



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 07:28 PM EST

PDB ID : 6MSJ  
EMDB ID : EMD-9221  
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

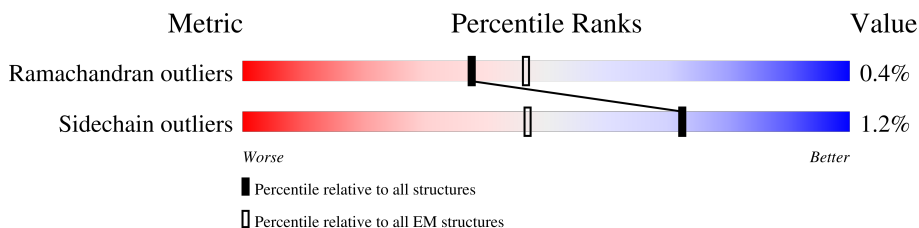
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	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	

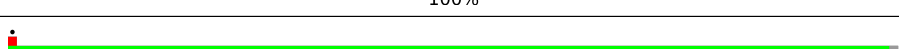
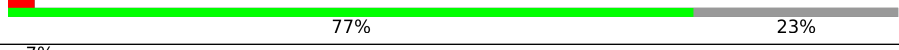


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Mol	Chain	Length	Quality of chain
10	d	349	62% 72% 26%
11	e	70	40% 53% 43%
12	f	892	70% 95%
13	A	433	44% 93% 5%
14	B	440	25% 91% 7%
15	C	398	17% 95% 5%
16	D	418	13% 86% 9%
17	E	403	28% 92%
18	F	439	61% 87% 10%
19	v	36	78% 100%
20	G	245	7% 95%
21	H	233	• 99%
21	h	233	15% 100%
22	I	260	10% 93% 5%
22	i	260	24% 96%
23	J	247	10% 96%
23	j	247	31% 97%
24	K	240	7% 92% 5%
24	k	240	21% 94% 5%
25	L	268	5% 89% 11%
25	l	268	12% 89% 11%
26	M	254	6% 94% 6%
26	m	254	14% 94% 6%
27	N	238	• 80% 20%
27	n	238	• 80% 20%

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Mol	Chain	Length	Quality of chain
28	O	276	 79% 20%
28	o	276	 8% 79% 20%
29	P	204	 100%
29	p	204	 100%
30	Q	201	 99%
30	q	201	 99%
31	R	262	 77% 23%
31	r	262	 77% 23%
32	S	240	 7% 88% 11%
32	s	240	 5% 88% 11%
33	T	263	 81% 18%
33	t	263	 81% 18%
34	g	240	 16% 100%

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 105316 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
			Total	C	N	O	S		
1	U	872	6828	4328	1157	1298	45	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	413	3229	2034	566	611	18	0	0

- Molecule 14 is a protein called Rpt2, NP\_002793.2 (26SHA chain B).

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	395	3098	1951	533	596	18	0	0

- Molecule 19 is a protein called substrate.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	G	239	1836	1168	305	350	13	0	0

- 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
			1723	1097	289	332	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
			1908	1204	326	369	9		
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
			1739	1077	317	340	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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
32	S	213	1641	1036	282	313	10	0	0
32	s	213	1641	1036	282	313	10	0	0

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

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

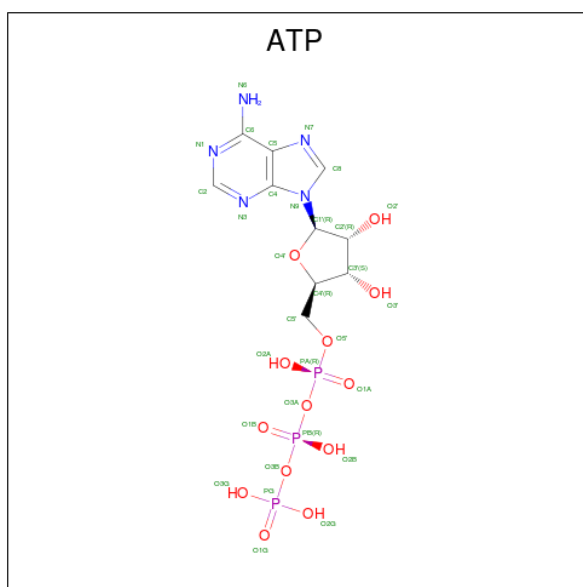
- Molecule 34 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

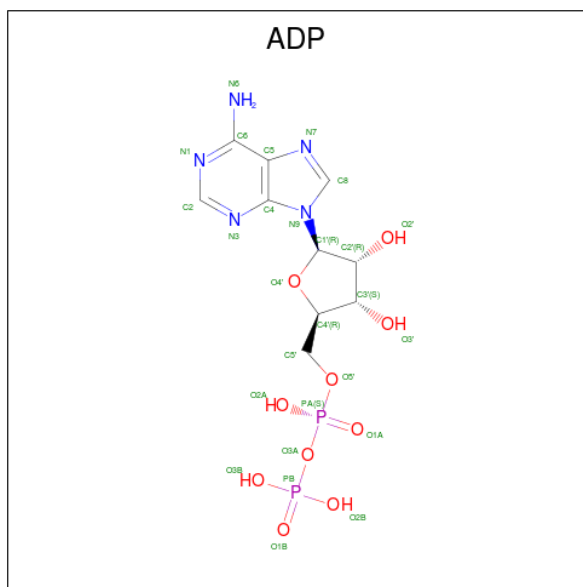


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

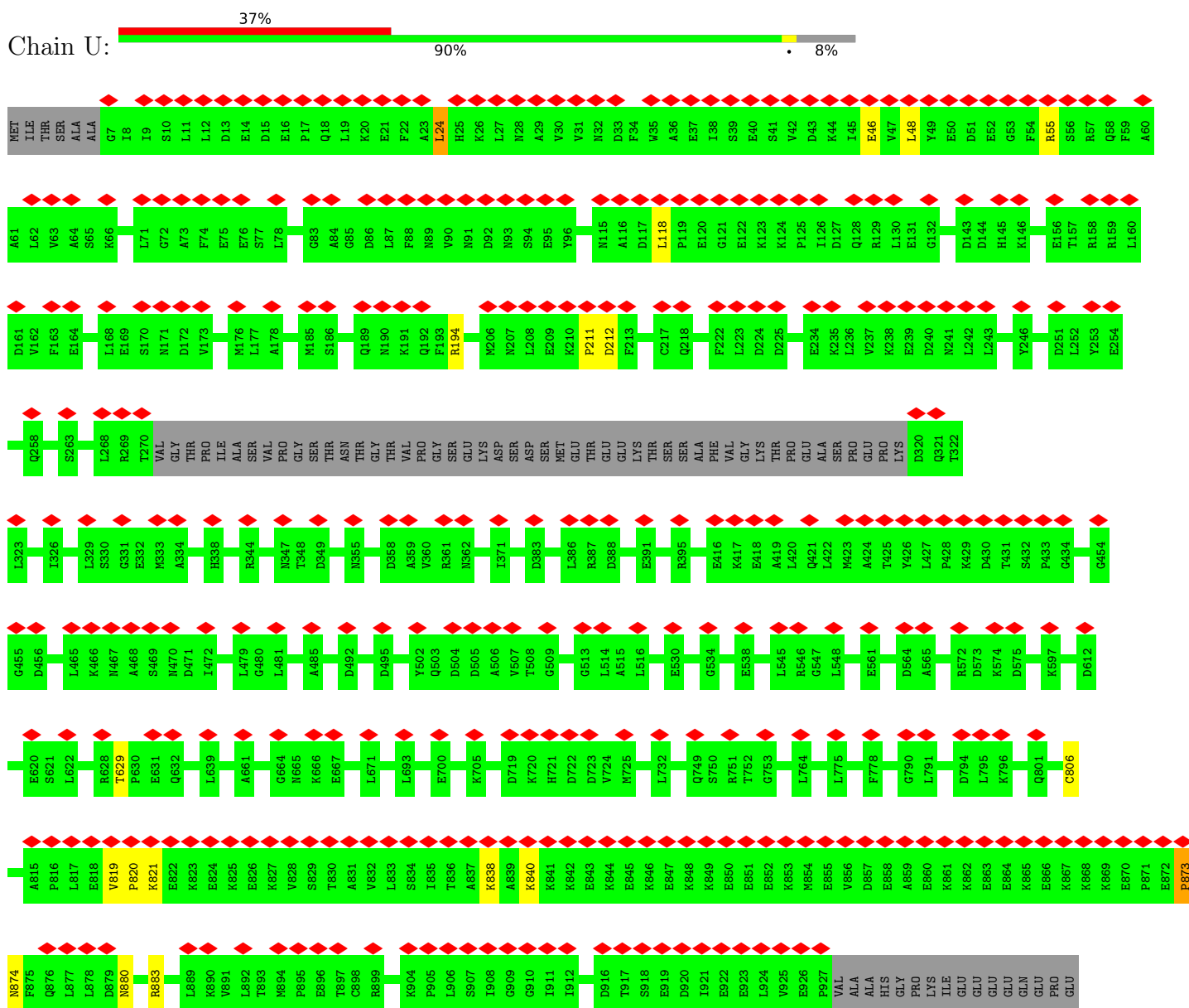


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	E	1	27	10	5	10	2	0

### 3 Residue-property plots [i](#)

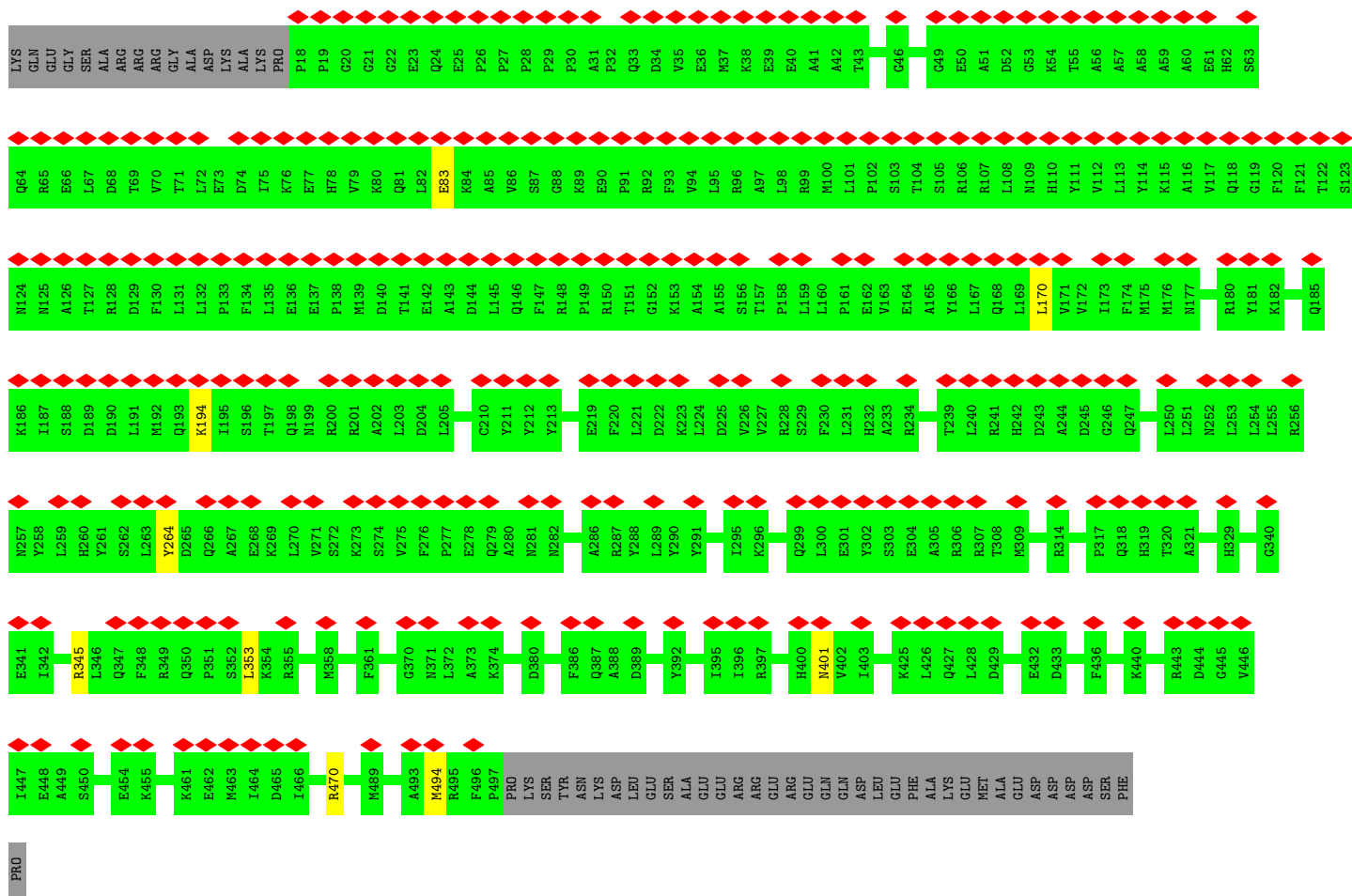
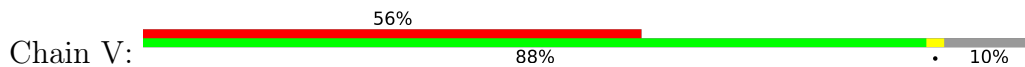
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

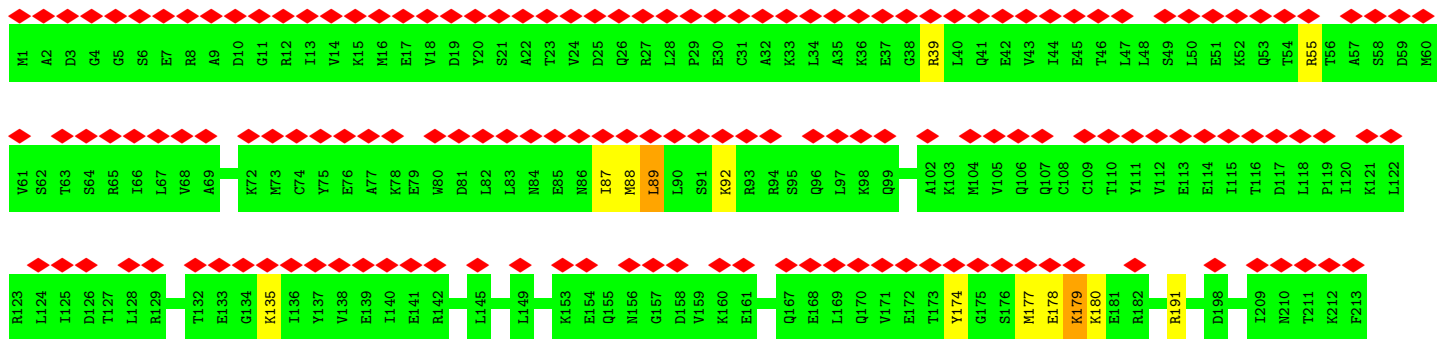


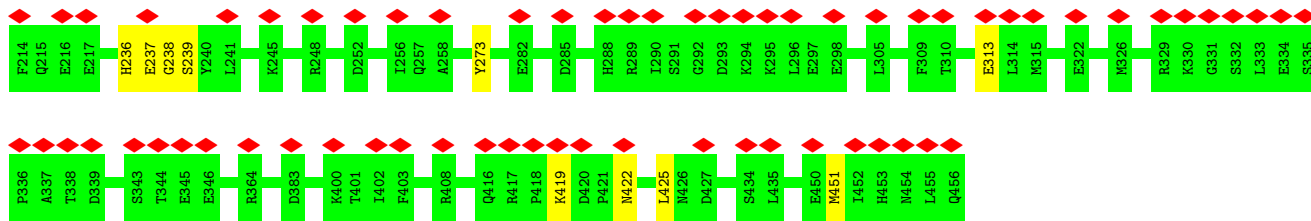
PRO  
 PRO  
 GLN  
 GLU  
 GLY  
 PRO  
 PHE  
 GLU  
 TYR  
 ILE  
 ASP  
 ASP

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

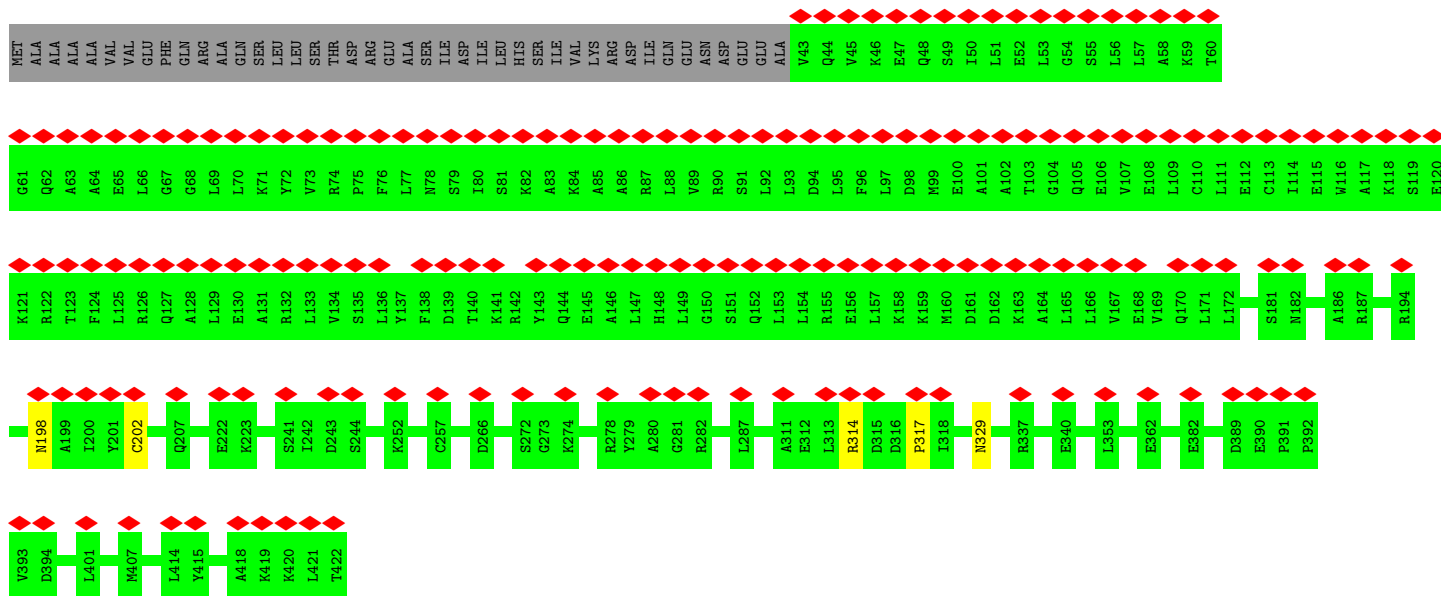
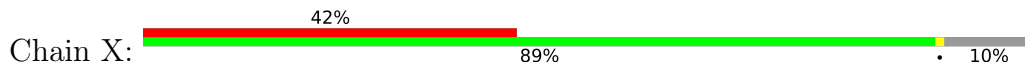


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

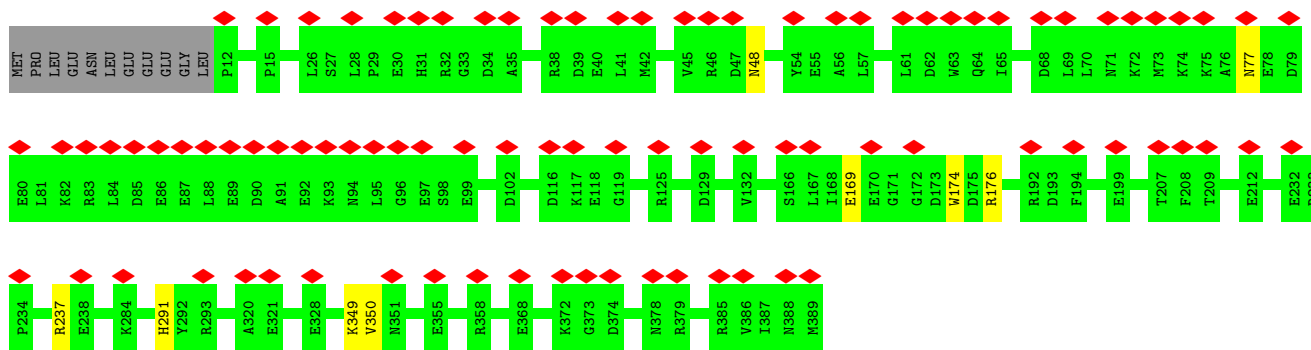




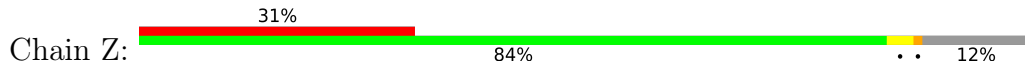
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

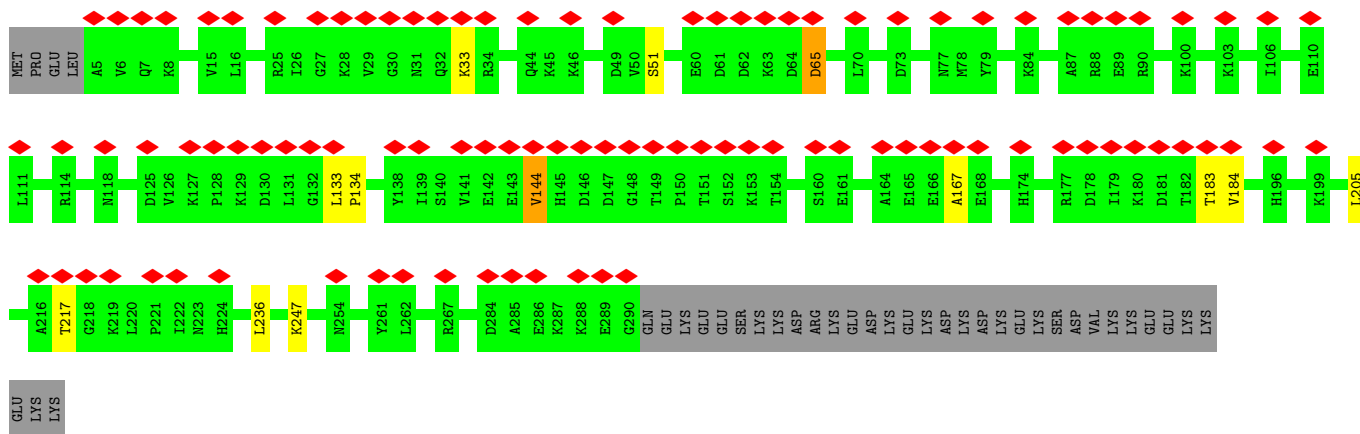


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



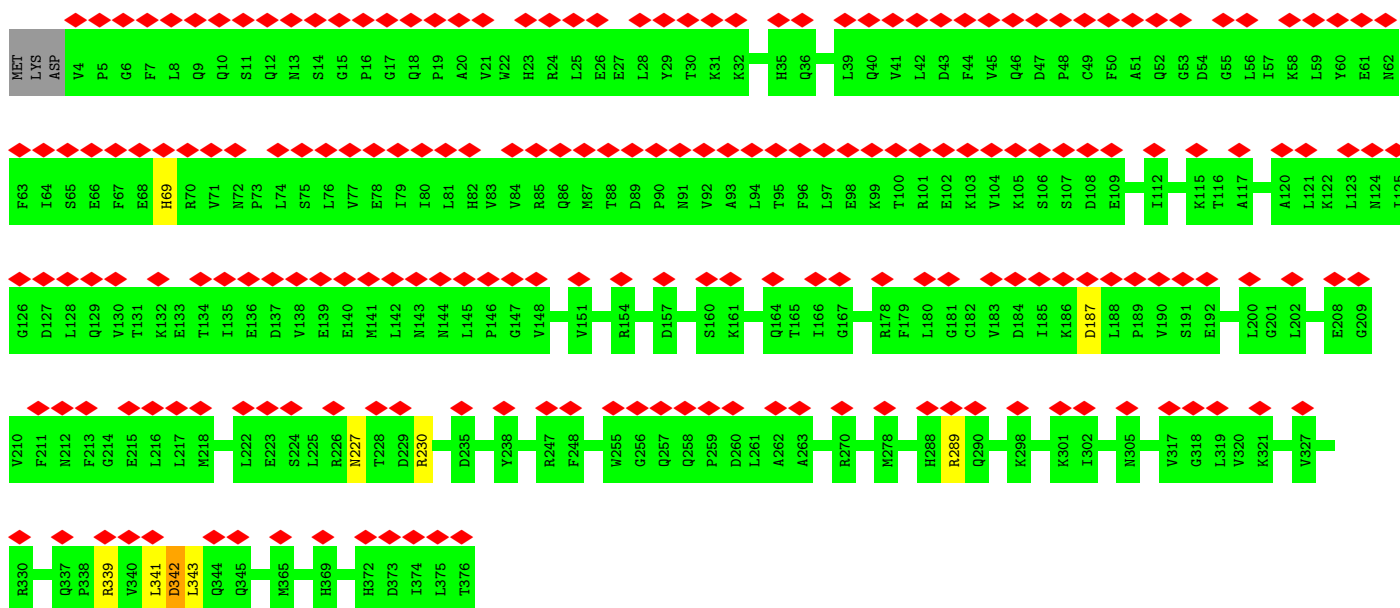
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7





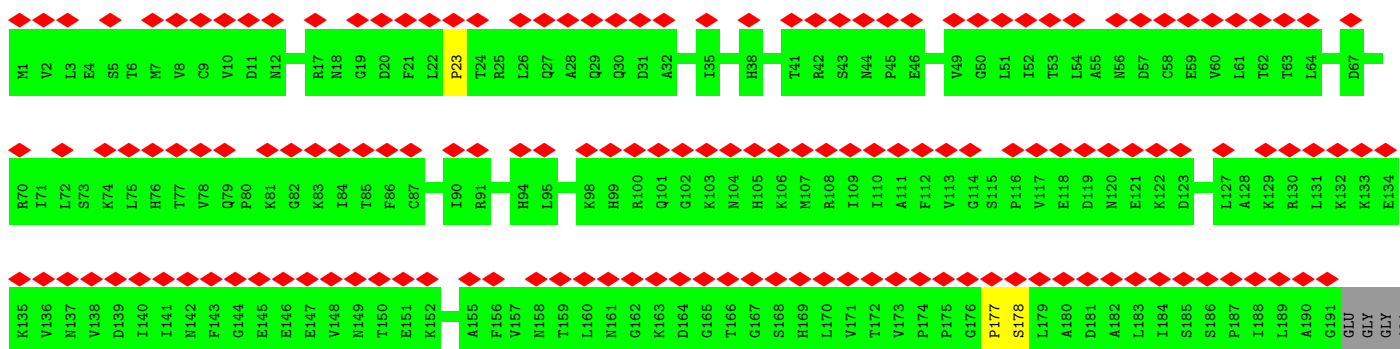
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



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

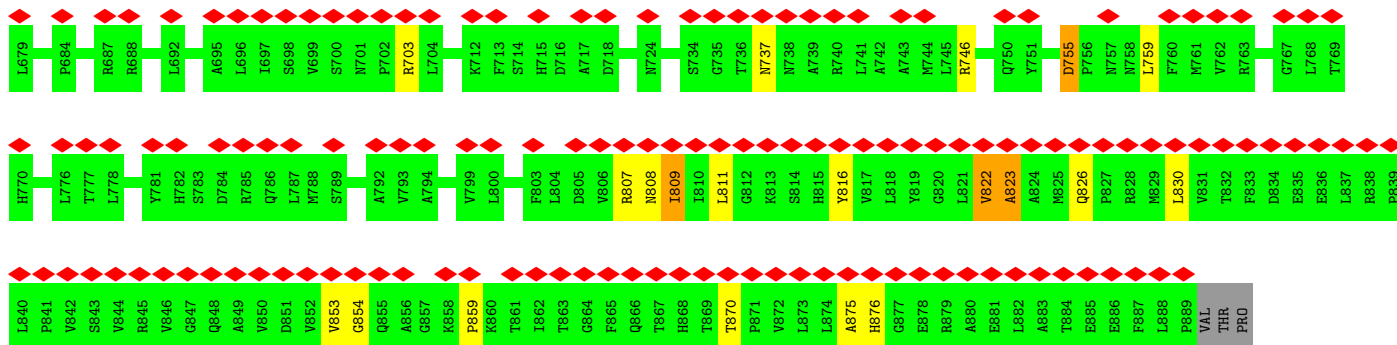
Chain b:



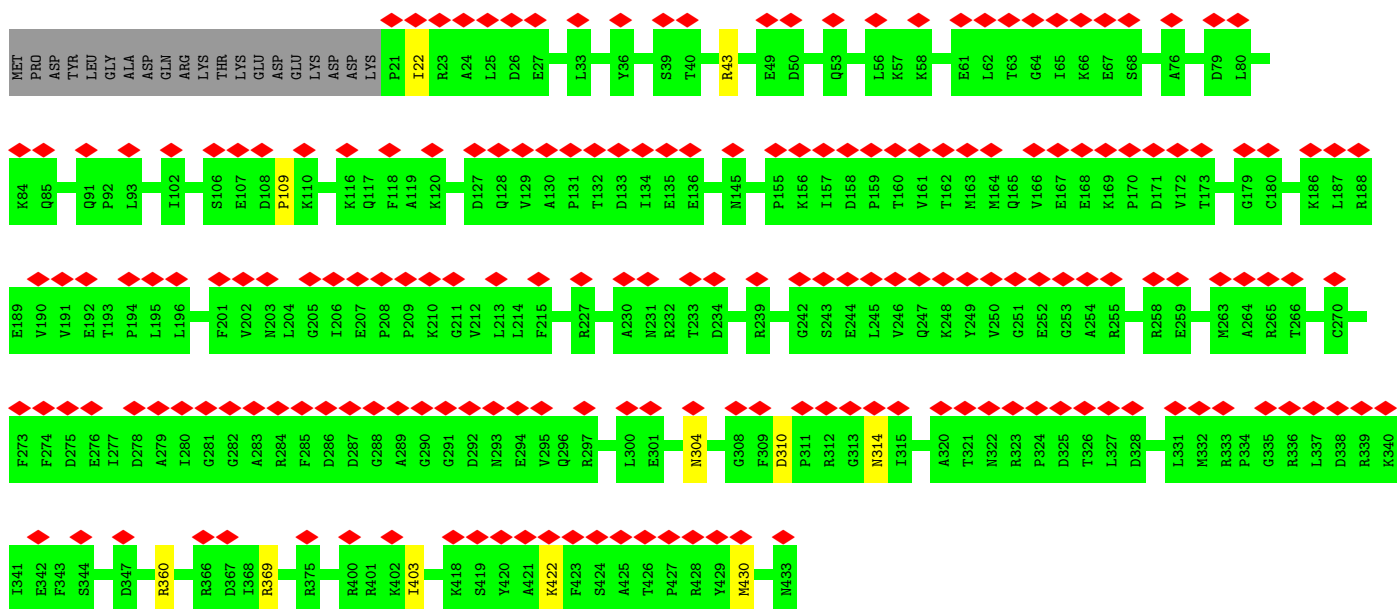
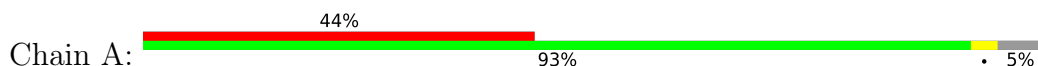




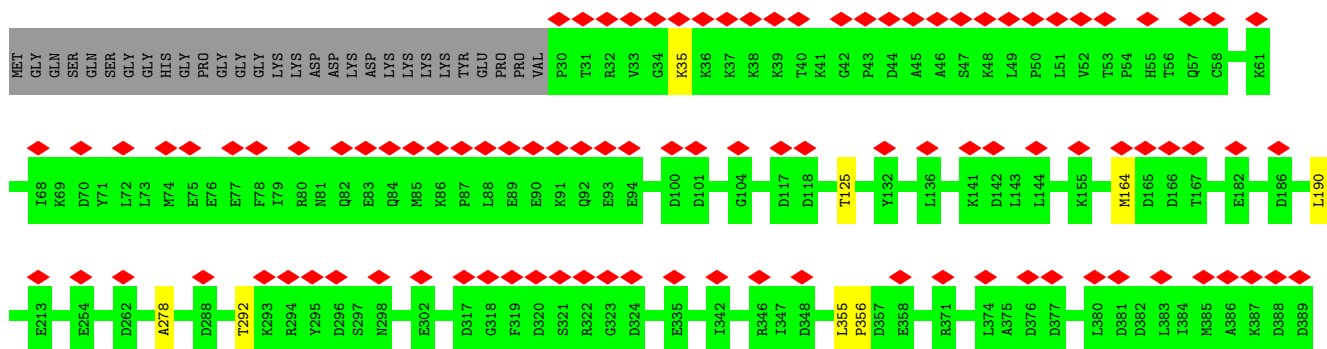
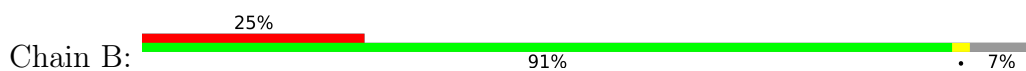


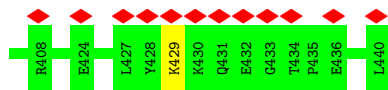


• Molecule 13: 26S proteasome regulatory subunit 7



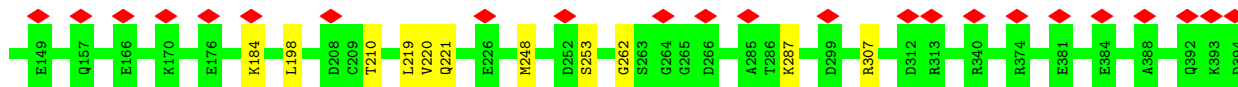
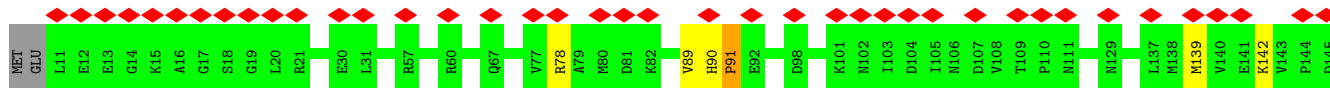
• Molecule 14: Rpt2, NP\_002793.2 (26SHA chain B)





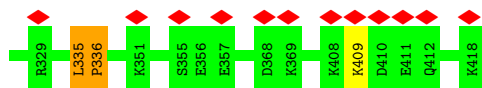
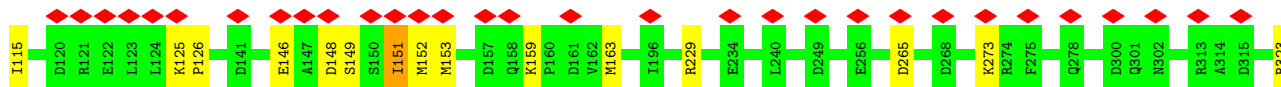
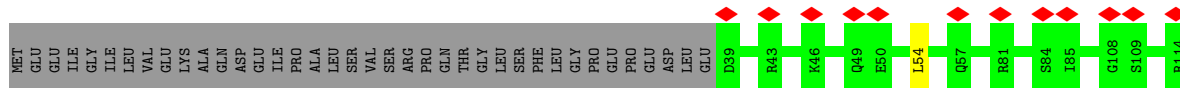
- Molecule 15: 26S proteasome regulatory subunit 8

Chain C: 17% 95% 5%



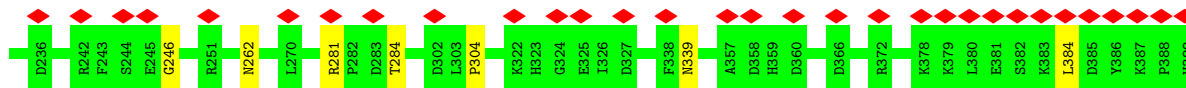
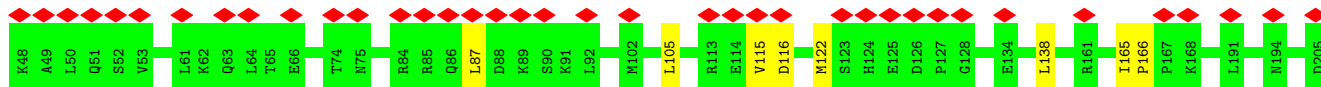
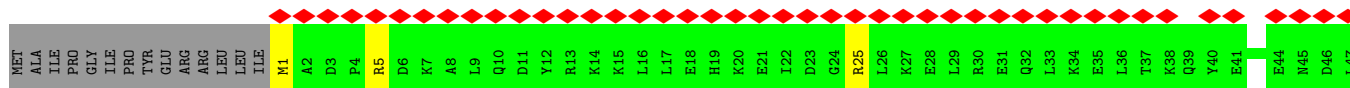
- Molecule 16: 26S proteasome regulatory subunit 6B

Chain D: 13% 86% 9%

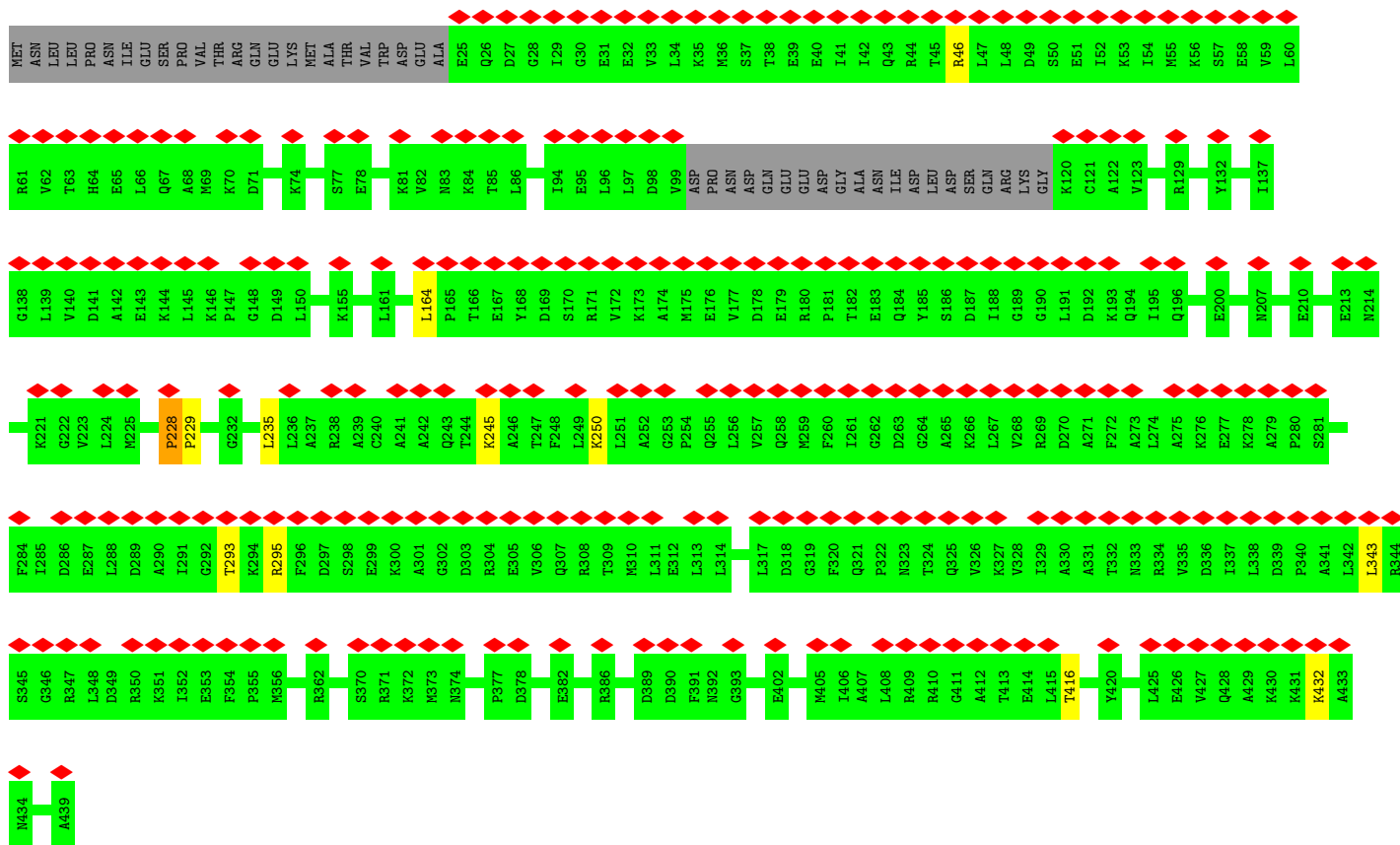
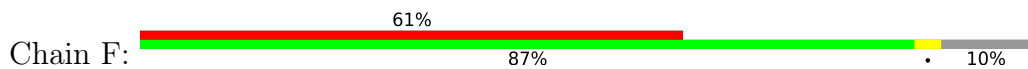


- Molecule 17: 26S proteasome regulatory subunit 10B

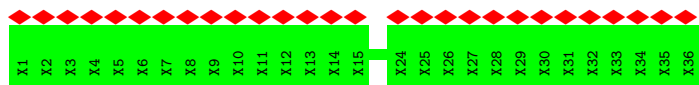
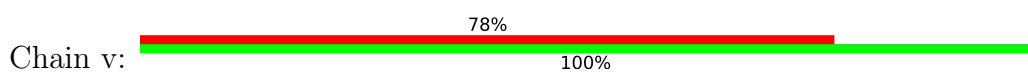
Chain E: 28% 92%



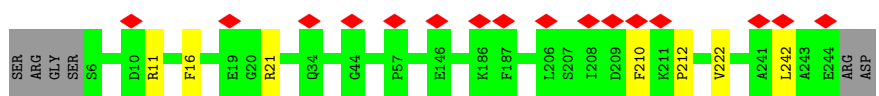
- Molecule 18: 26S proteasome regulatory subunit 6A



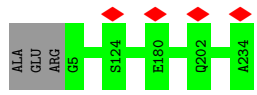
• Molecule 19: substrate



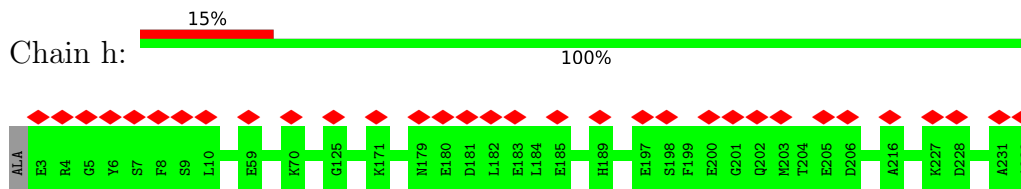
• Molecule 20: Proteasome subunit alpha type-6



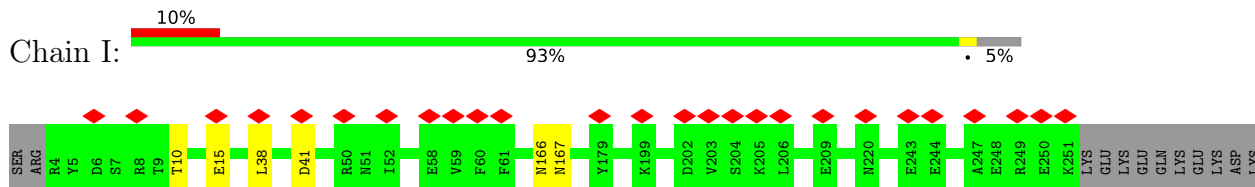
• Molecule 21: Proteasome subunit alpha type-2



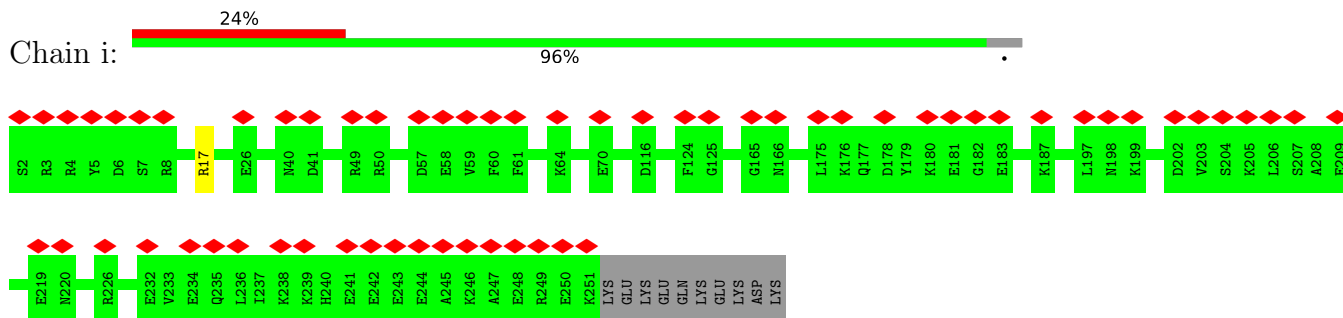
• Molecule 21: Proteasome subunit alpha type-2



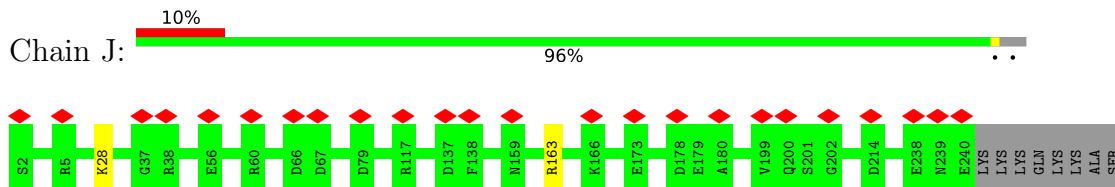
• Molecule 22: Proteasome subunit alpha type-4



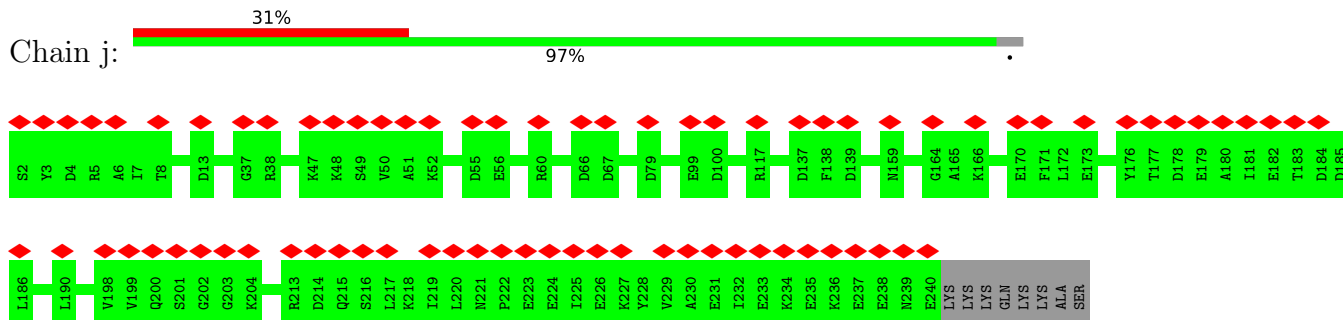
• Molecule 22: Proteasome subunit alpha type-4



• Molecule 23: Proteasome subunit alpha type-7

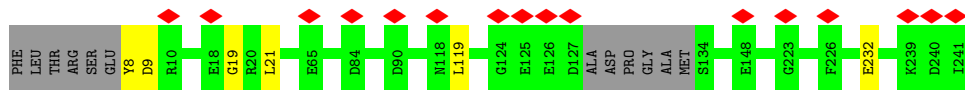


• Molecule 23: Proteasome subunit alpha type-7

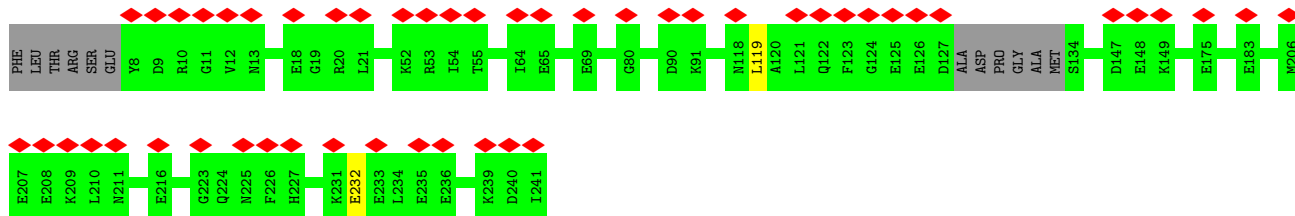


• Molecule 24: Proteasome subunit alpha type-5

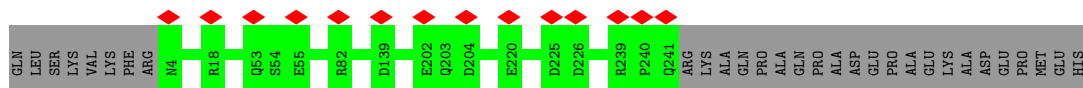
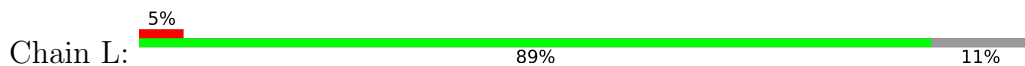




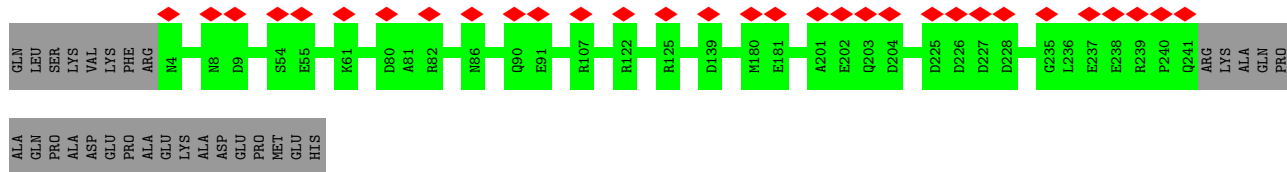
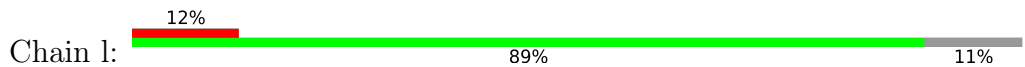
• Molecule 24: Proteasome subunit alpha type-5



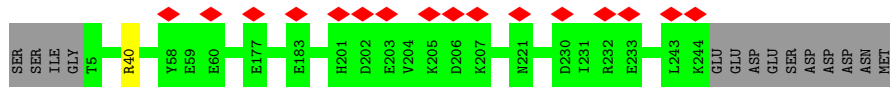
• Molecule 25: Proteasome subunit alpha type-1



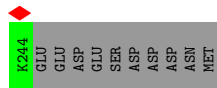
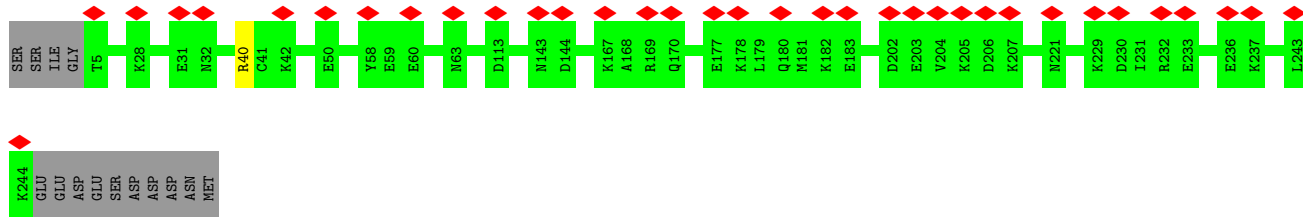
• Molecule 25: Proteasome subunit alpha type-1



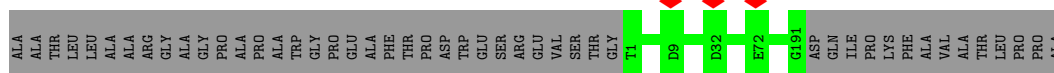
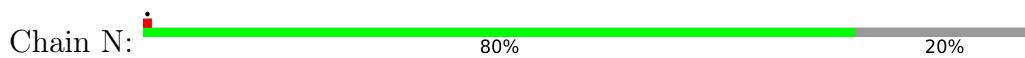
• Molecule 26: Proteasome subunit alpha type-3



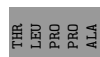
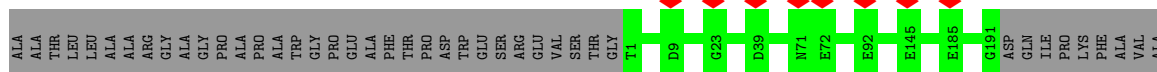
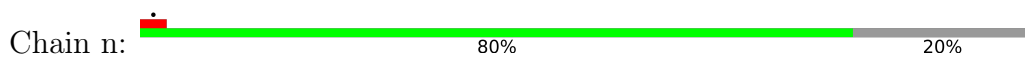
• Molecule 26: Proteasome subunit alpha type-3



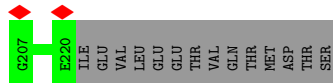
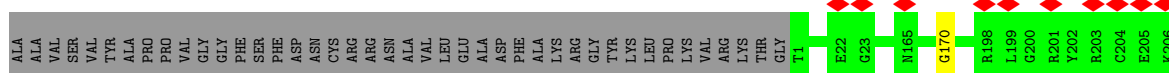
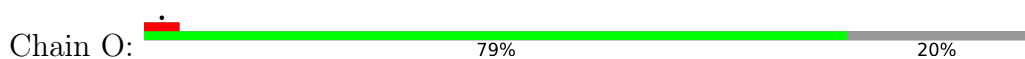
• Molecule 27: Proteasome subunit beta type-6



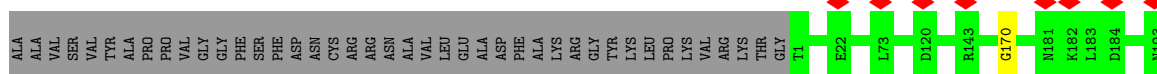
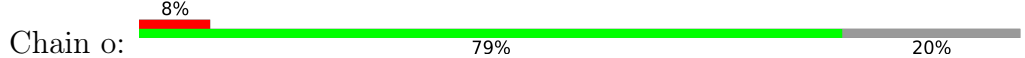
• Molecule 27: Proteasome subunit beta type-6



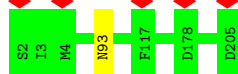
• Molecule 28: Proteasome subunit beta type-7



• Molecule 28: Proteasome subunit beta type-7

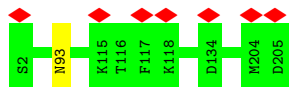


• Molecule 29: Proteasome subunit beta type-3

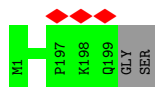


• Molecule 29: Proteasome subunit beta type-3

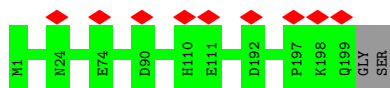




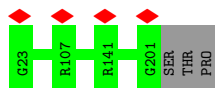
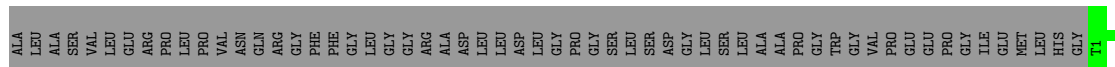
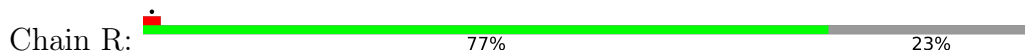
- Molecule 30: Proteasome subunit beta type-2



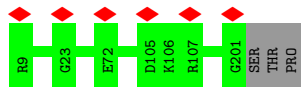
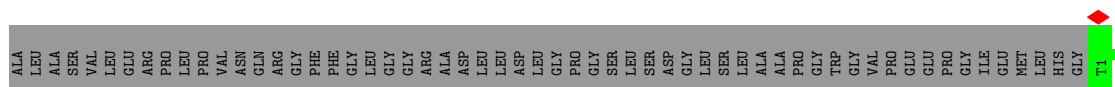
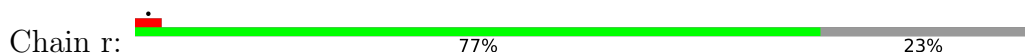
- Molecule 30: Proteasome subunit beta type-2



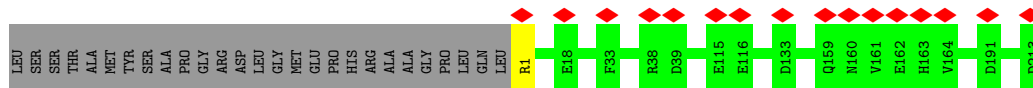
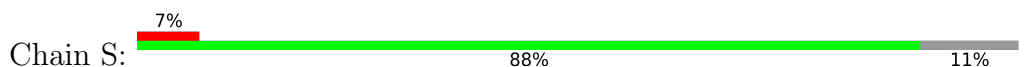
- Molecule 31: Proteasome subunit beta type-5



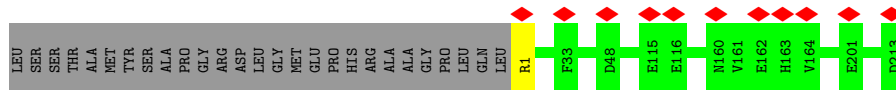
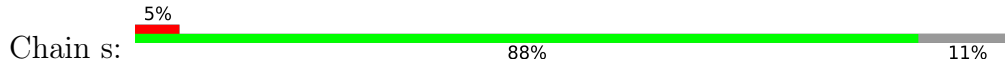
- Molecule 31: Proteasome subunit beta type-5



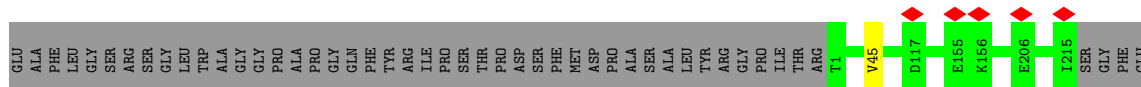
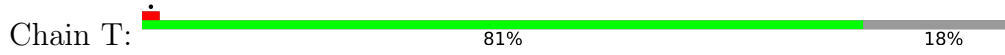
- Molecule 32: Proteasome subunit beta type-1



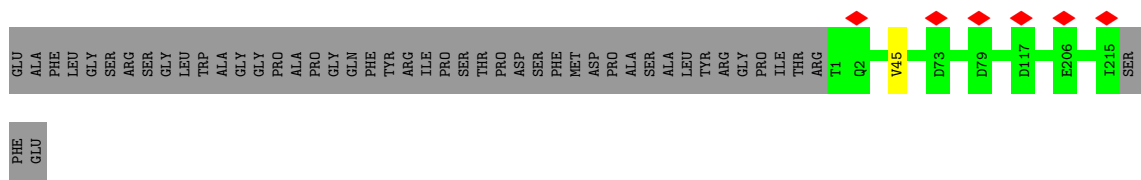
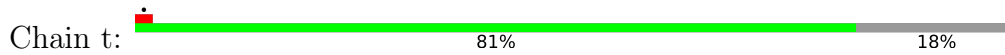
• Molecule 32: Proteasome subunit beta type-1



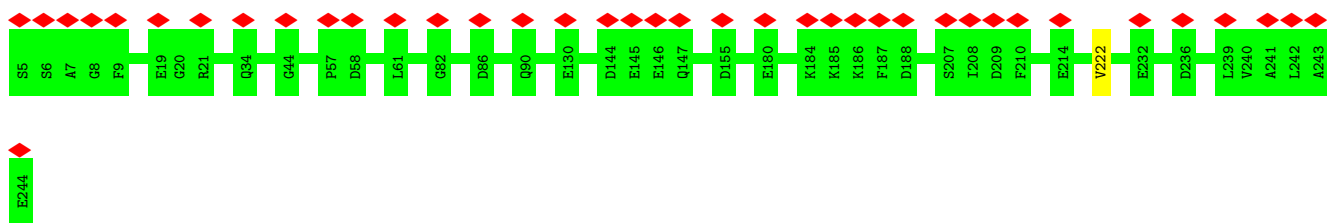
• Molecule 33: Proteasome subunit beta type-4



• Molecule 33: Proteasome subunit beta type-4



• Molecule 34: Proteasome subunit alpha type-6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288915	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 ( $\text{\AA}$ )	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 i

### 5.1 Standard geometry i

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

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	0.33	0/6945	0.61	1/9382 (0.0%)
2	V	0.32	0/3929	0.67	2/5309 (0.0%)
3	W	0.33	0/3751	0.67	2/5042 (0.0%)
4	X	0.31	0/3053	0.56	0/4115
5	Y	0.36	0/3173	0.65	0/4273
6	Z	0.33	0/2324	0.67	3/3150 (0.1%)
7	a	0.32	0/3053	0.65	2/4133 (0.0%)
8	b	0.29	0/1478	0.63	0/2001
9	c	0.34	0/2302	0.68	1/3110 (0.0%)
10	d	0.31	0/2162	0.59	1/2919 (0.0%)
11	e	0.33	0/338	0.72	1/450 (0.2%)
12	f	0.35	1/6980 (0.0%)	0.72	5/9433 (0.1%)
13	A	0.34	0/3283	0.61	0/4433
14	B	0.36	0/3254	0.61	0/4388
15	C	0.40	0/3146	0.66	3/4226 (0.1%)
16	D	0.40	0/3090	0.67	1/4168 (0.0%)
17	E	0.35	0/3145	0.64	4/4233 (0.1%)
18	F	0.33	0/3137	0.63	2/4223 (0.0%)
20	G	0.43	0/1870	0.62	1/2536 (0.0%)
21	H	0.47	0/1759	0.59	0/2389
21	h	0.38	0/1743	0.53	0/2372
22	I	0.41	0/1938	0.67	3/2621 (0.1%)
22	i	0.34	0/1942	0.58	0/2628
23	J	0.43	0/1763	0.58	0/2398
23	j	0.36	0/1728	0.55	0/2358
24	K	0.41	0/1755	0.64	2/2375 (0.1%)
24	k	0.34	0/1747	0.56	0/2364
25	L	0.40	0/1885	0.59	0/2552
25	l	0.40	0/1885	0.59	0/2552
26	M	0.40	0/1891	0.56	0/2552
26	m	0.40	0/1891	0.56	0/2552
27	N	0.39	0/1454	0.54	0/1967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	n	0.39	0/1454	0.54	0/1967
28	O	0.37	0/1670	0.54	0/2265
28	o	0.37	0/1670	0.54	0/2265
29	P	0.37	0/1614	0.52	0/2177
29	p	0.37	0/1614	0.52	0/2177
30	Q	0.39	0/1603	0.57	0/2174
30	q	0.39	0/1603	0.57	0/2174
31	R	0.40	0/1579	0.48	0/2134
31	r	0.40	0/1579	0.49	0/2134
32	S	0.37	0/1671	0.52	0/2253
32	s	0.37	0/1671	0.52	0/2253
33	T	0.39	0/1700	0.52	0/2305
33	t	0.39	0/1700	0.52	0/2305
34	g	0.36	0/1859	0.58	0/2523
All	All	0.37	1/106781 (0.0%)	0.61	34/144310 (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	7
2	V	0	2
3	W	0	2
4	X	0	1
5	Y	0	4
6	Z	0	4
7	a	0	1
9	c	0	4
10	d	0	4
11	e	0	1
12	f	0	14
13	A	0	2
14	B	0	2
15	C	0	3
16	D	0	5
17	E	0	5
18	F	0	3
20	G	0	3
22	I	0	1
24	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	k	0	1
28	O	0	1
28	o	0	1
33	T	0	1
33	t	0	1
34	g	0	1
All	All	0	77

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	6.03	1.45	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	56	LEU	CA-CB-CG	8.38	134.58	115.30
22	I	15	GLU	C-N-CA	7.24	137.50	122.30
6	Z	133	LEU	CA-CB-CG	7.08	131.58	115.30
18	F	235	LEU	CA-CB-CG	6.98	131.34	115.30
17	E	116	ASP	CB-CG-OD1	6.92	124.53	118.30
24	K	21	LEU	C-N-CA	6.78	138.65	121.70
12	f	759	LEU	CA-CB-CG	6.67	130.65	115.30
12	f	612	LEU	CA-CB-CG	6.63	130.56	115.30
3	W	425	LEU	CB-CG-CD2	-6.62	99.75	111.00
7	a	342	ASP	CB-CG-OD1	6.41	124.07	118.30
22	I	38	LEU	CA-CB-CG	6.37	129.96	115.30
7	a	187	ASP	CB-CG-OD1	6.36	124.03	118.30
3	W	89	LEU	CA-CB-CG	6.33	129.87	115.30
18	F	164	LEU	CA-CB-CG	6.25	129.67	115.30
24	K	119	LEU	CA-CB-CG	6.07	129.25	115.30
16	D	54	LEU	CA-CB-CG	6.03	129.16	115.30
22	I	41	ASP	CB-CG-OD1	5.96	123.67	118.30
17	E	105	LEU	CA-CB-CG	5.95	128.99	115.30
12	f	811	LEU	CA-CB-CG	5.95	128.99	115.30
12	f	830	LEU	CA-CB-CG	5.82	128.69	115.30
2	V	170	LEU	CA-CB-CG	5.60	128.17	115.30
15	C	404	LEU	CA-CB-CG	5.55	128.07	115.30
6	Z	205	LEU	CA-CB-CG	5.44	127.82	115.30
20	G	16	PHE	C-N-CA	5.44	135.30	121.70
15	C	139	MET	CA-CB-CG	5.41	122.50	113.30
6	Z	65	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	384	LEU	CA-CB-CG	5.29	127.46	115.30
9	c	212	LEU	CA-CB-CG	5.18	127.21	115.30
2	V	353	LEU	CA-CB-CG	5.17	127.20	115.30
17	E	115	VAL	C-N-CA	5.17	134.63	121.70
10	d	190	LEU	CA-CB-CG	5.17	127.18	115.30
1	U	24	LEU	CA-CB-CG	5.09	127.01	115.30
15	C	198	LEU	CA-CB-CG	5.04	126.90	115.30
12	f	217	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	22	ILE	Peptide
13	A	310	ASP	Peptide
14	B	278	ALA	Peptide
14	B	355	LEU	Peptide
15	C	220	VAL	Peptide
15	C	262	GLY	Peptide
15	C	403	LYS	Peptide
16	D	125	LYS	Peptide
16	D	159	LYS	Peptide
16	D	265	ASP	Peptide
16	D	335	LEU	Peptide
16	D	336	PRO	Peptide
17	E	165	ILE	Peptide
17	E	166	PRO	Peptide
17	E	246	GLY	Peptide
17	E	281	ARG	Peptide
17	E	304	PRO	Peptide
18	F	228	PRO	Peptide
18	F	295	ARG	Peptide
18	F	343	LEU	Peptide
20	G	210	PHE	Peptide
20	G	222	VAL	Peptide
20	G	242	LEU	Peptide
22	I	10	THR	Peptide
24	K	19	GLY	Peptide
24	K	232	GLU	Peptide
24	K	8	TYR	Peptide
28	O	170	GLY	Peptide
33	T	45	VAL	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	U	211	PRO	Peptide
1	U	212	ASP	Peptide
1	U	24	LEU	Peptide
1	U	806	CYS	Peptide
1	U	821	LYS	Peptide
1	U	873	PRO	Peptide
1	U	880	ASN	Peptide
2	V	264	TYR	Peptide
2	V	83	GLU	Peptide
3	W	273	TYR	Peptide
3	W	313	GLU	Peptide
4	X	202	CYS	Peptide
5	Y	169	GLU	Peptide
5	Y	174	TRP	Peptide
5	Y	291	HIS	Peptide
5	Y	349	LYS	Peptide
6	Z	144	VAL	Peptide
6	Z	167	ALA	Peptide
6	Z	183	THR	Peptide
6	Z	184	VAL	Peptide
7	a	341	LEU	Peptide
9	c	185	ASN	Peptide
9	c	232	GLN	Peptide
9	c	279	ASP	Peptide
9	c	65	TYR	Peptide
10	d	186	TYR	Peptide
10	d	198	LEU	Peptide
10	d	201	ASN	Peptide
10	d	88	GLN	Peptide
11	e	6	GLN	Peptide
12	f	249	LEU	Peptide
12	f	340	MET	Peptide
12	f	620	PHE	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

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Mol	Chain	Res	Type	Group
12	f	870	THR	Peptide
12	f	875	ALA	Peptide
34	g	222	VAL	Peptide
24	k	232	GLU	Peptide
28	o	170	GLY	Peptide
33	t	45	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	868/953 (91%)	785 (90%)	79 (9%)	4 (0%)	29	61
2	V	478/533 (90%)	420 (88%)	58 (12%)	0	100	100
3	W	454/456 (100%)	411 (90%)	36 (8%)	7 (2%)	10	38
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	41	71
5	Y	376/389 (97%)	340 (90%)	35 (9%)	1 (0%)	41	71
6	Z	284/324 (88%)	242 (85%)	39 (14%)	3 (1%)	14	45
7	a	371/376 (99%)	332 (90%)	36 (10%)	3 (1%)	19	51
8	b	189/377 (50%)	164 (87%)	22 (12%)	3 (2%)	9	36
9	c	285/309 (92%)	241 (85%)	41 (14%)	3 (1%)	14	45
10	d	255/349 (73%)	215 (84%)	39 (15%)	1 (0%)	34	66
11	e	36/70 (51%)	25 (69%)	11 (31%)	0	100	100
12	f	887/892 (99%)	715 (81%)	158 (18%)	14 (2%)	9	36
13	A	411/433 (95%)	361 (88%)	48 (12%)	2 (0%)	29	61
14	B	409/440 (93%)	343 (84%)	65 (16%)	1 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	C	394/398 (99%)	340 (86%)	49 (12%)	5 (1%)	12	40
16	D	378/418 (90%)	323 (85%)	49 (13%)	6 (2%)	9	36
17	E	387/403 (96%)	341 (88%)	46 (12%)	0	100	100
18	F	391/439 (89%)	347 (89%)	42 (11%)	2 (0%)	29	61
20	G	237/245 (97%)	214 (90%)	22 (9%)	1 (0%)	34	66
21	H	228/233 (98%)	222 (97%)	6 (3%)	0	100	100
21	h	230/233 (99%)	223 (97%)	7 (3%)	0	100	100
22	I	246/260 (95%)	228 (93%)	18 (7%)	0	100	100
22	i	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
23	J	237/247 (96%)	214 (90%)	23 (10%)	0	100	100
23	j	237/247 (96%)	217 (92%)	20 (8%)	0	100	100
24	K	224/240 (93%)	202 (90%)	21 (9%)	1 (0%)	34	66
24	k	224/240 (93%)	204 (91%)	20 (9%)	0	100	100
25	L	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
25	l	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
26	M	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
26	m	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
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%)	202 (93%)	16 (7%)	0	100	100
28	o	218/276 (79%)	202 (93%)	16 (7%)	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%)	190 (96%)	9 (4%)	0	100	100
31	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
32	S	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
32	s	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
33	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
33	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	g	238/240 (99%)	221 (93%)	17 (7%)	0	100	100
All	All	13386/14838 (90%)	12070 (90%)	1258 (9%)	58 (0%)	38	66

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	874	ASN
7	a	343	LEU
8	b	178	SER
9	c	285	GLU
12	f	665	GLU
12	f	808	ASN
12	f	853	VAL
13	A	430	MET
16	D	335	LEU
1	U	48	LEU
3	W	88	MET
3	W	178	GLU
3	W	180	LYS
3	W	239	SER
5	Y	350	VAL
12	f	118	ASN
12	f	657	ILE
12	f	876	HIS
16	D	146	GLU
3	W	238	GLY
7	a	69	HIS
7	a	342	ASP
9	c	233	ASP
9	c	284	LEU
12	f	476	THR
12	f	659	LEU
12	f	823	ALA
14	B	356	PRO
16	D	149	SER
18	F	228	PRO
24	K	9	ASP
1	U	820	PRO
1	U	873	PRO
4	X	317	PRO
10	d	199	PHE
15	C	90	HIS

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Mol	Chain	Res	Type
15	C	253	SER
3	W	179	LYS
6	Z	65	ASP
12	f	475	ASN
12	f	662	MET
12	f	809	ILE
15	C	221	GLN
16	D	126	PRO
16	D	336	PRO
12	f	859	PRO
13	A	109	PRO
16	D	151	ILE
6	Z	134	PRO
12	f	755	ASP
15	C	91	PRO
18	F	229	PRO
20	G	212	PRO
15	C	89	VAL
6	Z	144	VAL
8	b	177	PRO
3	W	87	ILE
8	b	23	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	748/816 (92%)	739 (99%)	9 (1%)	71	83
2	V	414/459 (90%)	409 (99%)	5 (1%)	71	83
3	W	416/416 (100%)	402 (97%)	14 (3%)	37	65
4	X	327/362 (90%)	324 (99%)	3 (1%)	78	87
5	Y	334/344 (97%)	330 (99%)	4 (1%)	71	83
6	Z	257/295 (87%)	252 (98%)	5 (2%)	57	77
7	a	333/336 (99%)	329 (99%)	4 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	243 (96%)	9 (4%)	35	63
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	37 (97%)	1 (3%)	46	71
12	f	745/748 (100%)	727 (98%)	18 (2%)	49	73
13	A	348/372 (94%)	341 (98%)	7 (2%)	55	76
14	B	357/385 (93%)	351 (98%)	6 (2%)	60	78
15	C	340/346 (98%)	331 (97%)	9 (3%)	46	71
16	D	333/366 (91%)	323 (97%)	10 (3%)	41	68
17	E	341/353 (97%)	332 (97%)	9 (3%)	46	71
18	F	340/379 (90%)	334 (98%)	6 (2%)	59	78
20	G	196/209 (94%)	194 (99%)	2 (1%)	76	86
21	H	172/190 (90%)	172 (100%)	0	100	100
21	h	164/190 (86%)	164 (100%)	0	100	100
22	I	195/220 (89%)	193 (99%)	2 (1%)	76	86
22	i	193/220 (88%)	192 (100%)	1 (0%)	88	93
23	J	161/210 (77%)	159 (99%)	2 (1%)	71	83
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%)	88	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%)	88	93
26	m	192/211 (91%)	191 (100%)	1 (0%)	88	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%)	86	91
29	p	172/173 (99%)	171 (99%)	1 (1%)	86	91
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%)	86	91
32	s	174/198 (88%)	173 (99%)	1 (1%)	86	91
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
34	g	193/205 (94%)	193 (100%)	0	100	100
All	All	11226/12578 (89%)	11093 (99%)	133 (1%)	72	83

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	46	GLU
1	U	55	ARG
1	U	118	LEU
1	U	194	ARG
1	U	629	THR
1	U	819	VAL
1	U	838	LYS
1	U	840	LYS
1	U	883	ARG
2	V	194	LYS
2	V	345	ARG
2	V	401	ASN
2	V	470	ARG
2	V	494	MET
3	W	39	ARG
3	W	55	ARG
3	W	89	LEU
3	W	92	LYS
3	W	135	LYS
3	W	174	TYR
3	W	177	MET
3	W	179	LYS
3	W	191	ARG
3	W	236	HIS
3	W	237	GLU
3	W	419	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	W	422	ASN
3	W	451	MET
4	X	198	ASN
4	X	314	ARG
4	X	329	ASN
5	Y	48	ASN
5	Y	77	ASN
5	Y	176	ARG
5	Y	237	ARG
6	Z	33	LYS
6	Z	51	SER
6	Z	217	THR
6	Z	236	LEU
6	Z	247	LYS
7	a	227	ASN
7	a	230	ARG
7	a	289	ARG
7	a	339	ARG
9	c	49	VAL
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
9	c	284	LEU
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	657	ILE
12	f	662	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	43	ARG
13	A	304	ASN
13	A	314	ASN
13	A	360	ARG
13	A	369	ARG
13	A	403	ILE
13	A	422	LYS
14	B	35	LYS
14	B	125	THR
14	B	164	MET
14	B	190	LEU
14	B	292	THR
14	B	429	LYS
15	C	78	ARG
15	C	91	PRO
15	C	142	LYS
15	C	184	LYS
15	C	210	THR
15	C	219	LEU
15	C	248	MET
15	C	287	LYS
15	C	307	ARG
16	D	115	ILE
16	D	148	ASP
16	D	151	ILE
16	D	152	MET
16	D	153	MET
16	D	163	MET
16	D	229	ARG
16	D	273	LYS
16	D	323	ARG
16	D	409	LYS
17	E	1	MET
17	E	5	ARG
17	E	25	ARG
17	E	87	LEU
17	E	122	MET
17	E	138	LEU

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Mol	Chain	Res	Type
17	E	262	ASN
17	E	284	THR
17	E	339	ASN
18	F	46	ARG
18	F	245	LYS
18	F	250	LYS
18	F	293	THR
18	F	416	THR
18	F	432	LYS
20	G	11	ARG
20	G	21	ARG
22	I	166	ASN
22	I	167	ASN
23	J	28	LYS
23	J	163	ARG
26	M	40	ARG
29	P	93	ASN
32	S	1	ARG
22	i	17	ARG
24	k	119	LEU
26	m	40	ARG
29	p	93	ASN
32	s	1	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	18	GLN
1	U	89	ASN
1	U	189	GLN
1	U	207	ASN
1	U	218	GLN
1	U	366	HIS
1	U	377	HIS
1	U	421	GLN
1	U	541	HIS
1	U	596	ASN
1	U	632	GLN
1	U	665	ASN
1	U	768	GLN
1	U	888	GLN
2	V	62	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	V	177	ASN
2	V	214	HIS
2	V	257	ASN
2	V	473	GLN
3	W	84	ASN
3	W	228	ASN
3	W	257	GLN
3	W	362	ASN
4	X	62	GLN
4	X	198	ASN
4	X	329	ASN
5	Y	48	ASN
5	Y	71	ASN
5	Y	77	ASN
5	Y	136	HIS
6	Z	12	HIS
6	Z	229	GLN
6	Z	278	ASN
7	a	86	GLN
7	a	143	ASN
7	a	152	HIS
7	a	227	ASN
7	a	332	HIS
7	a	370	GLN
8	b	76	HIS
8	b	137	ASN
9	c	92	GLN
9	c	128	ASN
9	c	130	GLN
9	c	149	GLN
9	c	185	ASN
9	c	197	ASN
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
10	d	116	HIS
10	d	245	GLN
11	e	63	HIS
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	291	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
12	f	614	HIS
12	f	737	ASN
12	f	752	HIS
12	f	786	GLN
12	f	815	HIS
13	A	38	GLN
13	A	60	ASN
13	A	314	ASN
13	A	358	HIS
13	A	414	ASN
14	B	57	GLN
14	B	195	GLN
14	B	332	ASN
15	C	36	ASN
15	C	53	ASN
15	C	205	HIS
15	C	278	ASN
15	C	377	HIS
15	C	380	GLN
16	D	67	ASN
16	D	173	GLN
16	D	237	GLN
16	D	257	ASN
16	D	302	ASN
16	D	414	HIS
17	E	194	ASN
17	E	225	HIS
17	E	226	GLN
17	E	262	ASN
17	E	300	HIS
17	E	339	ASN
18	F	207	ASN
18	F	333	ASN
20	G	123	GLN
21	H	119	GLN

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Mol	Chain	Res	Type
22	I	119	GLN
22	I	146	GLN
22	I	166	ASN
22	I	167	ASN
24	K	155	HIS
24	K	214	ASN
28	O	172	ASN
31	R	38	ASN
22	i	119	GLN
22	i	167	ASN
23	j	116	GLN
24	k	23	GLN
24	k	155	HIS
24	k	214	ASN
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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 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	D	440	37	26,33,33	0.93	1 (3%)	31,52,52	1.82	5 (16%)
36	ATP	B	441	37	26,33,33	0.93	1 (3%)	31,52,52	1.70	5 (16%)
36	ATP	A	434	37	26,33,33	0.90	1 (3%)	31,52,52	1.73	7 (22%)
36	ATP	C	407	37	26,33,33	0.88	1 (3%)	31,52,52	1.77	7 (22%)
38	ADP	E	419	-	24,29,29	0.95	1 (4%)	29,45,45	1.60	4 (13%)

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	D	440	37	-	0/18/38/38	0/3/3/3
36	ATP	B	441	37	-	3/18/38/38	0/3/3/3
36	ATP	A	434	37	-	1/18/38/38	0/3/3/3
36	ATP	C	407	37	-	0/18/38/38	0/3/3/3
38	ADP	E	419	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	434	ATP	C5-C4	2.34	1.47	1.40
36	D	440	ATP	C5-C4	2.29	1.47	1.40
38	E	419	ADP	C5-C4	2.26	1.46	1.40
36	B	441	ATP	C5-C4	2.16	1.46	1.40
36	C	407	ATP	C5-C4	2.13	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	407	ATP	PA-O3A-PB	-5.57	113.70	132.83
36	D	440	ATP	PB-O3B-PG	-4.85	116.17	132.83
36	B	441	ATP	PA-O3A-PB	-4.80	116.34	132.83
36	D	440	ATP	PA-O3A-PB	-4.70	116.71	132.83
38	E	419	ADP	PA-O3A-PB	-4.53	117.29	132.83
36	C	407	ATP	C3'-C2'-C1'	3.96	106.94	100.98
36	D	440	ATP	C3'-C2'-C1'	3.94	106.90	100.98
36	A	434	ATP	PB-O3B-PG	-3.82	119.73	132.83
36	A	434	ATP	PA-O3A-PB	-3.81	119.75	132.83
36	A	434	ATP	C3'-C2'-C1'	3.76	106.64	100.98
36	B	441	ATP	C3'-C2'-C1'	3.69	106.53	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	441	ATP	PB-O3B-PG	-3.66	120.28	132.83
38	E	419	ADP	C3'-C2'-C1'	3.47	106.20	100.98
36	C	407	ATP	N3-C2-N1	-3.47	123.26	128.68
36	A	434	ATP	N3-C2-N1	-3.15	123.75	128.68
36	D	440	ATP	N3-C2-N1	-3.10	123.83	128.68
36	B	441	ATP	N3-C2-N1	-3.03	123.94	128.68
38	E	419	ADP	C4-C5-N7	-2.84	106.44	109.40
38	E	419	ADP	N3-C2-N1	-2.84	124.24	128.68
36	D	440	ATP	C4-C5-N7	-2.43	106.86	109.40
36	B	441	ATP	C4-C5-N7	-2.42	106.88	109.40
36	C	407	ATP	PB-O3B-PG	-2.24	125.15	132.83
36	A	434	ATP	C1'-N9-C4	2.18	130.47	126.64
36	C	407	ATP	O2B-PB-O1B	2.08	122.53	112.24
36	A	434	ATP	O3G-PG-O2G	2.05	115.47	107.64
36	C	407	ATP	C4-C5-N7	-2.04	107.28	109.40
36	C	407	ATP	C2-N1-C6	2.01	122.20	118.75
36	A	434	ATP	C4-C5-N7	-2.01	107.30	109.40

There are no chirality outliers.

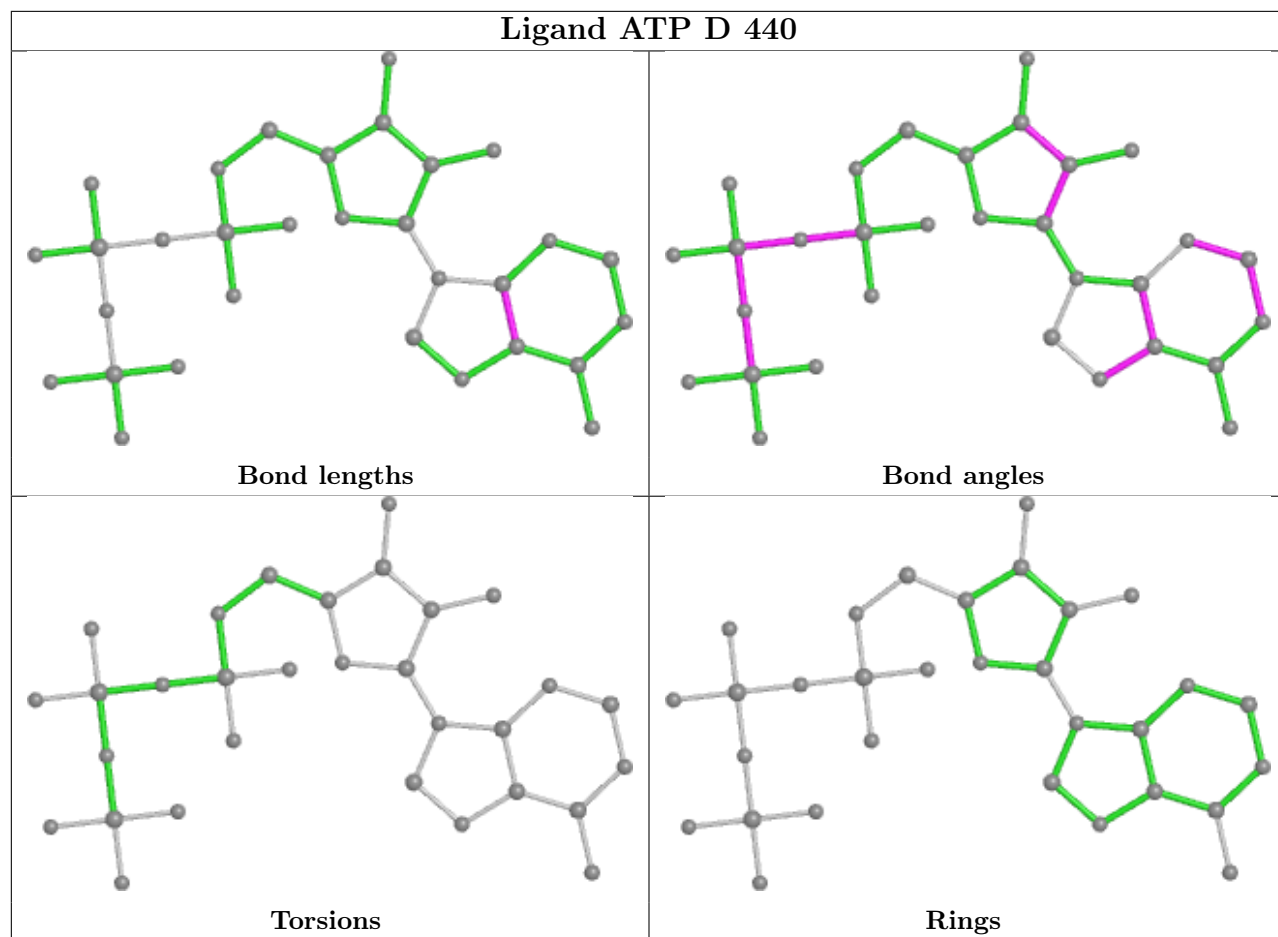
All (4) torsion outliers are listed below:

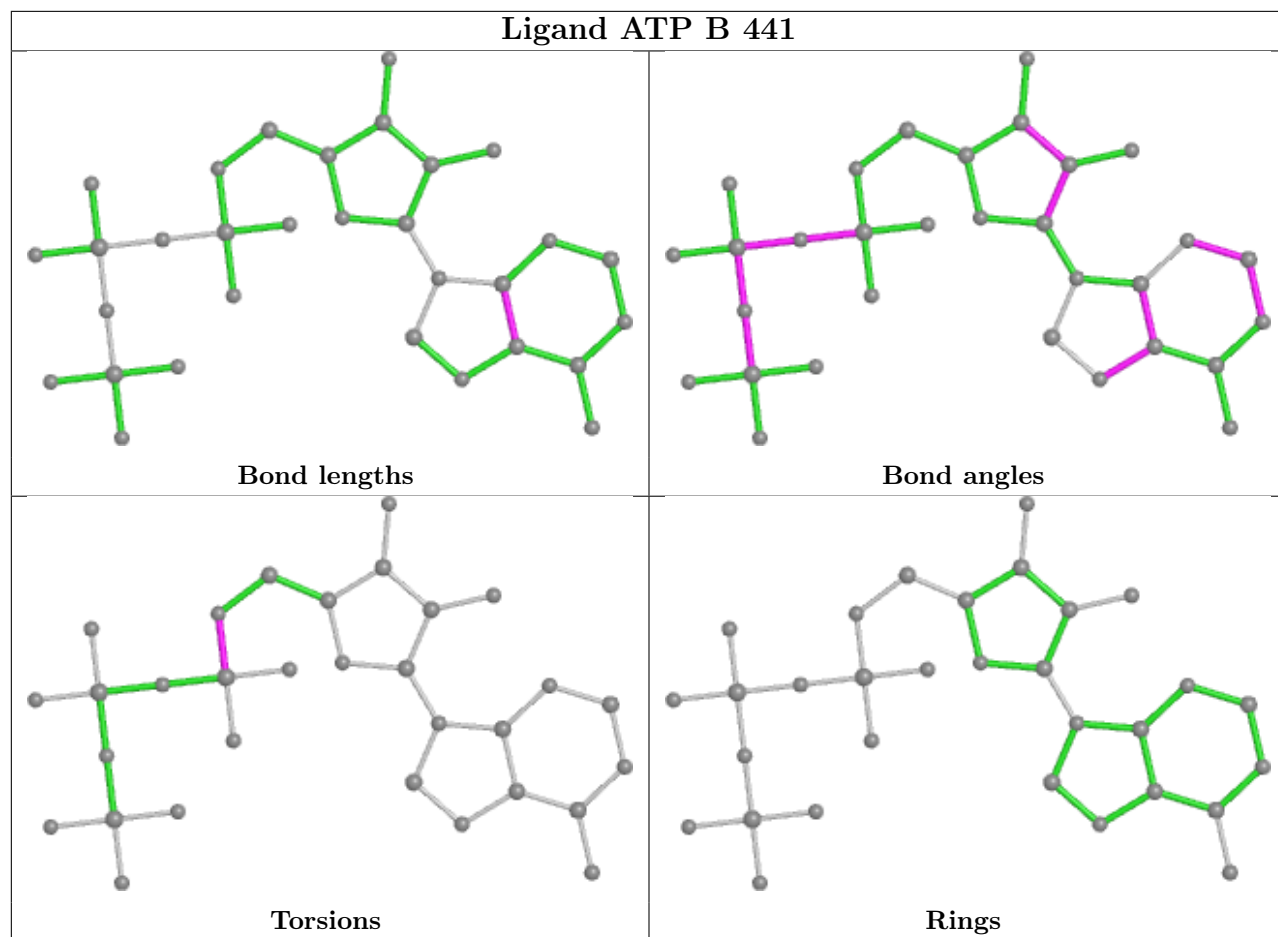
Mol	Chain	Res	Type	Atoms
36	B	441	ATP	C5'-O5'-PA-O1A
36	B	441	ATP	C5'-O5'-PA-O2A
36	A	434	ATP	C5'-O5'-PA-O3A
36	B	441	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

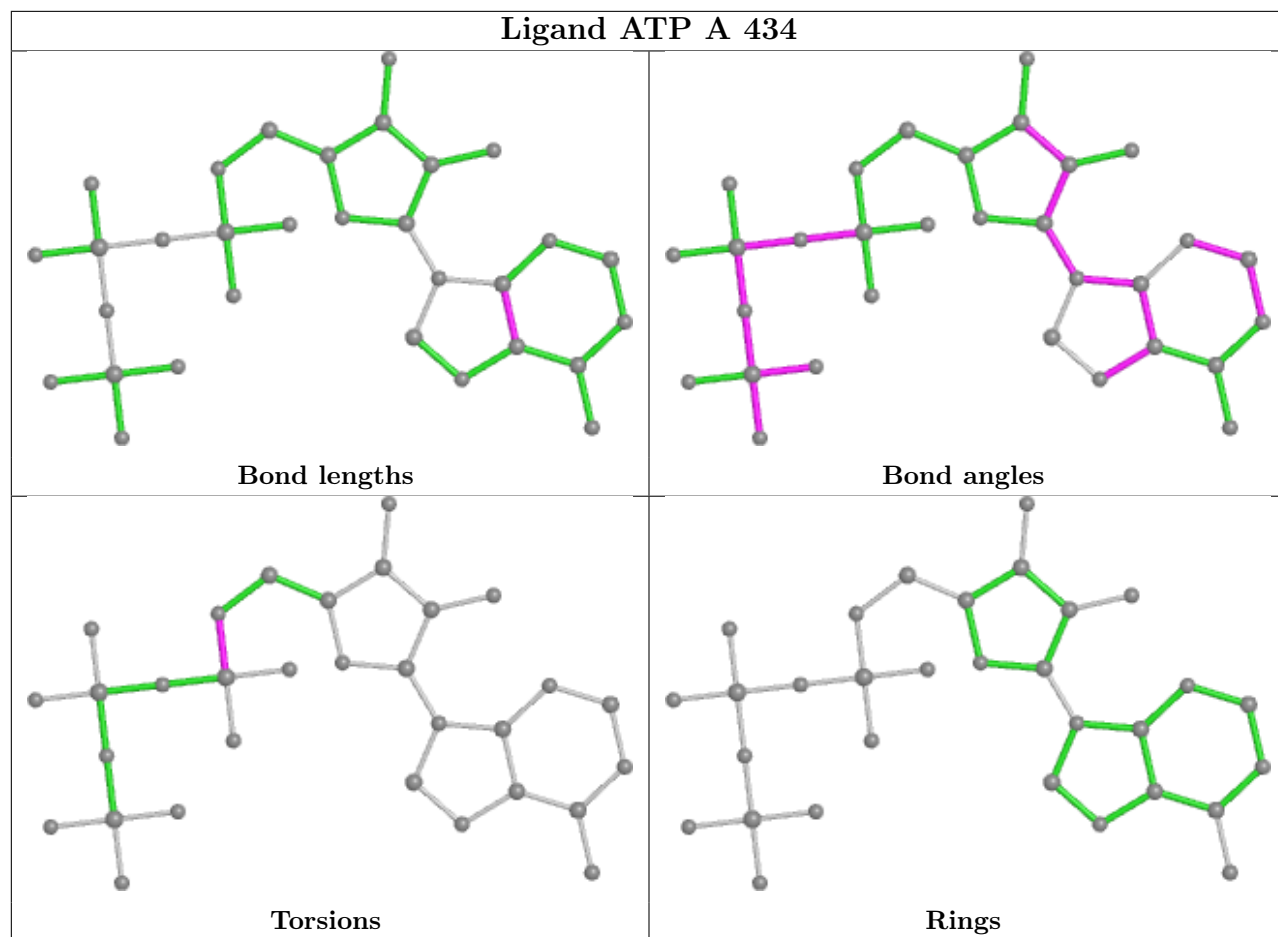
No monomer is involved in short contacts.

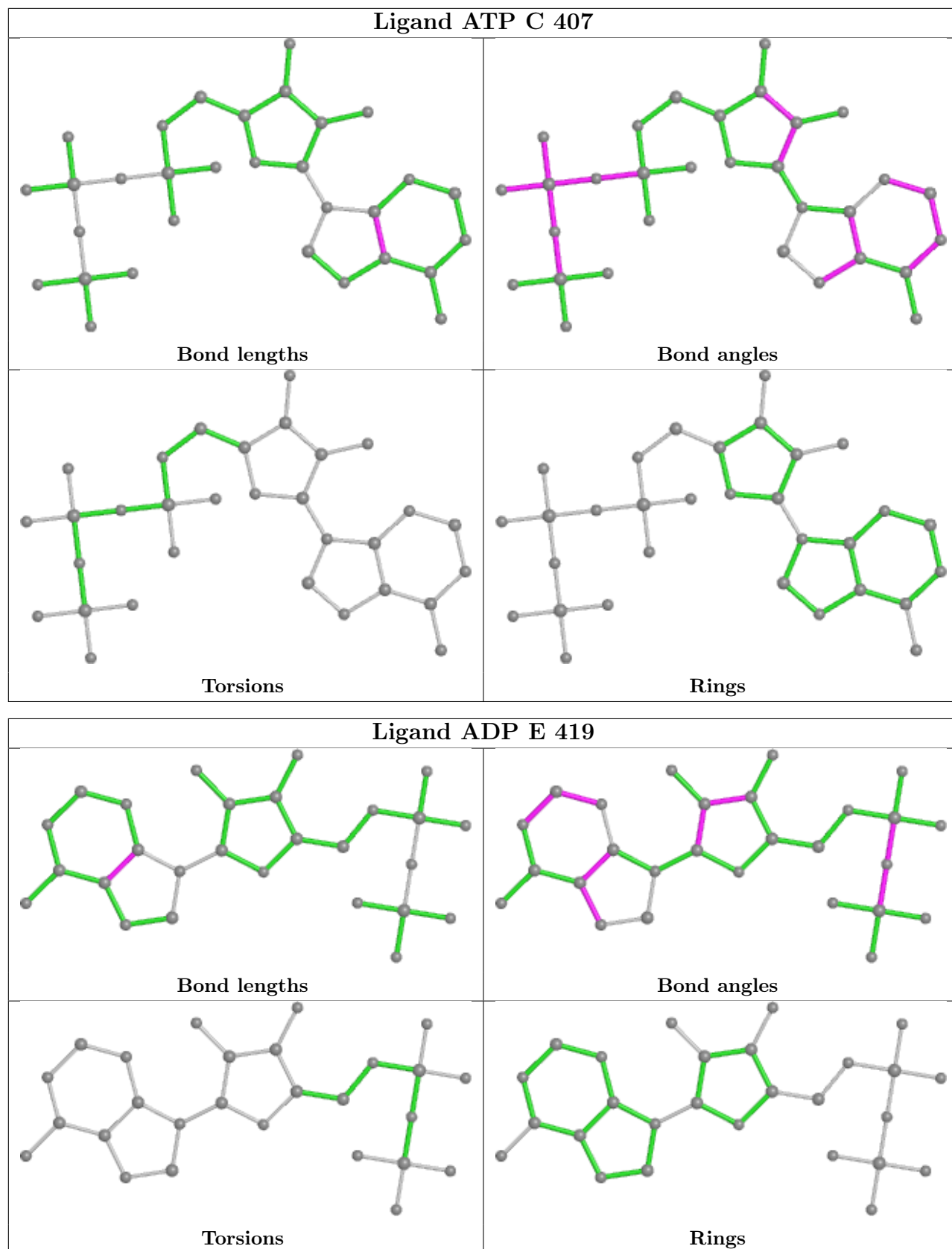
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

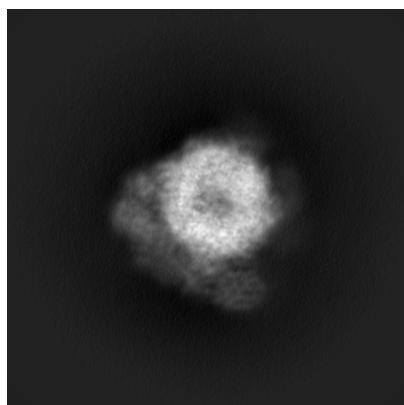
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9221. These allow visual inspection of the internal detail of the map and identification of artifacts.

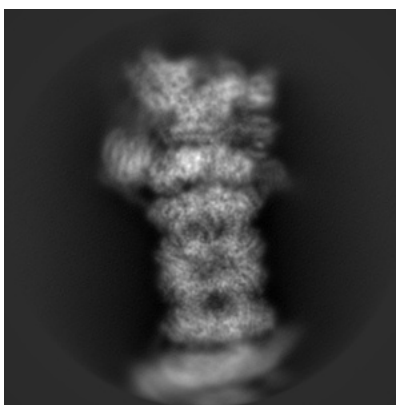
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

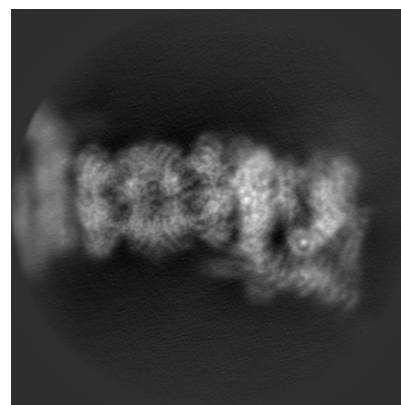
#### 6.1.1 Primary map



X



Y

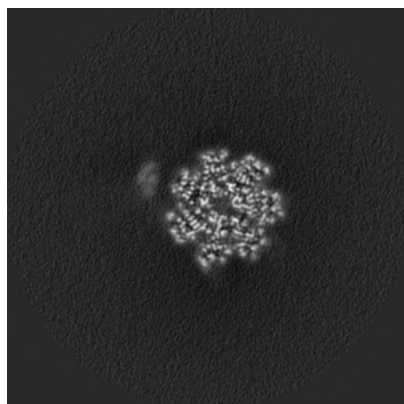


Z

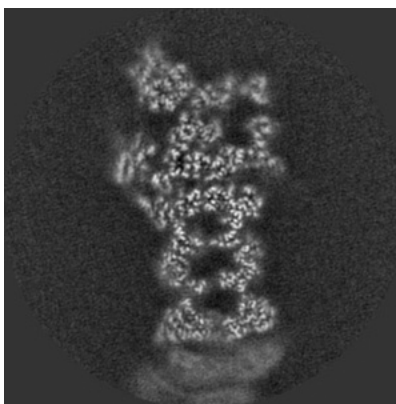
The images above show the map projected in three orthogonal directions.

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

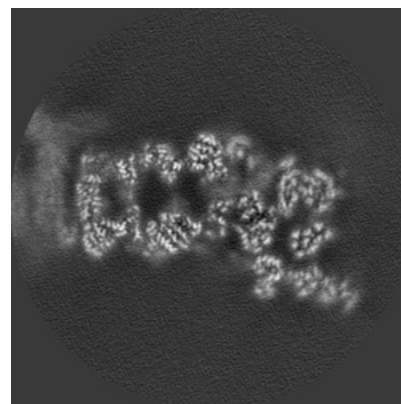
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

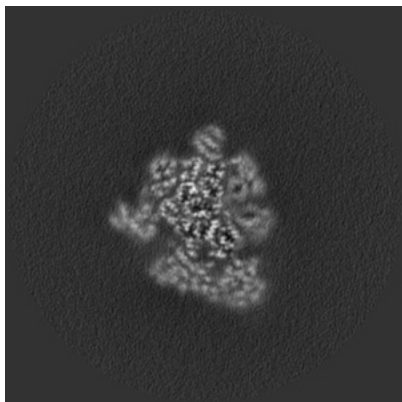


Z Index: 300

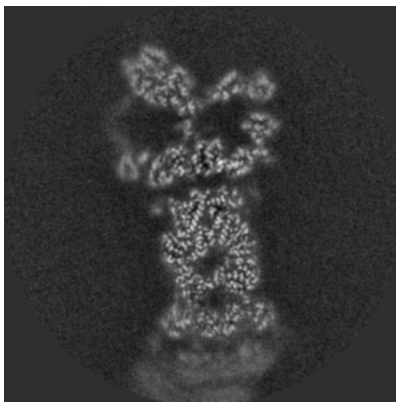
The images above show central slices of the map in three orthogonal directions.

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

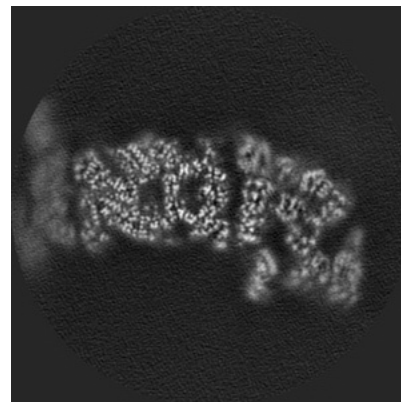
### 6.3.1 Primary map



X Index: 366



Y Index: 283

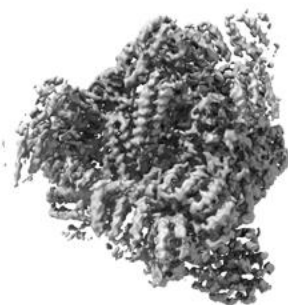


Z Index: 275

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

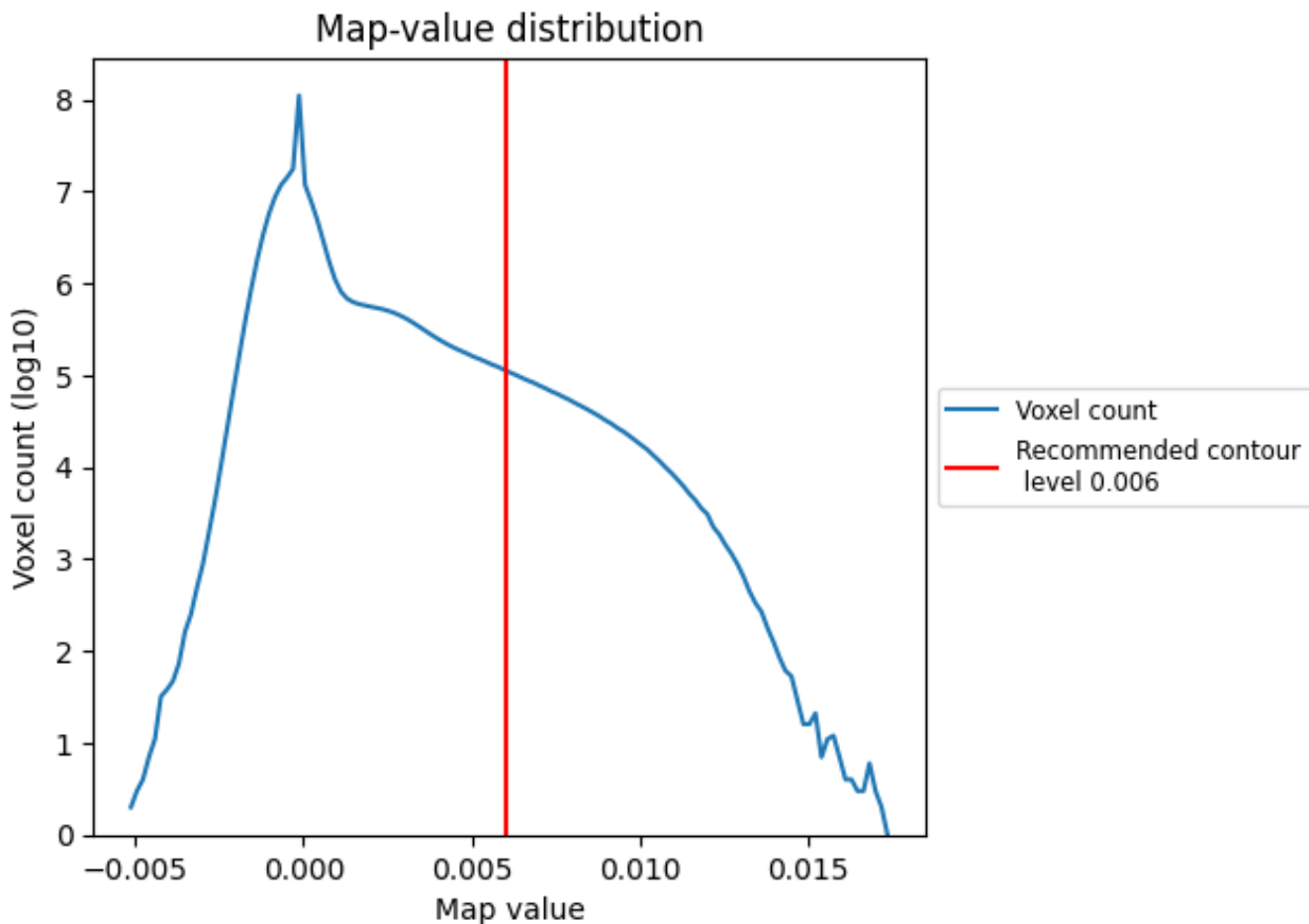
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

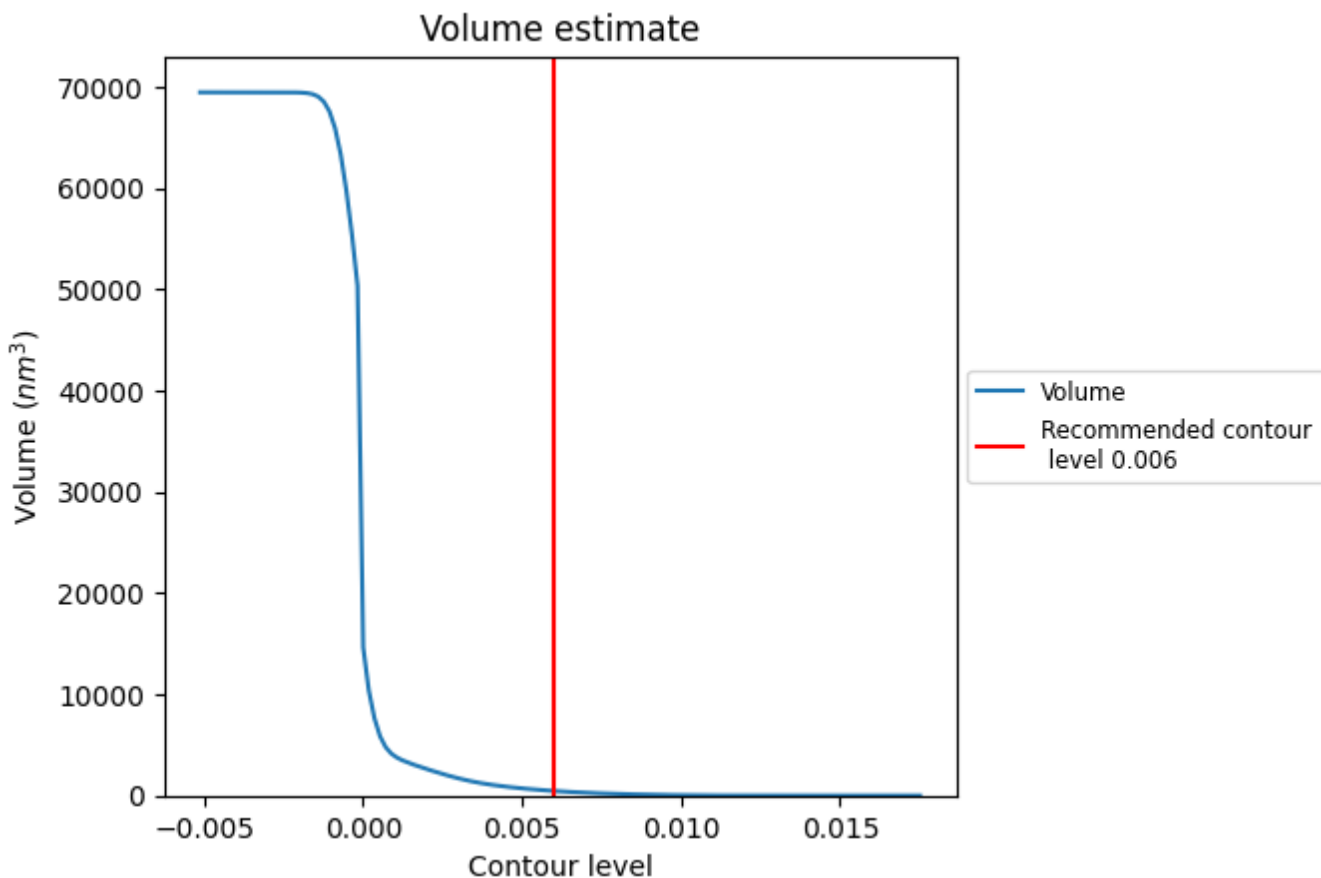
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

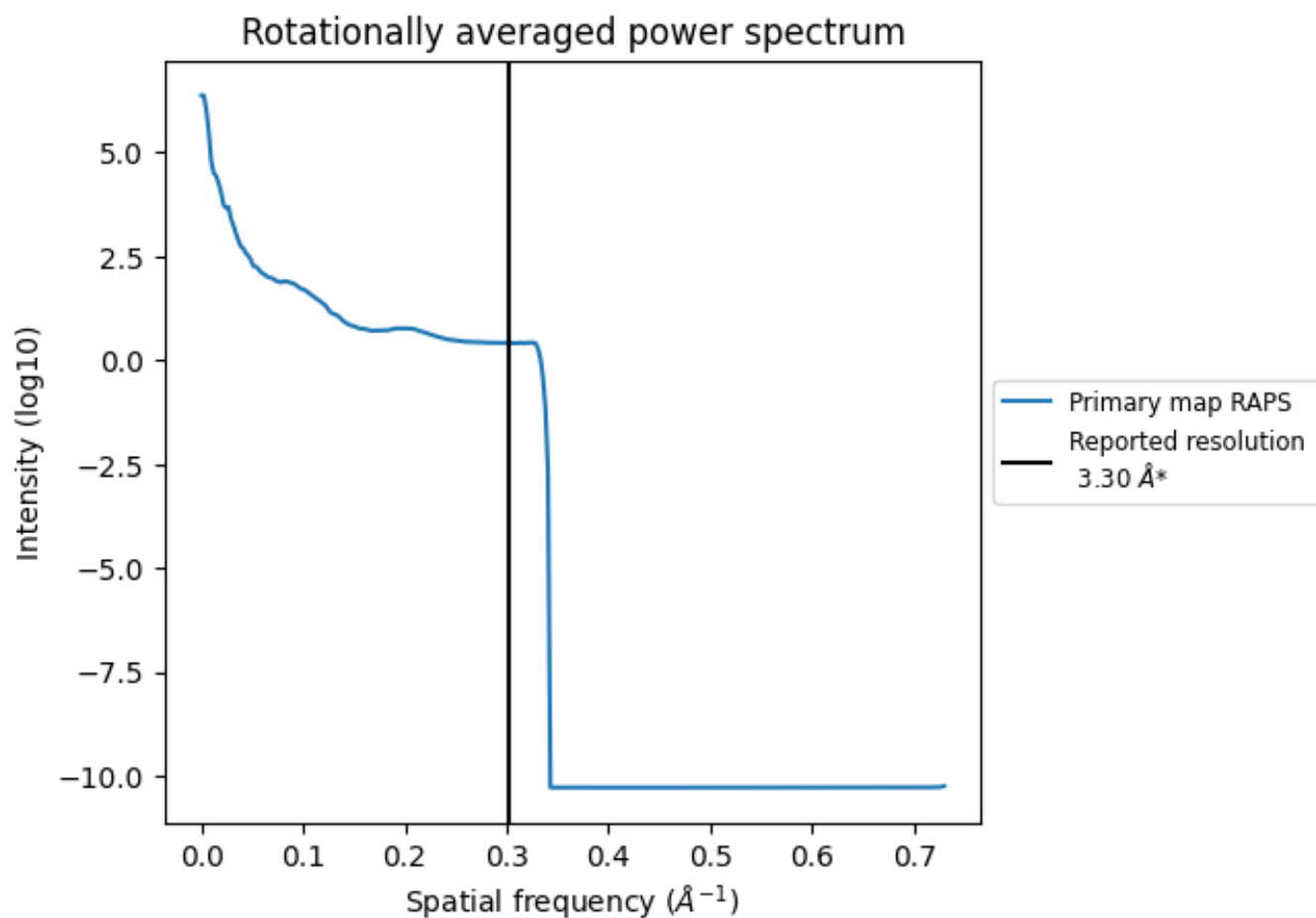


The volume at the recommended contour level is 456 nm<sup>3</sup>; this corresponds to an approximate mass of 412 kDa.

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



### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

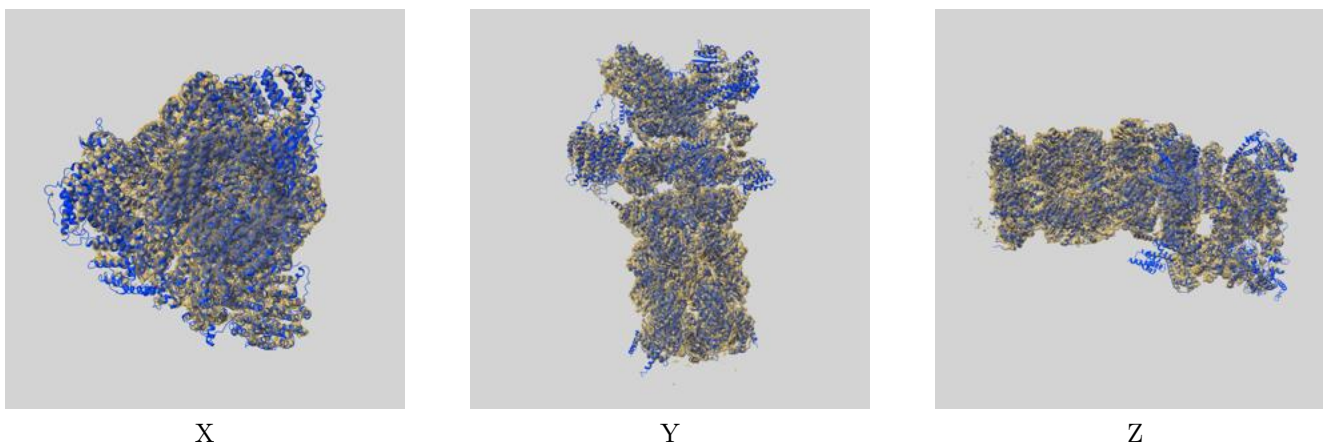
## 8 Fourier-Shell correlation

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

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

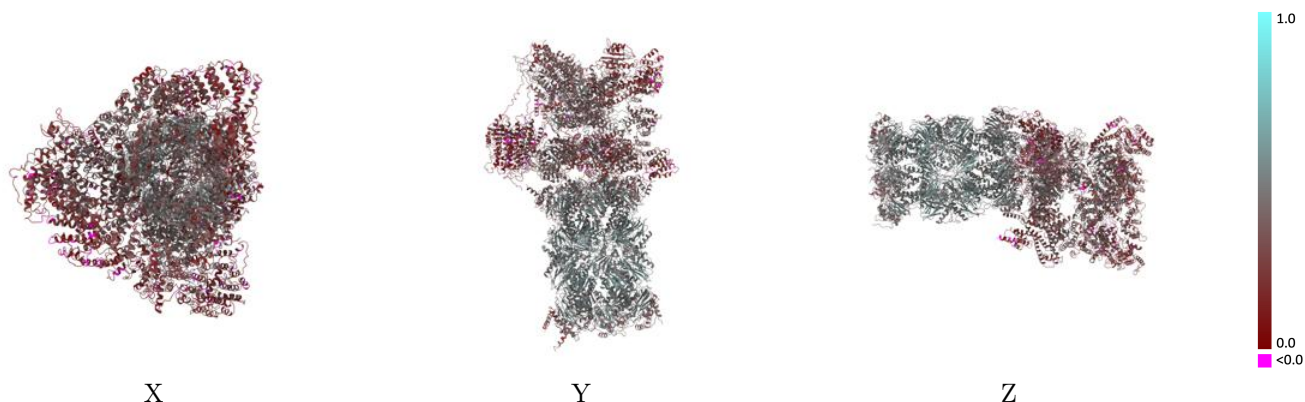
This section contains information regarding the fit between EMDB map EMD-9221 and PDB model 6MSJ. Per-residue inclusion information can be found in section 3 on page 13.

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



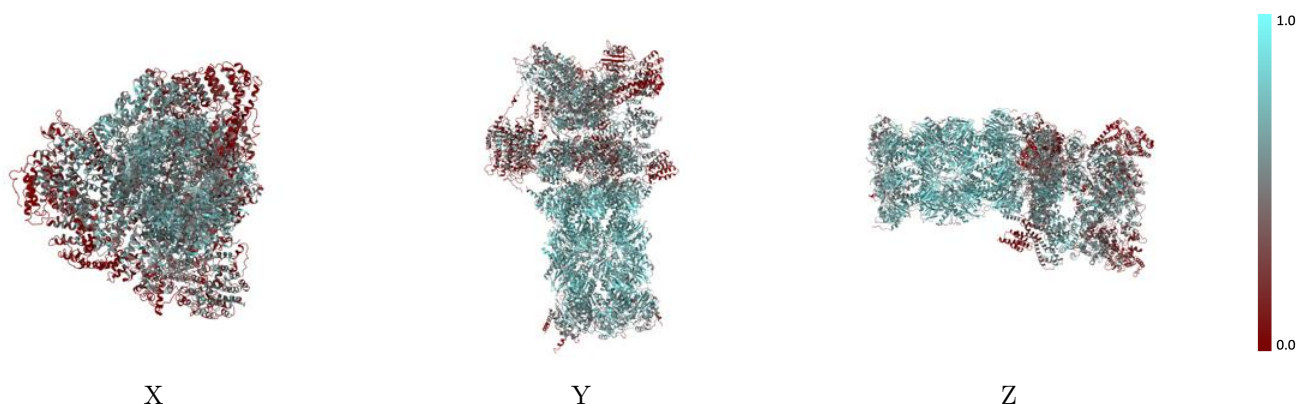
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



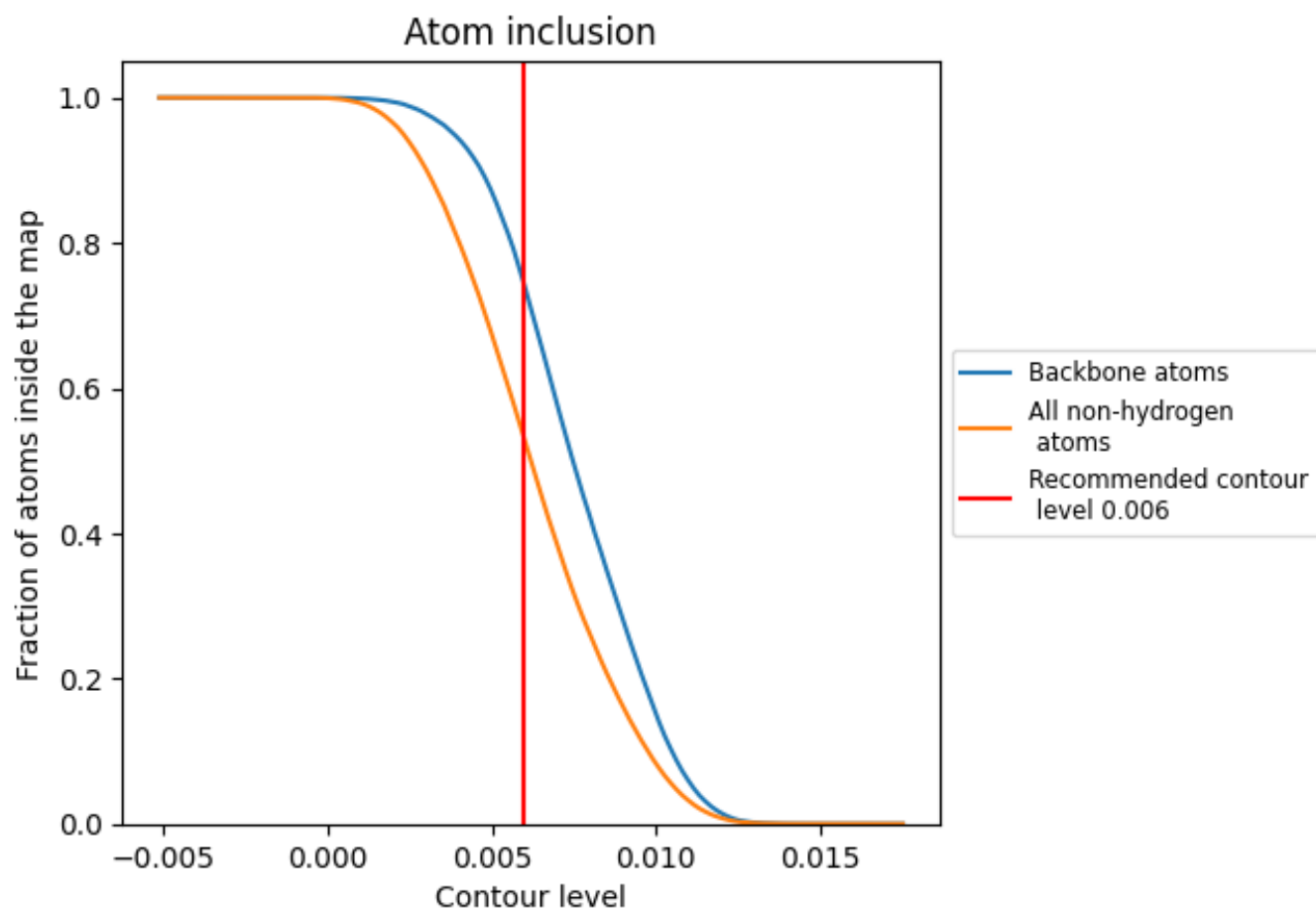
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 53% 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	 0.5284	 0.3730
A	 0.3999	 0.2830
B	 0.5099	 0.3550
C	 0.5818	 0.3780
D	 0.6021	 0.3820
E	 0.4995	 0.3530
F	 0.2689	 0.2310
G	 0.6955	 0.4450
H	 0.7428	 0.4760
I	 0.6768	 0.4390
J	 0.6700	 0.4350
K	 0.6764	 0.4420
L	 0.7205	 0.4670
M	 0.6962	 0.4400
N	 0.7682	 0.5000
O	 0.7354	 0.4940
P	 0.7458	 0.5090
Q	 0.7388	 0.4910
R	 0.7637	 0.5110
S	 0.6978	 0.5000
T	 0.7535	 0.5010
U	 0.4372	 0.3230
V	 0.3018	 0.2280
W	 0.3972	 0.2770
X	 0.3799	 0.2970
Y	 0.5612	 0.3080
Z	 0.4495	 0.3320
a	 0.3635	 0.2620
b	 0.2103	 0.2630
c	 0.4928	 0.3490
d	 0.1700	 0.2210
e	 0.3273	 0.2450
f	 0.2594	 0.2020
g	 0.5896	 0.4550
h	 0.5918	 0.4570



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Chain	Atom inclusion	Q-score
i	 0.5395	 0.4240
j	 0.5114	 0.4090
k	 0.5498	 0.4340
l	 0.6425	 0.4670
m	 0.6186	 0.4380
n	 0.7432	 0.5100
o	 0.6735	 0.4930
p	 0.7182	 0.5160
q	 0.7179	 0.5030
r	 0.7463	 0.5130
s	 0.7171	 0.5090
t	 0.7523	 0.5110
v	 0.1722	 0.2710