



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:48 AM UTC

PDB ID : 6MSE / pdb_00006mse
EMDB ID : EMD-9218
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

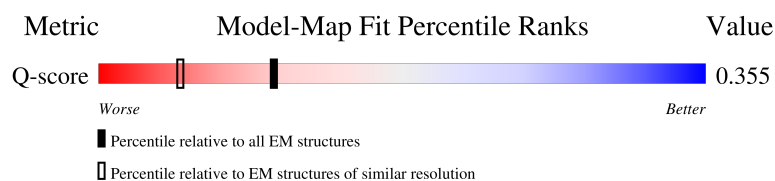
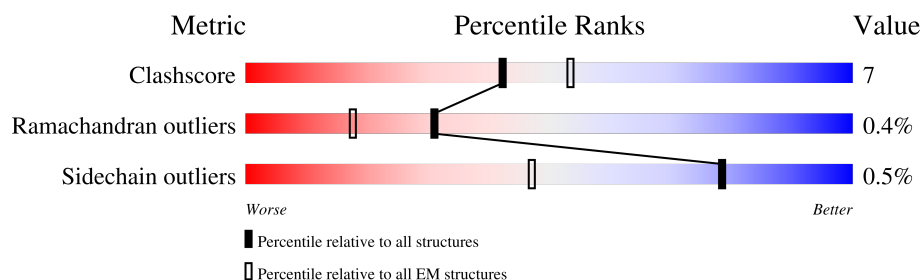
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	U	953	50% 68% 17% 15%
2	V	533	66% 64% 26% 10%
3	W	456	47% 75% 24%
4	X	422	50% 82% 9% 10%

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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	u	76	
20	v	28	
21	G	245	
21	g	245	
22	H	233	
22	h	233	
23	I	260	
23	i	260	
24	J	247	
24	j	247	
25	K	240	

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Mol	Chain	Length	Quality of chain
25	k	240	
26	L	268	
26	l	268	
27	M	254	
27	m	254	
28	N	238	
28	n	238	
29	O	276	
29	o	276	
30	P	204	
30	p	204	
31	Q	201	
31	q	201	
32	R	262	
32	r	262	
33	S	240	
33	s	240	
34	T	263	
34	t	263	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 105062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 19 is a protein called Ubiquitin.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called substrate.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

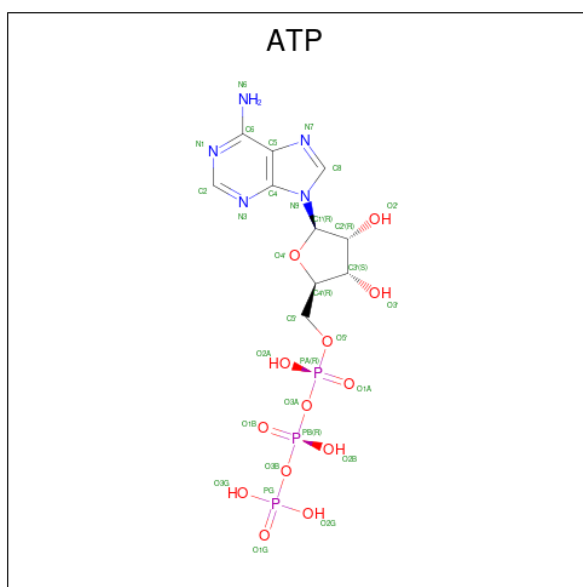
- Molecule 34 is a protein called Proteasome subunit beta type-4.

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

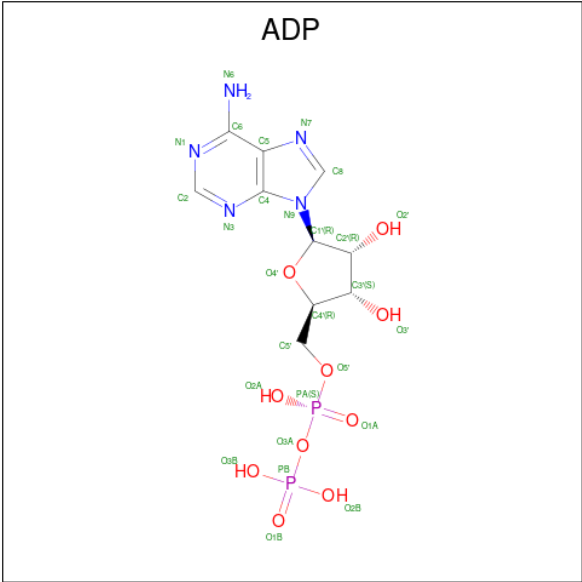


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

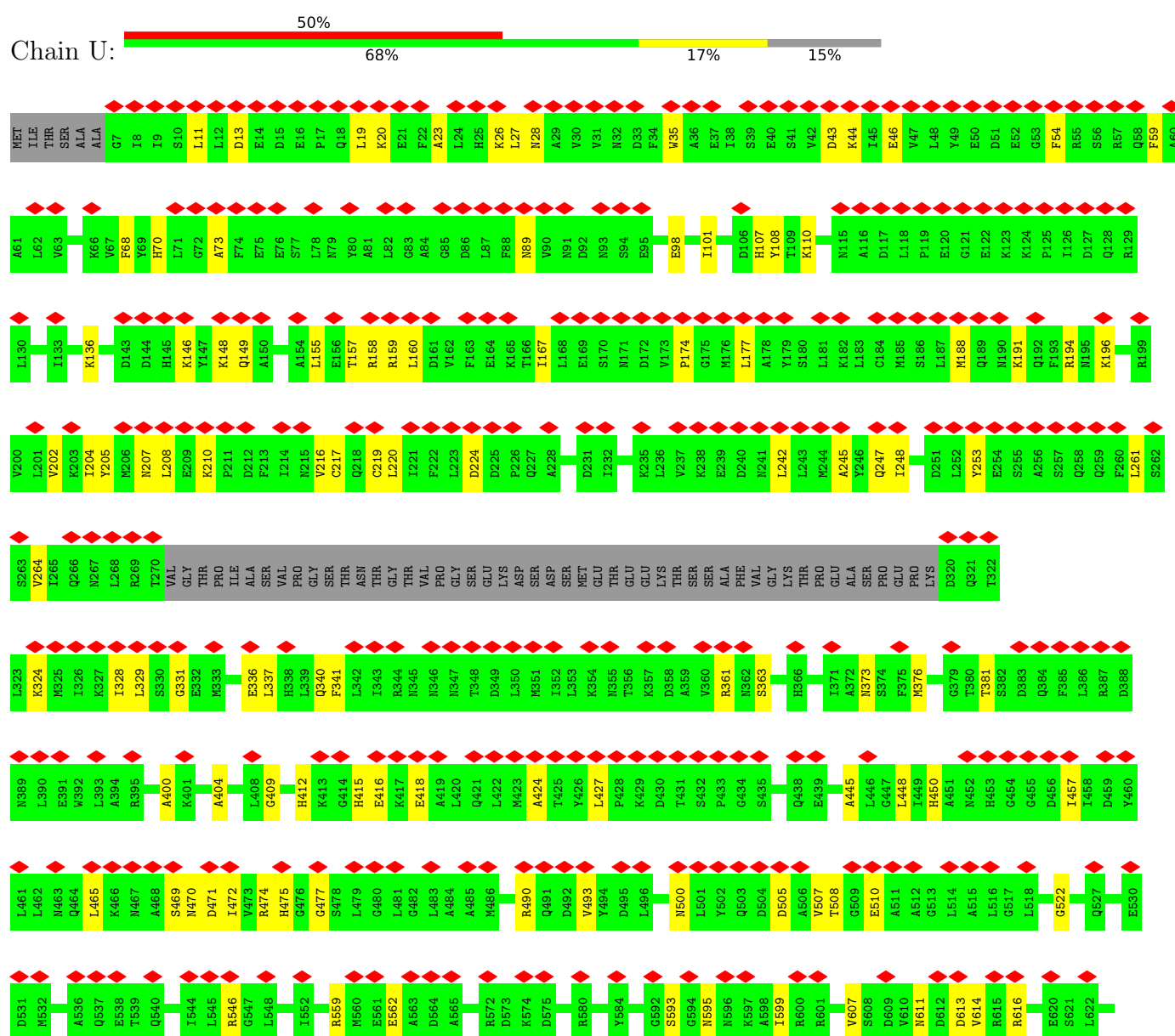


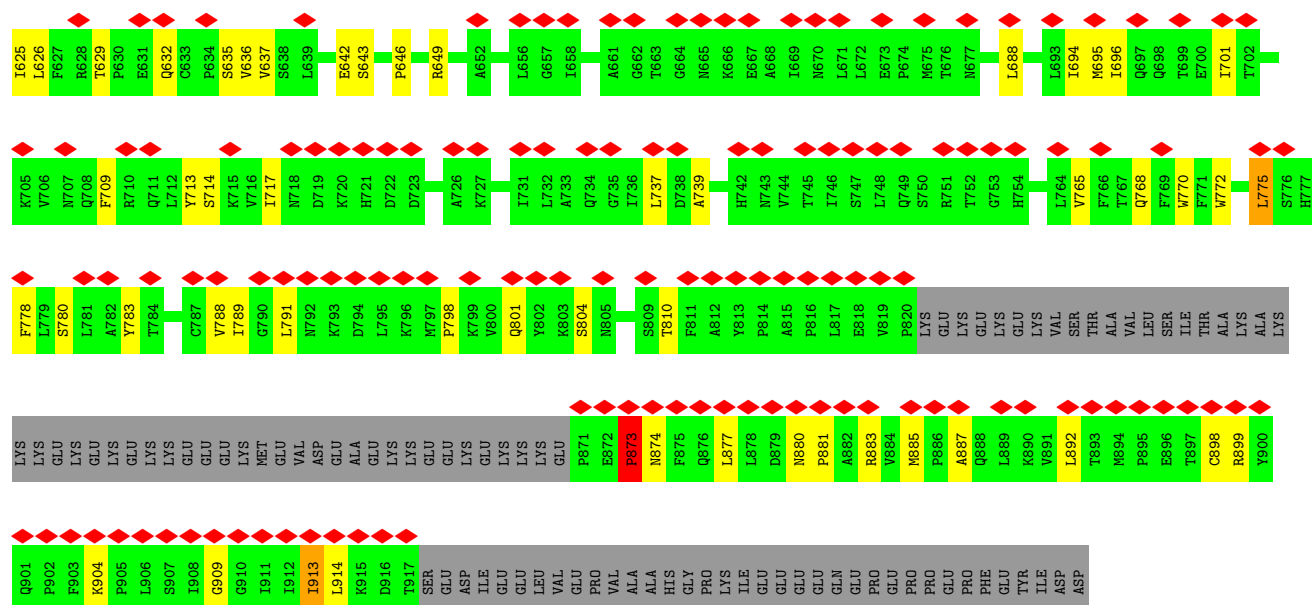
Mol	Chain	Residues	Atoms					AltConf
38	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

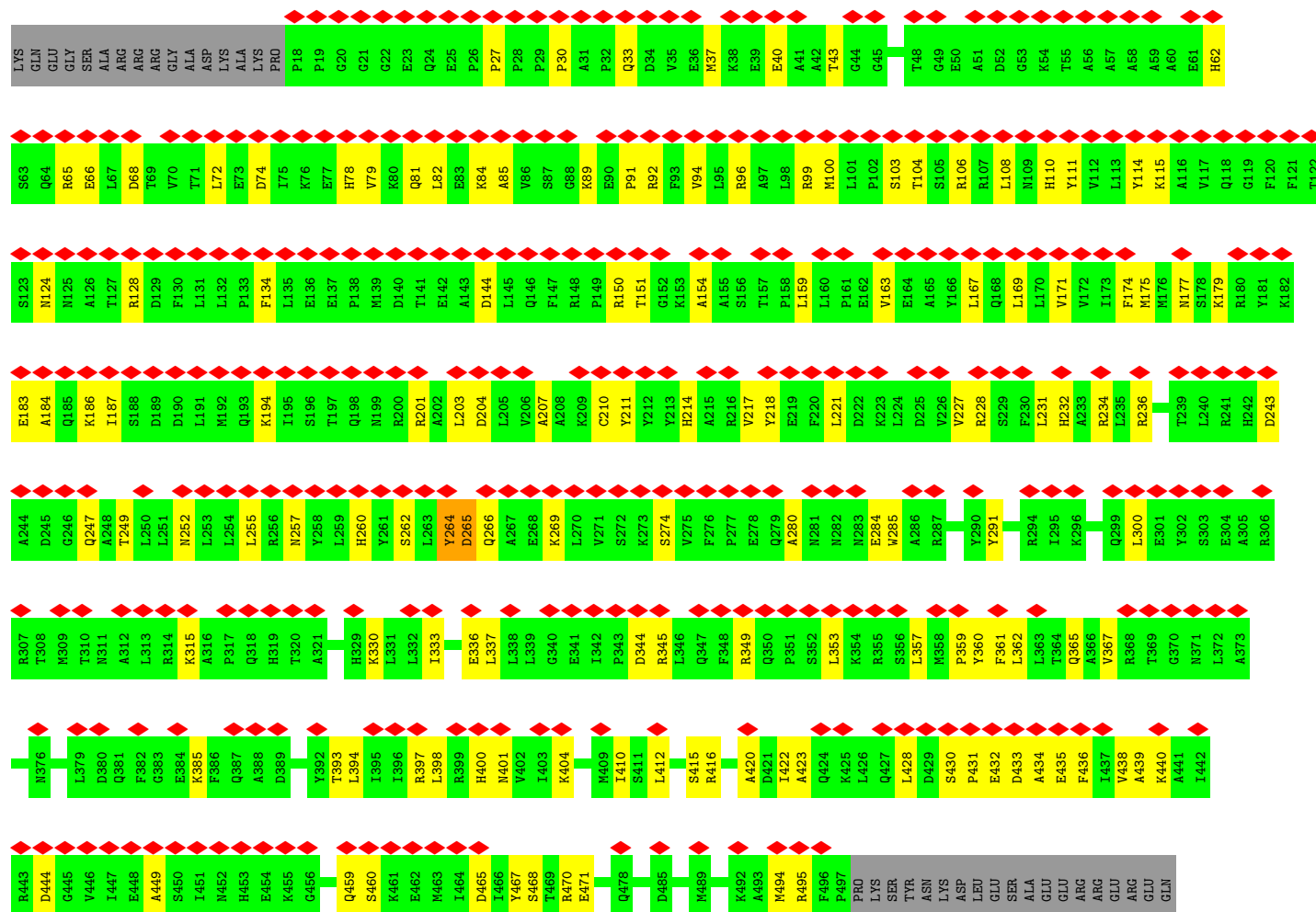
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



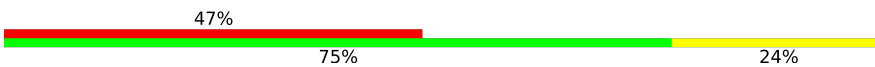


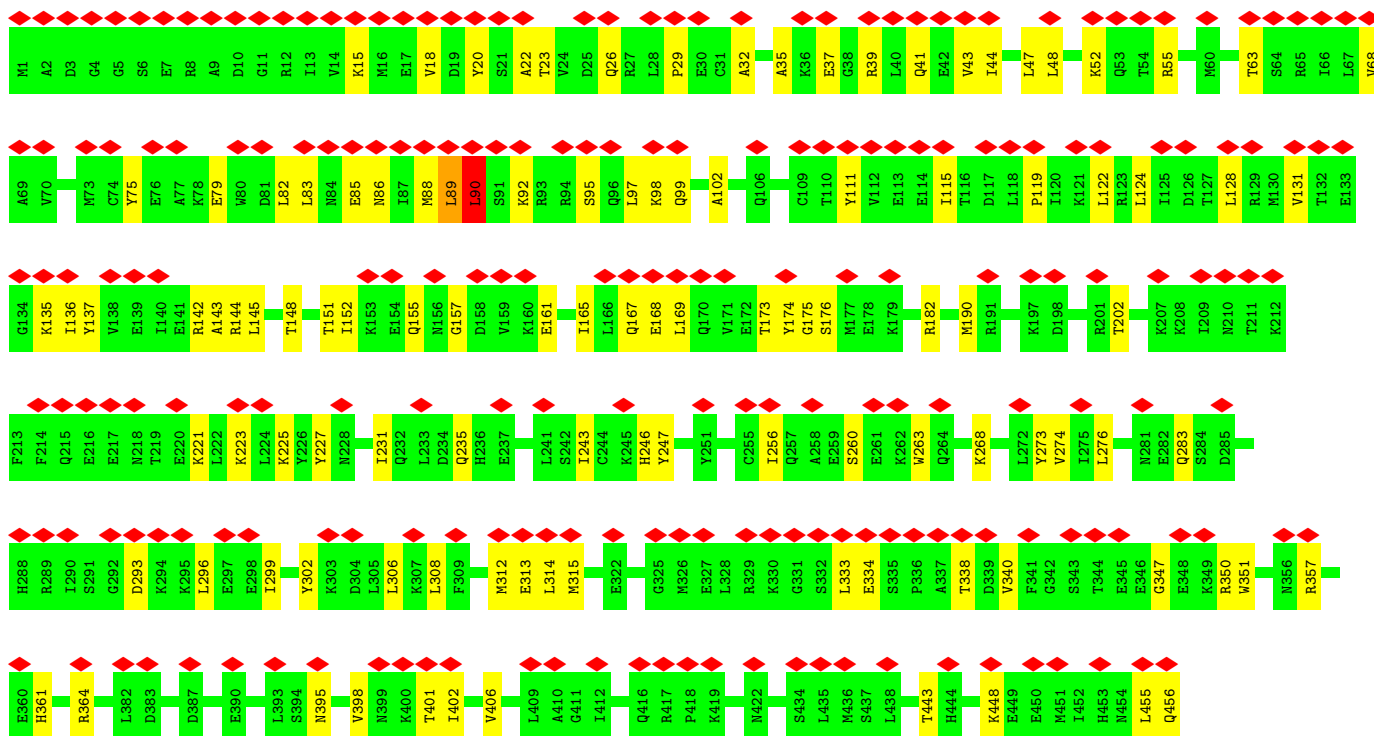
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



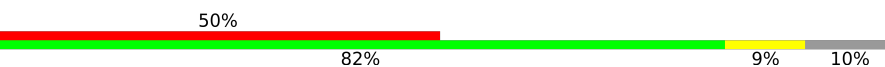
GLN
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LEU
GLU
PHE
ALA
LYS
GLU
MET
ALA
GLU
ASP
ASP
SER
PHE
PRO

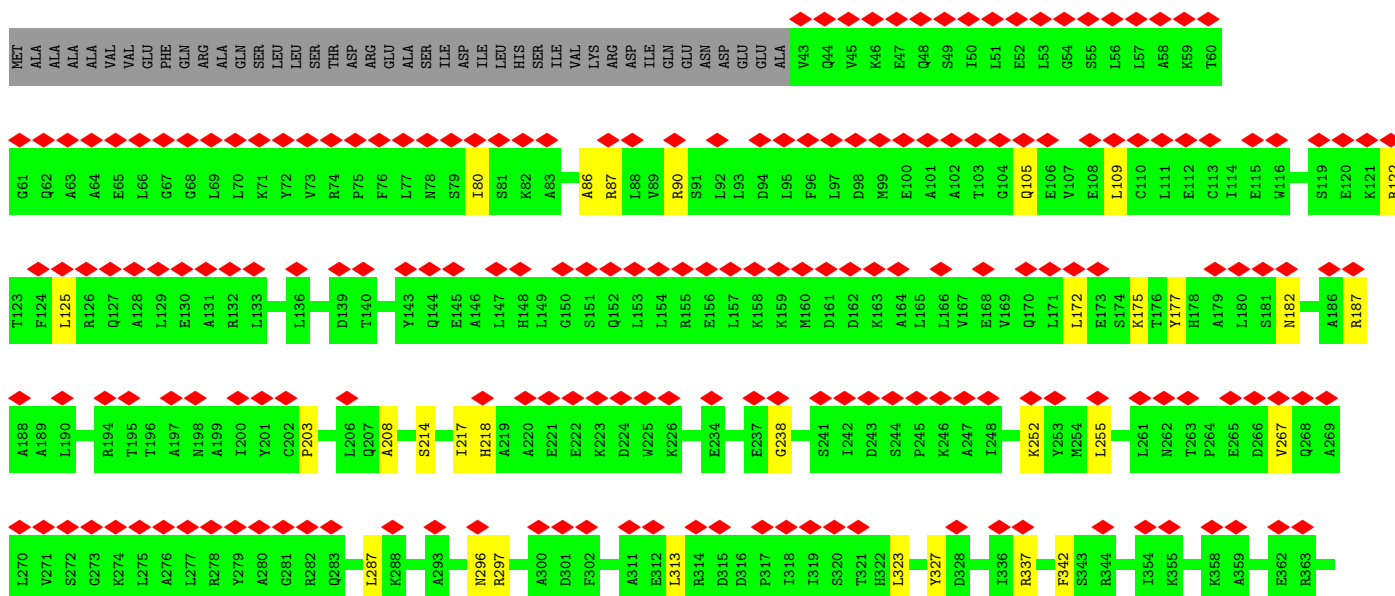
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

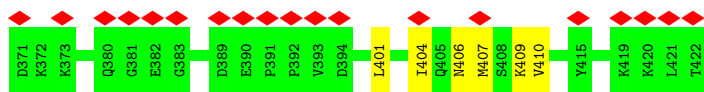
Chain W: 



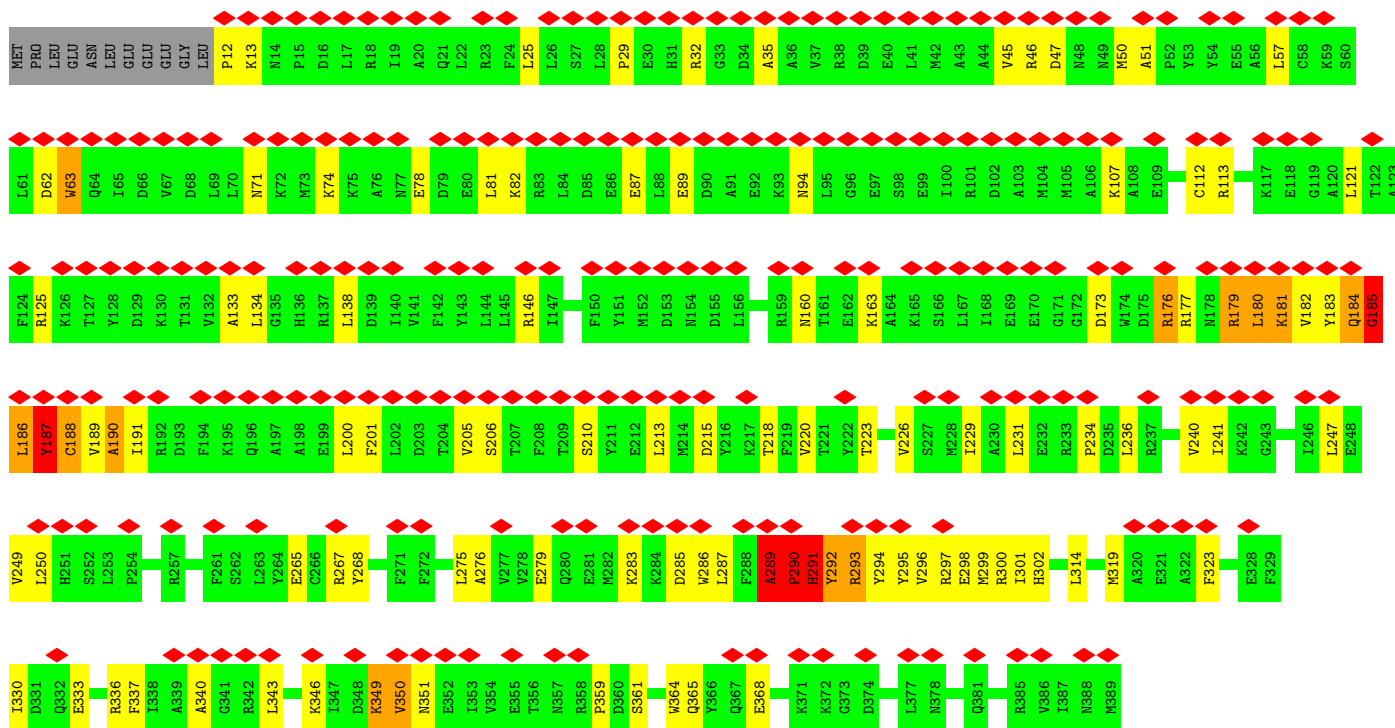
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 

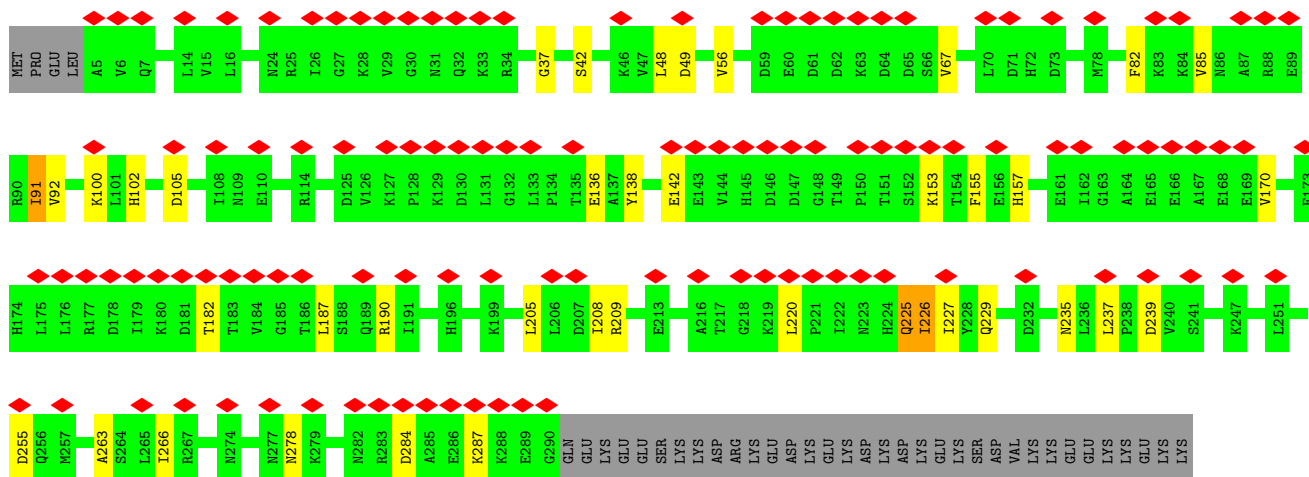
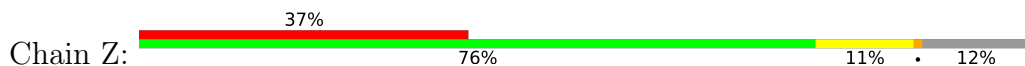




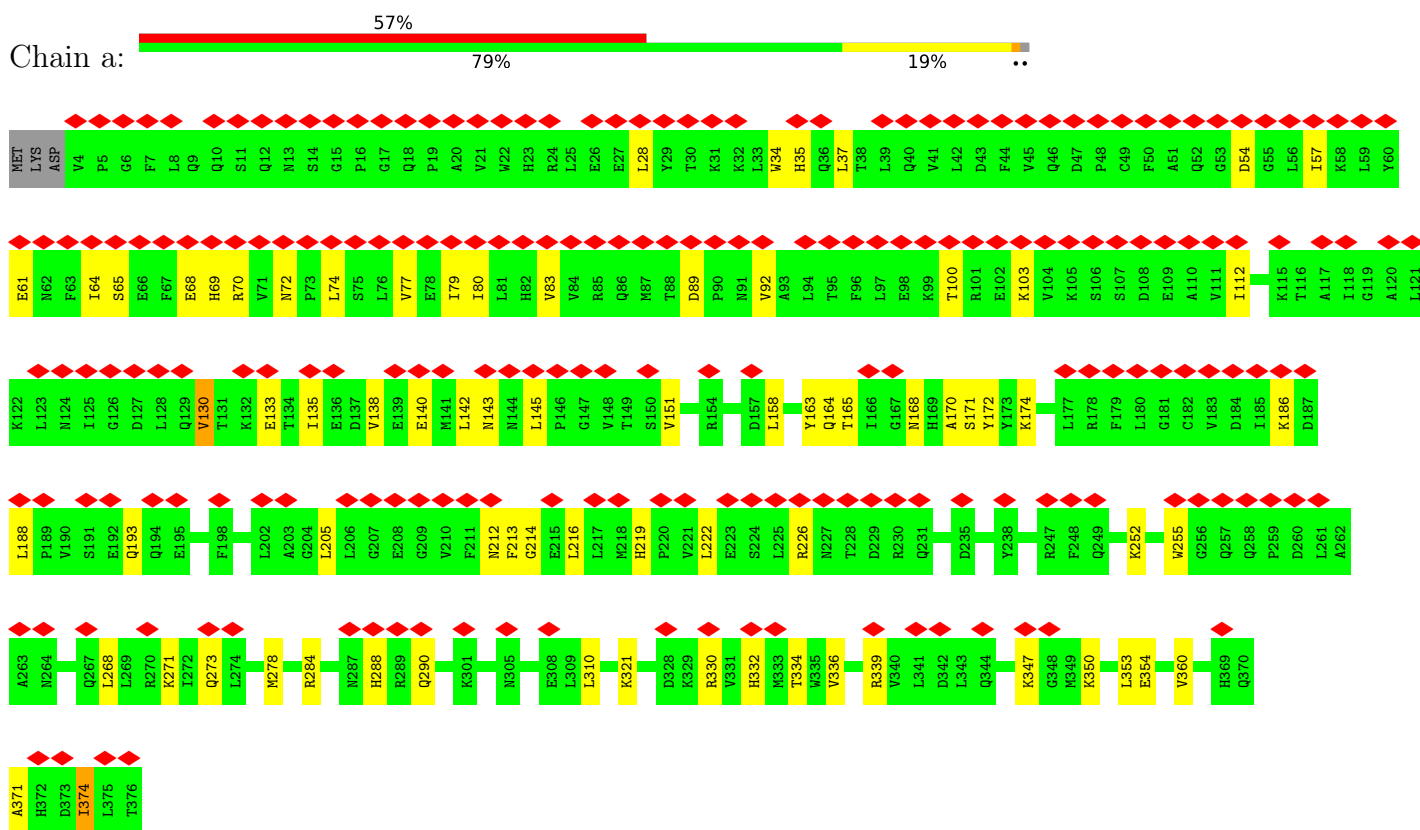
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



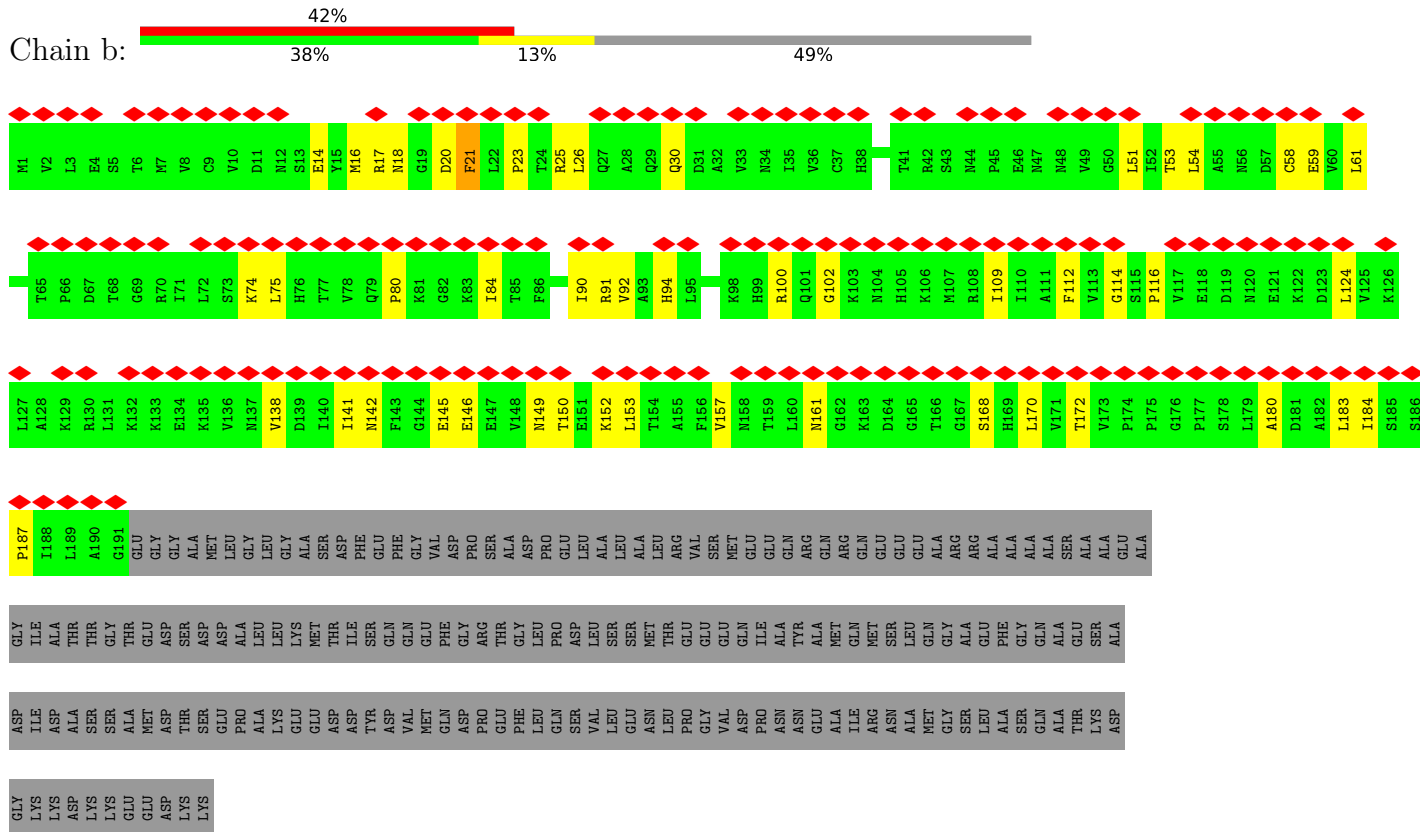
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

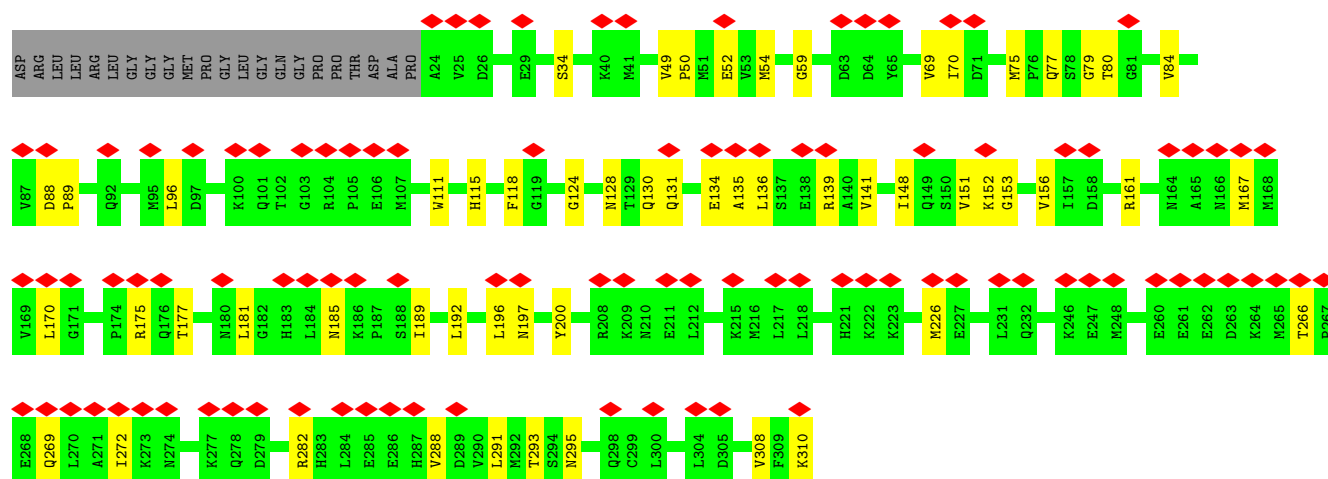
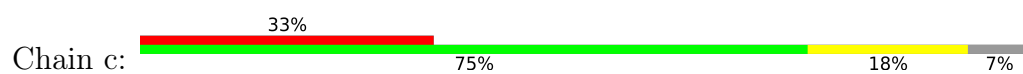


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

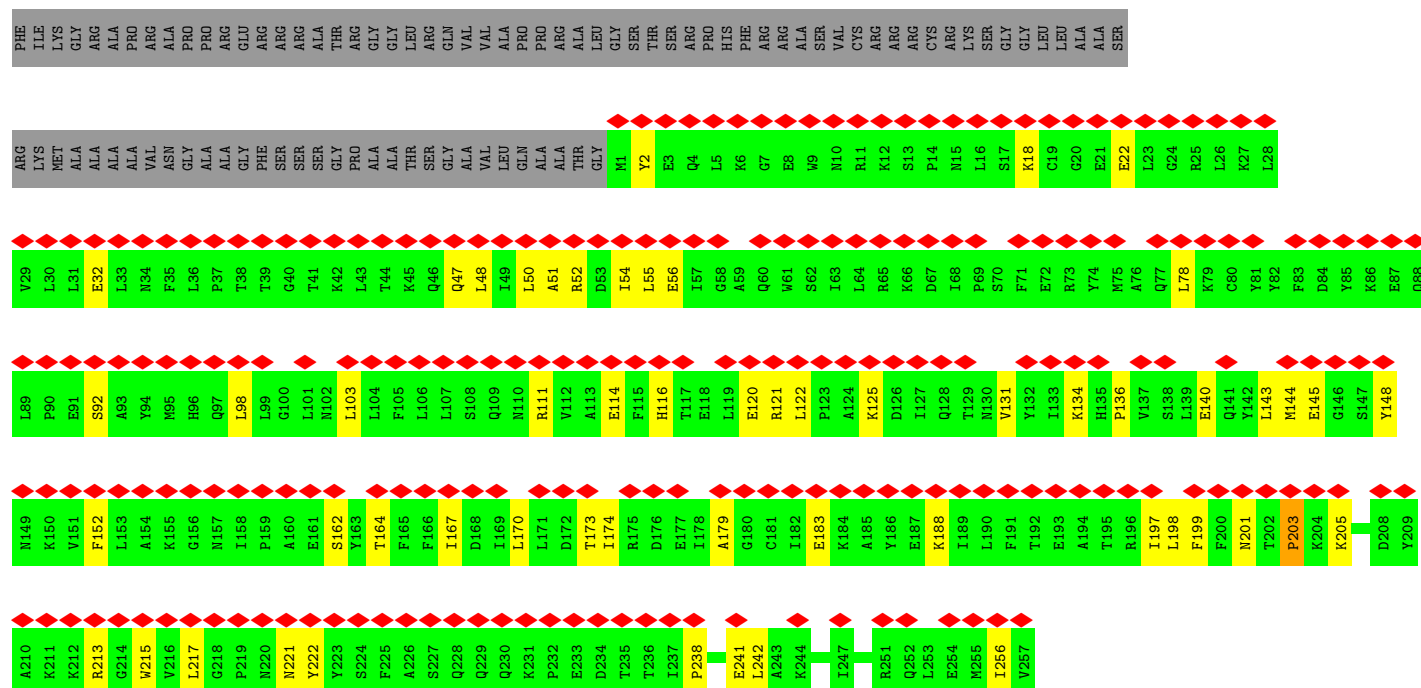


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

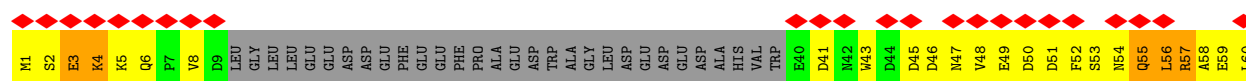


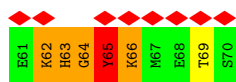


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

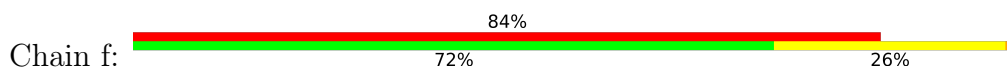


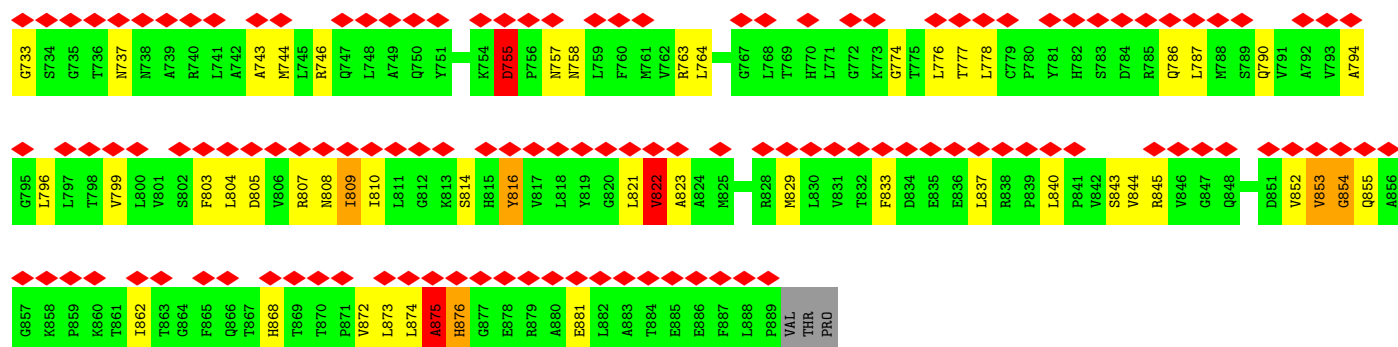
• Molecule 11: 26S proteasome complex subunit SEM1



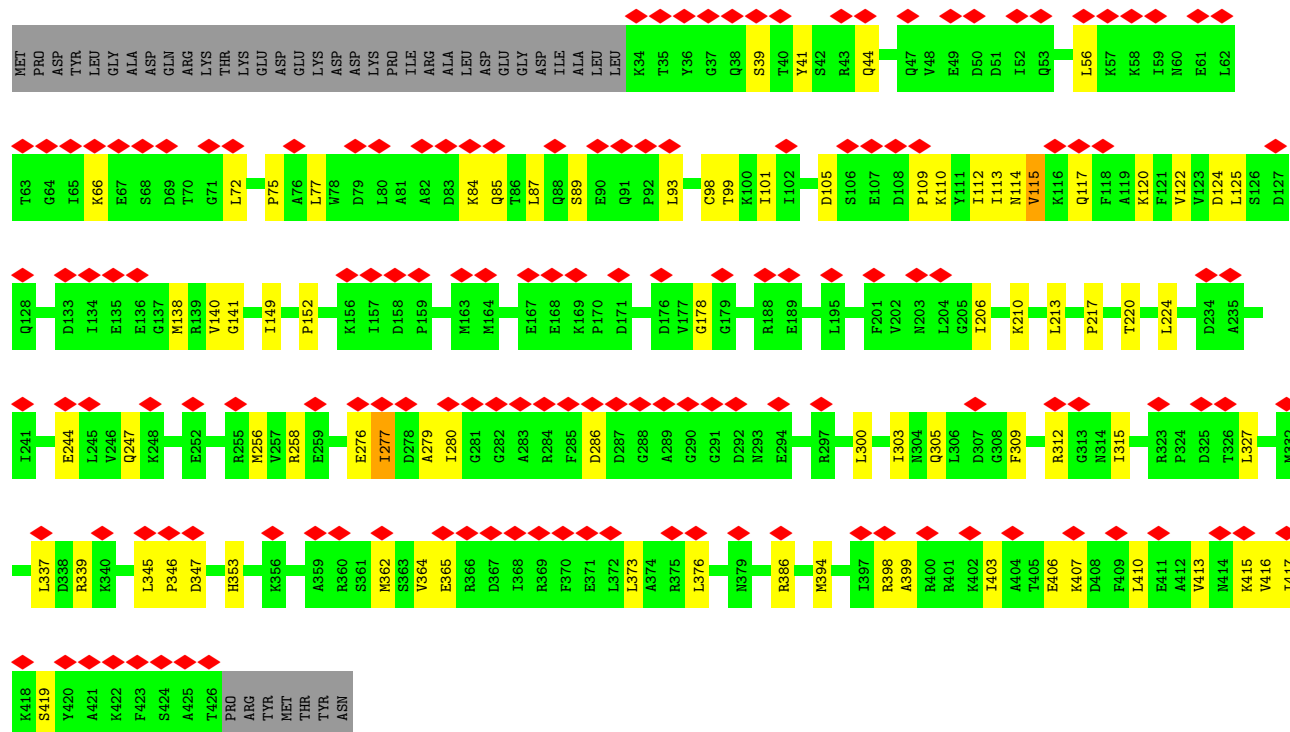


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

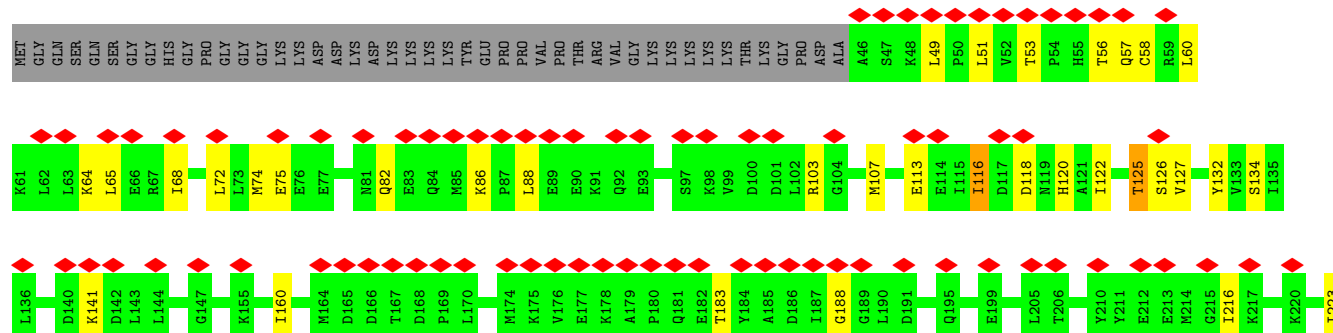
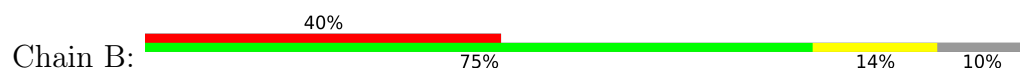


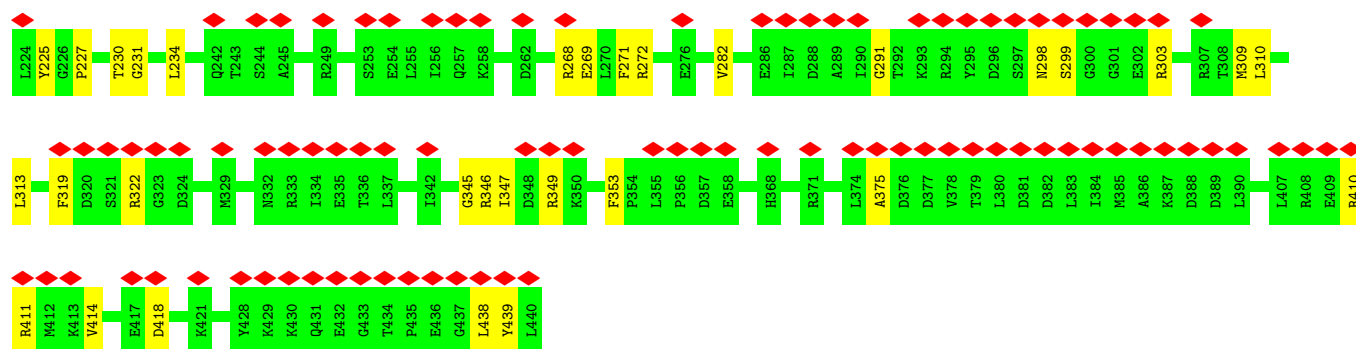


• Molecule 13: 26S proteasome regulatory subunit 7

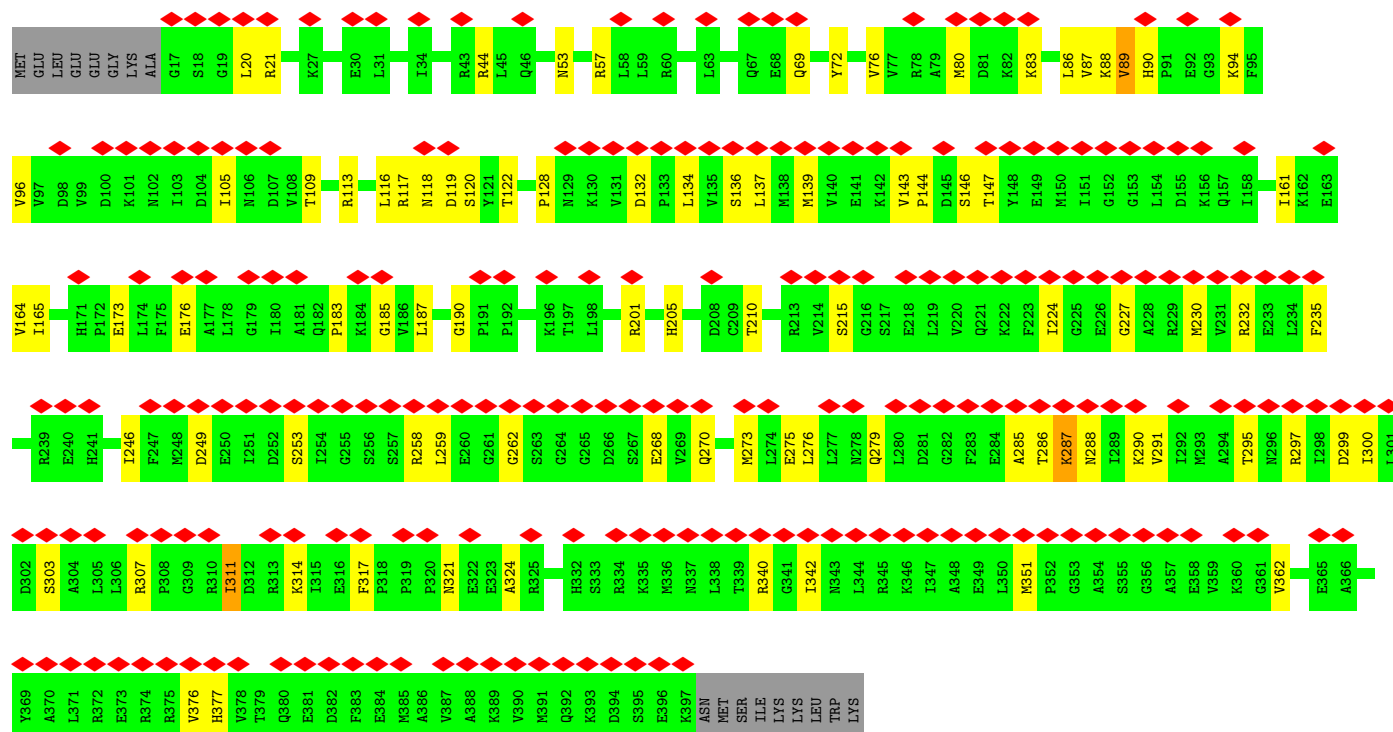


• Molecule 14: 26S proteasome regulatory subunit 4

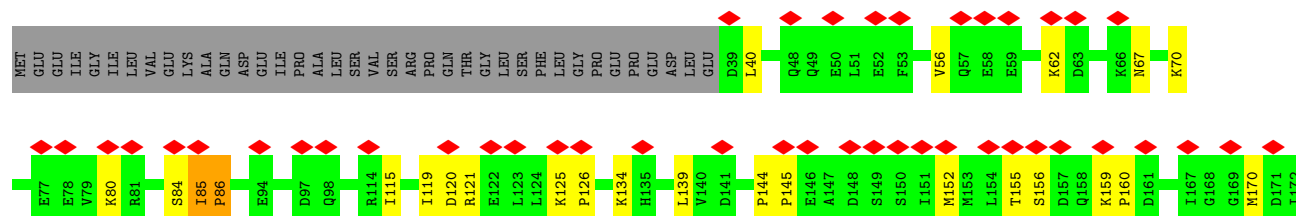
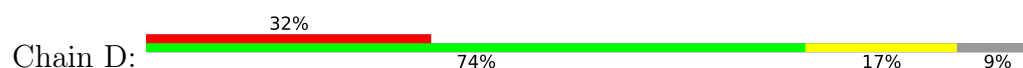


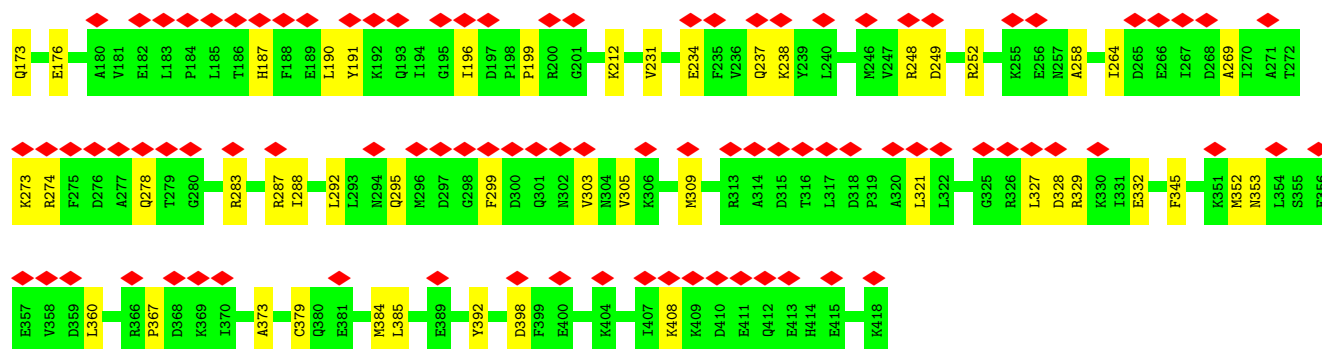


• Molecule 15: 26S proteasome regulatory subunit 8



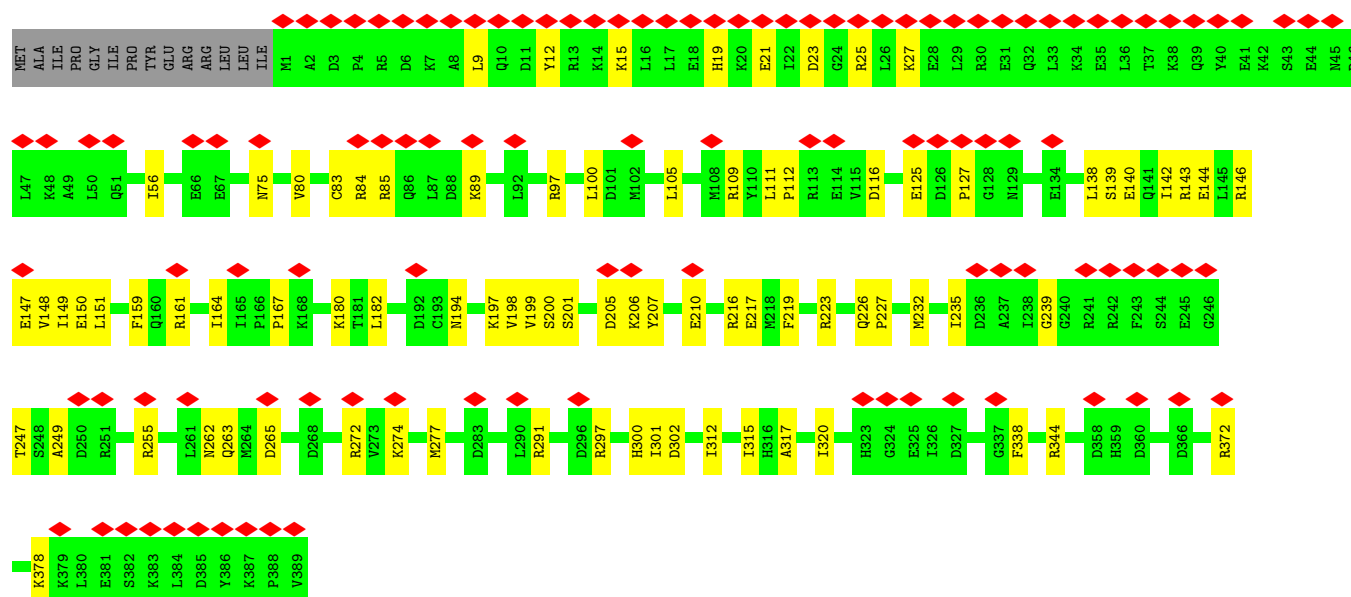
• Molecule 16: 26S proteasome regulatory subunit 6B





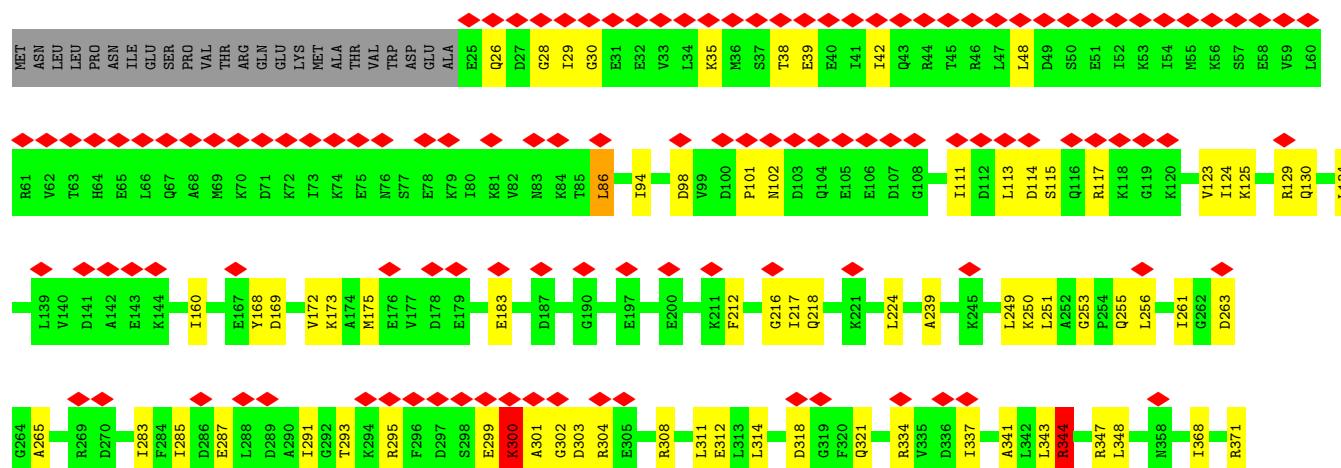
• Molecule 17: 26S proteasome regulatory subunit 10B

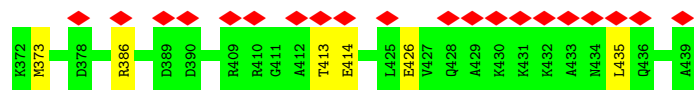
Chain E: 28% 76% 21% .



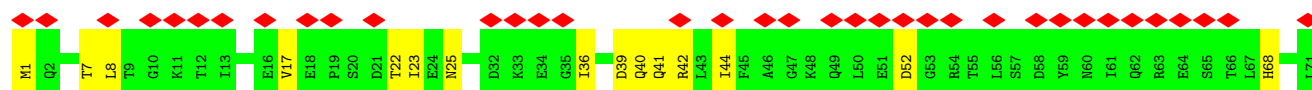
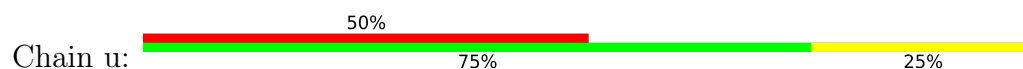
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F: 32% 76% 18% 5%

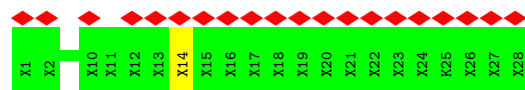




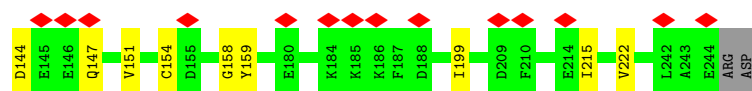
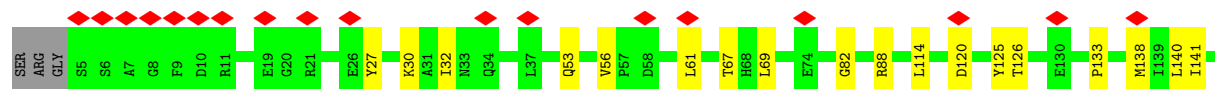
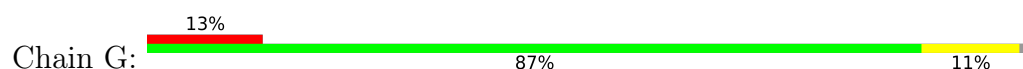
- Molecule 19: Ubiquitin



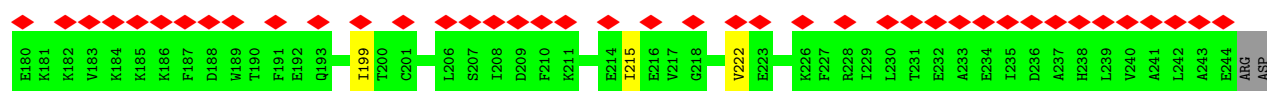
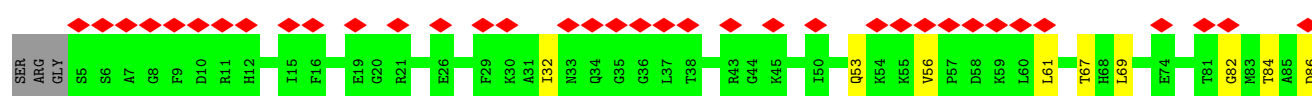
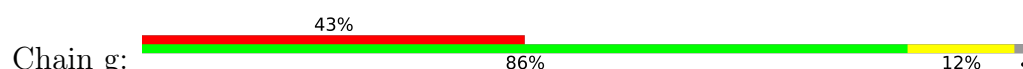
- Molecule 20: substrate



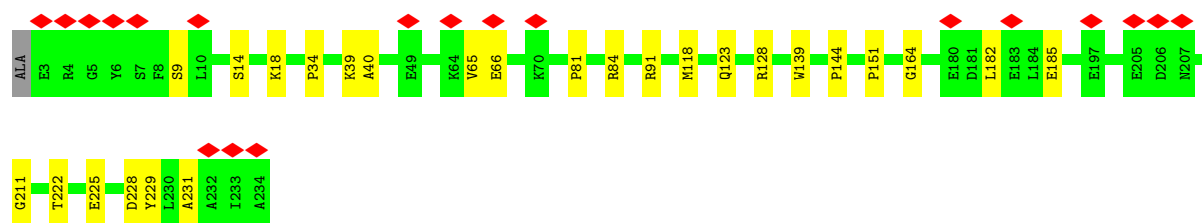
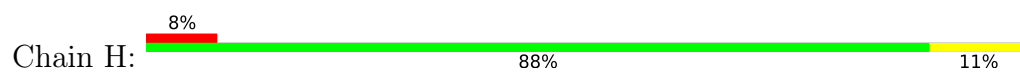
- Molecule 21: Proteasome subunit alpha type-6



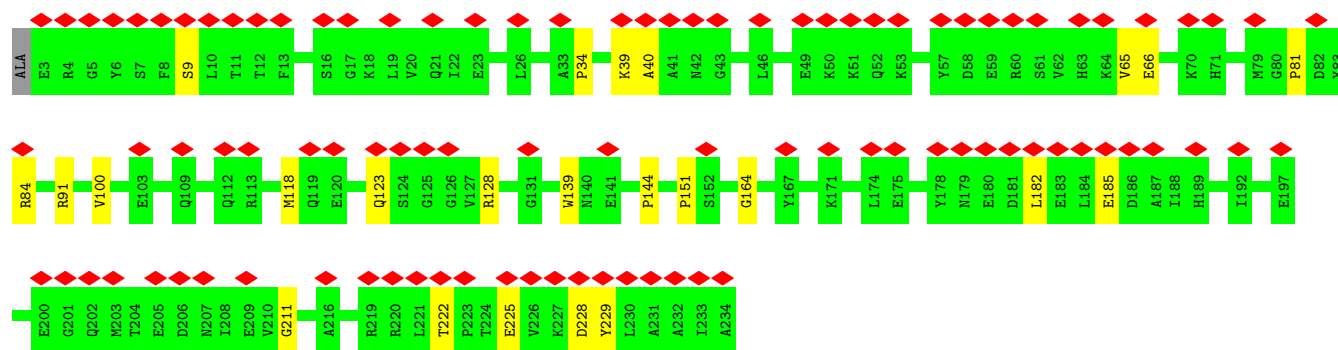
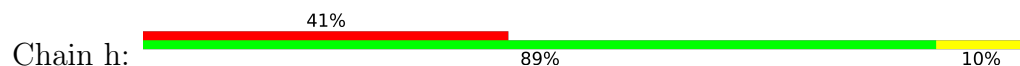
- Molecule 21: Proteasome subunit alpha type-6



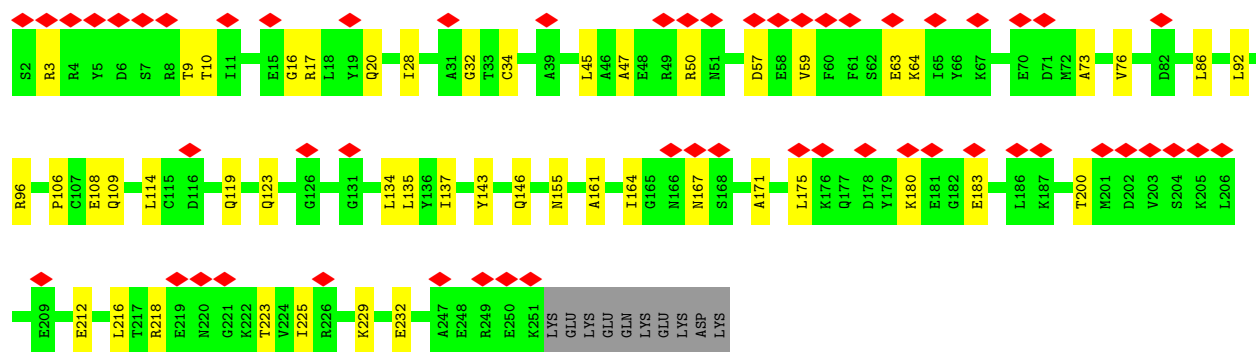
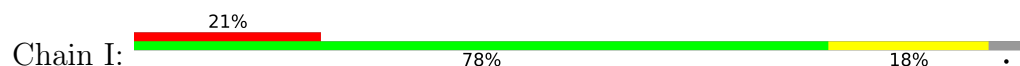
- Molecule 22: Proteasome subunit alpha type-2



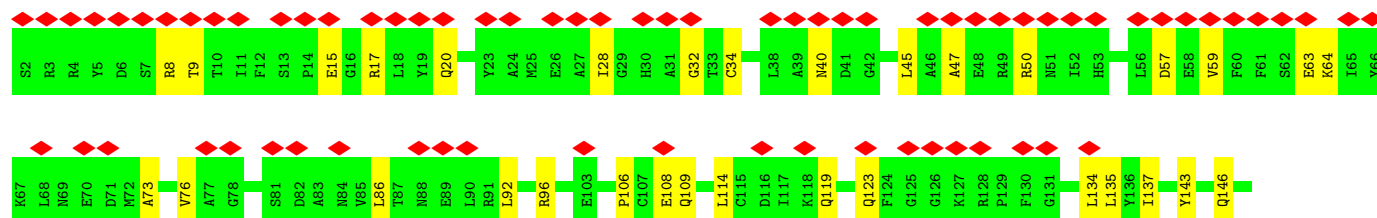
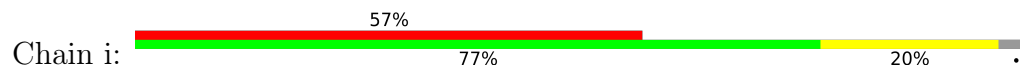
• Molecule 22: Proteasome subunit alpha type-2

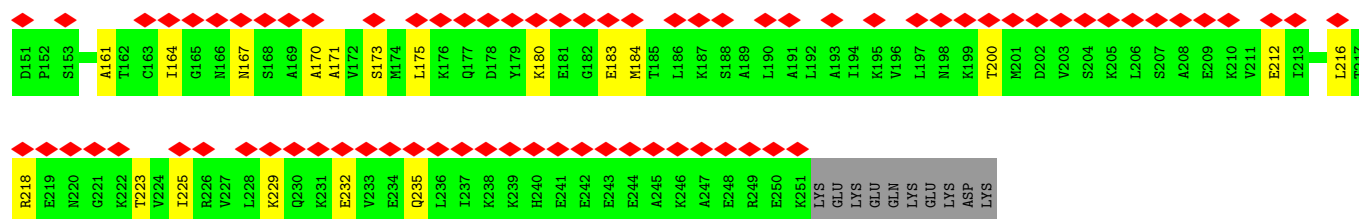


• Molecule 23: Proteasome subunit alpha type-4

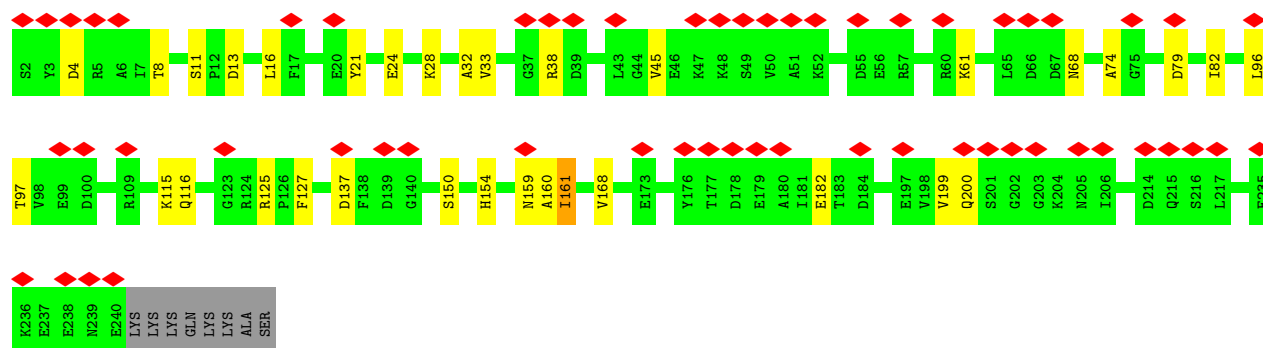
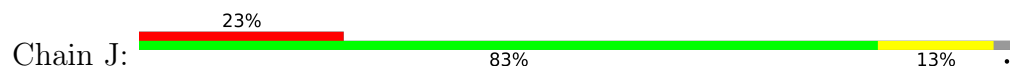


• Molecule 23: Proteasome subunit alpha type-4

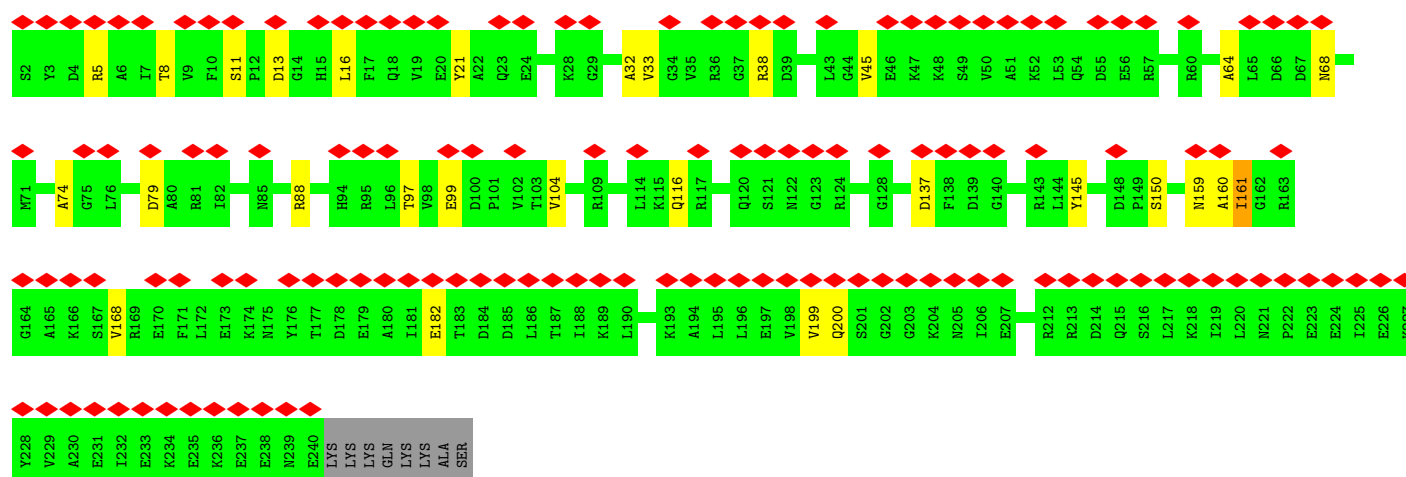
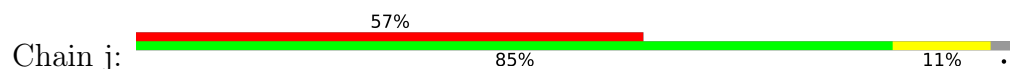




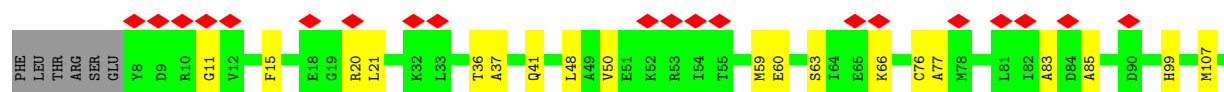
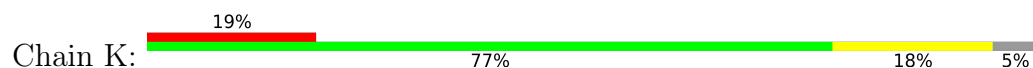
• Molecule 24: Proteasome subunit alpha type-7

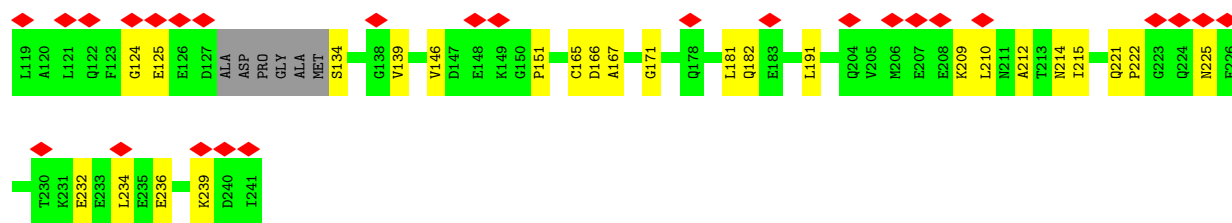


• Molecule 24: Proteasome subunit alpha type-7



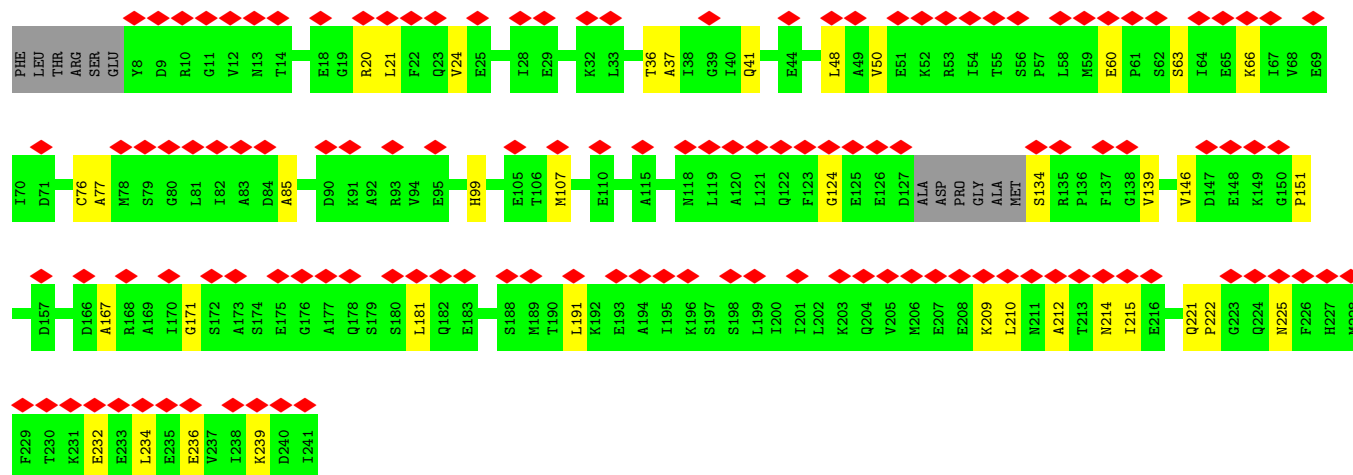
• Molecule 25: Proteasome subunit alpha type-5





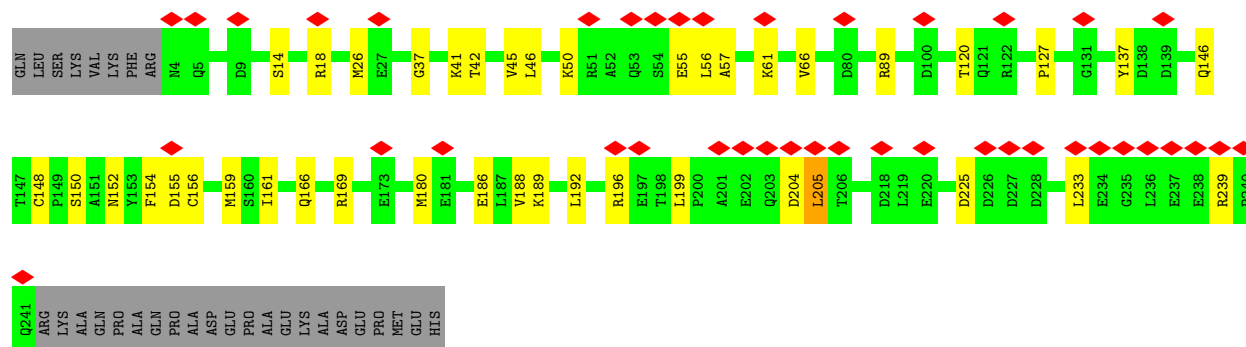
• Molecule 25: Proteasome subunit alpha type-5

Chain k: 53% 80% 15% 5%



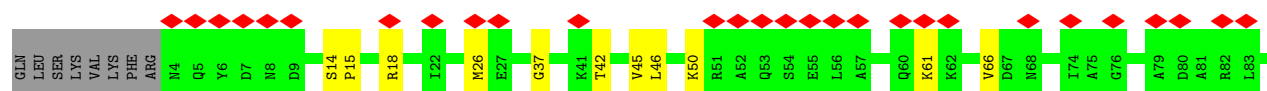
• Molecule 26: Proteasome subunit alpha type-1

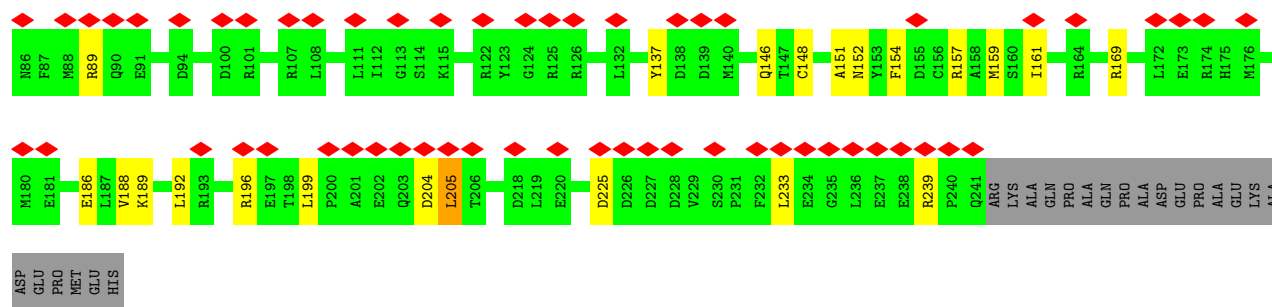
Chain L: 15% 74% 15% 11%



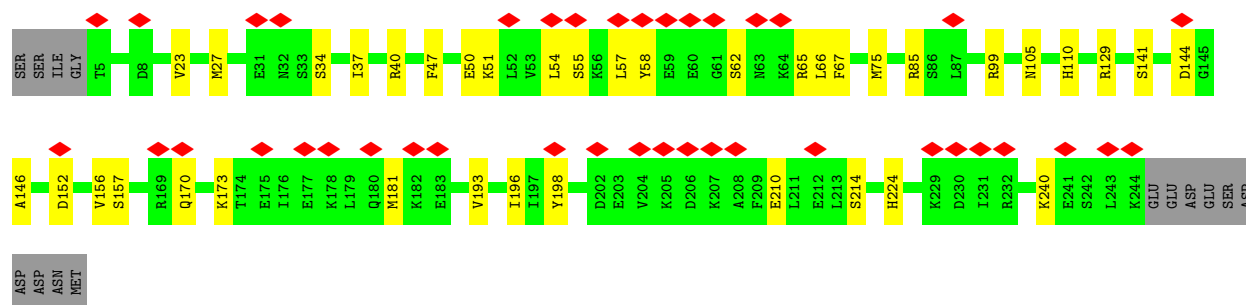
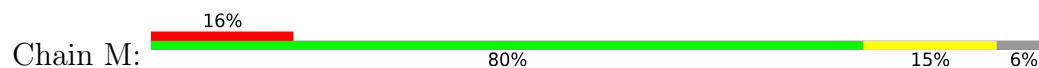
• Molecule 26: Proteasome subunit alpha type-1

Chain I: 32% 76% 12% 11%

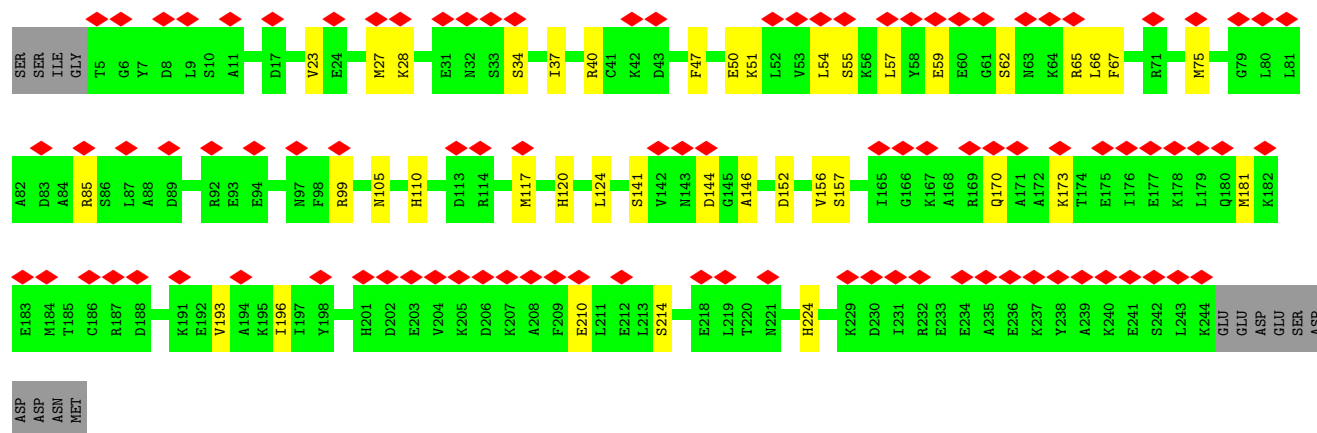
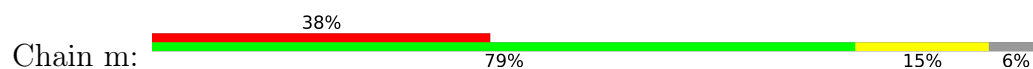




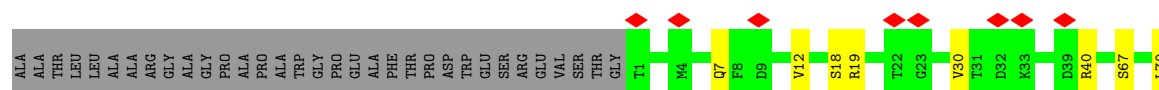
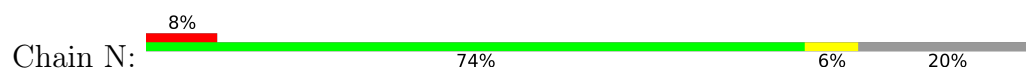
• Molecule 27: Proteasome subunit alpha type-3

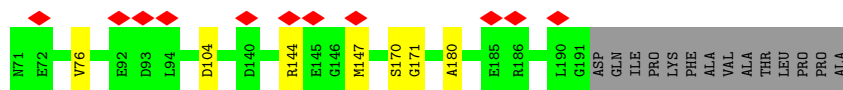


• Molecule 27: Proteasome subunit alpha type-3

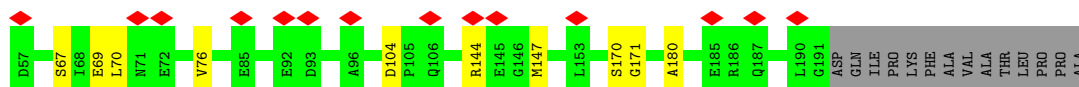
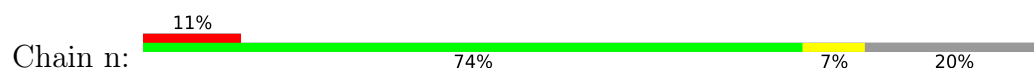


• Molecule 28: Proteasome subunit beta type-6

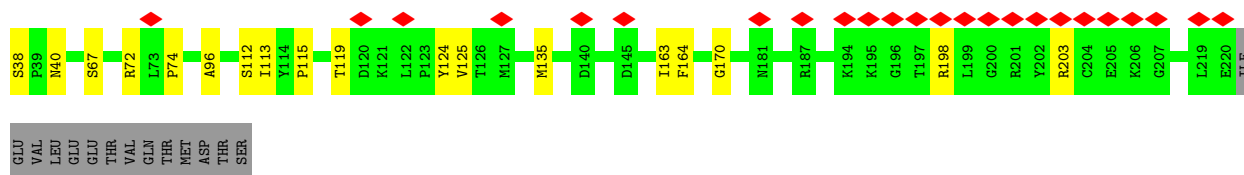
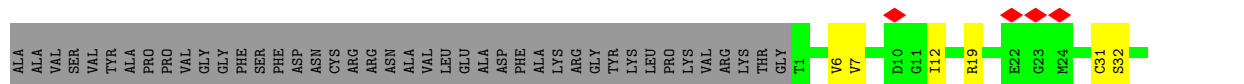




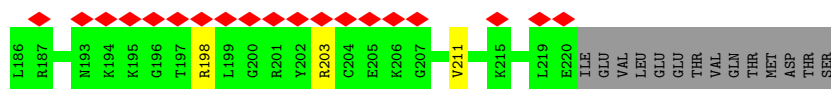
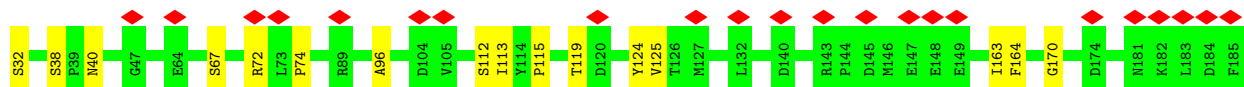
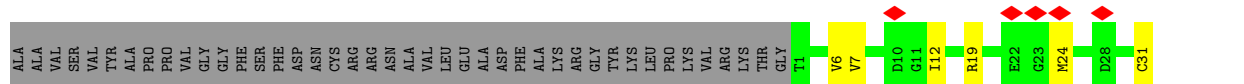
- Molecule 28: Proteasome subunit beta type-6



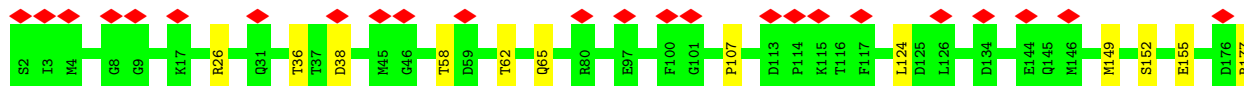
- Molecule 29: Proteasome subunit beta type-7



- Molecule 29: Proteasome subunit beta type-7

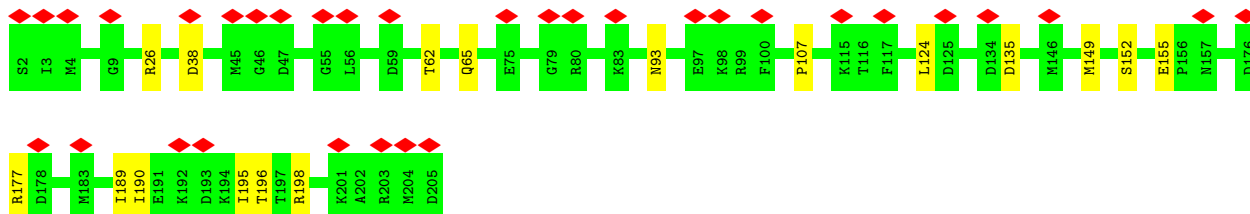
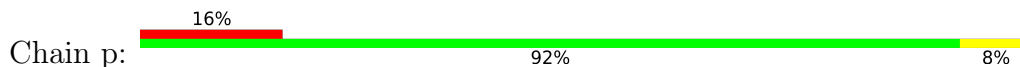


- Molecule 30: Proteasome subunit beta type-3

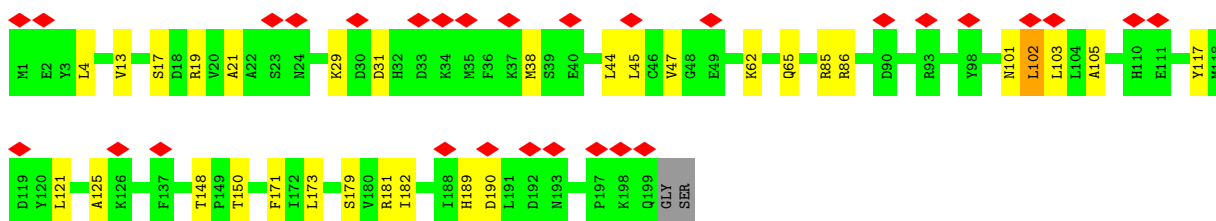
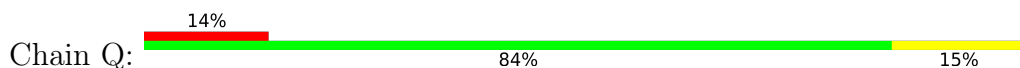




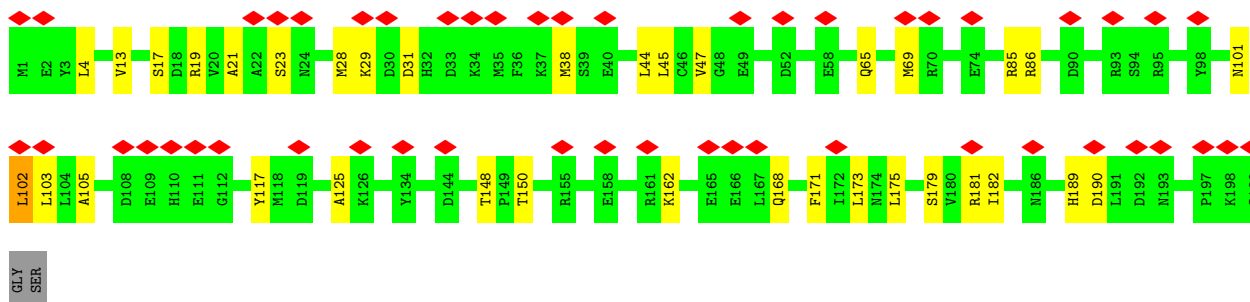
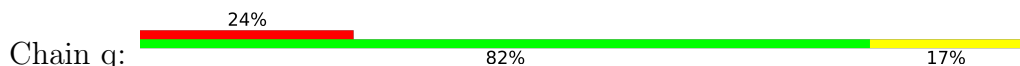
• Molecule 30: Proteasome subunit beta type-3



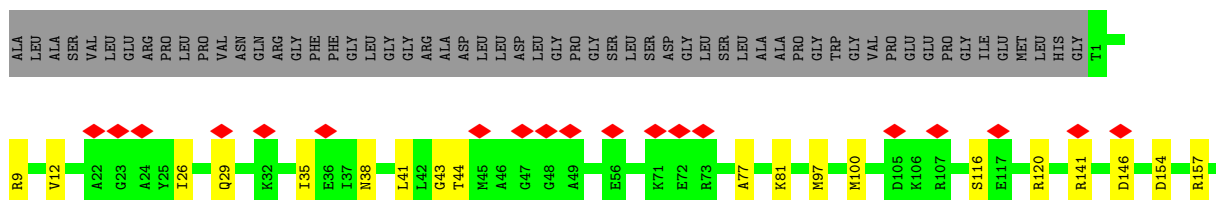
• Molecule 31: Proteasome subunit beta type-2

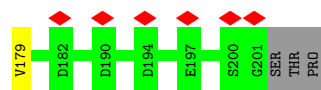


• Molecule 31: Proteasome subunit beta type-2

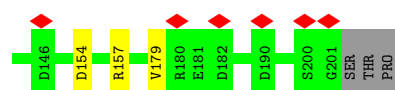
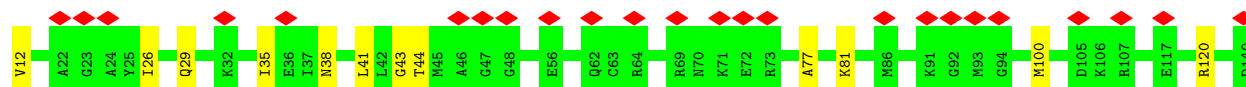
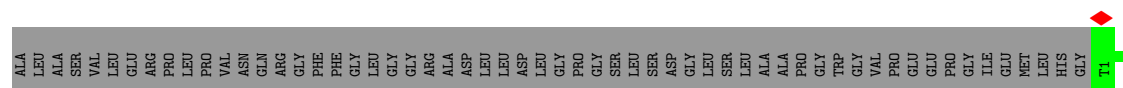


• Molecule 32: Proteasome subunit beta type-5

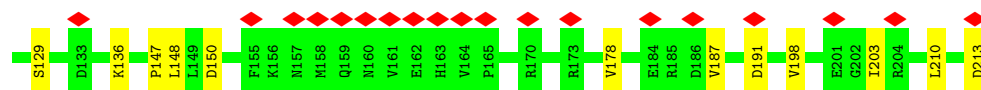
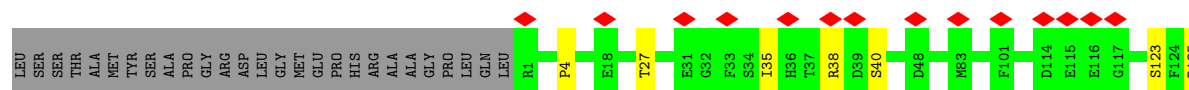
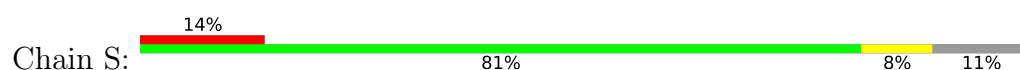




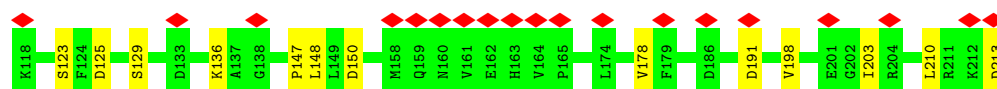
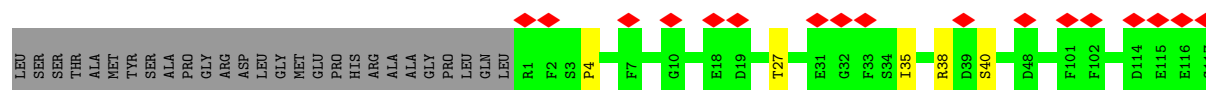
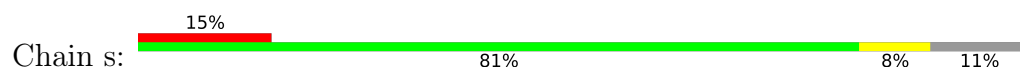
- Molecule 32: Proteasome subunit beta type-5



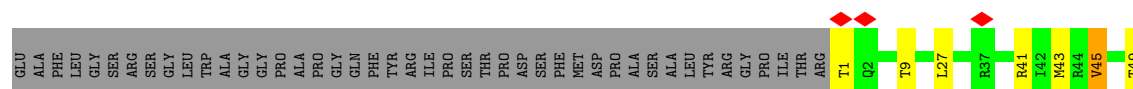
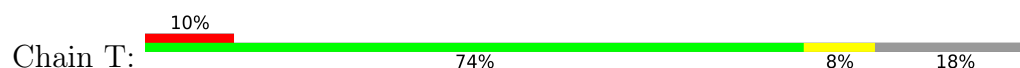
- Molecule 33: Proteasome subunit beta type-1

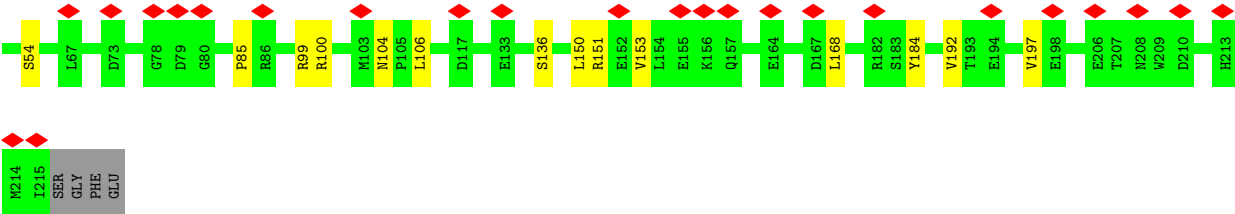


- Molecule 33: Proteasome subunit beta type-1

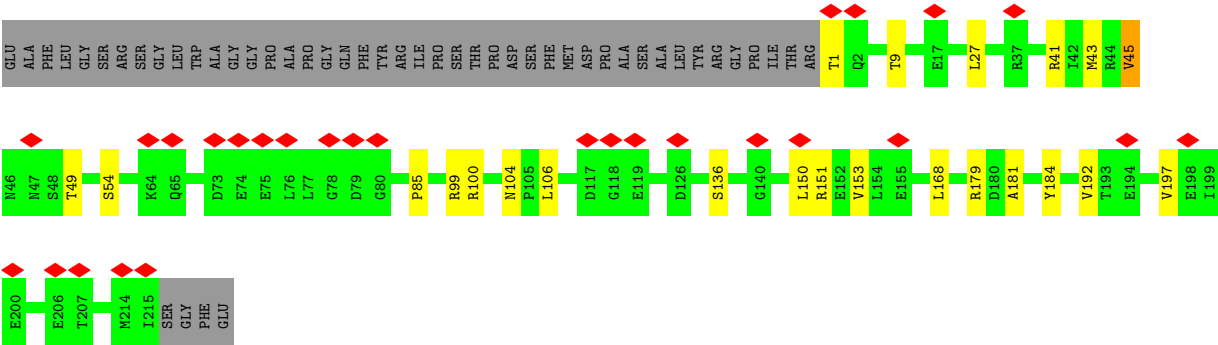


- Molecule 34: Proteasome subunit beta type-4





• Molecule 34: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.22	0/6449	0.55	3/8729 (0.0%)
2	V	0.30	1/3929 (0.0%)	0.73	1/5309 (0.0%)
3	W	0.25	0/3751	0.65	2/5042 (0.0%)
4	X	0.21	0/3053	0.50	0/4115
5	Y	0.59	8/3173 (0.3%)	0.98	23/4273 (0.5%)
6	Z	0.25	0/2324	0.68	0/3150
7	a	0.25	0/3053	0.64	3/4133 (0.1%)
8	b	0.23	0/1478	0.61	0/2001
9	c	0.27	0/2302	0.65	0/3110
10	d	0.25	0/2162	0.62	0/2919
11	e	1.12	3/338 (0.9%)	2.24	15/450 (3.3%)
12	f	0.28	0/6980	0.75	8/9433 (0.1%)
13	A	0.26	0/3117	0.64	0/4207
14	B	0.26	0/3131	0.58	0/4227
15	C	0.24	0/3017	0.65	3/4058 (0.1%)
16	D	0.26	0/3089	0.55	0/4168
17	E	0.26	0/3145	0.55	0/4233
18	F	0.28	1/3292 (0.0%)	0.53	0/4435
19	u	0.26	0/609	0.65	2/819 (0.2%)
20	v	0.02	0/8	0.05	0/8
21	G	0.23	0/1859	0.51	0/2523
21	g	0.23	0/1859	0.51	0/2523
22	H	0.24	0/1743	0.48	0/2372
22	h	0.24	0/1743	0.48	0/2372
23	I	0.22	0/1942	0.51	0/2628
23	i	0.22	0/1942	0.52	0/2628
24	J	0.22	0/1728	0.54	1/2358 (0.0%)
24	j	0.22	0/1728	0.54	1/2358 (0.0%)
25	K	0.22	0/1747	0.48	0/2364
25	k	0.22	0/1747	0.48	0/2364
26	L	0.26	0/1885	0.55	0/2552
26	l	0.26	0/1885	0.55	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	M	0.24	0/1891	0.54	0/2552
27	m	0.24	0/1891	0.54	0/2552
28	N	0.21	0/1454	0.41	0/1967
28	n	0.21	0/1454	0.41	0/1967
29	O	0.22	0/1670	0.40	0/2265
29	o	0.22	0/1670	0.40	0/2265
30	P	0.22	0/1614	0.41	0/2177
30	p	0.22	0/1614	0.41	0/2177
31	Q	0.26	0/1603	0.51	0/2174
31	q	0.26	0/1603	0.51	0/2174
32	R	0.22	0/1579	0.36	0/2134
32	r	0.22	0/1579	0.36	0/2134
33	S	0.22	0/1671	0.40	0/2253
33	s	0.22	0/1671	0.40	0/2253
34	T	0.23	0/1700	0.43	0/2305
34	t	0.23	0/1700	0.43	0/2305
All	All	0.27	13/106572 (0.0%)	0.59	62/144067 (0.0%)

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

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	184	GLN	CA-C	10.26	1.65	1.52
5	Y	184	GLN	N-CA	8.23	1.54	1.46
5	Y	186	LEU	CA-C	7.89	1.60	1.52
5	Y	185	GLY	CA-C	7.88	1.62	1.51
11	e	64	GLY	CA-C	6.56	1.61	1.51

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	185	GLY	CA-C-N	14.68	144.78	122.17
5	Y	185	GLY	C-N-CA	14.68	144.78	122.17
11	e	63	HIS	CA-C-N	13.50	147.86	121.41
11	e	63	HIS	C-N-CA	13.50	147.86	121.41
11	e	63	HIS	CB-CA-C	12.66	135.61	110.42

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	344	ASP	Peptide
2	V	82	LEU	Peptide
3	W	137	TYR	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6334	0	6366	97	0
2	V	3852	0	3893	99	0
3	W	3703	0	3822	73	0
4	X	3009	0	3113	22	0
5	Y	3115	0	3120	102	0
6	Z	2281	0	2312	28	0
7	a	2995	0	3012	42	0
8	b	1458	0	1505	28	0
9	c	2260	0	2276	39	0
10	d	2116	0	2146	39	0
11	e	334	0	294	51	0
12	f	6866	0	6866	154	0
13	A	3067	0	3100	56	0
14	B	3086	0	3134	46	0
15	C	2978	0	3075	51	0
16	D	3039	0	3075	43	0
17	E	3097	0	3174	65	0
18	F	3251	0	3318	58	0
19	u	603	0	629	14	0
20	v	143	0	44	1	0
21	G	1826	0	1796	16	0
21	g	1826	0	1796	19	0
22	H	1708	0	1594	17	0
22	h	1708	0	1594	16	0
23	I	1912	0	1851	30	0
23	i	1912	0	1851	29	0
24	J	1704	0	1517	22	0
24	j	1704	0	1517	16	0
25	K	1722	0	1673	29	0
25	k	1722	0	1673	20	0
26	L	1850	0	1822	31	0
26	l	1850	0	1822	22	0
27	M	1856	0	1814	26	0
27	m	1856	0	1814	28	0
28	N	1430	0	1398	10	0
28	n	1430	0	1398	9	0
29	O	1643	0	1644	15	0
29	o	1643	0	1644	16	0
30	P	1585	0	1598	12	0
30	p	1585	0	1598	13	0
31	Q	1570	0	1547	19	0
31	q	1570	0	1547	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	1548	0	1499	11	0
32	r	1548	0	1499	8	0
33	S	1641	0	1618	15	0
33	s	1641	0	1618	13	0
34	T	1667	0	1628	15	0
34	t	1667	0	1628	16	0
35	c	1	0	0	0	0
36	A	31	0	12	1	0
36	D	31	0	12	2	0
36	F	31	0	12	0	0
37	A	1	0	0	0	0
37	D	1	0	0	0	0
37	F	1	0	0	0	0
38	B	27	0	12	3	0
38	E	27	0	12	2	0
All	All	105062	0	104332	1392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1392 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:206:LYS:HE2	18:F:263:ASP:OD2	1.62	0.97
17:E:206:LYS:HE3	18:F:263:ASP:OD1	1.65	0.96
17:E:206:LYS:CE	18:F:263:ASP:OD1	2.30	0.79
5:Y:177:ARG:HA	5:Y:180:LEU:HB2	1.68	0.76
5:Y:184:GLN:HB2	11:e:66:LYS:HB3	1.67	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	748 (93%)	55 (7%)	3 (0%)	30	60
2	V	478/533 (90%)	412 (86%)	65 (14%)	1 (0%)	43	71
3	W	454/456 (100%)	409 (90%)	45 (10%)	0	100	100
4	X	378/422 (90%)	362 (96%)	15 (4%)	1 (0%)	36	65
5	Y	376/389 (97%)	317 (84%)	51 (14%)	8 (2%)	5	26
6	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	30	60
7	a	371/376 (99%)	334 (90%)	35 (9%)	2 (0%)	24	55
8	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	24	55
9	c	285/309 (92%)	256 (90%)	29 (10%)	0	100	100
10	d	255/349 (73%)	213 (84%)	41 (16%)	1 (0%)	30	60
11	e	36/70 (51%)	16 (44%)	18 (50%)	2 (6%)	1	9
12	f	887/892 (99%)	714 (80%)	164 (18%)	9 (1%)	12	40
13	A	391/433 (90%)	335 (86%)	53 (14%)	3 (1%)	16	45
14	B	393/440 (89%)	343 (87%)	50 (13%)	0	100	100
15	C	379/398 (95%)	334 (88%)	42 (11%)	3 (1%)	16	45
16	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	9	35
17	E	387/403 (96%)	349 (90%)	38 (10%)	0	100	100
18	F	413/439 (94%)	374 (91%)	36 (9%)	3 (1%)	18	49
19	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
20	v	1/28 (4%)	0	1 (100%)	0	100	100
21	G	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
21	g	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
22	H	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
22	h	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
23	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
23	i	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
24	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	45
24	j	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	45
25	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
26	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
26	l	236/268 (88%)	222 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
27	m	238/254 (94%)	215 (90%)	23 (10%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
30	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
31	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
31	q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
32	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
33	S	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
33	s	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
34	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
34	t	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
All	All	13375/14947 (90%)	12160 (91%)	1168 (9%)	47 (0%)	31	60

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	e	65	TYR
12	f	808	ASN
12	f	853	VAL
1	U	874	ASN
5	Y	89	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	689 (100%)	3 (0%)	84	84
2	V	414/459 (90%)	414 (100%)	0	100	100
3	W	416/416 (100%)	413 (99%)	3 (1%)	76	80
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	86
5	Y	334/344 (97%)	332 (99%)	2 (1%)	78	81
6	Z	257/295 (87%)	254 (99%)	3 (1%)	63	75
7	a	333/336 (99%)	329 (99%)	4 (1%)	63	75
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	251 (100%)	1 (0%)	84	84
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	740 (99%)	5 (1%)	76	80
13	A	332/372 (89%)	329 (99%)	3 (1%)	70	78
14	B	344/385 (89%)	341 (99%)	3 (1%)	70	78
15	C	326/346 (94%)	322 (99%)	4 (1%)	63	75
16	D	333/366 (91%)	332 (100%)	1 (0%)	86	86
17	E	341/353 (97%)	339 (99%)	2 (1%)	78	81
18	F	357/379 (94%)	354 (99%)	3 (1%)	73	79
19	u	68/68 (100%)	68 (100%)	0	100	100
20	v	1/1 (100%)	1 (100%)	0	100	100
21	G	193/209 (92%)	192 (100%)	1 (0%)	81	83
21	g	193/209 (92%)	192 (100%)	1 (0%)	81	83
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	192 (100%)	1 (0%)	81	83
23	i	193/220 (88%)	192 (100%)	1 (0%)	81	83
24	J	152/210 (72%)	151 (99%)	1 (1%)	76	80
24	j	152/210 (72%)	151 (99%)	1 (1%)	76	80
25	K	186/202 (92%)	186 (100%)	0	100	100
25	k	186/202 (92%)	186 (100%)	0	100	100
26	L	198/229 (86%)	196 (99%)	2 (1%)	68	76
26	l	198/229 (86%)	196 (99%)	2 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	M	192/211 (91%)	191 (100%)	1 (0%)	81	83
27	m	192/211 (91%)	191 (100%)	1 (0%)	81	83
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	163 (99%)	1 (1%)	78	81
31	q	164/171 (96%)	163 (99%)	1 (1%)	78	81
32	R	153/201 (76%)	153 (100%)	0	100	100
32	r	153/201 (76%)	153 (100%)	0	100	100
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	175 (100%)	0	100	100
34	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11190/12651 (88%)	11138 (100%)	52 (0%)	78	83

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	C	109	THR
18	F	86	LEU
26	l	205	LEU
15	C	137	LEU
16	D	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
17	E	220	ASN
23	I	30	HIS
29	o	116	HIS
17	E	263	GLN
19	u	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ATP	A	501	37	32,33,33	1.29	5 (15%)	48,52,52	1.83	9 (18%)
36	ATP	D	501	37	32,33,33	1.32	3 (9%)	48,52,52	1.99	9 (18%)
38	ADP	E	401	-	28,29,29	1.36	4 (14%)	43,45,45	1.96	9 (20%)
38	ADP	B	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.91	8 (18%)
36	ATP	F	501	37	32,33,33	1.30	4 (12%)	48,52,52	1.89	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	A	501	37	-	0/22/38/38	0/3/3/3
36	ATP	D	501	37	-	7/22/38/38	0/3/3/3
38	ADP	E	401	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	ADP	B	501	-	-	3/16/32/32	0/3/3/3
36	ATP	F	501	37	-	3/22/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	4.70	1.47	1.39
36	F	501	ATP	C5-C4	4.58	1.47	1.39
38	B	501	ADP	C5-C4	4.55	1.47	1.39
38	E	401	ADP	C5-C4	4.44	1.47	1.39
36	A	501	ATP	C5-C4	4.39	1.46	1.39

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ATP	C5-C4-N3	-7.06	117.00	126.72
38	E	401	ADP	C5-C4-N3	-6.59	117.64	126.72
36	F	501	ATP	C5-C4-N3	-6.58	117.65	126.72
38	B	501	ADP	C5-C4-N3	-6.23	118.14	126.72
36	A	501	ATP	C5-C4-N3	-5.96	118.51	126.72

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

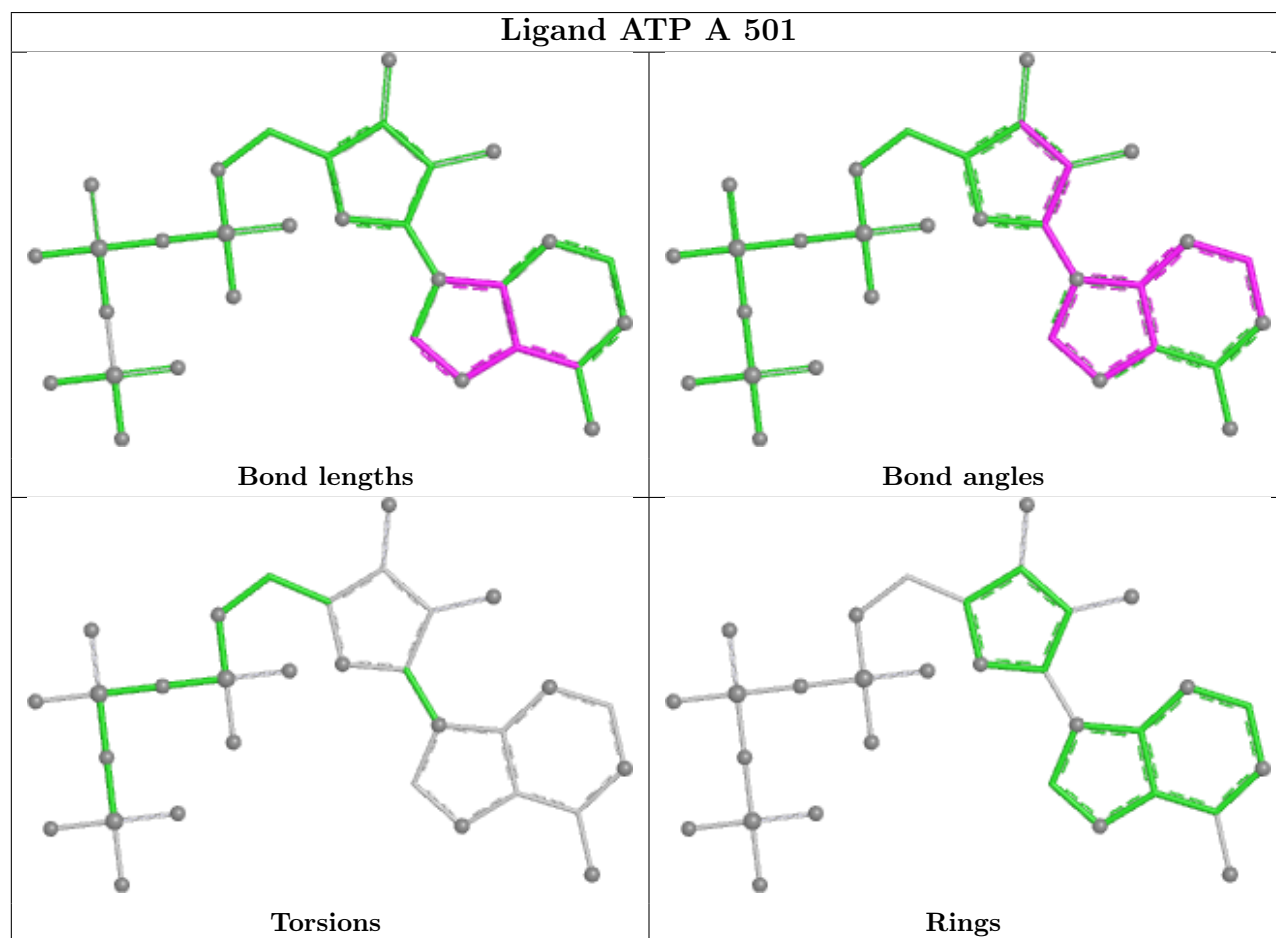
There are no ring outliers.

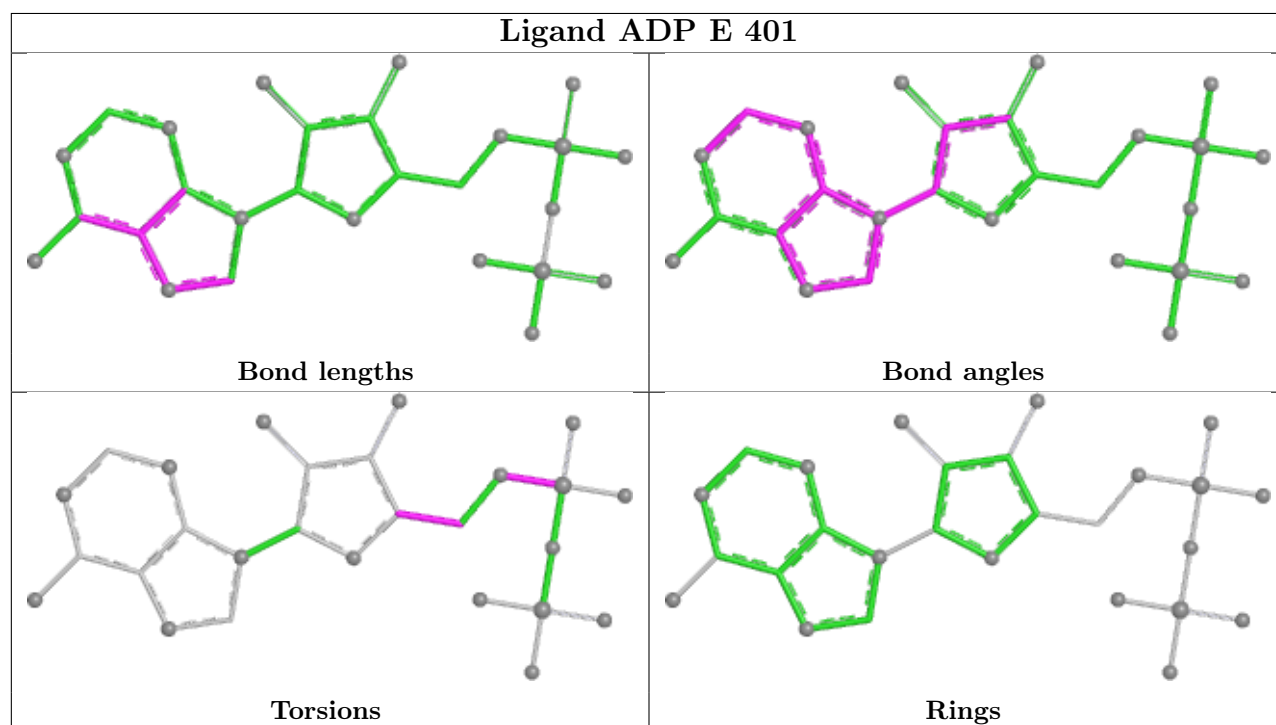
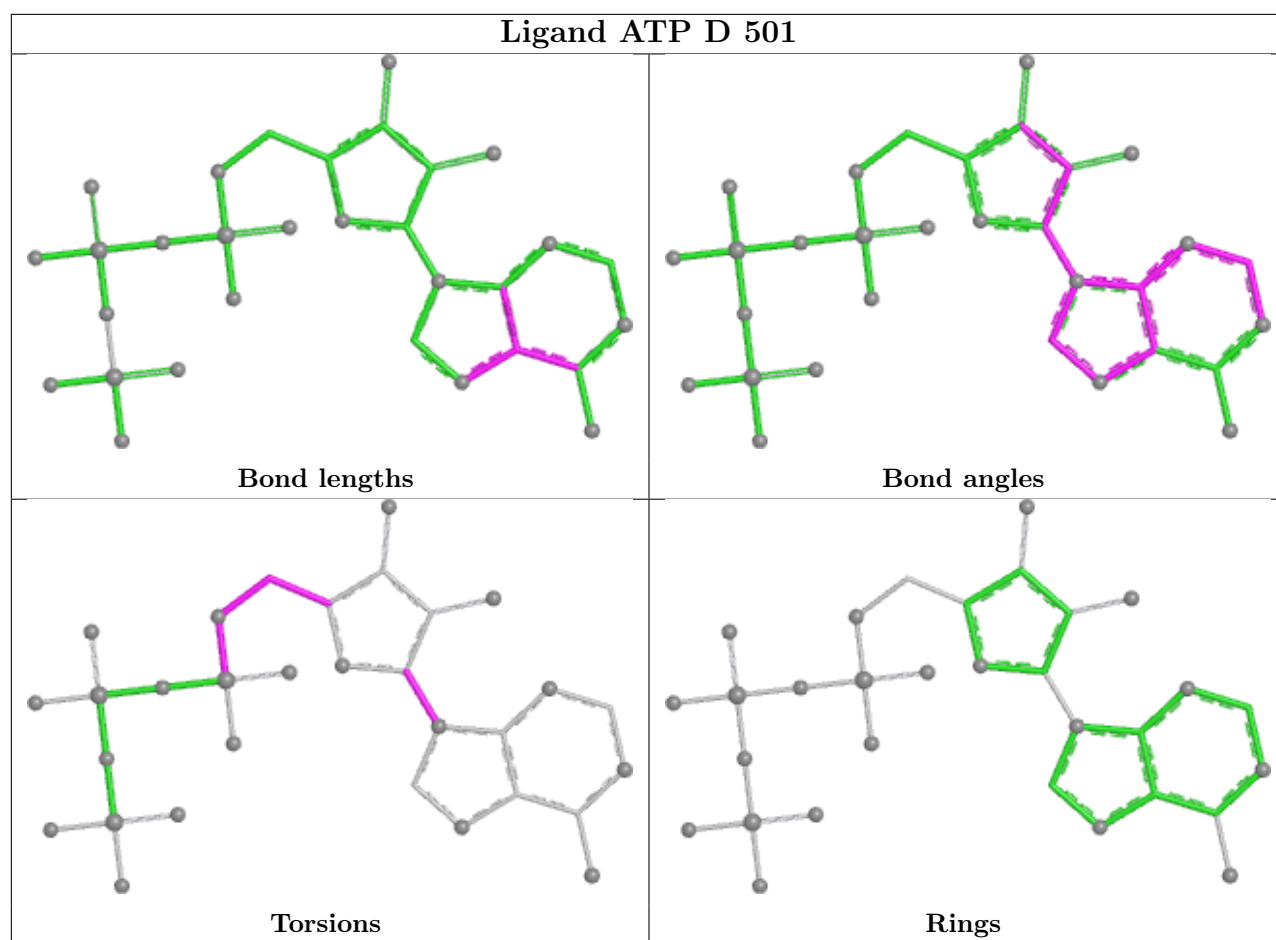
4 monomers are involved in 8 short contacts:

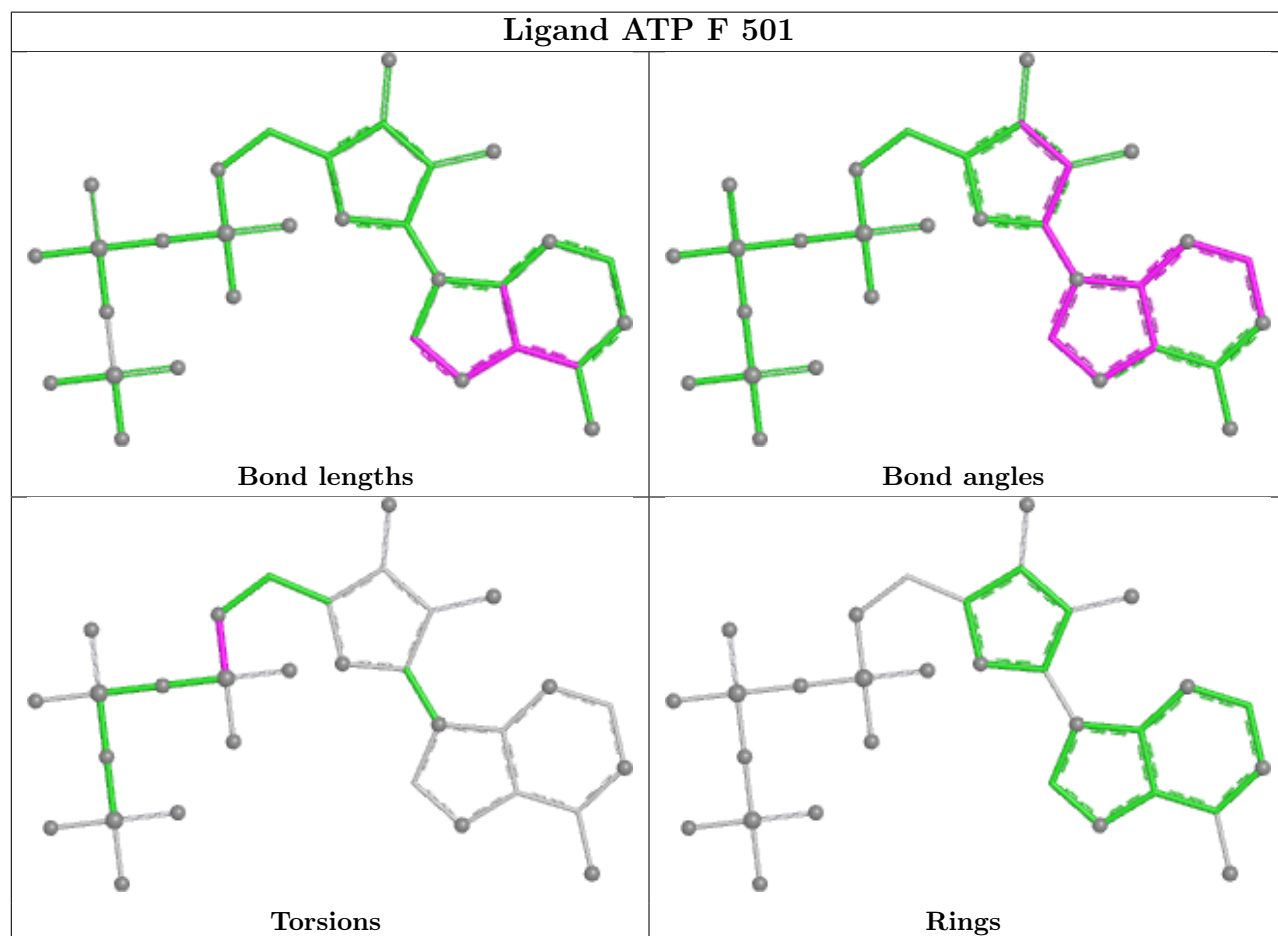
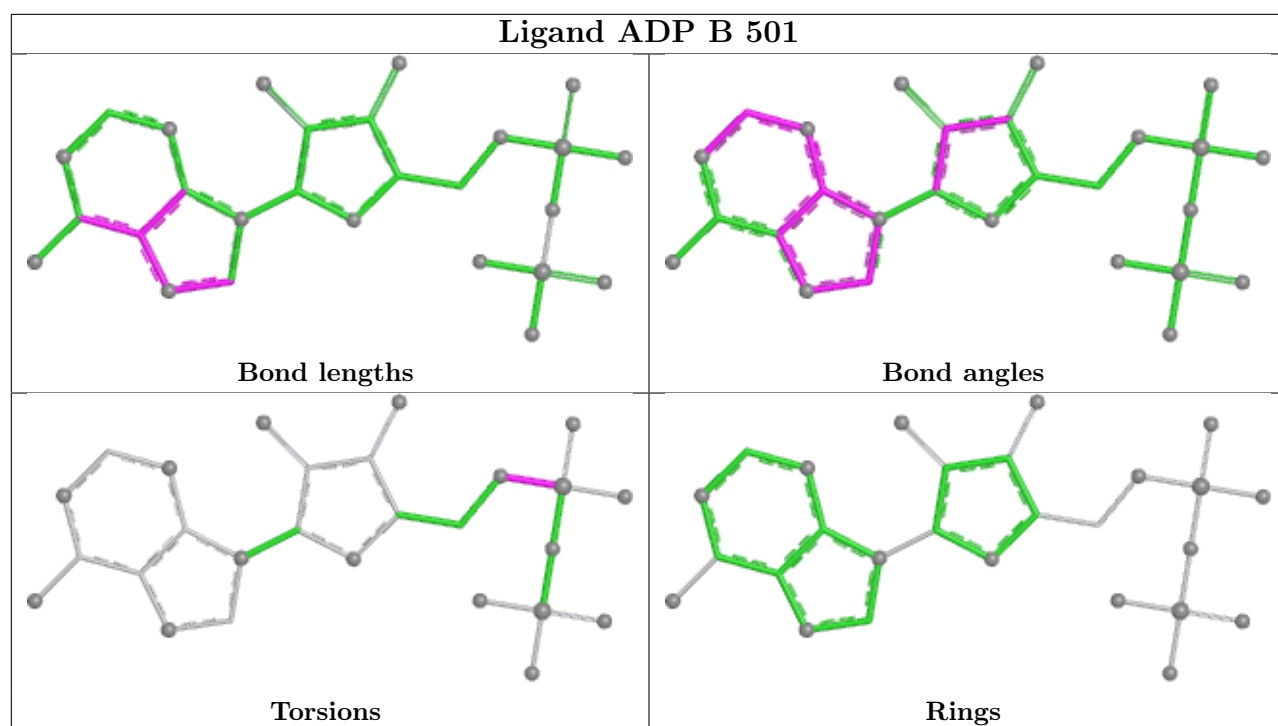
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	501	ATP	1	0
36	D	501	ATP	2	0
38	E	401	ADP	2	0
38	B	501	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

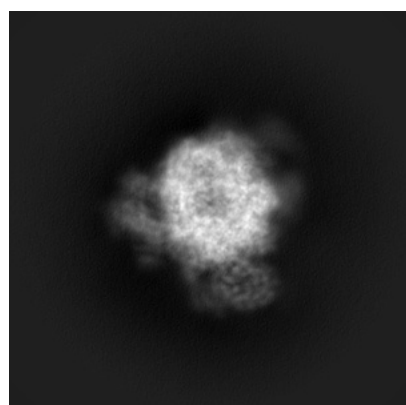
6 Map visualisation [i](#)

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

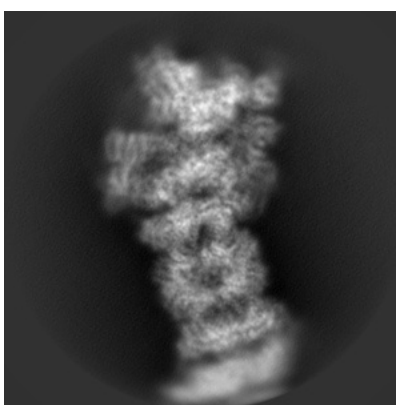
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

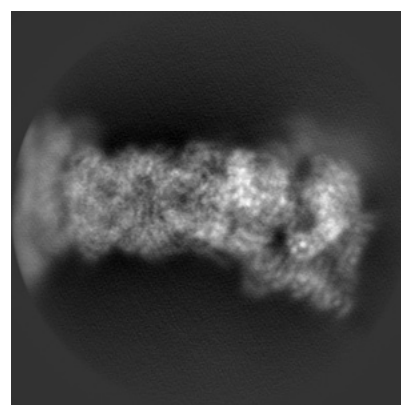
6.1.1 Primary map



X



Y

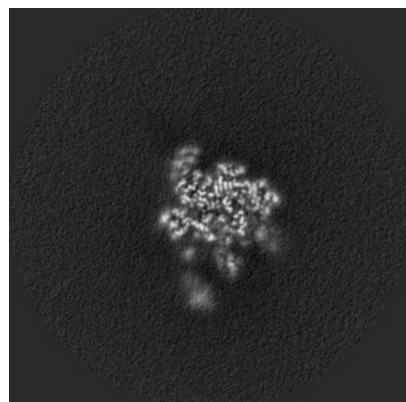


Z

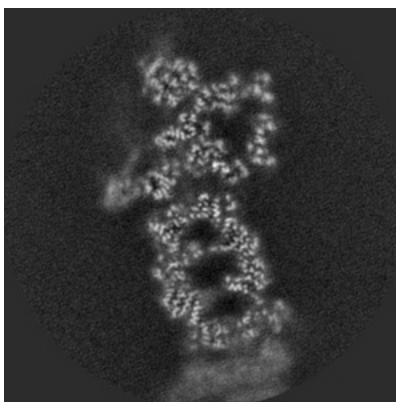
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

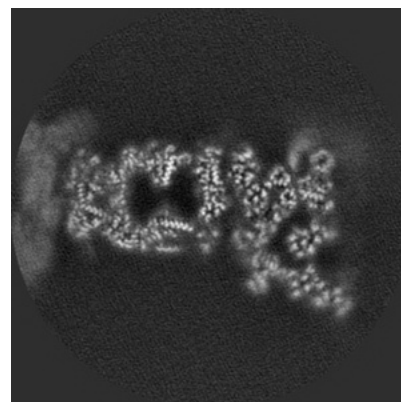
6.2.1 Primary map



X Index: 300



Y Index: 300

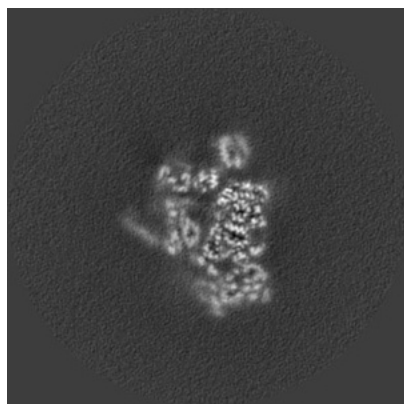


Z Index: 300

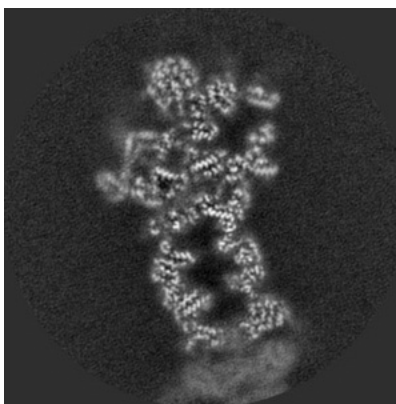
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

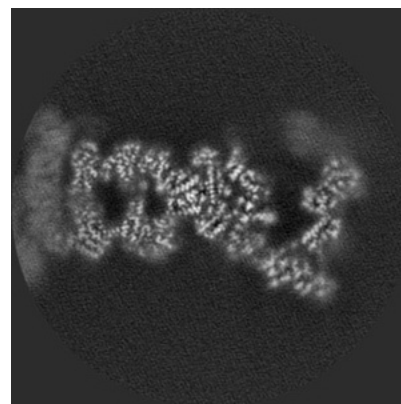
6.3.1 Primary map



X Index: 344



Y Index: 313

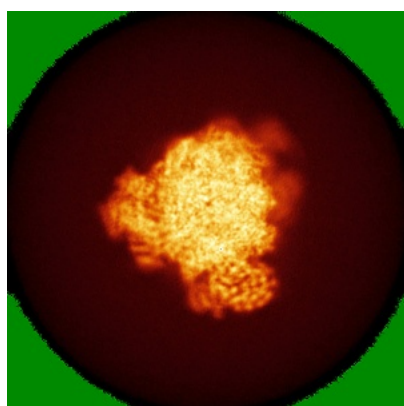


Z Index: 335

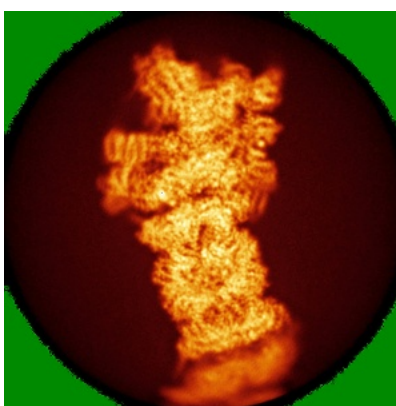
The images above show the largest variance slices of the map in three orthogonal directions.

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

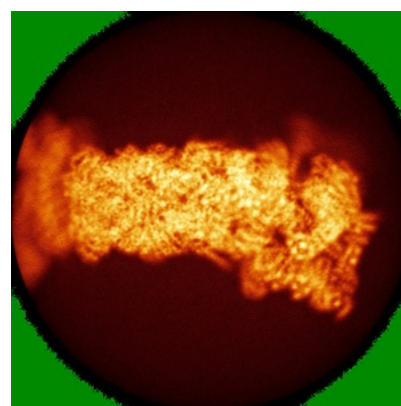
6.4.1 Primary map



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

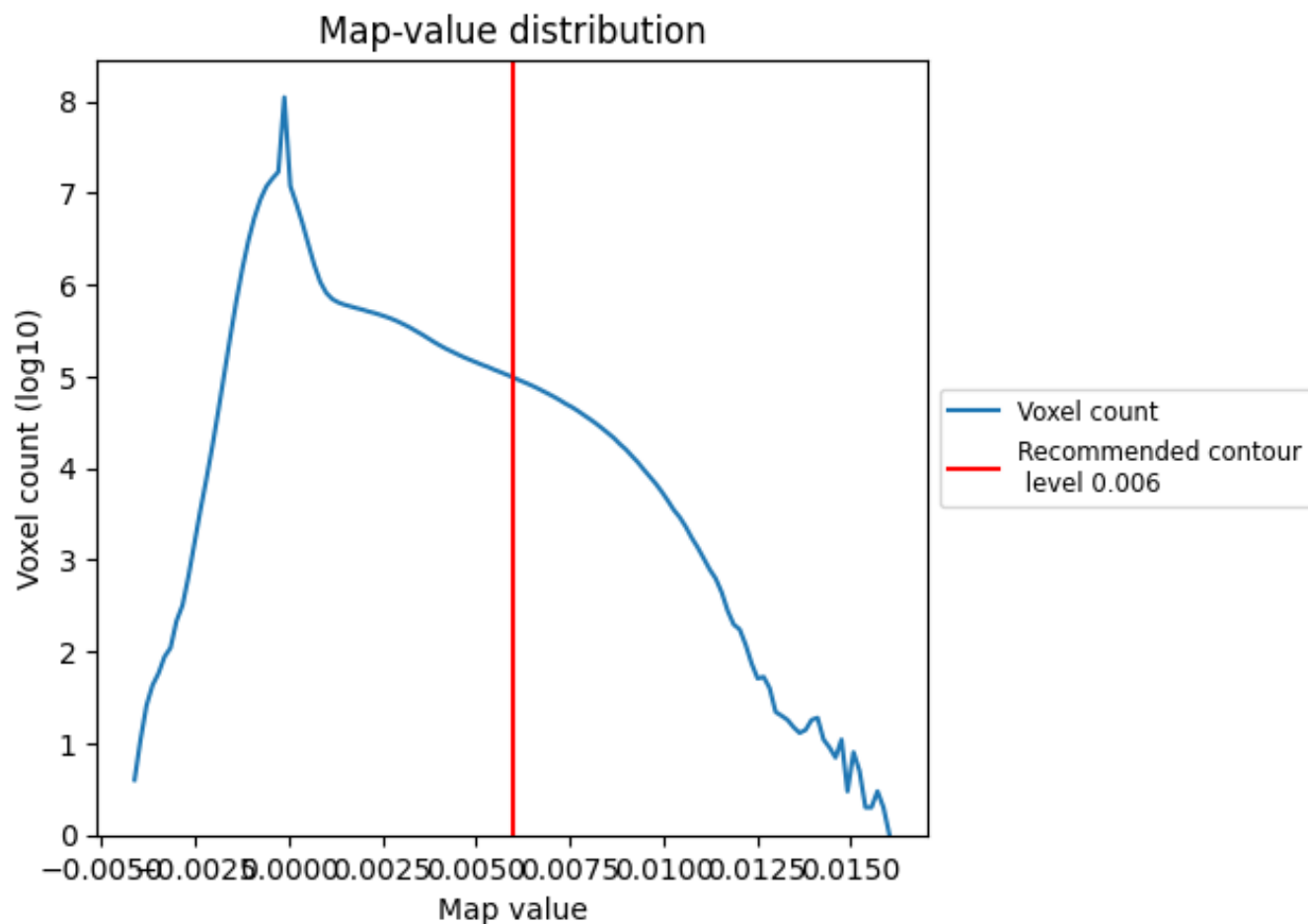
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

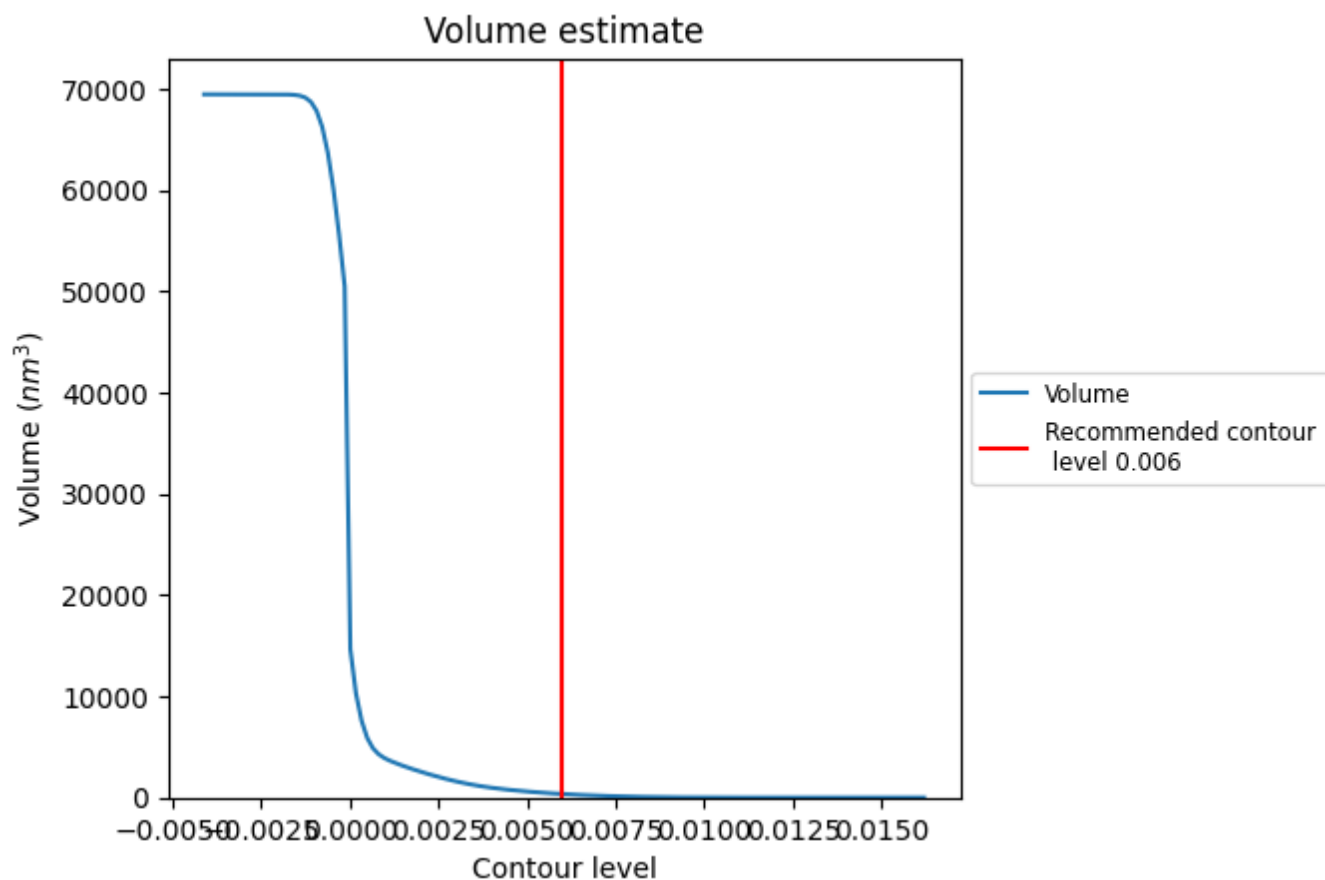
This section contains the results of statistical analysis of the map.

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.

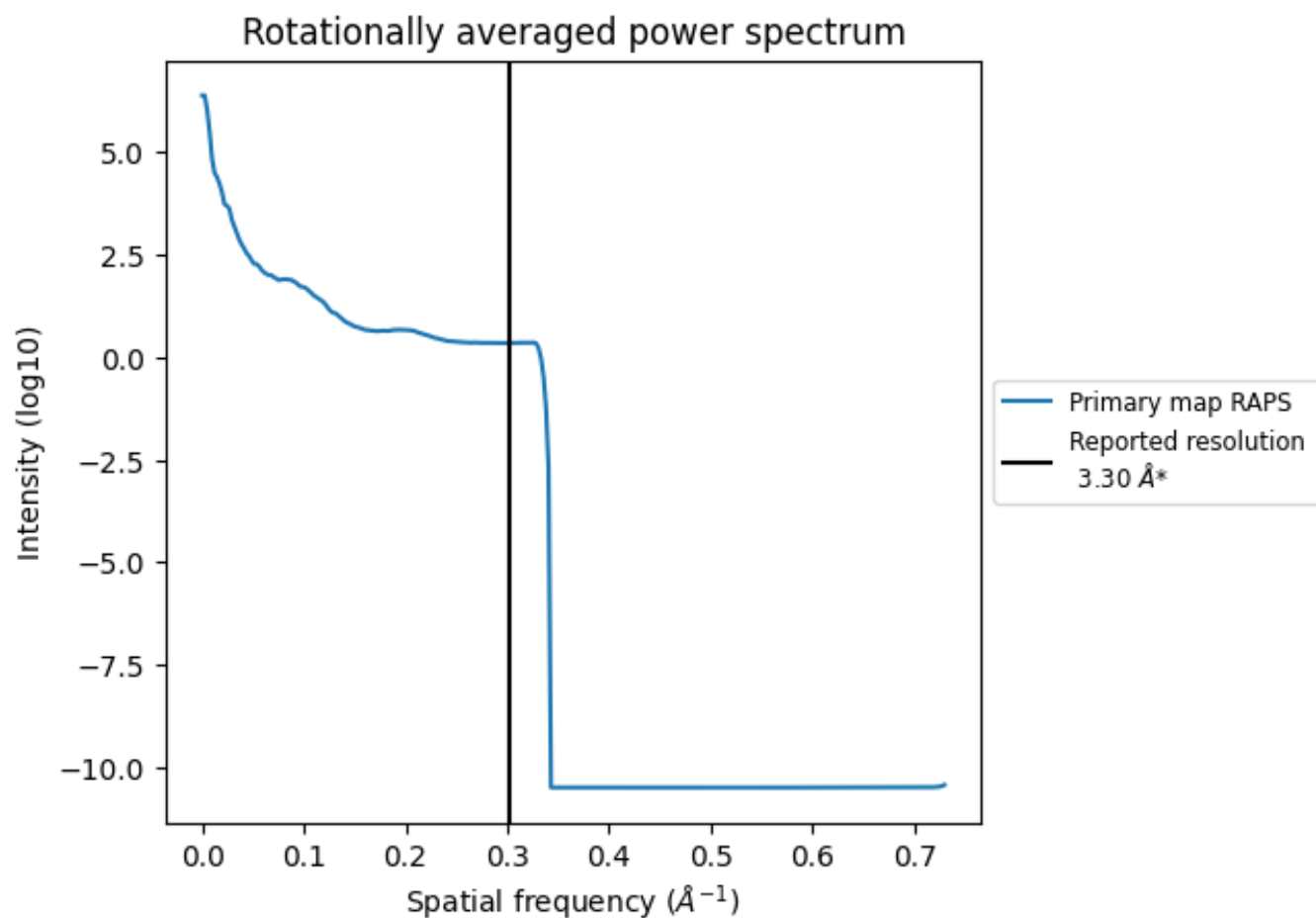
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm³; this corresponds to an approximate mass of 316 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

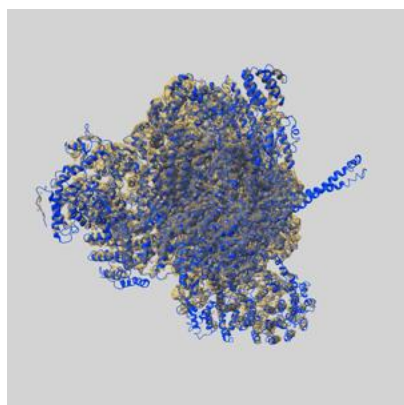
8 Fourier-Shell correlation

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

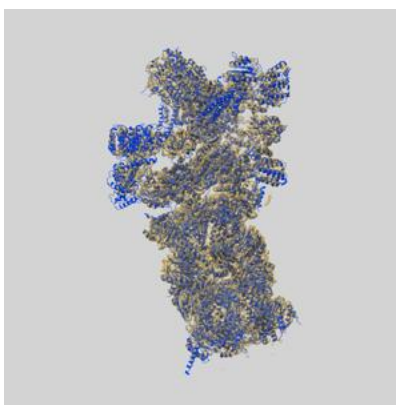
9 Map-model fit [i](#)

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

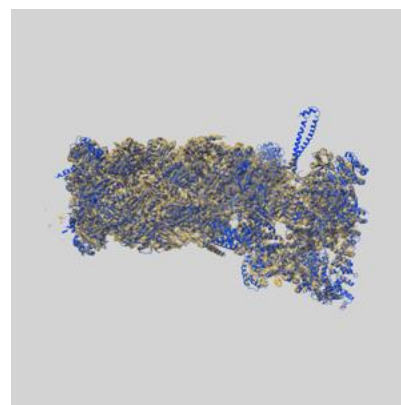
9.1 Map-model overlay [i](#)



X



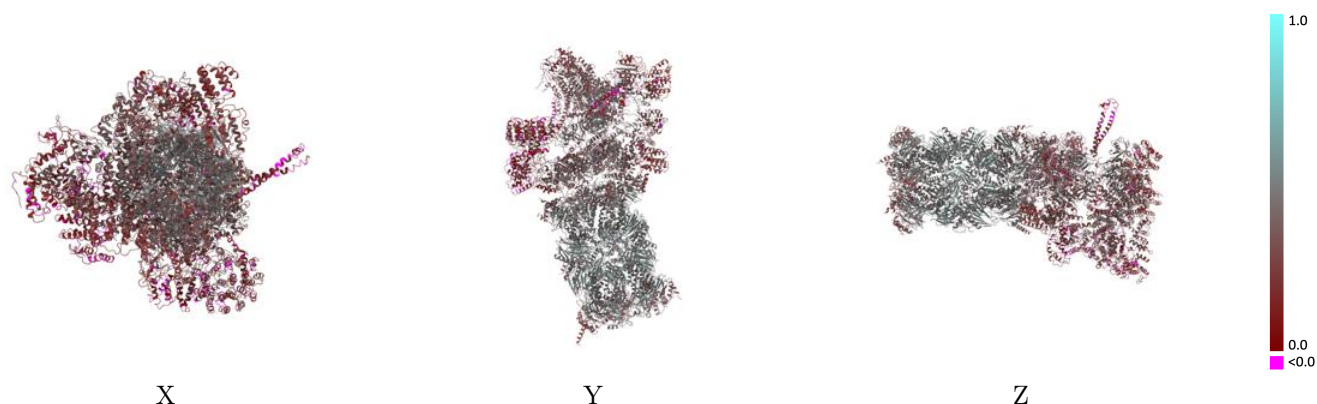
Y



Z

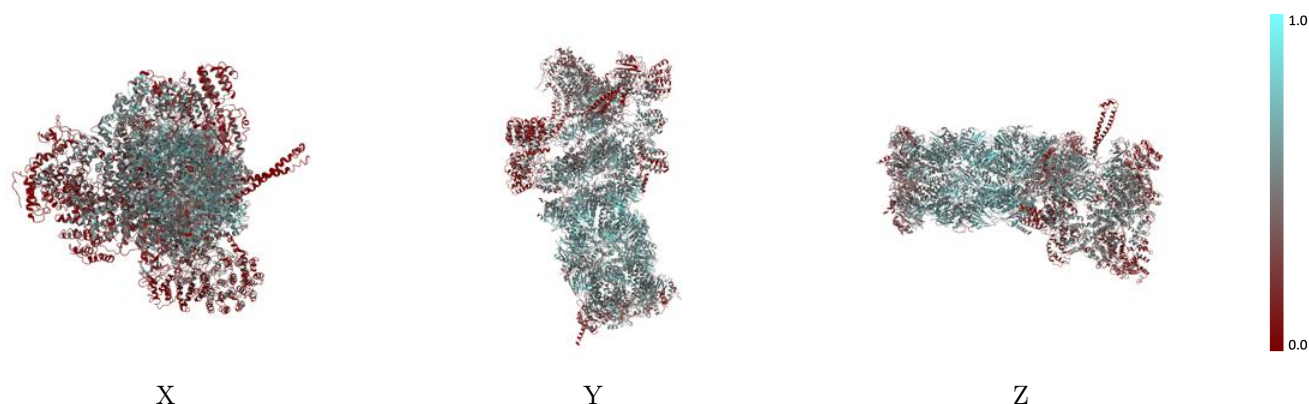
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



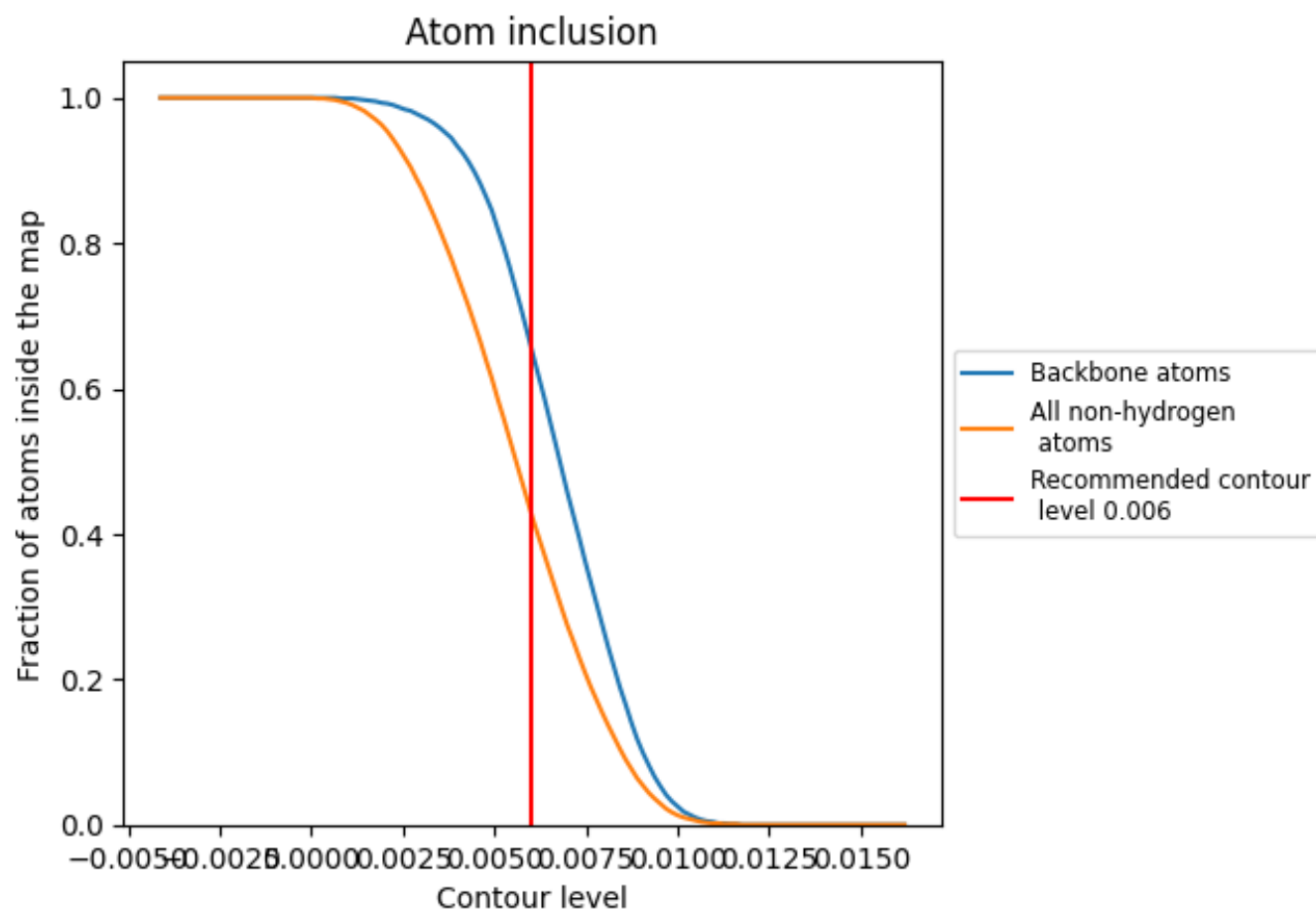
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4290	 0.3550
A	 0.4580	 0.3390
B	 0.4140	 0.3210
C	 0.3400	 0.2970
D	 0.4810	 0.3710
E	 0.4870	 0.3650
F	 0.4560	 0.3530
G	 0.5960	 0.4380
H	 0.6250	 0.4410
I	 0.5590	 0.4010
J	 0.5320	 0.4010
K	 0.5250	 0.4120
L	 0.5830	 0.4330
M	 0.5600	 0.4060
N	 0.6290	 0.4730
O	 0.5980	 0.4690
P	 0.6030	 0.4800
Q	 0.5880	 0.4490
R	 0.6260	 0.4810
S	 0.5680	 0.4790
T	 0.6250	 0.4790
U	 0.3490	 0.2980
V	 0.2460	 0.2070
W	 0.3920	 0.2490
X	 0.3600	 0.3020
Y	 0.2940	 0.2070
Z	 0.4290	 0.3590
a	 0.3340	 0.2620
b	 0.2140	 0.2880
c	 0.4650	 0.3730
d	 0.1510	 0.2060
e	 0.1760	 0.0300
f	 0.1610	 0.1760
g	 0.4240	 0.4320
h	 0.4280	 0.4300



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Chain	Atom inclusion	Q-score
i	 0.3430	 0.3770
j	 0.3260	 0.3800
k	 0.3780	 0.3940
l	 0.4730	 0.4310
m	 0.4410	 0.4120
n	 0.5840	 0.4840
o	 0.5270	 0.4760
p	 0.5520	 0.4810
q	 0.5320	 0.4560
r	 0.5850	 0.4920
s	 0.5460	 0.4780
t	 0.6080	 0.4860
u	 0.3830	 0.3900
v	 0.2520	 0.3740