



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 10:47 PM EDT

PDB ID : 6MSK
EMDB ID : EMD-9222
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

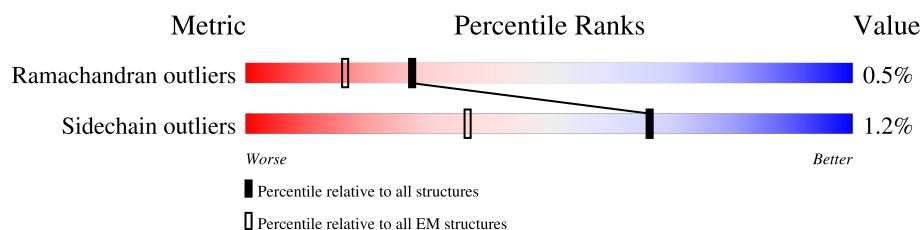
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	U	953	
2	V	533	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	

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Mol	Chain	Length	Quality of chain
10	d	349	
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	v	36	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	

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Mol	Chain	Length	Quality of chain
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105222 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	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- 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	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 14 is a protein called Rpt2, NP_002793.2 (26SHA chain B).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- 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
			3040	1923	524	580	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	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 19 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	230	Total	C	N	O	S	0	0
			1692	1073	285	329	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

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

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

- Molecule 27 is a protein called Proteasome subunit beta type-6.

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

- Molecule 28 is a protein called Proteasome subunit beta type-7.

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

- Molecule 29 is a protein called Proteasome subunit beta type-3.

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

- Molecule 30 is a protein called Proteasome subunit beta type-2.

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

- Molecule 31 is a protein called Proteasome subunit beta type-5.

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

- Molecule 32 is a protein called Proteasome subunit beta type-1.

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

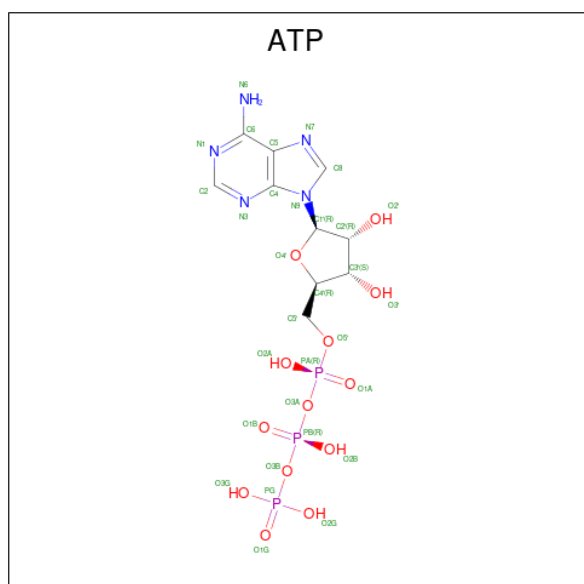
- Molecule 33 is a protein called Proteasome subunit beta type-4.

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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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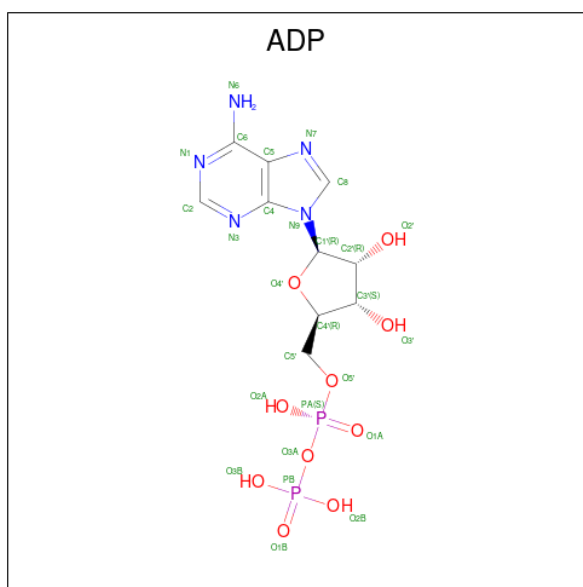
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Mol	Chain	Residues	Atoms					AltConf
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

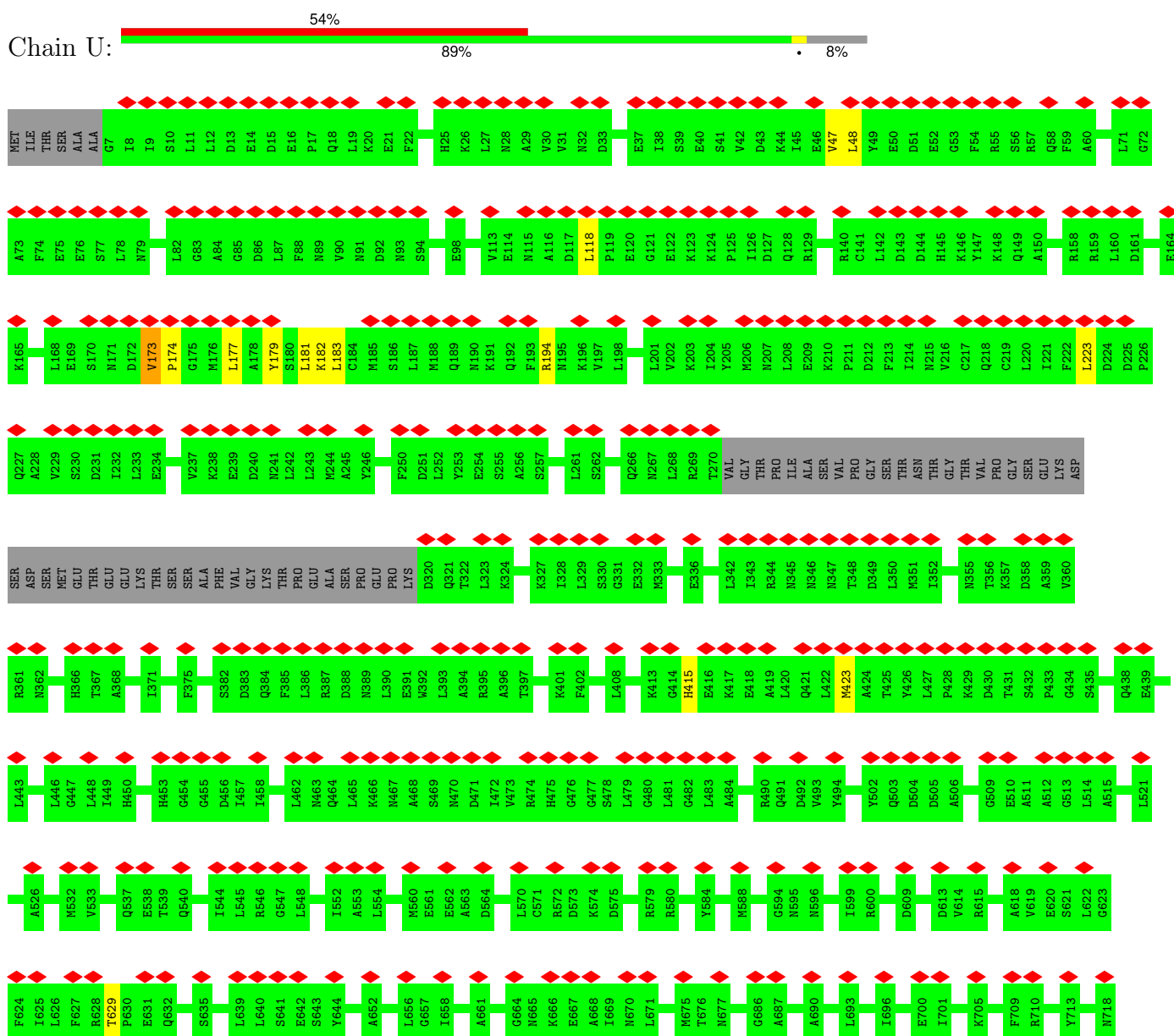


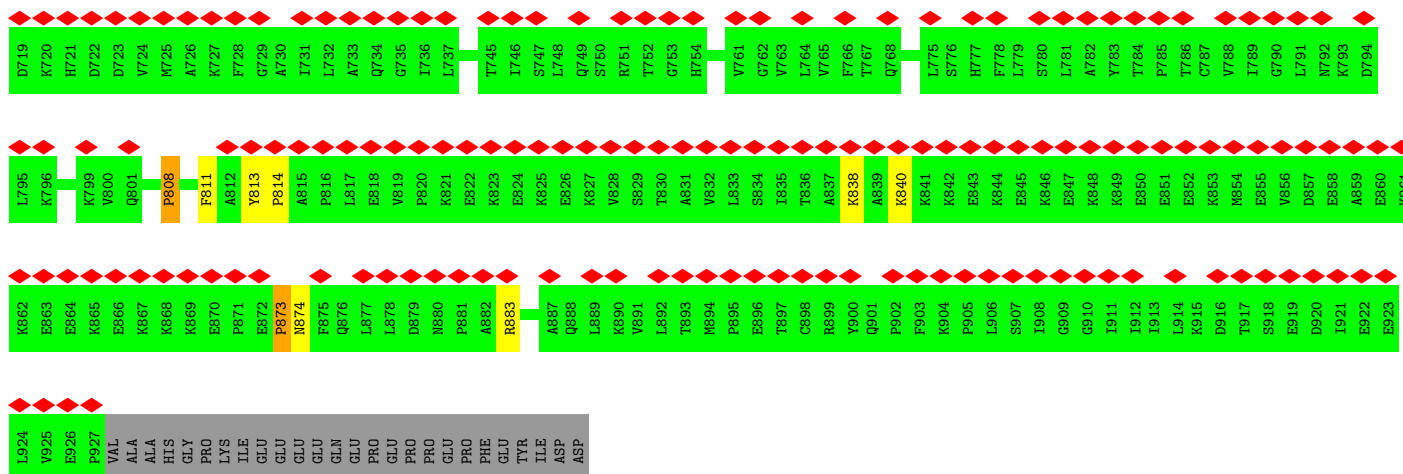
Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots [i](#)

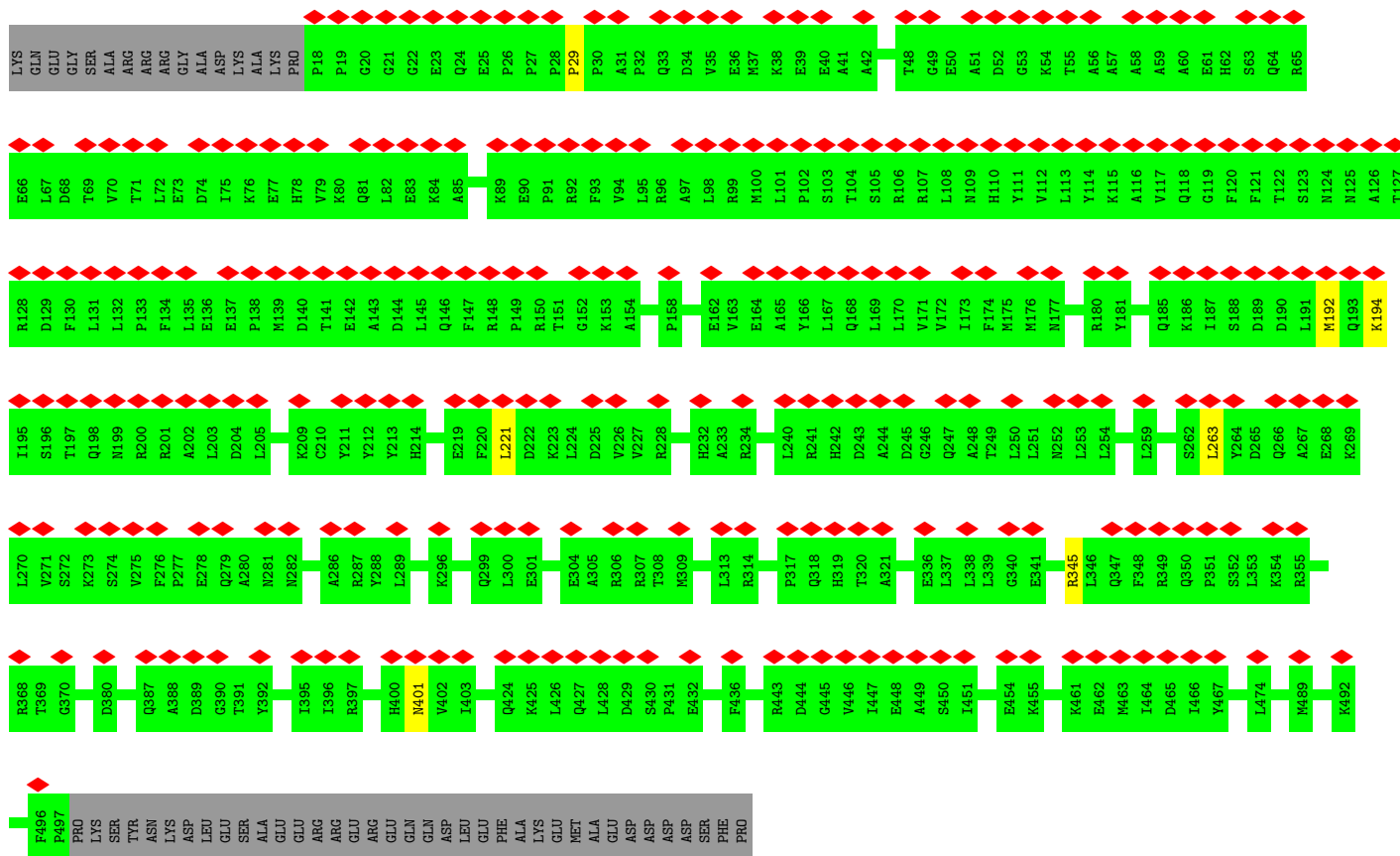
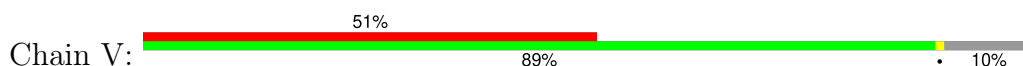
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome non-ATPase regulatory subunit 1



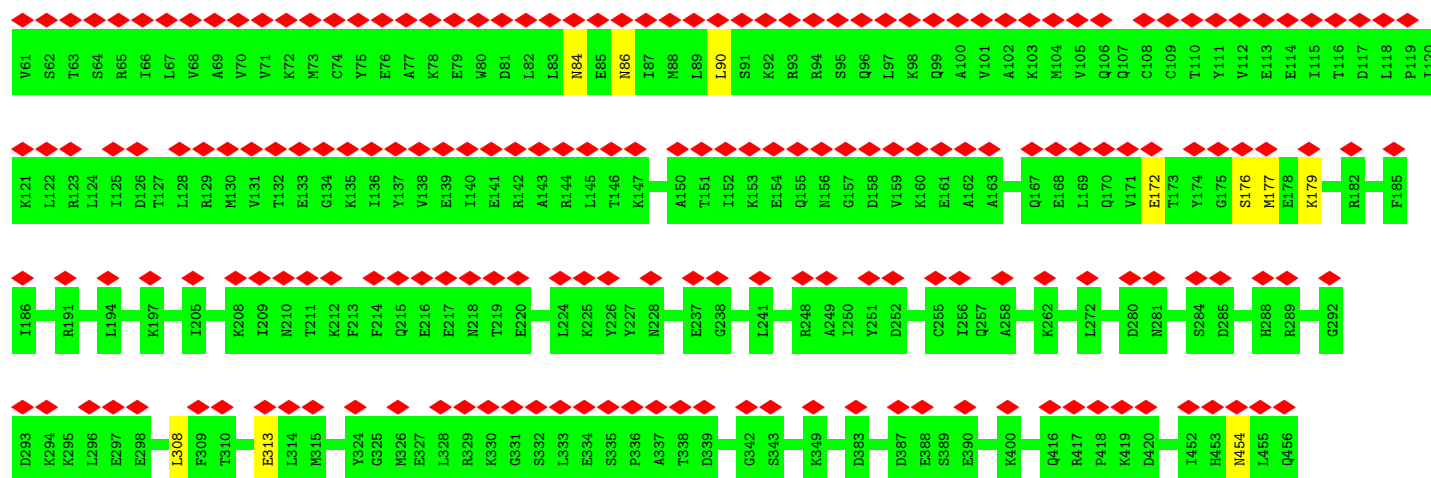


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



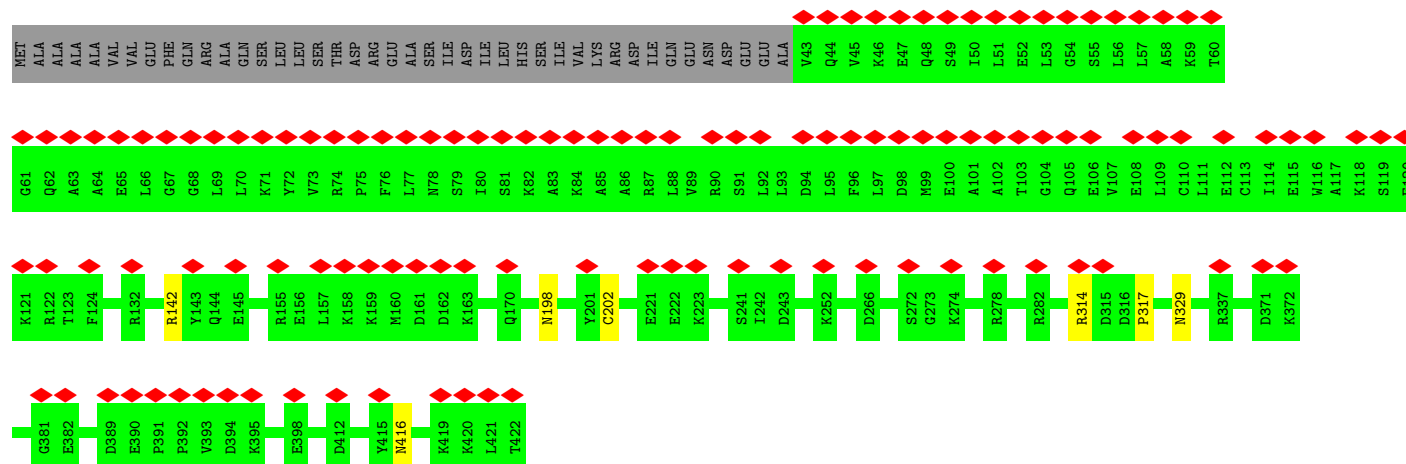
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12





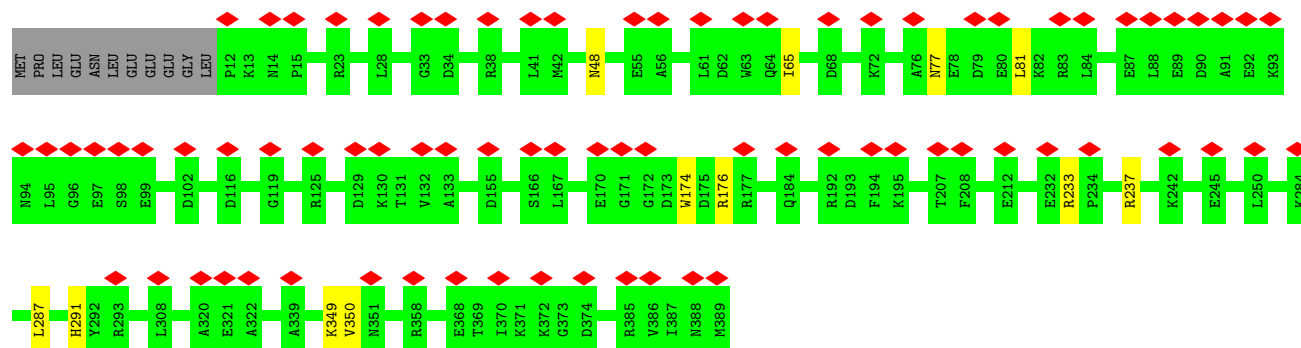
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 28% 88% 10%

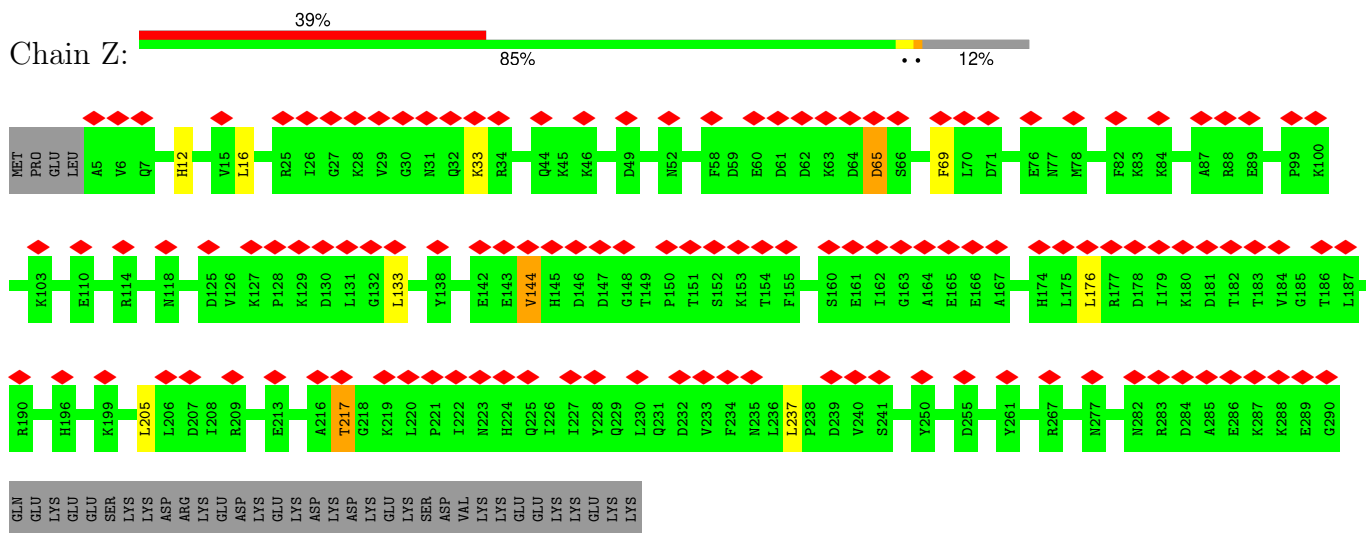


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

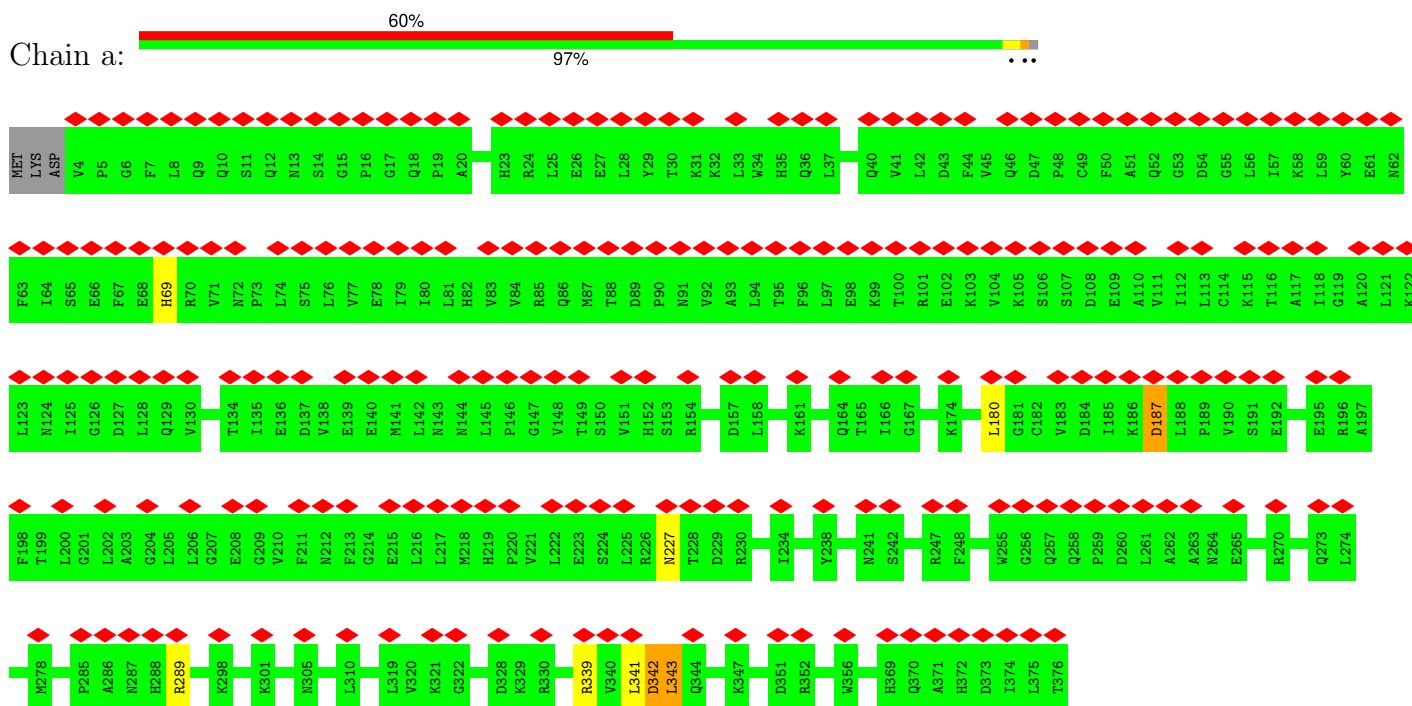
Chain Y: 20% 94% 6%



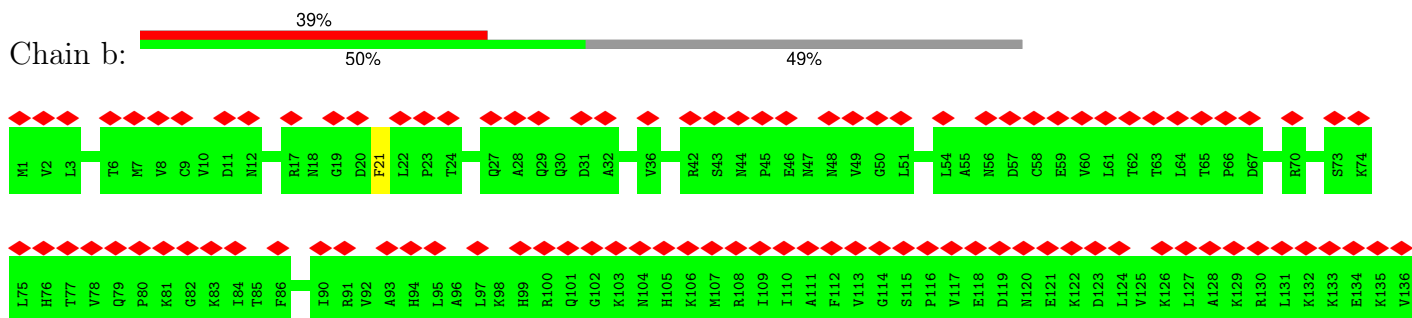
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

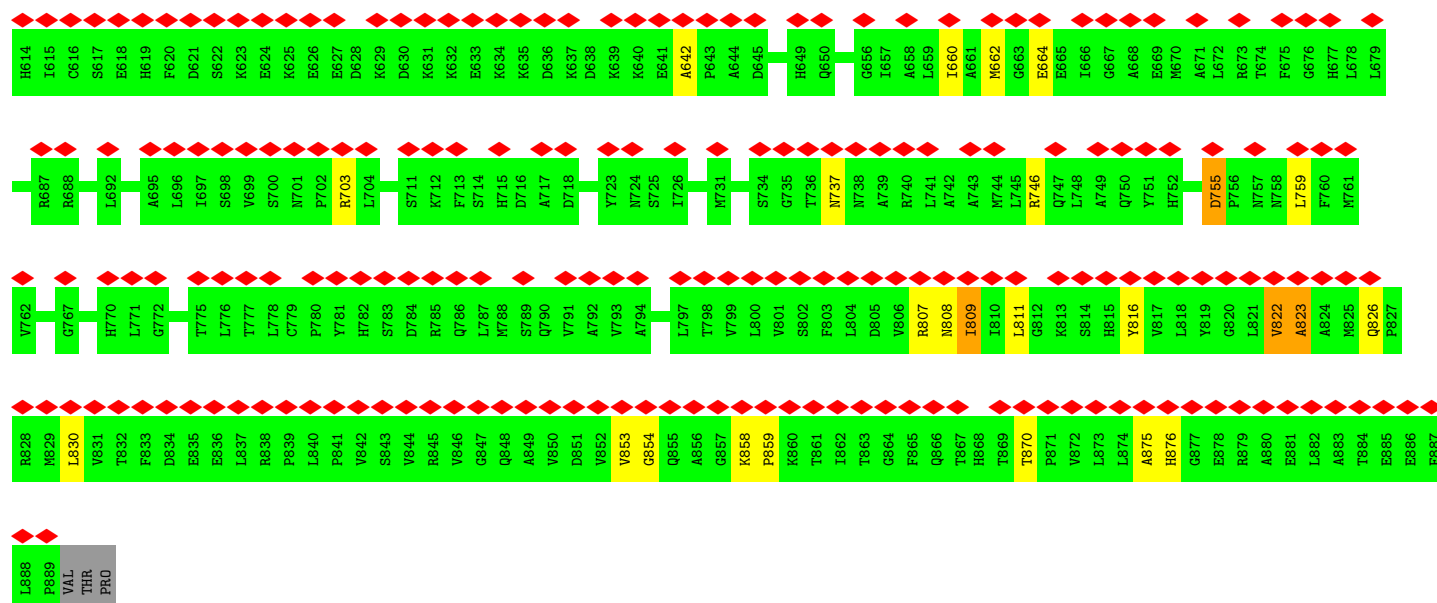


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



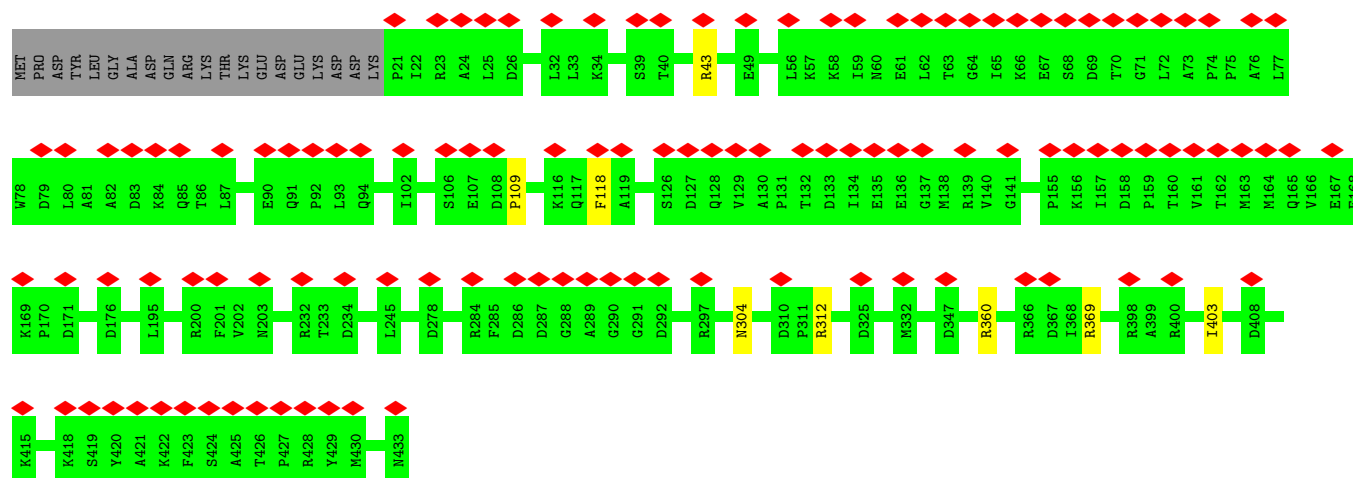
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4





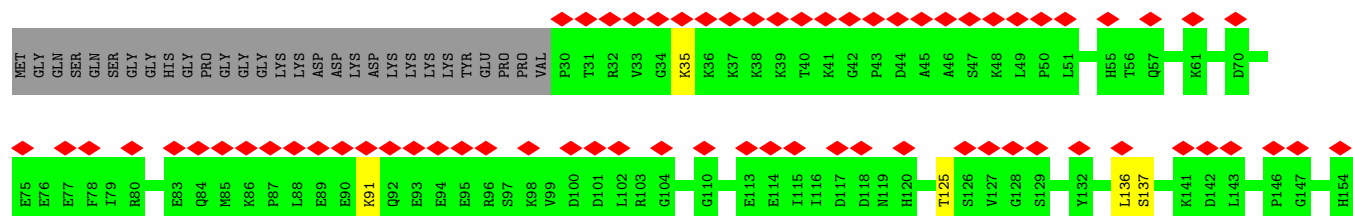
- Molecule 13: 26S proteasome regulatory subunit 7

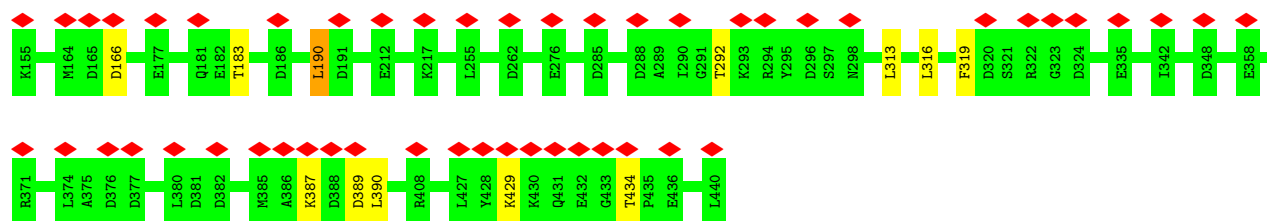
Chain A: 27% 94% 5%



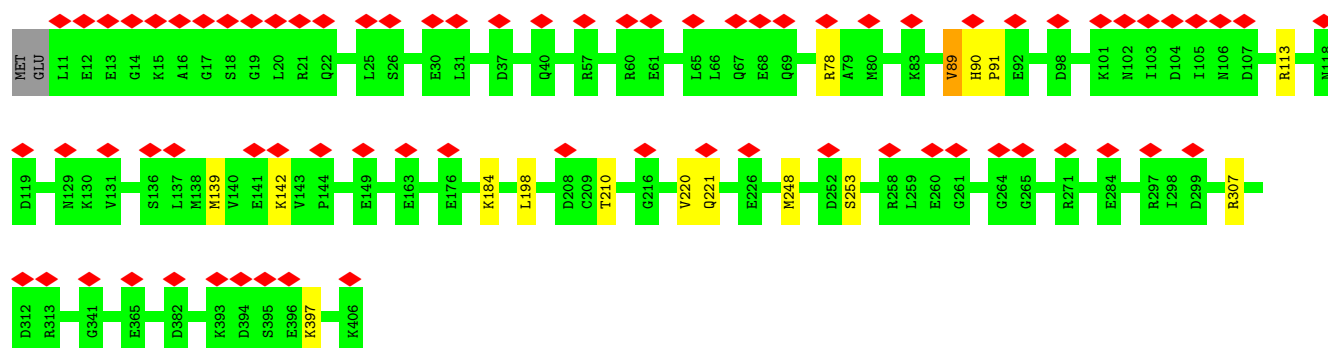
- Molecule 14: Rpt2, NP_002793.2 (26SHA chain B)

Chain B: 27% 90% 7%

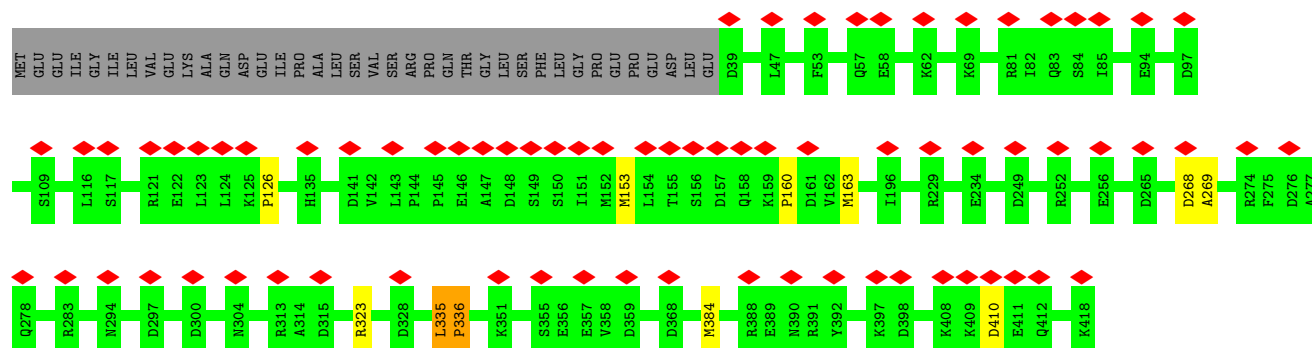
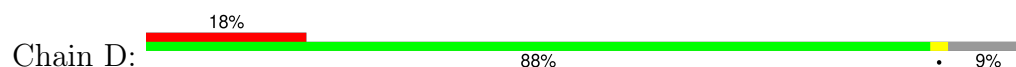




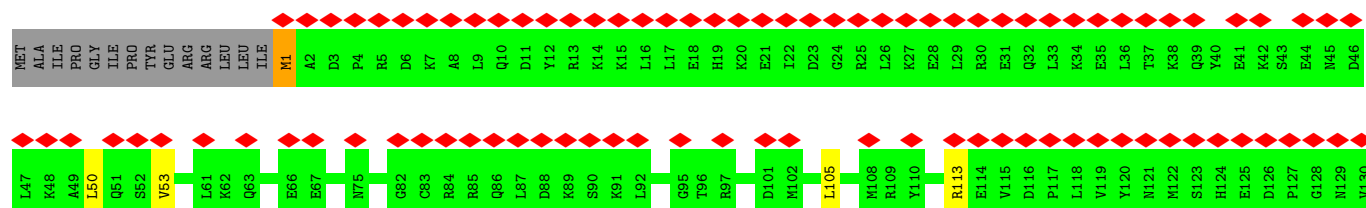
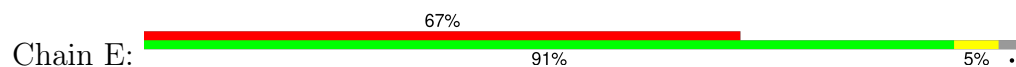
• Molecule 15: 26S proteasome regulatory subunit 8

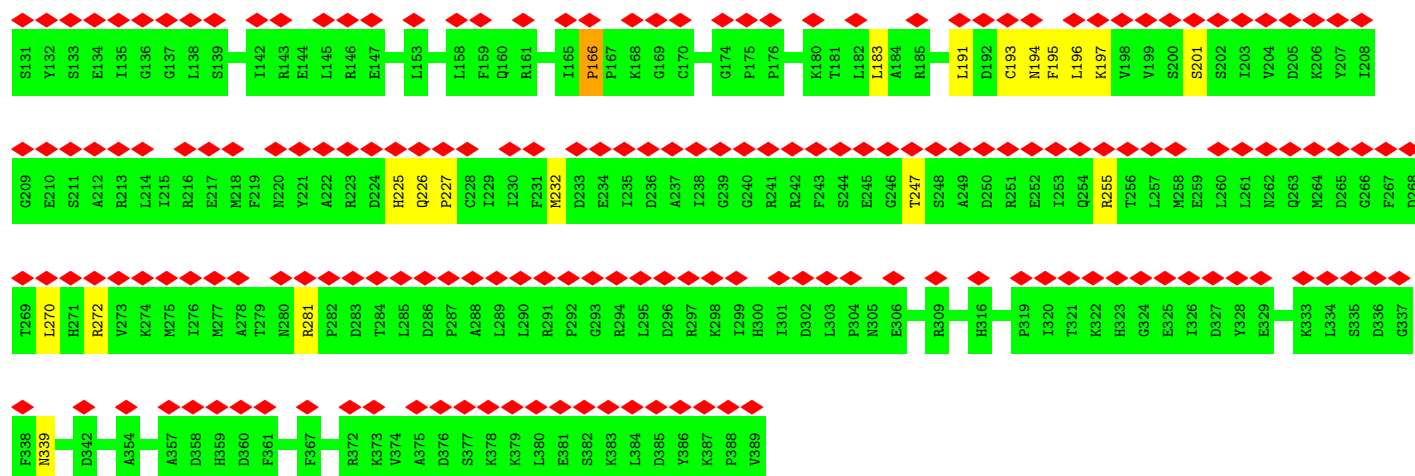


• Molecule 16: 26S proteasome regulatory subunit 6B



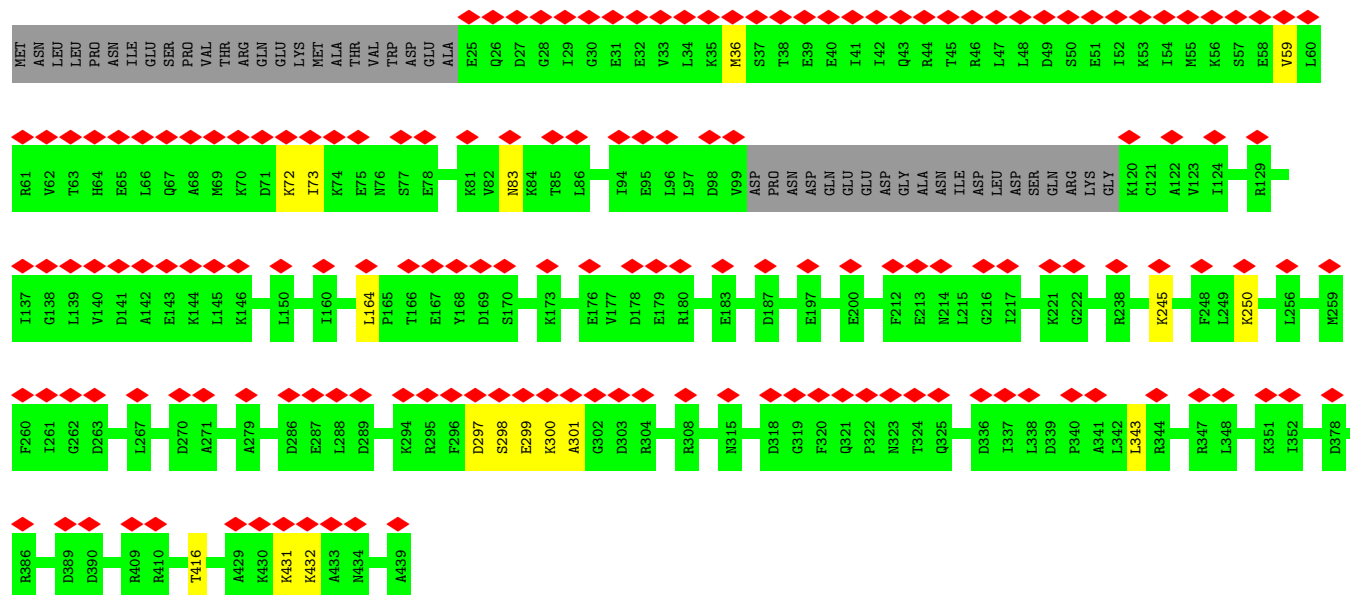
• Molecule 17: 26S proteasome regulatory subunit 10B





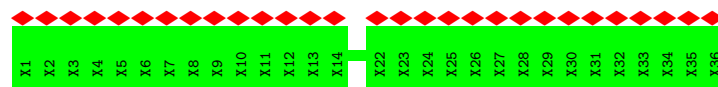
- Molecule 18: 26S proteasome regulatory subunit 6A

Chain F: 37% 86% 10%



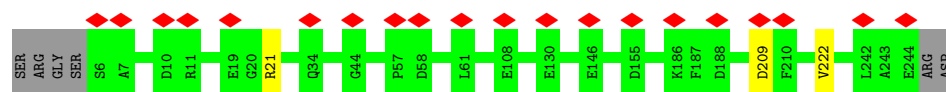
- Molecule 19: substrate

Chain v: 81% 100%

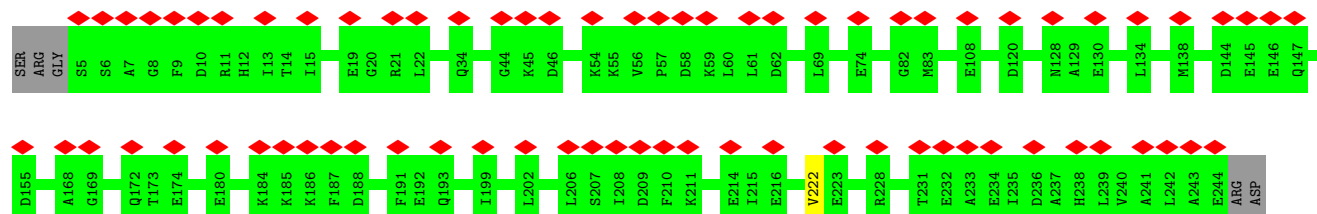


- Molecule 20: Proteasome subunit alpha type-6

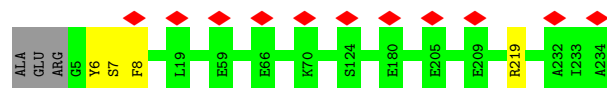
Chain G: 8% 96%



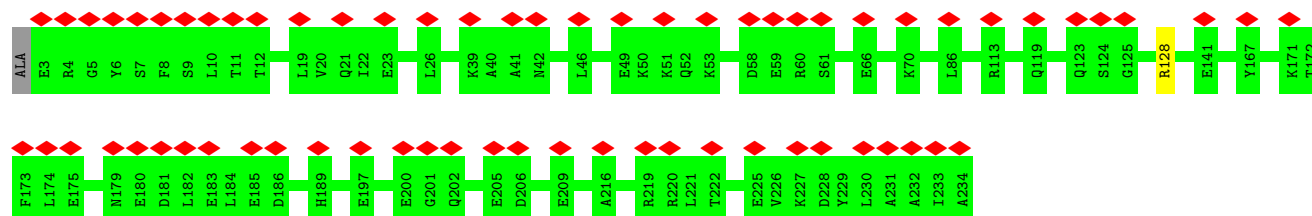
- Molecule 20: Proteasome subunit alpha type-6



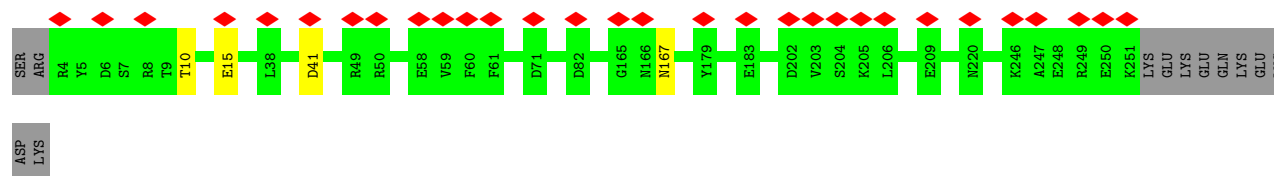
- Molecule 21: Proteasome subunit alpha type-2



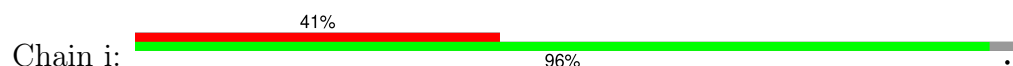
- Molecule 21: Proteasome subunit alpha type-2

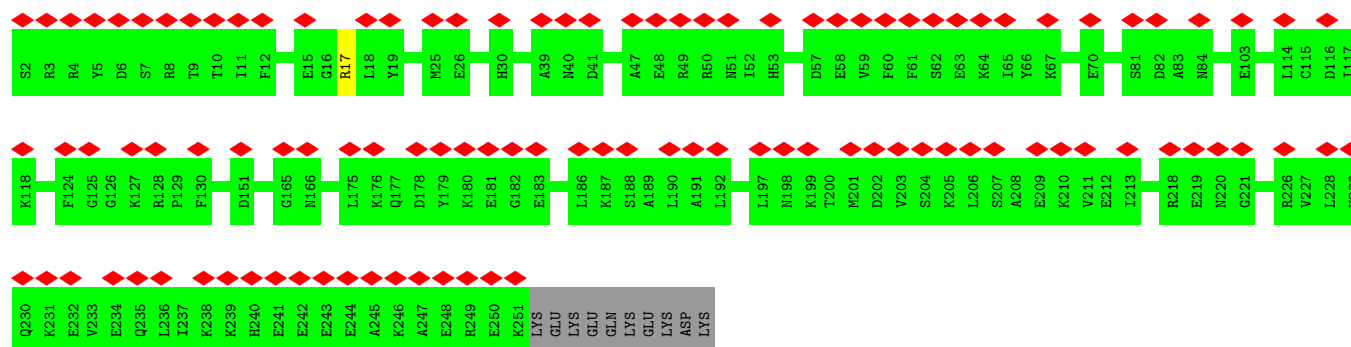


- Molecule 22: Proteasome subunit alpha type-4

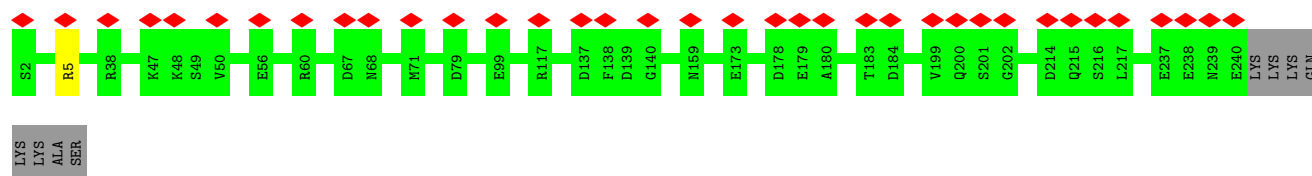


- Molecule 22: Proteasome subunit alpha type-4

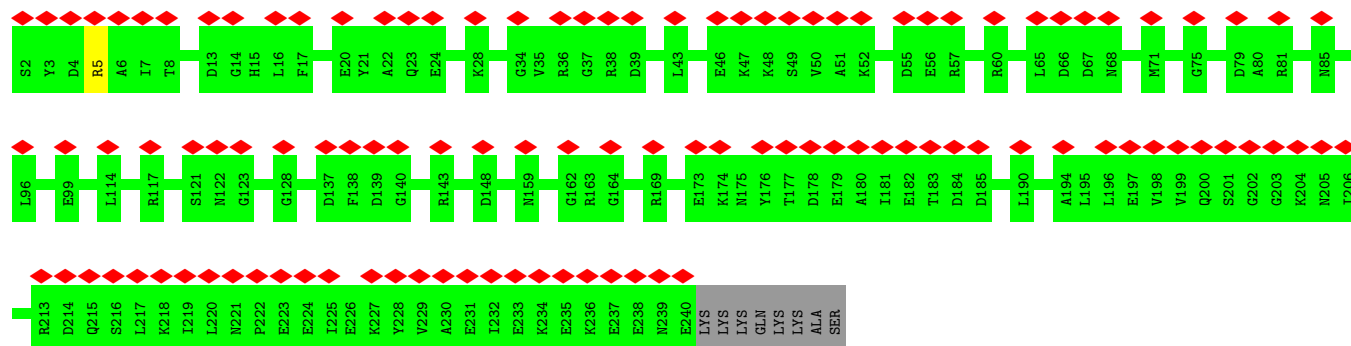




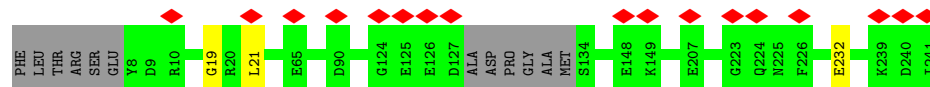
- Molecule 23: Proteasome subunit alpha type-7



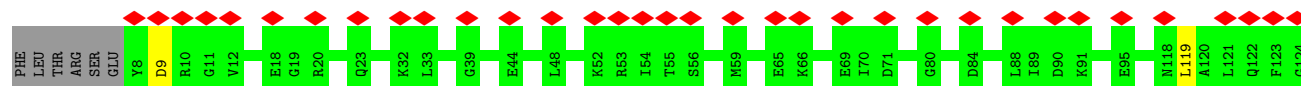
- Molecule 23: Proteasome subunit alpha type-7

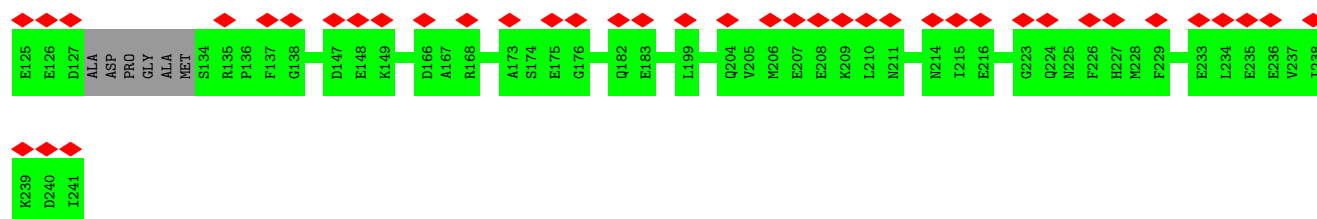


- Molecule 24: Proteasome subunit alpha type-5

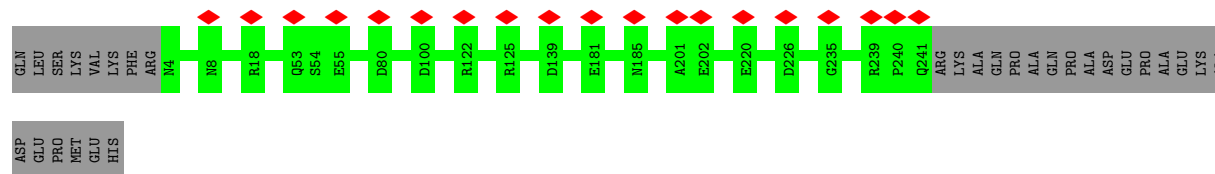
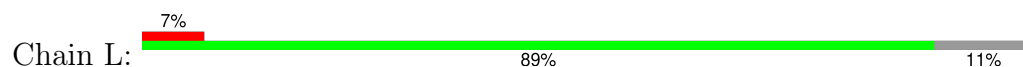


- Molecule 24: Proteasome subunit alpha type-5

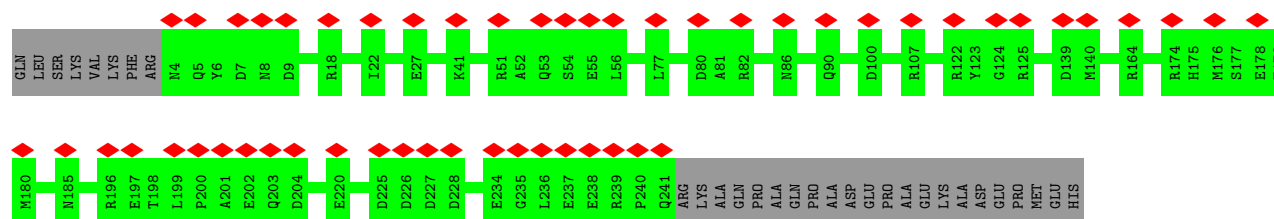
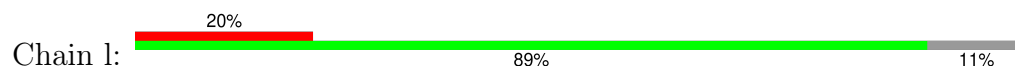




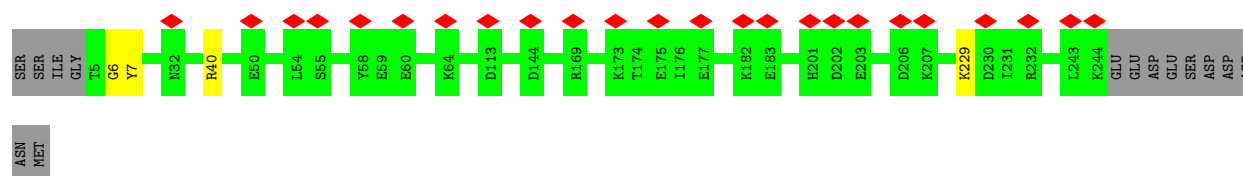
• Molecule 25: Proteasome subunit alpha type-1



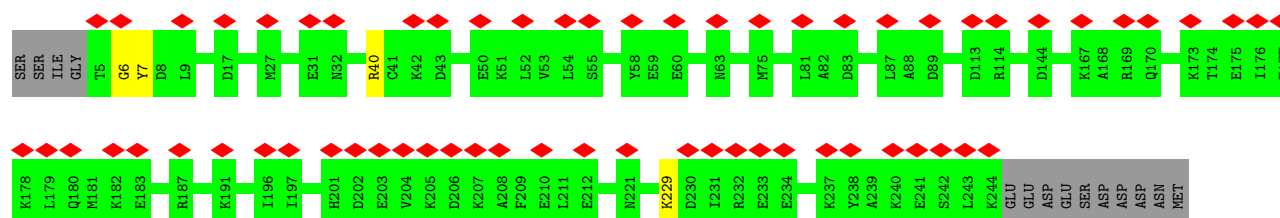
• Molecule 25: Proteasome subunit alpha type-1



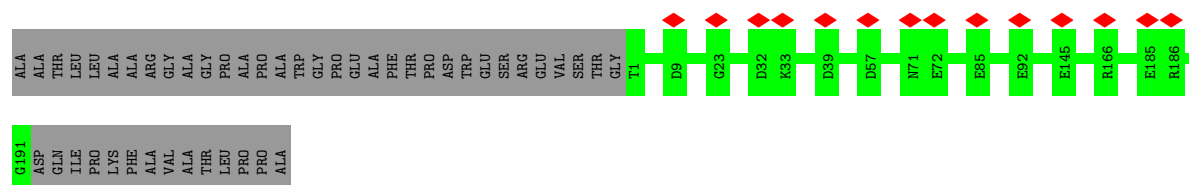
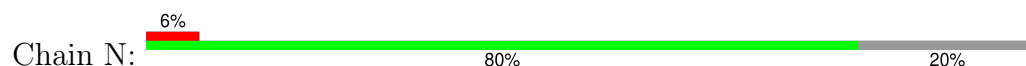
• Molecule 26: Proteasome subunit alpha type-3



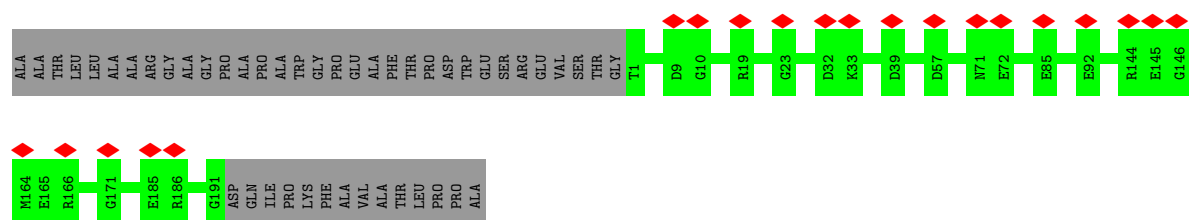
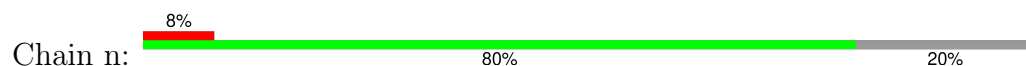
• Molecule 26: Proteasome subunit alpha type-3



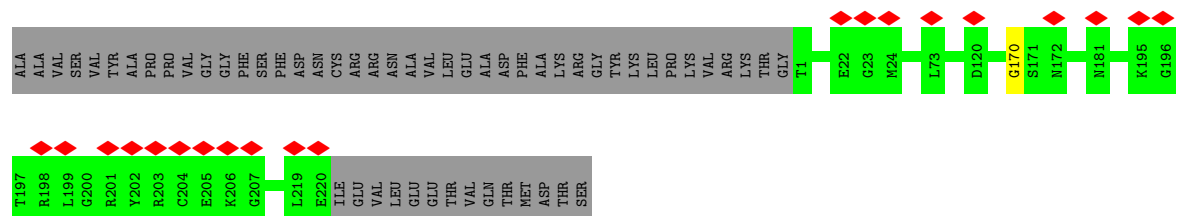
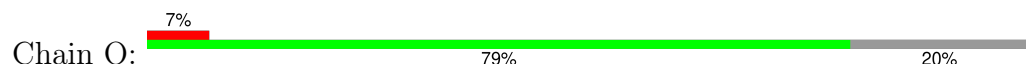
- Molecule 27: Proteasome subunit beta type-6



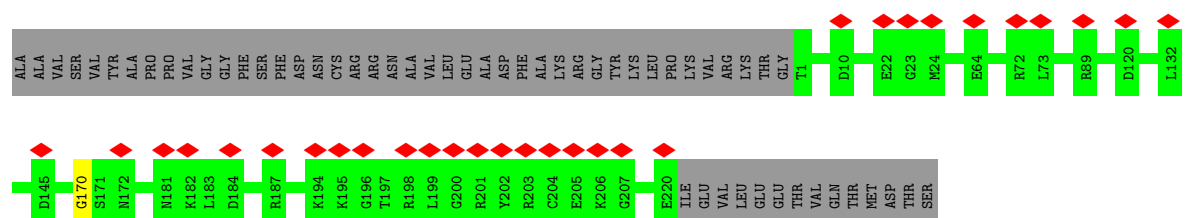
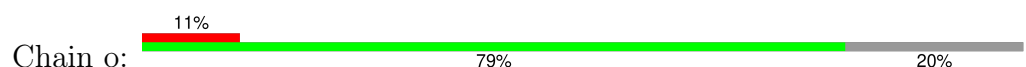
- Molecule 27: Proteasome subunit beta type-6



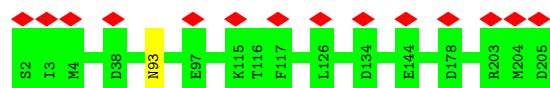
- Molecule 28: Proteasome subunit beta type-7



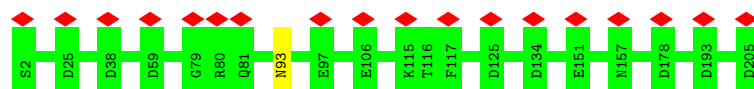
- Molecule 28: Proteasome subunit beta type-7



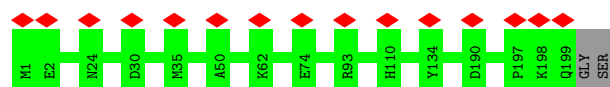
- Molecule 29: Proteasome subunit beta type-3



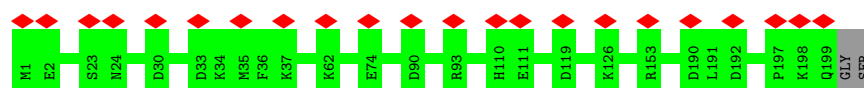
- Molecule 29: Proteasome subunit beta type-3



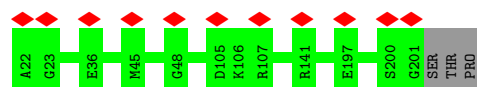
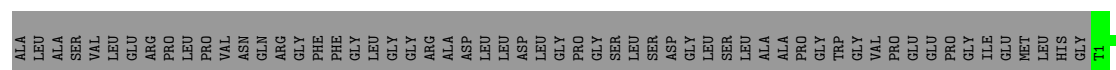
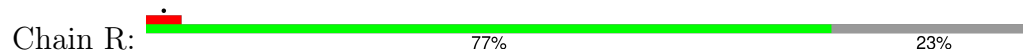
- Molecule 30: Proteasome subunit beta type-2



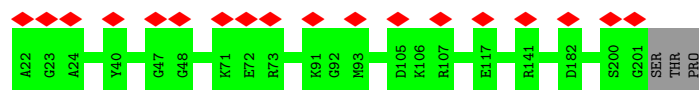
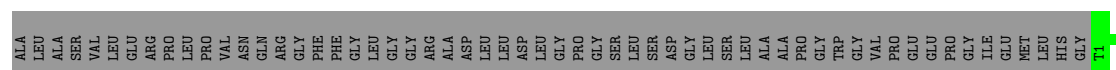
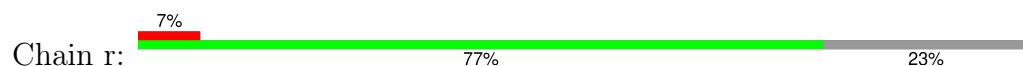
- Molecule 30: Proteasome subunit beta type-2



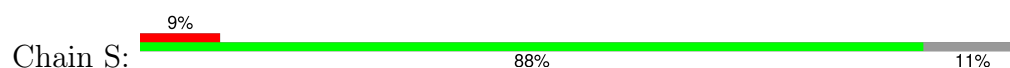
- Molecule 31: Proteasome subunit beta type-5

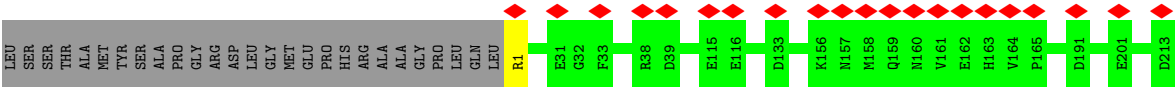


- Molecule 31: Proteasome subunit beta type-5

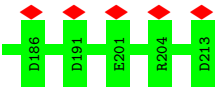
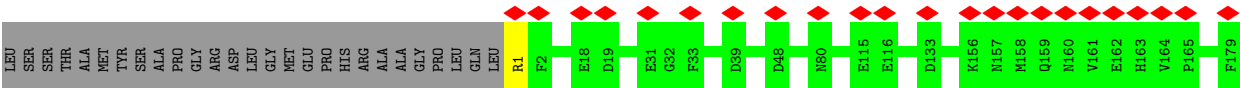
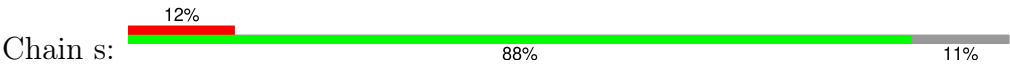


- Molecule 32: Proteasome subunit beta type-1

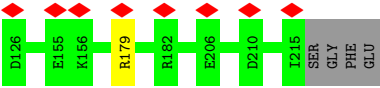
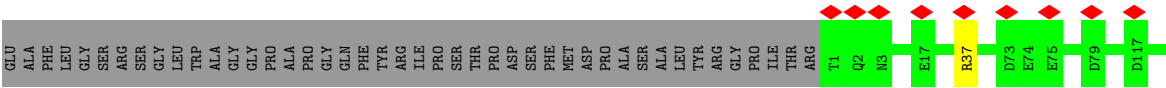
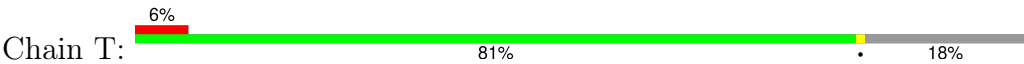




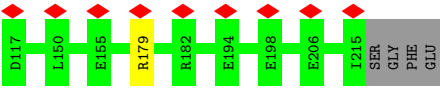
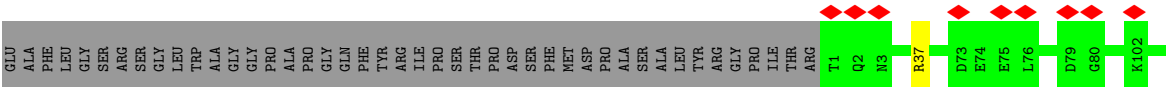
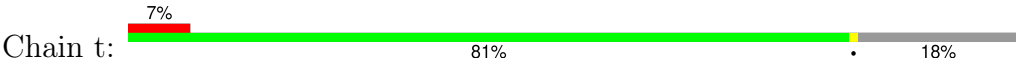
• Molecule 32: Proteasome subunit beta type-1



• Molecule 33: Proteasome subunit beta type-4



• Molecule 33: 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	348646	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	0.018	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (\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 (\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: ZN, ATP, MG, 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	U	0.29	0/6945	0.61	2/9382 (0.0%)
2	V	0.30	0/3929	0.65	2/5309 (0.0%)
3	W	0.28	0/3751	0.61	0/5042
4	X	0.27	0/3053	0.55	0/4115
5	Y	0.30	0/3173	0.62	1/4273 (0.0%)
6	Z	0.29	0/2324	0.66	5/3150 (0.2%)
7	a	0.28	0/3053	0.64	4/4133 (0.1%)
8	b	0.28	0/1478	0.62	0/2001
9	c	0.31	0/2302	0.68	1/3110 (0.0%)
10	d	0.29	0/2162	0.57	0/2919
11	e	0.29	0/338	0.66	1/450 (0.2%)
12	f	0.32	1/6980 (0.0%)	0.71	6/9433 (0.1%)
13	A	0.29	0/3283	0.57	0/4433
14	B	0.30	0/3254	0.64	2/4388 (0.0%)
15	C	0.30	0/3146	0.60	3/4226 (0.1%)
16	D	0.31	0/3090	0.61	0/4168
17	E	0.28	0/3145	0.64	4/4233 (0.1%)
18	F	0.28	0/3137	0.58	1/4223 (0.0%)
20	G	0.29	0/1853	0.56	0/2515
20	g	0.27	0/1859	0.56	0/2523
21	H	0.31	0/1727	0.55	0/2350
21	h	0.29	0/1743	0.50	0/2372
22	I	0.30	0/1925	0.64	3/2606 (0.1%)
22	i	0.26	0/1942	0.58	0/2628
23	J	0.27	0/1728	0.54	0/2358
23	j	0.27	0/1728	0.54	0/2358
24	K	0.29	0/1755	0.58	1/2375 (0.0%)
24	k	0.27	0/1747	0.53	0/2364
25	L	0.30	0/1885	0.56	0/2552
25	l	0.30	0/1885	0.56	0/2552
26	M	0.29	0/1891	0.54	0/2552
26	m	0.29	0/1891	0.54	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	N	0.26	0/1454	0.51	0/1967
27	n	0.26	0/1454	0.51	0/1967
28	O	0.27	0/1670	0.50	0/2265
28	o	0.27	0/1670	0.50	0/2265
29	P	0.27	0/1614	0.48	0/2177
29	p	0.27	0/1614	0.48	0/2177
30	Q	0.27	0/1603	0.54	0/2174
30	q	0.27	0/1603	0.54	0/2174
31	R	0.27	0/1579	0.46	0/2134
31	r	0.27	0/1579	0.46	0/2134
32	S	0.27	0/1671	0.49	0/2253
32	s	0.27	0/1671	0.49	0/2253
33	T	0.27	0/1700	0.49	0/2305
33	t	0.27	0/1700	0.49	0/2305
All	All	0.29	1/106684 (0.0%)	0.59	36/144195 (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	5
2	V	0	2
3	W	0	3
4	X	0	2
5	Y	0	5
6	Z	0	3
7	a	0	1
8	b	0	1
9	c	0	2
10	d	0	3
11	e	0	1
12	f	0	12
14	B	0	4
15	C	0	2
16	D	0	4
17	E	0	3
18	F	0	1
20	G	0	2
20	g	0	1
21	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	I	0	1
24	K	0	2
24	k	0	1
26	M	0	2
26	m	0	2
28	O	0	1
28	o	0	1
All	All	0	68

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	5.94	1.45	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	830	LEU	CA-CB-CG	7.98	133.65	115.30
6	Z	176	LEU	CA-CB-CG	7.46	132.47	115.30
14	B	313	LEU	CA-CB-CG	7.36	132.22	115.30
1	U	813	TYR	CA-CB-CG	7.30	127.28	113.40
7	a	342	ASP	CB-CG-OD1	7.25	124.82	118.30
11	e	56	LEU	CA-CB-CG	6.95	131.27	115.30
12	f	759	LEU	CA-CB-CG	6.76	130.85	115.30
12	f	612	LEU	CA-CB-CG	6.71	130.73	115.30
24	K	21	LEU	C-N-CA	6.62	138.26	121.70
18	F	164	LEU	CA-CB-CG	6.39	130.00	115.30
17	E	105	LEU	CA-CB-CG	6.38	129.97	115.30
6	Z	133	LEU	CA-CB-CG	6.16	129.47	115.30
12	f	811	LEU	CA-CB-CG	6.11	129.34	115.30
7	a	187	ASP	CB-CG-OD1	6.06	123.75	118.30
7	a	343	LEU	CA-CB-CG	6.05	129.22	115.30
22	I	41	ASP	CB-CG-OD1	6.05	123.74	118.30
6	Z	205	LEU	CA-CB-CG	6.03	129.17	115.30
14	B	190	LEU	CA-CB-CG	5.86	128.78	115.30
17	E	270	LEU	CA-CB-CG	5.84	128.73	115.30
22	I	15	GLU	C-N-CA	5.82	134.52	122.30
2	V	221	LEU	CA-CB-CG	5.66	128.33	115.30
7	a	180	LEU	CA-CB-CG	5.66	128.32	115.30
15	C	397	LYS	C-N-CA	5.46	135.35	121.70
12	f	217	LEU	CA-CB-CG	5.44	127.82	115.30
17	E	183	LEU	CA-CB-CG	5.37	127.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	223	LEU	CA-CB-CG	5.35	127.61	115.30
5	Y	287	LEU	CA-CB-CG	5.34	127.57	115.30
17	E	225	HIS	C-N-CA	5.33	135.02	121.70
6	Z	65	ASP	CB-CG-OD1	5.28	123.05	118.30
15	C	139	MET	CA-CB-CG	5.22	122.17	113.30
6	Z	217	THR	N-CA-C	-5.17	97.04	111.00
12	f	858	LYS	C-N-CD	5.15	139.21	128.40
9	c	212	LEU	CA-CB-CG	5.07	126.97	115.30
15	C	198	LEU	CA-CB-CG	5.06	126.93	115.30
2	V	263	LEU	CA-CB-CG	5.01	126.81	115.30
22	I	15	GLU	CA-C-N	5.00	126.20	116.20

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	B	136	LEU	Peptide
14	B	319	PHE	Peptide
14	B	434	THR	Peptide
14	B	91	LYS	Peptide
15	C	220	VAL	Peptide
15	C	89	VAL	Peptide
16	D	268	ASP	Peptide
16	D	335	LEU	Peptide
16	D	336	PRO	Peptide
16	D	410	ASP	Peptide
17	E	1	MET	Peptide
17	E	166	PRO	Peptide
17	E	281	ARG	Peptide
18	F	343	LEU	Peptide
20	G	209	ASP	Peptide
20	G	222	VAL	Peptide
21	H	6	TYR	Peptide
22	I	10	THR	Peptide
24	K	19	GLY	Peptide
24	K	232	GLU	Peptide
26	M	229	LYS	Peptide
26	M	6	GLY	Peptide
28	O	170	GLY	Peptide
1	U	415	HIS	Peptide
1	U	423	MET	Peptide
1	U	808	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	U	811	PHE	Peptide
1	U	873	PRO	Peptide
2	V	192	MET	Peptide
2	V	29	PRO	Peptide
3	W	172	GLU	Peptide
3	W	313	GLU	Peptide
3	W	90	LEU	Peptide
4	X	142	ARG	Peptide
4	X	202	CYS	Peptide
5	Y	174	TRP	Peptide
5	Y	233	ARG	Peptide
5	Y	291	HIS	Peptide
5	Y	349	LYS	Peptide
5	Y	65	ILE	Peptide
6	Z	144	VAL	Peptide
6	Z	237	LEU	Peptide
6	Z	69	PHE	Peptide
7	a	341	LEU	Peptide
8	b	21	PHE	Peptide
9	c	232	GLN	Peptide
9	c	279	ASP	Peptide
10	d	201	ASN	Peptide
10	d	202	THR	Peptide
10	d	88	GLN	Peptide
11	e	6	GLN	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide
20	g	222	VAL	Peptide
24	k	9	ASP	Peptide
26	m	229	LYS	Peptide
26	m	6	GLY	Peptide
28	o	170	GLY	Peptide

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	U	868/953 (91%)	781 (90%)	78 (9%)	9 (1%)	13	47
2	V	478/533 (90%)	414 (87%)	64 (13%)	0	100	100
3	W	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	30	64
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	37	69
5	Y	376/389 (97%)	336 (89%)	39 (10%)	1 (0%)	37	69
6	Z	284/324 (88%)	242 (85%)	40 (14%)	2 (1%)	19	54
7	a	371/376 (99%)	333 (90%)	34 (9%)	4 (1%)	12	44
8	b	189/377 (50%)	165 (87%)	24 (13%)	0	100	100
9	c	285/309 (92%)	248 (87%)	33 (12%)	4 (1%)	9	40
10	d	255/349 (73%)	212 (83%)	42 (16%)	1 (0%)	30	64
11	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
12	f	887/892 (99%)	710 (80%)	166 (19%)	11 (1%)	11	43
13	A	411/433 (95%)	364 (89%)	46 (11%)	1 (0%)	44	75
14	B	409/440 (93%)	355 (87%)	51 (12%)	3 (1%)	19	54
15	C	394/398 (99%)	353 (90%)	36 (9%)	5 (1%)	10	41
16	D	378/418 (90%)	317 (84%)	56 (15%)	5 (1%)	10	41
17	E	387/403 (96%)	323 (84%)	56 (14%)	8 (2%)	5	31
18	F	391/439 (89%)	339 (87%)	49 (12%)	3 (1%)	16	51
20	G	237/245 (97%)	207 (87%)	30 (13%)	0	100	100
20	g	238/245 (97%)	220 (92%)	18 (8%)	0	100	100
21	H	228/233 (98%)	218 (96%)	8 (4%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	h	230/233 (99%)	222 (96%)	8 (4%)	0	100	100
22	I	246/260 (95%)	221 (90%)	25 (10%)	0	100	100
22	i	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
23	J	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	64
23	j	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	64
24	K	224/240 (93%)	207 (92%)	17 (8%)	0	100	100
24	k	224/240 (93%)	210 (94%)	14 (6%)	0	100	100
25	L	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
25	l	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
26	M	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	30	64
26	m	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	30	64
27	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
27	n	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
28	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
29	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
29	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
30	q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
31	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
31	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	S	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
32	s	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
33	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
33	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	13386/14843 (90%)	12069 (90%)	1251 (9%)	66 (0%)	27	60

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	48	LEU
3	W	176	SER
3	W	179	LYS

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Mol	Chain	Res	Type
7	a	343	LEU
9	c	285	GLU
12	f	808	ASN
12	f	853	VAL
16	D	335	LEU
17	E	53	VAL
17	E	194	ASN
18	F	73	ILE
23	J	5	ARG
23	j	5	ARG
1	U	47	VAL
1	U	183	LEU
1	U	874	ASN
7	a	69	HIS
7	a	187	ASP
9	c	233	ASP
12	f	876	HIS
14	B	390	LEU
26	M	7	TYR
26	m	7	TYR
5	Y	350	VAL
7	a	342	ASP
10	d	199	PHE
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	823	ALA
12	f	859	PRO
14	B	166	ASP
16	D	160	PRO
17	E	191	LEU
17	E	197	LYS
18	F	72	LYS
21	H	7	SER
4	X	317	PRO
6	Z	65	ASP
9	c	201	TYR
12	f	809	ILE
14	B	137	SER
15	C	89	VAL
15	C	90	HIS
15	C	221	GLN

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Mol	Chain	Res	Type
16	D	269	ALA
17	E	193	CYS
18	F	301	ALA
21	H	8	PHE
1	U	173	VAL
1	U	808	PRO
1	U	873	PRO
9	c	284	LEU
12	f	475	ASN
16	D	336	PRO
12	f	755	ASP
13	A	109	PRO
15	C	253	SER
17	E	227	PRO
1	U	174	PRO
1	U	814	PRO
6	Z	144	VAL
16	D	126	PRO
17	E	166	PRO
15	C	91	PRO
17	E	226	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	748/816 (92%)	737 (98%)	11 (2%)	60	81
2	V	414/459 (90%)	411 (99%)	3 (1%)	81	92
3	W	416/416 (100%)	410 (99%)	6 (1%)	62	82
4	X	327/362 (90%)	323 (99%)	4 (1%)	67	85
5	Y	334/344 (97%)	329 (98%)	5 (2%)	60	81
6	Z	257/295 (87%)	253 (98%)	4 (2%)	58	79
7	a	333/336 (99%)	330 (99%)	3 (1%)	75	89
8	b	167/312 (54%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	c	252/267 (94%)	244 (97%)	8 (3%)	34	65
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	37 (97%)	1 (3%)	41	70
12	f	745/748 (100%)	727 (98%)	18 (2%)	44	71
13	A	348/372 (94%)	341 (98%)	7 (2%)	50	75
14	B	357/385 (93%)	348 (98%)	9 (2%)	42	71
15	C	340/346 (98%)	333 (98%)	7 (2%)	48	74
16	D	333/366 (91%)	329 (99%)	4 (1%)	67	85
17	E	341/353 (97%)	330 (97%)	11 (3%)	34	65
18	F	340/379 (90%)	328 (96%)	12 (4%)	31	63
20	G	192/209 (92%)	191 (100%)	1 (0%)	86	93
20	g	193/209 (92%)	193 (100%)	0	100	100
21	H	163/190 (86%)	162 (99%)	1 (1%)	84	92
21	h	164/190 (86%)	163 (99%)	1 (1%)	84	92
22	I	191/220 (87%)	190 (100%)	1 (0%)	86	93
22	i	193/220 (88%)	192 (100%)	1 (0%)	86	93
23	J	152/210 (72%)	152 (100%)	0	100	100
23	j	152/210 (72%)	152 (100%)	0	100	100
24	K	187/202 (93%)	187 (100%)	0	100	100
24	k	186/202 (92%)	185 (100%)	1 (0%)	86	93
25	L	198/229 (86%)	198 (100%)	0	100	100
25	l	198/229 (86%)	198 (100%)	0	100	100
26	M	192/211 (91%)	191 (100%)	1 (0%)	86	93
26	m	192/211 (91%)	191 (100%)	1 (0%)	86	93
27	N	148/180 (82%)	148 (100%)	0	100	100
27	n	148/180 (82%)	148 (100%)	0	100	100
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	172/173 (99%)	171 (99%)	1 (1%)	84	92
29	p	172/173 (99%)	171 (99%)	1 (1%)	84	92
30	Q	164/171 (96%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	q	164/171 (96%)	164 (100%)	0	100	100
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	173 (99%)	1 (1%)	84	92
32	s	174/198 (88%)	173 (99%)	1 (1%)	84	92
33	T	175/214 (82%)	173 (99%)	2 (1%)	70	86
33	t	175/214 (82%)	173 (99%)	2 (1%)	70	86
All	All	11200/12582 (89%)	11071 (99%)	129 (1%)	66	85

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	118	LEU
1	U	173	VAL
1	U	177	LEU
1	U	179	TYR
1	U	181	LEU
1	U	182	LYS
1	U	194	ARG
1	U	629	THR
1	U	838	LYS
1	U	840	LYS
1	U	883	ARG
2	V	194	LYS
2	V	345	ARG
2	V	401	ASN
3	W	39	ARG
3	W	84	ASN
3	W	86	ASN
3	W	177	MET
3	W	308	LEU
3	W	454	ASN
4	X	198	ASN
4	X	314	ARG
4	X	329	ASN
4	X	416	ASN
5	Y	48	ASN
5	Y	77	ASN
5	Y	81	LEU
5	Y	176	ARG

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Mol	Chain	Res	Type
5	Y	237	ARG
6	Z	12	HIS
6	Z	16	LEU
6	Z	33	LYS
6	Z	217	THR
7	a	227	ASN
7	a	289	ARG
7	a	339	ARG
9	c	115	HIS
9	c	154	LYS
9	c	175	ARG
9	c	185	ASN
9	c	197	ASN
9	c	198	ARG
9	c	254	ASN
9	c	274	ASN
11	e	57	ARG
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	267	ARG
12	f	297	MET
12	f	327	ASN
12	f	344	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	660	ILE
12	f	662	MET
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	43	ARG
13	A	118	PHE
13	A	304	ASN
13	A	312	ARG
13	A	360	ARG
13	A	369	ARG
13	A	403	ILE

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Mol	Chain	Res	Type
14	B	35	LYS
14	B	125	THR
14	B	183	THR
14	B	190	LEU
14	B	292	THR
14	B	316	LEU
14	B	387	LYS
14	B	389	ASP
14	B	429	LYS
15	C	78	ARG
15	C	113	ARG
15	C	142	LYS
15	C	184	LYS
15	C	210	THR
15	C	248	MET
15	C	307	ARG
16	D	153	MET
16	D	163	MET
16	D	323	ARG
16	D	384	MET
17	E	1	MET
17	E	50	LEU
17	E	113	ARG
17	E	195	PHE
17	E	196	LEU
17	E	201	SER
17	E	232	MET
17	E	247	THR
17	E	255	ARG
17	E	272	ARG
17	E	339	ASN
18	F	36	MET
18	F	59	VAL
18	F	83	ASN
18	F	245	LYS
18	F	250	LYS
18	F	297	ASP
18	F	298	SER
18	F	299	GLU
18	F	300	LYS
18	F	416	THR
18	F	431	LYS

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Mol	Chain	Res	Type
18	F	432	LYS
20	G	21	ARG
21	H	219	ARG
22	I	167	ASN
26	M	40	ARG
29	P	93	ASN
32	S	1	ARG
33	T	37	ARG
33	T	179	ARG
21	h	128	ARG
22	i	17	ARG
24	k	119	LEU
26	m	40	ARG
29	p	93	ASN
32	s	1	ARG
33	t	37	ARG
33	t	179	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	89	ASN
1	U	189	GLN
1	U	218	GLN
1	U	338	HIS
1	U	366	HIS
1	U	377	HIS
1	U	421	GLN
1	U	595	ASN
1	U	596	ASN
1	U	768	GLN
1	U	888	GLN
2	V	62	HIS
2	V	198	GLN
2	V	252	ASN
2	V	257	ASN
2	V	319	HIS
2	V	401	ASN
2	V	487	HIS
3	W	362	ASN
3	W	454	ASN
4	X	170	GLN

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Mol	Chain	Res	Type
4	X	198	ASN
4	X	329	ASN
4	X	349	HIS
4	X	416	ASN
5	Y	48	ASN
5	Y	49	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	291	HIS
5	Y	344	HIS
6	Z	109	ASN
6	Z	193	ASN
6	Z	243	GLN
7	a	9	GLN
7	a	86	GLN
7	a	124	ASN
7	a	227	ASN
7	a	249	GLN
8	b	30	GLN
8	b	161	ASN
9	c	92	GLN
9	c	115	HIS
9	c	130	GLN
9	c	185	ASN
9	c	197	ASN
9	c	237	HIS
9	c	254	ASN
9	c	274	ASN
10	d	15	ASN
10	d	46	GLN
10	d	96	HIS
12	f	43	GLN
12	f	118	ASN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN

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Mol	Chain	Res	Type
12	f	619	HIS
12	f	737	ASN
12	f	815	HIS
13	A	38	GLN
13	A	60	ASN
13	A	85	GLN
13	A	94	GLN
13	A	304	ASN
13	A	353	HIS
14	B	154	HIS
14	B	195	GLN
15	C	36	ASN
15	C	69	GLN
15	C	205	HIS
15	C	279	GLN
16	D	301	GLN
16	D	414	HIS
17	E	121	ASN
17	E	194	ASN
17	E	300	HIS
17	E	339	ASN
18	F	64	HIS
18	F	83	ASN
18	F	243	GLN
18	F	325	GLN
21	H	102	GLN
22	I	119	GLN
22	I	167	ASN
23	J	116	GLN
24	K	155	HIS
24	K	214	ASN
28	O	172	ASN
31	R	38	ASN
20	g	123	GLN
21	h	102	GLN
22	i	119	GLN
22	i	167	ASN
23	j	116	GLN
24	k	23	GLN
24	k	152	GLN
24	k	164	GLN
24	k	214	ASN

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Mol	Chain	Res	Type
25	l	152	ASN
28	o	172	ASN
31	r	38	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 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	$\# Z > 2$
35	ATP	F	501	36	28,33,33	0.87	0	34,52,52	1.27	2 (5%)
37	ADP	D	501	36	24,29,29	0.82	0	29,45,45	1.34	3 (10%)
35	ATP	B	501	36	28,33,33	0.85	0	34,52,52	1.32	3 (8%)
35	ATP	A	501	36	28,33,33	0.84	0	34,52,52	1.17	2 (5%)
35	ATP	C	501	36	28,33,33	0.82	0	34,52,52	1.19	2 (5%)

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	ATP	F	501	36	-	4/18/38/38	0/3/3/3
37	ADP	D	501	36	-	1/12/32/32	0/3/3/3
35	ATP	B	501	36	-	3/18/38/38	0/3/3/3
35	ATP	A	501	36	-	3/18/38/38	0/3/3/3
35	ATP	C	501	36	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	501	ATP	N3-C2-N1	-3.91	123.36	128.67
35	B	501	ATP	N3-C2-N1	-3.79	123.52	128.67
37	D	501	ADP	N3-C2-N1	-3.73	123.61	128.67
35	A	501	ATP	N3-C2-N1	-3.71	123.64	128.67
35	F	501	ATP	N3-C2-N1	-3.65	123.72	128.67
35	A	501	ATP	C4-C5-N7	-2.61	106.57	109.34
37	D	501	ADP	C4'-O4'-C1'	2.58	112.29	109.92
35	B	501	ATP	C4'-O4'-C1'	2.45	112.17	109.92
37	D	501	ADP	C4-C5-N7	-2.39	106.81	109.34
35	C	501	ATP	C4-C5-N7	-2.33	106.87	109.34
35	F	501	ATP	C4-C5-N7	-2.29	106.91	109.34
35	B	501	ATP	C4-C5-N7	-2.16	107.06	109.34

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	O4'-C4'-C5'-O5'
35	C	501	ATP	PB-O3A-PA-O1A
35	F	501	ATP	PB-O3A-PA-O1A
35	C	501	ATP	PB-O3A-PA-O2A
35	F	501	ATP	PB-O3A-PA-O2A

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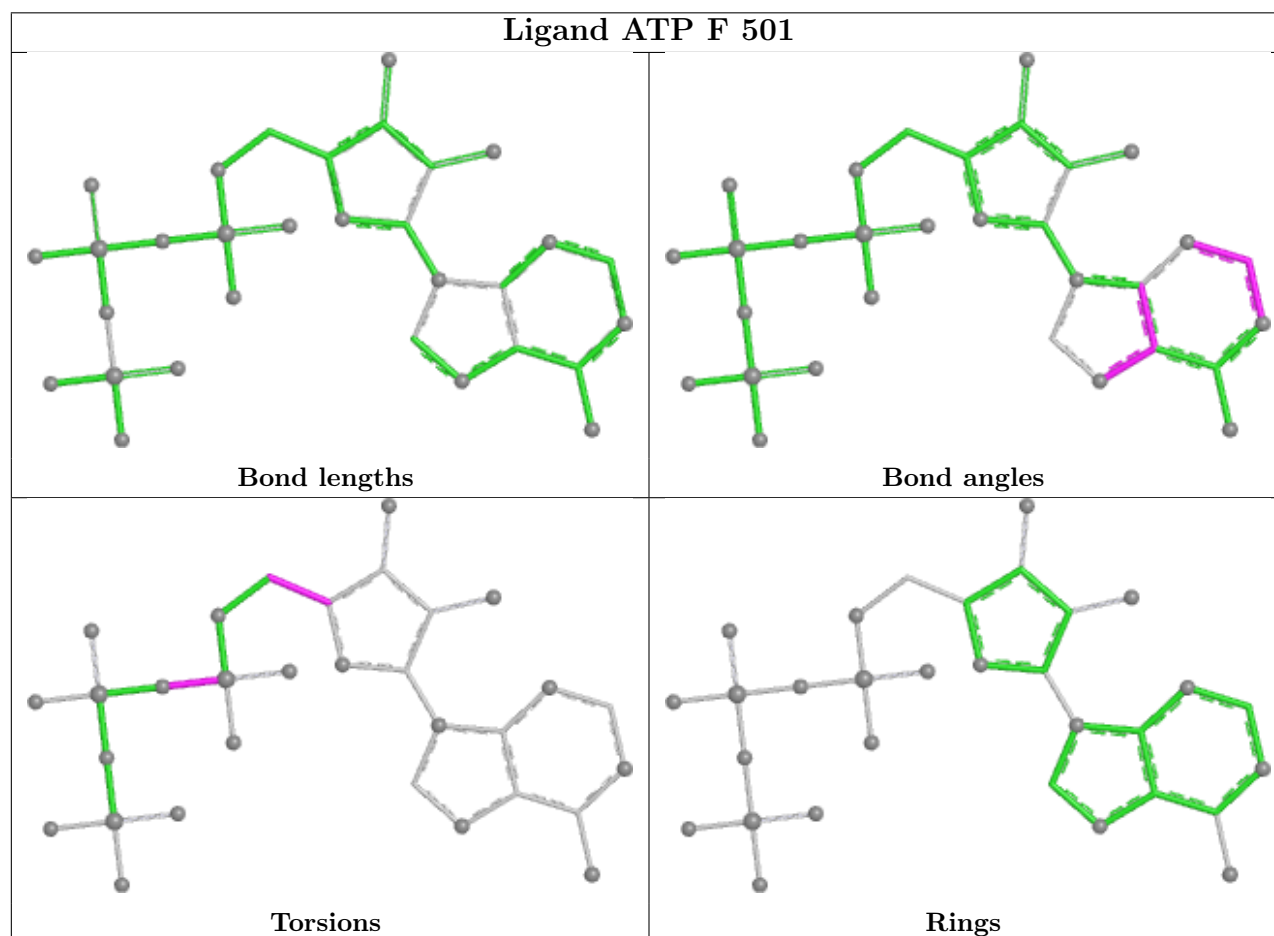
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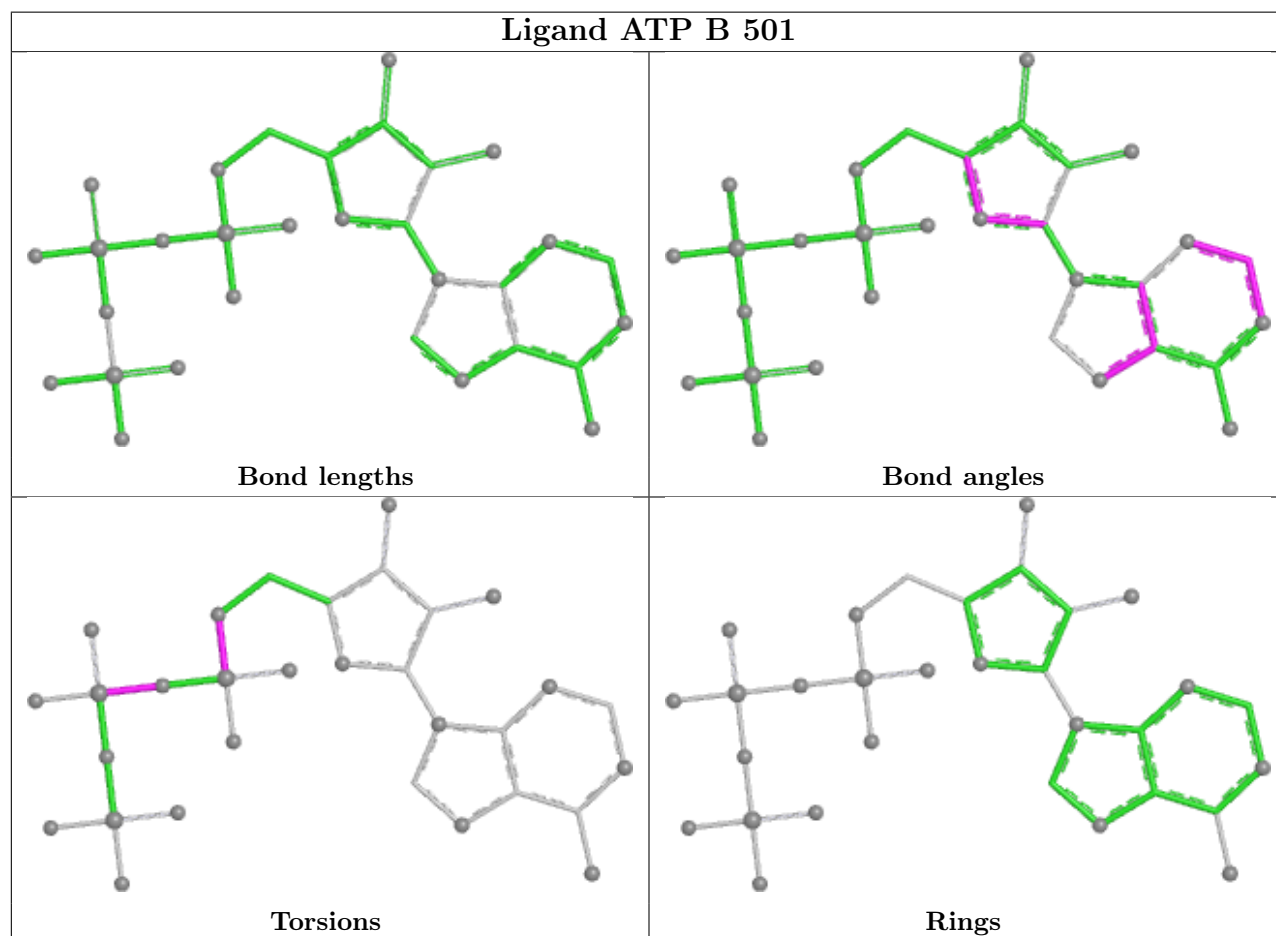
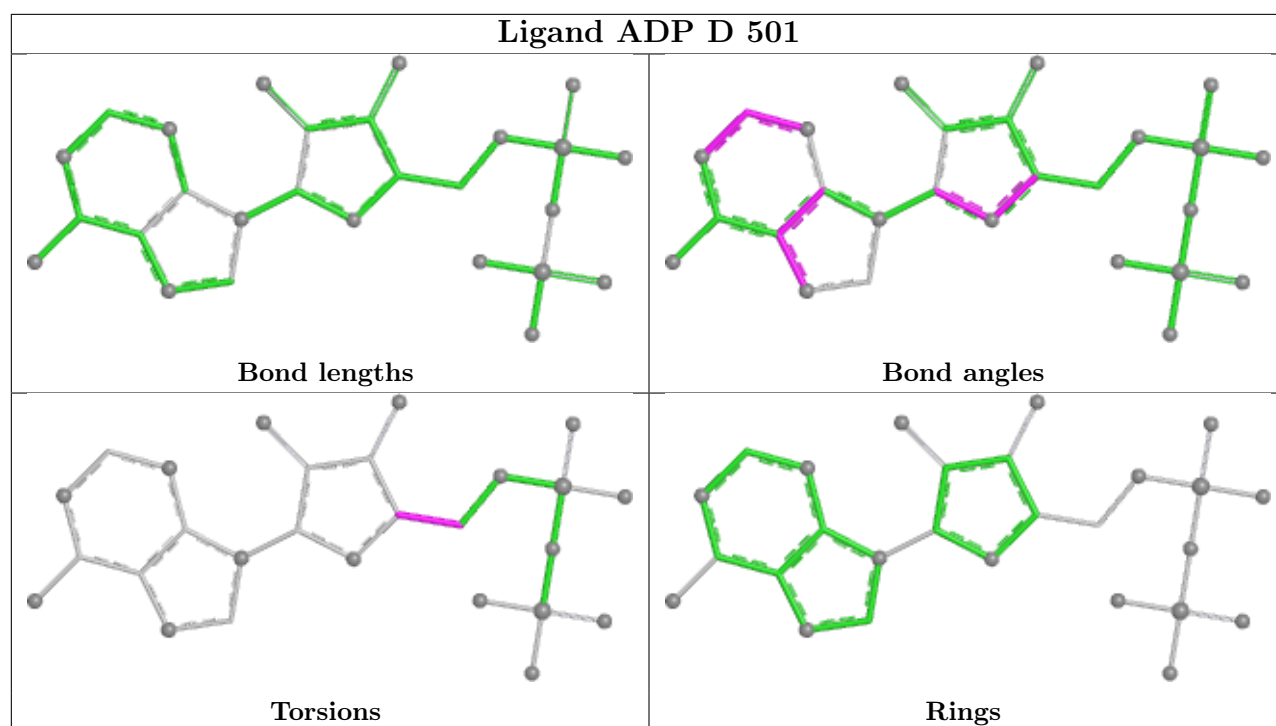
Mol	Chain	Res	Type	Atoms
37	D	501	ADP	O4'-C4'-C5'-O5'
35	B	501	ATP	PA-O3A-PB-O2B

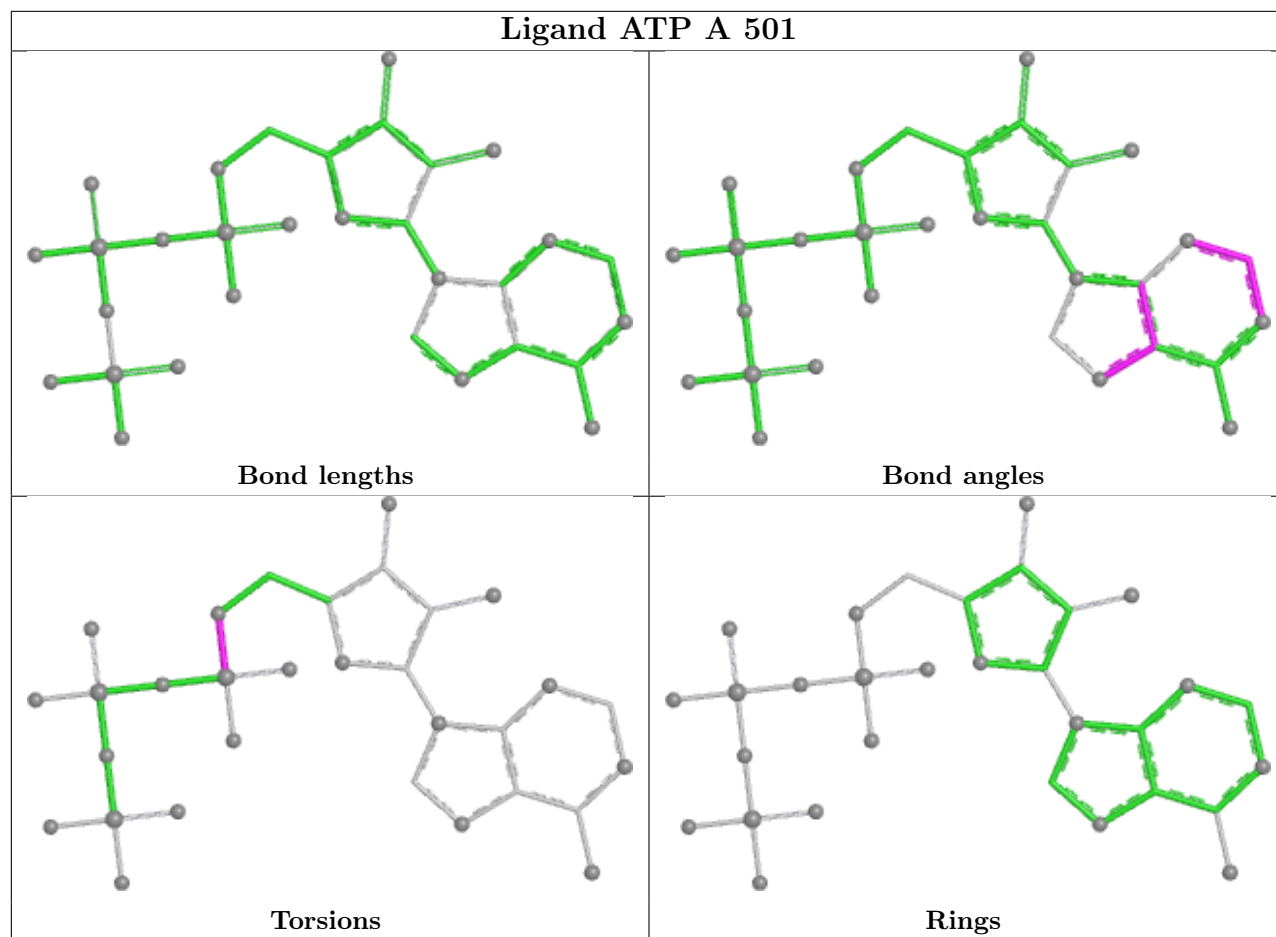
There are no ring outliers.

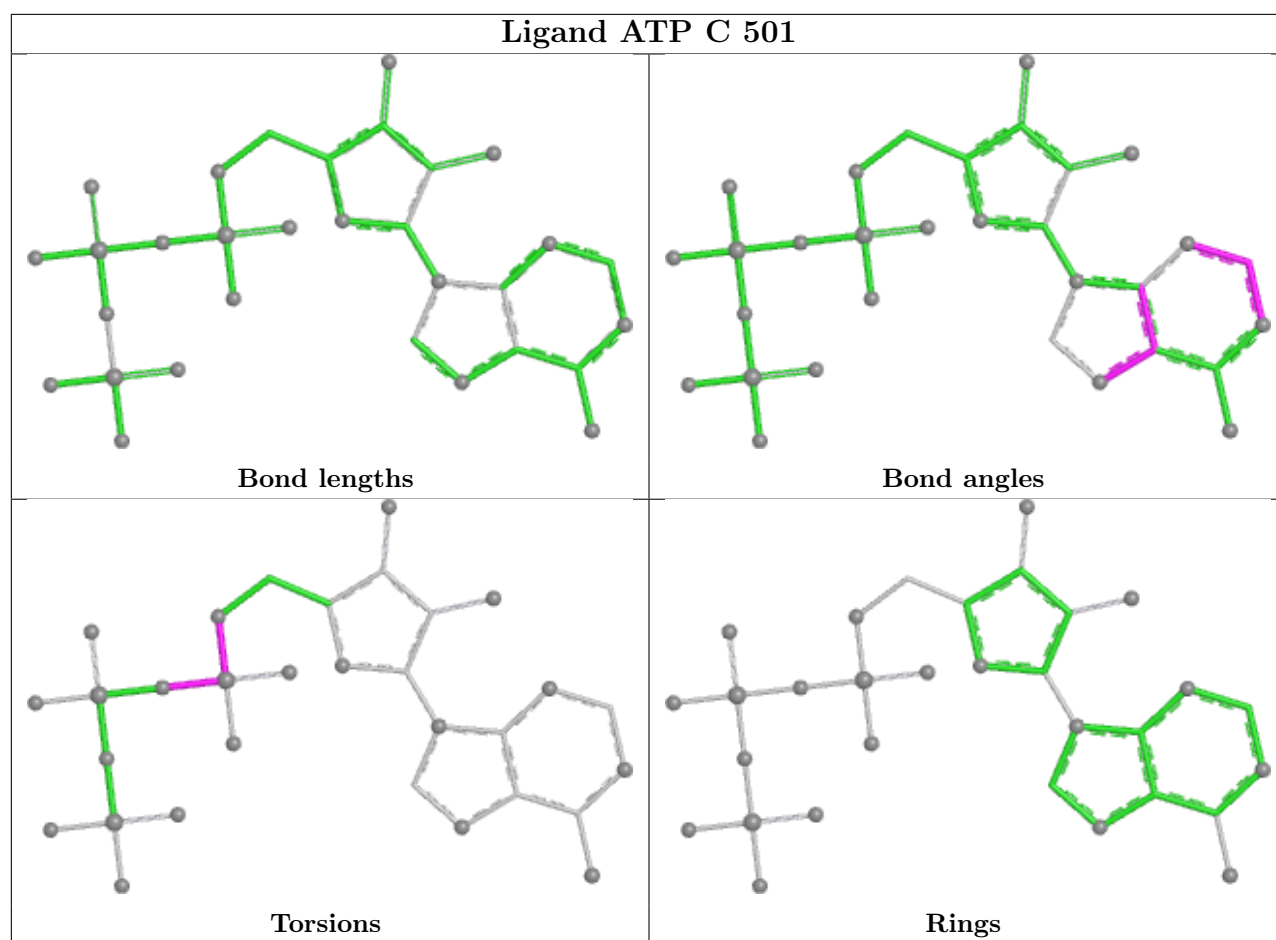
No monomer is involved in short contacts.

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 [i](#)

There are no chain breaks in this entry.

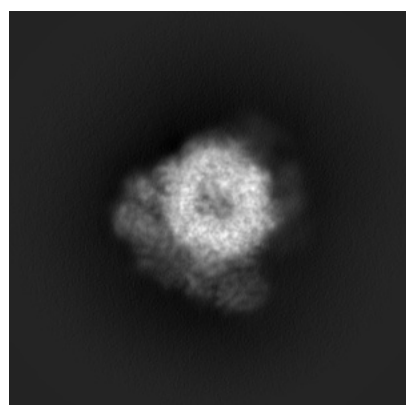
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9222. These allow visual inspection of the internal detail of the map and identification of artifacts.

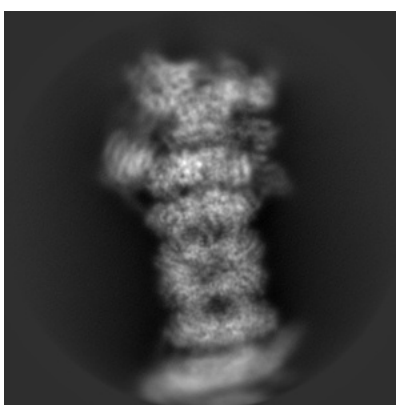
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

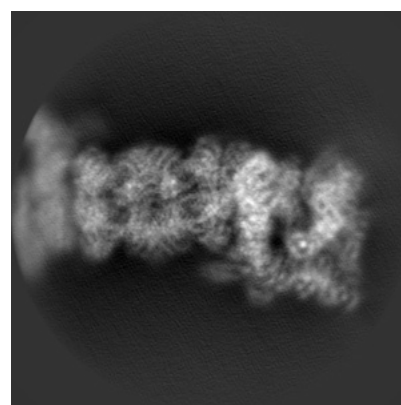
6.1.1 Primary map



X



Y

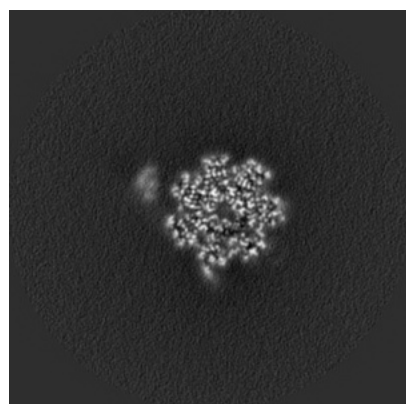


Z

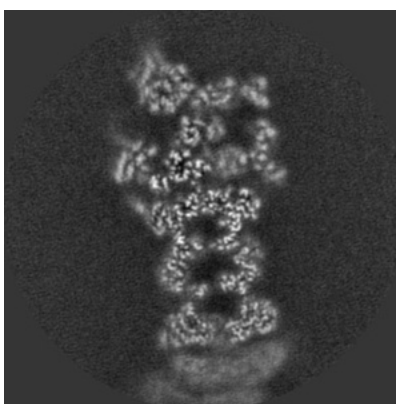
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

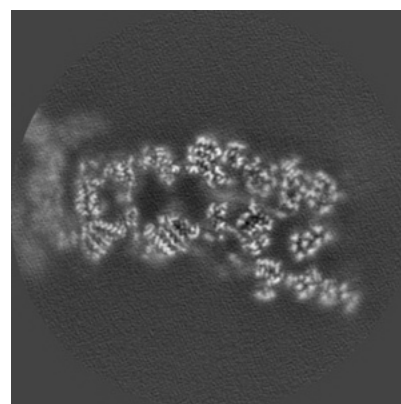
6.2.1 Primary map



X Index: 300



Y Index: 300

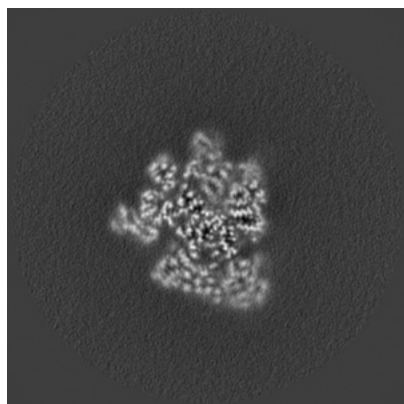


Z Index: 300

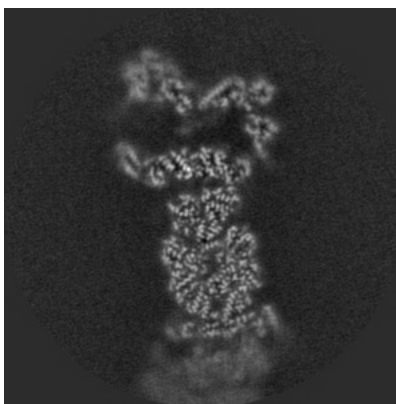
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

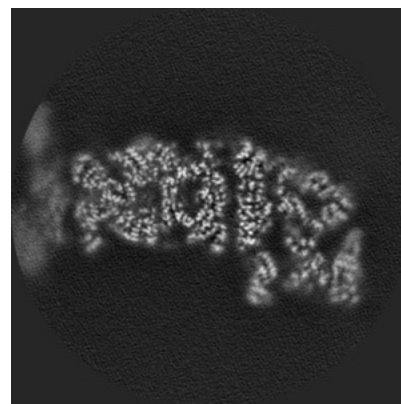
6.3.1 Primary map



X Index: 369



Y Index: 274

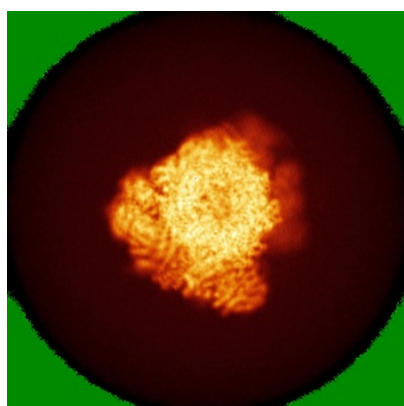


Z Index: 273

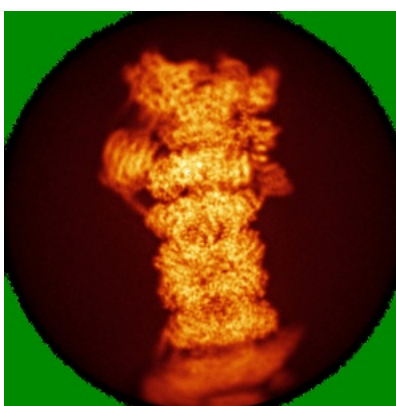
The images above show the largest variance slices of the map in three orthogonal directions.

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

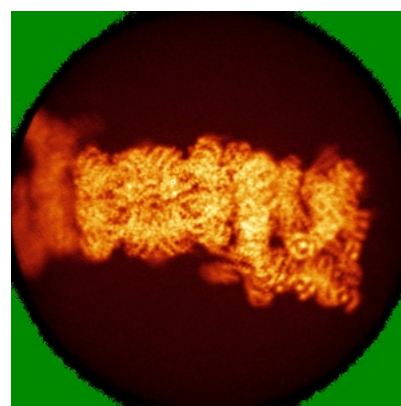
6.4.1 Primary map



X



Y

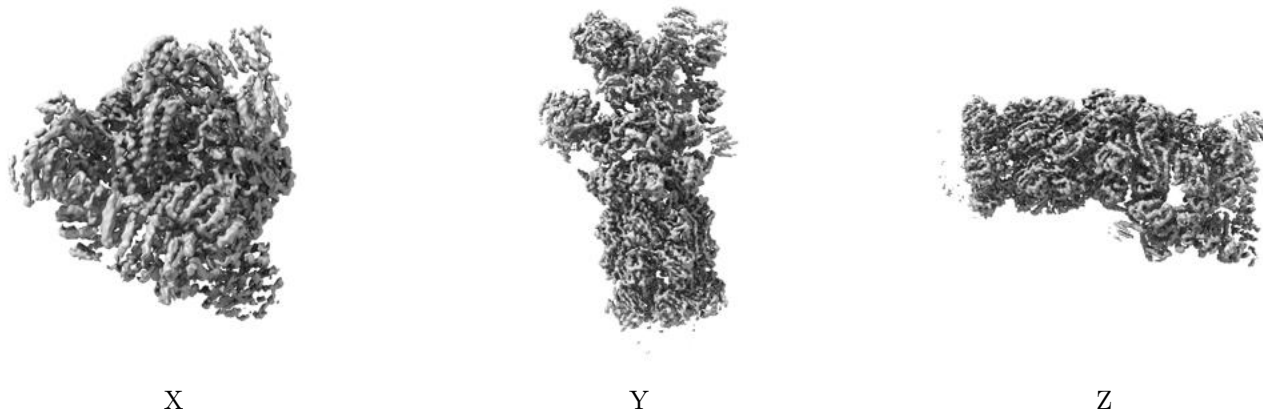


Z

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.

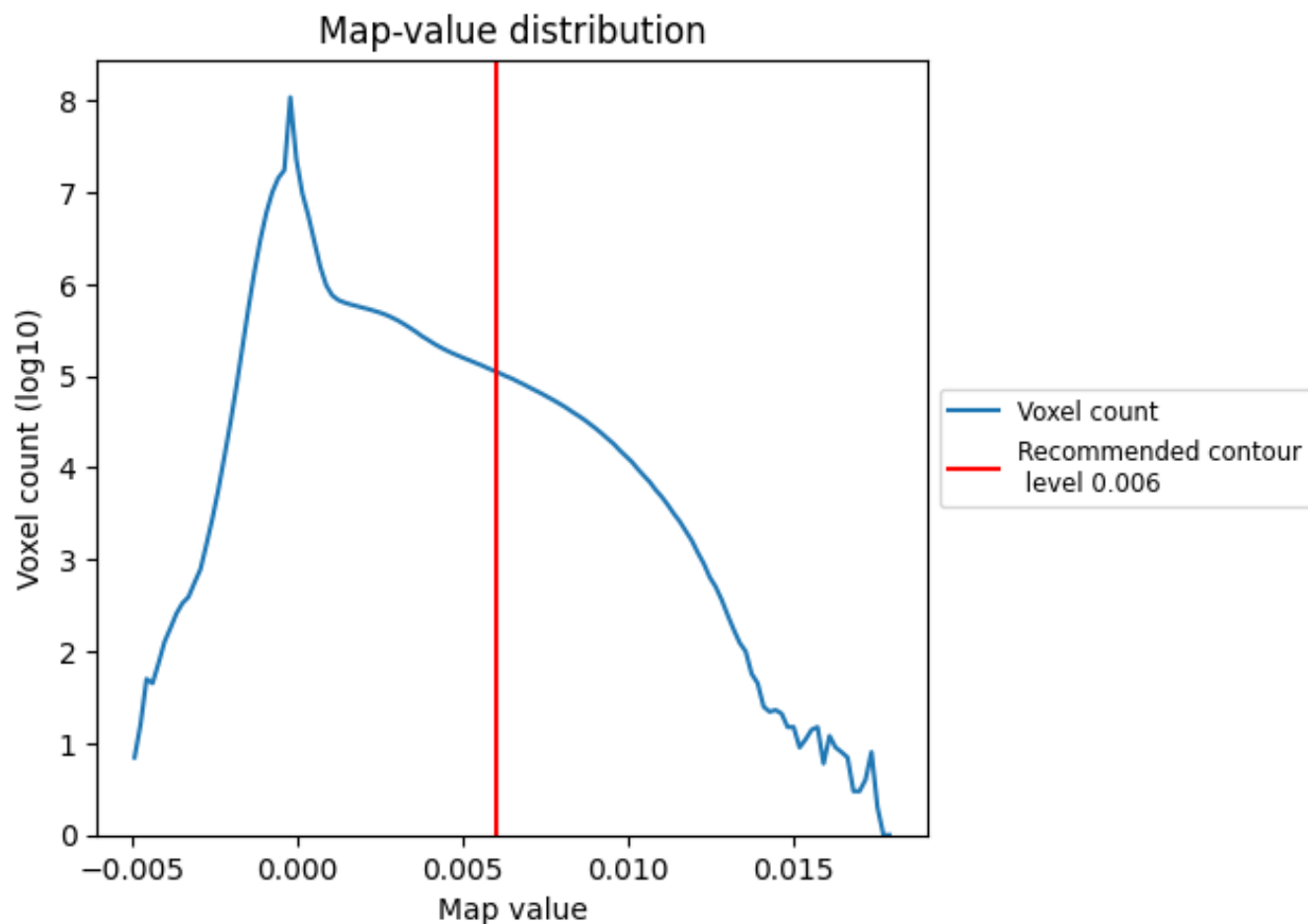
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

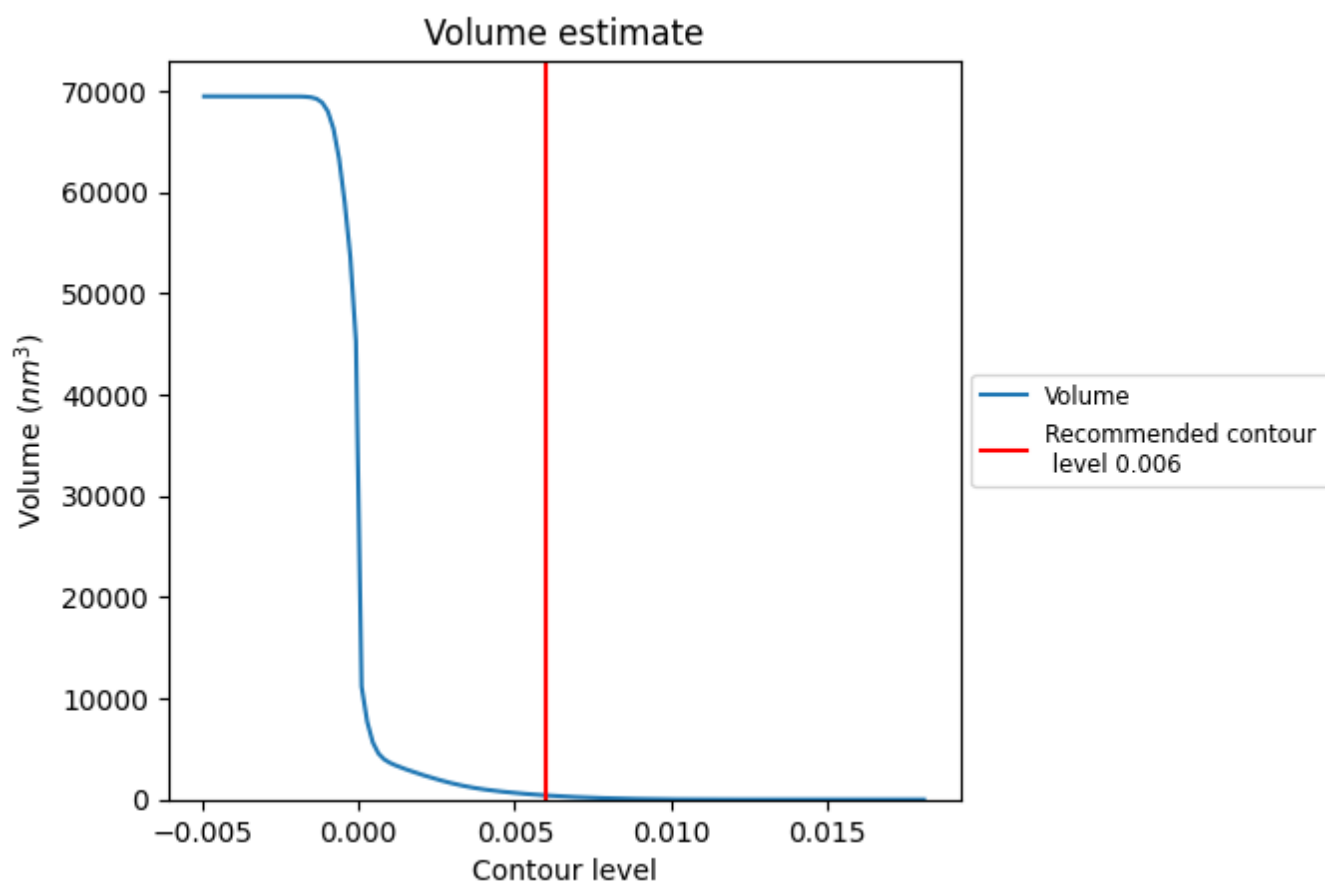
This section contains the results of statistical analysis of the map.

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.

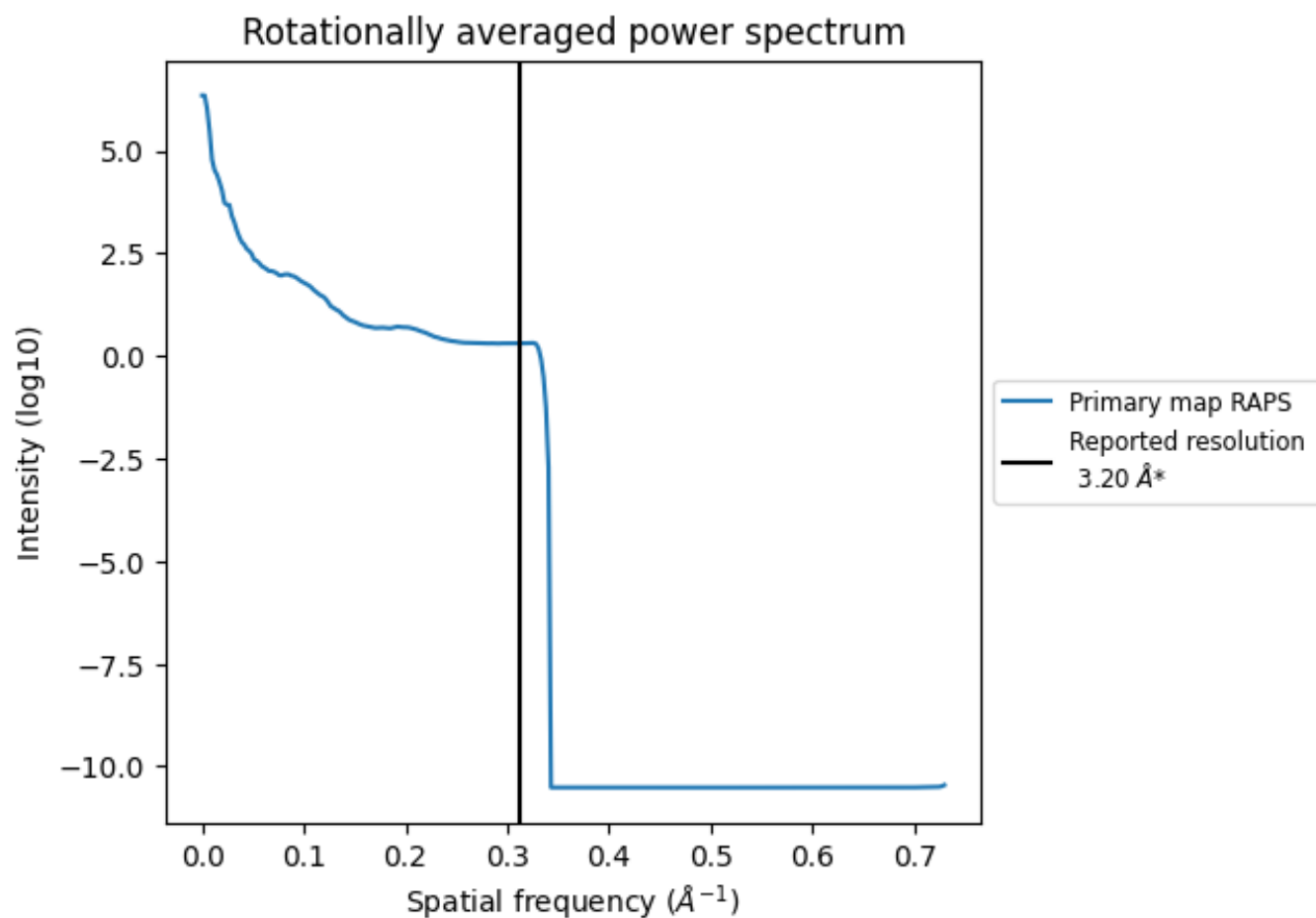
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm³; this corresponds to an approximate mass of 374 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 0.312 Å⁻¹

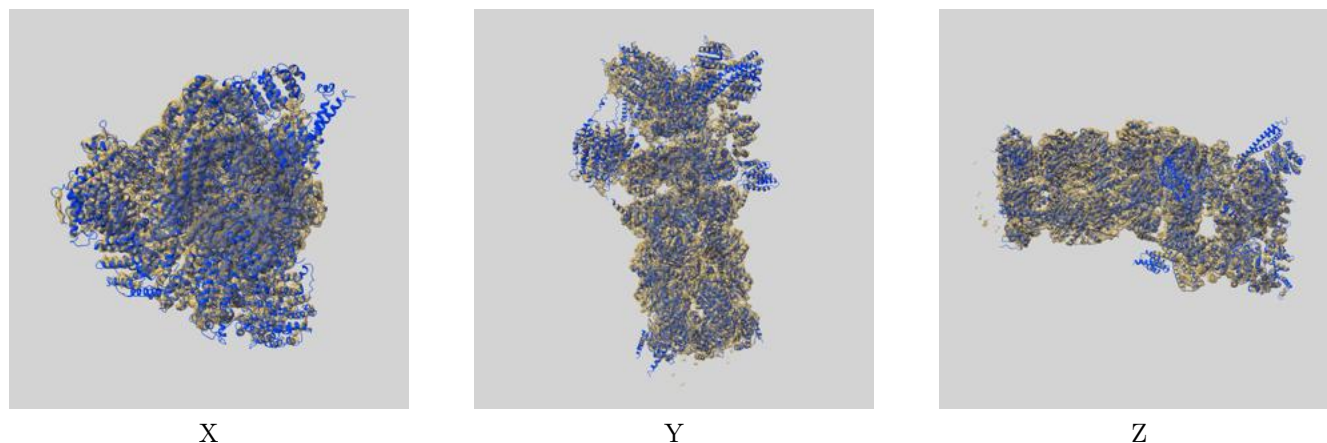
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

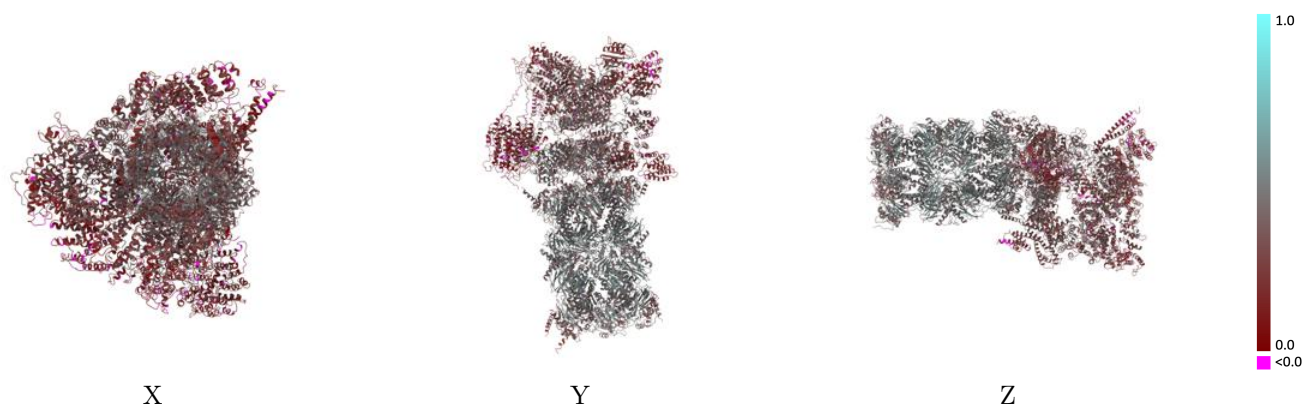
This section contains information regarding the fit between EMDB map EMD-9222 and PDB model 6MSK. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



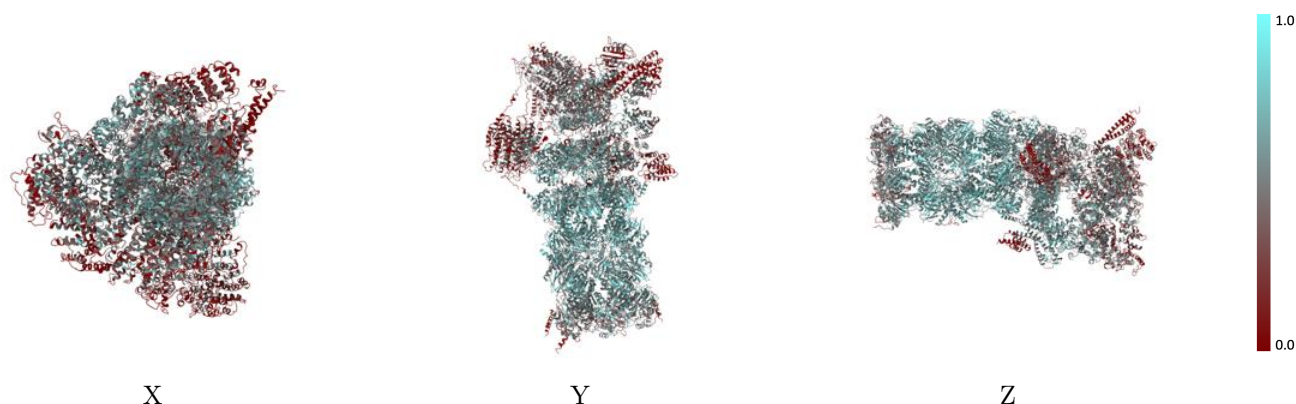
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



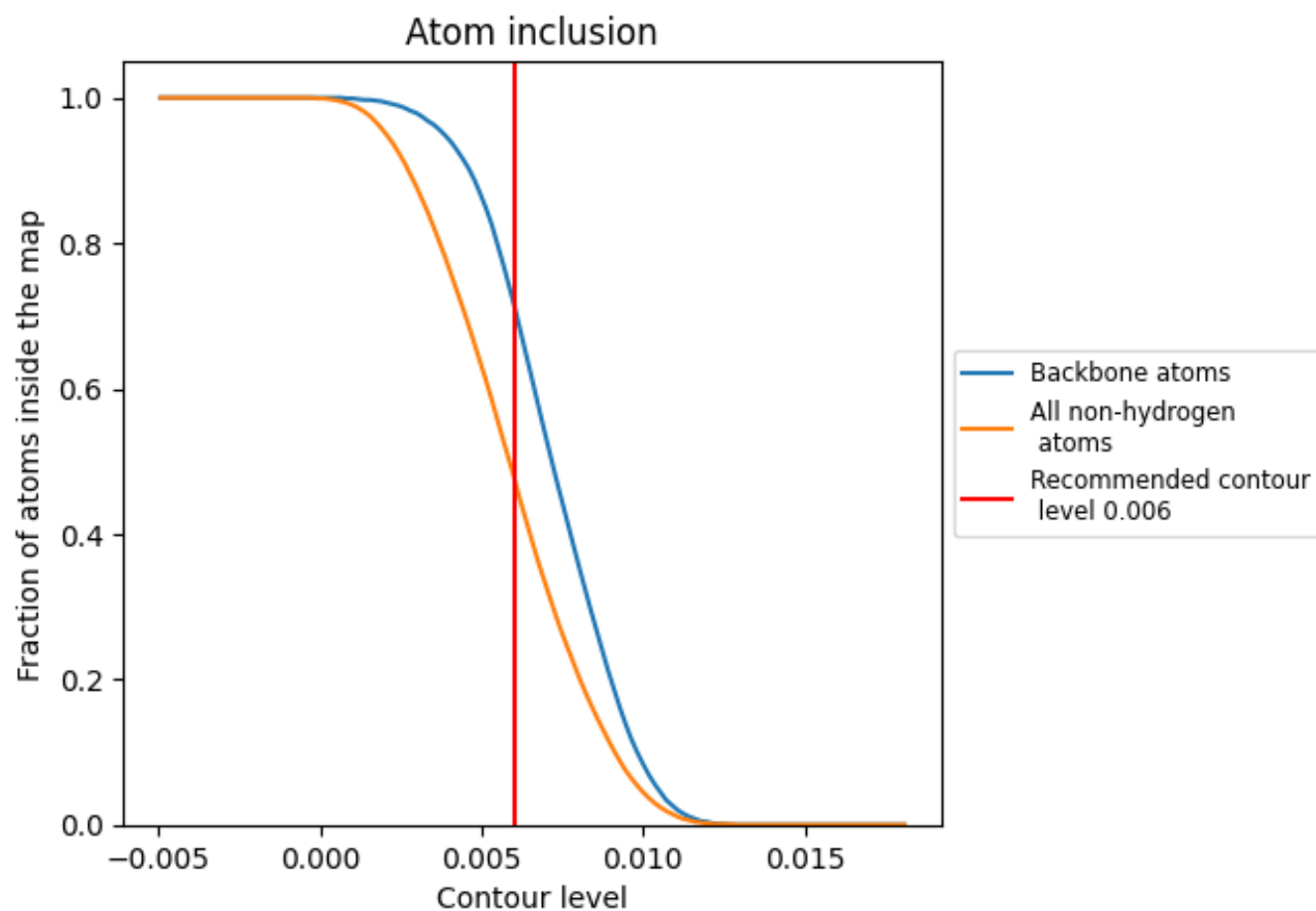
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 48% 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	 0.4800	 0.3550
A	 0.5110	 0.3670
B	 0.5060	 0.3540
C	 0.5670	 0.3740
D	 0.5510	 0.3600
E	 0.2520	 0.2210
F	 0.4420	 0.3240
G	 0.6380	 0.4290
H	 0.6810	 0.4480
I	 0.6260	 0.4150
J	 0.6210	 0.4190
K	 0.6240	 0.4300
L	 0.6550	 0.4470
M	 0.6260	 0.4200
N	 0.6620	 0.4650
O	 0.6350	 0.4620
P	 0.6600	 0.4810
Q	 0.6510	 0.4610
R	 0.6800	 0.4780
S	 0.6210	 0.4710
T	 0.6570	 0.4700
U	 0.3420	 0.2650
V	 0.3360	 0.2260
W	 0.3360	 0.2390
X	 0.4560	 0.3010
Y	 0.5410	 0.3010
Z	 0.4070	 0.3110
a	 0.3350	 0.2510
b	 0.2480	 0.2570
c	 0.3930	 0.3120
d	 0.2700	 0.2220
e	 0.3580	 0.2290
f	 0.2380	 0.1820
g	 0.4810	 0.4330
h	 0.4950	 0.4390



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Chain	Atom inclusion	Q-score
i	 0.4320	 0.4040
j	 0.4030	 0.3860
k	 0.4720	 0.4140
l	 0.5350	 0.4460
m	 0.5170	 0.4140
n	 0.6270	 0.4770
o	 0.5940	 0.4690
p	 0.6070	 0.4790
q	 0.6020	 0.4740
r	 0.6500	 0.4880
s	 0.5970	 0.4840
t	 0.6510	 0.4800
v	 0.1500	 0.3230