



# wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 06:50 PM EDT

PDB ID : 6MSH  
EMDB ID : EMD-9220  
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome  
Authors : Mao, Y.D.  
Deposited on : 2018-10-16  
Resolution : 3.60 Å(reported)

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

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

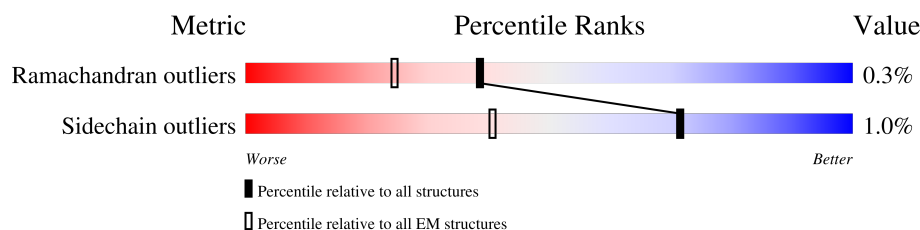
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	U	953	<div> <div>64%</div> <div>85%</div> <div>14%</div> </div>
2	V	533	<div> <div>75%</div> <div>89%</div> <div>10%</div> </div>
3	W	456	<div> <div>71%</div> <div>97%</div> <div>.</div> </div>
4	X	422	<div> <div>17%</div> <div>90%</div> <div>10%</div> </div>
5	Y	389	<div> <div>27%</div> <div>96%</div> <div>..</div> </div>
6	Z	324	<div> <div>67%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
7	a	376	<div> <div>82%</div> <div>98%</div> <div>..</div> </div>
8	b	377	<div> <div>50%</div> <div>51%</div> <div>49%</div> </div>
9	c	309	<div> <div>61%</div> <div>90%</div> <div>7%</div> </div>

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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	22	
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 36 unique types of molecules in this entry. The entry contains 103729 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	820	Total	C	N	O	S	0	0
			6398	4062	1086	1206	44		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	886	Total	C	N	O	S	0	0
			6840	4300	1171	1324	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	356	Total	C	N	O	S	0	0
			2767	1741	488	521	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

- 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	22	Total	C	N	O	0	0
			110	66	22	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	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	232	Total	C	N	O	S	0	0
			1708	1081	289	333	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	250	Total	C	N	O	S	0	0
			1912	1204	329	371	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
			1722	1080	284	348	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		

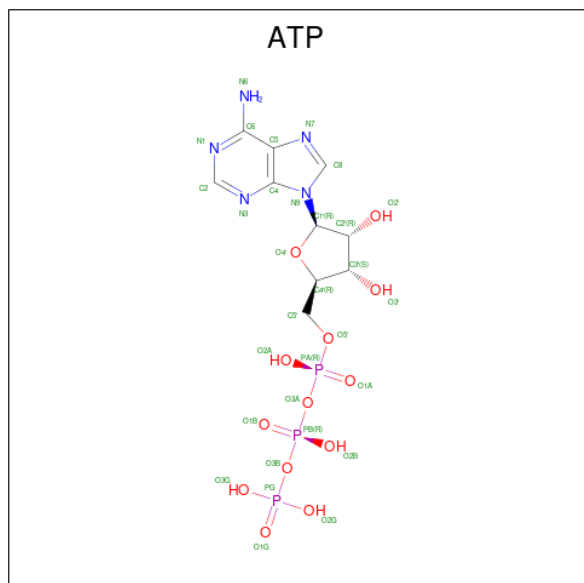
- Molecule 33 is a protein called Proteasome subunit beta type-4.

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:  $C_{10}H_{16}N_5O_{13}P_3$ ).



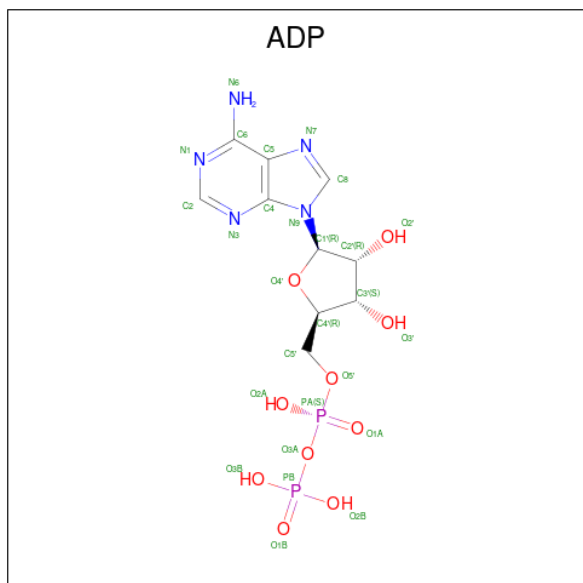
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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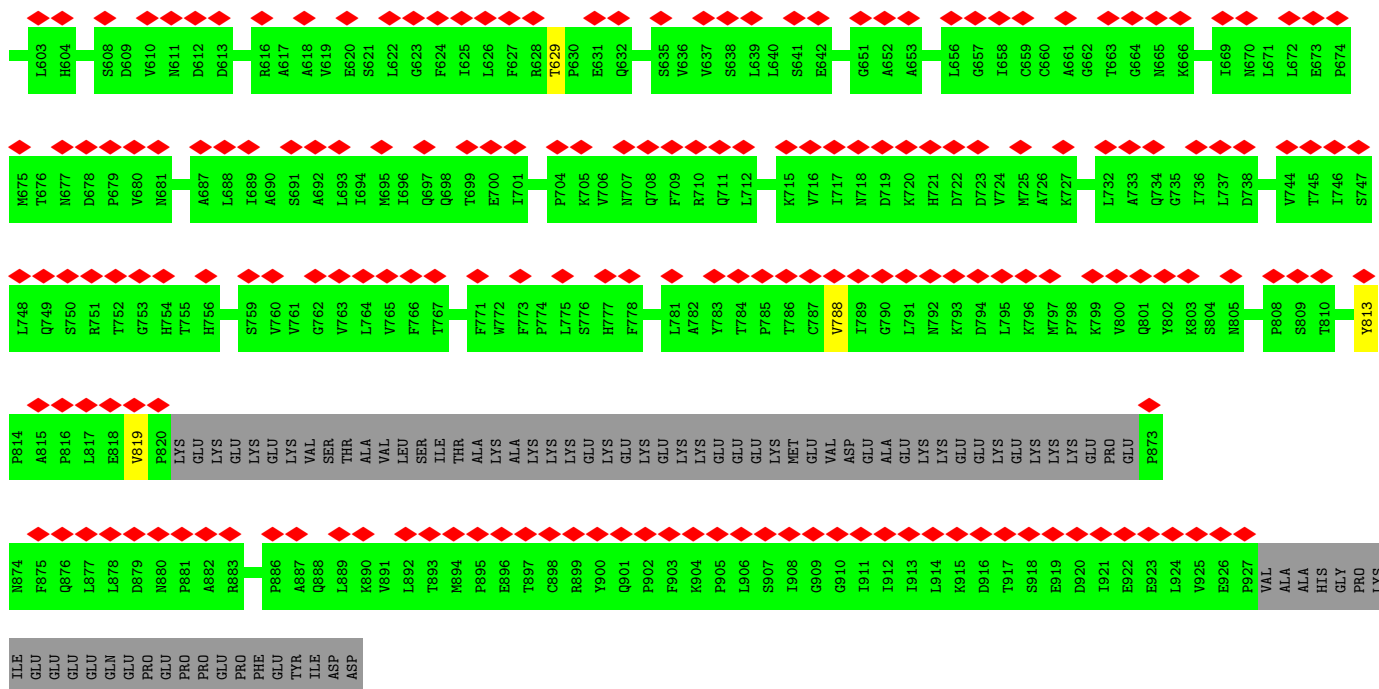
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Mol	Chain	Residues	Atoms					AltConf
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

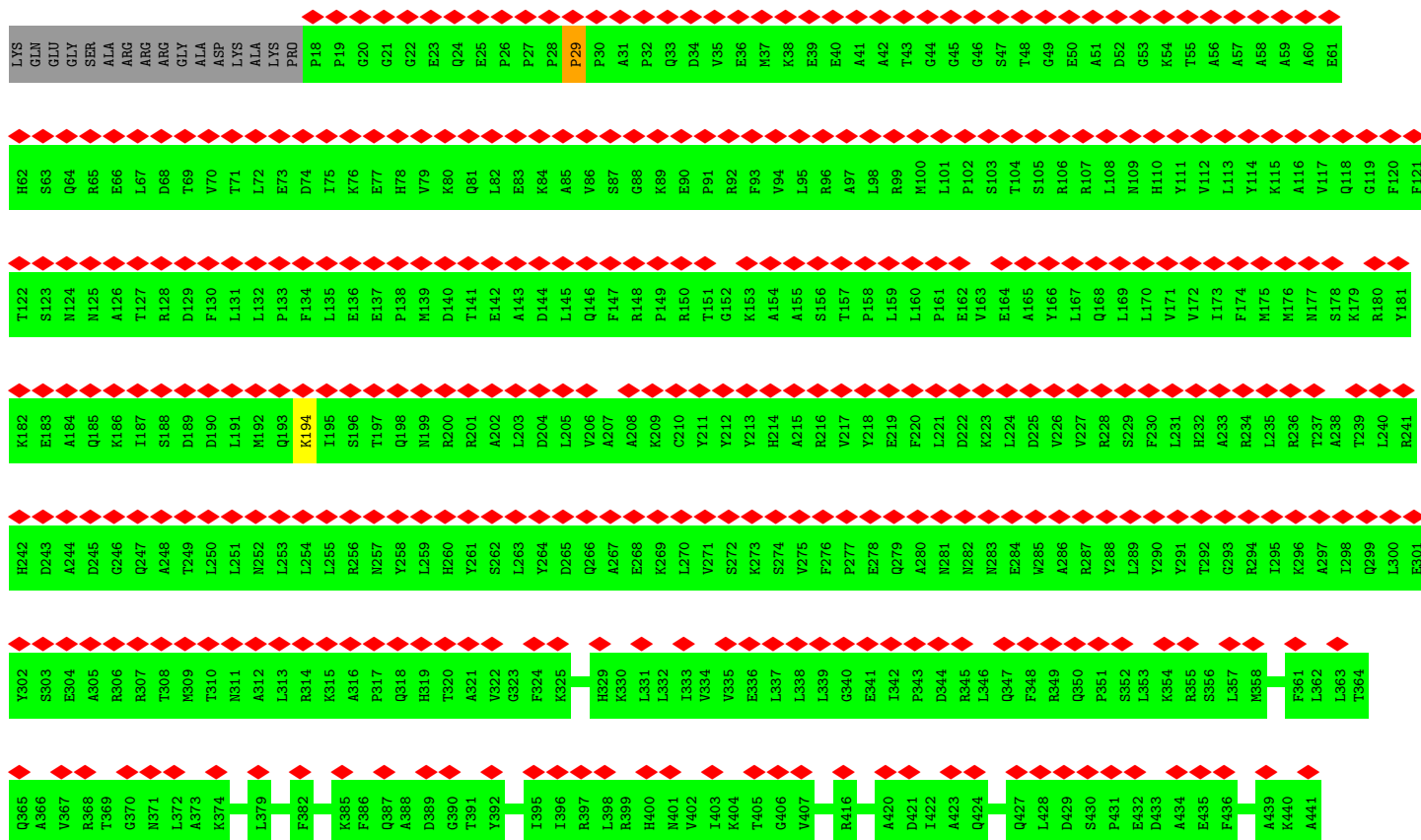
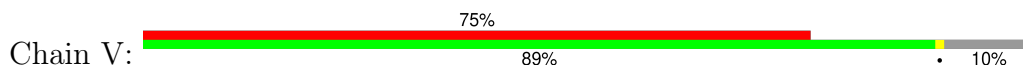
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

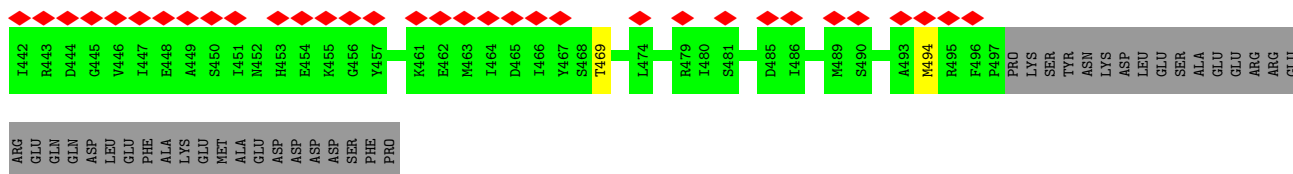




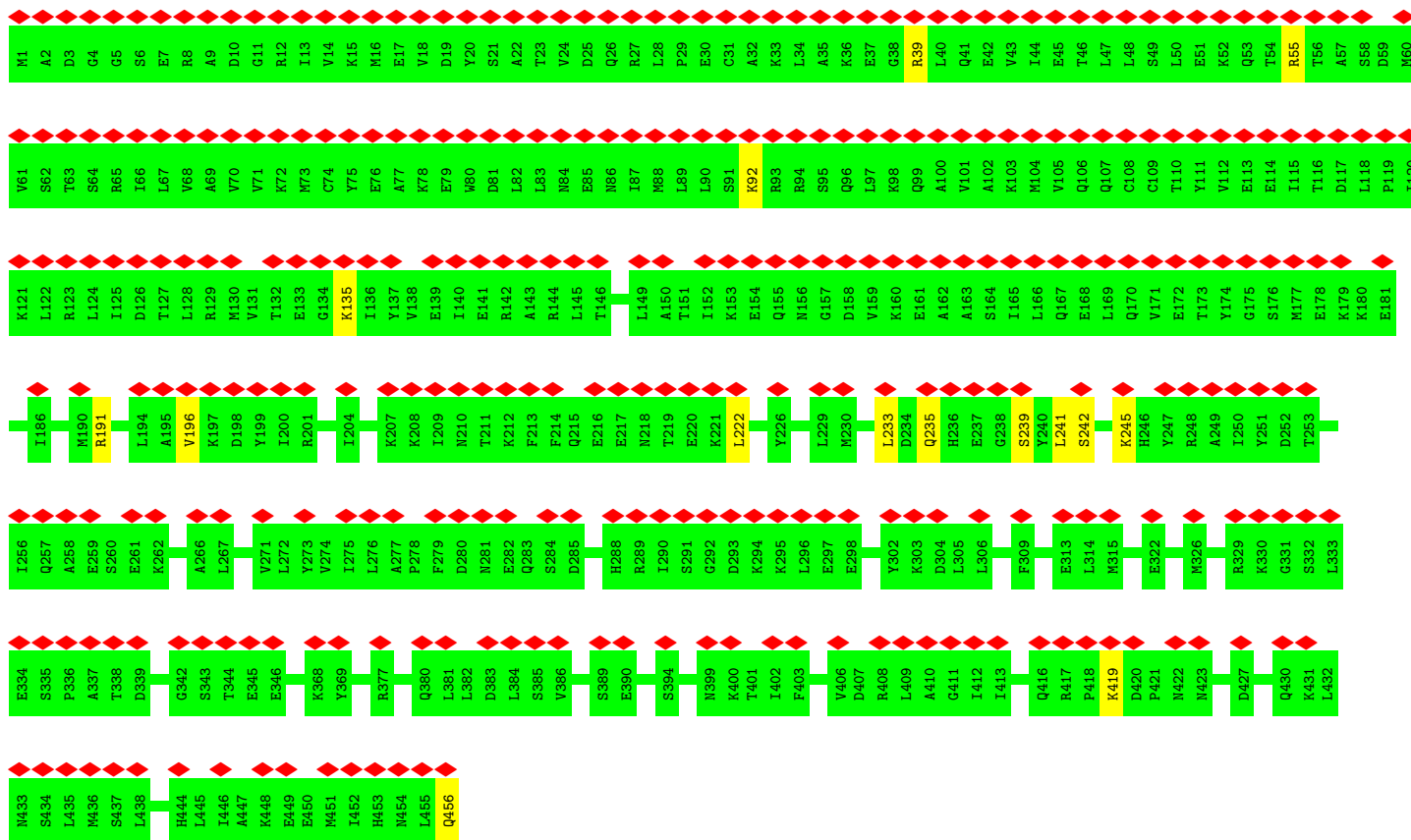


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

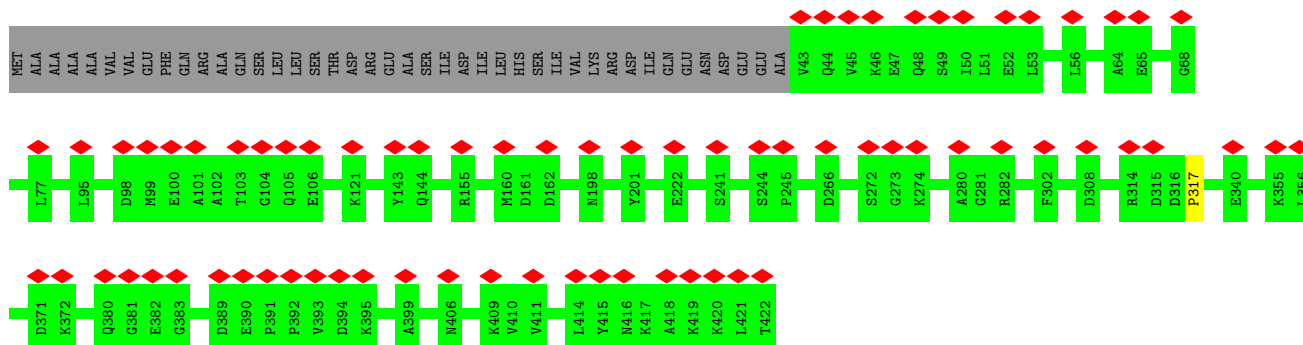
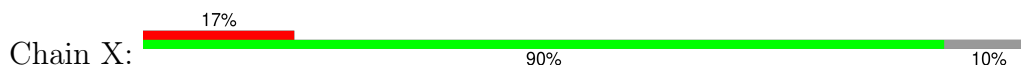




• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

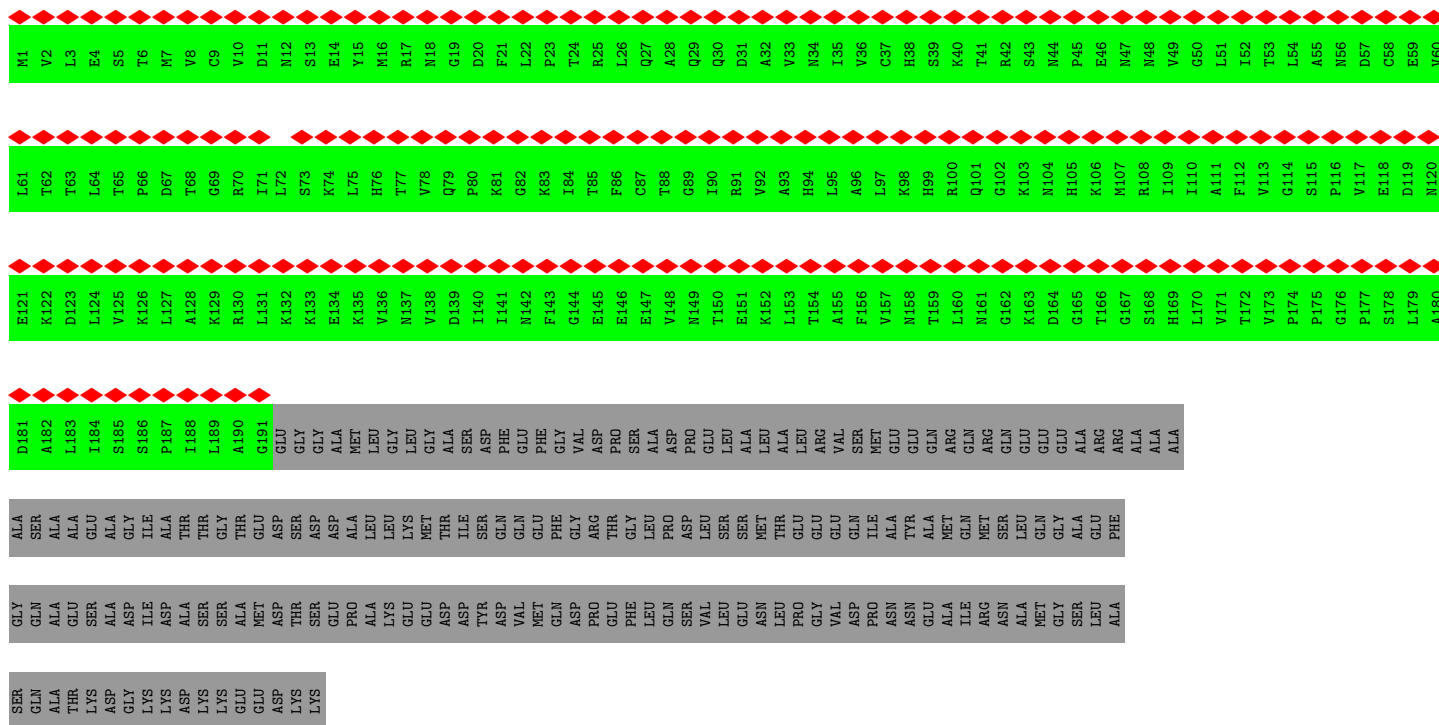


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

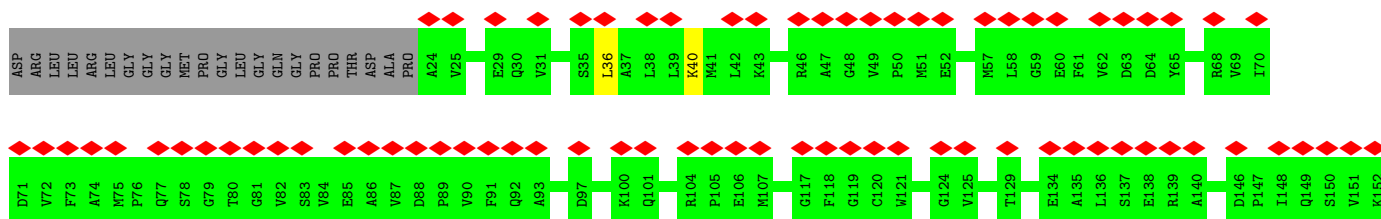
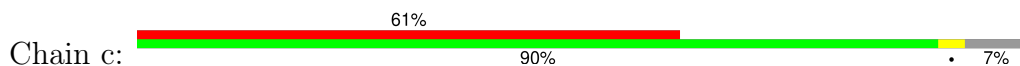


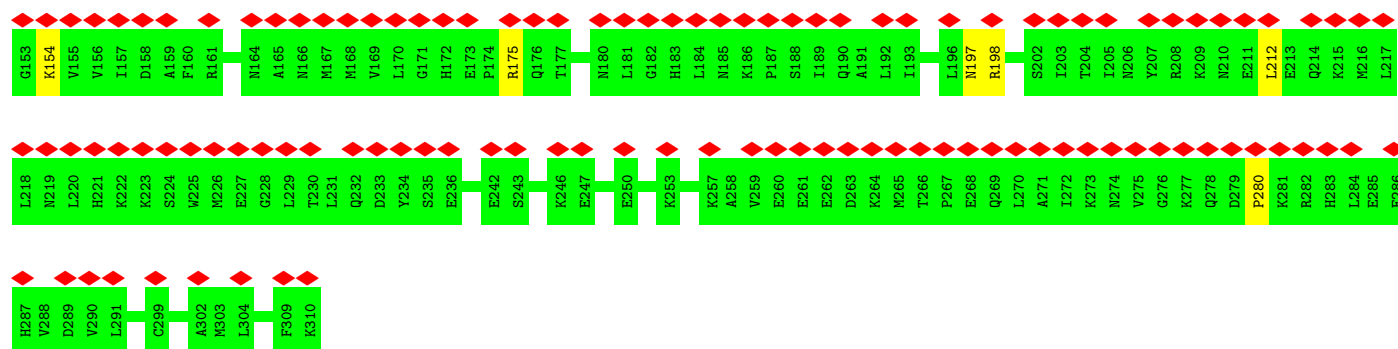


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



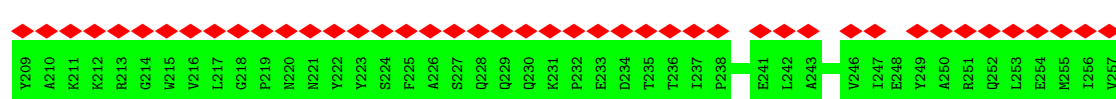
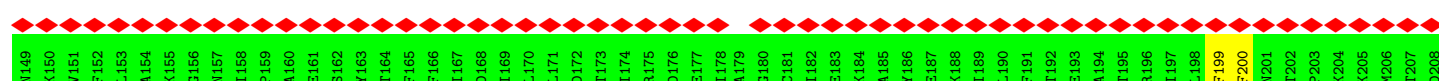
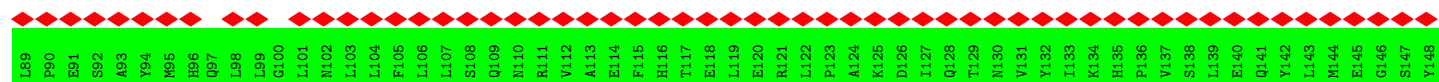
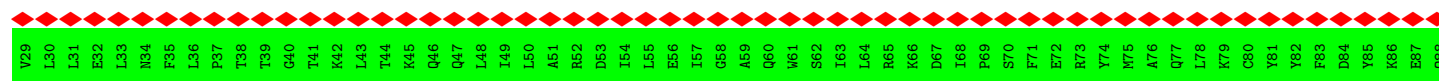
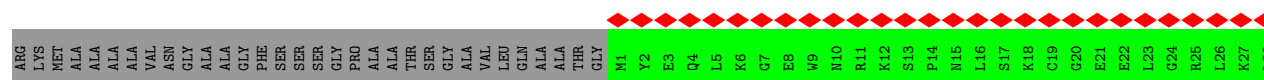
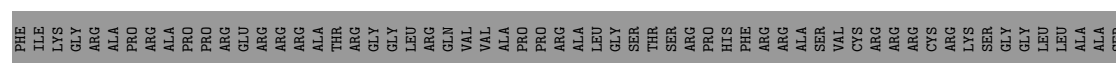
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14





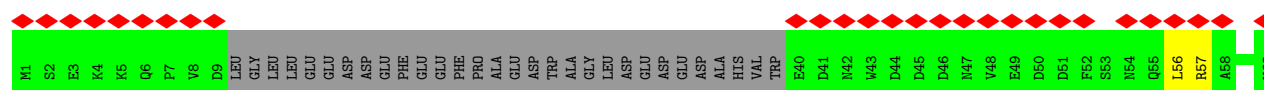
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 71%  
73% 26%



- Molecule 11: 26S proteasome complex subunit SEM1

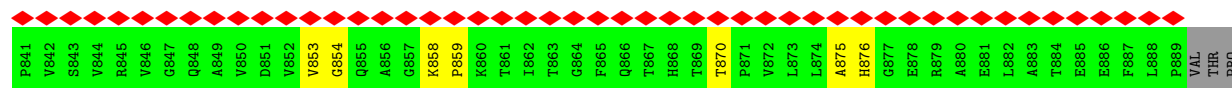
Chain e: 40%  
54% 43%



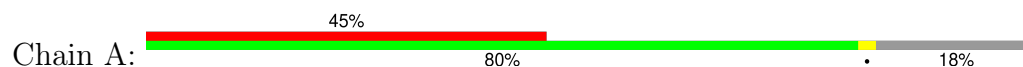
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 99%  
94%

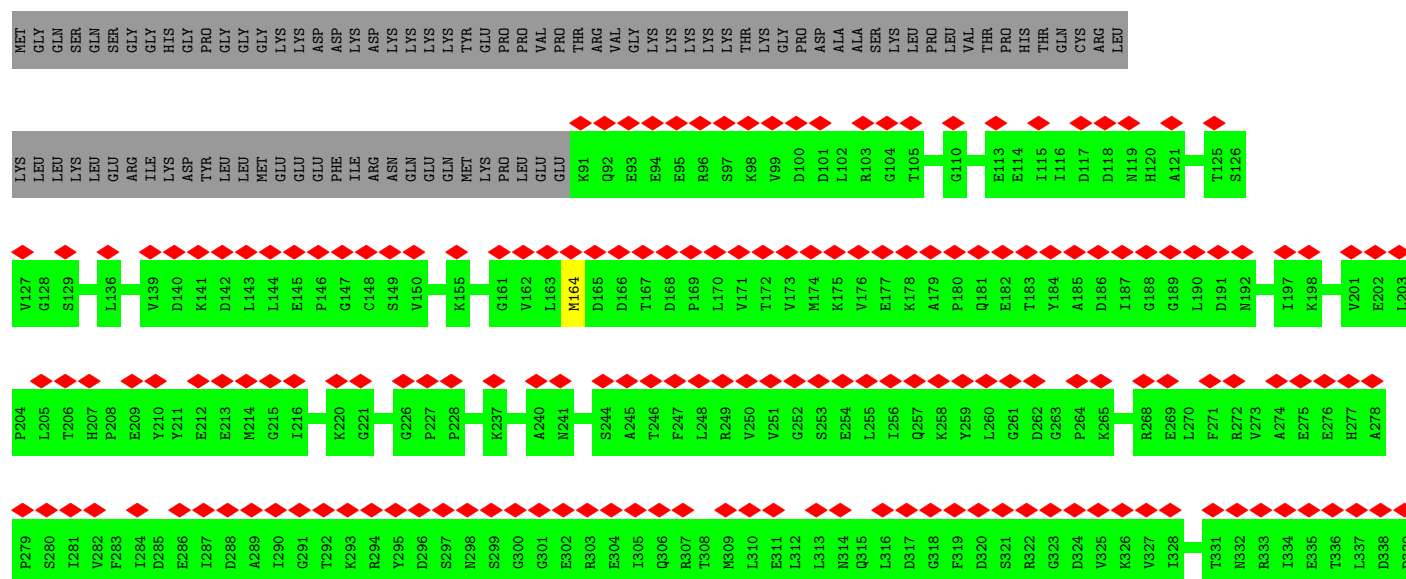
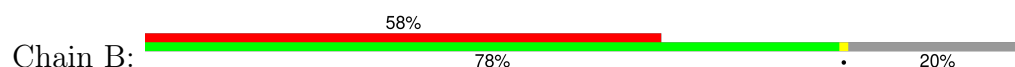


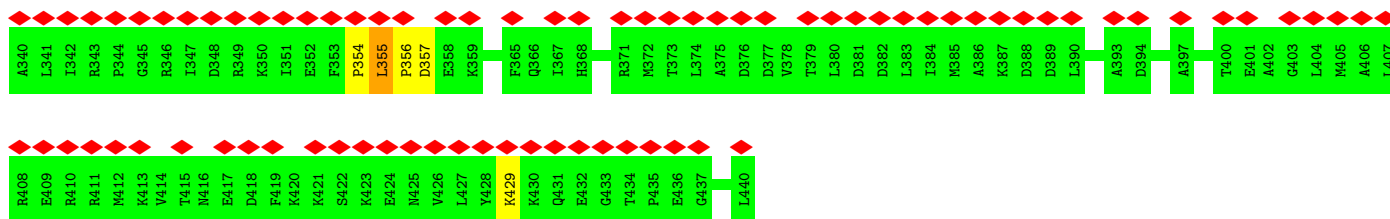


• Molecule 13: 26S proteasome regulatory subunit 7

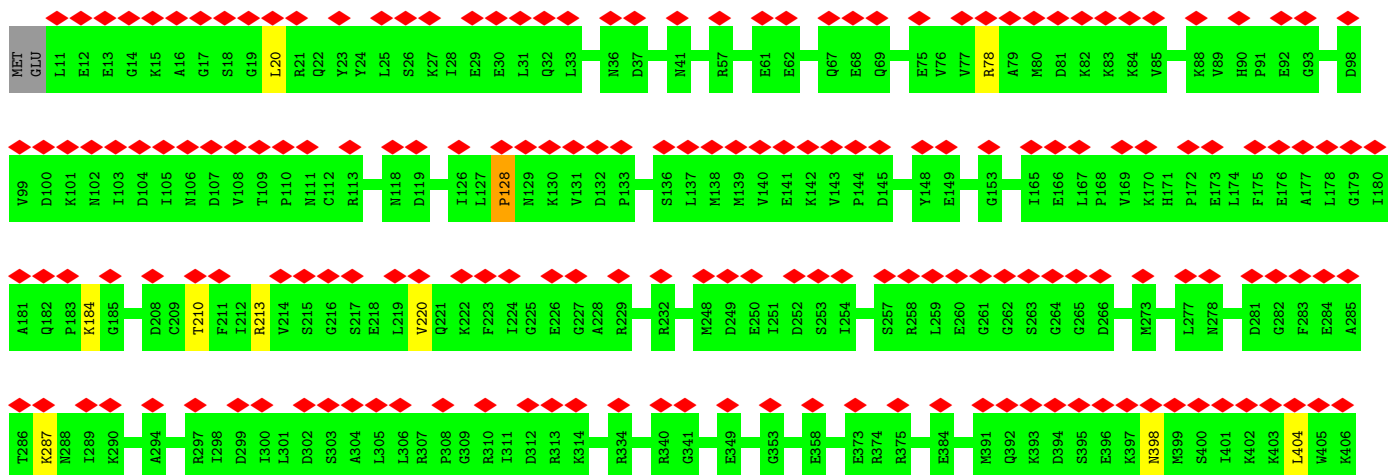


• Molecule 14: 26S proteasome regulatory subunit 4

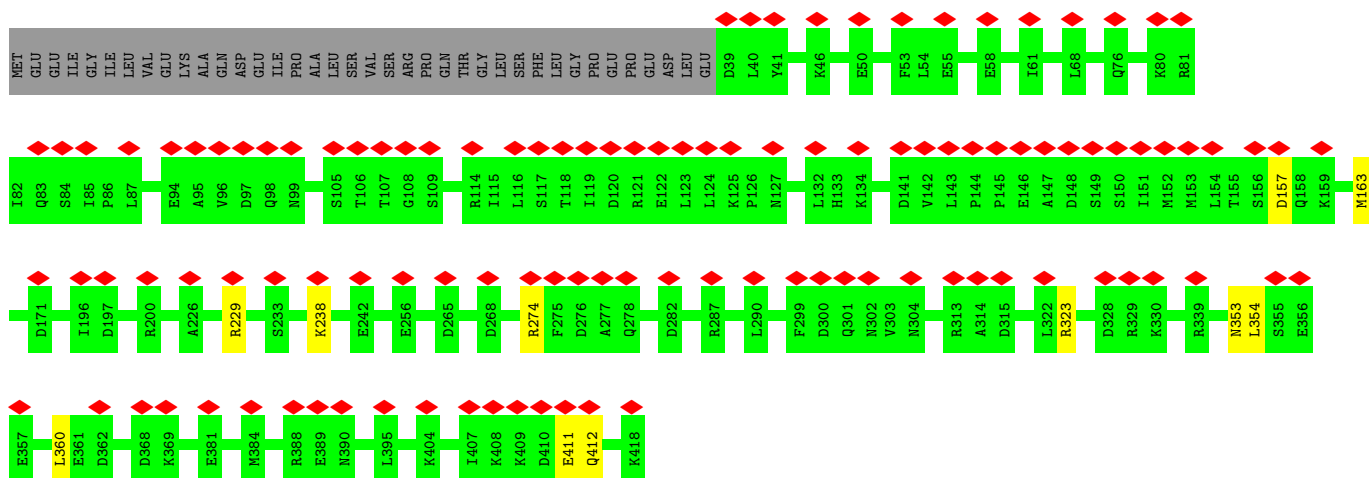
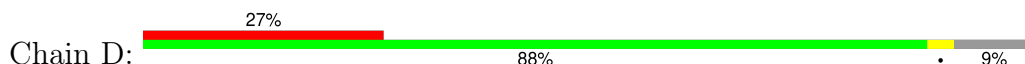




• Molecule 15: 26S proteasome regulatory subunit 8

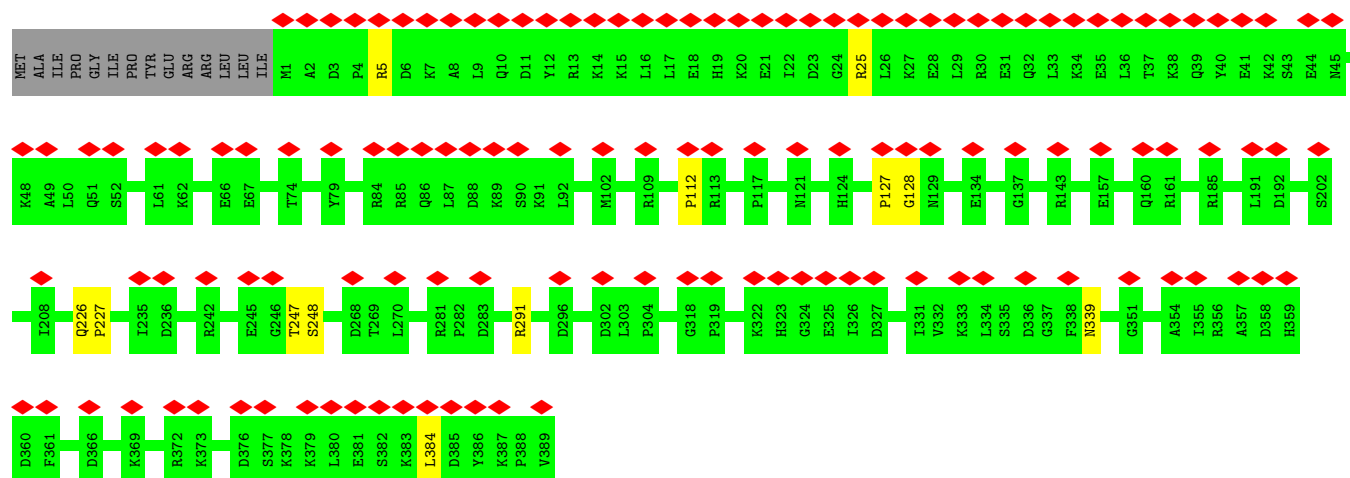


• Molecule 16: 26S proteasome regulatory subunit 6B

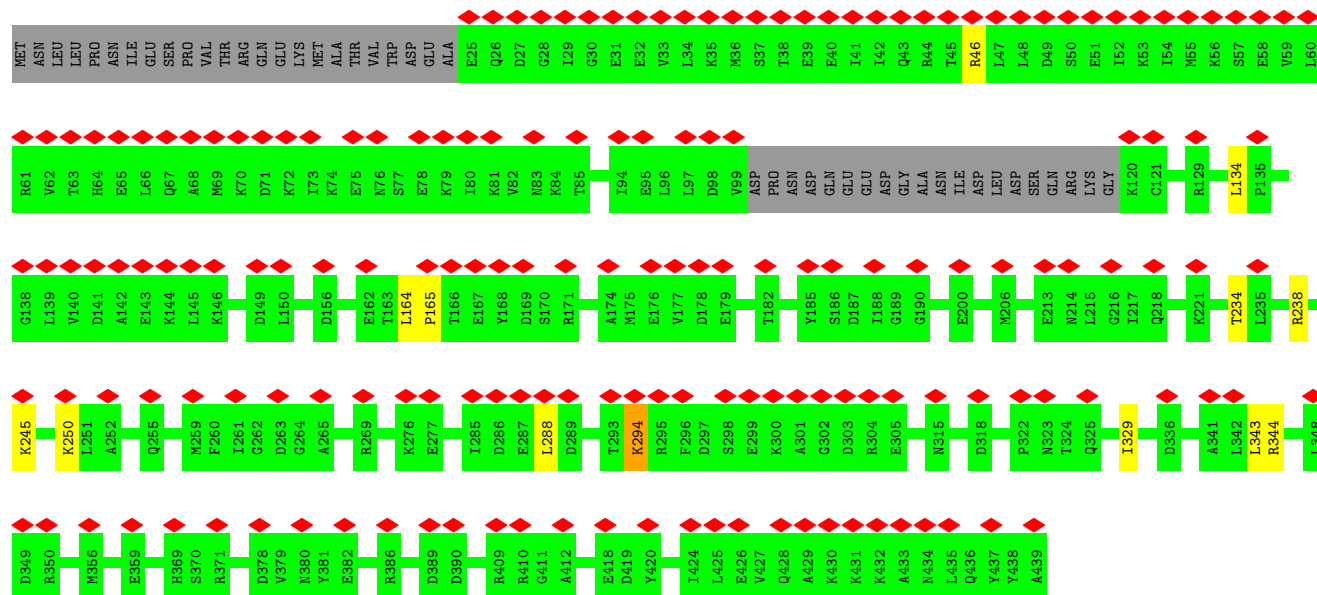
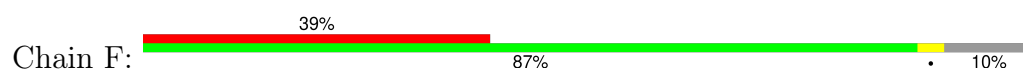


• Molecule 17: 26S proteasome regulatory subunit 10B

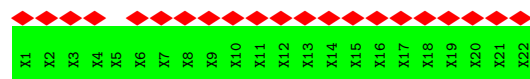




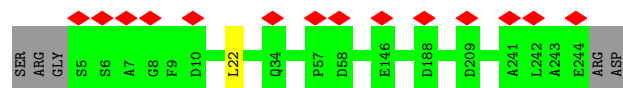
- Molecule 18: 26S proteasome regulatory subunit 6A



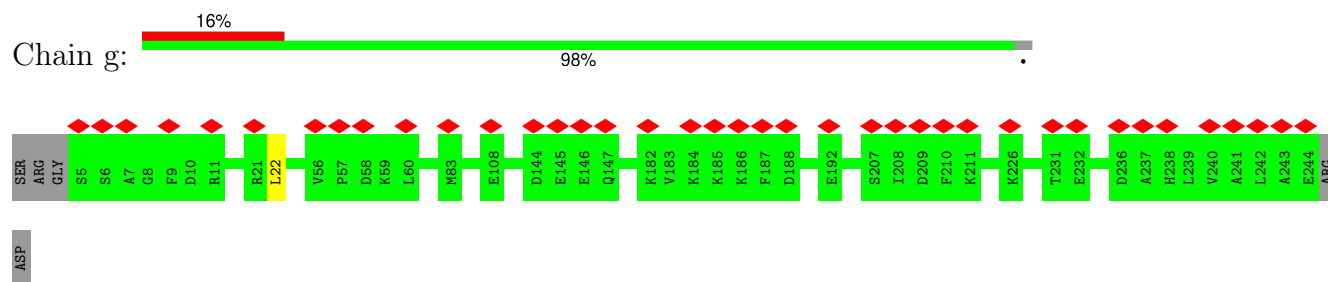
- Molecule 19: substrate



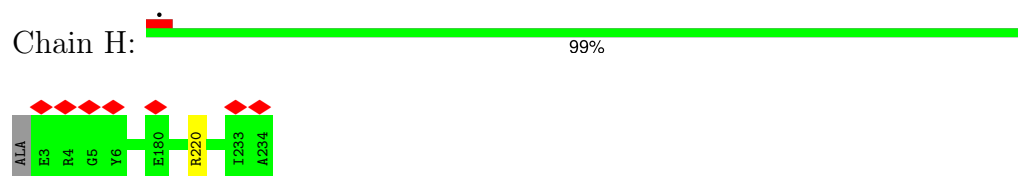
- Molecule 20: Proteasome subunit alpha type-6



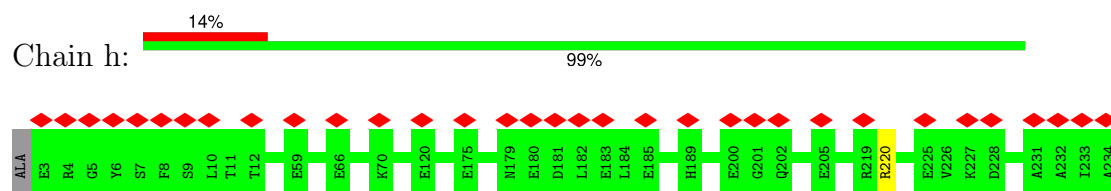
- Molecule 20: Proteasome subunit alpha type-6



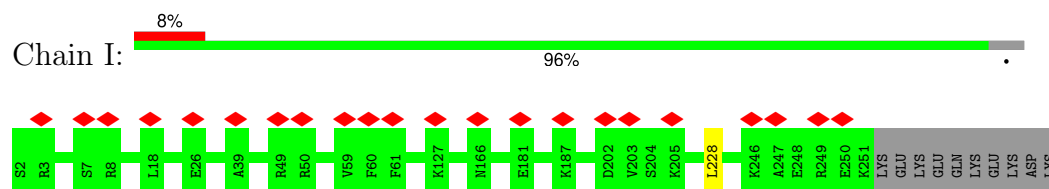
- Molecule 21: Proteasome subunit alpha type-2



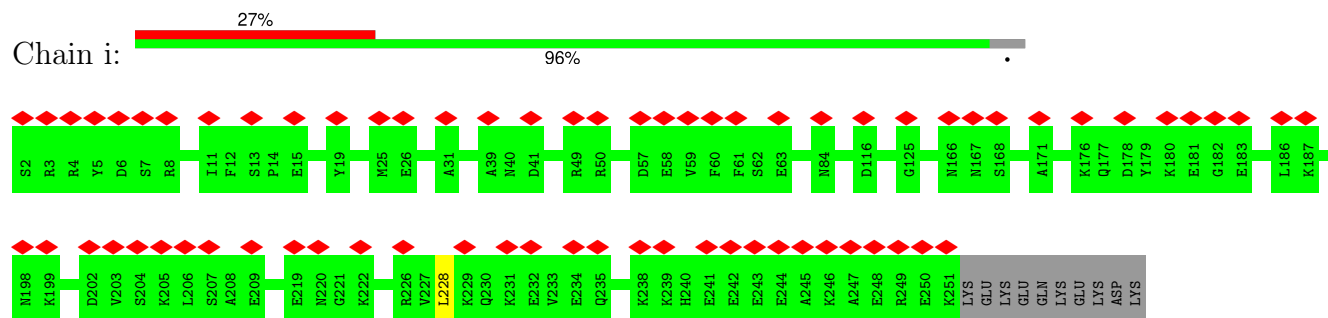
- Molecule 21: Proteasome subunit alpha type-2



- Molecule 22: Proteasome subunit alpha type-4

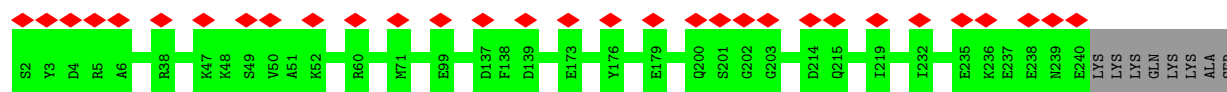


- Molecule 22: Proteasome subunit alpha type-4

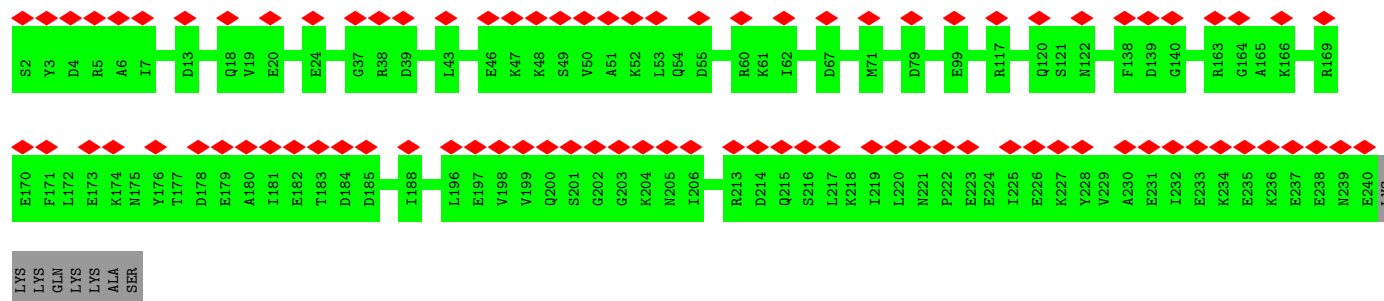


- Molecule 23: Proteasome subunit alpha type-7

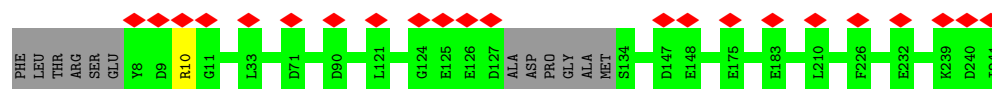




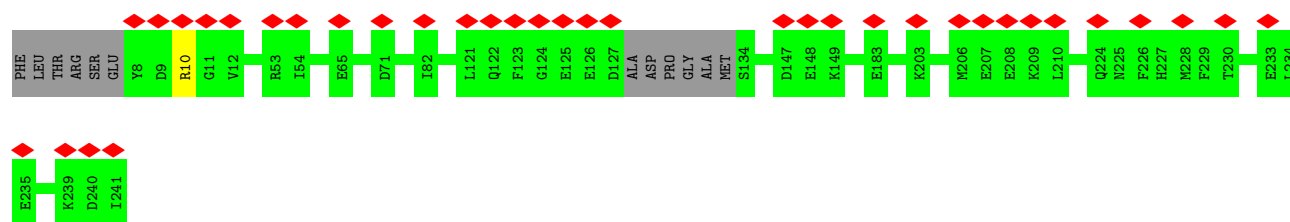
• Molecule 23: Proteasome subunit alpha type-7



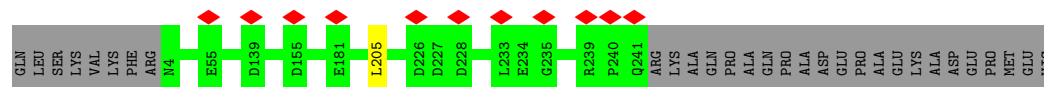
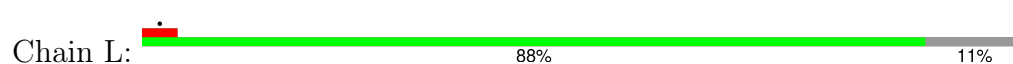
• Molecule 24: Proteasome subunit alpha type-5



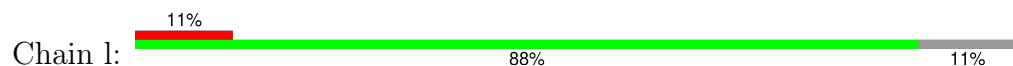
• Molecule 24: Proteasome subunit alpha type-5

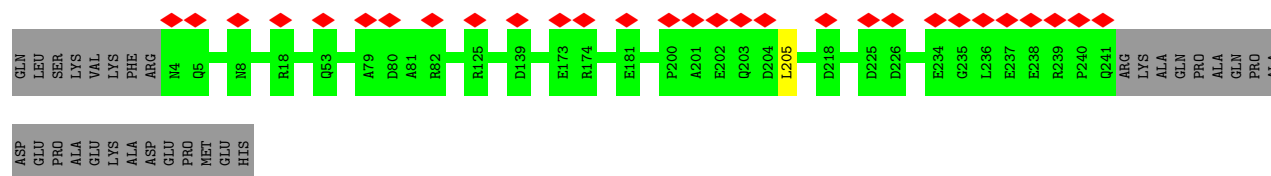


• Molecule 25: Proteasome subunit alpha type-1



• Molecule 25: Proteasome subunit alpha type-1

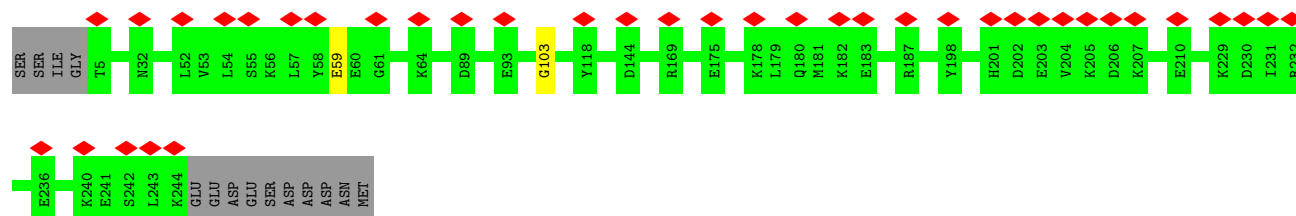




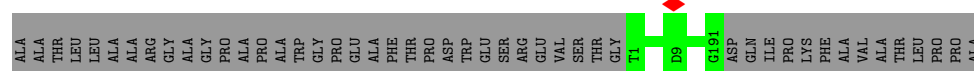
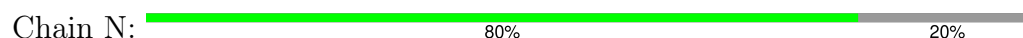
- Molecule 26: Proteasome subunit alpha type-3



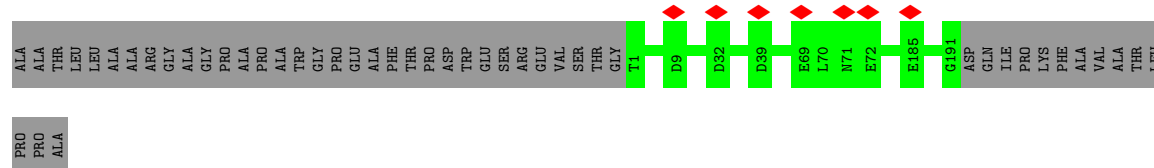
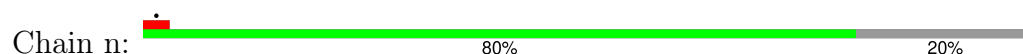
- Molecule 26: Proteasome subunit alpha type-3



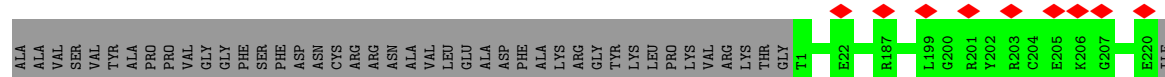
- Molecule 27: Proteasome subunit beta type-6



- Molecule 27: Proteasome subunit beta type-6




- Molecule 28: Proteasome subunit beta type-7



GLU VAL  
LEU GLU  
THR VAL  
GLN THR  
MET ASP  
THR SER

- Molecule 28: Proteasome subunit beta type-7

Chain o:  5% 80% 20%

ALA ALA VAL SER VAL THR ALA PRO PRO VAL GLY PHE SER PHE ASP ASN CYS ARG ARG ASN ALA VAL LEU GLU ALA ASP PHE PHE LYS ARG GLY TYR LYS LEU PRO LYS VAL ARG LYS THR GLY T1 G23 R143 N181 D184 K194 K196 G196 T197 R198 L199 G200 R201

E205 K206 G207 E220 ILE GLU VAL LEU GLU GLU THR VAL GLN THR MET ASP THR SER

- Molecule 29: Proteasome subunit beta type-3

Chain P:  100%

S2 F117 D205

- Molecule 29: Proteasome subunit beta type-3

Chain p:  100%

S2 D47 D59 K115 T116 F117 N157 D205

- Molecule 30: Proteasome subunit beta type-2

Chain Q:  98% ..


M1 E2 N24 E49 R93 L102 P176 P197 K198 Q199 GLY SER

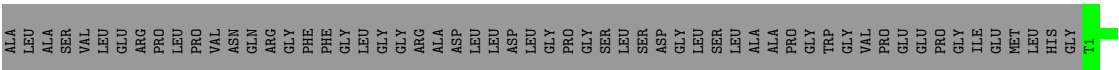
- Molecule 30: Proteasome subunit beta type-2

Chain q:  98% ..

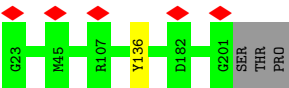
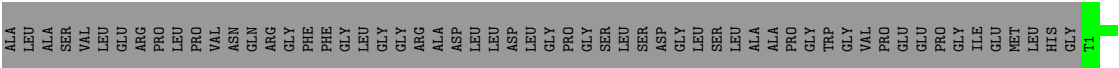
H1 D33 K34 K35 L102 H110 E111 R155 P176 D190 N193 K198 Q199 GLY SER

- Molecule 31: Proteasome subunit beta type-5

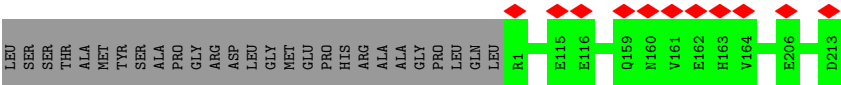
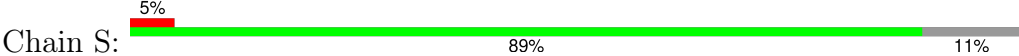
Chain R:  76% 23%



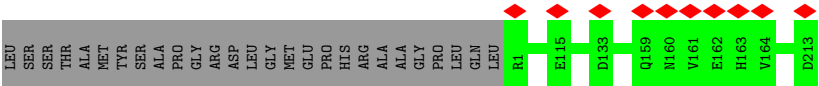
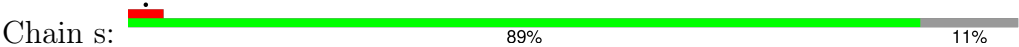
• Molecule 31: Proteasome subunit beta type-5



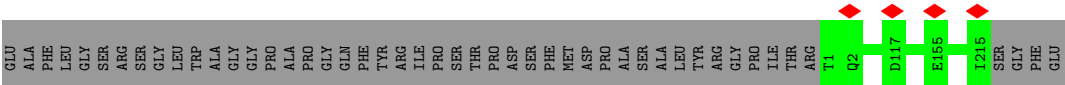
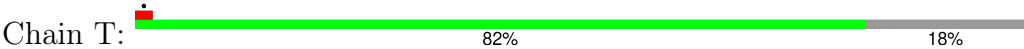
• Molecule 32: Proteasome subunit beta type-1



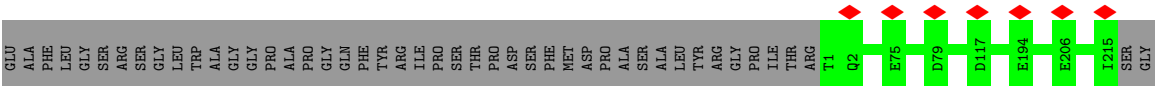
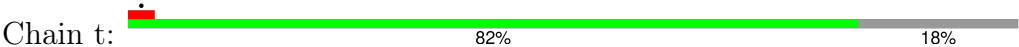
• Molecule 32: Proteasome subunit beta type-1



• 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	71651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ( $\text{\AA}$ )	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.685, 0.685, 0.685	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, 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	0.31	0/6513	0.56	1/8816 (0.0%)
2	V	0.34	0/3929	0.63	0/5309
3	W	0.31	0/3751	0.59	1/5042 (0.0%)
4	X	0.39	0/3053	0.57	0/4115
5	Y	0.38	0/3173	0.61	0/4273
6	Z	0.30	0/2324	0.61	2/3150 (0.1%)
7	a	0.31	0/3053	0.59	1/4133 (0.0%)
8	b	0.29	0/1478	0.58	0/2001
9	c	0.33	0/2302	0.63	1/3110 (0.0%)
10	d	0.32	0/2162	0.59	0/2919
11	e	0.32	0/338	0.65	1/450 (0.2%)
12	f	0.33	1/6954 (0.0%)	0.71	6/9399 (0.1%)
13	A	0.34	0/2814	0.55	0/3801
14	B	0.32	0/2745	0.57	0/3709
15	C	0.35	0/3146	0.60	1/4226 (0.0%)
16	D	0.41	0/3090	0.63	1/4168 (0.0%)
17	E	0.37	0/3145	0.62	1/4233 (0.0%)
18	F	0.37	0/3137	0.63	3/4223 (0.1%)
20	G	0.47	0/1859	0.57	0/2523
20	g	0.47	0/1859	0.57	0/2523
21	H	0.50	0/1743	0.59	1/2372 (0.0%)
21	h	0.50	0/1743	0.59	1/2372 (0.0%)
22	I	0.43	0/1942	0.59	0/2628
22	i	0.43	0/1942	0.59	0/2628
23	J	0.41	0/1728	0.54	0/2358
23	j	0.41	0/1728	0.54	0/2358
24	K	0.39	0/1747	0.56	0/2364
24	k	0.39	0/1747	0.56	0/2364
25	L	0.43	0/1885	0.59	0/2552
25	l	0.43	0/1885	0.59	0/2552
26	M	0.46	0/1891	0.59	0/2552
26	m	0.46	0/1891	0.59	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	N	0.43	0/1454	0.53	0/1967
27	n	0.43	0/1454	0.53	0/1967
28	O	0.42	0/1670	0.55	0/2265
28	o	0.42	0/1670	0.55	0/2265
29	P	0.45	0/1614	0.54	0/2177
29	p	0.45	0/1614	0.54	0/2177
30	Q	0.47	0/1603	0.62	0/2174
30	q	0.47	0/1603	0.62	0/2174
31	R	0.46	0/1579	0.52	0/2134
31	r	0.46	0/1579	0.52	0/2134
32	S	0.42	0/1671	0.54	0/2253
32	s	0.42	0/1671	0.54	0/2253
33	T	0.44	0/1700	0.53	0/2305
33	t	0.44	0/1700	0.53	0/2305
All	All	0.39	1/105279 (0.0%)	0.59	21/142325 (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
2	V	0	1
6	Z	0	2
7	a	0	1
10	d	0	1
12	f	0	12
13	A	0	2
15	C	0	2
16	D	0	2
17	E	0	1
18	F	0	1
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	5.92	1.45	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	830	LEU	CA-CB-CG	7.96	133.61	115.30
18	F	343	LEU	CA-CB-CG	7.43	132.40	115.30
11	e	56	LEU	CA-CB-CG	7.33	132.15	115.30
12	f	759	LEU	CA-CB-CG	6.76	130.84	115.30
12	f	612	LEU	CA-CB-CG	6.74	130.79	115.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	29	PRO	Peptide
6	Z	144	VAL	Peptide
6	Z	183	THR	Peptide
7	a	18	GLN	Peptide
10	d	199	PHE	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	814/953 (85%)	760 (93%)	53 (6%)	1 (0%)	48	79
2	V	478/533 (90%)	436 (91%)	41 (9%)	1 (0%)	44	73
3	W	454/456 (100%)	420 (92%)	34 (8%)	0	100	100
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	37	67
5	Y	376/389 (97%)	340 (90%)	36 (10%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	33
7	a	371/376 (99%)	338 (91%)	32 (9%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
9	c	285/309 (92%)	241 (85%)	43 (15%)	1 (0%)	30	63
10	d	255/349 (73%)	216 (85%)	38 (15%)	1 (0%)	30	63
11	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
12	f	884/892 (99%)	709 (80%)	164 (19%)	11 (1%)	11	43
13	A	354/433 (82%)	310 (88%)	42 (12%)	2 (1%)	22	55
14	B	348/440 (79%)	300 (86%)	44 (13%)	4 (1%)	12	45
15	C	394/398 (99%)	342 (87%)	51 (13%)	1 (0%)	37	67
16	D	378/418 (90%)	335 (89%)	42 (11%)	1 (0%)	37	67
17	E	387/403 (96%)	338 (87%)	43 (11%)	6 (2%)	8	38
18	F	391/439 (89%)	350 (90%)	40 (10%)	1 (0%)	37	67
20	G	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
20	g	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
21	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
21	h	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
22	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
22	i	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
23	J	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
23	j	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
24	K	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
25	L	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
25	l	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
26	M	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	51
26	m	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	51
27	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
28	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	25	59
30	q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	25	59
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%)	202 (96%)	9 (4%)	0	100	100
32	s	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
33	T	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
33	t	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
All	All	13216/14843 (89%)	12036 (91%)	1136 (9%)	44 (0%)	38	67

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	217	THR
10	d	200	PHE
12	f	808	ASN
12	f	853	VAL
14	B	354	PRO

### 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	700/816 (86%)	696 (99%)	4 (1%)	84	92
2	V	414/459 (90%)	411 (99%)	3 (1%)	81	90
3	W	416/416 (100%)	402 (97%)	14 (3%)	32	60
4	X	327/362 (90%)	327 (100%)	0	100	100
5	Y	334/344 (97%)	330 (99%)	4 (1%)	67	82
6	Z	257/295 (87%)	247 (96%)	10 (4%)	27	57
7	a	333/336 (99%)	330 (99%)	3 (1%)	75	87
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%)	246 (98%)	6 (2%)	44	67
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	37 (97%)	1 (3%)	41	65
12	f	742/748 (99%)	724 (98%)	18 (2%)	44	67
13	A	298/372 (80%)	293 (98%)	5 (2%)	56	75
14	B	300/385 (78%)	297 (99%)	3 (1%)	73	85
15	C	340/346 (98%)	333 (98%)	7 (2%)	48	71
16	D	333/366 (91%)	326 (98%)	7 (2%)	48	71
17	E	341/353 (97%)	337 (99%)	4 (1%)	67	82
18	F	340/379 (90%)	331 (97%)	9 (3%)	41	65
20	G	193/209 (92%)	192 (100%)	1 (0%)	86	93
20	g	193/209 (92%)	192 (100%)	1 (0%)	86	93
21	H	164/190 (86%)	164 (100%)	0	100	100
21	h	164/190 (86%)	164 (100%)	0	100	100
22	I	193/220 (88%)	192 (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	186/202 (92%)	185 (100%)	1 (0%)	86	93
24	k	186/202 (92%)	185 (100%)	1 (0%)	86	93
25	L	198/229 (86%)	197 (100%)	1 (0%)	86	93
25	l	198/229 (86%)	197 (100%)	1 (0%)	86	93
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100
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%)	172 (100%)	0	100	100
29	p	172/173 (99%)	172 (100%)	0	100	100
30	Q	164/171 (96%)	163 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	q	164/171 (96%)	163 (99%)	1 (1%)	84	92
31	R	153/201 (76%)	152 (99%)	1 (1%)	81	90
31	r	153/201 (76%)	152 (99%)	1 (1%)	81	90
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	174/198 (88%)	174 (100%)	0	100	100
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11045/12582 (88%)	10935 (99%)	110 (1%)	71	85

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	f	660	ILE
15	C	20	LEU
31	r	136	TYR
22	I	228	LEU
12	f	703	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
14	B	277	HIS
17	E	271	HIS
30	q	82	ASN
14	B	416	ASN
16	D	187	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
35	ATP	C	501	-	28,33,33	0.79	0	34,52,52	1.22	3 (8%)
35	ATP	D	501	-	28,33,33	0.78	0	34,52,52	1.37	4 (11%)
35	ATP	E	401	-	28,33,33	0.82	0	34,52,52	1.42	6 (17%)
36	ADP	F	501	-	24,29,29	0.79	0	29,45,45	1.38	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
35	ATP	C	501	-	-	2/18/38/38	0/3/3/3
35	ATP	D	501	-	-	6/18/38/38	0/3/3/3
35	ATP	E	401	-	-	1/18/38/38	0/3/3/3
36	ADP	F	501	-	-	7/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	501	ATP	N3-C2-N1	-4.16	123.03	128.67
36	F	501	ADP	N3-C2-N1	-3.87	123.41	128.67
35	E	401	ATP	N3-C2-N1	-3.42	124.03	128.67
35	D	501	ATP	N3-C2-N1	-3.40	124.06	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	501	ATP	O4'-C1'-N9	-2.77	105.07	108.75

There are no chirality outliers.

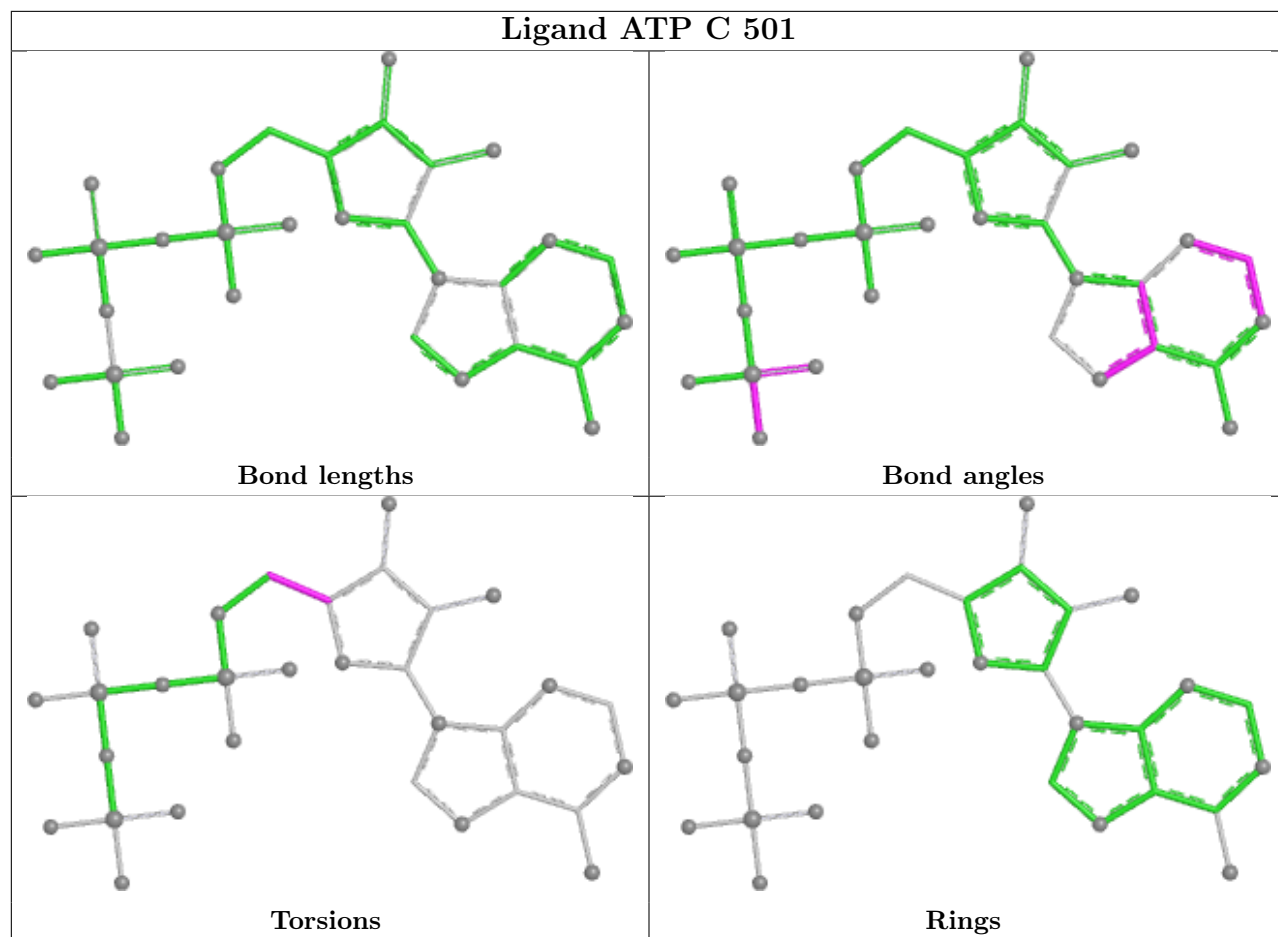
5 of 16 torsion outliers are listed below:

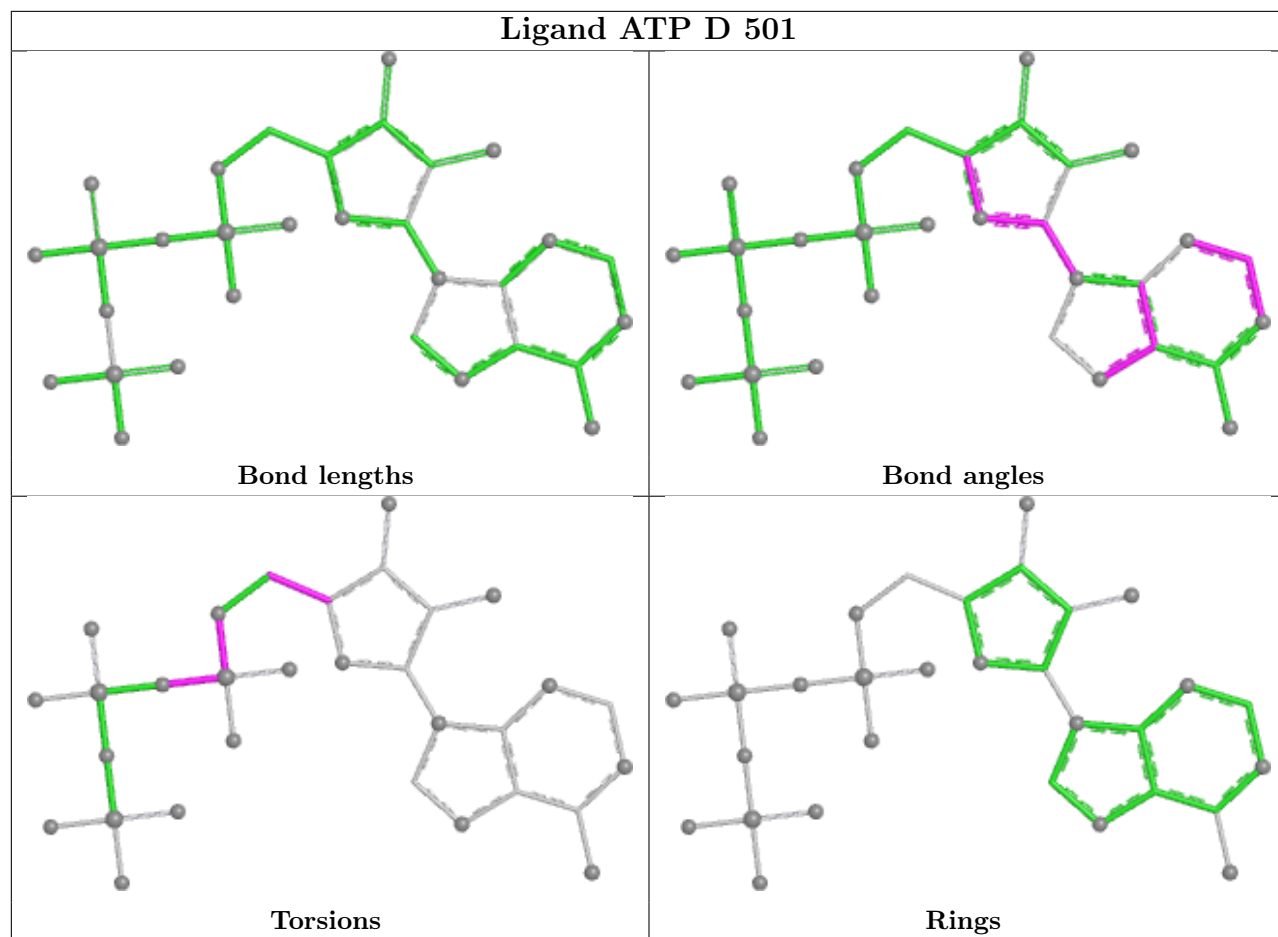
Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A
36	F	501	ADP	PA-O3A-PB-O2B
36	F	501	ADP	PA-O3A-PB-O3B

There are no ring outliers.

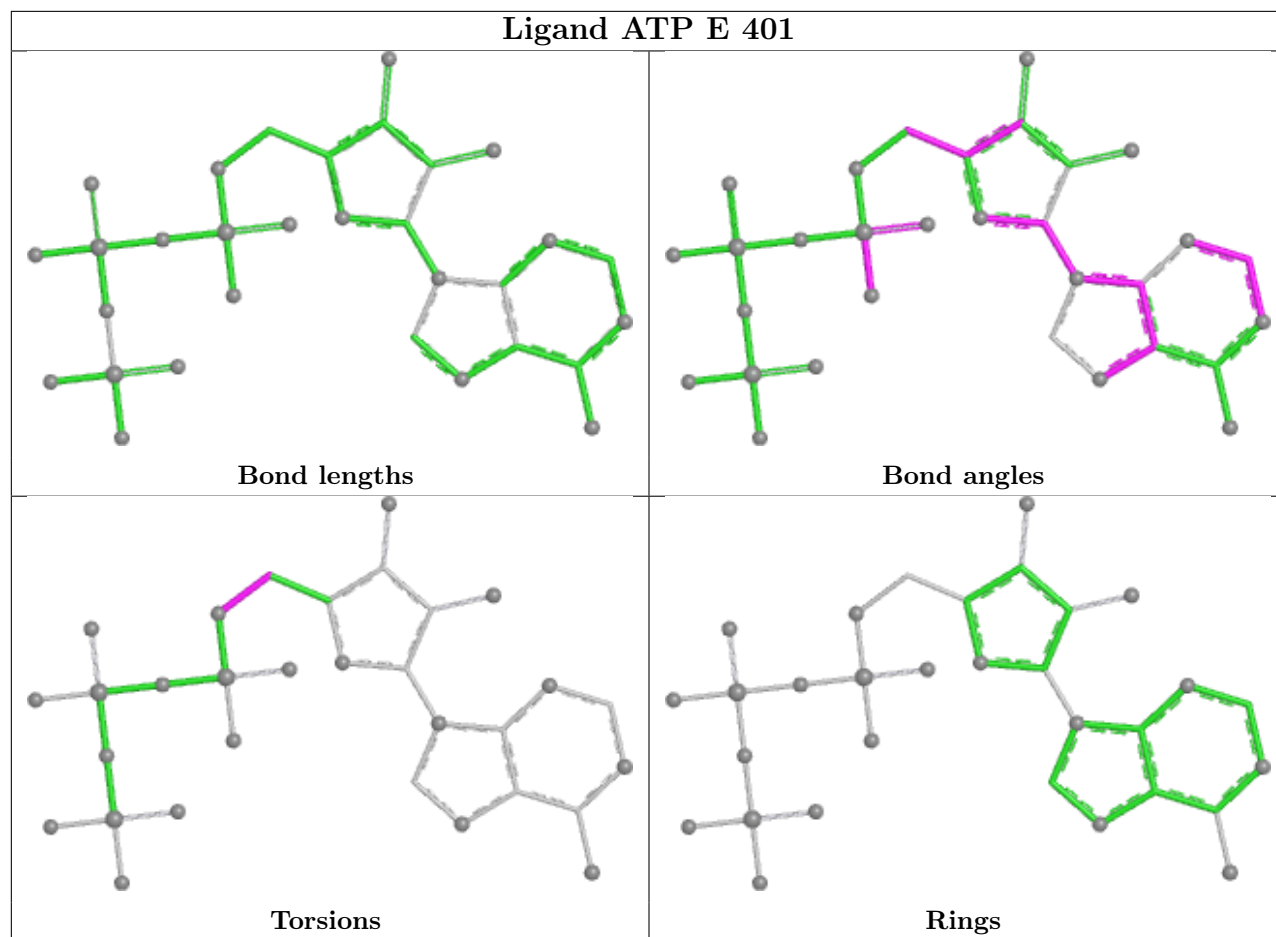
No monomer is involved in short contacts.

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.

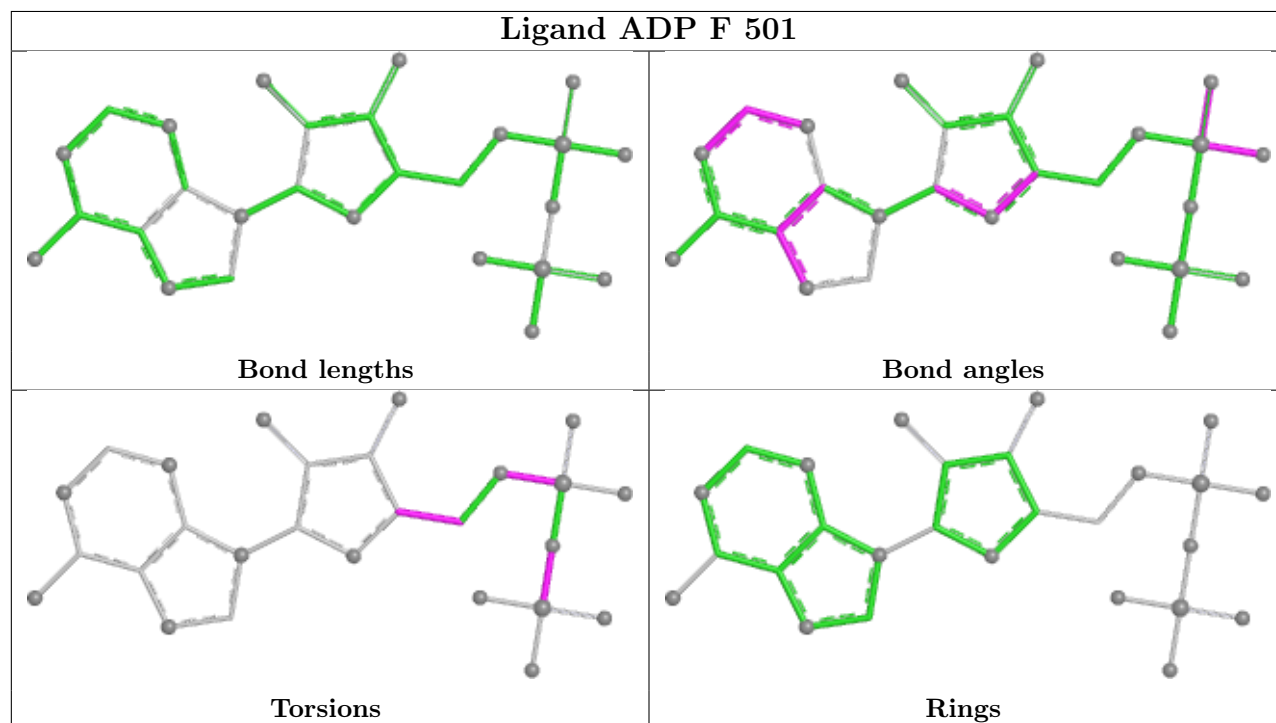




## Ligand ATP E 401



## Ligand ADP F 501



## 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.

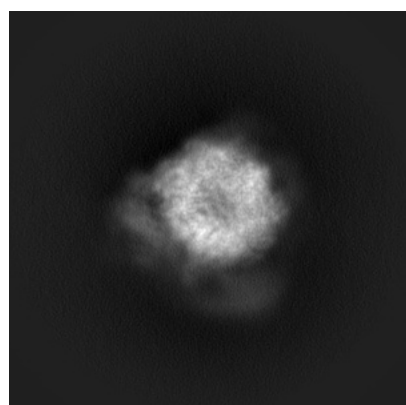
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9220. These allow visual inspection of the internal detail of the map and identification of artifacts.

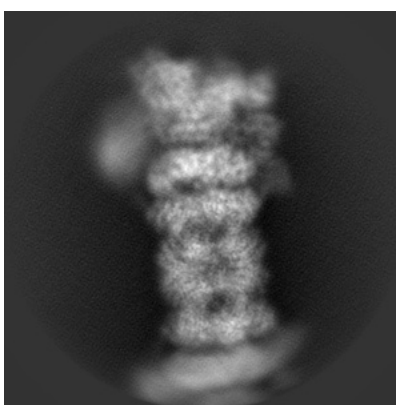
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

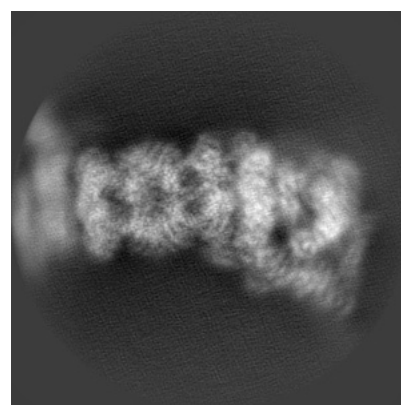
#### 6.1.1 Primary map



X



Y

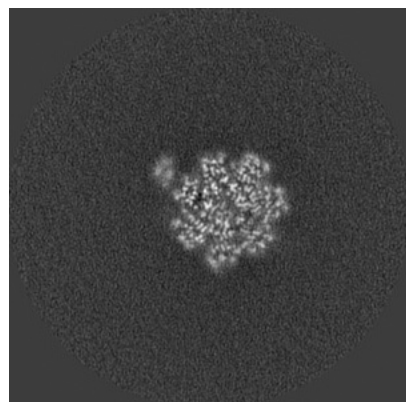


Z

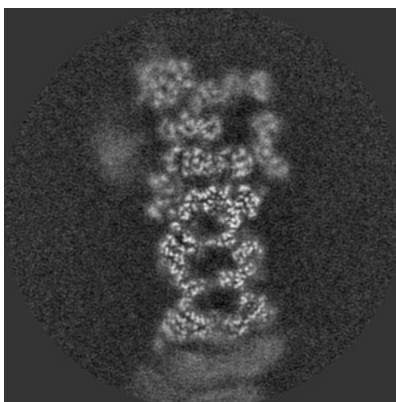
The images above show the map projected in three orthogonal directions.

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

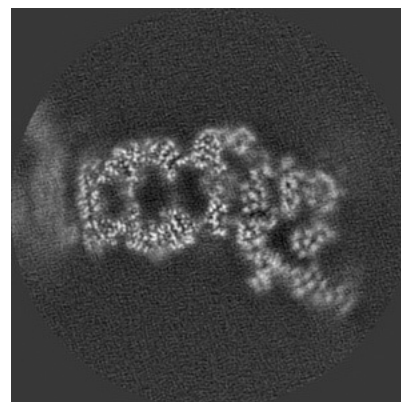
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

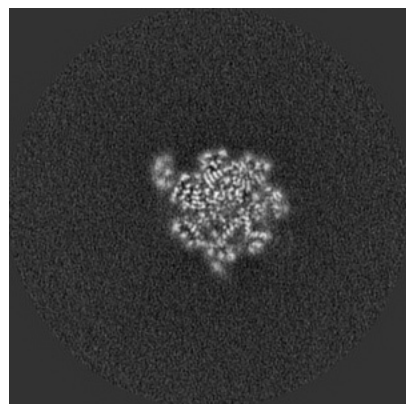


Z Index: 300

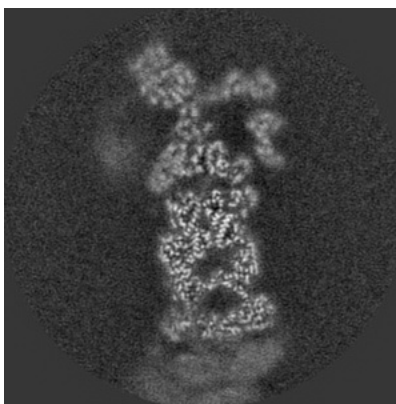
The images above show central slices of the map in three orthogonal directions.

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

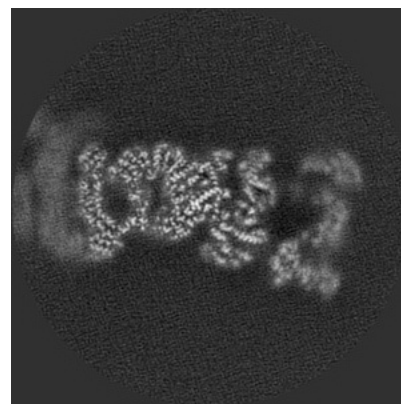
### 6.3.1 Primary map



X Index: 307



Y Index: 287

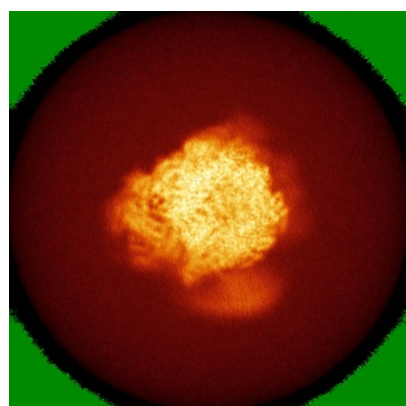


Z Index: 343

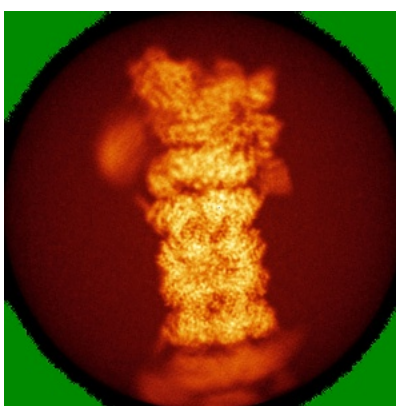
The images above show the largest variance slices of the map in three orthogonal directions.

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

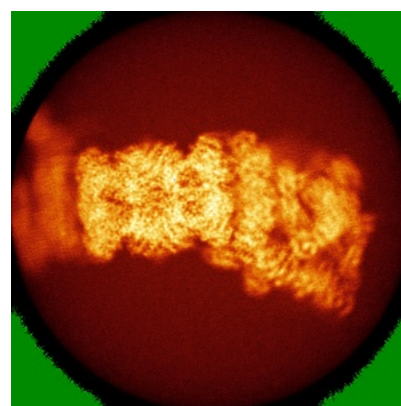
### 6.4.1 Primary map



X



Y

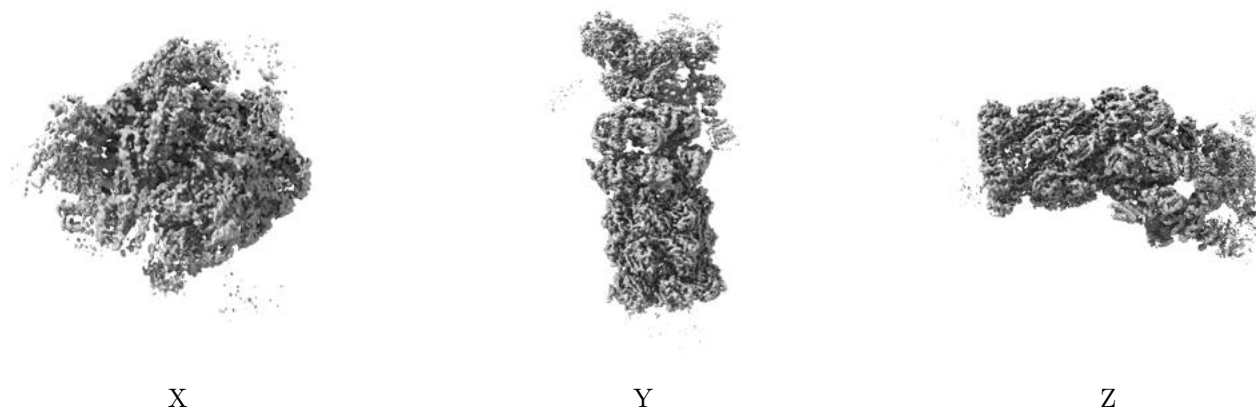


Z

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.

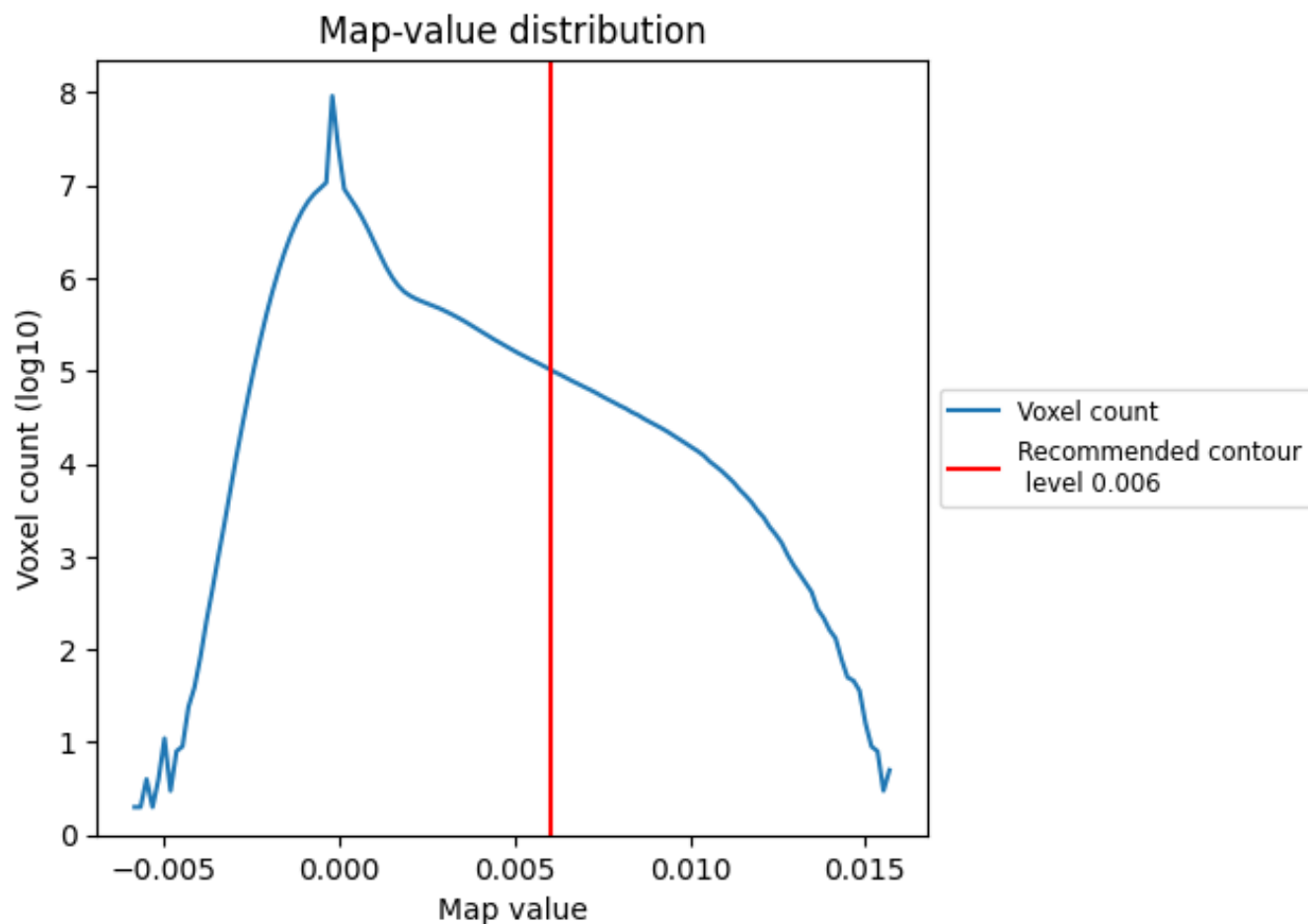
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

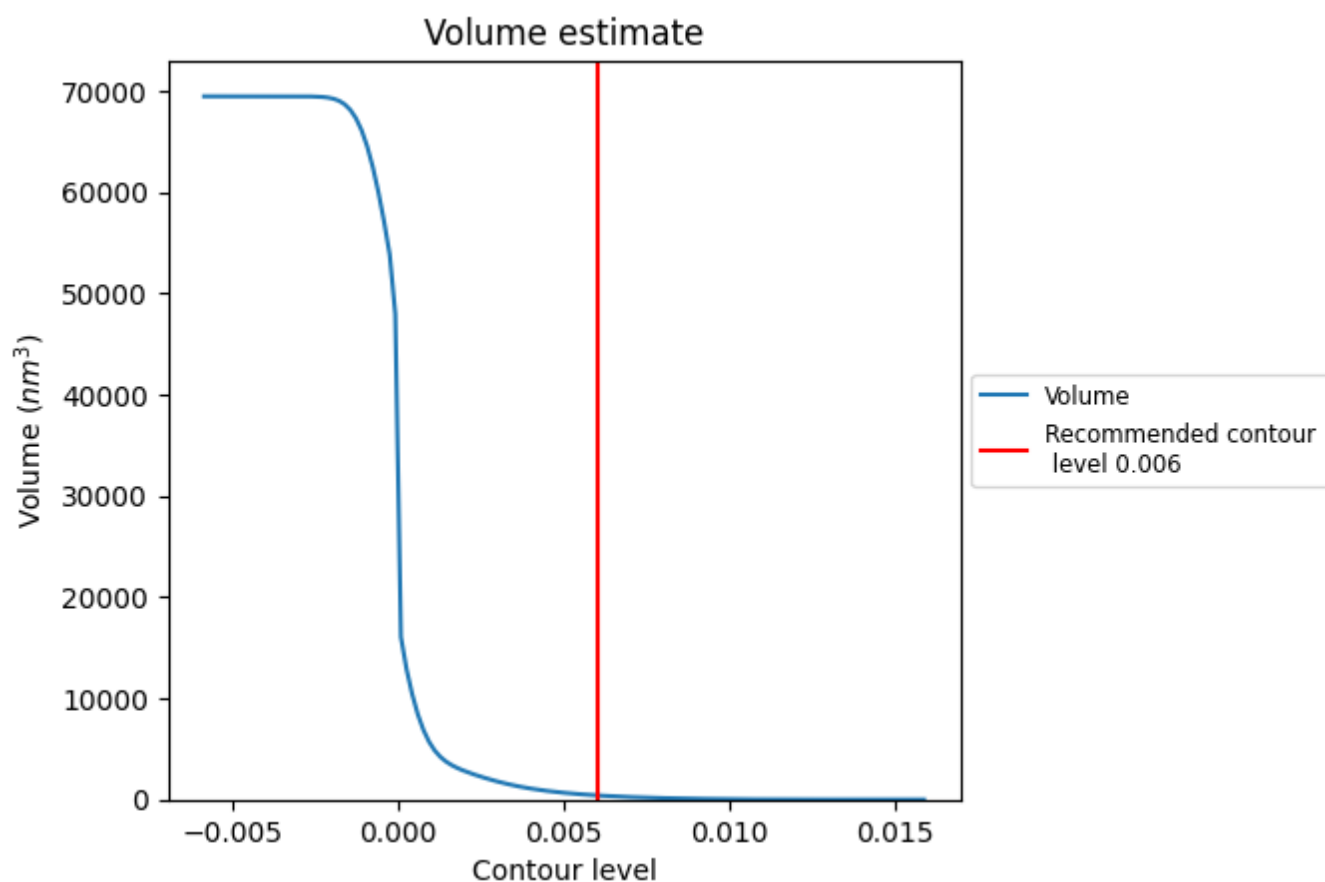
This section contains the results of statistical analysis of the map.

### 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.

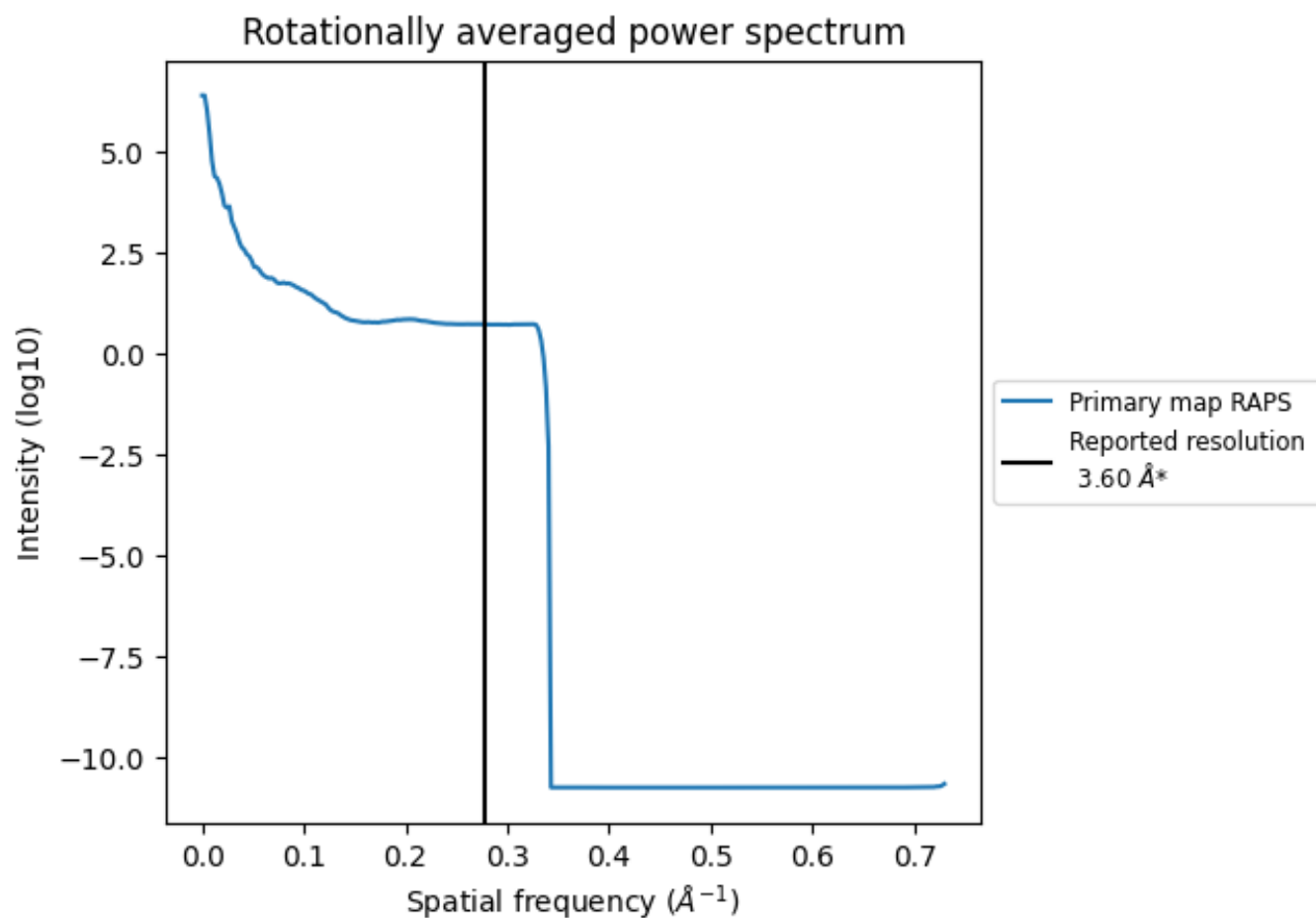
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm<sup>3</sup>; 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 0.278 Å<sup>-1</sup>

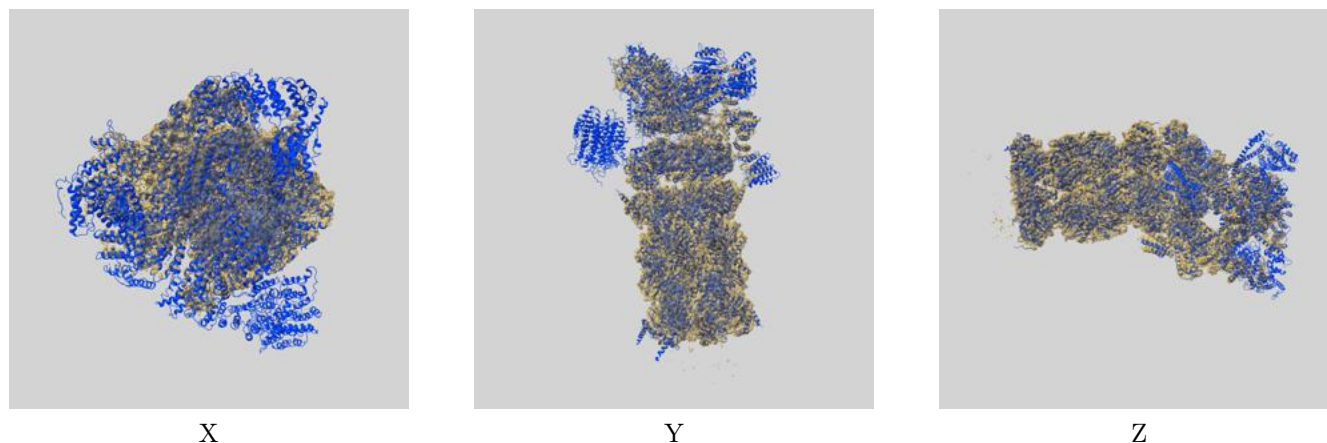
## 8 Fourier-Shell correlation

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

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

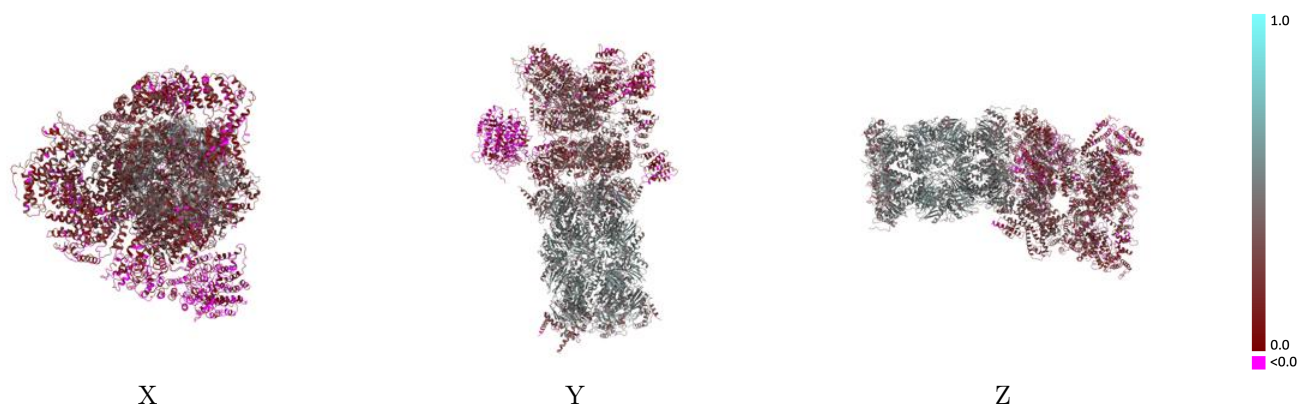
This section contains information regarding the fit between EMDB map EMD-9220 and PDB model 6MSH. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

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



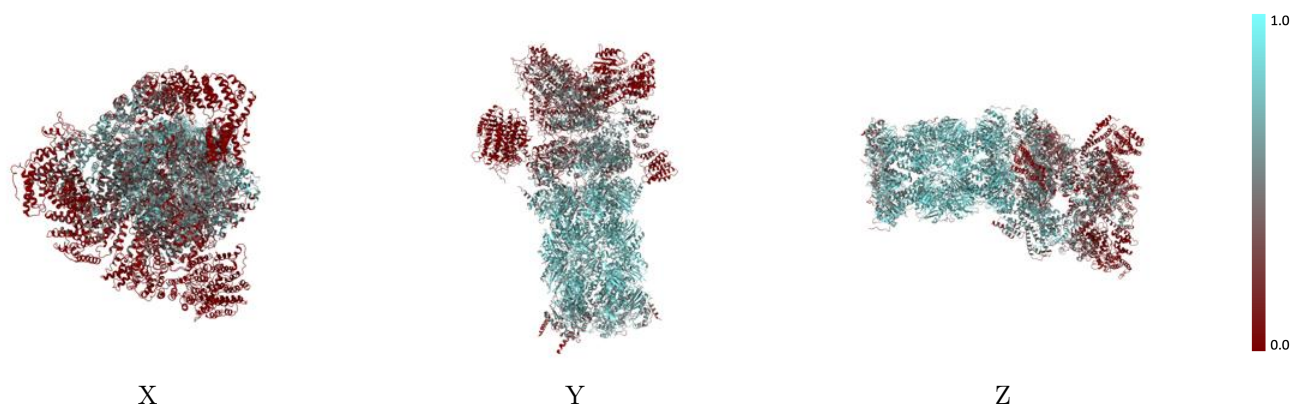
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



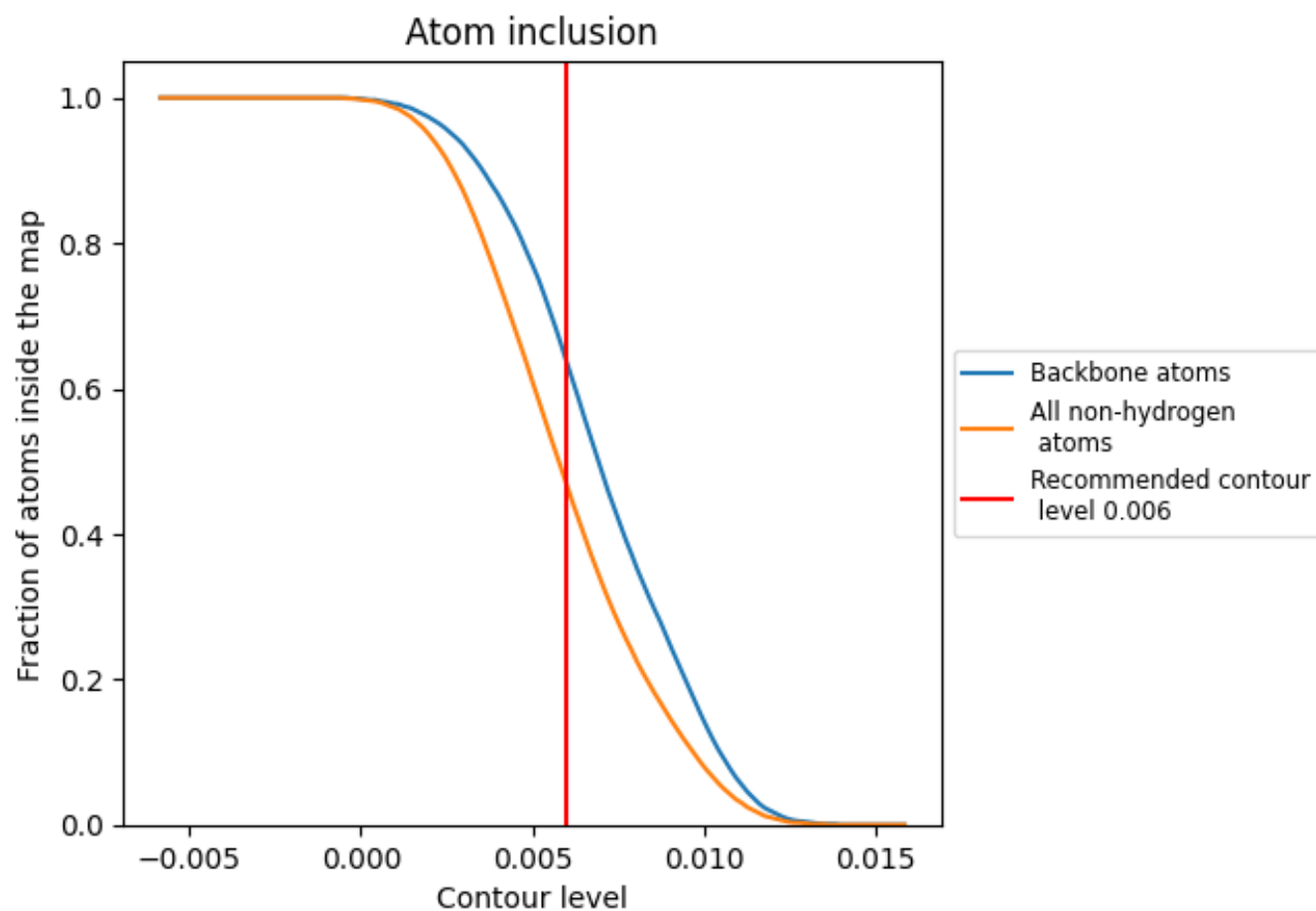
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 64% of all backbone atoms, 47% 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	 0.4680	 0.3220
A	 0.3550	 0.2230
B	 0.2200	 0.1930
C	 0.4110	 0.2770
D	 0.5110	 0.3430
E	 0.4630	 0.3010
F	 0.4250	 0.2540
G	 0.7230	 0.4480
H	 0.7700	 0.4580
I	 0.6950	 0.4170
J	 0.6640	 0.4090
K	 0.6590	 0.4270
L	 0.7160	 0.4530
M	 0.6960	 0.4230
N	 0.7810	 0.4940
O	 0.7640	 0.4890
P	 0.7680	 0.4970
Q	 0.7500	 0.4730
R	 0.7840	 0.5020
S	 0.7250	 0.4900
T	 0.7680	 0.4990
U	 0.2320	 0.2070
V	 0.1610	 0.1790
W	 0.2420	 0.1690
X	 0.5600	 0.2920
Y	 0.5320	 0.2640
Z	 0.2610	 0.2130
a	 0.1620	 0.1660
b	 0.0210	 0.1490
c	 0.3060	 0.2540
d	 0.0730	 0.1700
e	 0.2580	 0.1920
f	 0.0000	 0.0170
g	 0.6010	 0.4430
h	 0.6160	 0.4520



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Chain	Atom inclusion	Q-score
i	 0.5360	 0.4160
j	 0.4980	 0.3920
k	 0.5690	 0.4300
l	 0.6780	 0.4630
m	 0.6230	 0.4350
n	 0.7570	 0.5040
o	 0.7220	 0.4950
p	 0.7370	 0.5030
q	 0.7320	 0.4850
r	 0.7780	 0.5130
s	 0.7450	 0.4980
t	 0.7790	 0.5080
v	 0.0730	 0.2000