



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:21 PM EST

PDB ID : 6MSE  
EMDB ID : EMD-9218  
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome  
Authors : Mao, Y.D.  
Deposited on : 2018-10-16  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

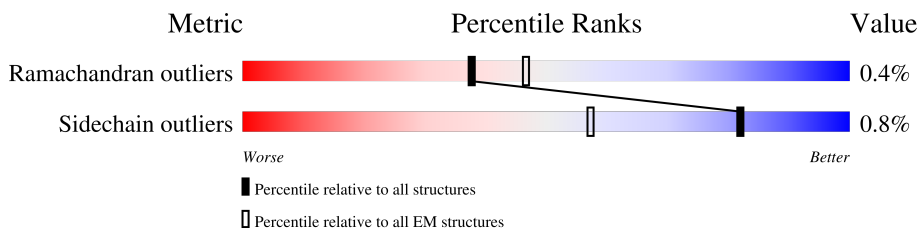
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	U	953	
2	V	533	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	

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Mol	Chain	Length	Quality of chain
10	d	349	65% 72% 26%
11	e	70	46% 36% 20% 43%
12	f	892	84% 95%
13	A	433	34% 88% 9%
14	B	440	40% 88% 10%
15	C	398	57% 92%
16	D	418	32% 88% 9%
17	E	403	28% 95%
18	F	439	32% 92% 5%
19	u	76	50% 99%
20	v	28	71% 100%
21	G	245	13% 98%
21	g	245	43% 98%
22	H	233	8% 100%
22	h	233	41% 100%
23	I	260	21% 96%
23	i	260	57% 96%
24	J	247	23% 96%
24	j	247	57% 96%
25	K	240	19% 94% 5%
25	k	240	53% 94% 5%
26	L	268	15% 89% 11%
26	l	268	32% 89% 11%
27	M	254	16% 94% 6%
27	m	254	38% 94% 6%

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Mol	Chain	Length	Quality of chain
28	N	238	 8% 80% 20%
28	n	238	 11% 80% 20%
29	O	276	 10% 80% 20%
29	o	276	 17% 80% 20%
30	P	204	 14% 100%
30	p	204	 16% 100%
31	Q	201	 14% 98% ..
31	q	201	 24% 98% ..
32	R	262	 10% 77% 23%
32	r	262	 12% 77% 23%
33	S	240	 14% 89% 11%
33	s	240	 15% 89% 11%
34	T	263	 10% 81% • 18%
34	t	263	 11% 81% • 18%

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 105062 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	812	6334	4023	1078	1189	44	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3852	2444	684	710	14	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3703	2339	635	704	25	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	380	3009	1918	509	570	12	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	334	200	55	77	2	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	f	889	6866	4315	1174	1331	46	0	0

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	393	3067	1930	539	581	17	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	395	3086	1946	523	602	15	0	0

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

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

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

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

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

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

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	76	603	378	107	117	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called substrate.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
21	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 22 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
22	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
23	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 24 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
24	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 25 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
25	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		



- Molecule 26 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
26	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 27 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
27	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 28 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
28	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 29 is a protein called Proteasome subunit beta type-7.

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

- Molecule 30 is a protein called Proteasome subunit beta type-3.

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

- Molecule 31 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
31	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 32 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
32	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 33 is a protein called Proteasome subunit beta type-1.

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

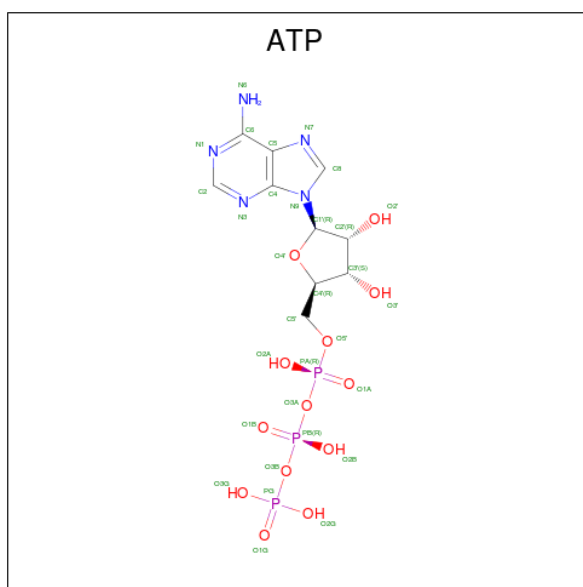
- Molecule 34 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
34	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

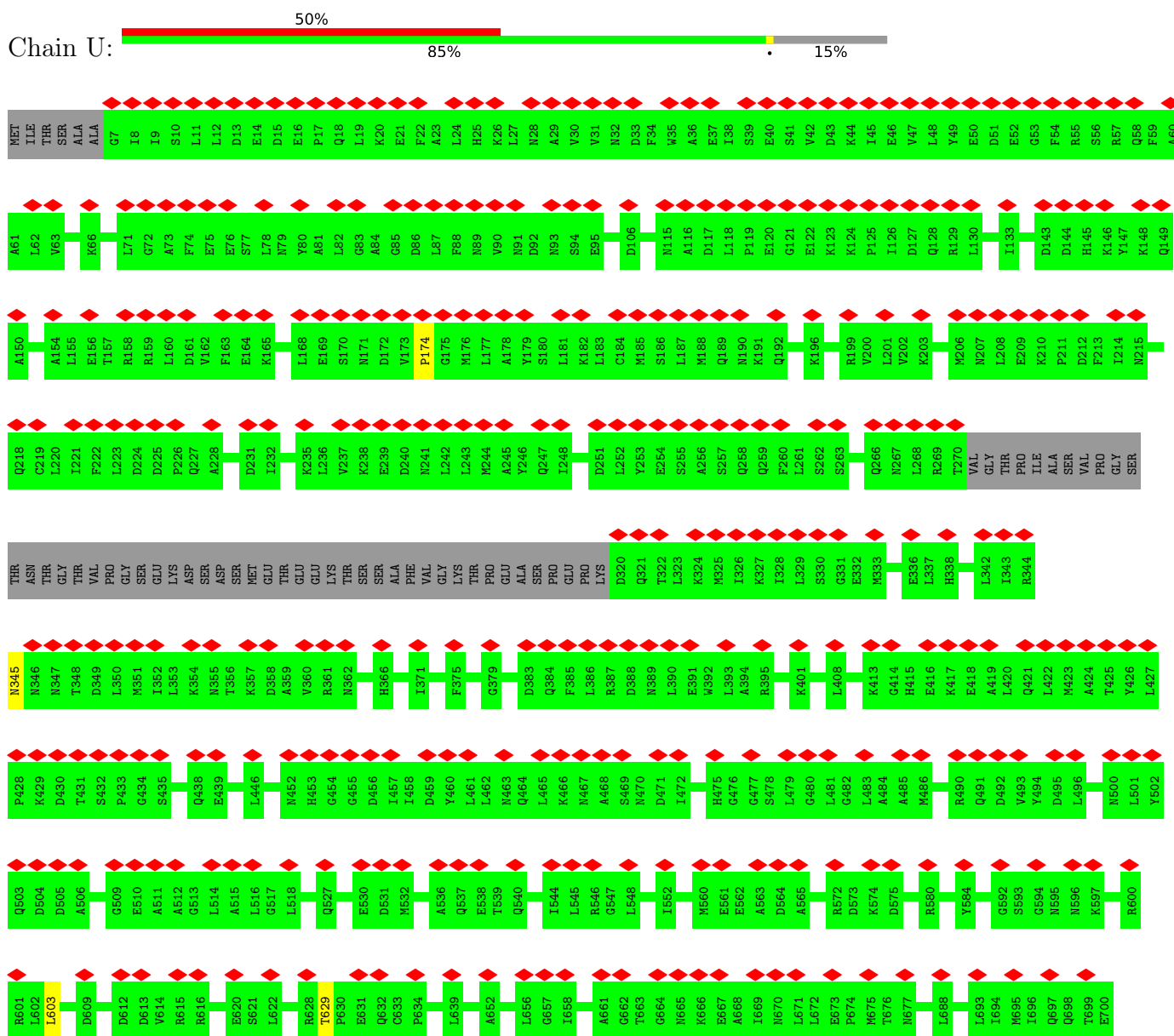
- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

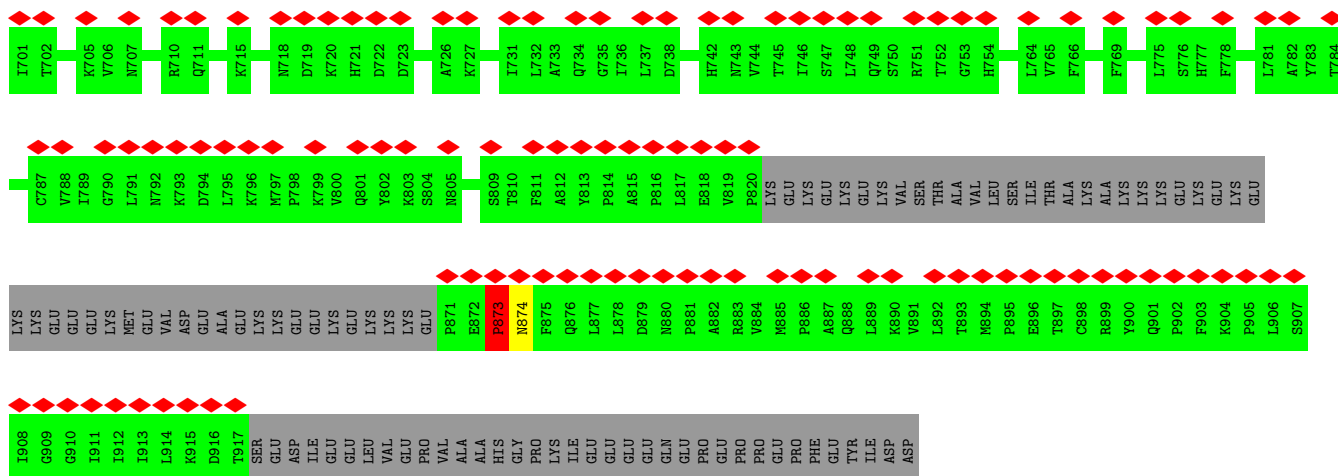


### 3 Residue-property plots

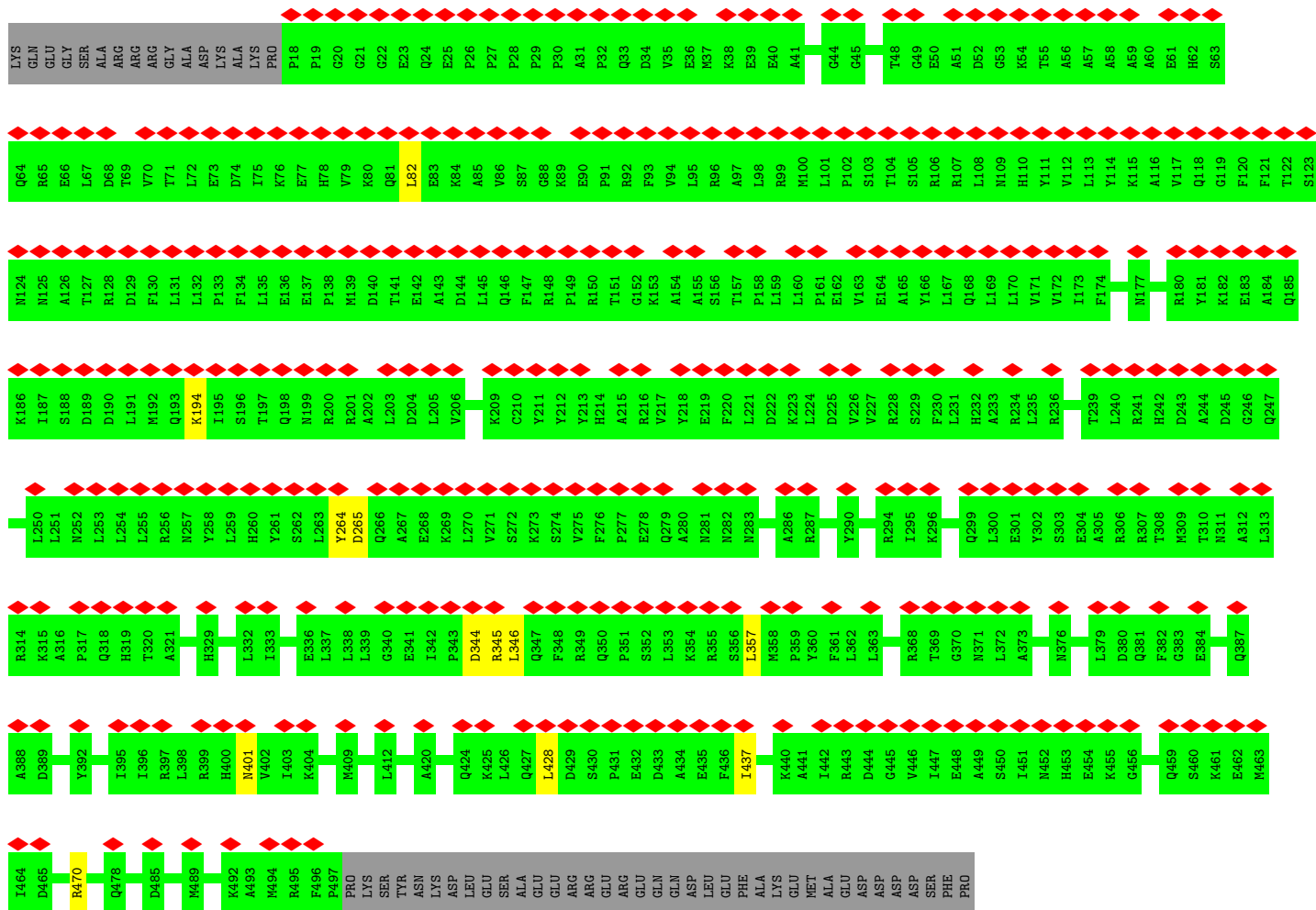
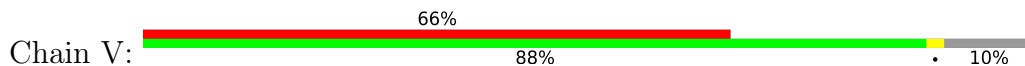
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

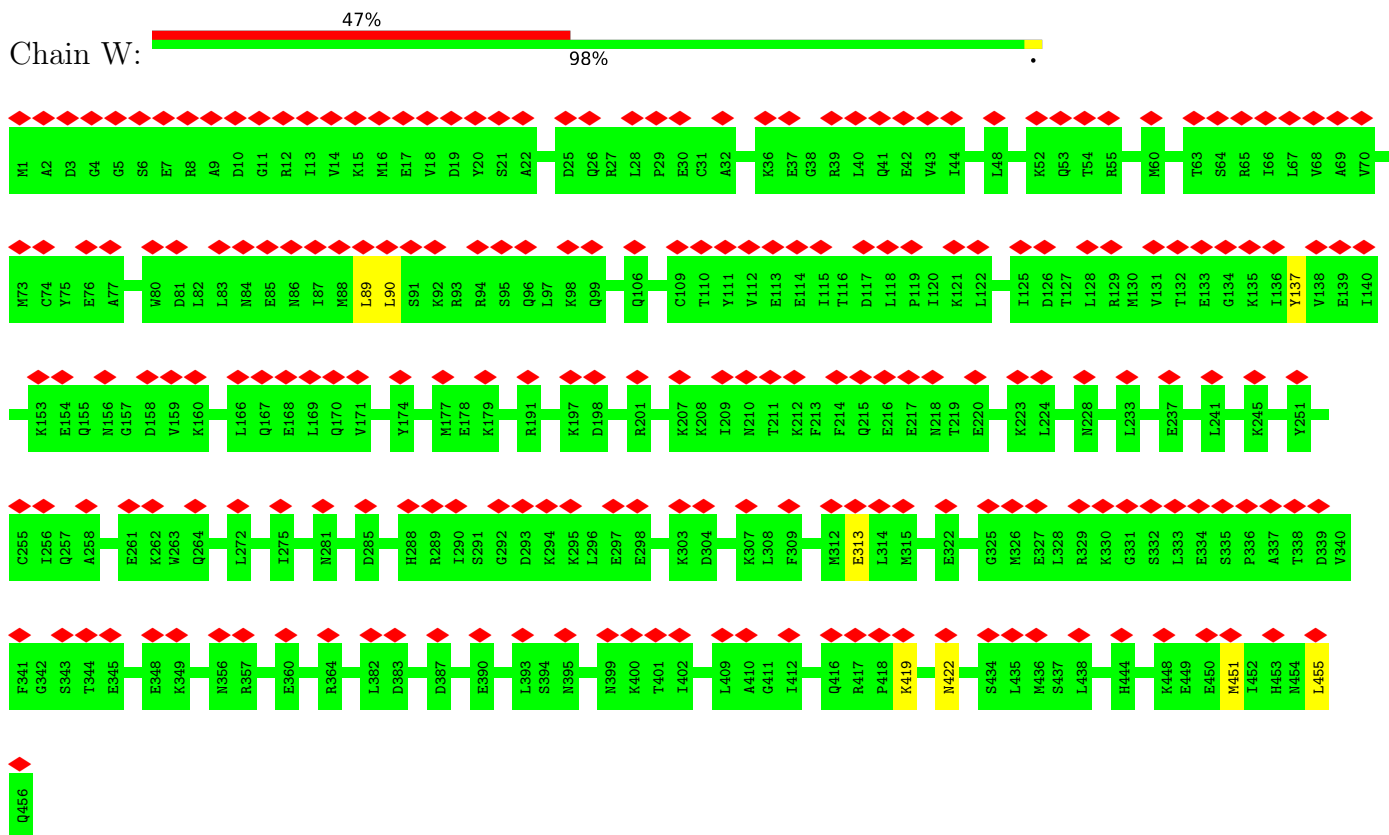




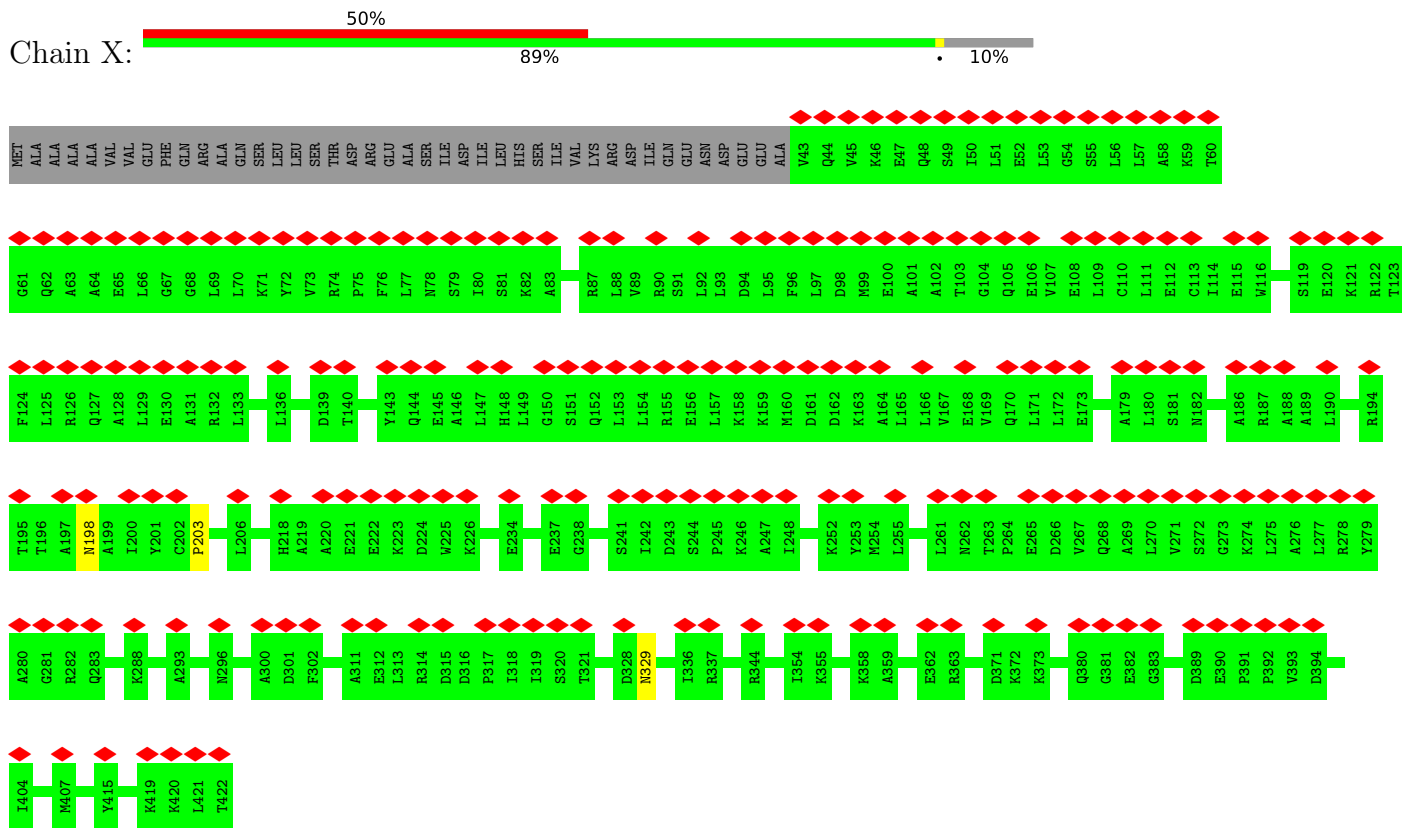
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

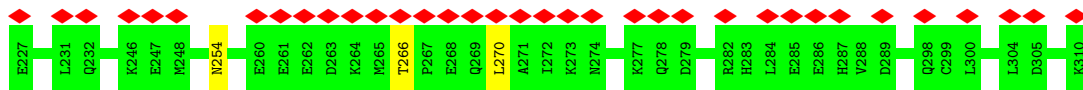


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

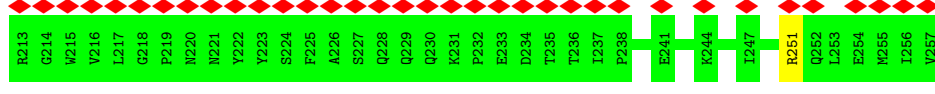
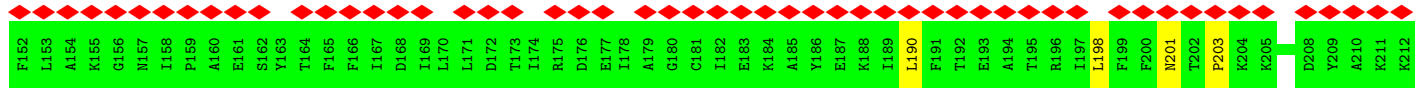
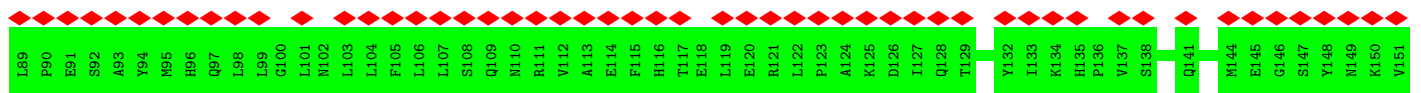
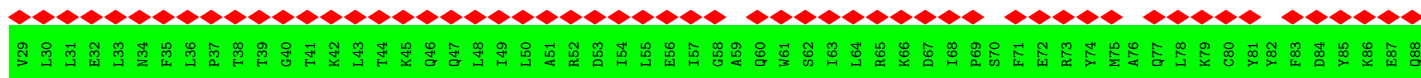
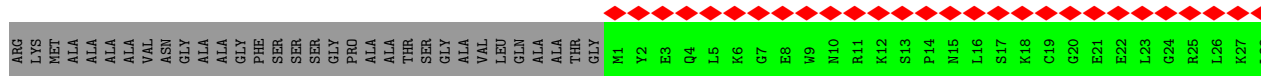
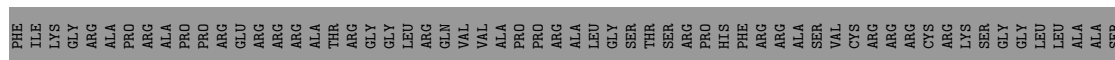
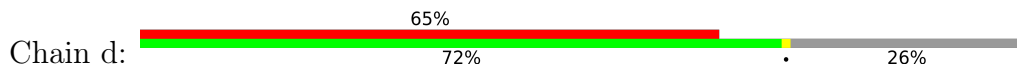




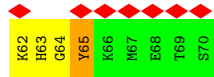
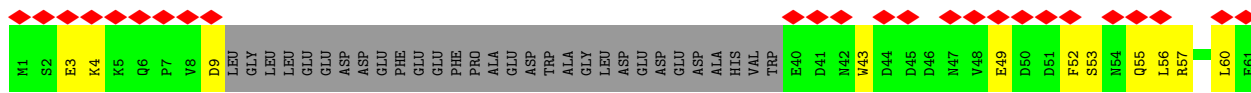
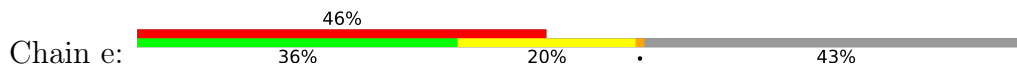




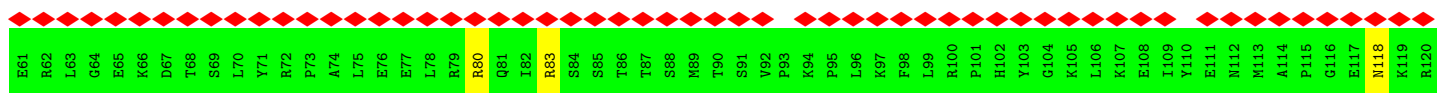
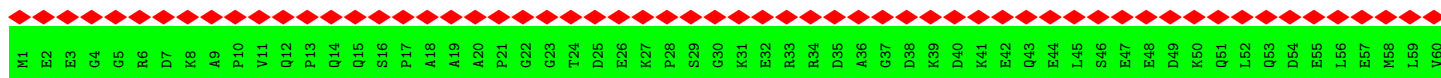
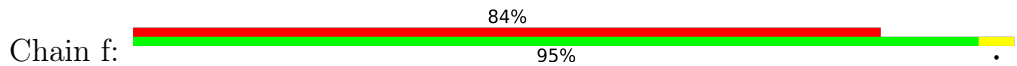
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

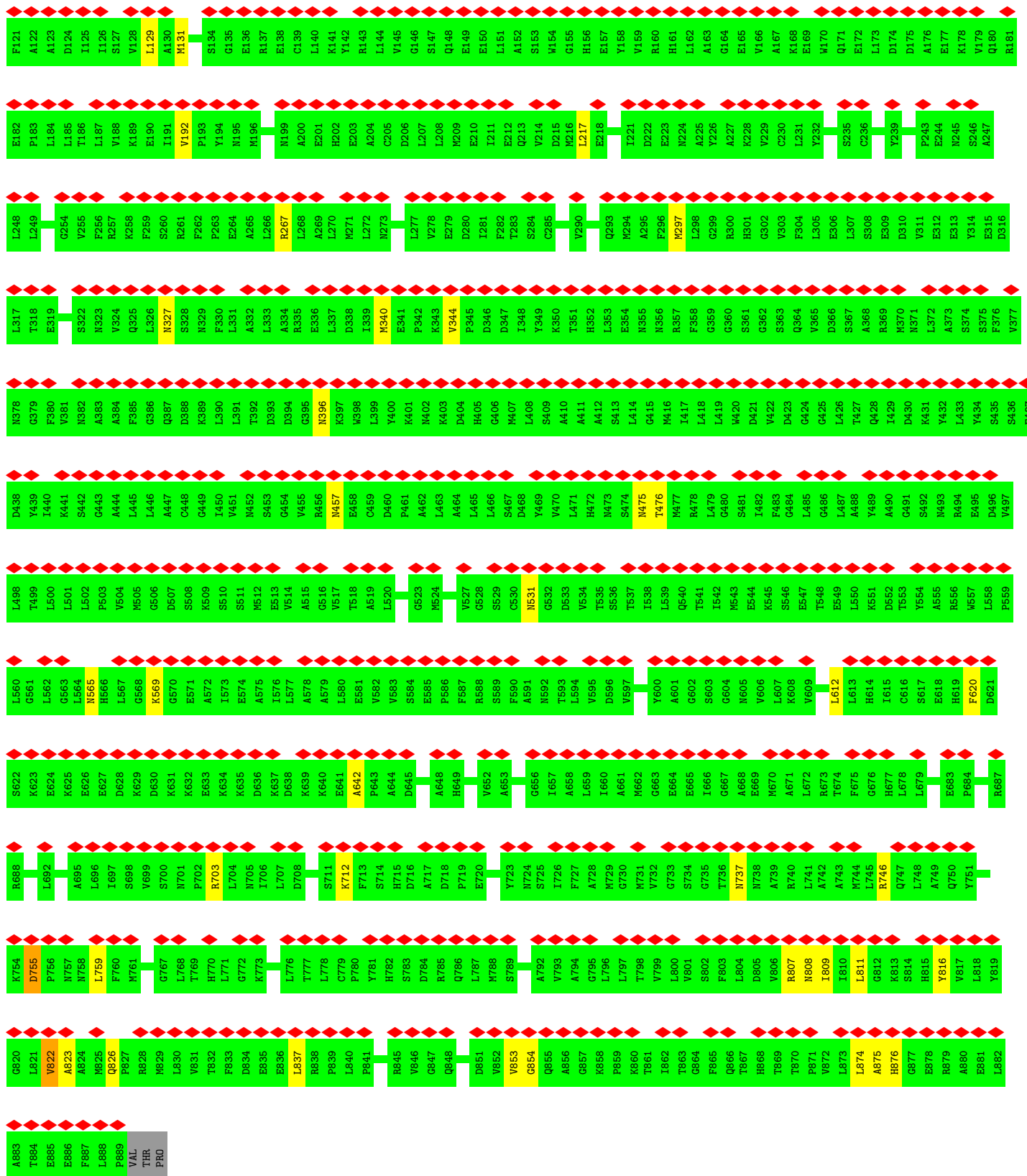


• Molecule 11: 26S proteasome complex subunit SEM1

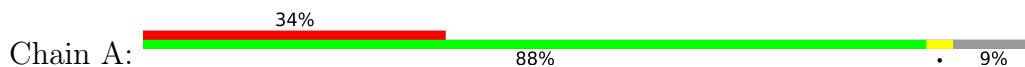


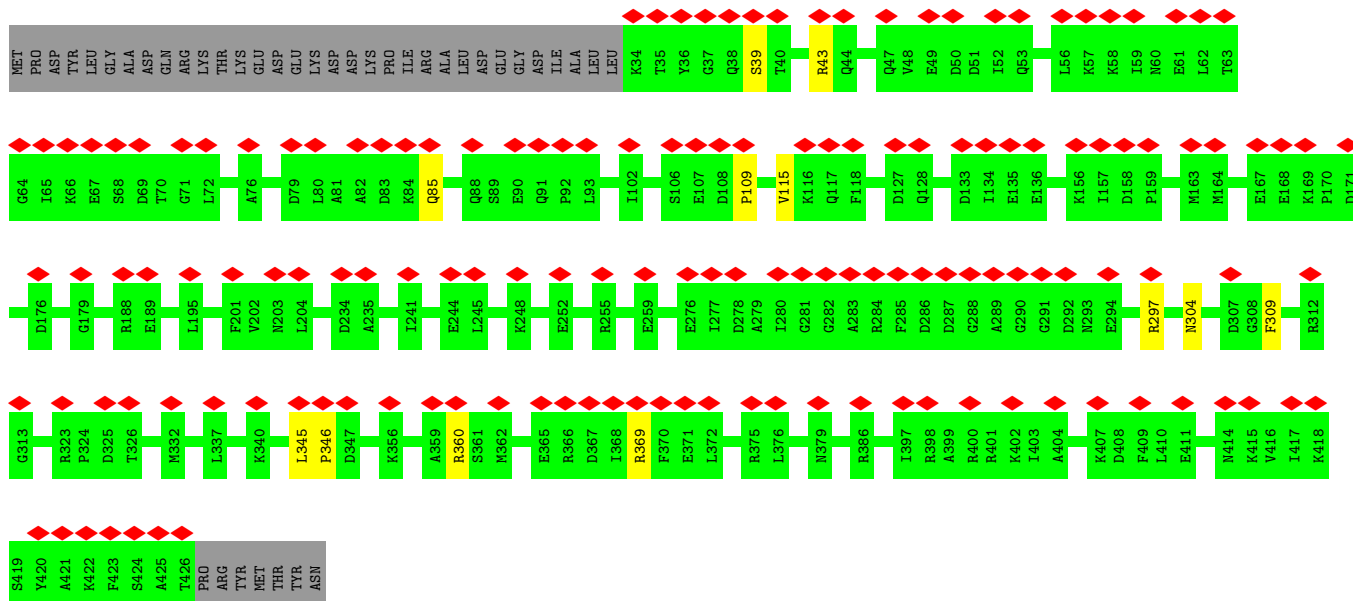
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2



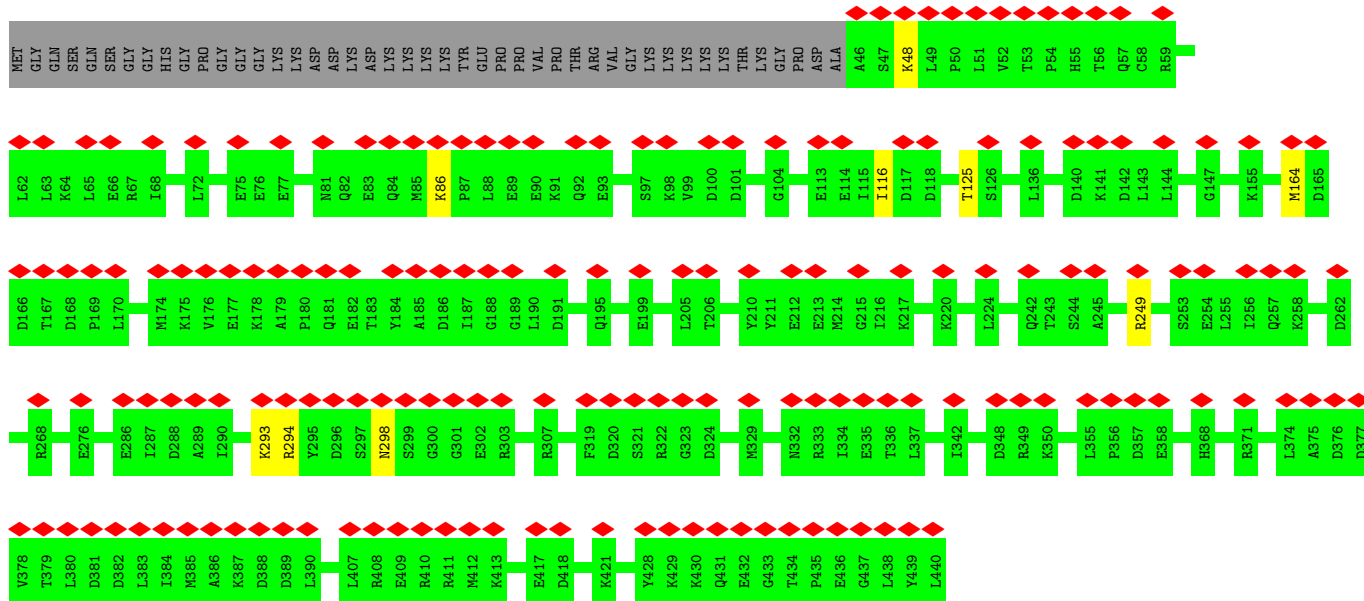
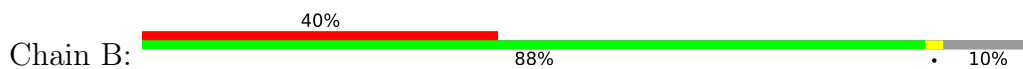


• Molecule 13: 26S proteasome regulatory subunit 7

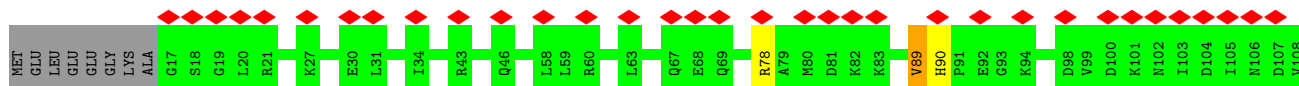
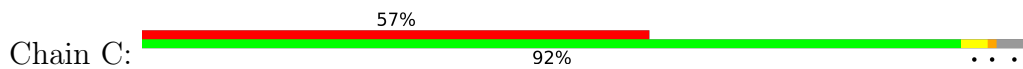


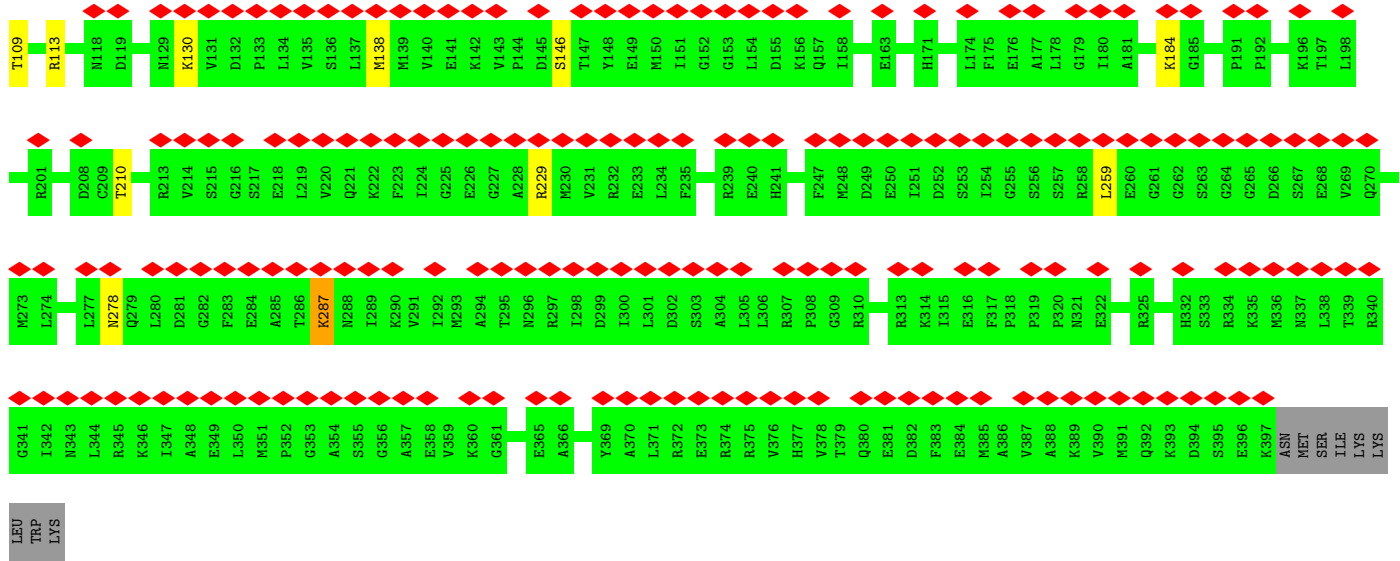


• Molecule 14: 26S proteasome regulatory subunit 4

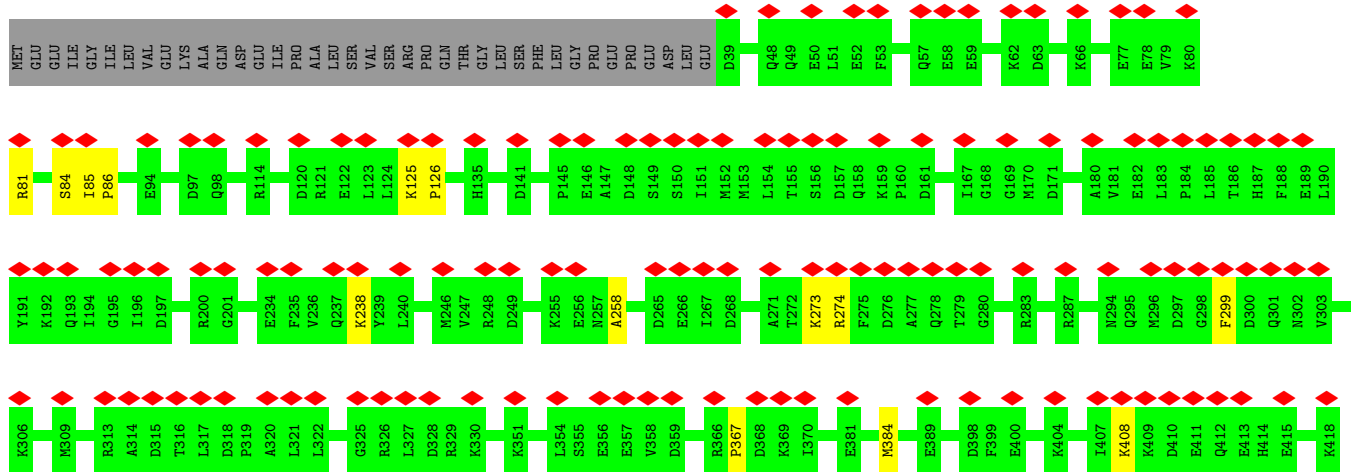
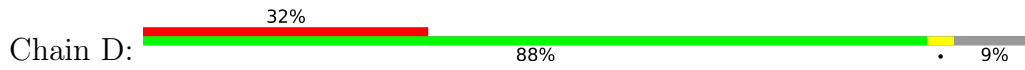


• Molecule 15: 26S proteasome regulatory subunit 8

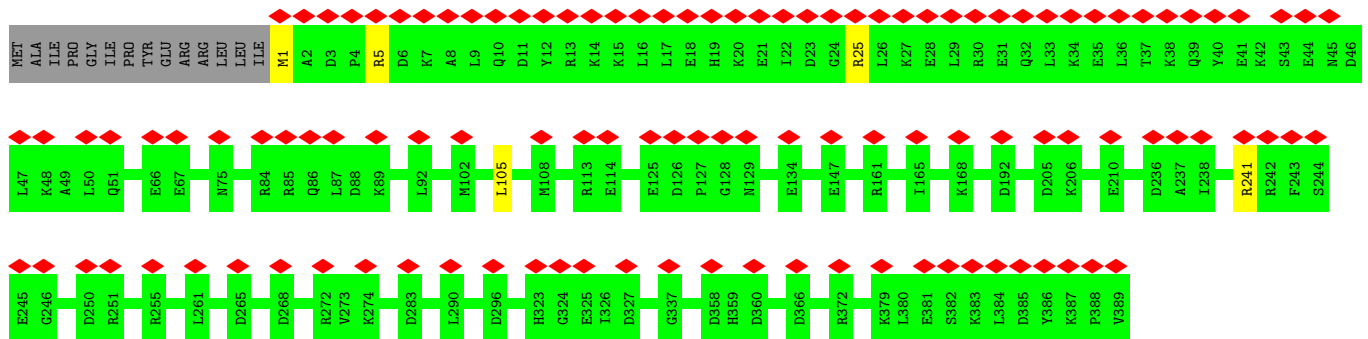




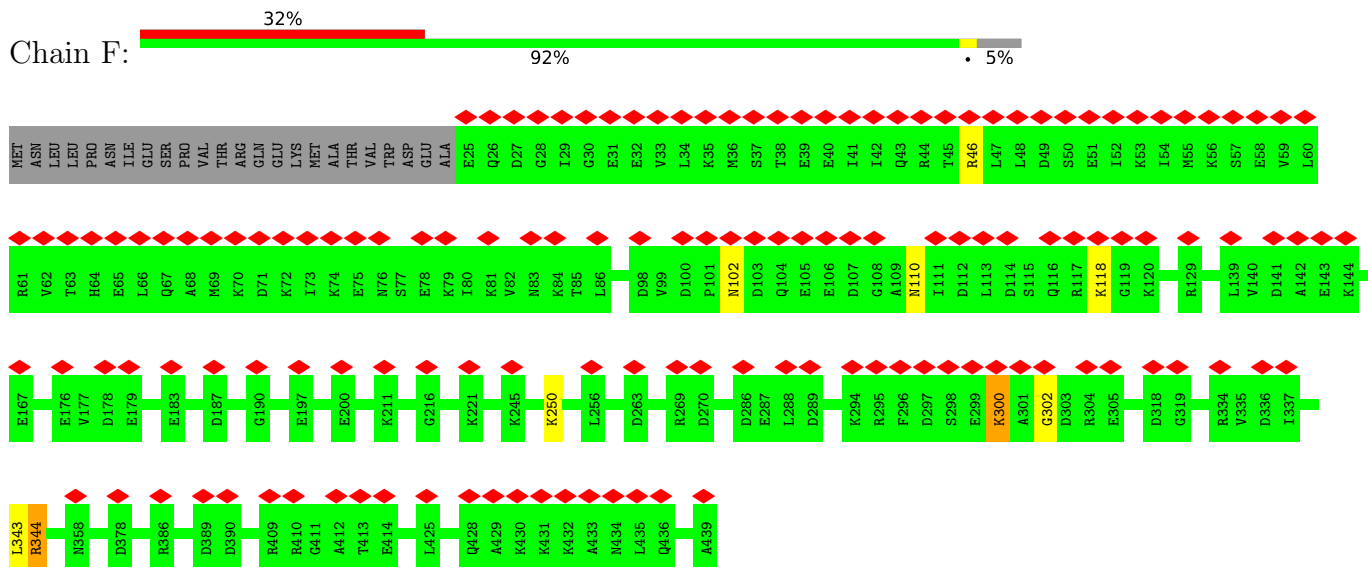
• Molecule 16: 26S proteasome regulatory subunit 6B



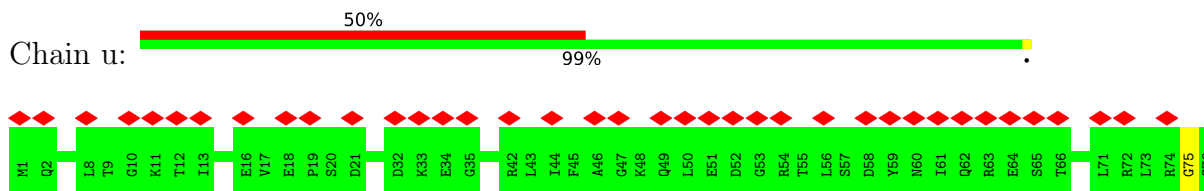
• Molecule 17: 26S proteasome regulatory subunit 10B



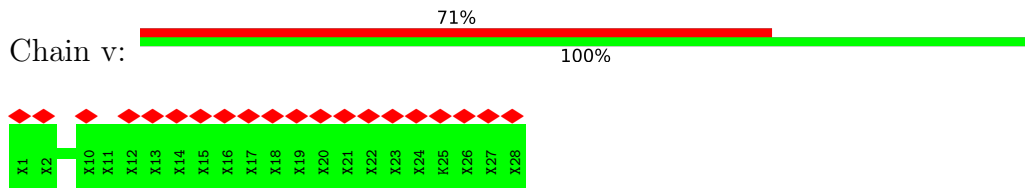
• Molecule 18: 26S proteasome regulatory subunit 6A



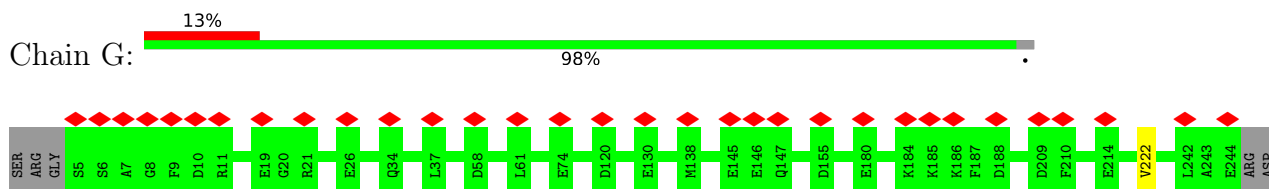
• Molecule 19: Ubiquitin



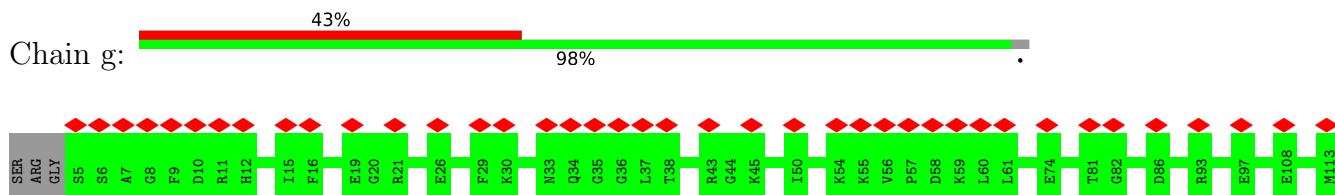
• Molecule 20: substrate

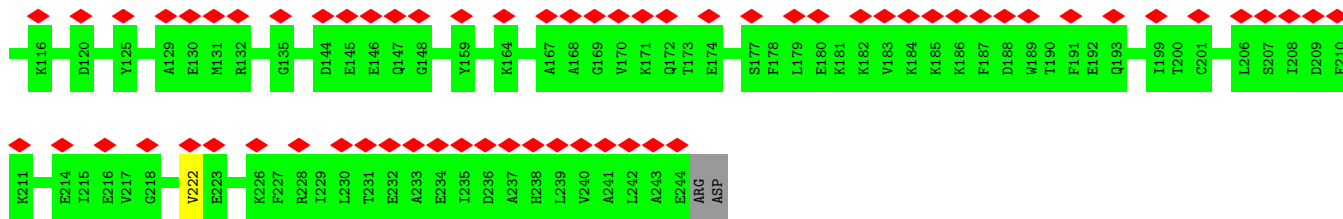


• Molecule 21: Proteasome subunit alpha type-6

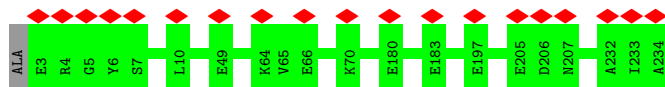


• Molecule 21: Proteasome subunit alpha type-6

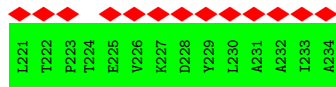
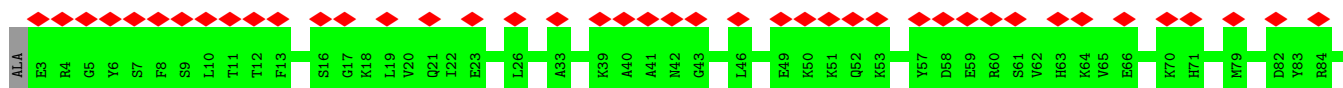
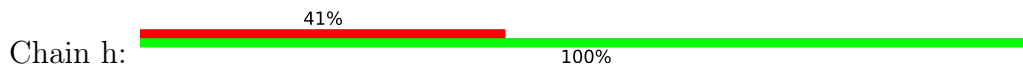




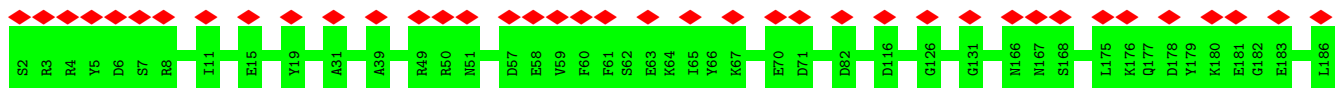
• Molecule 22: Proteasome subunit alpha type-2



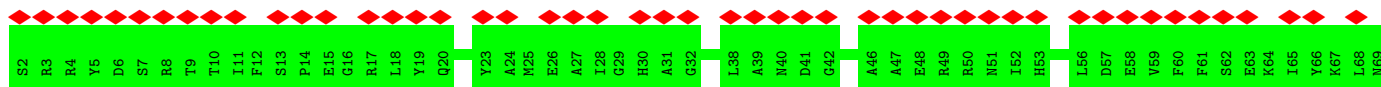
• Molecule 22: Proteasome subunit alpha type-2

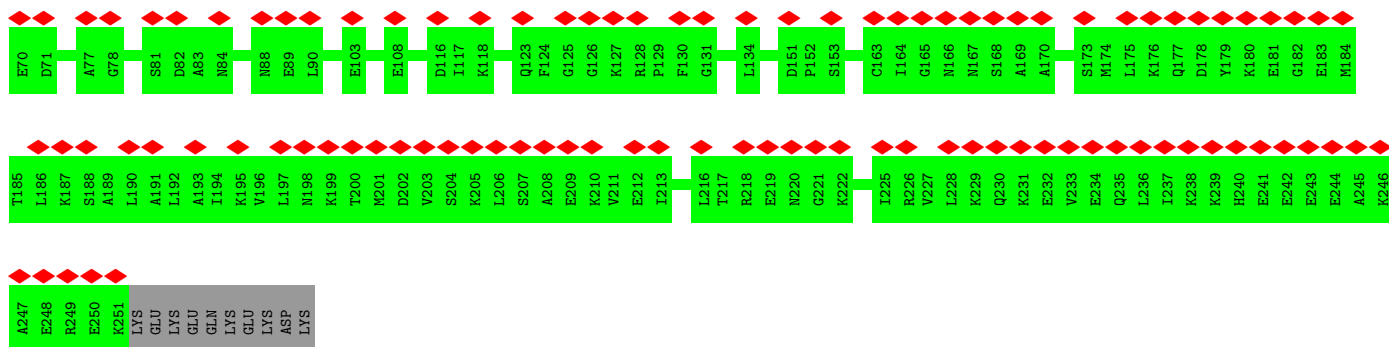


• Molecule 23: Proteasome subunit alpha type-4

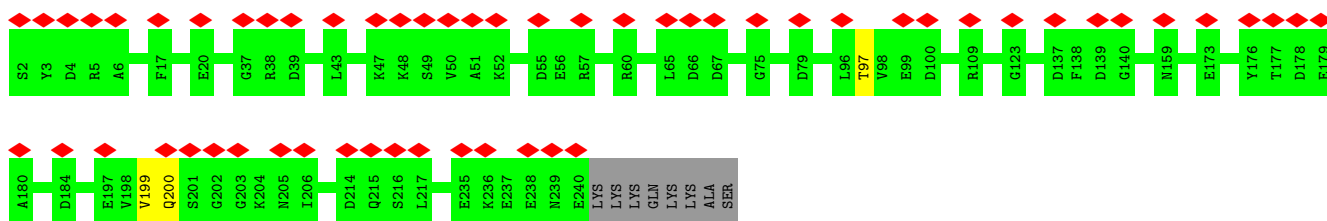


• Molecule 23: Proteasome subunit alpha type-4

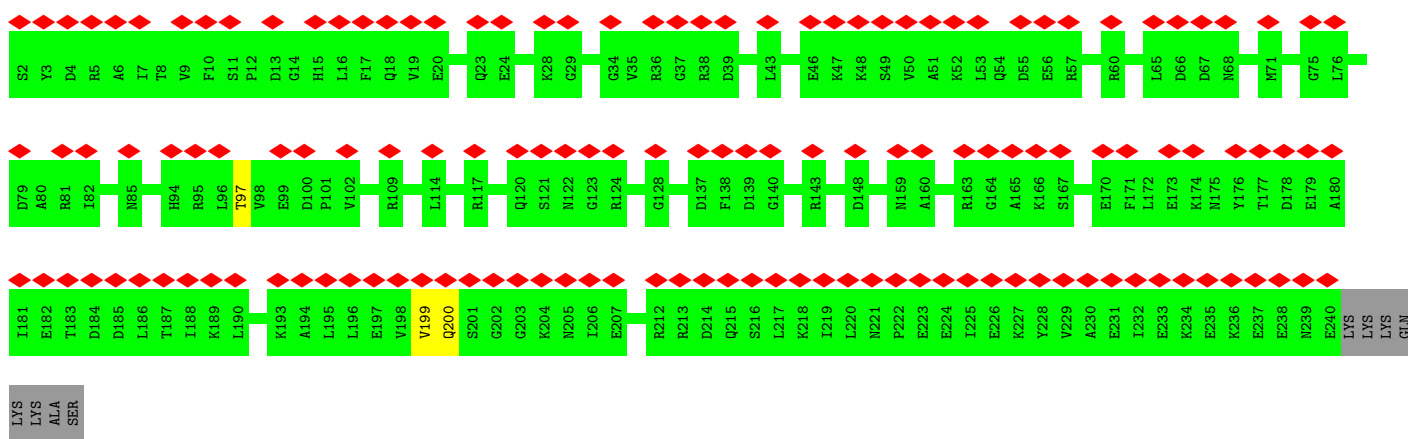




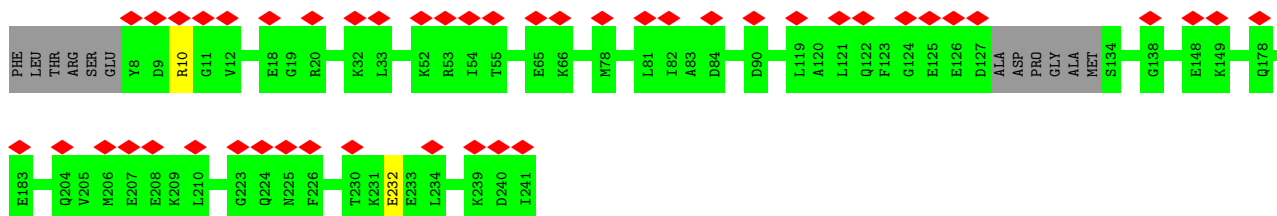
• Molecule 24: Proteasome subunit alpha type-7



• Molecule 24: Proteasome subunit alpha type-7

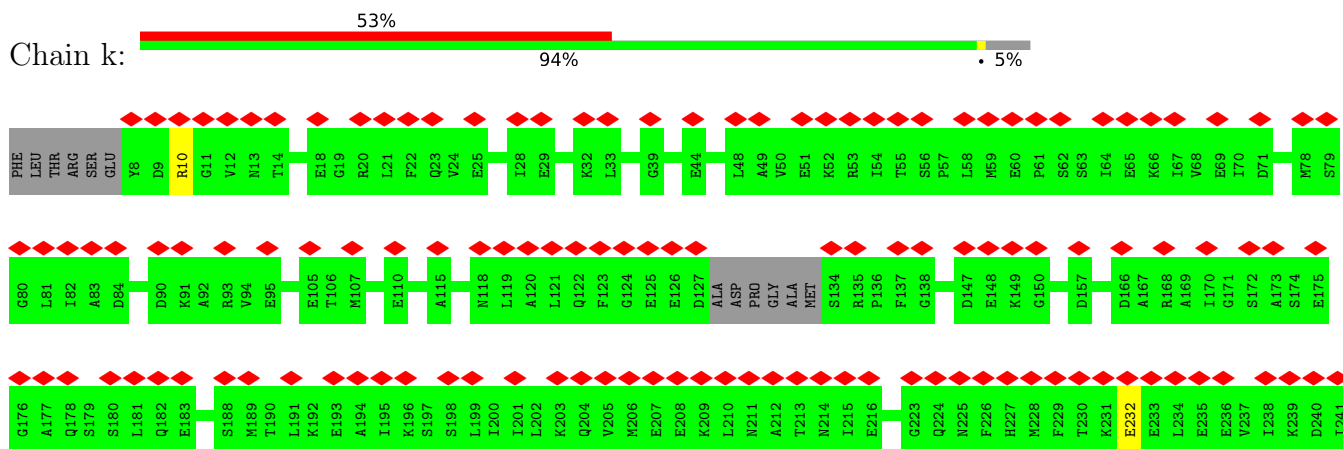


• Molecule 25: Proteasome subunit alpha type-5

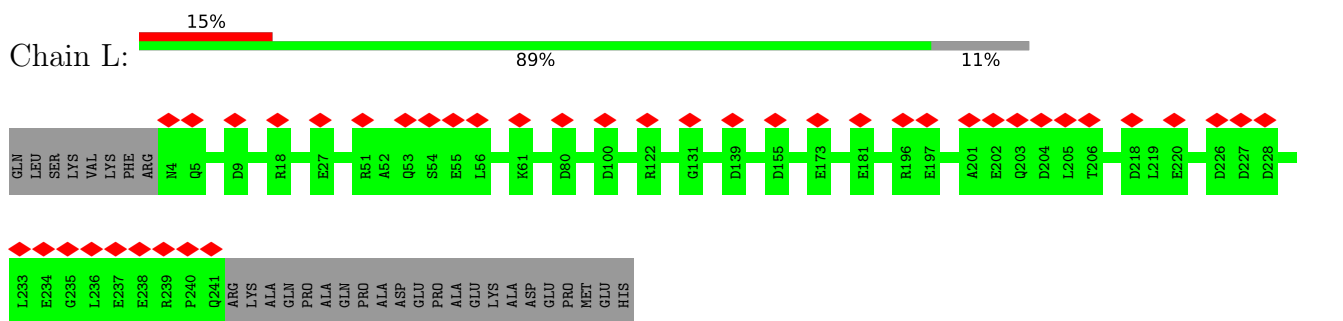




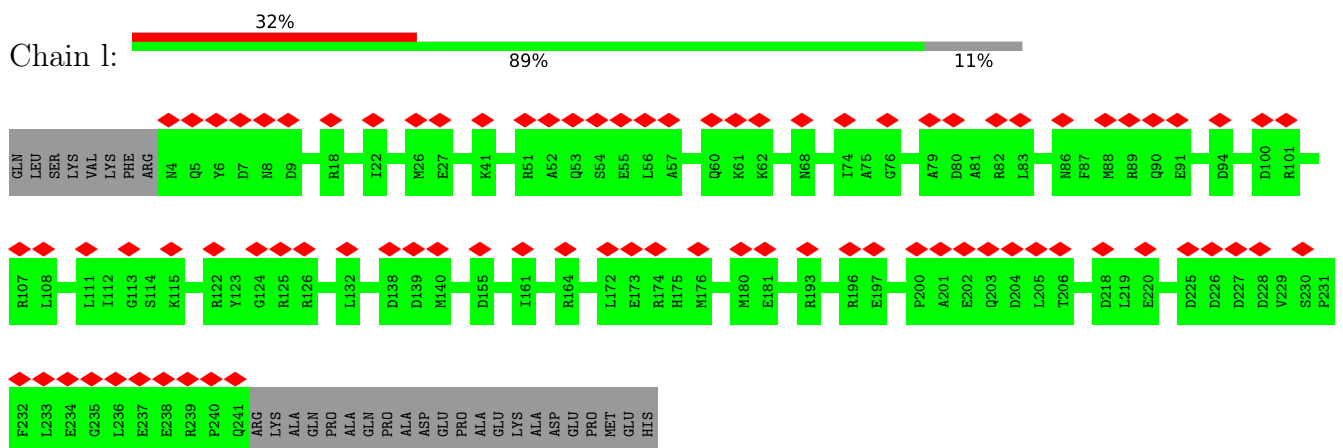
- Molecule 25: Proteasome subunit alpha type-5



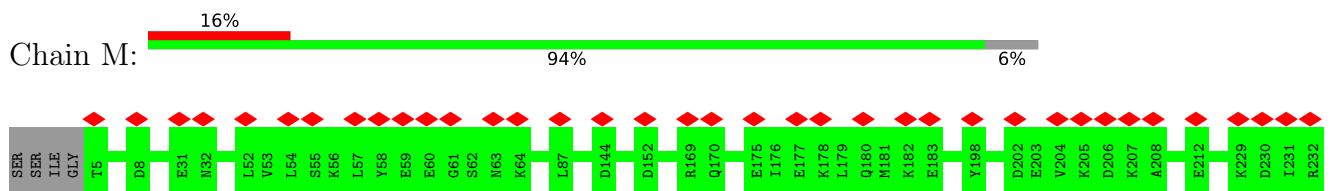
- Molecule 26: Proteasome subunit alpha type-1

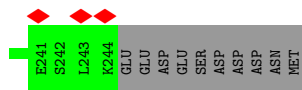


- Molecule 26: Proteasome subunit alpha type-1

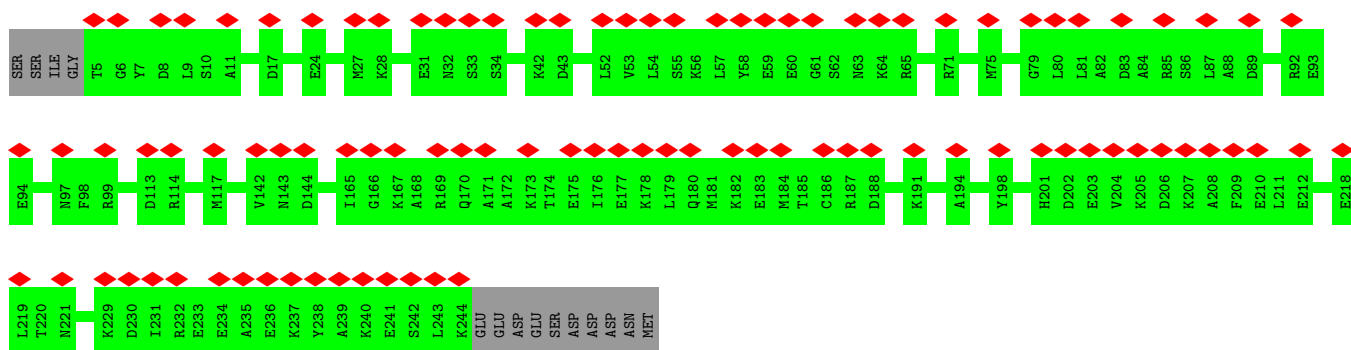
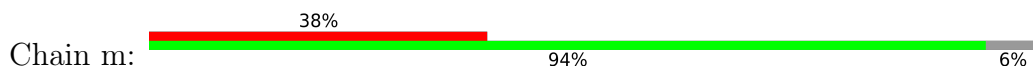


- Molecule 27: Proteasome subunit alpha type-3

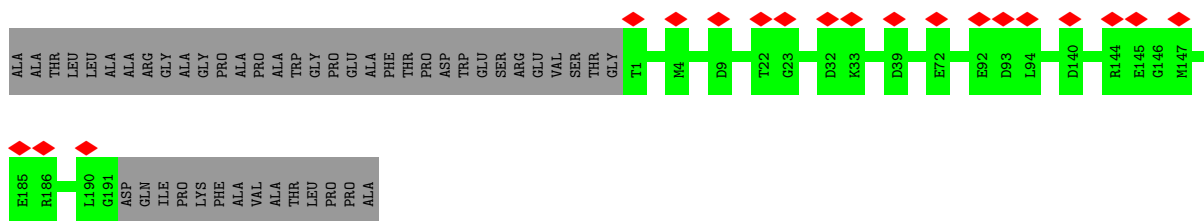
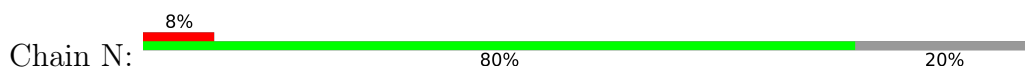




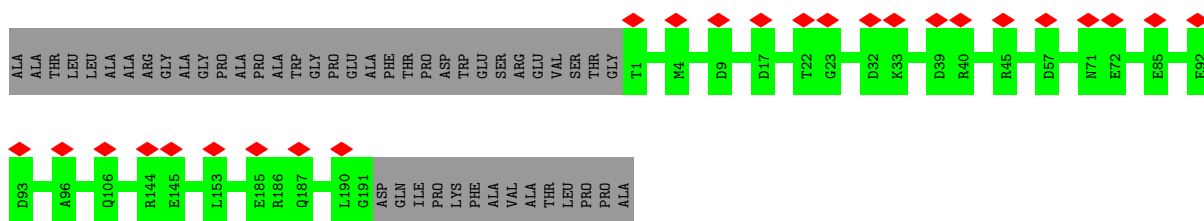
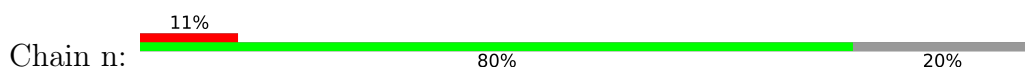
• Molecule 27: Proteasome subunit alpha type-3



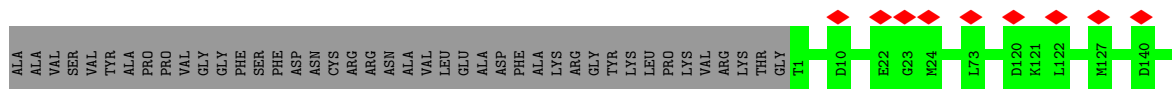
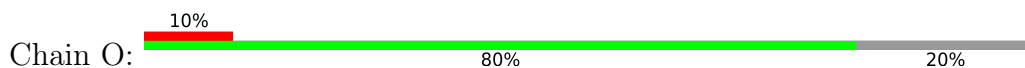
• Molecule 28: Proteasome subunit beta type-6

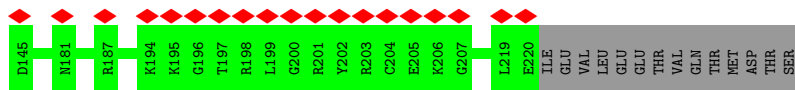


• Molecule 28: Proteasome subunit beta type-6

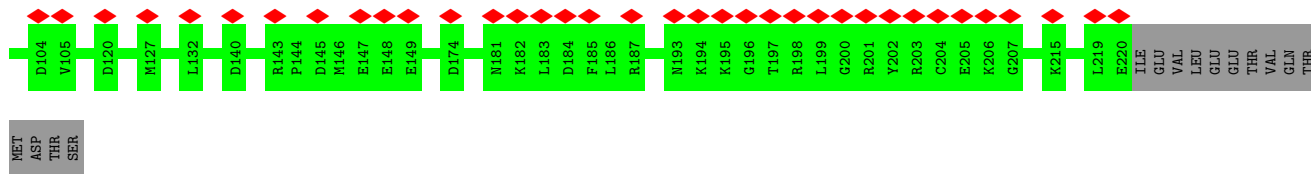
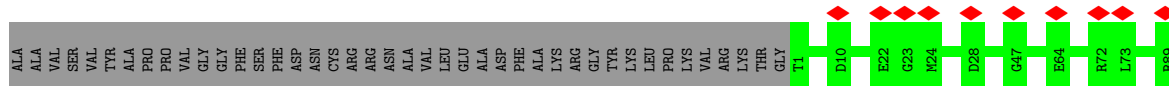
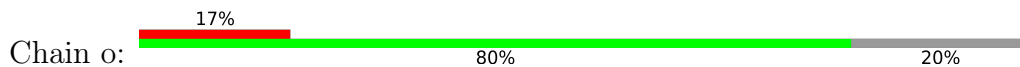


• Molecule 29: Proteasome subunit beta type-7

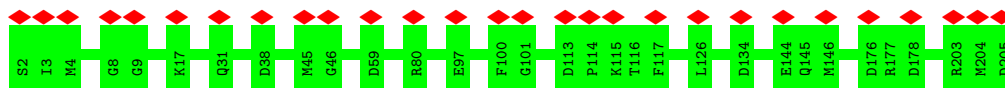




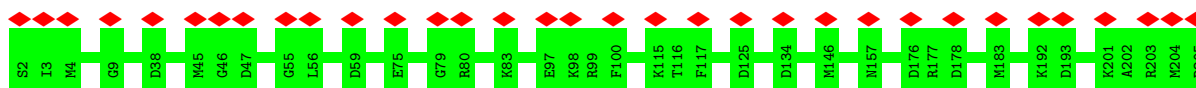
• Molecule 29: Proteasome subunit beta type-7



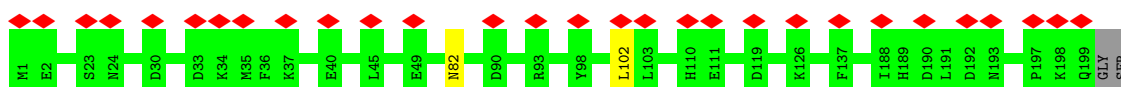
• Molecule 30: Proteasome subunit beta type-3



• Molecule 30: Proteasome subunit beta type-3



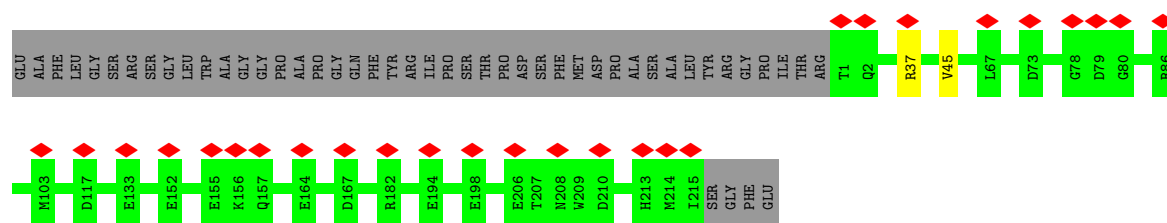
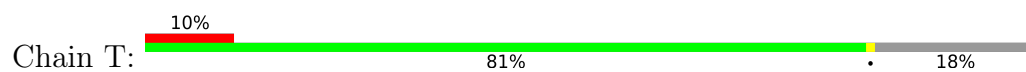
• Molecule 31: Proteasome subunit beta type-2



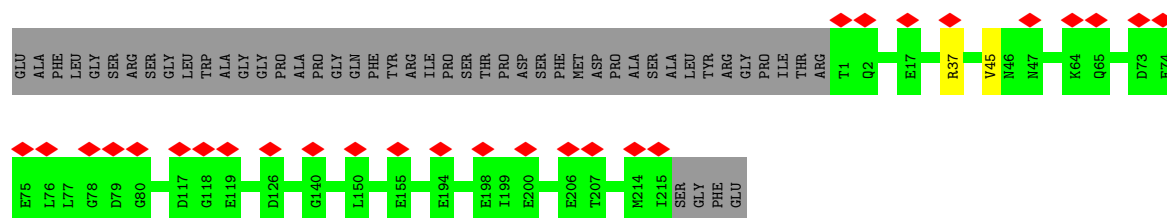
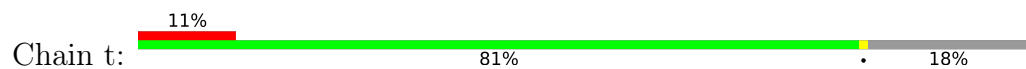
• Molecule 31: Proteasome subunit beta type-2







- Molecule 34: Proteasome subunit beta type-4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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, 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	U	0.30	0/6449	0.56	3/8729 (0.0%)
2	V	0.34	0/3929	0.68	4/5309 (0.1%)
3	W	0.31	0/3751	0.65	2/5042 (0.0%)
4	X	0.28	0/3053	0.54	0/4115
5	Y	0.49	4/3173 (0.1%)	0.85	11/4273 (0.3%)
6	Z	0.32	0/2324	0.68	4/3150 (0.1%)
7	a	0.31	0/3053	0.60	2/4133 (0.0%)
8	b	0.30	0/1478	0.61	0/2001
9	c	0.32	0/2302	0.63	1/3110 (0.0%)
10	d	0.31	0/2162	0.59	1/2919 (0.0%)
11	e	0.91	2/338 (0.6%)	1.98	17/450 (3.8%)
12	f	0.33	1/6980 (0.0%)	0.71	7/9433 (0.1%)
13	A	0.32	0/3117	0.61	1/4207 (0.0%)
14	B	0.32	0/3131	0.60	0/4227
15	C	0.31	0/3017	0.62	1/4058 (0.0%)
16	D	0.32	0/3089	0.57	0/4168
17	E	0.32	0/3145	0.56	1/4233 (0.0%)
18	F	0.34	0/3292	0.56	0/4435
19	u	0.30	0/609	0.60	1/819 (0.1%)
20	v	0.20	0/8	0.18	0/8
21	G	0.31	0/1859	0.54	0/2523
21	g	0.31	0/1859	0.54	0/2523
22	H	0.34	0/1743	0.53	0/2372
22	h	0.34	0/1743	0.53	0/2372
23	I	0.31	0/1942	0.55	0/2628
23	i	0.31	0/1942	0.55	0/2628
24	J	0.30	0/1728	0.56	0/2358
24	j	0.30	0/1728	0.56	0/2358
25	K	0.30	0/1747	0.54	0/2364
25	k	0.30	0/1747	0.54	0/2364
26	L	0.32	0/1885	0.56	0/2552
26	l	0.32	0/1885	0.56	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	M	0.33	0/1891	0.54	0/2552
27	m	0.33	0/1891	0.54	0/2552
28	N	0.30	0/1454	0.51	0/1967
28	n	0.30	0/1454	0.51	0/1967
29	O	0.30	0/1670	0.49	0/2265
29	o	0.30	0/1670	0.49	0/2265
30	P	0.30	0/1614	0.49	0/2177
30	p	0.30	0/1614	0.49	0/2177
31	Q	0.33	0/1603	0.56	0/2174
31	q	0.33	0/1603	0.56	0/2174
32	R	0.32	0/1579	0.45	0/2134
32	r	0.32	0/1579	0.46	0/2134
33	S	0.31	0/1671	0.49	0/2253
33	s	0.31	0/1671	0.49	0/2253
34	T	0.31	0/1700	0.50	0/2305
34	t	0.31	0/1700	0.50	0/2305
All	All	0.33	7/106572 (0.0%)	0.59	56/144067 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
2	V	0	3
3	W	0	2
5	Y	0	12
6	Z	0	2
7	a	0	1
8	b	0	2
9	c	0	2
10	d	0	2
11	e	0	5
12	f	0	11
13	A	0	3
14	B	0	1
15	C	0	3
16	D	0	6
18	F	0	2
21	G	0	1
21	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	J	0	1
24	j	0	1
25	K	0	1
25	k	0	1
34	T	0	1
34	t	0	1
All	All	0	66

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	289	ALA	C-N	7.22	1.48	1.34
5	Y	185	GLY	CA-C	6.97	1.62	1.51
11	e	64	GLY	CA-C	5.80	1.61	1.51
12	f	192	VAL	C-N	5.75	1.45	1.34
5	Y	292	TYR	CB-CG	5.62	1.60	1.51
11	e	64	GLY	N-CA	5.38	1.54	1.46
5	Y	185	GLY	N-CA	5.32	1.54	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	63	HIS	CB-CA-C	12.60	135.61	110.40
11	e	63	HIS	C-N-CA	12.17	147.86	122.30
5	Y	292	TYR	CA-CB-CG	10.89	134.09	113.40
11	e	57	ARG	CG-CD-NE	10.77	134.41	111.80
11	e	63	HIS	N-CA-CB	-10.55	91.61	110.60
5	Y	185	GLY	C-N-CA	9.23	144.78	121.70
5	Y	186	LEU	CA-CB-CG	9.12	136.28	115.30
11	e	56	LEU	CA-CB-CG	8.30	134.39	115.30
3	W	89	LEU	CA-CB-CG	7.65	132.90	115.30
2	V	428	LEU	CA-CB-CG	7.54	132.64	115.30
19	u	75	GLY	C-N-CA	-7.45	106.65	122.30
5	Y	291	HIS	N-CA-C	7.43	131.07	111.00
5	Y	287	LEU	CA-CB-CG	7.30	132.08	115.30
6	Z	187	LEU	CA-CB-CG	6.99	131.38	115.30
5	Y	185	GLY	N-CA-C	6.98	130.56	113.10
11	e	63	HIS	CA-CB-CG	6.69	124.97	113.60
1	U	603	LEU	CA-CB-CG	6.63	130.55	115.30
11	e	9	ASP	CB-CG-OD1	6.54	124.19	118.30
12	f	129	LEU	CA-CB-CG	6.43	130.09	115.30
6	Z	16	LEU	CA-CB-CG	6.40	130.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	270	LEU	CA-CB-CG	6.36	129.93	115.30
11	e	57	ARG	NE-CZ-NH1	6.34	123.47	120.30
11	e	64	GLY	N-CA-C	6.32	128.90	113.10
11	e	52	PHE	CB-CG-CD1	6.23	125.16	120.80
2	V	437	ILE	CG1-CB-CG2	-6.16	97.85	111.40
11	e	53	SER	N-CA-C	6.11	127.49	111.00
5	Y	184	GLN	C-N-CA	6.05	135.00	122.30
5	Y	292	TYR	N-CA-CB	6.03	121.46	110.60
12	f	837	LEU	CA-CB-CG	6.02	129.15	115.30
5	Y	138	LEU	CA-CB-CG	5.95	128.98	115.30
12	f	612	LEU	CA-CB-CG	5.91	128.88	115.30
15	C	259	LEU	CA-CB-CG	5.86	128.77	115.30
3	W	455	LEU	CA-CB-CG	5.80	128.63	115.30
7	a	187	ASP	CB-CG-OD1	5.78	123.50	118.30
12	f	811	LEU	CA-CB-CG	5.77	128.57	115.30
12	f	759	LEU	CA-CB-CG	5.75	128.53	115.30
11	e	65	TYR	CB-CA-C	-5.74	98.92	110.40
11	e	64	GLY	O-C-N	-5.66	113.64	122.70
2	V	357	LEU	CA-CB-CG	5.56	128.09	115.30
17	E	105	LEU	CA-CB-CG	5.54	128.05	115.30
13	A	85	GLN	C-N-CA	5.51	135.48	121.70
6	Z	220	LEU	CB-CG-CD1	5.50	120.36	111.00
11	e	65	TYR	CA-CB-CG	5.45	123.75	113.40
5	Y	290	PRO	N-CA-C	5.37	126.07	112.10
1	U	603	LEU	CB-CG-CD2	-5.36	101.90	111.00
11	e	64	GLY	CA-C-N	5.32	128.91	117.20
7	a	188	LEU	CA-CB-CG	5.31	127.52	115.30
11	e	49	GLU	CA-C-N	5.27	128.79	117.20
1	U	873	PRO	C-N-CA	5.23	134.77	121.70
10	d	190	LEU	CA-CB-CG	5.23	127.33	115.30
2	V	346	LEU	CA-CB-CG	5.22	127.31	115.30
6	Z	230	LEU	CA-CB-CG	5.17	127.19	115.30
5	Y	84	LEU	CA-CB-CG	5.11	127.04	115.30
11	e	57	ARG	CD-NE-CZ	5.09	130.72	123.60
12	f	874	LEU	CA-CB-CG	5.03	126.88	115.30
12	f	217	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	115	VAL	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
13	A	345	LEU	Peptide
13	A	39	SER	Peptide
14	B	116	ILE	Peptide
15	C	146	SER	Peptide
15	C	287	LYS	Peptide
15	C	89	VAL	Peptide
16	D	125	LYS	Peptide
16	D	126	PRO	Peptide
16	D	258	ALA	Peptide
16	D	273	LYS	Peptide
16	D	408	LYS	Peptide
16	D	85	ILE	Peptide
18	F	343	LEU	Peptide
18	F	344	ARG	Peptide
21	G	222	VAL	Peptide
24	J	199	VAL	Peptide
25	K	232	GLU	Peptide
34	T	45	VAL	Peptide
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	344	ASP	Peptide
2	V	82	LEU	Peptide
3	W	137	TYR	Peptide
3	W	313	GLU	Peptide
5	Y	173	ASP	Peptide
5	Y	179	ARG	Peptide
5	Y	180	LEU	Peptide
5	Y	181	LYS	Peptide
5	Y	185	GLY	Peptide
5	Y	187	TYR	Peptide
5	Y	293	ARG	Peptide
5	Y	294	TYR	Peptide
5	Y	349	LYS	Peptide
5	Y	51	ALA	Peptide
5	Y	62	ASP	Peptide
5	Y	87	GLU	Peptide
6	Z	225	GLN	Peptide
6	Z	239	ASP	Peptide
7	a	164	GLN	Peptide
8	b	149	ASN	Peptide
8	b	21	PHE	Peptide
9	c	185	ASN	Peptide

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Mol	Chain	Res	Type	Group
9	c	266	THR	Peptide
10	d	198	LEU	Peptide
10	d	201	ASN	Peptide
11	e	4	LYS	Peptide
11	e	43	TRP	Peptide
11	e	55	GLN	Peptide
11	e	60	LEU	Peptide
11	e	62	LYS	Peptide
12	f	340	MET	Peptide
12	f	620	PHE	Peptide
12	f	642	ALA	Peptide
12	f	712	LYS	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	854	GLY	Peptide
12	f	875	ALA	Peptide
21	g	222	VAL	Peptide
24	j	199	VAL	Peptide
25	k	232	GLU	Peptide
34	t	45	VAL	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	U	806/953 (85%)	748 (93%)	55 (7%)	3 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	478/533 (90%)	412 (86%)	65 (14%)	1 (0%)	47	77
3	W	454/456 (100%)	409 (90%)	45 (10%)	0	100	100
4	X	378/422 (90%)	362 (96%)	15 (4%)	1 (0%)	41	71
5	Y	376/389 (97%)	317 (84%)	51 (14%)	8 (2%)	7	31
6	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	34	66
7	a	371/376 (99%)	334 (90%)	35 (9%)	2 (0%)	29	61
8	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	29	61
9	c	285/309 (92%)	256 (90%)	29 (10%)	0	100	100
10	d	255/349 (73%)	213 (84%)	41 (16%)	1 (0%)	34	66
11	e	36/70 (51%)	16 (44%)	18 (50%)	2 (6%)	2	11
12	f	887/892 (99%)	714 (80%)	164 (18%)	9 (1%)	15	46
13	A	391/433 (90%)	335 (86%)	53 (14%)	3 (1%)	19	51
14	B	393/440 (89%)	343 (87%)	50 (13%)	0	100	100
15	C	379/398 (95%)	334 (88%)	42 (11%)	3 (1%)	19	51
16	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	12	40
17	E	387/403 (96%)	349 (90%)	38 (10%)	0	100	100
18	F	413/439 (94%)	374 (91%)	36 (9%)	3 (1%)	22	54
19	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
20	v	1/28 (4%)	0	1 (100%)	0	100	100
21	G	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
21	g	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
22	H	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
22	h	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
23	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
23	i	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
24	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	19	51
24	j	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	19	51
25	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
26	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
26	l	236/268 (88%)	222 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
27	m	238/254 (94%)	215 (90%)	23 (10%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
30	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
31	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
31	q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
32	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
33	S	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
33	s	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
34	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
34	t	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
All	All	13375/14947 (90%)	12160 (91%)	1168 (9%)	47 (0%)	38	66

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	e	65	TYR
12	f	808	ASN
12	f	853	VAL
1	U	874	ASN
5	Y	89	GLU
5	Y	290	PRO
5	Y	350	VAL
6	Z	226	ILE
13	A	346	PRO
18	F	302	GLY
5	Y	176	ARG
5	Y	188	CYS
7	a	69	HIS
12	f	118	ASN
12	f	476	THR

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Mol	Chain	Res	Type
12	f	876	HIS
16	D	86	PRO
18	F	344	ARG
1	U	873	PRO
2	V	265	ASP
5	Y	63	TRP
5	Y	291	HIS
11	e	3	GLU
12	f	823	ALA
16	D	299	PHE
18	F	300	LYS
24	J	97	THR
24	J	200	GLN
24	j	97	THR
24	j	200	GLN
13	A	309	PHE
15	C	90	HIS
15	C	287	LYS
16	D	84	SER
16	D	274	ARG
12	f	475	ASN
10	d	203	PRO
12	f	809	ILE
13	A	109	PRO
15	C	89	VAL
4	X	203	PRO
8	b	23	PRO
5	Y	289	ALA
16	D	367	PRO
1	U	174	PRO
7	a	214	GLY
12	f	755	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	690 (100%)	2 (0%)	92	96
2	V	414/459 (90%)	410 (99%)	4 (1%)	76	86
3	W	416/416 (100%)	412 (99%)	4 (1%)	76	86
4	X	327/362 (90%)	325 (99%)	2 (1%)	86	91
5	Y	334/344 (97%)	329 (98%)	5 (2%)	65	81
6	Z	257/295 (87%)	256 (100%)	1 (0%)	91	95
7	a	333/336 (99%)	331 (99%)	2 (1%)	86	91
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	245 (97%)	7 (3%)	43	70
10	d	231/293 (79%)	230 (100%)	1 (0%)	91	95
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	729 (98%)	16 (2%)	53	75
13	A	332/372 (89%)	327 (98%)	5 (2%)	65	81
14	B	344/385 (89%)	336 (98%)	8 (2%)	50	73
15	C	326/346 (94%)	317 (97%)	9 (3%)	43	70
16	D	333/366 (91%)	330 (99%)	3 (1%)	78	87
17	E	341/353 (97%)	337 (99%)	4 (1%)	71	83
18	F	357/379 (94%)	351 (98%)	6 (2%)	60	78
19	u	68/68 (100%)	68 (100%)	0	100	100
20	v	1/1 (100%)	1 (100%)	0	100	100
21	G	193/209 (92%)	193 (100%)	0	100	100
21	g	193/209 (92%)	193 (100%)	0	100	100
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	193 (100%)	0	100	100
23	i	193/220 (88%)	193 (100%)	0	100	100
24	J	152/210 (72%)	152 (100%)	0	100	100
24	j	152/210 (72%)	152 (100%)	0	100	100
25	K	186/202 (92%)	185 (100%)	1 (0%)	88	93
25	k	186/202 (92%)	185 (100%)	1 (0%)	88	93
26	L	198/229 (86%)	198 (100%)	0	100	100
26	l	198/229 (86%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	M	192/211 (91%)	192 (100%)	0	100	100
27	m	192/211 (91%)	192 (100%)	0	100	100
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	162 (99%)	2 (1%)	71	83
31	q	164/171 (96%)	162 (99%)	2 (1%)	71	83
32	R	153/201 (76%)	153 (100%)	0	100	100
32	r	153/201 (76%)	153 (100%)	0	100	100
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	174 (99%)	1 (1%)	86	91
34	t	175/214 (82%)	174 (99%)	1 (1%)	86	91
All	All	11190/12651 (88%)	11103 (99%)	87 (1%)	82	89

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	345	ASN
1	U	629	THR
2	V	194	LYS
2	V	345	ARG
2	V	401	ASN
2	V	470	ARG
3	W	90	LEU
3	W	419	LYS
3	W	422	ASN
3	W	451	MET
4	X	198	ASN
4	X	329	ASN
5	Y	48	ASN
5	Y	77	ASN
5	Y	83	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	Y	297	ARG
5	Y	358	ARG
6	Z	180	LYS
7	a	230	ARG
7	a	289	ARG
9	c	104	ARG
9	c	139	ARG
9	c	156	VAL
9	c	186	LYS
9	c	197	ASN
9	c	222	LYS
9	c	254	ASN
10	d	251	ARG
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	267	ARG
12	f	297	MET
12	f	327	ASN
12	f	344	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	43	ARG
13	A	297	ARG
13	A	304	ASN
13	A	360	ARG
13	A	369	ARG
14	B	48	LYS
14	B	86	LYS
14	B	125	THR
14	B	164	MET
14	B	249	ARG
14	B	293	LYS
14	B	294	ARG
14	B	298	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	C	78	ARG
15	C	109	THR
15	C	113	ARG
15	C	130	LYS
15	C	138	MET
15	C	184	LYS
15	C	210	THR
15	C	229	ARG
15	C	278	ASN
16	D	81	ARG
16	D	238	LYS
16	D	384	MET
17	E	1	MET
17	E	5	ARG
17	E	25	ARG
17	E	241	ARG
18	F	46	ARG
18	F	102	ASN
18	F	110	ASN
18	F	118	LYS
18	F	250	LYS
18	F	300	LYS
25	K	10	ARG
31	Q	82	ASN
31	Q	102	LEU
34	T	37	ARG
25	k	10	ARG
31	q	82	ASN
31	q	102	LEU
34	t	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	U	70	HIS
1	U	91	ASN
1	U	345	ASN
1	U	377	HIS
1	U	415	HIS
1	U	595	ASN
1	U	647	HIS
1	U	768	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	V	33	GLN
2	V	177	ASN
2	V	214	HIS
2	V	242	HIS
2	V	247	GLN
3	W	41	GLN
3	W	235	GLN
3	W	246	HIS
3	W	362	ASN
3	W	422	ASN
4	X	198	ASN
4	X	213	GLN
4	X	292	GLN
4	X	296	ASN
4	X	329	ASN
4	X	333	GLN
4	X	334	ASN
4	X	349	HIS
4	X	406	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	291	HIS
6	Z	96	HIS
6	Z	102	HIS
6	Z	229	GLN
7	a	23	HIS
7	a	129	GLN
7	a	143	ASN
7	a	168	ASN
7	a	193	GLN
7	a	249	GLN
7	a	369	HIS
8	b	142	ASN
9	c	128	ASN
9	c	183	HIS
9	c	197	ASN
9	c	241	ASN
9	c	254	ASN
9	c	256	ASN
10	d	116	HIS
11	e	6	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	171	GLN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	619	HIS
12	f	752	HIS
12	f	786	GLN
12	f	848	GLN
13	A	304	ASN
13	A	305	GLN
13	A	353	HIS
14	B	131	HIS
14	B	193	GLN
14	B	241	ASN
14	B	277	HIS
14	B	298	ASN
14	B	368	HIS
15	C	270	GLN
15	C	278	ASN
16	D	67	ASN
16	D	187	HIS
16	D	257	ASN
17	E	19	HIS
17	E	45	ASN
17	E	121	ASN
17	E	194	ASN
17	E	220	ASN
17	E	225	HIS
17	E	262	ASN
17	E	263	GLN
18	F	102	ASN
18	F	110	ASN
18	F	255	GLN
18	F	315	ASN

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Mol	Chain	Res	Type
18	F	321	GLN
19	u	25	ASN
19	u	41	GLN
22	H	102	GLN
23	I	119	GLN
23	I	123	GLN
24	J	68	ASN
24	J	116	GLN
25	K	99	HIS
25	K	164	GLN
25	K	214	ASN
25	K	225	ASN
26	L	146	GLN
26	L	166	GLN
28	N	154	GLN
31	Q	101	ASN
32	R	29	GLN
32	R	38	ASN
34	T	81	HIS
22	h	102	GLN
23	i	20	GLN
23	i	119	GLN
23	i	123	GLN
24	j	68	ASN
24	j	116	GLN
25	k	99	HIS
25	k	164	GLN
25	k	214	ASN
25	k	225	ASN
26	l	146	GLN
28	n	154	GLN
30	p	93	ASN
31	q	101	ASN
32	r	29	GLN
32	r	38	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	ATP	A	501	37	26,33,33	0.89	1 (3%)	31,52,52	1.67	5 (16%)
36	ATP	F	501	37	26,33,33	0.94	1 (3%)	31,52,52	1.64	5 (16%)
38	ADP	B	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.57	4 (13%)
38	ADP	E	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.60	4 (13%)
36	ATP	D	501	37	26,33,33	0.94	1 (3%)	31,52,52	1.71	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	A	501	37	-	0/18/38/38	0/3/3/3
36	ATP	F	501	37	-	3/18/38/38	0/3/3/3
38	ADP	B	501	-	-	4/12/32/32	0/3/3/3
38	ADP	E	401	-	-	3/12/32/32	0/3/3/3
36	ATP	D	501	37	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	2.47	1.47	1.40
36	F	501	ATP	C5-C4	2.39	1.47	1.40
38	B	501	ADP	C5-C4	2.37	1.47	1.40
38	E	401	ADP	C5-C4	2.30	1.47	1.40
36	A	501	ATP	C5-C4	2.26	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	501	ATP	PA-O3A-PB	-4.66	116.84	132.83
36	F	501	ATP	PA-O3A-PB	-4.59	117.08	132.83
38	E	401	ADP	PA-O3A-PB	-4.26	118.20	132.83
36	D	501	ATP	C3'-C2'-C1'	4.17	107.25	100.98
38	B	501	ADP	C3'-C2'-C1'	4.12	107.18	100.98
38	B	501	ADP	PA-O3A-PB	-4.07	118.85	132.83
36	D	501	ATP	PA-O3A-PB	-3.96	119.24	132.83
38	E	401	ADP	C3'-C2'-C1'	3.94	106.92	100.98
36	A	501	ATP	C3'-C2'-C1'	3.85	106.77	100.98
36	F	501	ATP	C3'-C2'-C1'	3.43	106.14	100.98
36	D	501	ATP	N3-C2-N1	-3.27	123.57	128.68
36	F	501	ATP	N3-C2-N1	-3.26	123.59	128.68
36	A	501	ATP	PB-O3B-PG	-3.13	122.09	132.83
38	E	401	ADP	N3-C2-N1	-3.12	123.81	128.68
36	A	501	ATP	N3-C2-N1	-3.11	123.83	128.68
36	D	501	ATP	PB-O3B-PG	-3.03	122.44	132.83
38	B	501	ADP	N3-C2-N1	-2.92	124.12	128.68
36	F	501	ATP	PB-O3B-PG	-2.81	123.17	132.83
36	D	501	ATP	C1'-N9-C4	2.73	131.44	126.64
36	A	501	ATP	C4-C5-N7	-2.44	106.85	109.40
38	E	401	ADP	C4-C5-N7	-2.29	107.01	109.40
38	B	501	ADP	C4-C5-N7	-2.19	107.12	109.40
36	F	501	ATP	C4-C5-N7	-2.03	107.29	109.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	D	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C3'-C4'-C5'-O5'
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O2A
38	B	501	ADP	C5'-O5'-PA-O1A

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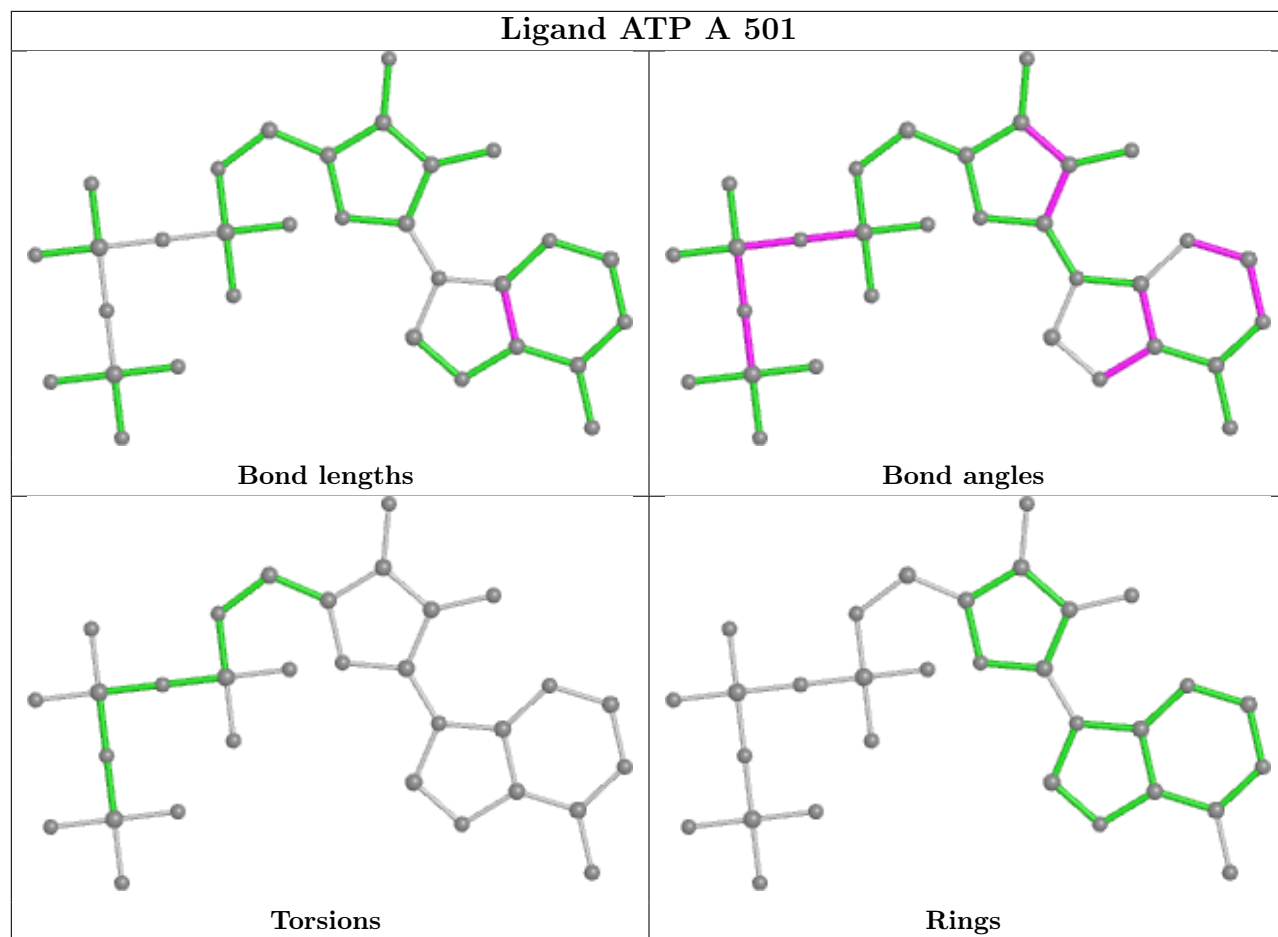
*Continued from previous page...*

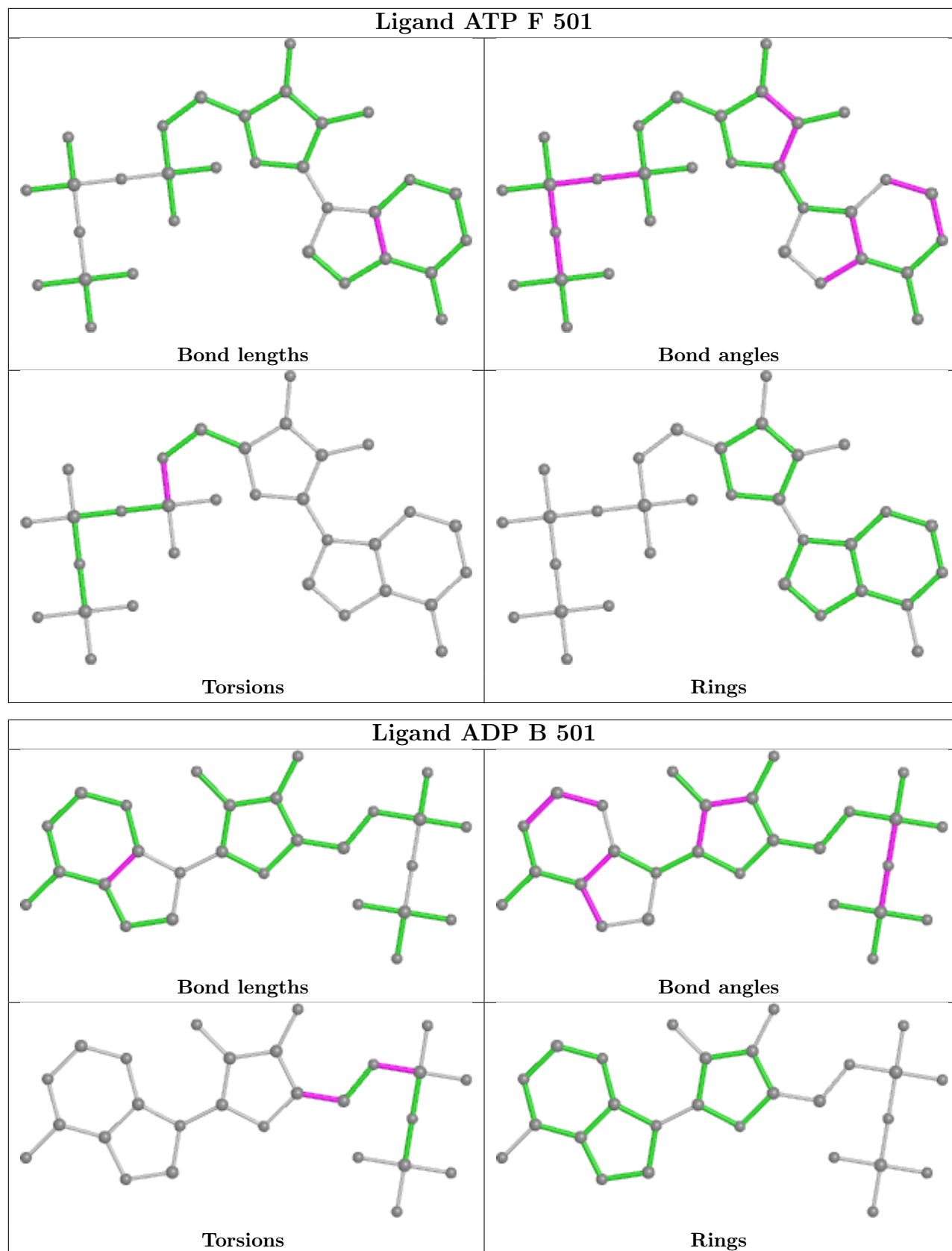
Mol	Chain	Res	Type	Atoms
38	B	501	ADP	C5'-O5'-PA-O2A
38	E	401	ADP	C5'-O5'-PA-O1A
36	D	501	ATP	C4'-C5'-O5'-PA
36	D	501	ATP	O4'-C4'-C5'-O5'
38	E	401	ADP	C3'-C4'-C5'-O5'
36	D	501	ATP	C5'-O5'-PA-O1A
38	E	401	ADP	O4'-C4'-C5'-O5'
36	F	501	ATP	C5'-O5'-PA-O3A
38	B	501	ADP	C5'-O5'-PA-O3A
38	B	501	ADP	O4'-C4'-C5'-O5'

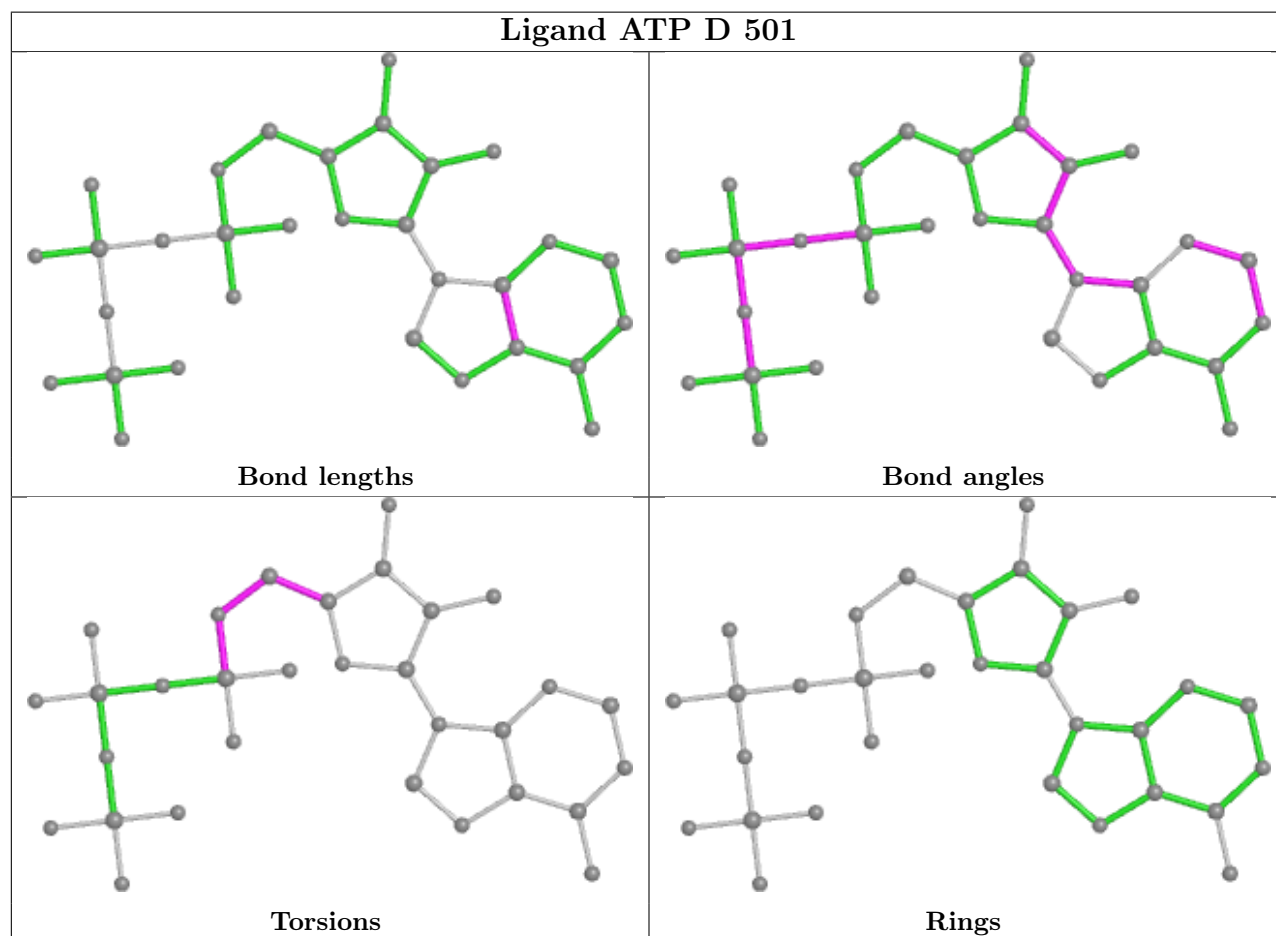
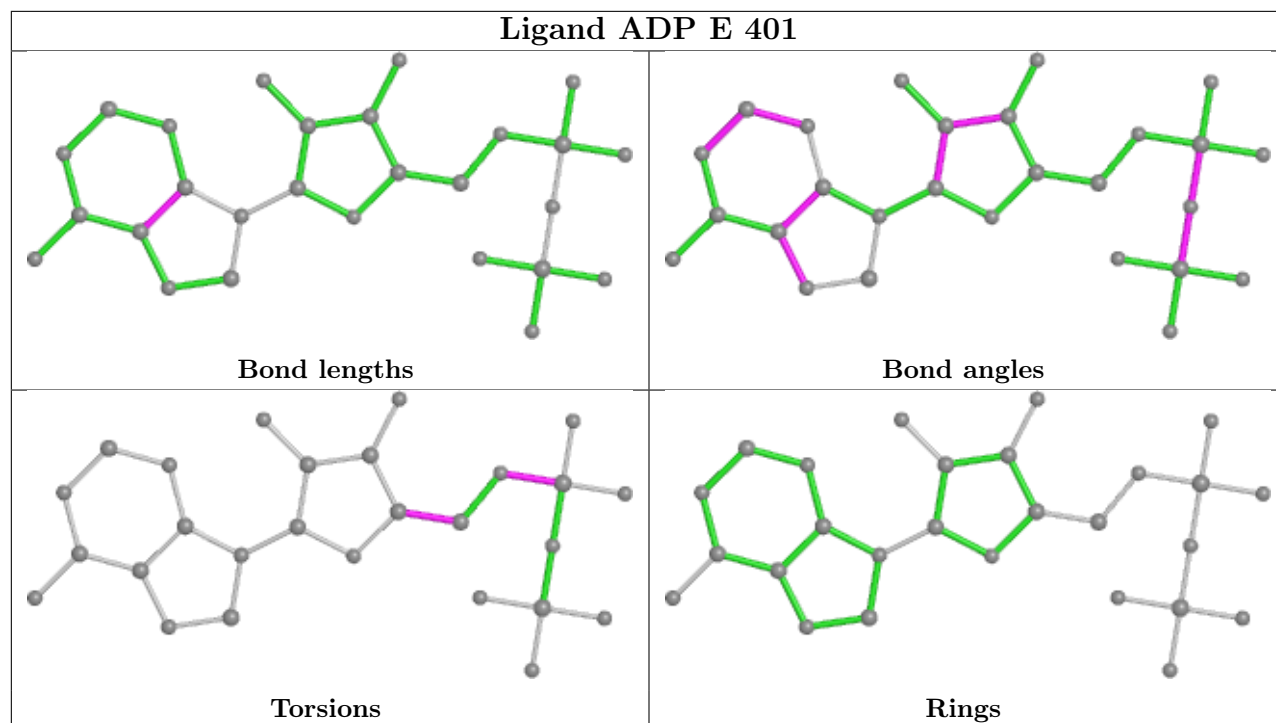
There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

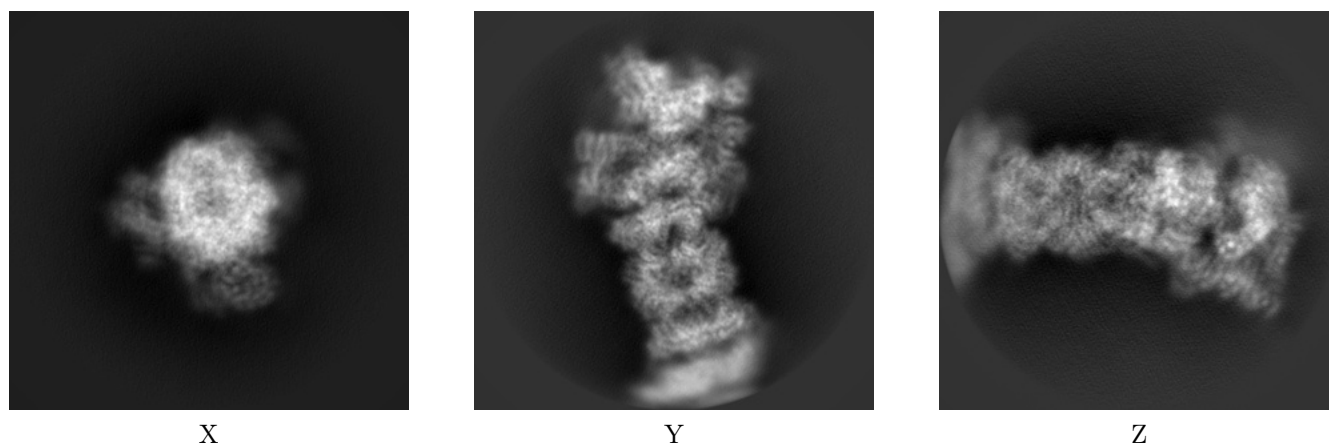
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9218. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

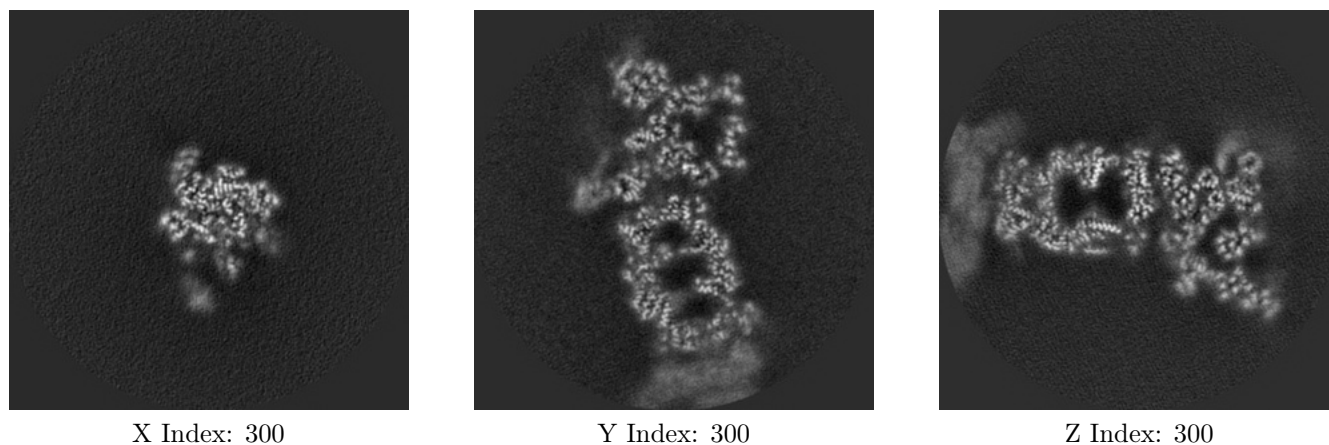
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

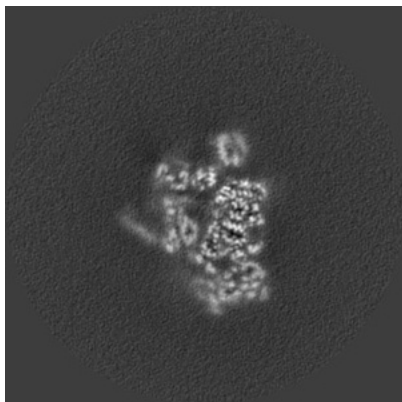
#### 6.2.1 Primary map



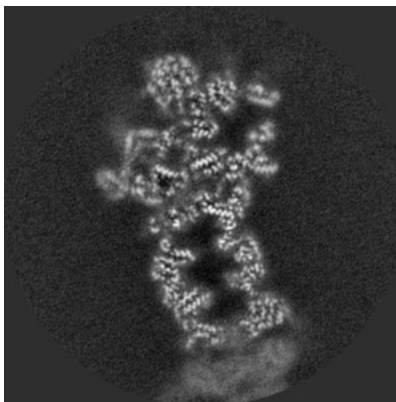
The images above show central slices of the map in three orthogonal directions.

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

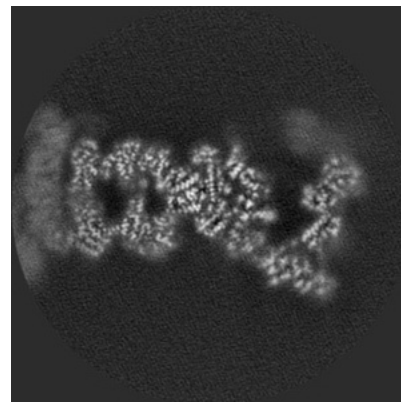
### 6.3.1 Primary map



X Index: 344



Y Index: 313

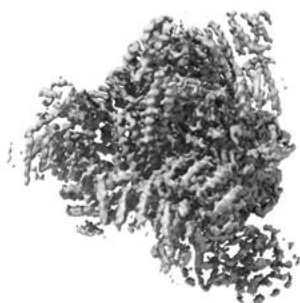


Z Index: 335

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

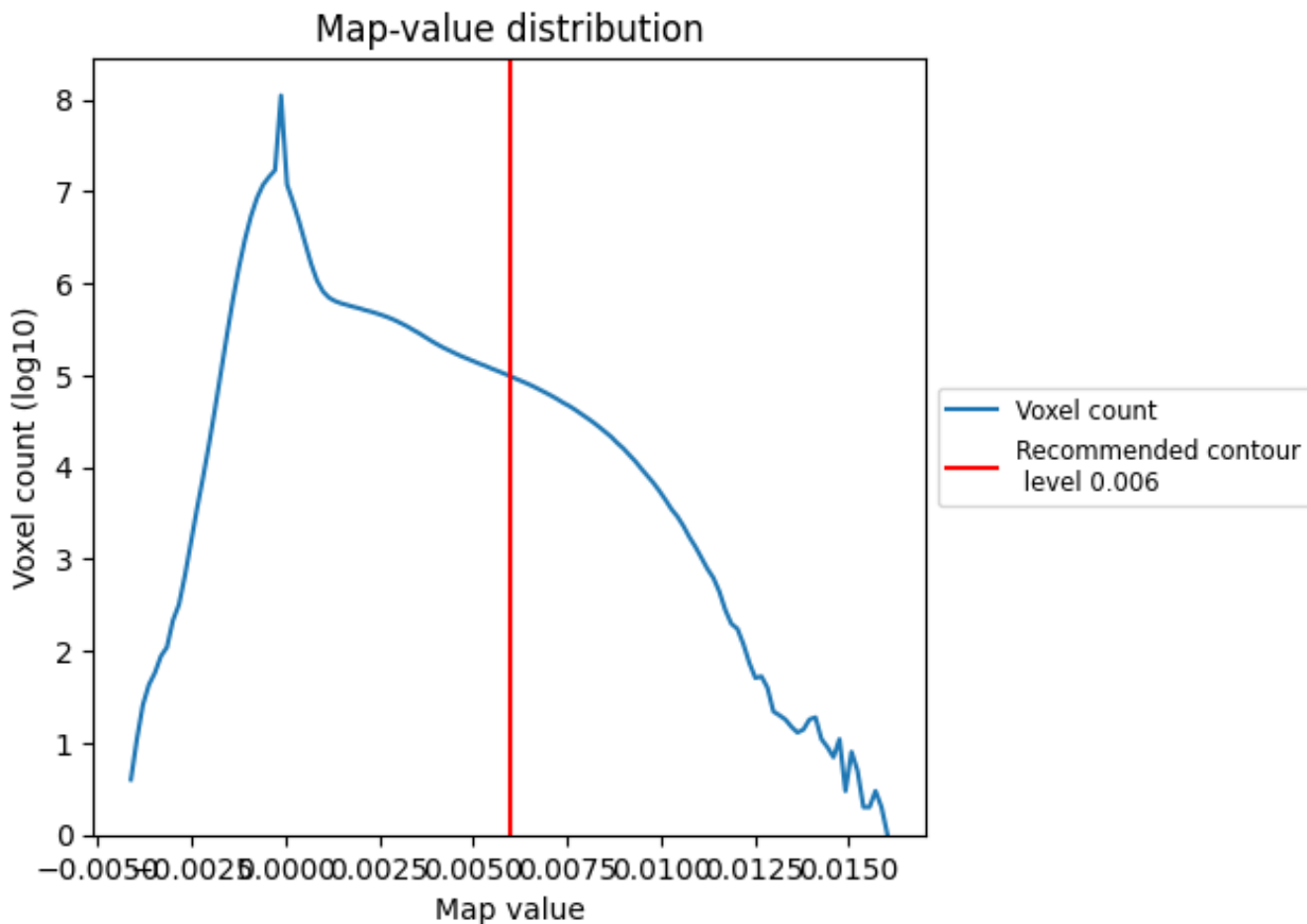
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

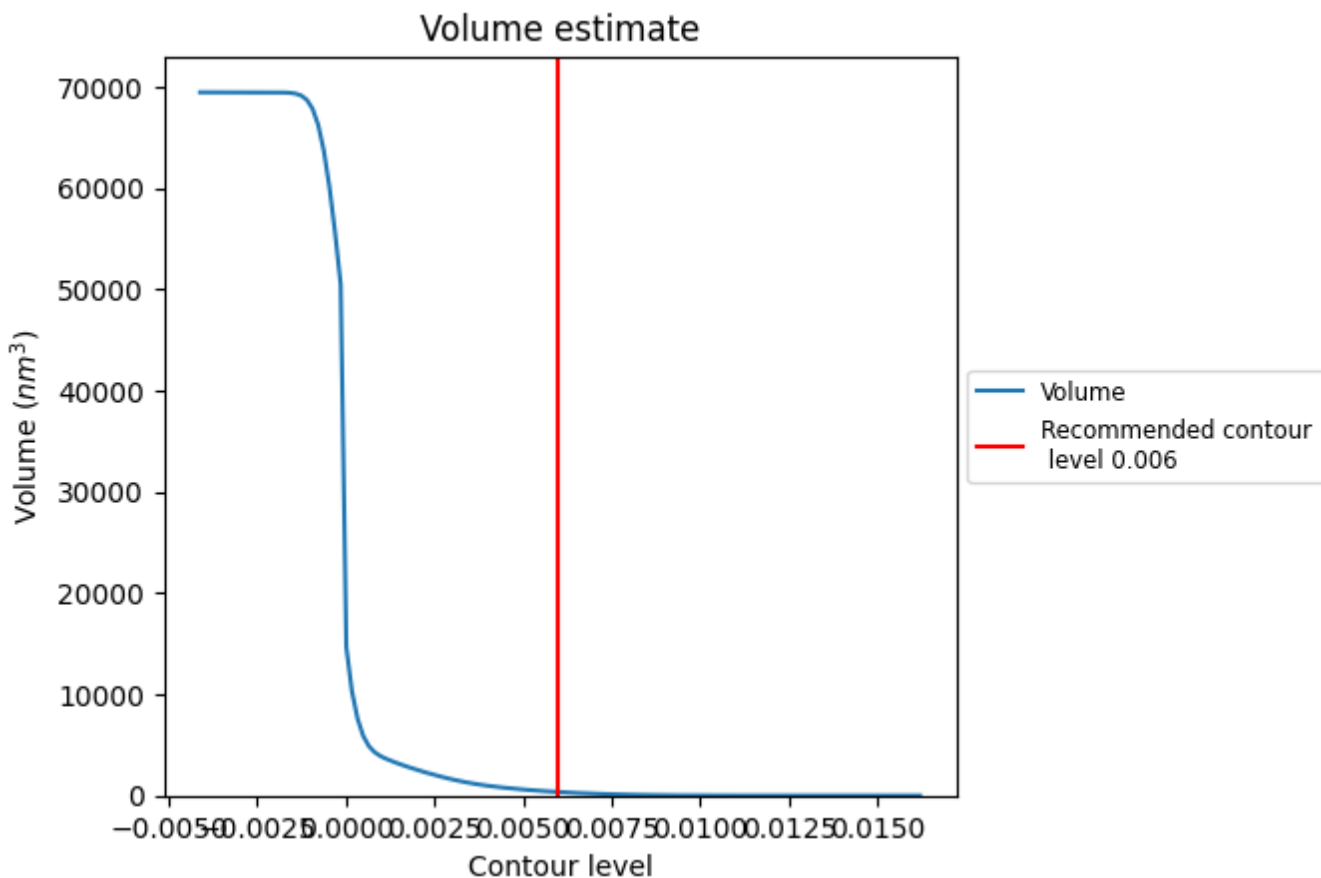
This section contains the results of statistical analysis of the map.

### 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.

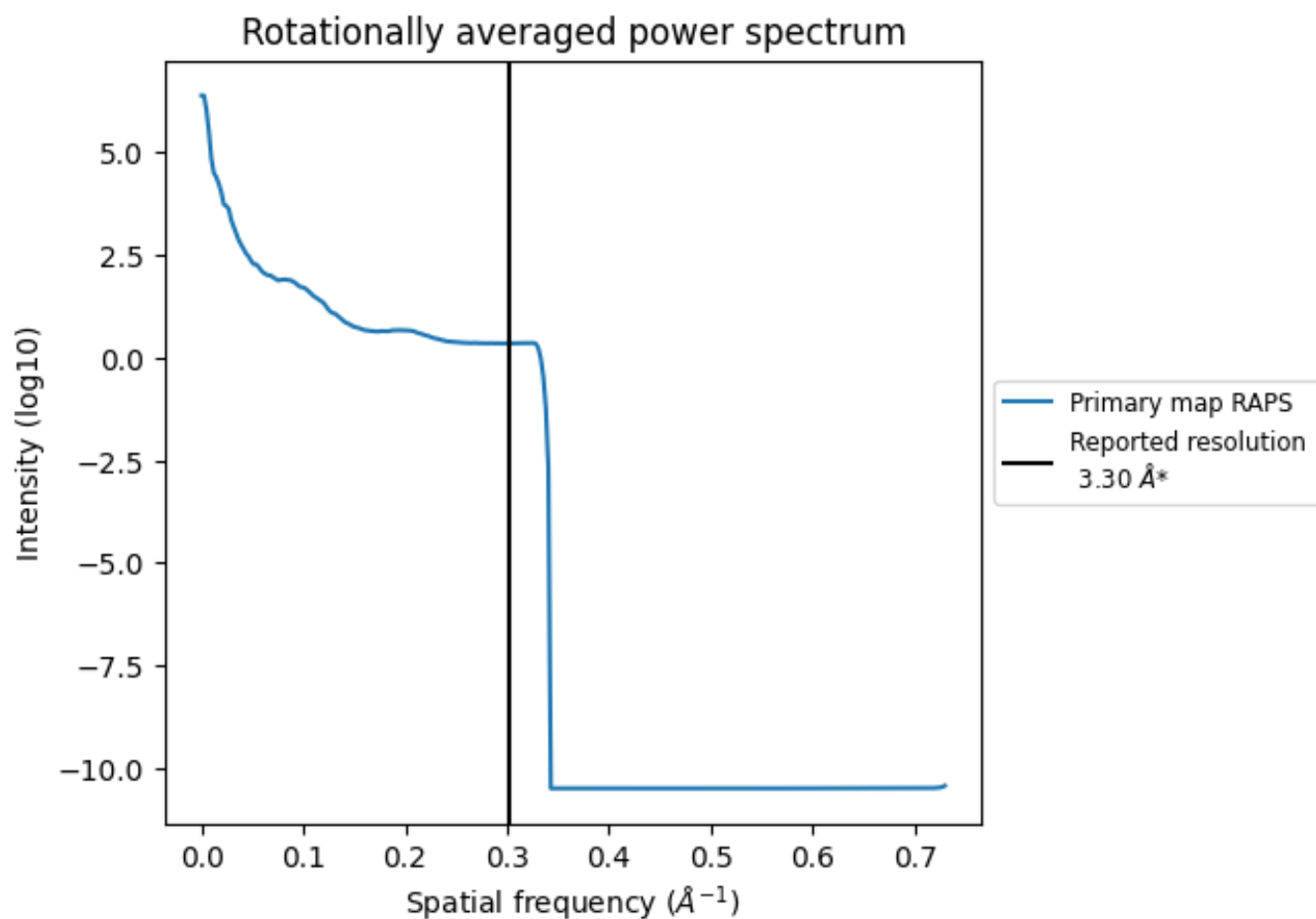
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm<sup>3</sup>; this corresponds to an approximate mass of 316 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 0.303 Å<sup>-1</sup>

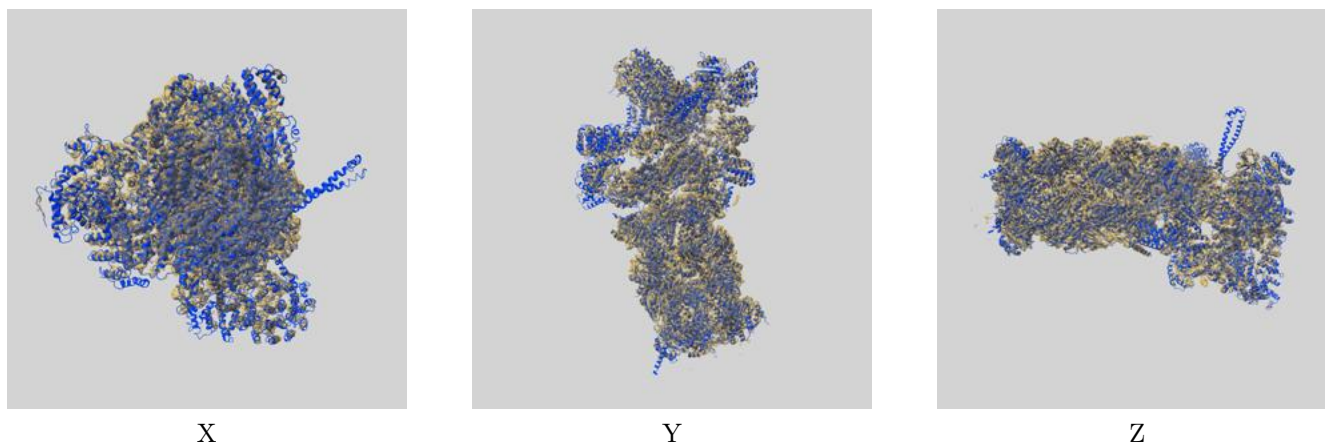
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

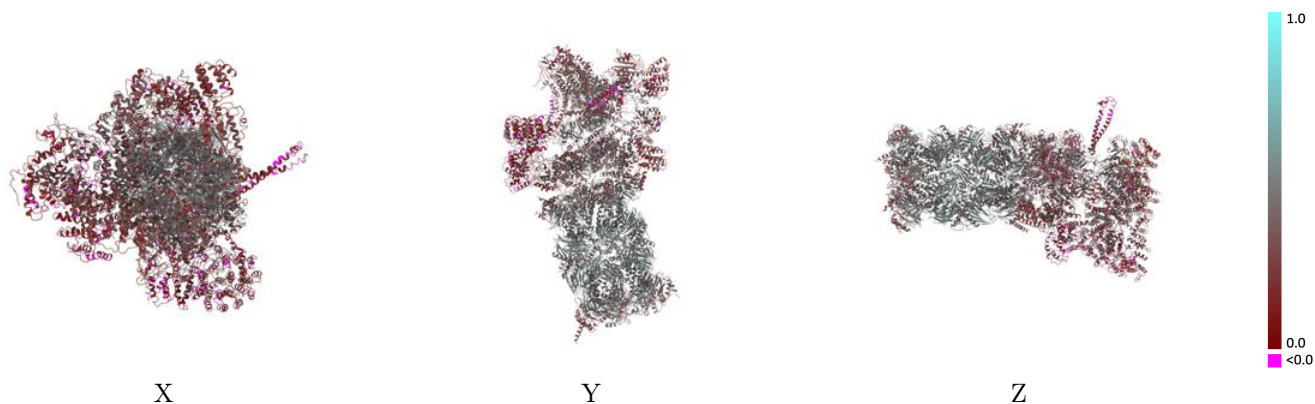
This section contains information regarding the fit between EMDB map EMD-9218 and PDB model 6MSE. Per-residue inclusion information can be found in section 3 on page 13.

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



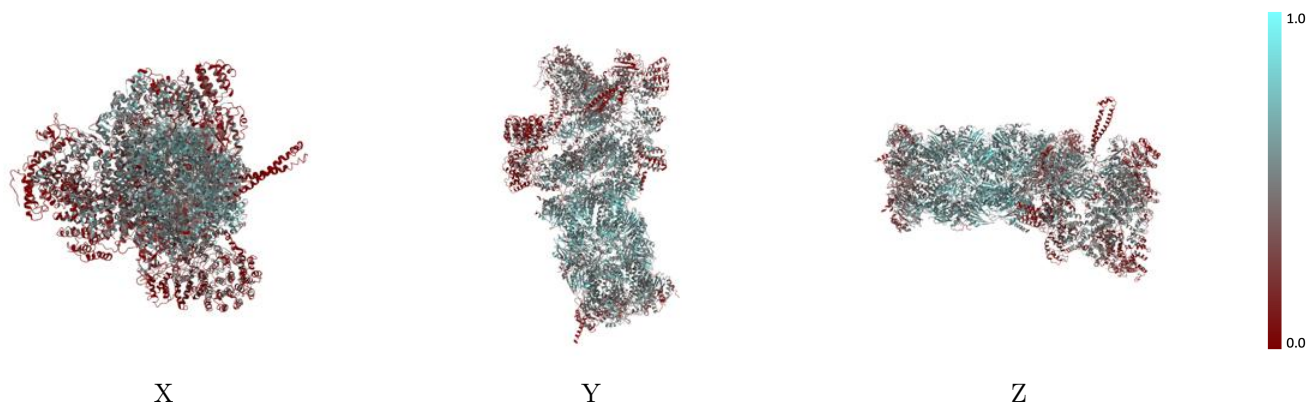
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



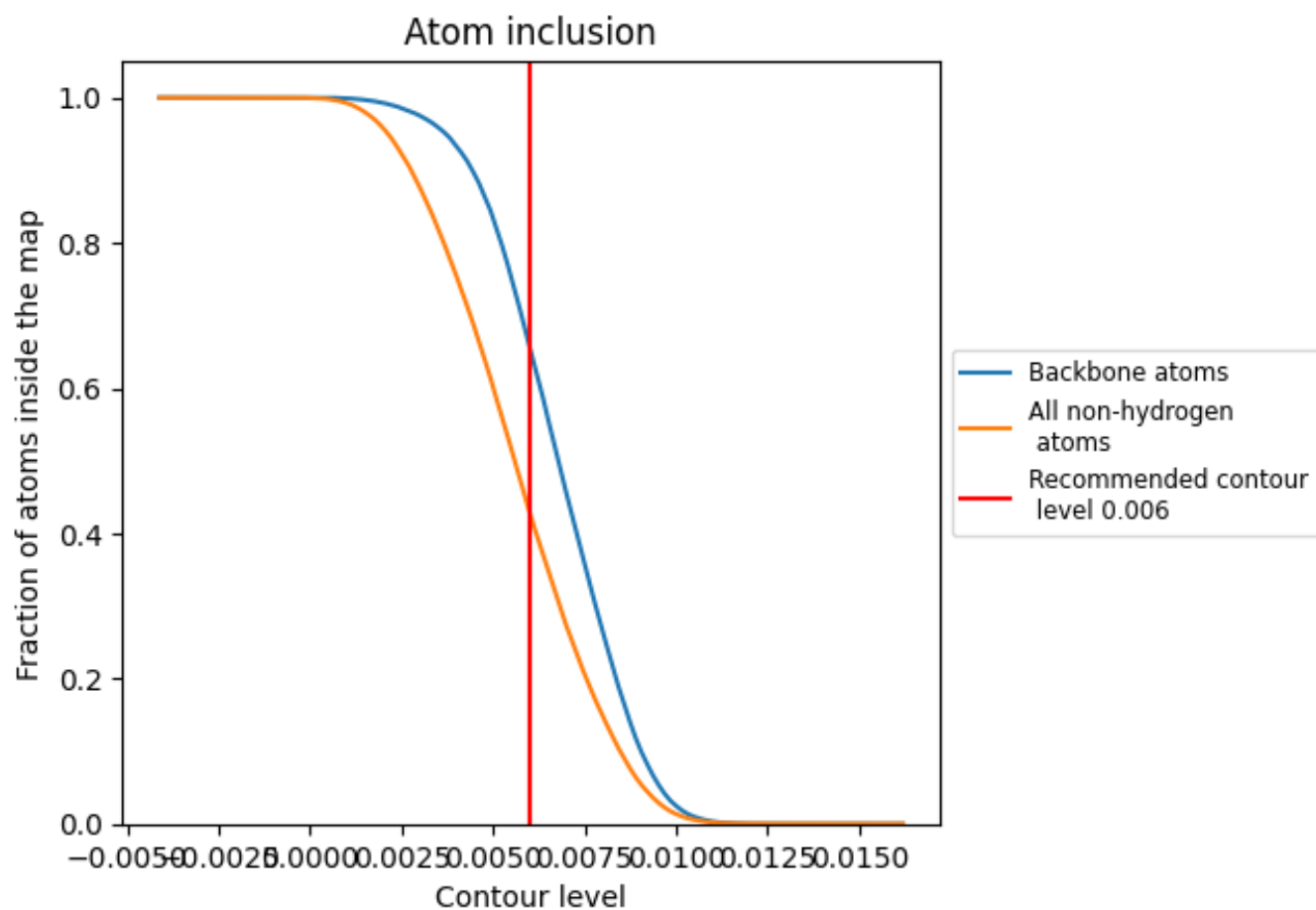
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 43% 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 (0.006) and Q-score for the entire model and for each chain.





























Chain	Atom inclusion	Q-score
All	 0.4288	 0.3550
A	 0.4580	 0.3390
B	 0.4143	 0.3210
C	 0.3404	 0.2970
D	 0.4814	 0.3710
E	 0.4874	 0.3650
F	 0.4562	 0.3530
G	 0.5958	 0.4380
H	 0.6251	 0.4410
I	 0.5587	 0.4010
J	 0.5318	 0.4010
K	 0.5252	 0.4120
L	 0.5833	 0.4330
M	 0.5597	 0.4060
N	 0.6295	 0.4730
O	 0.5979	 0.4690
P	 0.6033	 0.4800
Q	 0.5883	 0.4490
R	 0.6262	 0.4810
S	 0.5676	 0.4790
T	 0.6254	 0.4790
U	 0.3494	 0.2980
V	 0.2465	 0.2070
W	 0.3923	 0.2490
X	 0.3599	 0.3020
Y	 0.2943	 0.2070
Z	 0.4291	 0.3590
a	 0.3337	 0.2620
b	 0.2137	 0.2880
c	 0.4646	 0.3730
d	 0.1508	 0.2060
e	 0.1758	 0.0300
f	 0.1609	 0.1760
g	 0.4237	 0.4320
h	 0.4279	 0.4300



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Chain	Atom inclusion	Q-score
i	 0.3426	 0.3770
j	 0.3259	 0.3800
k	 0.3775	 0.3940
l	 0.4726	 0.4310
m	 0.4414	 0.4120
n	 0.5844	 0.4840
o	 0.5273	 0.4760
p	 0.5520	 0.4810
q	 0.5322	 0.4560
r	 0.5854	 0.4920
s	 0.5458	 0.4780
t	 0.6075	 0.4860
u	 0.3834	 0.3900
v	 0.2517	 0.3740