



## Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 12:03 PM EDT

PDB ID : 5T0J  
EMDB ID : EMD-8337  
Title : Structural basis for dynamic regulation of the human 26S proteasome  
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;  
Kirschner, M.W.; Mao, Y.  
Deposited on : 2016-08-16  
Resolution : 8.00 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>.

---

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

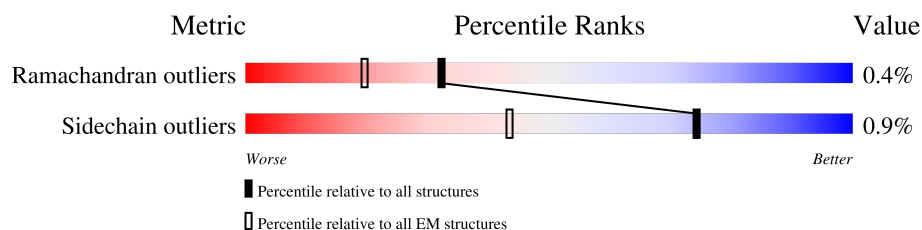
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 8.00 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	207382	16835
Sidechain outliers	206894	16415

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	f	749	<div> <div>61%</div> <div>91%</div> <div>7%</div> </div>
2	G	245	<div> <div>31%</div> <div>96%</div> <div>2%</div> </div>
3	H	233	<div> <div>38%</div> <div>98%</div> <div>2%</div> </div>
4	I	260	<div> <div>37%</div> <div>95%</div> <div>2%</div> </div>
5	J	247	<div> <div>29%</div> <div>95%</div> <div>2%</div> </div>
6	K	240	<div> <div>27%</div> <div>94%</div> <div>5%</div> </div>
7	L	268	<div> <div>25%</div> <div>89%</div> <div>11%</div> </div>
8	M	254	<div> <div>28%</div> <div>94%</div> <div>6%</div> </div>
9	N	238	<div> <div>24%</div> <div>80%</div> <div>20%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	O	276	
11	P	204	
12	Q	201	
13	R	262	
14	S	240	
15	T	263	
16	A	433	
17	B	440	
18	D	418	
19	E	403	
20	F	439	
21	C	398	
22	U	953	
23	V	533	
24	W	456	
25	X	422	
26	Y	389	
27	Z	324	
28	a	376	
29	b	377	
30	c	309	
31	d	349	
32	e	70	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 76674 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

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

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

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

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 9 is a protein called Proteasome subunit beta type-6.

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-3.

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

- Molecule 12 is a protein called Proteasome subunit beta type-2.

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

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

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is a protein called Proteasome subunit beta type-4.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 17 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	348	Total	C	N	O	S	0	0
			2717	1708	460	537	12		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	392	Total	C	N	O	S	0	0
			3078	1932	551	577	18		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

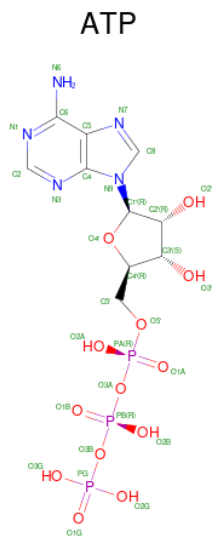
Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 32 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 33 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
33	A	1	Total 31	C 10	N 5	O 13	P 3	0
33	D	1	Total 31	C 10	N 5	O 13	P 3	0
33	E	1	Total 31	C 10	N 5	O 13	P 3	0
33	F	1	Total 31	C 10	N 5	O 13	P 3	0

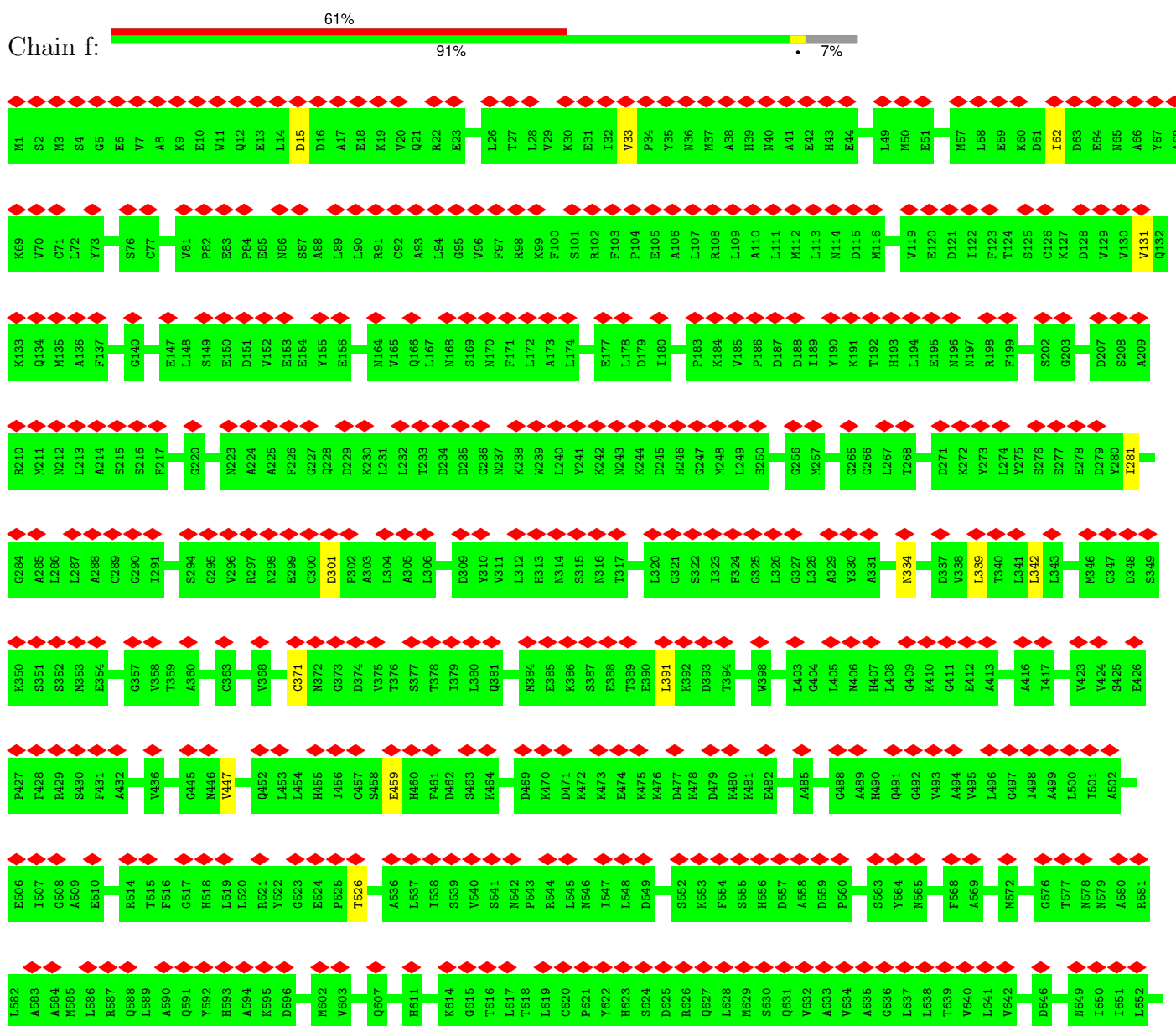
- Molecule 34 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

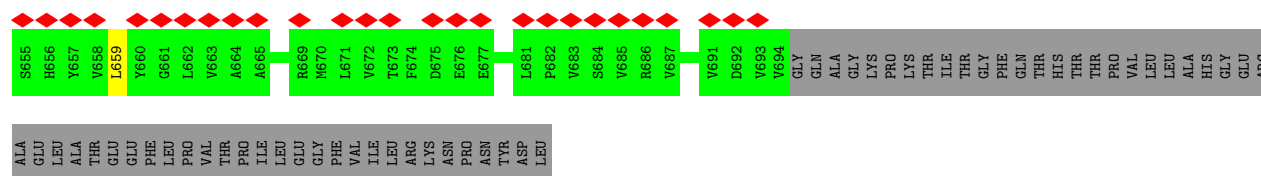
Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0

### 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.

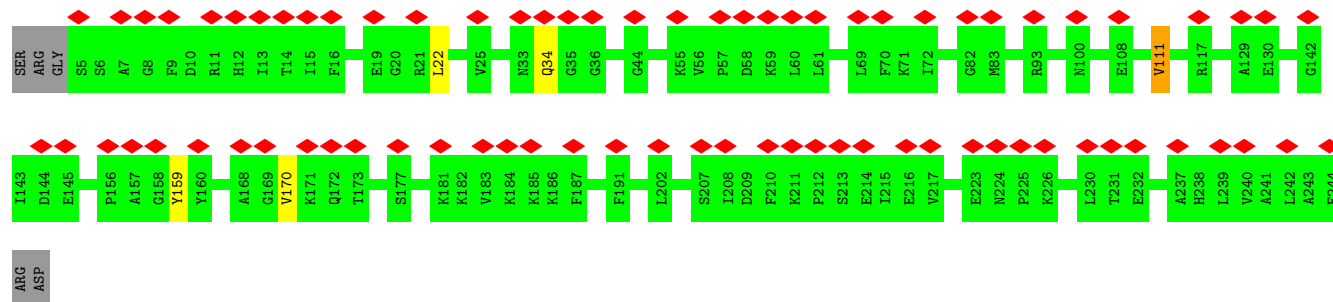
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 2





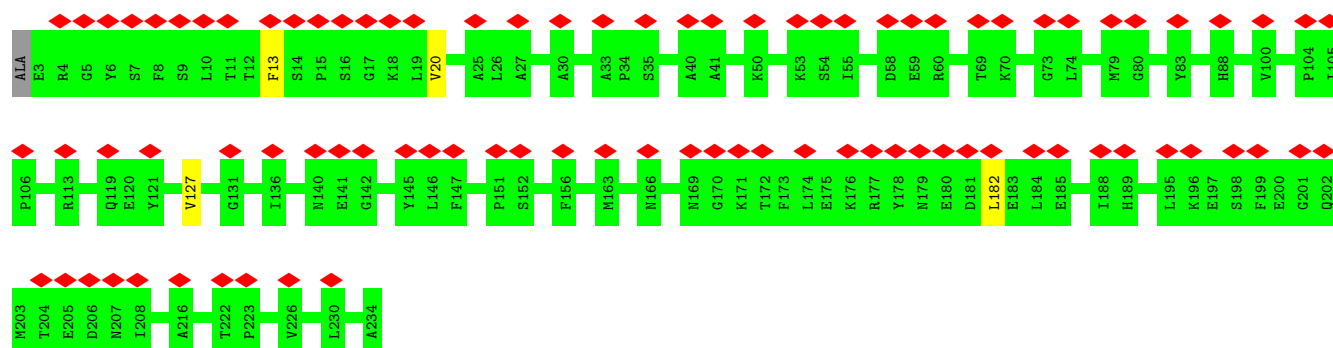
• Molecule 2: Proteasome subunit alpha type-6

Chain G: 31% 96%



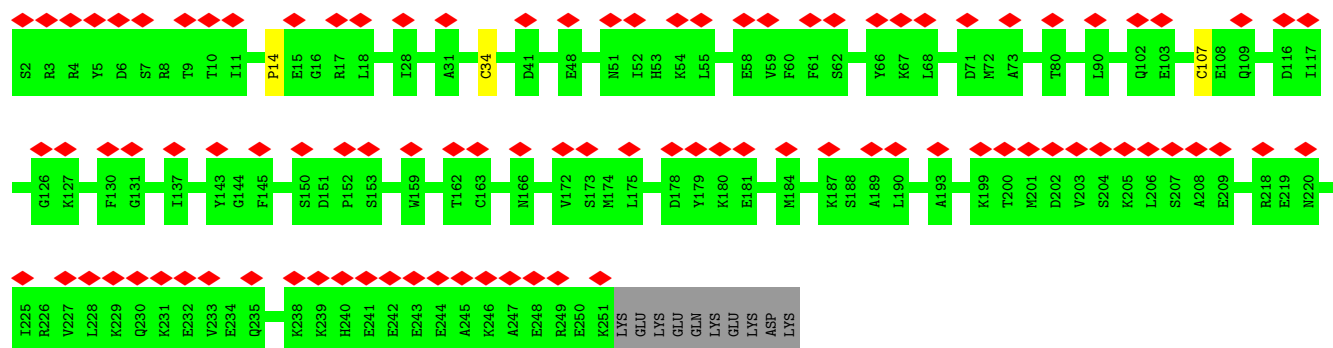
• Molecule 3: Proteasome subunit alpha type-2

Chain H: 38% 98%

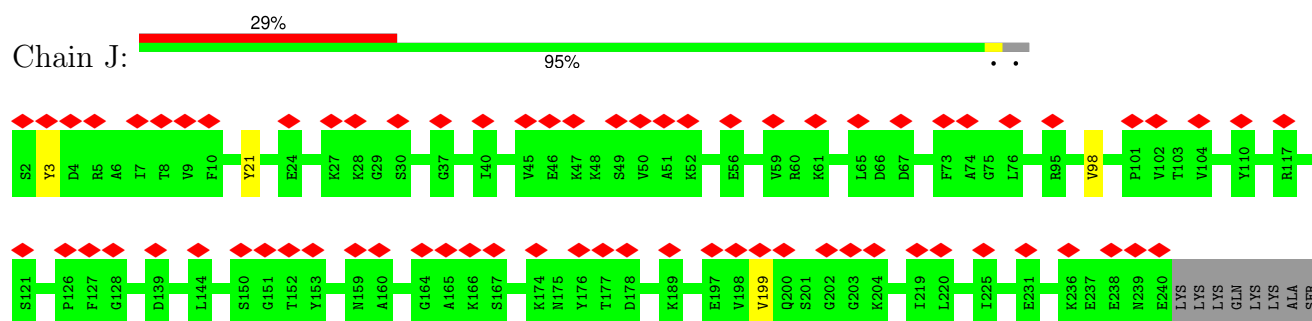


• Molecule 4: Proteasome subunit alpha type-4

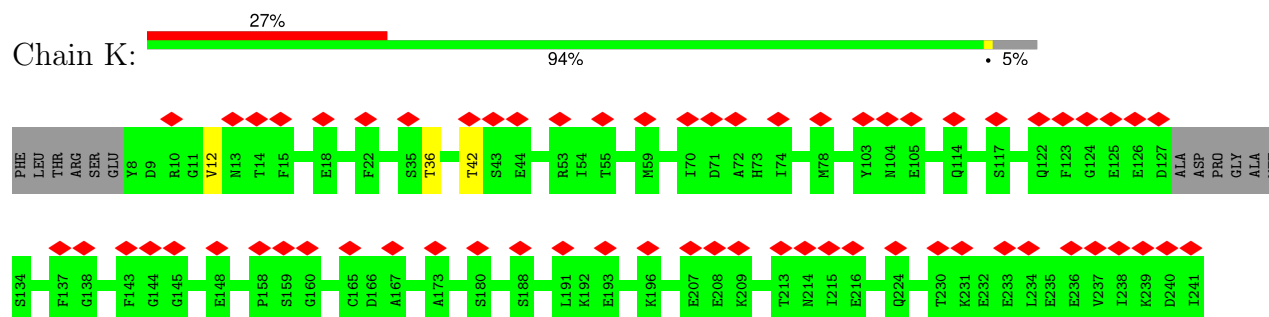
Chain I: 37% 95%



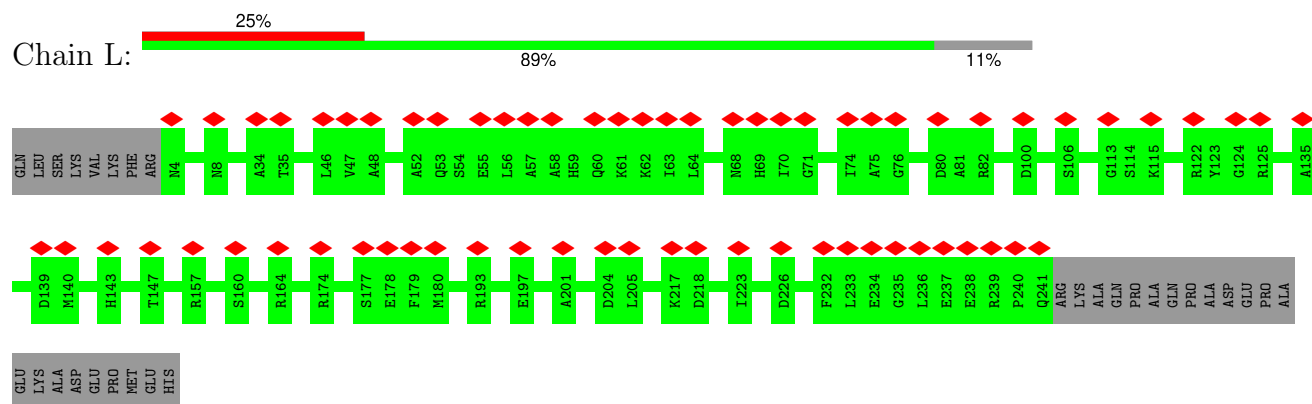
• Molecule 5: Proteasome subunit alpha type-7



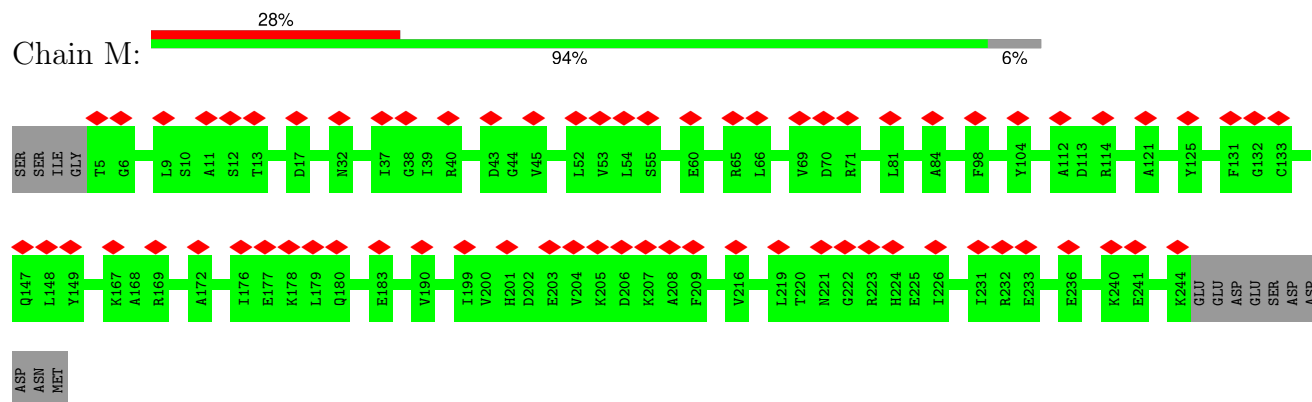
- Molecule 6: Proteasome subunit alpha type-5



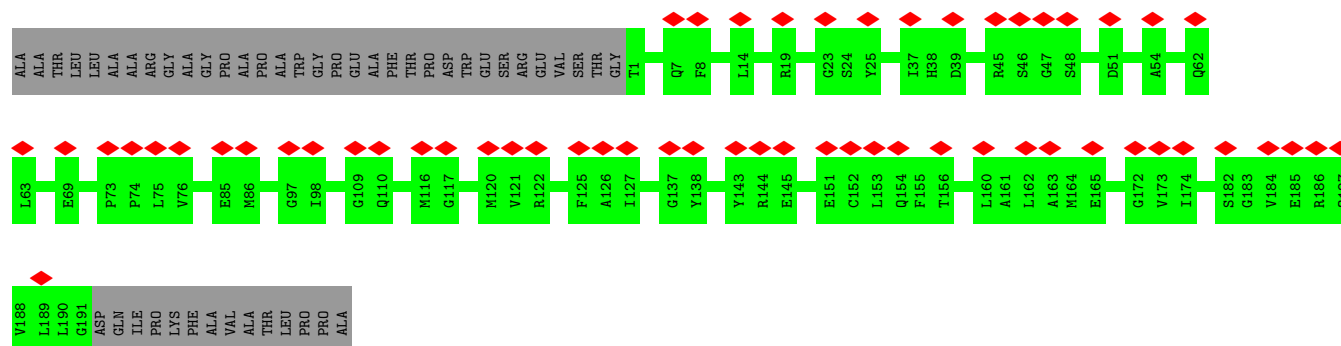
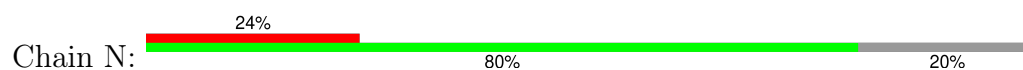
- Molecule 7: Proteasome subunit alpha type-1



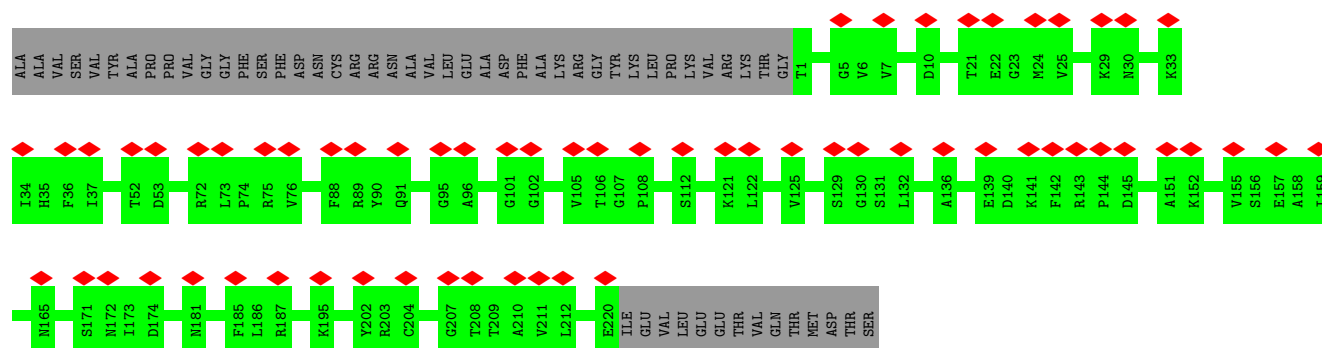
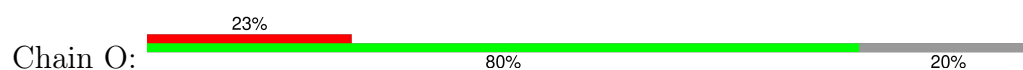
- Molecule 8: Proteasome subunit alpha type-3



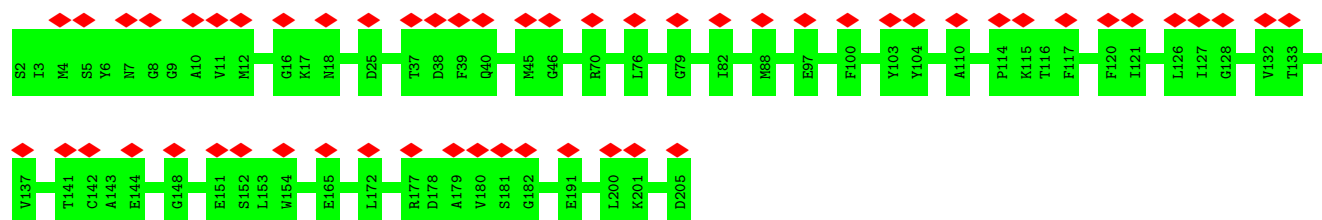
- Molecule 9: Proteasome subunit beta type-6



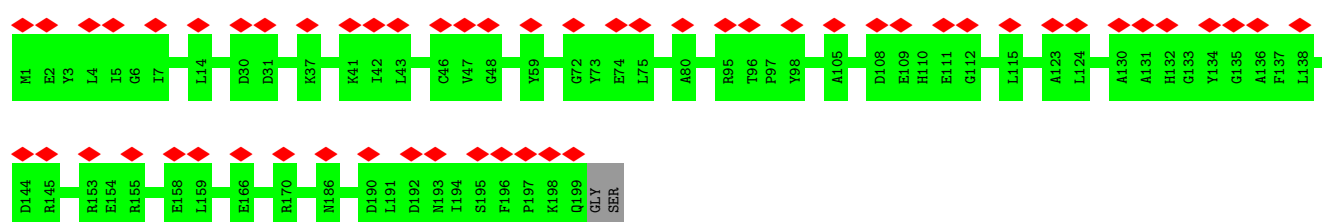
• Molecule 10: Proteasome subunit beta type-7



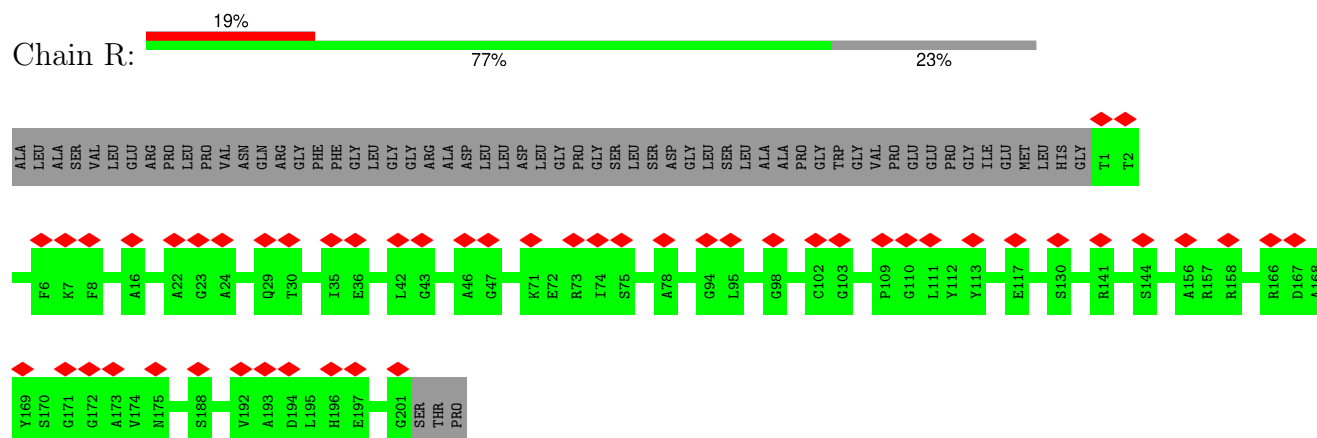
• Molecule 11: Proteasome subunit beta type-3



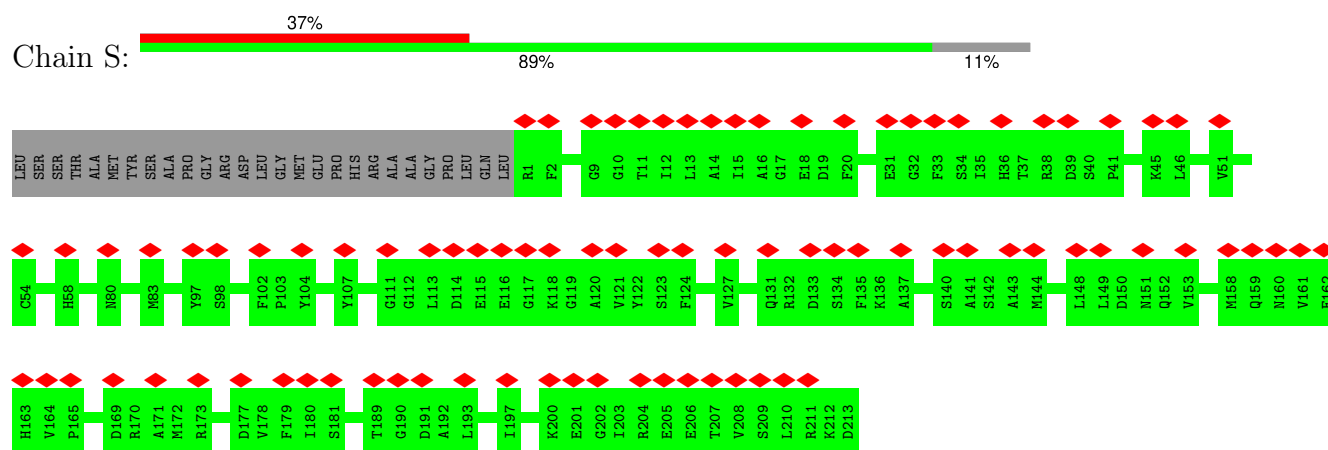
• Molecule 12: Proteasome subunit beta type-2



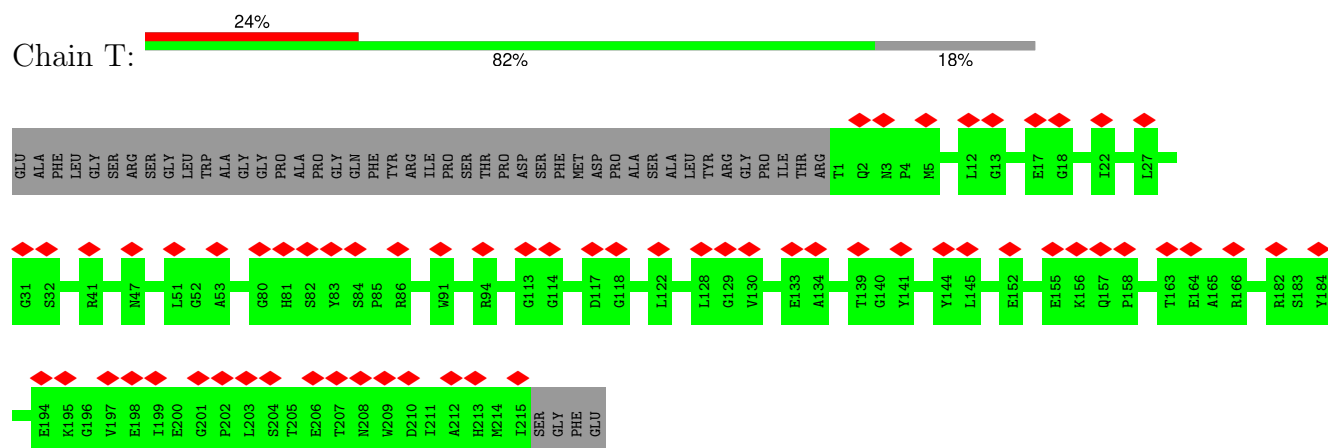
- Molecule 13: Proteasome subunit beta type-5



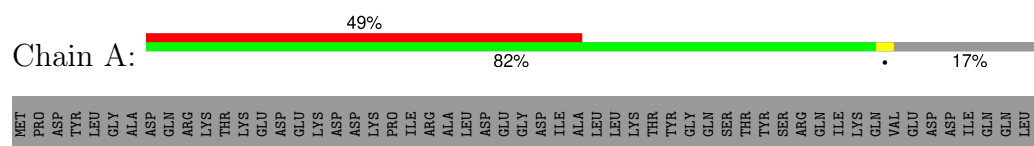
- Molecule 14: Proteasome subunit beta type-1

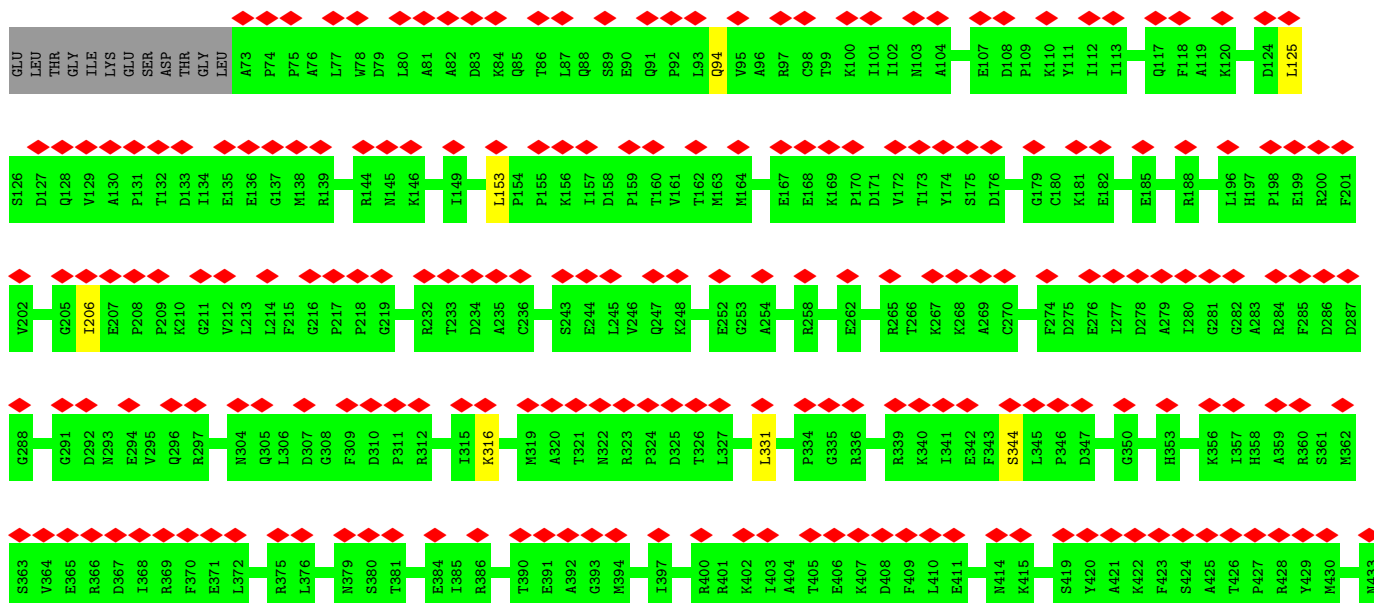


- Molecule 15: Proteasome subunit beta type-4

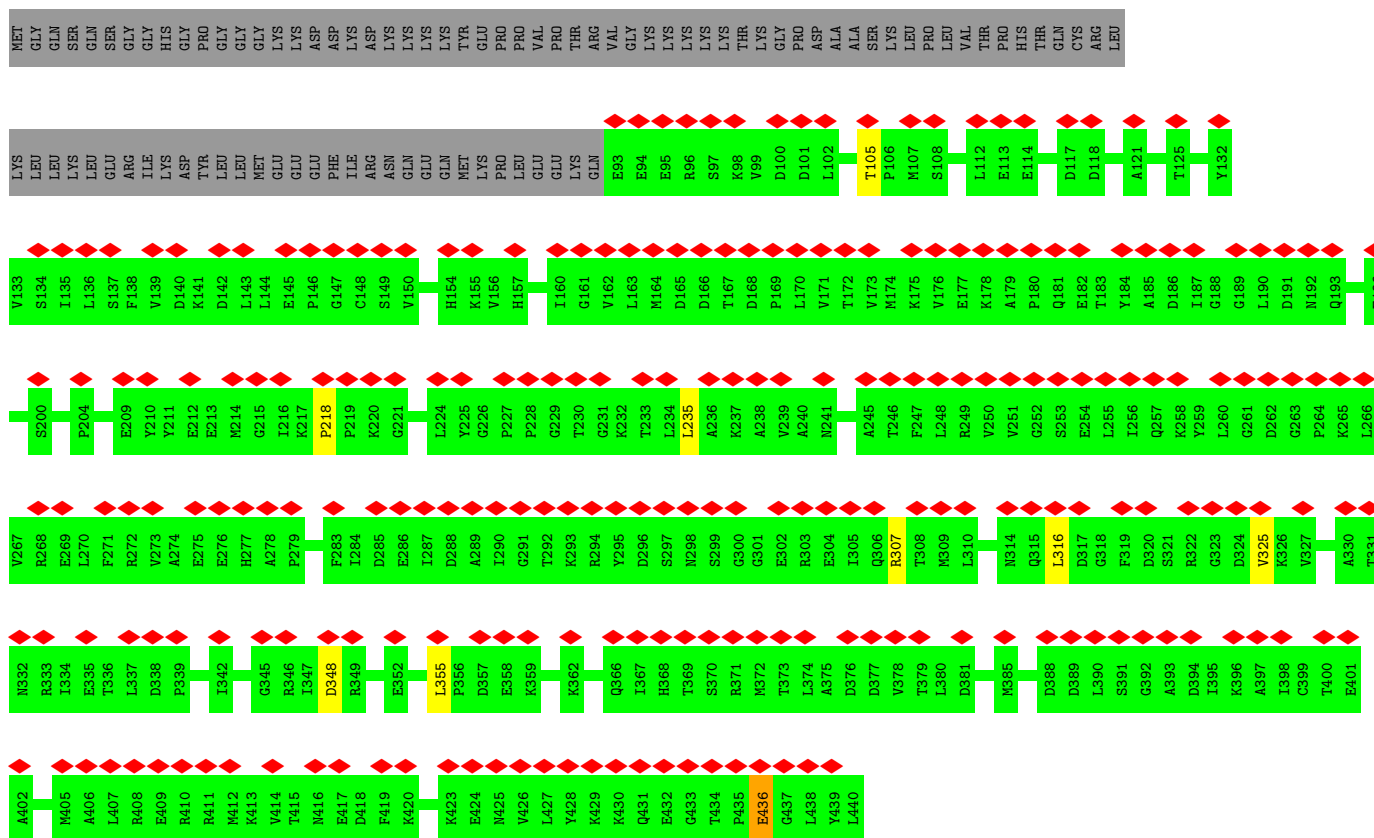
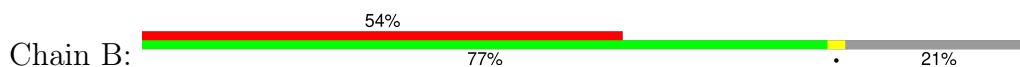


- Molecule 16: 26S protease regulatory subunit 7





• Molecule 17: 26S protease regulatory subunit 4

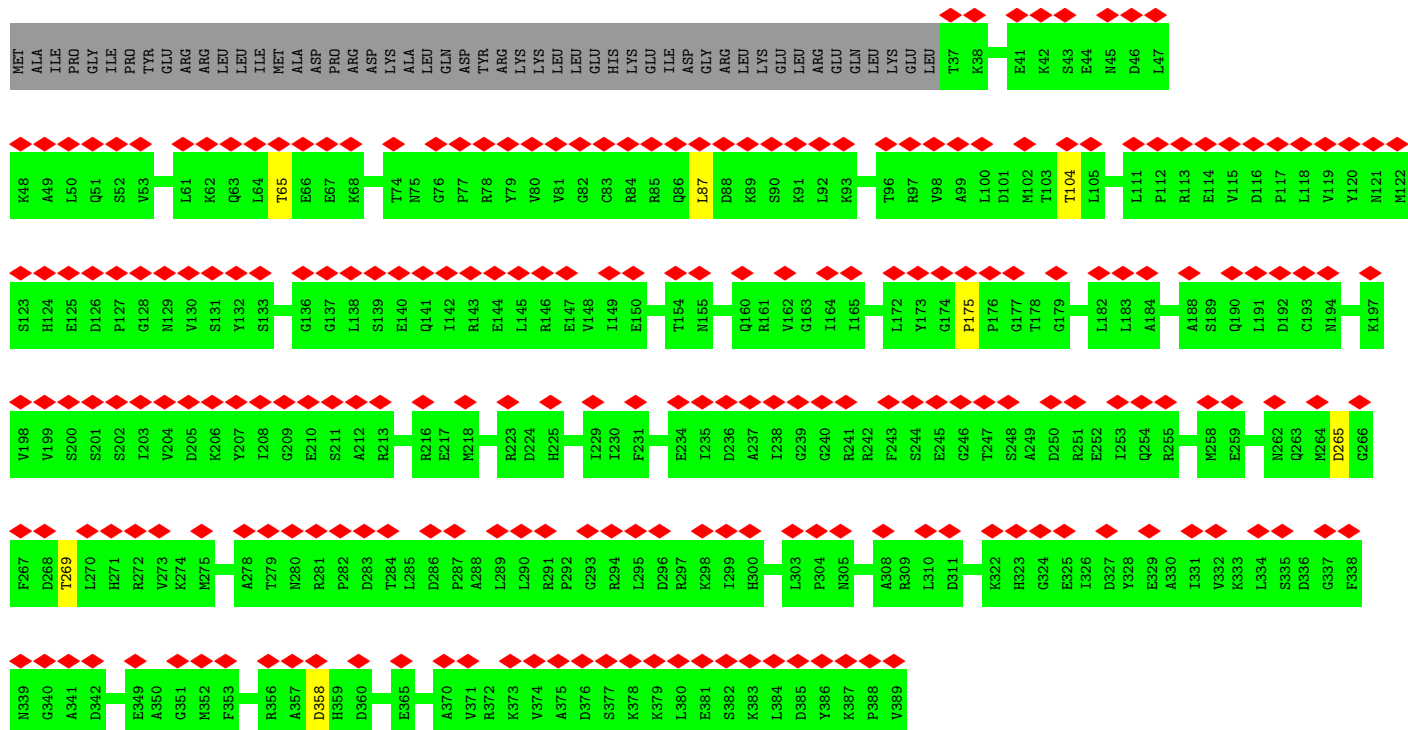
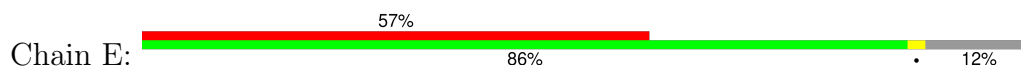


• Molecule 18: 26S protease regulatory subunit 6B



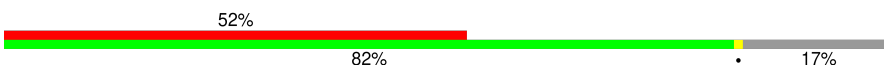


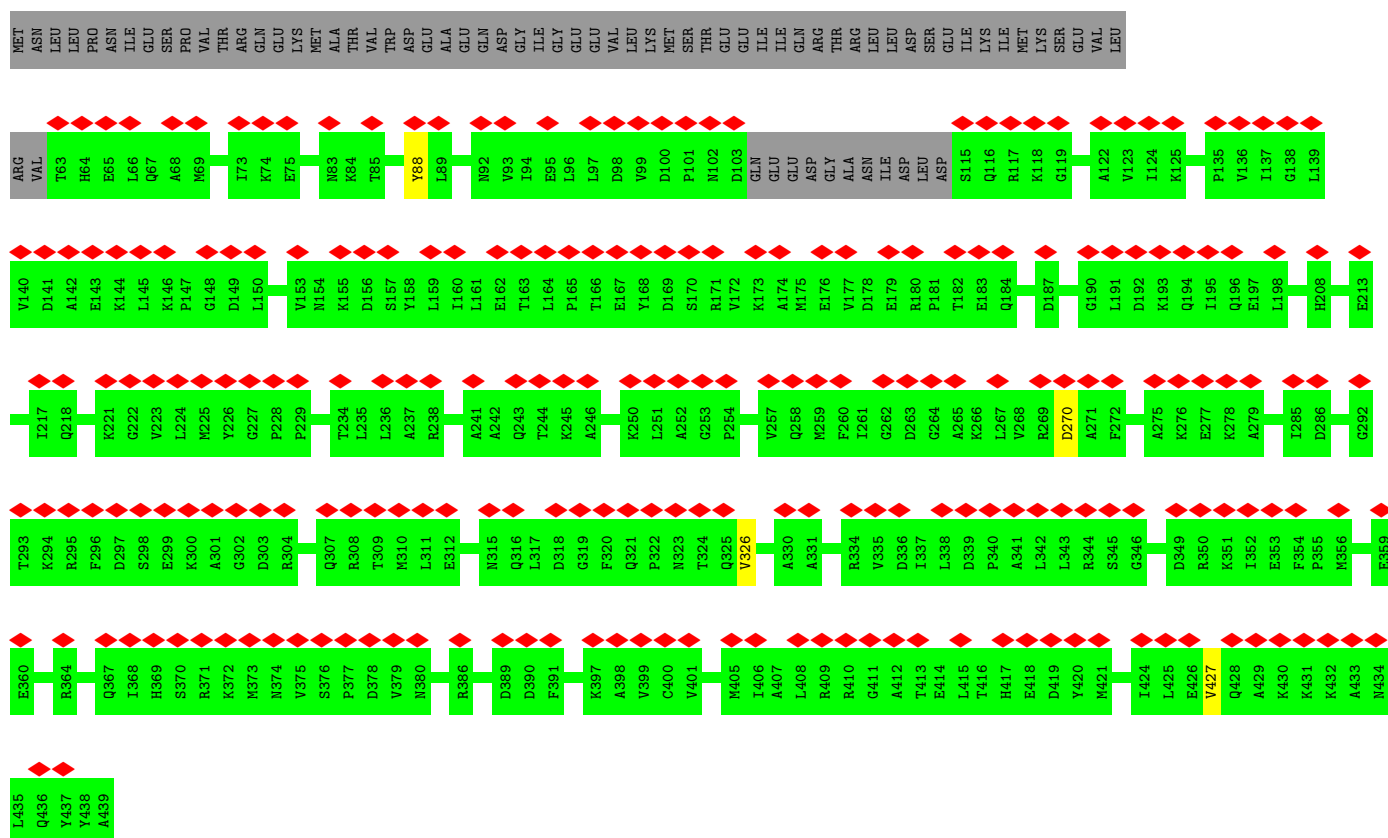
• Molecule 19: 26S protease regulatory subunit 10B



• Molecule 20: 26S protease regulatory subunit 6A

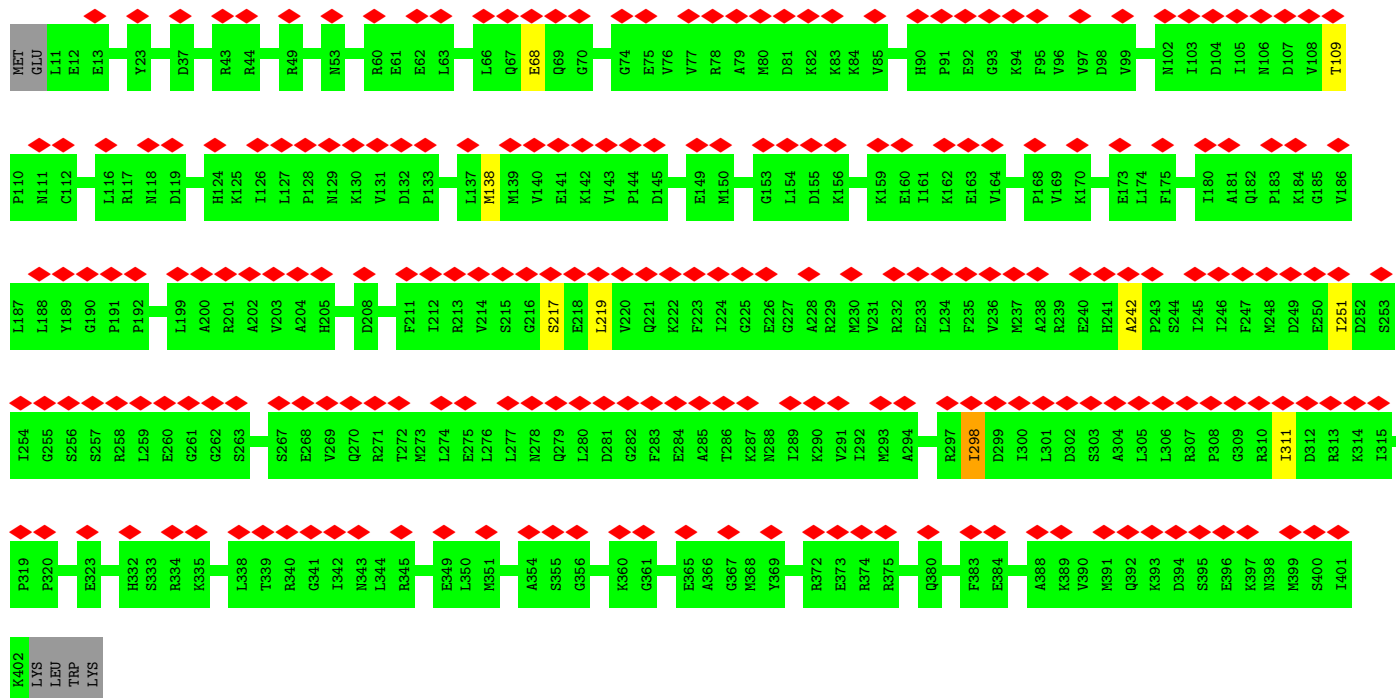


Chain F: 

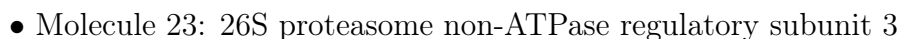


• Molecule 21: 26S protease regulatory subunit 8

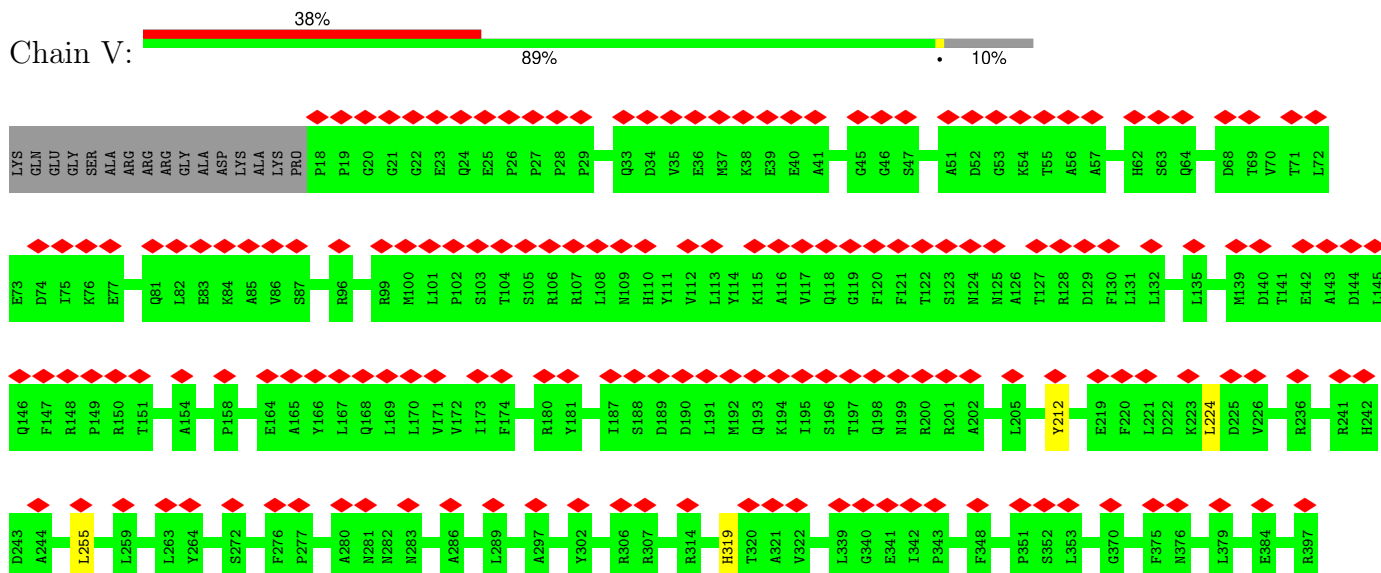
Chain C: 



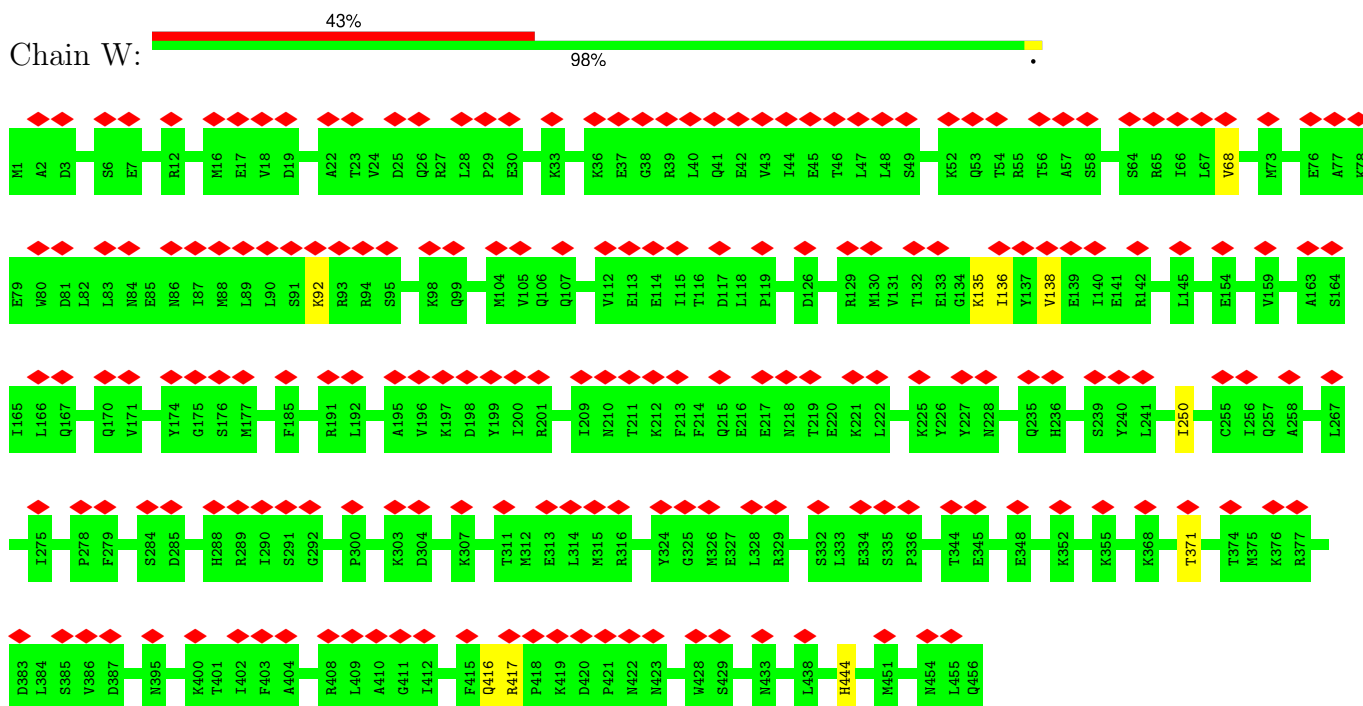
Chain U:



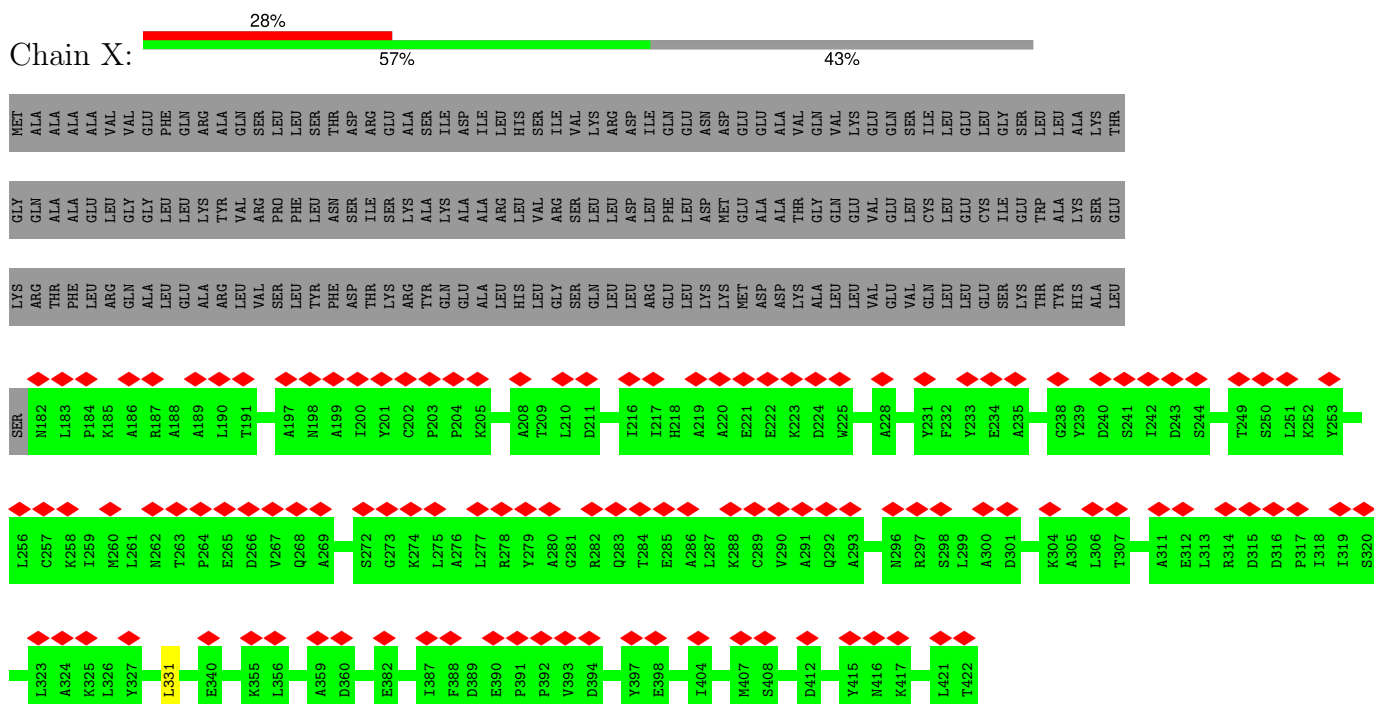
Chain V:



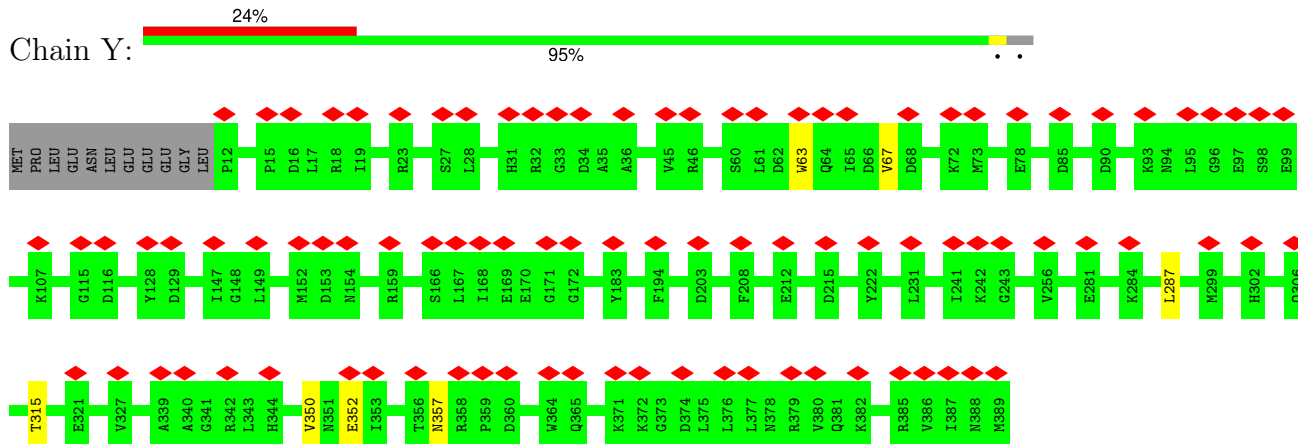
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 12



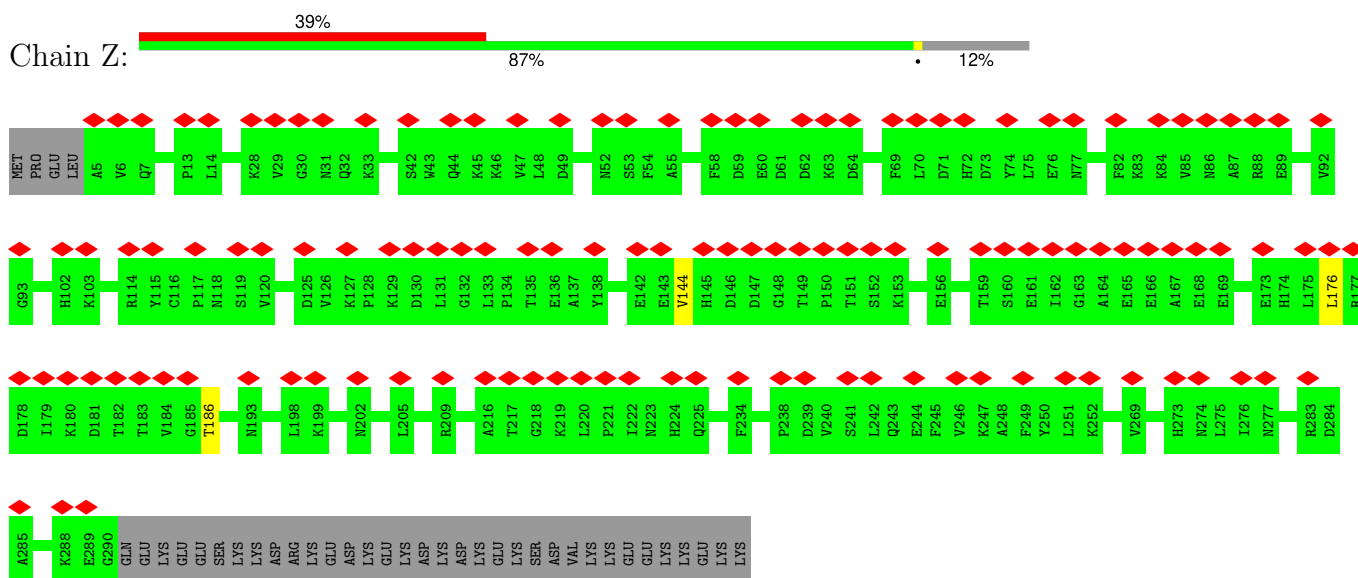
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 11



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

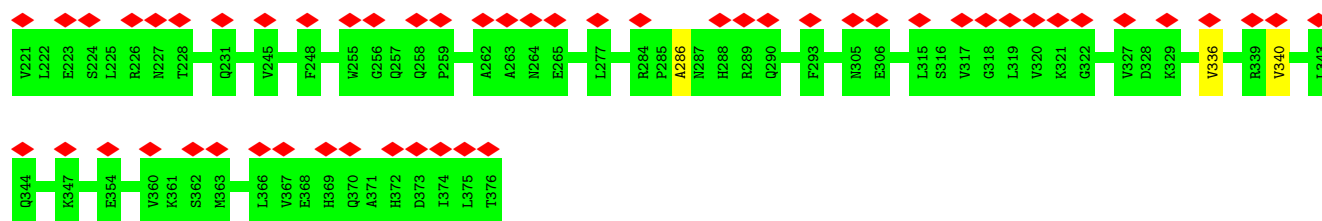


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 7



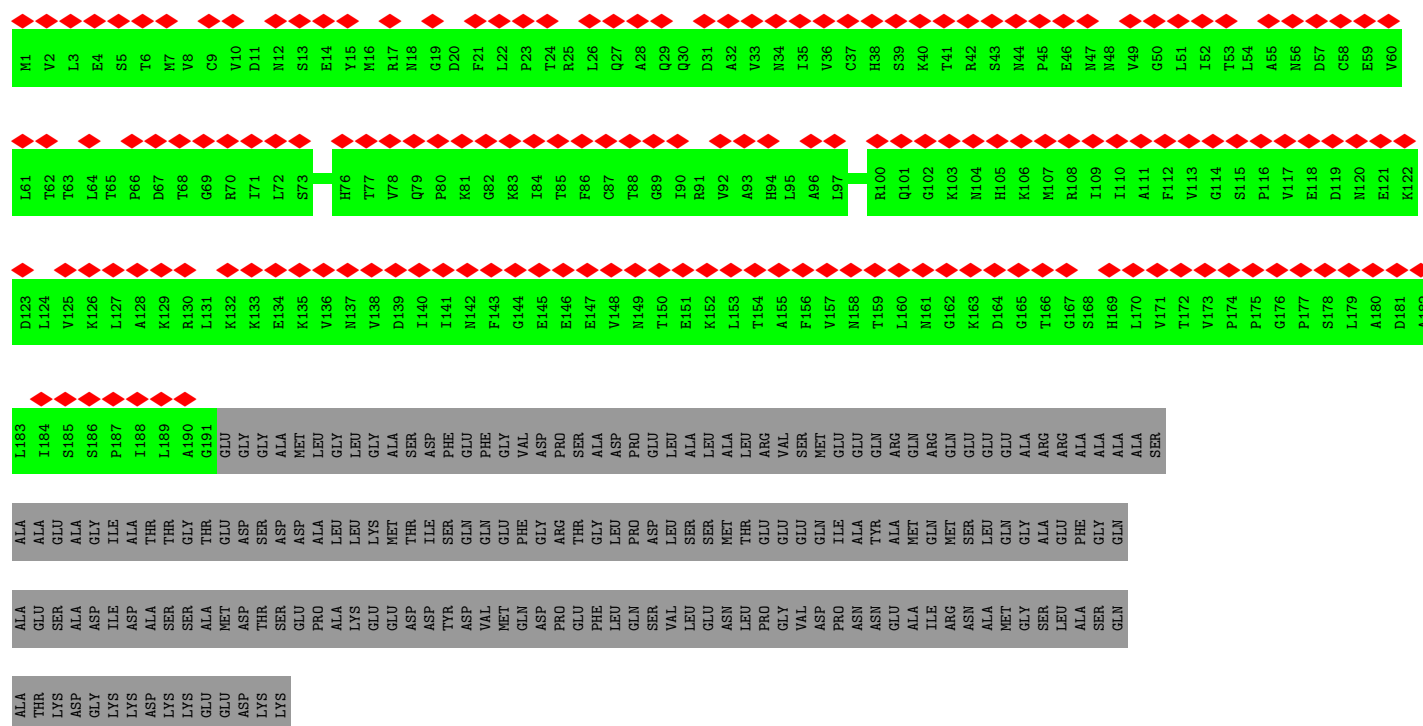
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 13



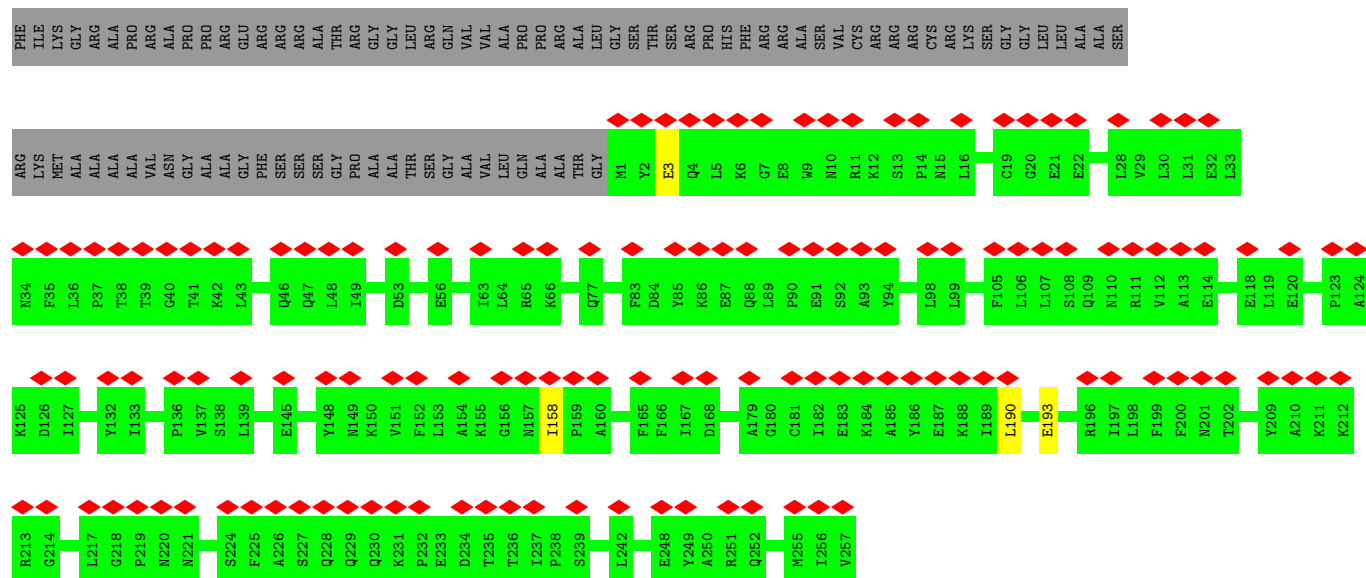
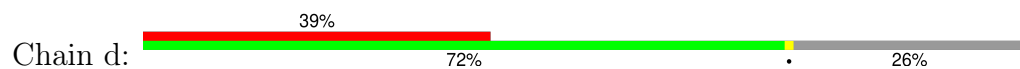


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 4

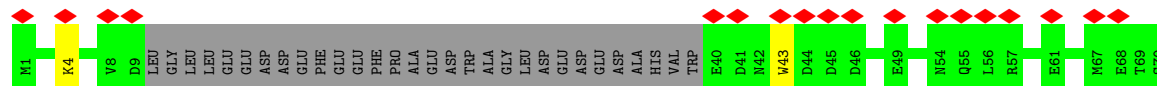
Chain b: 45% 51% 49%



• Molecule 31: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 32: 26S proteasome complex subunit DSS1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14382	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	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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, 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	f	0.24	0/5413	0.50	1/7317 (0.0%)
2	G	0.24	0/1859	0.45	0/2523
3	H	0.25	0/1743	0.49	0/2372
4	I	0.60	1/1942 (0.1%)	0.59	4/2628 (0.2%)
5	J	3.05	6/1728 (0.3%)	0.48	0/2358
6	K	0.24	0/1747	0.43	0/2364
7	L	0.23	0/1885	0.43	0/2552
8	M	0.23	0/1891	0.40	0/2552
9	N	0.23	0/1454	0.41	0/1967
10	O	0.23	0/1670	0.43	0/2265
11	P	0.23	0/1614	0.40	0/2177
12	Q	0.24	0/1603	0.41	0/2174
13	R	0.23	0/1579	0.39	0/2134
14	S	0.24	0/1671	0.41	0/2253
15	T	0.24	0/1700	0.41	0/2305
16	A	0.25	0/2886	0.50	0/3899
17	B	0.25	0/2756	0.50	0/3721
18	D	0.25	0/3090	0.51	1/4168 (0.0%)
19	E	0.39	1/2835 (0.0%)	0.45	0/3821
20	F	0.26	0/2903	0.50	0/3912
21	C	0.27	1/3117 (0.0%)	0.50	2/4189 (0.0%)
22	U	0.23	0/6396	0.40	0/8646
23	V	1.26	6/3929 (0.2%)	0.50	0/5309
24	W	0.24	0/3751	0.47	2/5042 (0.0%)
25	X	0.23	0/1936	0.41	0/2614
26	Y	0.24	0/3173	0.47	2/4273 (0.0%)
27	Z	0.24	0/2324	0.48	0/3150
28	a	0.23	0/3053	0.42	0/4133
29	b	0.26	0/1478	0.44	0/2001
30	c	0.26	1/2226 (0.0%)	0.46	0/3007
31	d	0.25	0/2162	0.48	0/2919
32	e	3.67	1/338 (0.3%)	0.75	2/450 (0.4%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.64	17/77852 (0.0%)	0.46	14/105195 (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
17	B	0	1
18	D	0	3
23	V	0	1
24	W	0	1
26	Y	0	1
28	a	0	1
31	d	0	1
All	All	0	9

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	4	LYS	CD-CE	67.17	3.19	1.51
5	J	21	TYR	CD2-CE2	67.11	2.40	1.39
5	J	21	TYR	CD1-CE1	65.88	2.38	1.39
5	J	21	TYR	CE1-CZ	49.34	2.02	1.38
5	J	21	TYR	CE2-CZ	45.57	1.97	1.38
23	V	212	TYR	CD2-CE2	40.57	2.00	1.39
23	V	212	TYR	CD1-CE1	40.40	2.00	1.39
5	J	21	TYR	CG-CD2	36.47	1.86	1.39
5	J	21	TYR	CG-CD1	35.86	1.85	1.39
23	V	212	TYR	CE1-CZ	29.51	1.76	1.38
23	V	212	TYR	CE2-CZ	28.92	1.76	1.38
4	I	14	PRO	CA-C	23.61	2.00	1.52
23	V	212	TYR	CG-CD2	23.07	1.69	1.39
23	V	212	TYR	CG-CD1	22.77	1.68	1.39
19	E	175	PRO	C-N	16.65	1.65	1.34
21	C	242	ALA	C-N	7.00	1.47	1.34
30	c	104	ARG	C-N	5.89	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	14	PRO	O-C-N	-15.43	98.01	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	e	4	LYS	CD-CE-NZ	8.24	130.65	111.70
4	I	14	PRO	CA-C-N	7.71	134.15	117.20
32	e	4	LYS	CG-CD-CE	7.23	133.60	111.90
4	I	14	PRO	N-CA-CB	-7.13	94.75	103.30
1	f	459	GLU	N-CA-C	6.14	127.58	111.00
4	I	14	PRO	N-CA-C	6.01	127.73	112.10
21	C	217	SER	C-N-CA	5.74	136.05	121.70
26	Y	63	TRP	C-N-CA	5.73	136.03	121.70
26	Y	287	LEU	CA-CB-CG	5.41	127.73	115.30
24	W	92	LYS	C-N-CA	5.22	134.76	121.70
24	W	135	LYS	C-N-CA	5.21	134.72	121.70
18	D	409	LYS	C-N-CA	5.19	134.68	121.70
21	C	217	SER	CA-C-N	5.12	128.47	117.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	B	436	GLU	Peptide
18	D	258	ALA	Peptide
18	D	406	VAL	Peptide
18	D	412	GLN	Peptide
23	V	319	HIS	Peptide
24	W	416	GLN	Peptide
26	Y	357	ASN	Peptide
28	a	286	ALA	Peptide
31	d	3	GLU	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	f	686/749 (92%)	575 (84%)	107 (16%)	4 (1%)	22	60
2	G	238/245 (97%)	221 (93%)	15 (6%)	2 (1%)	16	55
3	H	230/233 (99%)	200 (87%)	28 (12%)	2 (1%)	14	52
4	I	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
5	J	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	16	55
6	K	224/240 (93%)	196 (88%)	27 (12%)	1 (0%)	30	68
7	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
8	M	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
9	N	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
10	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
11	P	202/204 (99%)	187 (93%)	15 (7%)	0	100	100
12	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
13	R	199/262 (76%)	185 (93%)	14 (7%)	0	100	100
14	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
15	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
16	A	359/433 (83%)	307 (86%)	51 (14%)	1 (0%)	37	73
17	B	344/440 (78%)	304 (88%)	38 (11%)	2 (1%)	22	60
18	D	378/418 (90%)	323 (85%)	51 (14%)	4 (1%)	12	47
19	E	351/403 (87%)	317 (90%)	34 (10%)	0	100	100
20	F	362/439 (82%)	327 (90%)	34 (9%)	1 (0%)	37	73
21	C	390/398 (98%)	344 (88%)	42 (11%)	4 (1%)	13	49
22	U	798/953 (84%)	738 (92%)	59 (7%)	1 (0%)	48	83
23	V	478/533 (90%)	421 (88%)	57 (12%)	0	100	100
24	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	19	57
25	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
26	Y	376/389 (97%)	332 (88%)	42 (11%)	2 (0%)	25	64
27	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	30	68
28	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	25	64
29	b	189/377 (50%)	175 (93%)	14 (7%)	0	100	100
30	c	274/309 (89%)	246 (90%)	25 (9%)	3 (1%)	12	47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	d	255/349 (73%)	229 (90%)	26 (10%)	0	100	100
32	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
All	All	9704/11269 (86%)	8711 (90%)	958 (10%)	35 (0%)	32	68

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	62	ILE
1	f	447	VAL
2	G	111	VAL
22	U	364	VAL
24	W	68	VAL
24	W	136	ILE
26	Y	350	VAL
1	f	131	VAL
30	c	157	ILE
1	f	281	ILE
5	J	199	VAL
21	C	298	ILE
28	a	340	VAL
3	H	127	VAL
6	K	12	VAL
18	D	151	ILE
21	C	68	GLU
21	C	219	LEU
24	W	138	VAL
26	Y	67	VAL
27	Z	144	VAL
30	c	156	VAL
17	B	218	PRO
18	D	411	GLU
18	D	406	VAL
18	D	259	PRO
28	a	336	VAL
30	c	189	ILE
2	G	170	VAL
3	H	20	VAL
21	C	251	ILE
16	A	206	ILE
17	B	325	VAL
20	F	326	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	J	98	VAL

### 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	f	582/628 (93%)	572 (98%)	10 (2%)	56	72
2	G	193/209 (92%)	189 (98%)	4 (2%)	48	66
3	H	164/190 (86%)	162 (99%)	2 (1%)	67	78
4	I	193/220 (88%)	191 (99%)	2 (1%)	73	82
5	J	152/210 (72%)	151 (99%)	1 (1%)	81	87
6	K	186/202 (92%)	184 (99%)	2 (1%)	70	80
7	L	198/229 (86%)	198 (100%)	0	100	100
8	M	192/211 (91%)	192 (100%)	0	100	100
9	N	148/180 (82%)	148 (100%)	0	100	100
10	O	177/227 (78%)	177 (100%)	0	100	100
11	P	172/173 (99%)	172 (100%)	0	100	100
12	Q	164/171 (96%)	164 (100%)	0	100	100
13	R	153/201 (76%)	153 (100%)	0	100	100
14	S	174/198 (88%)	174 (100%)	0	100	100
15	T	175/214 (82%)	175 (100%)	0	100	100
16	A	308/372 (83%)	302 (98%)	6 (2%)	52	69
17	B	304/385 (79%)	297 (98%)	7 (2%)	45	64
18	D	333/366 (91%)	330 (99%)	3 (1%)	75	83
19	E	308/353 (87%)	302 (98%)	6 (2%)	52	69
20	F	312/379 (82%)	309 (99%)	3 (1%)	73	82
21	C	340/346 (98%)	336 (99%)	4 (1%)	67	78
22	U	685/816 (84%)	681 (99%)	4 (1%)	84	88
23	V	414/459 (90%)	412 (100%)	2 (0%)	86	89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	416/416 (100%)	412 (99%)	4 (1%)	73	82
25	X	208/362 (58%)	207 (100%)	1 (0%)	86	89
26	Y	334/344 (97%)	332 (99%)	2 (1%)	84	88
27	Z	257/295 (87%)	255 (99%)	2 (1%)	79	85
28	a	333/336 (99%)	331 (99%)	2 (1%)	84	88
29	b	167/312 (54%)	167 (100%)	0	100	100
30	c	243/267 (91%)	239 (98%)	4 (2%)	58	73
31	d	231/293 (79%)	228 (99%)	3 (1%)	65	77
32	e	38/63 (60%)	37 (97%)	1 (3%)	41	59
All	All	8254/9627 (86%)	8179 (99%)	75 (1%)	74	83

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	15	ASP
1	f	33	VAL
1	f	301	ASP
1	f	334	ASN
1	f	339	LEU
1	f	342	LEU
1	f	371	CYS
1	f	391	LEU
1	f	526	THR
1	f	659	LEU
2	G	22	LEU
2	G	34	GLN
2	G	111	VAL
2	G	159	TYR
3	H	13	PHE
3	H	182	LEU
4	I	34	CYS
4	I	107	CYS
5	J	3	TYR
6	K	36	THR
6	K	42	THR
16	A	94	GLN
16	A	125	LEU
16	A	153	LEU
16	A	316	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	A	331	LEU
16	A	344	SER
17	B	105	THR
17	B	235	LEU
17	B	307	ARG
17	B	316	LEU
17	B	348	ASP
17	B	355	LEU
17	B	436	GLU
18	D	186	THR
18	D	234	GLU
18	D	303	VAL
19	E	65	THR
19	E	87	LEU
19	E	104	THR
19	E	265	ASP
19	E	269	THR
19	E	358	ASP
20	F	88	TYR
20	F	270	ASP
20	F	427	VAL
21	C	109	THR
21	C	138	MET
21	C	298	ILE
21	C	311	ILE
22	U	336	GLU
22	U	479	LEU
22	U	554	LEU
22	U	895	PRO
23	V	224	LEU
23	V	255	LEU
24	W	250	ILE
24	W	371	THR
24	W	417	ARG
24	W	444	HIS
25	X	331	LEU
26	Y	315	THR
26	Y	352	GLU
27	Z	176	LEU
27	Z	186	THR
28	a	28	LEU
28	a	158	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	c	194	HIS
30	c	229	LEU
30	c	273	LYS
30	c	309	PHE
31	d	158	ILE
31	d	190	LEU
31	d	193	GLU
32	e	43	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	246	HIS
1	f	269	GLN
1	f	293	ASN
1	f	491	GLN
1	f	565	ASN
2	G	53	GLN
2	G	100	ASN
4	I	95	GLN
4	I	109	GLN
4	I	119	GLN
6	K	23	GLN
6	K	97	GLN
6	K	164	GLN
7	L	166	GLN
7	L	190	HIS
9	N	187	GLN
11	P	33	GLN
12	Q	8	GLN
12	Q	99	HIS
13	R	29	GLN
13	R	85	ASN
15	T	2	GLN
15	T	69	GLN
16	A	414	ASN
17	B	157	HIS
17	B	314	ASN
18	D	57	GLN
18	D	137	ASN
18	D	286	GLN
18	D	301	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
18	D	302	ASN
18	D	304	ASN
18	D	376	ASN
19	E	190	GLN
19	E	316	HIS
20	F	194	GLN
21	C	50	ASN
21	C	129	ASN
21	C	205	HIS
21	C	270	GLN
21	C	278	ASN
21	C	288	ASN
22	U	189	GLN
22	U	345	ASN
22	U	389	ASN
22	U	421	GLN
22	U	698	GLN
22	U	756	HIS
23	V	62	HIS
23	V	299	GLN
23	V	326	GLN
23	V	427	GLN
23	V	459	GLN
23	V	477	HIS
23	V	487	HIS
24	W	155	GLN
24	W	235	GLN
24	W	362	ASN
24	W	430	GLN
25	X	406	ASN
26	Y	136	HIS
26	Y	363	ASN
26	Y	378	ASN
27	Z	44	GLN
27	Z	102	HIS
27	Z	223	ASN
27	Z	224	HIS
28	a	23	HIS
28	a	257	GLN
28	a	273	GLN
28	a	290	GLN
28	a	337	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	c	115	HIS
32	e	6	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	$\# Z  > 2$
33	ATP	F	501	-	28,33,33	0.97	0	34,52,52	1.17	2 (5%)
33	ATP	E	401	-	28,33,33	1.00	1 (3%)	34,52,52	1.16	2 (5%)
33	ATP	A	501	-	28,33,33	0.98	0	34,52,52	1.18	2 (5%)
33	ATP	D	501	-	28,33,33	0.98	0	34,52,52	1.23	3 (8%)

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
33	ATP	F	501	-	-	4/18/38/38	0/3/3/3
33	ATP	E	401	-	-	2/18/38/38	0/3/3/3
33	ATP	A	501	-	-	1/18/38/38	0/3/3/3
33	ATP	D	501	-	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	401	ATP	PB-O3A	2.03	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	501	ATP	N3-C2-N1	-3.76	123.56	128.67
33	F	501	ATP	N3-C2-N1	-3.70	123.65	128.67
33	A	501	ATP	N3-C2-N1	-3.65	123.71	128.67
33	E	401	ATP	N3-C2-N1	-3.61	123.77	128.67
33	D	501	ATP	O4'-C1'-N9	2.88	112.57	108.75
33	A	501	ATP	C4-C5-N7	-2.72	106.46	109.34
33	D	501	ATP	C4-C5-N7	-2.67	106.52	109.34
33	F	501	ATP	C4-C5-N7	-2.65	106.54	109.34
33	E	401	ATP	C4-C5-N7	-2.45	106.75	109.34

There are no chirality outliers.

All (9) torsion outliers are listed below:

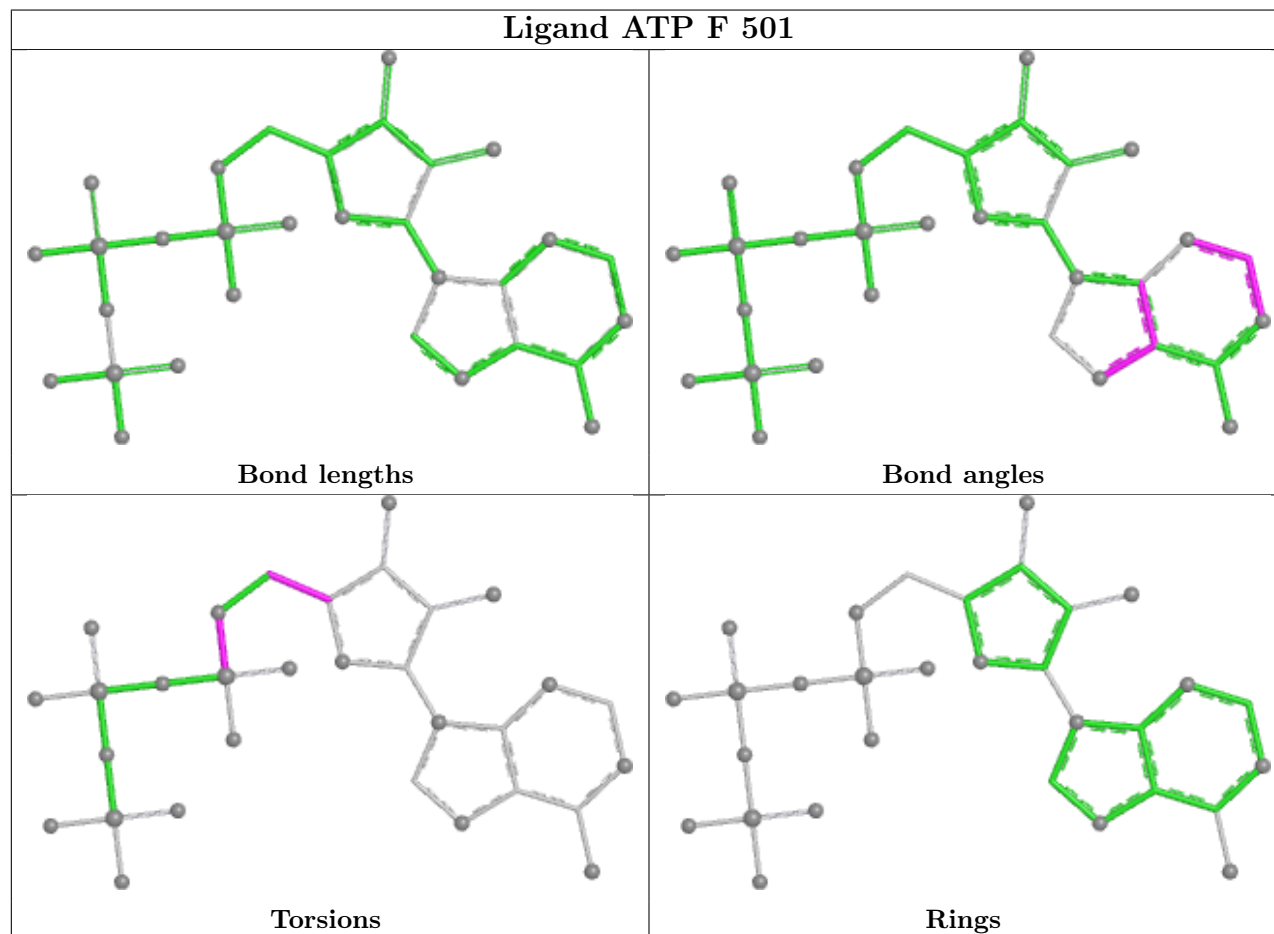
Mol	Chain	Res	Type	Atoms
33	F	501	ATP	C5'-O5'-PA-O1A
33	F	501	ATP	C5'-O5'-PA-O3A
33	F	501	ATP	O4'-C4'-C5'-O5'
33	E	401	ATP	PB-O3A-PA-O1A
33	F	501	ATP	C3'-C4'-C5'-O5'
33	A	501	ATP	C5'-O5'-PA-O1A
33	D	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	O4'-C4'-C5'-O5'
33	E	401	ATP	PB-O3A-PA-O2A

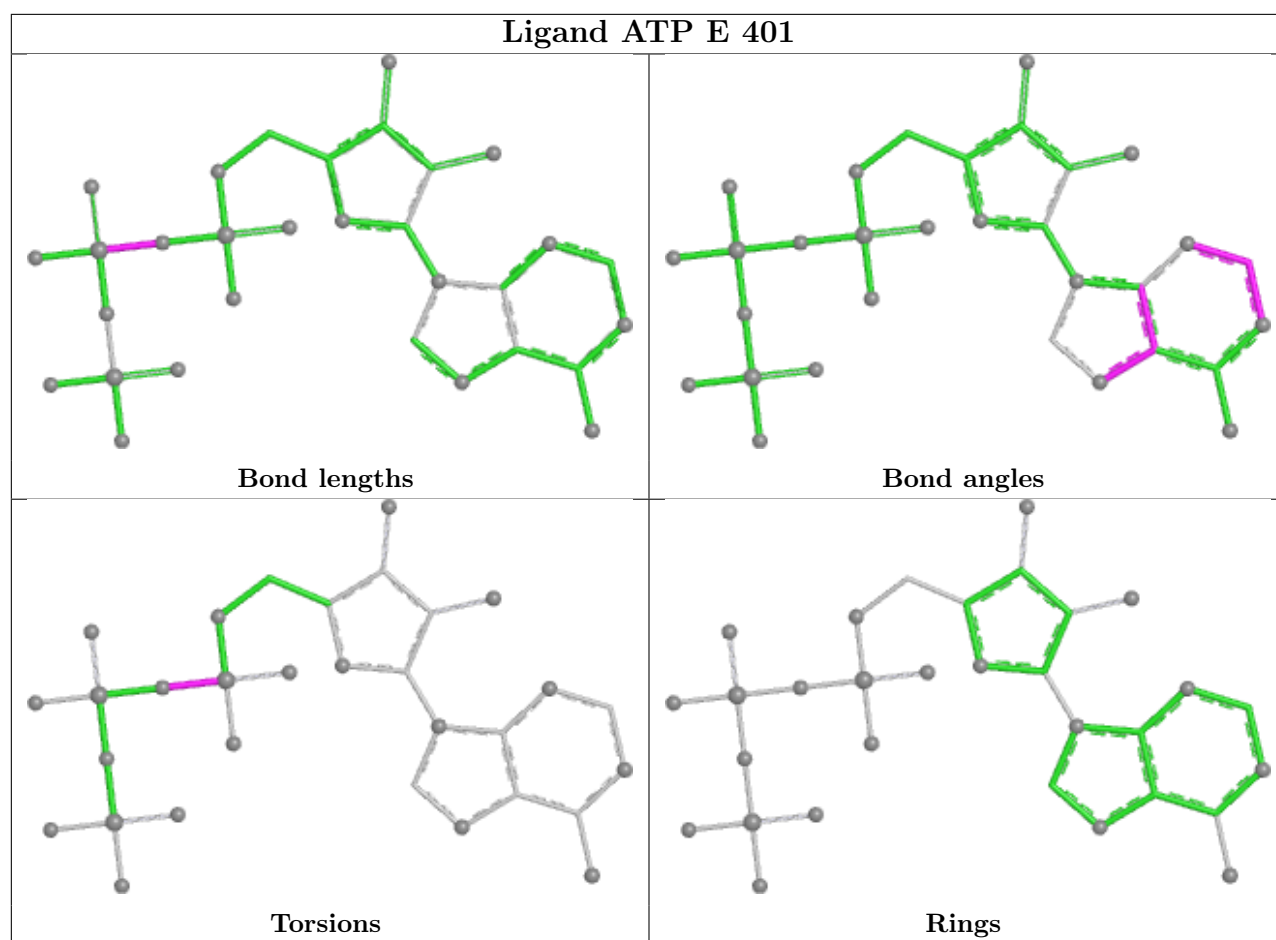
There are no ring outliers.

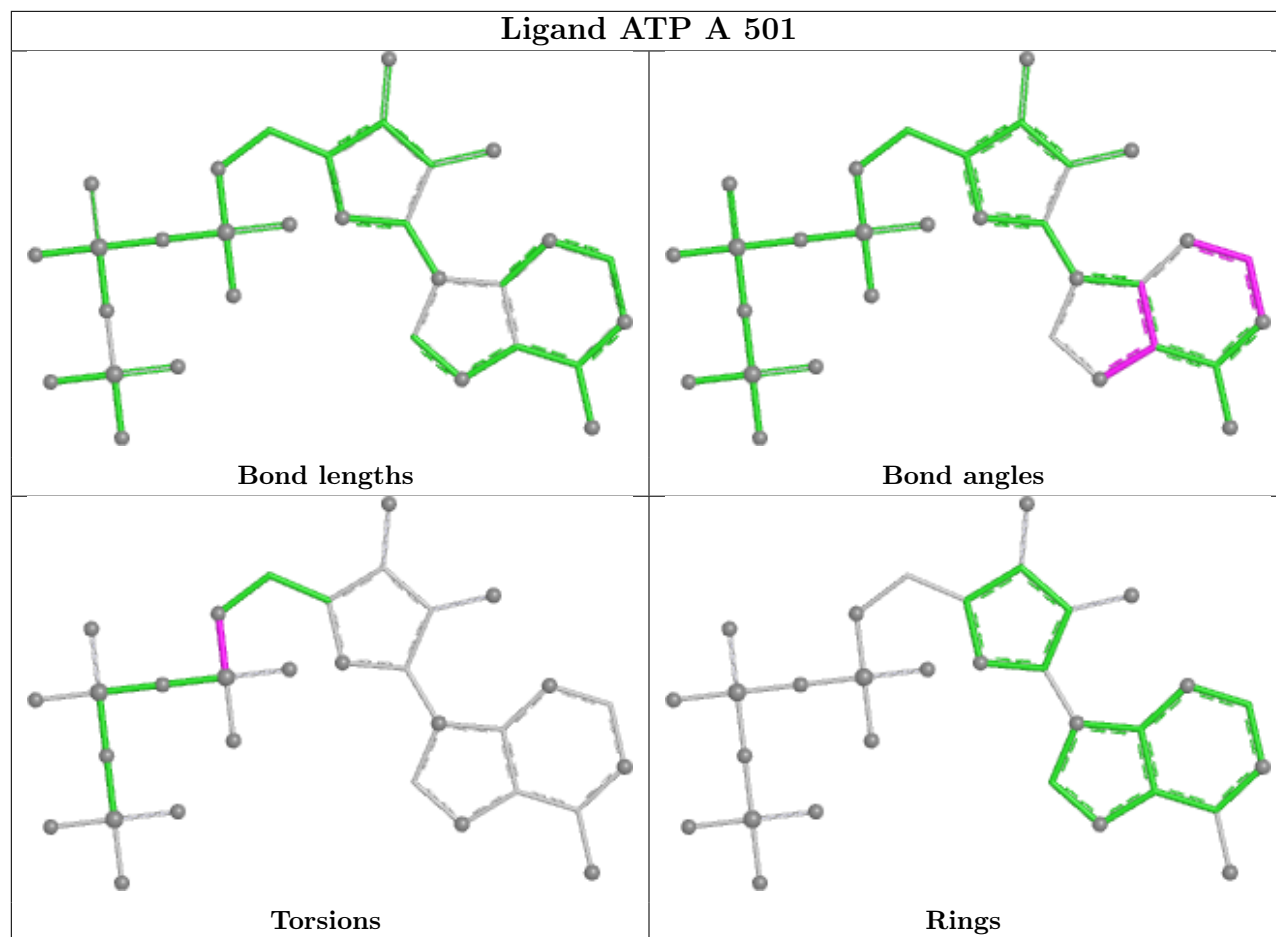
No monomer is involved in short contacts.

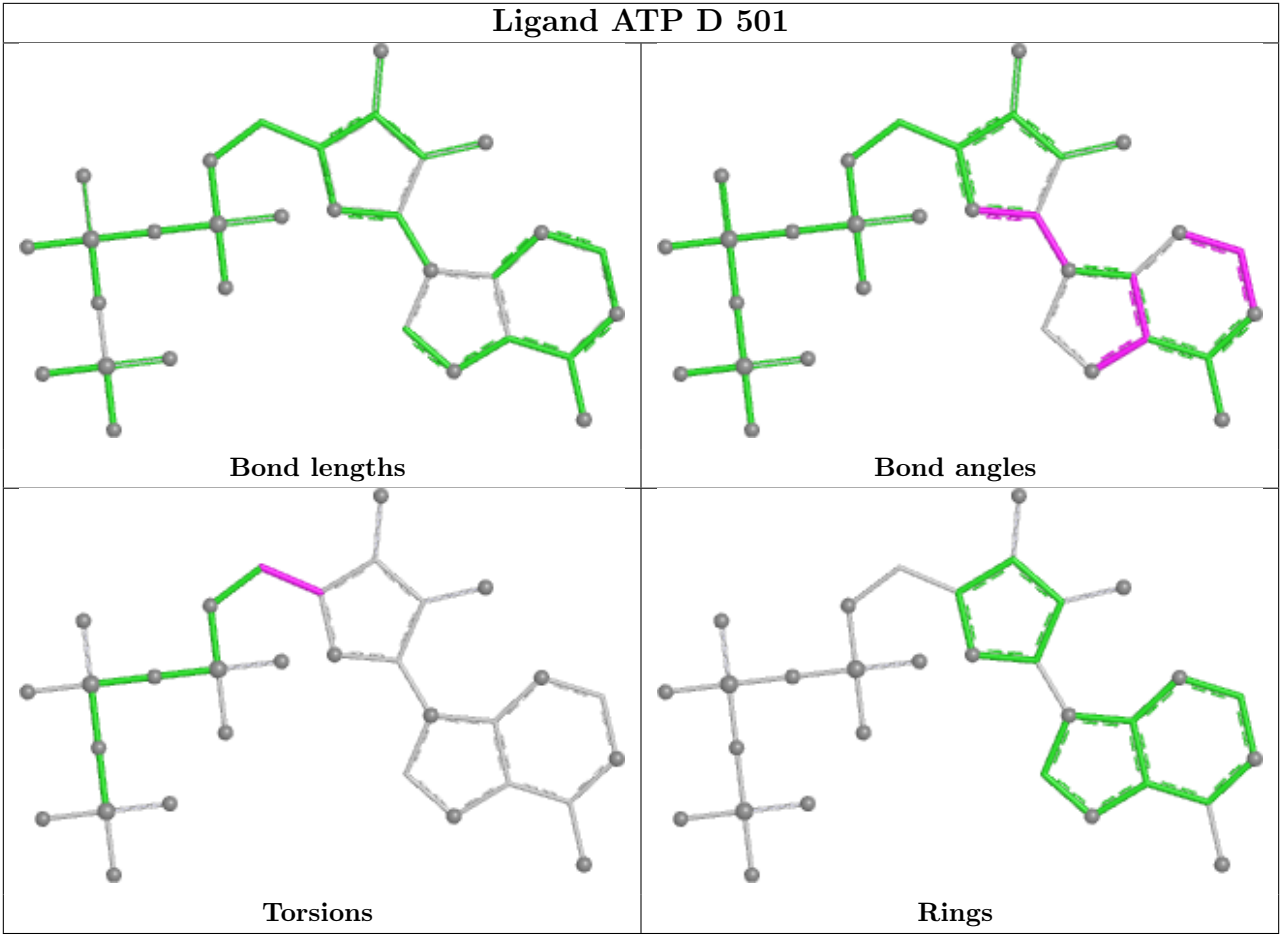
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	3
17	B	1
19	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.87
1	f	79:ASN	C	80:TYR	N	7.82
1	f	348:ASP	C	349:SER	N	6.24

Continued on next page...

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	216:ILE	C	217:LYS	N	4.90
1	E	175:PRO	C	176:PRO	N	1.65



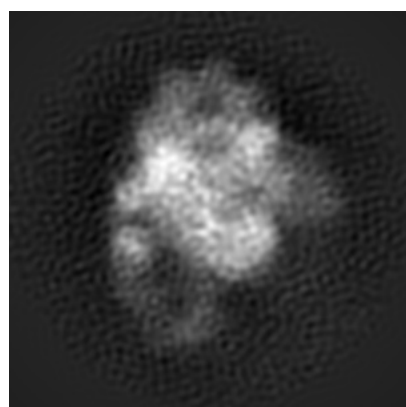
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8337. These allow visual inspection of the internal detail of the map and identification of artifacts.

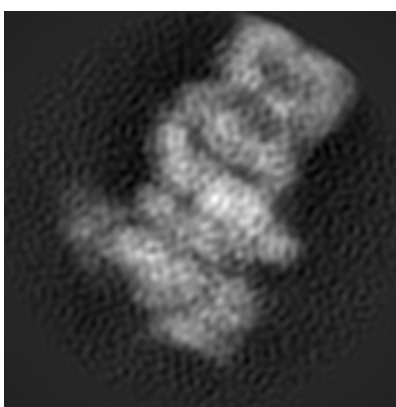
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

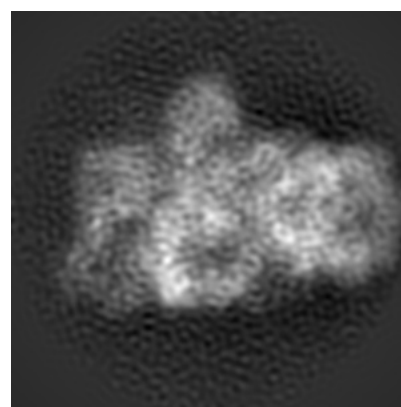
#### 6.1.1 Primary map



X



Y

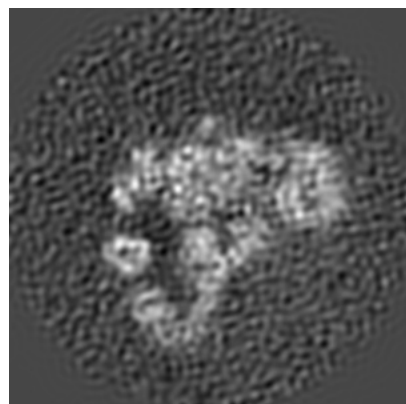


Z

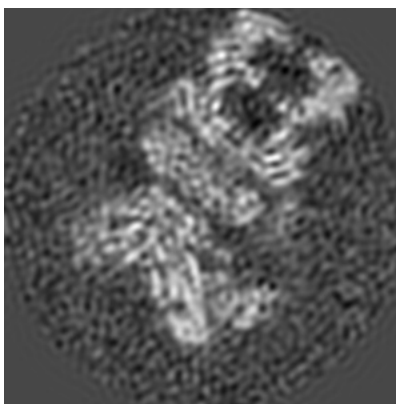
The images above show the map projected in three orthogonal directions.

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

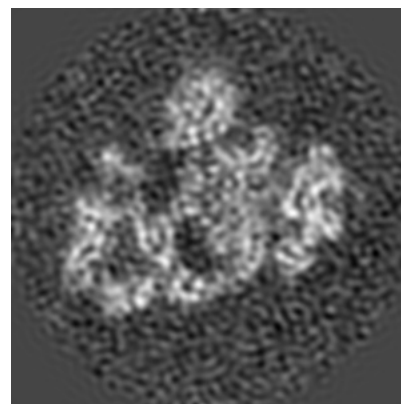
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

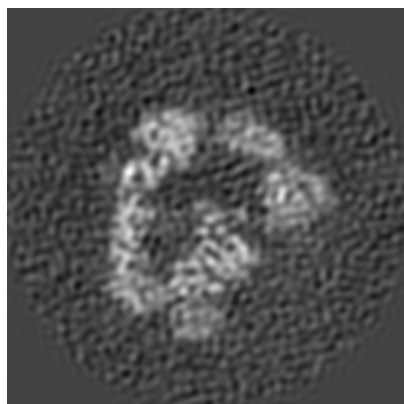


Z Index: 180

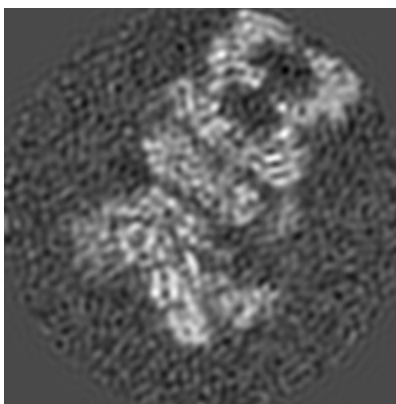
The images above show central slices of the map in three orthogonal directions.

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

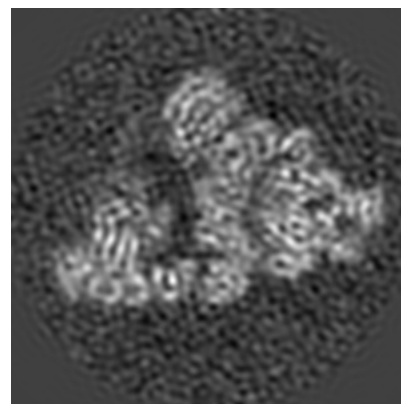
### 6.3.1 Primary map



X Index: 150



Y Index: 182

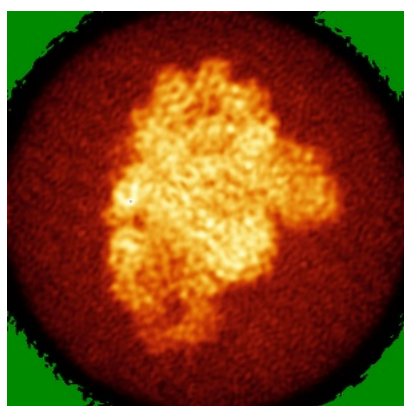


Z Index: 197

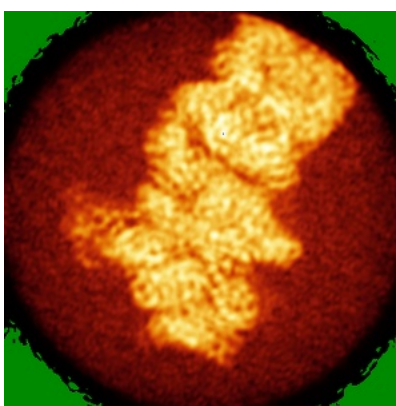
The images above show the largest variance slices of the map in three orthogonal directions.

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

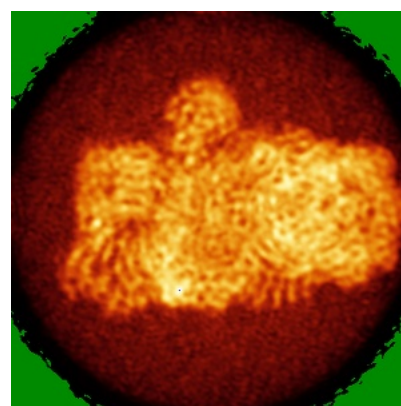
### 6.4.1 Primary map



X



Y

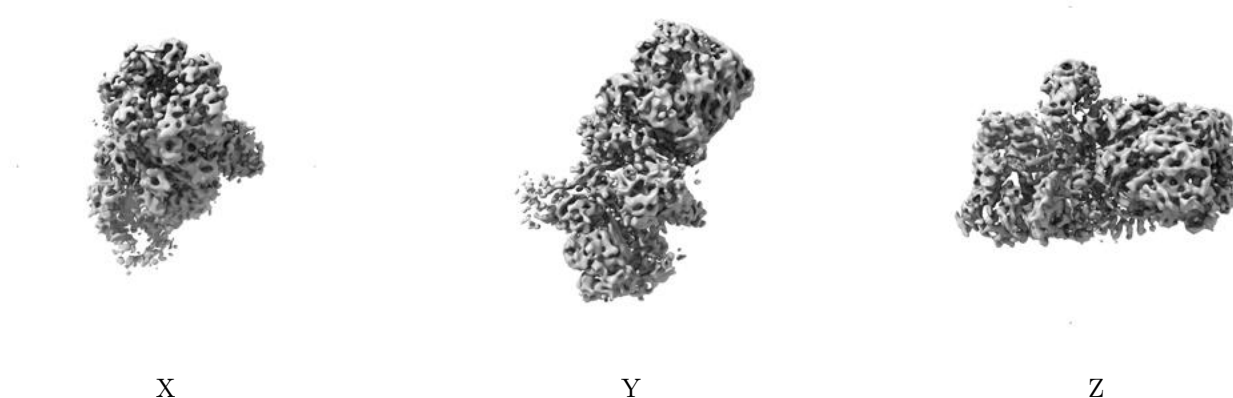


Z

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 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

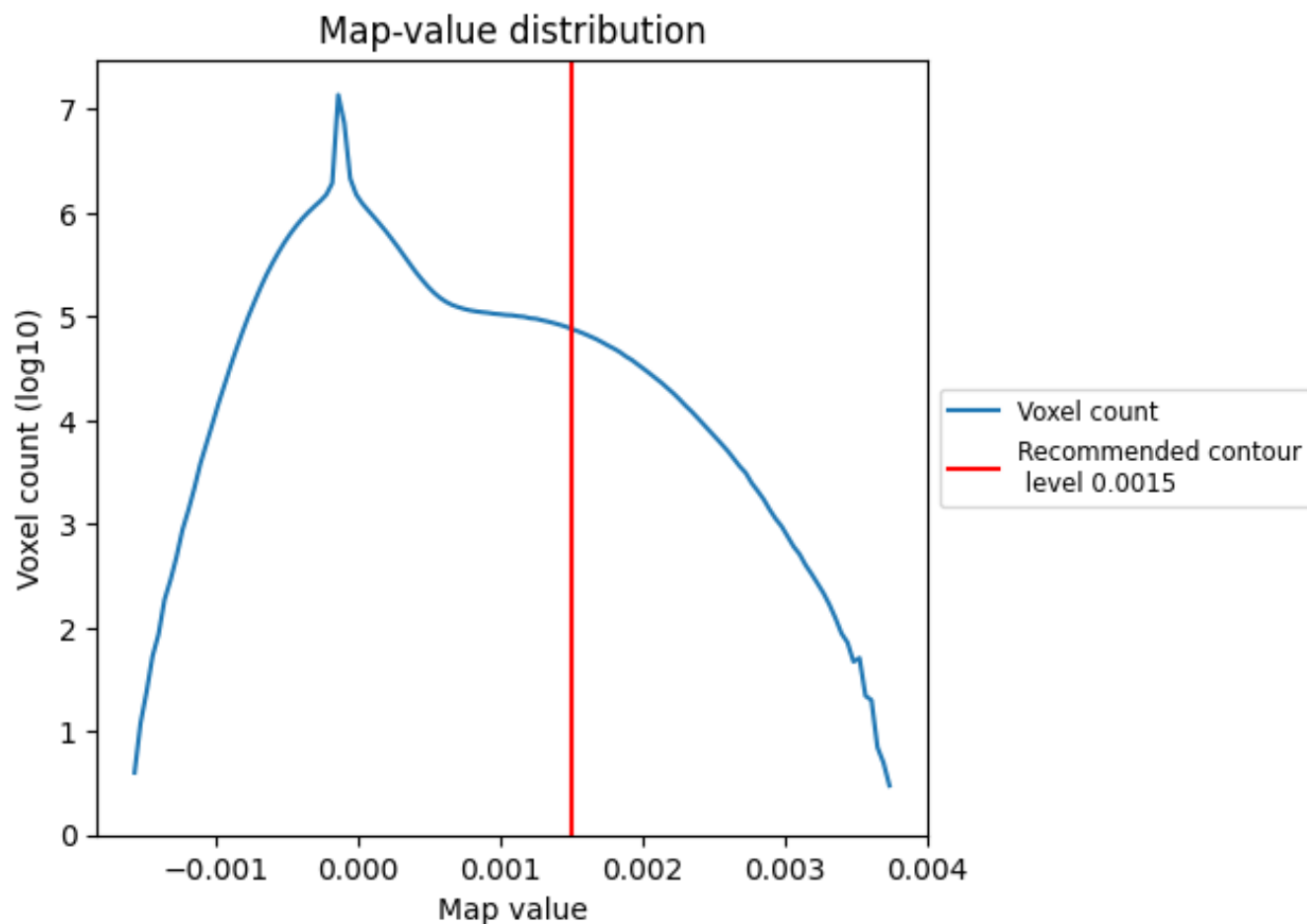
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

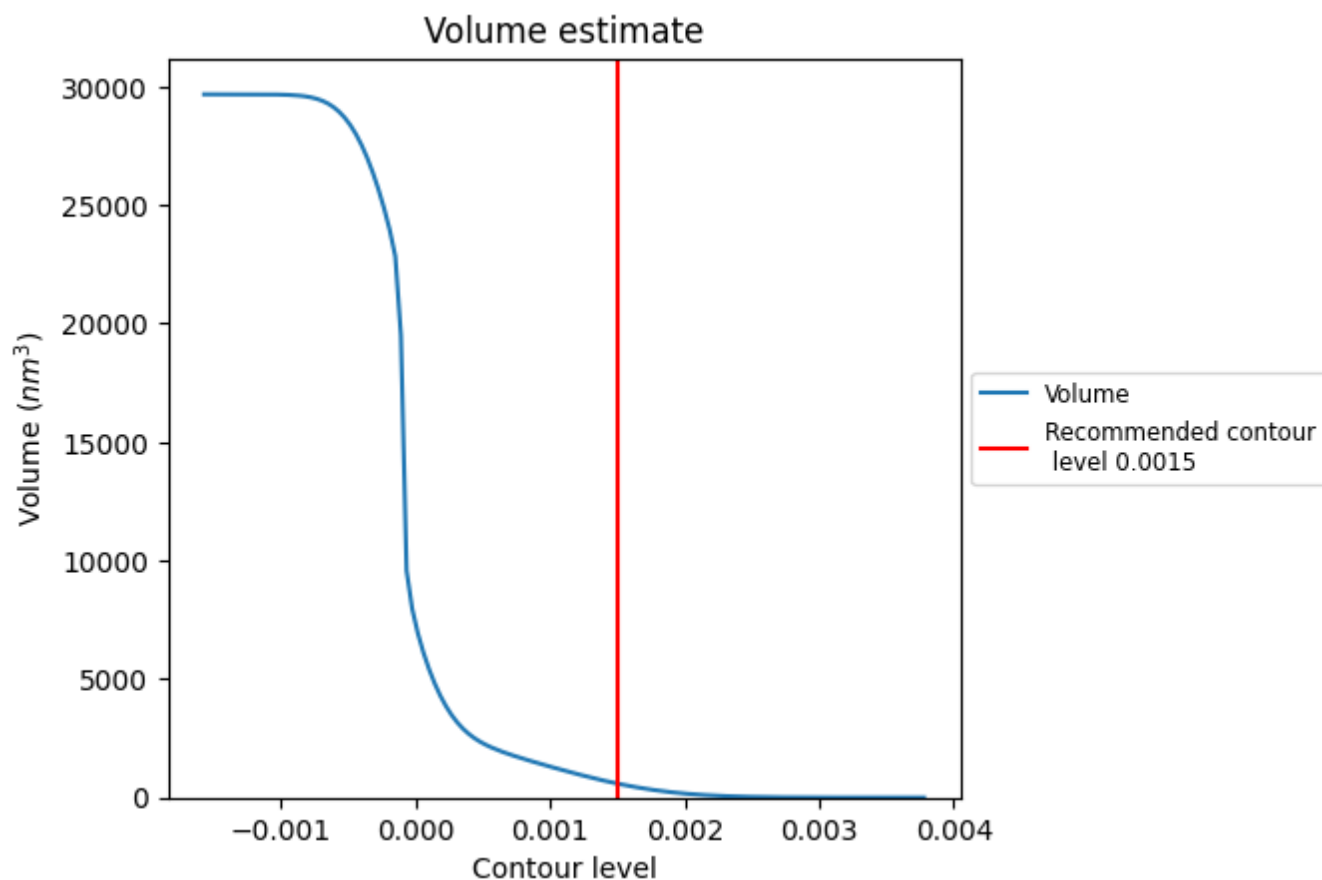
This section contains the results of statistical analysis of the map.

### 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.

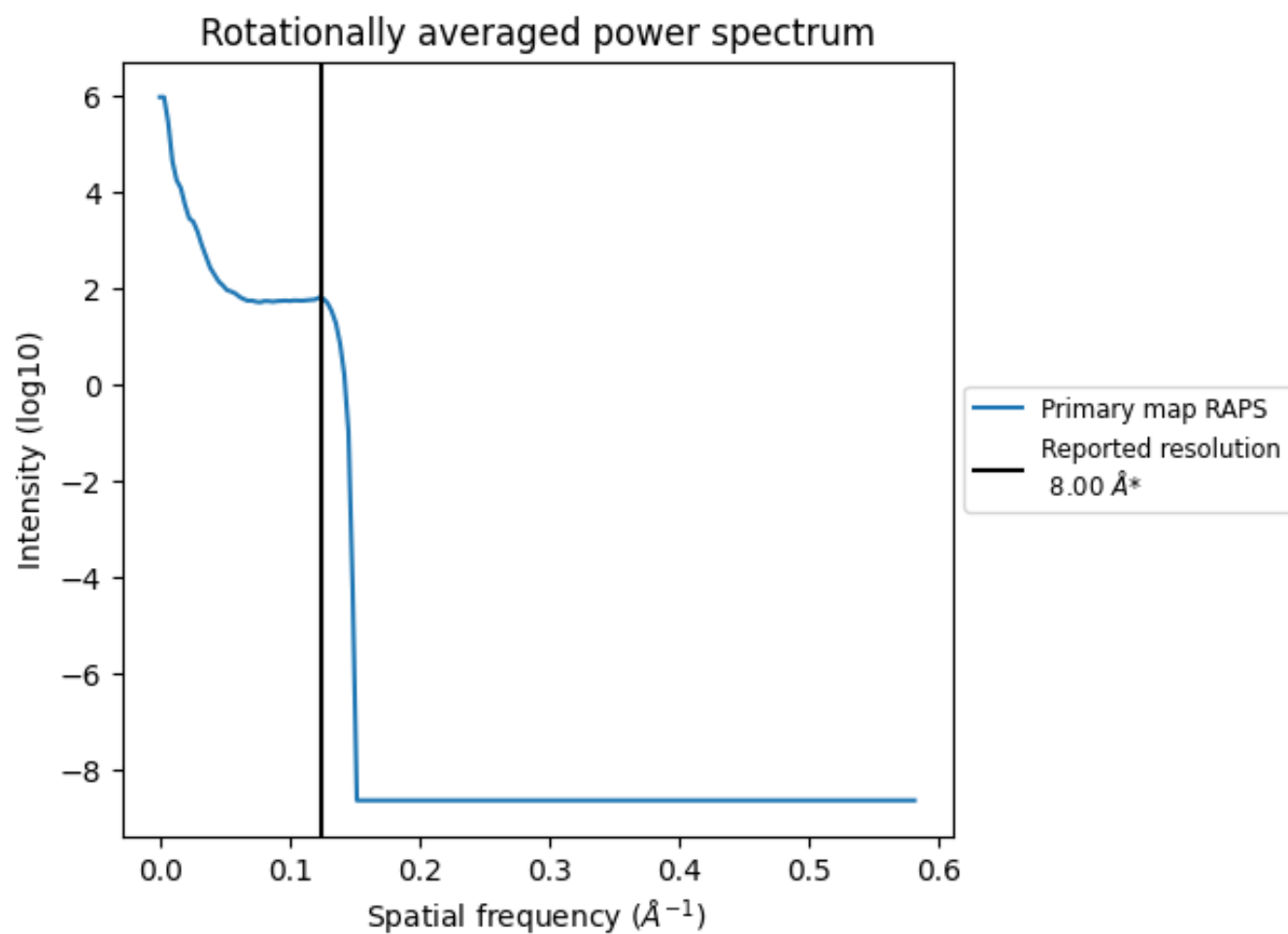
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 590 nm<sup>3</sup>; this corresponds to an approximate mass of 533 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 0.125 Å<sup>-1</sup>

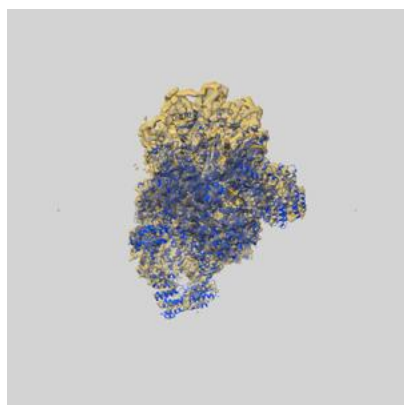
## 8 Fourier-Shell correlation

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

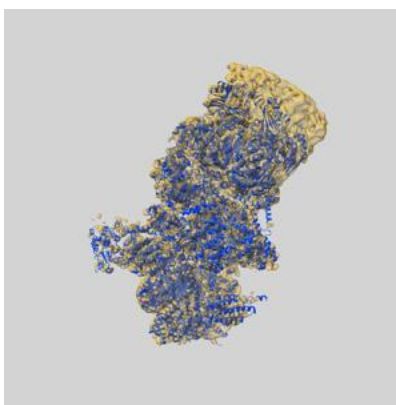
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8337 and PDB model 5T0J. Per-residue inclusion information can be found in section [3](#) on page [10](#).

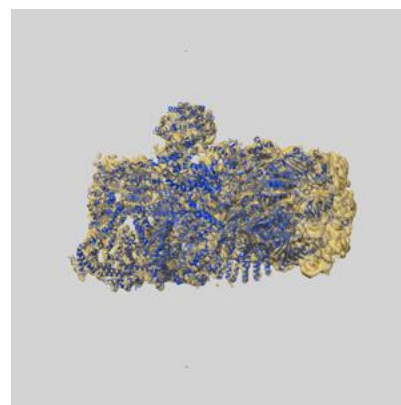
### 9.1 Map-model overlay [i](#)



X



Y

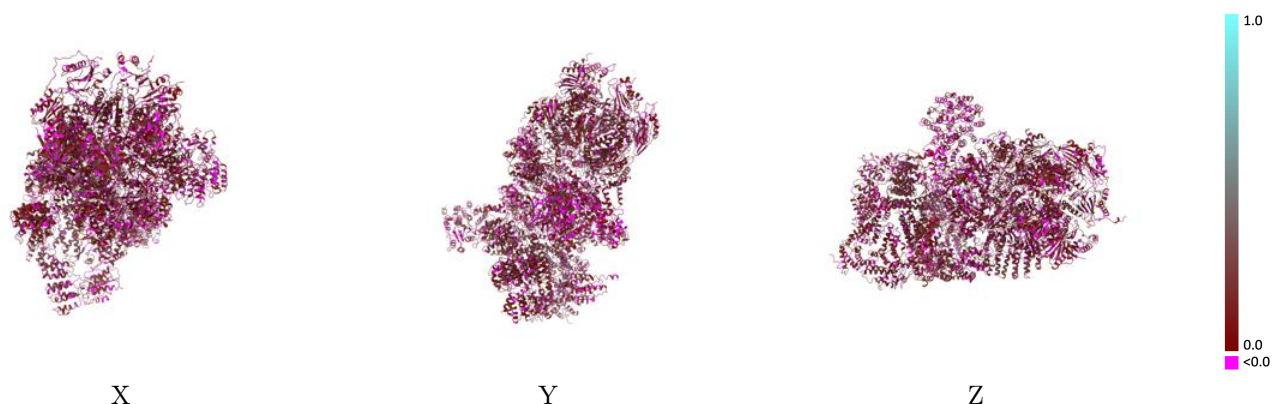


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

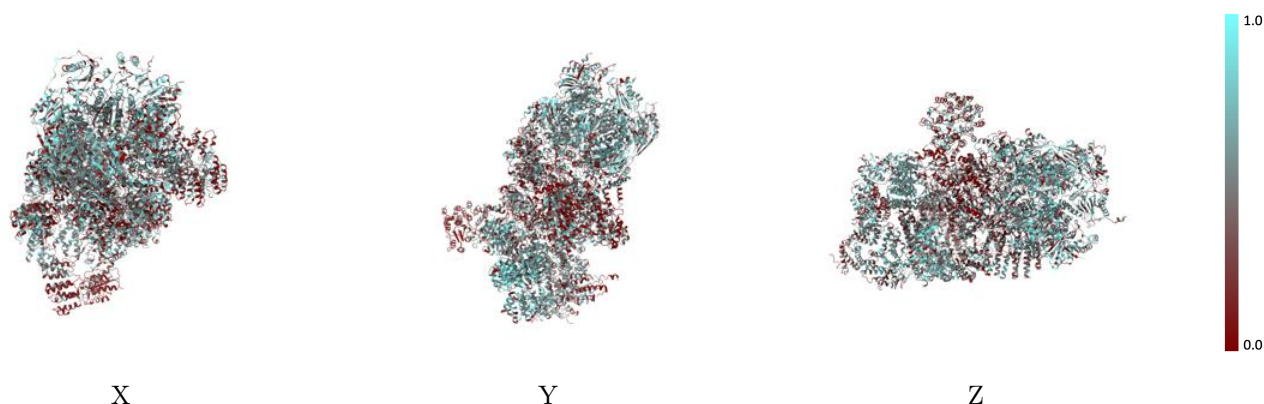


## 9.2 Q-score mapped to coordinate model [i](#)



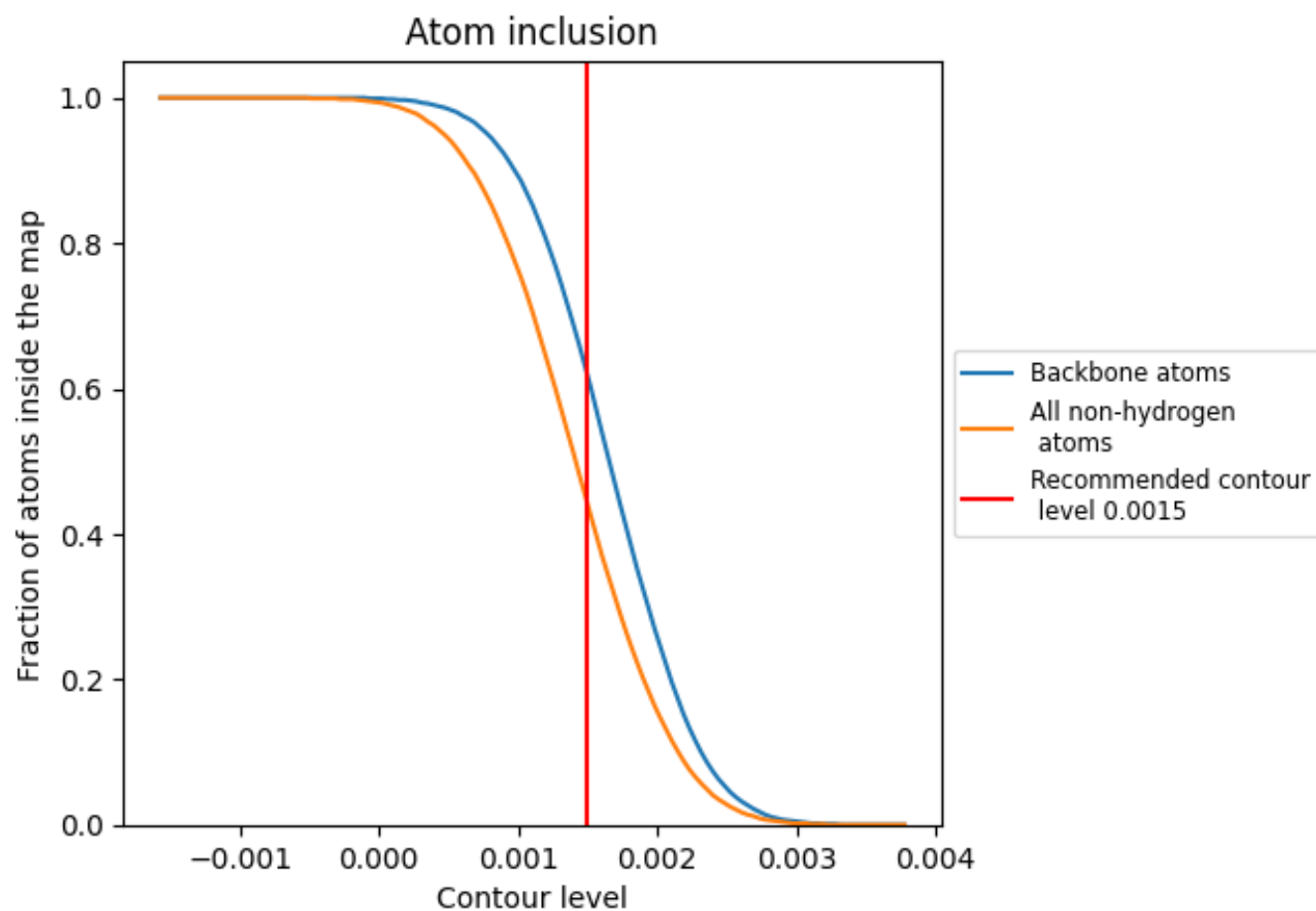
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0015).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 44% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4410	 0.1160
A	 0.3420	 0.1020
B	 0.2650	 0.0920
C	 0.3460	 0.1040
D	 0.3310	 0.1040
E	 0.3040	 0.1130
F	 0.3190	 0.0980
G	 0.5310	 0.1330
H	 0.4920	 0.1230
I	 0.4770	 0.1330
J	 0.5460	 0.1470
K	 0.5390	 0.1500
L	 0.5570	 0.1390
M	 0.5620	 0.1380
N	 0.5390	 0.1190
O	 0.5450	 0.1130
P	 0.5530	 0.1160
Q	 0.5570	 0.1320
R	 0.5630	 0.1260
S	 0.4690	 0.1140
T	 0.5510	 0.1280
U	 0.5970	 0.1300
V	 0.4370	 0.1210
W	 0.4440	 0.1300
X	 0.4100	 0.1040
Y	 0.5830	 0.1320
Z	 0.4460	 0.1170
a	 0.3730	 0.1160
b	 0.1300	 0.0790
c	 0.4680	 0.1300
d	 0.3760	 0.1200
e	 0.4550	 0.1270
f	 0.3070	 0.0710

