



# Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 05:39 am BST

PDB ID : 7QYA  
EMDB ID : EMD-14210  
Title : Proteasome-ZFAND5 Complex Z-B state  
Authors : Zhu, Y.; Lu, Y.  
Deposited on : 2022-01-27  
Resolution : 4.80 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>.

---

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

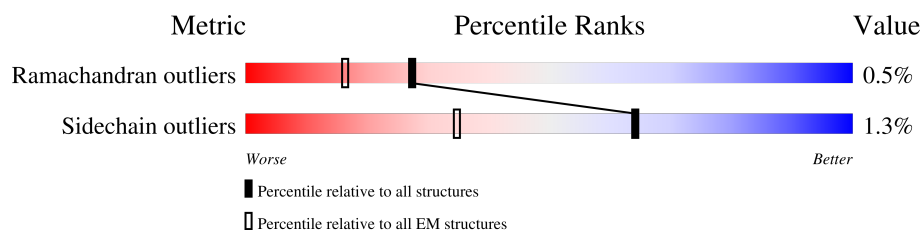
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 4.80 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.



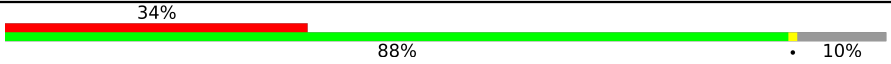
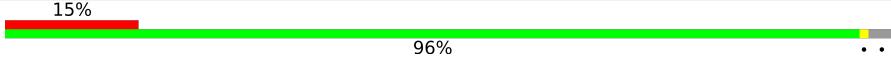
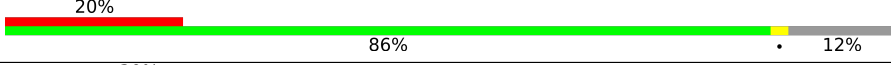

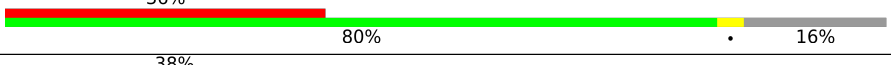
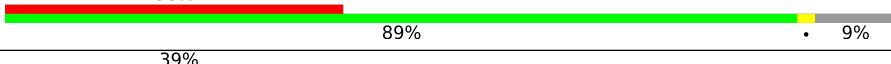
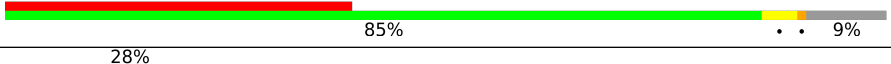
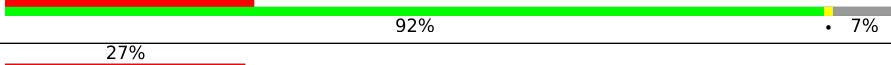
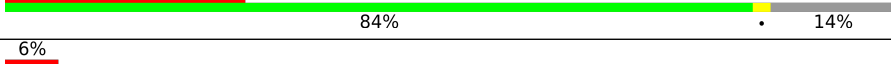
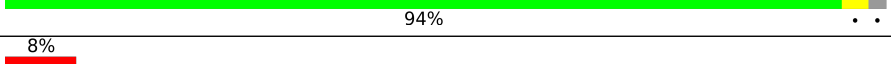
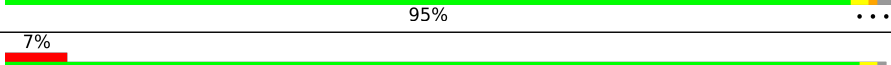
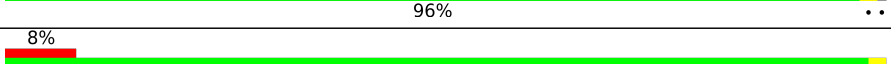
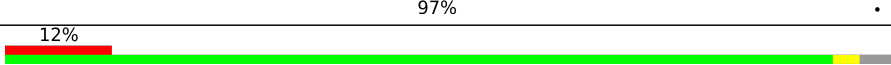
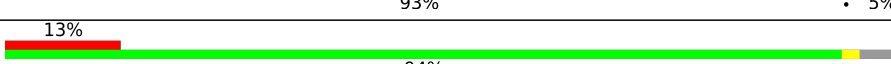
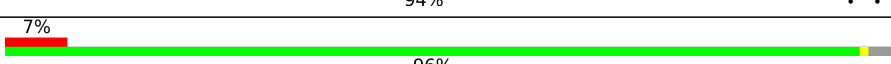
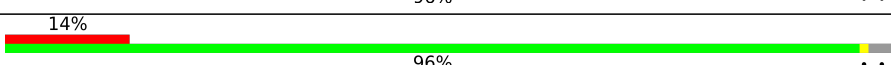
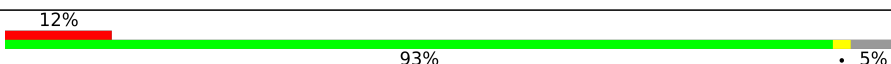
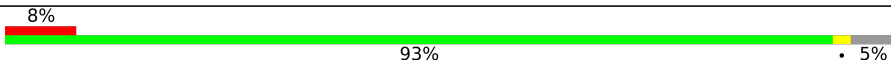
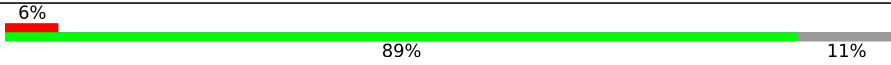
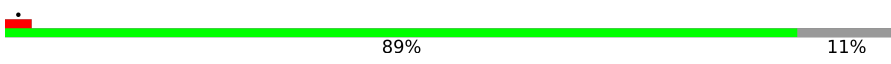
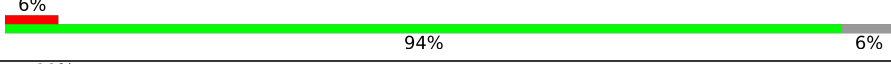
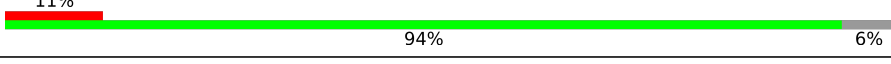
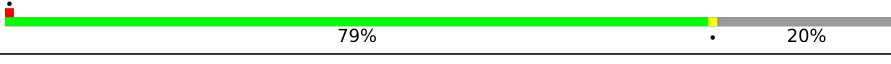


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	a	376	
2	b	377	
3	c	309	
4	d	349	
5	e	70	
6	f	908	
7	U	953	
8	V	533	
9	W	456	


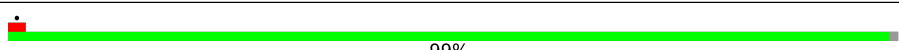
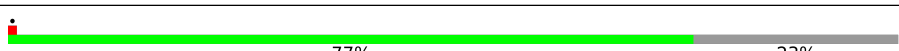

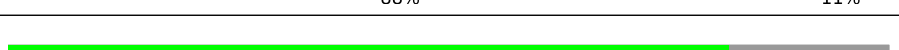

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	X	422	
11	Y	389	
12	Z	324	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	

Continued on next page...

*Continued from previous page...*

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

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 101325 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 13.

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

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	191	Total	C	N	O	S	0	0
			1457	910	260	279	8		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	278	Total	C	N	O	S	0	0
			2186	1389	373	406	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	257	Total	C	N	O	S	0	0
			2115	1371	345	390	9		

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	40	Total	C	N	O	S	0	0
			333	200	54	77	2		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	689	Total	C	N	O	S	0	0
			5318	3343	903	1037	35		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	806	Total	C	N	O	S	0	0
			6286	3990	1074	1178	44		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	473	Total	C	N	O	S	0	0
			3807	2418	675	700	14		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	456	Total	C	N	O	S	0	0
			3702	2339	634	704	25		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	380	Total	C	N	O	S	0	0
			3008	1918	508	570	12		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	378	Total	C	N	O	S	0	0
			3114	1987	532	578	17		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	286	Total	C	N	O	S	0	0
			2280	1457	391	427	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	380	Total	C	N	O	S	0	0
			2892	1817	514	543	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	370	Total	C	N	O	S	0	0
			2805	1763	477	553	12		

- Molecule 15 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	363	Total	C	N	O	S	0	0
			2858	1804	512	525	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3039	1923	523	580	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	375	Total	C	N	O	S	0	0
			2859	1796	511	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	376	Total	C	N	O	S	0	0
			2858	1802	495	546	15		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		
20	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 24 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 26 is a protein called Proteasome subunit beta type-6.



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

- Molecule 27 is a protein called Proteasome subunit beta type-7.

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

- Molecule 28 is a protein called Proteasome subunit beta type-3.

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

- Molecule 29 is a protein called Proteasome subunit beta type-2.

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

- Molecule 30 is a protein called Proteasome subunit beta type-5.

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

- Molecule 31 is a protein called Proteasome subunit beta type-1.

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

*Continued on next page...*

Continued from previous page...

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

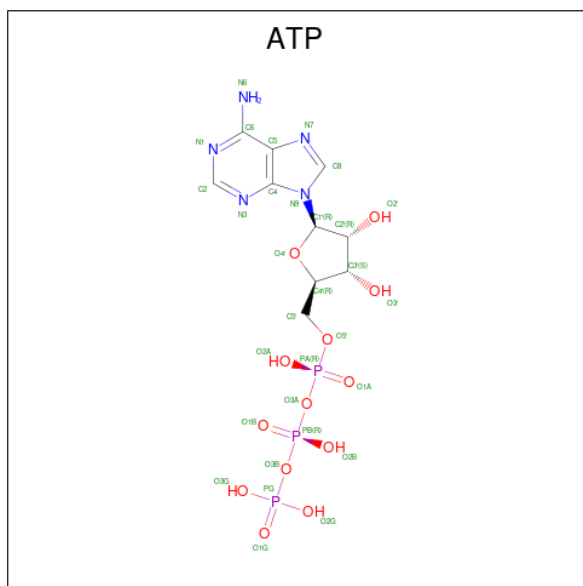
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

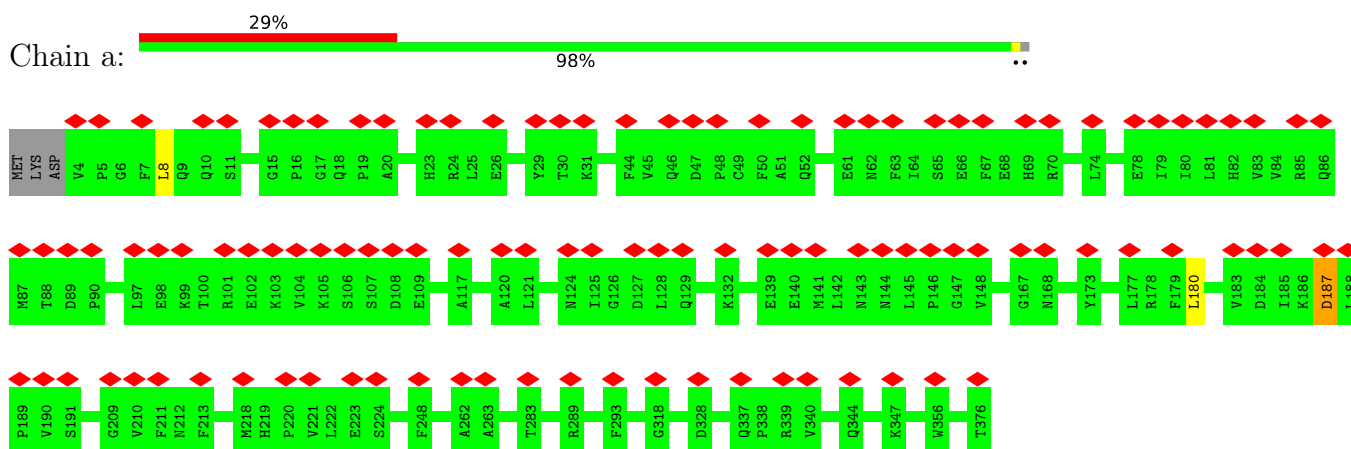
*Continued from previous page...*

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

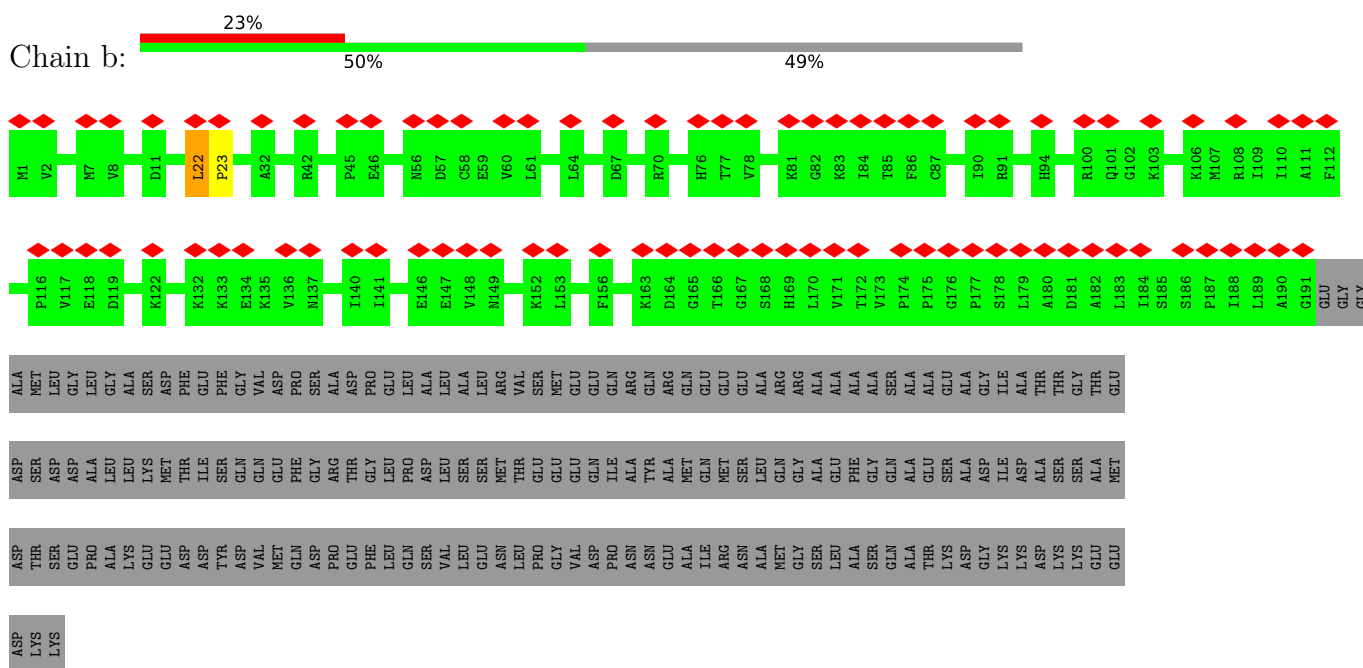
### 3 Residue-property plots

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

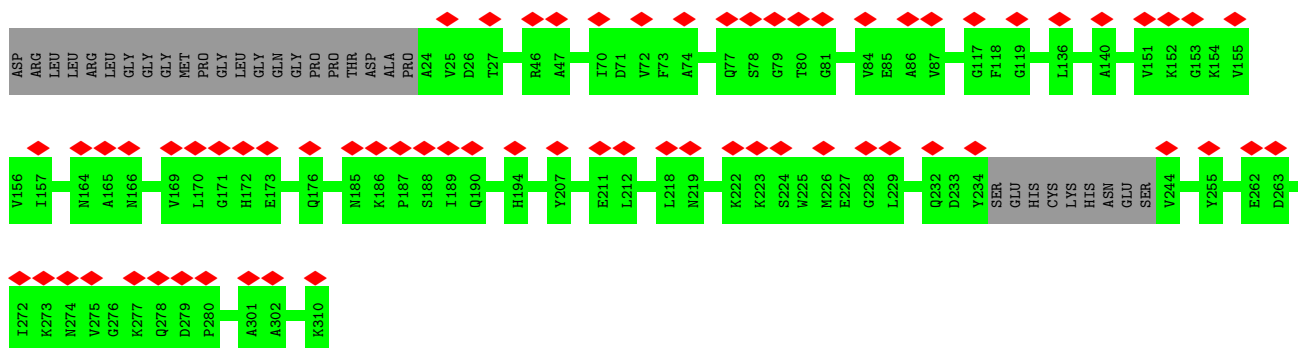
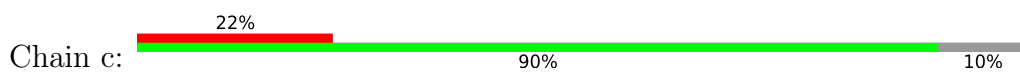
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 13



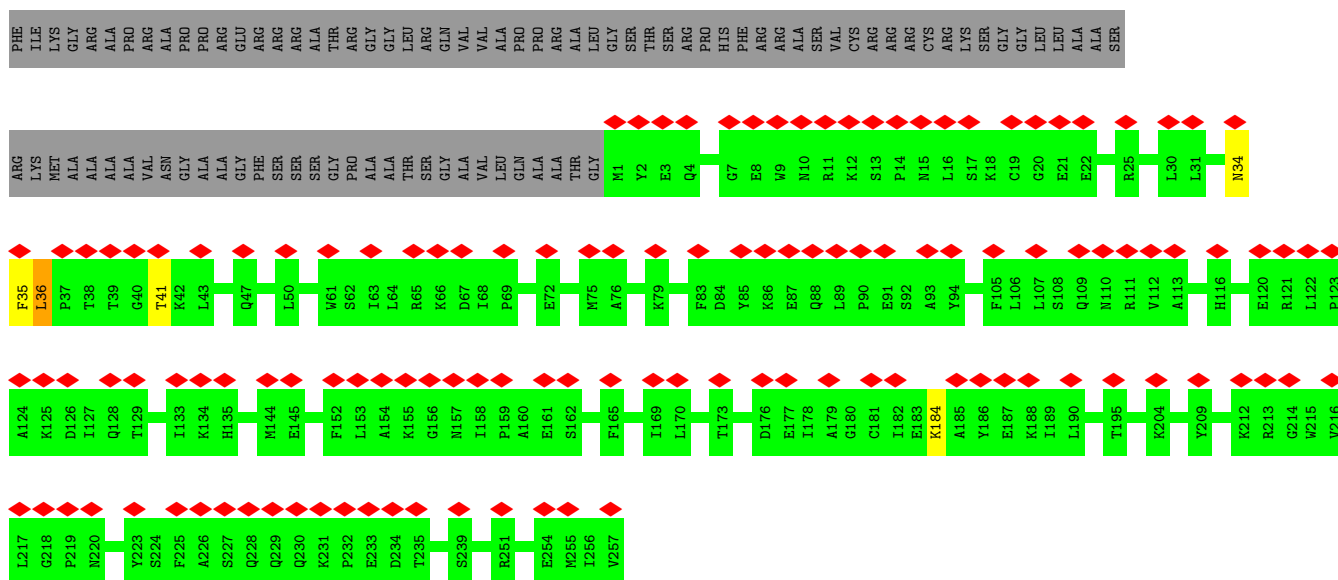
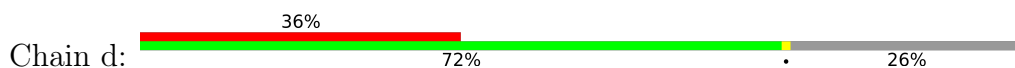
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 4



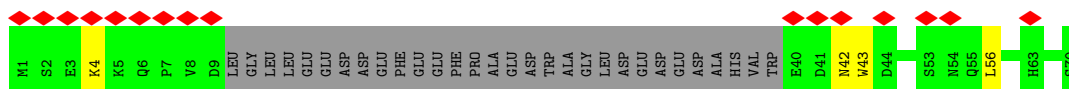
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 14



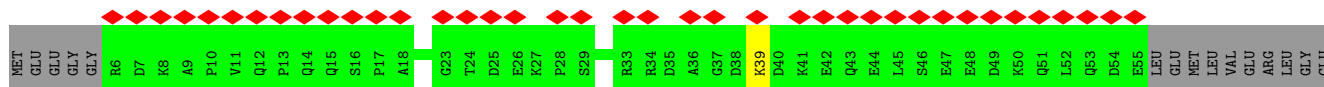
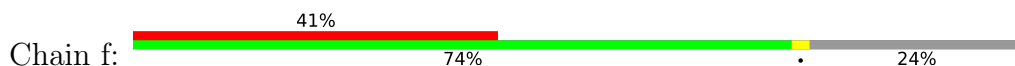
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 8

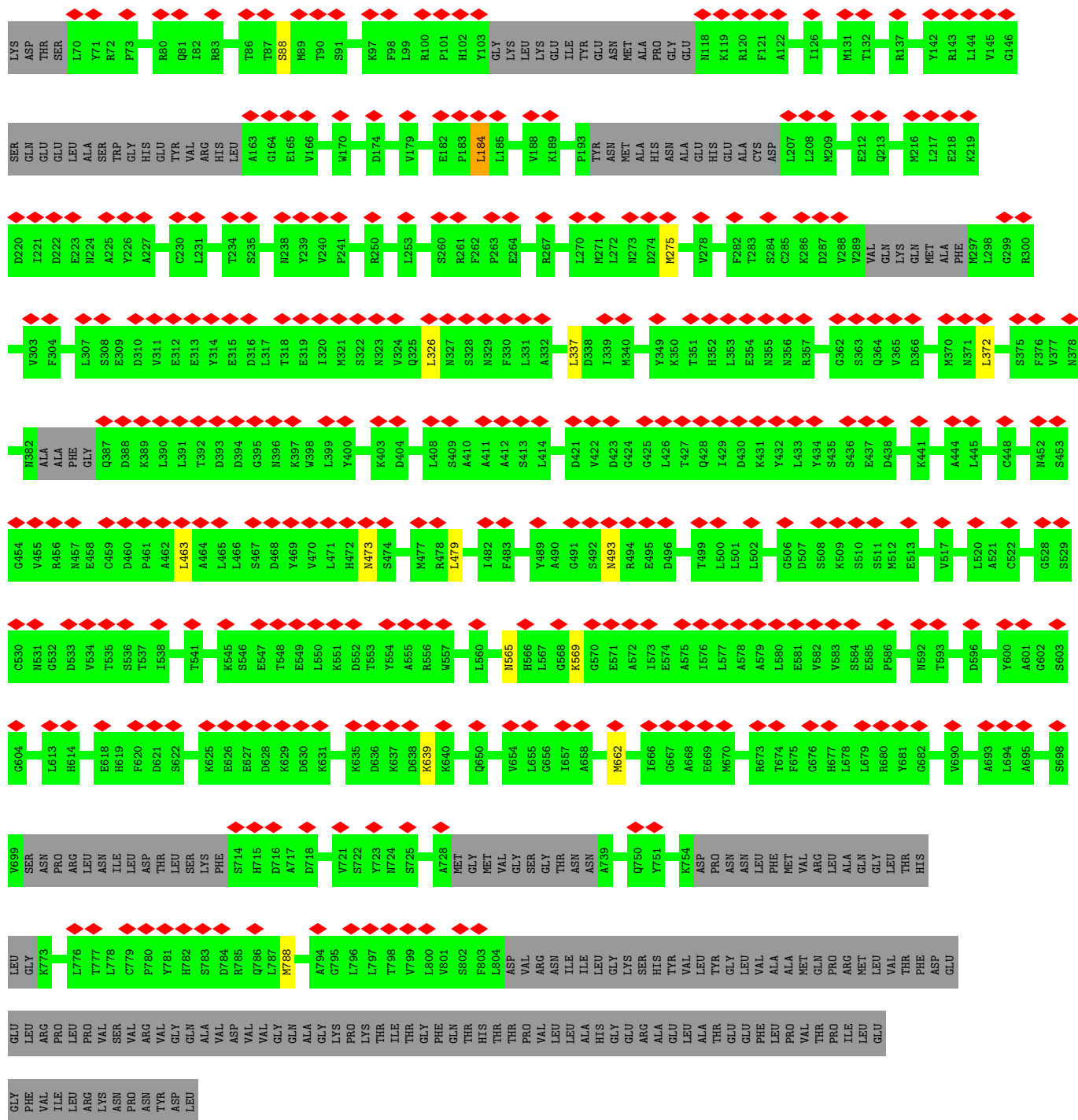


• Molecule 5: 26S proteasome complex subunit SEM1



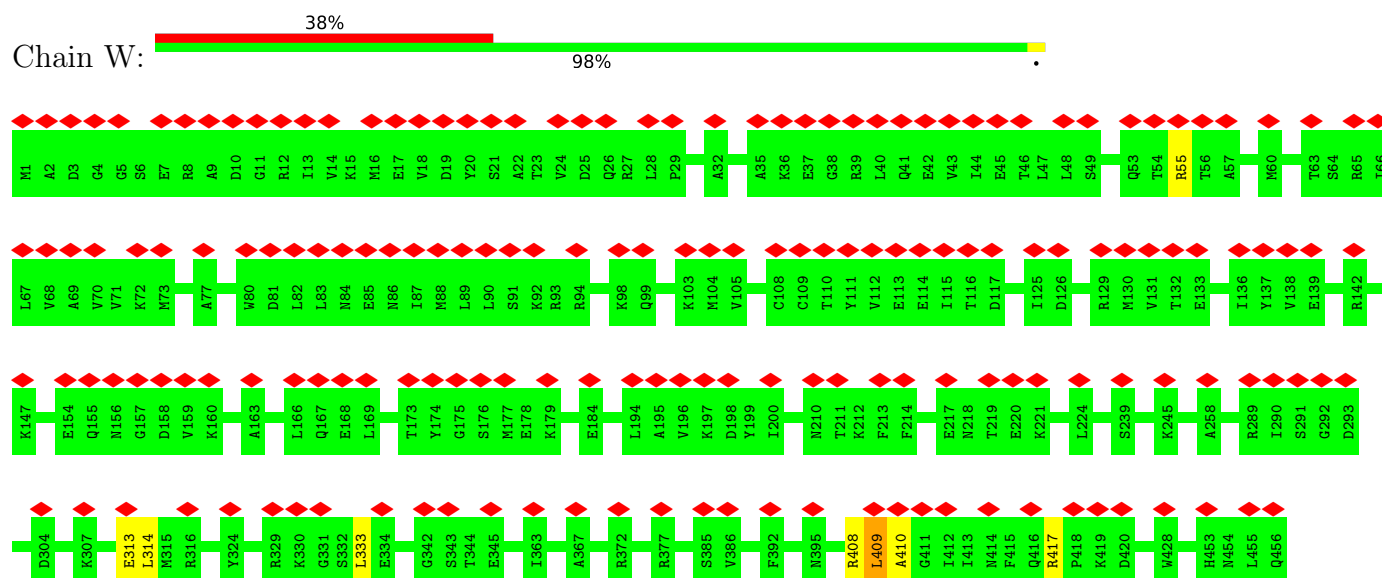
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 2



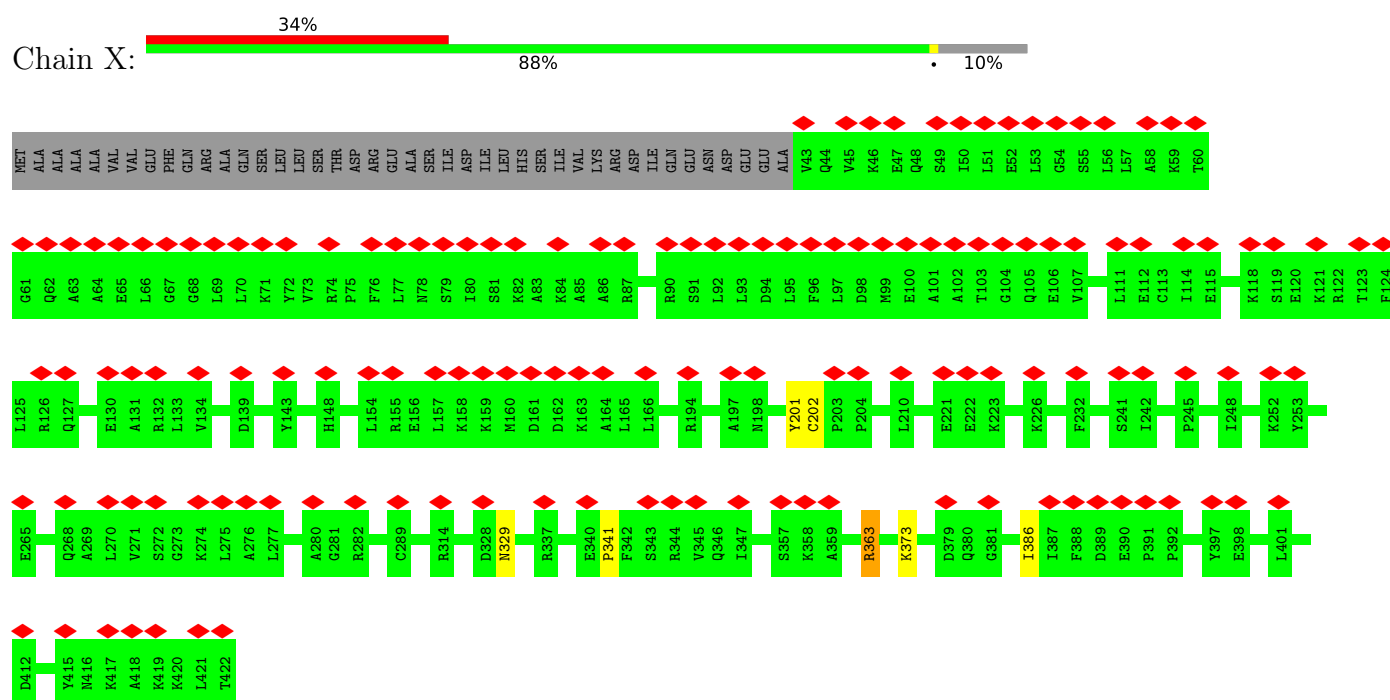




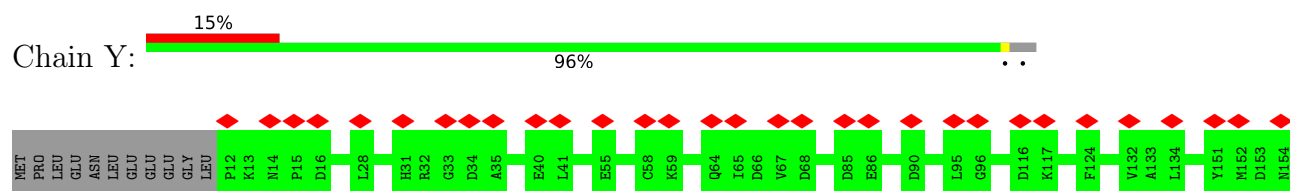
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



- Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



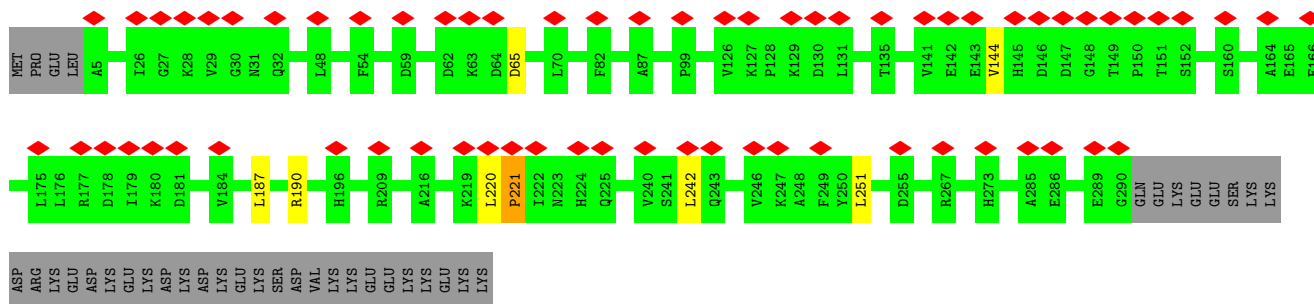
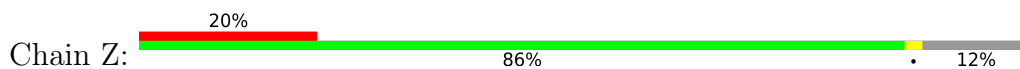
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6



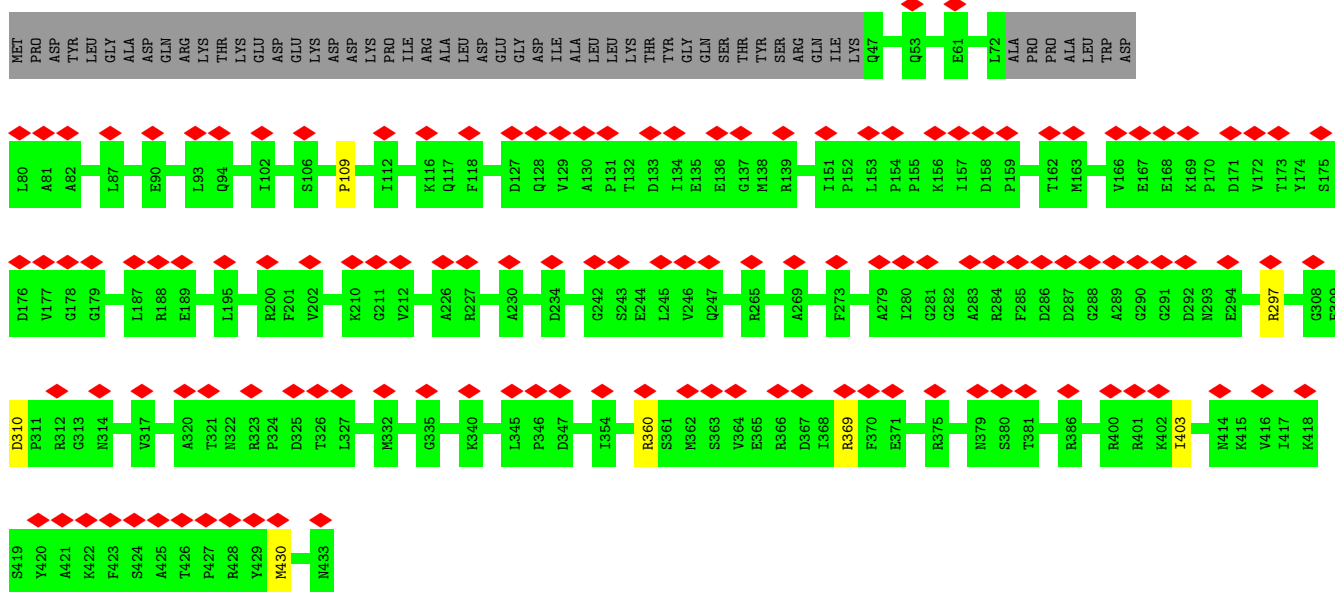
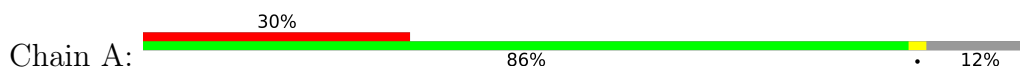




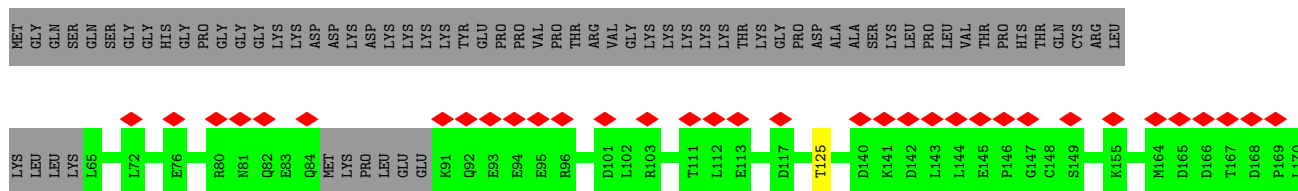
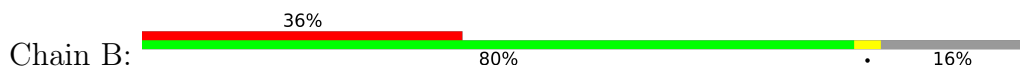
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

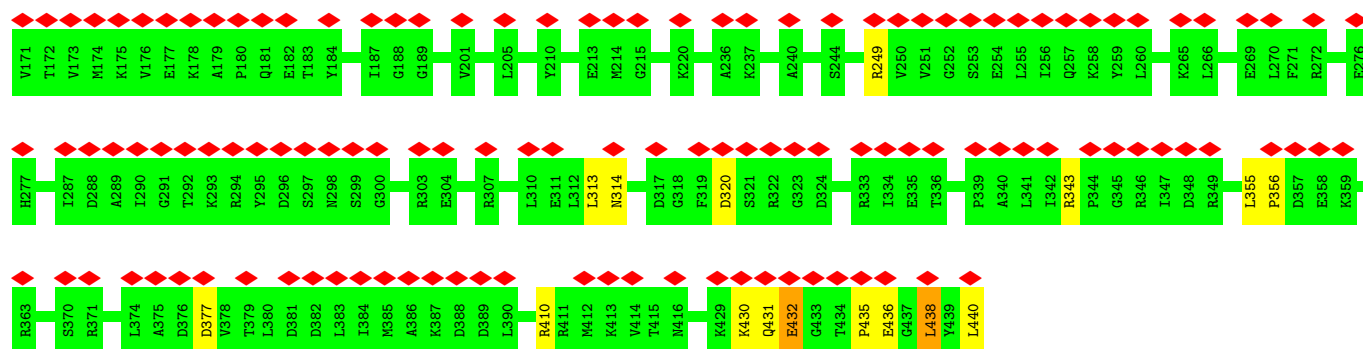


- Molecule 13: 26S protease regulatory subunit 7



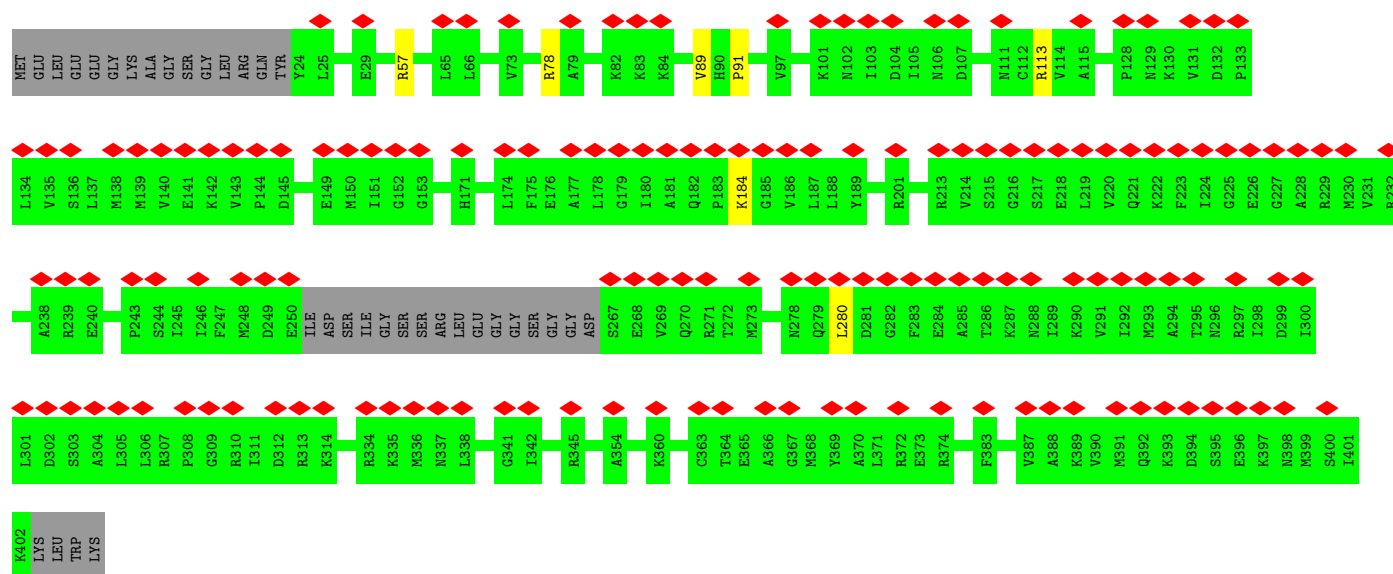
- Molecule 14: 26S protease regulatory subunit 4





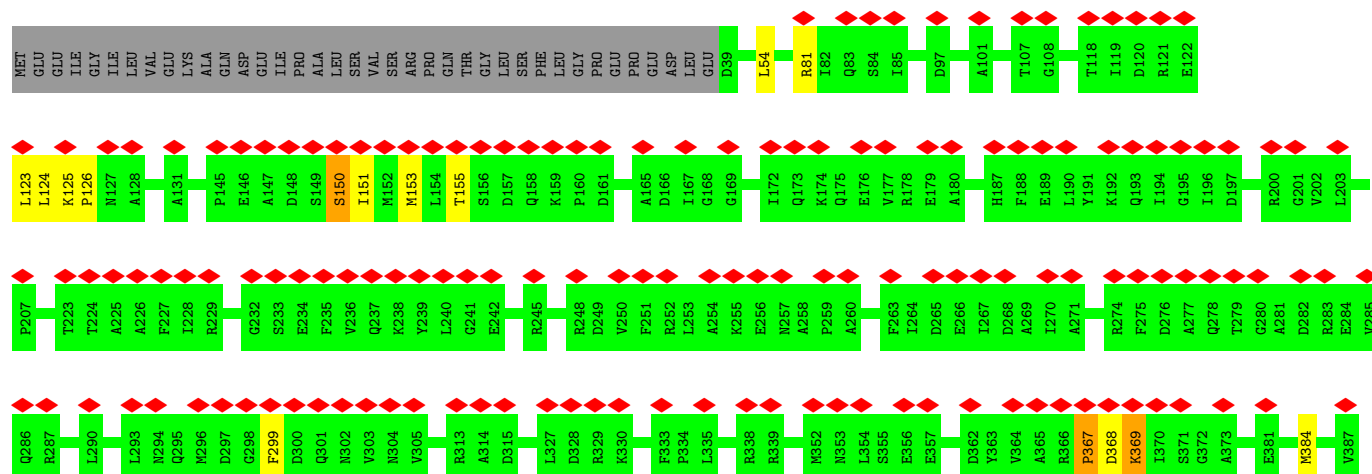
• Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8

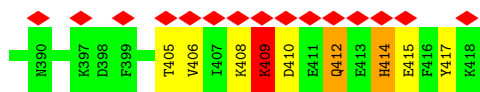
Chain C: 38% 89% 9%



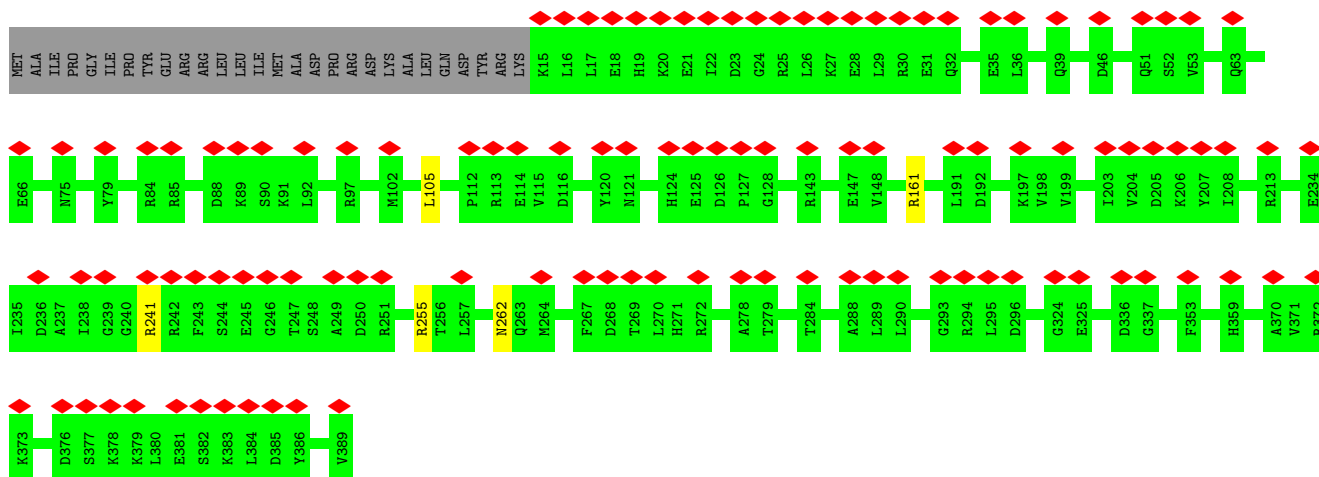
• Molecule 16: 26S protease regulatory subunit 6B

Chain D: 39% 85% 9%

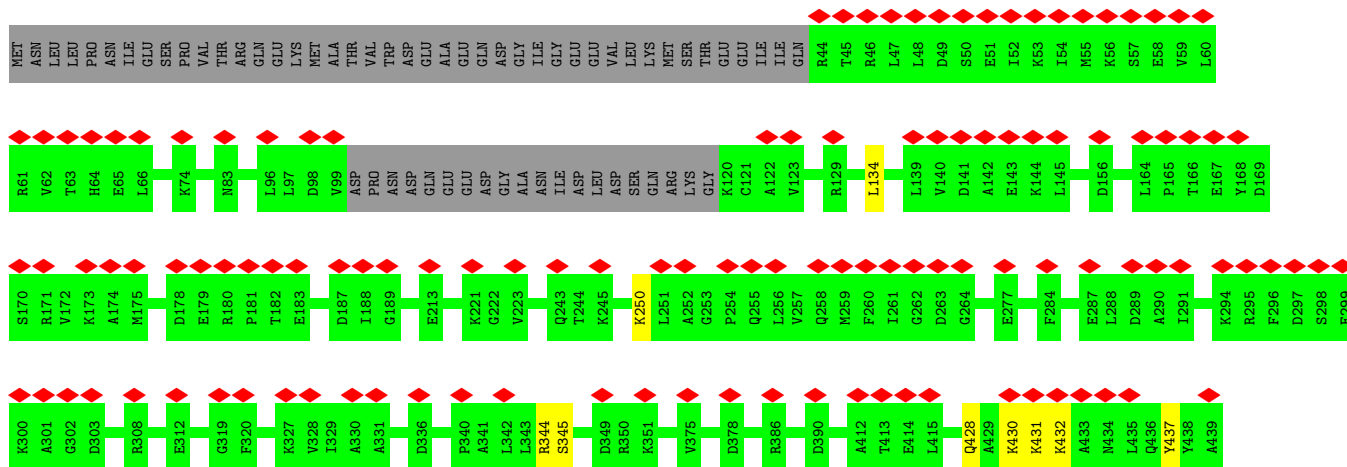
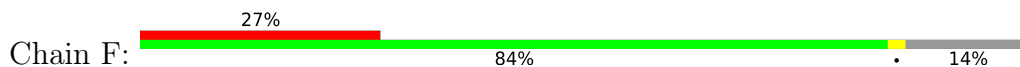




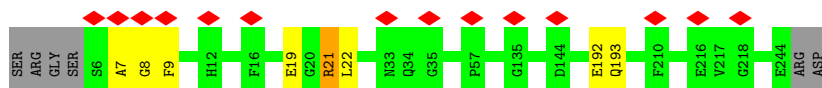
- Molecule 17: 26S proteasome regulatory subunit 10B



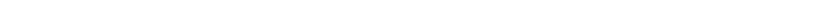
- Molecule 18: 26S protease regulatory subunit 6A

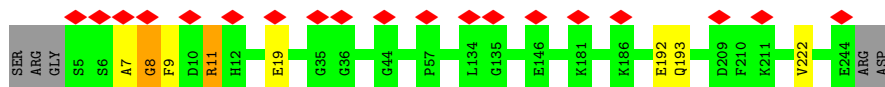


- Molecule 19: Proteasome subunit alpha type-6



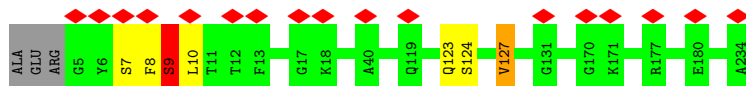
- Molecule 19: Proteasome subunit alpha type-6

Chain g: 



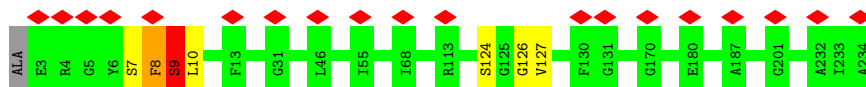
- Molecule 20: Proteasome subunit alpha type-2

Chain H:  7% 96%

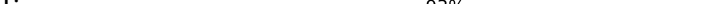


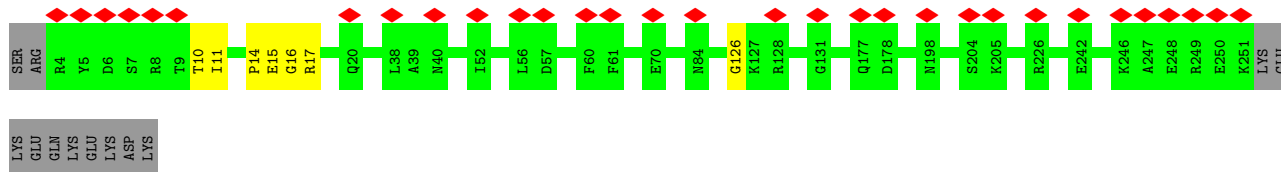
- Molecule 20: Proteasome subunit alpha type-2

Chain h:  8% 97%



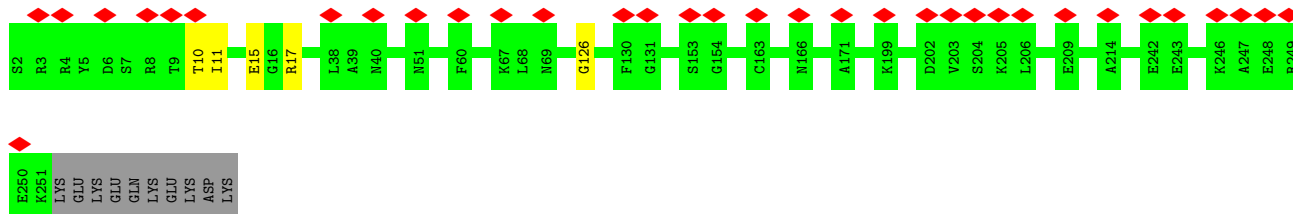
- Molecule 21: Proteasome subunit alpha type-4

Chain I:  12% 93% 5%



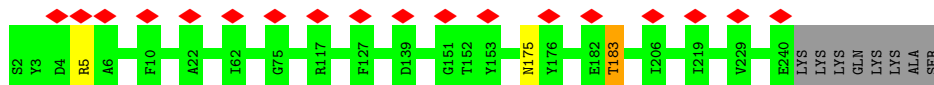
- Molecule 21: Proteasome subunit alpha type-4

Chain i:  13% 94% . .

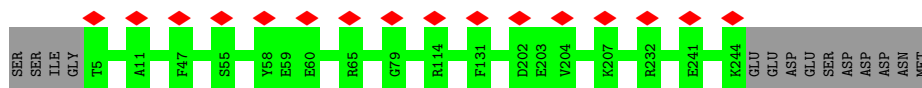


- Molecule 22: Proteasome subunit alpha type-7

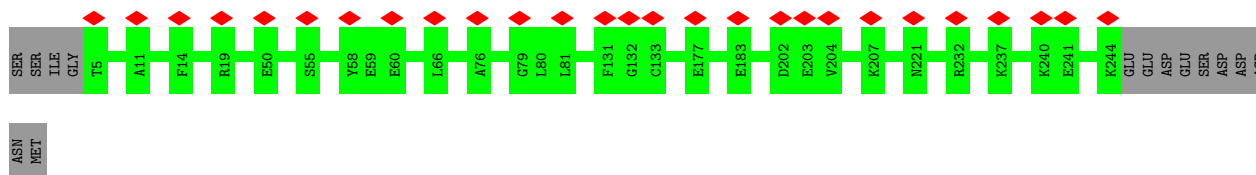
Chain J:  7% 96% ..



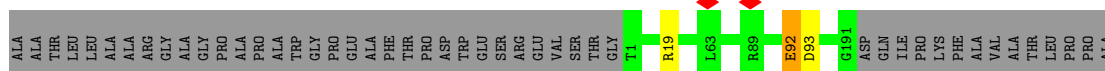
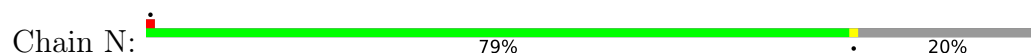




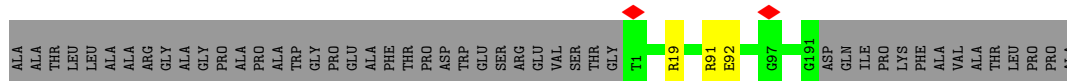
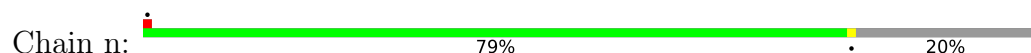
- Molecule 25: Proteasome subunit alpha type-3



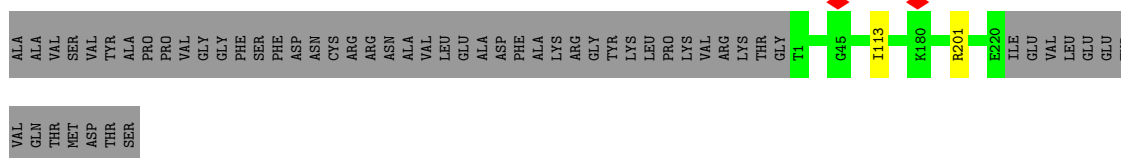
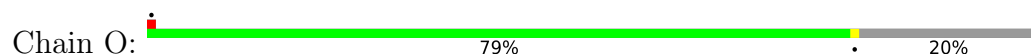
- Molecule 26: Proteasome subunit beta type-6



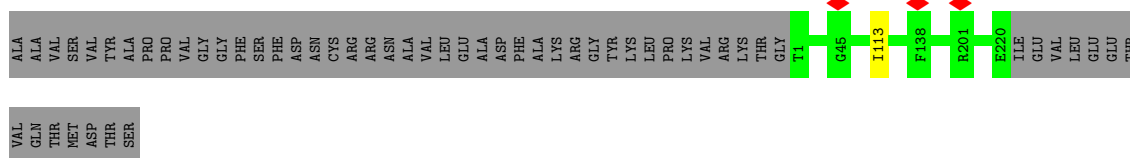
- Molecule 26: Proteasome subunit beta type-6



- Molecule 27: Proteasome subunit beta type-7



- Molecule 27: Proteasome subunit beta type-7



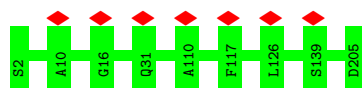
- Molecule 28: Proteasome subunit beta type-3

Chain P:  100%



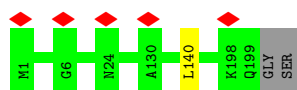
- Molecule 28: Proteasome subunit beta type-3

Chain p:  100%



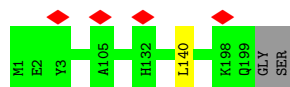
- Molecule 29: Proteasome subunit beta type-2

Chain Q:  99%


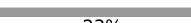


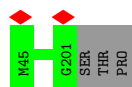
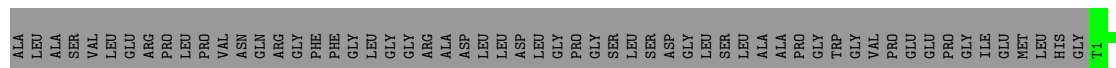
- Molecule 29: Proteasome subunit beta type-2

Chain q:  99%


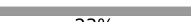


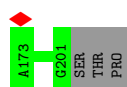
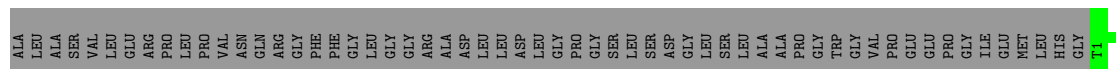
- Molecule 30: Proteasome subunit beta type-5

Chain R:  77%  23%




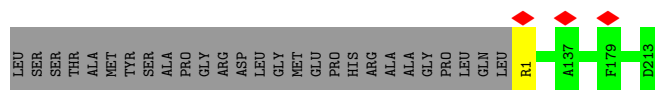
- Molecule 30: Proteasome subunit beta type-5

Chain r:  77%  23%




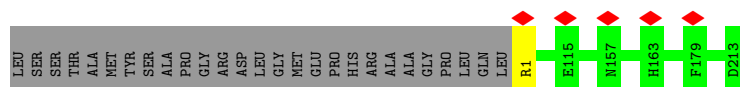
- Molecule 31: Proteasome subunit beta type-1

Chain S:  88% 11%




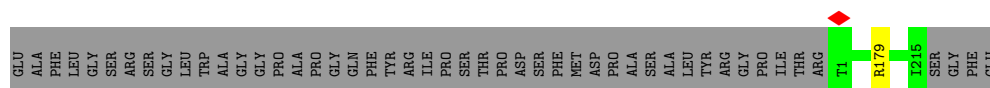
- Molecule 31: Proteasome subunit beta type-1

Chain s:  88% 11%




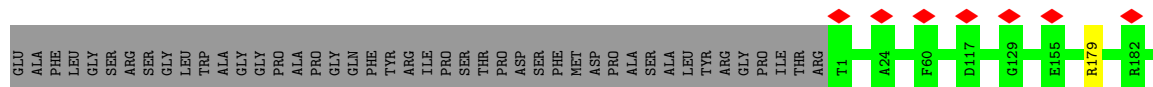
- Molecule 32: Proteasome subunit beta type-4

Chain T:  81% 18%



- Molecule 32: Proteasome subunit beta type-4

Chain t:  81% 18%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	a	0.31	0/3053	0.65	4/4133 (0.1%)
2	b	0.30	0/1477	0.63	1/1999 (0.1%)
3	c	0.32	0/2225	0.67	0/3005
4	d	0.32	0/2161	0.68	0/2917
5	e	0.36	0/337	0.84	1/448 (0.2%)
6	f	0.32	0/5392	0.71	5/7269 (0.1%)
7	U	0.32	0/6395	0.63	7/8645 (0.1%)
8	V	0.34	0/3882	0.68	3/5245 (0.1%)
9	W	0.32	0/3750	0.65	0/5040
10	X	0.31	0/3052	0.62	1/4113 (0.0%)
11	Y	0.33	0/3171	0.65	1/4269 (0.0%)
12	Z	0.34	0/2323	0.70	5/3148 (0.2%)
13	A	0.29	0/2938	0.57	0/3968
14	B	0.29	0/2843	0.60	3/3844 (0.1%)
15	C	0.31	0/2895	0.60	1/3893 (0.0%)
16	D	0.32	0/3089	0.62	2/4166 (0.0%)
17	E	0.30	0/2903	0.55	1/3922 (0.0%)
18	F	0.30	0/2896	0.54	1/3910 (0.0%)
19	G	0.32	0/1853	0.58	0/2515
19	g	0.31	0/1859	0.59	1/2523 (0.0%)
20	H	0.32	0/1723	0.59	2/2346 (0.1%)
20	h	0.32	0/1743	0.59	2/2372 (0.1%)
21	I	0.31	0/1925	0.60	0/2606
21	i	0.31	0/1942	0.60	0/2628
22	J	0.30	0/1728	0.54	1/2358 (0.0%)
22	j	0.30	0/1728	0.52	0/2358
23	K	0.31	0/1755	0.57	0/2375
23	k	0.31	0/1747	0.56	0/2364
24	L	0.32	0/1885	0.57	0/2552
24	l	0.32	0/1885	0.57	0/2552
25	M	0.33	0/1891	0.56	0/2552
25	m	0.33	0/1891	0.56	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
26	N	0.32	0/1454	0.55	0/1967
26	n	0.32	0/1454	0.54	0/1967
27	O	0.31	0/1670	0.55	1/2265 (0.0%)
27	o	0.31	0/1670	0.55	1/2265 (0.0%)
28	P	0.32	0/1614	0.52	0/2177
28	p	0.32	0/1614	0.53	0/2177
29	Q	0.34	0/1603	0.58	0/2174
29	q	0.34	0/1603	0.58	0/2174
30	R	0.33	0/1579	0.51	0/2134
30	r	0.33	0/1579	0.51	0/2134
31	S	0.32	0/1671	0.52	0/2253
31	s	0.32	0/1671	0.52	0/2253
32	T	0.32	0/1700	0.52	0/2305
32	t	0.32	0/1700	0.52	0/2305
All	All	0.32	0/102919	0.60	44/139137 (0.0%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	56	LEU	CA-CB-CG	7.90	133.48	115.30
11	Y	287	LEU	CA-CB-CG	7.33	132.16	115.30
16	D	54	LEU	CA-CB-CG	6.83	131.01	115.30
6	f	479	LEU	CA-CB-CG	6.76	130.84	115.30
20	H	8	PHE	N-CA-C	-6.73	92.82	111.00
1	a	8	LEU	CA-CB-CG	6.71	130.73	115.30
20	h	8	PHE	N-CA-C	-6.61	93.16	111.00
16	D	409	LYS	N-CA-C	6.59	128.79	111.00
1	a	180	LEU	CA-CB-CG	6.56	130.38	115.30
8	V	254	LEU	CA-CB-CG	6.52	130.30	115.30
6	f	184	LEU	CA-CB-CG	6.47	130.19	115.30
10	X	363	ARG	N-CA-C	-6.40	93.71	111.00
8	V	357	LEU	CA-CB-CG	6.34	129.87	115.30
12	Z	187	LEU	CA-CB-CG	6.33	129.86	115.30
22	J	183	THR	N-CA-C	-6.30	94.00	111.00
6	f	372	LEU	CA-CB-CG	6.26	129.70	115.30
7	U	187	LEU	CA-CB-CG	6.14	129.43	115.30
1	a	187	ASP	CB-CG-OD1	5.92	123.62	118.30
12	Z	221	PRO	N-CA-C	-5.87	96.84	112.10
8	V	170	LEU	CA-CB-CG	5.68	128.37	115.30
12	Z	65	ASP	CB-CG-OD1	5.67	123.41	118.30
14	B	320	ASP	CB-CG-OD1	5.57	123.31	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	242	LEU	CA-CB-CG	5.51	127.97	115.30
14	B	313	LEU	CA-CB-CG	5.50	127.95	115.30
19	g	8	GLY	N-CA-C	5.50	126.84	113.10
7	U	168	LEU	CA-CB-CG	5.49	127.94	115.30
14	B	355	LEU	N-CA-C	-5.43	96.33	111.00
27	O	113	ILE	C-N-CA	5.43	135.28	121.70
27	o	113	ILE	C-N-CA	5.43	135.27	121.70
6	f	337	LEU	CA-CB-CG	5.41	127.75	115.30
7	U	220	LEU	CA-CB-CG	5.38	127.67	115.30
17	E	105	LEU	CA-CB-CG	5.35	127.61	115.30
2	b	22	LEU	C-N-CD	-5.31	108.92	120.60
7	U	223	LEU	CA-CB-CG	5.23	127.33	115.30
20	h	9	SER	C-N-CA	5.23	134.78	121.70
7	U	224	ASP	CB-CG-OD1	5.18	122.96	118.30
7	U	797	MET	CA-CB-CG	5.12	122.00	113.30
18	F	134	LEU	CA-CB-CG	5.11	127.05	115.30
6	f	463	LEU	CA-CB-CG	5.08	126.99	115.30
20	H	9	SER	C-N-CA	5.08	134.39	121.70
7	U	371	ILE	CG1-CB-CG2	-5.05	100.30	111.40
15	C	280	LEU	CA-CB-CG	5.04	126.88	115.30
12	Z	251	LEU	CA-CB-CG	5.01	126.83	115.30
1	a	180	LEU	CB-CG-CD1	-5.01	102.48	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	a	371/376 (99%)	334 (90%)	36 (10%)	1 (0%)	37	72
2	b	189/377 (50%)	165 (87%)	23 (12%)	1 (0%)	25	64
3	c	274/309 (89%)	230 (84%)	44 (16%)	0	100	100
4	d	255/349 (73%)	220 (86%)	32 (12%)	3 (1%)	11	44
5	e	36/70 (51%)	27 (75%)	8 (22%)	1 (3%)	4	24
6	f	669/908 (74%)	582 (87%)	86 (13%)	1 (0%)	48	83
7	U	798/953 (84%)	721 (90%)	76 (10%)	1 (0%)	48	83
8	V	471/533 (88%)	400 (85%)	70 (15%)	1 (0%)	44	78
9	W	454/456 (100%)	392 (86%)	58 (13%)	4 (1%)	14	50
10	X	378/422 (90%)	336 (89%)	38 (10%)	4 (1%)	12	46
11	Y	376/389 (97%)	329 (88%)	47 (12%)	0	100	100
12	Z	284/324 (88%)	245 (86%)	37 (13%)	2 (1%)	19	56
13	A	376/433 (87%)	328 (87%)	46 (12%)	2 (0%)	25	64
14	B	366/440 (83%)	324 (88%)	36 (10%)	6 (2%)	8	37
15	C	359/398 (90%)	317 (88%)	40 (11%)	2 (1%)	22	59
16	D	378/418 (90%)	324 (86%)	41 (11%)	13 (3%)	3	20
17	E	373/403 (93%)	330 (88%)	43 (12%)	0	100	100
18	F	372/439 (85%)	329 (88%)	41 (11%)	2 (0%)	25	64
19	G	237/245 (97%)	204 (86%)	29 (12%)	4 (2%)	7	35
19	g	238/245 (97%)	207 (87%)	28 (12%)	3 (1%)	10	42
20	H	228/233 (98%)	213 (93%)	12 (5%)	3 (1%)	10	42
20	h	230/233 (99%)	213 (93%)	14 (6%)	3 (1%)	10	42
21	I	246/260 (95%)	220 (89%)	22 (9%)	4 (2%)	8	37
21	i	248/260 (95%)	222 (90%)	24 (10%)	2 (1%)	16	53
22	J	237/247 (96%)	219 (92%)	17 (7%)	1 (0%)	30	68
22	j	237/247 (96%)	221 (93%)	16 (7%)	0	100	100
23	K	224/240 (93%)	202 (90%)	22 (10%)	0	100	100
23	k	224/240 (93%)	202 (90%)	22 (10%)	0	100	100
24	L	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
24	l	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
25	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
25	m	238/254 (94%)	218 (92%)	20 (8%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	N	189/238 (79%)	174 (92%)	13 (7%)	2 (1%)	12	46
26	n	189/238 (79%)	176 (93%)	12 (6%)	1 (0%)	25	64
27	O	218/276 (79%)	208 (95%)	10 (5%)	0	100	100
27	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	P	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
28	p	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
29	Q	197/201 (98%)	179 (91%)	18 (9%)	0	100	100
29	q	197/201 (98%)	179 (91%)	18 (9%)	0	100	100
30	R	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
30	r	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
31	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
31	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
32	T	213/263 (81%)	200 (94%)	13 (6%)	0	100	100
32	t	213/263 (81%)	200 (94%)	13 (6%)	0	100	100
All	All	12934/14859 (87%)	11629 (90%)	1238 (10%)	67 (0%)	27	64

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	23	PRO
4	d	34	ASN
9	W	410	ALA
10	X	363	ARG
10	X	386	ILE
12	Z	221	PRO
14	B	435	PRO
15	C	91	PRO
16	D	125	LYS
16	D	153	MET
16	D	367	PRO
16	D	409	LYS
16	D	410	ASP
16	D	417	TYR
18	F	344	ARG
18	F	437	TYR
19	G	7	ALA
20	H	10	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	I	126	GLY
22	J	183	THR
26	N	92	GLU
19	g	8	GLY
19	g	11	ARG
20	h	10	LEU
21	i	126	GLY
12	Z	144	VAL
14	B	438	LEU
19	G	8	GLY
19	G	9	PHE
20	H	9	SER
20	H	127	VAL
19	g	7	ALA
20	h	9	SER
20	h	126	GLY
1	a	187	ASP
6	f	326	LEU
8	V	81	GLN
9	W	313	GLU
10	X	202	CYS
14	B	432	GLU
16	D	369	LYS
16	D	412	GLN
16	D	414	HIS
19	G	21	ARG
7	U	561	GLU
9	W	314	LEU
9	W	409	LEU
14	B	356	PRO
16	D	126	PRO
16	D	150	SER
16	D	299	PHE
21	I	14	PRO
26	n	19	ARG
4	d	35	PHE
10	X	201	TYR
14	B	377	ASP
21	I	10	THR
26	N	19	ARG
21	i	10	THR
5	e	4	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	A	109	PRO
14	B	436	GLU
16	D	155	THR
21	I	16	GLY
4	d	36	LEU
15	C	89	VAL
13	A	310	ASP

### 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	a	333/336 (99%)	333 (100%)	0	100	100
2	b	166/312 (53%)	165 (99%)	1 (1%)	84	88
3	c	243/267 (91%)	243 (100%)	0	100	100
4	d	230/293 (78%)	227 (99%)	3 (1%)	65	77
5	e	37/63 (59%)	35 (95%)	2 (5%)	18	40
6	f	579/763 (76%)	568 (98%)	11 (2%)	52	70
7	U	685/816 (84%)	678 (99%)	7 (1%)	73	82
8	V	409/459 (89%)	402 (98%)	7 (2%)	56	72
9	W	415/416 (100%)	410 (99%)	5 (1%)	67	79
10	X	326/362 (90%)	323 (99%)	3 (1%)	75	83
11	Y	333/344 (97%)	331 (99%)	2 (1%)	84	88
12	Z	257/295 (87%)	255 (99%)	2 (1%)	79	85
13	A	297/372 (80%)	292 (98%)	5 (2%)	56	72
14	B	300/385 (78%)	290 (97%)	10 (3%)	33	53
15	C	314/346 (91%)	310 (99%)	4 (1%)	65	77
16	D	332/366 (91%)	316 (95%)	16 (5%)	21	43
17	E	298/353 (84%)	294 (99%)	4 (1%)	65	77
18	F	296/379 (78%)	290 (98%)	6 (2%)	50	69

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	G	192/209 (92%)	187 (97%)	5 (3%)	41	60
19	g	193/209 (92%)	187 (97%)	6 (3%)	35	55
20	H	162/190 (85%)	157 (97%)	5 (3%)	35	55
20	h	164/190 (86%)	159 (97%)	5 (3%)	36	56
21	I	191/220 (87%)	188 (98%)	3 (2%)	58	74
21	i	193/220 (88%)	190 (98%)	3 (2%)	58	74
22	J	152/210 (72%)	150 (99%)	2 (1%)	65	77
22	j	152/210 (72%)	150 (99%)	2 (1%)	65	77
23	K	187/202 (93%)	182 (97%)	5 (3%)	40	59
23	k	186/202 (92%)	182 (98%)	4 (2%)	47	66
24	L	198/229 (86%)	198 (100%)	0	100	100
24	l	198/229 (86%)	198 (100%)	0	100	100
25	M	192/211 (91%)	192 (100%)	0	100	100
25	m	192/211 (91%)	192 (100%)	0	100	100
26	N	148/180 (82%)	146 (99%)	2 (1%)	62	76
26	n	148/180 (82%)	146 (99%)	2 (1%)	62	76
27	O	177/227 (78%)	176 (99%)	1 (1%)	84	88
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	172/173 (99%)	172 (100%)	0	100	100
28	p	172/173 (99%)	172 (100%)	0	100	100
29	Q	164/171 (96%)	163 (99%)	1 (1%)	84	88
29	q	164/171 (96%)	163 (99%)	1 (1%)	84	88
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100
31	S	174/198 (88%)	173 (99%)	1 (1%)	84	88
31	s	174/198 (88%)	173 (99%)	1 (1%)	84	88
32	T	175/214 (82%)	174 (99%)	1 (1%)	84	88
32	t	175/214 (82%)	174 (99%)	1 (1%)	84	88
All	All	10728/12597 (85%)	10589 (99%)	139 (1%)	64	77

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	22	LEU
4	d	36	LEU
4	d	41	THR
4	d	184	LYS
5	e	42	ASN
5	e	43	TRP
6	f	39	LYS
6	f	88	SER
6	f	184	LEU
6	f	275	MET
6	f	473	ASN
6	f	493	ASN
6	f	565	ASN
6	f	569	LYS
6	f	639	LYS
6	f	662	MET
6	f	788	MET
7	U	129	ARG
7	U	223	LEU
7	U	345	ASN
7	U	429	LYS
7	U	561	GLU
7	U	629	THR
7	U	797	MET
8	V	54	LYS
8	V	79	VAL
8	V	80	LYS
8	V	86	VAL
8	V	328	VAL
8	V	346	LEU
8	V	347	GLN
9	W	55	ARG
9	W	333	LEU
9	W	408	ARG
9	W	409	LEU
9	W	417	ARG
10	X	329	ASN
10	X	341	PRO
10	X	373	LYS
11	Y	297	ARG
11	Y	357	ASN
12	Z	190	ARG
12	Z	220	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	A	297	ARG
13	A	360	ARG
13	A	369	ARG
13	A	403	ILE
13	A	430	MET
14	B	125	THR
14	B	249	ARG
14	B	314	ASN
14	B	343	ARG
14	B	410	ARG
14	B	430	LYS
14	B	431	GLN
14	B	432	GLU
14	B	438	LEU
14	B	440	LEU
15	C	57	ARG
15	C	78	ARG
15	C	113	ARG
15	C	184	LYS
16	D	81	ARG
16	D	123	LEU
16	D	124	LEU
16	D	150	SER
16	D	151	ILE
16	D	367	PRO
16	D	368	ASP
16	D	369	LYS
16	D	384	MET
16	D	405	THR
16	D	406	VAL
16	D	408	LYS
16	D	409	LYS
16	D	412	GLN
16	D	414	HIS
16	D	415	GLU
17	E	161	ARG
17	E	241	ARG
17	E	255	ARG
17	E	262	ASN
18	F	250	LYS
18	F	345	SER
18	F	428	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	F	430	LYS
18	F	431	LYS
18	F	432	LYS
19	G	19	GLU
19	G	21	ARG
19	G	22	LEU
19	G	192	GLU
19	G	193	GLN
20	H	7	SER
20	H	9	SER
20	H	123	GLN
20	H	124	SER
20	H	127	VAL
21	I	11	ILE
21	I	15	GLU
21	I	17	ARG
22	J	5	ARG
22	J	175	ASN
23	K	9	ASP
23	K	10	ARG
23	K	20	ARG
23	K	21	LEU
23	K	22	PHE
26	N	92	GLU
26	N	93	ASP
27	O	201	ARG
29	Q	140	LEU
31	S	1	ARG
32	T	179	ARG
19	g	9	PHE
19	g	11	ARG
19	g	19	GLU
19	g	192	GLU
19	g	193	GLN
19	g	222	VAL
20	h	7	SER
20	h	8	PHE
20	h	9	SER
20	h	124	SER
20	h	127	VAL
21	i	11	ILE
21	i	15	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	i	17	ARG
22	j	7	ILE
22	j	175	ASN
23	k	9	ASP
23	k	20	ARG
23	k	21	LEU
23	k	22	PHE
26	n	91	ARG
26	n	92	GLU
29	q	140	LEU
31	s	1	ARG
32	t	179	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	35	HIS
1	a	86	GLN
1	a	193	GLN
1	a	231	GLN
2	b	79	GLN
3	c	101	GLN
3	c	256	ASN
4	d	4	GLN
4	d	135	HIS
6	f	102	HIS
6	f	180	GLN
6	f	329	ASN
6	f	452	ASN
6	f	493	ASN
6	f	540	GLN
6	f	565	ASN
7	U	345	ASN
7	U	768	GLN
7	U	880	ASN
8	V	81	GLN
8	V	118	GLN
8	V	199	ASN
8	V	347	GLN
8	V	453	HIS
8	V	473	GLN
9	W	235	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	X	148	HIS
10	X	296	ASN
10	X	349	HIS
11	Y	363	ASN
11	Y	365	GLN
12	Z	243	GLN
13	A	150	HIS
13	A	247	GLN
14	B	241	ASN
15	C	90	HIS
15	C	278	ASN
15	C	332	HIS
16	D	49	GLN
16	D	74	HIS
16	D	133	HIS
16	D	173	GLN
16	D	353	ASN
16	D	412	GLN
17	E	194	ASN
17	E	263	GLN
17	E	323	HIS
17	E	339	ASN
18	F	255	GLN
18	F	333	ASN
19	G	100	ASN
19	G	123	GLN
20	H	119	GLN
21	I	119	GLN
21	I	146	GLN
22	J	175	ASN
23	K	41	GLN
23	K	98	ASN
23	K	152	GLN
23	K	164	GLN
23	K	214	ASN
23	K	227	HIS
24	L	117	GLN
27	O	62	ASN
27	O	91	GLN
28	P	173	ASN
29	Q	65	GLN
29	Q	101	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	Q	168	GLN
30	R	38	ASN
30	R	119	ASN
32	T	69	GLN
21	i	119	GLN
21	i	146	GLN
22	j	122	ASN
22	j	154	HIS
22	j	175	ASN
23	k	41	GLN
23	k	114	GLN
23	k	152	GLN
23	k	164	GLN
23	k	214	ASN
23	k	227	HIS
24	l	8	ASN
27	o	62	ASN
27	o	91	GLN
29	q	65	GLN
29	q	101	ASN
29	q	168	GLN
30	r	38	ASN
32	t	2	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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$
34	ATP	D	501	-	26,33,33	2.79	1 (3%)	31,52,52	1.37	3 (9%)
34	ATP	F	501	-	26,33,33	2.77	1 (3%)	31,52,52	1.46	4 (12%)
34	ATP	E	401	-	26,33,33	2.77	1 (3%)	31,52,52	1.56	3 (9%)
34	ATP	A	501	-	26,33,33	2.78	1 (3%)	31,52,52	1.30	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	D	501	-	-	6/18/38/38	0/3/3/3
34	ATP	F	501	-	-	9/18/38/38	0/3/3/3
34	ATP	E	401	-	-	7/18/38/38	0/3/3/3
34	ATP	A	501	-	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	ATP	PG-O1G	13.90	1.95	1.50
34	F	501	ATP	PG-O1G	13.84	1.95	1.50
34	A	501	ATP	PG-O1G	13.84	1.95	1.50
34	E	401	ATP	PG-O1G	13.81	1.95	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	401	ATP	PA-O3A-PB	-5.74	113.13	132.83
34	E	401	ATP	PB-O3B-PG	-5.37	114.42	132.83
34	D	501	ATP	PA-O3A-PB	-5.16	115.11	132.83
34	F	501	ATP	PB-O3B-PG	-4.88	116.08	132.83
34	A	501	ATP	PA-O3A-PB	-4.38	117.80	132.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	501	ATP	PB-O3B-PG	-4.19	118.44	132.83
34	F	501	ATP	PA-O3A-PB	-4.04	118.98	132.83
34	A	501	ATP	PB-O3B-PG	-3.75	119.95	132.83
34	F	501	ATP	C3'-C2'-C1'	2.74	105.10	100.98
34	F	501	ATP	C5-C6-N6	2.26	123.79	120.35
34	E	401	ATP	C5-C6-N6	2.24	123.76	120.35
34	A	501	ATP	C5-C6-N6	2.17	123.64	120.35
34	D	501	ATP	C5-C6-N6	2.05	123.47	120.35

There are no chirality outliers.

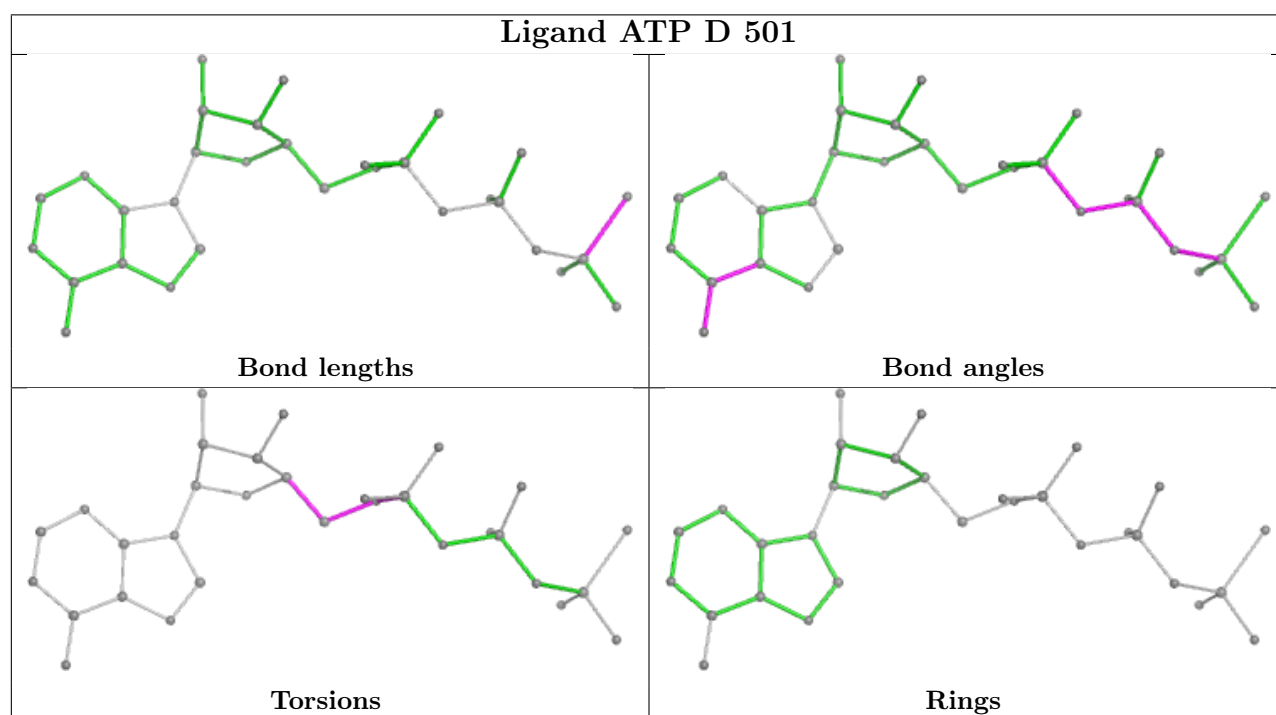
All (27) torsion outliers are listed below:

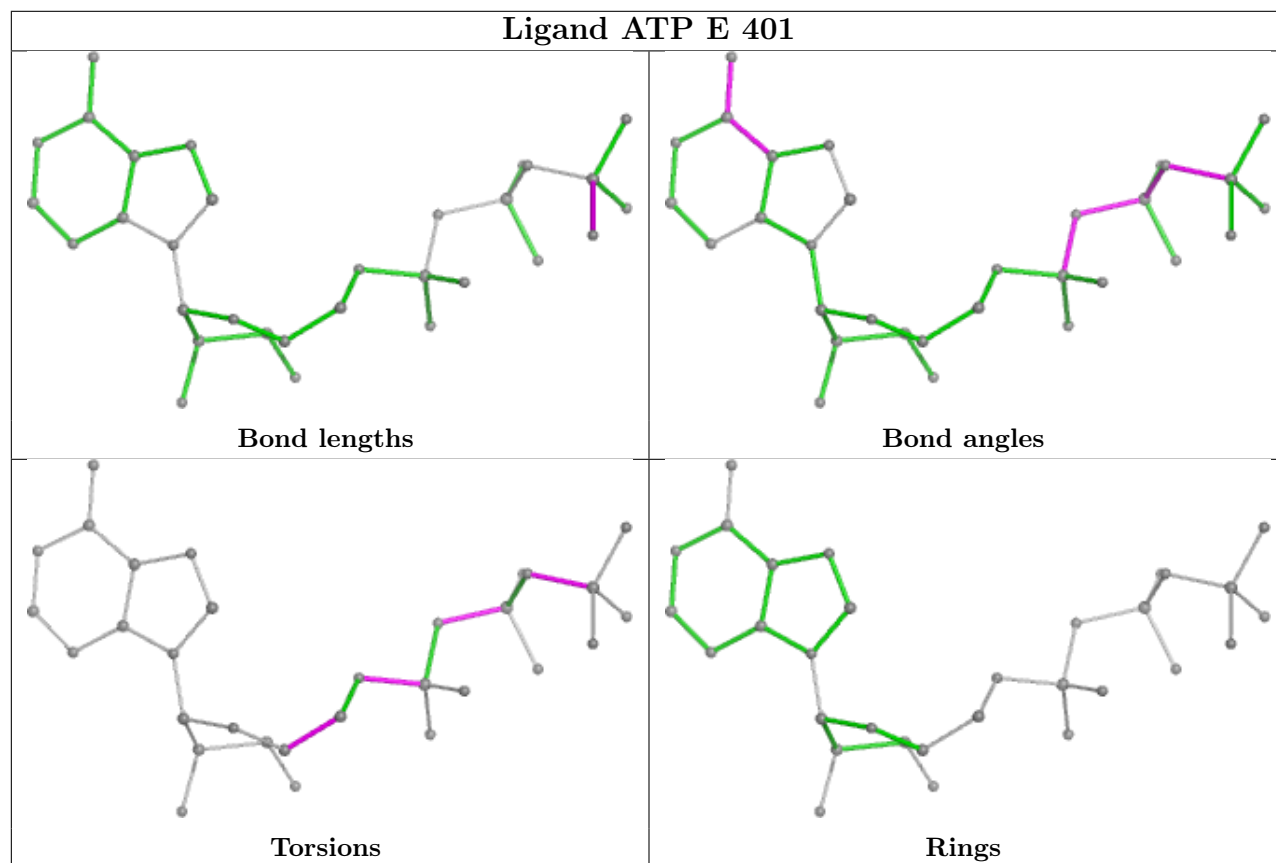
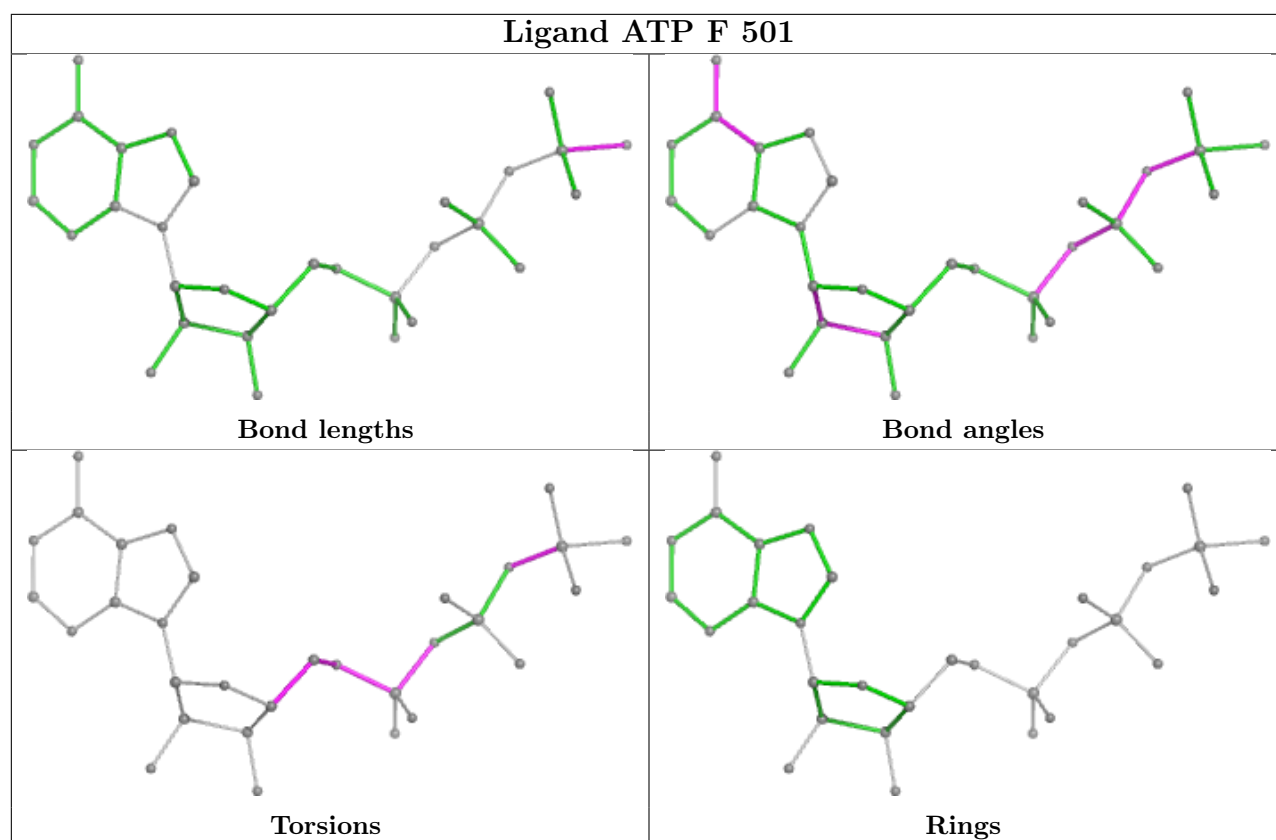
Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C3'-C4'-C5'-O5'
34	D	501	ATP	C5'-O5'-PA-O1A
34	E	401	ATP	PB-O3B-PG-O2G
34	E	401	ATP	PB-O3B-PG-O3G
34	F	501	ATP	PB-O3B-PG-O2G
34	F	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	O4'-C4'-C5'-O5'
34	D	501	ATP	O4'-C4'-C5'-O5'
34	D	501	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	C3'-C4'-C5'-O5'
34	D	501	ATP	C4'-C5'-O5'-PA
34	F	501	ATP	C4'-C5'-O5'-PA
34	D	501	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	C5'-O5'-PA-O3A
34	D	501	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	C5'-O5'-PA-O2A
34	F	501	ATP	C5'-O5'-PA-O2A
34	A	501	ATP	C4'-C5'-O5'-PA
34	E	401	ATP	PA-O3A-PB-O1B
34	F	501	ATP	PB-O3B-PG-O1G
34	A	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	PB-O3A-PA-O2A

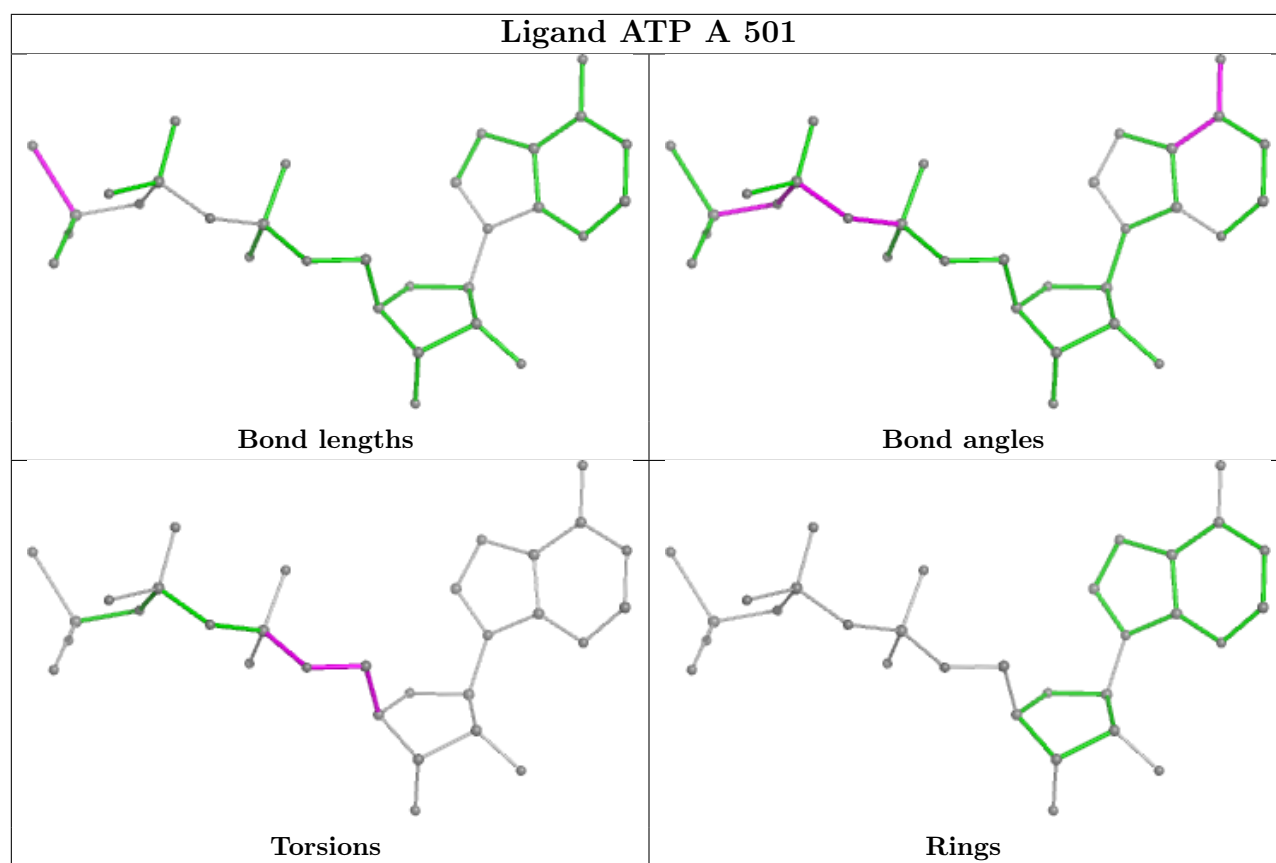
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

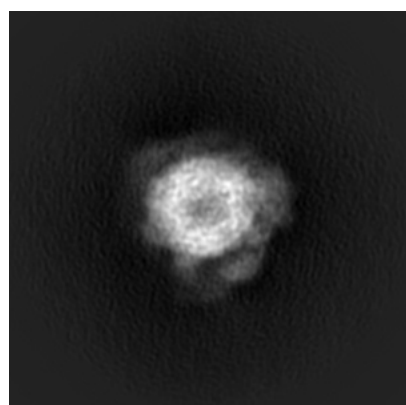
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14210. These allow visual inspection of the internal detail of the map and identification of artifacts.

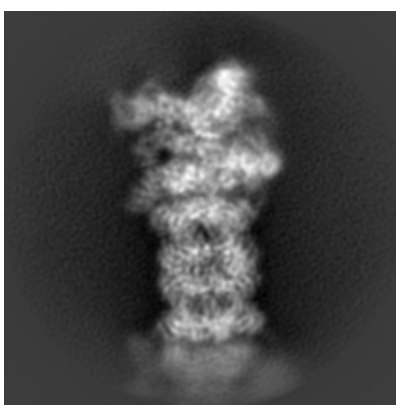
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

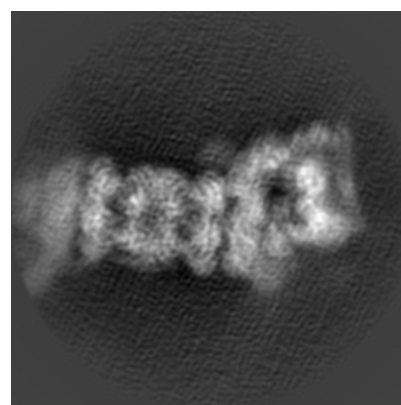
#### 6.1.1 Primary map



X



Y

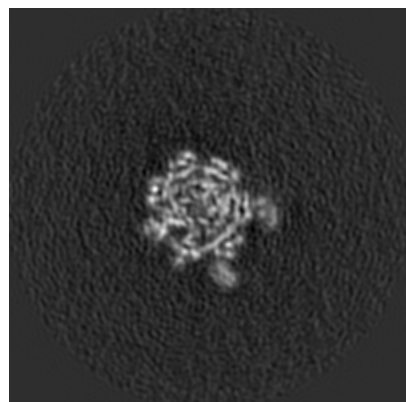


Z

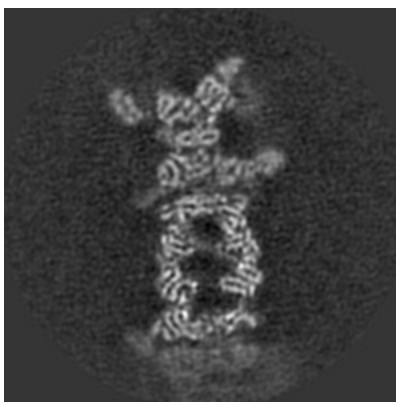
The images above show the map projected in three orthogonal directions.

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

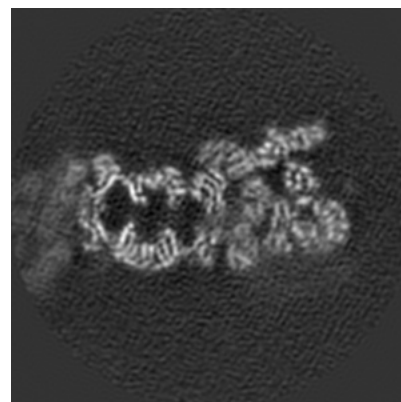
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

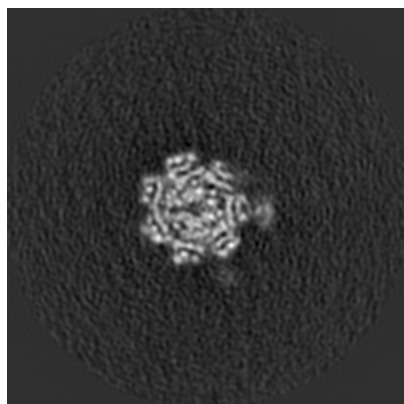


Z Index: 160

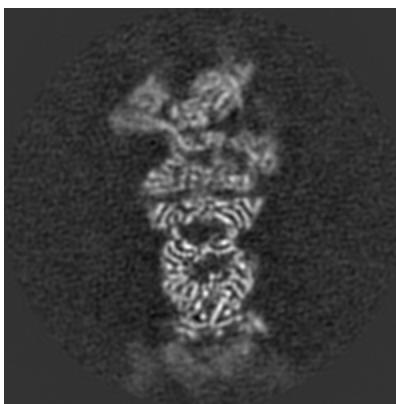
The images above show central slices of the map in three orthogonal directions.

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

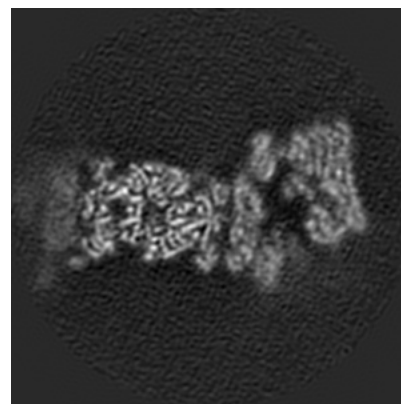
### 6.3.1 Primary map



X Index: 156



Y Index: 140

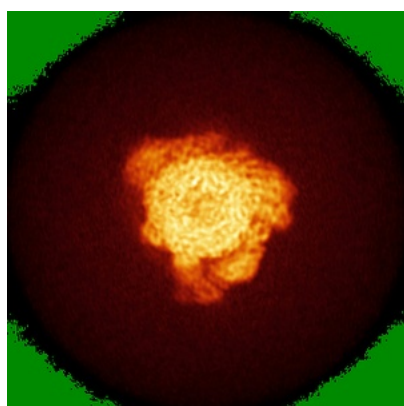


Z Index: 181

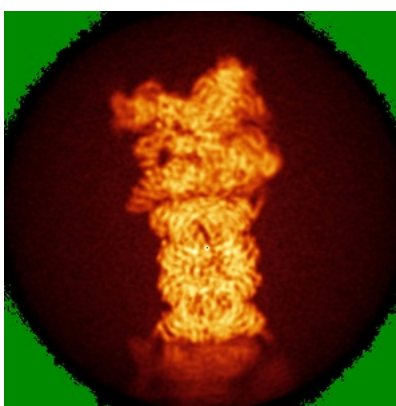
The images above show the largest variance slices of the map in three orthogonal directions.

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

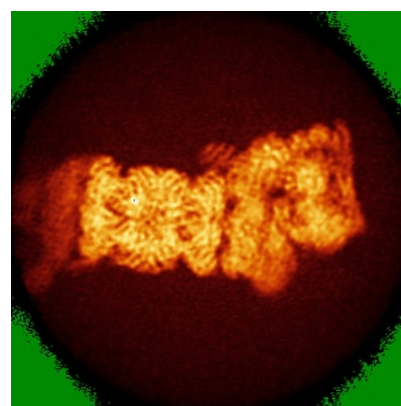
### 6.4.1 Primary map



X



Y

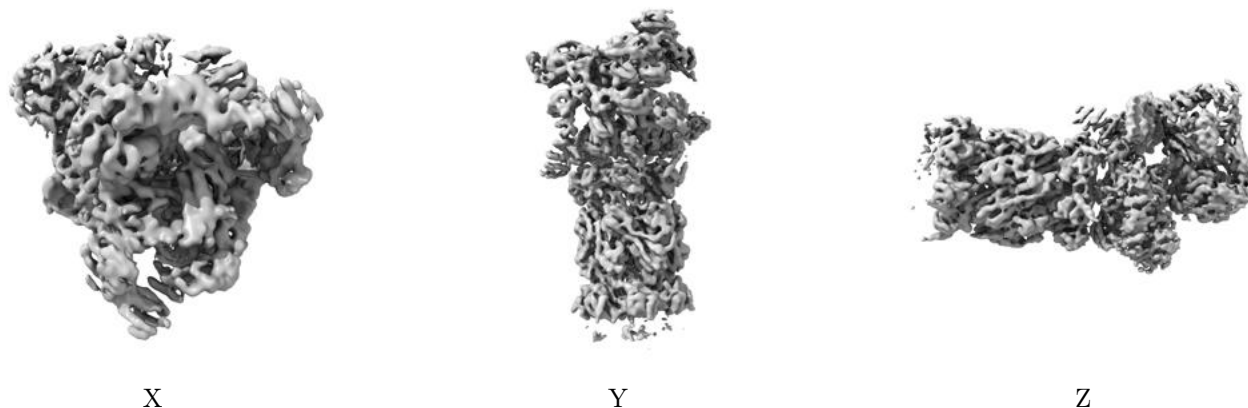


Z

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

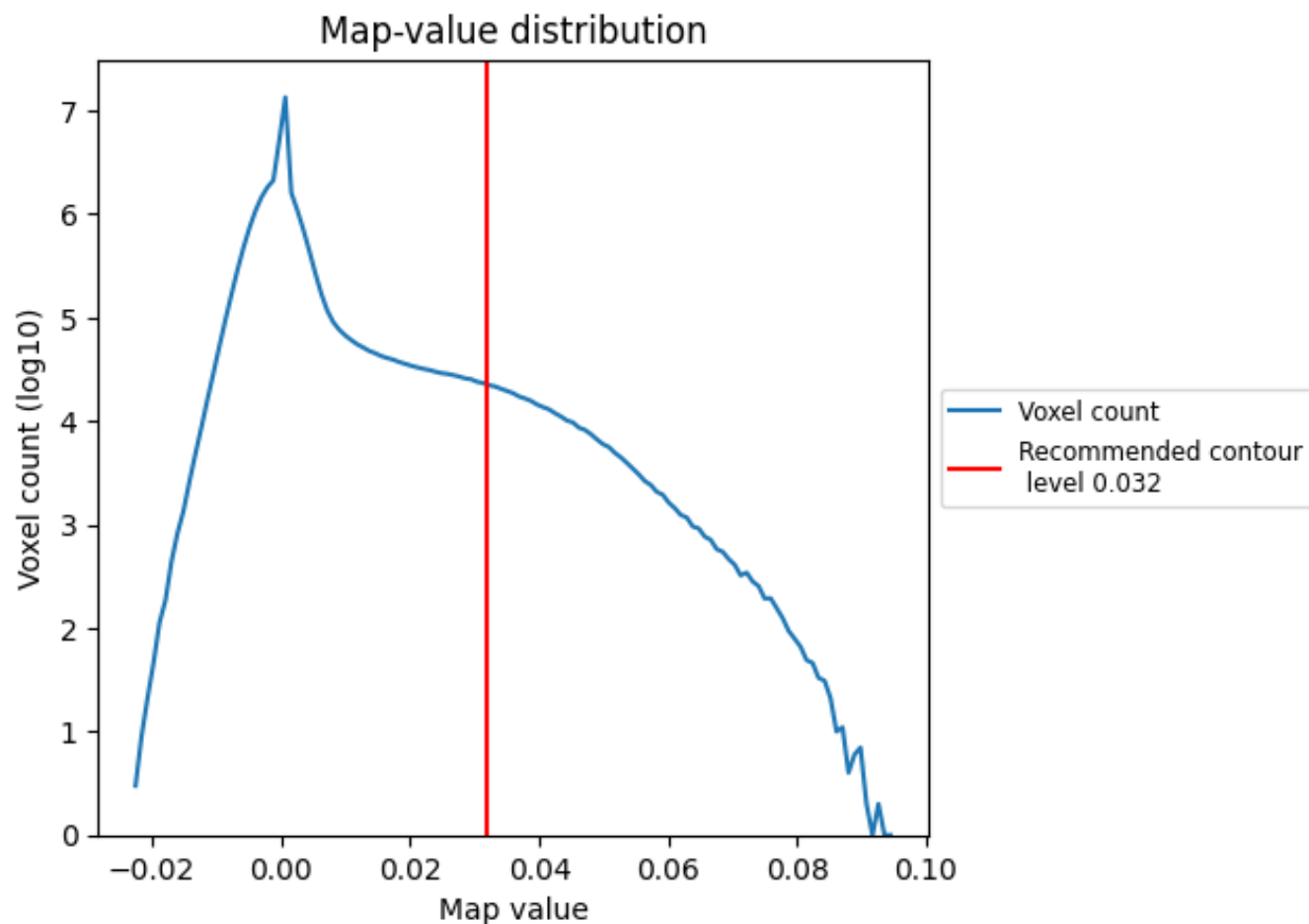
## 6.6 Mask visualisation [i](#)

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.

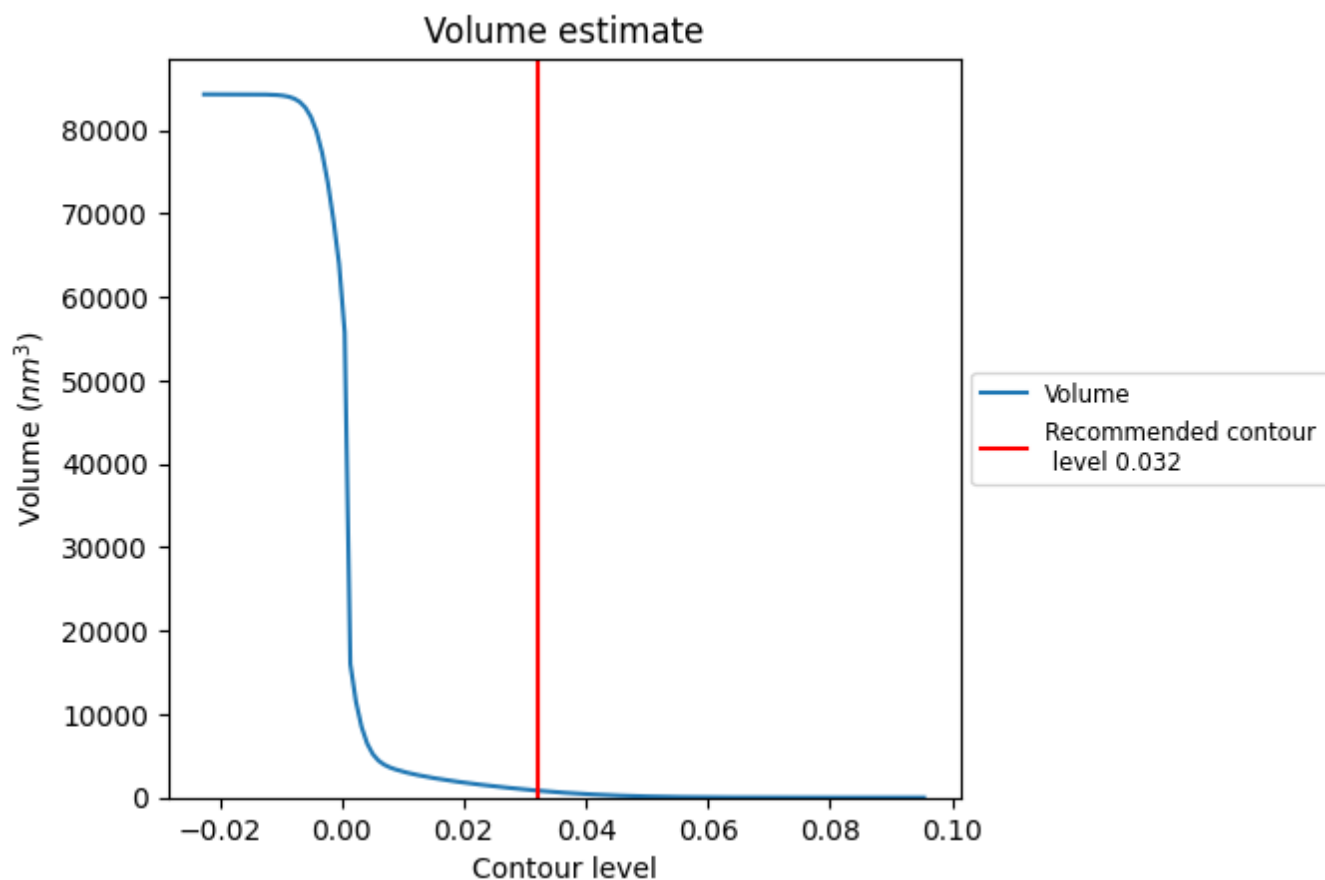
### 7.1 Map-value distribution [i](#)



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.



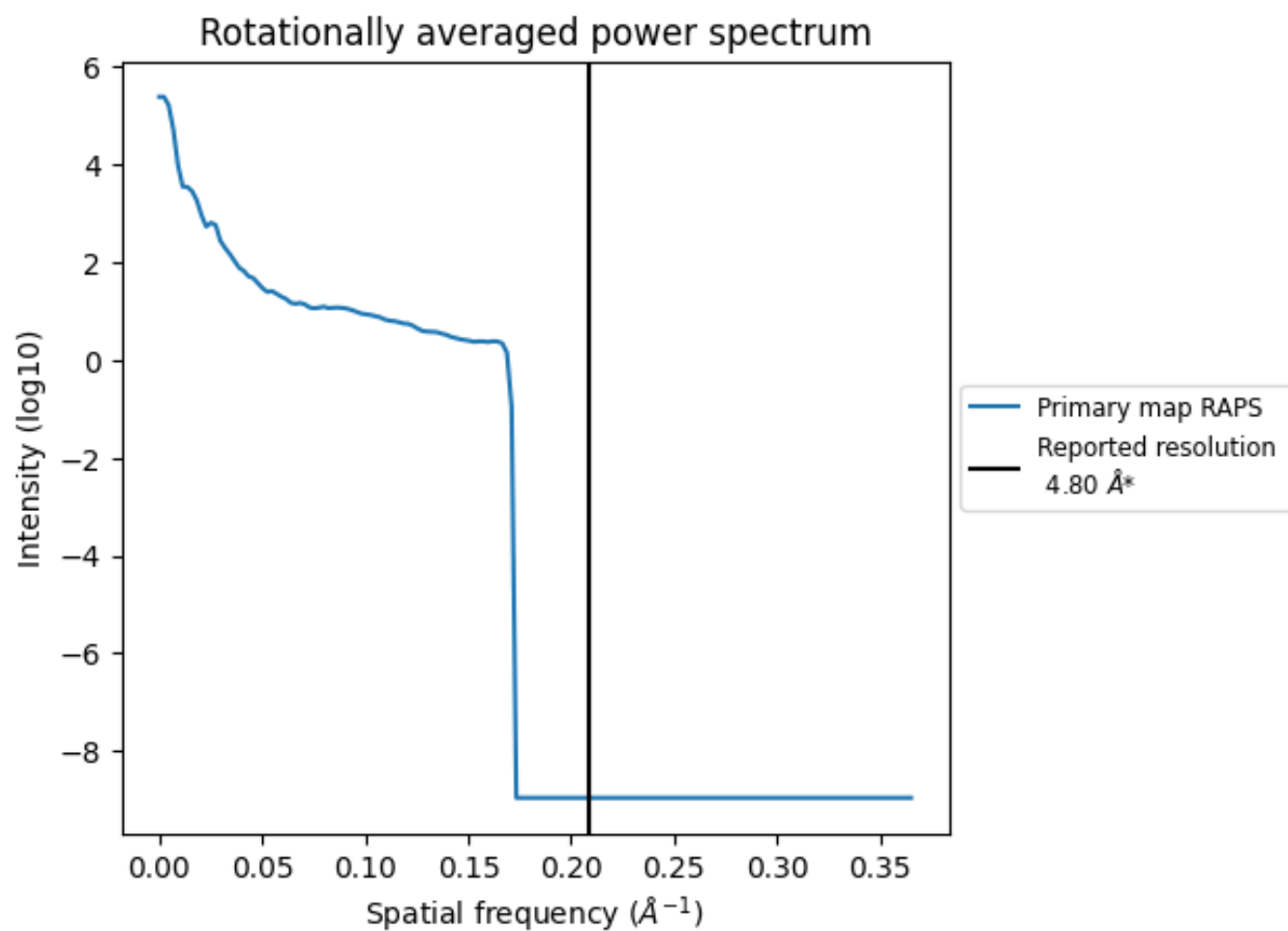
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 840 nm<sup>3</sup>; this corresponds to an approximate mass of 759 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 0.208 Å<sup>-1</sup>

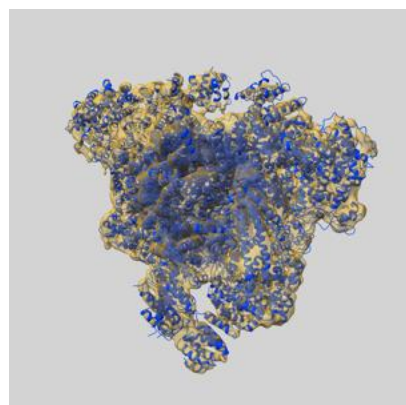
## 8 Fourier-Shell correlation ⓘ

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

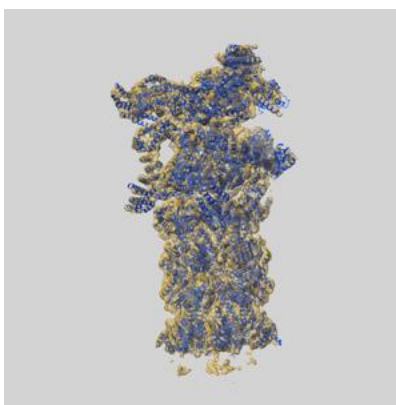
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14210 and PDB model 7QYA. Per-residue inclusion information can be found in section [3](#) on page [12](#).

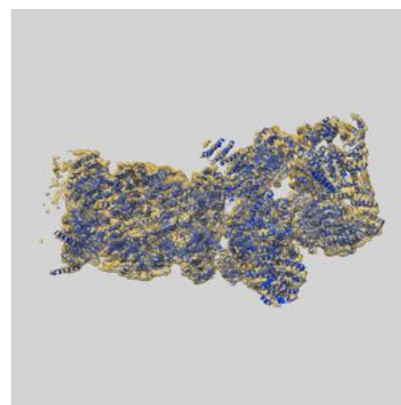
### 9.1 Map-model overlay [i](#)



X



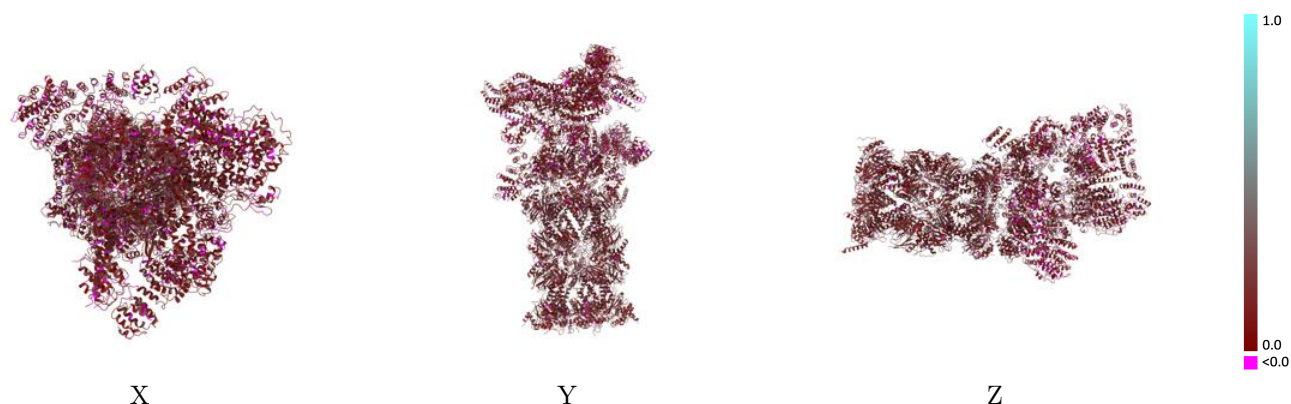
Y



Z

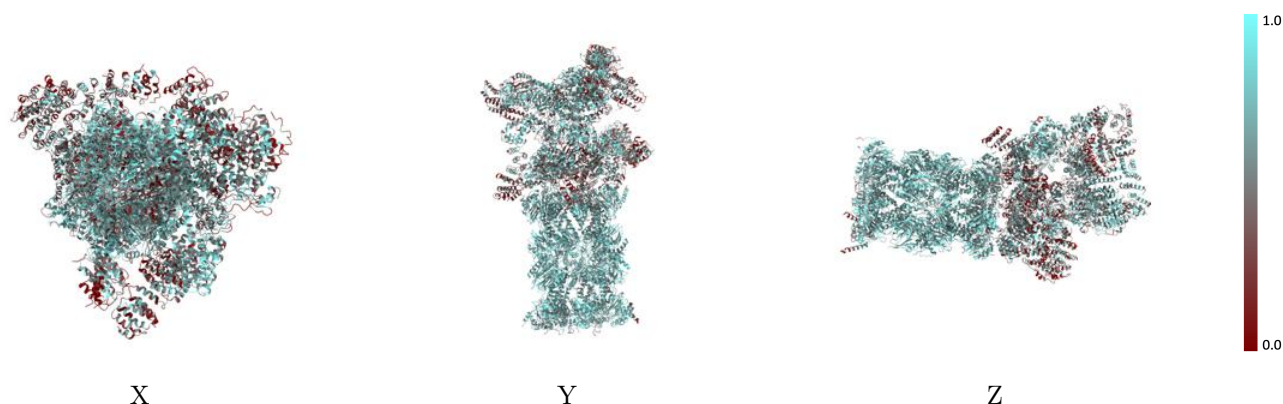
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



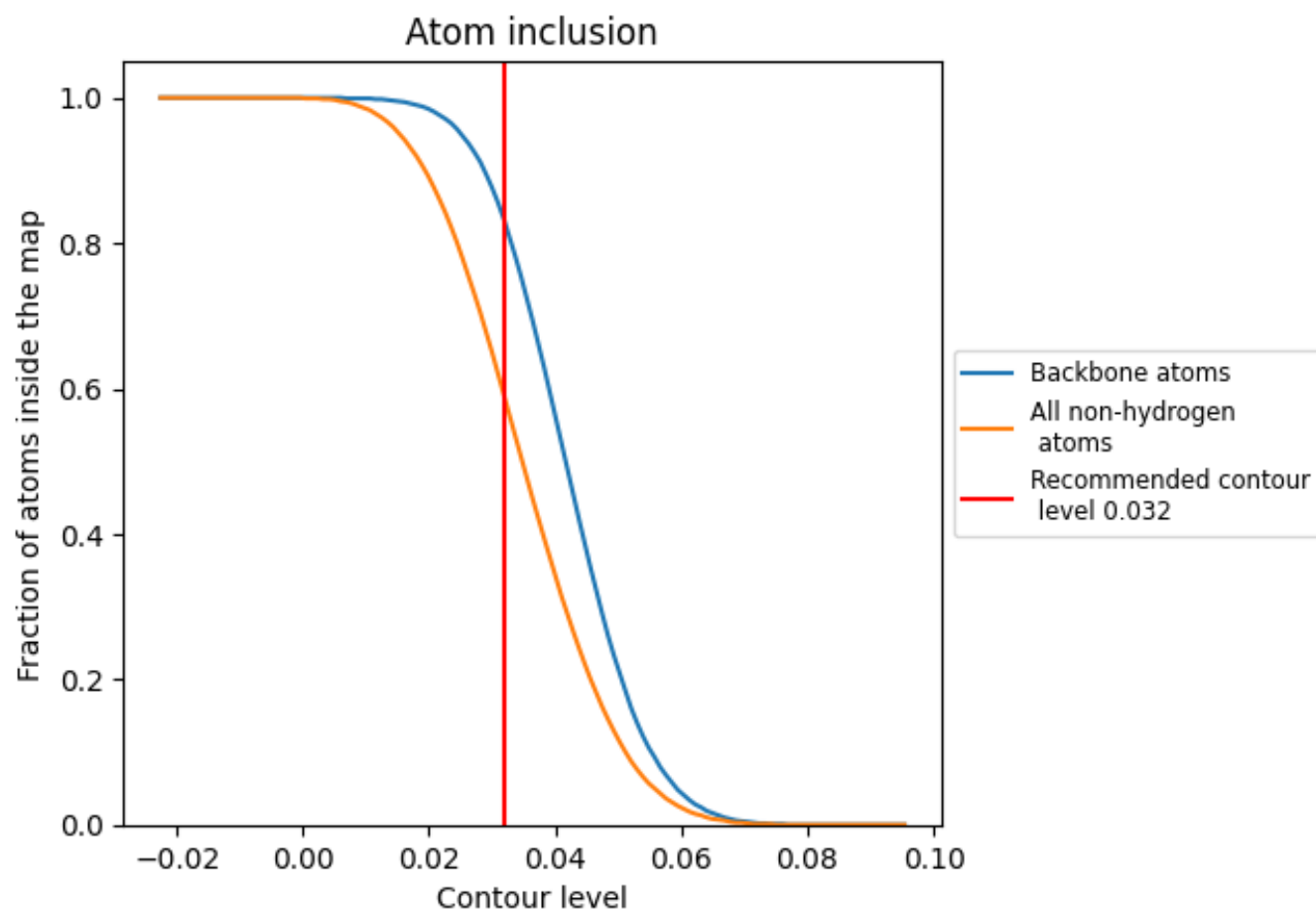
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 59% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.1760
A	 0.5090	 0.1800
B	 0.4240	 0.1710
C	 0.4500	 0.1670
D	 0.4330	 0.1680
E	 0.5330	 0.1740
F	 0.5370	 0.1730
G	 0.6810	 0.1990
H	 0.6750	 0.1950
I	 0.6250	 0.1920
J	 0.6850	 0.2140
K	 0.6280	 0.1850
L	 0.6960	 0.1940
M	 0.6800	 0.1930
N	 0.7300	 0.2040
O	 0.7310	 0.2110
P	 0.7010	 0.1940
Q	 0.7130	 0.2050
R	 0.7460	 0.2070
S	 0.7100	 0.2060
T	 0.7440	 0.2160
U	 0.6130	 0.1570
V	 0.4190	 0.1360
W	 0.4870	 0.1530
X	 0.4800	 0.1620
Y	 0.6400	 0.1500
Z	 0.5610	 0.1580
a	 0.5330	 0.1520
b	 0.4190	 0.1420
c	 0.5770	 0.1560
d	 0.4090	 0.1400
e	 0.4470	 0.0890
f	 0.3630	 0.1210
g	 0.6560	 0.2010
h	 0.6560	 0.2010



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.6210	 0.1940
j	 0.6430	 0.1980
k	 0.6560	 0.1980
l	 0.6960	 0.2070
m	 0.6580	 0.1830
n	 0.7470	 0.2070
o	 0.7390	 0.2140
p	 0.7060	 0.1930
q	 0.7240	 0.2090
r	 0.7580	 0.2070
s	 0.7290	 0.2110
t	 0.7330	 0.2130