



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 09:44 AM JST

PDB ID : 5GJQ
EMDB ID : EMD-9511
Title : Structure of the human 26S proteasome bound to USP14-UbA1
Authors : Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.
Deposited on : 2016-07-01
Resolution : 4.50 Å (reported)

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

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

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

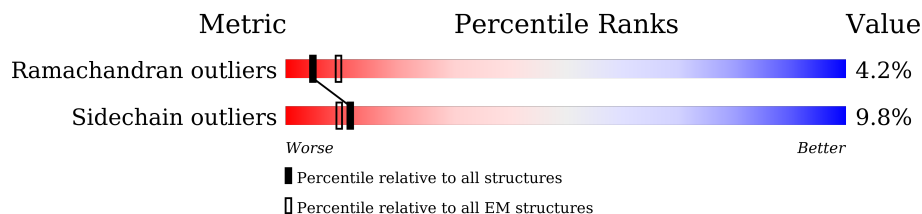
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	a	239	
1	o	239	
2	B	246	
2	h	246	
3	b	277	
3	p	277	
4	C	234	
4	i	234	
5	c	205	

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Mol	Chain	Length	Quality of chain
5	q	205	90% 10%
6	D	261	91% . .
6	j	261	89% 7% .
7	d	201	93% 5% ..
7	r	201	89% 9% .
8	E	248	8% 90% 8% .
8	k	248	10% 90% 8% .
9	e	263	72% 5% 24%
9	s	263	71% 6% 24%
10	F	241	94% . .
10	l	241	93% . .
11	f	241	84% 5% 12%
11	t	241	83% 5% 12%
12	G	263	86% . . 10%
12	m	263	82% 9% 10%
13	g	264	75% 7% 18%
13	u	264	75% 7% 18%
14	H	433	15% 67% 18% . 12%
15	I	440	15% 61% 18% . 18%
16	J	406	16% 66% 20% . 12%
17	K	418	11% 65% 23% . 9%
18	L	389	19% 74% 19% . . .
19	M	439	17% 65% 19% . 14%
20	N	953	49% 80% 5% . 14%
21	X	255	91% . 5%

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Mol	Chain	Length	Quality of chain
21	n	255	89% 5% 5%
22	O	376	73% 87% 11%
23	P	456	57% 83% 7% 9%
24	Q	422	44% 83% 15%
25	R	389	24% 82% 13%
26	S	534	52% 69% 26%
27	T	350	59% 64% 9% 26%
28	U	324	64% 74% 12% 13%
29	V	310	52% 69% 12% 17%
30	W	377	51% 45% 5% 49%
31	Y	70	60% 70% 14% 16%
32	Z	908	76% 75% 6% 19%
33	x	494	39% 55% 15% 28%
34	y	76	68% 93% 7%

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 98461 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 Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		
1	o	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	244	Total	C	N	O	S	0	0
			1845	1171	309	352	13		
2	h	244	Total	C	N	O	S	0	0
			1853	1177	311	352	13		

- Molecule 3 is a protein called Proteasome subunit beta type-7.

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

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	233	Total	C	N	O	S	0	0
			1707	1081	287	334	5		
4	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
5	q	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 6 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
6	j	250	Total	C	N	O	S	0	0
			1913	1203	330	372	8		

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
7	r	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	243	Total	C	N	O	S	0	0
			1724	1068	312	339	5		
8	k	243	Total	C	N	O	S	0	0
			1691	1051	309	327	4		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
9	s	201	Total	C	N	O	S	0	0
			1551	977	273	292	9		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	234	Total	C	N	O	S	0	0
			1766	1108	290	357	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	234	1726	1107	291	317	11	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	f	213	1641	1036	282	313	10	0	0
11	t	213	1644	1039	282	313	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	238	1850	1159	334	346	11	0	0
12	m	238	1850	1159	334	346	11	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	g	216	1672	1055	286	319	12	0	0
13	u	217	1678	1058	290	318	12	0	0

- Molecule 14 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	380	2879	1809	513	539	18	0	0

- Molecule 15 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I	359	2720	1708	465	535	12	0	0

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	358	2820	1780	506	518	16	0	0

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	M	376	2858	1802	496	545	15	0	0

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	823	5462	3499	933	1012	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	n	243	1873	1189	317	356	11	0	0
21	X	243	1873	1189	317	356	11	0	0

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	372	2372	1518	405	438	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	413	2828	1819	489	514	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	421	2948	1864	509	567	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	376	2767	1794	461	503	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	395	2600	1662	463	472	3	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	258	1702	1102	280	315	5	0	0

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	283	2131	1370	369	388	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	257	2011	1276	341	377	17	0	0

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	193	1300	818	228	250	4	0	0

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	Y	59	308	184	60	64	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	Z	732	3608	2144	732	732	0	0

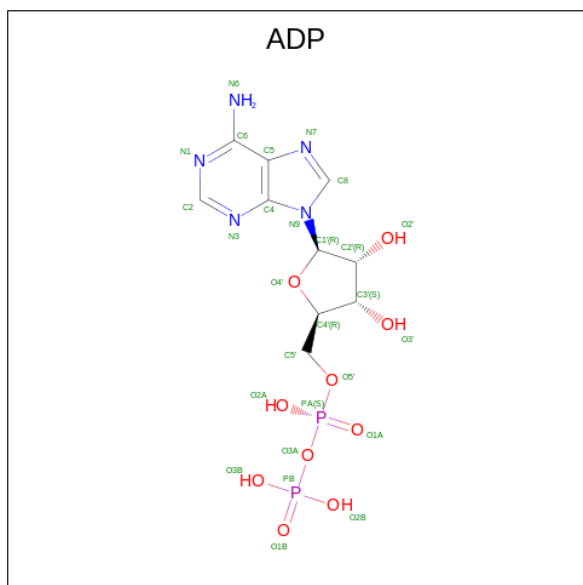
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	x	355	2810	1782	470	538	20	0	0

- Molecule 34 is a protein called Polyubiquitin-B.

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

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

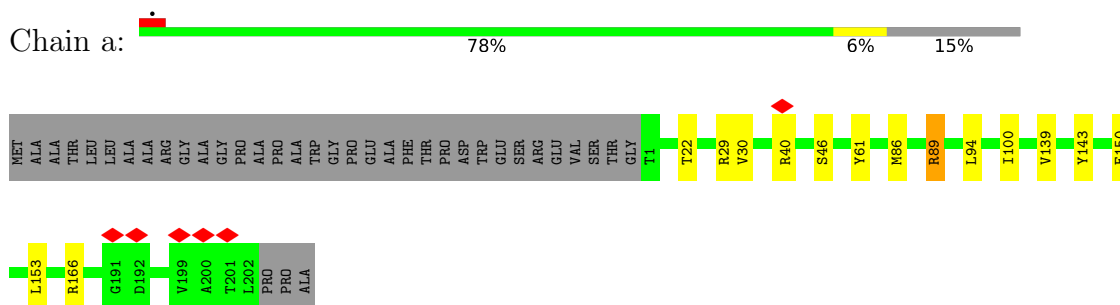


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

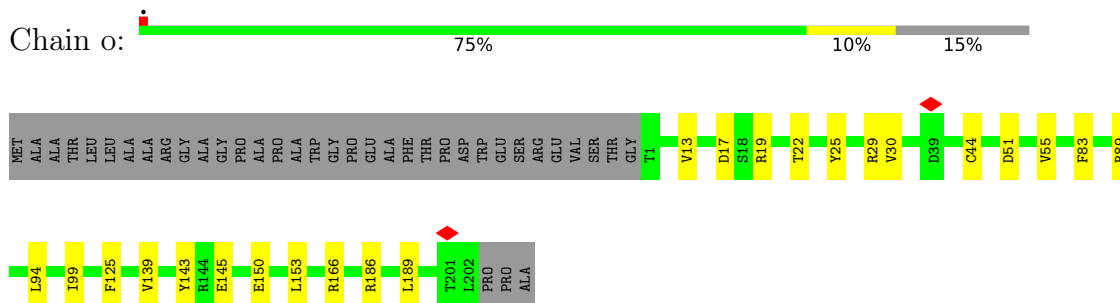
3 Residue-property plots [i](#)

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.

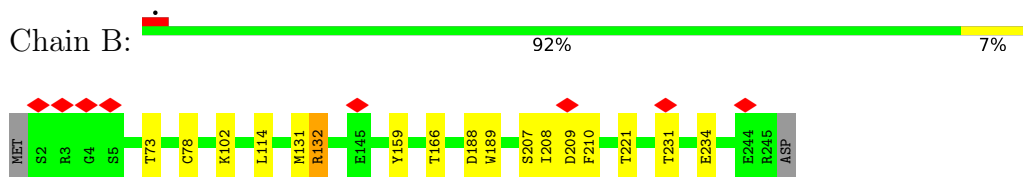
- Molecule 1: Proteasome subunit beta type-6



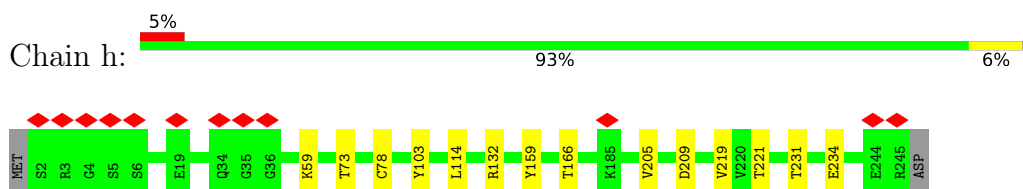
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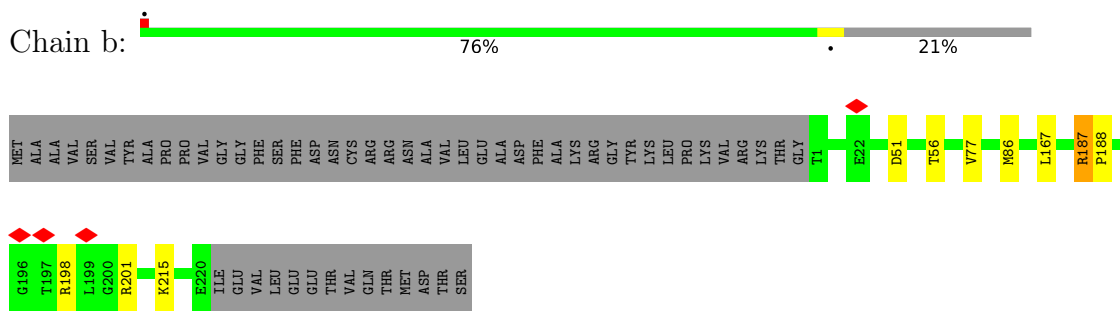
- Molecule 2: Proteasome subunit alpha type-6



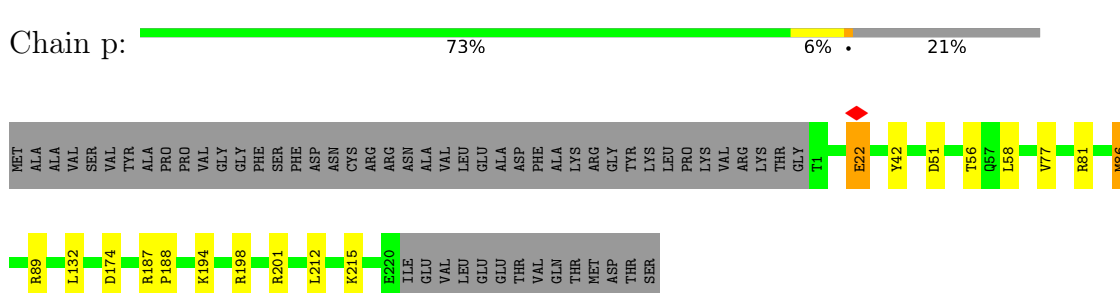
- Molecule 2: Proteasome subunit alpha type-6



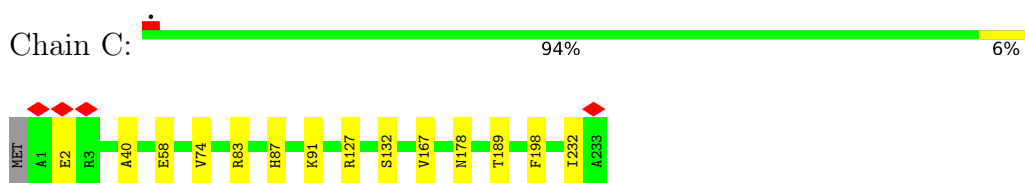
• Molecule 3: Proteasome subunit beta type-7



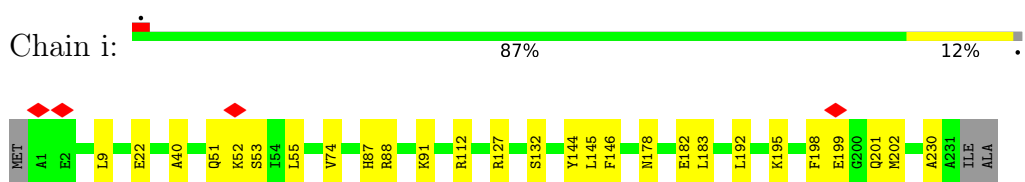
• Molecule 3: Proteasome subunit beta type-7



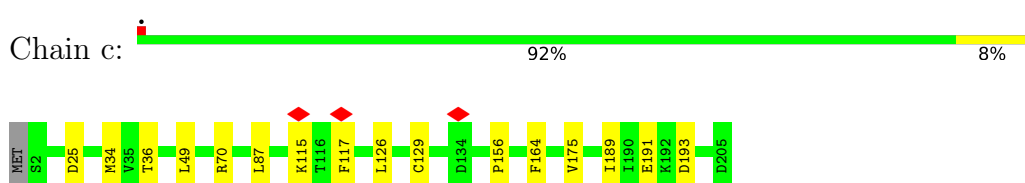
• Molecule 4: Proteasome subunit alpha type-2



• Molecule 4: Proteasome subunit alpha type-2



• Molecule 5: Proteasome subunit beta type-3

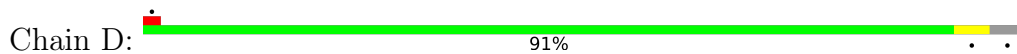


• Molecule 5: Proteasome subunit beta type-3

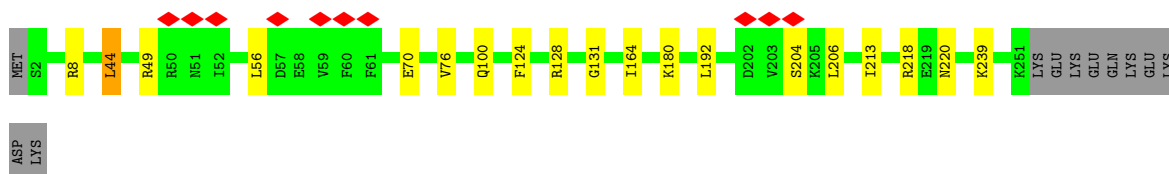
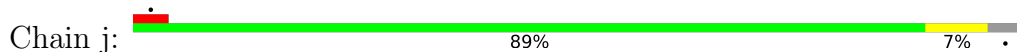




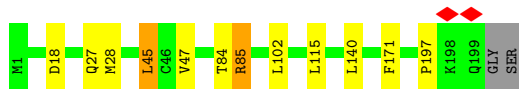
• Molecule 6: Proteasome subunit alpha type-4



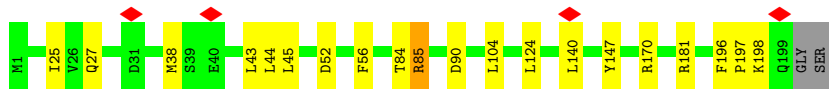
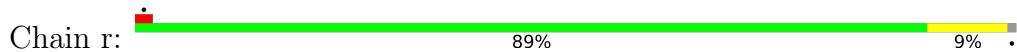
• Molecule 6: Proteasome subunit alpha type-4



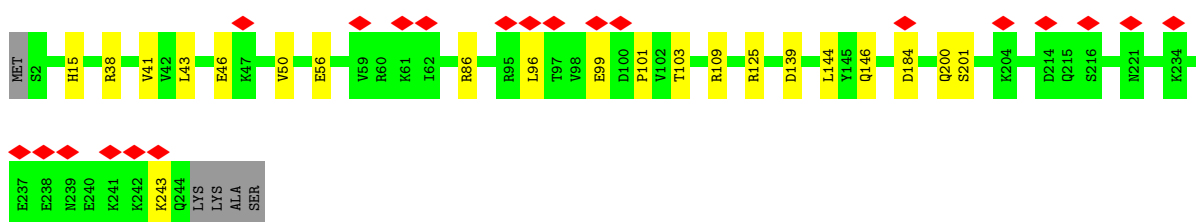
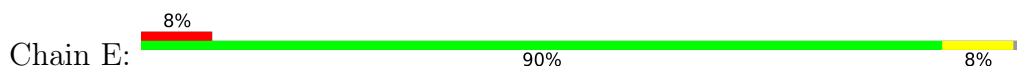
• Molecule 7: Proteasome subunit beta type-2



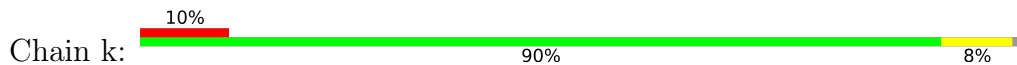
• Molecule 7: Proteasome subunit beta type-2

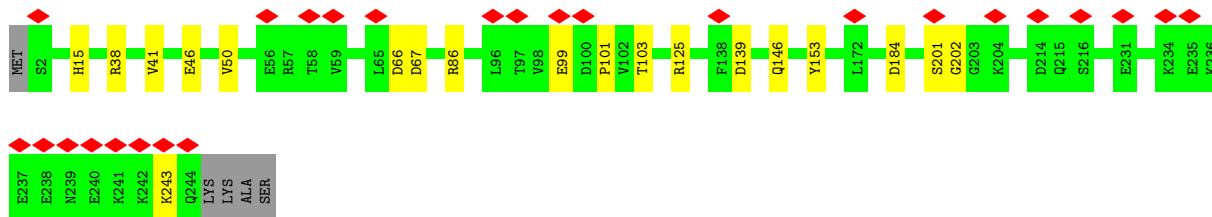


• Molecule 8: Proteasome subunit alpha type-7

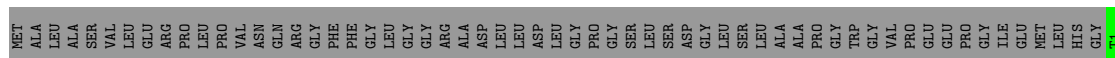


• Molecule 8: Proteasome subunit alpha type-7

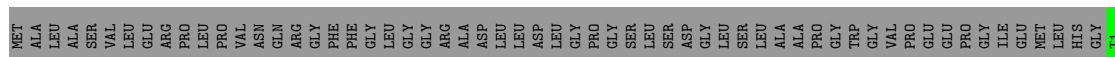




• Molecule 9: Proteasome subunit beta type-5



• Molecule 9: Proteasome subunit beta type-5



• Molecule 10: Proteasome subunit alpha type-5



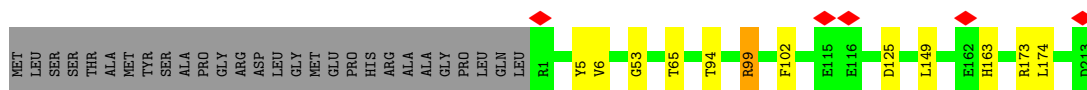
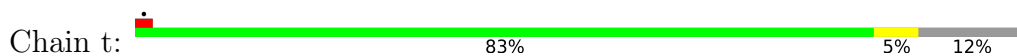
• Molecule 10: Proteasome subunit alpha type-5



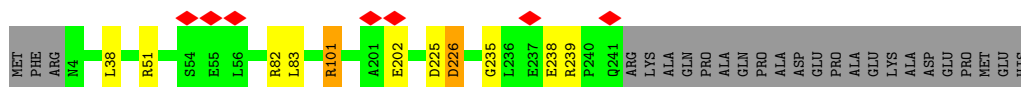
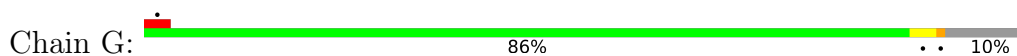
• Molecule 11: Proteasome subunit beta type-1



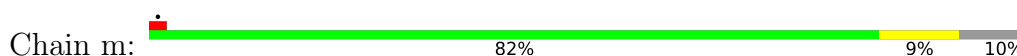
• Molecule 11: Proteasome subunit beta type-1



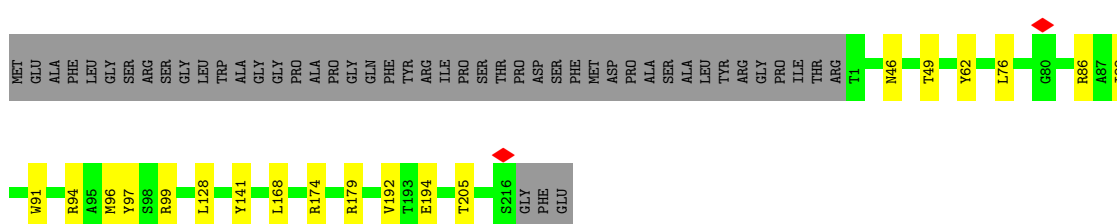
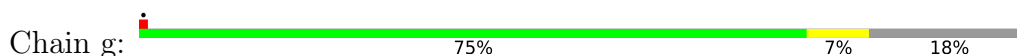
• Molecule 12: Proteasome subunit alpha type-1



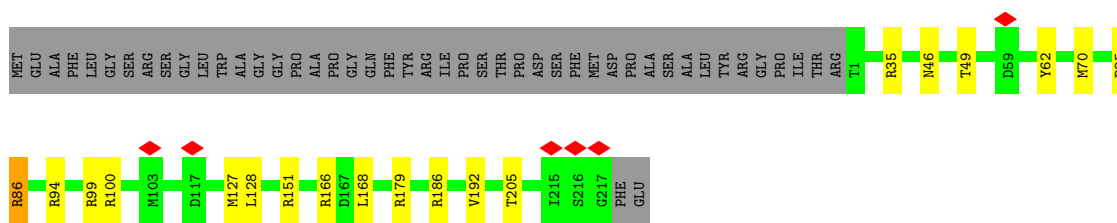
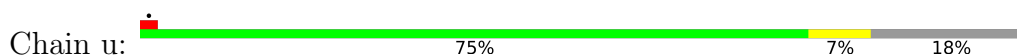
• Molecule 12: Proteasome subunit alpha type-1



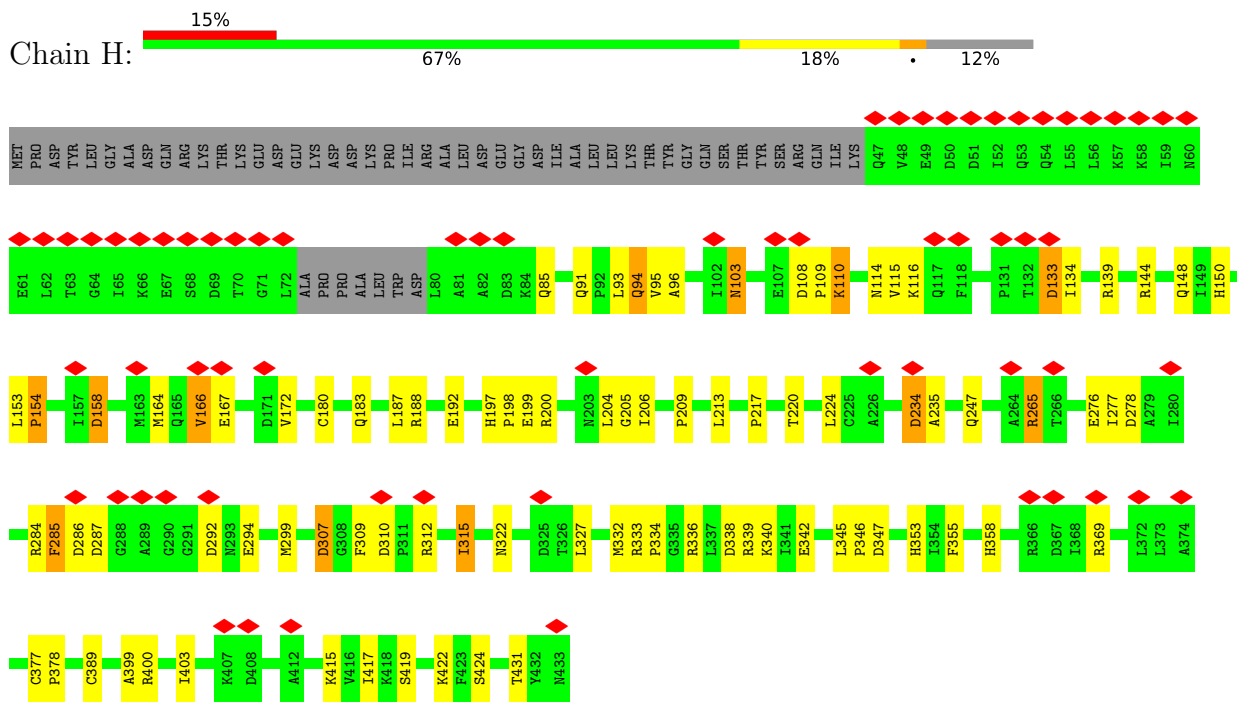
• Molecule 13: Proteasome subunit beta type-4



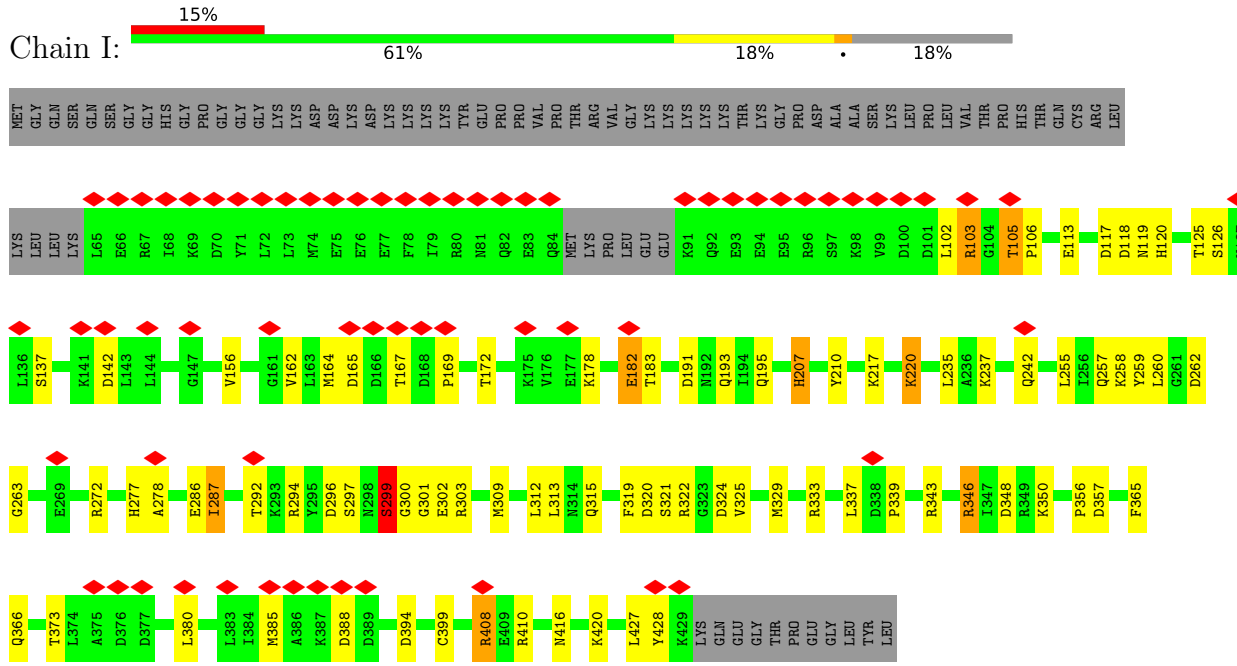
• Molecule 13: Proteasome subunit beta type-4



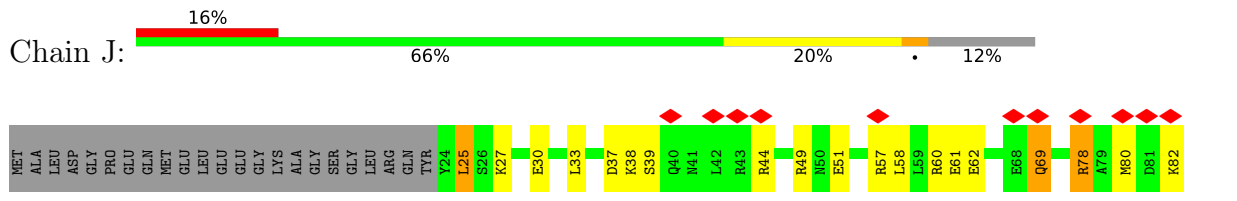
• Molecule 14: 26S protease regulatory subunit 7

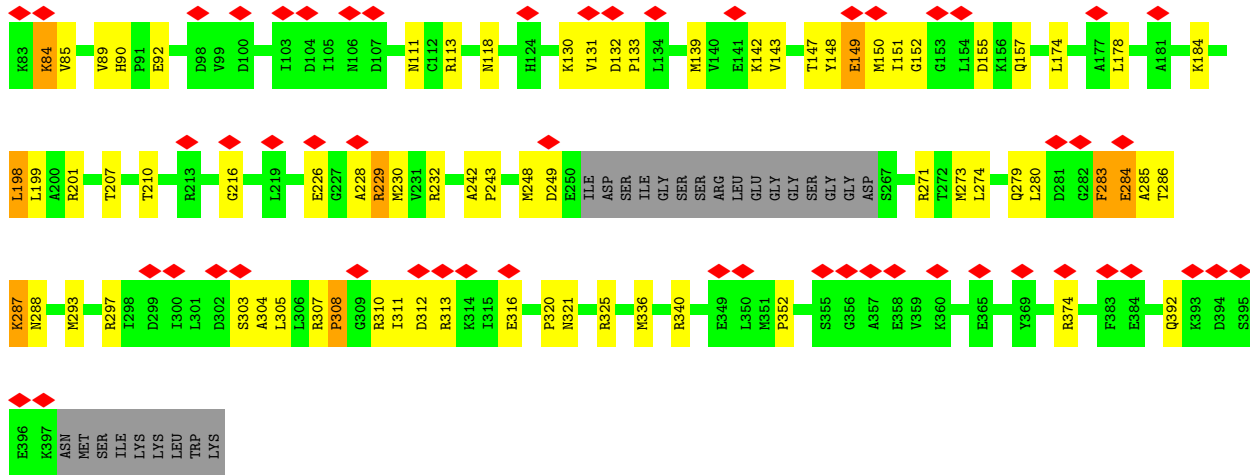


• Molecule 15: 26S protease regulatory subunit 4

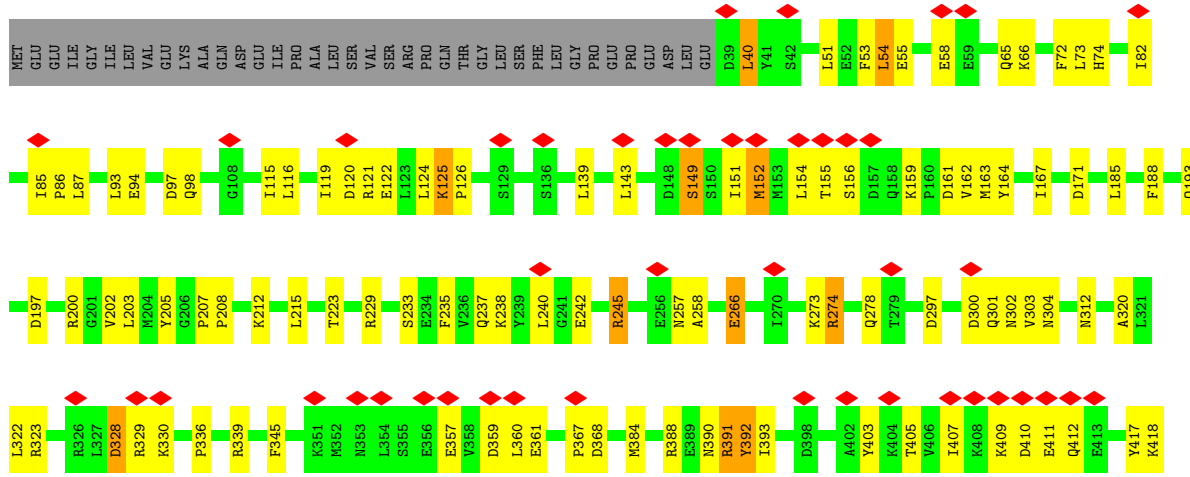


• Molecule 16: 26S protease regulatory subunit 8

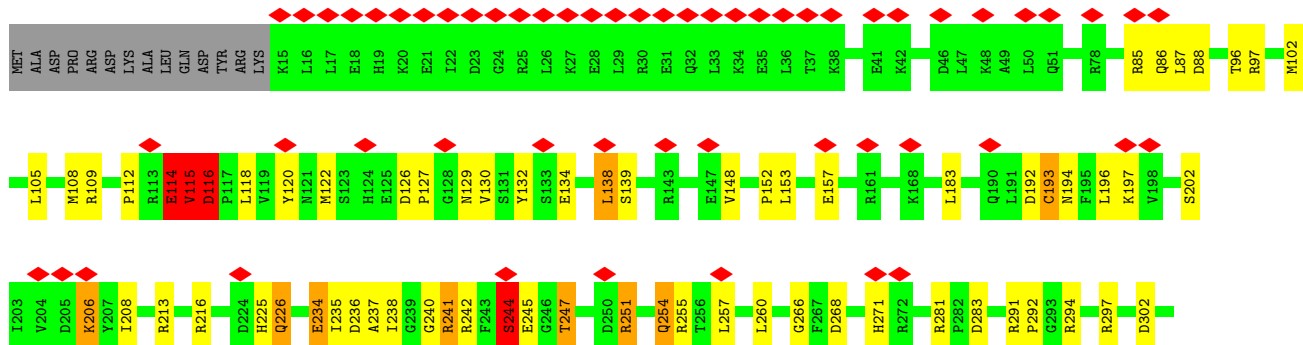
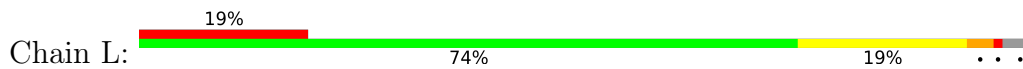




• Molecule 17: 26S protease regulatory subunit 6B

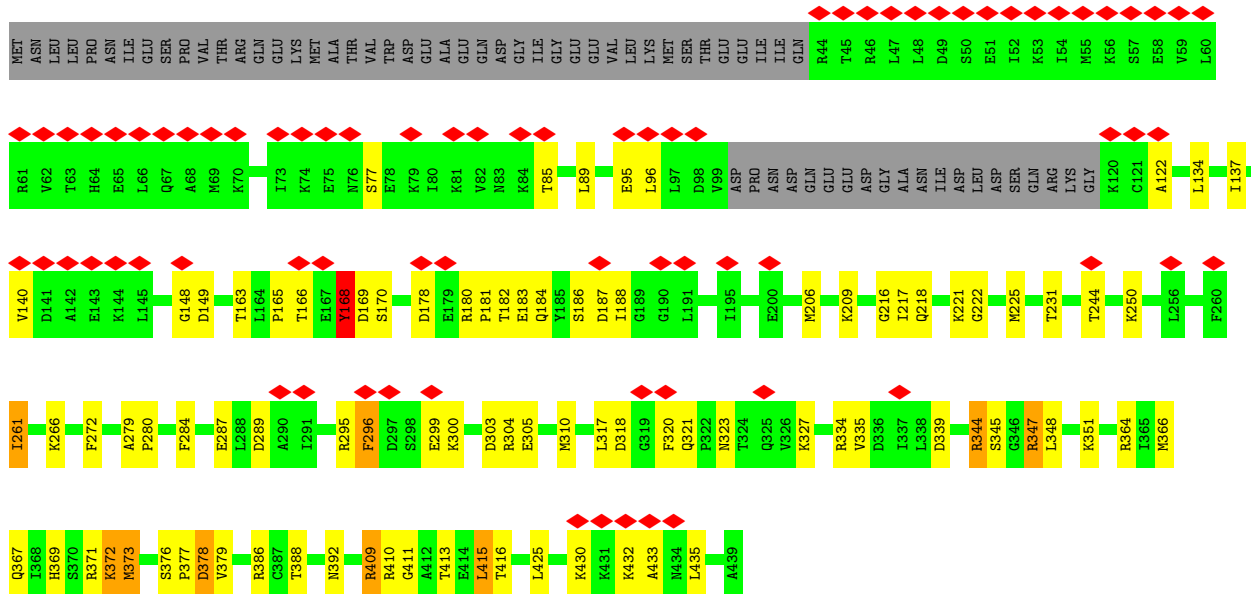


• Molecule 18: 26S protease regulatory subunit 10B

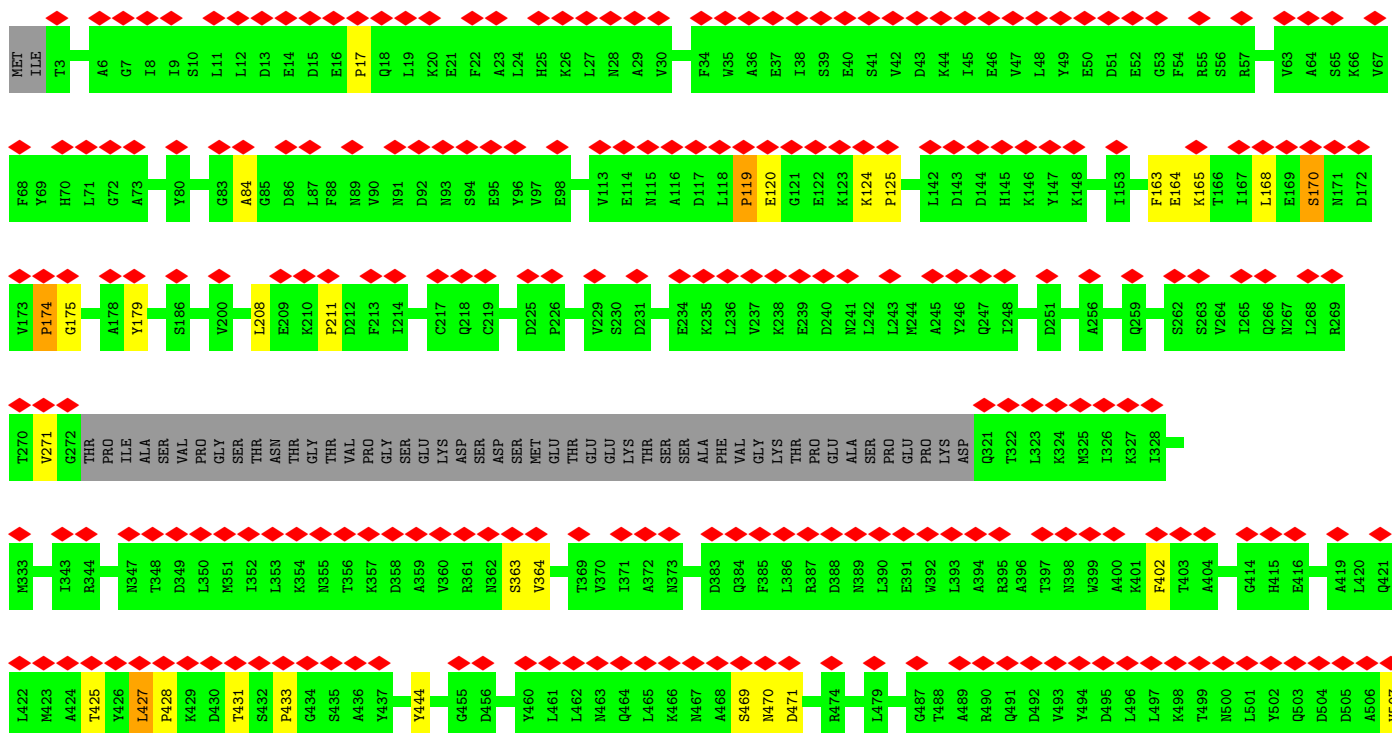
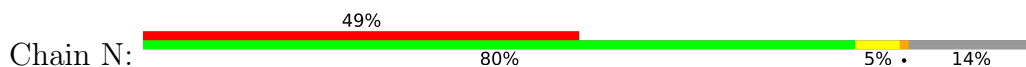


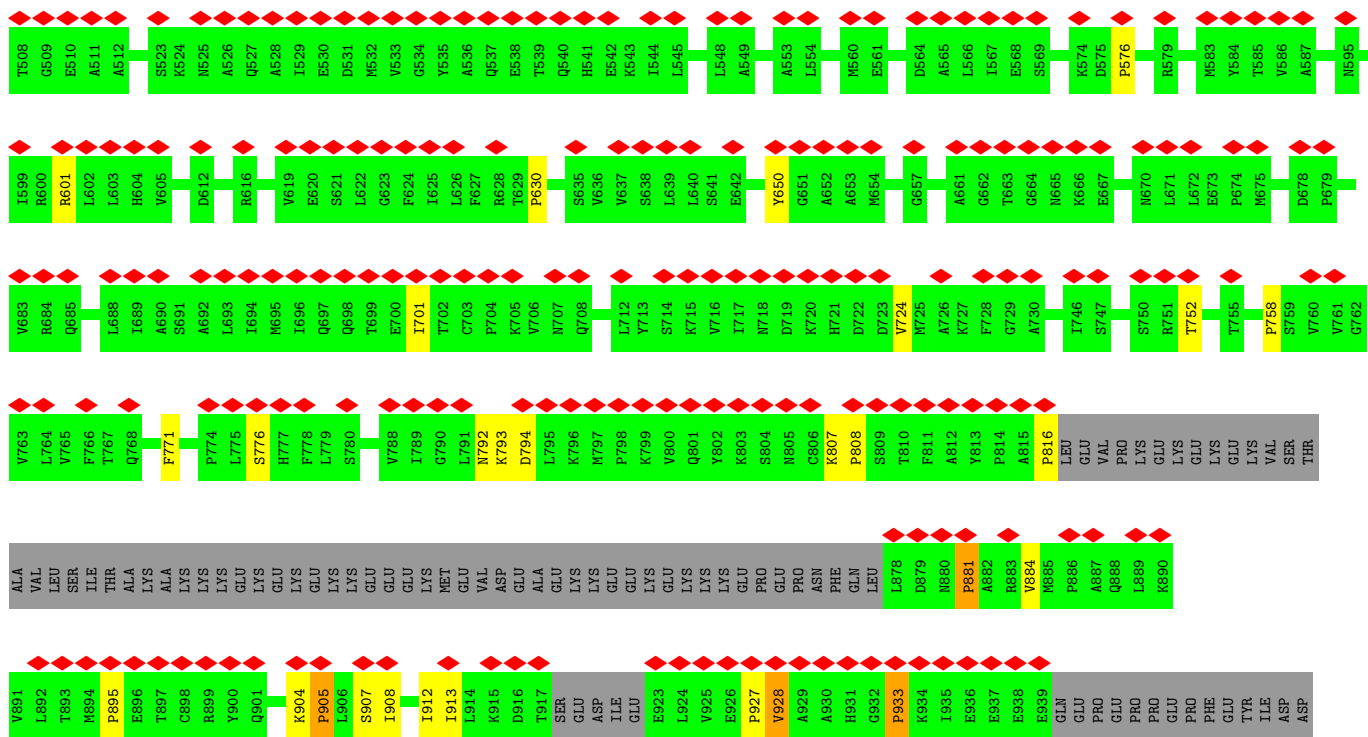


• Molecule 19: 26S protease regulatory subunit 6A

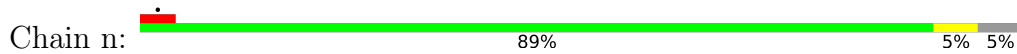


• Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

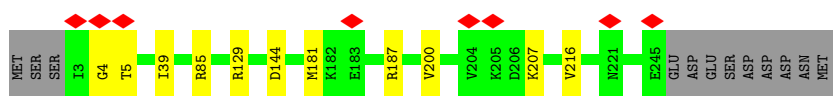
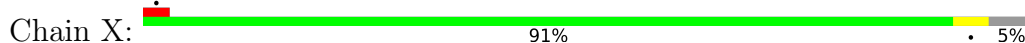




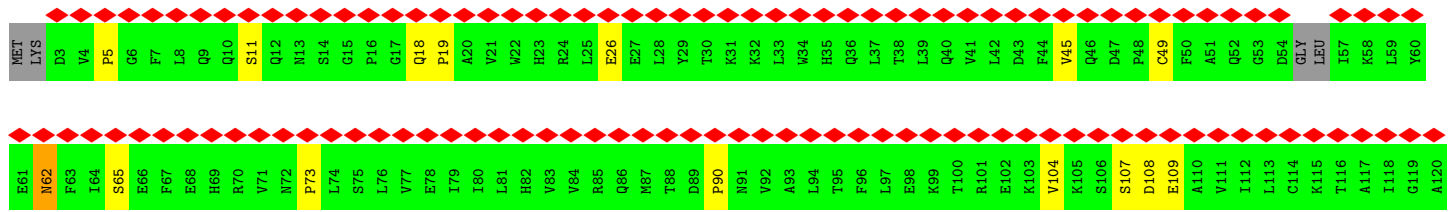
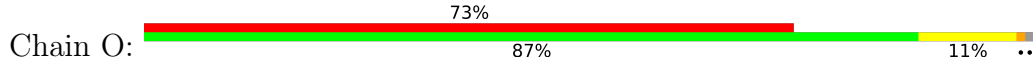
• Molecule 21: Proteasome subunit alpha type-3

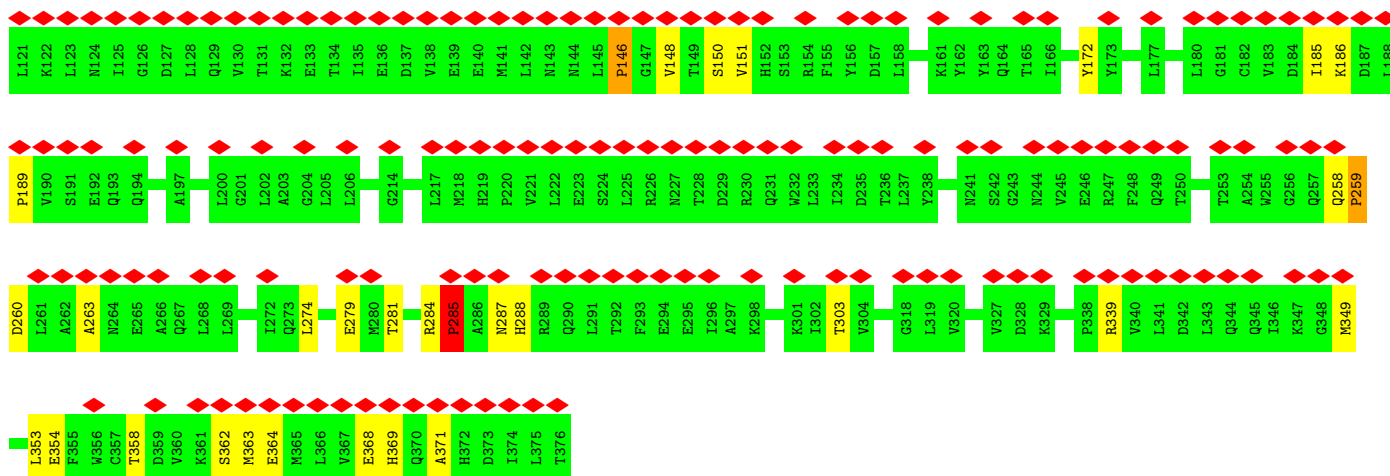


• Molecule 21: Proteasome subunit alpha type-3

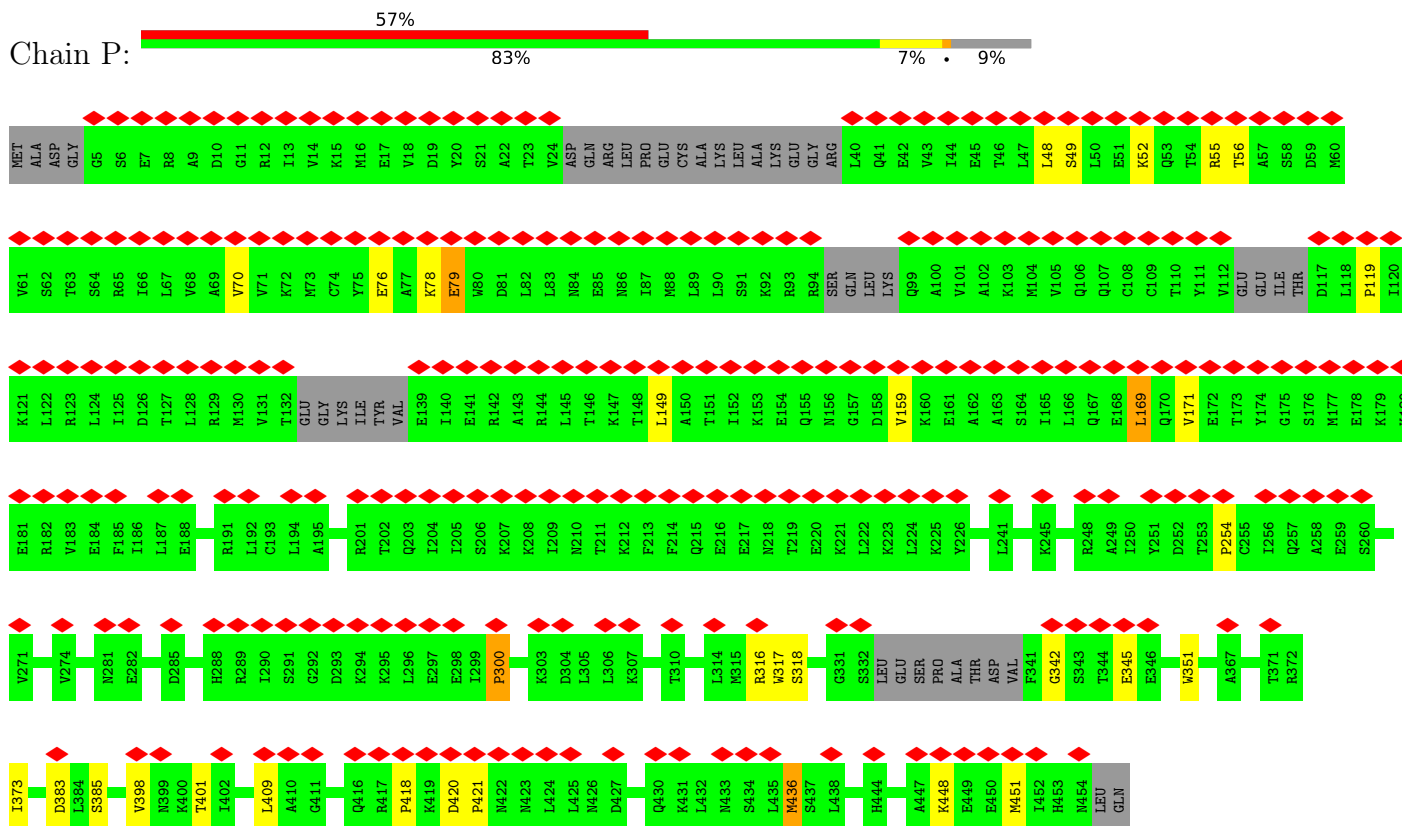


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

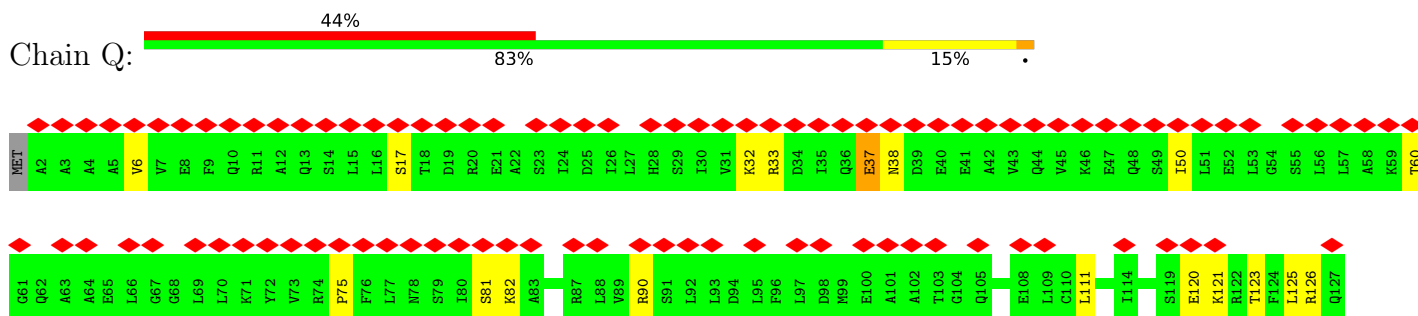


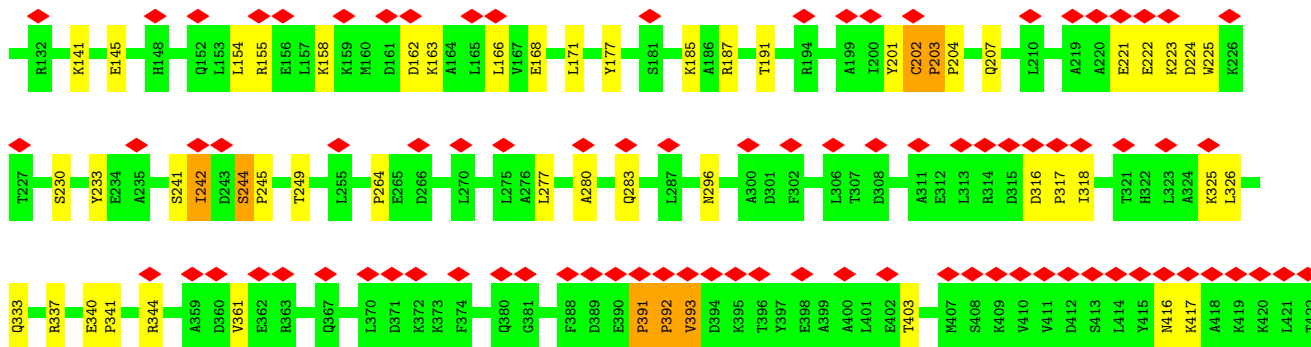


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

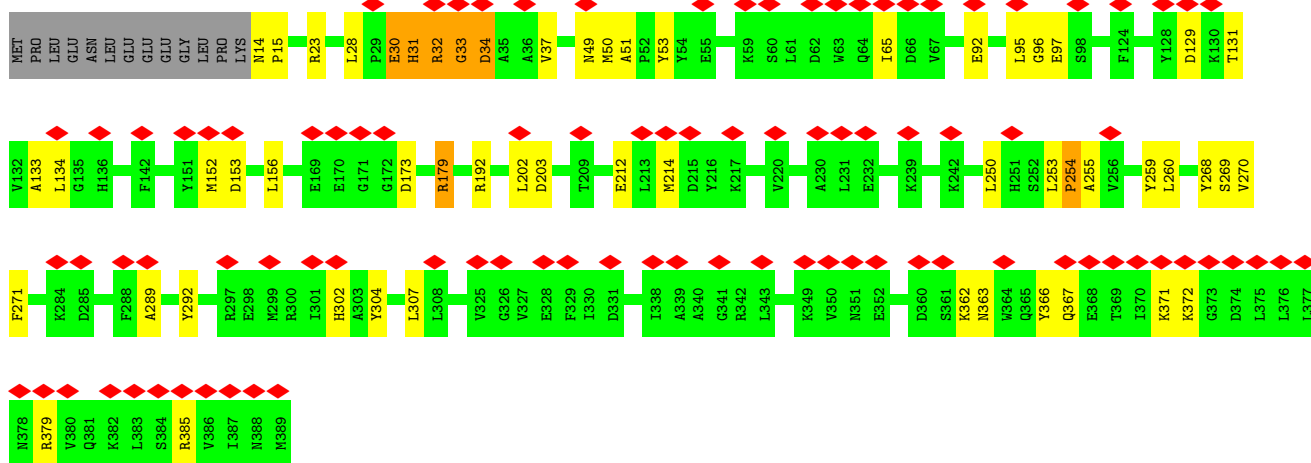
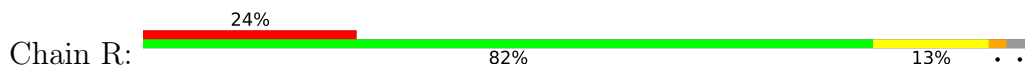


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

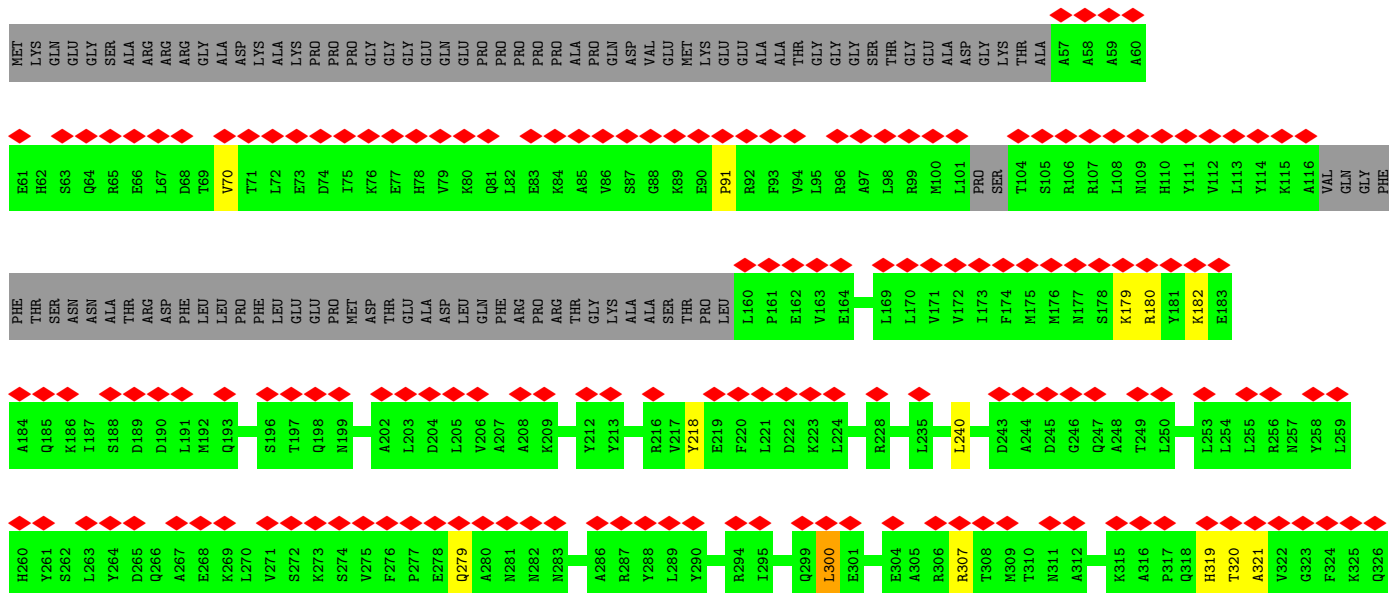


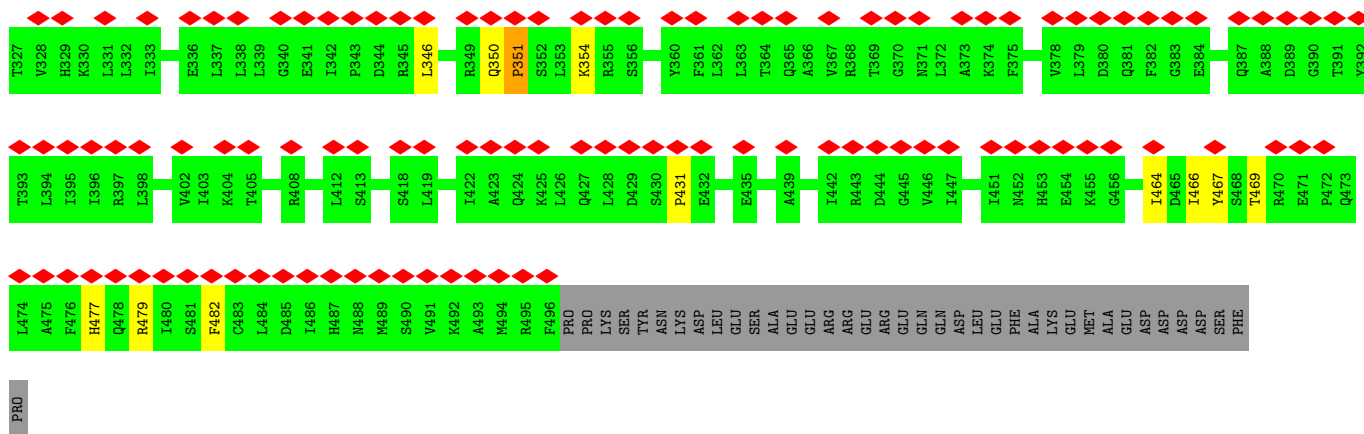


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

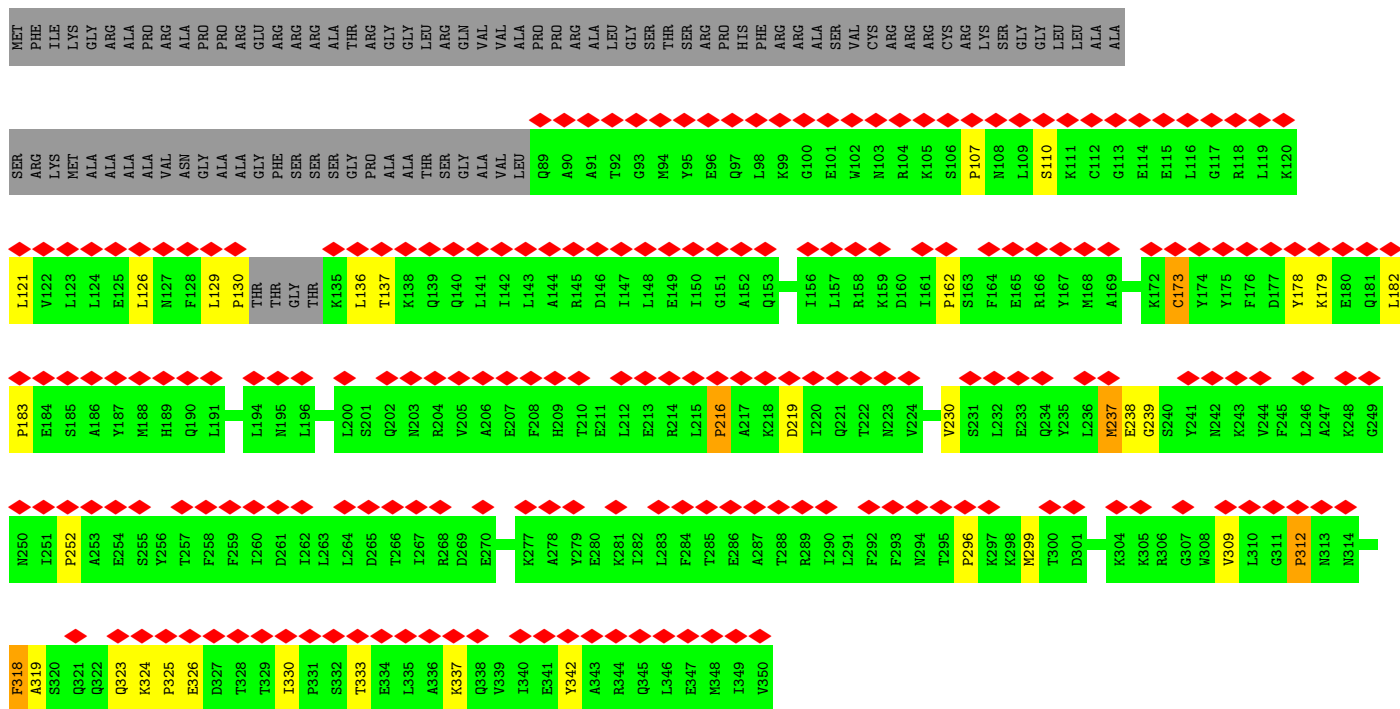


• Molecule 26: 26S proteasome non-ATPase regulatory subunit 3

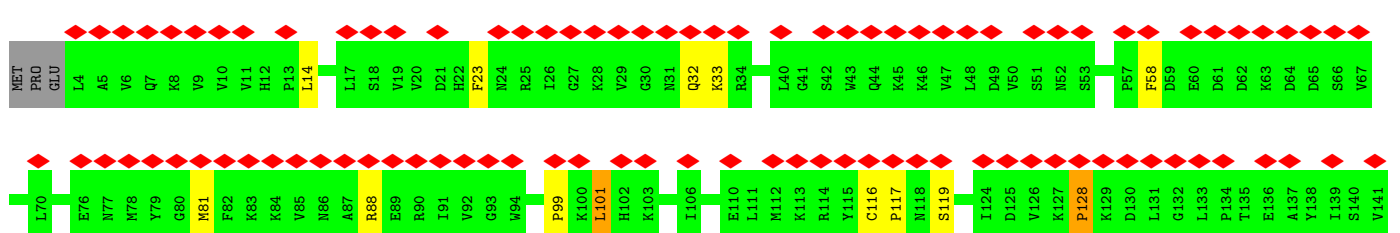
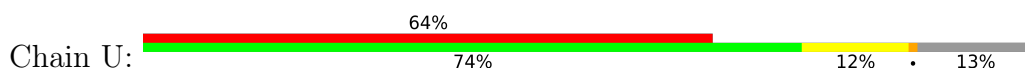


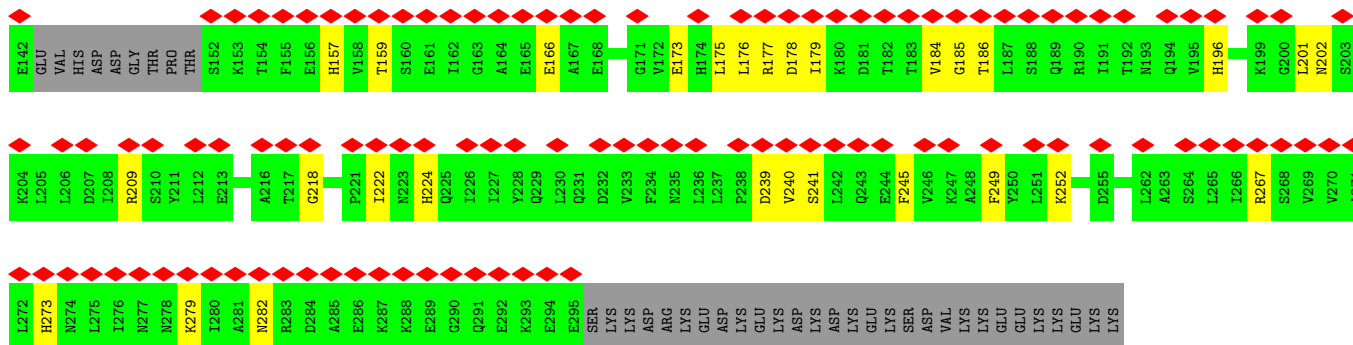


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 8

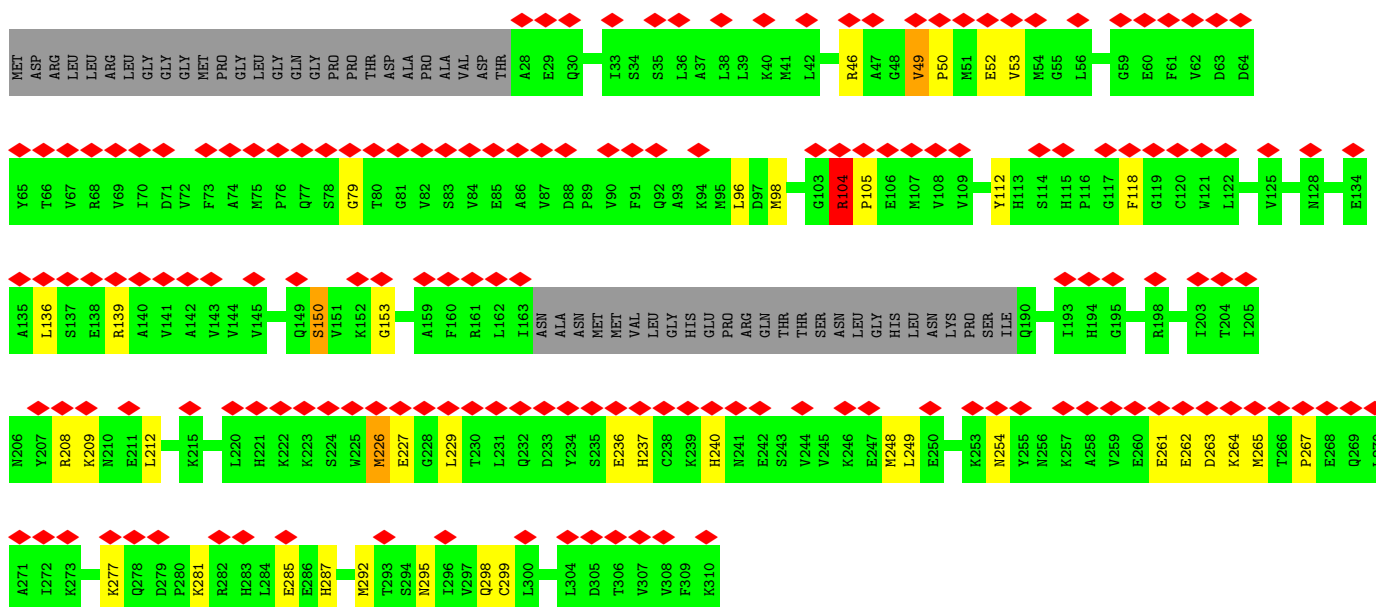


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 7

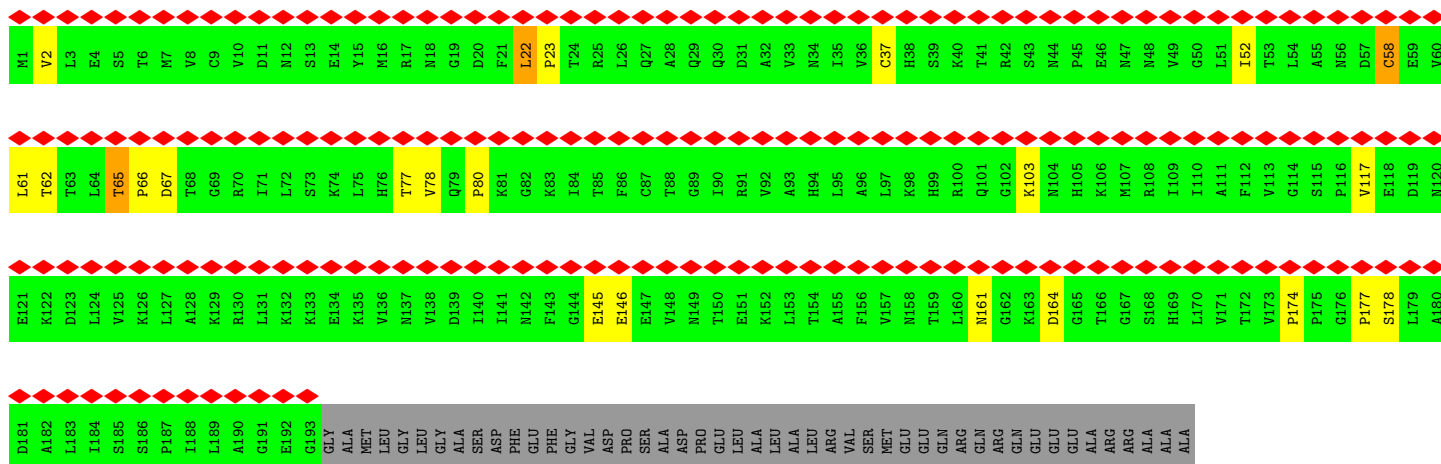


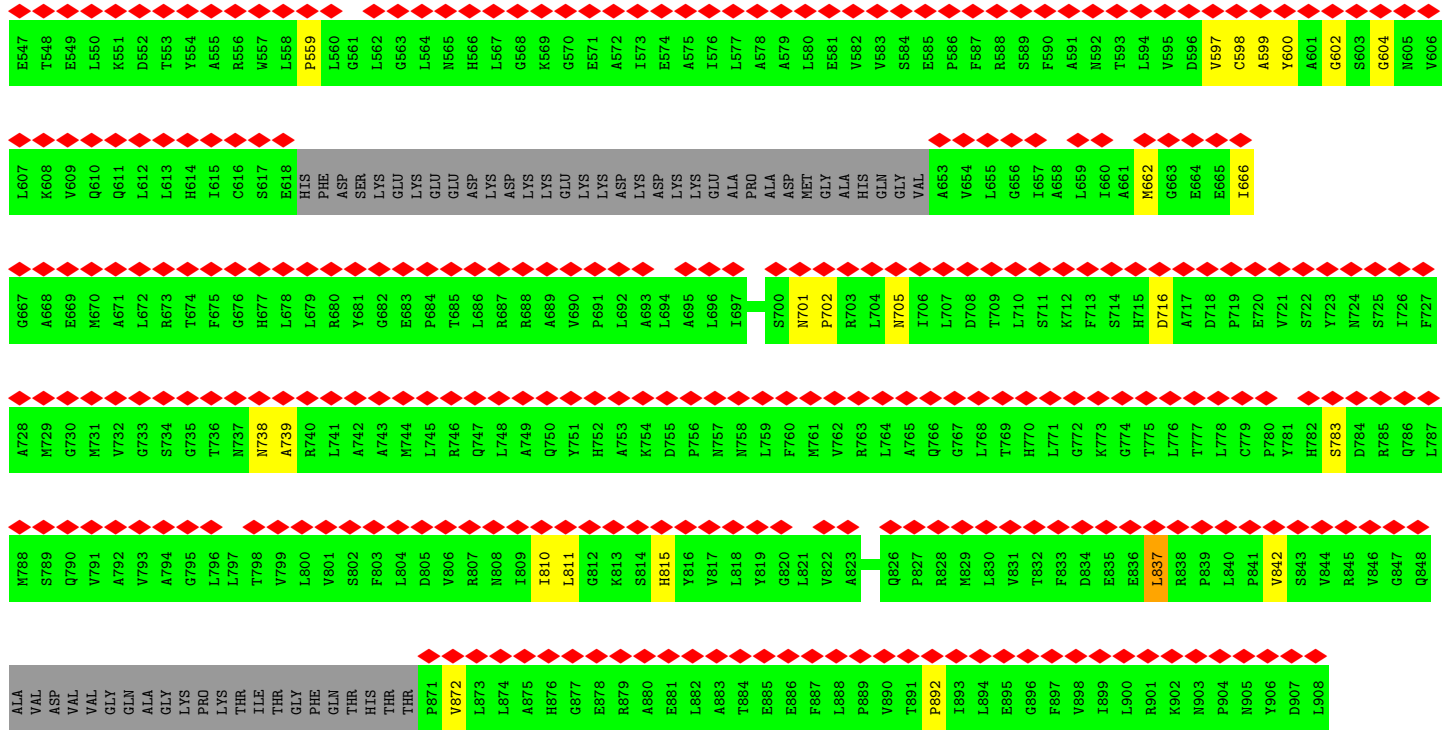


• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

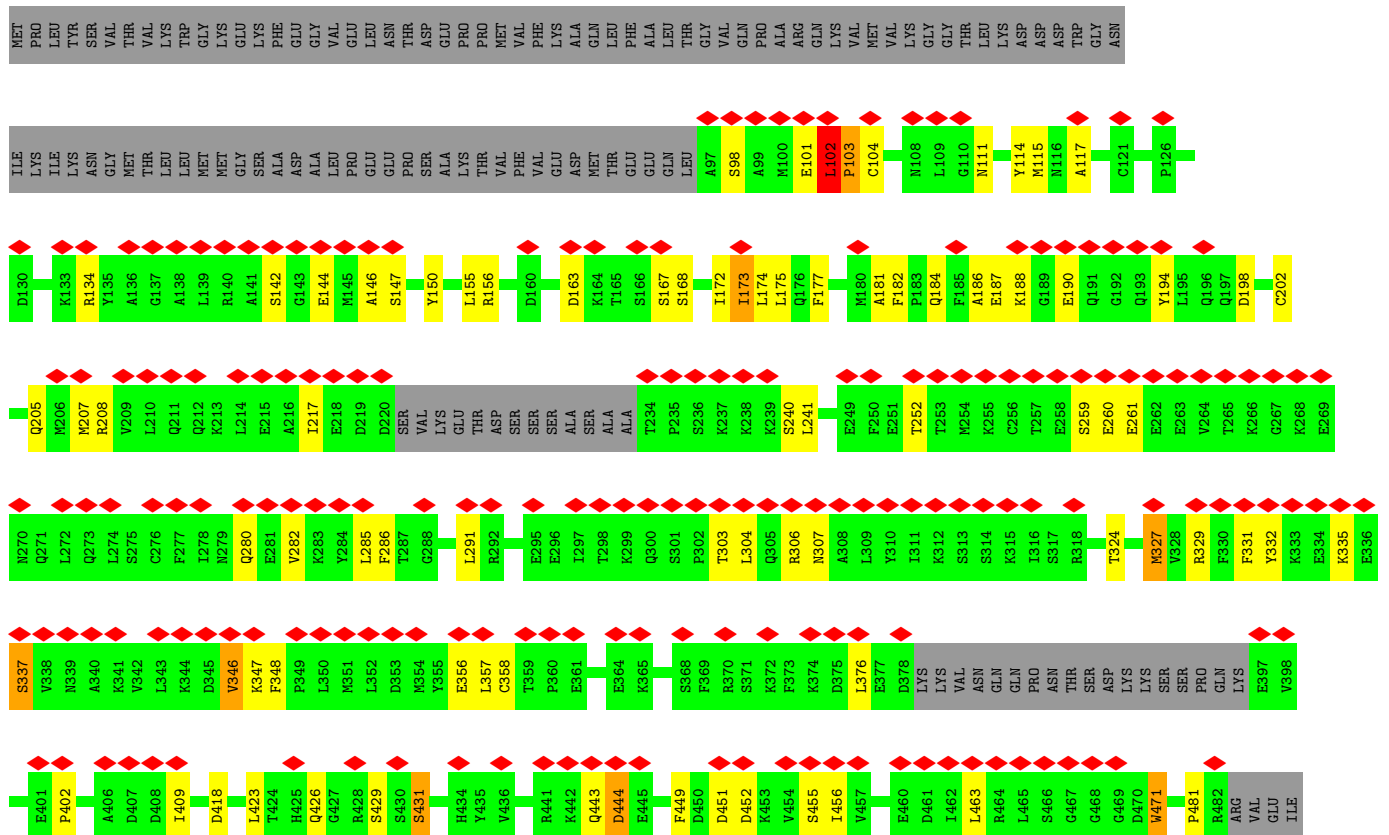
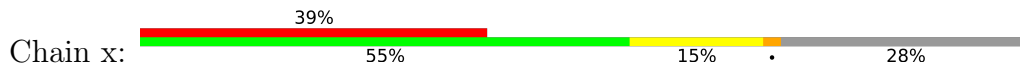


• Molecule 30: 26S proteasome non-ATPase regulatory subunit 4



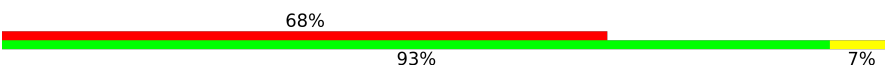


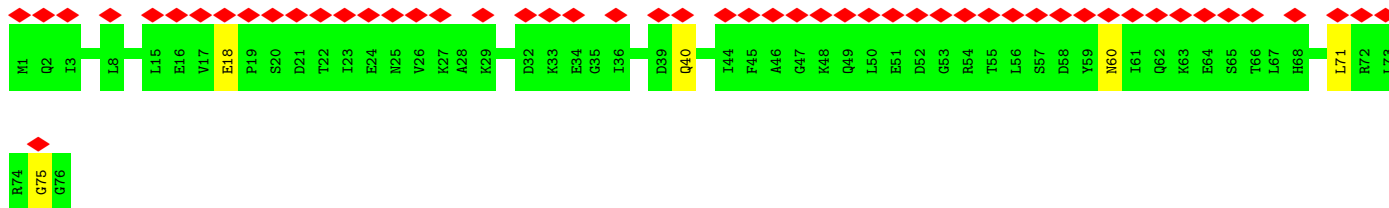
● Molecule 33: Ubiquitin carboxyl-terminal hydrolase 14



MET
GLU
GLU
GLU
SER
GLU
GLN

• Molecule 34: Polyubiquitin-B

Chain y: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	1.10	3/1535 (0.2%)	1.10	6/2078 (0.3%)
1	o	1.13	4/1535 (0.3%)	1.18	13/2078 (0.6%)
2	B	0.83	1/1878 (0.1%)	0.88	2/2549 (0.1%)
2	h	1.01	0/1886	1.00	2/2557 (0.1%)
3	b	0.98	0/1670	1.06	2/2265 (0.1%)
3	p	1.06	2/1670 (0.1%)	1.15	8/2265 (0.4%)
4	C	0.82	0/1742	0.89	4/2372 (0.2%)
4	i	1.11	5/1780 (0.3%)	1.10	7/2417 (0.3%)
5	c	1.08	2/1614 (0.1%)	1.11	6/2177 (0.3%)
5	q	1.21	5/1614 (0.3%)	1.19	4/2177 (0.2%)
6	D	0.81	2/1942 (0.1%)	0.89	1/2628 (0.0%)
6	j	0.99	1/1943 (0.1%)	1.04	7/2629 (0.3%)
7	d	0.99	0/1603	1.09	6/2174 (0.3%)
7	r	1.12	2/1603 (0.1%)	1.17	10/2174 (0.5%)
8	E	0.78	0/1748	0.88	5/2386 (0.2%)
8	k	0.95	2/1716 (0.1%)	1.04	5/2347 (0.2%)
9	e	1.08	2/1579 (0.1%)	1.11	7/2134 (0.3%)
9	s	1.13	4/1582 (0.3%)	1.10	6/2138 (0.3%)
10	F	0.76	0/1794	0.84	0/2430
10	l	0.95	1/1753 (0.1%)	1.01	4/2346 (0.2%)
11	f	1.03	1/1671 (0.1%)	1.05	2/2253 (0.1%)
11	t	1.08	2/1674 (0.1%)	1.14	4/2257 (0.2%)
12	G	0.77	0/1885	0.88	3/2552 (0.1%)
12	m	0.95	1/1885 (0.1%)	1.01	4/2552 (0.2%)
13	g	1.01	3/1705 (0.2%)	1.06	7/2312 (0.3%)
13	u	1.04	1/1711 (0.1%)	1.10	9/2319 (0.4%)
14	H	0.82	1/2925 (0.0%)	1.09	8/3952 (0.2%)
15	I	0.80	1/2756 (0.0%)	1.01	8/3727 (0.2%)
16	J	0.77	0/2857	0.95	4/3844 (0.1%)
17	K	0.81	1/3089 (0.0%)	0.99	7/4168 (0.2%)
18	L	0.79	4/2904 (0.1%)	1.09	12/3924 (0.3%)
19	M	0.75	0/2896	0.91	3/3912 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	N	0.41	1/5520 (0.0%)	0.60	1/7446 (0.0%)
21	X	0.83	0/1908	0.87	1/2575 (0.0%)
21	n	0.93	2/1908 (0.1%)	0.98	4/2575 (0.2%)
22	O	0.56	0/2387	0.74	3/3211 (0.1%)
23	P	0.54	0/2857	0.72	4/3855 (0.1%)
24	Q	0.62	1/2981 (0.0%)	0.76	4/4045 (0.1%)
25	R	0.65	1/2817 (0.0%)	0.80	6/3811 (0.2%)
26	S	0.57	0/2623	0.70	2/3545 (0.1%)
27	T	0.56	0/1716	0.68	3/2310 (0.1%)
28	U	0.58	0/2167	0.75	2/2936 (0.1%)
29	V	0.60	0/2047	0.83	4/2763 (0.1%)
30	W	0.52	0/1312	0.76	3/1769 (0.2%)
31	Y	0.58	0/307	0.84	1/424 (0.2%)
32	Z	0.32	0/3603	0.53	1/5005 (0.0%)
33	x	0.67	0/2860	0.90	2/3852 (0.1%)
34	y	0.60	0/603	0.75	0/811
All	All	0.83	56/99761 (0.1%)	0.94	217/135026 (0.2%)

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
3	b	0	2
4	i	0	1
6	j	0	1
7	r	0	1
14	H	0	1
15	I	0	4
16	J	0	1
17	K	0	1
18	L	0	4
19	M	0	2
20	N	0	3
22	O	0	2
23	P	0	2
24	Q	0	6
25	R	0	5
27	T	0	1
28	U	0	1
29	V	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	W	0	7
31	Y	0	2
32	Z	0	7
34	y	0	2
All	All	0	59

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	q	155	GLU	CD-OE2	13.15	1.40	1.25
18	L	116	ASP	N-CA	-10.28	1.25	1.46
4	i	22	GLU	CG-CD	8.89	1.65	1.51
3	p	81	ARG	CZ-NH2	8.66	1.44	1.33
5	c	164	PHE	CG-CD1	-8.04	1.26	1.38

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	115	VAL	CA-C-N	-22.22	68.32	117.20
14	H	336	ARG	NE-CZ-NH1	-21.51	109.54	120.30
18	L	115	VAL	C-N-CA	-18.03	76.64	121.70
14	H	336	ARG	NE-CZ-NH2	16.39	128.50	120.30
17	K	200	ARG	NE-CZ-NH1	14.57	127.59	120.30

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	H	154	PRO	Peptide
15	I	105	THR	Peptide
15	I	137	SER	Peptide
15	I	299	SER	Mainchain
3	b	187	ARG	Peptide,Mainchain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
1	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
2	B	242/246 (98%)	228 (94%)	9 (4%)	5 (2%)	7	39
2	h	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
3	b	218/277 (79%)	210 (96%)	7 (3%)	1 (0%)	29	68
3	p	218/277 (79%)	207 (95%)	9 (4%)	2 (1%)	17	56
4	C	231/234 (99%)	204 (88%)	24 (10%)	3 (1%)	12	48
4	i	229/234 (98%)	202 (88%)	24 (10%)	3 (1%)	12	48
5	c	202/205 (98%)	189 (94%)	11 (5%)	2 (1%)	15	54
5	q	202/205 (98%)	188 (93%)	11 (5%)	3 (2%)	10	46
6	D	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	34	72
6	j	248/261 (95%)	233 (94%)	12 (5%)	3 (1%)	13	50
7	d	197/201 (98%)	186 (94%)	10 (5%)	1 (0%)	29	68
7	r	197/201 (98%)	186 (94%)	9 (5%)	2 (1%)	15	54
8	E	241/248 (97%)	223 (92%)	12 (5%)	6 (2%)	5	35
8	k	241/248 (97%)	224 (93%)	11 (5%)	6 (2%)	5	35
9	e	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
9	s	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
10	F	232/241 (96%)	216 (93%)	14 (6%)	2 (1%)	17	56
10	l	232/241 (96%)	215 (93%)	15 (6%)	2 (1%)	17	56
11	f	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
11	t	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
12	G	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	12	48
12	m	236/263 (90%)	222 (94%)	10 (4%)	4 (2%)	9	43
13	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	u	215/264 (81%)	205 (95%)	9 (4%)	1 (0%)	29	68
14	H	376/433 (87%)	254 (68%)	81 (22%)	41 (11%)	0	8
15	I	355/440 (81%)	264 (74%)	63 (18%)	28 (8%)	1	14
16	J	354/406 (87%)	253 (72%)	68 (19%)	33 (9%)	0	12
17	K	378/418 (90%)	260 (69%)	73 (19%)	45 (12%)	0	6
18	L	373/389 (96%)	268 (72%)	69 (18%)	36 (10%)	0	11
19	M	372/439 (85%)	257 (69%)	72 (19%)	43 (12%)	0	6
20	N	815/953 (86%)	610 (75%)	176 (22%)	29 (4%)	3	28
21	X	241/255 (94%)	233 (97%)	5 (2%)	3 (1%)	13	50
21	n	241/255 (94%)	232 (96%)	7 (3%)	2 (1%)	19	60
22	O	368/376 (98%)	292 (79%)	55 (15%)	21 (6%)	1	20
23	P	401/456 (88%)	333 (83%)	55 (14%)	13 (3%)	4	30
24	Q	419/422 (99%)	324 (77%)	67 (16%)	28 (7%)	1	18
25	R	374/389 (96%)	292 (78%)	60 (16%)	22 (6%)	1	20
26	S	389/534 (73%)	332 (85%)	42 (11%)	15 (4%)	3	26
27	T	254/350 (73%)	191 (75%)	44 (17%)	19 (8%)	1	15
28	U	279/324 (86%)	224 (80%)	42 (15%)	13 (5%)	2	24
29	V	253/310 (82%)	210 (83%)	32 (13%)	11 (4%)	2	25
30	W	191/377 (51%)	143 (75%)	38 (20%)	10 (5%)	2	22
31	Y	55/70 (79%)	36 (66%)	12 (22%)	7 (13%)	0	5
32	Z	722/908 (80%)	560 (78%)	113 (16%)	49 (7%)	1	17
33	x	349/494 (71%)	245 (70%)	62 (18%)	42 (12%)	0	6
34	y	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	13374/15440 (87%)	11297 (84%)	1514 (11%)	563 (4%)	5	25

5 of 563 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	120	ALA
12	G	238	GLU
14	H	95	VAL
14	H	108	ASP
14	H	109	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	155/181 (86%)	148 (96%)	7 (4%)	27	54
1	o	155/181 (86%)	148 (96%)	7 (4%)	27	54
2	B	193/210 (92%)	182 (94%)	11 (6%)	20	48
2	h	195/210 (93%)	183 (94%)	12 (6%)	18	45
3	b	177/228 (78%)	170 (96%)	7 (4%)	31	56
3	p	177/228 (78%)	168 (95%)	9 (5%)	24	50
4	C	163/191 (85%)	155 (95%)	8 (5%)	25	51
4	i	177/191 (93%)	163 (92%)	14 (8%)	12	38
5	c	172/174 (99%)	163 (95%)	9 (5%)	23	50
5	q	172/174 (99%)	163 (95%)	9 (5%)	23	50
6	D	193/221 (87%)	182 (94%)	11 (6%)	20	48
6	j	193/221 (87%)	183 (95%)	10 (5%)	23	50
7	d	164/171 (96%)	156 (95%)	8 (5%)	25	51
7	r	164/171 (96%)	157 (96%)	7 (4%)	29	55
8	E	152/211 (72%)	142 (93%)	10 (7%)	16	43
8	k	142/211 (67%)	134 (94%)	8 (6%)	21	48
9	e	153/202 (76%)	149 (97%)	4 (3%)	46	67
9	s	154/202 (76%)	148 (96%)	6 (4%)	32	57
10	F	190/203 (94%)	185 (97%)	5 (3%)	46	67
10	l	191/203 (94%)	185 (97%)	6 (3%)	40	63
11	f	174/199 (87%)	166 (95%)	8 (5%)	27	53
11	t	175/199 (88%)	168 (96%)	7 (4%)	31	56
12	G	198/224 (88%)	191 (96%)	7 (4%)	36	60
12	m	198/224 (88%)	183 (92%)	15 (8%)	13	40
13	g	175/215 (81%)	166 (95%)	9 (5%)	24	50
13	u	175/215 (81%)	164 (94%)	11 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	292/372 (78%)	238 (82%)	54 (18%)	1	10
15	I	291/385 (76%)	231 (79%)	60 (21%)	1	7
16	J	310/352 (88%)	246 (79%)	64 (21%)	1	7
17	K	333/366 (91%)	268 (80%)	65 (20%)	1	9
18	L	298/341 (87%)	239 (80%)	59 (20%)	1	9
19	M	296/379 (78%)	240 (81%)	56 (19%)	1	9
20	N	377/816 (46%)	345 (92%)	32 (8%)	10	36
21	X	193/212 (91%)	186 (96%)	7 (4%)	35	60
21	n	193/212 (91%)	184 (95%)	9 (5%)	26	52
22	O	144/336 (43%)	119 (83%)	25 (17%)	2	12
23	P	202/416 (49%)	182 (90%)	20 (10%)	8	28
24	Q	249/362 (69%)	207 (83%)	42 (17%)	2	13
25	R	226/344 (66%)	196 (87%)	30 (13%)	4	20
26	S	163/460 (35%)	153 (94%)	10 (6%)	18	46
27	T	109/294 (37%)	92 (84%)	17 (16%)	2	16
28	U	212/295 (72%)	184 (87%)	28 (13%)	4	20
29	V	219/268 (82%)	188 (86%)	31 (14%)	3	18
30	W	109/312 (35%)	102 (94%)	7 (6%)	17	44
31	Y	4/63 (6%)	4 (100%)	0	100	100
33	x	305/439 (70%)	254 (83%)	51 (17%)	2	14
34	y	68/68 (100%)	64 (94%)	4 (6%)	19	47
All	All	9120/12352 (74%)	8224 (90%)	896 (10%)	11	28

5 of 896 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	M	168	TYR
33	x	431	SER
22	O	65	SER
33	x	337	SER
29	V	98	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
30	W	169	HIS
33	x	197	GLN
34	y	25	ASN
17	K	302	ASN
17	K	286	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	GLZ	y	76	34	3,3,3	0.74	0	0,2,2	-	-

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	GLZ	y	76	34	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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
35	ADP	H	501	-	24,29,29	1.58	4 (16%)	29,45,45	2.76	10 (34%)
35	ADP	L	401	-	24,29,29	1.02	1 (4%)	29,45,45	1.74	8 (27%)
35	ADP	I	501	-	24,29,29	1.47	3 (12%)	29,45,45	1.90	6 (20%)
35	ADP	K	501	-	24,29,29	1.34	3 (12%)	29,45,45	1.92	11 (37%)
35	ADP	J	501	-	24,29,29	1.35	4 (16%)	29,45,45	2.15	9 (31%)
35	ADP	M	501	-	24,29,29	1.16	3 (12%)	29,45,45	1.81	10 (34%)

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
35	ADP	H	501	-	-	2/12/32/32	0/3/3/3
35	ADP	L	401	-	-	2/12/32/32	0/3/3/3
35	ADP	I	501	-	-	3/12/32/32	0/3/3/3
35	ADP	K	501	-	-	5/12/32/32	0/3/3/3
35	ADP	J	501	-	-	5/12/32/32	0/3/3/3
35	ADP	M	501	-	-	3/12/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H	501	ADP	O4'-C1'	4.76	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	I	501	ADP	C5-C4	4.40	1.52	1.40
35	J	501	ADP	C2'-C1'	-2.91	1.49	1.53
35	H	501	ADP	C6-C5	2.90	1.54	1.43
35	K	501	ADP	O4'-C1'	2.80	1.45	1.41

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	H	501	ADP	C3'-C2'-C1'	7.83	112.77	100.98
35	H	501	ADP	O4'-C1'-C2'	-5.76	98.51	106.93
35	I	501	ADP	C3'-C2'-C1'	5.66	109.49	100.98
35	H	501	ADP	C4-C5-N7	-5.00	104.19	109.40
35	J	501	ADP	N3-C2-N1	-4.59	121.50	128.68

There are no chirality outliers.

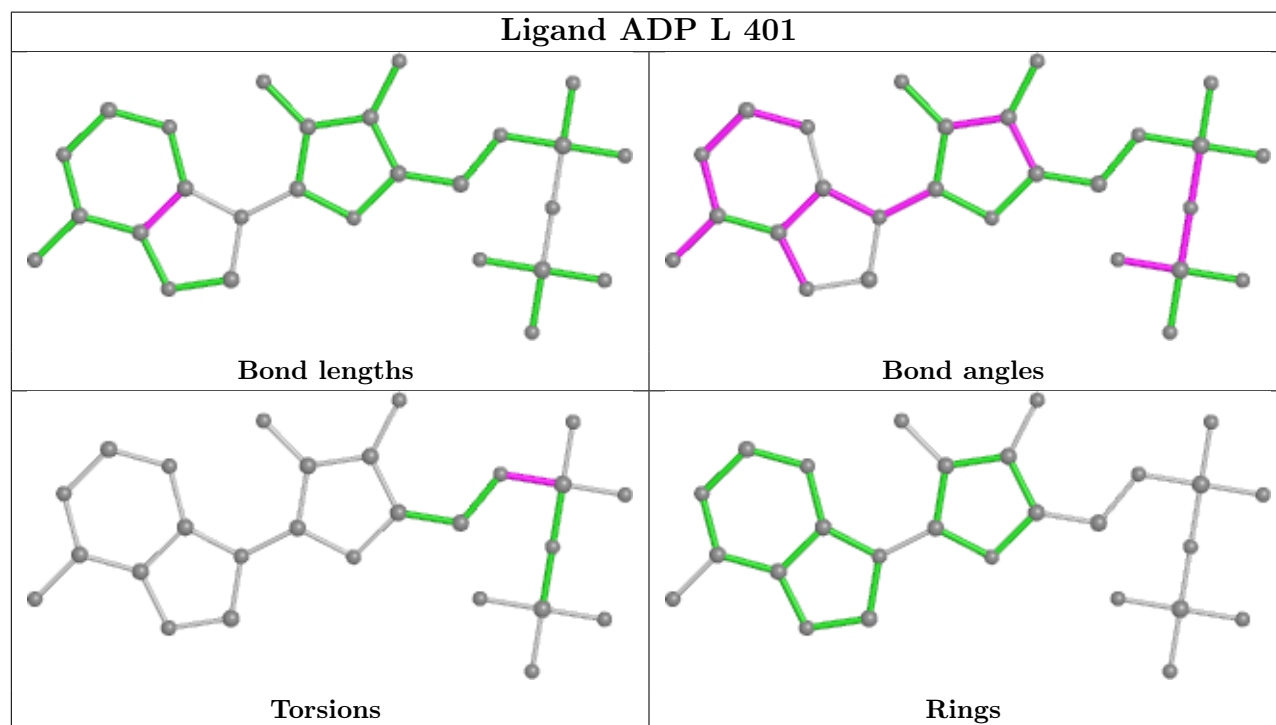
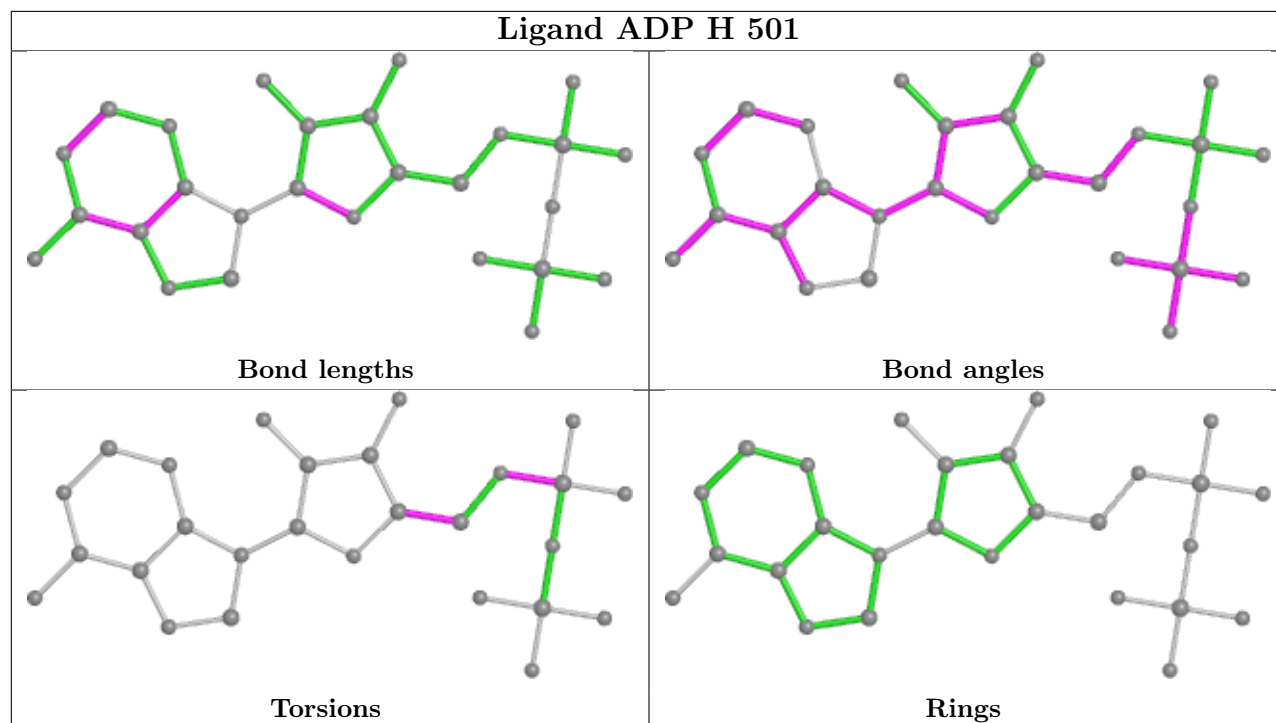
5 of 20 torsion outliers are listed below:

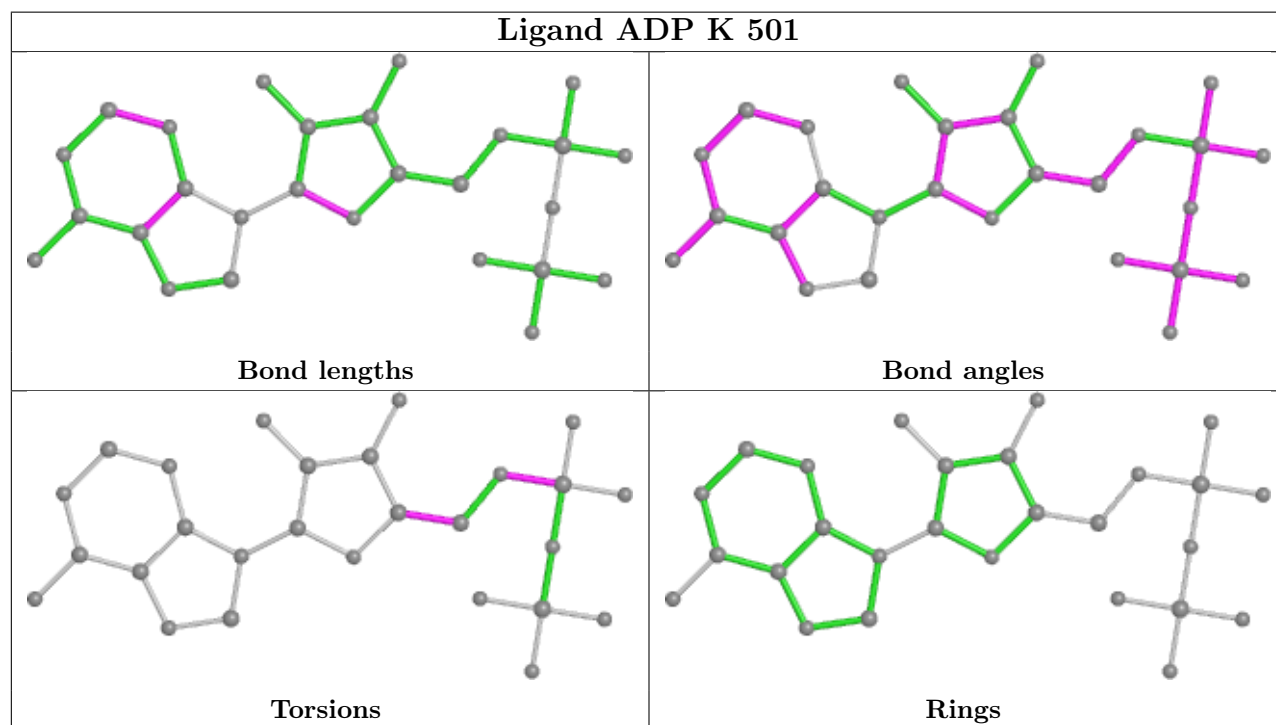
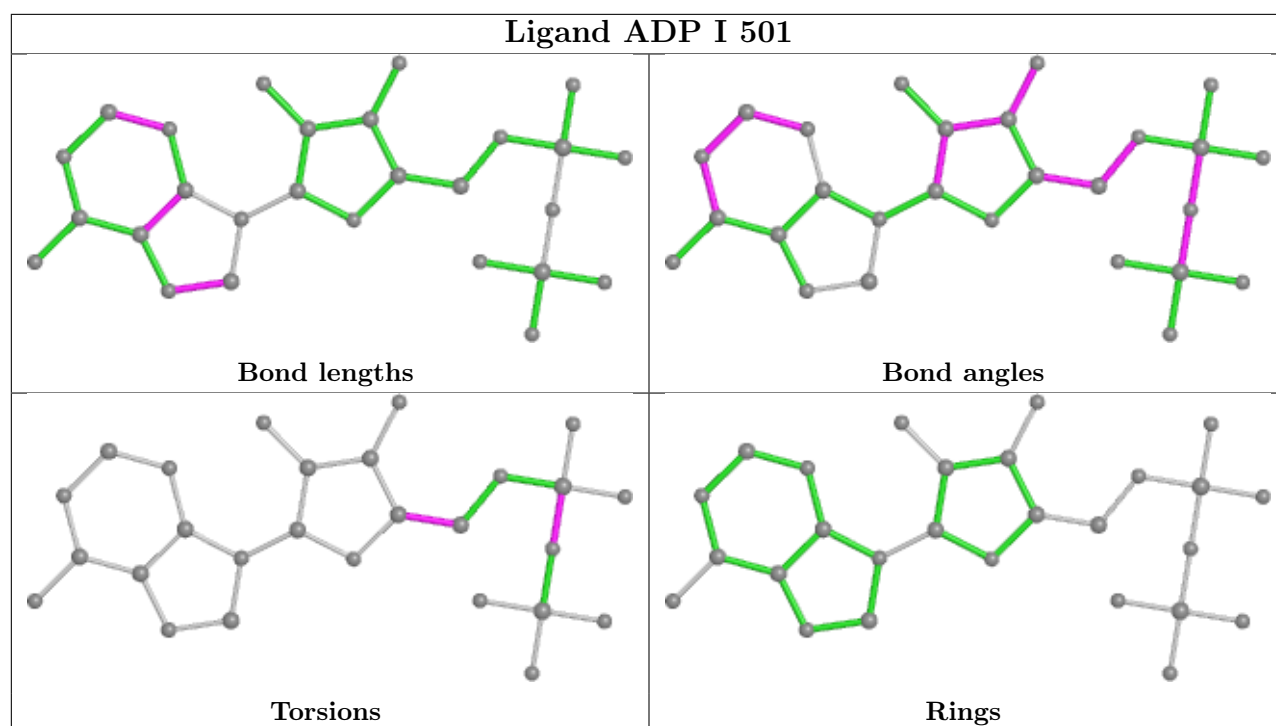
Mol	Chain	Res	Type	Atoms
35	H	501	ADP	O4'-C4'-C5'-O5'
35	I	501	ADP	O4'-C4'-C5'-O5'
35	J	501	ADP	C5'-O5'-PA-O1A
35	J	501	ADP	C5'-O5'-PA-O2A
35	J	501	ADP	C5'-O5'-PA-O3A

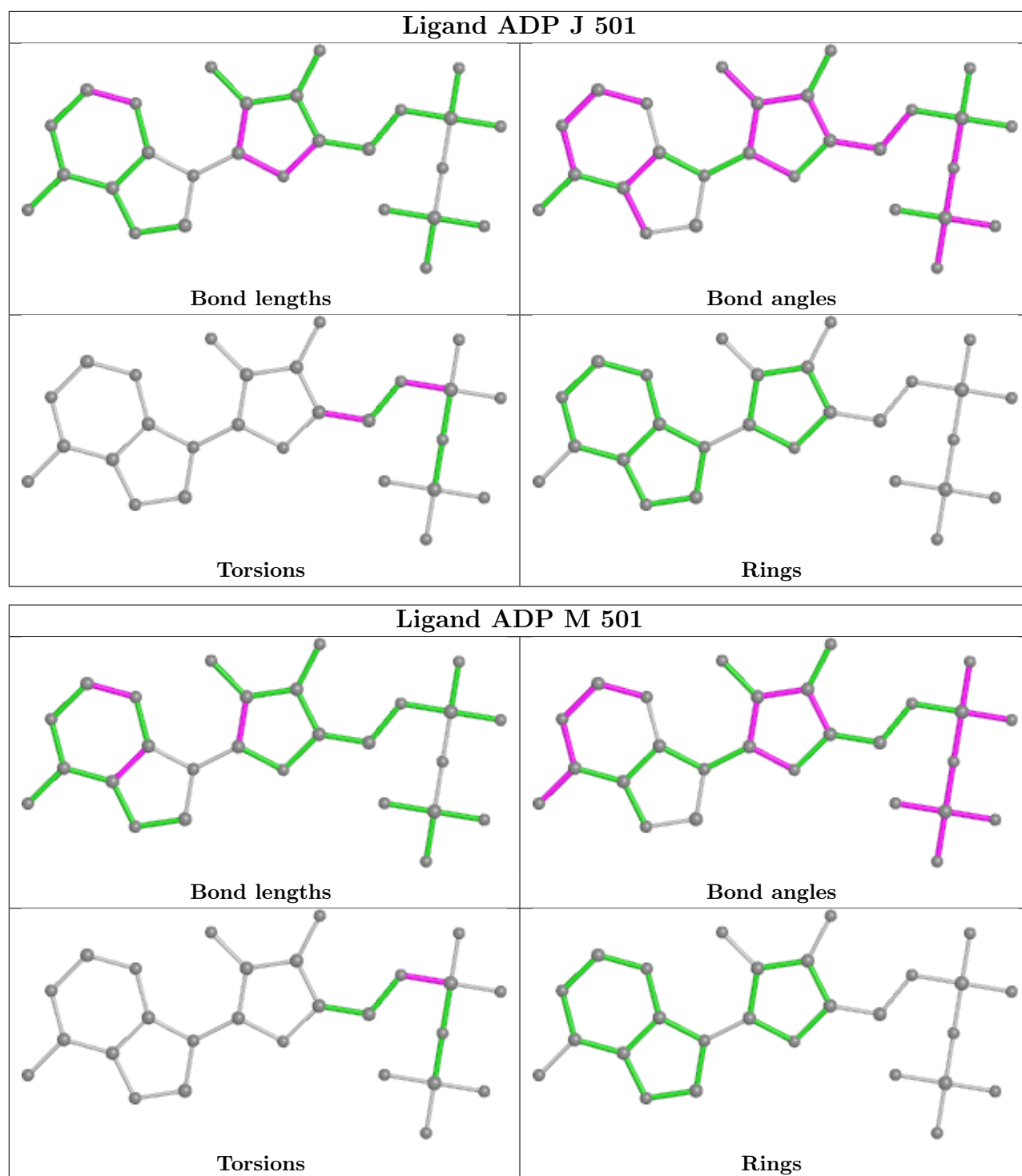
There are no ring outliers.

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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

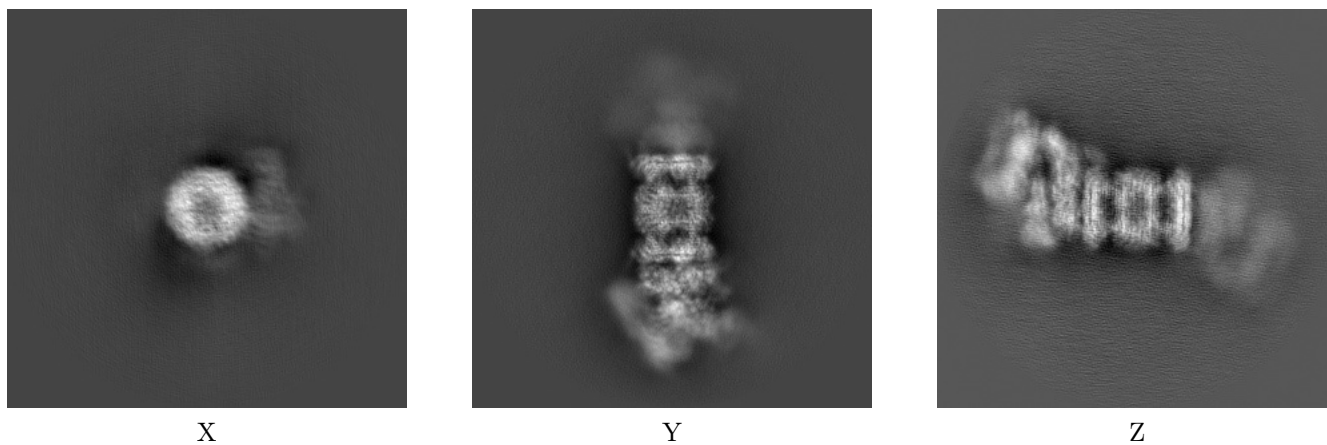
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9511. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

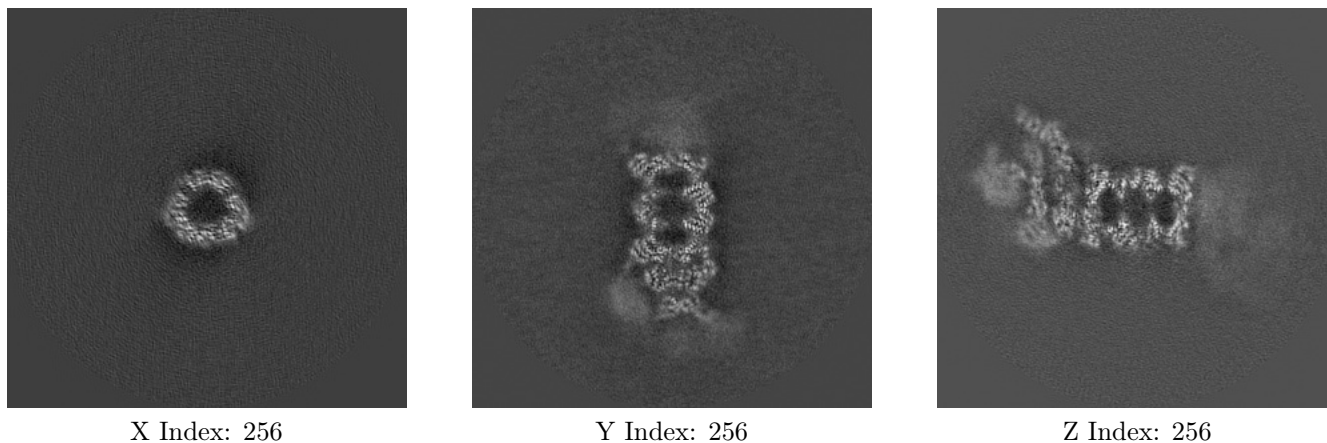
6.1.1 Primary map



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

6.2 Central slices [i](#)

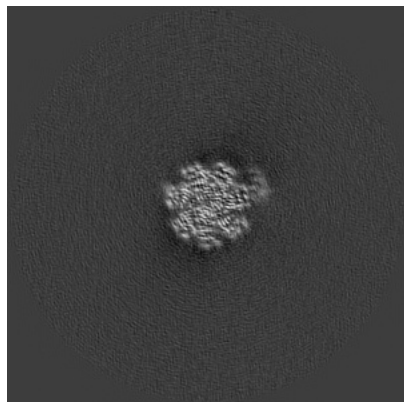
6.2.1 Primary map



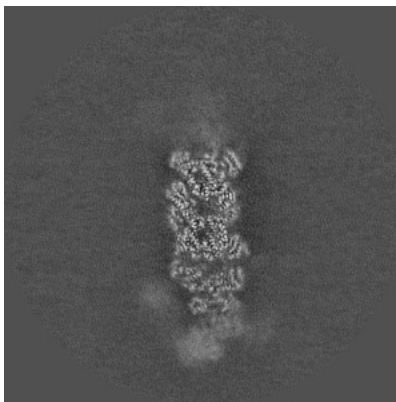
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

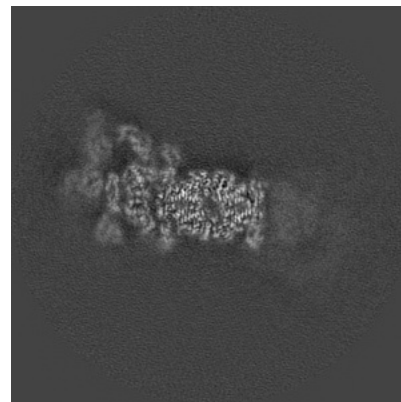
6.3.1 Primary map



X Index: 202



Y Index: 278

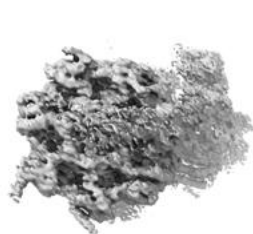


Z Index: 280

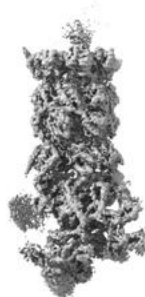
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

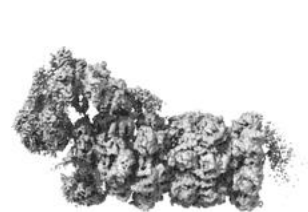
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

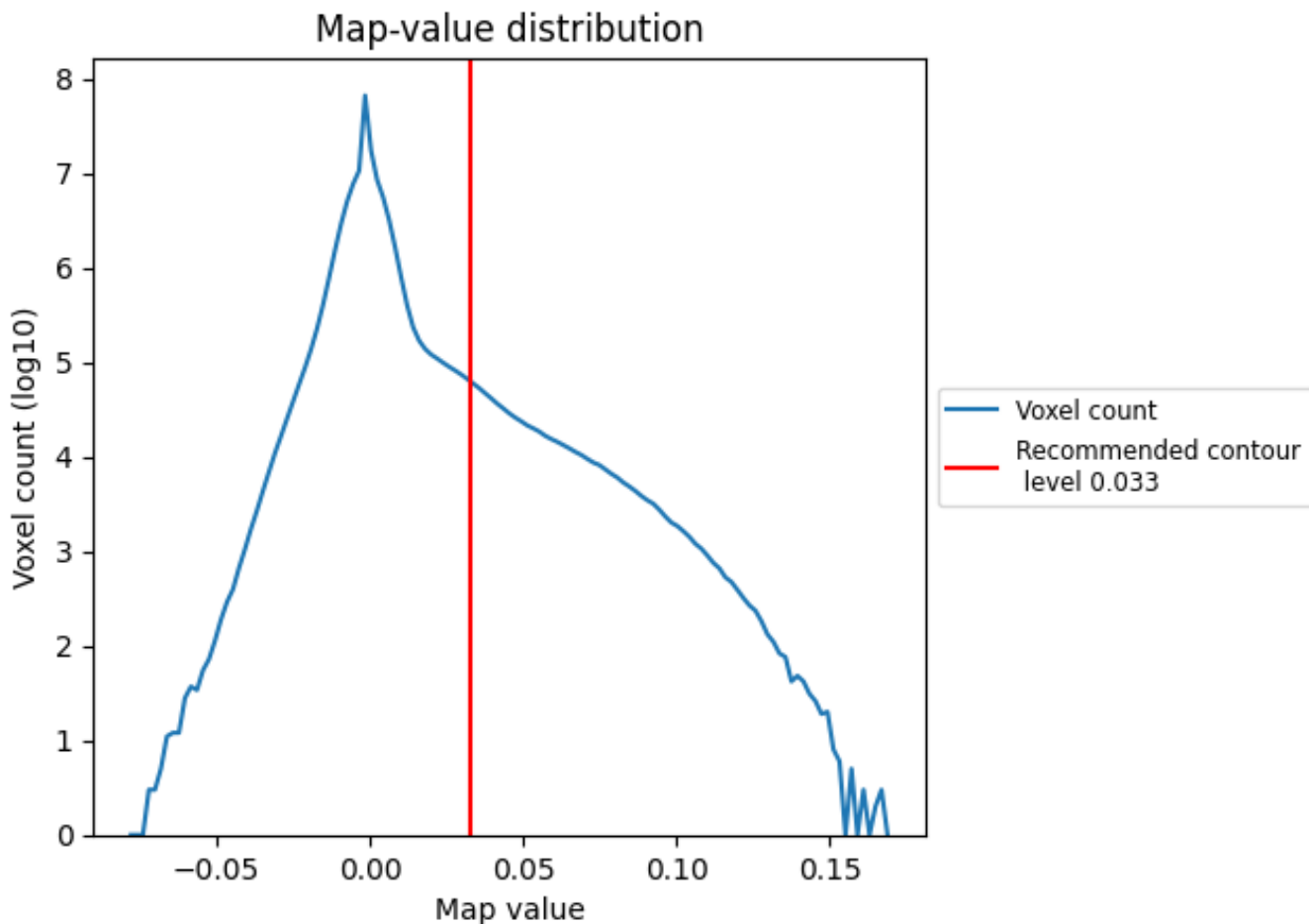
6.5 Mask visualisation

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

7 Map analysis [i](#)

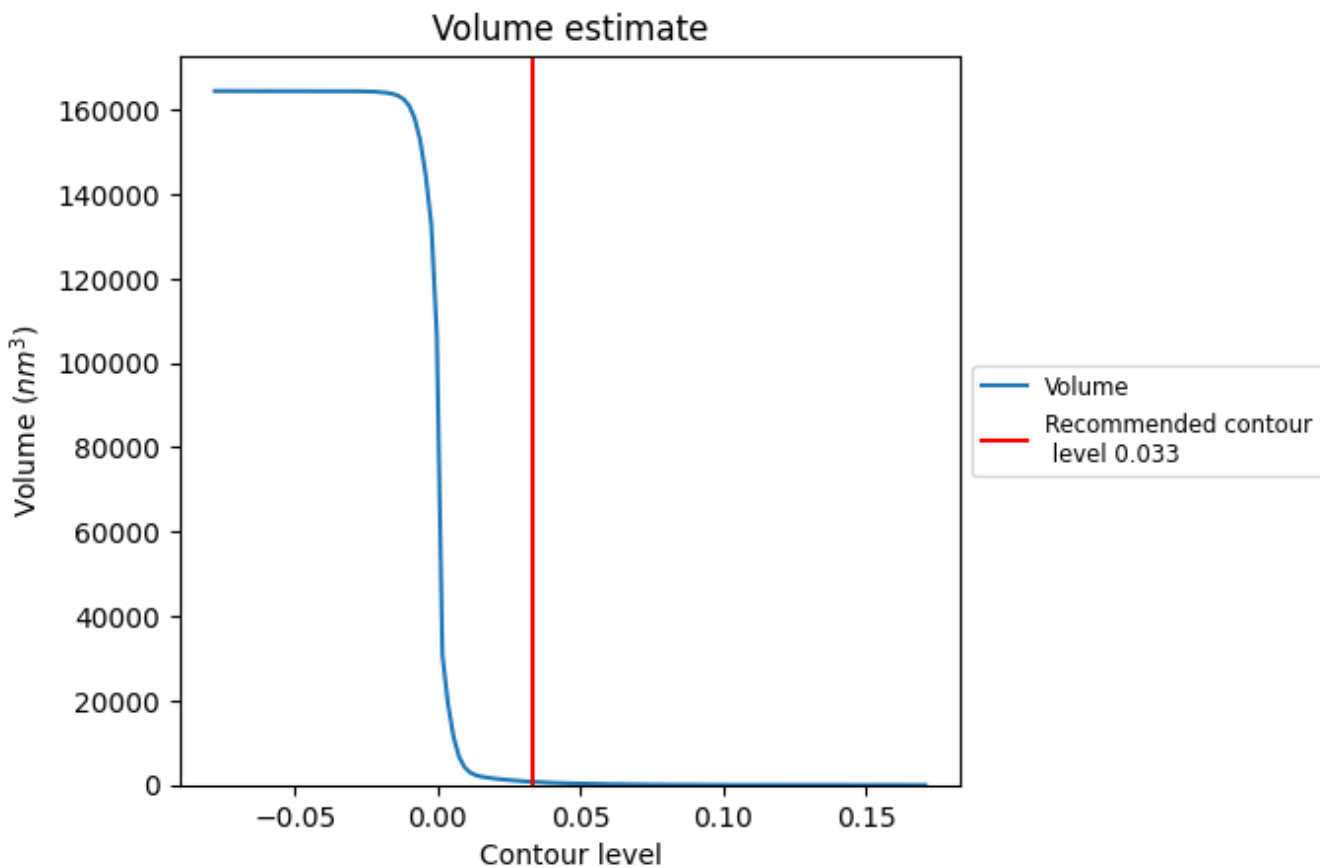
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

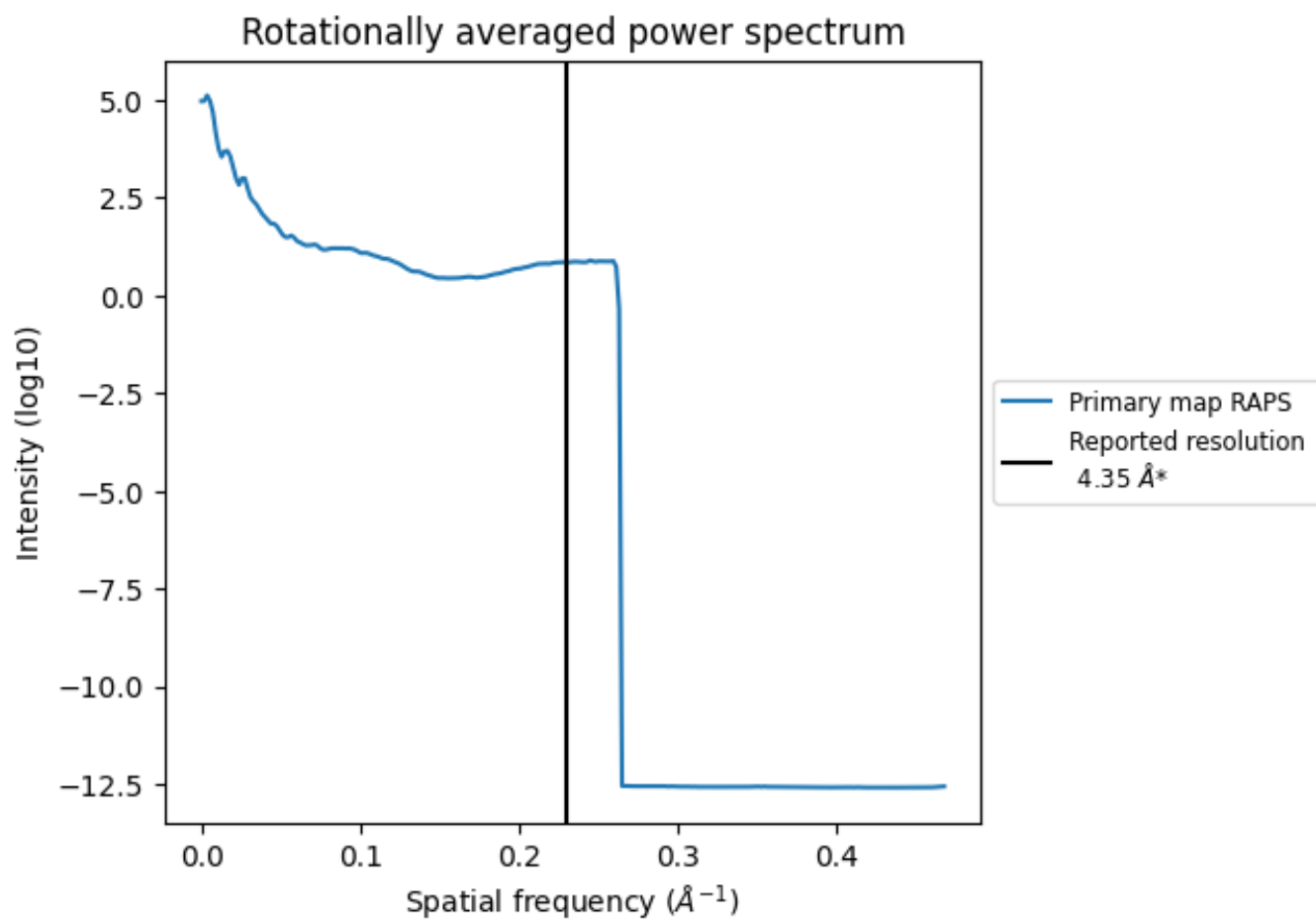
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 752 nm^3 ; this corresponds to an approximate mass of 679 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.230 Å⁻¹

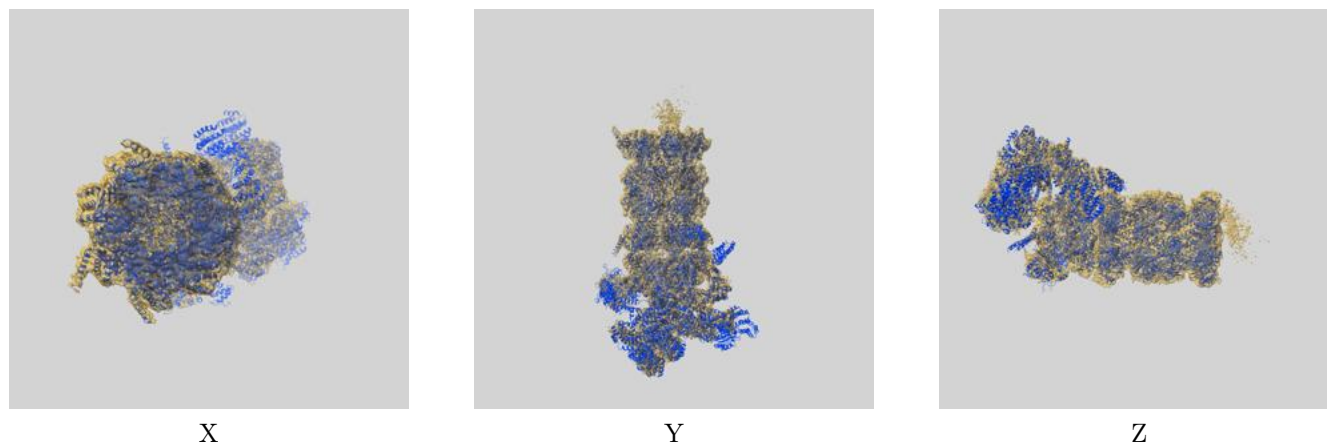
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

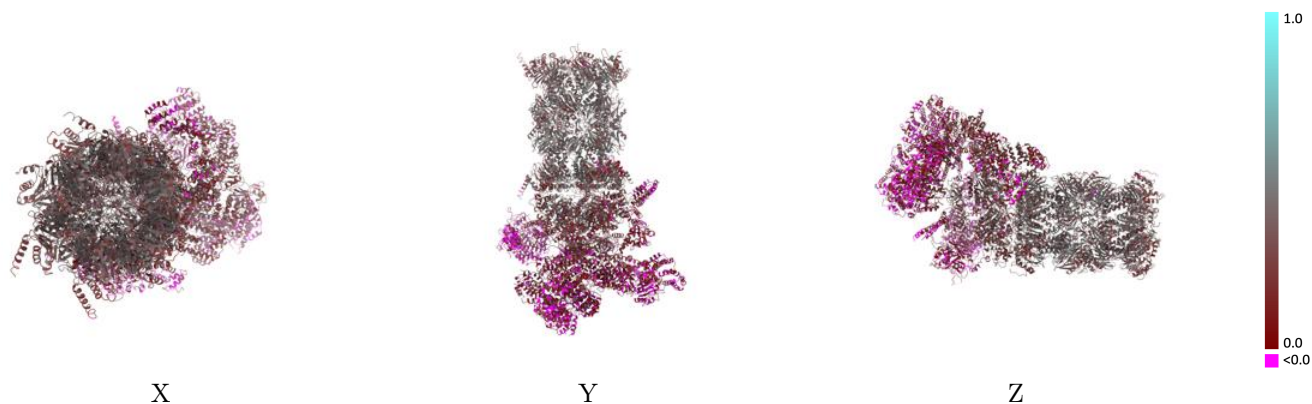
This section contains information regarding the fit between EMDB map EMD-9511 and PDB model 5GJQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



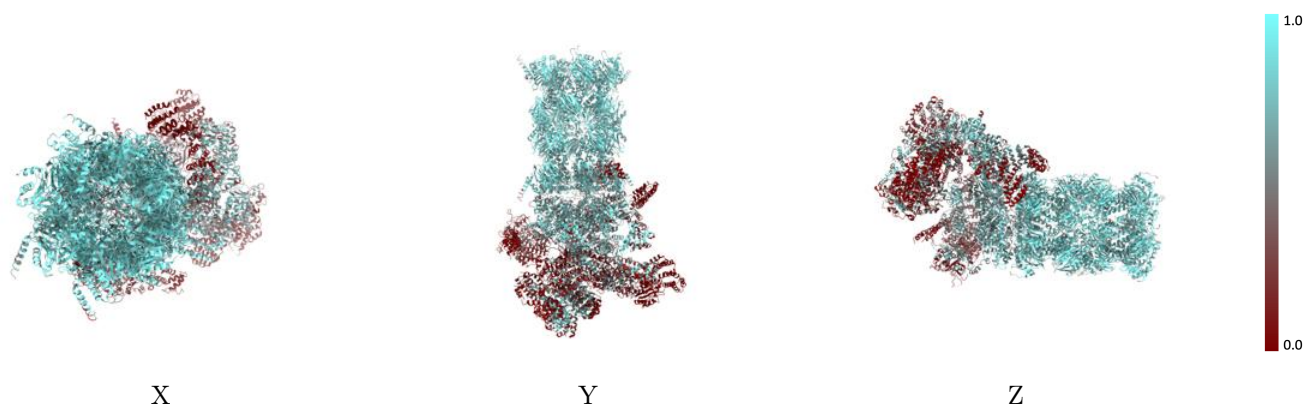
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



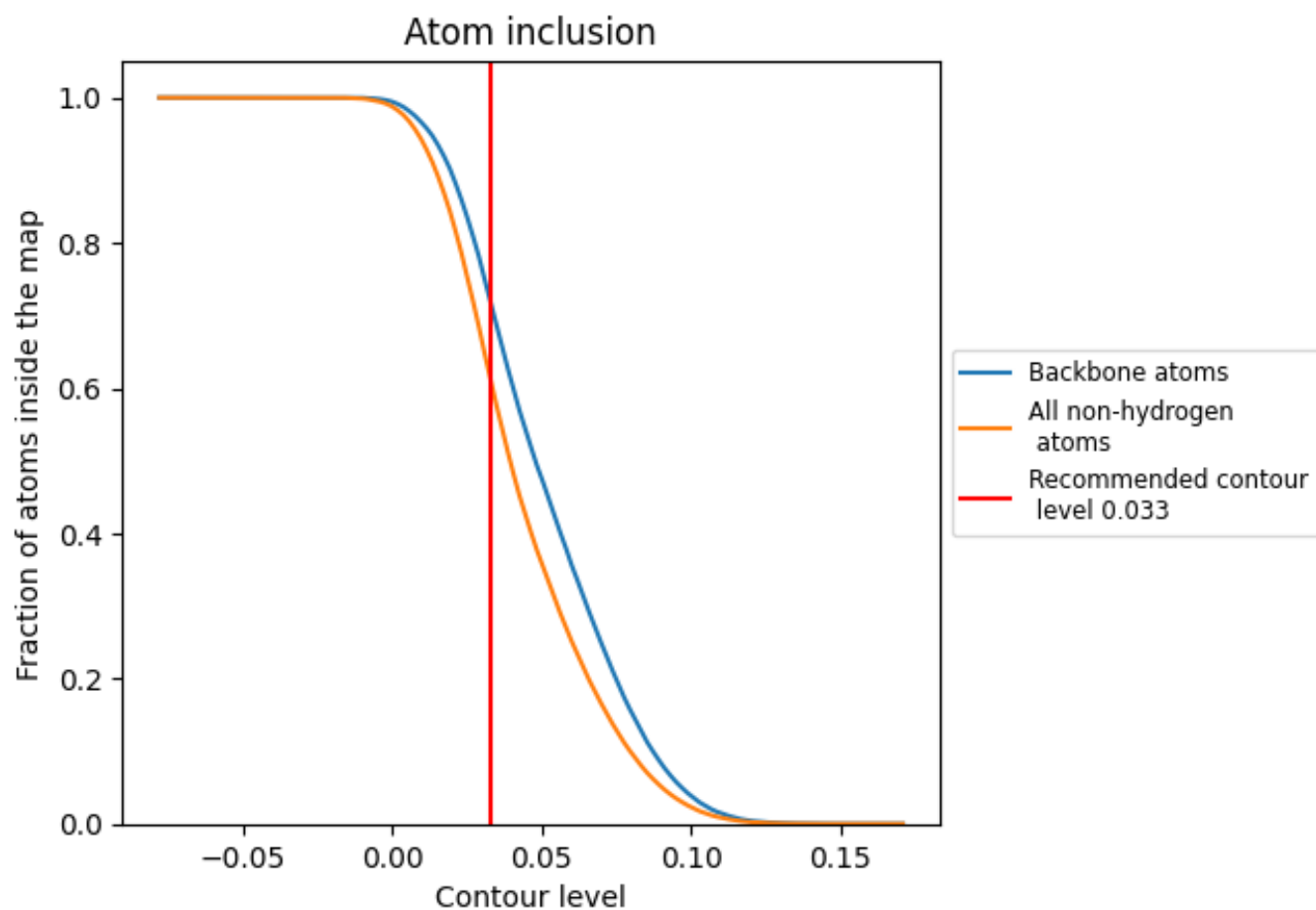
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.033).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





























The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6086	 0.2740
B	 0.7939	 0.3520
C	 0.8172	 0.3590
D	 0.8031	 0.3480
E	 0.7651	 0.3130
F	 0.7885	 0.3570
G	 0.8008	 0.3490
H	 0.6429	 0.3090
I	 0.6237	 0.3070
J	 0.6241	 0.2940
K	 0.6551	 0.2840
L	 0.6175	 0.2840
M	 0.6228	 0.2930
N	 0.3863	 0.0710
O	 0.2563	 0.1060
P	 0.3282	 0.1410
Q	 0.4816	 0.2210
R	 0.5944	 0.2160
S	 0.2863	 0.1500
T	 0.1912	 0.1140
U	 0.2700	 0.1230
V	 0.3095	 0.1700
W	 0.0054	 0.0270
X	 0.8119	 0.3640
Y	 0.2760	 0.2040
Z	 0.0793	 0.0230
a	 0.8084	 0.3870
b	 0.8042	 0.3810
c	 0.8055	 0.3870
d	 0.8300	 0.3760
e	 0.8264	 0.3890
f	 0.8467	 0.3860
g	 0.8618	 0.4020
h	 0.7822	 0.3800
i	 0.7943	 0.3970



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Chain	Atom inclusion	Q-score
j	 0.7643	 0.3570
k	 0.7647	 0.3420
l	 0.7860	 0.3670
m	 0.8124	 0.3770
n	 0.7874	 0.3670
o	 0.8395	 0.3930
p	 0.8346	 0.3940
q	 0.8350	 0.4030
r	 0.8143	 0.3910
s	 0.8594	 0.3920
t	 0.7998	 0.3950
u	 0.8162	 0.3960
x	 0.3774	 0.1260
y	 0.2703	 0.0860