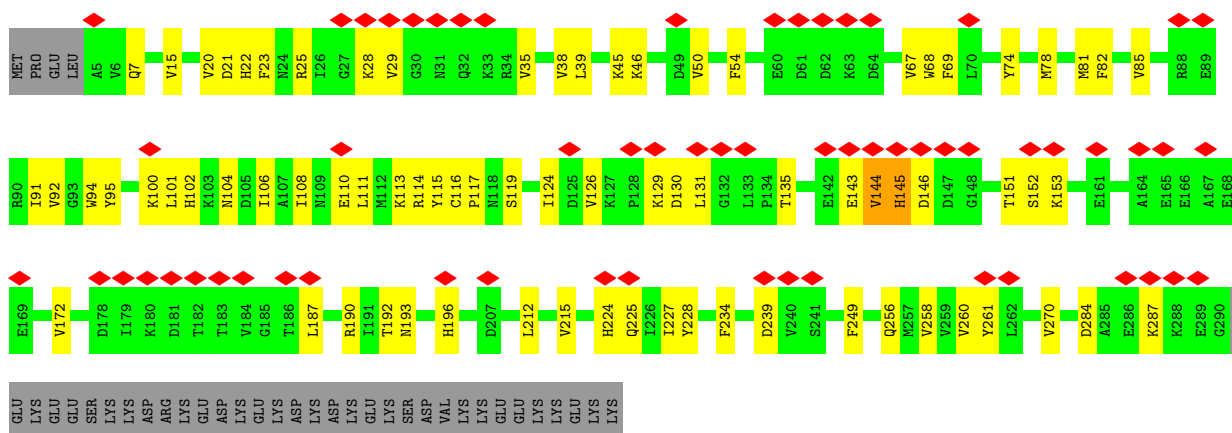
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



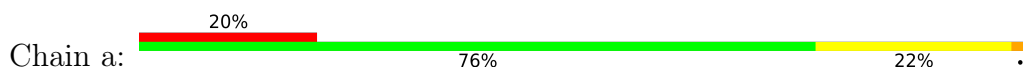
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

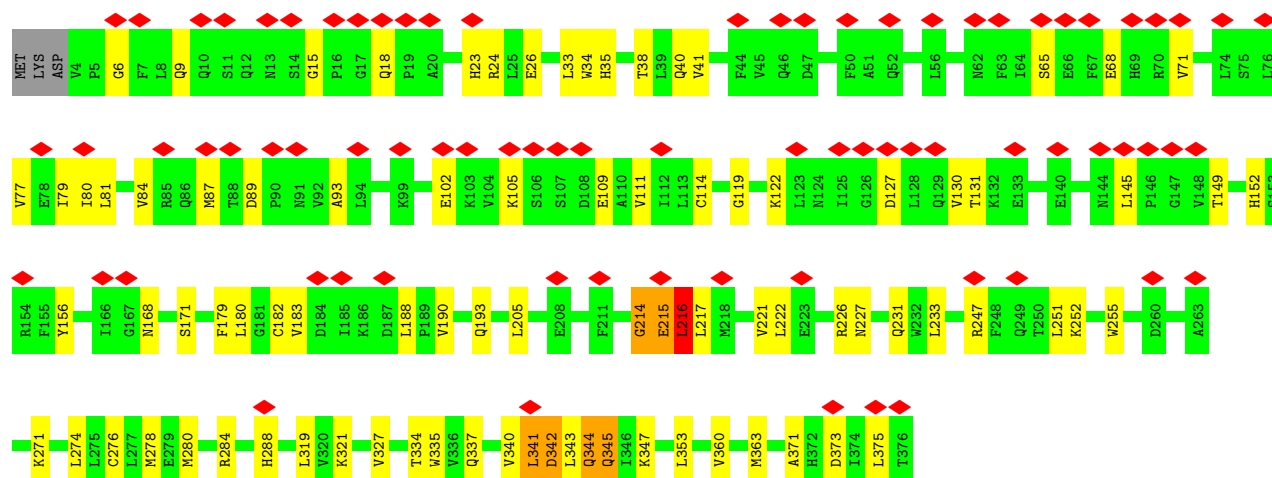


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

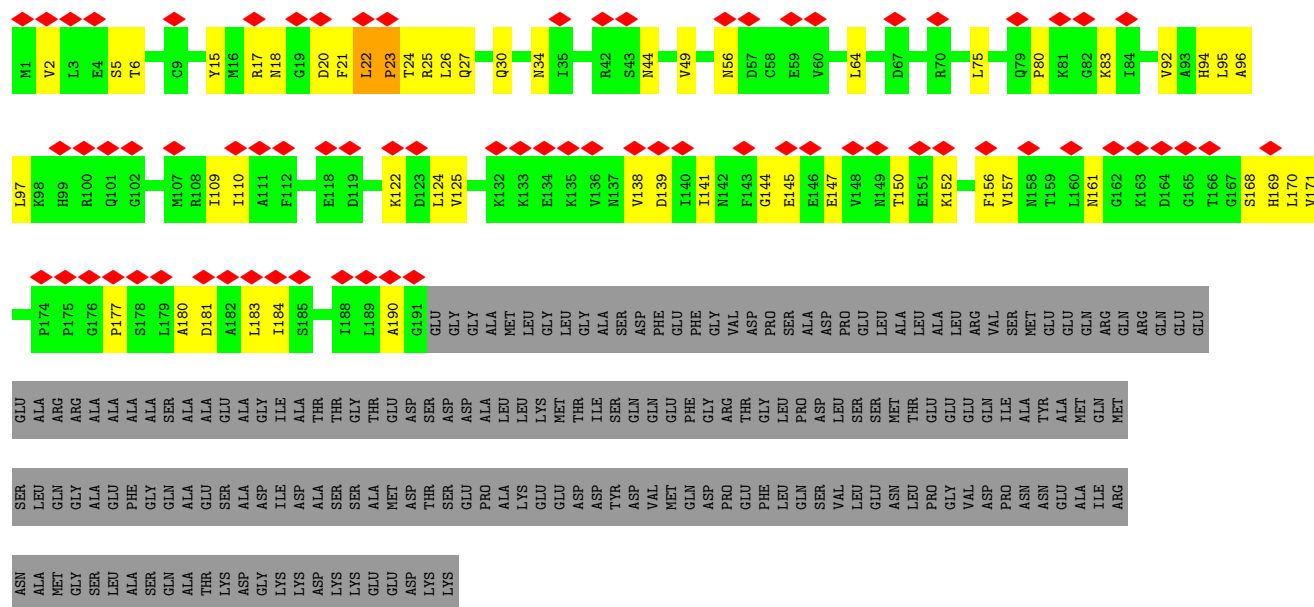
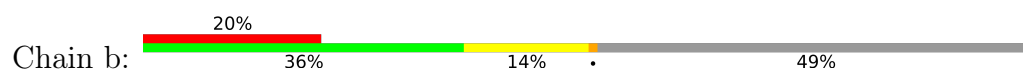


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

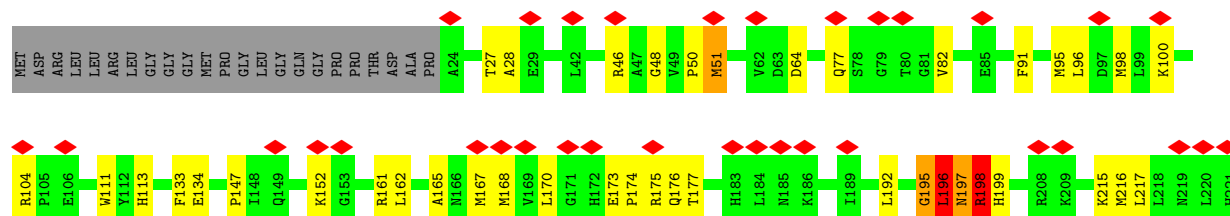




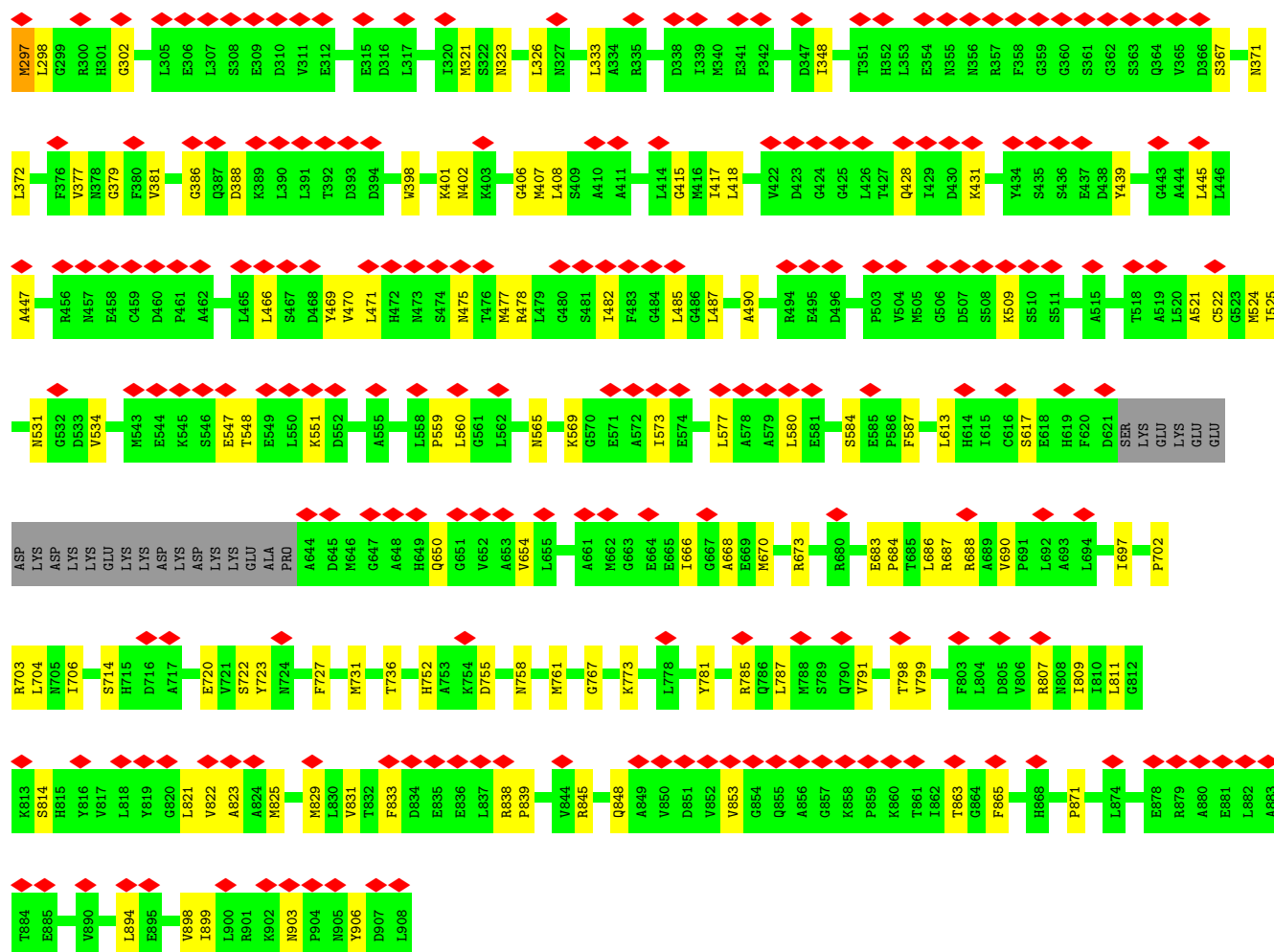
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4



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







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113188	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	0.018	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00538	Depositor
Map size (\AA)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.685, 0.685, 0.685	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ZN, 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	0.21	0/3283	0.52	0/4433
2	B	0.24	0/3254	0.57	0/4388
3	C	0.25	0/3146	0.56	0/4226
4	D	0.26	0/3090	0.63	1/4168 (0.0%)
5	E	0.26	0/3145	0.61	1/4233 (0.0%)
6	F	0.25	0/3137	0.57	0/4223
7	G	0.28	0/1901	0.49	0/2572
7	g	0.23	0/1913	0.47	0/2589
8	H	0.27	0/1840	0.52	0/2495
8	h	0.24	0/1844	0.49	1/2497 (0.0%)
9	I	0.27	0/1963	0.47	0/2650
9	i	0.22	0/1985	0.46	0/2677
10	J	0.26	0/1887	0.48	0/2553
10	j	0.23	0/1887	0.48	0/2549
11	K	0.23	0/1841	0.43	0/2486
11	k	0.22	0/1809	0.46	0/2444
12	L	0.25	0/1911	0.46	0/2584
12	l	0.24	0/1896	0.47	0/2565
13	M	0.24	0/1925	0.46	0/2592
13	m	0.22	0/1916	0.45	0/2580
14	N	0.26	0/1548	0.41	0/2097
14	n	0.29	0/1536	0.48	0/2080
15	O	0.24	0/1672	0.44	0/2267
15	o	0.24	0/1686	0.49	0/2282
16	P	0.28	0/1616	0.52	1/2180 (0.0%)
16	p	0.25	0/1620	0.52	0/2184
17	Q	0.30	0/1621	0.44	0/2194
17	q	0.24	0/1611	0.47	2/2182 (0.1%)
18	R	0.26	0/1590	0.47	0/2147
18	r	0.26	0/1580	0.46	0/2135
19	S	0.25	0/1671	0.48	0/2252
19	s	0.25	0/1680	0.51	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.25	0/1716	0.47	0/2323
20	t	0.25	0/1720	0.46	0/2328
21	U	0.20	0/6984	0.48	0/9435
22	V	0.21	0/3681	0.46	0/4969
23	W	0.19	0/3644	0.50	0/4901
24	X	0.20	0/3381	0.50	0/4558
25	Y	0.24	0/3261	0.52	0/4393
26	Z	0.27	0/2324	0.68	1/3150 (0.0%)
27	a	0.26	0/3053	0.59	1/4133 (0.0%)
28	b	0.23	0/1478	0.62	1/2001 (0.0%)
29	c	0.32	0/2302	0.70	1/3110 (0.0%)
30	d	0.29	1/2162 (0.0%)	0.65	3/2919 (0.1%)
31	e	0.25	0/437	0.49	0/595
32	f	0.19	0/6640	0.51	2/8988 (0.0%)
All	All	0.24	1/107787 (0.0%)	0.52	15/145571 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	204	LYS	CA-C	5.50	1.60	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	113	MET	CA-C-N	9.17	133.14	120.39
32	f	113	MET	C-N-CA	9.17	133.14	120.39
30	d	88	GLN	N-CA-C	-7.83	103.80	112.72
5	E	166	PRO	N-CA-C	7.45	119.79	110.70
28	b	20	ASP	N-CA-C	-7.43	103.48	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	44	0
2	B	3207	0	3278	58	0
3	C	3105	0	3219	59	0
4	D	3040	0	3076	61	0
5	E	3097	0	3174	75	0
6	F	3098	0	3187	52	0
7	G	1867	0	1867	21	0
7	g	1879	0	1872	13	0
8	H	1801	0	1773	18	0
8	h	1805	0	1798	18	0
9	I	1933	0	1923	18	0
9	i	1955	0	1955	16	0
10	J	1861	0	1846	23	0
10	j	1861	0	1865	31	0
11	K	1813	0	1796	22	0
11	k	1782	0	1766	18	0
12	L	1876	0	1856	18	0
12	l	1861	0	1839	18	0
13	M	1890	0	1880	12	0
13	m	1881	0	1868	19	0
14	N	1521	0	1494	7	0
14	n	1510	0	1483	8	0
15	O	1645	0	1648	12	0
15	o	1659	0	1681	19	0
16	P	1587	0	1598	19	0
16	p	1591	0	1609	15	0
17	Q	1588	0	1584	19	0
17	q	1578	0	1569	18	0
18	R	1559	0	1523	8	0
18	r	1549	0	1506	8	0
19	S	1641	0	1639	23	0
19	s	1650	0	1645	22	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	18	0
21	U	6867	0	6929	95	0
22	V	3612	0	3685	55	0
23	W	3596	0	3716	50	0
24	X	3335	0	3435	41	0
25	Y	3202	0	3204	44	0
26	Z	2281	0	2312	72	0
27	a	2995	0	3012	59	0
28	b	1458	0	1505	41	0
29	c	2260	0	2276	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	53	0
31	e	425	0	331	11	0
32	f	6529	0	6541	92	0
33	v	180	0	45	0	0
34	A	31	0	12	0	0
34	B	31	0	12	3	0
34	C	31	0	12	2	0
34	F	31	0	12	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	F	1	0	0	0	0
36	D	27	0	12	1	0
37	c	1	0	0	0	0
All	All	106302	0	106603	1343	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 1343 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)
21:U:885:MET:H	21:U:888:GLN:HE21	1.10	0.96
29:c:231:LEU:C	29:c:233:ASP:H	1.70	0.96
3:C:90:HIS:CD2	3:C:91:PRO:HD3	2.13	0.83
5:E:242:ARG:HB3	5:E:281:ARG:HH12	1.42	0.83
5:E:168:LYS:HD2	5:E:274:LYS:HA	1.60	0.82

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	411/433 (95%)	375 (91%)	36 (9%)	0	100	100
2	B	409/440 (93%)	362 (88%)	47 (12%)	0	100	100
3	C	394/398 (99%)	354 (90%)	37 (9%)	3 (1%)	16	48
4	D	378/418 (90%)	319 (84%)	54 (14%)	5 (1%)	9	38
5	E	387/403 (96%)	330 (85%)	54 (14%)	3 (1%)	16	48
6	F	391/439 (89%)	351 (90%)	37 (10%)	3 (1%)	16	48
7	G	238/246 (97%)	220 (92%)	16 (7%)	2 (1%)	16	48
7	g	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	246/261 (94%)	233 (95%)	13 (5%)	0	100	100
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	227 (96%)	9 (4%)	1 (0%)	30	60
11	K	236/241 (98%)	224 (95%)	12 (5%)	0	100	100
11	k	232/241 (96%)	221 (95%)	11 (5%)	0	100	100
12	L	238/263 (90%)	226 (95%)	12 (5%)	0	100	100
12	l	236/263 (90%)	226 (96%)	10 (4%)	0	100	100
13	M	240/255 (94%)	232 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	24	56
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	197/201 (98%)	190 (96%)	6 (3%)	1 (0%)	24	56
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
19	s	211/241 (88%)	200 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
20	t	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
21	U	874/953 (92%)	807 (92%)	67 (8%)	0	100	100
22	V	442/534 (83%)	422 (96%)	20 (4%)	0	100	100
23	W	439/456 (96%)	431 (98%)	8 (2%)	0	100	100
24	X	420/422 (100%)	404 (96%)	16 (4%)	0	100	100
25	Y	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	36	65
26	Z	284/324 (88%)	246 (87%)	37 (13%)	1 (0%)	30	60
27	a	371/376 (99%)	339 (91%)	31 (8%)	1 (0%)	36	65
28	b	189/377 (50%)	170 (90%)	17 (9%)	2 (1%)	11	42
29	c	285/310 (92%)	233 (82%)	47 (16%)	5 (2%)	6	34
30	d	255/350 (73%)	215 (84%)	39 (15%)	1 (0%)	30	60
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	804 (96%)	36 (4%)	0	100	100
All	All	13415/14876 (90%)	12529 (93%)	856 (6%)	30 (0%)	44	72

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	73	ILE
28	b	22	LEU
29	c	50	PRO
29	c	279	ASP
29	c	280	PRO

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	348/372 (94%)	347 (100%)	1 (0%)	86	83
2	B	357/385 (93%)	357 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
3	C	340/346 (98%)	336 (99%)	4 (1%)	63	72	
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	72	
5	E	341/353 (97%)	337 (99%)	4 (1%)	63	72	
6	F	340/379 (90%)	334 (98%)	6 (2%)	51	67	
7	G	202/210 (96%)	201 (100%)	1 (0%)	81	80	
7	g	201/210 (96%)	201 (100%)	0	100	100	
8	H	187/191 (98%)	187 (100%)	0	100	100	
8	h	188/191 (98%)	185 (98%)	3 (2%)	55	68	
9	I	202/221 (91%)	201 (100%)	1 (0%)	81	80	
9	i	206/221 (93%)	206 (100%)	0	100	100	
10	J	197/211 (93%)	195 (99%)	2 (1%)	68	74	
10	j	196/211 (93%)	196 (100%)	0	100	100	
11	K	197/203 (97%)	197 (100%)	0	100	100	
11	k	195/203 (96%)	195 (100%)	0	100	100	
12	L	202/224 (90%)	201 (100%)	1 (0%)	81	80	
12	l	201/224 (90%)	201 (100%)	0	100	100	
13	M	198/212 (93%)	198 (100%)	0	100	100	
13	m	198/212 (93%)	198 (100%)	0	100	100	
14	N	158/181 (87%)	157 (99%)	1 (1%)	78	79	
14	n	156/181 (86%)	155 (99%)	1 (1%)	78	79	
15	O	178/228 (78%)	178 (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%)	166 (99%)	2 (1%)	63	72	
17	q	166/171 (97%)	166 (100%)	0	100	100	
18	R	156/202 (77%)	156 (100%)	0	100	100	
18	r	154/202 (76%)	154 (100%)	0	100	100	
19	S	175/199 (88%)	175 (100%)	0	100	100	
19	s	177/199 (89%)	177 (100%)	0	100	100	
20	T	178/215 (83%)	178 (100%)	0	100	100	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	752 (100%)	0	100	100
22	V	390/460 (85%)	387 (99%)	3 (1%)	73	76
23	W	406/416 (98%)	406 (100%)	0	100	100
24	X	362/362 (100%)	361 (100%)	1 (0%)	86	83
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	79
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	81
27	a	333/336 (99%)	326 (98%)	7 (2%)	47	64
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	242 (96%)	10 (4%)	28	52
30	d	231/294 (79%)	227 (98%)	4 (2%)	53	67
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	88
All	All	11449/12614 (91%)	11389 (100%)	60 (0%)	78	80

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	248	GLU
32	f	297	MET
27	a	216	LEU
30	d	202	THR
14	n	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	380	GLN
27	a	193	GLN
14	n	110	GLN
24	X	416	ASN
26	Z	196	HIS

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](#)

Of 11 ligands modelled in this entry, 6 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	$\# Z > 2$
36	ADP	D	501	35	27,29,29	1.34	4 (14%)	42,45,45	2.04	9 (21%)
34	ATP	C	501	35	29,33,33	0.31	0	44,52,52	0.51	0
34	ATP	B	501	35	29,33,33	0.32	0	44,52,52	0.49	0
34	ATP	F	501	35	29,33,33	0.32	0	44,52,52	0.47	1 (2%)
34	ATP	A	501	35	29,33,33	0.32	0	44,52,52	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	D	501	35	-	2/16/32/32	0/3/3/3
34	ATP	C	501	35	-	6/22/38/38	0/3/3/3
34	ATP	B	501	35	-	2/22/38/38	0/3/3/3
34	ATP	F	501	35	-	2/22/38/38	0/3/3/3
34	ATP	A	501	35	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ADP	C5-C4	4.47	1.47	1.39
36	D	501	ADP	C5-C6	2.51	1.48	1.41
36	D	501	ADP	C5-N7	-2.36	1.34	1.39
36	D	501	ADP	C8-N7	2.14	1.35	1.31

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ADP	C5-C4-N3	-6.52	118.24	126.75
36	D	501	ADP	N3-C4-N9	5.41	136.00	127.08
36	D	501	ADP	C2-N3-C4	3.91	120.98	111.75
36	D	501	ADP	PA-O3A-PB	-3.40	121.15	132.83
36	D	501	ADP	N3-C2-N1	-3.02	123.89	128.60

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	PB-O3B-PG-O3G
34	C	501	ATP	PB-O3B-PG-O3G
34	C	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	O4'-C4'-C5'-O5'
34	A	501	ATP	C3'-C4'-C5'-O5'

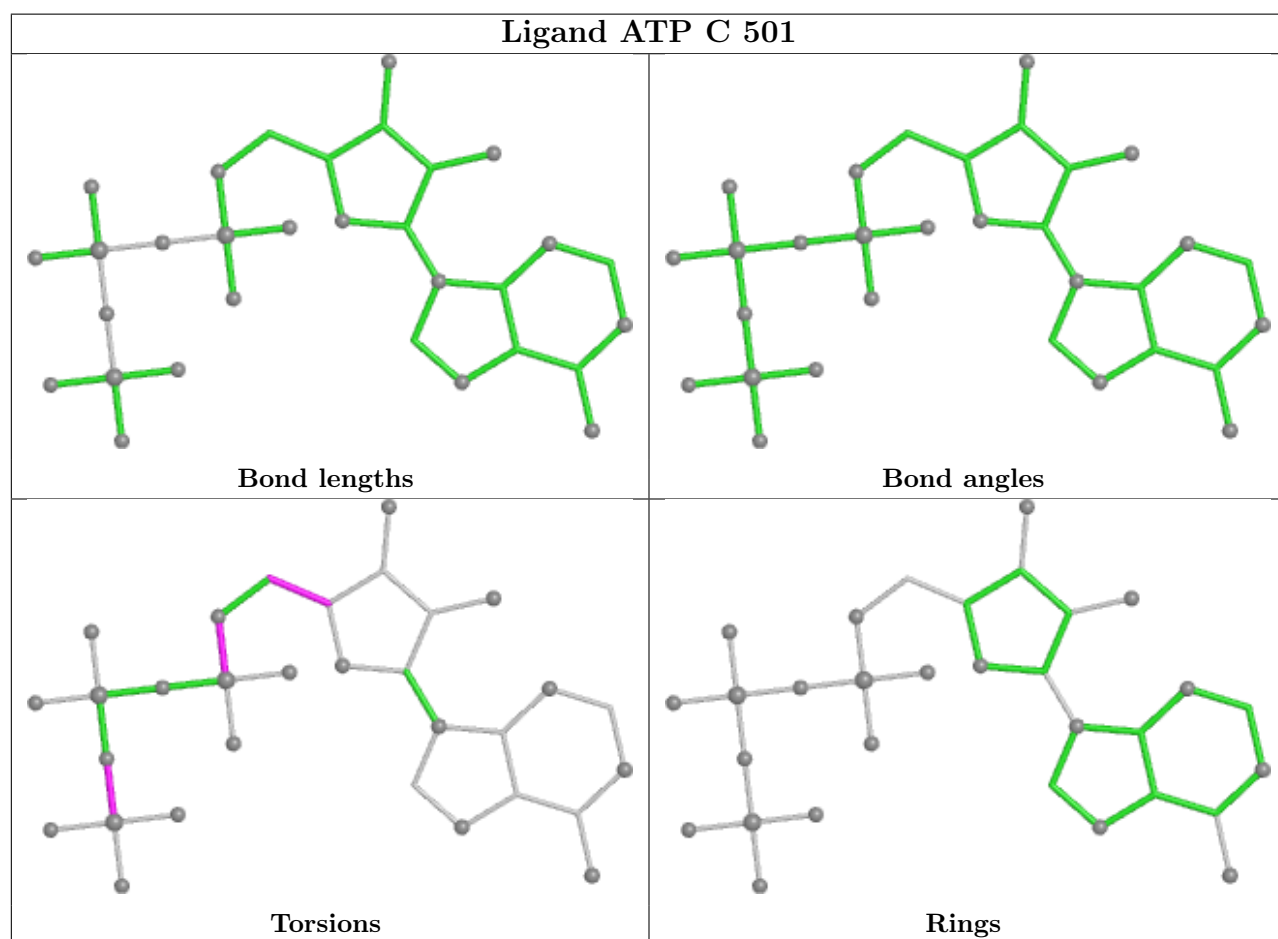
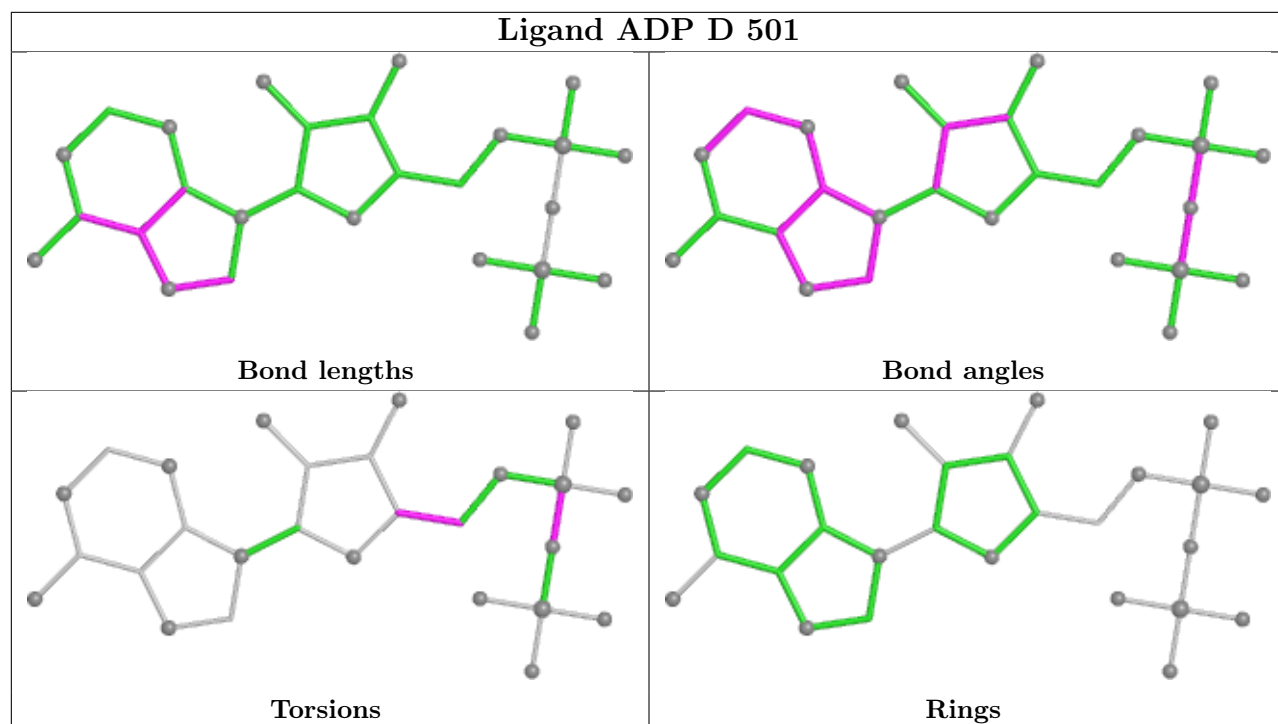
There are no ring outliers.

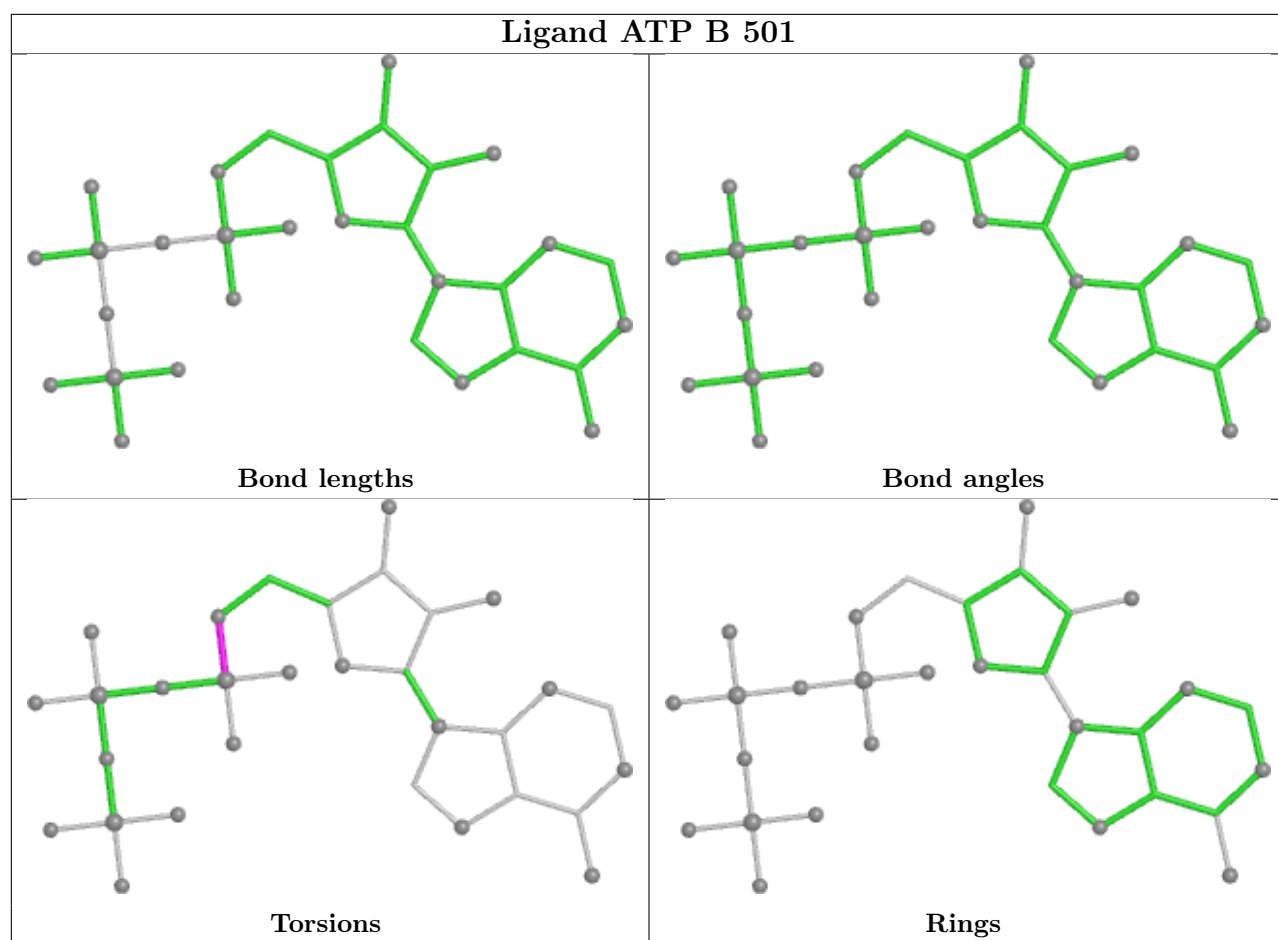
3 monomers are involved in 6 short contacts:

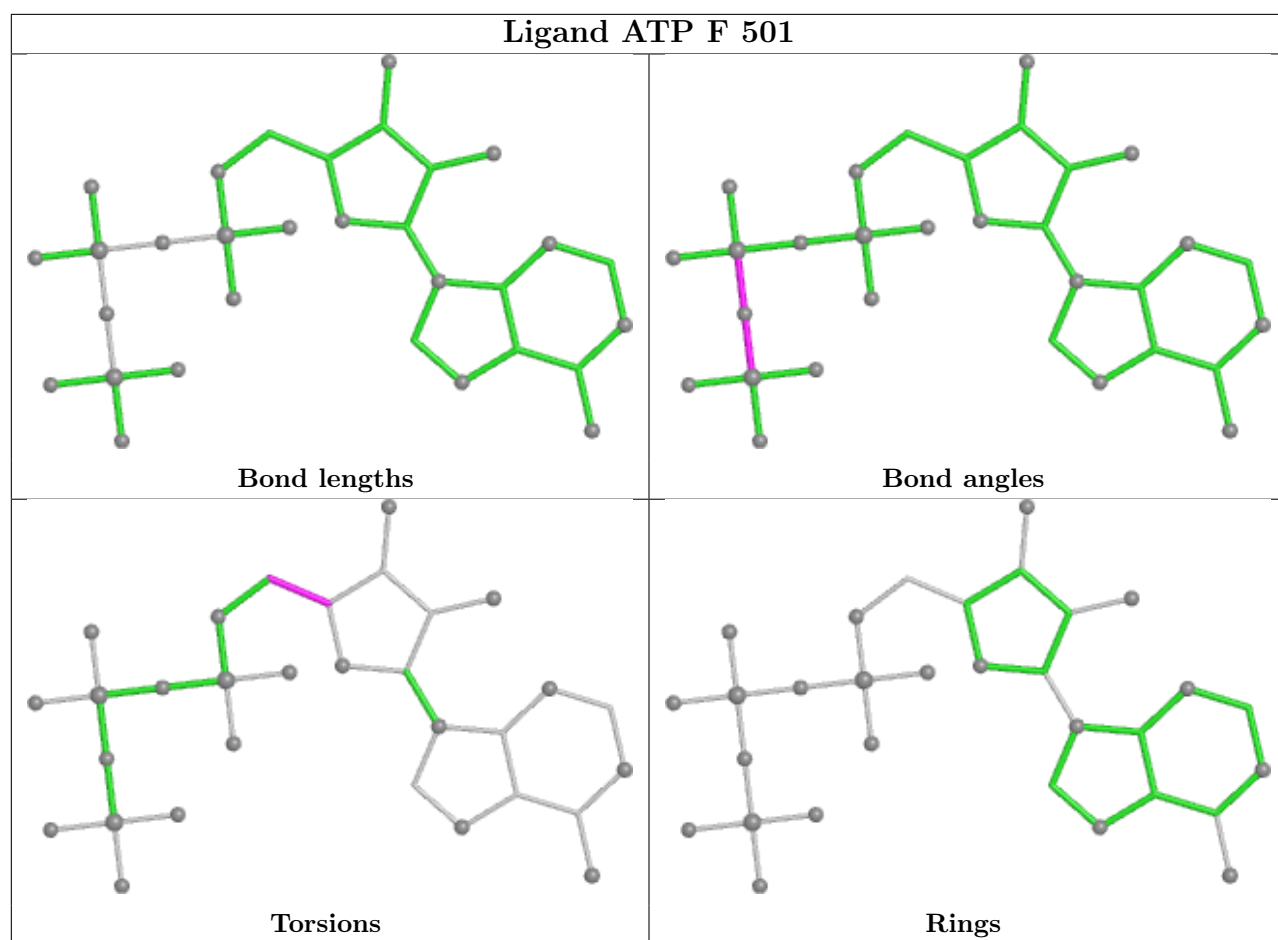
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	D	501	ADP	1	0
34	C	501	ATP	2	0
34	B	501	ATP	3	0

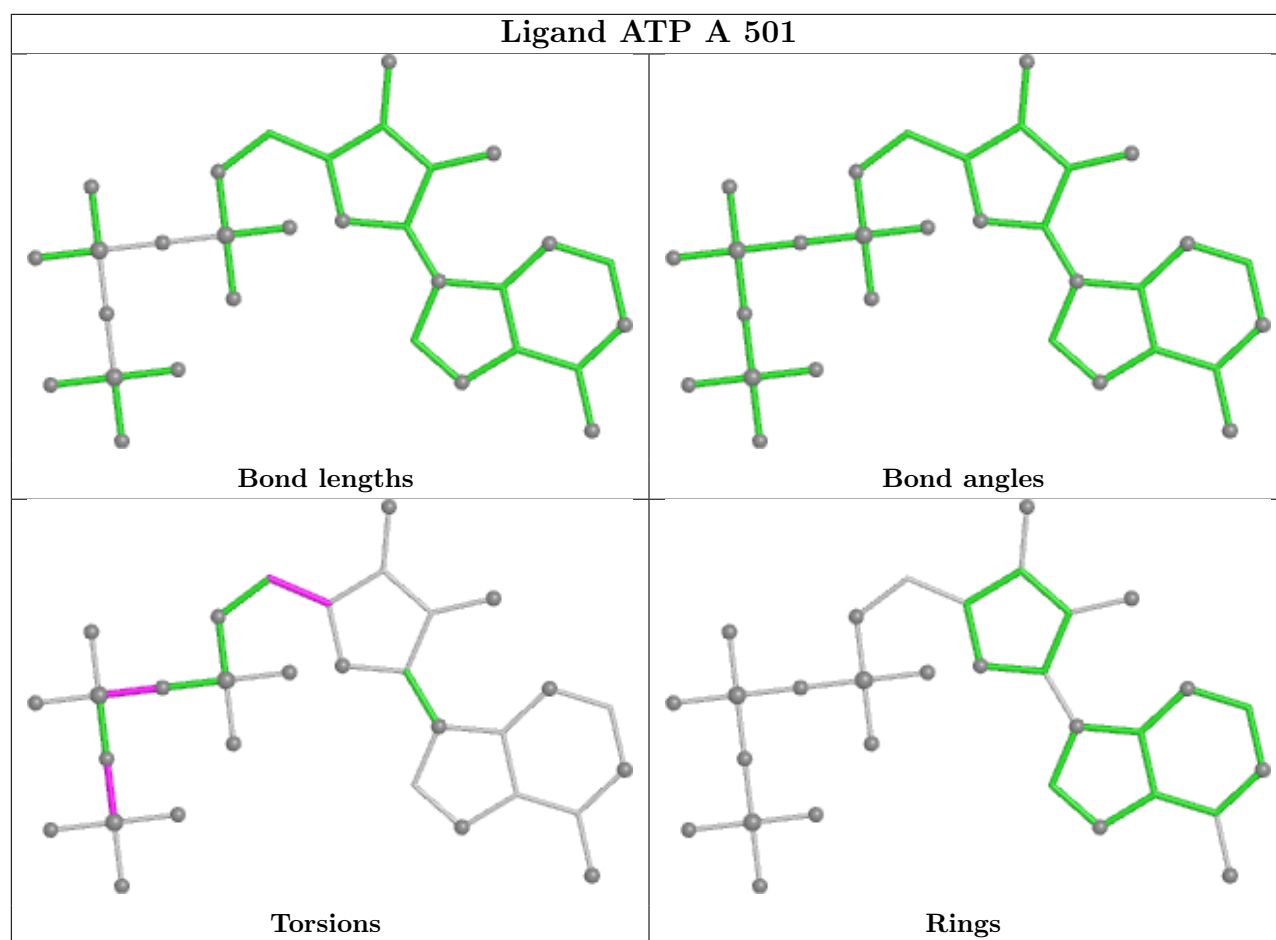
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

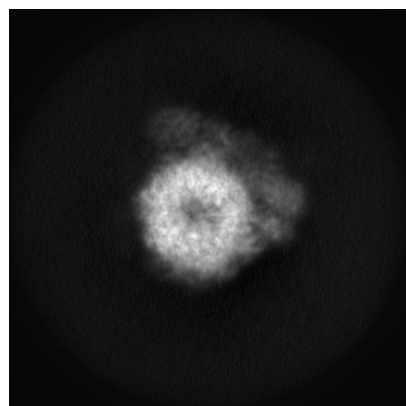
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62089. These allow visual inspection of the internal detail of the map and identification of artifacts.

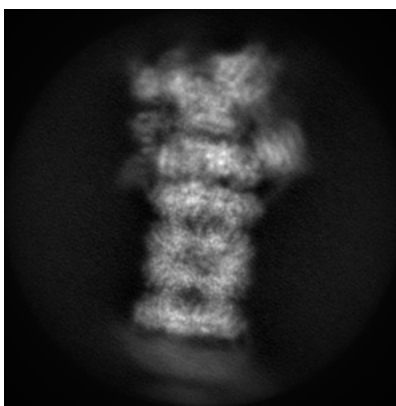
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

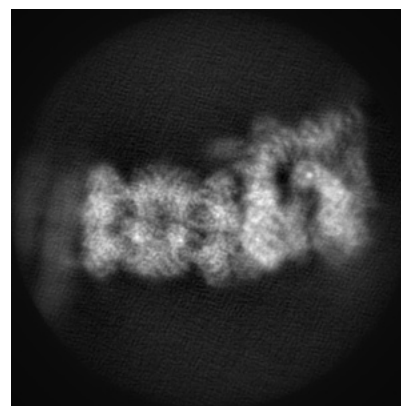
6.1.1 Primary map



X

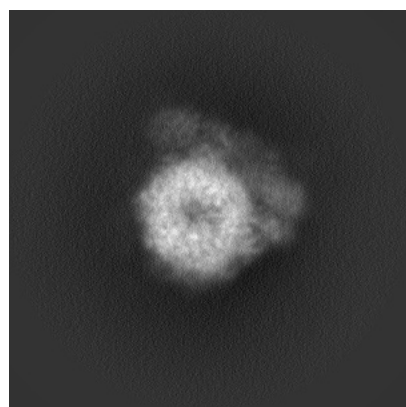


Y

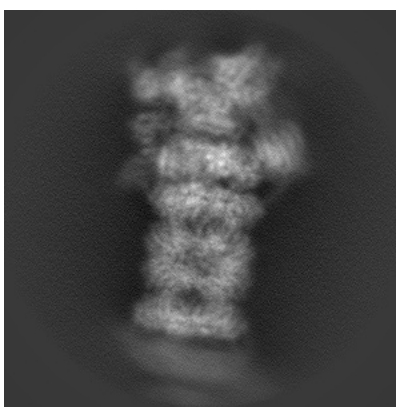


Z

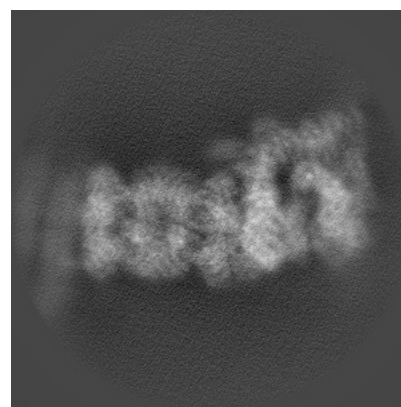
6.1.2 Raw map



X



Y

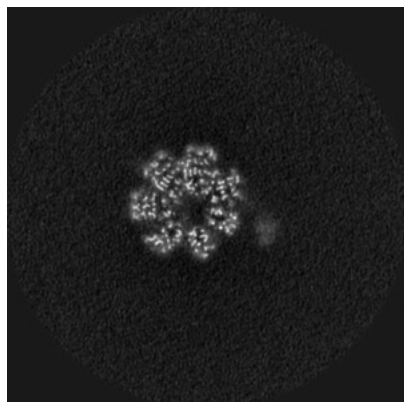


Z

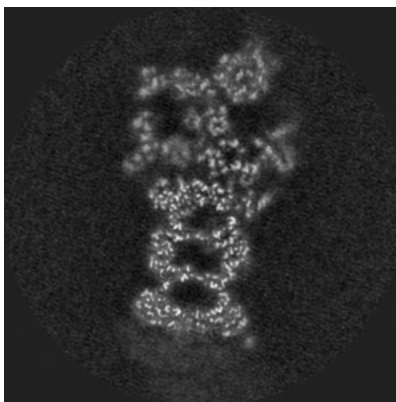
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

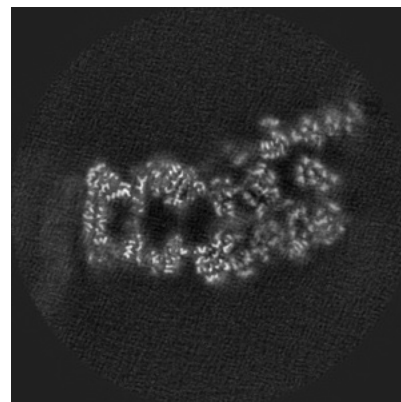
6.2.1 Primary map



X Index: 300

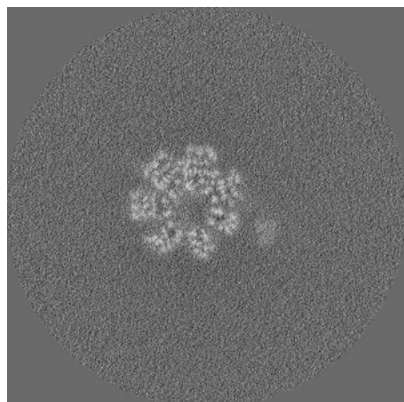


Y Index: 300

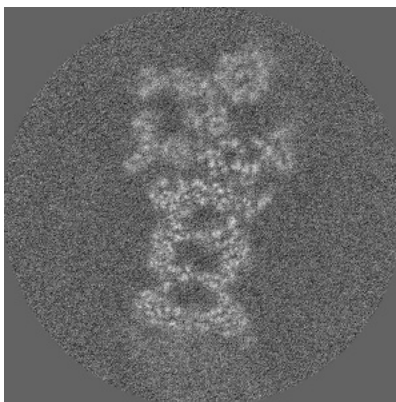


Z Index: 300

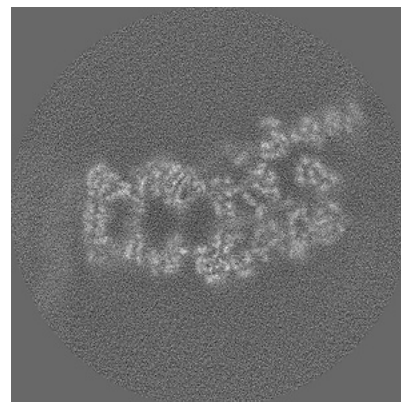
6.2.2 Raw map



X Index: 300



Y Index: 300

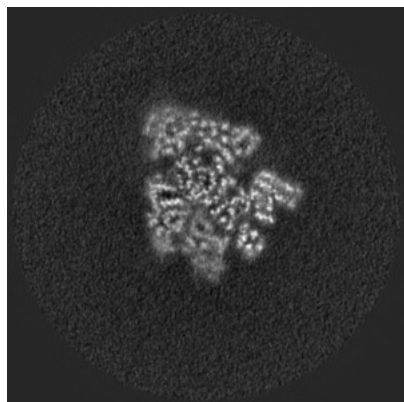


Z Index: 300

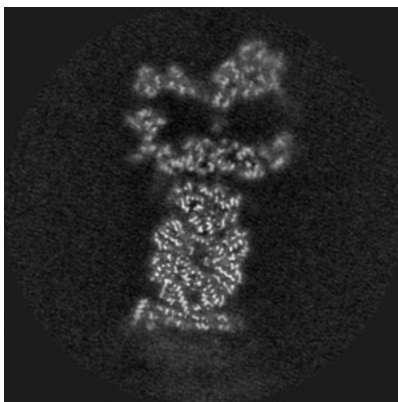
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

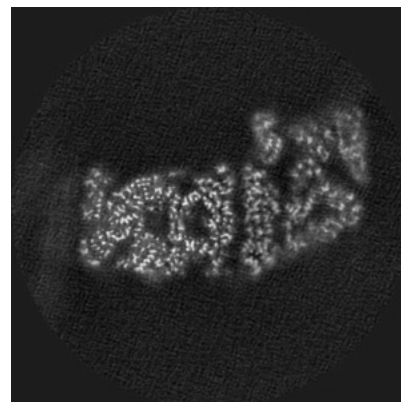
6.3.1 Primary map



X Index: 381

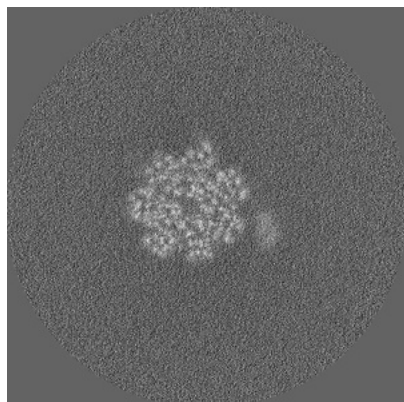


Y Index: 319

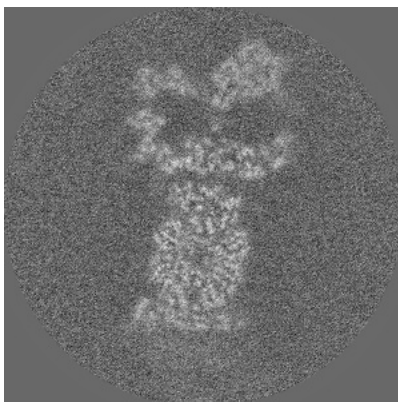


Z Index: 327

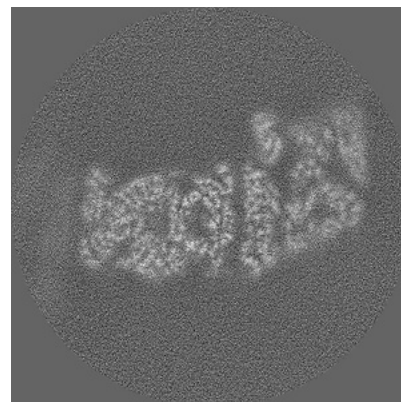
6.3.2 Raw map



X Index: 309



Y Index: 318

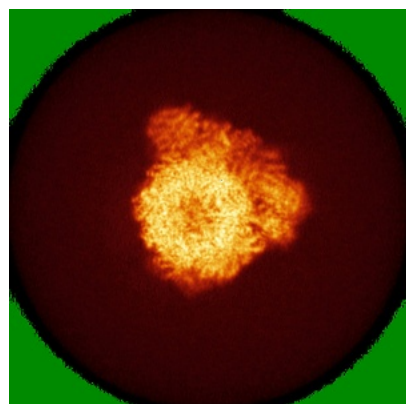


Z Index: 328

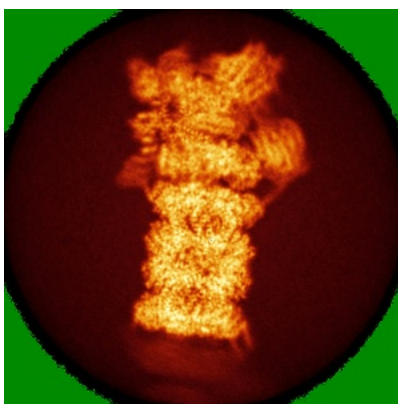
The images above show the largest variance slices of the map in three orthogonal directions.

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

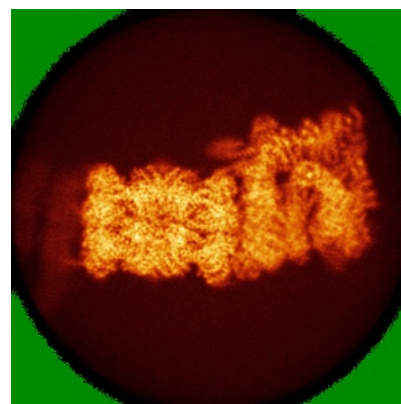
6.4.1 Primary map



X

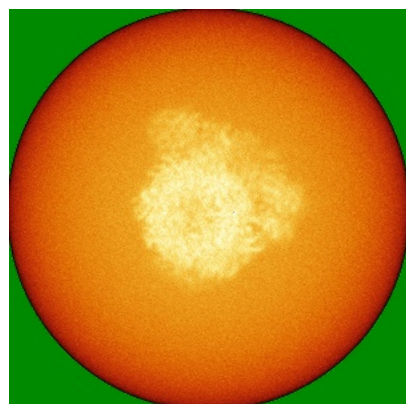


Y

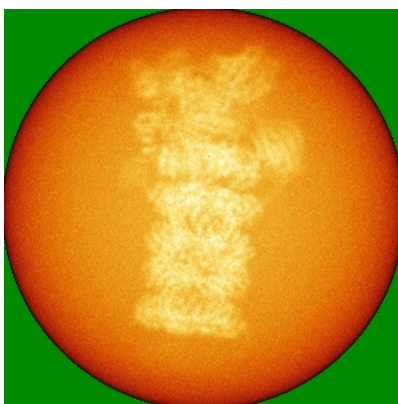


Z

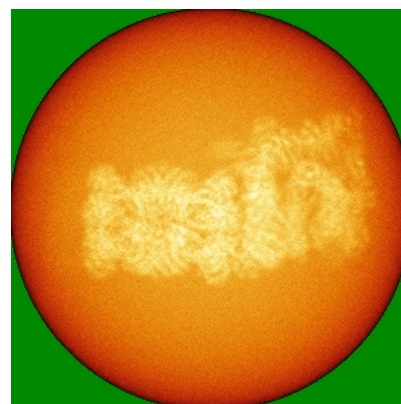
6.4.2 Raw map



X



Y

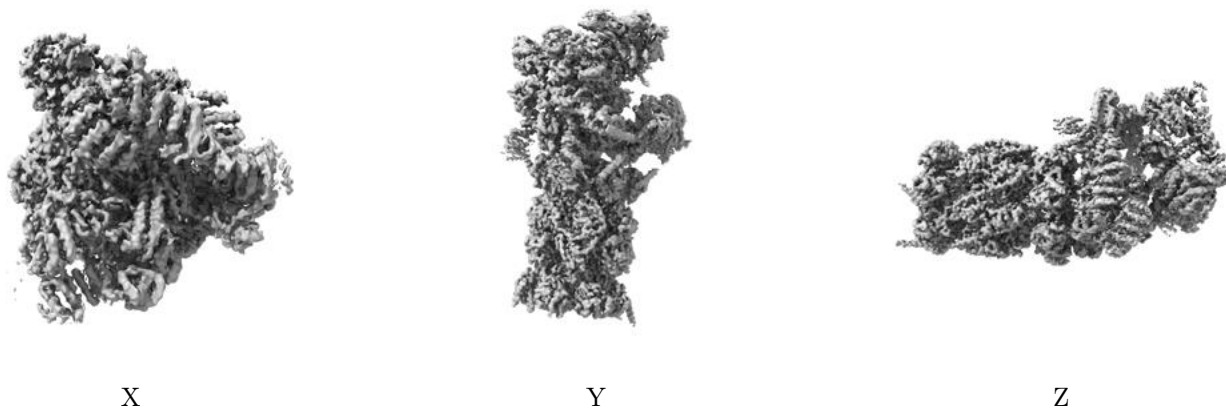


Z

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.

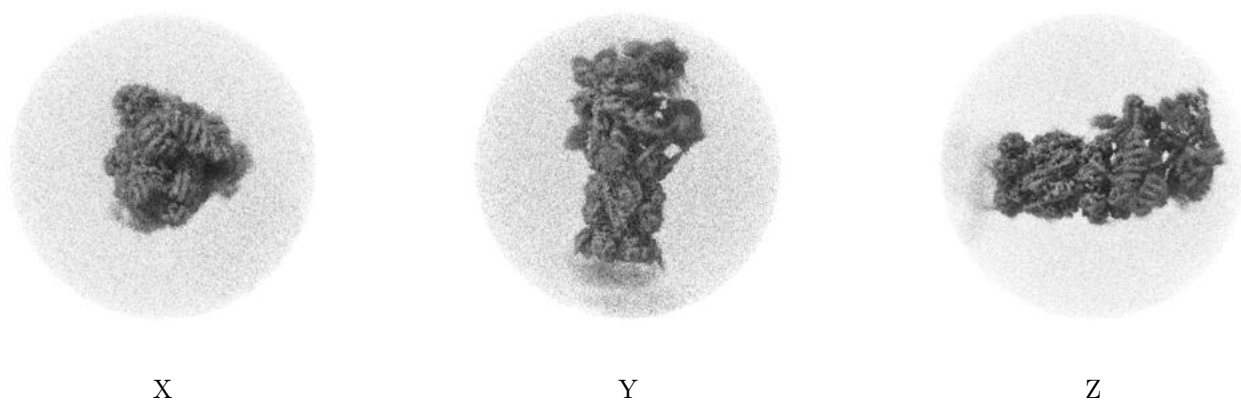
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00538. 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.

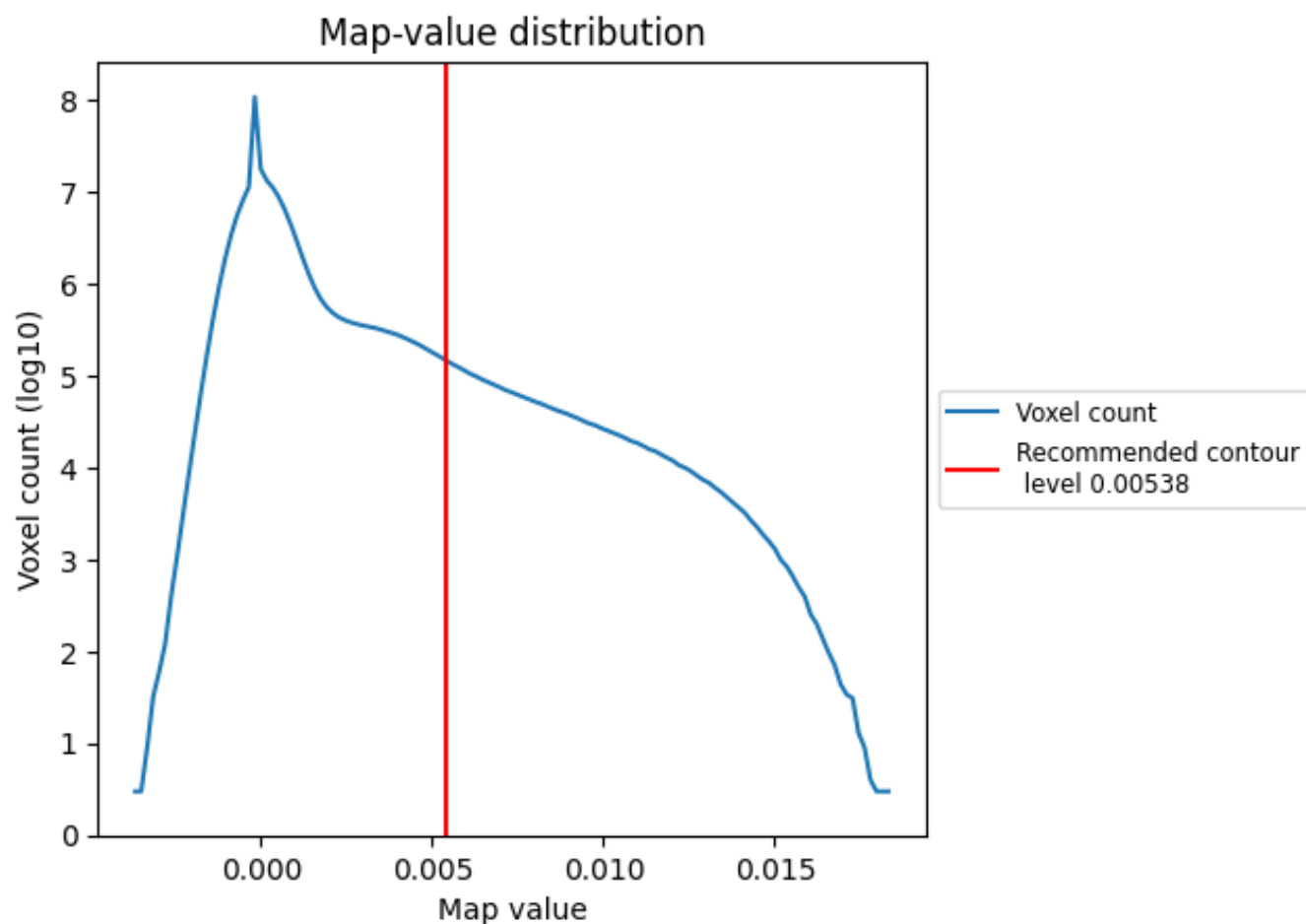
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

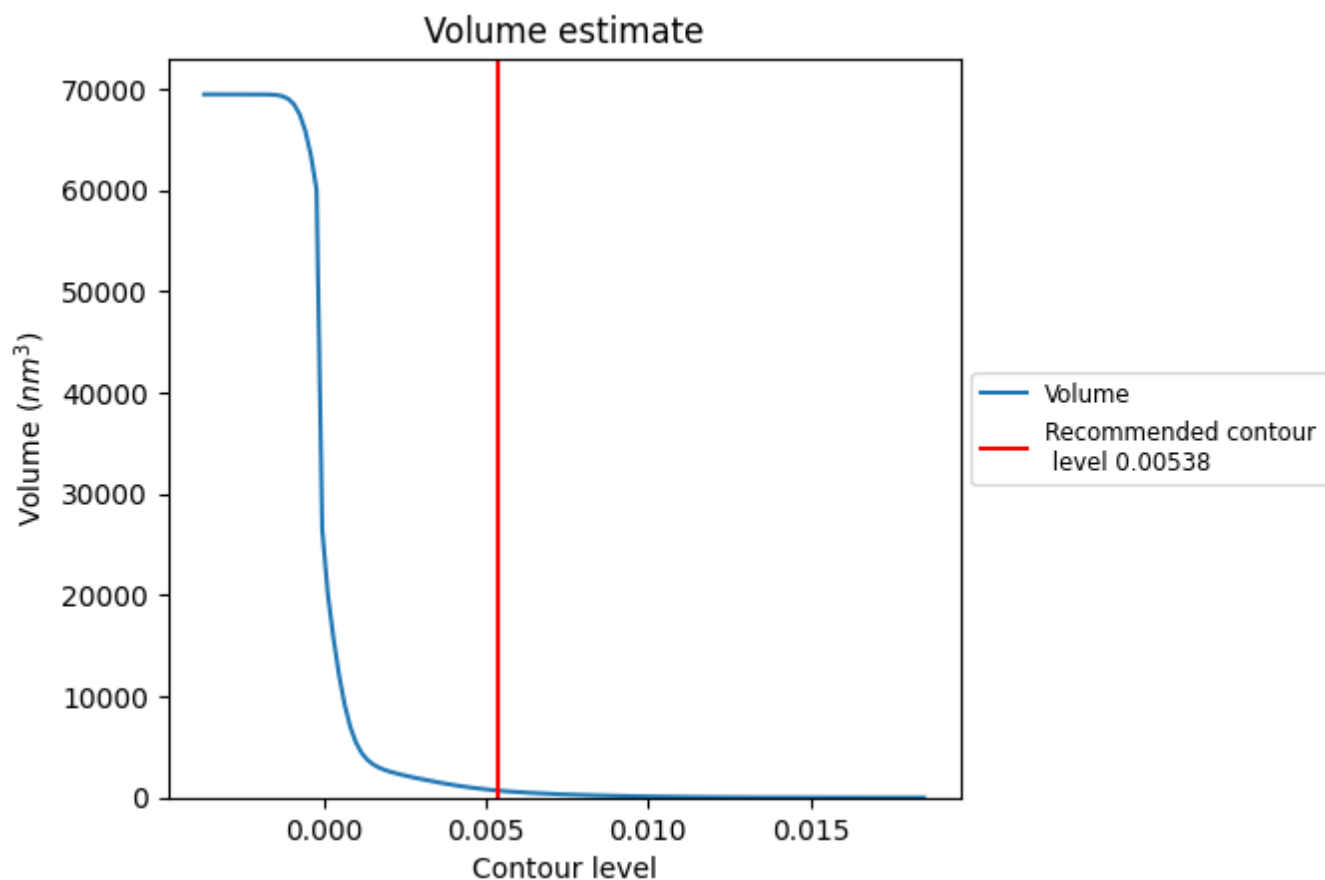
This section contains the results of statistical analysis of the map.

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.

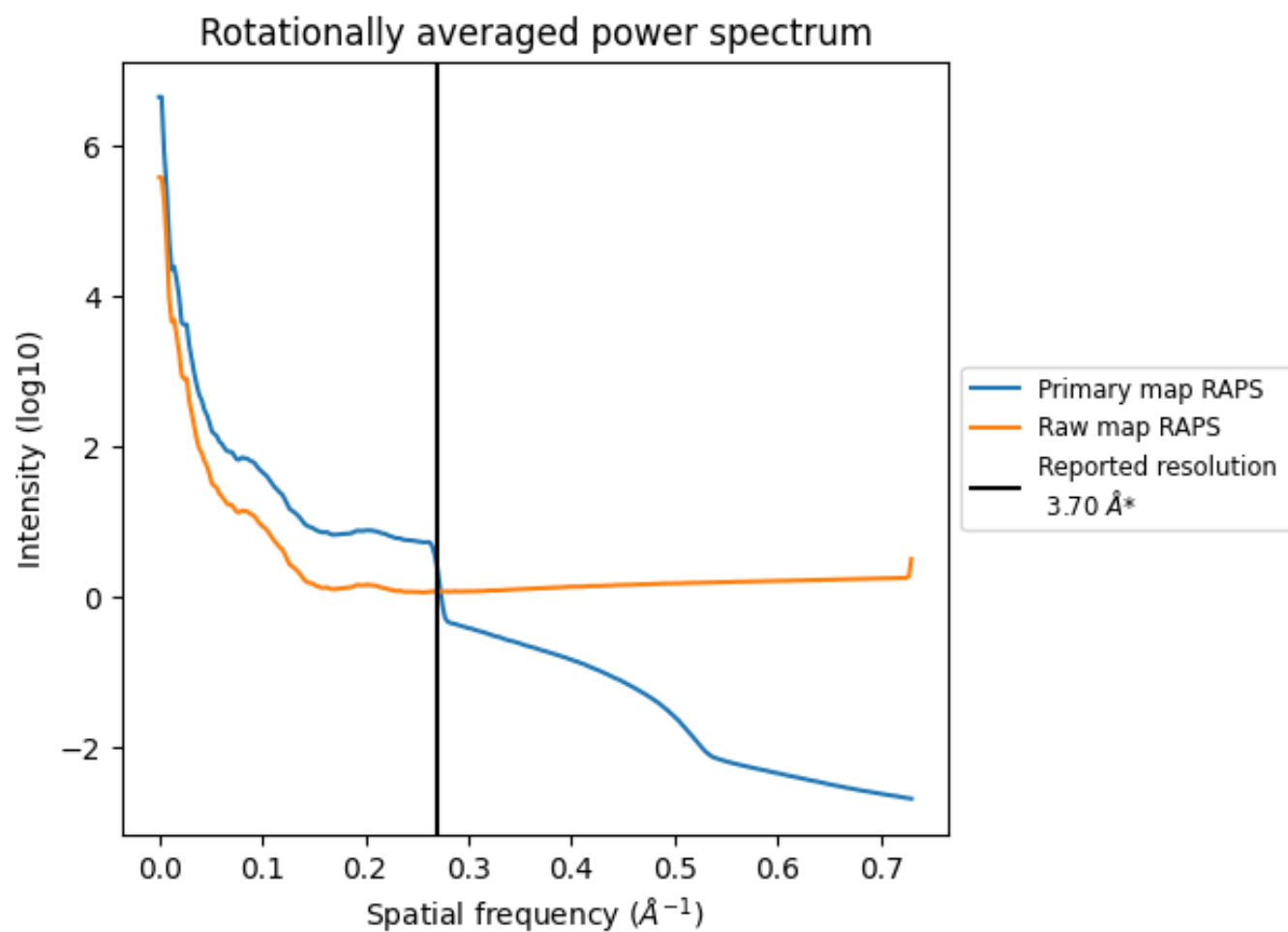
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 690 nm³; this corresponds to an approximate mass of 623 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 [i](#)

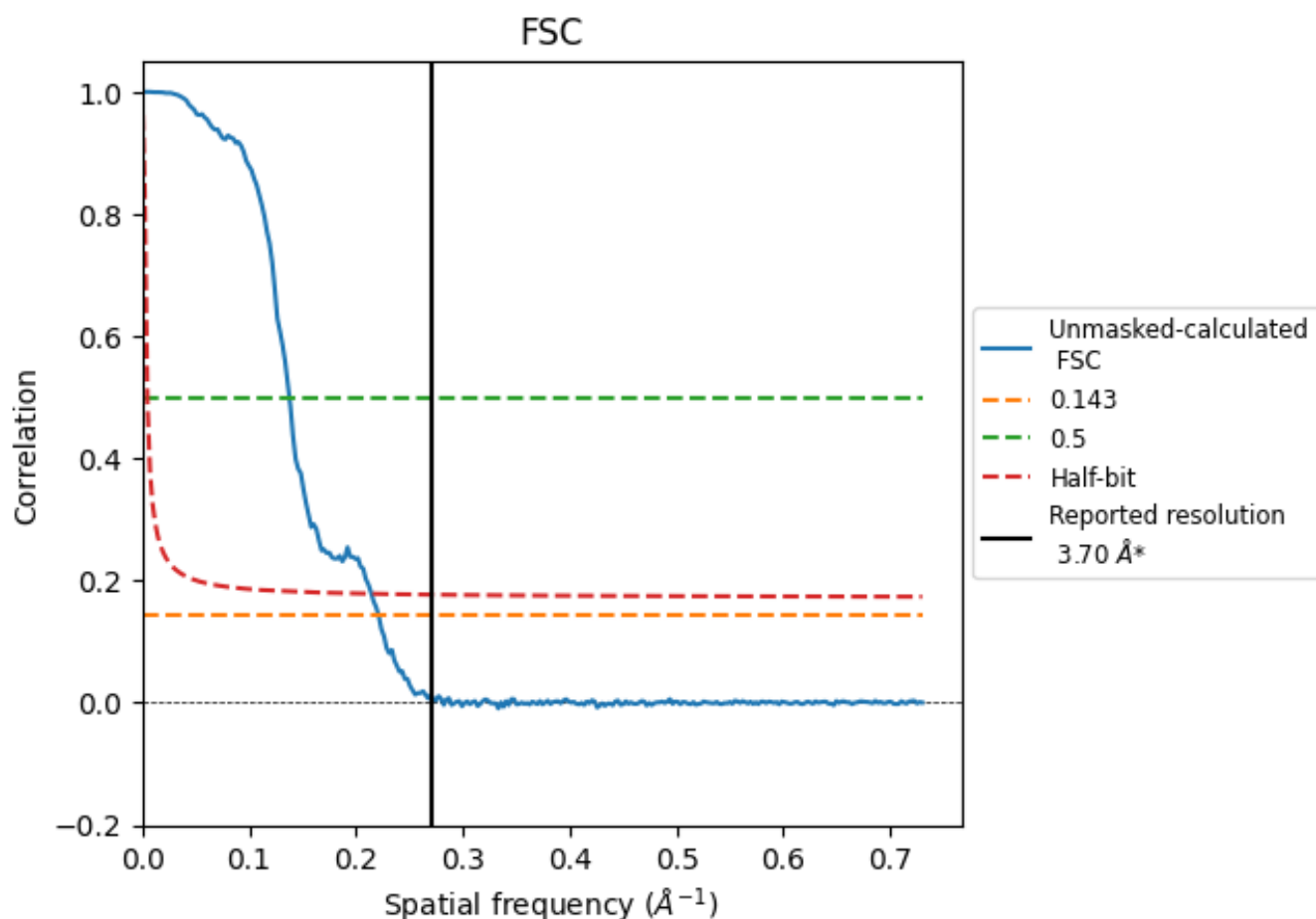


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

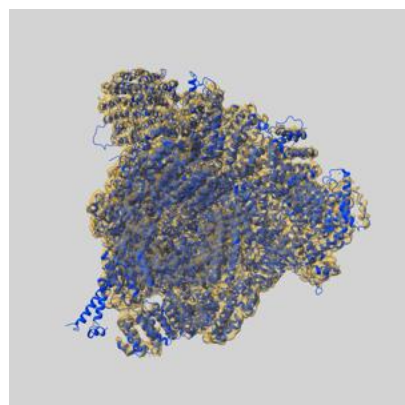
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.52	7.26	4.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.7 by more than 10 %

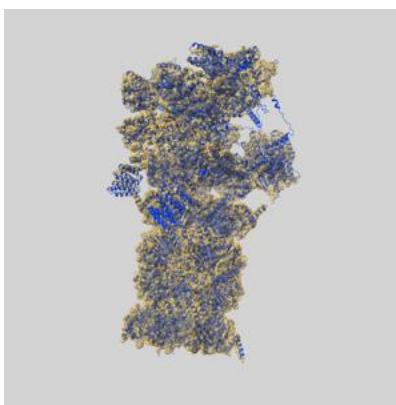
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62089 and PDB model 9K5D. Per-residue inclusion information can be found in section 3 on page 13.

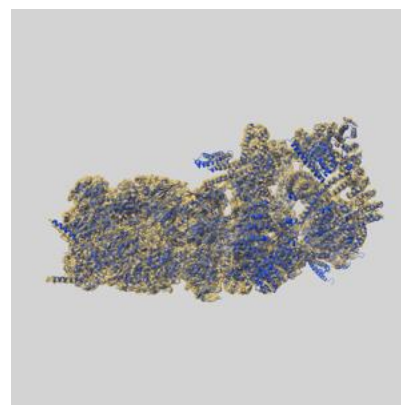
9.1 Map-model overlay [i](#)



X



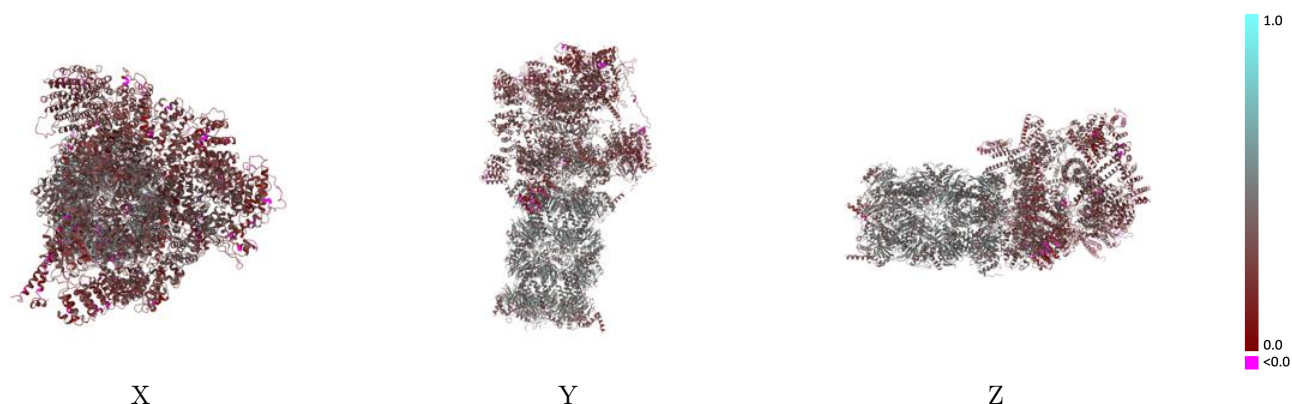
Y



Z

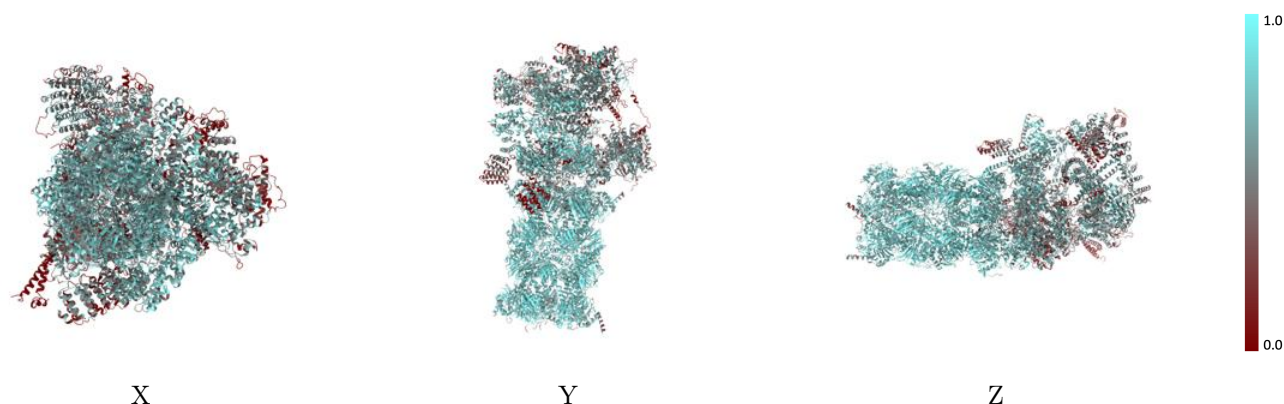
The images above show the 3D surface view of the map at the recommended contour level 0.00538 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



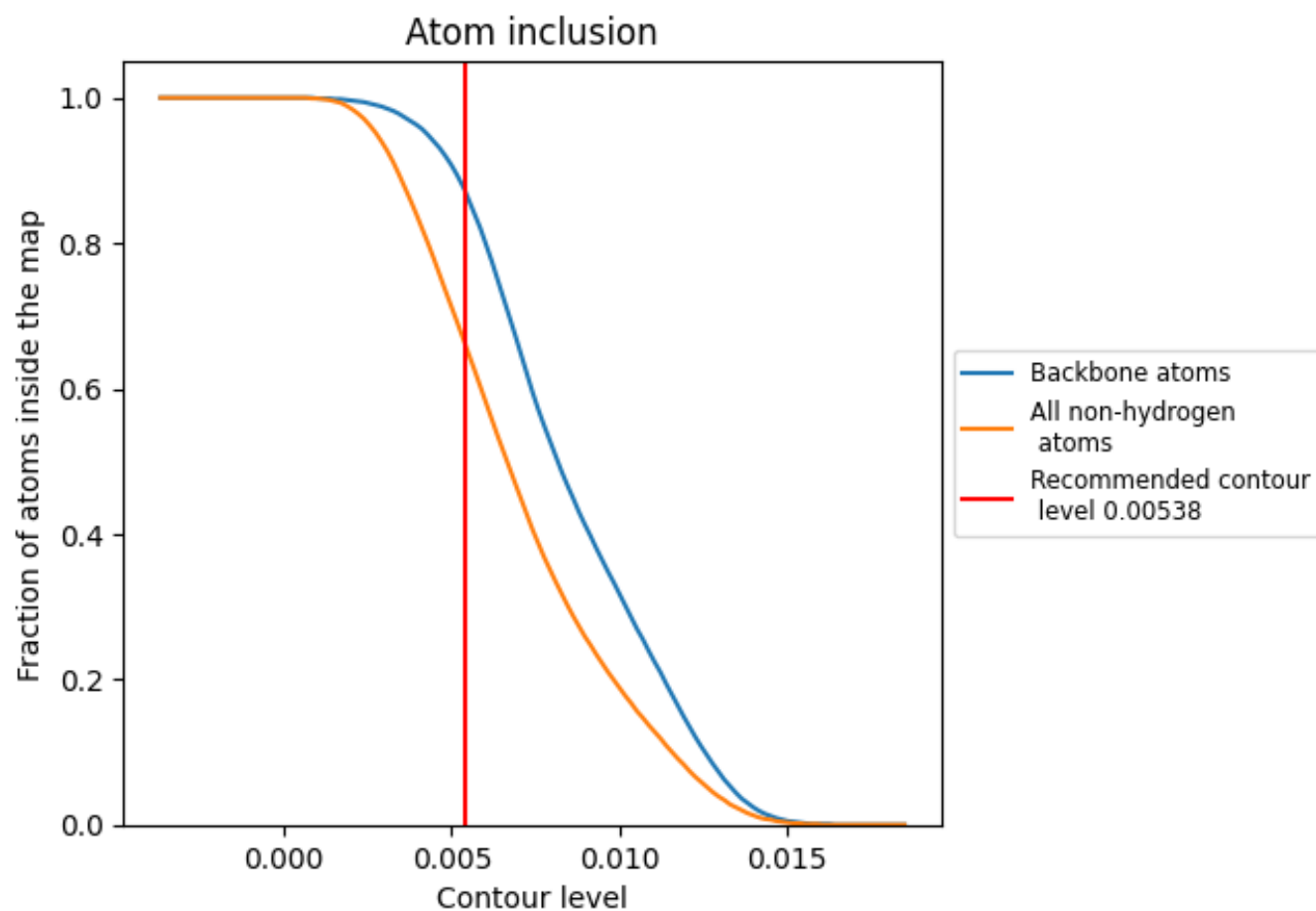
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00538).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 66% 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 (0.00538) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3630
A	 0.6090	 0.3520
B	 0.5850	 0.3490
C	 0.6570	 0.3670
D	 0.6350	 0.3480
E	 0.3550	 0.2080
F	 0.5440	 0.3160
G	 0.7920	 0.4460
H	 0.8130	 0.4540
I	 0.7850	 0.4420
J	 0.7680	 0.4330
K	 0.7660	 0.4370
L	 0.8180	 0.4580
M	 0.8040	 0.4470
N	 0.8390	 0.4630
O	 0.8390	 0.4610
P	 0.8520	 0.4660
Q	 0.8380	 0.4610
R	 0.8630	 0.4650
S	 0.8360	 0.4570
T	 0.8450	 0.4680
U	 0.5350	 0.2630
V	 0.4960	 0.2870
W	 0.5010	 0.2790
X	 0.5330	 0.2990
Y	 0.7120	 0.3340
Z	 0.5750	 0.3110
a	 0.5400	 0.2570
b	 0.4650	 0.2720
c	 0.5740	 0.3020
d	 0.3830	 0.2170
e	 0.4870	 0.3110
f	 0.4980	 0.2560
g	 0.7940	 0.4310
h	 0.8070	 0.4320



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Chain	Atom inclusion	Q-score
i	 0.7520	 0.4170
j	 0.7140	 0.3790
k	 0.7560	 0.4260
l	 0.8120	 0.4390
m	 0.8040	 0.4270
n	 0.8310	 0.4530
o	 0.8440	 0.4510
p	 0.8410	 0.4560
q	 0.8500	 0.4590
r	 0.8600	 0.4640
s	 0.8300	 0.4560
t	 0.8540	 0.4590
v	 0.2060	 0.3570