



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:21 PM UTC

PDB ID : 5VFR / pdb_00005vfr
EMDB ID : EMD-8665
Title : Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on : 2017-04-09
Resolution : 4.90 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:

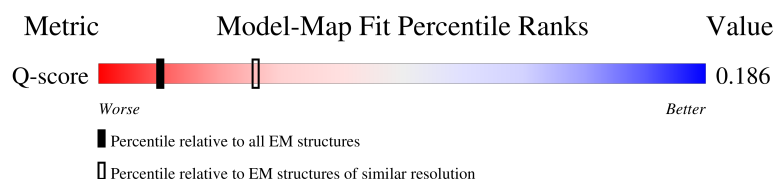
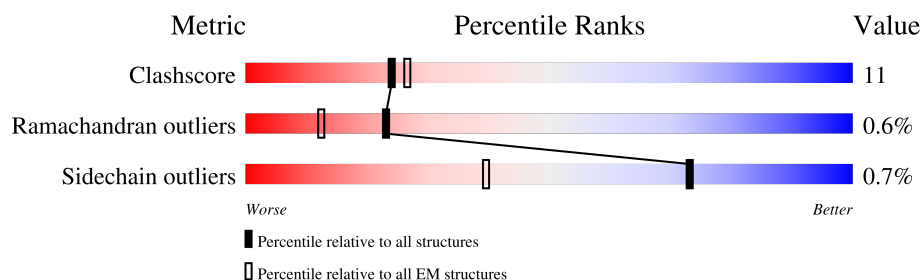
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 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	1274 (4.40 - 5.40)

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

Mol	Chain	Length	Quality of chain
1	U	911	83% 61% 27% 12%
2	V	480	95% 68% 30% ..
3	W	456	94% 65% 34%
4	X	380	60% 47% 15% 37%

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Mol	Chain	Length	Quality of chain
5	Y	378	
6	Z	286	
7	a	373	
8	b	191	
9	c	287	
10	d	257	
11	e	70	
12	G	240	
12	g	240	
13	H	232	
13	h	232	
14	I	250	
14	i	250	
15	J	243	
15	j	243	
16	K	234	
16	k	234	
17	L	238	
17	l	238	
18	M	245	
18	m	245	
19	N	191	
19	n	191	
20	O	220	
20	o	220	

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Mol	Chain	Length	Quality of chain
21	P	204	
21	p	204	
22	Q	199	
22	q	199	
23	R	201	
23	r	201	
24	S	213	
24	s	213	
25	T	215	
25	t	215	
26	A	399	
27	B	389	
28	C	392	
29	D	380	
30	E	375	
31	F	396	
32	f	908	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	AGS	F	501	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 99908 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
1	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	472	Total	C	N	O	S	0	0
			3799	2413	675	697	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

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

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

- Molecule 11 is a protein called Sem1.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
12	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 13 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		

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

- Molecule 14 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
14	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

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

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

- Molecule 16 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
16	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 17 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 18 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 19 is a protein called Proteasome subunit beta type-6.

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

- Molecule 20 is a protein called Proteasome subunit beta type-7.

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

- Molecule 21 is a protein called Proteasome subunit beta type-3.

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

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

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

- Molecule 23 is a protein called Proteasome subunit beta type-5.

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

- Molecule 24 is a protein called Proteasome subunit beta type-1.

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

- Molecule 25 is a protein called Proteasome subunit beta type-4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	342	Total	C	N	O	S	0	0
			2672	1684	475	497	16		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	363	Total	C	N	O	S	0	0
			2859	1804	513	525	17		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	376	Total	C	N	O	S	0	0
			2859	1802	496	546	15		

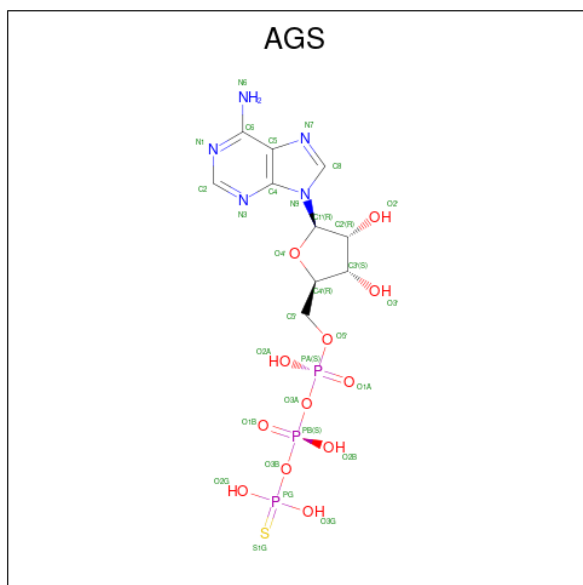
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
34	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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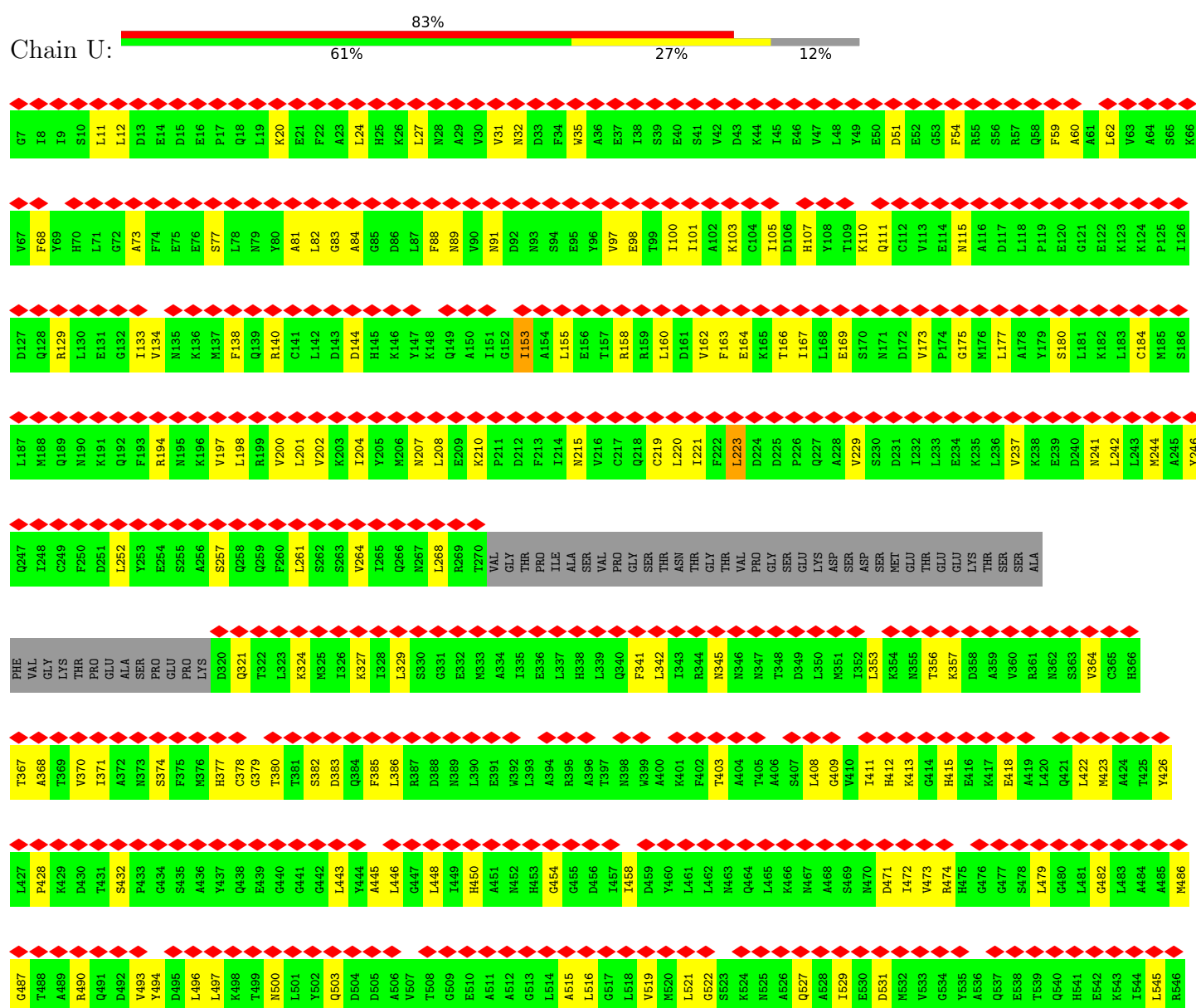
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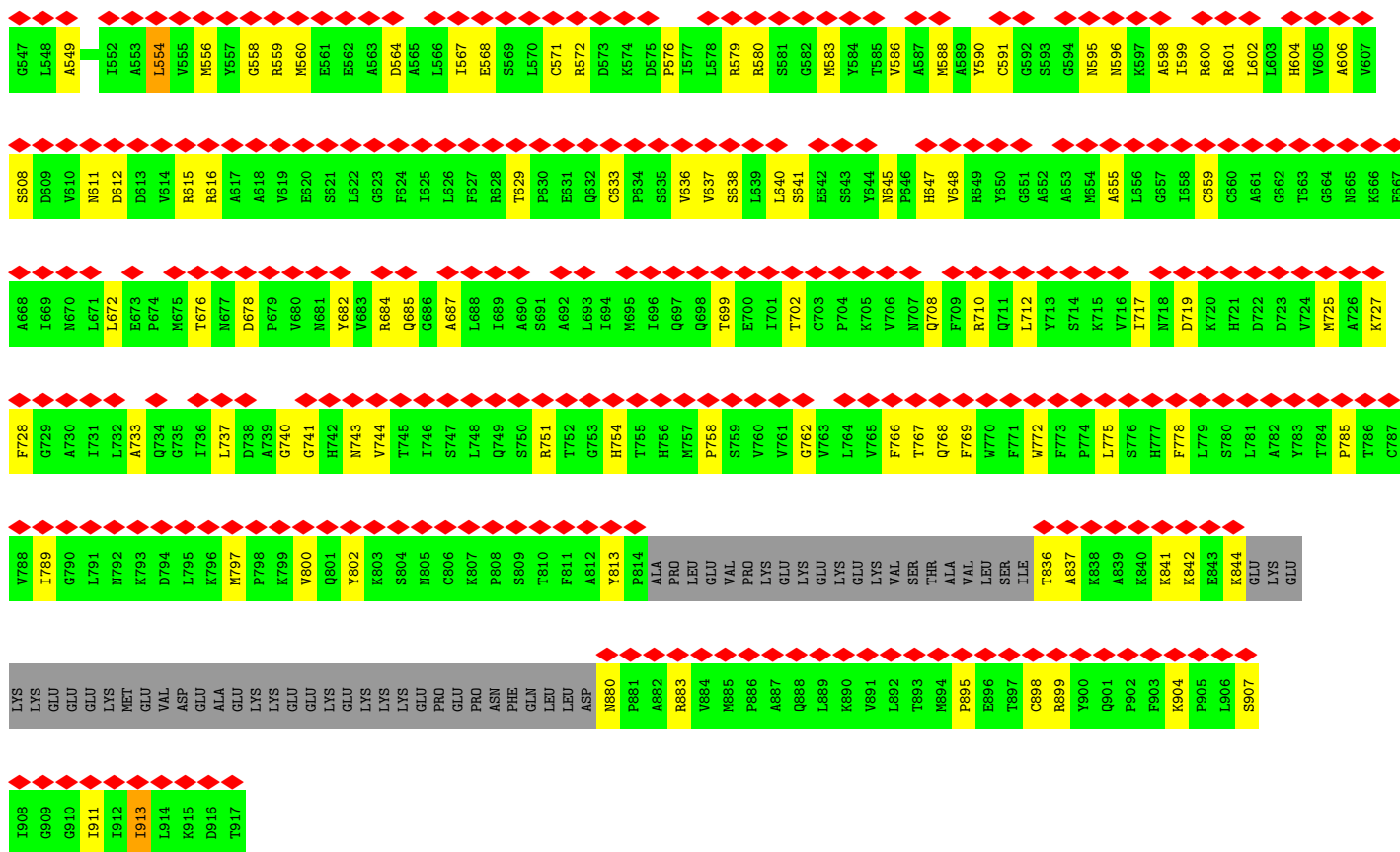
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
34	F	1	31	10	5	12	3	1	0

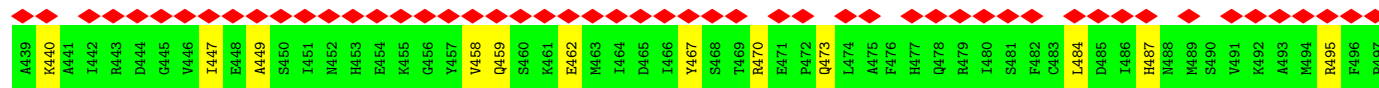
3 Residue-property plots

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.

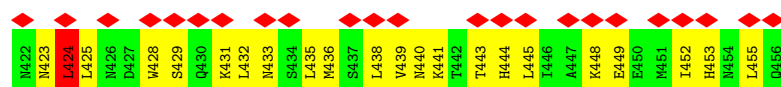
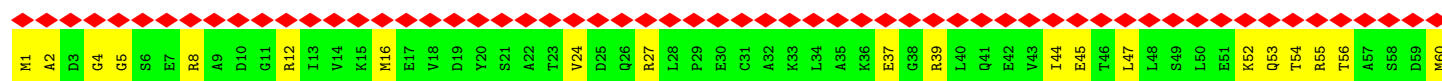
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



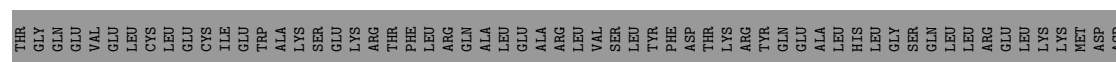
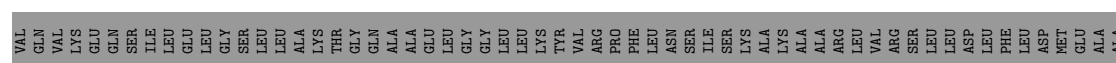


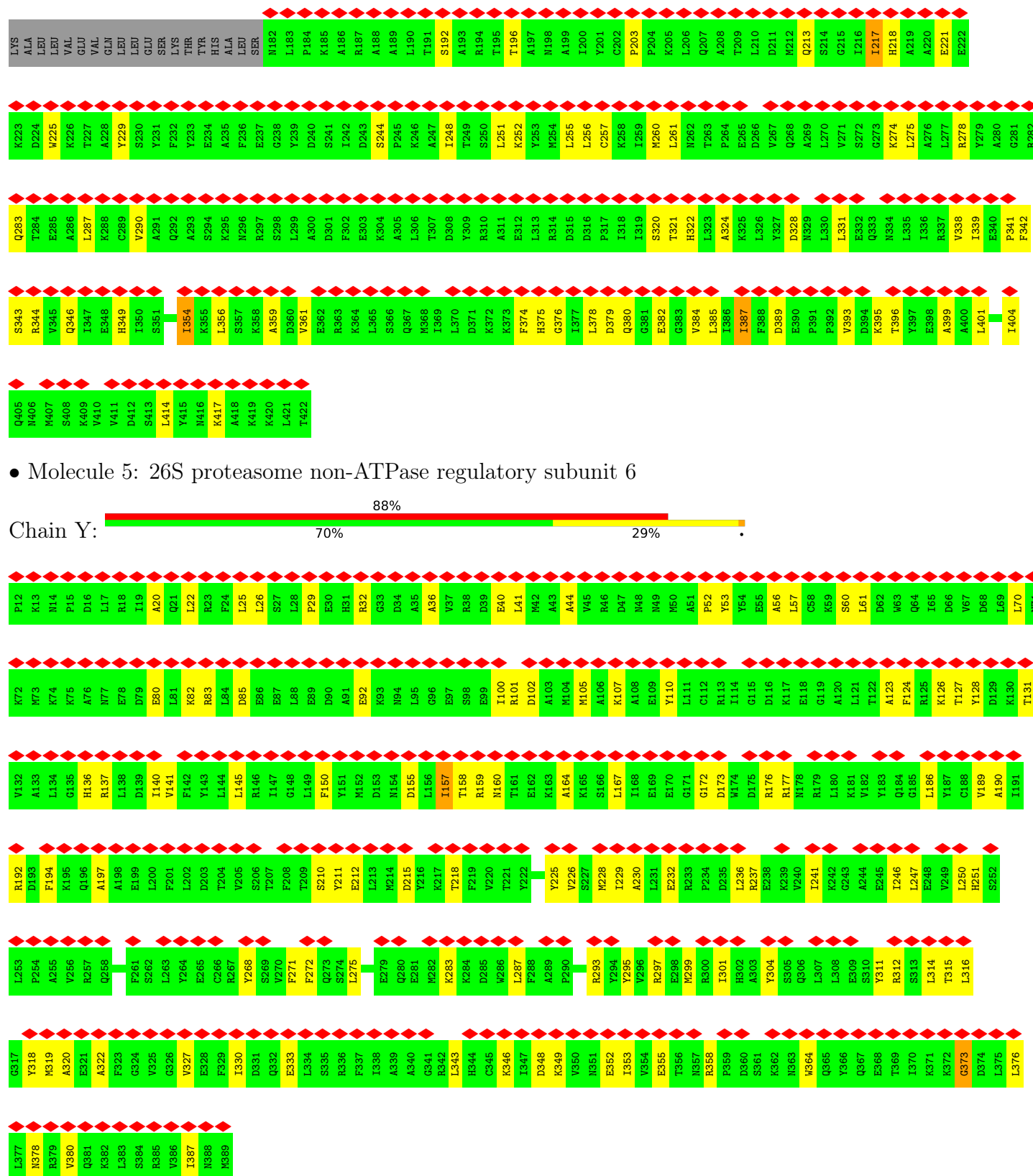


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



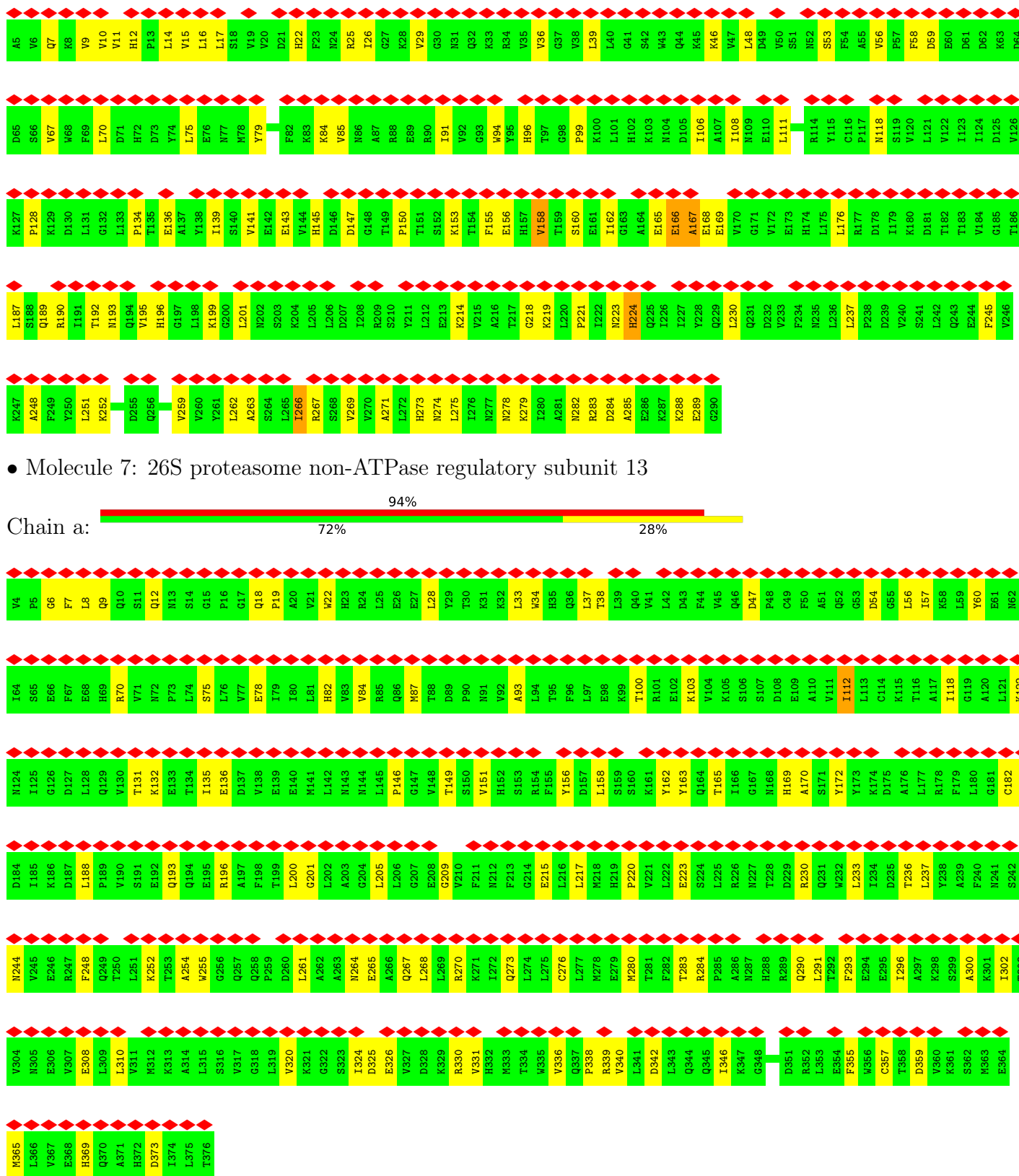
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11





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

• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

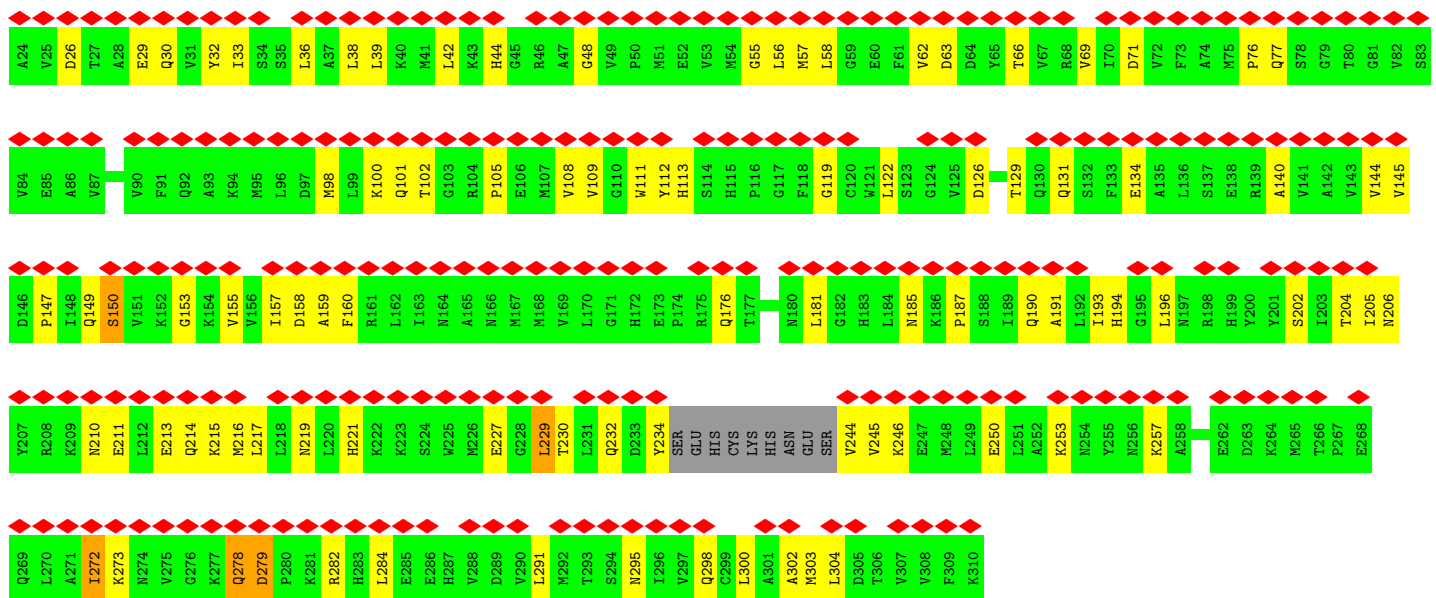
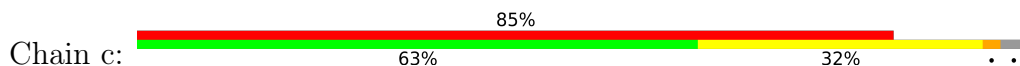


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

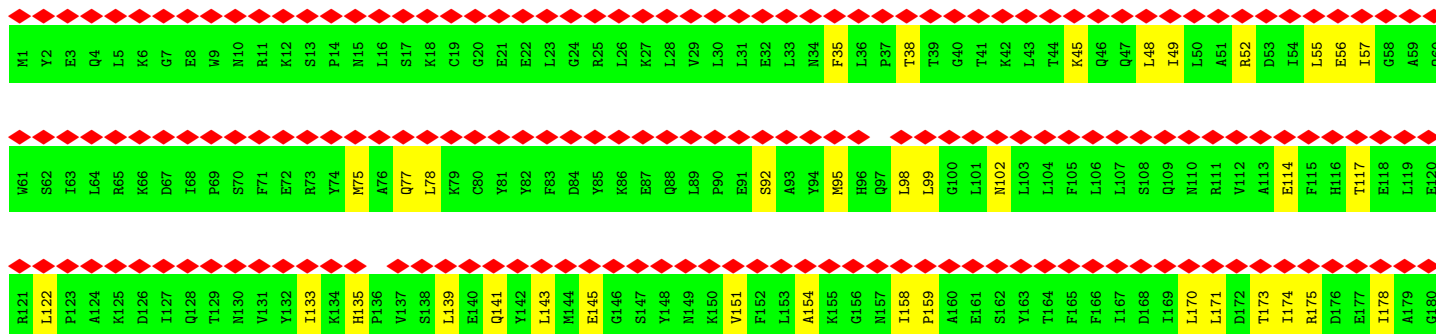
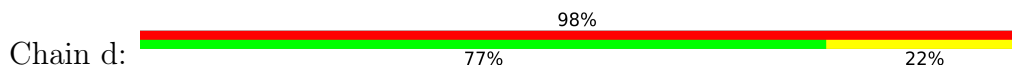


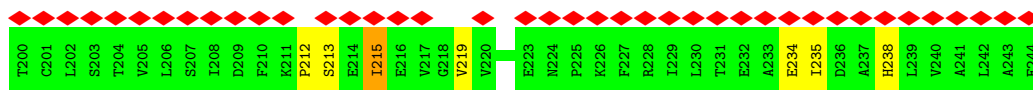


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

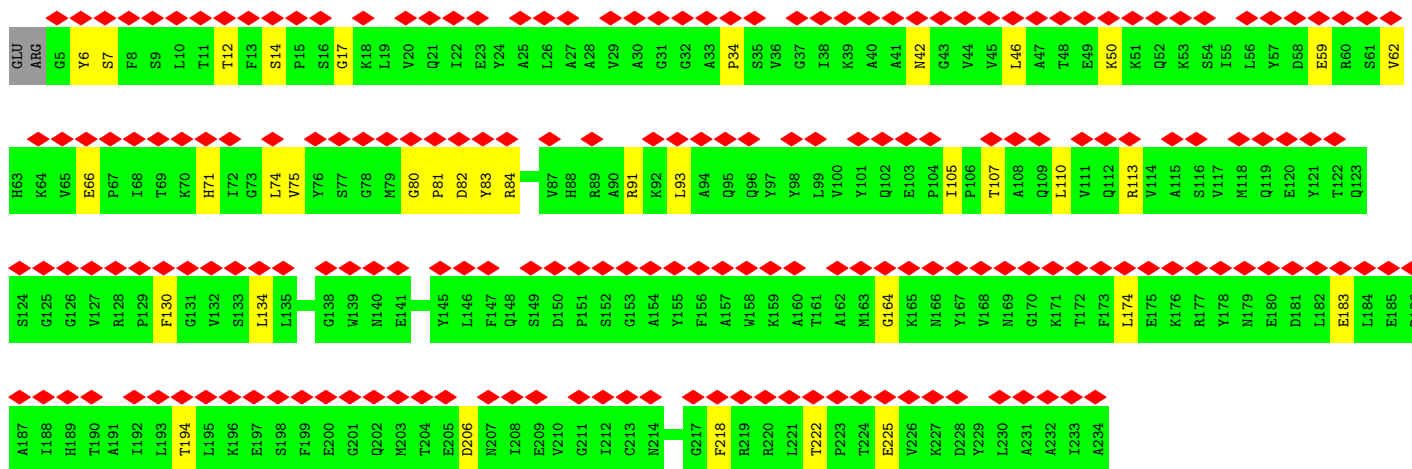
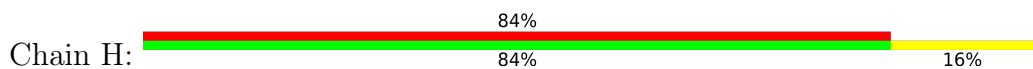


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

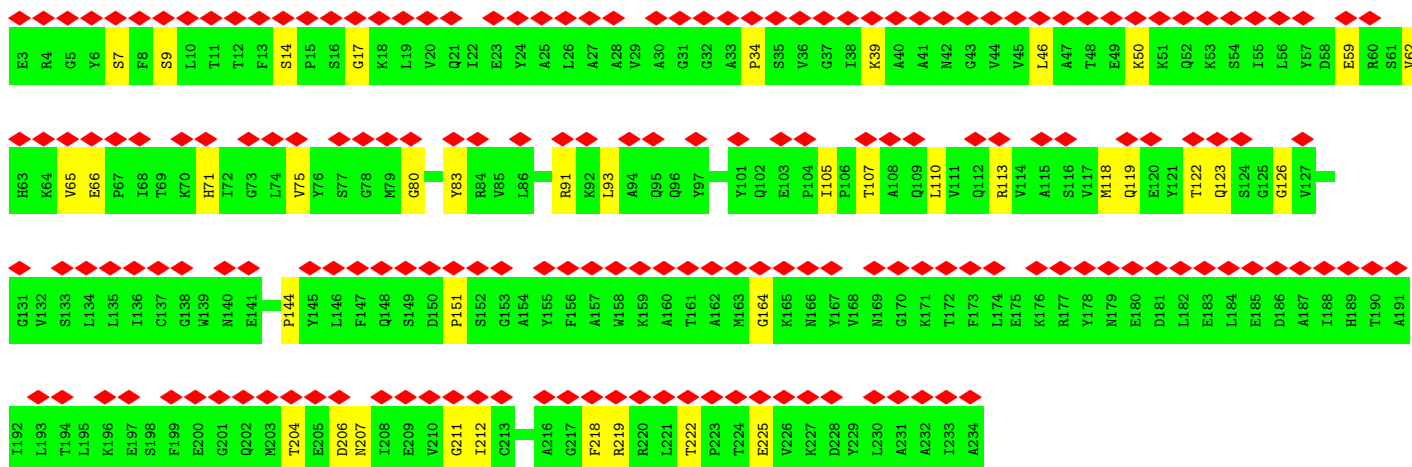
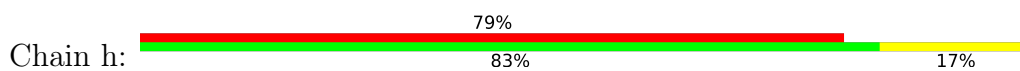




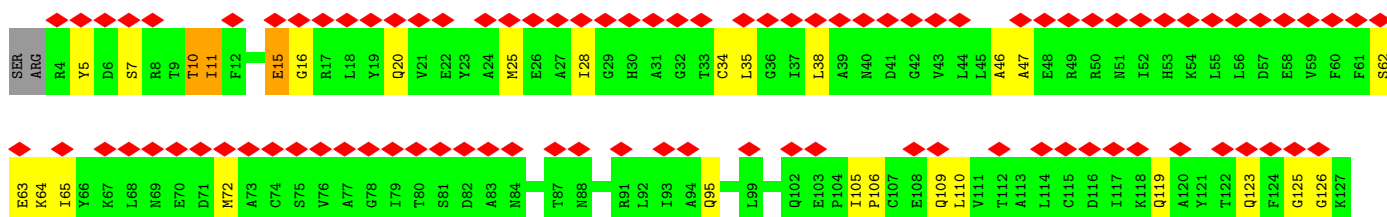
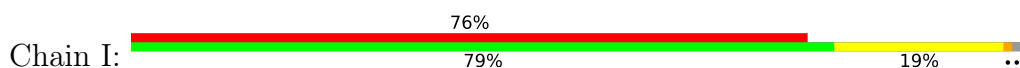
• Molecule 13: Proteasome subunit alpha type-2

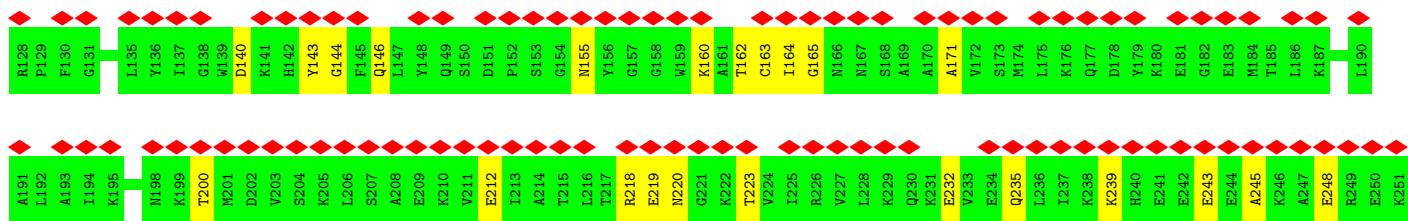


• Molecule 13: Proteasome subunit alpha type-2

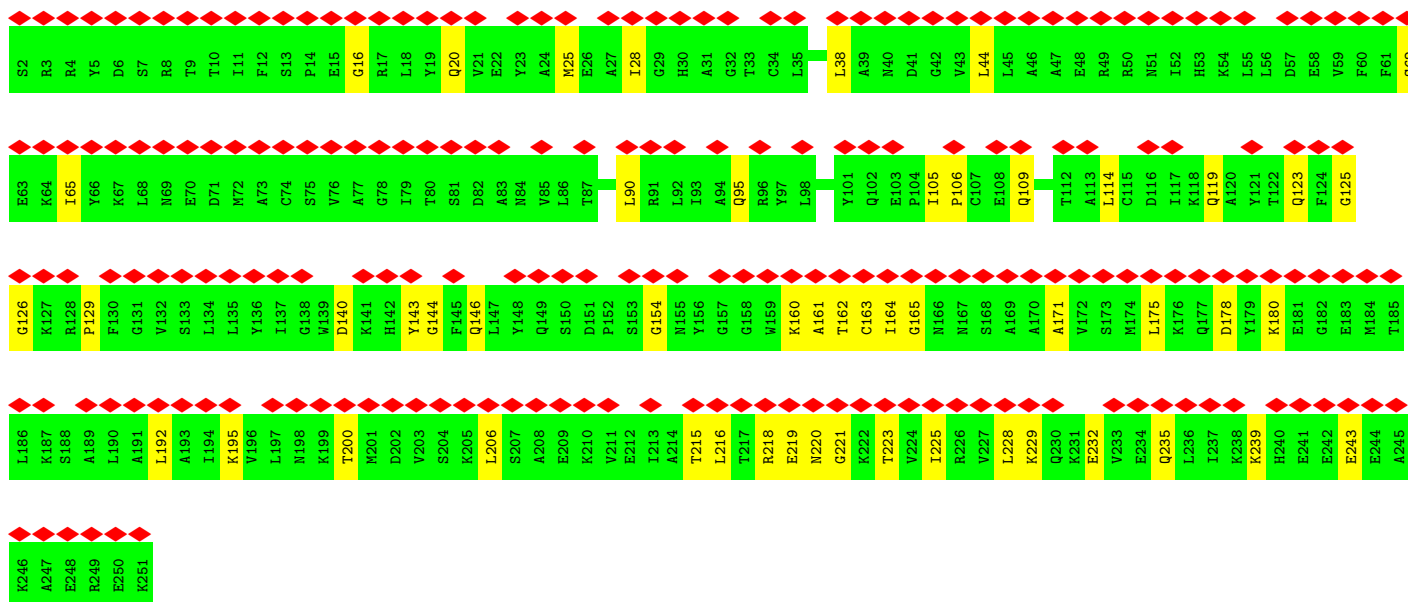
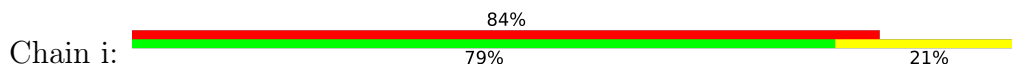


• Molecule 14: Proteasome subunit alpha type-4

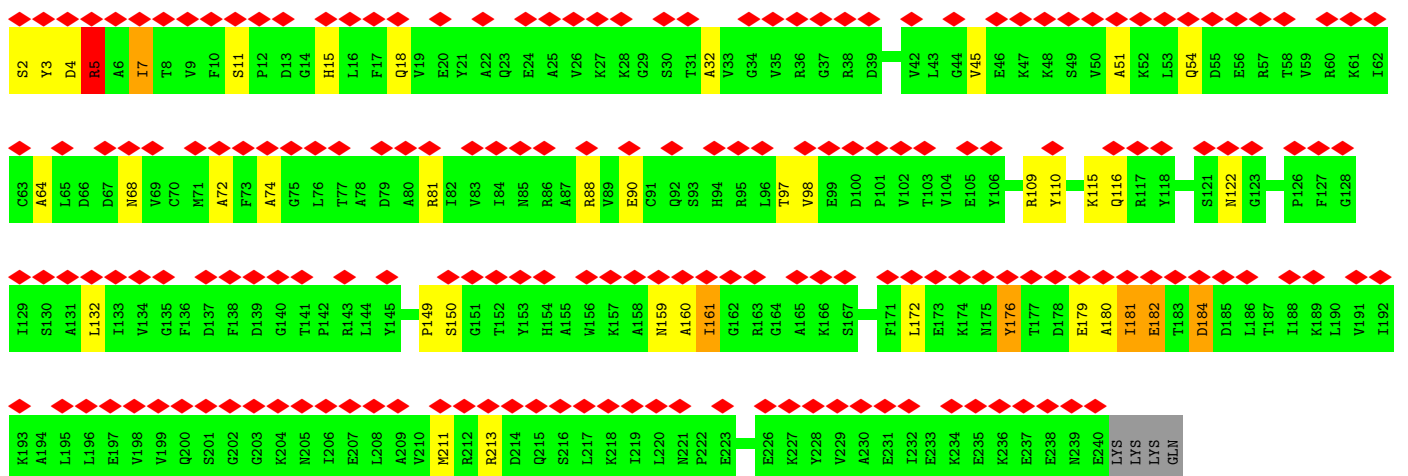
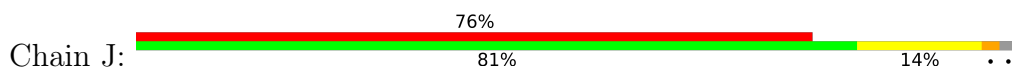




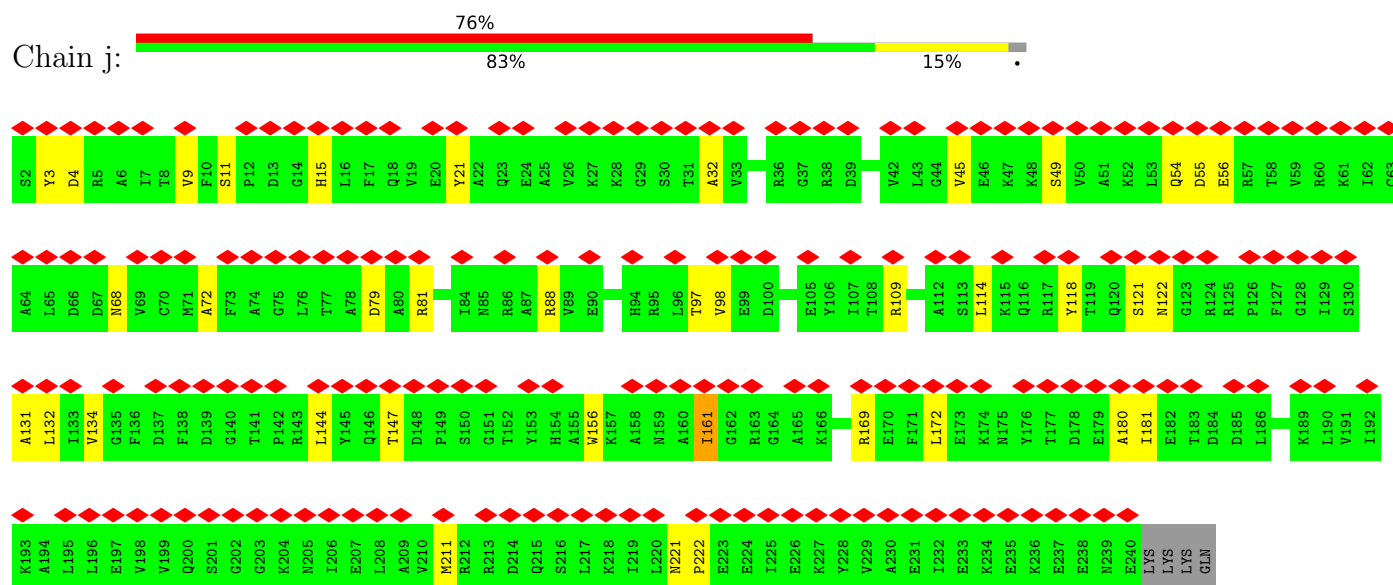
• Molecule 14: Proteasome subunit alpha type-4



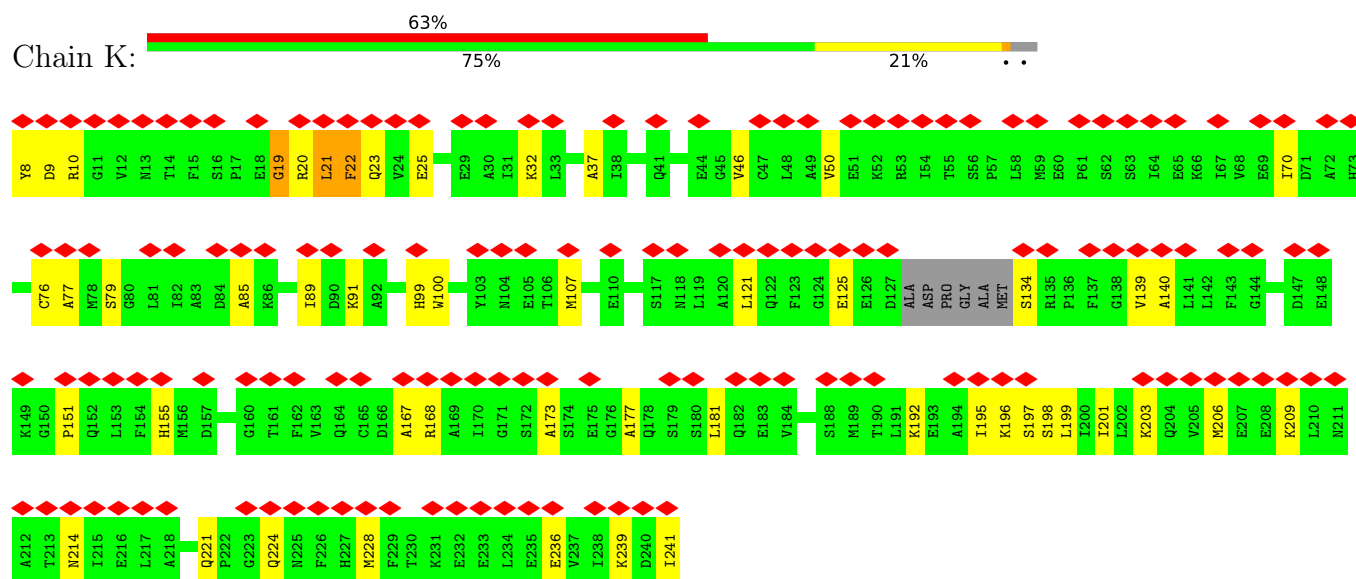
• Molecule 15: Proteasome subunit alpha type-7



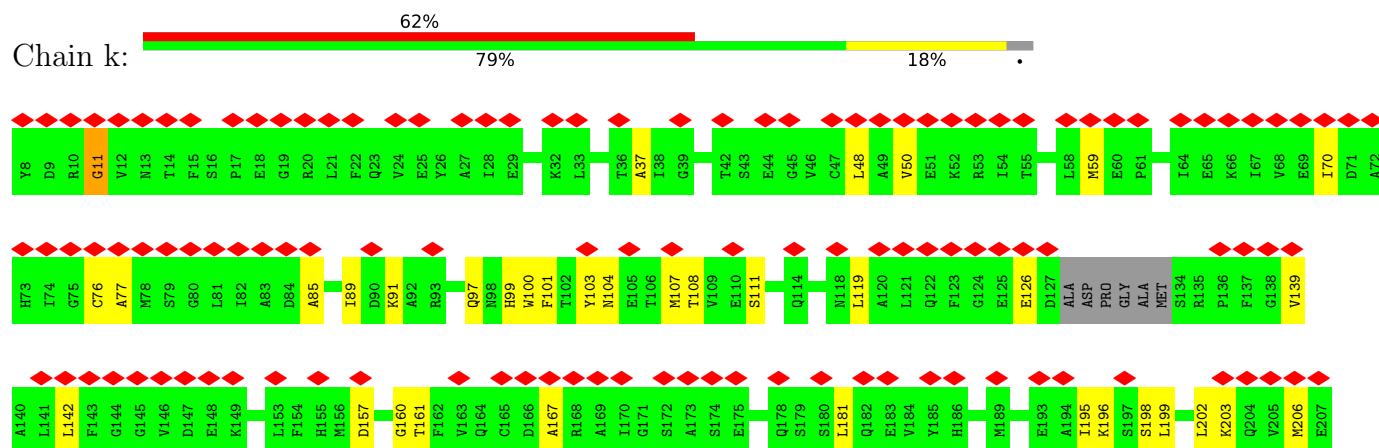
• Molecule 15: Proteasome subunit alpha type-7



• Molecule 16: Proteasome subunit alpha type-5

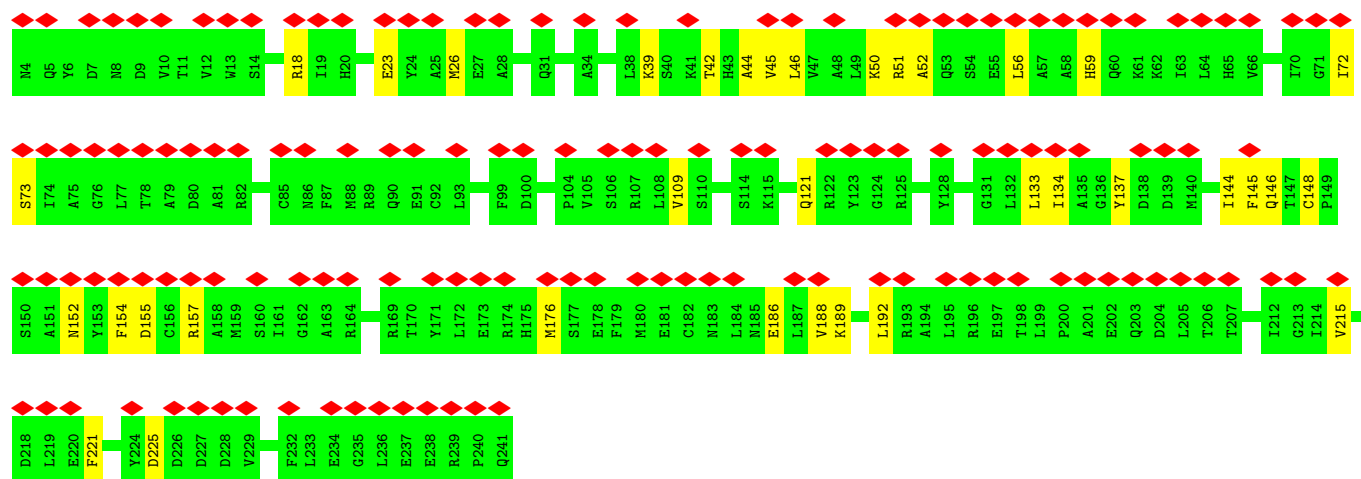
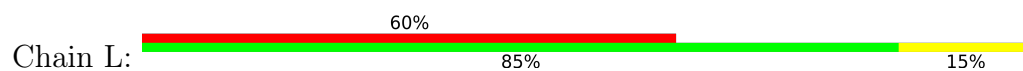


• Molecule 16: Proteasome subunit alpha type-5

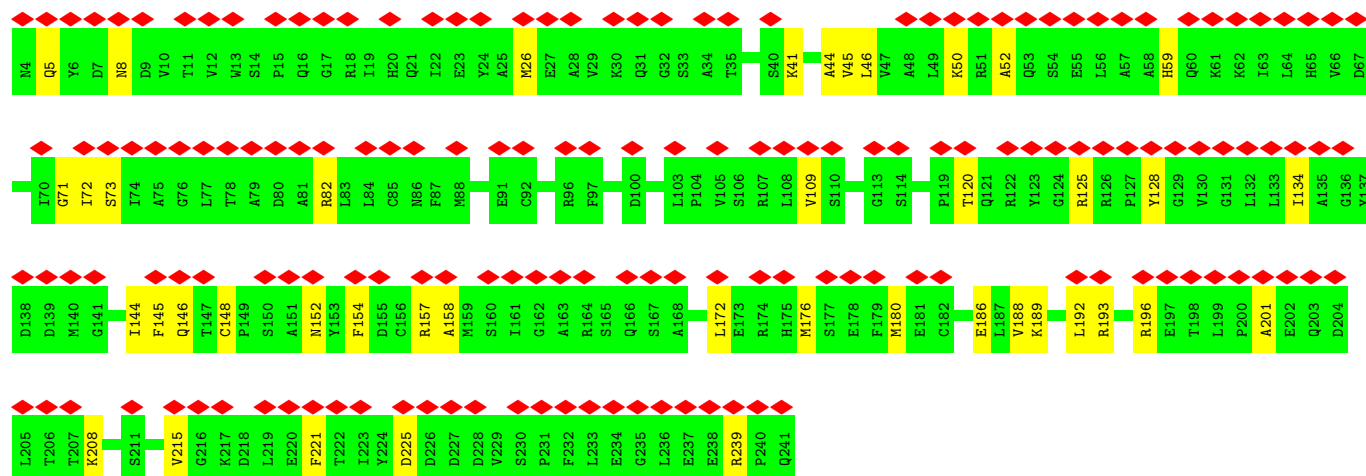
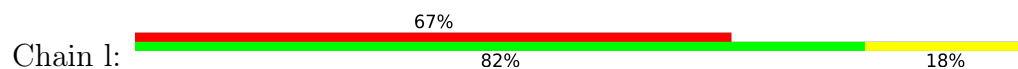




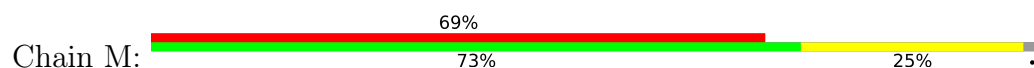
• Molecule 17: Proteasome subunit alpha type-1

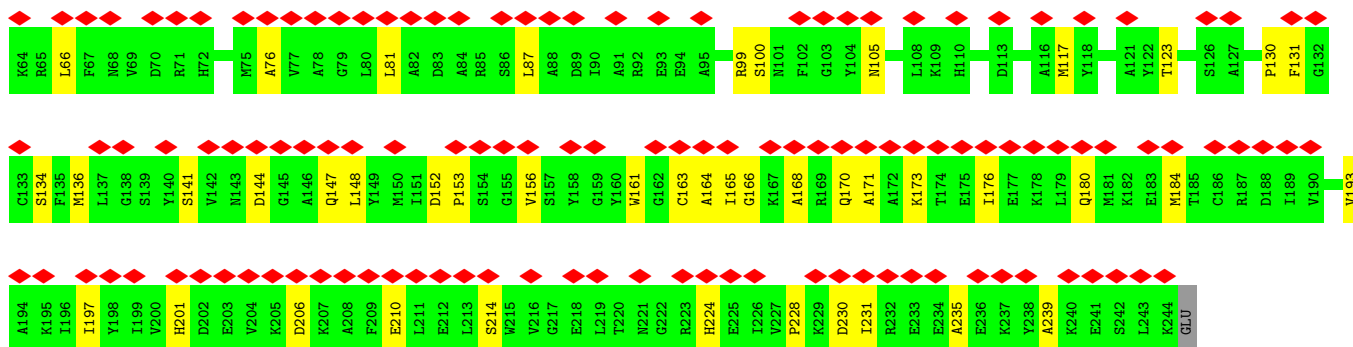


• Molecule 17: Proteasome subunit alpha type-1

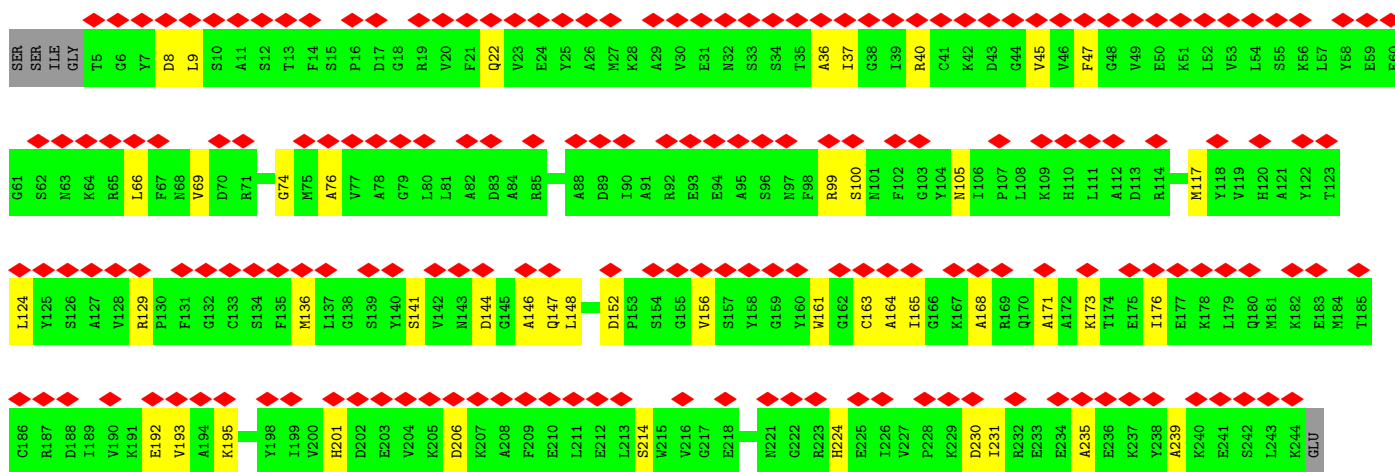
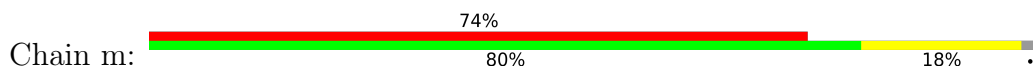


• Molecule 18: Proteasome subunit alpha type-3

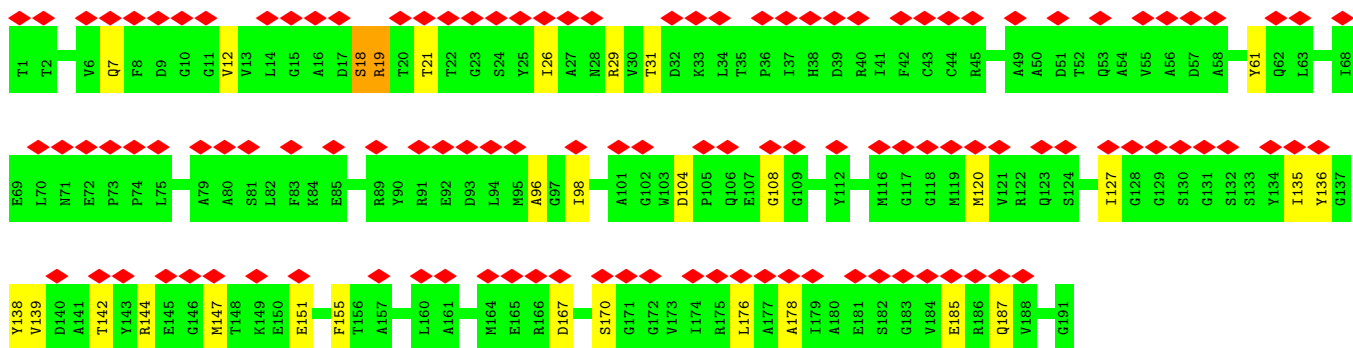
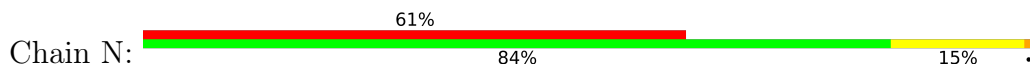




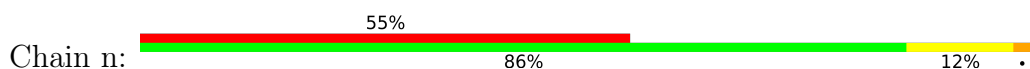
• Molecule 18: Proteasome subunit alpha type-3

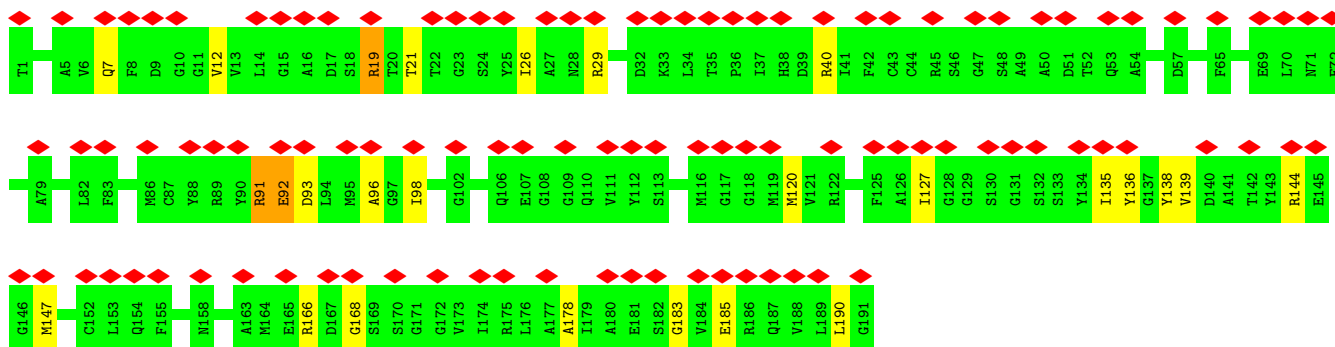


• Molecule 19: Proteasome subunit beta type-6

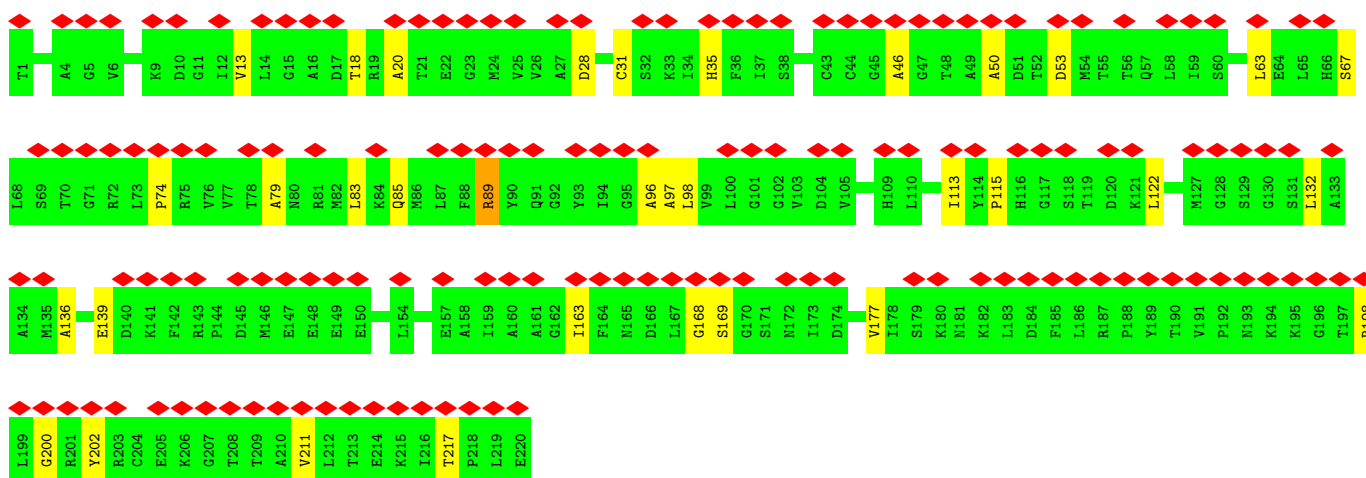
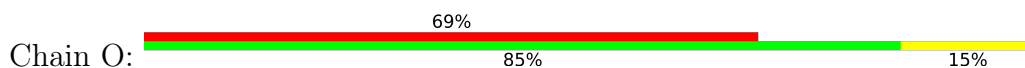


• Molecule 19: Proteasome subunit beta type-6

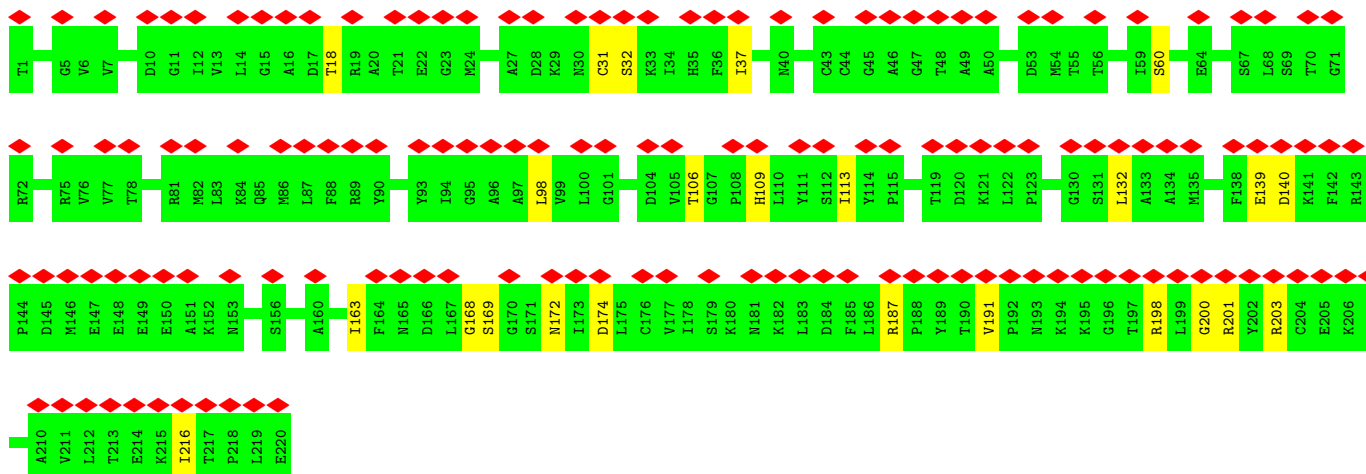
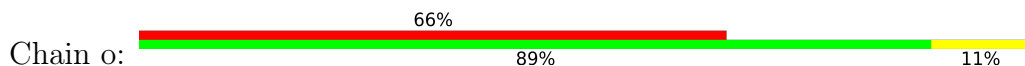




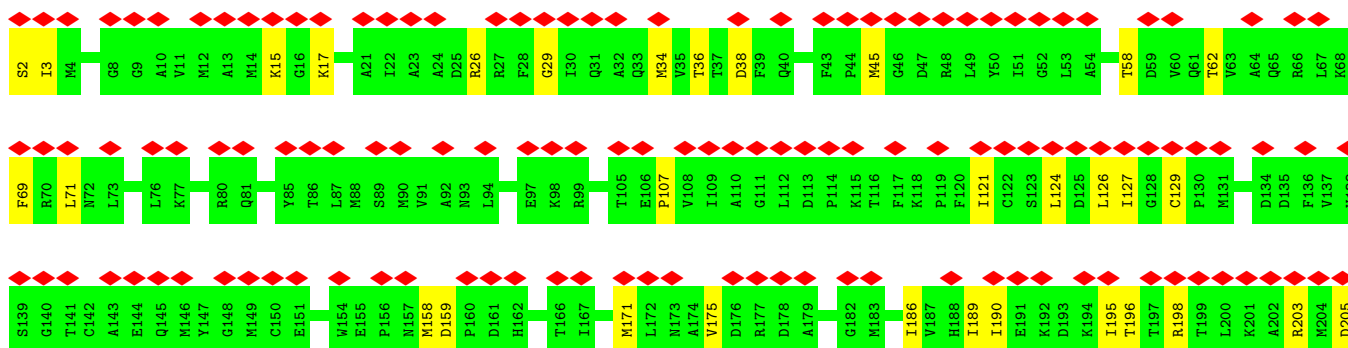
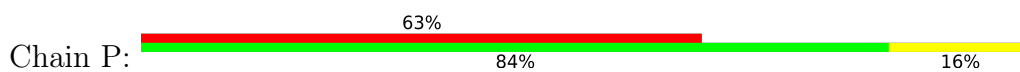
• Molecule 20: Proteasome subunit beta type-7



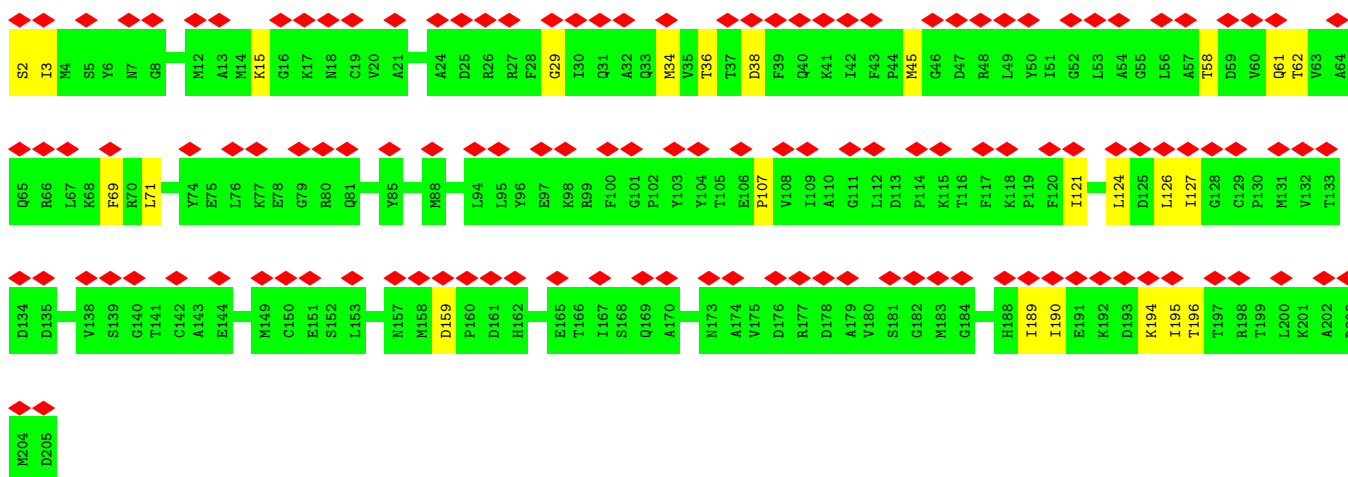
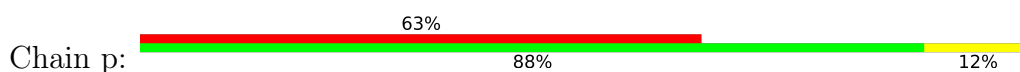
• Molecule 20: Proteasome subunit beta type-7



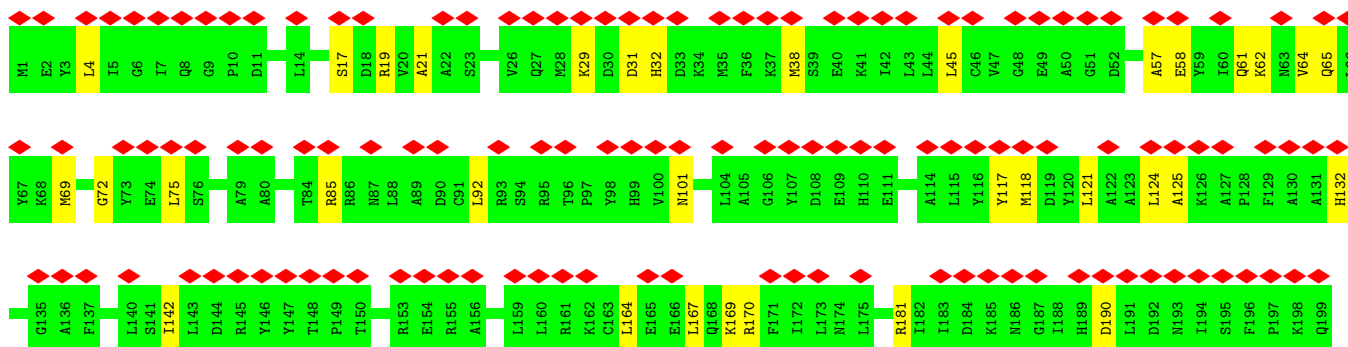
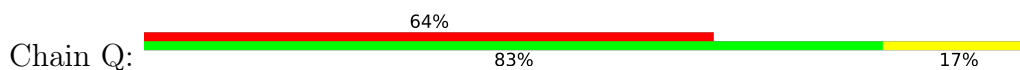
• Molecule 21: Proteasome subunit beta type-3



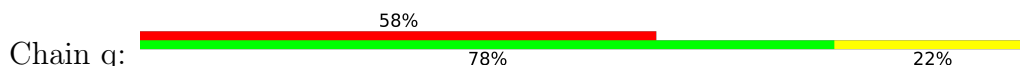
• Molecule 21: Proteasome subunit beta type-3

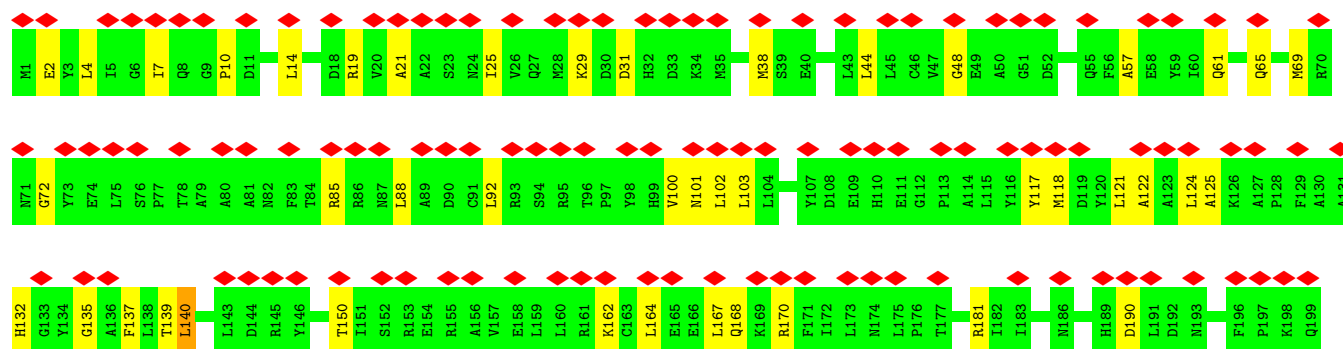


• Molecule 22: Proteasome subunit beta type-2

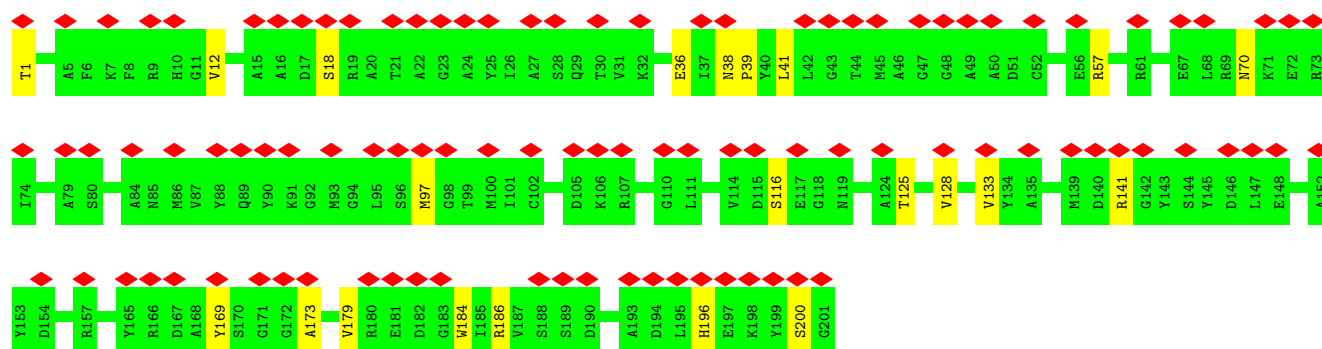


• Molecule 22: Proteasome subunit beta type-2

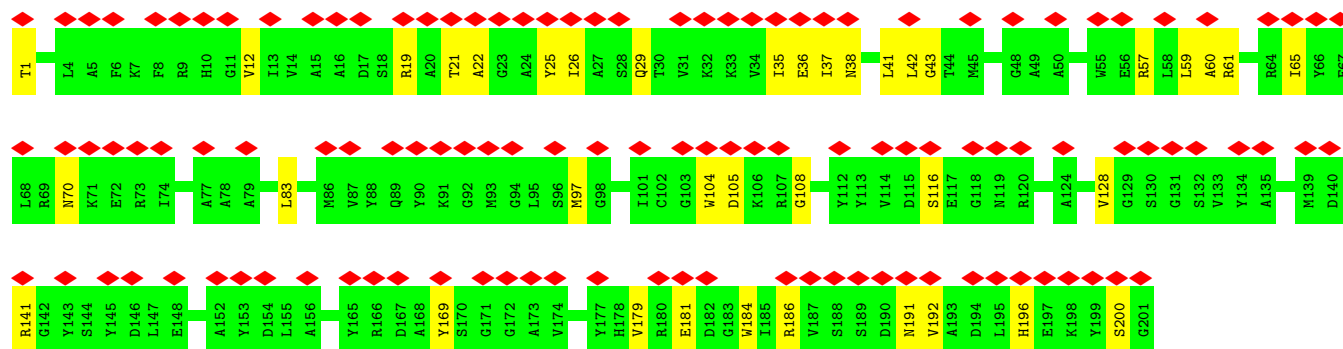
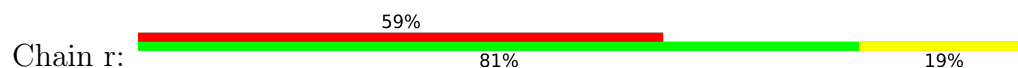




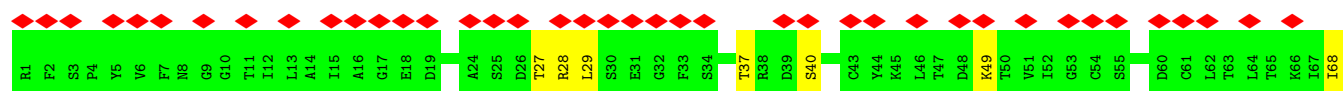
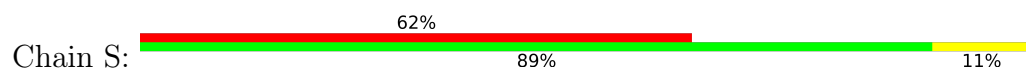
• Molecule 23: Proteasome subunit beta type-5

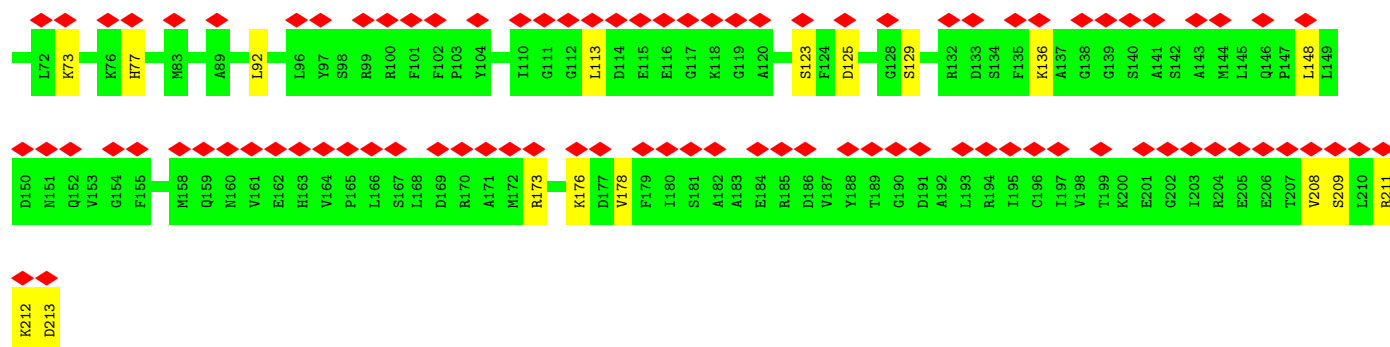


• Molecule 23: Proteasome subunit beta type-5

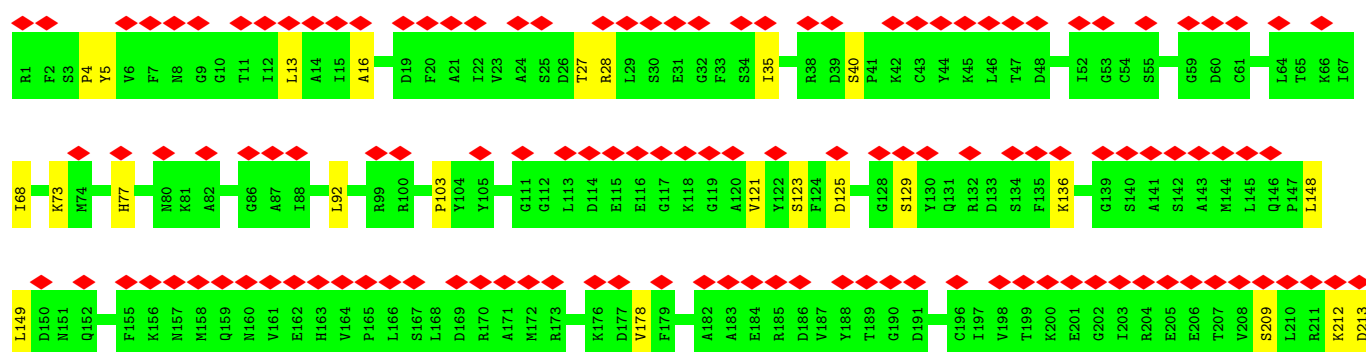
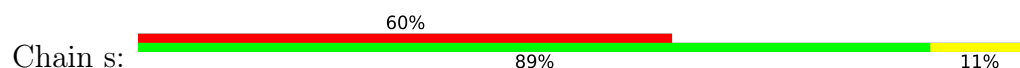


• Molecule 24: Proteasome subunit beta type-1

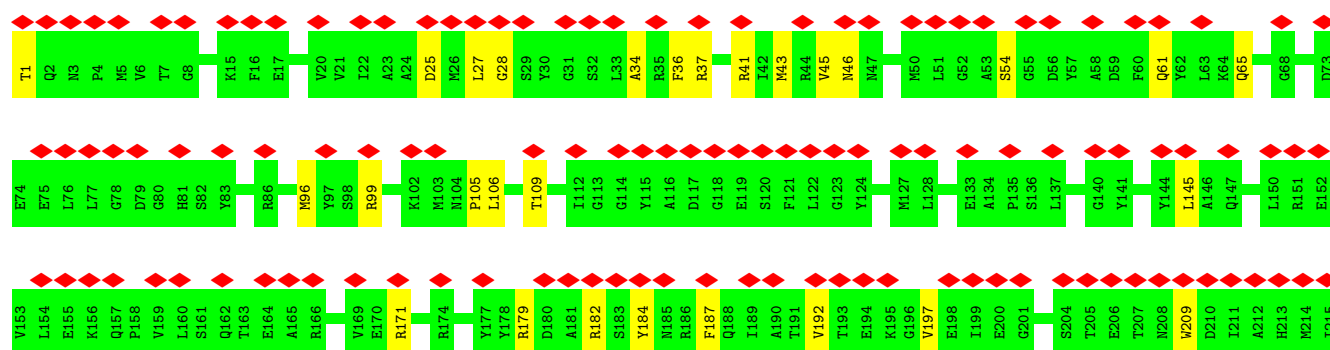
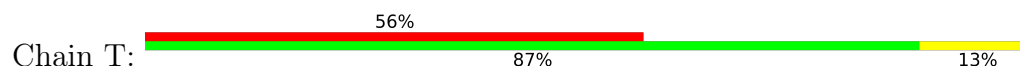




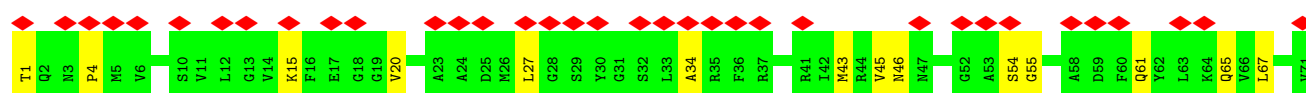
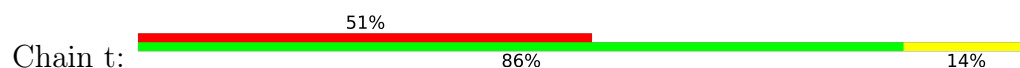
• Molecule 24: Proteasome subunit beta type-1

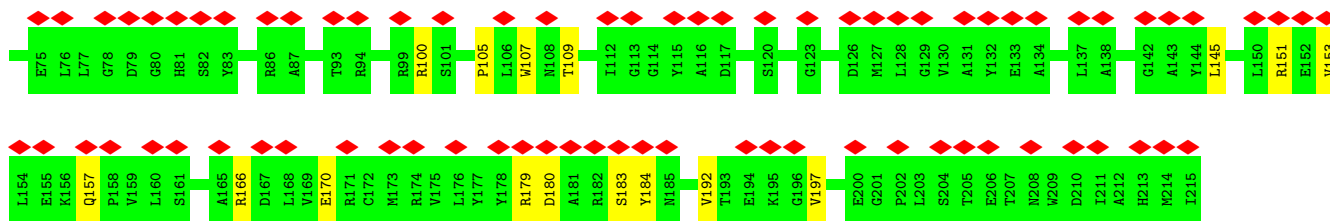


• Molecule 25: Proteasome subunit beta type-4



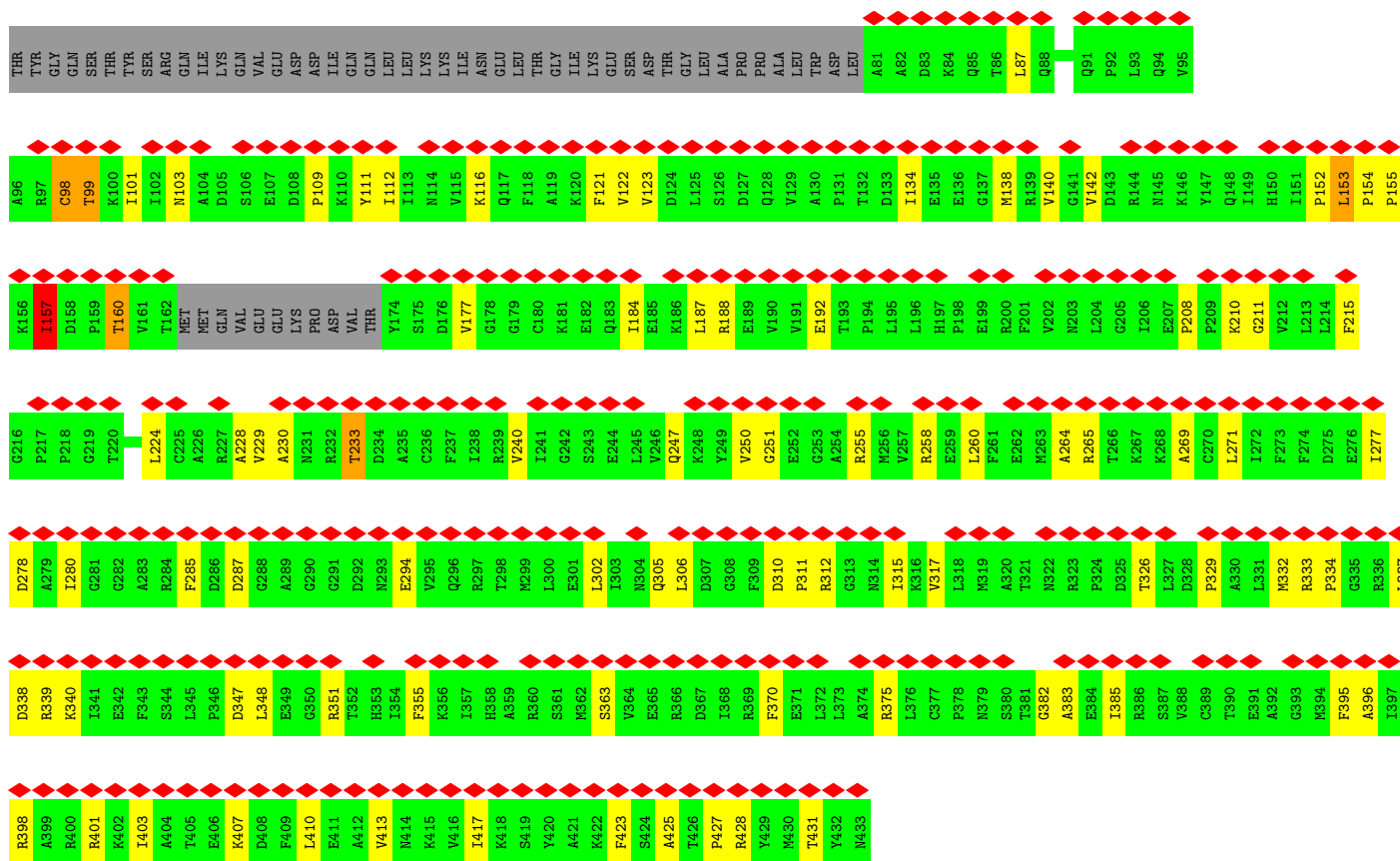
• Molecule 25: Proteasome subunit beta type-4





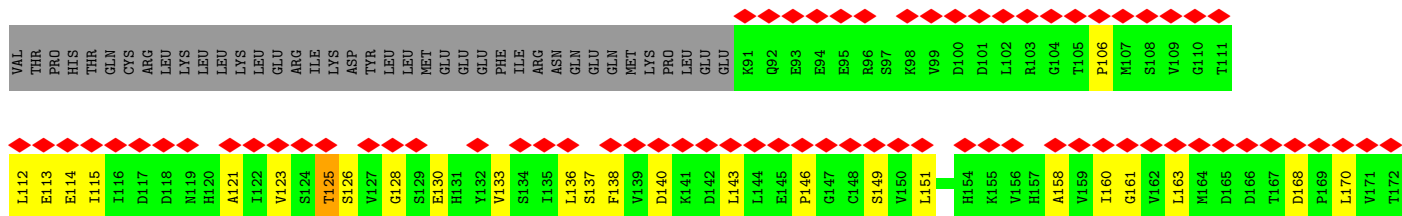
• Molecule 26: 26S proteasome regulatory subunit 7

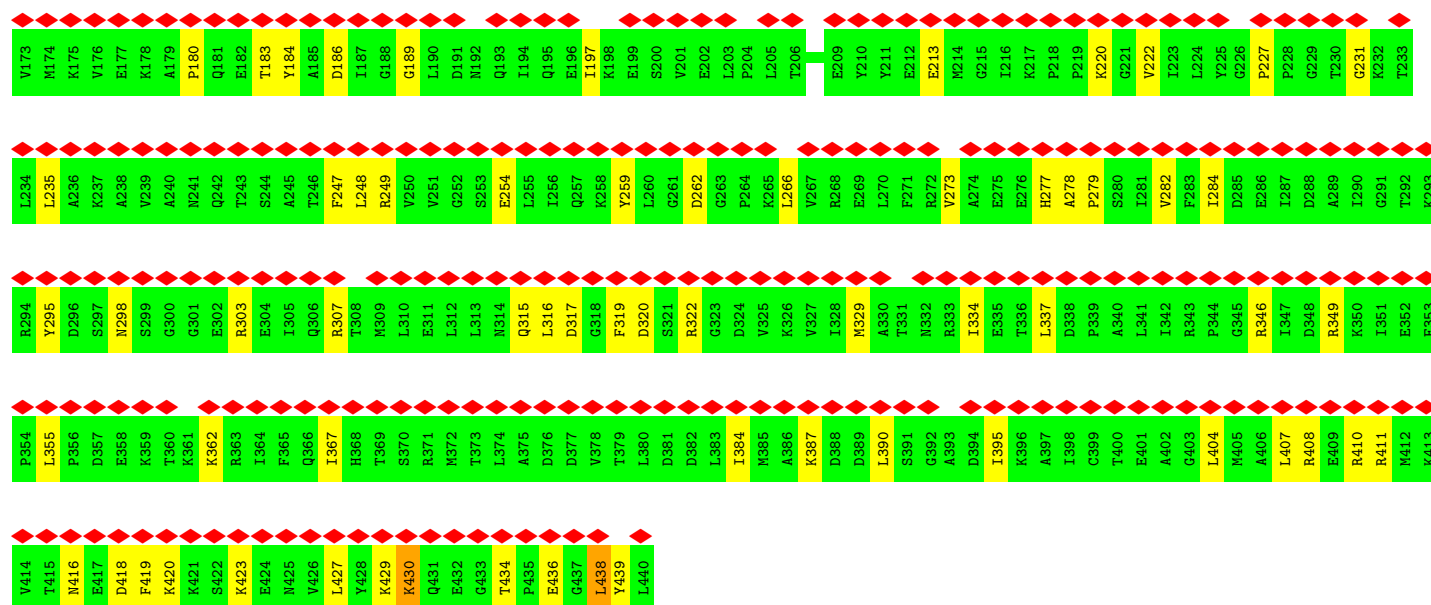
Chain A: 75% 62% 22% 14%



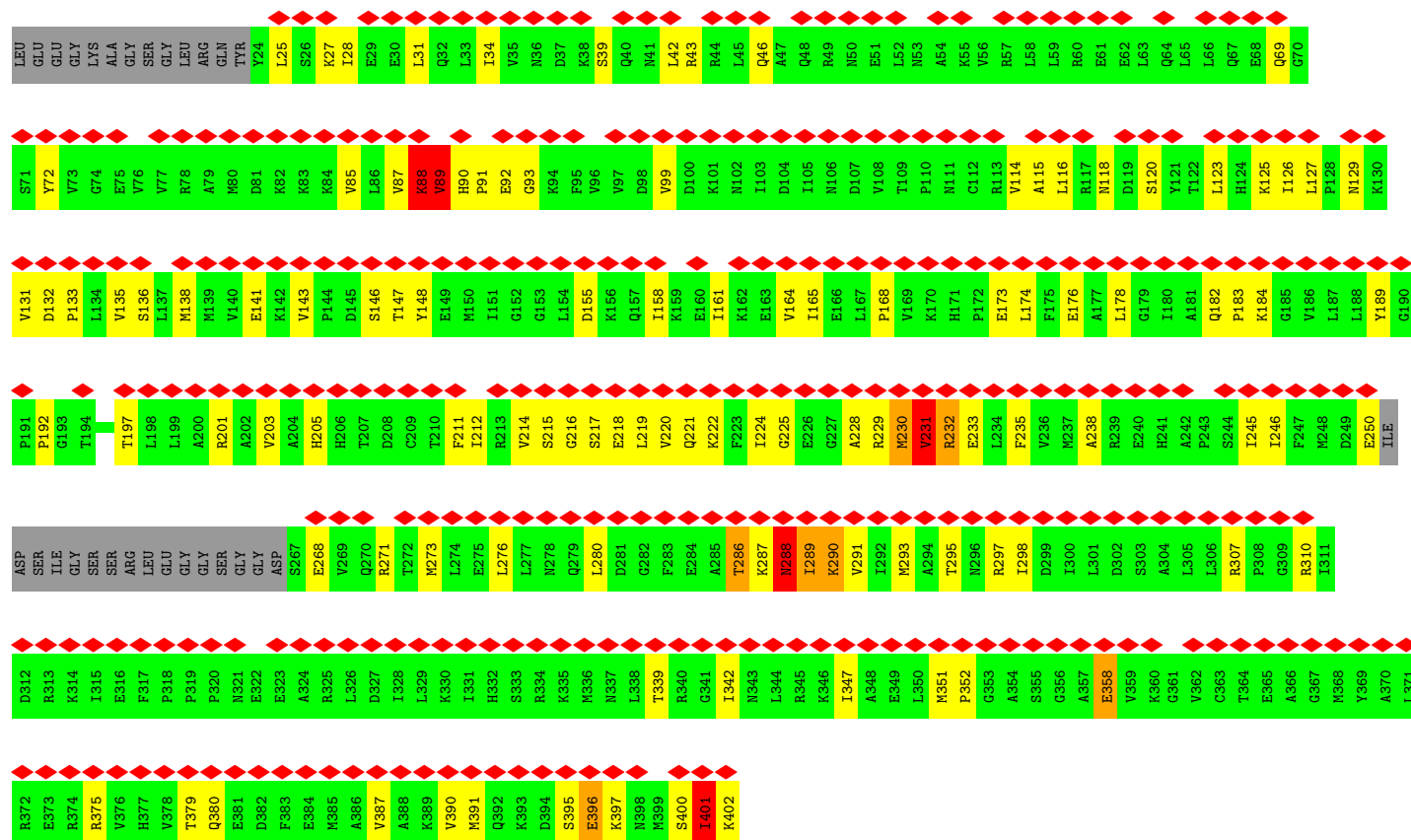
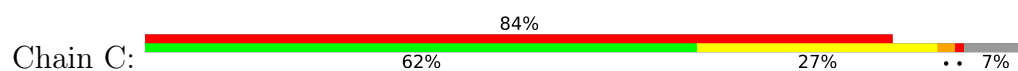
• Molecule 27: 26S proteasome regulatory subunit 4

Chain B: 84% 67% 22% 10%

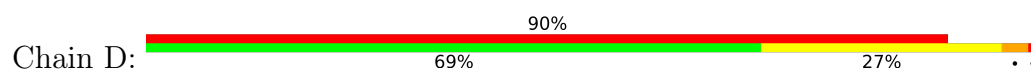


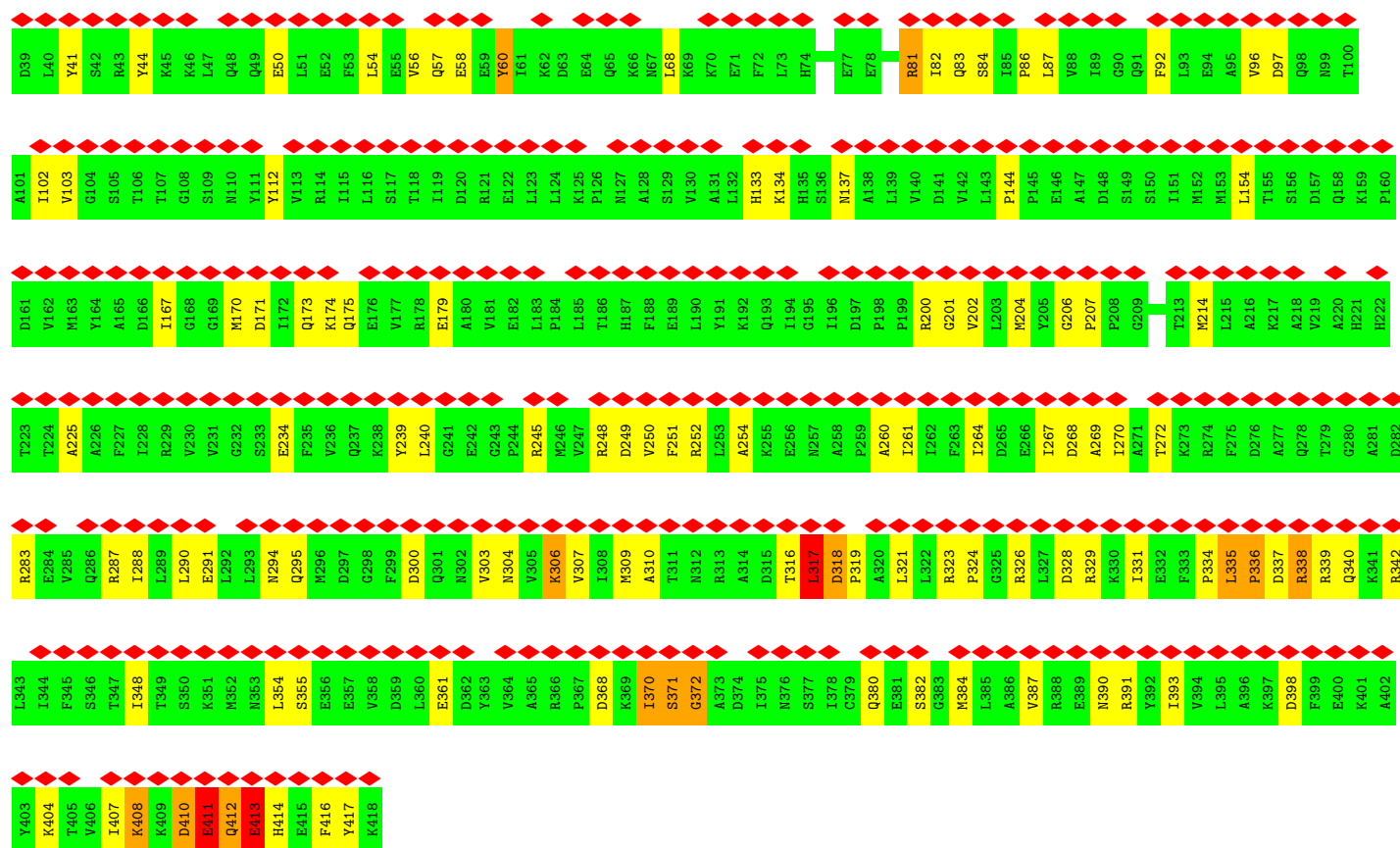


• Molecule 28: 26S proteasome regulatory subunit 8

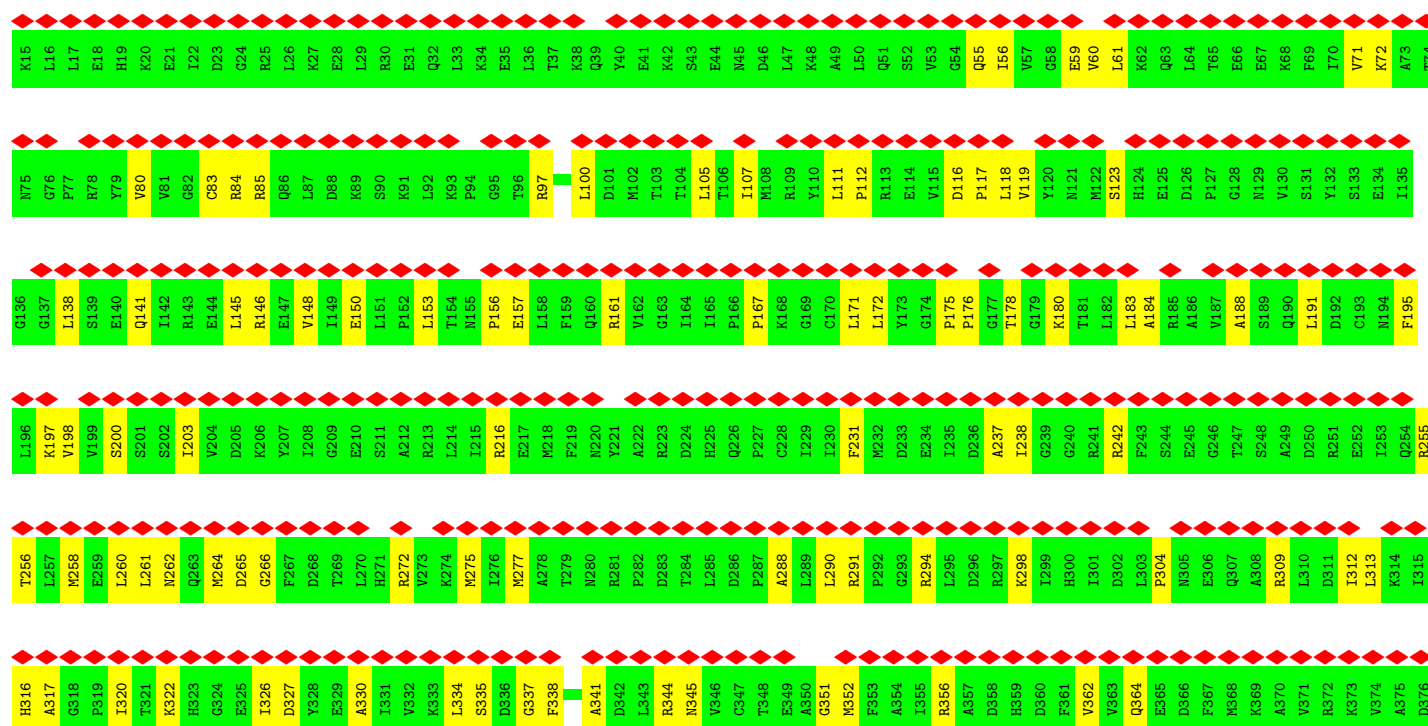
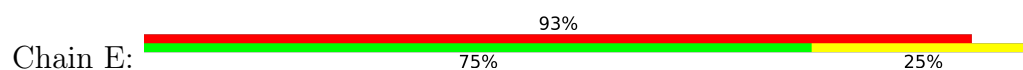


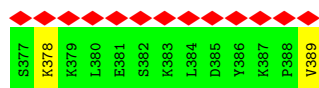
• Molecule 29: 26S proteasome regulatory subunit 6B



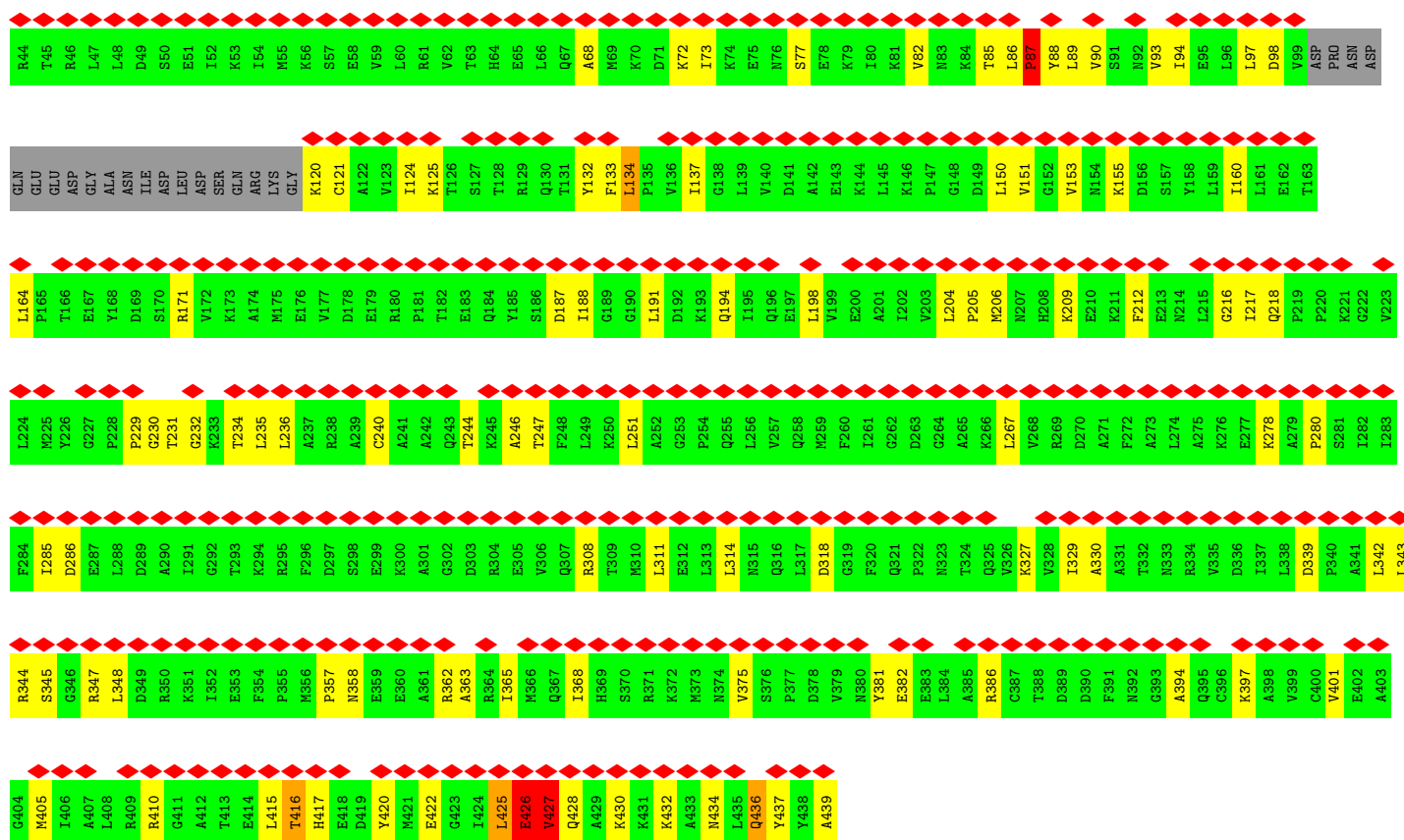
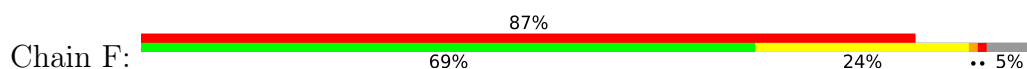


• Molecule 30: 26S proteasome regulatory subunit 10B

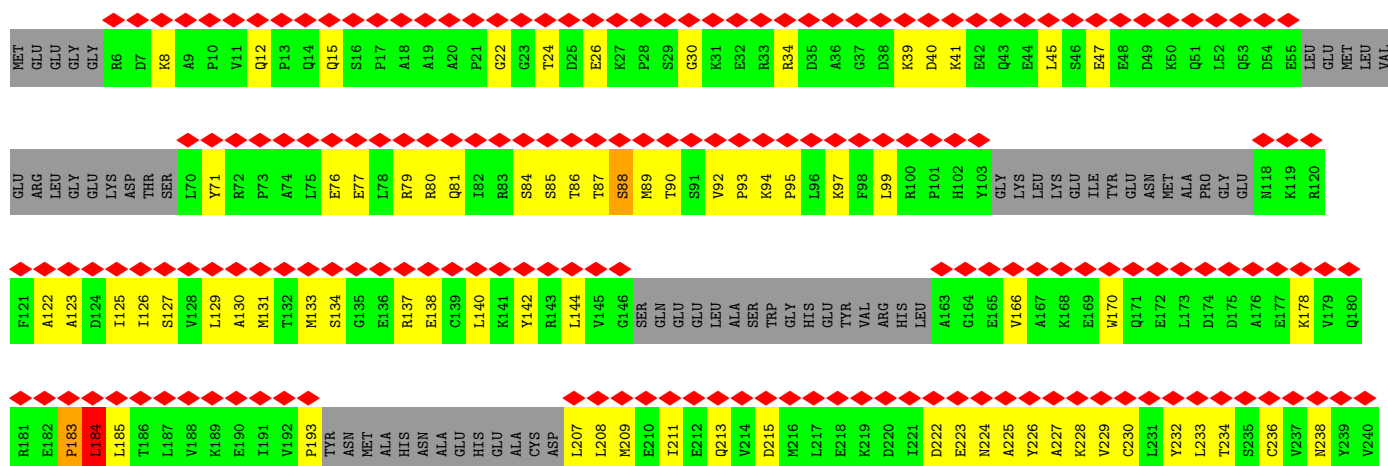
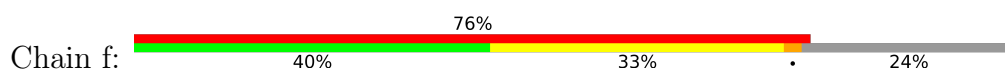




• Molecule 31: 26S proteasome regulatory subunit 6A



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33278	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	0.017	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.29	0/6396	0.74	5/8646 (0.1%)
2	V	0.34	0/3874	0.81	2/5234 (0.0%)
3	W	0.31	0/3751	0.82	1/5042 (0.0%)
4	X	0.30	0/1936	0.73	1/2614 (0.0%)
5	Y	0.31	0/3173	0.75	0/4273
6	Z	0.31	0/2324	0.84	1/3150 (0.0%)
7	a	0.30	0/3053	0.78	0/4133
8	b	0.32	0/1478	0.79	4/2001 (0.2%)
9	c	0.36	1/2226 (0.0%)	0.87	4/3007 (0.1%)
10	d	0.31	0/2162	0.79	2/2919 (0.1%)
11	e	0.39	0/338	1.03	2/450 (0.4%)
12	G	0.28	0/1853	0.69	0/2515
12	g	0.26	0/1859	0.61	0/2523
13	H	0.27	0/1723	0.65	2/2346 (0.1%)
13	h	0.25	0/1743	0.57	0/2372
14	I	0.29	0/1925	0.77	3/2606 (0.1%)
14	i	0.28	0/1942	0.70	0/2628
15	J	0.36	0/1728	0.87	7/2358 (0.3%)
15	j	0.34	0/1728	0.80	2/2358 (0.1%)
16	K	0.29	0/1755	0.79	9/2375 (0.4%)
16	k	0.26	0/1747	0.61	0/2364
17	L	0.30	0/1885	0.65	0/2552
17	l	0.27	0/1885	0.64	0/2552
18	M	0.27	0/1891	0.67	2/2552 (0.1%)
18	m	0.26	0/1891	0.62	2/2552 (0.1%)
19	N	0.26	0/1454	0.66	2/1967 (0.1%)
19	n	0.28	0/1454	0.68	0/1967
20	O	0.26	0/1670	0.59	0/2265
20	o	0.29	0/1670	0.67	0/2265
21	P	0.25	0/1614	0.54	0/2177
21	p	0.28	0/1614	0.56	0/2177
22	Q	0.34	0/1603	0.73	0/2174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	q	0.34	0/1603	0.71	1/2174 (0.0%)
23	R	0.27	0/1579	0.51	0/2134
23	r	0.25	0/1579	0.51	0/2134
24	S	0.27	0/1671	0.57	0/2253
24	s	0.27	0/1671	0.55	0/2253
25	T	0.27	0/1700	0.57	0/2305
25	t	0.26	0/1700	0.57	0/2305
26	A	0.29	0/2717	0.81	6/3665 (0.2%)
27	B	0.28	0/2745	0.78	3/3709 (0.1%)
28	C	0.35	0/2896	0.94	14/3895 (0.4%)
29	D	0.39	1/3090 (0.0%)	1.00	17/4168 (0.4%)
30	E	0.27	0/2904	0.67	0/3924
31	F	0.28	0/2897	0.76	12/3912 (0.3%)
32	f	0.33	1/5393 (0.0%)	0.87	20/7271 (0.3%)
All	All	0.30	3/101490 (0.0%)	0.74	124/137216 (0.1%)

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	2
2	V	0	1
3	W	0	1
5	Y	0	1
6	Z	0	5
8	b	0	1
9	c	0	5
15	J	0	2
15	j	0	1
16	K	0	3
16	k	0	1
20	O	0	1
26	A	0	3
27	B	0	1
28	C	0	10
29	D	0	8
31	F	0	5
All	All	0	51

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	279	ASP	C-N	6.82	1.42	1.33
29	D	144	PRO	C-N	5.23	1.39	1.33
32	f	494	ARG	CA-C	5.21	1.59	1.52

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	414	HIS	N-CA-C	10.74	126.71	113.50
32	f	488	ALA	N-CA-C	10.52	122.82	111.36
16	K	21	LEU	CA-C-N	9.92	139.56	121.70
16	K	21	LEU	C-N-CA	9.92	139.56	121.70
29	D	335	LEU	CA-C-N	9.72	129.67	119.85

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	432	SER	Peptide
1	U	598	ALA	Peptide
2	V	194	LYS	Peptide
3	W	313	GLU	Peptide
5	Y	373	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6287	0	6338	154	0
2	V	3799	0	3850	100	0
3	W	3703	0	3822	106	0
4	X	1905	0	1951	45	0
5	Y	3115	0	3120	80	0
6	Z	2281	0	2312	73	0
7	a	2995	0	3012	71	0
8	b	1458	0	1505	42	0
9	c	2187	0	2215	66	0
10	d	2116	0	2146	38	0
11	e	334	0	294	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	1820	0	1791	23	0
12	g	1826	0	1796	20	0
13	H	1688	0	1575	21	0
13	h	1708	0	1594	21	0
14	I	1895	0	1833	30	0
14	i	1912	0	1851	30	0
15	J	1704	0	1517	24	0
15	j	1704	0	1517	27	0
16	K	1729	0	1680	30	0
16	k	1722	0	1673	30	0
17	L	1850	0	1822	25	0
17	l	1850	0	1822	27	0
18	M	1856	0	1814	38	0
18	m	1856	0	1814	30	0
19	N	1430	0	1398	19	0
19	n	1430	0	1398	19	0
20	O	1643	0	1644	21	0
20	o	1643	0	1644	16	0
21	P	1585	0	1598	22	0
21	p	1585	0	1598	17	0
22	Q	1570	0	1547	21	0
22	q	1570	0	1547	27	0
23	R	1548	0	1499	14	0
23	r	1548	0	1499	28	0
24	S	1641	0	1618	13	0
24	s	1641	0	1618	14	0
25	T	1667	0	1628	20	0
25	t	1667	0	1628	22	0
26	A	2672	0	2700	57	0
27	B	2706	0	2731	64	0
28	C	2859	0	2971	79	0
29	D	3040	0	3076	94	0
30	E	2860	0	2828	60	0
31	F	2859	0	2853	85	0
32	f	5319	0	5329	461	0
33	c	1	0	0	0	0
34	A	31	0	12	3	0
34	B	31	0	12	4	0
34	D	31	0	12	7	0
34	F	31	0	12	9	0
All	All	99908	0	99064	2151	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 11.

The worst 5 of 2151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:494:ARG:HD3	32:f:496:ASP:OD1	1.26	1.35
32:f:753:ALA:O	32:f:754:LYS:HE2	1.27	1.31
31:F:230:GLY:O	34:F:501:AGS:H8	1.14	1.29
32:f:796:LEU:O	32:f:799:VAL:HG22	1.30	1.26
32:f:742:ALA:HA	32:f:745:LEU:CD2	1.66	1.25

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	798/911 (88%)	735 (92%)	63 (8%)	0	100	100
2	V	470/480 (98%)	400 (85%)	68 (14%)	2 (0%)	30	67
3	W	454/456 (100%)	394 (87%)	58 (13%)	2 (0%)	30	67
4	X	239/380 (63%)	222 (93%)	16 (7%)	1 (0%)	30	67
5	Y	376/378 (100%)	336 (89%)	40 (11%)	0	100	100
6	Z	284/286 (99%)	240 (84%)	39 (14%)	5 (2%)	6	33
7	a	371/373 (100%)	339 (91%)	31 (8%)	1 (0%)	36	71
8	b	189/191 (99%)	160 (85%)	29 (15%)	0	100	100
9	c	274/287 (96%)	237 (86%)	33 (12%)	4 (2%)	8	38
10	d	255/257 (99%)	219 (86%)	34 (13%)	2 (1%)	16	52
11	e	36/70 (51%)	26 (72%)	9 (25%)	1 (3%)	4	24
12	G	237/240 (99%)	215 (91%)	22 (9%)	0	100	100
12	g	238/240 (99%)	220 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	H	228/232 (98%)	210 (92%)	18 (8%)	0	100	100
13	h	230/232 (99%)	219 (95%)	11 (5%)	0	100	100
14	I	246/250 (98%)	222 (90%)	23 (9%)	1 (0%)	30	67
14	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	30	67
15	J	237/243 (98%)	222 (94%)	12 (5%)	3 (1%)	9	41
15	j	237/243 (98%)	220 (93%)	15 (6%)	2 (1%)	16	52
16	K	224/234 (96%)	205 (92%)	18 (8%)	1 (0%)	30	67
16	k	224/234 (96%)	203 (91%)	20 (9%)	1 (0%)	30	67
17	L	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
17	l	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
18	M	238/245 (97%)	216 (91%)	22 (9%)	0	100	100
18	m	238/245 (97%)	219 (92%)	19 (8%)	0	100	100
19	N	189/191 (99%)	179 (95%)	9 (5%)	1 (0%)	24	63
19	n	189/191 (99%)	179 (95%)	7 (4%)	3 (2%)	7	37
20	O	218/220 (99%)	204 (94%)	14 (6%)	0	100	100
20	o	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
21	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
21	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
22	Q	197/199 (99%)	181 (92%)	15 (8%)	1 (0%)	24	63
22	q	197/199 (99%)	179 (91%)	16 (8%)	2 (1%)	12	47
23	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
23	r	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
24	S	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
24	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
25	T	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
25	t	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
26	A	338/399 (85%)	269 (80%)	64 (19%)	5 (2%)	8	38
27	B	348/389 (90%)	300 (86%)	46 (13%)	2 (1%)	21	58
28	C	359/392 (92%)	290 (81%)	59 (16%)	10 (3%)	4	24
29	D	378/380 (100%)	298 (79%)	74 (20%)	6 (2%)	7	37
30	E	373/375 (100%)	343 (92%)	29 (8%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	F	372/396 (94%)	334 (90%)	33 (9%)	5 (1%)	9	41
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	10	42
All	All	12738/13558 (94%)	11445 (90%)	1222 (10%)	71 (1%)	23	58

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	424	LEU
9	c	279	ASP
11	e	60	LEU
15	J	184	ASP
16	K	10	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	685/779 (88%)	682 (100%)	3 (0%)	84	83
2	V	409/414 (99%)	406 (99%)	3 (1%)	76	79
3	W	416/416 (100%)	411 (99%)	5 (1%)	63	74
4	X	208/327 (64%)	206 (99%)	2 (1%)	68	76
5	Y	334/334 (100%)	332 (99%)	2 (1%)	78	81
6	Z	257/257 (100%)	253 (98%)	4 (2%)	55	69
7	a	333/333 (100%)	331 (99%)	2 (1%)	78	81
8	b	167/167 (100%)	165 (99%)	2 (1%)	63	74
9	c	243/252 (96%)	239 (98%)	4 (2%)	55	69
10	d	231/231 (100%)	230 (100%)	1 (0%)	84	83
11	e	38/63 (60%)	38 (100%)	0	100	100
12	G	192/205 (94%)	189 (98%)	3 (2%)	55	69
12	g	193/205 (94%)	191 (99%)	2 (1%)	68	76
13	H	162/190 (85%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	h	164/190 (86%)	164 (100%)	0	100	100
14	I	191/210 (91%)	190 (100%)	1 (0%)	81	82
14	i	193/210 (92%)	191 (99%)	2 (1%)	68	76
15	J	152/207 (73%)	149 (98%)	3 (2%)	48	66
15	j	152/207 (73%)	151 (99%)	1 (1%)	76	79
16	K	187/196 (95%)	186 (100%)	1 (0%)	81	82
16	k	186/196 (95%)	186 (100%)	0	100	100
17	L	198/204 (97%)	198 (100%)	0	100	100
17	l	198/204 (97%)	198 (100%)	0	100	100
18	M	192/202 (95%)	191 (100%)	1 (0%)	81	82
18	m	192/202 (95%)	192 (100%)	0	100	100
19	N	148/148 (100%)	148 (100%)	0	100	100
19	n	148/148 (100%)	148 (100%)	0	100	100
20	O	177/181 (98%)	176 (99%)	1 (1%)	78	81
20	o	177/181 (98%)	177 (100%)	0	100	100
21	P	172/173 (99%)	172 (100%)	0	100	100
21	p	172/173 (99%)	172 (100%)	0	100	100
22	Q	164/170 (96%)	164 (100%)	0	100	100
22	q	164/170 (96%)	160 (98%)	4 (2%)	43	63
23	R	153/156 (98%)	152 (99%)	1 (1%)	76	79
23	r	153/156 (98%)	152 (99%)	1 (1%)	76	79
24	S	174/178 (98%)	174 (100%)	0	100	100
24	s	174/178 (98%)	174 (100%)	0	100	100
25	T	175/178 (98%)	175 (100%)	0	100	100
25	t	175/178 (98%)	175 (100%)	0	100	100
26	A	286/343 (83%)	284 (99%)	2 (1%)	76	79
27	B	300/345 (87%)	298 (99%)	2 (1%)	76	79
28	C	315/340 (93%)	312 (99%)	3 (1%)	68	76
29	D	333/333 (100%)	329 (99%)	4 (1%)	63	74
30	E	298/329 (91%)	297 (100%)	1 (0%)	86	84
31	F	296/340 (87%)	294 (99%)	2 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	f	580/763 (76%)	564 (97%)	16 (3%)	38	59
All	All	10607/11562 (92%)	10528 (99%)	79 (1%)	73	79

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	D	306	LYS
32	f	391	LEU
29	D	411	GLU
32	f	207	LEU
32	f	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
25	t	81	HIS
27	B	195	GLN
30	E	86	GLN
11	e	63	HIS
10	d	228	GLN

5.3.3 RNA [i](#)

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
34	AGS	B	501	-	32,33,33	0.84	2 (6%)	45,52,52	1.06	1 (2%)
34	AGS	D	501	-	32,33,33	0.60	1 (3%)	45,52,52	0.83	1 (2%)
34	AGS	A	501	-	32,33,33	0.72	1 (3%)	45,52,52	0.78	1 (2%)
34	AGS	F	501	-	32,33,33	0.54	0	45,52,52	0.76	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	AGS	B	501	-	-	4/21/38/38	0/3/3/3
34	AGS	D	501	-	-	2/21/38/38	0/3/3/3
34	AGS	A	501	-	-	8/21/38/38	0/3/3/3
34	AGS	F	501	-	-	5/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PA-O3A	-2.26	1.57	1.59
34	B	501	AGS	PB-O3A	-2.15	1.57	1.59
34	A	501	AGS	PA-O3A	-2.09	1.57	1.59
34	D	501	AGS	PG-S1G	2.06	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	AGS	PB-O3B-PG	-5.16	114.27	133.17
34	A	501	AGS	PB-O3B-PG	-4.41	117.01	133.17
34	D	501	AGS	PB-O3B-PG	-4.22	117.73	133.17
34	F	501	AGS	PB-O3B-PG	-2.87	122.65	133.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O2A
34	A	501	AGS	C5'-O5'-PA-O3A
34	B	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O1A

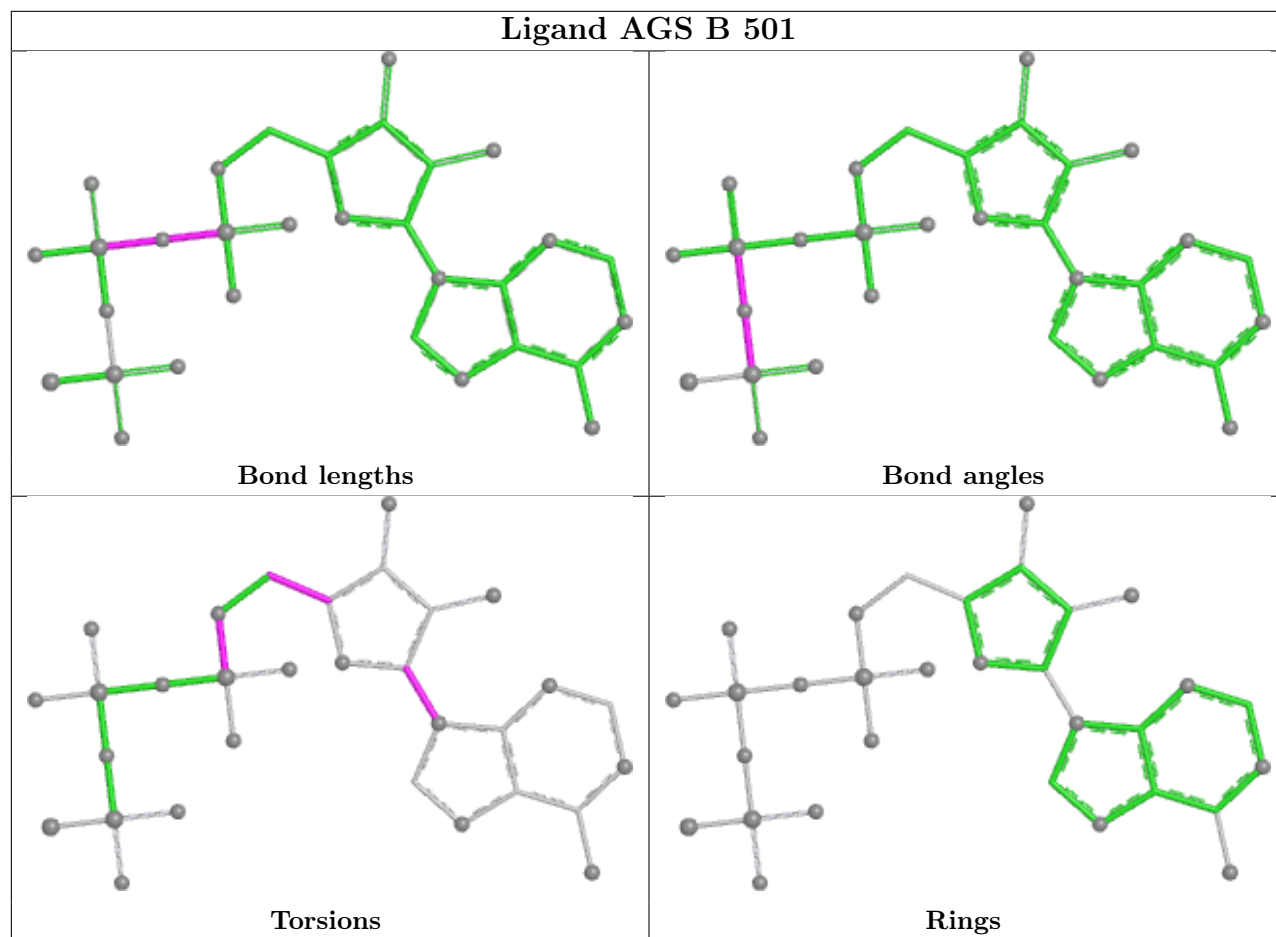
There are no ring outliers.

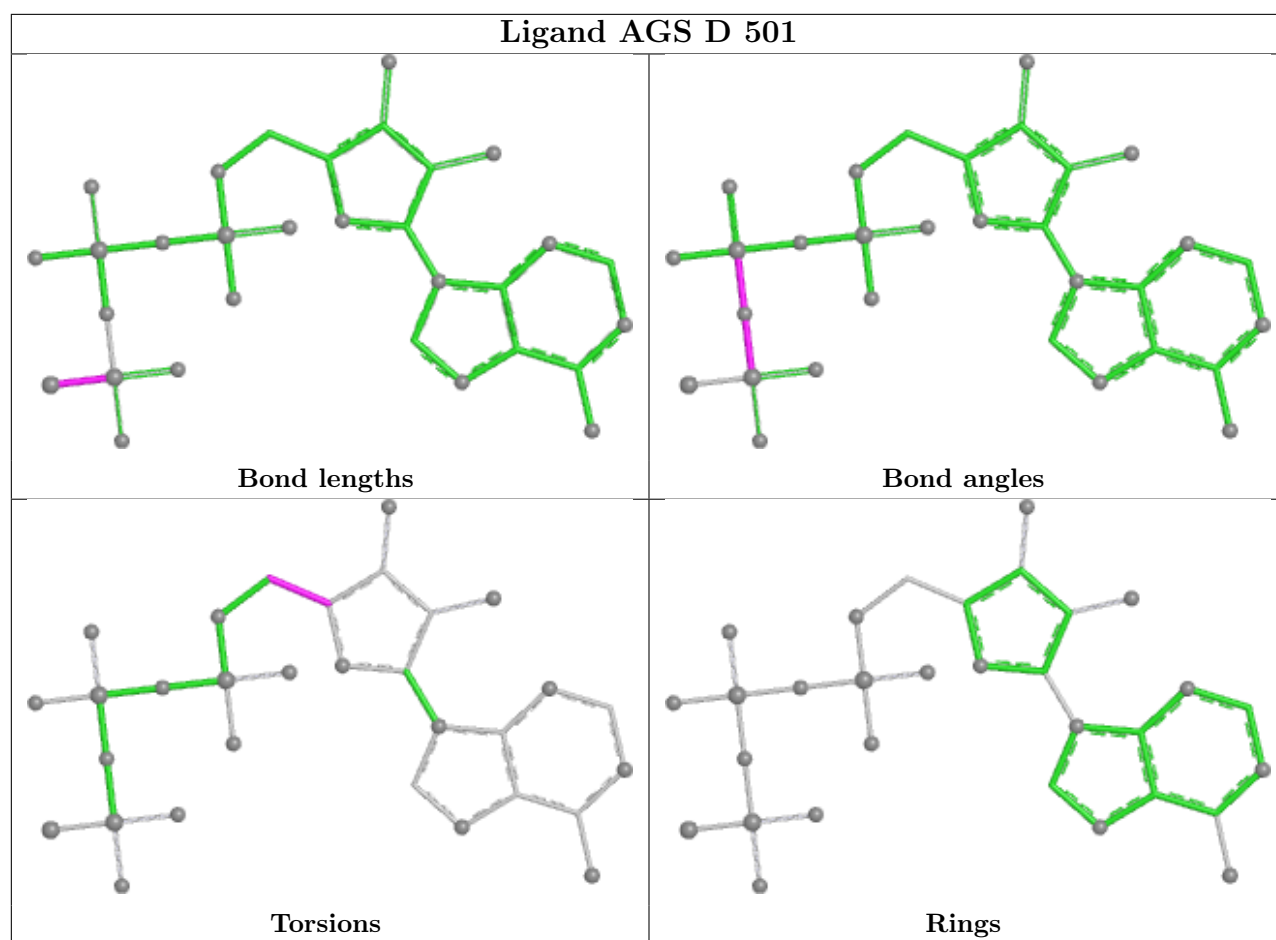
4 monomers are involved in 23 short contacts:

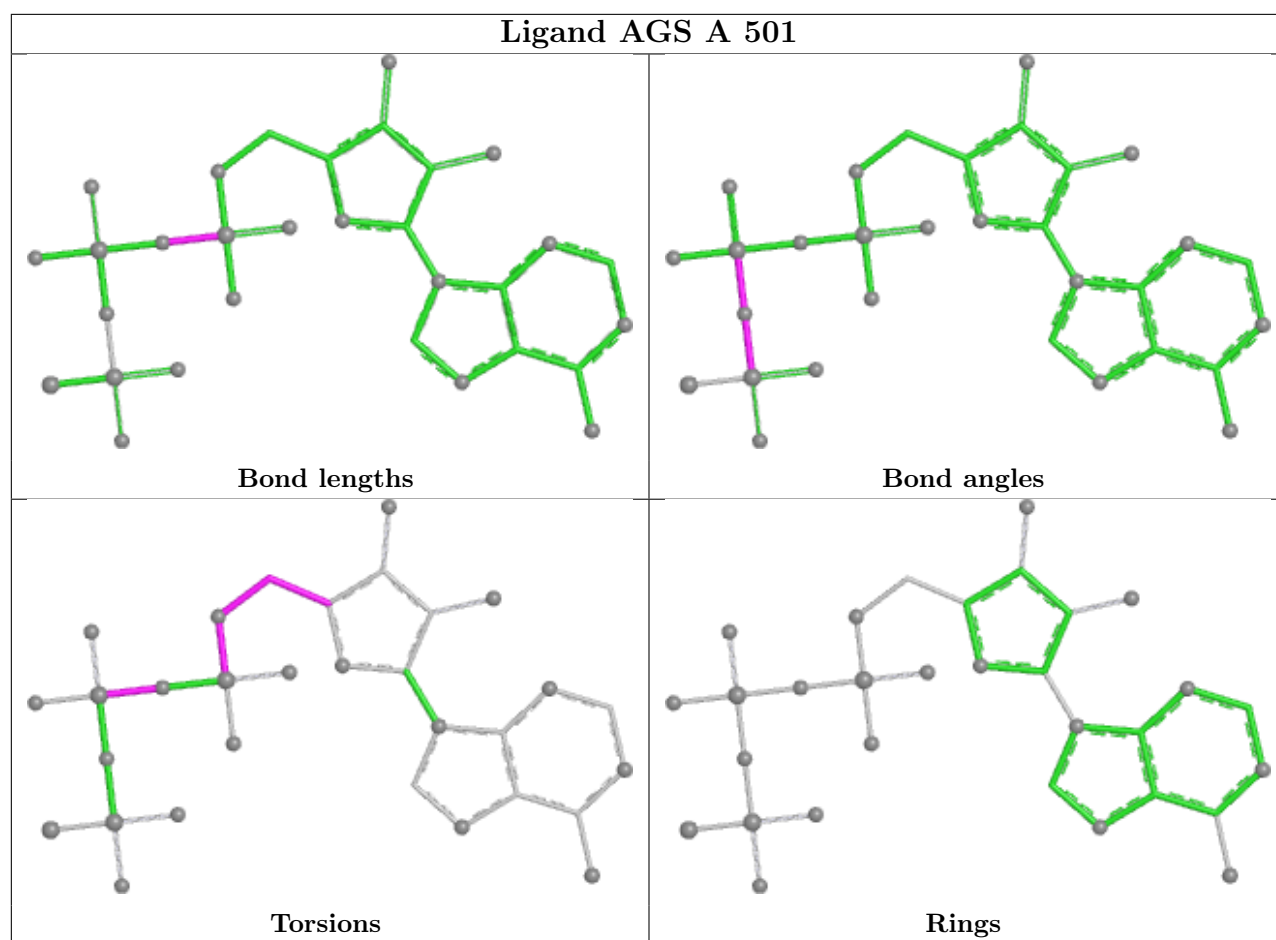
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	501	AGS	4	0
34	D	501	AGS	7	0
34	A	501	AGS	3	0
34	F	501	AGS	9	0

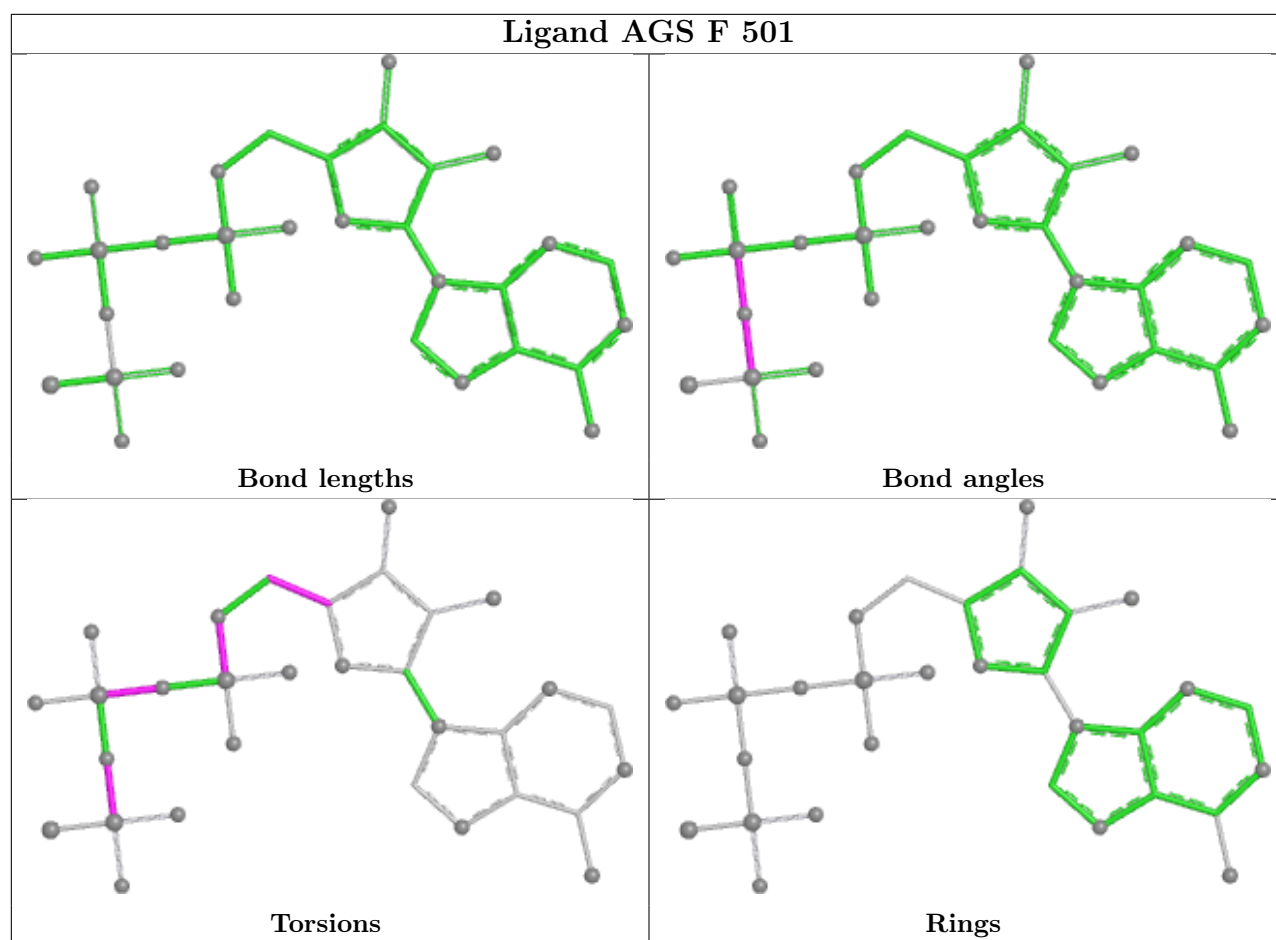
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS B 501









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.

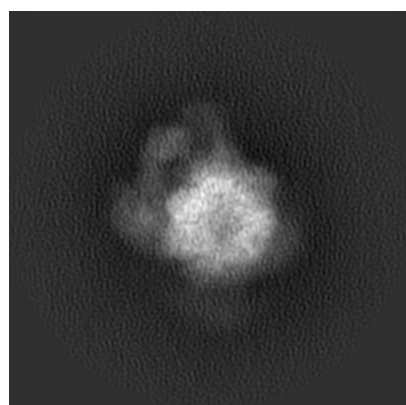
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8665. These allow visual inspection of the internal detail of the map and identification of artifacts.

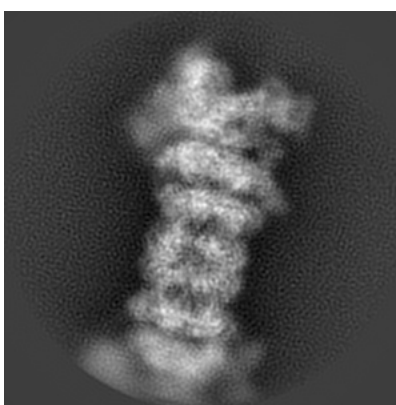
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

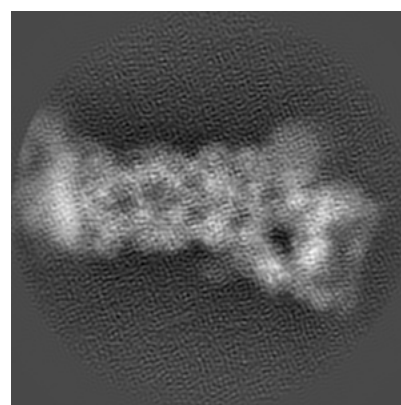
6.1.1 Primary map



X



Y

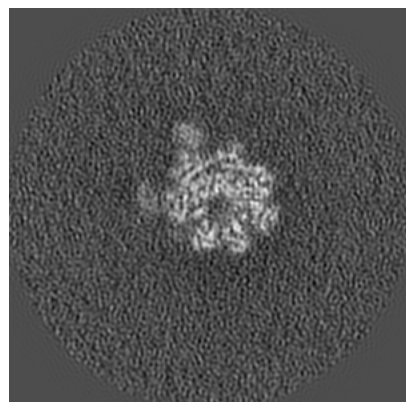


Z

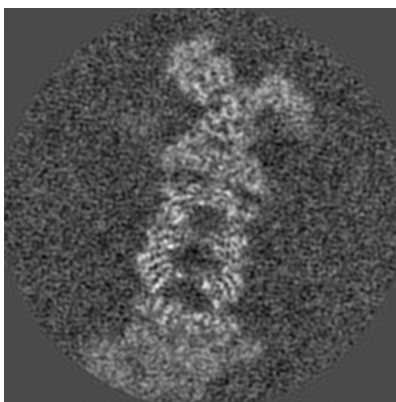
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

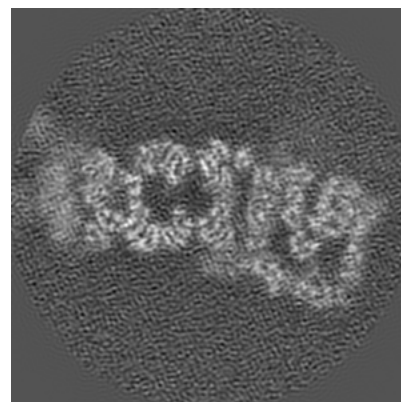
6.2.1 Primary map



X Index: 280



Y Index: 280

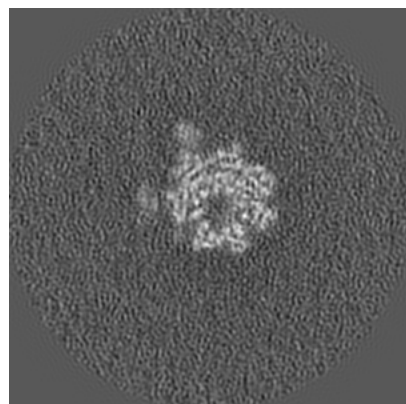


Z Index: 280

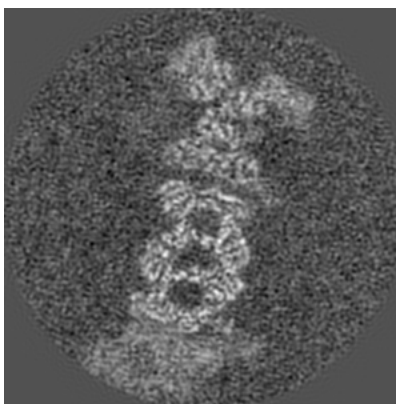
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

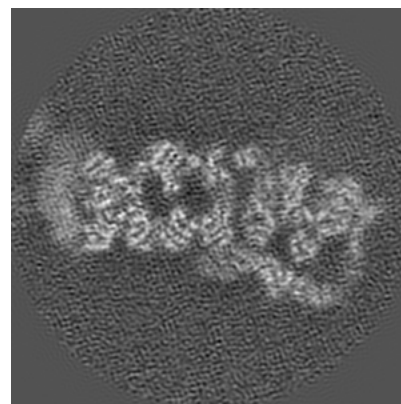
6.3.1 Primary map



X Index: 278



Y Index: 273

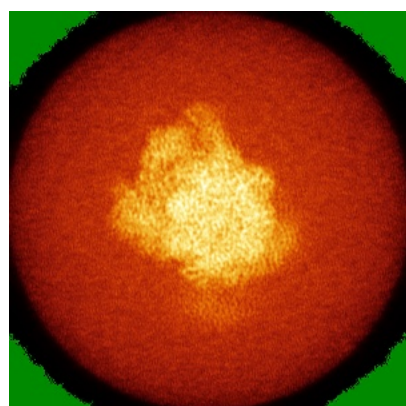


Z Index: 286

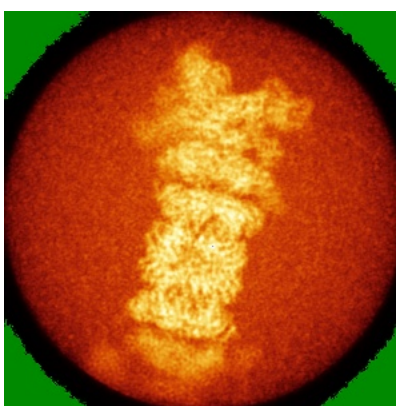
The images above show the largest variance slices of the map in three orthogonal directions.

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

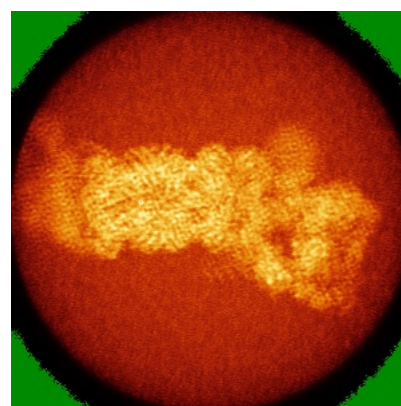
6.4.1 Primary map



X



Y

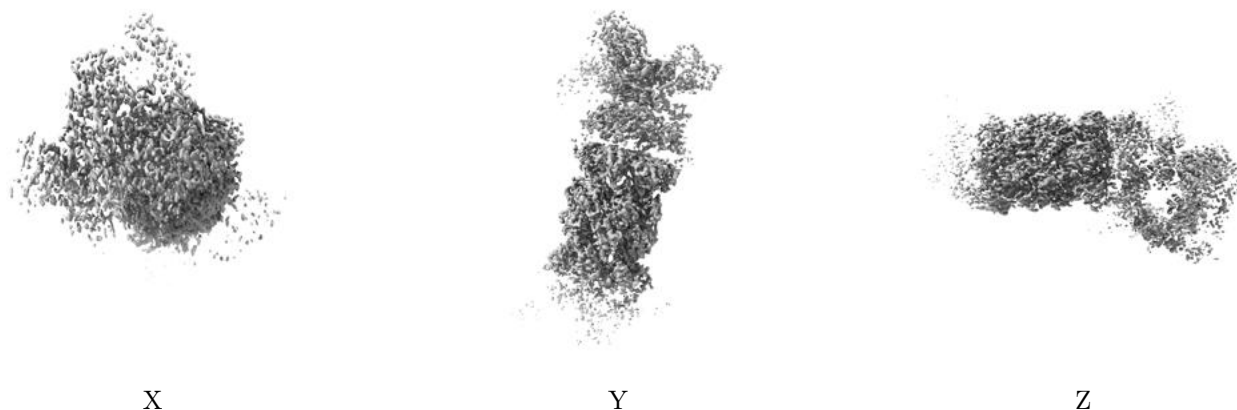


Z

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

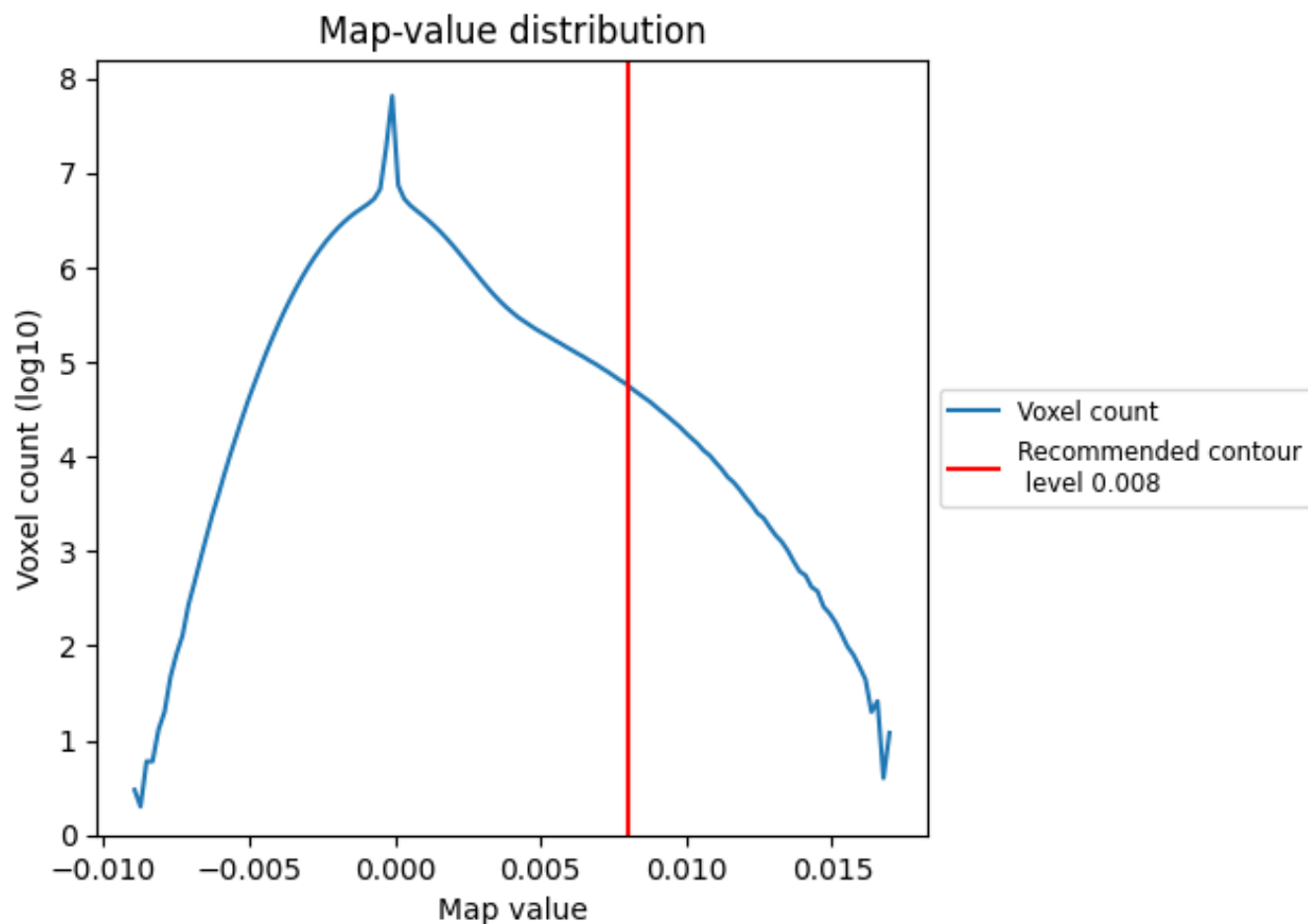
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

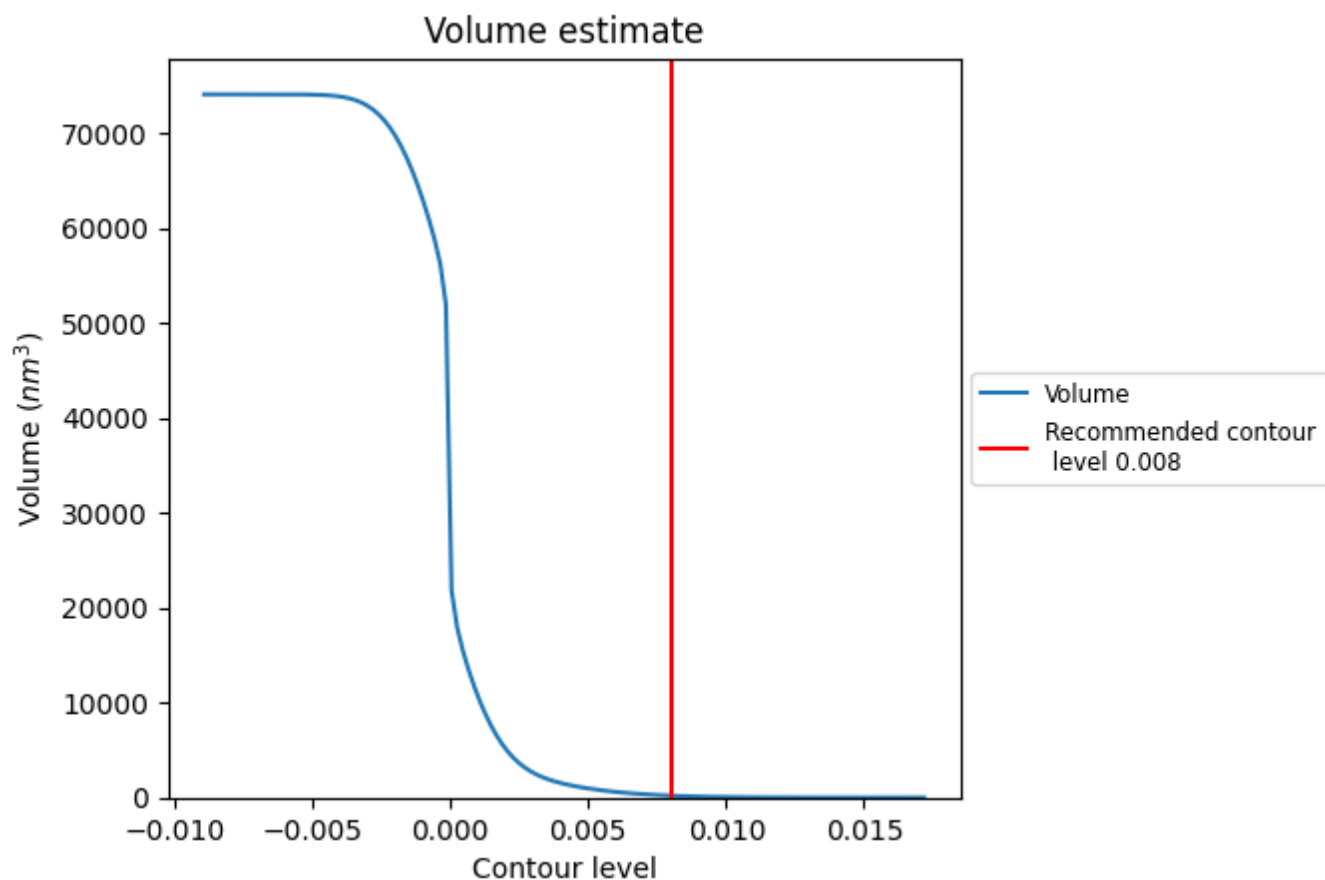
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

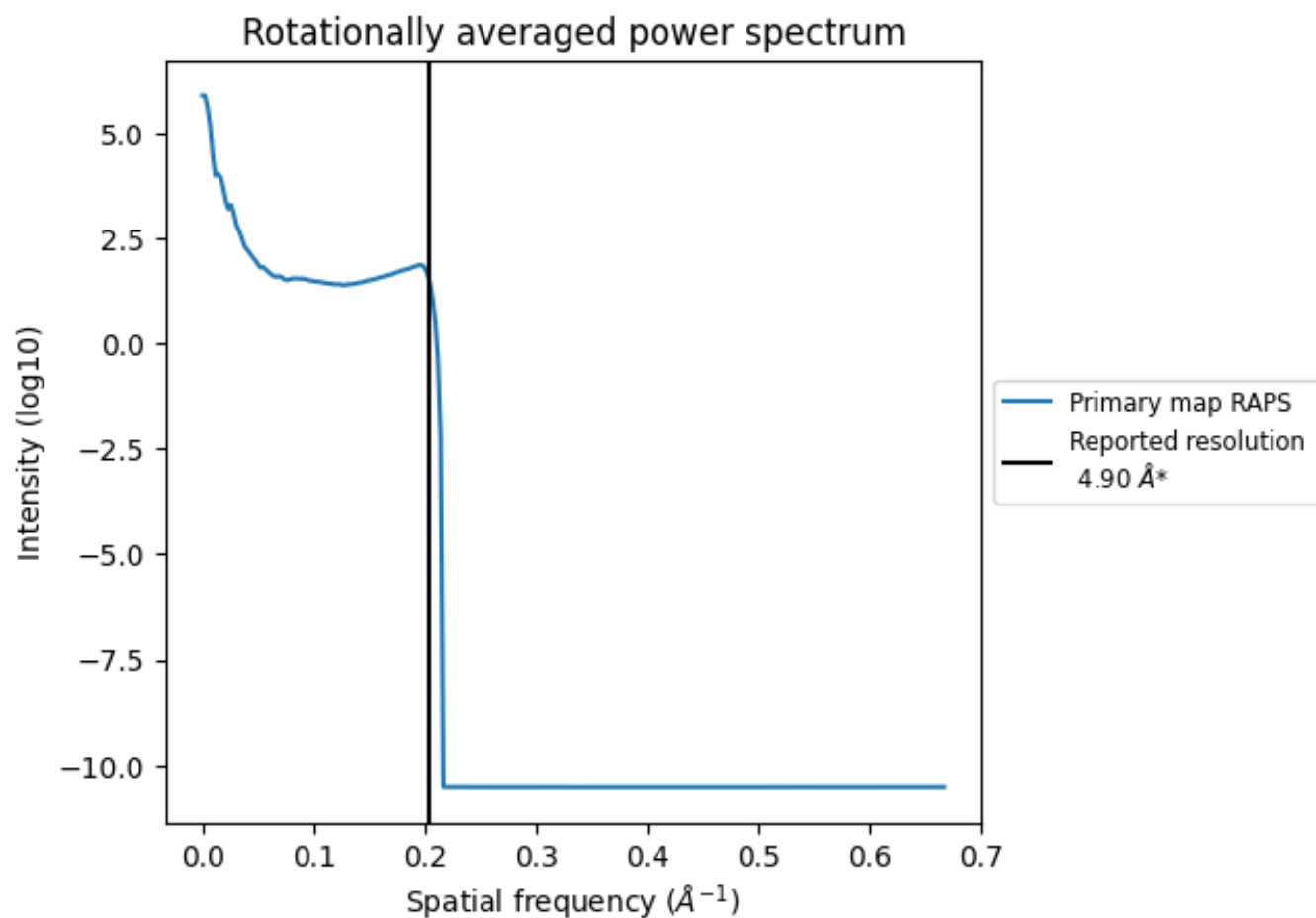
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.204 $\text{\AA}^{-1}$

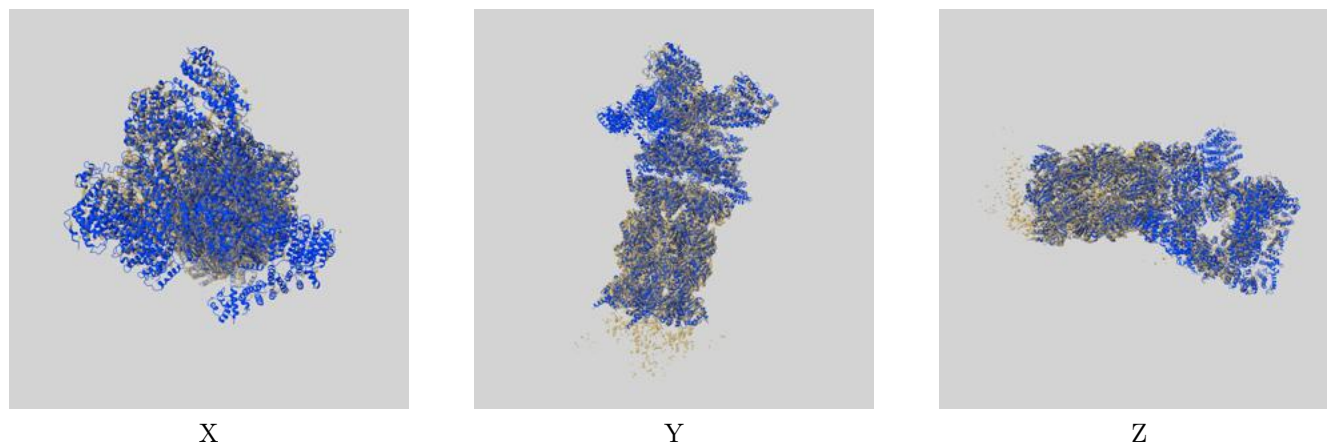
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

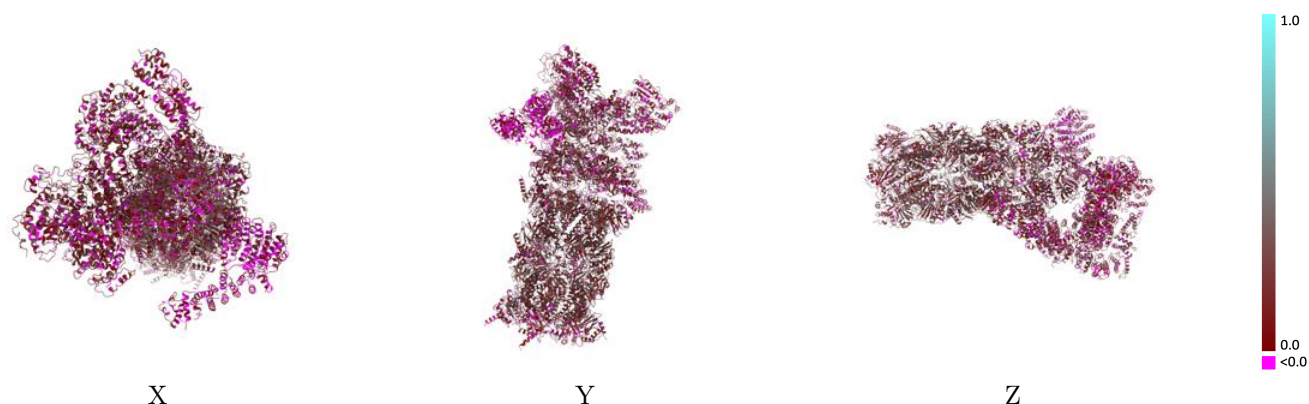
This section contains information regarding the fit between EMDB map EMD-8665 and PDB model 5VFR. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



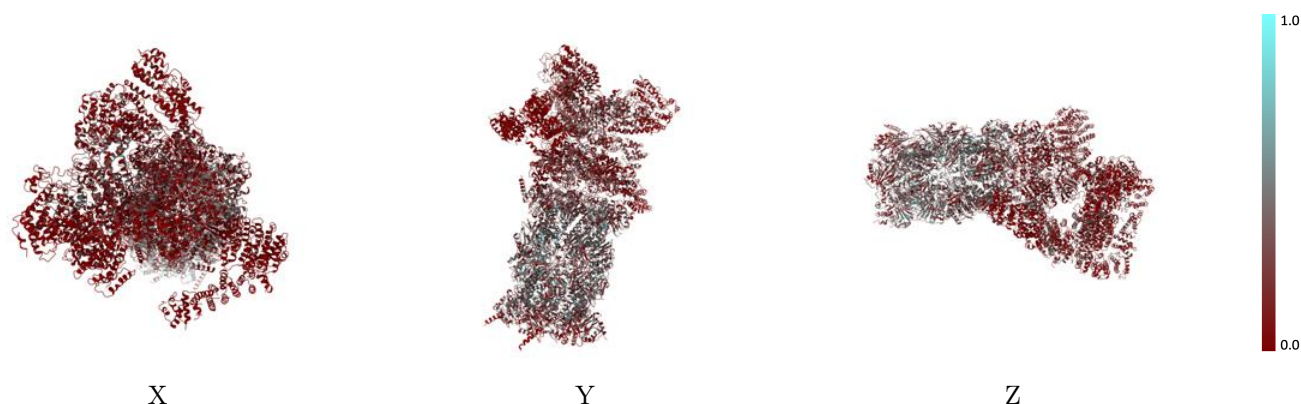
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



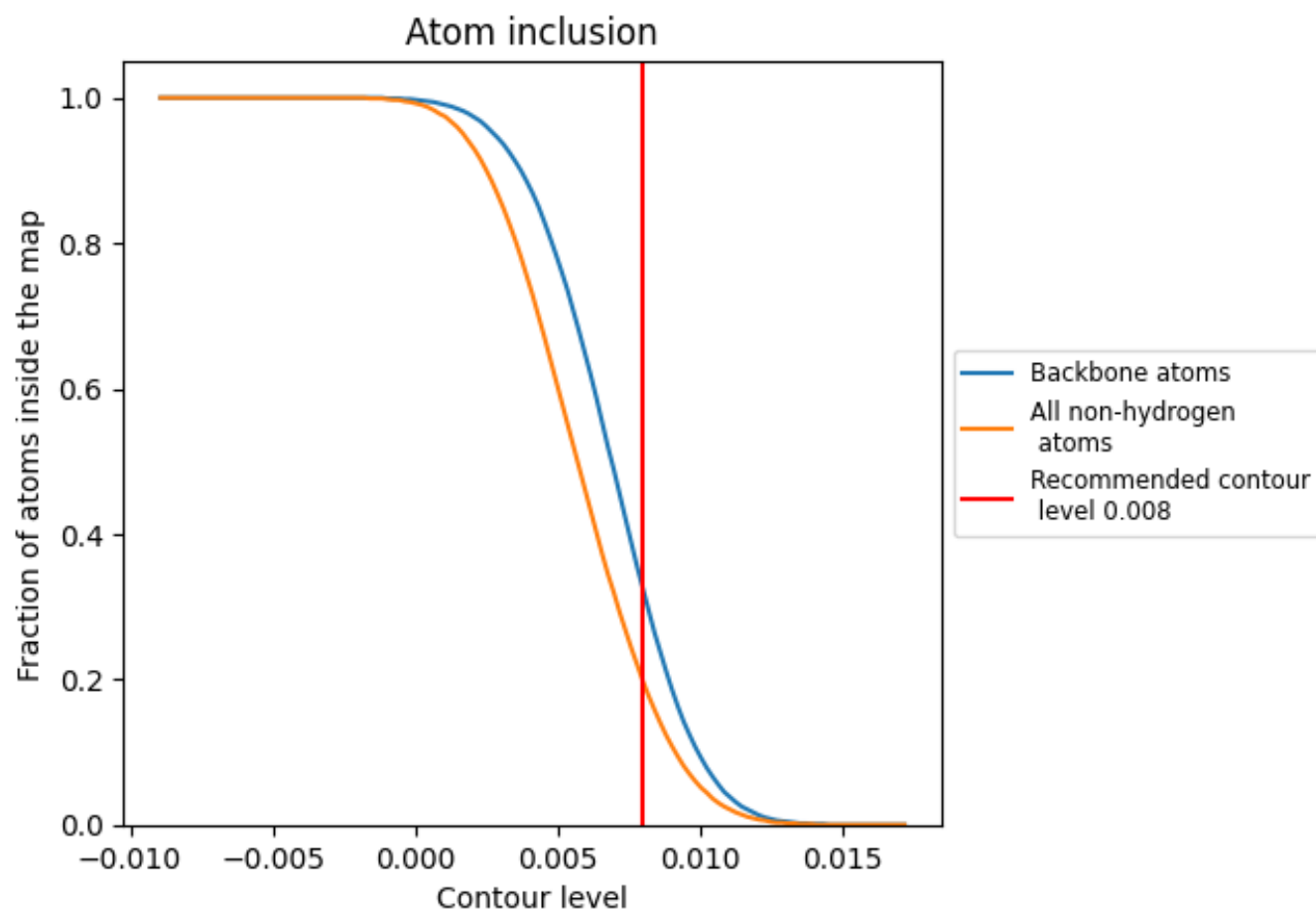
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 20% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1970	 0.1860
A	 0.1520	 0.1910
B	 0.1050	 0.1900
C	 0.1190	 0.1960
D	 0.1460	 0.1980
E	 0.1200	 0.2070
F	 0.1280	 0.2010
G	 0.2490	 0.2070
H	 0.2100	 0.2030
I	 0.2340	 0.2090
J	 0.2470	 0.2200
K	 0.3090	 0.2120
L	 0.3360	 0.2280
M	 0.2830	 0.2150
N	 0.3350	 0.2540
O	 0.2910	 0.2390
P	 0.3380	 0.2470
Q	 0.3400	 0.2390
R	 0.4270	 0.2710
S	 0.3460	 0.2450
T	 0.3900	 0.2640
U	 0.1060	 0.1580
V	 0.0700	 0.1380
W	 0.0870	 0.1360
X	 0.0740	 0.1310
Y	 0.1580	 0.1480
Z	 0.1580	 0.1450
a	 0.0980	 0.1480
b	 0.0490	 0.0980
c	 0.1770	 0.1640
d	 0.0480	 0.1520
e	 0.0700	 0.1860
f	 0.0040	 0.0220
g	 0.2400	 0.2120
h	 0.2190	 0.2030



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Chain	Atom inclusion	Q-score
i	 0.1970	 0.1760
j	 0.2430	 0.1990
k	 0.2920	 0.2100
l	 0.3080	 0.2060
m	 0.2660	 0.2030
n	 0.3570	 0.2410
o	 0.3190	 0.2460
p	 0.3480	 0.2360
q	 0.3720	 0.2570
r	 0.3810	 0.2470
s	 0.3510	 0.2470
t	 0.3820	 0.2450