



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:34 pm BST

PDB ID : 7QXW  
EMDB ID : EMD-14204  
Title : Proteasome-ZFAND5 Complex Z+D state  
Authors : Zhu, Y.; Lu, Y.  
Deposited on : 2022-01-27  
Resolution : 4.10 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:

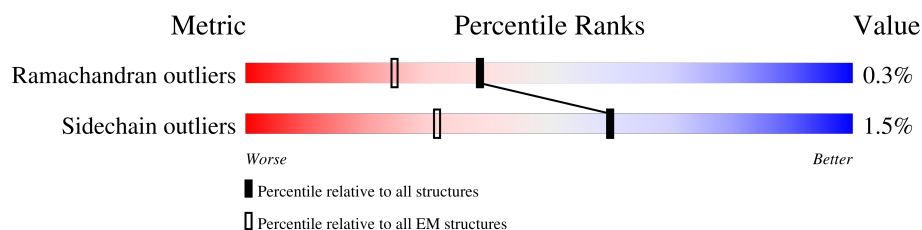
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	U	953	<div> <div>36%</div> <div>84%</div> <div>15%</div> </div>
2	V	533	<div> <div>33%</div> <div>89%</div> <div>10%</div> </div>
3	W	456	<div> <div>20%</div> <div>98%</div> <div>.</div> </div>
4	X	422	<div> <div>54%</div> <div>90%</div> <div>10%</div> </div>
5	Y	389	<div> <div>24%</div> <div>95%</div> <div>..</div> </div>
6	Z	324	<div> <div>15%</div> <div>88%</div> <div>12%</div> </div>
7	a	376	<div> <div>30%</div> <div>98%</div> <div>..</div> </div>
8	b	377	<div> <div>27%</div> <div>49%</div> <div>49%</div> </div>
9	c	309	<div> <div>10%</div> <div>87%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
10	d	349	
11	f	908	
12	A	433	
13	B	432	
14	C	398	
15	D	418	
16	E	403	
17	F	439	
18	e	70	
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	 80% 20%
27	o	276	 80% 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	 89% 11%
31	s	240	 89% 11%
32	T	263	 81% 18%
32	t	263	 81% 18%
33	v	213	 8% 22% 7% 71%

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 103867 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	282	Total	C	N	O	S	0	0
			2232	1414	384	415	19		

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

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

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 12 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	393	Total	C	N	O	S	0	0
			3067	1930	539	581	17		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	387	Total	C	N	O	S	0	0
			3027	1907	515	590	15		

- Molecule 14 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	376	Total	C	N	O	S	0	0
			2936	1846	531	544	15		

- Molecule 15 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	351	Total	C	N	O	S	0	0
			2773	1745	491	521	16		

- Molecule 17 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	354	Total	C	N	O	S	0	0
			2763	1745	476	527	15		

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	39	Total	C	N	O	S	0	0
			327	197	54	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	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	232	Total	C	N	O	S	0	0
			1708	1081	289	333	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	250	Total	C	N	O	S	0	0
			1912	1204	329	371	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
			1722	1080	284	348	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 a protein called AN1-type zinc finger protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	v	62	Total	C	N	O	S	0	0
			499	311	96	85	7		

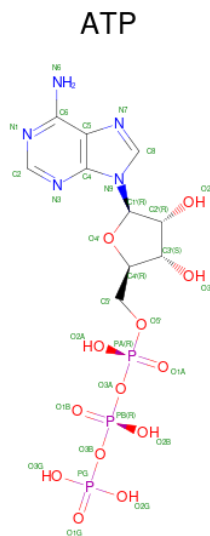
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	66	ILE	VAL	conflict	UNP O76080
v	70	GLU	ASP	conflict	UNP O76080
v	71	ALA	THR	conflict	UNP O76080

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<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
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	D	1	Total 31	C 10	N 5	O 13	P 3	0
35	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

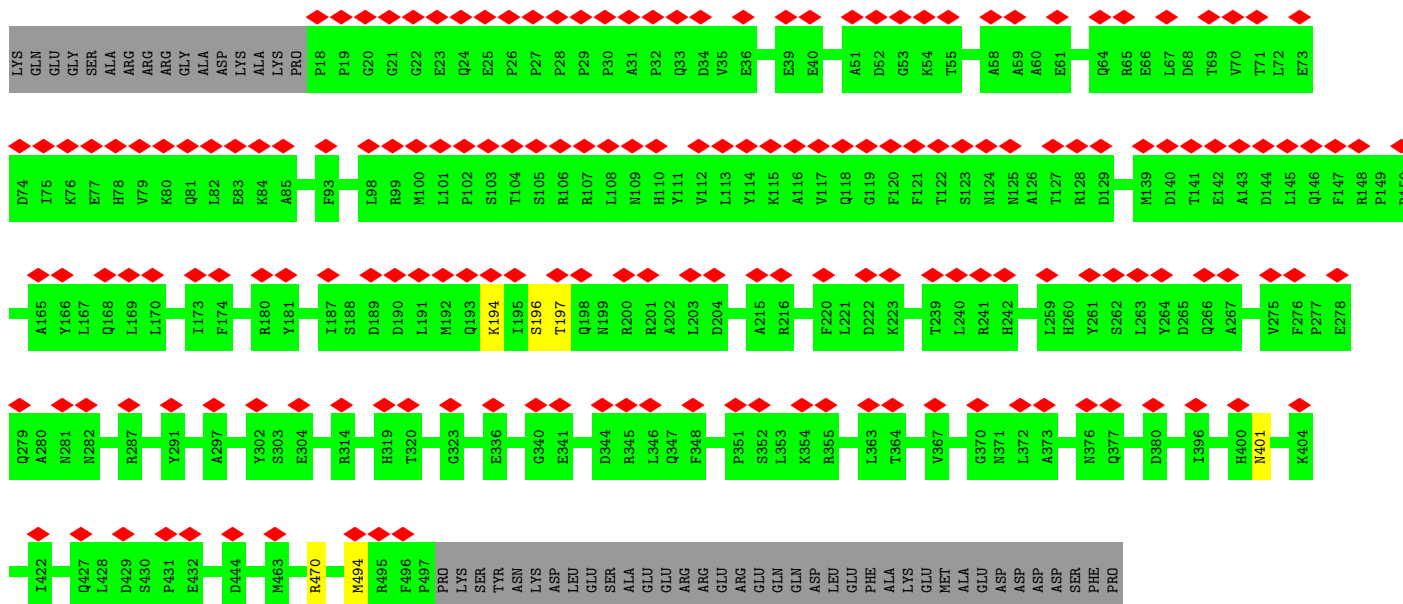
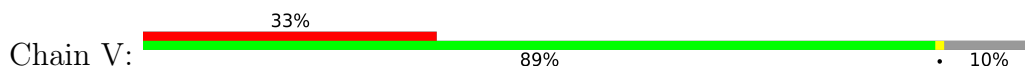
Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total Mg 1 1	0
36	D	1	Total Mg 1 1	0
36	F	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

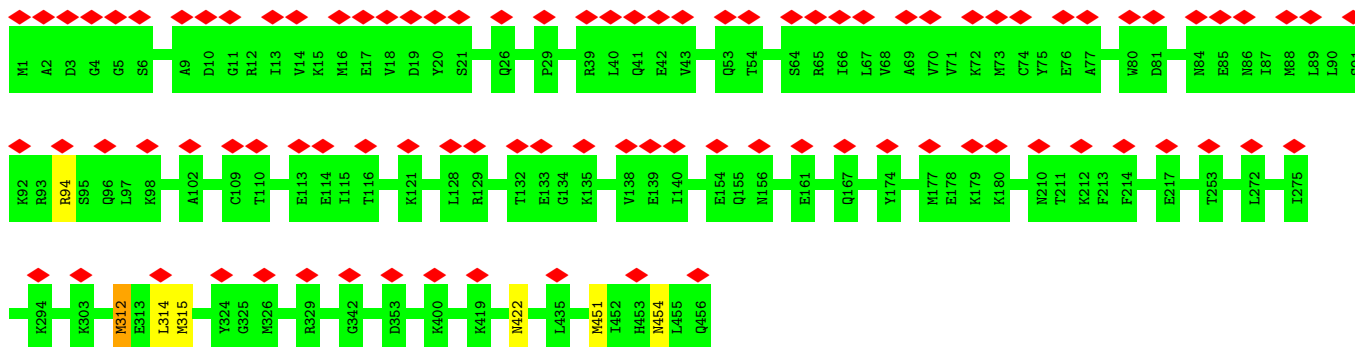




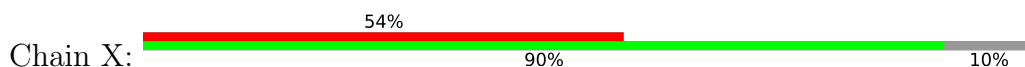
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

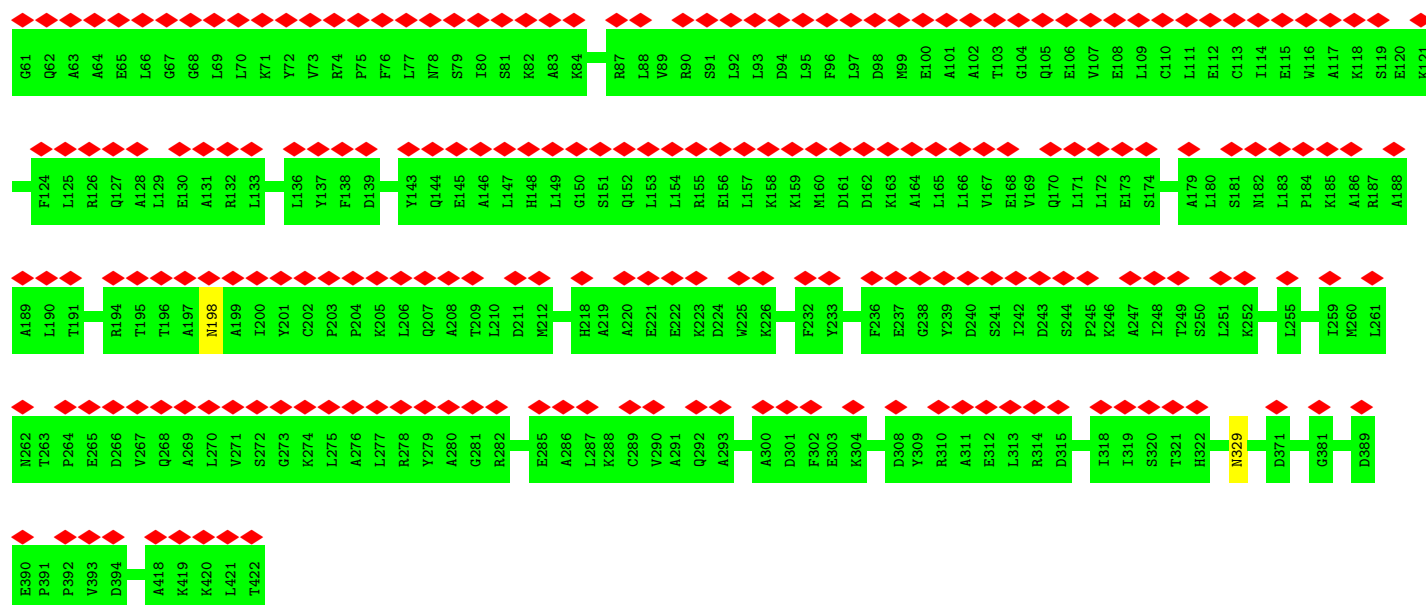


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



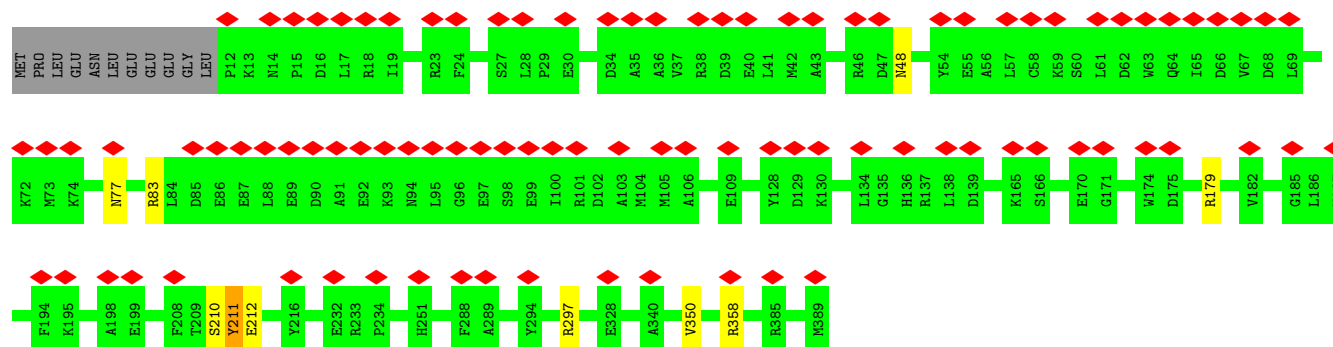
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11





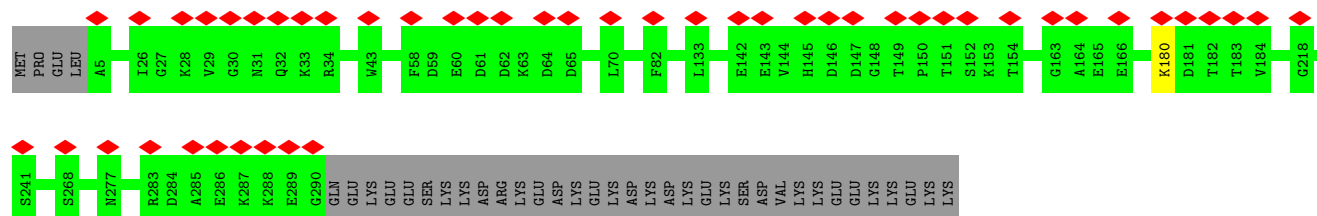
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 24% 95%



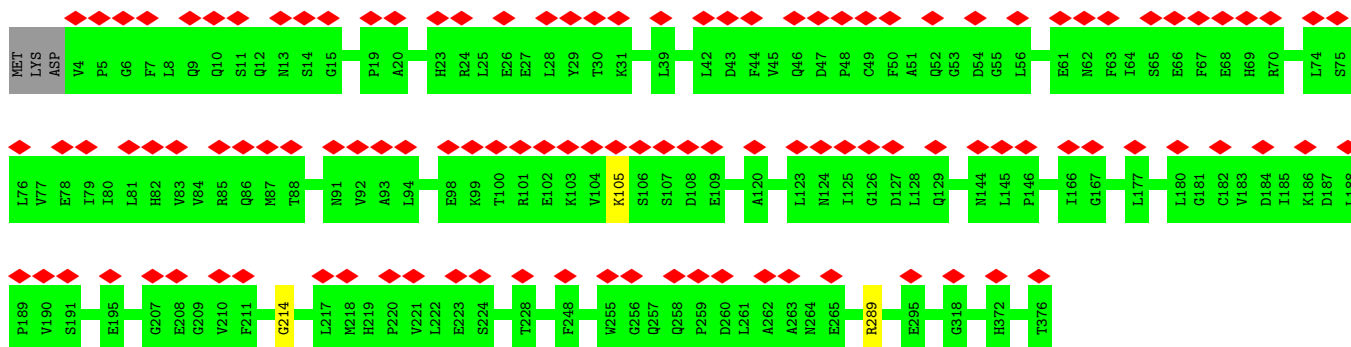
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 15% 88% 12%

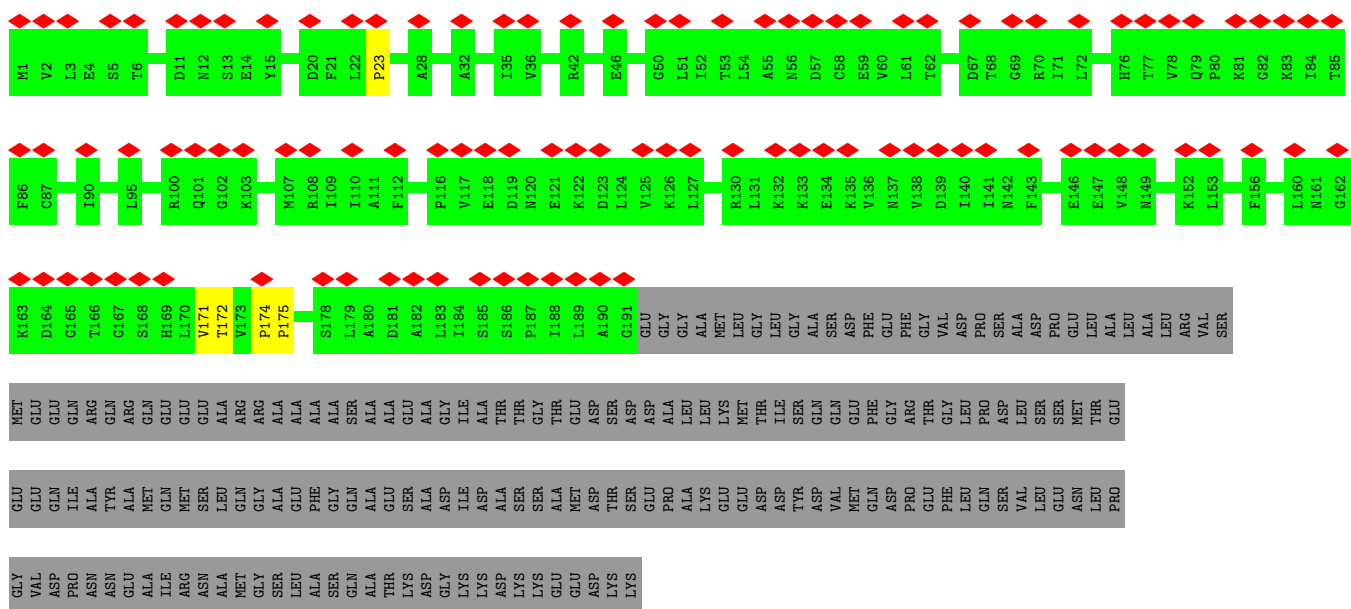


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

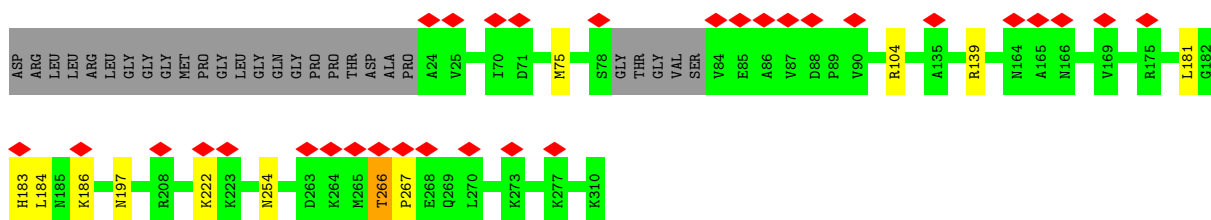
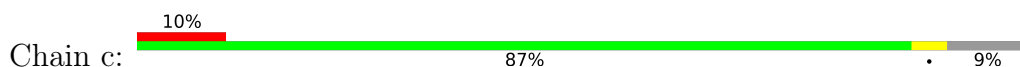
Chain a: 30% 98%



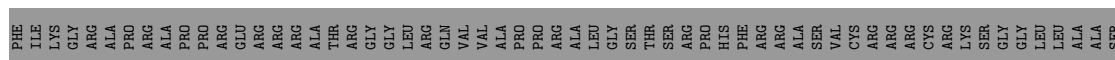
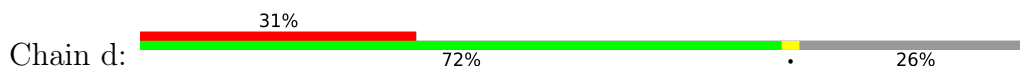
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



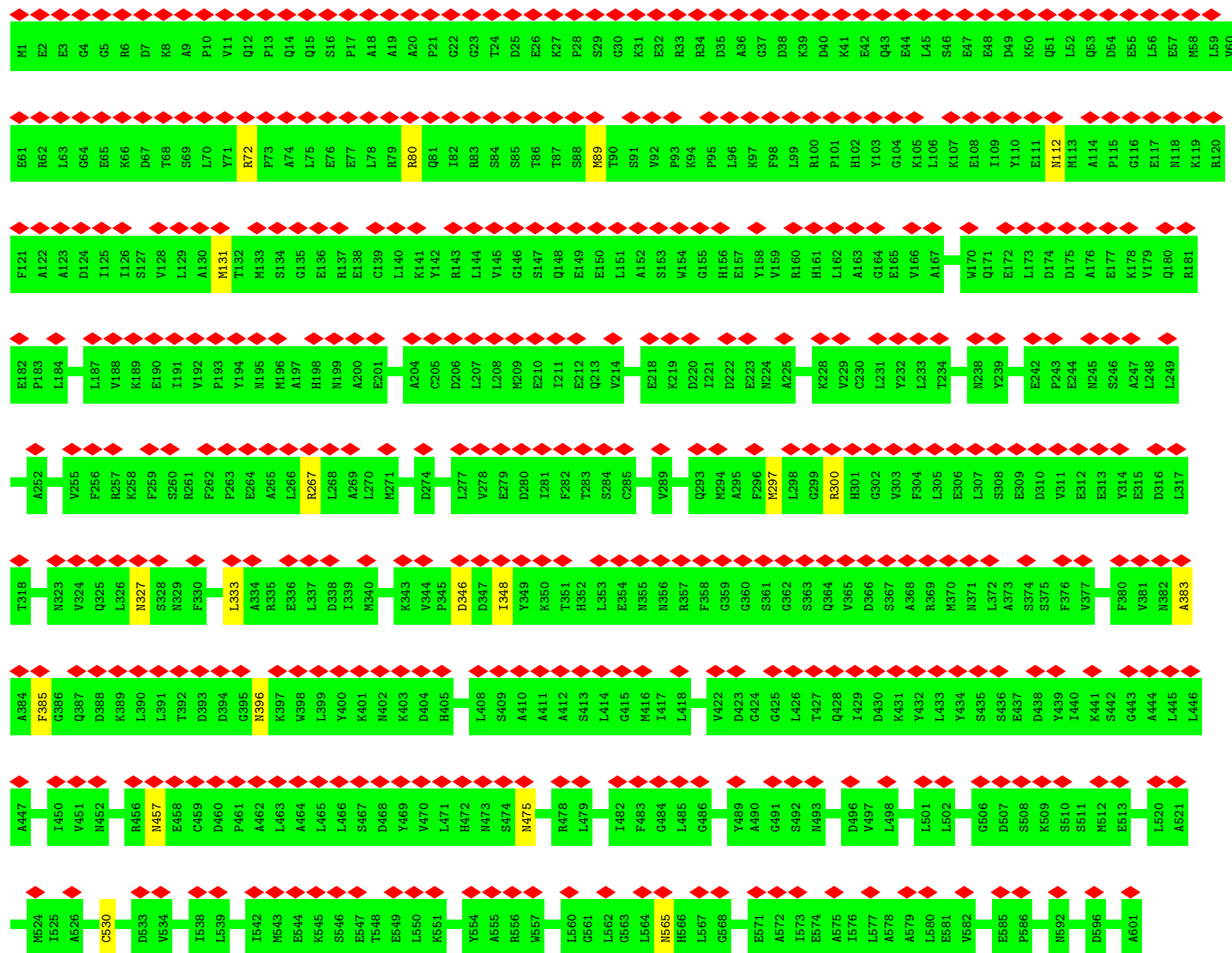
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

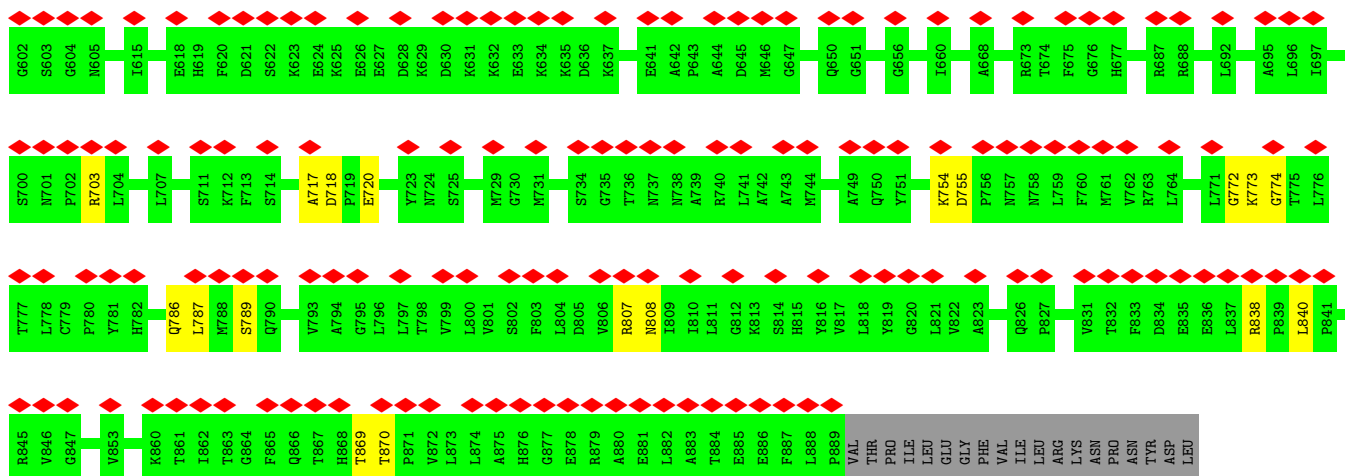


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

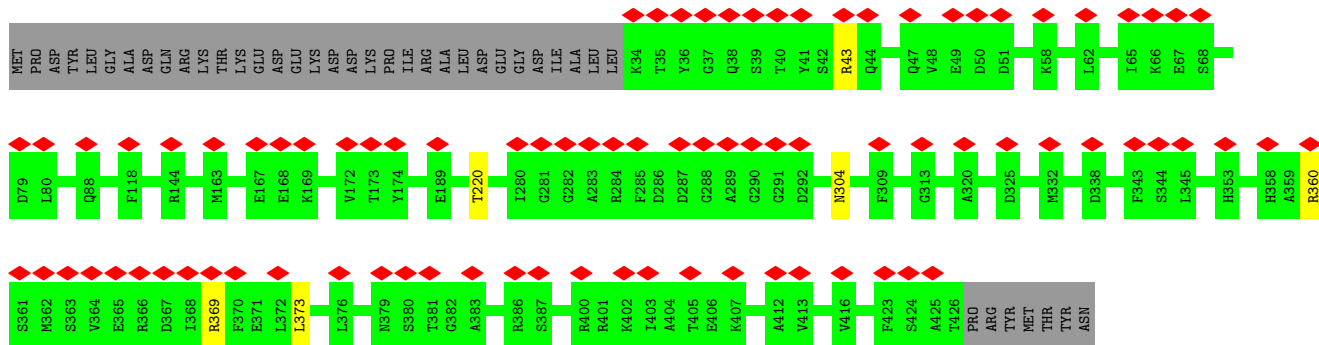
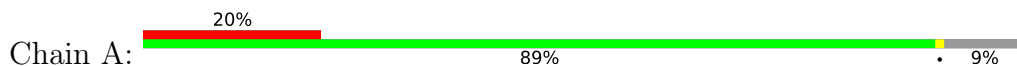




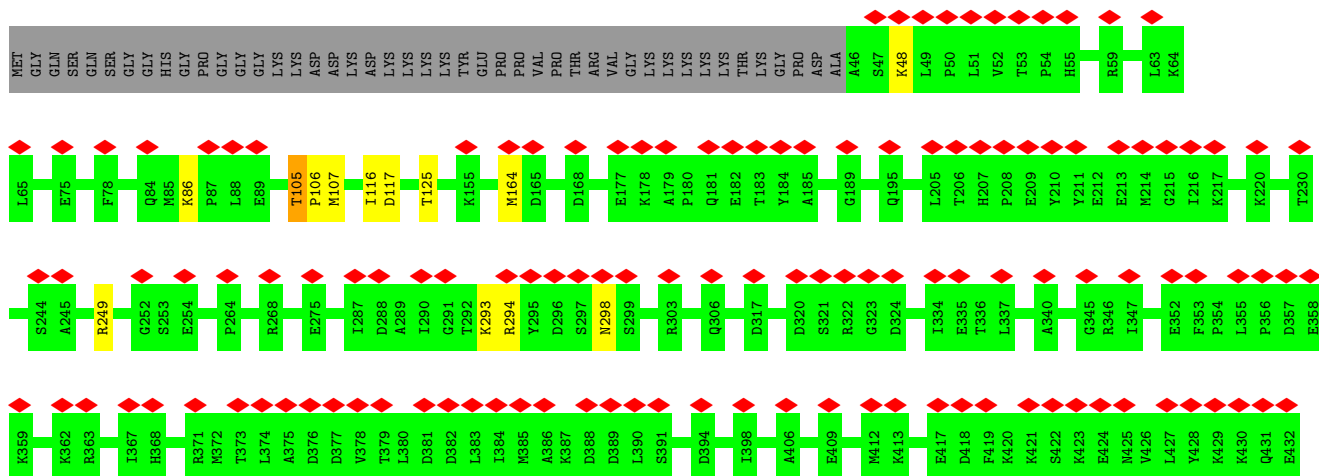
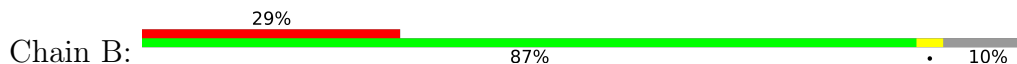




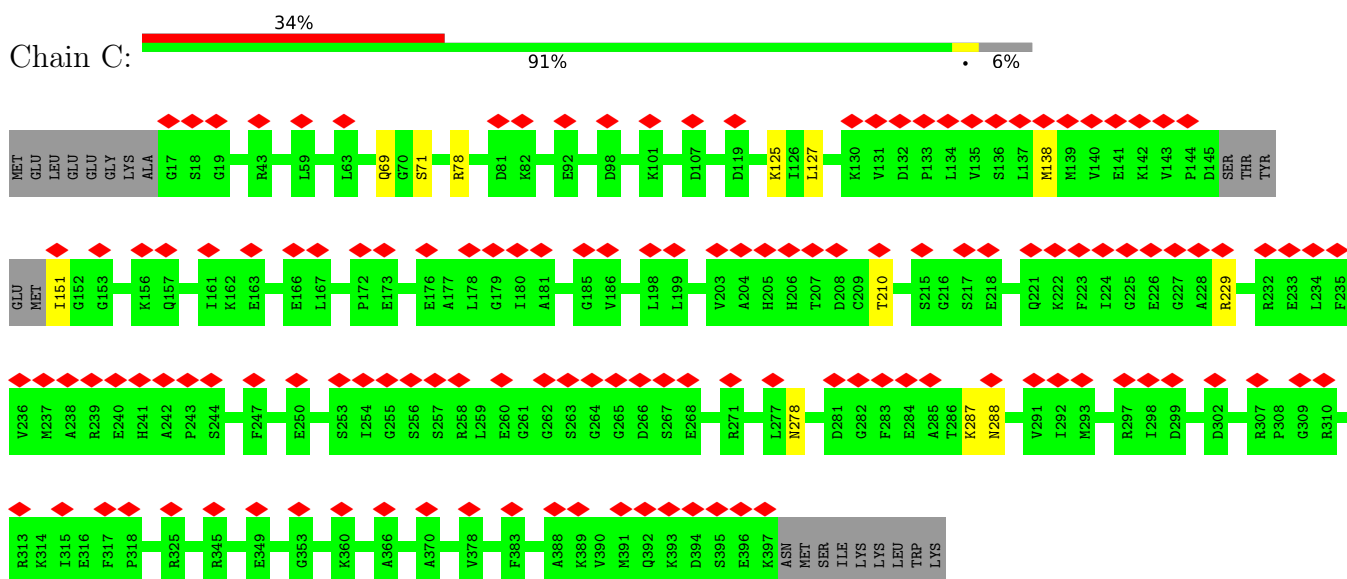
• Molecule 12: 26S protease regulatory subunit 7



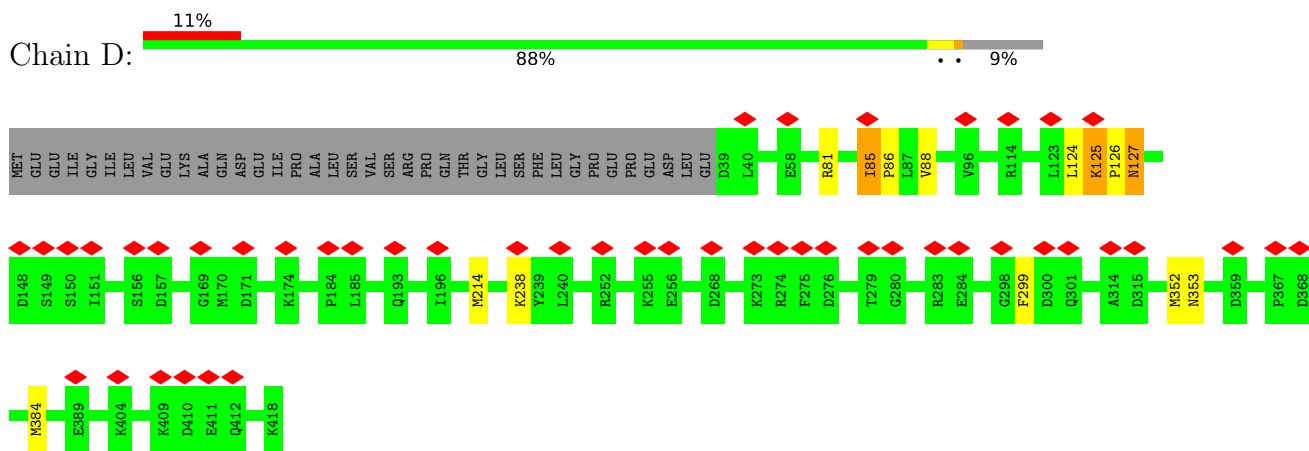
• Molecule 13: 26S proteasome regulatory subunit 4



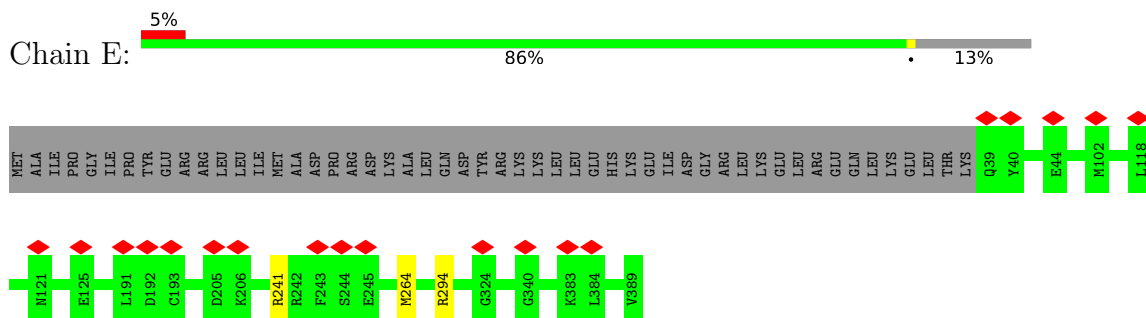
• Molecule 14: Isoform 2 of 26S proteasome regulatory subunit 8



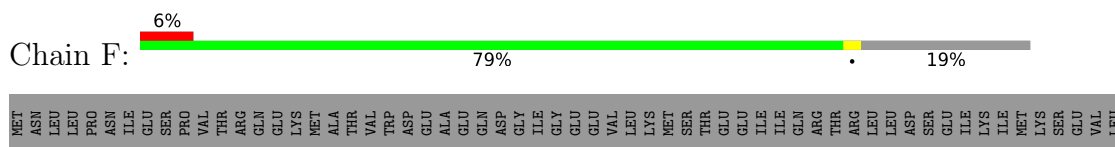
- Molecule 15: 26S protease regulatory subunit 6B

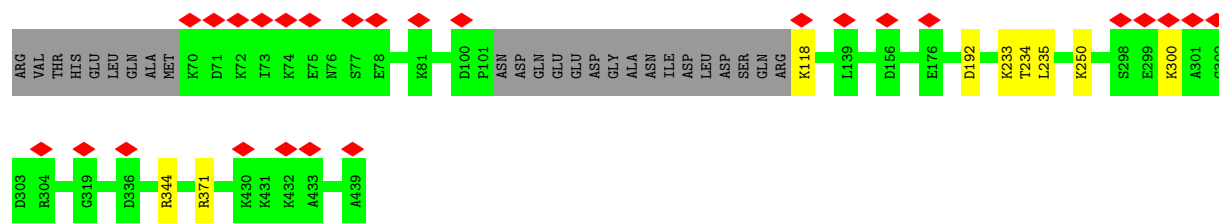


- Molecule 16: 26S proteasome regulatory subunit 10B

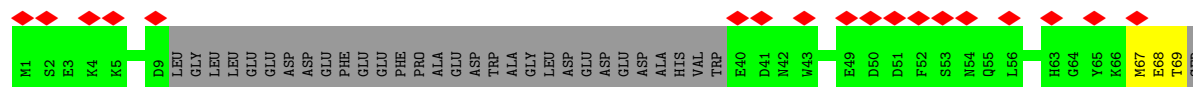


- Molecule 17: 26S protease regulatory subunit 6A

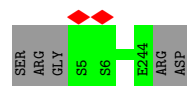




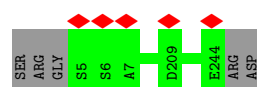
- Molecule 18: 26S proteasome complex subunit SEM1



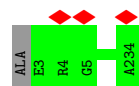
- Molecule 19: Proteasome subunit alpha type-6



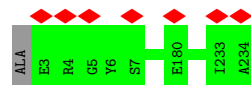
- Molecule 19: Proteasome subunit alpha type-6



- Molecule 20: Proteasome subunit alpha type-2

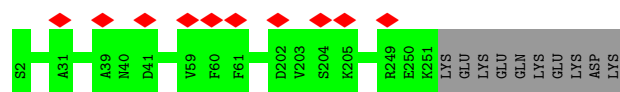


- Molecule 20: Proteasome subunit alpha type-2

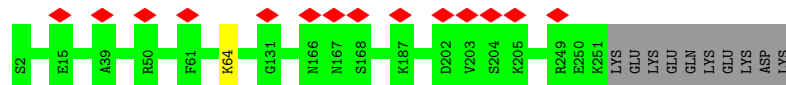


- Molecule 21: Proteasome subunit alpha type-4

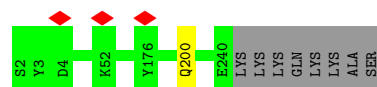




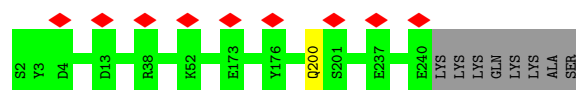
- Molecule 21: Proteasome subunit alpha type-4



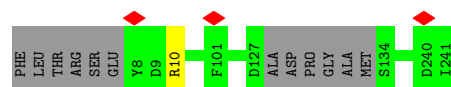
- Molecule 22: Proteasome subunit alpha type-7



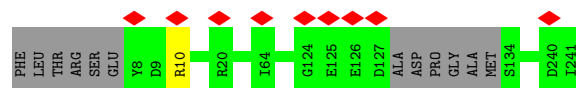
- Molecule 22: Proteasome subunit alpha type-7



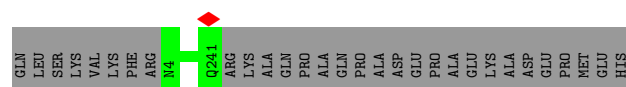
- Molecule 23: Proteasome subunit alpha type-5



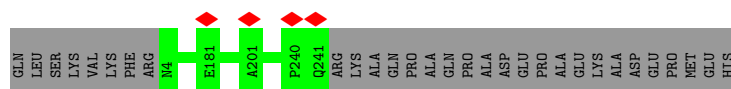
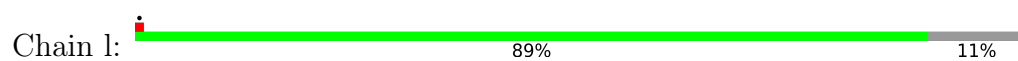
- Molecule 23: Proteasome subunit alpha type-5



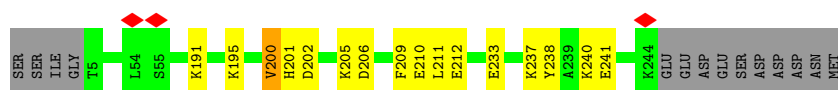
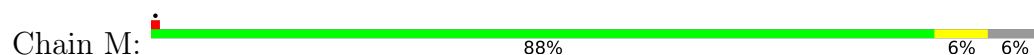
- Molecule 24: Isoform Long of Proteasome subunit alpha type-1



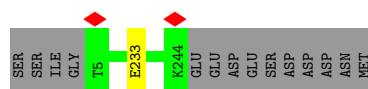
- Molecule 24: Isoform Long of Proteasome subunit alpha type-1



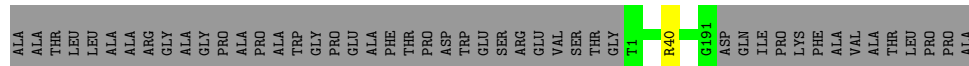
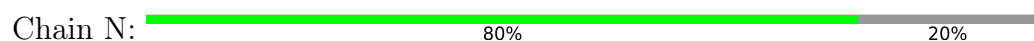
- Molecule 25: Proteasome subunit alpha type-3



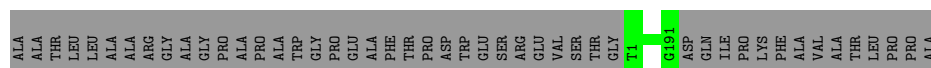
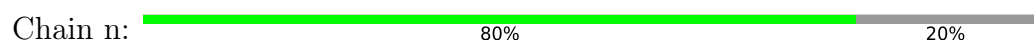
- Molecule 25: Proteasome subunit alpha type-3



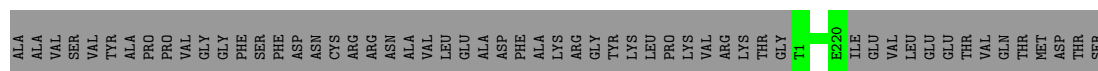
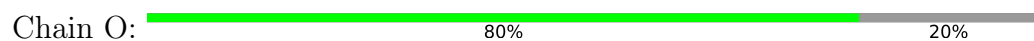
- Molecule 26: Proteasome subunit beta type-6



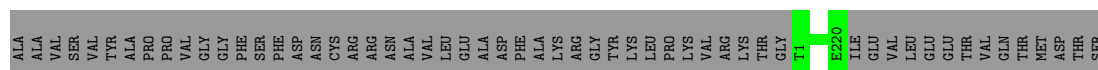
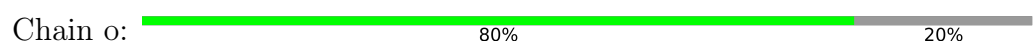
- Molecule 26: Proteasome subunit beta type-6



- 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: 

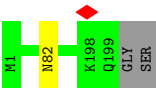
100%



- Molecule 29: Proteasome subunit beta type-2

Chain Q: 

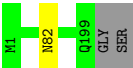
99%



- Molecule 29: Proteasome subunit beta type-2

Chain q: 

99%

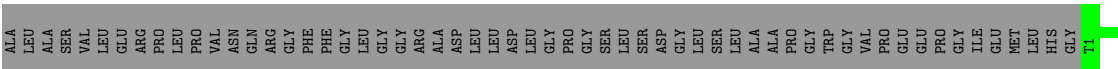


- Molecule 30: Proteasome subunit beta type-5

Chain R: 

77%

23%

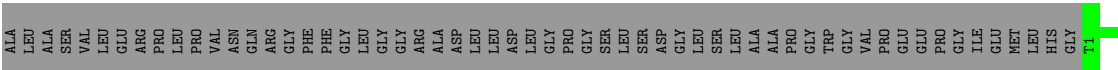


- Molecule 30: Proteasome subunit beta type-5

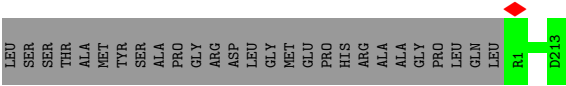
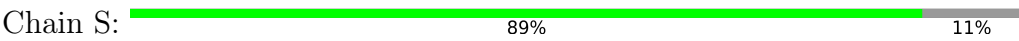
Chain r: 

77%

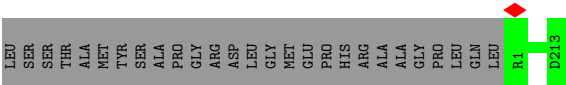
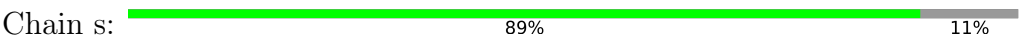
23%



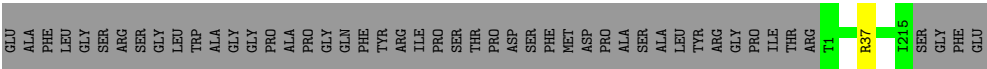
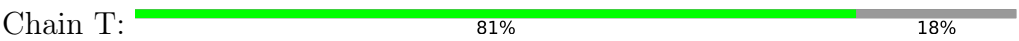
• Molecule 31: Proteasome subunit beta type-1



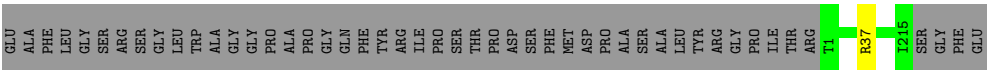
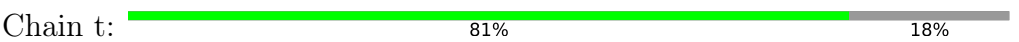
• Molecule 31: Proteasome subunit beta type-1



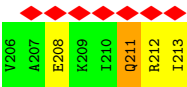
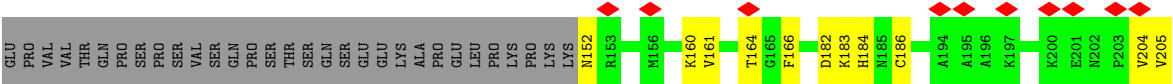
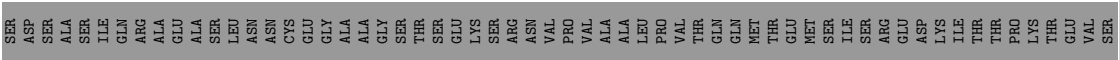
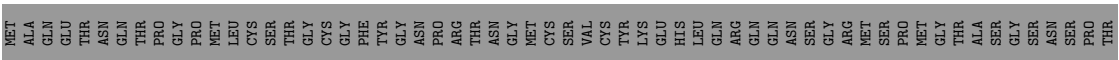
• Molecule 32: Proteasome subunit beta type-4



• Molecule 32: Proteasome subunit beta type-4



• Molecule 33: AN1-type zinc finger protein 5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28928	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	0.124	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0328	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP, 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	U	0.27	0/6449	0.43	0/8729
2	V	0.29	0/3929	0.47	0/5309
3	W	0.28	0/3751	0.46	0/5042
4	X	0.26	0/3053	0.41	0/4115
5	Y	0.30	0/3173	0.52	0/4273
6	Z	0.28	0/2324	0.47	0/3150
7	a	0.27	0/3053	0.42	0/4133
8	b	0.26	0/1478	0.46	0/2001
9	c	0.29	0/2273	0.49	0/3069
10	d	0.29	0/2162	0.50	0/2919
11	f	0.28	0/6980	0.53	0/9433
12	A	0.29	0/3117	0.48	2/4207 (0.0%)
13	B	0.28	0/3070	0.49	0/4143
14	C	0.28	0/2973	0.48	0/3997
15	D	0.29	0/3089	0.47	0/4168
16	E	0.29	0/2818	0.46	0/3800
17	F	0.31	0/2802	0.47	0/3777
18	e	0.28	0/331	0.45	0/442
19	G	0.32	0/1859	0.46	0/2523
19	g	0.32	0/1859	0.46	0/2523
20	H	0.33	0/1743	0.45	0/2372
20	h	0.33	0/1743	0.45	0/2372
21	I	0.31	0/1942	0.47	0/2628
21	i	0.31	0/1942	0.47	0/2628
22	J	0.31	0/1728	0.46	0/2358
22	j	0.30	0/1728	0.46	0/2358
23	K	0.31	0/1747	0.47	0/2364
23	k	0.31	0/1747	0.47	0/2364
24	L	0.32	0/1885	0.45	0/2552
24	l	0.32	0/1885	0.45	0/2552
25	M	0.33	0/1891	0.48	0/2552
25	m	0.33	0/1891	0.47	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
26	N	0.34	0/1454	0.47	0/1967
26	n	0.34	0/1454	0.47	0/1967
27	O	0.33	0/1670	0.46	0/2265
27	o	0.33	0/1670	0.46	0/2265
28	P	0.33	0/1614	0.45	0/2177
28	p	0.33	0/1614	0.45	0/2177
29	Q	0.34	0/1603	0.47	0/2174
29	q	0.34	0/1603	0.47	0/2174
30	R	0.35	0/1579	0.44	0/2134
30	r	0.35	0/1579	0.44	0/2134
31	S	0.34	0/1671	0.46	0/2253
31	s	0.34	0/1671	0.46	0/2253
32	T	0.34	0/1700	0.46	0/2305
32	t	0.34	0/1700	0.46	0/2305
33	v	0.48	0/508	0.69	0/676
All	All	0.31	0/105505	0.47	2/142631 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	220	THR	O-C-N	-5.51	113.83	123.20
12	A	220	THR	CA-C-N	5.30	126.80	116.20

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	U	806/953 (85%)	728 (90%)	76 (9%)	2 (0%)	44	77
2	V	478/533 (90%)	410 (86%)	68 (14%)	0	100	100
3	W	454/456 (100%)	413 (91%)	40 (9%)	1 (0%)	44	77
4	X	378/422 (90%)	353 (93%)	25 (7%)	0	100	100
5	Y	376/389 (97%)	317 (84%)	56 (15%)	3 (1%)	16	53
6	Z	284/324 (88%)	246 (87%)	38 (13%)	0	100	100
7	a	371/376 (99%)	335 (90%)	35 (9%)	1 (0%)	37	71
8	b	189/377 (50%)	166 (88%)	20 (11%)	3 (2%)	8	39
9	c	278/309 (90%)	240 (86%)	36 (13%)	2 (1%)	19	56
10	d	255/349 (73%)	215 (84%)	40 (16%)	0	100	100
11	f	887/908 (98%)	719 (81%)	158 (18%)	10 (1%)	12	46
12	A	391/433 (90%)	342 (88%)	49 (12%)	0	100	100
13	B	385/432 (89%)	332 (86%)	50 (13%)	3 (1%)	16	53
14	C	372/398 (94%)	320 (86%)	50 (13%)	2 (0%)	25	62
15	D	378/418 (90%)	319 (84%)	51 (14%)	8 (2%)	5	33
16	E	349/403 (87%)	298 (85%)	51 (15%)	0	100	100
17	F	350/439 (80%)	308 (88%)	41 (12%)	1 (0%)	37	71
18	e	35/70 (50%)	26 (74%)	9 (26%)	0	100	100
19	G	238/245 (97%)	224 (94%)	14 (6%)	0	100	100
19	g	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
20	H	230/233 (99%)	211 (92%)	19 (8%)	0	100	100
20	h	230/233 (99%)	211 (92%)	19 (8%)	0	100	100
21	I	248/260 (95%)	222 (90%)	26 (10%)	0	100	100
21	i	248/260 (95%)	222 (90%)	25 (10%)	1 (0%)	30	67
22	J	237/247 (96%)	212 (90%)	24 (10%)	1 (0%)	30	67
22	j	237/247 (96%)	212 (90%)	24 (10%)	1 (0%)	30	67
23	K	224/240 (93%)	203 (91%)	21 (9%)	0	100	100
23	k	224/240 (93%)	203 (91%)	21 (9%)	0	100	100
24	L	236/268 (88%)	207 (88%)	29 (12%)	0	100	100
24	l	236/268 (88%)	206 (87%)	30 (13%)	0	100	100
25	M	238/254 (94%)	201 (84%)	33 (14%)	4 (2%)	7	37
25	m	238/254 (94%)	210 (88%)	27 (11%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	N	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
26	n	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
27	O	218/276 (79%)	208 (95%)	10 (5%)	0	100	100
27	o	218/276 (79%)	208 (95%)	10 (5%)	0	100	100
28	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
28	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
29	Q	197/201 (98%)	172 (87%)	25 (13%)	0	100	100
29	q	197/201 (98%)	172 (87%)	25 (13%)	0	100	100
30	R	199/262 (76%)	189 (95%)	10 (5%)	0	100	100
30	r	199/262 (76%)	189 (95%)	10 (5%)	0	100	100
31	S	211/240 (88%)	193 (92%)	18 (8%)	0	100	100
31	s	211/240 (88%)	193 (92%)	18 (8%)	0	100	100
32	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
32	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
33	v	60/213 (28%)	46 (77%)	12 (20%)	2 (3%)	3	25
All	All	13236/15064 (88%)	11758 (89%)	1432 (11%)	46 (0%)	38	71

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	312	MET
8	b	175	PRO
11	f	717	ALA
11	f	718	ASP
11	f	789	SER
11	f	870	THR
13	B	105	THR
13	B	106	PRO
13	B	107	MET
15	D	85	ILE
15	D	126	PRO
22	J	200	GLN
22	j	200	GLN
5	Y	211	TYR
5	Y	212	GLU
8	b	174	PRO
11	f	475	ASN

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Mol	Chain	Res	Type
14	C	71	SER
14	C	288	ASN
15	D	125	LYS
25	M	241	GLU
33	v	208	GLU
5	Y	350	VAL
11	f	774	GLY
15	D	86	PRO
15	D	124	LEU
11	f	869	THR
15	D	299	PHE
17	F	344	ARG
25	M	205	LYS
33	v	211	GLN
1	U	10	SER
1	U	172	ASP
9	c	267	PRO
11	f	755	ASP
25	M	200	VAL
25	M	233	GLU
25	m	233	GLU
11	f	383	ALA
15	D	127	ASN
21	i	64	LYS
7	a	214	GLY
9	c	266	THR
15	D	88	VAL
8	b	23	PRO
11	f	772	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	685 (99%)	7 (1%)	73	81
2	V	414/459 (90%)	408 (99%)	6 (1%)	62	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W	416/416 (100%)	409 (98%)	7 (2%)	56	72
4	X	327/362 (90%)	325 (99%)	2 (1%)	84	88
5	Y	334/344 (97%)	326 (98%)	8 (2%)	44	63
6	Z	257/295 (87%)	256 (100%)	1 (0%)	89	91
7	a	333/336 (99%)	331 (99%)	2 (1%)	84	88
8	b	167/312 (54%)	165 (99%)	2 (1%)	67	79
9	c	249/267 (93%)	238 (96%)	11 (4%)	24	47
10	d	231/293 (79%)	224 (97%)	7 (3%)	36	57
11	f	745/763 (98%)	718 (96%)	27 (4%)	30	53
12	A	332/372 (89%)	327 (98%)	5 (2%)	60	75
13	B	338/379 (89%)	327 (97%)	11 (3%)	33	55
14	C	321/346 (93%)	311 (97%)	10 (3%)	35	56
15	D	333/366 (91%)	324 (97%)	9 (3%)	40	61
16	E	306/353 (87%)	303 (99%)	3 (1%)	73	81
17	F	301/379 (79%)	293 (97%)	8 (3%)	40	61
18	e	37/63 (59%)	34 (92%)	3 (8%)	9	31
19	G	193/209 (92%)	193 (100%)	0	100	100
19	g	193/209 (92%)	193 (100%)	0	100	100
20	H	164/190 (86%)	164 (100%)	0	100	100
20	h	164/190 (86%)	164 (100%)	0	100	100
21	I	193/220 (88%)	193 (100%)	0	100	100
21	i	193/220 (88%)	193 (100%)	0	100	100
22	J	152/210 (72%)	152 (100%)	0	100	100
22	j	152/210 (72%)	152 (100%)	0	100	100
23	K	186/202 (92%)	185 (100%)	1 (0%)	86	90
23	k	186/202 (92%)	185 (100%)	1 (0%)	86	90
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%)	179 (93%)	13 (7%)	13	36
25	m	192/211 (91%)	192 (100%)	0	100	100
26	N	148/180 (82%)	147 (99%)	1 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	n	148/180 (82%)	148 (100%)	0	100	100
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%)	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%)	174 (100%)	0	100	100
31	s	174/198 (88%)	174 (100%)	0	100	100
32	T	175/214 (82%)	174 (99%)	1 (1%)	84	88
32	t	175/214 (82%)	174 (99%)	1 (1%)	84	88
33	v	53/184 (29%)	39 (74%)	14 (26%)	0	3
All	All	11068/12775 (87%)	10905 (98%)	163 (2%)	60	75

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	8	ILE
1	U	9	ILE
1	U	345	ASN
1	U	574	LYS
1	U	580	ARG
1	U	583	MET
1	U	645	ASN
2	V	194	LYS
2	V	196	SER
2	V	197	THR
2	V	401	ASN
2	V	470	ARG
2	V	494	MET
3	W	94	ARG
3	W	312	MET
3	W	314	LEU
3	W	315	MET
3	W	422	ASN

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Mol	Chain	Res	Type
3	W	451	MET
3	W	454	ASN
4	X	198	ASN
4	X	329	ASN
5	Y	48	ASN
5	Y	77	ASN
5	Y	83	ARG
5	Y	179	ARG
5	Y	210	SER
5	Y	211	TYR
5	Y	297	ARG
5	Y	358	ARG
6	Z	180	LYS
7	a	105	LYS
7	a	289	ARG
8	b	171	VAL
8	b	172	THR
9	c	75	MET
9	c	104	ARG
9	c	139	ARG
9	c	181	LEU
9	c	183	HIS
9	c	184	LEU
9	c	186	LYS
9	c	197	ASN
9	c	222	LYS
9	c	254	ASN
9	c	266	THR
10	d	36	LEU
10	d	42	LYS
10	d	79	LYS
10	d	80	CYS
10	d	88	GLN
10	d	89	LEU
10	d	251	ARG
11	f	72	ARG
11	f	80	ARG
11	f	89	MET
11	f	112	ASN
11	f	131	MET
11	f	267	ARG
11	f	297	MET

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Mol	Chain	Res	Type
11	f	300	ARG
11	f	327	ASN
11	f	333	LEU
11	f	346	ASP
11	f	348	ILE
11	f	385	PHE
11	f	396	ASN
11	f	457	ASN
11	f	530	CYS
11	f	565	ASN
11	f	703	ARG
11	f	720	GLU
11	f	754	LYS
11	f	773	LYS
11	f	786	GLN
11	f	787	LEU
11	f	807	ARG
11	f	808	ASN
11	f	838	ARG
11	f	840	LEU
12	A	43	ARG
12	A	304	ASN
12	A	360	ARG
12	A	369	ARG
12	A	373	LEU
13	B	48	LYS
13	B	86	LYS
13	B	105	THR
13	B	116	ILE
13	B	117	ASP
13	B	125	THR
13	B	164	MET
13	B	249	ARG
13	B	293	LYS
13	B	294	ARG
13	B	298	ASN
14	C	69	GLN
14	C	78	ARG
14	C	125	LYS
14	C	127	LEU
14	C	138	MET
14	C	151	ILE

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Mol	Chain	Res	Type
14	C	210	THR
14	C	229	ARG
14	C	278	ASN
14	C	287	LYS
15	D	81	ARG
15	D	85	ILE
15	D	125	LYS
15	D	127	ASN
15	D	214	MET
15	D	238	LYS
15	D	352	MET
15	D	353	ASN
15	D	384	MET
16	E	241	ARG
16	E	264	MET
16	E	294	ARG
17	F	118	LYS
17	F	192	ASP
17	F	233	LYS
17	F	234	THR
17	F	235	LEU
17	F	250	LYS
17	F	300	LYS
17	F	371	ARG
18	e	67	MET
18	e	68	GLU
18	e	69	THR
23	K	10	ARG
25	M	191	LYS
25	M	195	LYS
25	M	200	VAL
25	M	201	HIS
25	M	202	ASP
25	M	206	ASP
25	M	209	PHE
25	M	210	GLU
25	M	211	LEU
25	M	212	GLU
25	M	237	LYS
25	M	238	TYR
25	M	240	LYS
26	N	40	ARG

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Mol	Chain	Res	Type
29	Q	82	ASN
32	T	37	ARG
23	k	10	ARG
29	q	82	ASN
32	t	37	ARG
33	v	152	ASN
33	v	160	LYS
33	v	161	VAL
33	v	164	THR
33	v	166	PHE
33	v	182	ASP
33	v	183	LYS
33	v	184	HIS
33	v	186	CYS
33	v	204	VAL
33	v	205	VAL
33	v	211	GLN
33	v	212	ARG
33	v	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	18	GLN
1	U	70	HIS
1	U	171	ASN
1	U	207	ASN
1	U	247	GLN
1	U	415	HIS
1	U	541	HIS
1	U	595	ASN
1	U	645	ASN
1	U	665	ASN
1	U	685	GLN
1	U	697	GLN
1	U	734	GLN
1	U	743	ASN
1	U	749	GLN
1	U	756	HIS
1	U	768	GLN
1	U	805	ASN
2	V	33	GLN

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Mol	Chain	Res	Type
2	V	124	ASN
2	V	247	GLN
2	V	318	GLN
2	V	319	HIS
2	V	401	ASN
2	V	473	GLN
3	W	86	ASN
3	W	203	GLN
3	W	235	GLN
3	W	265	GLN
3	W	361	HIS
3	W	362	ASN
3	W	380	GLN
3	W	454	ASN
3	W	456	GLN
4	X	213	GLN
4	X	292	GLN
4	X	296	ASN
4	X	329	ASN
4	X	334	ASN
4	X	406	ASN
5	Y	48	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	344	HIS
5	Y	363	ASN
6	Z	32	GLN
6	Z	193	ASN
6	Z	202	ASN
6	Z	229	GLN
7	a	12	GLN
7	a	23	HIS
7	a	129	GLN
7	a	143	ASN
7	a	231	GLN
7	a	249	GLN
7	a	258	GLN
7	a	287	ASN
7	a	369	HIS
7	a	370	GLN
9	c	92	GLN
9	c	128	ASN

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Mol	Chain	Res	Type
9	c	183	HIS
9	c	197	ASN
9	c	254	ASN
9	c	256	ASN
9	c	298	GLN
10	d	60	GLN
10	d	102	ASN
10	d	116	HIS
11	f	112	ASN
11	f	118	ASN
11	f	171	GLN
11	f	213	GLN
11	f	291	GLN
11	f	396	ASN
11	f	457	ASN
11	f	565	ASN
11	f	611	GLN
11	f	614	HIS
11	f	715	HIS
11	f	808	ASN
11	f	815	HIS
11	f	848	GLN
11	f	855	GLN
11	f	876	HIS
12	A	85	GLN
12	A	304	ASN
12	A	305	GLN
12	A	314	ASN
13	B	193	GLN
13	B	241	ASN
13	B	257	GLN
13	B	277	HIS
13	B	298	ASN
13	B	332	ASN
14	C	124	HIS
14	C	182	GLN
14	C	206	HIS
14	C	270	GLN
14	C	278	ASN
14	C	332	HIS
15	D	83	GLN
15	D	187	HIS

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Mol	Chain	Res	Type
15	D	257	ASN
15	D	353	ASN
15	D	414	HIS
16	E	45	ASN
16	E	225	HIS
16	E	263	GLN
16	E	364	GLN
17	F	83	ASN
17	F	196	GLN
17	F	255	GLN
17	F	315	ASN
17	F	321	GLN
18	e	6	GLN
19	G	33	ASN
19	G	123	GLN
20	H	102	GLN
21	I	119	GLN
21	I	123	GLN
21	I	235	GLN
22	J	18	GLN
22	J	116	GLN
22	J	175	ASN
22	J	200	GLN
23	K	99	HIS
23	K	118	ASN
23	K	214	ASN
24	L	146	GLN
24	L	152	ASN
24	L	166	GLN
26	N	28	ASN
26	N	154	GLN
29	Q	55	GLN
29	Q	65	GLN
29	Q	101	ASN
29	Q	132	HIS
30	R	38	ASN
30	R	85	ASN
32	T	61	GLN
19	g	33	ASN
19	g	123	GLN
20	h	102	GLN
21	i	119	GLN

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Mol	Chain	Res	Type
21	i	123	GLN
21	i	235	GLN
22	j	18	GLN
22	j	116	GLN
22	j	175	ASN
23	k	99	HIS
23	k	118	ASN
23	k	214	ASN
23	k	225	ASN
24	l	117	GLN
24	l	146	GLN
24	l	152	ASN
26	n	28	ASN
26	n	66	HIS
26	n	154	GLN
27	o	165	ASN
29	q	55	GLN
29	q	65	GLN
29	q	101	ASN
29	q	132	HIS
30	r	38	ASN
30	r	85	ASN
32	t	61	GLN
32	t	65	GLN
33	v	184	HIS
33	v	202	ASN
33	v	211	GLN

### 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	ATP	F	501	36	26,33,33	0.92	1 (3%)	31,52,52	1.51	4 (12%)
35	ATP	D	501	36	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
35	ATP	A	501	36	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)
37	ADP	B	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	5 (17%)
37	ADP	E	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	F	501	36	-	11/18/38/38	0/3/3/3
35	ATP	D	501	36	-	7/18/38/38	0/3/3/3
35	ATP	A	501	36	-	3/18/38/38	0/3/3/3
37	ADP	B	501	-	-	2/12/32/32	0/3/3/3
37	ADP	E	401	-	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	ATP	C5-C4	2.52	1.47	1.40
35	D	501	ATP	C5-C4	2.48	1.47	1.40
37	E	401	ADP	C5-C4	2.47	1.47	1.40
37	B	501	ADP	C5-C4	2.42	1.47	1.40
35	F	501	ATP	C5-C4	2.40	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	501	ATP	PB-O3B-PG	-4.28	118.14	132.83
37	B	501	ADP	C3'-C2'-C1'	3.63	106.44	100.98
35	A	501	ATP	PA-O3A-PB	-3.60	120.47	132.83
35	D	501	ATP	PA-O3A-PB	-3.60	120.48	132.83
35	D	501	ATP	PB-O3B-PG	-3.59	120.50	132.83
35	A	501	ATP	PB-O3B-PG	-3.59	120.50	132.83
37	E	401	ADP	PA-O3A-PB	-3.59	120.52	132.83
37	B	501	ADP	PA-O3A-PB	-3.52	120.74	132.83
37	E	401	ADP	C3'-C2'-C1'	3.45	106.17	100.98
35	A	501	ATP	C3'-C2'-C1'	3.42	106.13	100.98
35	D	501	ATP	C3'-C2'-C1'	3.42	106.13	100.98
35	A	501	ATP	N3-C2-N1	-3.18	123.70	128.68
35	D	501	ATP	N3-C2-N1	-3.17	123.73	128.68
37	E	401	ADP	N3-C2-N1	-3.17	123.73	128.68
35	F	501	ATP	N3-C2-N1	-3.16	123.73	128.68
37	B	501	ADP	N3-C2-N1	-3.05	123.92	128.68
35	F	501	ATP	C4-C5-N7	-2.80	106.48	109.40
35	A	501	ATP	C4-C5-N7	-2.73	106.55	109.40
35	D	501	ATP	C4-C5-N7	-2.66	106.62	109.40
37	E	401	ADP	C4-C5-N7	-2.65	106.64	109.40
37	B	501	ADP	C4-C5-N7	-2.60	106.69	109.40
35	F	501	ATP	C3'-C2'-C1'	2.54	104.80	100.98
37	B	501	ADP	O3B-PB-O2B	2.00	115.29	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

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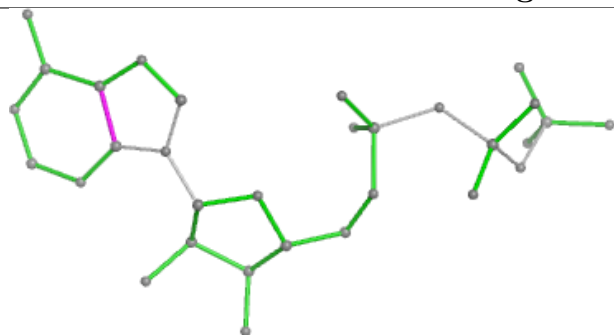
Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C4'-C5'-O5'-PA
35	A	501	ATP	C3'-C4'-C5'-O5'
37	E	401	ADP	PB-O3A-PA-O2A
35	F	501	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C3'-C4'-C5'-O5'
35	A	501	ATP	PA-O3A-PB-O1B
35	F	501	ATP	PA-O3A-PB-O1B
35	F	501	ATP	PA-O3A-PB-O2B
35	F	501	ATP	PB-O3A-PA-O1A
37	E	401	ADP	PB-O3A-PA-O1A

There are no ring outliers.

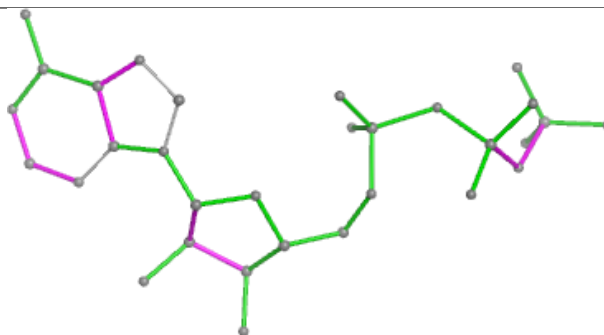
No monomer is involved in short contacts.

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

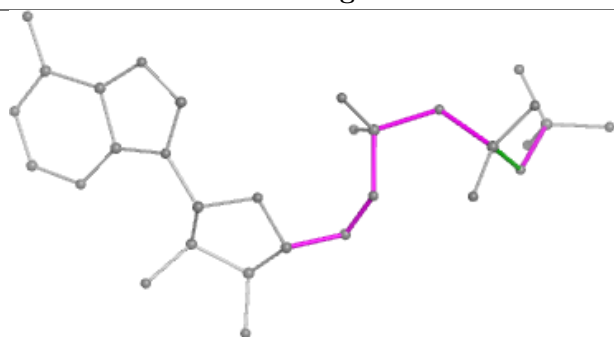
## Ligand ATP F 501



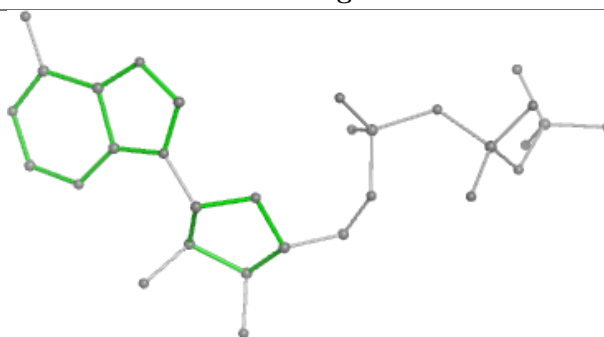
Bond lengths



Bond angles

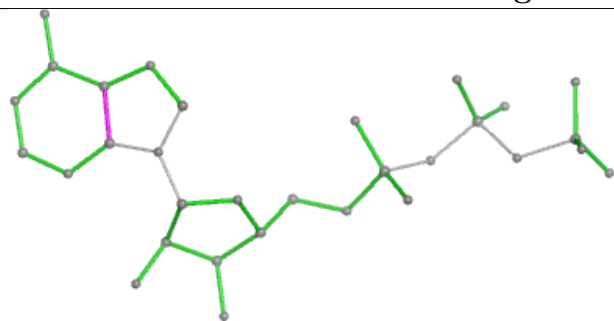


Torsions

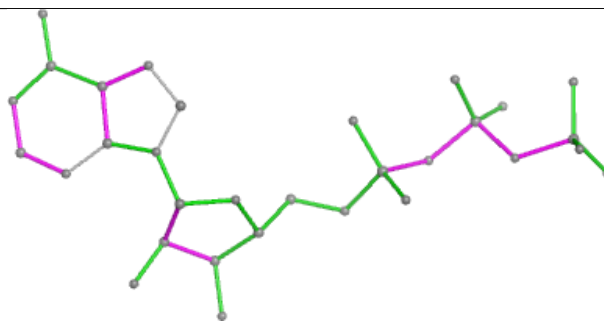


Rings

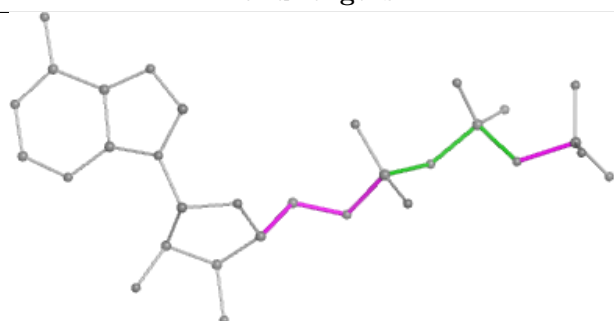
## Ligand ATP D 501



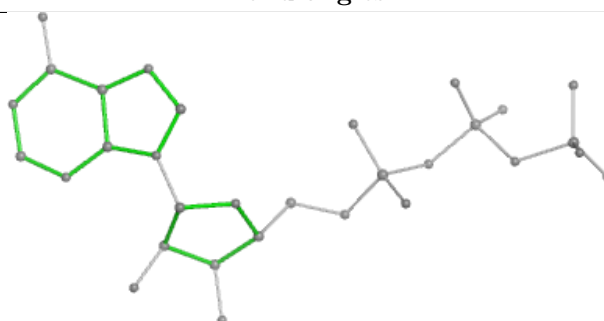
Bond lengths



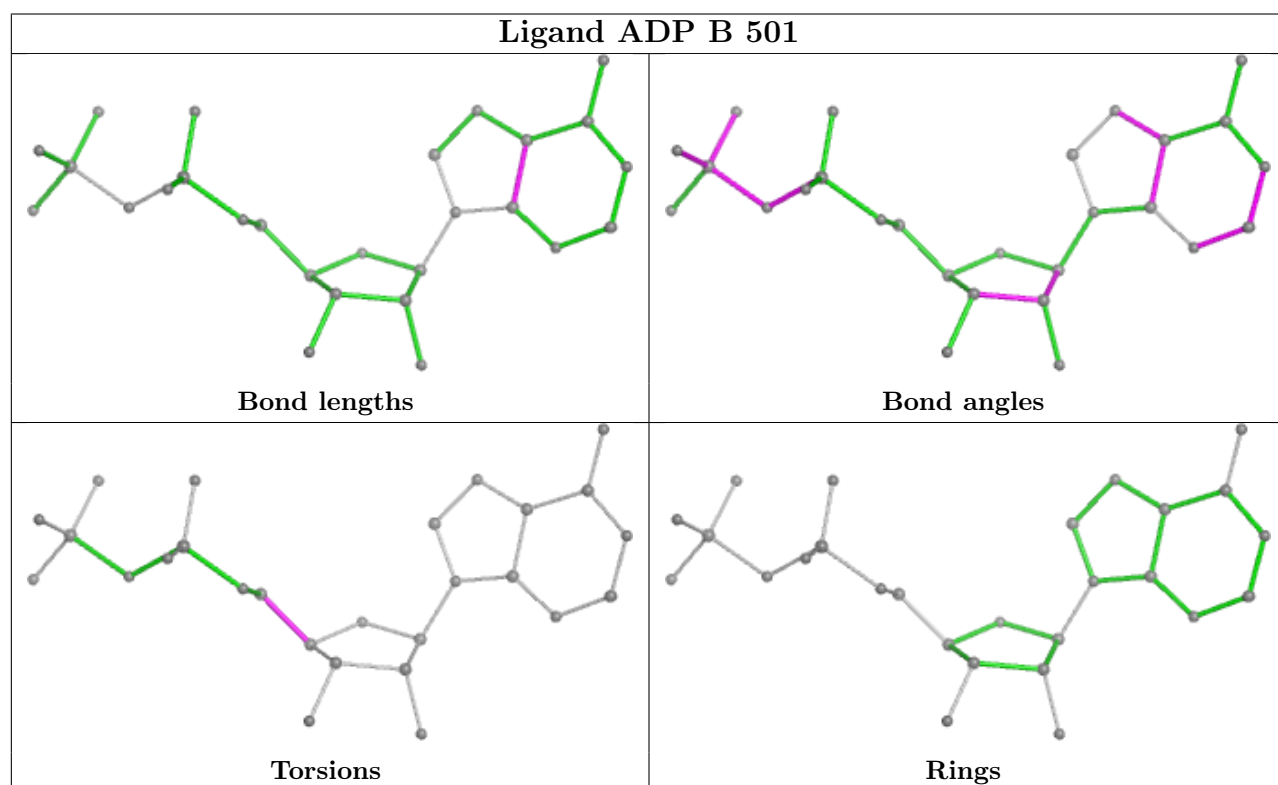
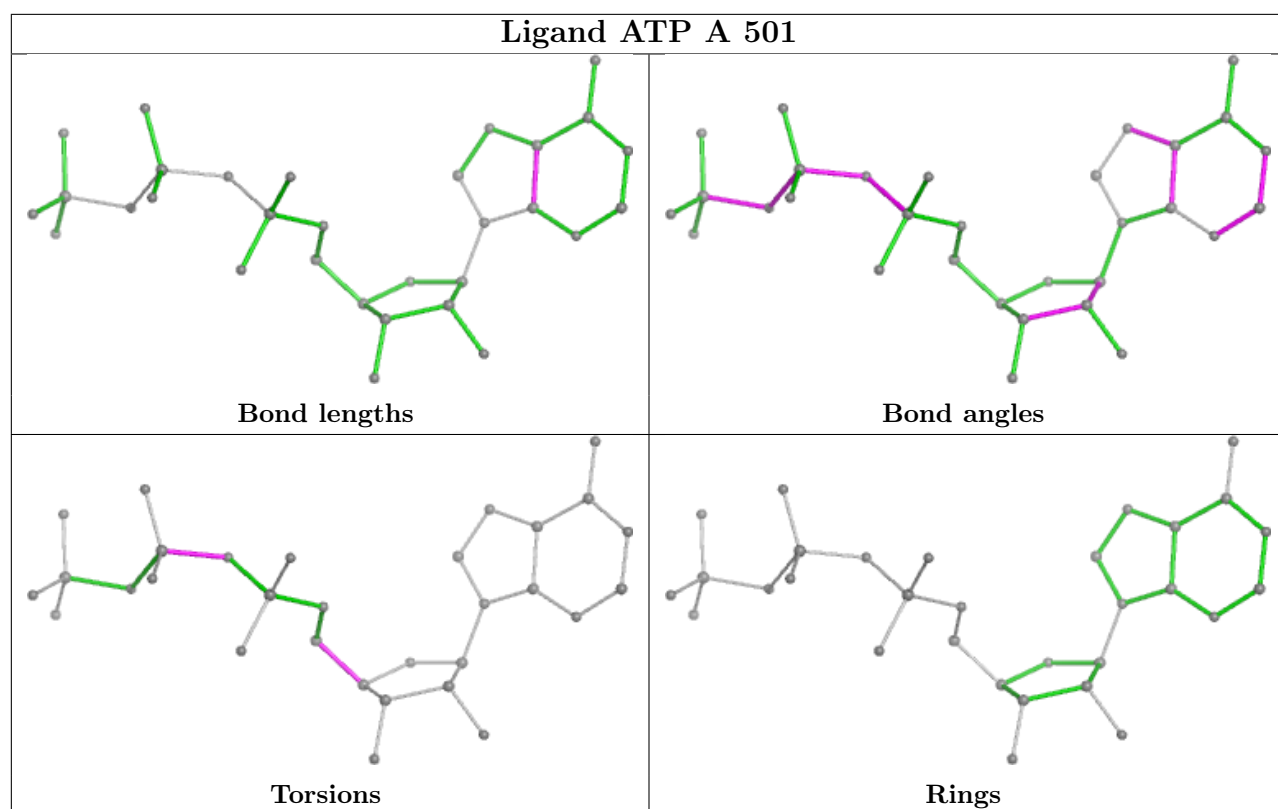
Bond angles

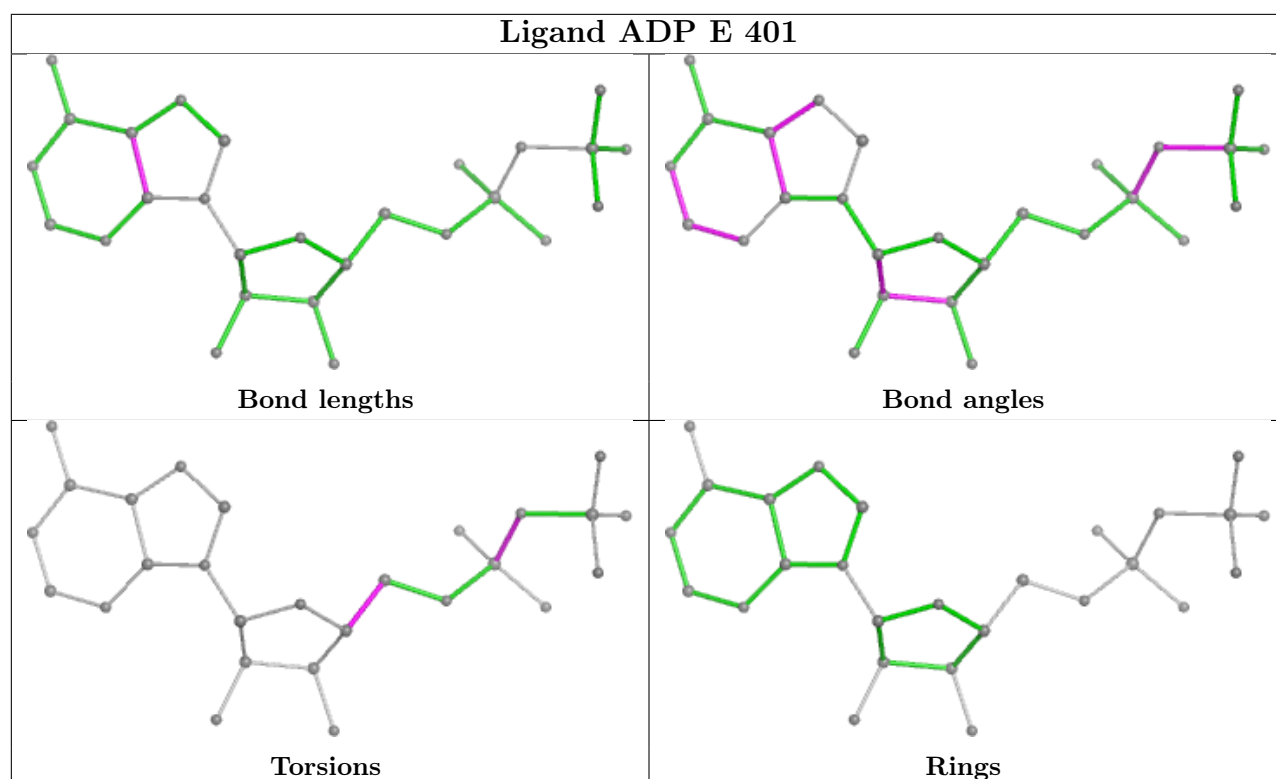


Torsions



Rings





## 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.

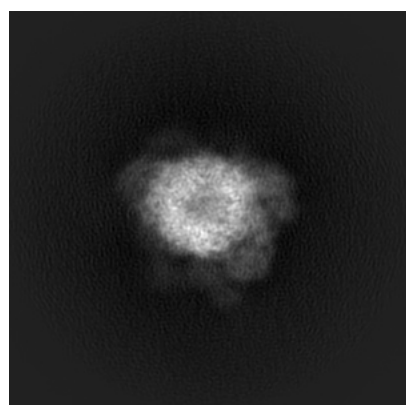
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14204. These allow visual inspection of the internal detail of the map and identification of artifacts.

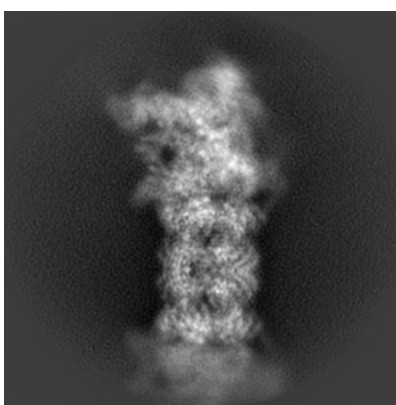
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

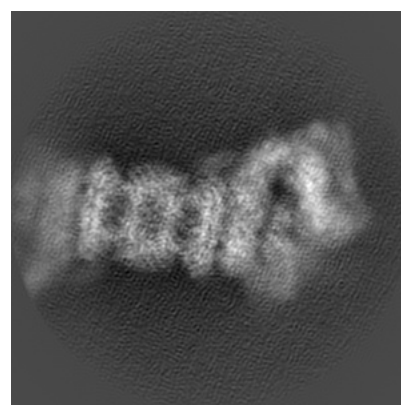
#### 6.1.1 Primary map



X



Y

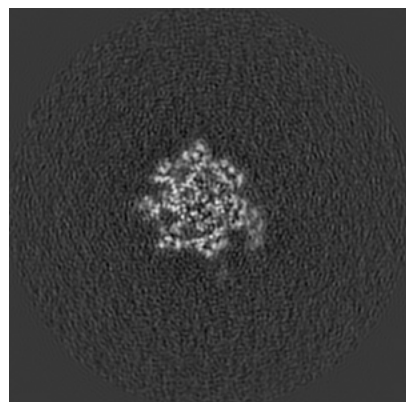


Z

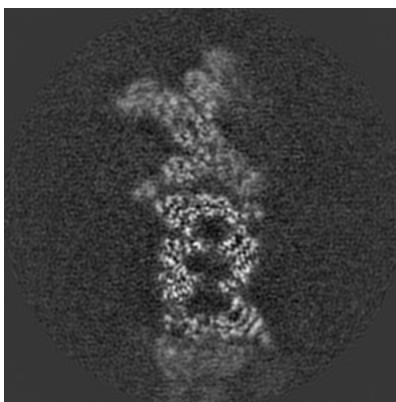
The images above show the map projected in three orthogonal directions.

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

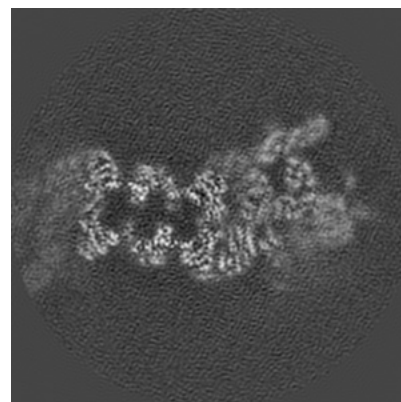
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



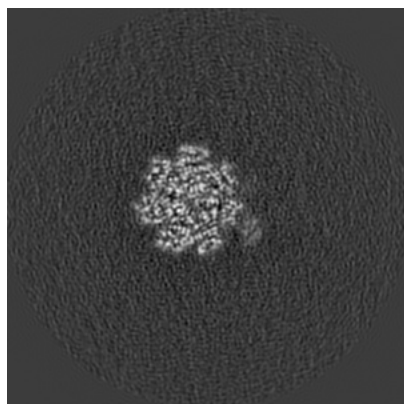
Z Index: 160



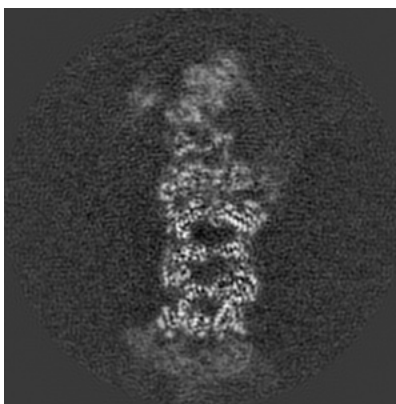
The images above show central slices of the map in three orthogonal directions.

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

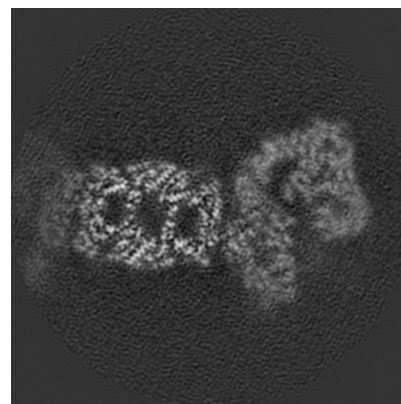
### 6.3.1 Primary map



X Index: 154



Y Index: 143

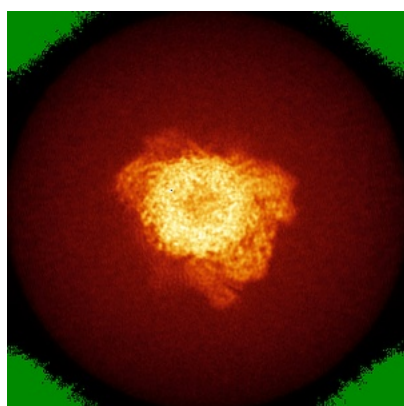


Z Index: 176

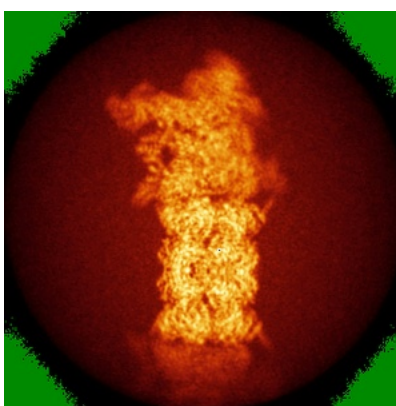
The images above show the largest variance slices of the map in three orthogonal directions.

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

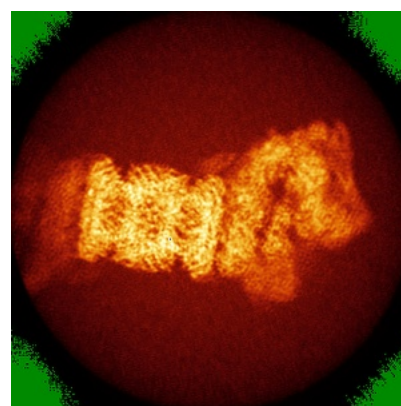
### 6.4.1 Primary map



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 0.0328. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

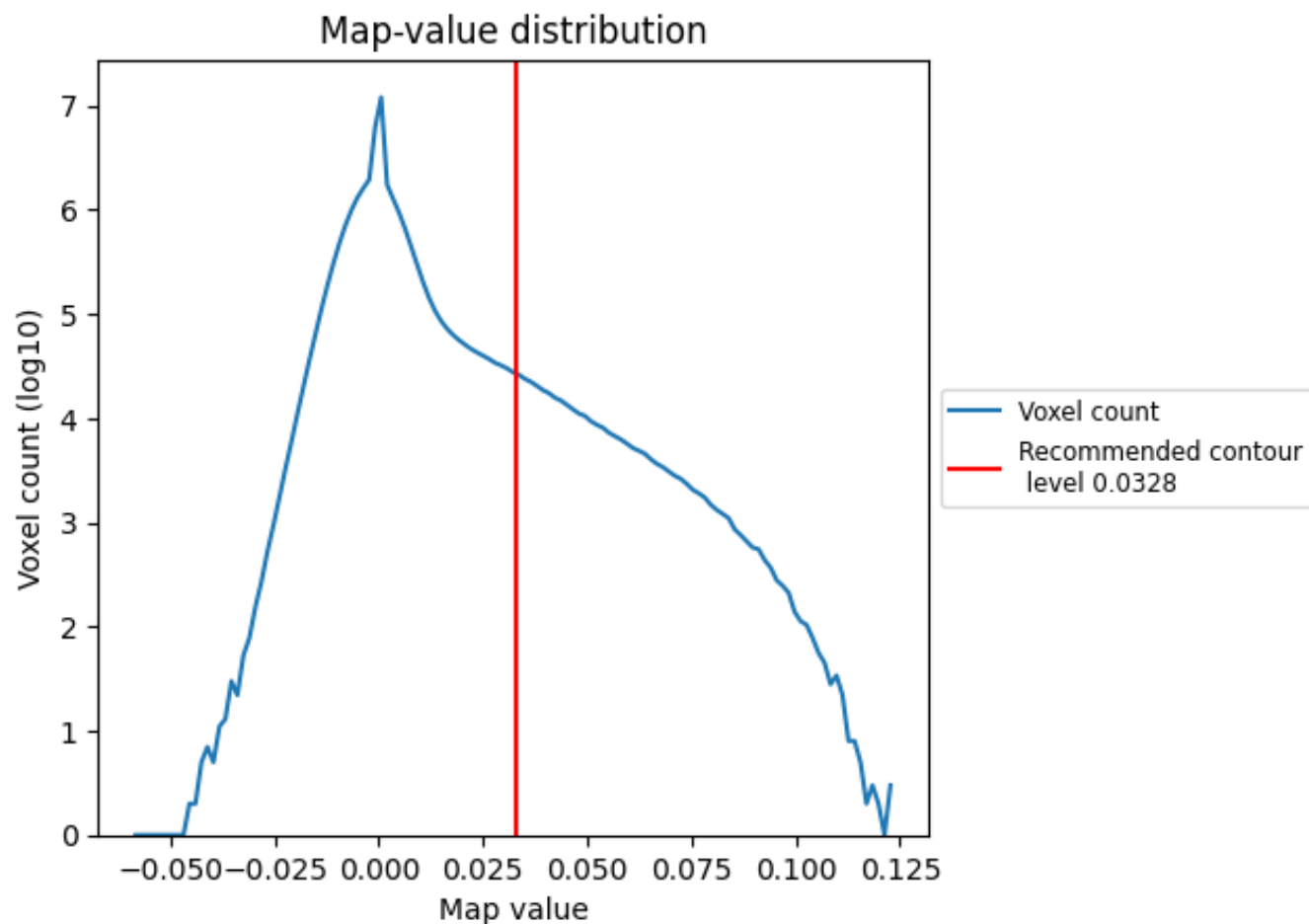
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

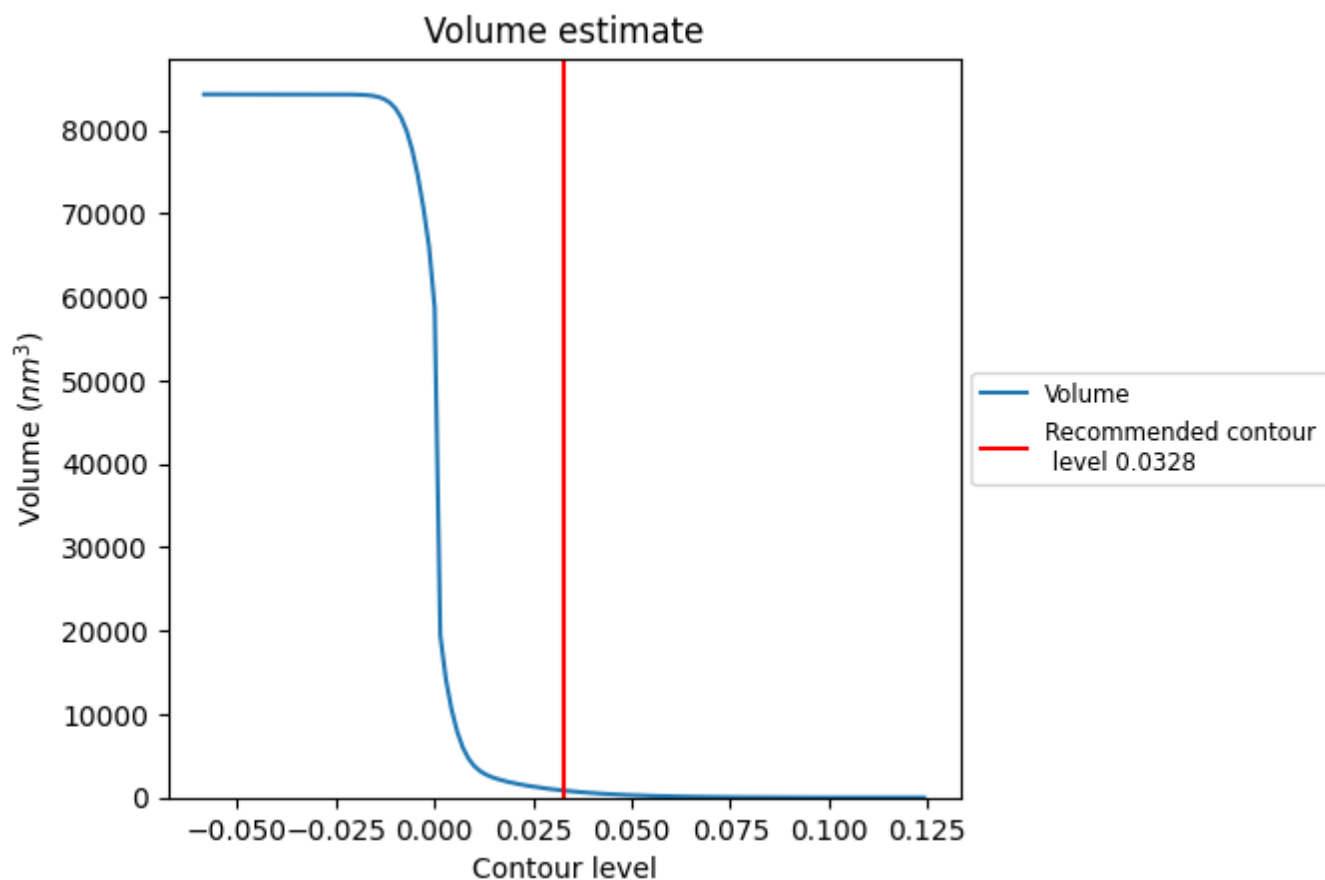
This section contains the results of statistical analysis of the map.

### 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.

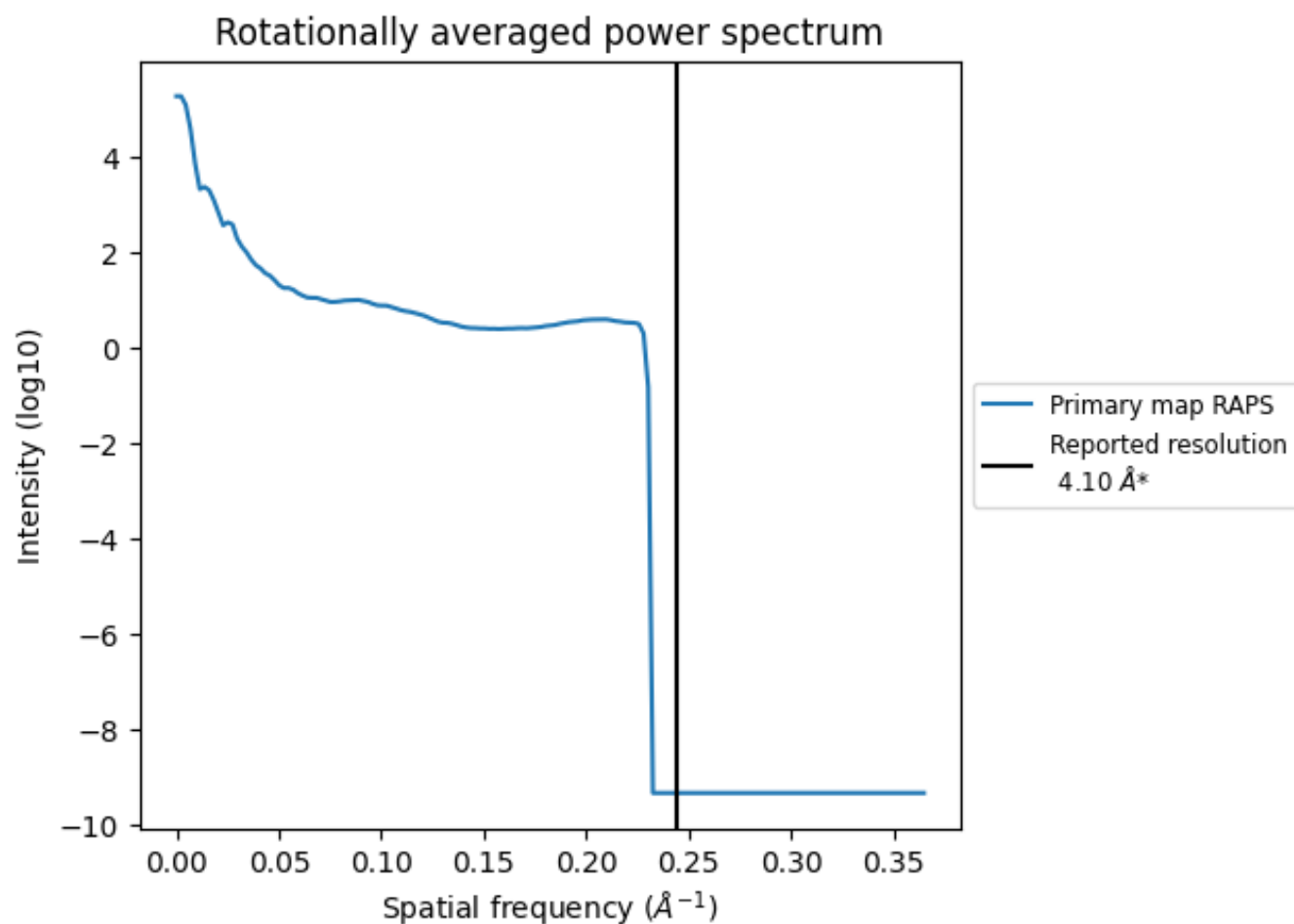
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 842 nm<sup>3</sup>; this corresponds to an approximate mass of 761 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 0.244 Å<sup>-1</sup>

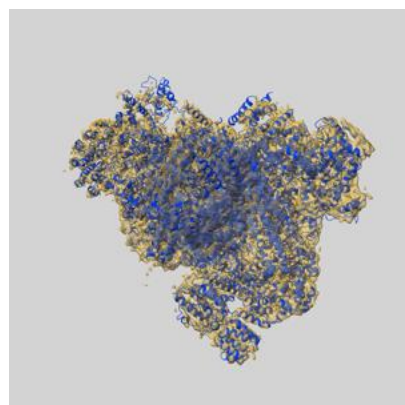
## 8 Fourier-Shell correlation ⓘ

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

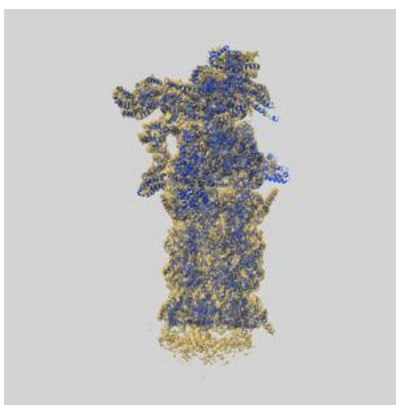
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14204 and PDB model 7QXW. Per-residue inclusion information can be found in section 3 on page 13.

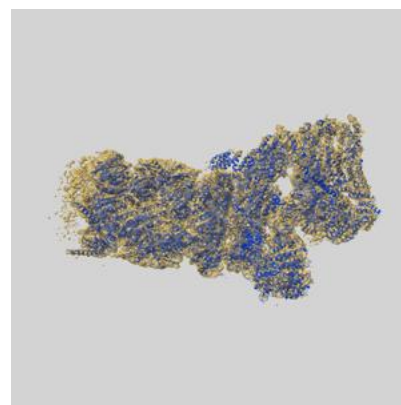
### 9.1 Map-model overlay [i](#)



X



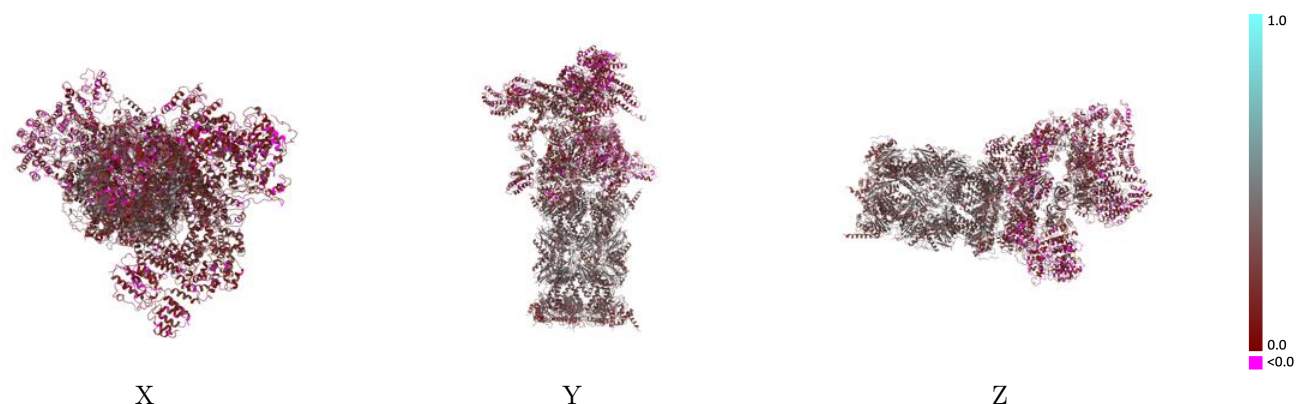
Y



Z

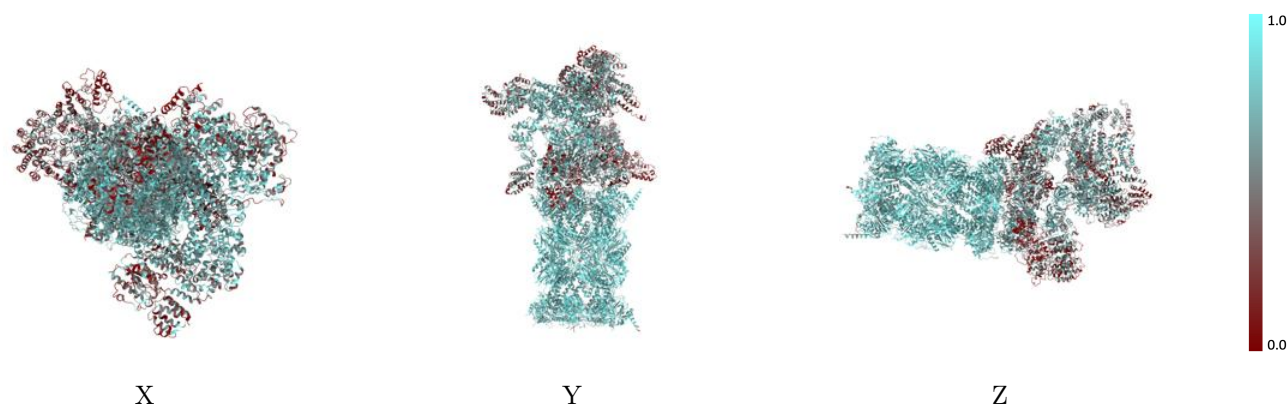
The images above show the 3D surface view of the map at the recommended contour level 0.0328 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



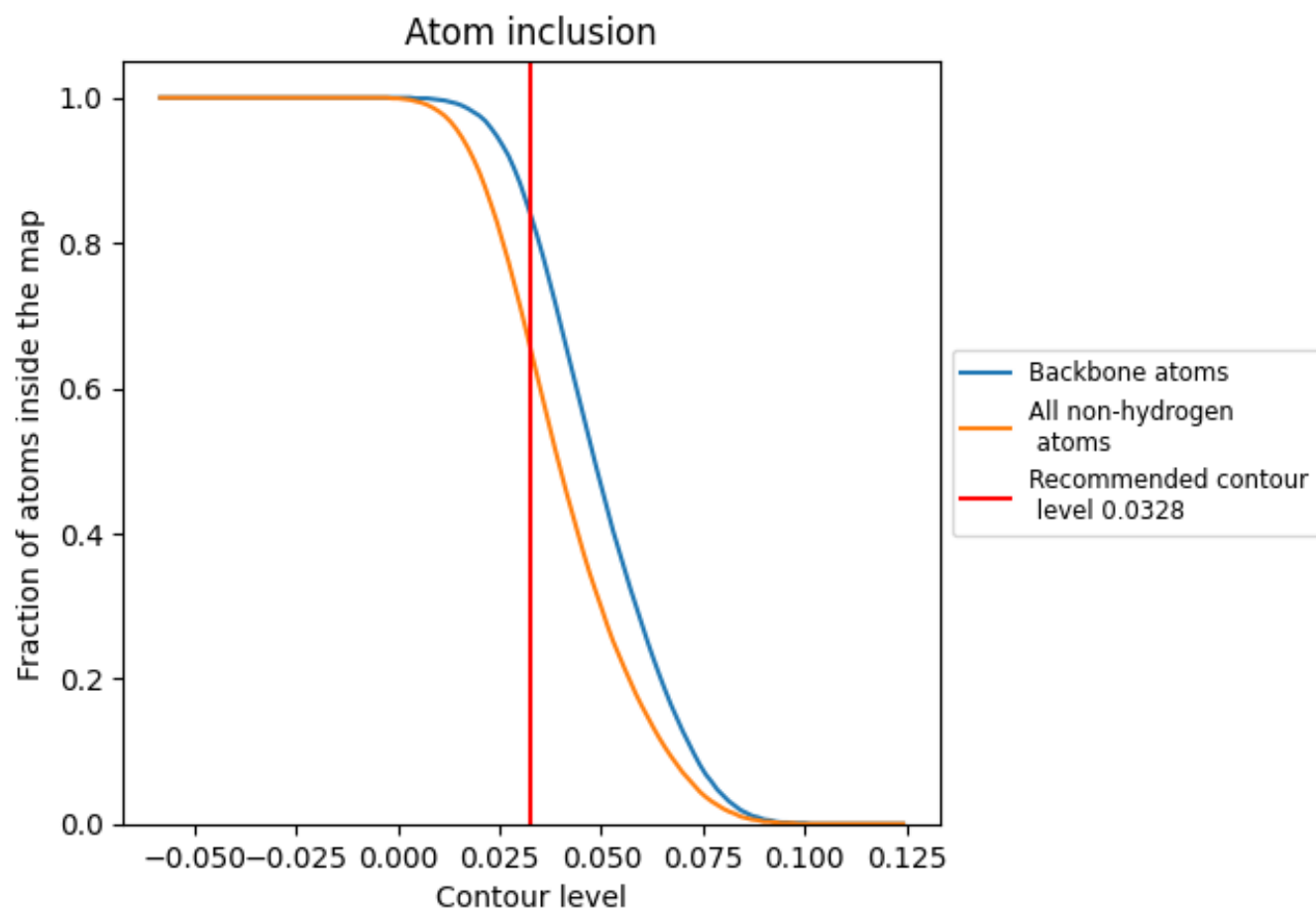
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0328).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.0328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6500	 0.2670
A	 0.5960	 0.2420
B	 0.5090	 0.2190
C	 0.4850	 0.1790
D	 0.6350	 0.2600
E	 0.7130	 0.2980
F	 0.7020	 0.3050
G	 0.7920	 0.3250
H	 0.8070	 0.3500
I	 0.7830	 0.3200
J	 0.8180	 0.3310
K	 0.7820	 0.3310
L	 0.8210	 0.3540
M	 0.7900	 0.3240
N	 0.8390	 0.3700
O	 0.8450	 0.3740
P	 0.8410	 0.3780
Q	 0.8330	 0.3600
R	 0.8690	 0.3820
S	 0.8480	 0.3850
T	 0.8720	 0.3900
U	 0.4710	 0.1610
V	 0.4750	 0.1480
W	 0.5840	 0.1920
X	 0.3670	 0.2060
Y	 0.5940	 0.1570
Z	 0.6320	 0.2470
a	 0.5250	 0.1830
b	 0.3660	 0.1380
c	 0.6550	 0.2460
d	 0.4650	 0.1390
e	 0.4490	 0.1280
f	 0.2820	 0.1350
g	 0.7610	 0.3310
h	 0.7710	 0.3280



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Chain	Atom inclusion	Q-score
i	 0.7250	 0.3150
j	 0.7710	 0.3210
k	 0.7470	 0.3180
l	 0.7970	 0.3440
m	 0.7610	 0.3130
n	 0.8650	 0.3830
o	 0.8530	 0.3860
p	 0.8430	 0.3830
q	 0.8360	 0.3610
r	 0.8620	 0.3760
s	 0.8370	 0.3670
t	 0.8610	 0.3820
v	 0.5870	 0.2850