



# Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 03:43 pm BST

PDB ID : 7QXN  
EMDB ID : EMD-14201  
Title : Proteasome-ZFAND5 Complex Z+A state  
Authors : Zhu, Y.; Lu, Y.  
Deposited on : 2022-01-26  
Resolution : 3.70 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:

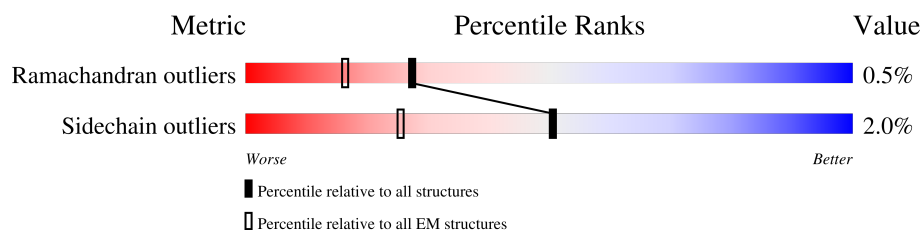
EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 3.70 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	U	953	
2	V	533	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	

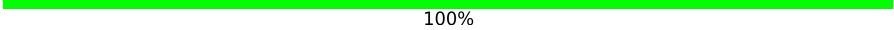
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Mol	Chain	Length	Quality of chain
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	

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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%

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103713 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	508	Total	C	N	O	S	0	0
			3994	2530	712	738	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
			3693	2332	635	701	25		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6857	4306	1174	1331	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	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
			2858	1802	496	545	15		

- 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
			1713	1062	311	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
			1591	1013	265	294	19		
28	p	204	Total	C	N	O	S	0	0
			1591	1013	265	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
			1644	1039	282	313	10		

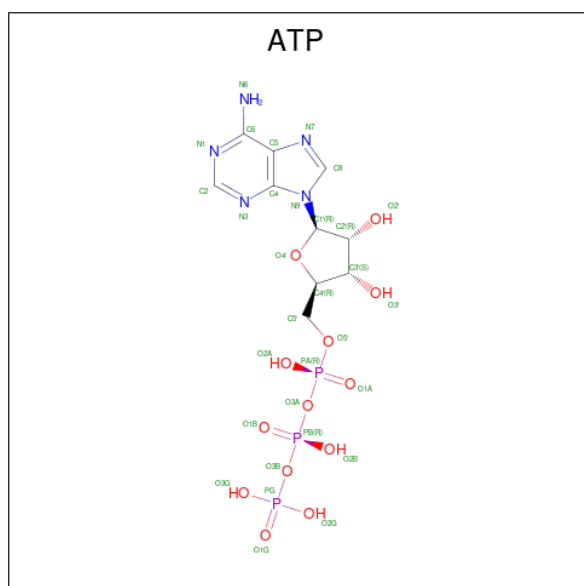
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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

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

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

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



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

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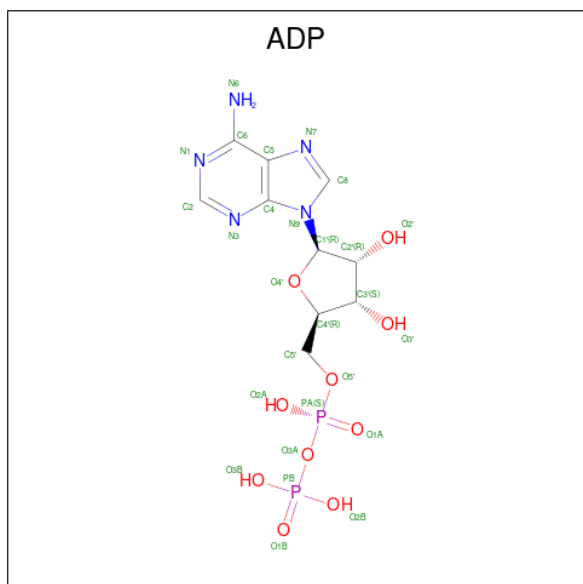
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Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



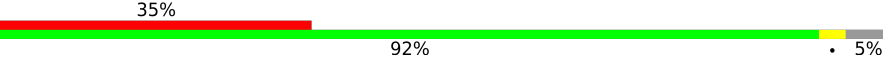
Mol	Chain	Residues	Atoms					AltConf
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

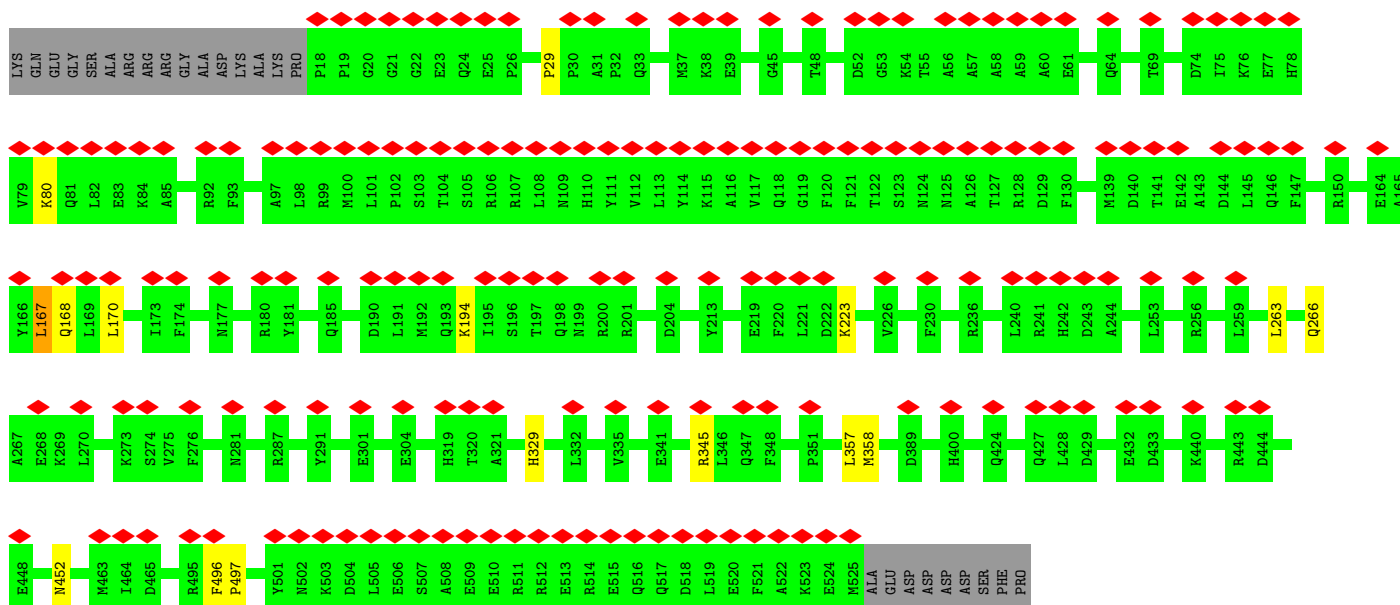
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	F	1	27	10	5	10	2	0

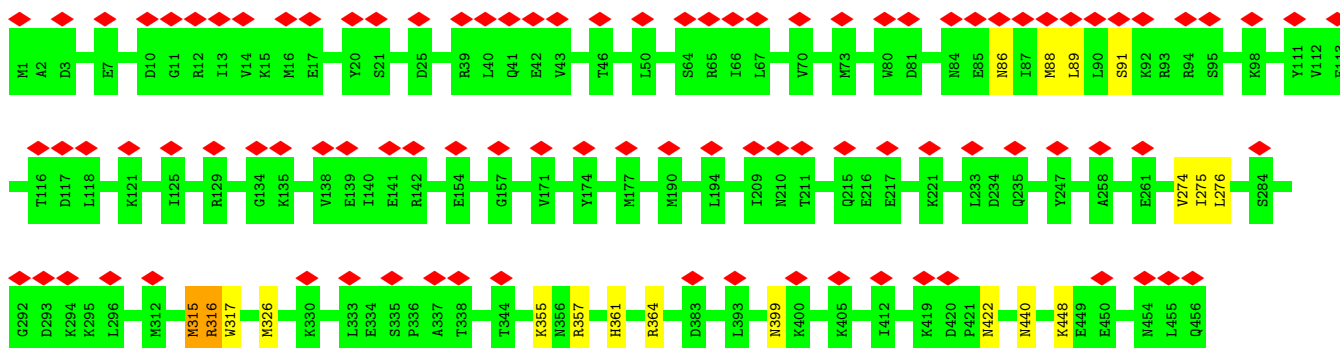


Chain V: 




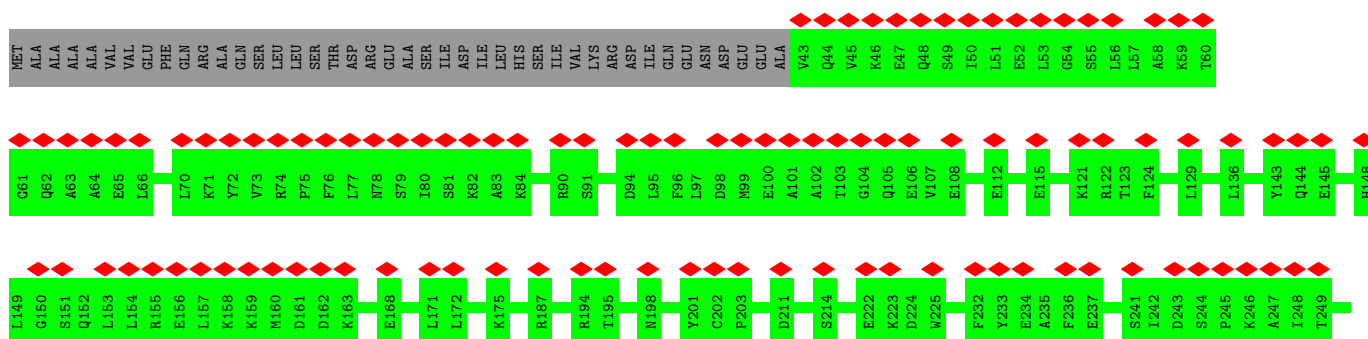
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

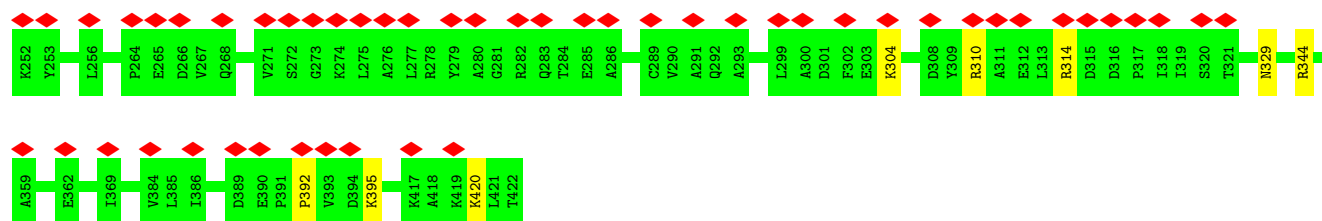
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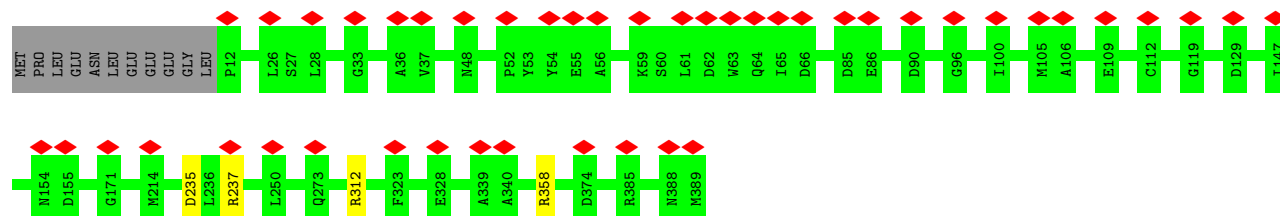
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 

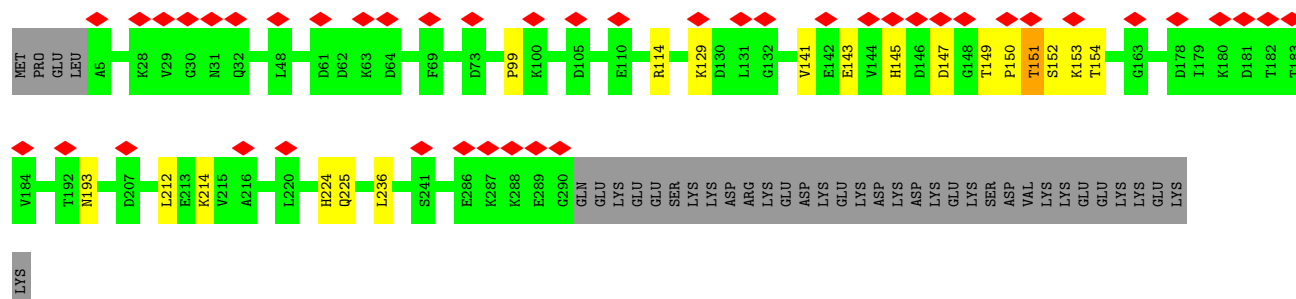
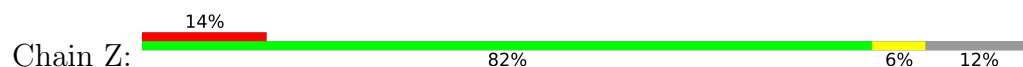




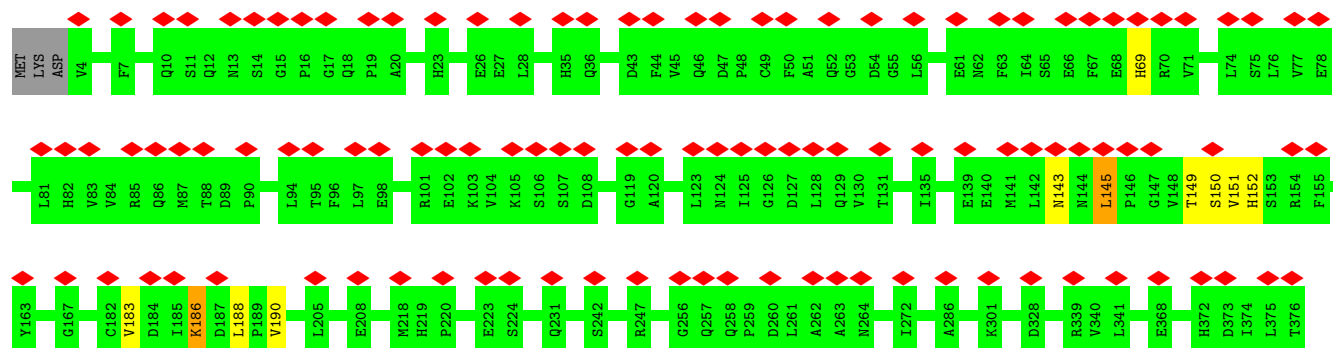
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



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

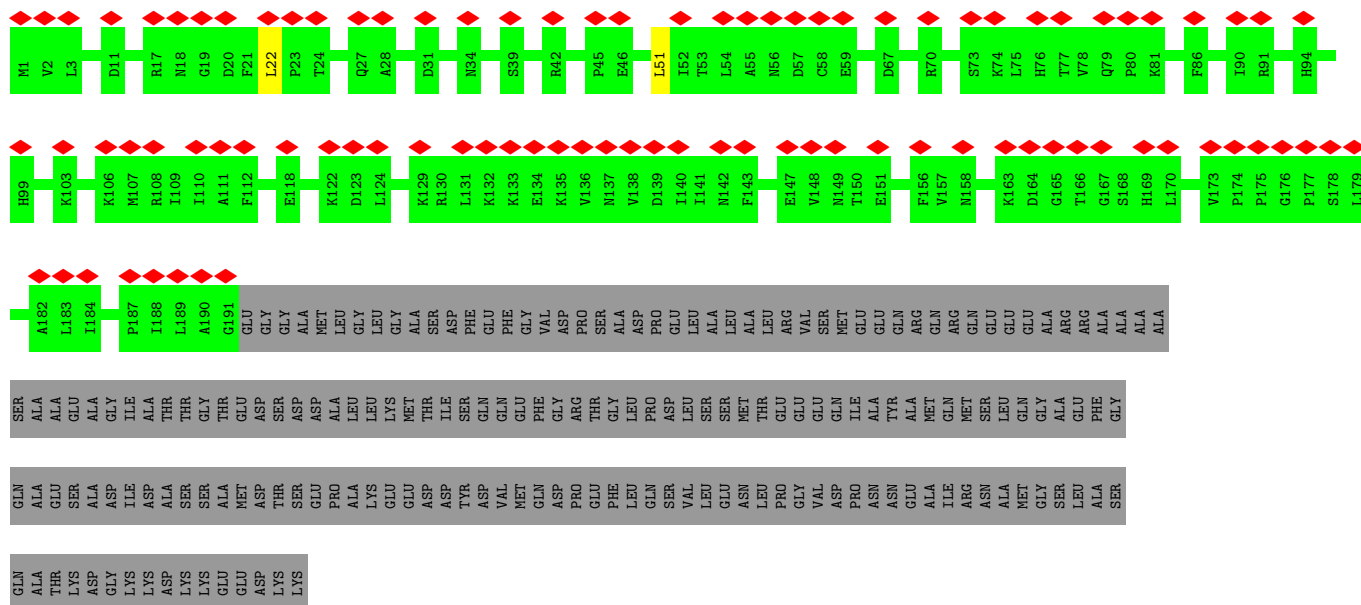


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

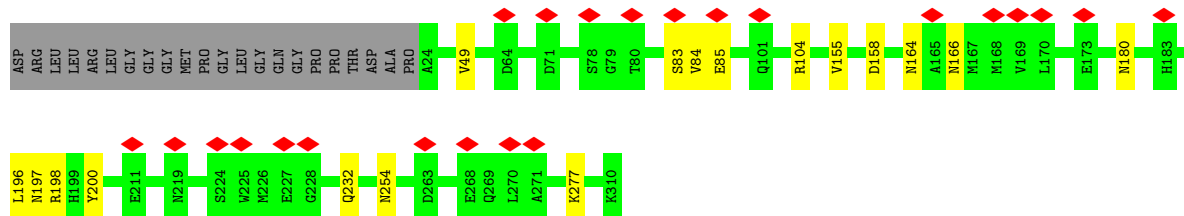
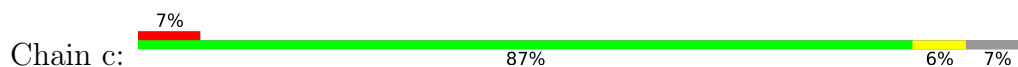


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

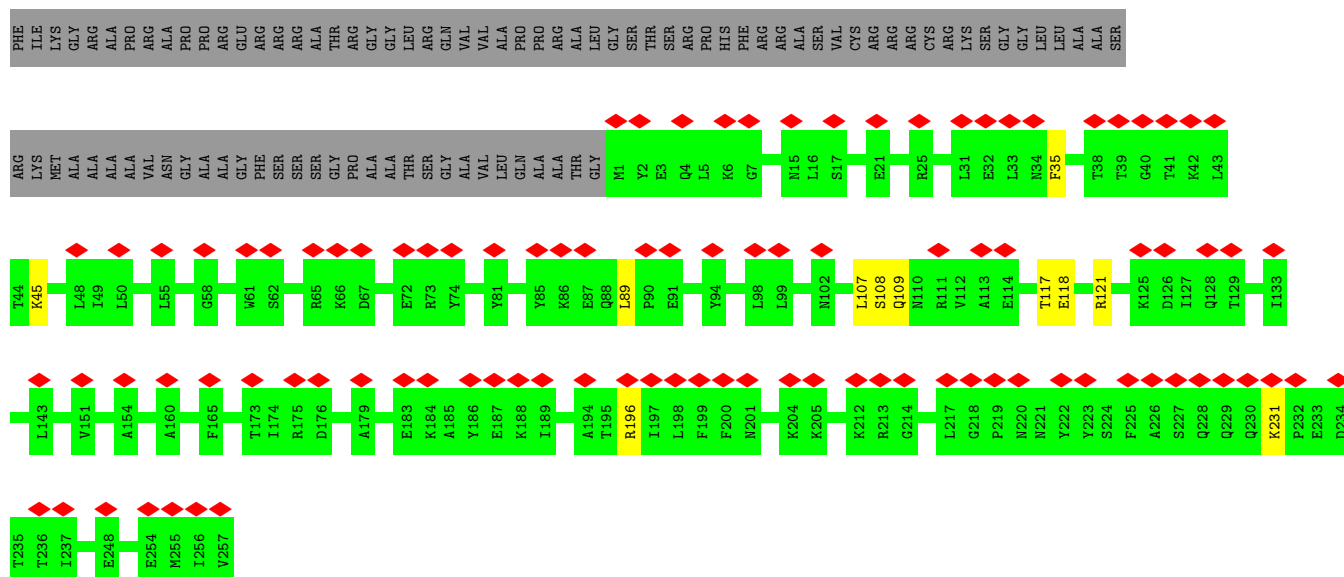




• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

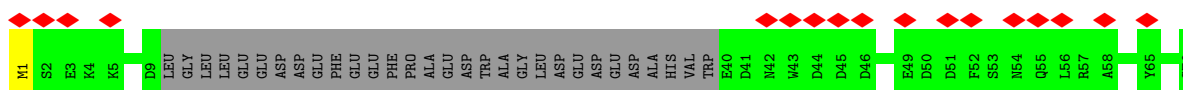


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

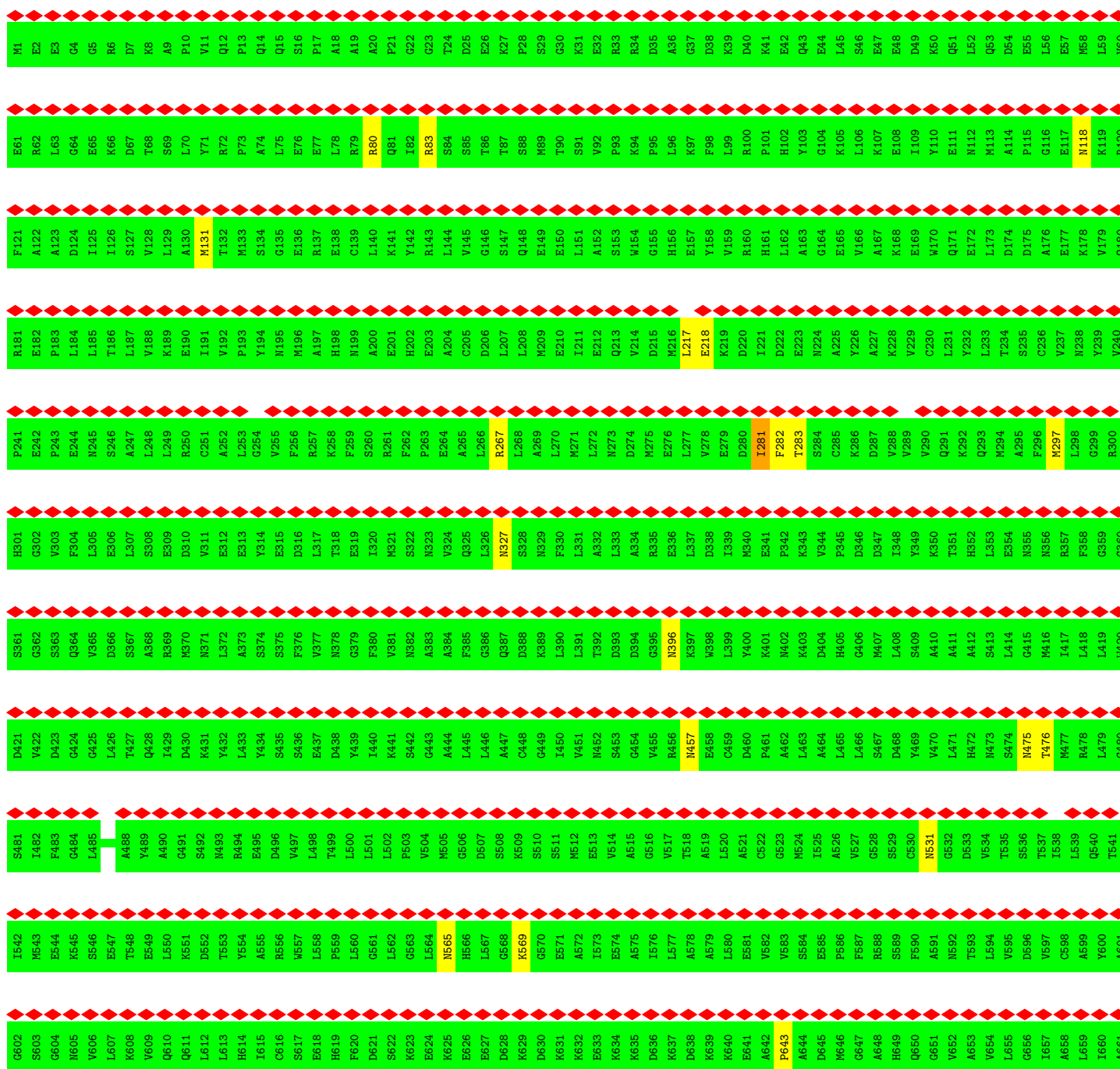
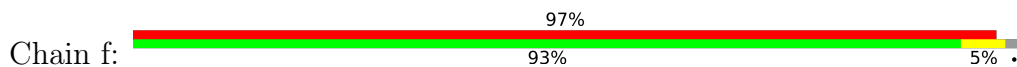


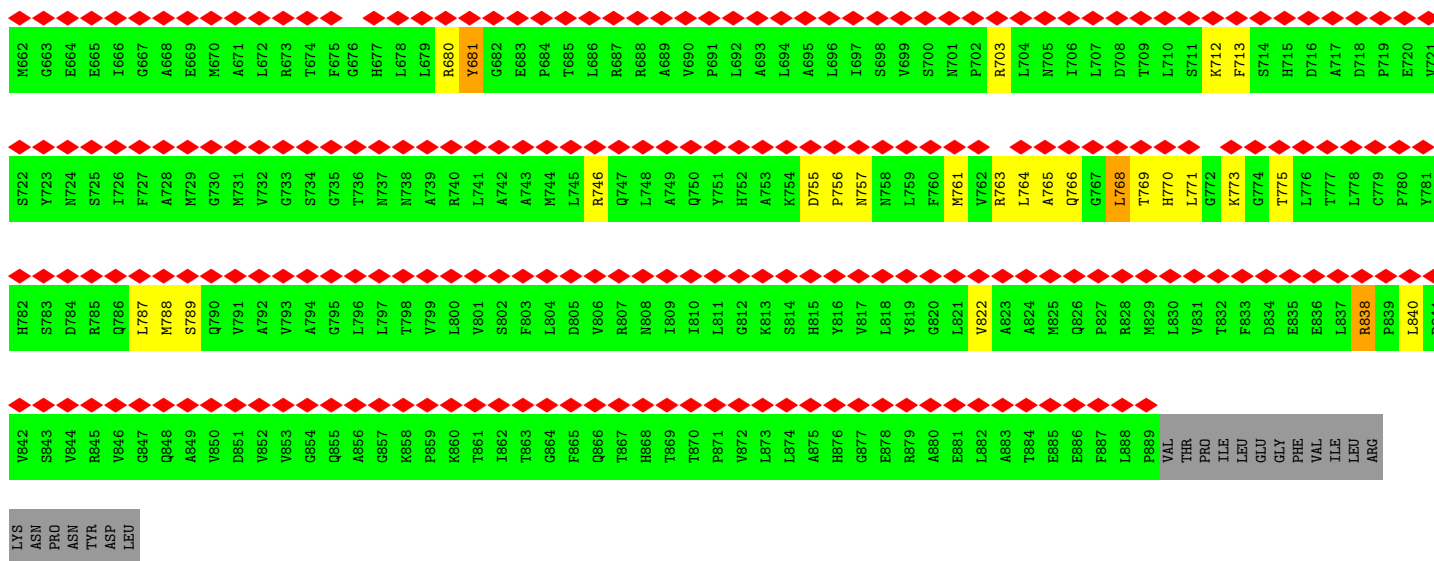


• Molecule 11: 26S proteasome complex subunit SEM1

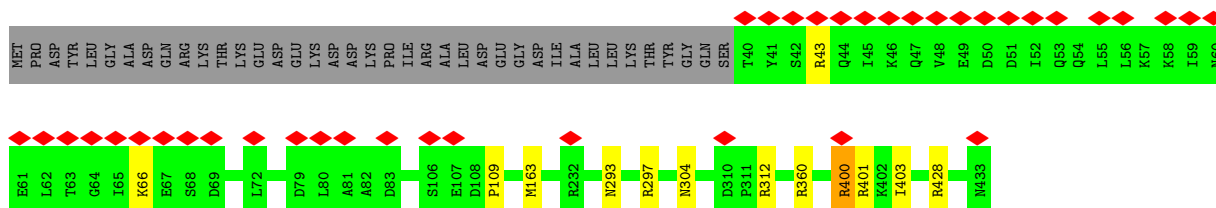
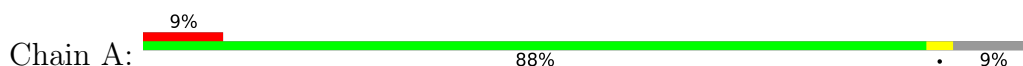


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

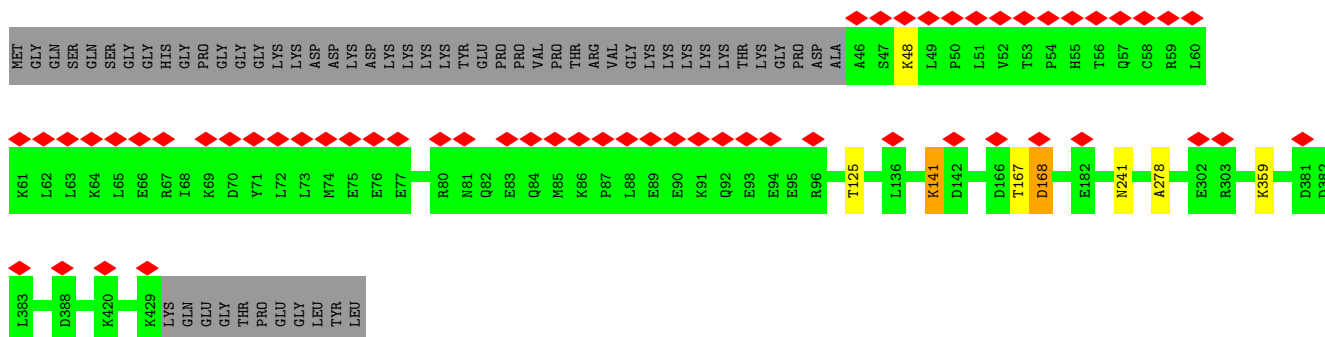
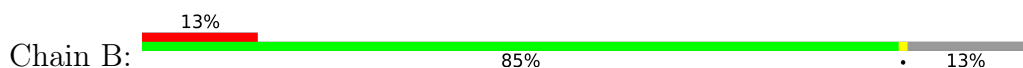




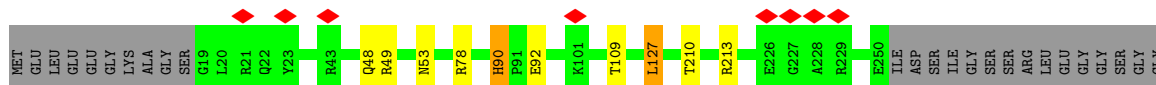
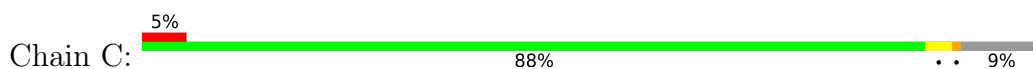
• Molecule 13: 26S protease regulatory subunit 7

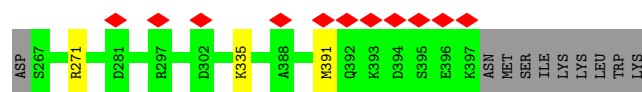


• Molecule 14: 26S protease regulatory subunit 4

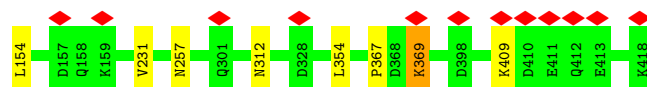
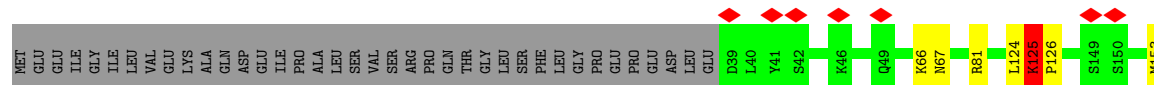
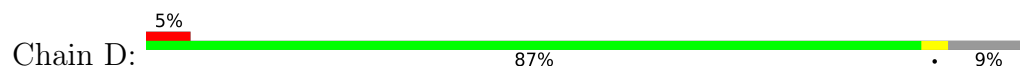


• Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8

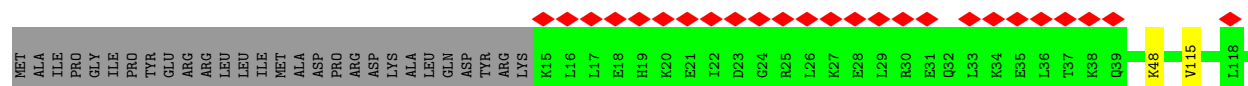




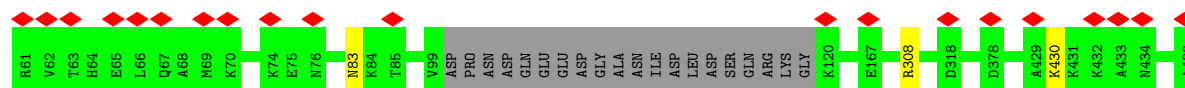
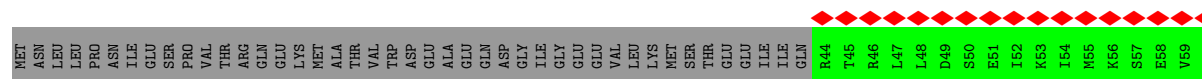
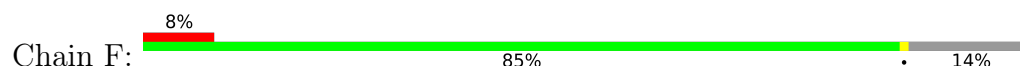
- Molecule 16: 26S protease regulatory subunit 6B



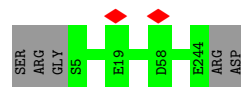
- Molecule 17: 26S proteasome regulatory subunit 10B



- Molecule 18: 26S protease regulatory subunit 6A

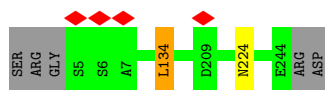


- Molecule 19: Proteasome subunit alpha type-6

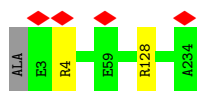


- Molecule 19: Proteasome subunit alpha type-6

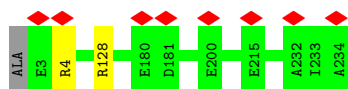




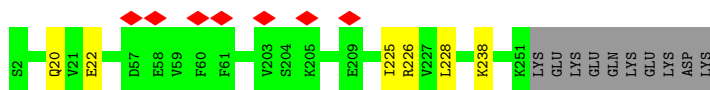
- Molecule 20: Proteasome subunit alpha type-2



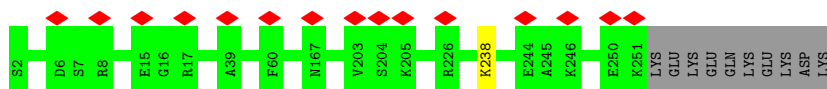
- Molecule 20: Proteasome subunit alpha type-2



- Molecule 21: Proteasome subunit alpha type-4



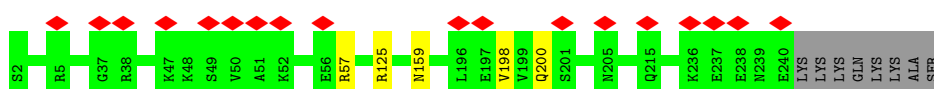
- Molecule 21: Proteasome subunit alpha type-4



- Molecule 22: Proteasome subunit alpha type-7

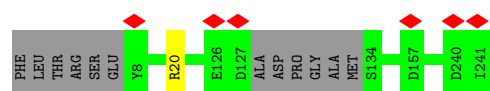


- Molecule 22: Proteasome subunit alpha type-7



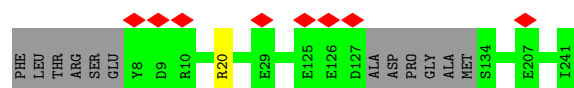
- Molecule 23: Proteasome subunit alpha type-5

Chain K:  95% 5%




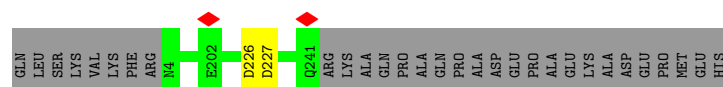
- Molecule 23: Proteasome subunit alpha type-5

Chain k:  95% 5%




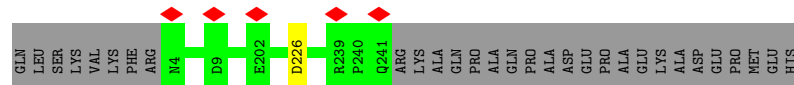
- Molecule 24: Isoform Long of Proteasome subunit alpha type-1

Chain L:  88% 11%



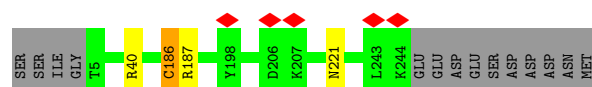
- Molecule 24: Isoform Long of Proteasome subunit alpha type-1

Chain l:  88% 11%



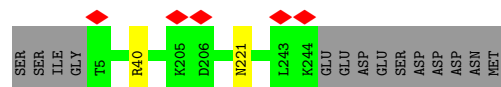
- Molecule 25: Proteasome subunit alpha type-3

Chain M:  93% 6%




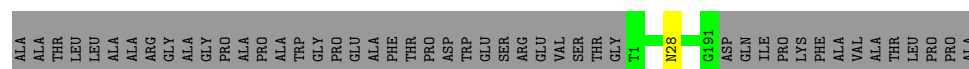
- Molecule 25: Proteasome subunit alpha type-3

Chain m:  94% 6%




- Molecule 26: Proteasome subunit beta type-6

Chain N:  80% 20%




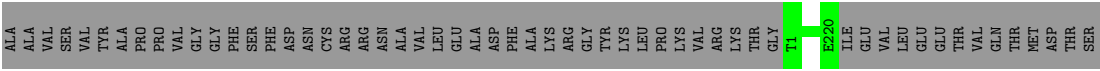
• Molecule 26: Proteasome subunit beta type-6

Chain n:  80% 20%




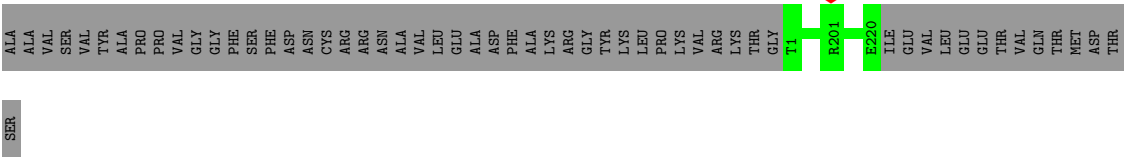
• Molecule 27: Proteasome subunit beta type-7

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%



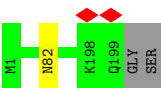
• Molecule 28: Proteasome subunit beta type-3

Chain p:  100%



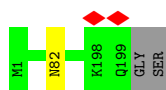
• Molecule 29: Proteasome subunit beta type-2

Chain Q:  99%



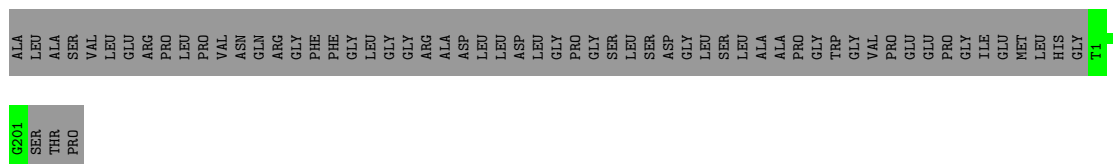
• Molecule 29: Proteasome subunit beta type-2

Chain q:  99%



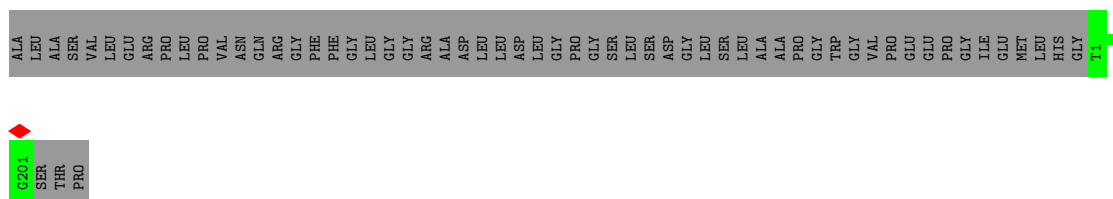
- Molecule 30: Proteasome subunit beta type-5

Chain R: 77% 23%



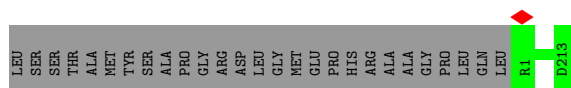
- Molecule 30: Proteasome subunit beta type-5

Chain r: 77% 23%



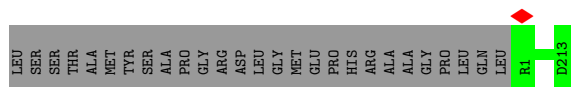
- Molecule 31: Proteasome subunit beta type-1

Chain S: 89% 11%



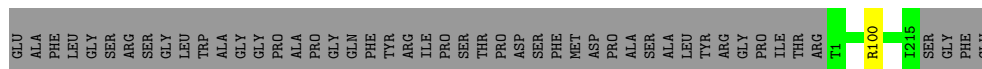
- Molecule 31: Proteasome subunit beta type-1

Chain s: 89% 11%



- Molecule 32: Proteasome subunit beta type-4

Chain T: 81% 18%



- Molecule 32: Proteasome subunit beta type-4

Chain t: 81% 18%

GLU	ALA	PHE	LEU	GLY	SER	ARG	SER	GLY	LEU	TRP	ALA	GLY	GLY	PRO	ALA	PRO	GLY	GLN	PHE	TYR	ARG	ILE	PRO	SER	THR	PRO	ASP	SER	PHE	MET	ASP	PRO	ALA	SER	ALA	LEU	TYR	ARG	GLY	PRO	ILE	THR	ARG	TH	R100	T215	SER	GLY	PHE	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	------	------	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.172	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0394	Depositor
Map size ( $\text{\AA}$ )	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: ZN, ADP, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	U	0.32	0/6449	0.58	1/8729 (0.0%)
2	V	0.34	0/4072	0.63	1/5510 (0.0%)
3	W	0.33	0/3740	0.64	0/5027
4	X	0.30	0/3053	0.58	0/4115
5	Y	0.35	0/3173	0.62	0/4273
6	Z	0.33	0/2324	0.60	0/3150
7	a	0.31	0/3053	0.59	0/4133
8	b	0.29	0/1478	0.60	0/2001
9	c	0.34	0/2302	0.63	0/3110
10	d	0.33	0/2162	0.64	0/2919
11	e	0.30	0/338	0.57	0/450
12	f	0.30	0/6970	0.67	0/9420
13	A	0.35	0/3148	0.60	0/4250
14	B	0.34	0/3061	0.60	0/4129
15	C	0.33	0/2902	0.58	0/3904
16	D	0.37	0/3089	0.62	1/4168 (0.0%)
17	E	0.33	0/2904	0.56	0/3924
18	F	0.35	0/2896	0.56	0/3912
19	G	0.33	0/1859	0.52	0/2523
19	g	0.33	0/1859	0.52	0/2523
20	H	0.35	0/1743	0.51	0/2372
20	h	0.35	0/1743	0.51	0/2372
21	I	0.35	0/1942	0.56	0/2628
21	i	0.35	0/1942	0.56	0/2628
22	J	0.34	0/1737	0.54	0/2369
22	j	0.34	0/1728	0.54	0/2358
23	K	0.33	0/1747	0.54	0/2364
23	k	0.33	0/1747	0.54	0/2364
24	L	0.35	0/1885	0.55	0/2552
24	l	0.35	0/1885	0.57	1/2552 (0.0%)
25	M	0.36	0/1891	0.55	0/2552
25	m	0.36	0/1891	0.53	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
26	N	0.35	0/1454	0.50	0/1967
26	n	0.35	0/1454	0.50	0/1967
27	O	0.36	0/1670	0.53	0/2265
27	o	0.36	0/1670	0.53	0/2265
28	P	0.35	0/1620	0.51	0/2184
28	p	0.35	0/1620	0.51	0/2184
29	Q	0.37	0/1603	0.55	0/2174
29	q	0.37	0/1603	0.55	0/2174
30	R	0.38	0/1579	0.49	0/2134
30	r	0.38	0/1579	0.49	0/2134
31	S	0.36	0/1671	0.51	0/2253
31	s	0.36	0/1674	0.51	0/2257
32	T	0.36	0/1700	0.52	0/2305
32	t	0.36	0/1700	0.52	0/2305
All	All	0.34	0/105310	0.57	4/142401 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	l	226	ASP	CB-CG-OD1	7.01	124.61	118.30
1	U	53	GLY	N-CA-C	-5.76	98.71	113.10
2	V	170	LEU	CA-CB-CG	5.58	128.12	115.30
16	D	125	LYS	N-CA-C	5.07	124.70	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	U	806/953 (85%)	731 (91%)	72 (9%)	3 (0%)	30	62
2	V	506/533 (95%)	445 (88%)	55 (11%)	6 (1%)	11	41
3	W	454/456 (100%)	401 (88%)	49 (11%)	4 (1%)	14	47
4	X	378/422 (90%)	352 (93%)	25 (7%)	1 (0%)	37	67
5	Y	376/389 (97%)	336 (89%)	40 (11%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	33
7	a	371/376 (99%)	324 (87%)	42 (11%)	5 (1%)	10	40
8	b	189/377 (50%)	170 (90%)	18 (10%)	1 (0%)	25	57
9	c	285/309 (92%)	244 (86%)	39 (14%)	2 (1%)	19	51
10	d	255/349 (73%)	208 (82%)	46 (18%)	1 (0%)	30	62
11	e	36/70 (51%)	27 (75%)	9 (25%)	0	100	100
12	f	887/908 (98%)	698 (79%)	176 (20%)	13 (2%)	8	38
13	A	392/433 (90%)	340 (87%)	50 (13%)	2 (0%)	25	57
14	B	382/440 (87%)	338 (88%)	41 (11%)	3 (1%)	16	49
15	C	359/398 (90%)	332 (92%)	25 (7%)	2 (1%)	22	54
16	D	378/418 (90%)	327 (86%)	46 (12%)	5 (1%)	10	40
17	E	373/403 (93%)	338 (91%)	35 (9%)	0	100	100
18	F	372/439 (85%)	339 (91%)	33 (9%)	0	100	100
19	G	238/245 (97%)	230 (97%)	8 (3%)	0	100	100
19	g	238/245 (97%)	228 (96%)	9 (4%)	1 (0%)	30	62
20	H	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
20	h	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
21	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
21	i	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
22	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	49
22	j	237/247 (96%)	217 (92%)	18 (8%)	2 (1%)	16	49
23	K	224/240 (93%)	213 (95%)	11 (5%)	0	100	100
23	k	224/240 (93%)	213 (95%)	11 (5%)	0	100	100
24	L	236/268 (88%)	218 (92%)	17 (7%)	1 (0%)	30	62
24	l	236/268 (88%)	217 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	M	238/254 (94%)	221 (93%)	16 (7%)	1 (0%)	30	62
25	m	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
26	N	189/238 (79%)	181 (96%)	8 (4%)	0	100	100
26	n	189/238 (79%)	181 (96%)	8 (4%)	0	100	100
27	O	218/276 (79%)	210 (96%)	8 (4%)	0	100	100
27	o	218/276 (79%)	210 (96%)	8 (4%)	0	100	100
28	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
28	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
29	q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
30	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
30	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
31	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
32	T	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
32	t	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
All	All	13243/14859 (89%)	11994 (91%)	1188 (9%)	61 (0%)	27	57

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	55	ARG
2	V	167	LEU
2	V	168	GLN
6	Z	149	THR
6	Z	150	PRO
7	a	145	LEU
7	a	152	HIS
7	a	186	LYS
8	b	22	LEU
9	c	158	ASP
12	f	281	ILE
12	f	766	GLN
12	f	789	SER
12	f	838	ARG
14	B	141	LYS

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Mol	Chain	Res	Type
14	B	168	ASP
16	D	125	LYS
16	D	126	PRO
16	D	369	LYS
24	L	226	ASP
3	W	91	SER
3	W	315	MET
6	Z	151	THR
9	c	196	LEU
12	f	756	PRO
12	f	761	MET
14	B	278	ALA
16	D	154	LEU
25	M	186	CYS
1	U	52	GLU
7	a	151	VAL
12	f	476	THR
12	f	768	LEU
3	W	316	ARG
3	W	317	TRP
6	Z	224	HIS
7	a	69	HIS
10	d	109	GLN
12	f	118	ASN
12	f	681	TYR
22	J	200	GLN
19	g	134	LEU
22	j	198	VAL
22	j	200	GLN
2	V	496	PHE
4	X	392	PRO
6	Z	212	LEU
12	f	475	ASN
12	f	765	ALA
13	A	109	PRO
13	A	400	ARG
2	V	263	LEU
16	D	367	PRO
6	Z	99	PRO
12	f	643	PRO
1	U	174	PRO
15	C	90	HIS

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Mol	Chain	Res	Type
2	V	29	PRO
22	J	198	VAL
2	V	497	PRO
15	C	127	LEU

### 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%)	687 (99%)	5 (1%)	81	88
2	V	415/459 (90%)	405 (98%)	10 (2%)	44	63
3	W	414/416 (100%)	397 (96%)	17 (4%)	26	52
4	X	327/362 (90%)	320 (98%)	7 (2%)	48	67
5	Y	334/344 (97%)	330 (99%)	4 (1%)	67	79
6	Z	257/295 (87%)	243 (95%)	14 (5%)	18	46
7	a	333/336 (99%)	325 (98%)	8 (2%)	44	63
8	b	167/312 (54%)	166 (99%)	1 (1%)	84	90
9	c	252/267 (94%)	237 (94%)	15 (6%)	16	43
10	d	231/293 (79%)	221 (96%)	10 (4%)	25	50
11	e	38/63 (60%)	37 (97%)	1 (3%)	41	61
12	f	743/763 (97%)	706 (95%)	37 (5%)	20	47
13	A	337/372 (91%)	325 (96%)	12 (4%)	30	55
14	B	339/385 (88%)	332 (98%)	7 (2%)	48	67
15	C	314/346 (91%)	301 (96%)	13 (4%)	26	52
16	D	333/366 (91%)	321 (96%)	12 (4%)	30	55
17	E	298/353 (84%)	293 (98%)	5 (2%)	56	73
18	F	296/379 (78%)	293 (99%)	3 (1%)	73	82
19	G	193/209 (92%)	193 (100%)	0	100	100
19	g	193/209 (92%)	191 (99%)	2 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	H	164/190 (86%)	162 (99%)	2 (1%)	67	79
20	h	164/190 (86%)	162 (99%)	2 (1%)	67	79
21	I	193/220 (88%)	187 (97%)	6 (3%)	35	57
21	i	193/220 (88%)	192 (100%)	1 (0%)	86	92
22	J	154/210 (73%)	147 (96%)	7 (4%)	23	50
22	j	152/210 (72%)	149 (98%)	3 (2%)	50	68
23	K	186/202 (92%)	185 (100%)	1 (0%)	86	92
23	k	186/202 (92%)	185 (100%)	1 (0%)	86	92
24	L	198/229 (86%)	197 (100%)	1 (0%)	86	92
24	l	198/229 (86%)	198 (100%)	0	100	100
25	M	192/211 (91%)	188 (98%)	4 (2%)	48	67
25	m	192/211 (91%)	190 (99%)	2 (1%)	73	82
26	N	148/180 (82%)	147 (99%)	1 (1%)	81	88
26	n	148/180 (82%)	147 (99%)	1 (1%)	81	88
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	173/173 (100%)	173 (100%)	0	100	100
28	p	173/173 (100%)	173 (100%)	0	100	100
29	Q	164/171 (96%)	163 (99%)	1 (1%)	84	90
29	q	164/171 (96%)	163 (99%)	1 (1%)	84	90
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	175/198 (88%)	175 (100%)	0	100	100
32	T	175/214 (82%)	174 (99%)	1 (1%)	84	90
32	t	175/214 (82%)	174 (99%)	1 (1%)	84	90
All	All	11007/12597 (87%)	10788 (98%)	219 (2%)	50	68

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	55	ARG
1	U	177	LEU

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Mol	Chain	Res	Type
1	U	345	ASN
1	U	603	LEU
1	U	605	VAL
2	V	80	LYS
2	V	167	LEU
2	V	194	LYS
2	V	223	LYS
2	V	266	GLN
2	V	329	HIS
2	V	345	ARG
2	V	357	LEU
2	V	358	MET
2	V	452	ASN
3	W	86	ASN
3	W	88	MET
3	W	89	LEU
3	W	274	VAL
3	W	275	ILE
3	W	276	LEU
3	W	315	MET
3	W	316	ARG
3	W	326	MET
3	W	355	LYS
3	W	357	ARG
3	W	361	HIS
3	W	364	ARG
3	W	399	ASN
3	W	422	ASN
3	W	440	ASN
3	W	448	LYS
4	X	304	LYS
4	X	310	ARG
4	X	314	ARG
4	X	329	ASN
4	X	344	ARG
4	X	395	LYS
4	X	420	LYS
5	Y	235	ASP
5	Y	237	ARG
5	Y	312	ARG
5	Y	358	ARG
6	Z	114	ARG

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Mol	Chain	Res	Type
6	Z	129	LYS
6	Z	141	VAL
6	Z	143	GLU
6	Z	145	HIS
6	Z	147	ASP
6	Z	151	THR
6	Z	152	SER
6	Z	153	LYS
6	Z	154	THR
6	Z	193	ASN
6	Z	214	LYS
6	Z	225	GLN
6	Z	236	LEU
7	a	143	ASN
7	a	145	LEU
7	a	149	THR
7	a	150	SER
7	a	183	VAL
7	a	186	LYS
7	a	188	LEU
7	a	190	VAL
8	b	51	LEU
9	c	49	VAL
9	c	83	SER
9	c	84	VAL
9	c	85	GLU
9	c	104	ARG
9	c	155	VAL
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN
9	c	197	ASN
9	c	198	ARG
9	c	200	TYR
9	c	232	GLN
9	c	254	ASN
9	c	277	LYS
10	d	35	PHE
10	d	45	LYS
10	d	89	LEU
10	d	107	LEU
10	d	108	SER

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Mol	Chain	Res	Type
10	d	117	THR
10	d	118	GLU
10	d	121	ARG
10	d	196	ARG
10	d	231	LYS
11	e	1	MET
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	217	LEU
12	f	218	GLU
12	f	267	ARG
12	f	281	ILE
12	f	282	PHE
12	f	283	THR
12	f	297	MET
12	f	327	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	680	ARG
12	f	681	TYR
12	f	703	ARG
12	f	712	LYS
12	f	713	PHE
12	f	746	ARG
12	f	755	ASP
12	f	757	ASN
12	f	763	ARG
12	f	764	LEU
12	f	768	LEU
12	f	769	THR
12	f	770	HIS
12	f	771	LEU
12	f	773	LYS
12	f	775	THR
12	f	787	LEU
12	f	788	MET
12	f	822	VAL
12	f	838	ARG

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Mol	Chain	Res	Type
12	f	840	LEU
13	A	43	ARG
13	A	66	LYS
13	A	163	MET
13	A	293	ASN
13	A	297	ARG
13	A	304	ASN
13	A	312	ARG
13	A	360	ARG
13	A	400	ARG
13	A	401	ARG
13	A	403	ILE
13	A	428	ARG
14	B	48	LYS
14	B	125	THR
14	B	141	LYS
14	B	167	THR
14	B	168	ASP
14	B	241	ASN
14	B	359	LYS
15	C	48	GLN
15	C	49	ARG
15	C	53	ASN
15	C	78	ARG
15	C	90	HIS
15	C	92	GLU
15	C	109	THR
15	C	127	LEU
15	C	210	THR
15	C	213	ARG
15	C	271	ARG
15	C	335	LYS
15	C	391	MET
16	D	66	LYS
16	D	67	ASN
16	D	81	ARG
16	D	124	LEU
16	D	125	LYS
16	D	153	MET
16	D	231	VAL
16	D	257	ASN
16	D	312	ASN

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Mol	Chain	Res	Type
16	D	354	LEU
16	D	369	LYS
16	D	409	LYS
17	E	48	LYS
17	E	115	VAL
17	E	197	LYS
17	E	223	ARG
17	E	384	LEU
18	F	83	ASN
18	F	308	ARG
18	F	430	LYS
20	H	4	ARG
20	H	128	ARG
21	I	20	GLN
21	I	22	GLU
21	I	225	ILE
21	I	226	ARG
21	I	228	LEU
21	I	238	LYS
22	J	53	LEU
22	J	54	GLN
22	J	56	GLU
22	J	57	ARG
22	J	125	ARG
22	J	159	ASN
22	J	200	GLN
23	K	20	ARG
24	L	227	ASP
25	M	40	ARG
25	M	186	CYS
25	M	187	ARG
25	M	221	ASN
26	N	28	ASN
29	Q	82	ASN
32	T	100	ARG
19	g	134	LEU
19	g	224	ASN
20	h	4	ARG
20	h	128	ARG
21	i	238	LYS
22	j	57	ARG
22	j	125	ARG

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Mol	Chain	Res	Type
22	j	159	ASN
23	k	20	ARG
25	m	40	ARG
25	m	221	ASN
26	n	28	ASN
29	q	82	ASN
32	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	247	GLN
1	U	345	ASN
1	U	389	ASN
1	U	415	HIS
1	U	595	ASN
1	U	768	GLN
1	U	777	HIS
2	V	62	HIS
2	V	257	ASN
2	V	260	HIS
2	V	329	HIS
2	V	400	HIS
2	V	401	ASN
2	V	427	GLN
2	V	452	ASN
3	W	96	GLN
3	W	228	ASN
3	W	356	ASN
3	W	361	HIS
3	W	362	ASN
3	W	399	ASN
3	W	440	ASN
4	X	198	ASN
4	X	213	GLN
4	X	262	ASN
4	X	322	HIS
4	X	329	ASN
4	X	333	GLN
5	Y	71	ASN
5	Y	306	GLN
5	Y	367	GLN

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Mol	Chain	Res	Type
6	Z	109	ASN
6	Z	202	ASN
6	Z	223	ASN
6	Z	225	GLN
6	Z	256	GLN
6	Z	273	HIS
6	Z	277	ASN
6	Z	278	ASN
7	a	144	ASN
7	a	193	GLN
7	a	231	GLN
7	a	258	GLN
7	a	264	ASN
7	a	267	GLN
7	a	290	GLN
7	a	345	GLN
7	a	370	GLN
8	b	101	GLN
8	b	142	ASN
9	c	44	HIS
9	c	101	GLN
9	c	113	HIS
9	c	130	GLN
9	c	149	GLN
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN
9	c	197	ASN
9	c	232	GLN
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
9	c	278	GLN
9	c	298	GLN
10	d	88	GLN
11	e	63	HIS
12	f	43	GLN
12	f	171	GLN
12	f	213	GLN
12	f	291	GLN
12	f	396	ASN
12	f	457	ASN

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Mol	Chain	Res	Type
12	f	475	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	619	HIS
12	f	715	HIS
12	f	737	ASN
12	f	782	HIS
12	f	808	ASN
12	f	826	GLN
13	A	85	GLN
13	A	293	ASN
13	A	304	ASN
14	B	81	ASN
14	B	241	ASN
14	B	368	HIS
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN
15	C	90	HIS
15	C	221	GLN
15	C	241	HIS
16	D	133	HIS
16	D	187	HIS
16	D	222	HIS
16	D	257	ASN
16	D	312	ASN
16	D	353	ASN
16	D	380	GLN
16	D	412	GLN
17	E	75	ASN
18	F	76	ASN
18	F	83	ASN
18	F	184	GLN
18	F	321	GLN
18	F	369	HIS
21	I	53	HIS
21	I	119	GLN
21	I	146	GLN
22	J	54	GLN
22	J	116	GLN
22	J	154	HIS

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Mol	Chain	Res	Type
22	J	159	ASN
22	J	200	GLN
22	J	205	ASN
23	K	99	HIS
23	K	224	GLN
24	L	190	HIS
25	M	180	GLN
25	M	221	ASN
26	N	28	ASN
27	O	165	ASN
28	P	93	ASN
29	Q	8	GLN
29	Q	55	GLN
29	Q	65	GLN
30	R	29	GLN
30	R	38	ASN
30	R	85	ASN
32	T	81	HIS
19	g	128	ASN
21	i	53	HIS
21	i	146	GLN
22	j	154	HIS
22	j	159	ASN
23	k	99	HIS
23	k	224	GLN
24	l	190	HIS
25	m	180	GLN
25	m	221	ASN
26	n	28	ASN
27	o	66	HIS
27	o	165	ASN
28	p	93	ASN
29	q	8	GLN
30	r	29	GLN
30	r	38	ASN
30	r	85	ASN
32	t	61	GLN
32	t	81	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
36	ADP	F	501	35	24,29,29	0.92	1 (4%)	29,45,45	1.51	5 (17%)
36	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)
34	ATP	A	501	35	26,33,33	0.91	1 (3%)	31,52,52	1.66	5 (16%)
34	ATP	D	501	35	26,33,33	0.90	1 (3%)	31,52,52	1.63	5 (16%)
34	ATP	E	401	35	26,33,33	0.91	1 (3%)	31,52,52	1.68	5 (16%)
34	ATP	B	501	35	26,33,33	0.90	1 (3%)	31,52,52	1.65	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	F	501	35	-	2/12/32/32	0/3/3/3
36	ADP	C	501	-	-	3/12/32/32	0/3/3/3
34	ATP	A	501	35	-	0/18/38/38	0/3/3/3
34	ATP	D	501	35	-	3/18/38/38	0/3/3/3
34	ATP	E	401	35	-	6/18/38/38	0/3/3/3
34	ATP	B	501	35	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-C4	2.37	1.47	1.40
34	E	401	ATP	C5-C4	2.34	1.47	1.40
36	F	501	ADP	C5-C4	2.30	1.47	1.40
34	D	501	ATP	C5-C4	2.27	1.46	1.40
34	A	501	ATP	C5-C4	2.23	1.46	1.40
34	B	501	ATP	C5-C4	2.21	1.46	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	401	ATP	PA-O3A-PB	-4.99	115.69	132.83
34	B	501	ATP	PA-O3A-PB	-4.83	116.25	132.83
34	D	501	ATP	PA-O3A-PB	-4.53	117.29	132.83
36	F	501	ADP	PA-O3A-PB	-4.37	117.84	132.83
34	A	501	ATP	PB-O3B-PG	-4.23	118.32	132.83
36	C	501	ADP	C3'-C2'-C1'	3.95	106.92	100.98
34	A	501	ATP	PA-O3A-PB	-3.78	119.86	132.83
36	C	501	ADP	PA-O3A-PB	-3.66	120.27	132.83
34	A	501	ATP	C3'-C2'-C1'	3.62	106.43	100.98
34	D	501	ATP	PB-O3B-PG	-3.59	120.51	132.83
34	B	501	ATP	N3-C2-N1	-3.41	123.34	128.68
34	B	501	ATP	C3'-C2'-C1'	3.38	106.06	100.98
34	D	501	ATP	N3-C2-N1	-3.28	123.55	128.68
34	E	401	ATP	PB-O3B-PG	-3.24	121.70	132.83
34	E	401	ATP	N3-C2-N1	-3.23	123.63	128.68
34	E	401	ATP	C3'-C2'-C1'	3.18	105.76	100.98
36	C	501	ADP	N3-C2-N1	-3.11	123.82	128.68
36	F	501	ADP	C3'-C2'-C1'	3.02	105.52	100.98
36	F	501	ADP	N3-C2-N1	-2.94	124.08	128.68
34	A	501	ATP	N3-C2-N1	-2.88	124.17	128.68
34	D	501	ATP	C3'-C2'-C1'	2.86	105.29	100.98
34	B	501	ATP	PB-O3B-PG	-2.71	123.52	132.83
34	A	501	ATP	C4-C5-N7	-2.68	106.60	109.40
34	D	501	ATP	C4-C5-N7	-2.41	106.89	109.40
36	F	501	ADP	C4-C5-N7	-2.36	106.94	109.40
36	C	501	ADP	C4-C5-N7	-2.35	106.95	109.40
34	B	501	ATP	C4-C5-N7	-2.28	107.03	109.40
34	E	401	ATP	C4-C5-N7	-2.23	107.08	109.40
36	F	501	ADP	O3B-PB-O2B	2.10	115.68	107.64

There are no chirality outliers.

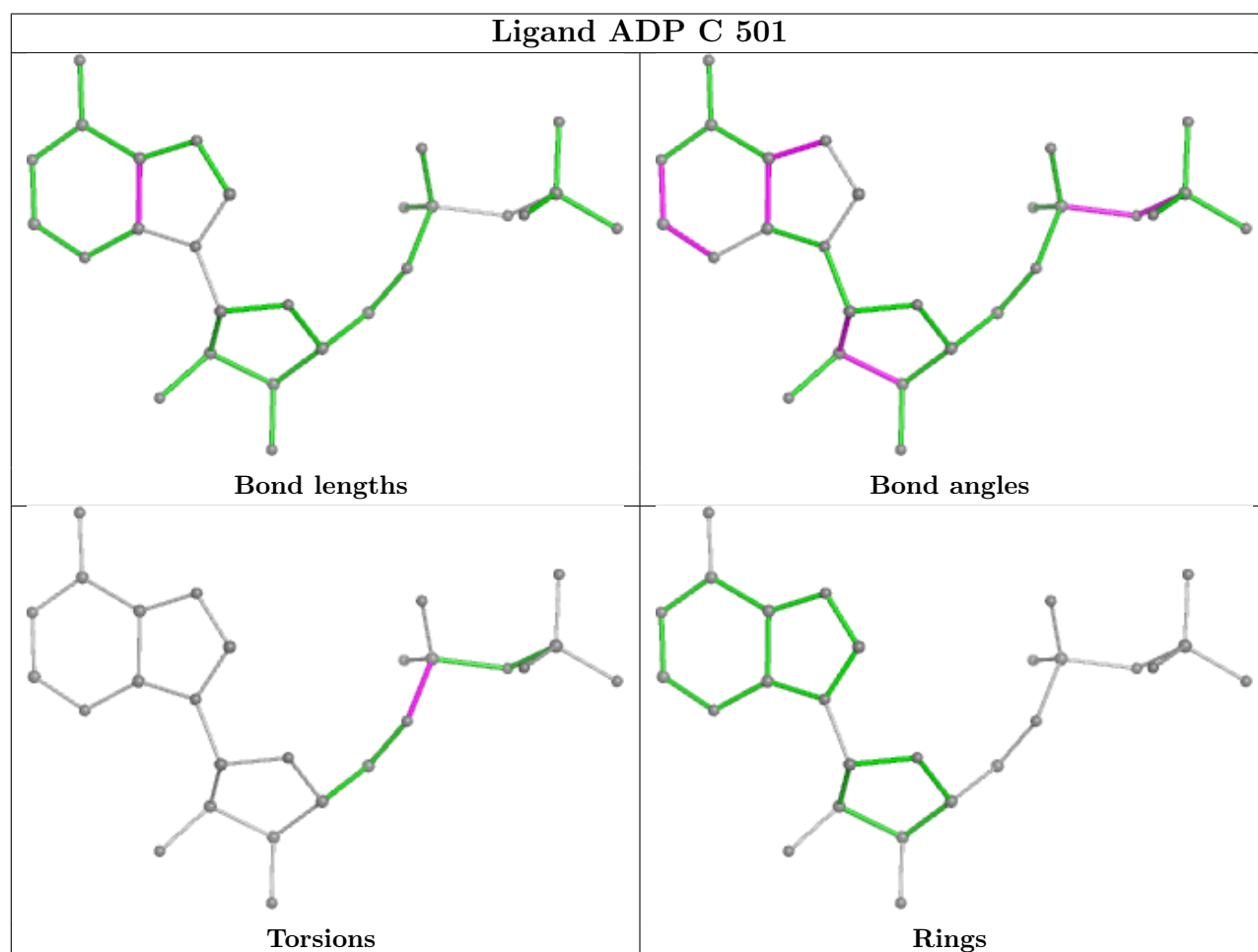
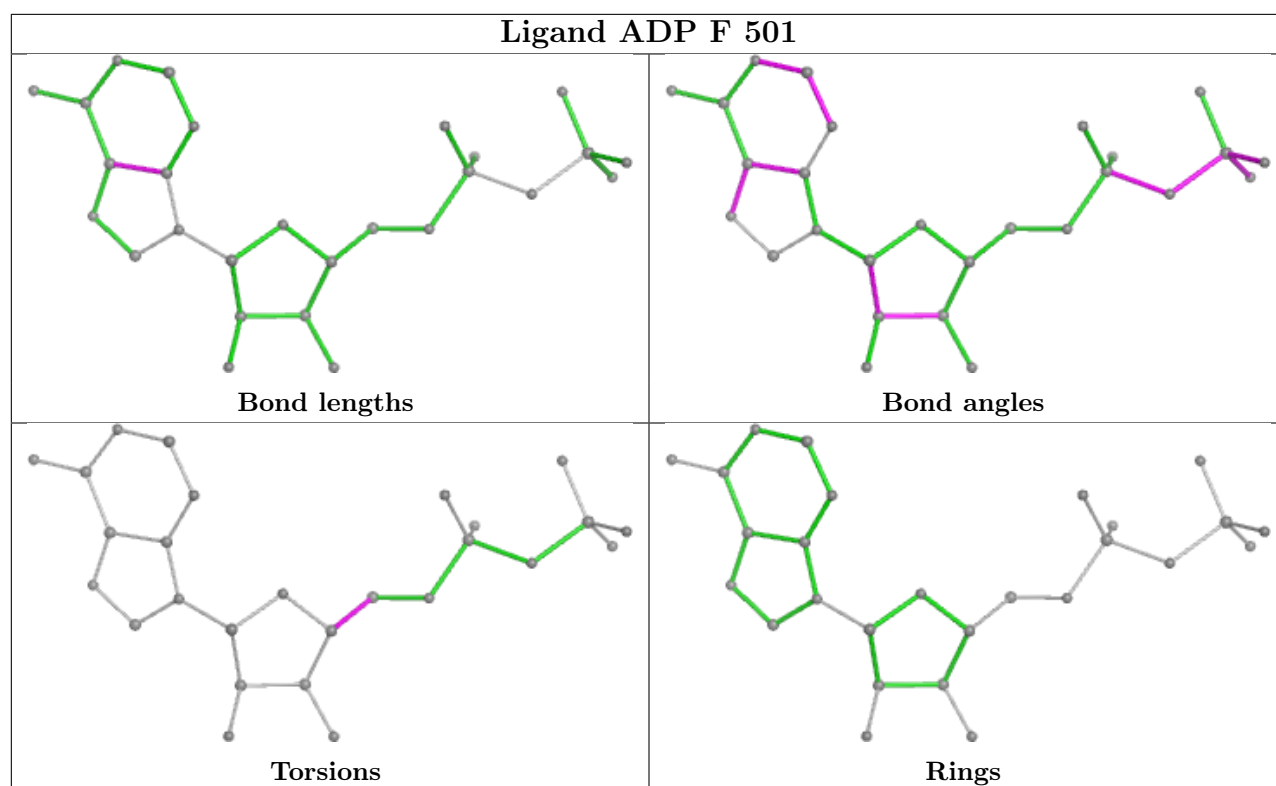
All (14) torsion outliers are listed below:

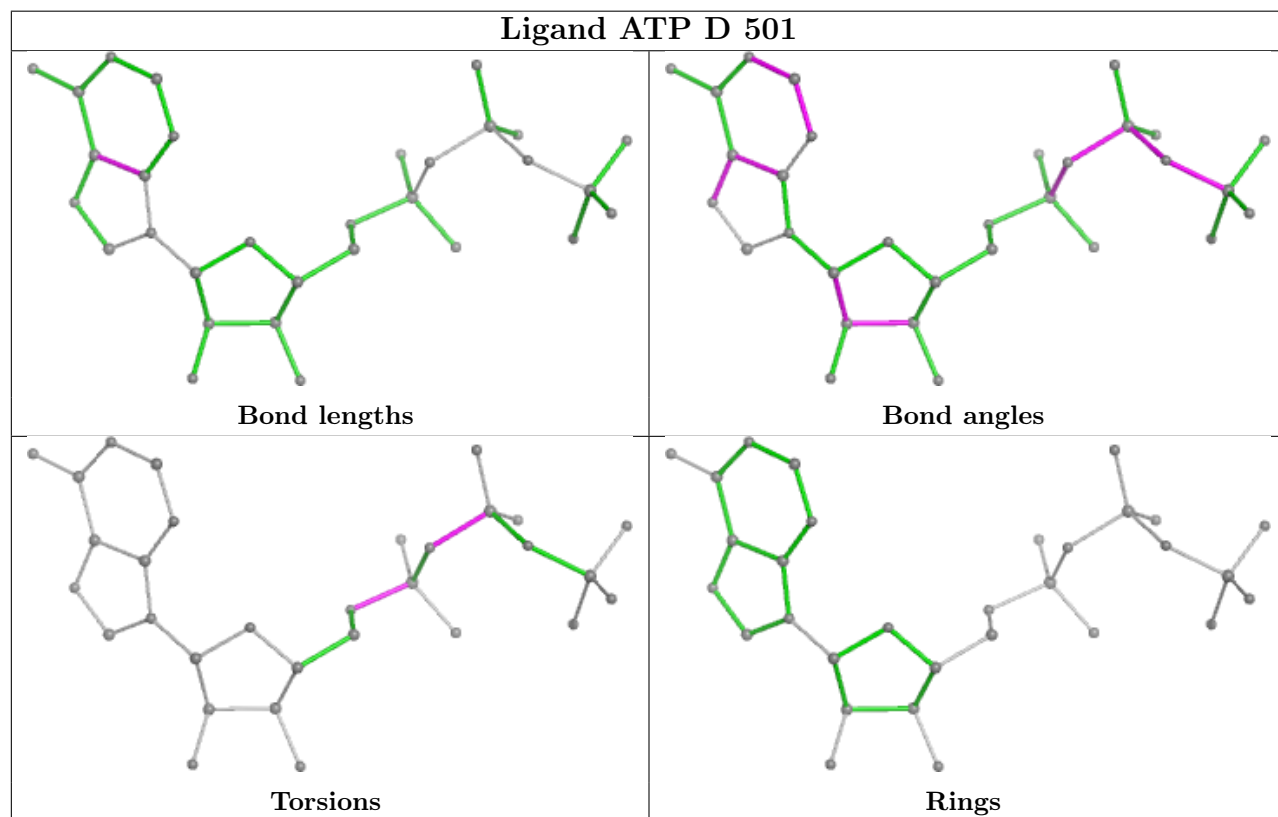
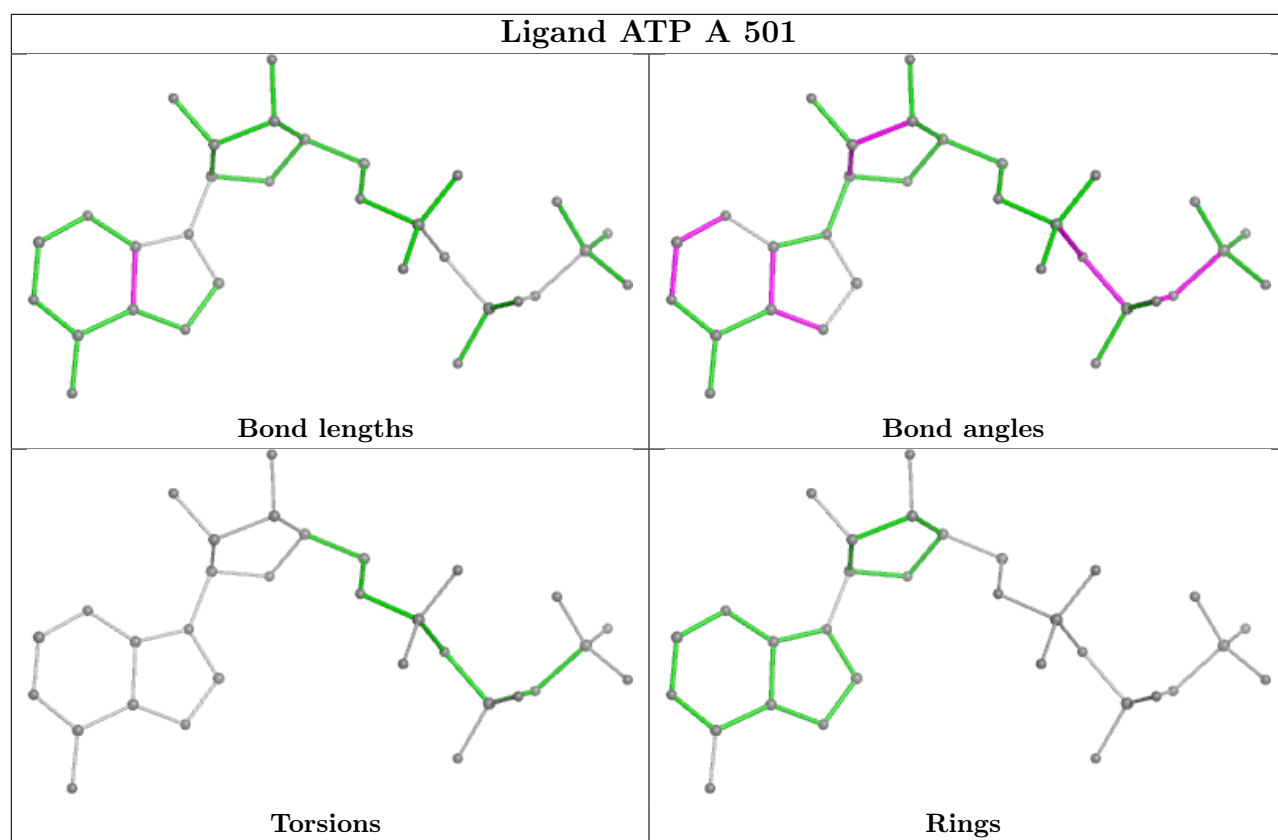
Mol	Chain	Res	Type	Atoms
34	E	401	ATP	PB-O3B-PG-O2G
34	E	401	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	F	501	ADP	O4'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'
36	C	501	ADP	C5'-O5'-PA-O3A
34	D	501	ATP	PA-O3A-PB-O1B
34	E	401	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	PB-O3B-PG-O1G
34	D	501	ATP	PA-O3A-PB-O2B
34	D	501	ATP	C5'-O5'-PA-O1A

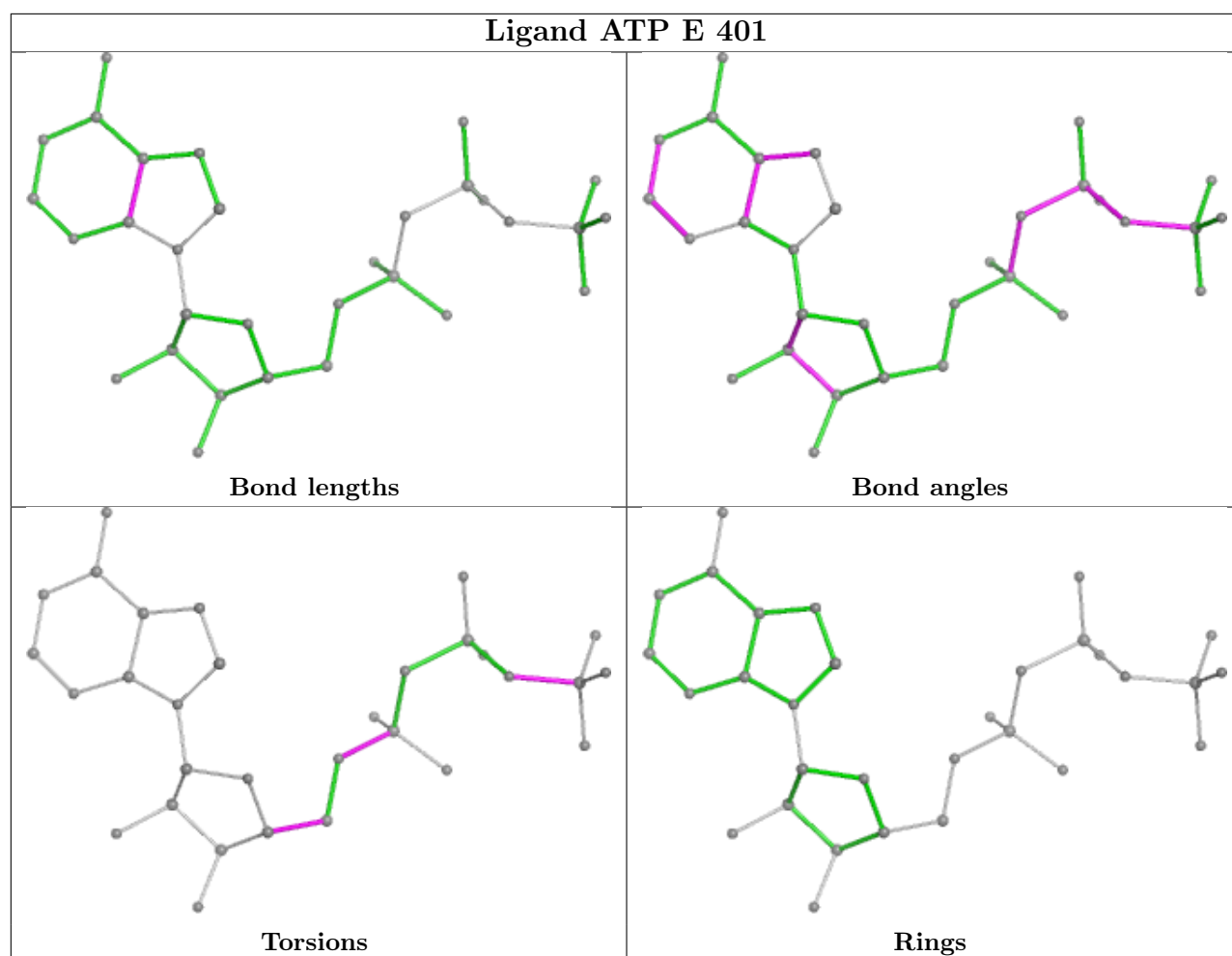
There are no ring outliers.

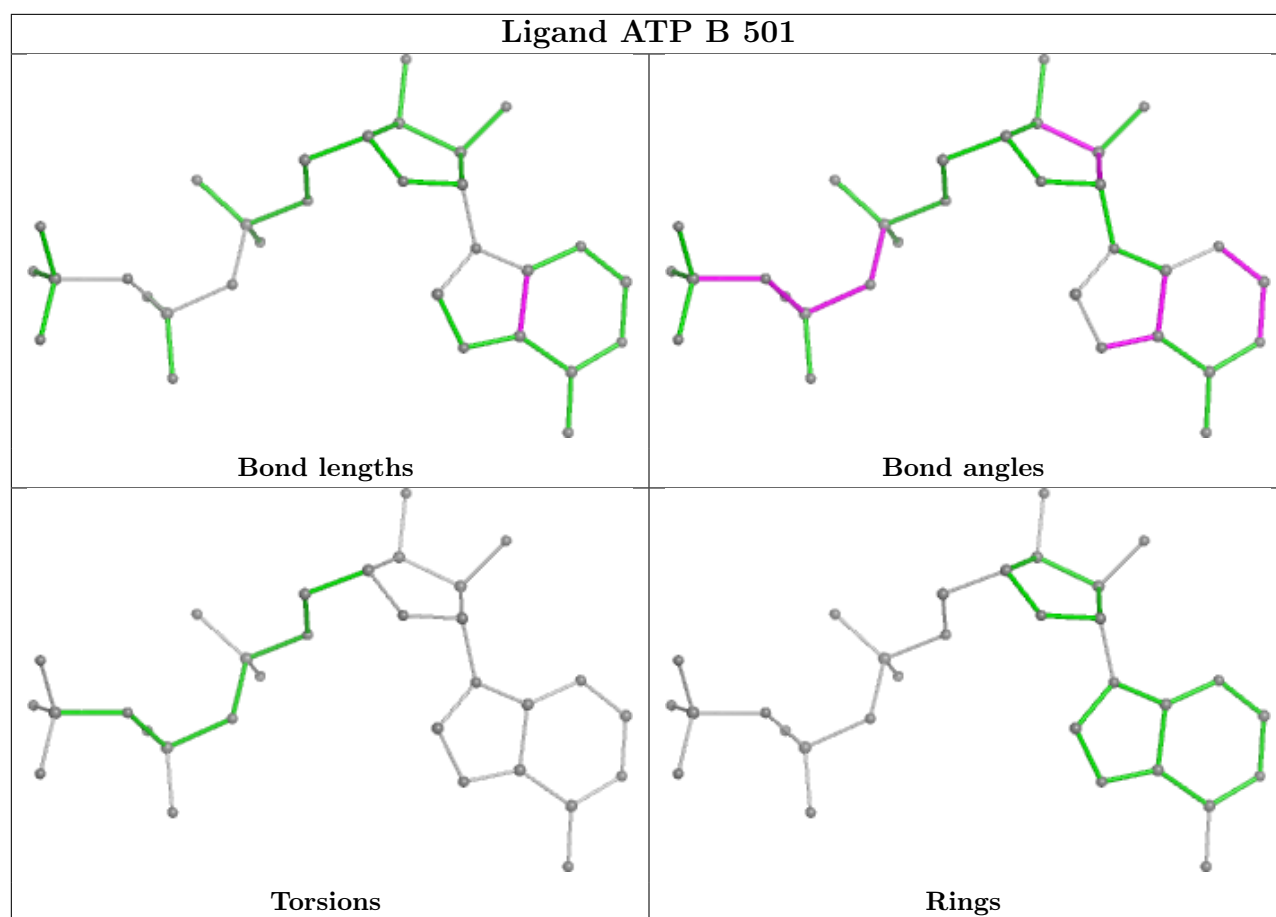
No monomer is involved in short contacts.

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.









## 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.



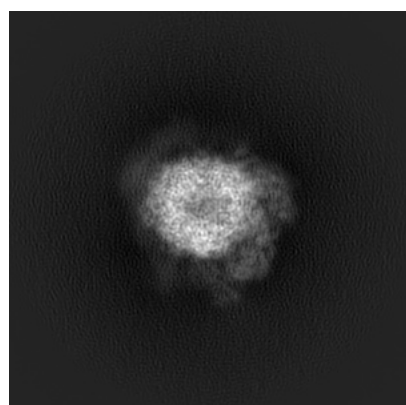
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14201. These allow visual inspection of the internal detail of the map and identification of artifacts.

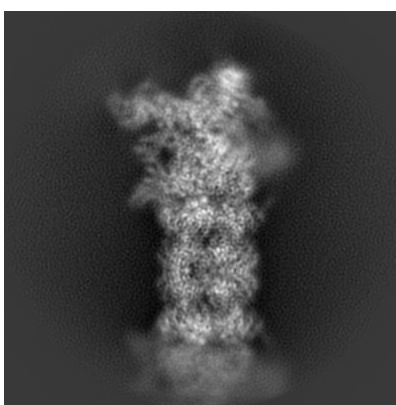
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

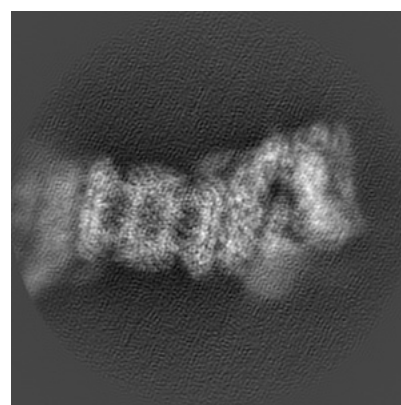
#### 6.1.1 Primary map



X



Y

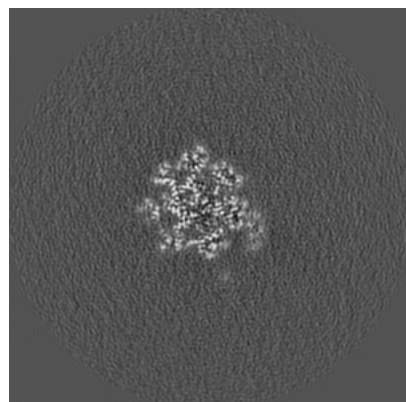


Z

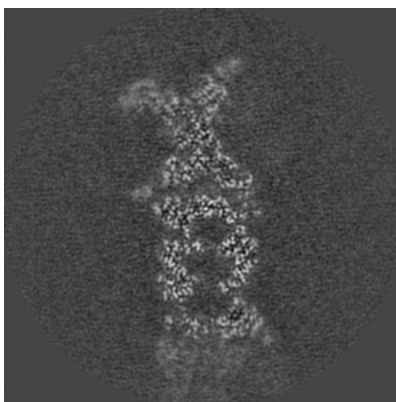
The images above show the map projected in three orthogonal directions.

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

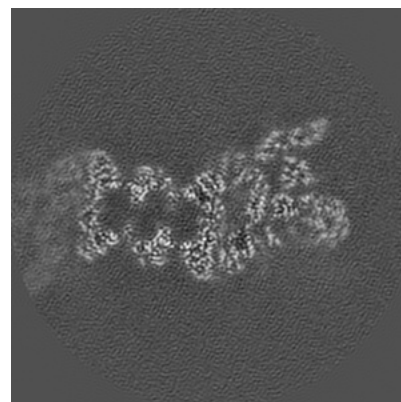
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

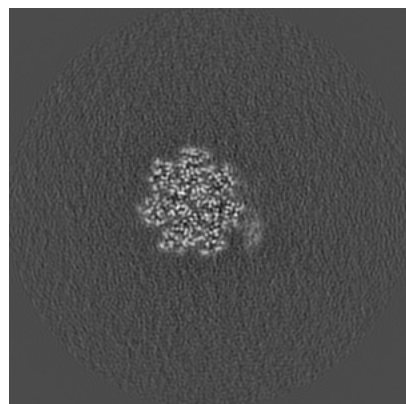


Z Index: 160

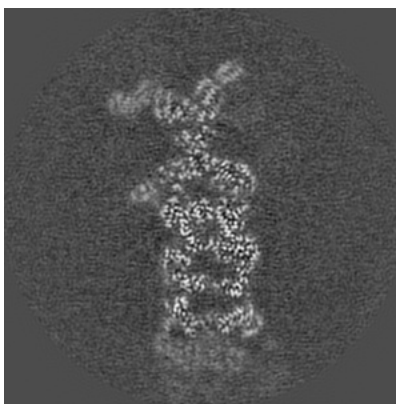
The images above show central slices of the map in three orthogonal directions.

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

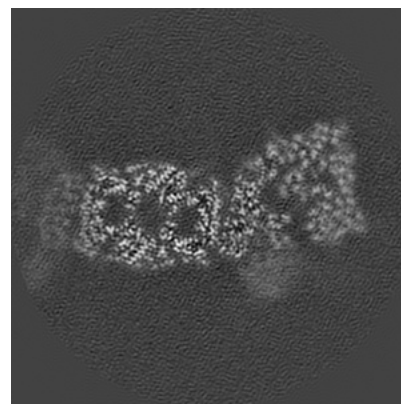
### 6.3.1 Primary map



X Index: 154



Y Index: 165

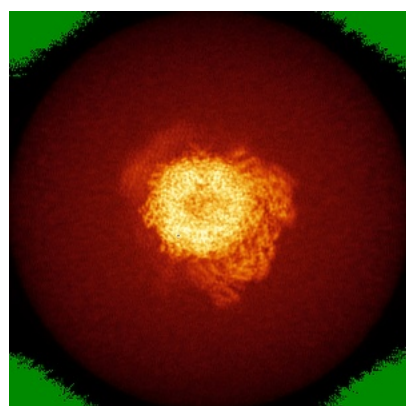


Z Index: 176

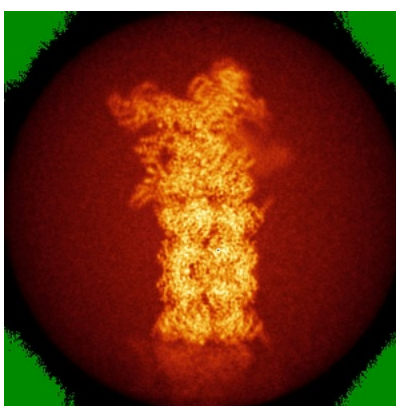
The images above show the largest variance slices of the map in three orthogonal directions.

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

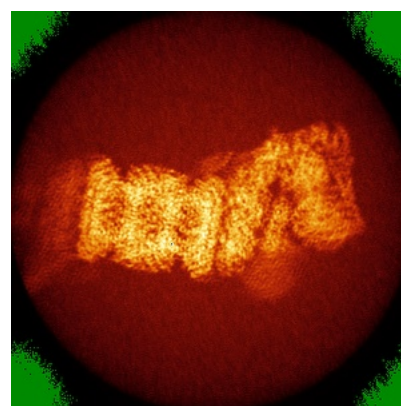
### 6.4.1 Primary map



X



Y

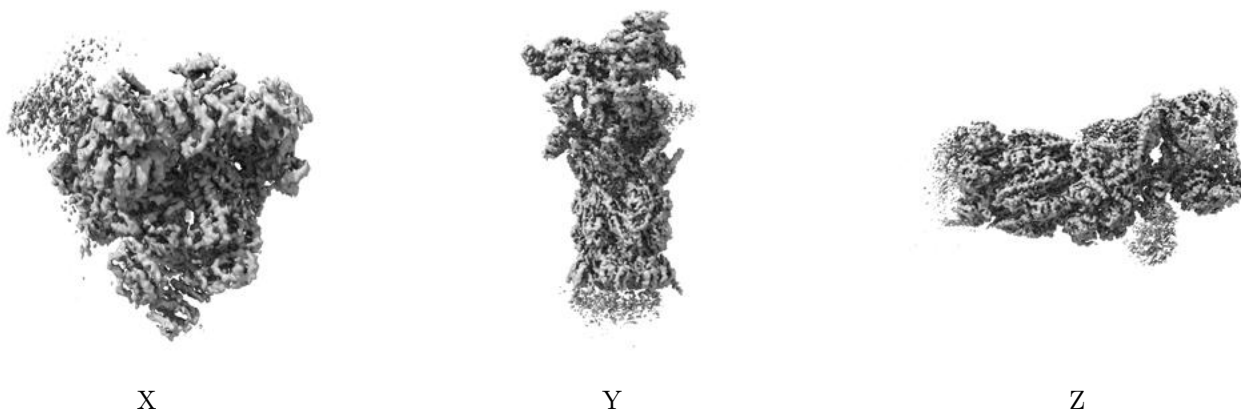


Z

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 0.0394. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

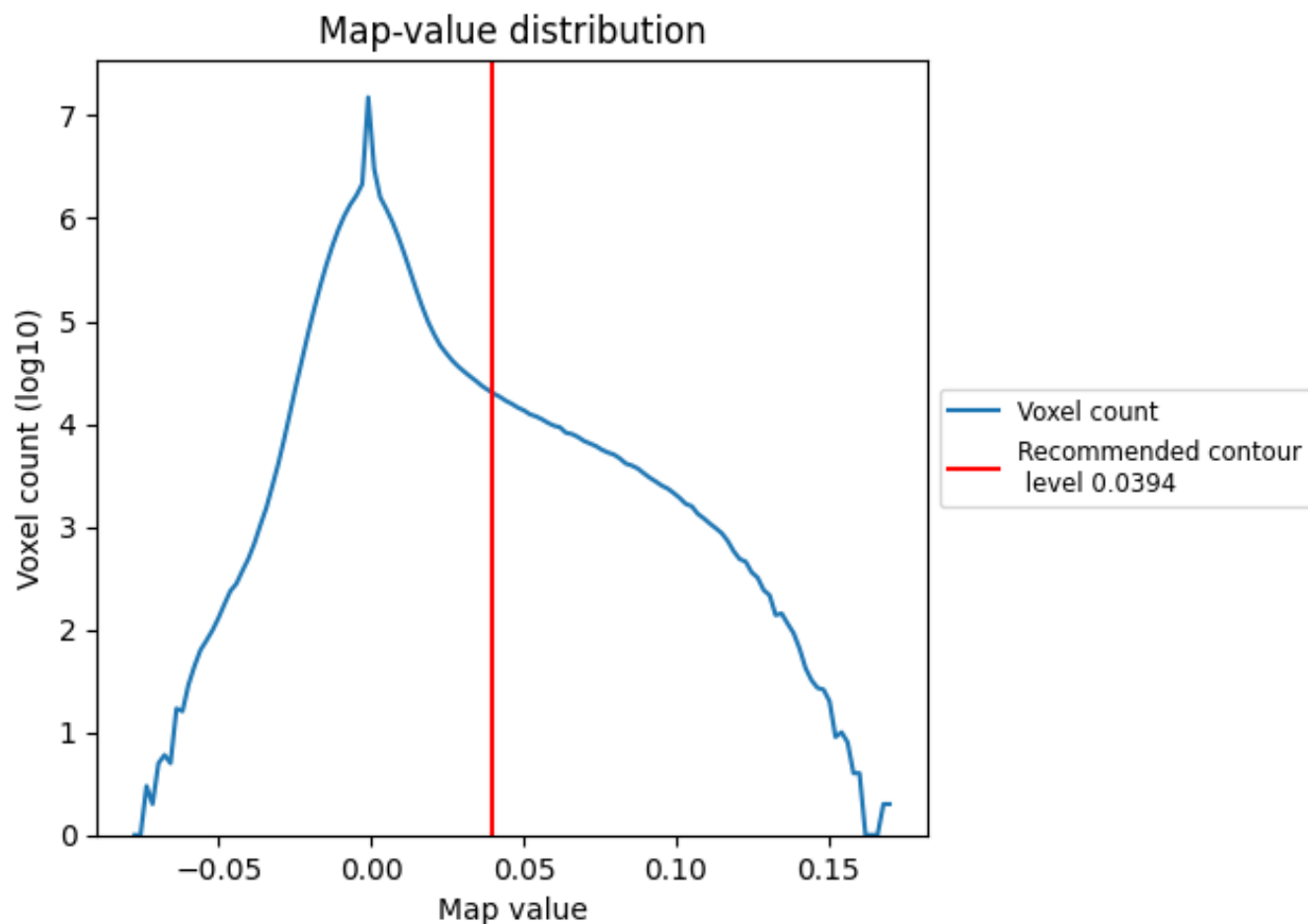
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

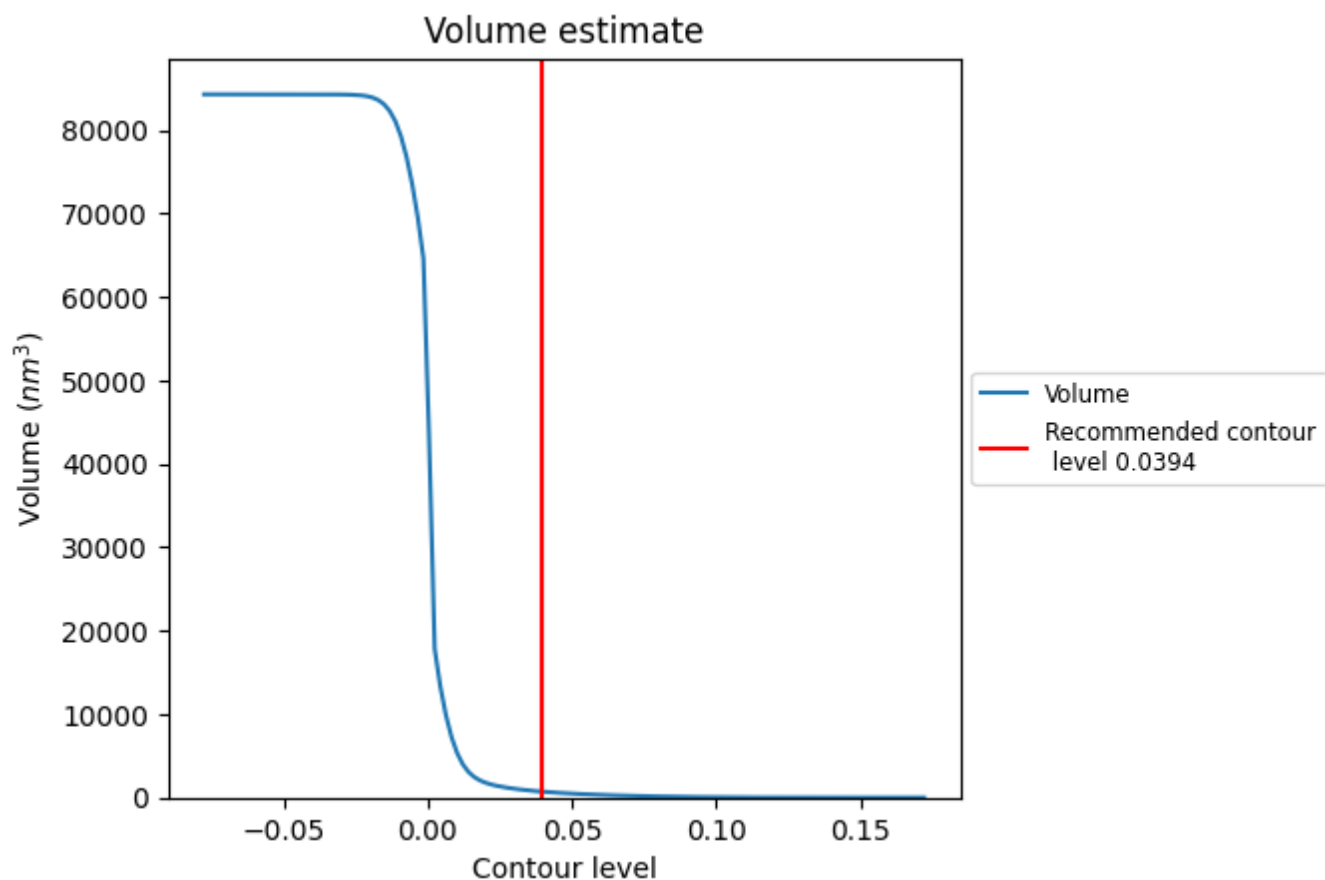
This section contains the results of statistical analysis of the map.

### 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.

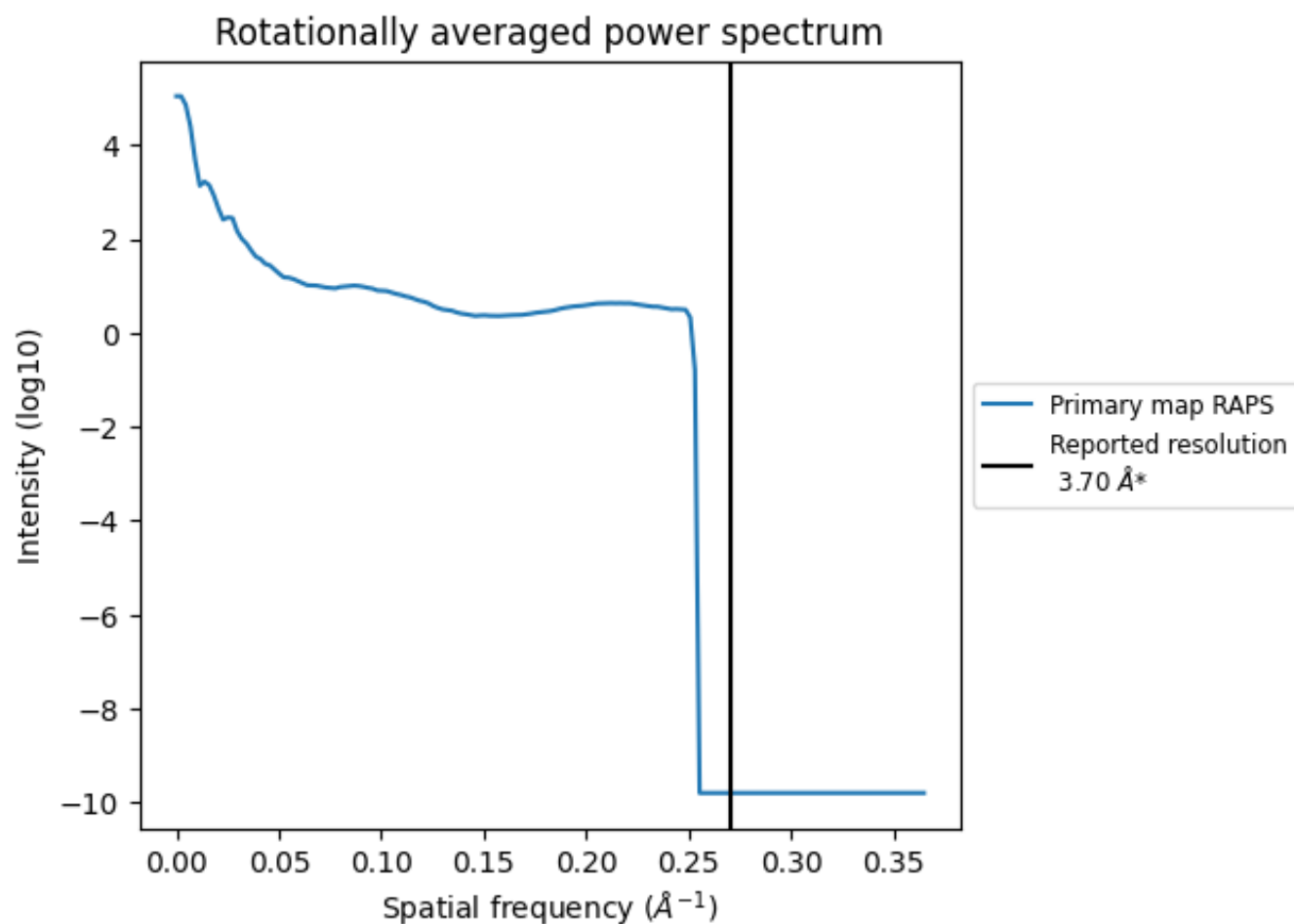
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 717 nm<sup>3</sup>; this corresponds to an approximate mass of 648 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 0.270  $\text{\AA}^{-1}$

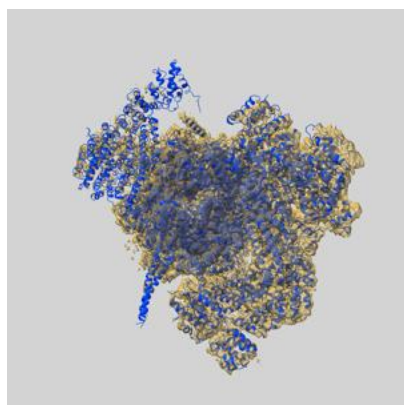
## 8 Fourier-Shell correlation

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

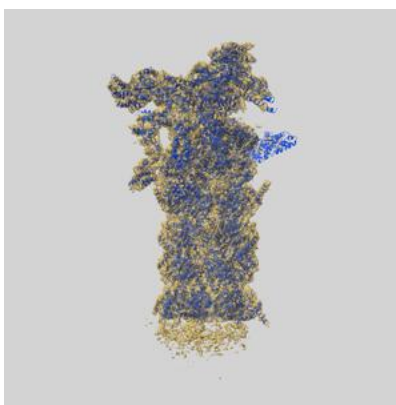
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14201 and PDB model 7QXN. Per-residue inclusion information can be found in section [3](#) on page [13](#).

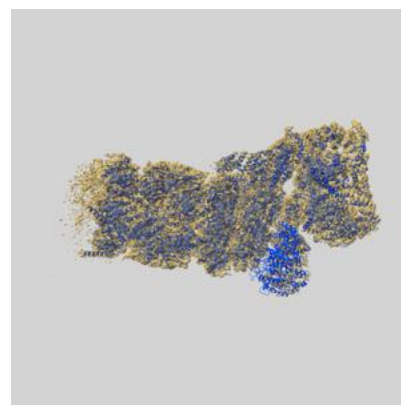
### 9.1 Map-model overlay [i](#)



X



Y

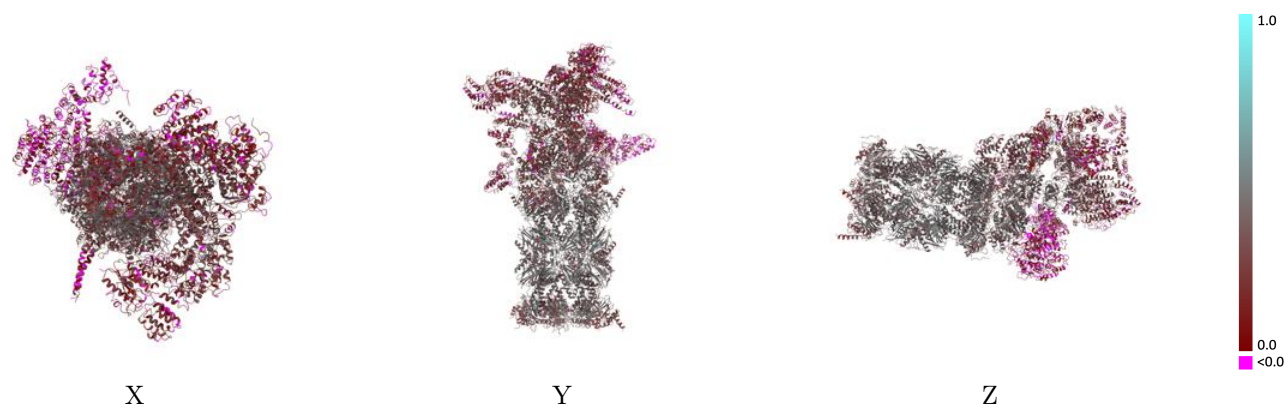


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0394 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.

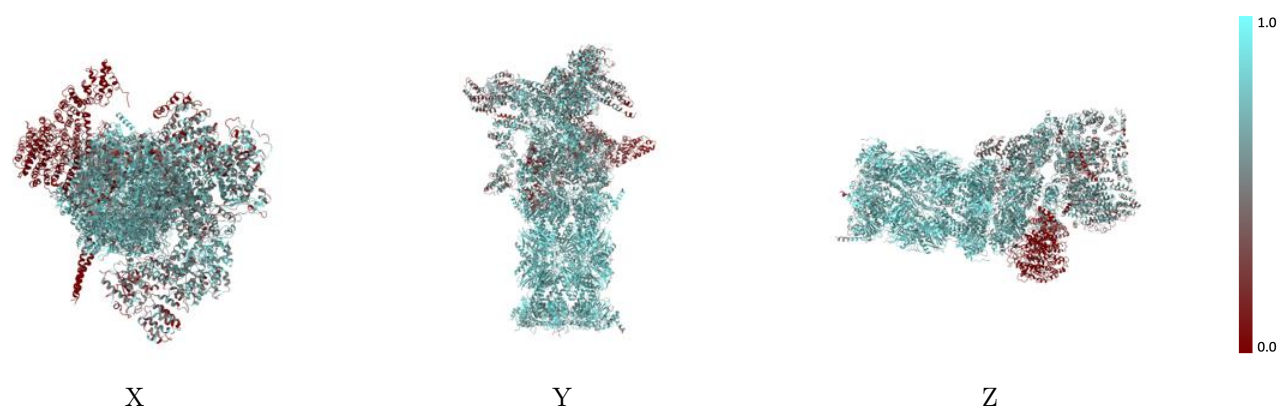


## 9.2 Q-score mapped to coordinate model [i](#)



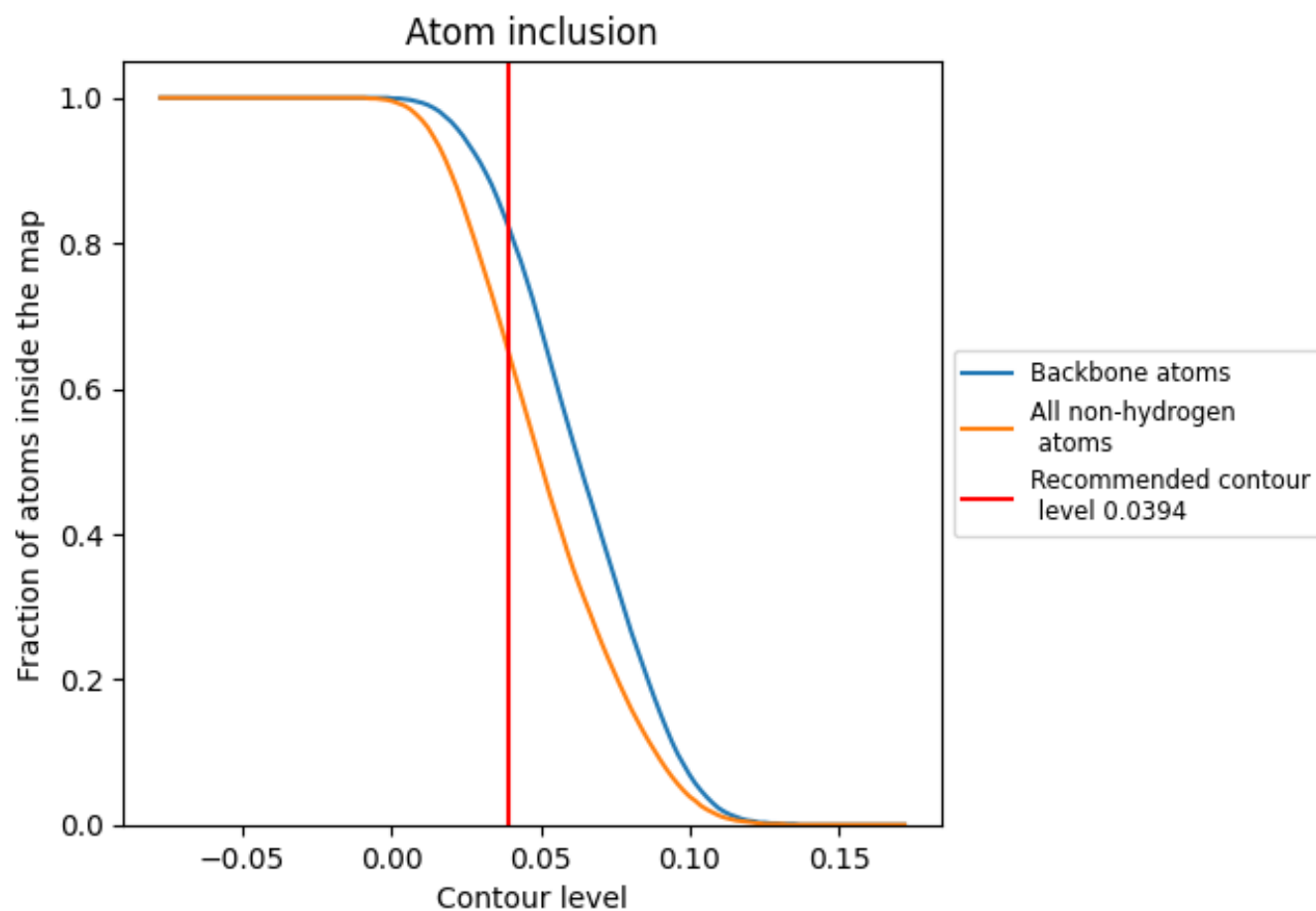
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0394).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% 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 (0.0394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.3190
A	 0.6810	 0.3510
B	 0.6280	 0.3260
C	 0.7050	 0.3540
D	 0.6960	 0.3530
E	 0.6960	 0.3440
F	 0.7030	 0.3630
G	 0.8000	 0.4100
H	 0.7980	 0.4130
I	 0.7730	 0.3880
J	 0.7850	 0.3870
K	 0.7830	 0.4010
L	 0.8060	 0.4150
M	 0.7880	 0.4030
N	 0.8280	 0.4300
O	 0.8250	 0.4290
P	 0.8200	 0.4350
Q	 0.8240	 0.4210
R	 0.8490	 0.4440
S	 0.8290	 0.4380
T	 0.8390	 0.4360
U	 0.5540	 0.2170
V	 0.4750	 0.1770
W	 0.5700	 0.2100
X	 0.4650	 0.2630
Y	 0.6530	 0.2480
Z	 0.6040	 0.2940
a	 0.5190	 0.2120
b	 0.3910	 0.1780
c	 0.6570	 0.3130
d	 0.4880	 0.1680
e	 0.4490	 0.1280
f	 0.0360	 0.0660
g	 0.7360	 0.3870
h	 0.7530	 0.3930



*Continued on next page...*

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Chain	Atom inclusion	Q-score
i	 0.7100	 0.3650
j	 0.7280	 0.3530
k	 0.7290	 0.3820
l	 0.7540	 0.3880
m	 0.7390	 0.3780
n	 0.8190	 0.4240
o	 0.8150	 0.4260
p	 0.8160	 0.4340
q	 0.8090	 0.4180
r	 0.8250	 0.4230
s	 0.8130	 0.4180
t	 0.8370	 0.4280