



## Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 02:44 pm BST

PDB ID : 7QY7  
EMDB ID : EMD-14209  
Title : Proteasome-ZFAND5 Complex Z-A state  
Authors : Zhu, Y.; Lu, Y.  
Deposited on : 2022-01-27  
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

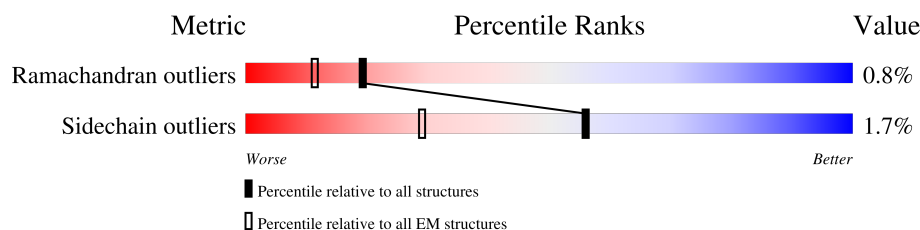
EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

# 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 4.70 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	<div> <div>37%</div> <div>98%</div> <div>..</div> </div>
2	b	377	<div> <div>32%</div> <div>50%</div> <div>.</div> <div>49%</div> </div>
3	c	309	<div> <div>21%</div> <div>87%</div> <div>..</div> <div>10%</div> </div>
4	d	349	<div> <div>32%</div> <div>71%</div> <div>.</div> <div>26%</div> </div>
5	e	70	<div> <div>37%</div> <div>51%</div> <div>..</div> <div>43%</div> </div>
6	f	908	<div> <div>53%</div> <div>74%</div> <div>.</div> <div>24%</div> </div>
7	U	953	<div> <div>16%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
8	V	533	<div> <div>30%</div> <div>86%</div> <div>.</div> <div>11%</div> </div>
9	W	456	<div> <div>53%</div> <div>97%</div> <div>.</div> </div>



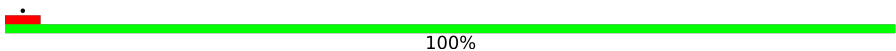

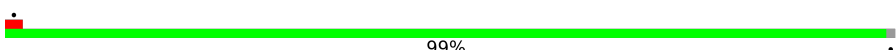
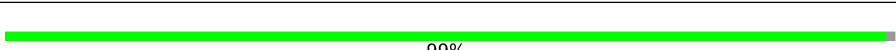
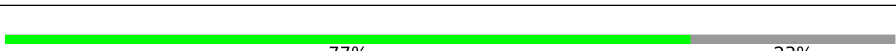

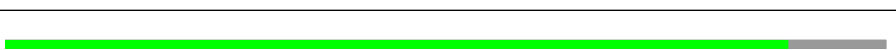

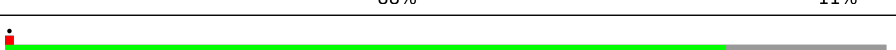

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Mol	Chain	Length	Quality of chain
10	X	422	
11	Y	389	
12	Z	324	
13	A	433	
14	B	440	
15	C	394	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	

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

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 99911 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
			1458	910	261	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
			2187	1389	374	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
			2116	1371	346	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
			334	200	55	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
			5319	3343	904	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
			6287	3990	1075	1178	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	472	Total	C	N	O	S	0	0
			3799	2413	675	697	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
			3703	2339	635	704	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

- 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
			3115	1987	533	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
			2281	1457	392	427	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	342	Total	C	N	O	S	0	0
			2672	1684	475	497	16		

- Molecule 14 is a protein called 26S protease 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 PSMC5 isoform 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	362	Total	C	N	O	S	0	0
			2850	1799	512	522	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	378	Total	C	N	O	S	0	0
			3021	1912	520	576	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
			2860	1796	512	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
			2859	1802	496	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		

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

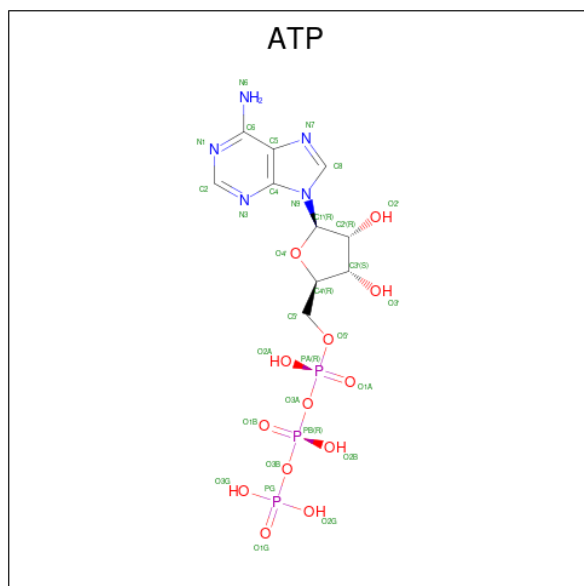
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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).

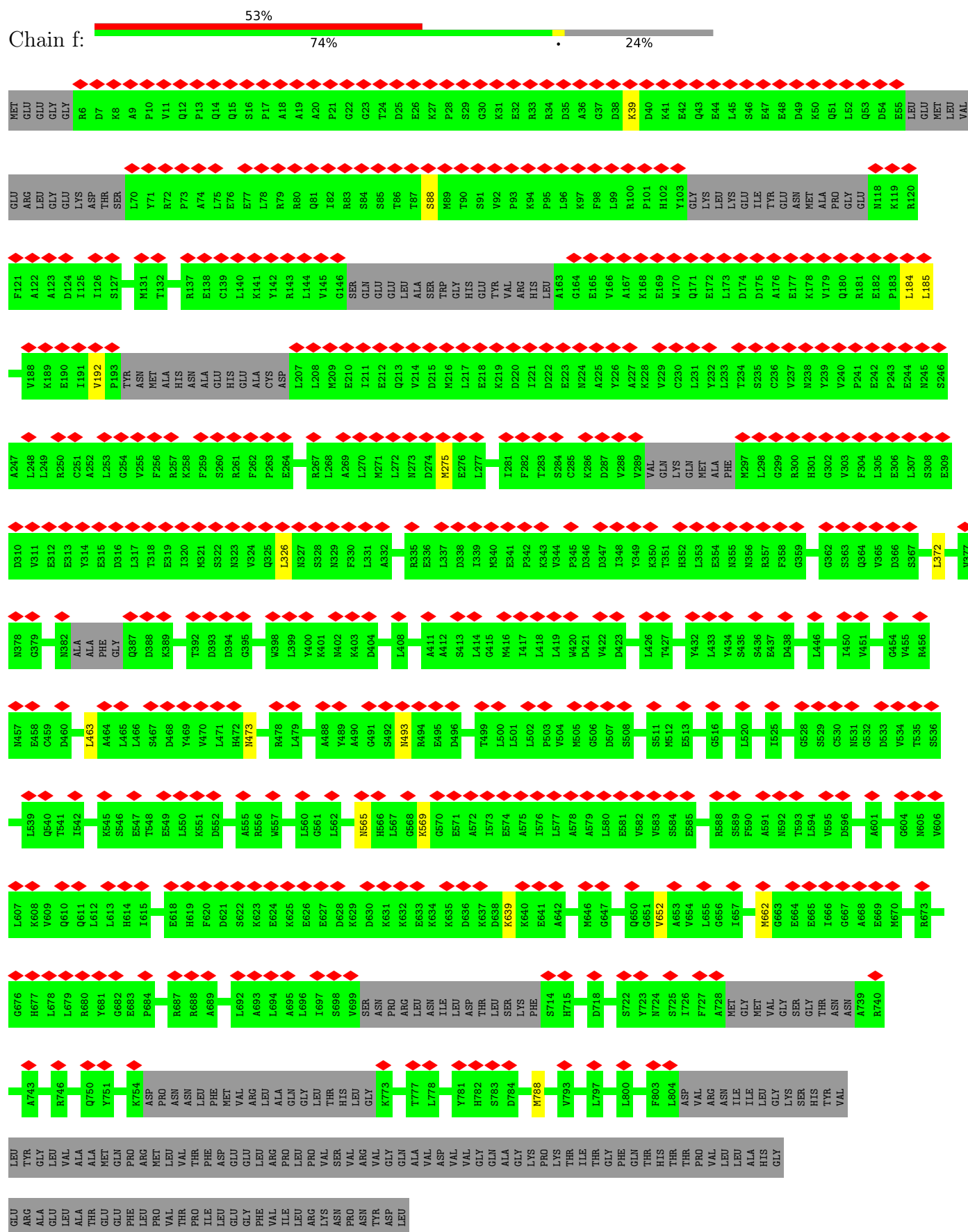


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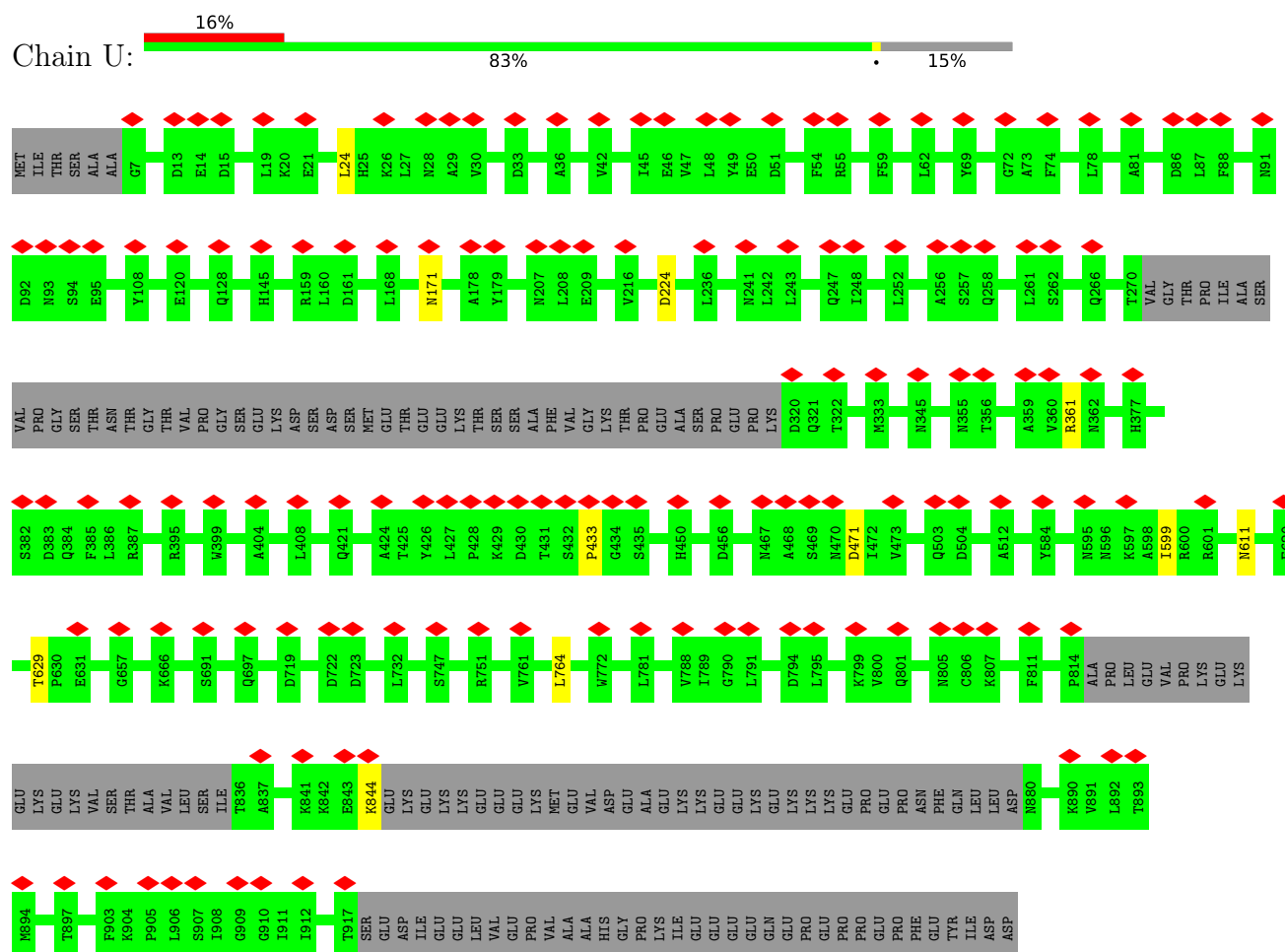
Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	



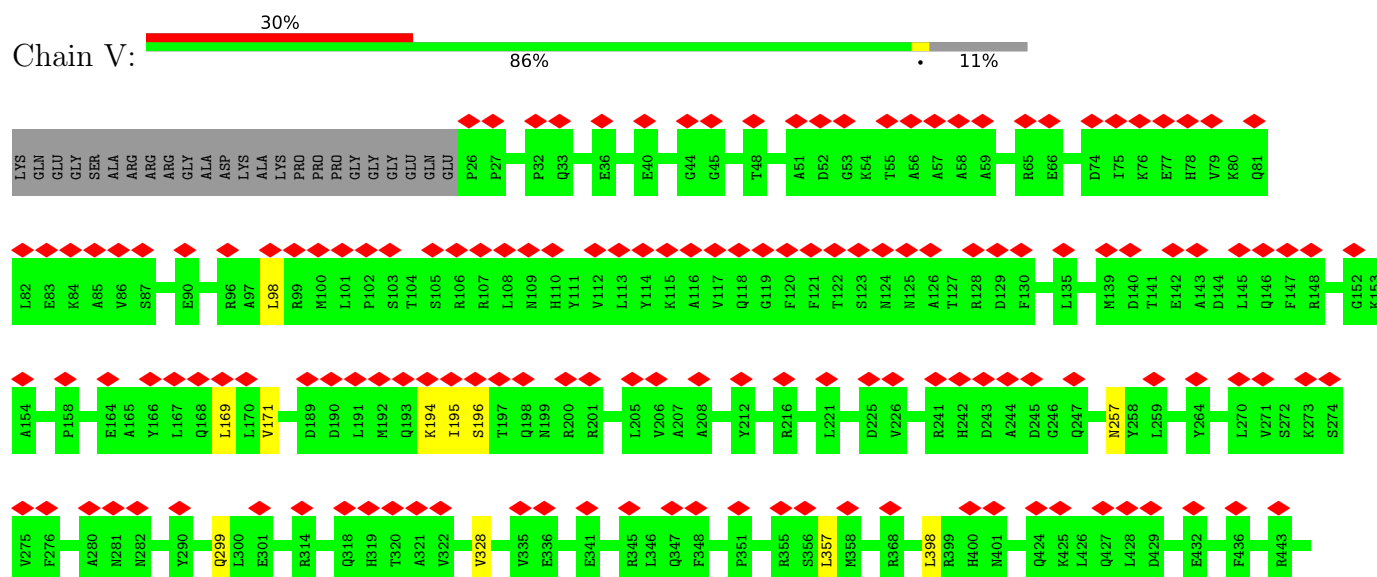




- Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



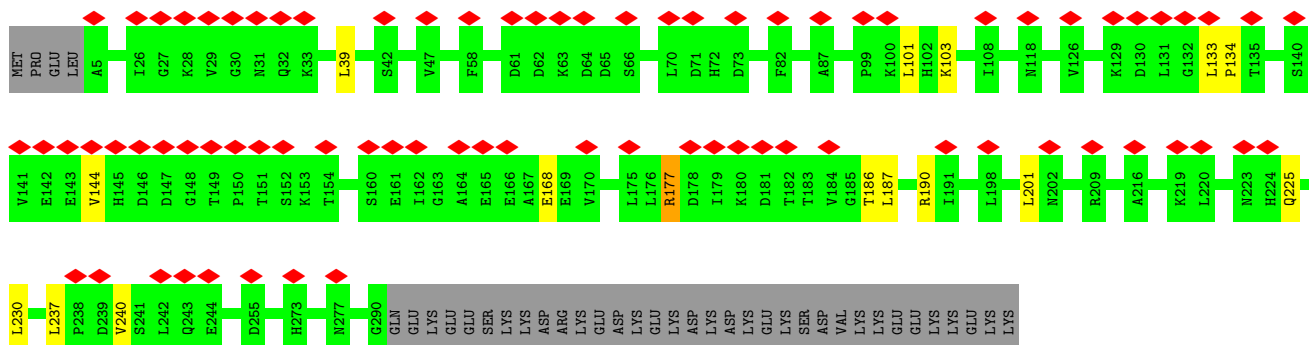
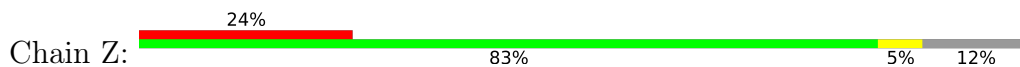
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 3



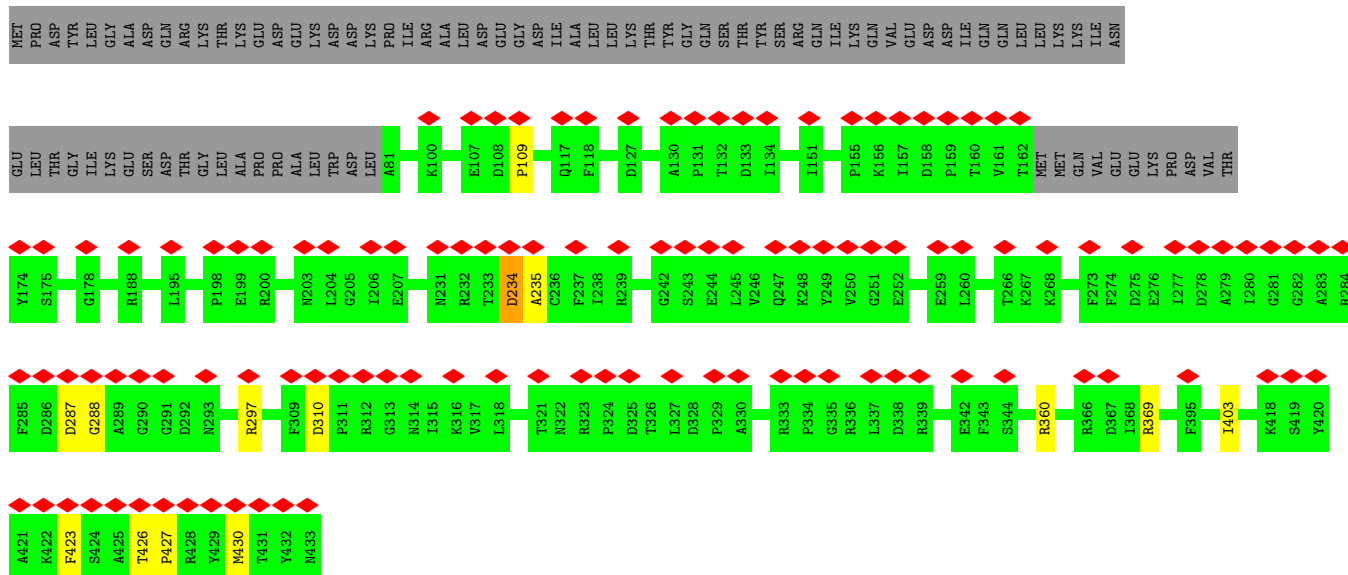
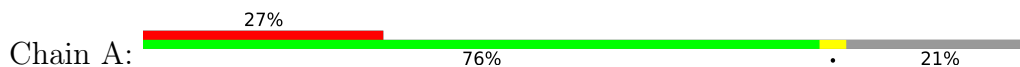




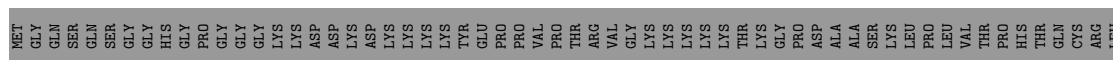
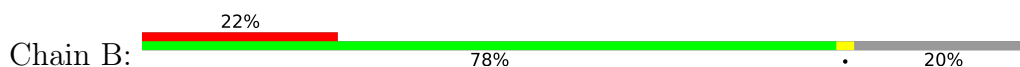
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

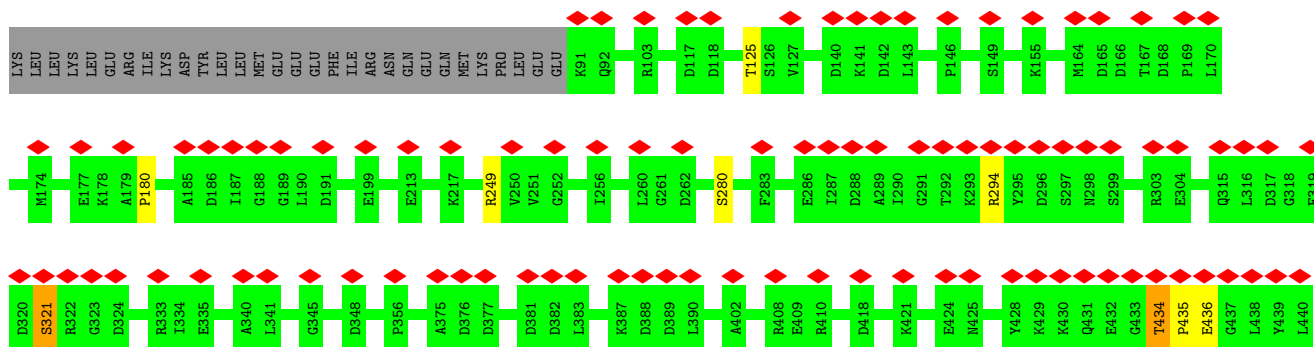


- Molecule 13: 26S protease regulatory subunit 7

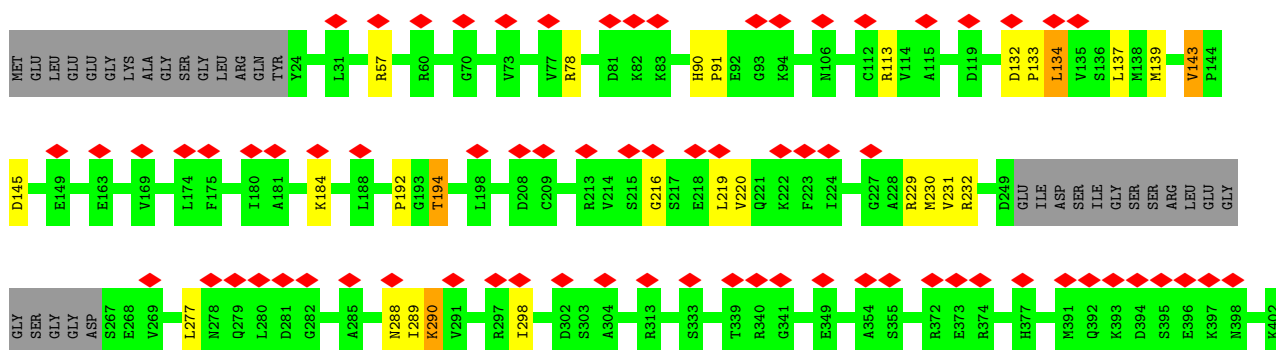
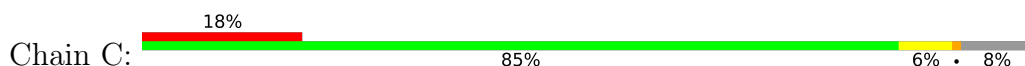


- Molecule 14: 26S protease regulatory subunit 4

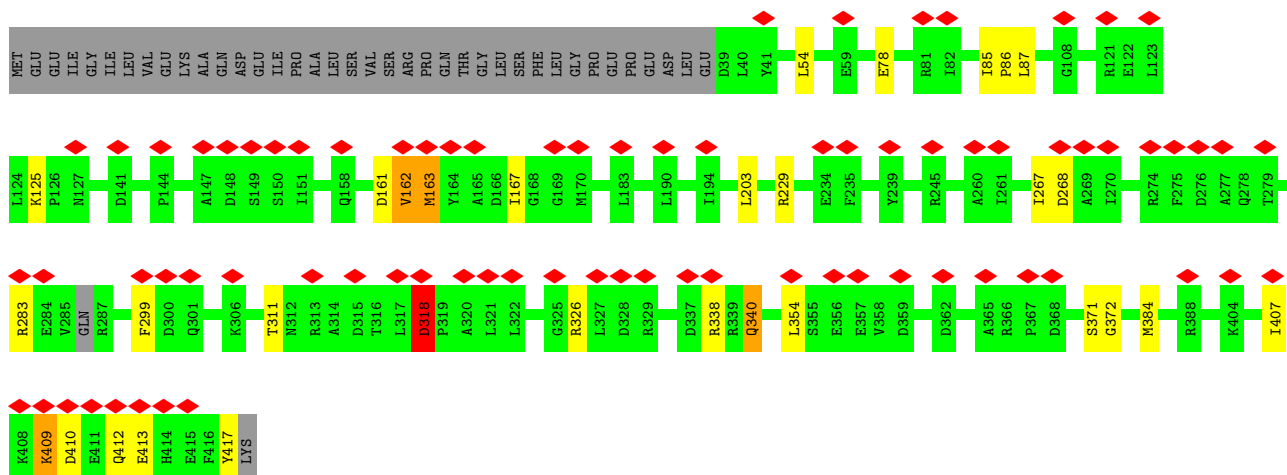
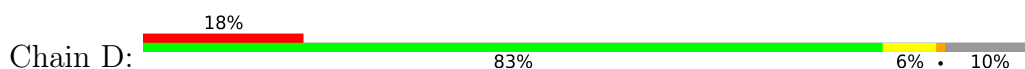




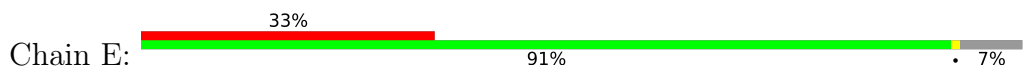
• Molecule 15: PSMC5 isoform 15

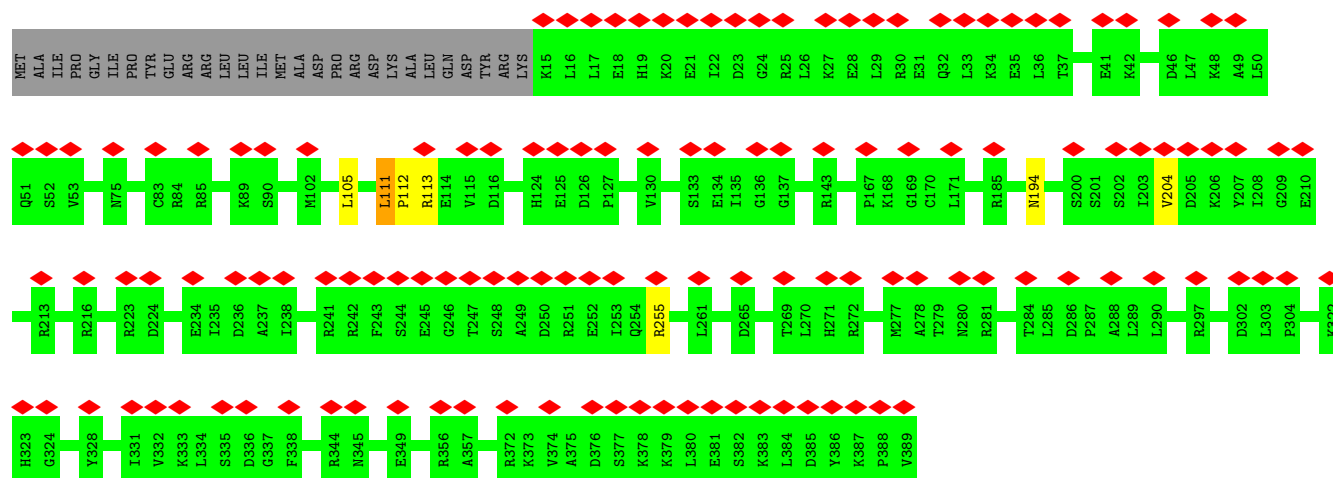


• Molecule 16: 26S protease regulatory subunit 6B



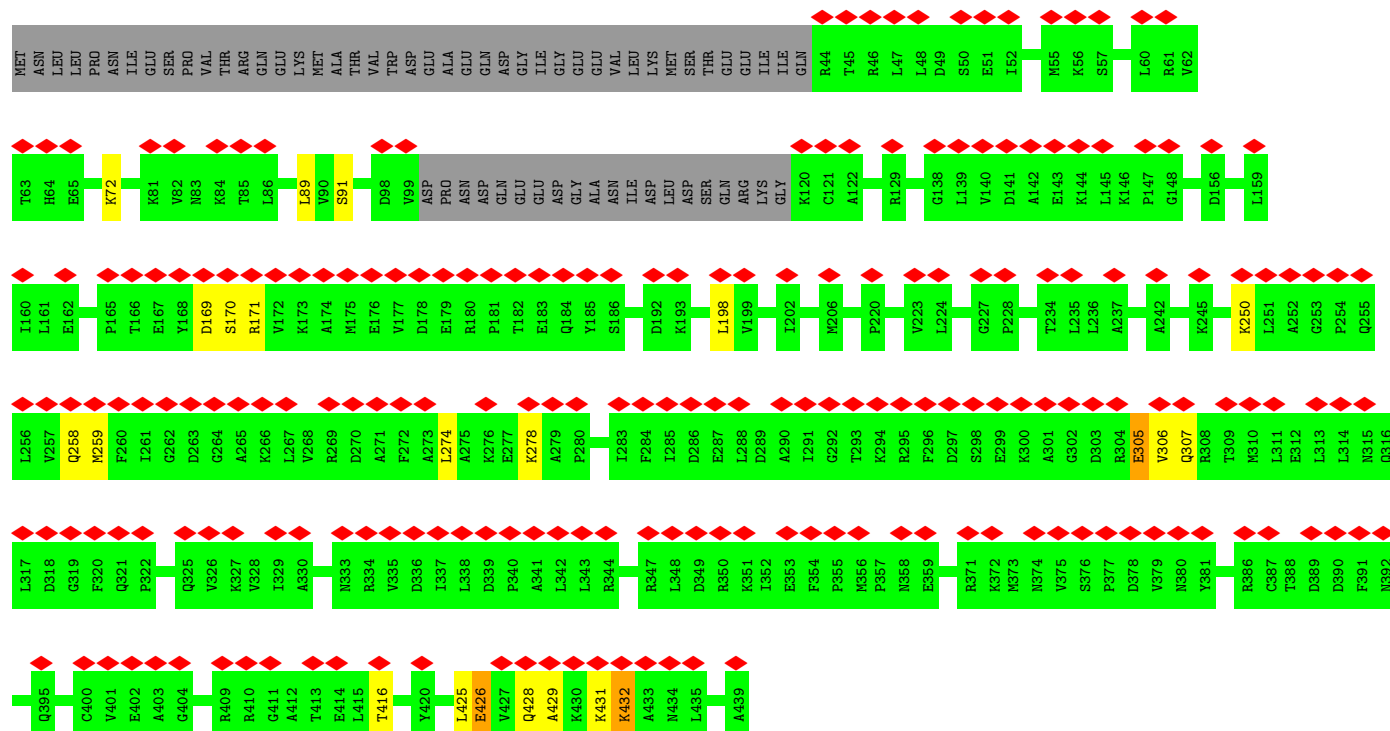
• Molecule 17: 26S proteasome regulatory subunit 10B





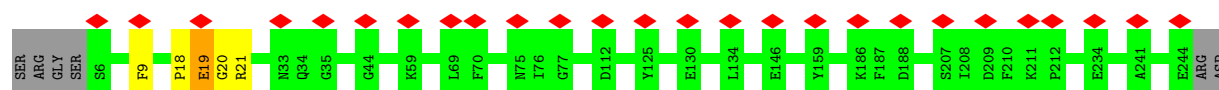
- Molecule 18: 26S protease regulatory subunit 6A

Chain F:

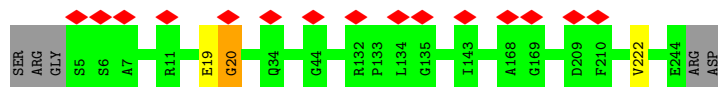


- Molecule 19: Proteasome subunit alpha type-6

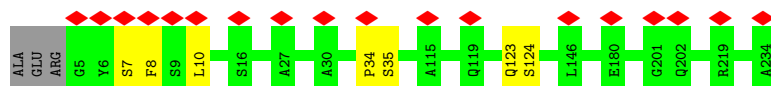
Chain G:



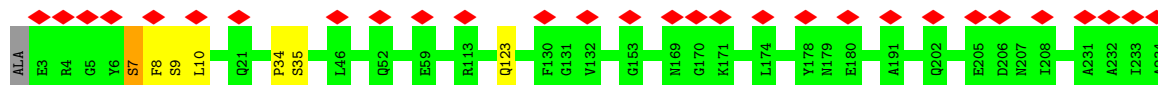
- Molecule 19: Proteasome subunit alpha type-6



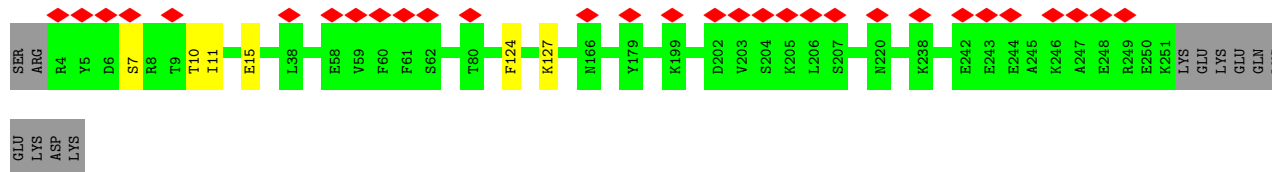
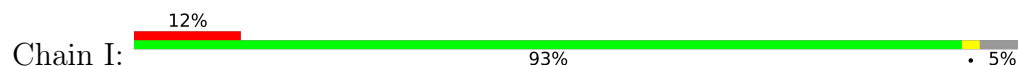
- Molecule 20: Proteasome subunit alpha type-2



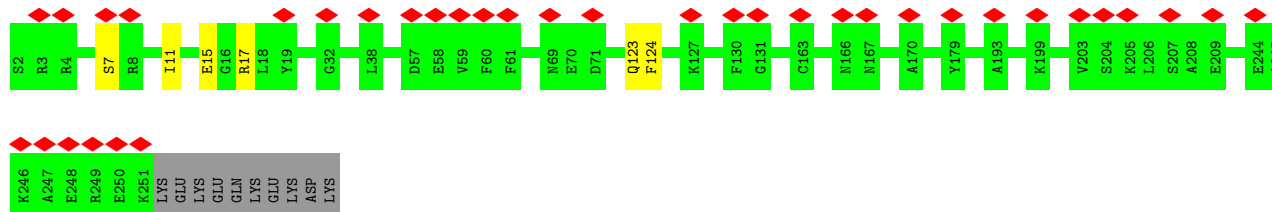
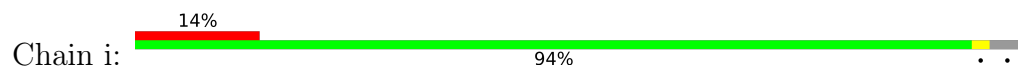
- Molecule 20: Proteasome subunit alpha type-2



- Molecule 21: Proteasome subunit alpha type-4



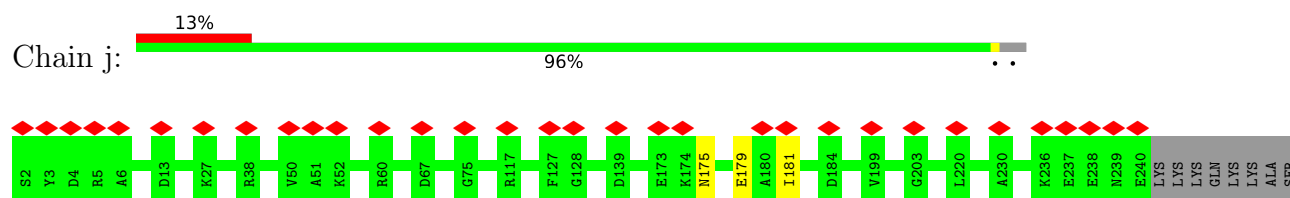
- Molecule 21: Proteasome subunit alpha type-4



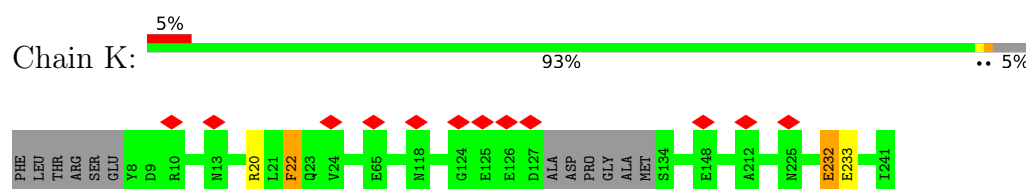
- Molecule 22: Proteasome subunit alpha type-7

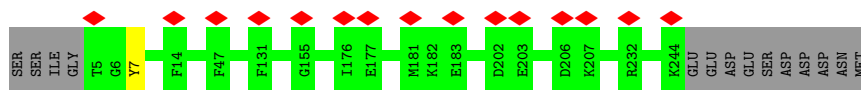


## • Molecule 22: Proteasome subunit alpha type-7



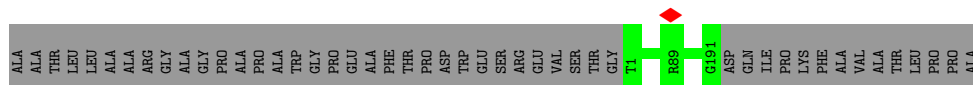
## • Molecule 23: Proteasome subunit alpha type-5





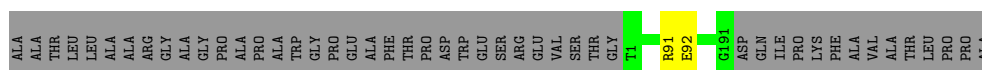
- Molecule 26: Proteasome subunit beta type-6

Chain N: 80% 20%



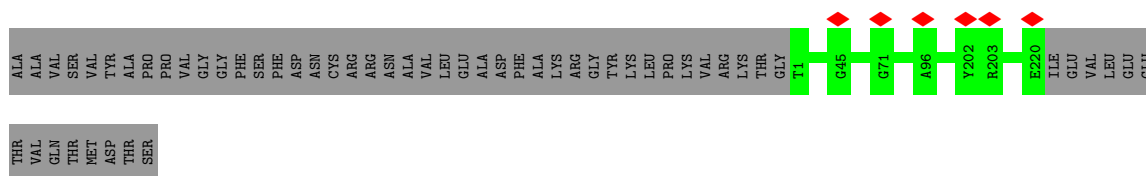
- Molecule 26: Proteasome subunit beta type-6

Chain n: 79% 20%



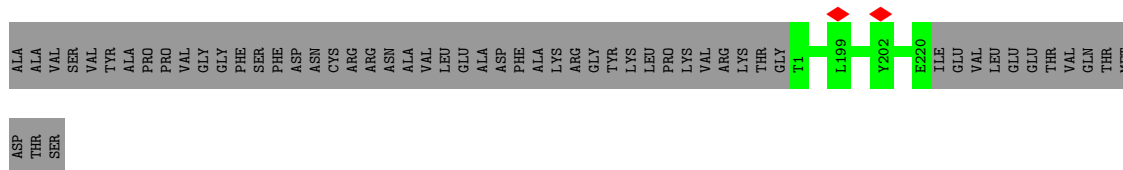
- Molecule 27: Proteasome subunit beta type-7

Chain O: 80% 20%



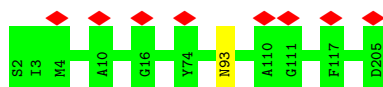
- Molecule 27: Proteasome subunit beta type-7

Chain o: 80% 20%



- Molecule 28: Proteasome subunit beta type-3

Chain P: 100%

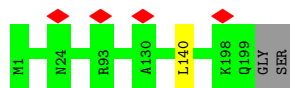


- Molecule 28: Proteasome subunit beta type-3

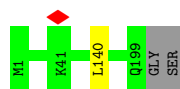
Chain p: 100%



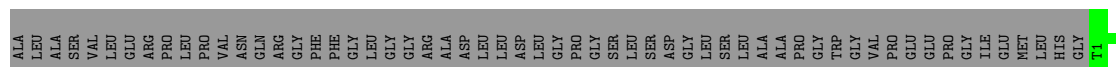
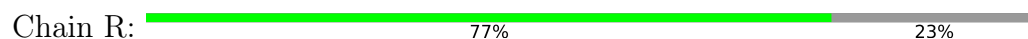
- Molecule 29: Proteasome subunit beta type-2



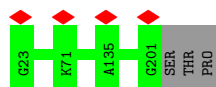
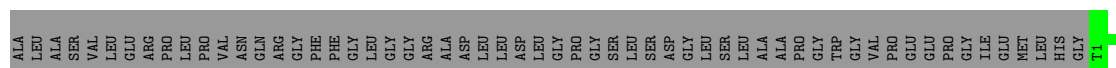
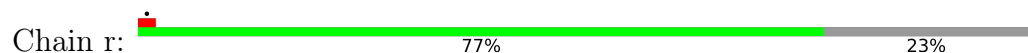
- Molecule 29: Proteasome subunit beta type-2



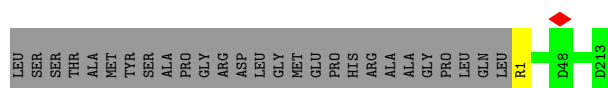
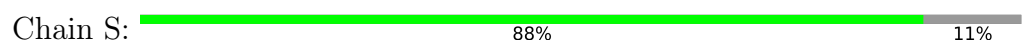
- Molecule 30: Proteasome subunit beta type-5



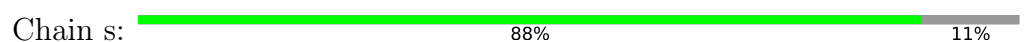
- Molecule 30: Proteasome subunit beta type-5

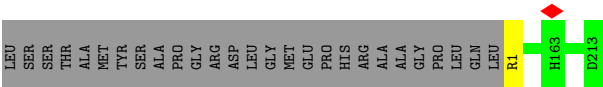


- Molecule 31: Proteasome subunit beta type-1

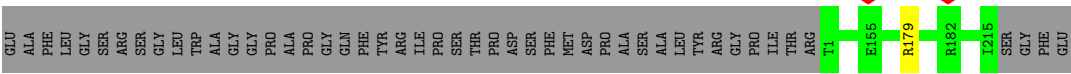
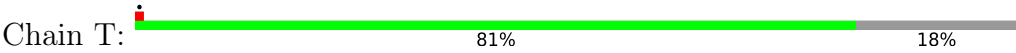


- Molecule 31: Proteasome subunit beta type-1

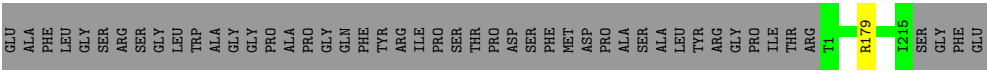
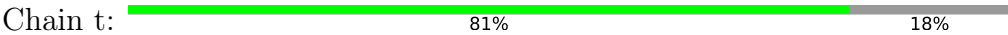




● Molecule 32: Proteasome subunit beta type-4



● Molecule 32: 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	34363	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	0.100	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0315	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: ZN, ATP

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	0.34	0/3053	0.65	1/4133 (0.0%)
2	b	0.33	0/1478	0.63	1/2001 (0.0%)
3	c	0.38	0/2226	0.70	1/3007 (0.0%)
4	d	0.36	0/2162	0.68	2/2919 (0.1%)
5	e	0.37	0/338	0.68	0/450
6	f	0.32	0/5393	0.68	2/7271 (0.0%)
7	U	0.36	0/6396	0.65	3/8646 (0.0%)
8	V	0.39	0/3874	0.71	2/5234 (0.0%)
9	W	0.35	0/3751	0.69	3/5042 (0.1%)
10	X	0.39	0/1936	0.64	0/2614
11	Y	0.41	0/3173	0.65	0/4273
12	Z	0.37	0/2324	0.72	3/3150 (0.1%)
13	A	0.36	0/2717	0.64	1/3665 (0.0%)
14	B	0.36	0/2745	0.59	0/3709
15	C	0.37	0/2887	0.74	4/3883 (0.1%)
16	D	0.43	0/3070	0.80	2/4142 (0.0%)
17	E	0.35	0/2904	0.61	0/3924
18	F	0.33	0/2897	0.63	2/3912 (0.1%)
19	G	0.37	0/1853	0.58	0/2515
19	g	0.38	0/1859	0.60	1/2523 (0.0%)
20	H	0.39	0/1723	0.61	1/2346 (0.0%)
20	h	0.39	0/1743	0.58	0/2372
21	I	0.38	0/1925	0.61	0/2606
21	i	0.37	0/1942	0.62	0/2628
22	J	0.35	0/1728	0.55	0/2358
22	j	0.35	0/1728	0.56	0/2358
23	K	0.38	0/1755	0.59	1/2375 (0.0%)
23	k	0.38	0/1747	0.59	1/2364 (0.0%)
24	L	0.39	0/1885	0.60	0/2552
24	l	0.39	0/1885	0.60	0/2552
25	M	0.41	0/1891	0.60	0/2552
25	m	0.40	0/1891	0.60	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
26	N	0.40	0/1454	0.57	0/1967
26	n	0.40	0/1454	0.57	0/1967
27	O	0.38	0/1670	0.56	0/2265
27	o	0.38	0/1670	0.56	0/2265
28	P	0.39	0/1614	0.56	0/2177
28	p	0.39	0/1614	0.56	0/2177
29	Q	0.42	0/1603	0.59	0/2174
29	q	0.42	0/1603	0.59	0/2174
30	R	0.42	0/1579	0.55	0/2134
30	r	0.42	0/1579	0.55	0/2134
31	S	0.41	0/1671	0.56	0/2253
31	s	0.41	0/1671	0.56	0/2253
32	T	0.41	0/1700	0.58	0/2305
32	t	0.41	0/1700	0.58	0/2305
All	All	0.38	0/101461	0.63	31/137178 (0.0%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	134	LEU	CA-CB-CG	9.15	136.35	115.30
6	f	372	LEU	CA-CB-CG	5.92	128.93	115.30
15	C	219	LEU	CA-CB-CG	5.91	128.89	115.30
18	F	198	LEU	CA-CB-CG	5.89	128.85	115.30
23	K	233	GLU	N-CA-C	-5.85	95.21	111.00
8	V	357	LEU	CA-CB-CG	5.84	128.72	115.30
20	H	8	PHE	N-CA-C	-5.77	95.43	111.00
3	c	229	LEU	CA-CB-CG	5.75	128.52	115.30
15	C	277	LEU	CA-CB-CG	-5.72	102.13	115.30
23	k	233	GLU	N-CA-C	-5.71	95.58	111.00
7	U	764	LEU	CA-CB-CG	5.68	128.37	115.30
1	a	187	ASP	CB-CG-OD1	5.66	123.40	118.30
2	b	102	GLY	N-CA-C	-5.66	98.95	113.10
7	U	224	ASP	CB-CG-OD1	5.52	123.27	118.30
15	C	298	ILE	CG1-CB-CG2	-5.50	99.29	111.40
18	F	274	LEU	CA-CB-CG	5.50	127.94	115.30
9	W	409	LEU	CA-CB-CG	5.49	127.92	115.30
8	V	98	LEU	CA-CB-CG	5.33	127.56	115.30
16	D	203	LEU	CA-CB-CG	5.32	127.54	115.30
6	f	463	LEU	CA-CB-CG	5.27	127.42	115.30
19	g	20	GLY	N-CA-C	5.25	126.23	113.10
4	d	55	LEU	CA-CB-CG	-5.23	103.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	39	LEU	CA-CB-CG	5.18	127.22	115.30
16	D	318	ASP	N-CA-CB	5.17	119.91	110.60
4	d	190	LEU	CA-CB-CG	5.17	127.19	115.30
12	Z	133	LEU	CA-CB-CG	5.13	127.11	115.30
13	A	234	ASP	N-CA-C	-5.12	97.18	111.00
7	U	471	ASP	CB-CG-OD1	5.10	122.89	118.30
9	W	370	TYR	C-N-CA	5.07	134.38	121.70
12	Z	201	LEU	CA-CB-CG	-5.04	103.70	115.30
9	W	40	LEU	N-CA-C	5.00	124.51	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%)	331 (89%)	38 (10%)	2 (0%)	25	64
2	b	189/377 (50%)	160 (85%)	28 (15%)	1 (0%)	25	64
3	c	274/309 (89%)	228 (83%)	40 (15%)	6 (2%)	5	29
4	d	255/349 (73%)	216 (85%)	36 (14%)	3 (1%)	11	44
5	e	36/70 (51%)	21 (58%)	14 (39%)	1 (3%)	4	24
6	f	669/908 (74%)	591 (88%)	75 (11%)	3 (0%)	30	68
7	U	798/953 (84%)	729 (91%)	68 (8%)	1 (0%)	48	83
8	V	470/533 (88%)	396 (84%)	70 (15%)	4 (1%)	14	51
9	W	454/456 (100%)	393 (87%)	56 (12%)	5 (1%)	12	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	239/422 (57%)	211 (88%)	25 (10%)	3 (1%)	10	42
11	Y	376/389 (97%)	331 (88%)	43 (11%)	2 (0%)	25	64
12	Z	284/324 (88%)	237 (84%)	42 (15%)	5 (2%)	7	34
13	A	338/433 (78%)	269 (80%)	63 (19%)	6 (2%)	7	34
14	B	348/440 (79%)	307 (88%)	37 (11%)	4 (1%)	12	46
15	C	358/394 (91%)	285 (80%)	58 (16%)	15 (4%)	2	18
16	D	374/418 (90%)	287 (77%)	72 (19%)	15 (4%)	2	18
17	E	373/403 (93%)	330 (88%)	40 (11%)	3 (1%)	16	54
18	F	372/439 (85%)	326 (88%)	38 (10%)	8 (2%)	5	29
19	G	237/245 (97%)	210 (89%)	23 (10%)	4 (2%)	7	36
19	g	238/245 (97%)	212 (89%)	24 (10%)	2 (1%)	16	54
20	H	228/233 (98%)	207 (91%)	19 (8%)	2 (1%)	14	51
20	h	230/233 (99%)	207 (90%)	21 (9%)	2 (1%)	14	51
21	I	246/260 (95%)	222 (90%)	23 (9%)	1 (0%)	30	68
21	i	248/260 (95%)	224 (90%)	23 (9%)	1 (0%)	30	68
22	J	237/247 (96%)	215 (91%)	20 (8%)	2 (1%)	16	54
22	j	237/247 (96%)	217 (92%)	18 (8%)	2 (1%)	16	54
23	K	224/240 (93%)	201 (90%)	21 (9%)	2 (1%)	14	51
23	k	224/240 (93%)	202 (90%)	21 (9%)	1 (0%)	30	68
24	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
24	l	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
25	M	238/254 (94%)	213 (90%)	25 (10%)	0	100	100
25	m	238/254 (94%)	214 (90%)	24 (10%)	0	100	100
26	N	189/238 (79%)	178 (94%)	11 (6%)	0	100	100
26	n	189/238 (79%)	178 (94%)	10 (5%)	1 (0%)	25	64
27	O	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
27	o	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
28	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
28	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
29	Q	197/201 (98%)	178 (90%)	19 (10%)	0	100	100
29	q	197/201 (98%)	178 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	R	199/262 (76%)	187 (94%)	12 (6%)	0	100	100
30	r	199/262 (76%)	187 (94%)	12 (6%)	0	100	100
31	S	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
31	s	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
32	T	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
32	t	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
All	All	12733/14855 (86%)	11318 (89%)	1308 (10%)	107 (1%)	19	54

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	103	LYS
4	d	201	ASN
9	W	314	LEU
9	W	424	LEU
10	X	203	PRO
10	X	300	ALA
11	Y	361	SER
13	A	427	PRO
14	B	434	THR
15	C	90	HIS
15	C	134	LEU
15	C	143	VAL
15	C	192	PRO
15	C	231	VAL
16	D	86	PRO
16	D	161	ASP
16	D	162	VAL
16	D	318	ASP
16	D	338	ARG
16	D	372	GLY
17	E	111	LEU
18	F	306	VAL
19	G	9	PHE
19	G	18	PRO
23	K	22	PHE
22	j	179	GLU
26	n	92	GLU
3	c	280	PRO
8	V	171	VAL

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Mol	Chain	Res	Type
9	W	40	LEU
12	Z	144	VAL
13	A	235	ALA
13	A	288	GLY
14	B	321	SER
15	C	194	THR
15	C	290	LYS
16	D	371	SER
17	E	113	ARG
18	F	89	LEU
18	F	429	ALA
19	G	19	GLU
22	j	181	ILE
3	c	273	LYS
5	e	61	GLU
6	f	185	LEU
8	V	196	SER
10	X	262	ASN
11	Y	357	ASN
15	C	145	ASP
15	C	288	ASN
16	D	299	PHE
16	D	340	GLN
16	D	407	ILE
18	F	305	GLU
18	F	432	LYS
20	H	10	LEU
23	K	232	GLU
19	g	19	GLU
19	g	20	GLY
1	a	187	ASP
3	c	187	PRO
6	f	326	LEU
8	V	195	ILE
9	W	423	ASN
12	Z	103	LYS
13	A	234	ASP
15	C	216	GLY
15	C	289	ILE
16	D	268	ASP
16	D	410	ASP
18	F	426	GLU

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Mol	Chain	Res	Type
22	J	181	ILE
20	h	7	SER
23	k	232	GLU
3	c	156	VAL
3	c	278	GLN
8	V	299	GLN
9	W	38	GLY
12	Z	177	ARG
14	B	435	PRO
15	C	232	ARG
16	D	163	MET
16	D	409	LYS
17	E	112	PRO
18	F	169	ASP
21	I	7	SER
21	i	7	SER
4	d	35	PHE
4	d	158	ILE
12	Z	168	GLU
18	F	307	GLN
19	G	20	GLY
22	J	183	THR
3	c	174	PRO
20	H	34	PRO
7	U	433	PRO
13	A	109	PRO
13	A	310	ASP
15	C	91	PRO
15	C	133	PRO
20	h	34	PRO
12	Z	134	PRO
14	B	180	PRO
16	D	267	ILE
1	a	338	PRO
6	f	652	VAL
15	C	220	VAL

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

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	333/336 (99%)	332 (100%)	1 (0%)	91	92
2	b	167/312 (54%)	165 (99%)	2 (1%)	67	79
3	c	243/267 (91%)	238 (98%)	5 (2%)	48	67
4	d	231/293 (79%)	227 (98%)	4 (2%)	56	73
5	e	38/63 (60%)	34 (90%)	4 (10%)	5	20
6	f	580/763 (76%)	568 (98%)	12 (2%)	48	67
7	U	685/816 (84%)	678 (99%)	7 (1%)	73	82
8	V	409/459 (89%)	403 (98%)	6 (2%)	60	75
9	W	416/416 (100%)	408 (98%)	8 (2%)	52	70
10	X	208/362 (58%)	203 (98%)	5 (2%)	44	63
11	Y	334/344 (97%)	331 (99%)	3 (1%)	75	83
12	Z	257/295 (87%)	248 (96%)	9 (4%)	31	52
13	A	286/372 (77%)	278 (97%)	8 (3%)	38	59
14	B	300/385 (78%)	293 (98%)	7 (2%)	45	65
15	C	314/342 (92%)	302 (96%)	12 (4%)	28	50
16	D	331/366 (90%)	311 (94%)	20 (6%)	16	38
17	E	298/353 (84%)	293 (98%)	5 (2%)	56	73
18	F	296/379 (78%)	281 (95%)	15 (5%)	20	42
19	G	192/209 (92%)	190 (99%)	2 (1%)	73	82
19	g	193/209 (92%)	192 (100%)	1 (0%)	86	90
20	H	162/190 (85%)	158 (98%)	4 (2%)	42	62
20	h	164/190 (86%)	158 (96%)	6 (4%)	29	51
21	I	191/220 (87%)	186 (97%)	5 (3%)	41	61
21	i	193/220 (88%)	188 (97%)	5 (3%)	41	61
22	J	152/210 (72%)	150 (99%)	2 (1%)	65	77
22	j	152/210 (72%)	151 (99%)	1 (1%)	81	87
23	K	187/202 (93%)	184 (98%)	3 (2%)	58	75
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	M	192/211 (91%)	192 (100%)	0	100	100
25	m	192/211 (91%)	191 (100%)	1 (0%)	86	90
26	N	148/180 (82%)	148 (100%)	0	100	100
26	n	148/180 (82%)	147 (99%)	1 (1%)	81	87
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	172/173 (99%)	171 (99%)	1 (1%)	84	88
28	p	172/173 (99%)	171 (99%)	1 (1%)	84	88
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	10604/12593 (84%)	10428 (98%)	176 (2%)	56	73

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	349	MET
2	b	101	GLN
2	b	103	LYS
3	c	154	LYS
3	c	249	LEU
3	c	272	ILE
3	c	273	LYS
3	c	278	GLN
4	d	158	ILE
4	d	161	GLU
4	d	162	SER
4	d	235	THR
5	e	56	LEU
5	e	57	ARG
5	e	59	GLU

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Mol	Chain	Res	Type
5	e	61	GLU
6	f	39	LYS
6	f	88	SER
6	f	184	LEU
6	f	192	VAL
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	24	LEU
7	U	171	ASN
7	U	361	ARG
7	U	599	ILE
7	U	611	ASN
7	U	629	THR
7	U	844	LYS
8	V	169	LEU
8	V	194	LYS
8	V	257	ASN
8	V	328	VAL
8	V	398	LEU
8	V	448	GLU
9	W	39	ARG
9	W	40	LEU
9	W	55	ARG
9	W	89	LEU
9	W	90	LEU
9	W	248	ARG
9	W	310	THR
9	W	429	SER
10	X	261	LEU
10	X	263	THR
10	X	299	LEU
10	X	313	LEU
10	X	314	ARG
11	Y	32	ARG
11	Y	287	LEU
11	Y	357	ASN

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Mol	Chain	Res	Type
12	Z	101	LEU
12	Z	177	ARG
12	Z	186	THR
12	Z	187	LEU
12	Z	190	ARG
12	Z	225	GLN
12	Z	230	LEU
12	Z	237	LEU
12	Z	240	VAL
13	A	287	ASP
13	A	297	ARG
13	A	360	ARG
13	A	369	ARG
13	A	403	ILE
13	A	423	PHE
13	A	426	THR
13	A	430	MET
14	B	125	THR
14	B	249	ARG
14	B	280	SER
14	B	294	ARG
14	B	321	SER
14	B	434	THR
14	B	436	GLU
15	C	57	ARG
15	C	78	ARG
15	C	113	ARG
15	C	132	ASP
15	C	137	LEU
15	C	139	MET
15	C	143	VAL
15	C	184	LYS
15	C	194	THR
15	C	229	ARG
15	C	230	MET
15	C	290	LYS
16	D	54	LEU
16	D	78	GLU
16	D	85	ILE
16	D	87	LEU
16	D	125	LYS
16	D	162	VAL

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Mol	Chain	Res	Type
16	D	163	MET
16	D	167	ILE
16	D	229	ARG
16	D	283	ARG
16	D	311	THR
16	D	318	ASP
16	D	326	ARG
16	D	340	GLN
16	D	354	LEU
16	D	384	MET
16	D	409	LYS
16	D	412	GLN
16	D	413	GLU
16	D	417	TYR
17	E	105	LEU
17	E	111	LEU
17	E	194	ASN
17	E	204	VAL
17	E	255	ARG
18	F	72	LYS
18	F	91	SER
18	F	170	SER
18	F	171	ARG
18	F	250	LYS
18	F	258	GLN
18	F	259	MET
18	F	278	LYS
18	F	305	GLU
18	F	416	THR
18	F	425	LEU
18	F	426	GLU
18	F	428	GLN
18	F	431	LYS
18	F	432	LYS
19	G	19	GLU
19	G	21	ARG
20	H	7	SER
20	H	35	SER
20	H	123	GLN
20	H	124	SER
21	I	10	THR
21	I	11	ILE

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Mol	Chain	Res	Type
21	I	15	GLU
21	I	124	PHE
21	I	127	LYS
22	J	175	ASN
22	J	179	GLU
23	K	20	ARG
23	K	22	PHE
23	K	232	GLU
28	P	93	ASN
29	Q	140	LEU
31	S	1	ARG
32	T	179	ARG
19	g	222	VAL
20	h	7	SER
20	h	8	PHE
20	h	9	SER
20	h	10	LEU
20	h	35	SER
20	h	123	GLN
21	i	11	ILE
21	i	15	GLU
21	i	17	ARG
21	i	123	GLN
21	i	124	PHE
22	j	175	ASN
23	k	20	ARG
23	k	21	LEU
23	k	22	PHE
23	k	232	GLU
25	m	7	TYR
26	n	91	ARG
28	p	93	ASN
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 (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	241	ASN
1	a	244	ASN
2	b	34	ASN

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Mol	Chain	Res	Type
3	c	77	GLN
3	c	101	GLN
3	c	176	GLN
3	c	199	HIS
3	c	295	ASN
6	f	102	HIS
6	f	329	ASN
6	f	405	HIS
6	f	452	ASN
6	f	473	ASN
6	f	493	ASN
6	f	540	GLN
6	f	565	ASN
6	f	782	HIS
7	U	207	ASN
7	U	247	GLN
7	U	421	GLN
7	U	698	GLN
7	U	880	ASN
8	V	177	ASN
8	V	487	HIS
9	W	218	ASN
9	W	236	HIS
9	W	361	HIS
9	W	414	ASN
9	W	440	ASN
10	X	292	GLN
11	Y	367	GLN
12	Z	96	HIS
12	Z	104	ASN
12	Z	145	HIS
12	Z	174	HIS
12	Z	224	HIS
12	Z	274	ASN
13	A	293	ASN
13	A	358	HIS
13	A	414	ASN
15	C	69	GLN
15	C	270	GLN
15	C	380	GLN
16	D	74	HIS
16	D	83	GLN

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Mol	Chain	Res	Type
16	D	187	HIS
16	D	222	HIS
16	D	412	GLN
17	E	339	ASN
18	F	214	ASN
18	F	258	GLN
19	G	127	GLN
20	H	112	GLN
20	H	123	GLN
21	I	88	ASN
21	I	119	GLN
21	I	146	GLN
22	J	116	GLN
22	J	146	GLN
22	J	175	ASN
23	K	214	ASN
23	K	221	GLN
24	L	152	ASN
25	M	101	ASN
26	N	154	GLN
27	O	62	ASN
28	P	93	ASN
29	Q	27	GLN
29	Q	87	ASN
29	Q	101	ASN
29	Q	168	GLN
29	Q	186	ASN
30	R	38	ASN
30	R	119	ASN
32	T	213	HIS
19	g	127	GLN
20	h	112	GLN
21	i	88	ASN
21	i	146	GLN
22	j	116	GLN
22	j	146	GLN
22	j	175	ASN
23	k	214	ASN
23	k	221	GLN
24	l	152	ASN
25	m	101	ASN
26	n	154	GLN

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Mol	Chain	Res	Type
27	o	62	ASN
28	p	169	GLN
29	q	27	GLN
29	q	87	ASN
29	q	101	ASN
29	q	168	GLN
30	r	38	ASN
30	r	119	ASN
32	t	61	GLN
32	t	81	HIS
32	t	213	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
34	ATP	D	502	-	26,33,33	2.77	1 (3%)	31,52,52	1.57	3 (9%)
34	ATP	A	501	-	26,33,33	2.77	1 (3%)	31,52,52	1.46	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	ATP	E	401	17	26,33,33	0.88	1 (3%)	31,52,52	1.78	7 (22%)
34	ATP	B	501	-	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)
34	ATP	D	501	16	26,33,33	0.88	1 (3%)	31,52,52	1.78	7 (22%)

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	502	-	-	6/18/38/38	0/3/3/3
34	ATP	A	501	-	-	8/18/38/38	0/3/3/3
34	ATP	E	401	17	-	0/18/38/38	0/3/3/3
34	ATP	B	501	-	-	4/18/38/38	0/3/3/3
34	ATP	D	501	16	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	501	ATP	PG-O1G	13.80	1.95	1.50
34	D	502	ATP	PG-O1G	13.79	1.95	1.50
34	B	501	ATP	C5-C4	2.49	1.47	1.40
34	D	501	ATP	C5-C4	2.15	1.46	1.40
34	E	401	ATP	C5-C4	2.13	1.46	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	502	ATP	PB-O3B-PG	-5.64	113.47	132.83
34	D	501	ATP	PA-O3A-PB	-5.58	113.68	132.83
34	E	401	ATP	PA-O3A-PB	-5.57	113.70	132.83
34	D	502	ATP	PA-O3A-PB	-5.53	113.86	132.83
34	A	501	ATP	PB-O3B-PG	-5.42	114.22	132.83
34	A	501	ATP	PA-O3A-PB	-4.41	117.69	132.83
34	E	401	ATP	C3'-C2'-C1'	3.98	106.97	100.98
34	D	501	ATP	C3'-C2'-C1'	3.97	106.96	100.98
34	B	501	ATP	PB-O3B-PG	-3.58	120.53	132.83
34	B	501	ATP	PA-O3A-PB	-3.57	120.56	132.83
34	E	401	ATP	N3-C2-N1	-3.50	123.20	128.68
34	D	501	ATP	N3-C2-N1	-3.49	123.22	128.68
34	B	501	ATP	C3'-C2'-C1'	3.41	106.12	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	ATP	N3-C2-N1	-3.17	123.72	128.68
34	B	501	ATP	C4-C5-N7	-2.73	106.56	109.40
34	E	401	ATP	PB-O3B-PG	-2.26	125.07	132.83
34	D	502	ATP	C5-C6-N6	2.25	123.77	120.35
34	D	501	ATP	PB-O3B-PG	-2.25	125.11	132.83
34	A	501	ATP	C5-C6-N6	2.24	123.76	120.35
34	E	401	ATP	C4-C5-N7	-2.09	107.22	109.40
34	E	401	ATP	O2B-PB-O1B	2.08	122.55	112.24
34	D	501	ATP	O2B-PB-O1B	2.08	122.53	112.24
34	D	501	ATP	C4-C5-N7	-2.06	107.25	109.40
34	E	401	ATP	C2-N1-C6	2.06	122.27	118.75
34	D	501	ATP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

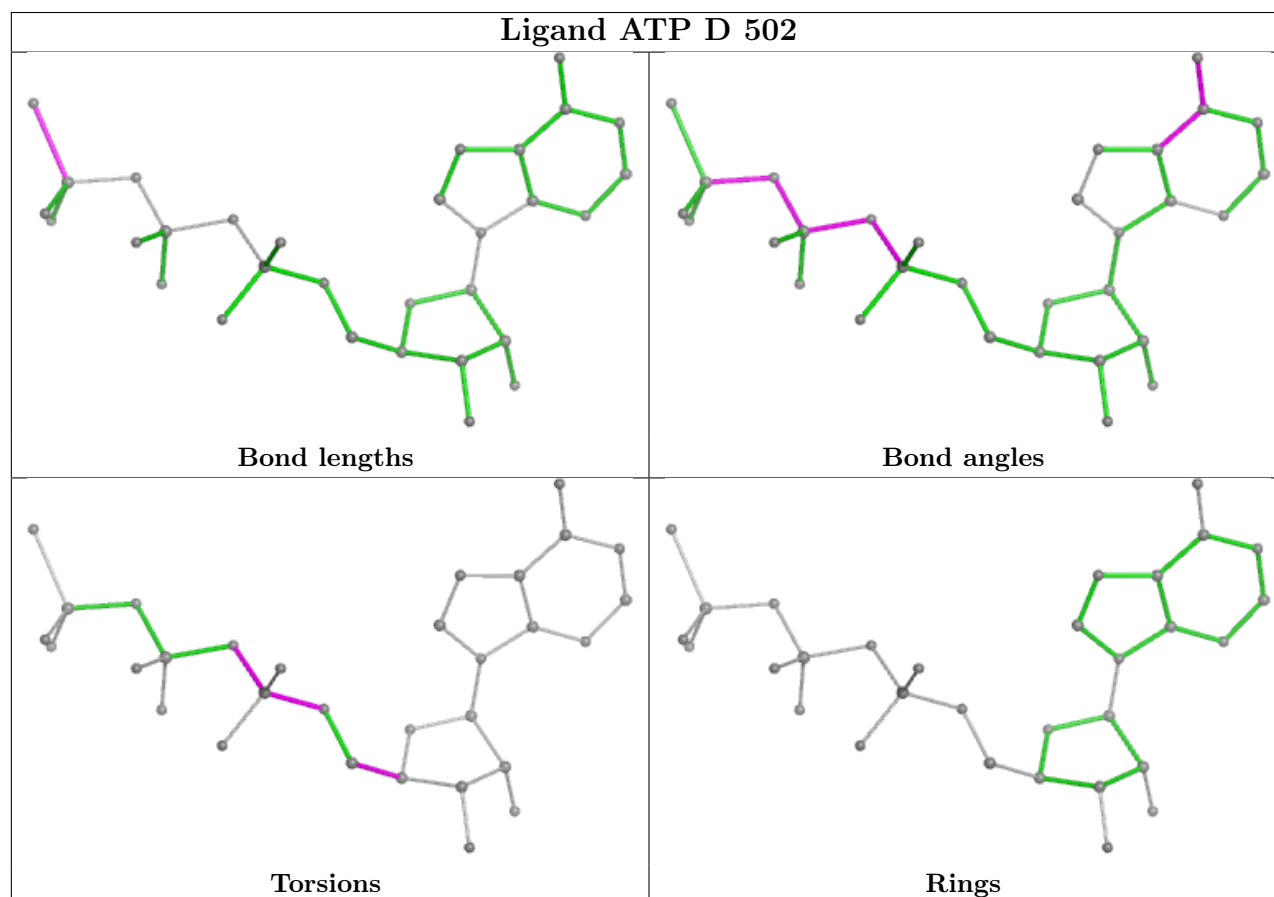
Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C5'-O5'-PA-O2A
34	B	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	C4'-C5'-O5'-PA
34	D	502	ATP	C5'-O5'-PA-O1A
34	D	502	ATP	O4'-C4'-C5'-O5'
34	D	502	ATP	C3'-C4'-C5'-O5'
34	A	501	ATP	C4'-C5'-O5'-PA
34	A	501	ATP	PA-O3A-PB-O2B
34	B	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	PB-O3B-PG-O1G
34	B	501	ATP	O4'-C4'-C5'-O5'
34	A	501	ATP	C5'-O5'-PA-O3A
34	D	502	ATP	C5'-O5'-PA-O3A
34	A	501	ATP	PA-O3A-PB-O1B
34	D	502	ATP	PB-O3A-PA-O1A
34	D	502	ATP	PB-O3A-PA-O2A
34	A	501	ATP	O4'-C4'-C5'-O5'

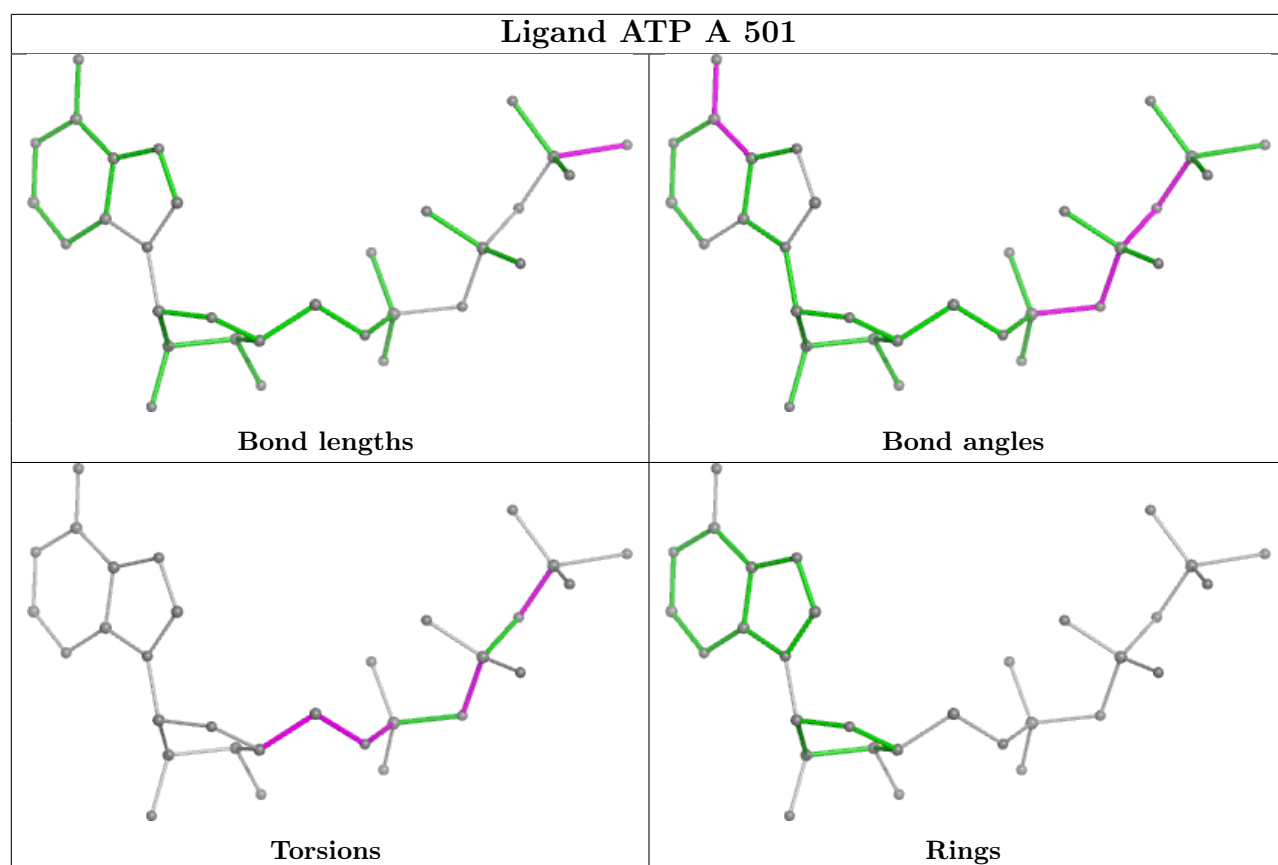
There are no ring outliers.

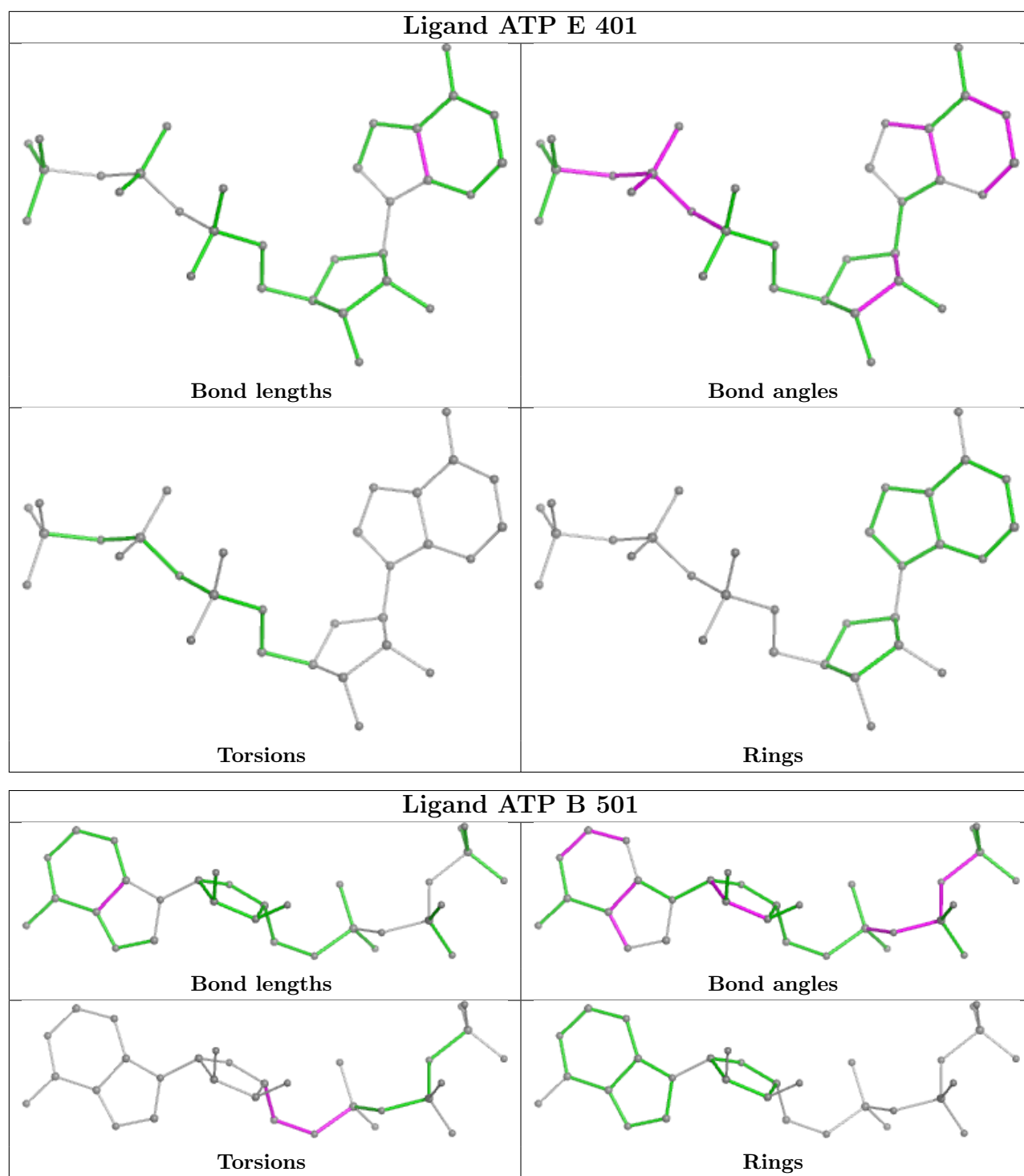
No monomer is involved in short contacts.

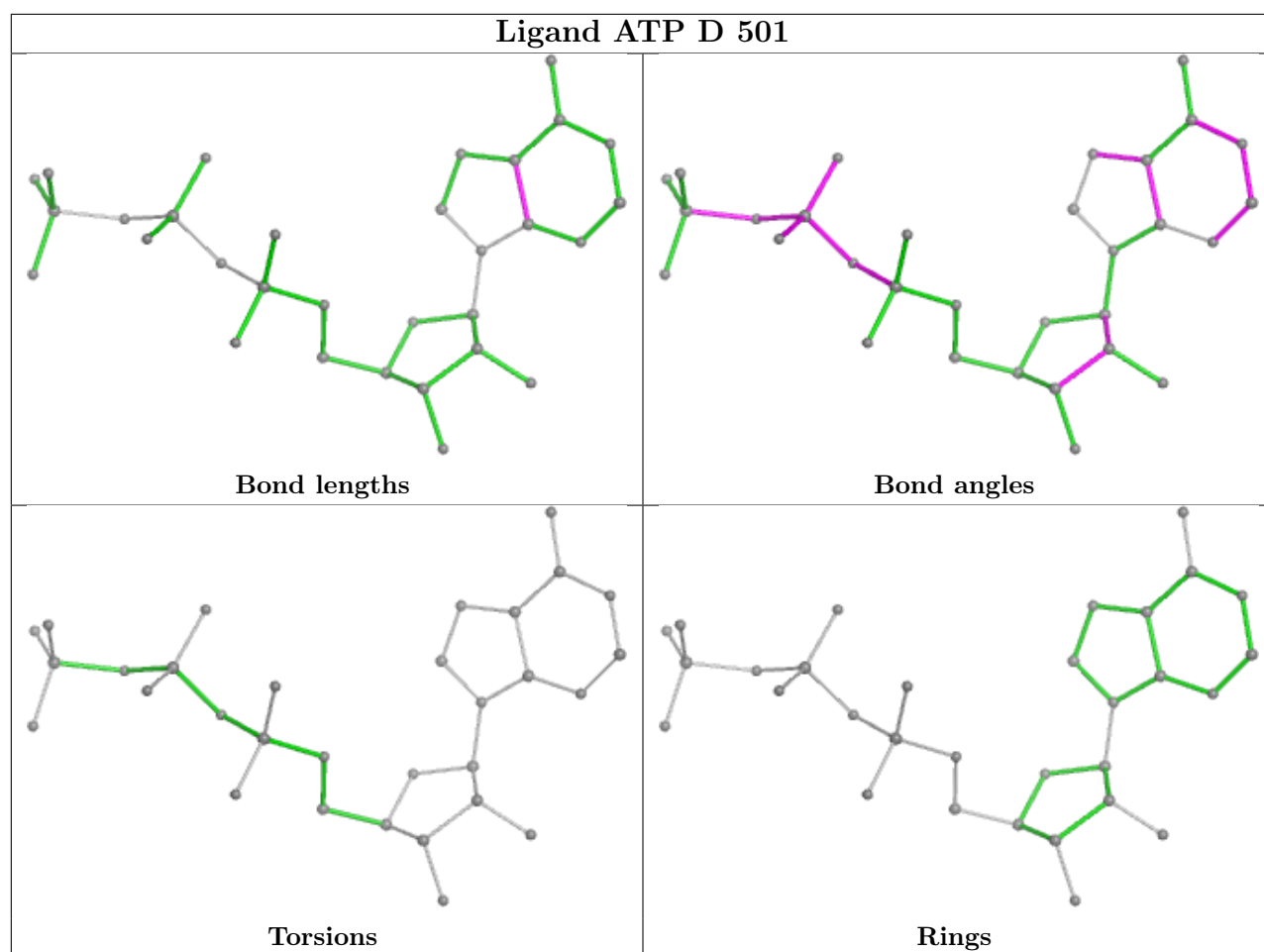
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

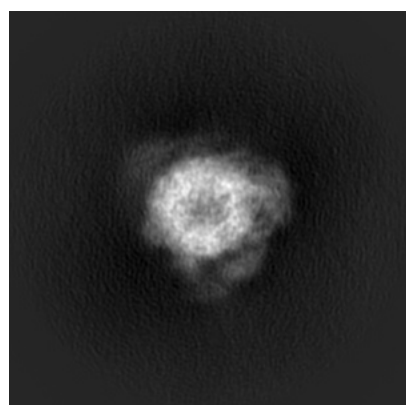
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14209. These allow visual inspection of the internal detail of the map and identification of artifacts.

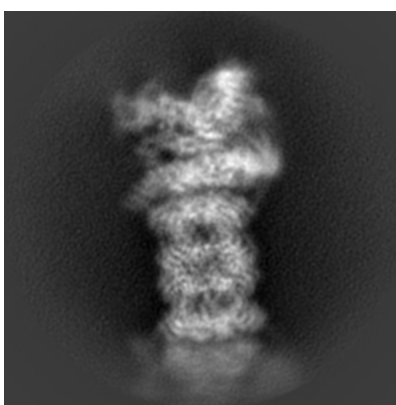
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

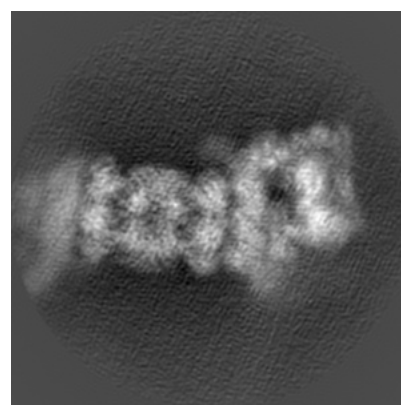
#### 6.1.1 Primary map



X



Y

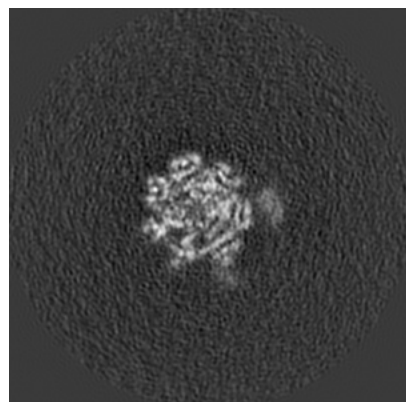


Z

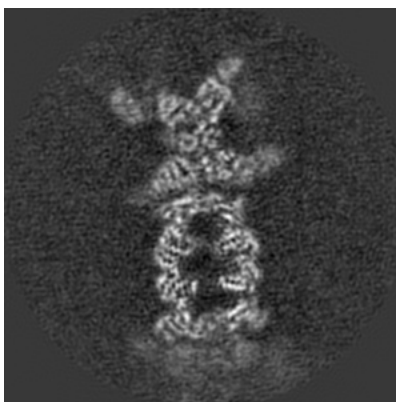
The images above show the map projected in three orthogonal directions.

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

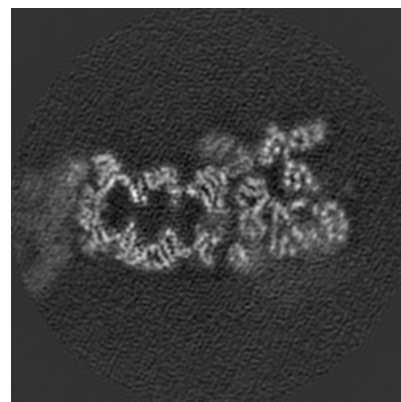
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



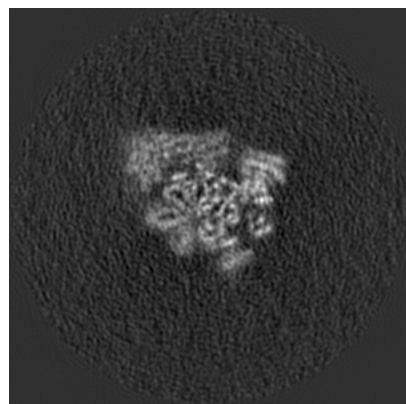
Z Index: 160



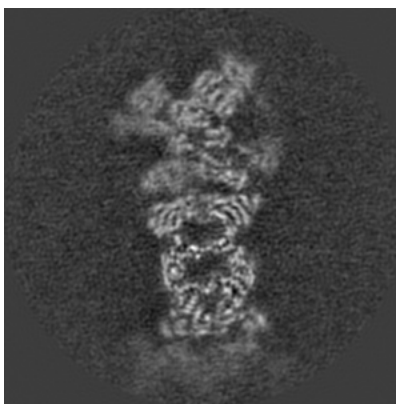
The images above show central slices of the map in three orthogonal directions.

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

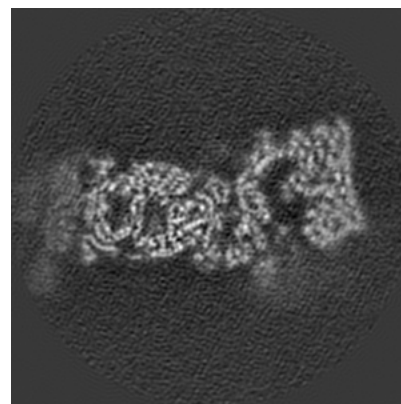
### 6.3.1 Primary map



X Index: 195



Y Index: 143

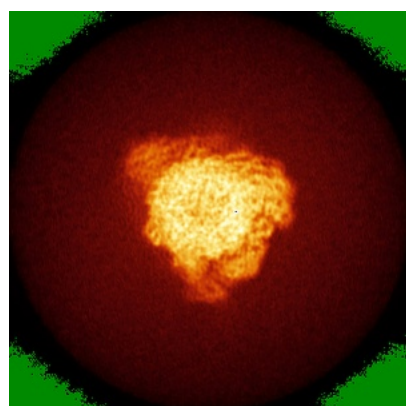


Z Index: 179

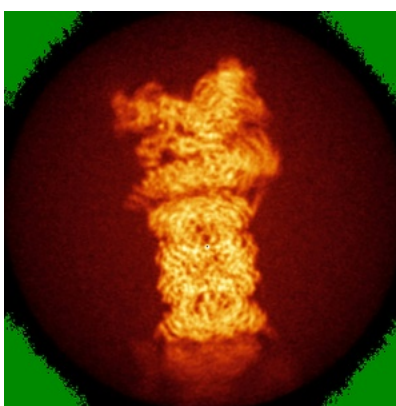
The images above show the largest variance slices of the map in three orthogonal directions.

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

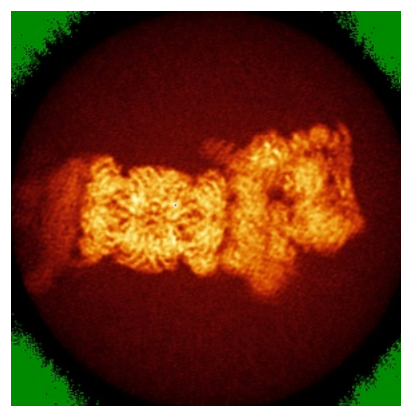
### 6.4.1 Primary map



X



Y

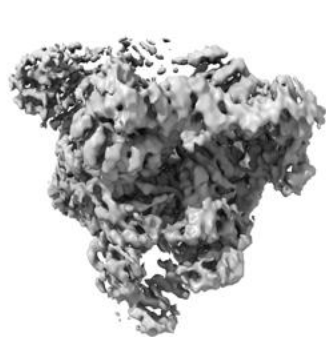


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0315. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

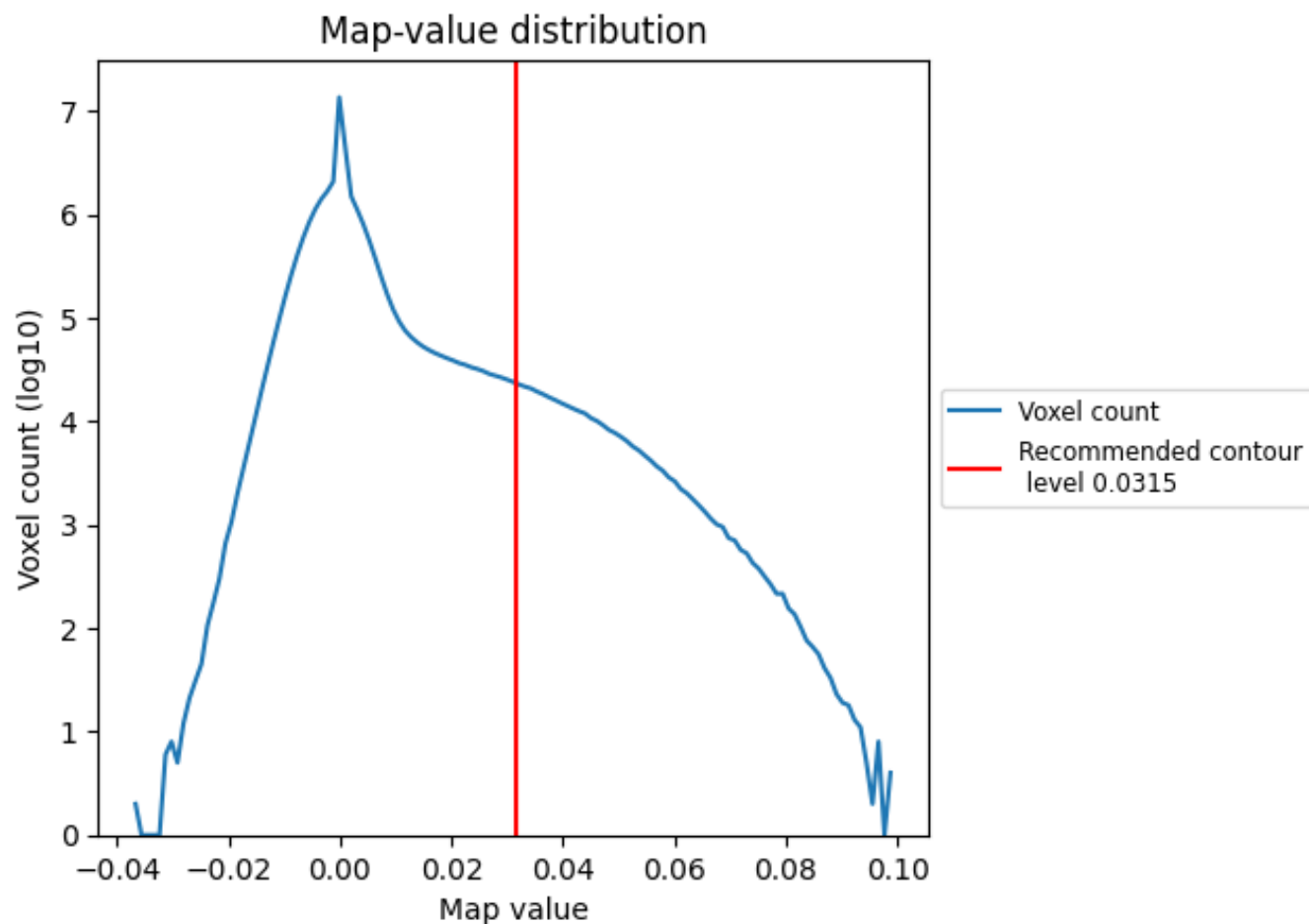
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

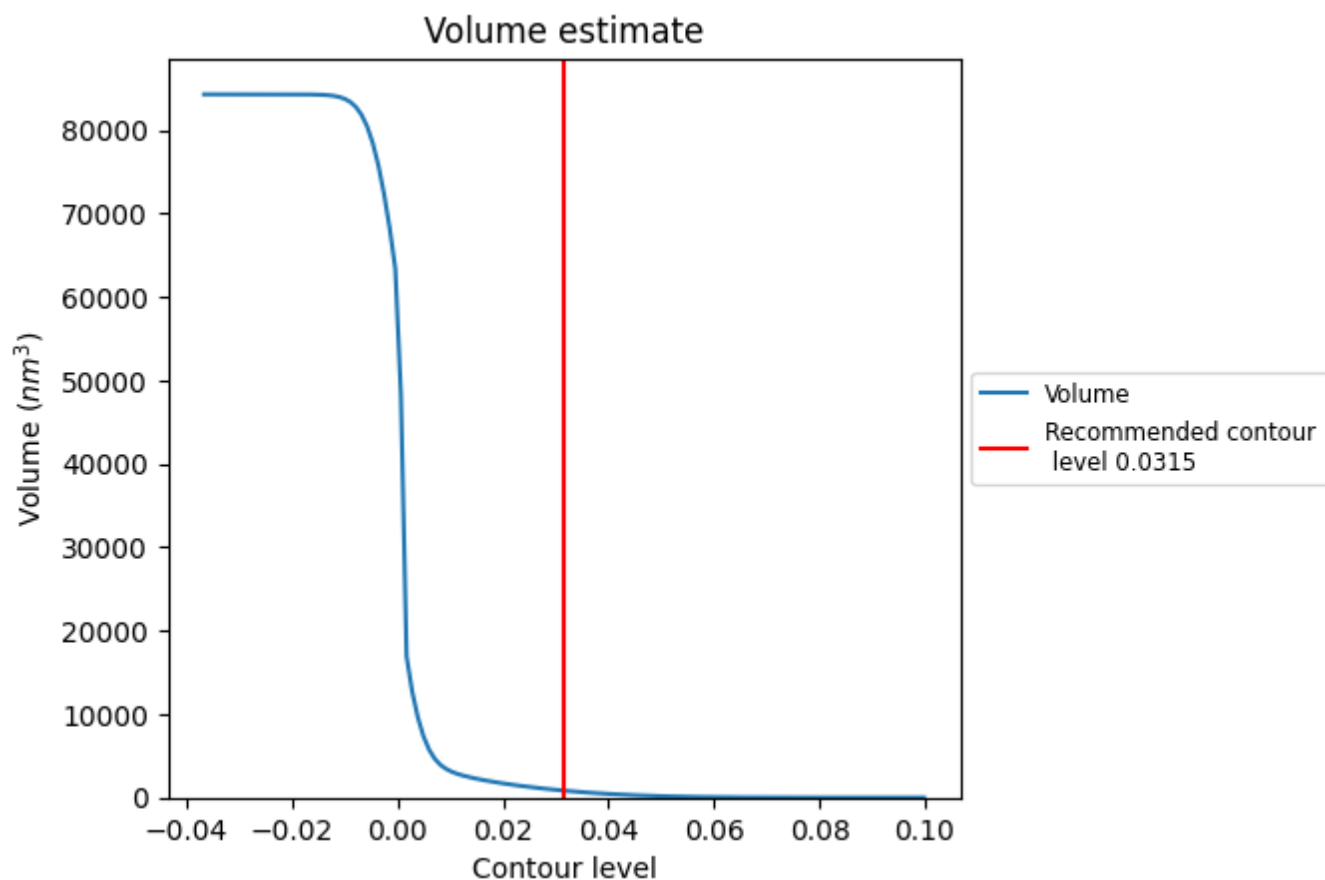
This section contains the results of statistical analysis of the map.

### 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.

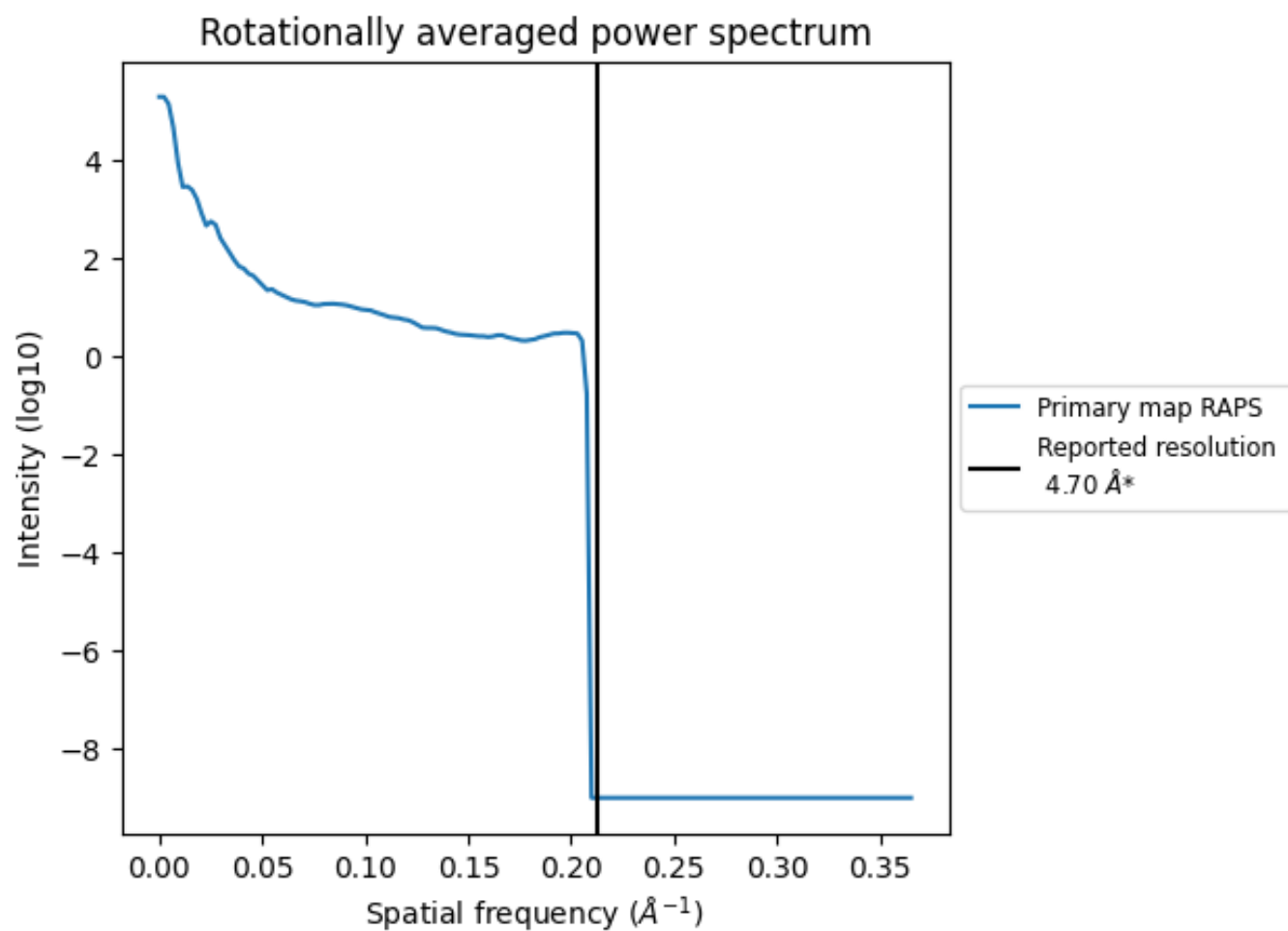
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm<sup>3</sup>; this corresponds to an approximate mass of 755 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 0.213 Å<sup>-1</sup>

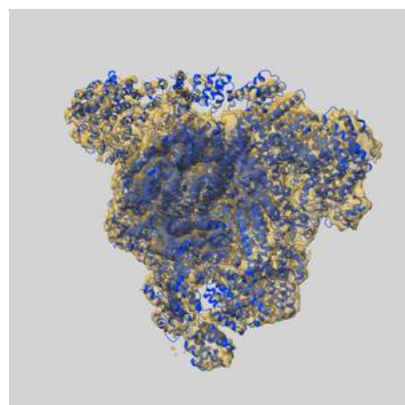
## 8 Fourier-Shell correlation ⓘ

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

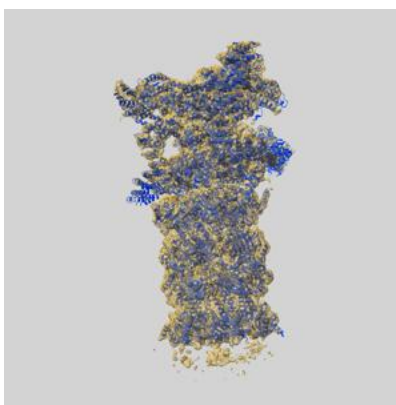
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14209 and PDB model 7QY7. Per-residue inclusion information can be found in section 3 on page 12.

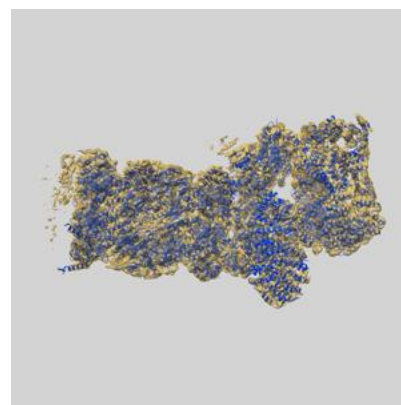
### 9.1 Map-model overlay [i](#)



X



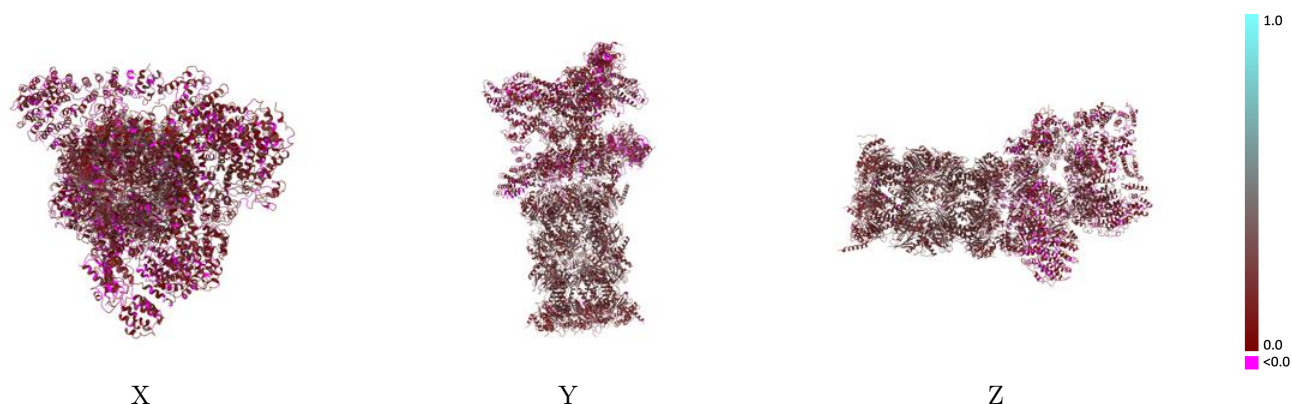
Y



Z

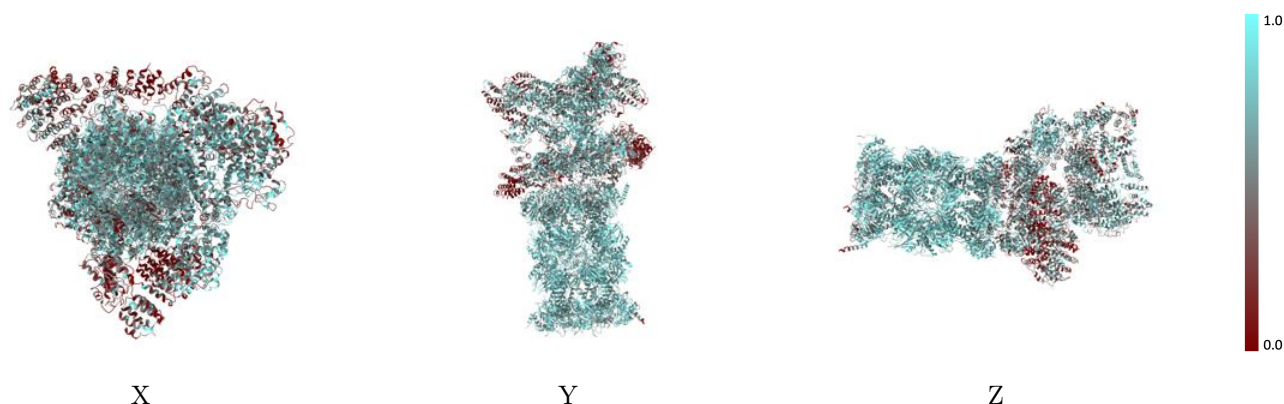
The images above show the 3D surface view of the map at the recommended contour level 0.0315 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

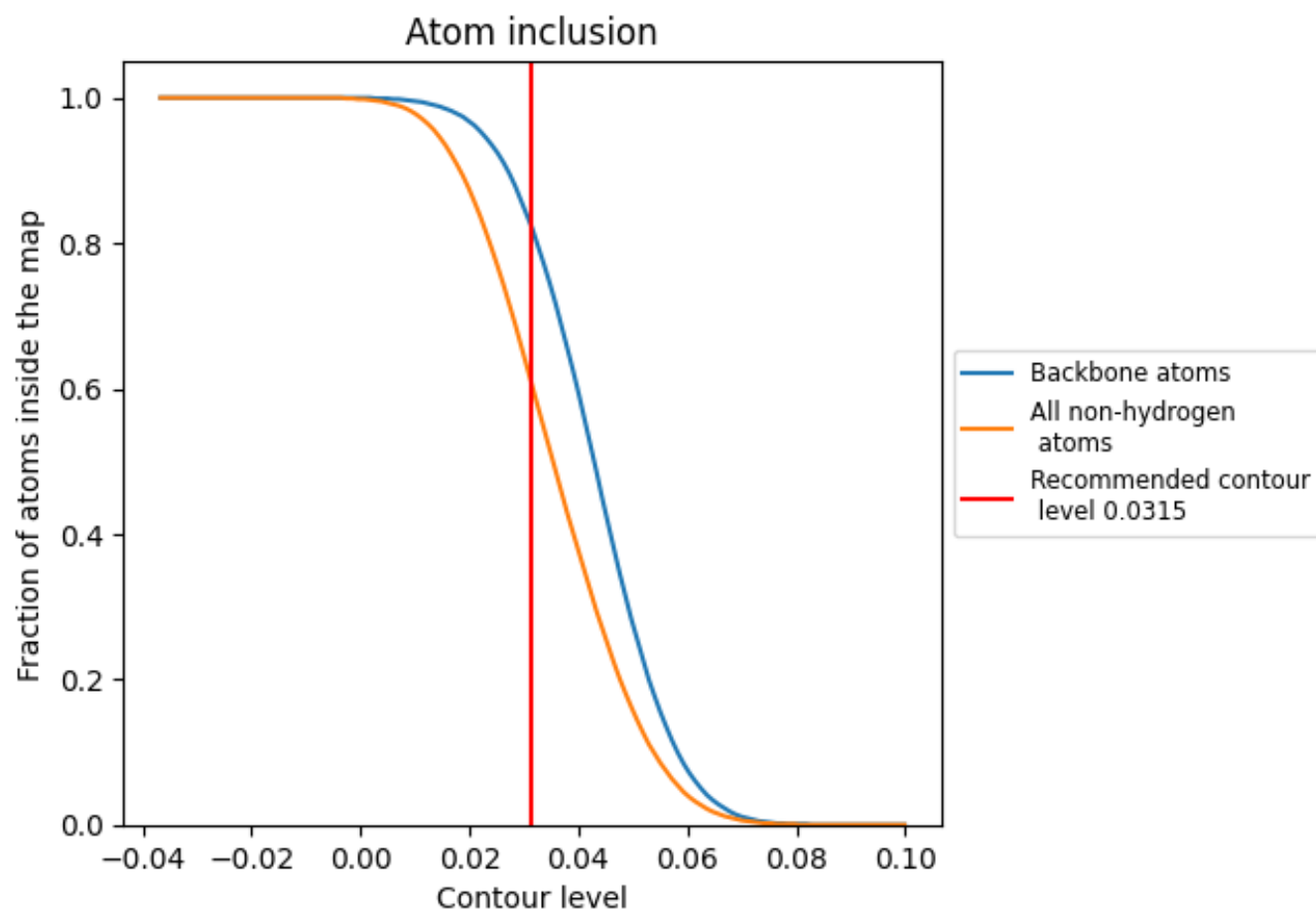
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0315).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 60% 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 (0.0315) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.1930
A	 0.5000	 0.1350
B	 0.5440	 0.1790
C	 0.5910	 0.1820
D	 0.5840	 0.1730
E	 0.5050	 0.1660
F	 0.3830	 0.1110
G	 0.6800	 0.2080
H	 0.7010	 0.2230
I	 0.6480	 0.2160
J	 0.7250	 0.2430
K	 0.7030	 0.2340
L	 0.7270	 0.2330
M	 0.6920	 0.2100
N	 0.7770	 0.2590
O	 0.7650	 0.2670
P	 0.7330	 0.2540
Q	 0.7820	 0.2680
R	 0.8130	 0.2830
S	 0.7710	 0.2790
T	 0.7900	 0.2730
U	 0.6140	 0.1540
V	 0.4960	 0.1370
W	 0.3670	 0.1230
X	 0.5550	 0.1560
Y	 0.6660	 0.1610
Z	 0.5620	 0.1470
a	 0.4960	 0.1340
b	 0.3020	 0.1100
c	 0.5870	 0.1650
d	 0.4570	 0.1350
e	 0.3300	 0.0690
f	 0.2640	 0.1140
g	 0.6730	 0.2300
h	 0.6530	 0.2190



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Chain	Atom inclusion	Q-score
i	 0.6310	 0.2150
j	 0.6730	 0.2230
k	 0.6740	 0.2290
l	 0.7260	 0.2420
m	 0.7070	 0.2320
n	 0.7800	 0.2620
o	 0.7710	 0.2720
p	 0.7530	 0.2720
q	 0.7620	 0.2770
r	 0.7820	 0.2610
s	 0.7810	 0.2770
t	 0.7820	 0.2750