



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:18 pm GMT

PDB ID : 7QXX  
EMDB ID : EMD-14205  
Title : Proteasome-ZFAND5 Complex Z+E state  
Authors : Zhu, Y.; Lu, Y.  
Deposited on : 2022-01-27  
Resolution : 4.40 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:

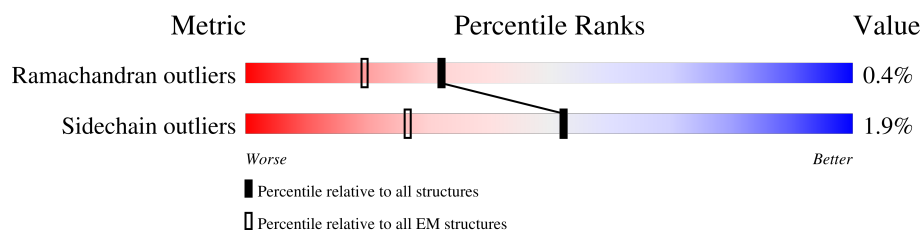
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 4.40 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.



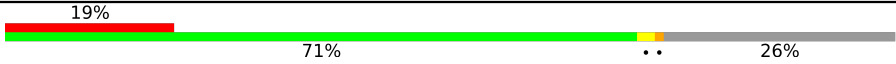

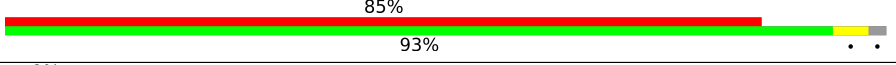

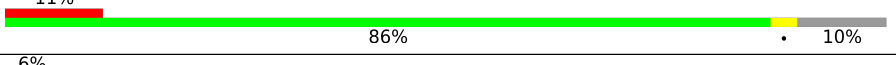
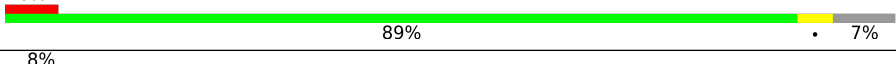
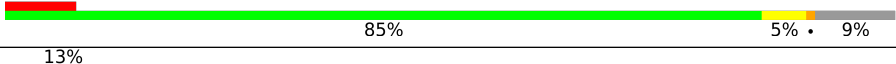
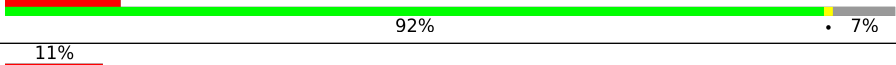
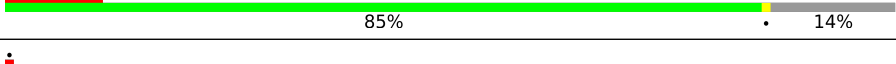
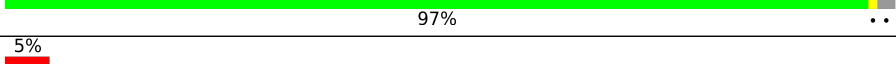
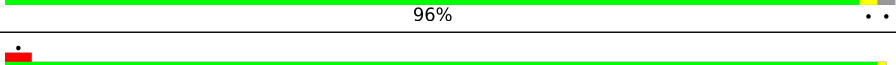
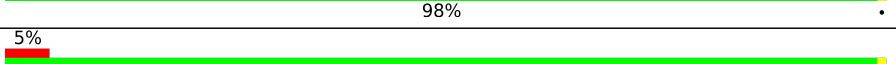
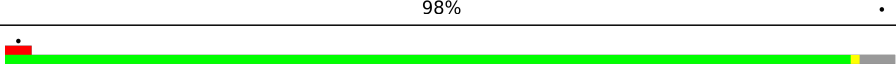
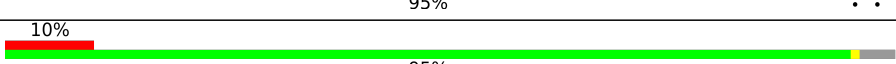
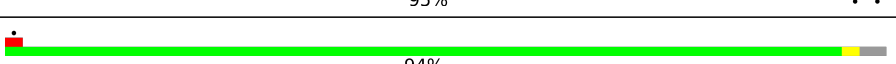
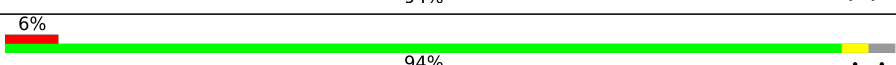
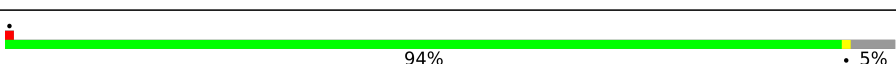
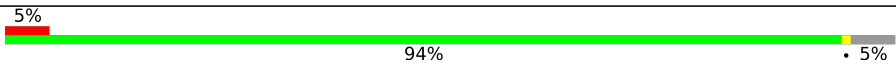
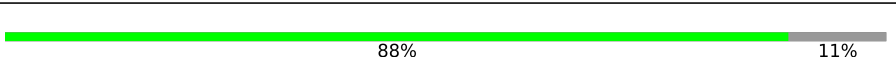

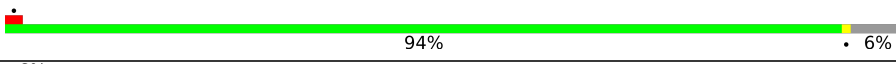
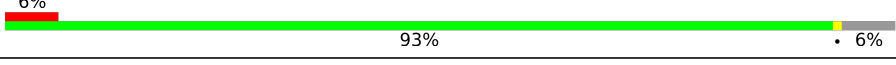
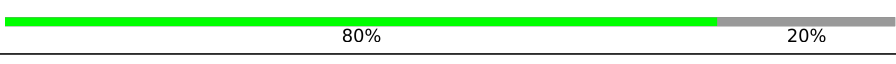


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>18%</div> <div>84%</div> <div>15%</div> </div>
2	V	533	<div> <div>32%</div> <div>92%</div> <div>5%</div> </div>
3	W	456	<div> <div>36%</div> <div>59%</div> <div>39%</div> </div>
4	X	422	<div> <div>6%</div> <div>23%</div> <div>77%</div> </div>
5	Y	389	<div> <div>11%</div> <div>96%</div> <div>•</div> </div>
6	Z	324	<div> <div>29%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
7	a	376	<div> <div>68%</div> <div>99%</div> <div>••</div> </div>
8	b	377	<div> <div>47%</div> <div>50%</div> <div>49%</div> </div>
9	c	309	<div> <div>15%</div> <div>89%</div> <div>7%</div> </div>












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Mol	Chain	Length	Quality of chain
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	429	
15	C	389	
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	 79% 20%
27	o	276	 79% 20%
28	P	204	 100%
28	p	204	 100%
29	Q	201	 98% ..
29	q	201	 98% ..
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 100121 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
			6328	4020	1075	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	279	Total	C	N	O	S	0	0
			2310	1473	394	430	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	99	Total	C	N	O	S	0	0
			797	511	132	152	2		

- 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
			6866	4315	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 proteasome 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 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		

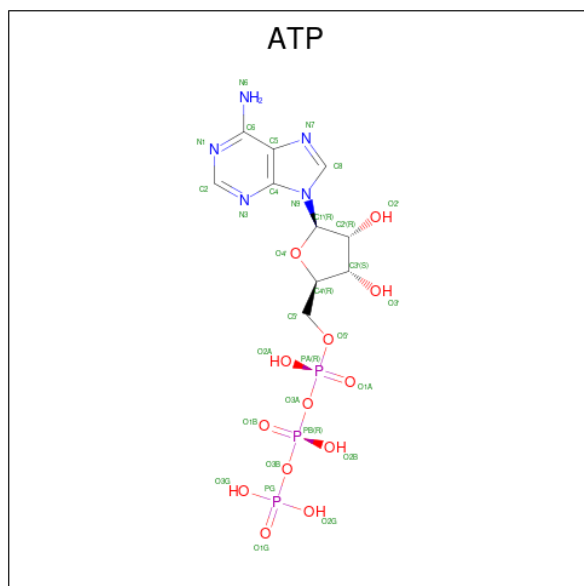
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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).



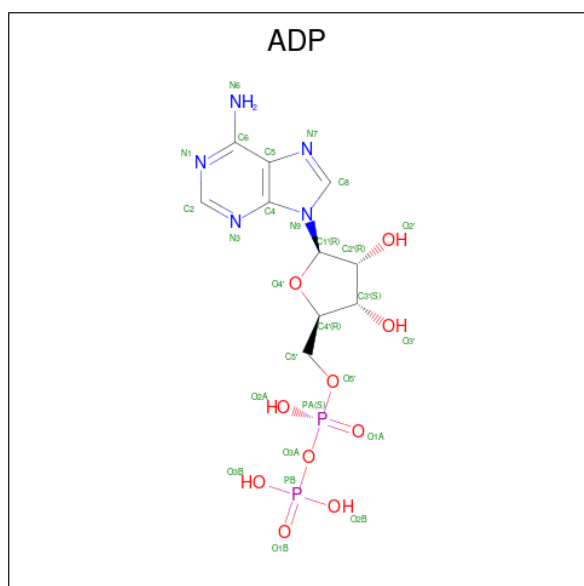
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Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	

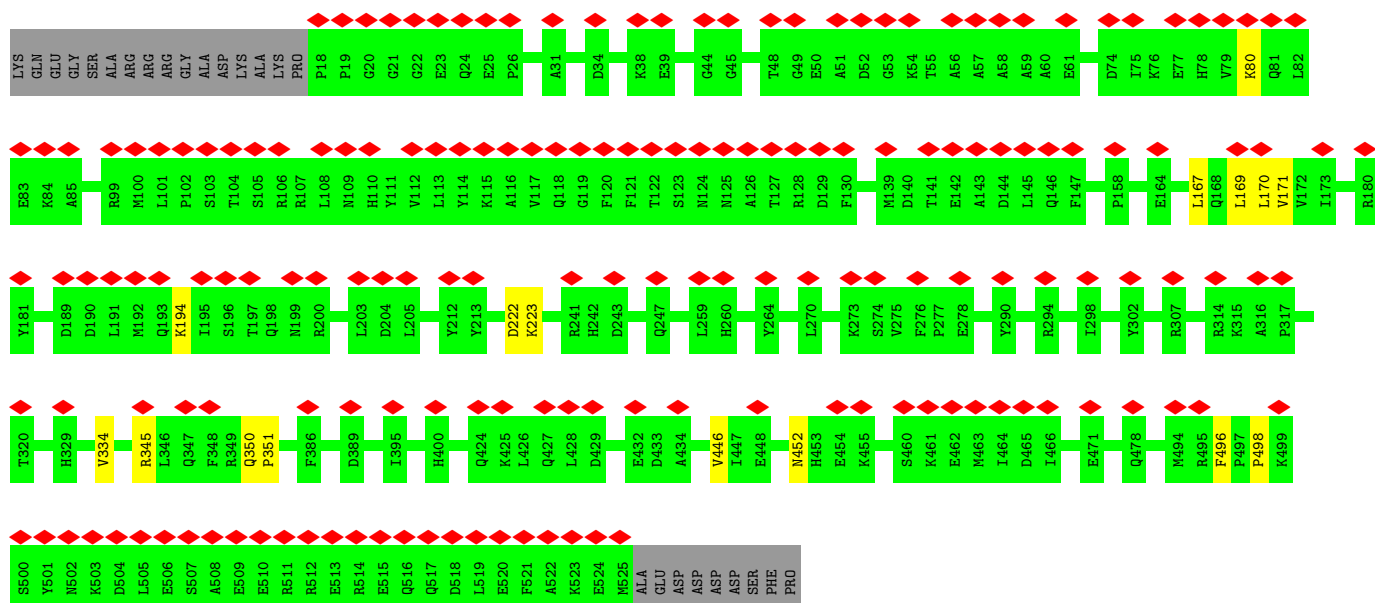
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



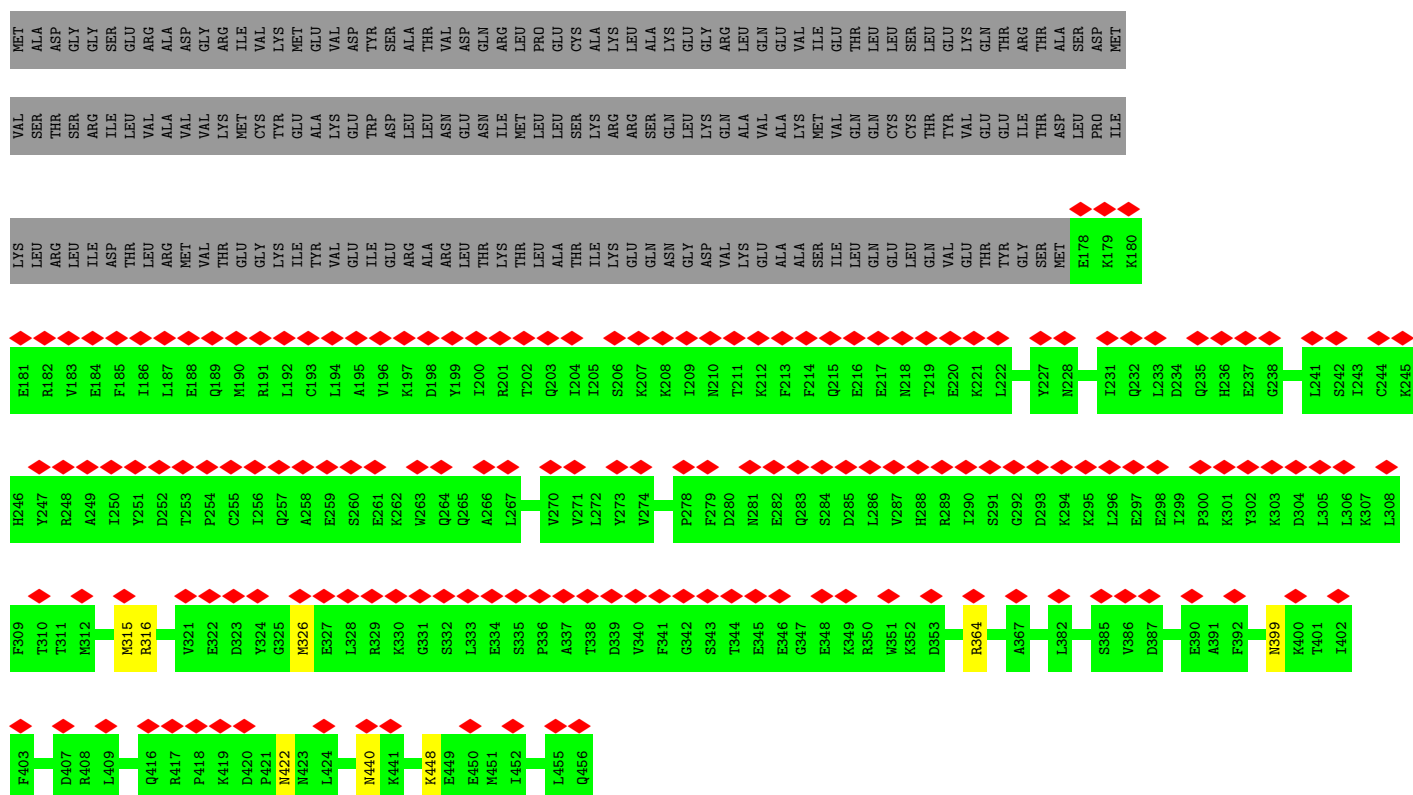
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	F	1	27	10	5	10	2	0



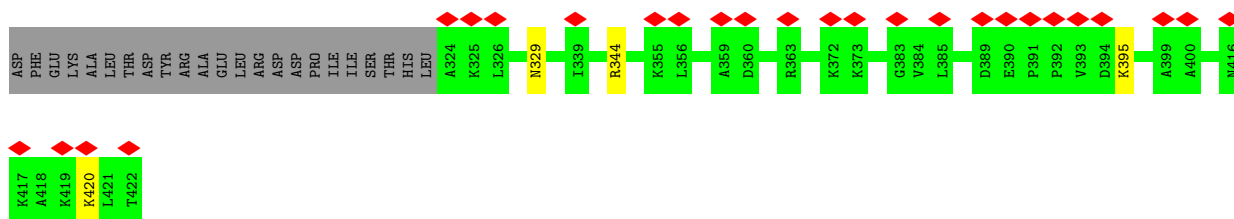


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

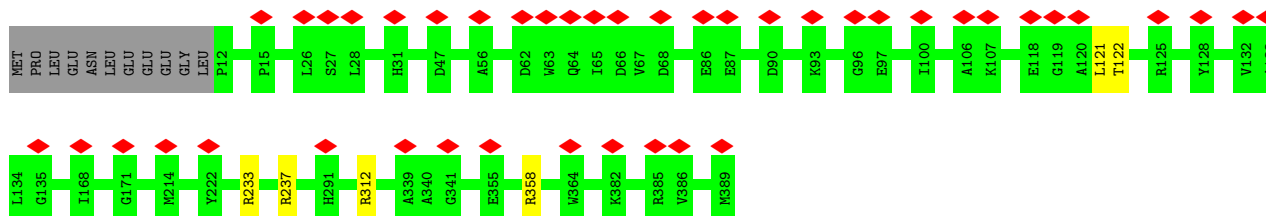


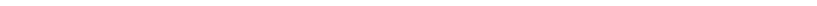
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

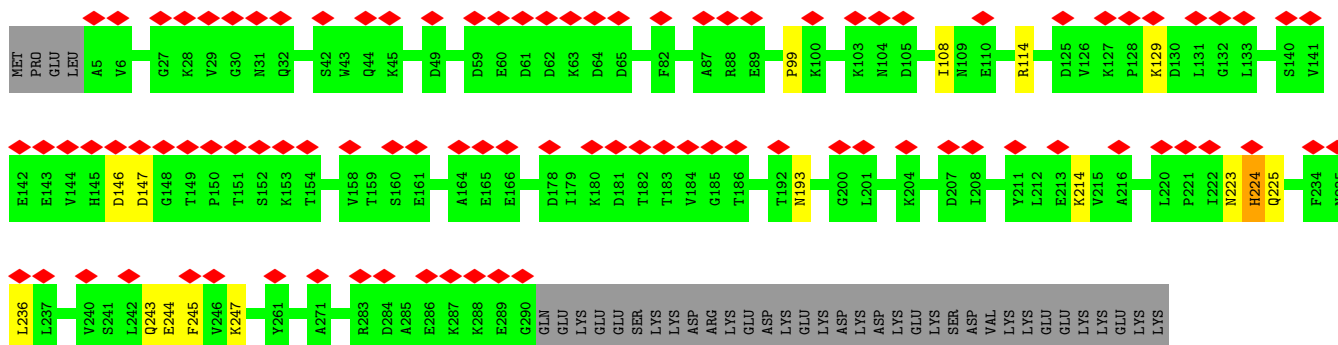




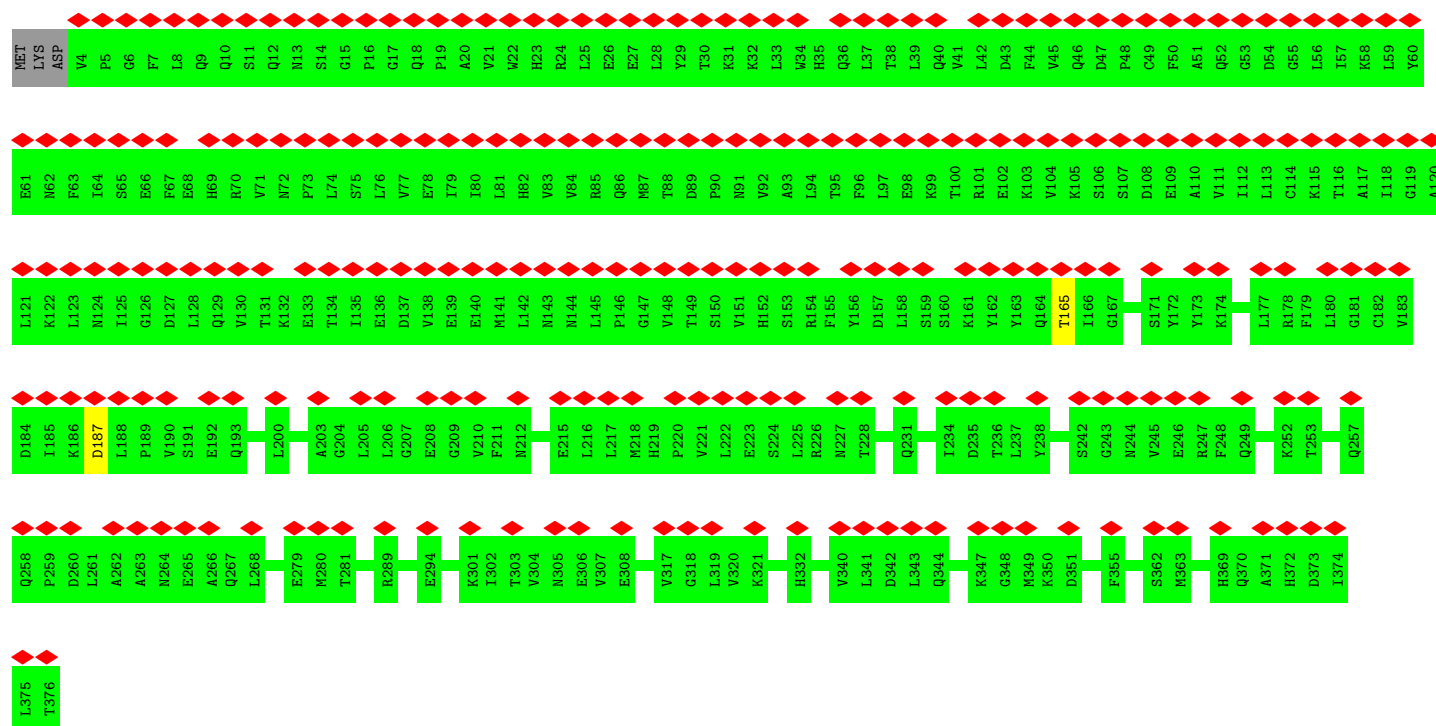
- Chain Y:  11% 96%



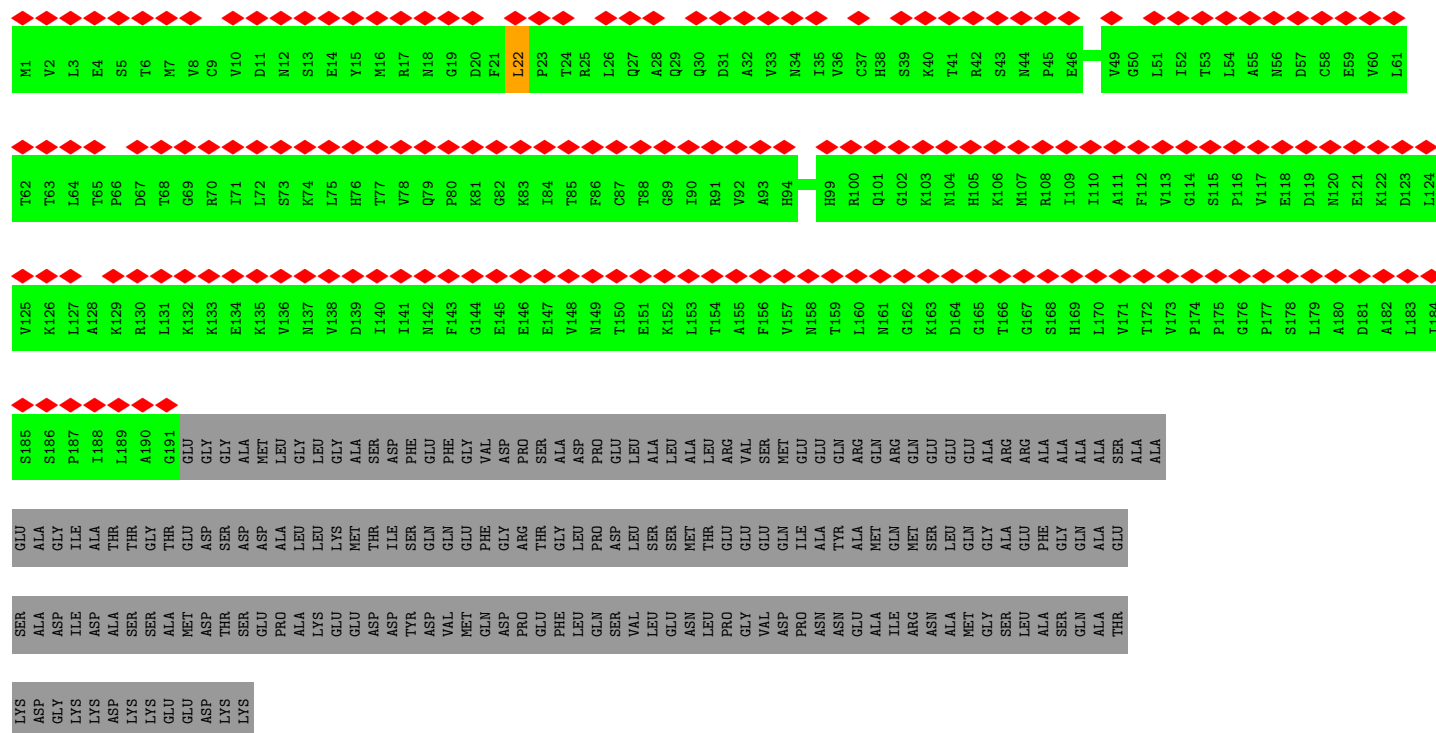
- Chain Z:  29% 83% 5% 12%



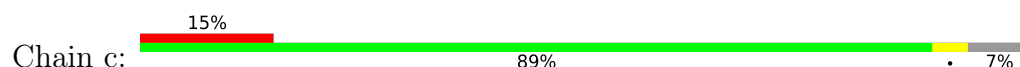
- Chain a:  68% 99%



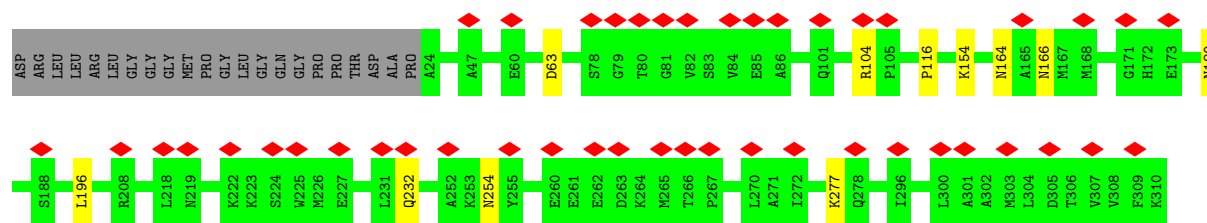
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



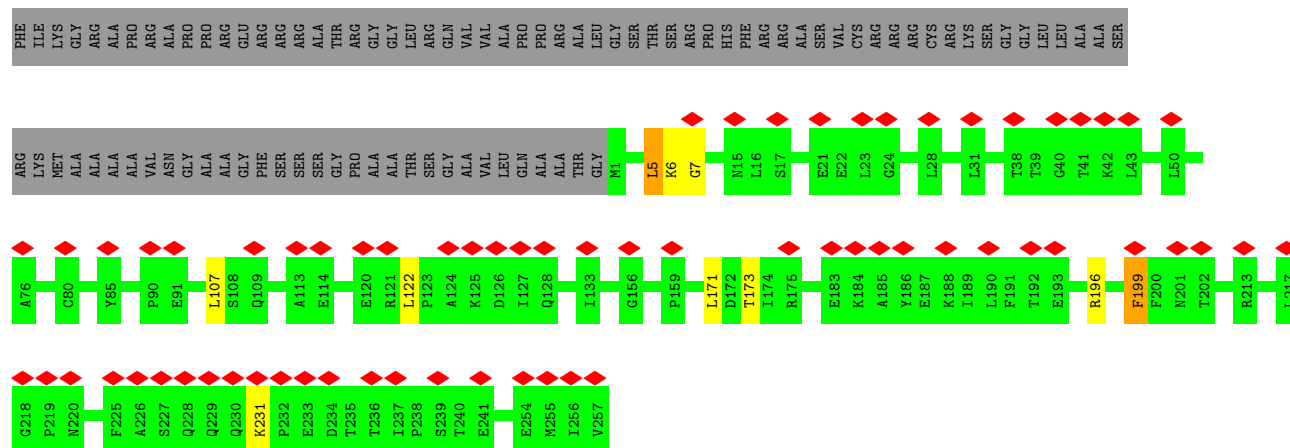
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



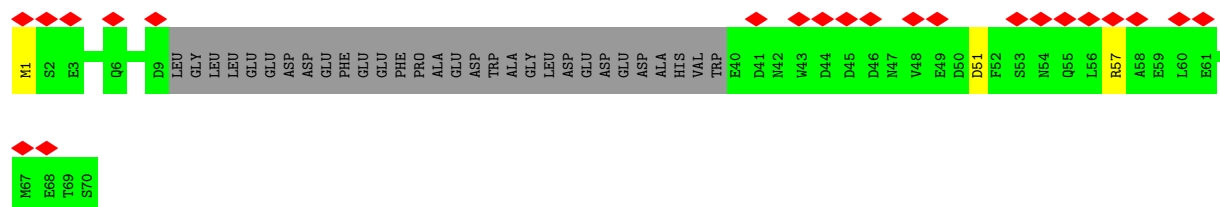




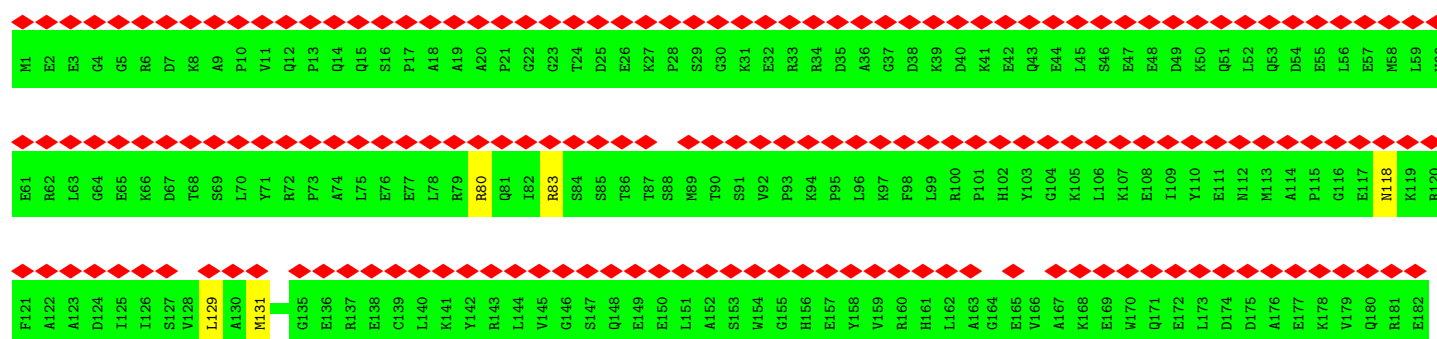
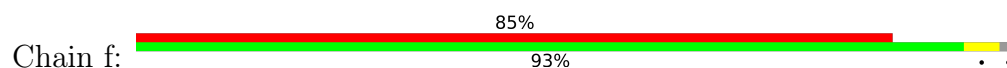
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



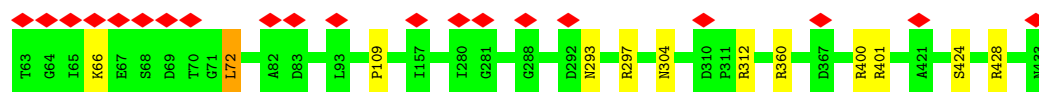
• Molecule 11: 26S proteasome complex subunit SEM1



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

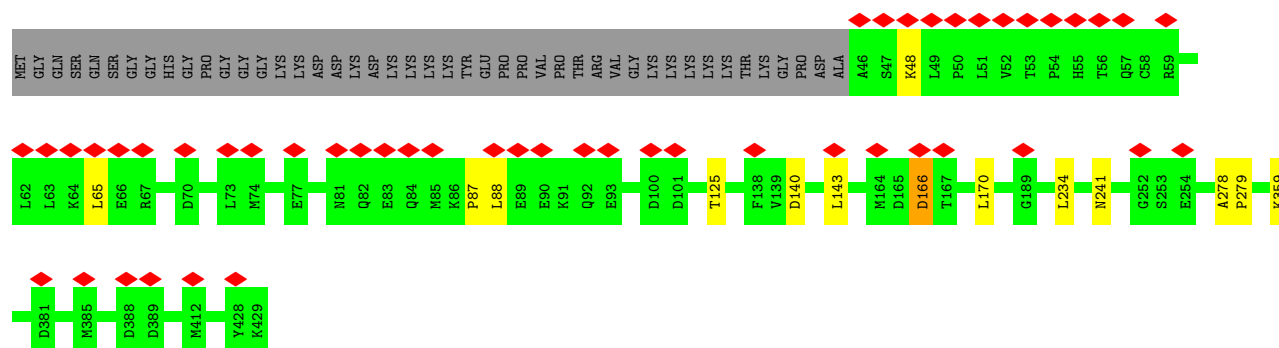






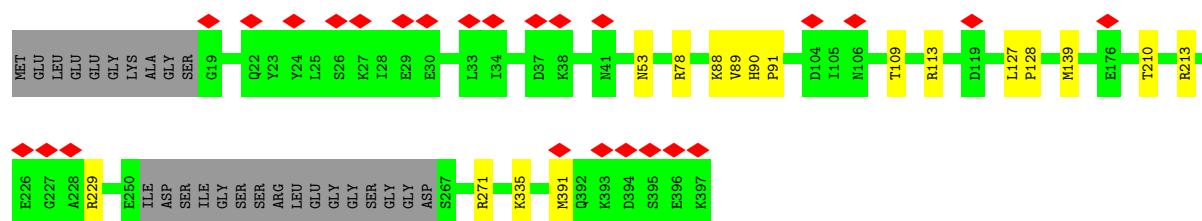
- Molecule 14: 26S proteasome regulatory subunit 4

Chain B: 11% 86% 10%



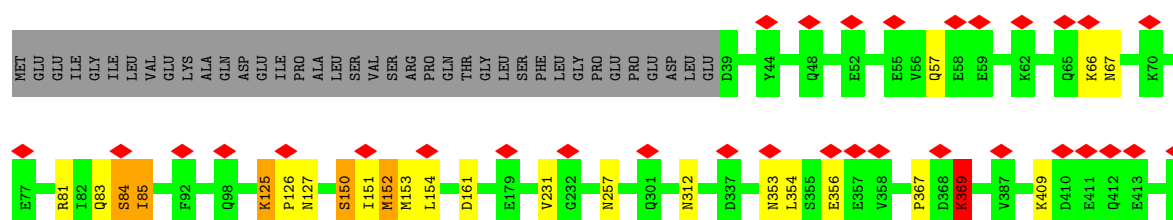
- Molecule 15: 26S proteasome regulatory subunit 8

Chain C: 6% 89% 7%



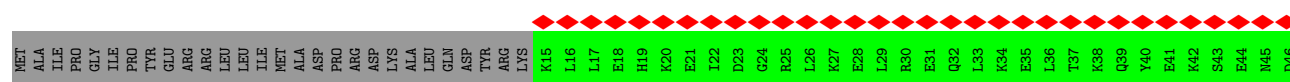
- Molecule 16: 26S protease regulatory subunit 6B

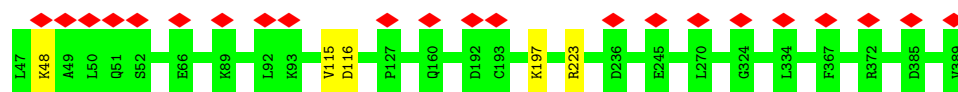
Chain D: 8% 85% 5% 9%



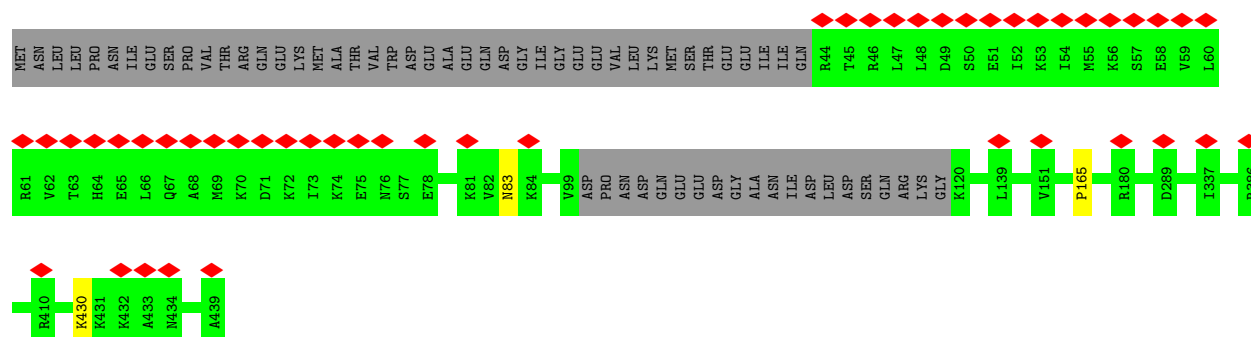
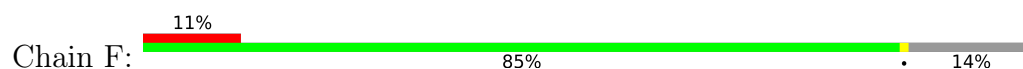
- Molecule 17: 26S proteasome regulatory subunit 10B

Chain E: 13% 92% 7%

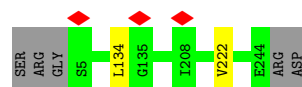




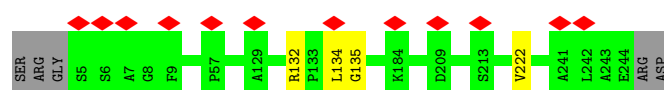
- Molecule 18: 26S protease regulatory subunit 6A



- Molecule 19: Proteasome subunit alpha type-6



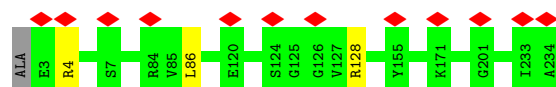
- Molecule 19: Proteasome subunit alpha type-6



- Molecule 20: Proteasome subunit alpha type-2

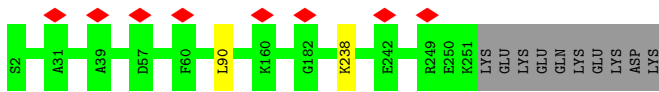


- Molecule 20: Proteasome subunit alpha type-2



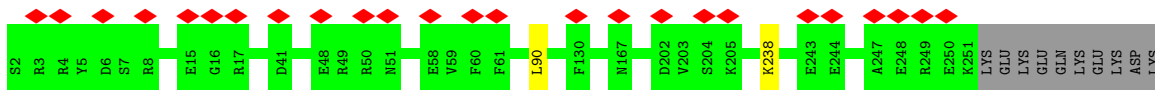
- Molecule 21: Proteasome subunit alpha type-4

Chain I: 



- Molecule 21: Proteasome subunit alpha type-4

Chain i: 



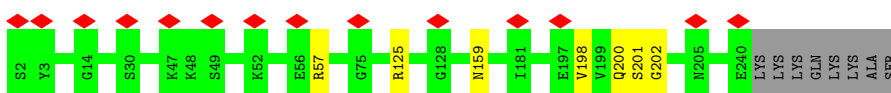
- Molecule 22: Proteasome subunit alpha type-7

Chain J: 



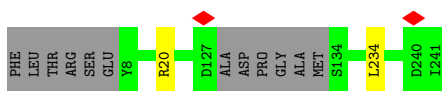
- Molecule 22: Proteasome subunit alpha type-7

Chain j:  6% 94%

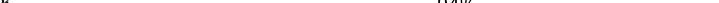


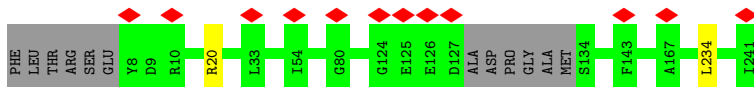
- Molecule 23: Proteasome subunit alpha type-5

Chain K:  94% • 5%

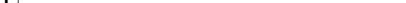


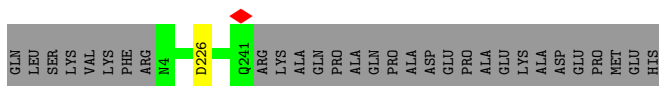
- Molecule 23: Proteasome subunit alpha type-5

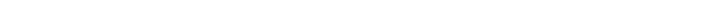
Chain k:  5% 94% 5%

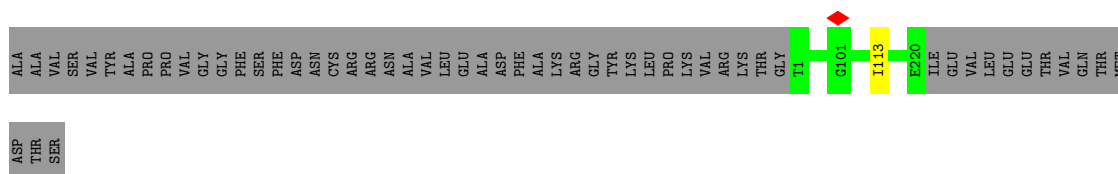


- Molecule 24: Isoform Long of Proteasome subunit alpha type-1

Chain L:  88% 11%



- Chain o:  79% 20%



- Molecule 28: Proteasome subunit beta type-3

Chain P: 100%

There are no outlier residues recorded for this chain.

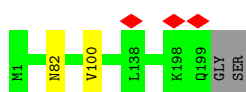
- Molecule 28: Proteasome subunit beta type-3

Chain p: 100%

There are no outlier residues recorded for this chain.

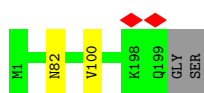
- Molecule 29: Proteasome subunit beta type-2

Chain Q: 98%



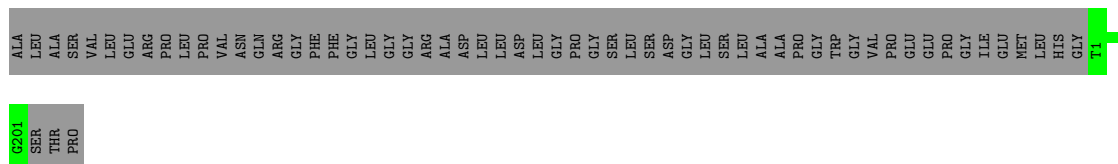
- Molecule 29: Proteasome subunit beta type-2

Chain q: 98%



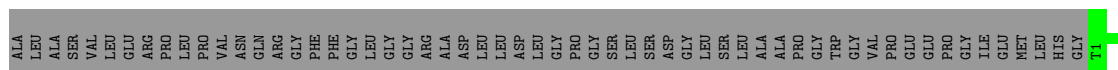
- Molecule 30: Proteasome subunit beta type-5

Chain R: 77% 23%



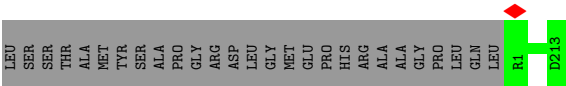
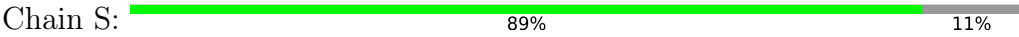
- Molecule 30: Proteasome subunit beta type-5

Chain r: 77% 23%

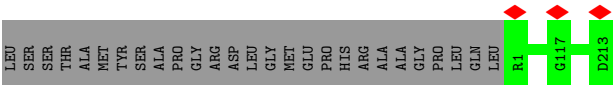
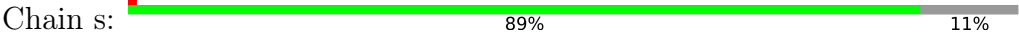




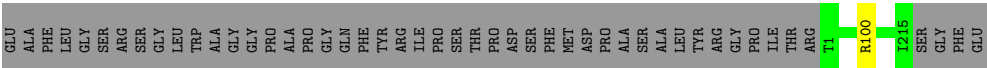
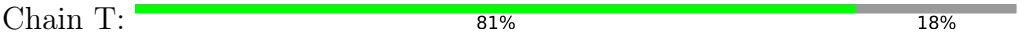
● Molecule 31: Proteasome subunit beta type-1



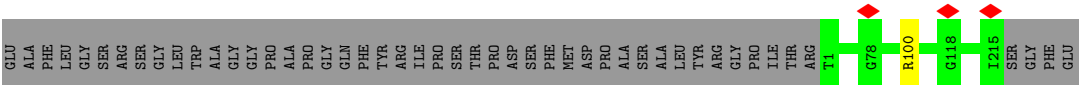
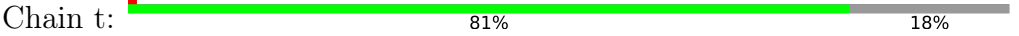
● Molecule 31: Proteasome subunit beta type-1



● Molecule 32: Proteasome subunit beta type-4



● Molecule 32: Proteasome subunit beta type-4





## 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	0.114	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0324	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: ADP, ATP, MG, 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	0.40	0/6443	0.61	0/8722
2	V	0.44	0/4072	0.69	0/5510
3	W	0.37	0/2349	0.63	0/3157
4	X	0.42	0/807	0.68	0/1084
5	Y	0.46	0/3173	0.68	0/4273
6	Z	0.39	0/2324	0.69	0/3150
7	a	0.35	0/3053	0.62	0/4133
8	b	0.32	0/1478	0.62	0/2001
9	c	0.43	0/2302	0.69	0/3110
10	d	0.41	0/2162	0.71	1/2919 (0.0%)
11	e	0.42	0/338	0.78	0/450
12	f	0.35	0/6980	0.72	5/9433 (0.1%)
13	A	0.47	0/3148	0.67	0/4250
14	B	0.46	0/3061	0.69	3/4129 (0.1%)
15	C	0.46	0/2902	0.65	0/3904
16	D	0.47	0/3089	0.71	5/4168 (0.1%)
17	E	0.45	0/2904	0.66	0/3924
18	F	0.48	0/2896	0.65	0/3912
19	G	0.47	0/1859	0.59	0/2523
19	g	0.47	0/1859	0.59	0/2523
20	H	0.51	0/1743	0.59	0/2372
20	h	0.51	0/1743	0.59	0/2372
21	I	0.48	0/1942	0.63	0/2628
21	i	0.48	0/1942	0.63	0/2628
22	J	0.44	0/1737	0.60	0/2369
22	j	0.44	0/1728	0.60	0/2358
23	K	0.46	0/1747	0.62	1/2364 (0.0%)
23	k	0.46	0/1747	0.62	1/2364 (0.0%)
24	L	0.50	0/1885	0.63	0/2552
24	l	0.50	0/1885	0.66	1/2552 (0.0%)
25	M	0.49	0/1891	0.62	0/2552
25	m	0.49	0/1891	0.62	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
26	N	0.48	0/1454	0.60	0/1967
26	n	0.48	0/1454	0.60	0/1967
27	O	0.49	1/1670 (0.1%)	0.62	0/2265
27	o	0.49	1/1670 (0.1%)	0.62	0/2265
28	P	0.48	0/1620	0.60	0/2184
28	p	0.48	0/1620	0.60	0/2184
29	Q	0.53	0/1603	0.62	0/2174
29	q	0.54	0/1603	0.62	0/2174
30	R	0.55	0/1579	0.61	0/2134
30	r	0.55	0/1579	0.61	0/2134
31	S	0.50	0/1671	0.60	0/2253
31	s	0.50	0/1674	0.60	0/2257
32	T	0.52	0/1700	0.62	0/2305
32	t	0.52	0/1700	0.62	0/2305
All	All	0.46	2/101677 (0.0%)	0.64	17/137506 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	o	113	ILE	C-N	-5.07	1.22	1.34
27	O	113	ILE	C-N	-5.02	1.22	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	l	226	ASP	CB-CG-OD1	8.19	125.67	118.30
16	D	126	PRO	C-N-CA	7.68	140.89	121.70
16	D	125	LYS	N-CA-C	7.54	131.37	111.00
12	f	680	ARG	N-CA-C	-7.43	90.93	111.00
14	B	140	ASP	CB-CG-OD1	6.63	124.27	118.30
14	B	279	PRO	N-CA-C	-6.29	95.75	112.10
12	f	759	LEU	CA-CB-CG	6.12	129.37	115.30
12	f	755	ASP	C-N-CD	-6.09	107.19	120.60
16	D	126	PRO	N-CA-C	-5.82	96.98	112.10
10	d	107	LEU	CA-CB-CG	5.76	128.54	115.30
16	D	150	SER	N-CA-C	-5.56	96.00	111.00
14	B	234	LEU	CA-CB-CG	5.29	127.46	115.30
12	f	471	LEU	CA-CB-CG	5.28	127.44	115.30
23	k	234	LEU	CA-CB-CG	5.16	127.17	115.30
23	K	234	LEU	CA-CB-CG	5.15	127.14	115.30
16	D	369	LYS	N-CA-C	5.06	124.66	111.00
12	f	672	LEU	CA-CB-CG	5.03	126.86	115.30

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%)	725 (90%)	77 (10%)	4 (0%)	25	63
2	V	506/533 (95%)	435 (86%)	67 (13%)	4 (1%)	16	53
3	W	277/456 (61%)	247 (89%)	30 (11%)	0	100	100
4	X	97/422 (23%)	93 (96%)	4 (4%)	0	100	100
5	Y	376/389 (97%)	345 (92%)	31 (8%)	0	100	100
6	Z	284/324 (88%)	239 (84%)	42 (15%)	3 (1%)	12	46
7	a	371/376 (99%)	325 (88%)	45 (12%)	1 (0%)	37	72
8	b	189/377 (50%)	167 (88%)	21 (11%)	1 (0%)	25	63
9	c	285/309 (92%)	241 (85%)	41 (14%)	3 (1%)	12	46
10	d	255/349 (73%)	206 (81%)	45 (18%)	4 (2%)	8	37
11	e	36/70 (51%)	25 (69%)	10 (28%)	1 (3%)	4	25
12	f	887/908 (98%)	713 (80%)	164 (18%)	10 (1%)	12	46
13	A	392/433 (90%)	333 (85%)	56 (14%)	3 (1%)	16	53
14	B	382/429 (89%)	338 (88%)	40 (10%)	4 (1%)	13	48
15	C	359/389 (92%)	328 (91%)	29 (8%)	2 (1%)	22	59
16	D	378/418 (90%)	322 (85%)	47 (12%)	9 (2%)	5	28
17	E	373/403 (93%)	330 (88%)	43 (12%)	0	100	100
18	F	372/439 (85%)	332 (89%)	39 (10%)	1 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	G	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
19	g	238/245 (97%)	228 (96%)	8 (3%)	2 (1%)	16	53
20	H	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
20	h	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
21	I	248/260 (95%)	219 (88%)	29 (12%)	0	100	100
21	i	248/260 (95%)	219 (88%)	29 (12%)	0	100	100
22	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	53
22	j	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	16	53
23	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
23	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
24	L	236/268 (88%)	212 (90%)	23 (10%)	1 (0%)	30	67
24	l	236/268 (88%)	212 (90%)	24 (10%)	0	100	100
25	M	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
25	m	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
26	N	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
26	n	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
27	O	218/276 (79%)	206 (94%)	12 (6%)	0	100	100
27	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	P	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
28	p	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
29	Q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
29	q	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
30	R	199/262 (76%)	184 (92%)	15 (8%)	0	100	100
30	r	199/262 (76%)	183 (92%)	16 (8%)	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%)	199 (93%)	14 (7%)	0	100	100
32	t	213/263 (81%)	199 (93%)	14 (7%)	0	100	100
All	All	12785/14839 (86%)	11476 (90%)	1252 (10%)	57 (0%)	32	67

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	351	PRO
2	V	446	VAL
6	Z	146	ASP
7	a	187	ASP
8	b	22	LEU
12	f	756	PRO
12	f	839	PRO
15	C	91	PRO
15	C	128	PRO
16	D	85	ILE
16	D	369	LYS
24	L	226	ASP
19	g	135	GLY
22	j	202	GLY
6	Z	224	HIS
2	V	350	GLN
2	V	498	PRO
9	c	196	LEU
10	d	7	GLY
12	f	118	ASN
12	f	680	ARG
13	A	424	SER
14	B	87	PRO
16	D	127	ASN
16	D	152	MET
16	D	154	LEU
16	D	161	ASP
1	U	57	ARG
10	d	5	LEU
10	d	173	THR
10	d	199	PHE
12	f	474	SER
12	f	476	THR
12	f	738	ASN
12	f	773	LYS
12	f	837	LEU
14	B	88	LEU
16	D	84	SER
16	D	367	PRO
19	g	134	LEU
1	U	128	GLN
1	U	174	PRO
1	U	178	ALA

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Mol	Chain	Res	Type
9	c	63	ASP
11	e	57	ARG
12	f	840	LEU
13	A	109	PRO
14	B	166	ASP
14	B	278	ALA
22	J	198	VAL
13	A	72	LEU
22	J	200	GLN
22	j	198	VAL
6	Z	99	PRO
9	c	116	PRO
16	D	151	ILE
18	F	165	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	691/816 (85%)	688 (100%)	3 (0%)	89	91
2	V	415/459 (90%)	403 (97%)	12 (3%)	37	58
3	W	260/416 (62%)	252 (97%)	8 (3%)	35	56
4	X	91/362 (25%)	87 (96%)	4 (4%)	24	46
5	Y	334/344 (97%)	328 (98%)	6 (2%)	54	71
6	Z	257/295 (87%)	243 (95%)	14 (5%)	18	40
7	a	333/336 (99%)	332 (100%)	1 (0%)	91	92
8	b	167/312 (54%)	166 (99%)	1 (1%)	84	88
9	c	252/267 (94%)	244 (97%)	8 (3%)	34	55
10	d	231/293 (79%)	224 (97%)	7 (3%)	36	57
11	e	38/63 (60%)	36 (95%)	2 (5%)	19	41
12	f	745/763 (98%)	713 (96%)	32 (4%)	25	47
13	A	337/372 (91%)	326 (97%)	11 (3%)	33	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	B	339/376 (90%)	331 (98%)	8 (2%)	44	63
15	C	314/337 (93%)	299 (95%)	15 (5%)	21	43
16	D	333/366 (91%)	314 (94%)	19 (6%)	17	39
17	E	298/353 (84%)	293 (98%)	5 (2%)	56	72
18	F	296/379 (78%)	294 (99%)	2 (1%)	81	87
19	G	193/209 (92%)	191 (99%)	2 (1%)	73	81
19	g	193/209 (92%)	191 (99%)	2 (1%)	73	81
20	H	164/190 (86%)	161 (98%)	3 (2%)	54	71
20	h	164/190 (86%)	161 (98%)	3 (2%)	54	71
21	I	193/220 (88%)	191 (99%)	2 (1%)	73	81
21	i	193/220 (88%)	191 (99%)	2 (1%)	73	81
22	J	154/210 (73%)	148 (96%)	6 (4%)	27	49
22	j	152/210 (72%)	147 (97%)	5 (3%)	33	54
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%)	190 (99%)	2 (1%)	73	81
25	m	192/211 (91%)	189 (98%)	3 (2%)	58	74
26	N	148/180 (82%)	147 (99%)	1 (1%)	81	87
26	n	148/180 (82%)	147 (99%)	1 (1%)	81	87
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	173/173 (100%)	173 (100%)	0	100	100
28	p	173/173 (100%)	173 (100%)	0	100	100
29	Q	164/171 (96%)	162 (99%)	2 (1%)	67	79
29	q	164/171 (96%)	162 (99%)	2 (1%)	67	79
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	T	175/214 (82%)	174 (99%)	1 (1%)	84	88
32	t	175/214 (82%)	174 (99%)	1 (1%)	84	88
All	All	10618/12579 (84%)	10420 (98%)	198 (2%)	52	70

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	176	MET
1	U	345	ASN
1	U	603	LEU
2	V	80	LYS
2	V	167	LEU
2	V	169	LEU
2	V	170	LEU
2	V	171	VAL
2	V	194	LYS
2	V	222	ASP
2	V	223	LYS
2	V	334	VAL
2	V	345	ARG
2	V	452	ASN
2	V	496	PHE
3	W	315	MET
3	W	316	ARG
3	W	326	MET
3	W	364	ARG
3	W	399	ASN
3	W	422	ASN
3	W	440	ASN
3	W	448	LYS
4	X	329	ASN
4	X	344	ARG
4	X	395	LYS
4	X	420	LYS
5	Y	121	LEU
5	Y	122	THR
5	Y	233	ARG
5	Y	237	ARG
5	Y	312	ARG
5	Y	358	ARG
6	Z	108	ILE

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Mol	Chain	Res	Type
6	Z	114	ARG
6	Z	129	LYS
6	Z	147	ASP
6	Z	193	ASN
6	Z	214	LYS
6	Z	223	ASN
6	Z	224	HIS
6	Z	225	GLN
6	Z	236	LEU
6	Z	243	GLN
6	Z	244	GLU
6	Z	245	PHE
6	Z	247	LYS
7	a	165	THR
8	b	22	LEU
9	c	104	ARG
9	c	154	LYS
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN
9	c	232	GLN
9	c	254	ASN
9	c	277	LYS
10	d	5	LEU
10	d	6	LYS
10	d	122	LEU
10	d	171	LEU
10	d	196	ARG
10	d	199	PHE
10	d	231	LYS
11	e	1	MET
11	e	51	ASP
12	f	80	ARG
12	f	83	ARG
12	f	129	LEU
12	f	131	MET
12	f	218	GLU
12	f	257	ARG
12	f	258	LYS
12	f	267	ARG
12	f	281	ILE
12	f	297	MET

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Mol	Chain	Res	Type
12	f	327	ASN
12	f	341	GLU
12	f	344	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	608	LYS
12	f	679	LEU
12	f	703	ARG
12	f	712	LYS
12	f	713	PHE
12	f	746	ARG
12	f	755	ASP
12	f	773	LYS
12	f	786	GLN
12	f	787	LEU
12	f	807	ARG
12	f	822	VAL
12	f	837	LEU
12	f	838	ARG
13	A	43	ARG
13	A	66	LYS
13	A	72	LEU
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	428	ARG
14	B	48	LYS
14	B	65	LEU
14	B	125	THR
14	B	143	LEU
14	B	166	ASP
14	B	170	LEU
14	B	241	ASN
14	B	359	LYS
15	C	53	ASN

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Mol	Chain	Res	Type
15	C	78	ARG
15	C	88	LYS
15	C	89	VAL
15	C	90	HIS
15	C	109	THR
15	C	113	ARG
15	C	127	LEU
15	C	139	MET
15	C	210	THR
15	C	213	ARG
15	C	229	ARG
15	C	271	ARG
15	C	335	LYS
15	C	391	MET
16	D	57	GLN
16	D	66	LYS
16	D	67	ASN
16	D	81	ARG
16	D	83	GLN
16	D	84	SER
16	D	85	ILE
16	D	125	LYS
16	D	150	SER
16	D	152	MET
16	D	153	MET
16	D	231	VAL
16	D	257	ASN
16	D	312	ASN
16	D	353	ASN
16	D	354	LEU
16	D	356	GLU
16	D	369	LYS
16	D	409	LYS
17	E	48	LYS
17	E	115	VAL
17	E	116	ASP
17	E	197	LYS
17	E	223	ARG
18	F	83	ASN
18	F	430	LYS
19	G	134	LEU
19	G	222	VAL

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Mol	Chain	Res	Type
20	H	4	ARG
20	H	86	LEU
20	H	128	ARG
21	I	90	LEU
21	I	238	LYS
22	J	52	LYS
22	J	53	LEU
22	J	57	ARG
22	J	125	ARG
22	J	159	ASN
22	J	200	GLN
23	K	20	ARG
25	M	40	ARG
25	M	221	ASN
26	N	28	ASN
29	Q	82	ASN
29	Q	100	VAL
32	T	100	ARG
19	g	132	ARG
19	g	222	VAL
20	h	4	ARG
20	h	86	LEU
20	h	128	ARG
21	i	90	LEU
21	i	238	LYS
22	j	57	ARG
22	j	125	ARG
22	j	159	ASN
22	j	200	GLN
22	j	201	SER
23	k	20	ARG
25	m	40	ARG
25	m	215	TRP
25	m	221	ASN
26	n	28	ASN
29	q	82	ASN
29	q	100	VAL
32	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	247	GLN
1	U	345	ASN
1	U	377	HIS
1	U	415	HIS
1	U	595	ASN
1	U	756	HIS
1	U	768	GLN
1	U	777	HIS
1	U	876	GLN
2	V	62	HIS
2	V	118	GLN
2	V	247	GLN
2	V	387	GLN
2	V	401	ASN
2	V	427	GLN
2	V	452	ASN
2	V	488	ASN
3	W	399	ASN
3	W	422	ASN
4	X	329	ASN
4	X	416	ASN
5	Y	363	ASN
5	Y	365	GLN
5	Y	367	GLN
6	Z	72	HIS
6	Z	109	ASN
6	Z	223	ASN
6	Z	225	GLN
6	Z	254	ASN
6	Z	256	GLN
7	a	35	HIS
7	a	193	GLN
7	a	212	ASN
7	a	231	GLN
7	a	258	GLN
7	a	267	GLN
7	a	345	GLN
7	a	370	GLN
8	b	142	ASN
9	c	44	HIS
9	c	113	HIS
9	c	128	ASN
9	c	130	GLN

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Mol	Chain	Res	Type
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	15	ASN
10	d	116	HIS
12	f	213	GLN
12	f	291	GLN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	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	738	ASN
12	f	766	GLN
12	f	782	HIS
12	f	808	ASN
12	f	848	GLN
13	A	85	GLN
13	A	293	ASN
13	A	304	ASN
14	B	81	ASN
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN
15	C	90	HIS
15	C	171	HIS
15	C	221	GLN
15	C	278	ASN
16	D	67	ASN

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Mol	Chain	Res	Type
16	D	110	ASN
16	D	133	HIS
16	D	173	GLN
16	D	187	HIS
16	D	257	ASN
16	D	353	ASN
17	E	280	ASN
18	F	83	ASN
19	G	24	GLN
19	G	33	ASN
21	I	53	HIS
21	I	146	GLN
22	J	54	GLN
22	J	85	ASN
22	J	154	HIS
22	J	159	ASN
23	K	99	HIS
23	K	214	ASN
25	M	101	ASN
25	M	221	ASN
26	N	28	ASN
27	O	62	ASN
27	O	91	GLN
27	O	193	ASN
29	Q	8	GLN
29	Q	32	HIS
29	Q	55	GLN
29	Q	63	ASN
29	Q	82	ASN
29	Q	87	ASN
30	R	29	GLN
30	R	38	ASN
30	R	85	ASN
30	R	162	GLN
32	T	2	GLN
32	T	61	GLN
32	T	69	GLN
19	g	33	ASN
21	i	146	GLN
22	j	85	ASN
22	j	159	ASN
22	j	205	ASN

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Mol	Chain	Res	Type
23	k	99	HIS
23	k	118	ASN
23	k	214	ASN
25	m	101	ASN
25	m	221	ASN
26	n	28	ASN
27	o	62	ASN
27	o	66	HIS
27	o	91	GLN
27	o	193	ASN
29	q	8	GLN
29	q	32	HIS
29	q	63	ASN
29	q	87	ASN
30	r	29	GLN
30	r	38	ASN
30	r	85	ASN
30	r	162	GLN
32	t	2	GLN
32	t	61	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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
34	ATP	E	401	35	26,33,33	0.95	1 (3%)	31,52,52	1.81	6 (19%)
36	ADP	F	501	35	24,29,29	0.94	1 (4%)	29,45,45	1.64	5 (17%)
34	ATP	B	501	35	26,33,33	0.95	1 (3%)	31,52,52	1.88	7 (22%)
34	ATP	A	501	35	26,33,33	1.00	1 (3%)	31,52,52	1.75	5 (16%)
34	ATP	D	501	35	26,33,33	0.92	1 (3%)	31,52,52	1.82	7 (22%)
36	ADP	C	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.61	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	E	401	35	-	5/18/38/38	0/3/3/3
36	ADP	F	501	35	-	4/12/32/32	0/3/3/3
34	ATP	B	501	35	-	2/18/38/38	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
36	ADP	C	501	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	401	ATP	C5-C4	2.34	1.47	1.40
36	C	501	ADP	C5-C4	2.30	1.47	1.40
34	A	501	ATP	C5-C4	2.18	1.46	1.40
34	D	501	ATP	C5-C4	2.15	1.46	1.40
34	B	501	ATP	C5-C4	2.12	1.46	1.40
36	F	501	ADP	C5-C4	2.09	1.46	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	ATP	PA-O3A-PB	-5.58	113.67	132.83
34	D	501	ATP	PA-O3A-PB	-4.92	115.93	132.83
34	A	501	ATP	PB-O3B-PG	-4.73	116.58	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	401	ATP	PA-O3A-PB	-4.72	116.64	132.83
34	D	501	ATP	PB-O3B-PG	-4.70	116.71	132.83
34	E	401	ATP	PB-O3B-PG	-4.46	117.51	132.83
36	F	501	ADP	PA-O3A-PB	-4.46	117.54	132.83
34	A	501	ATP	PA-O3A-PB	-4.40	117.73	132.83
36	C	501	ADP	PA-O3A-PB	-4.16	118.56	132.83
34	B	501	ATP	C3'-C2'-C1'	3.94	106.92	100.98
34	B	501	ATP	PB-O3B-PG	-3.92	119.39	132.83
36	C	501	ADP	C3'-C2'-C1'	3.83	106.75	100.98
34	E	401	ATP	C3'-C2'-C1'	3.73	106.60	100.98
34	B	501	ATP	N3-C2-N1	-3.63	123.00	128.68
34	D	501	ATP	N3-C2-N1	-3.30	123.52	128.68
36	F	501	ADP	N3-C2-N1	-3.19	123.69	128.68
34	E	401	ATP	N3-C2-N1	-3.15	123.75	128.68
34	A	501	ATP	C4-C5-N7	-3.14	106.13	109.40
34	A	501	ATP	C3'-C2'-C1'	3.06	105.59	100.98
36	C	501	ADP	N3-C2-N1	-2.93	124.11	128.68
34	A	501	ATP	N3-C2-N1	-2.85	124.23	128.68
34	E	401	ATP	C4-C5-N7	-2.73	106.56	109.40
36	C	501	ADP	C4-C5-N7	-2.67	106.61	109.40
36	F	501	ADP	C3'-C2'-C1'	2.64	104.96	100.98
34	D	501	ATP	C3'-C2'-C1'	2.64	104.95	100.98
34	D	501	ATP	O2B-PB-O1B	2.29	123.55	112.24
36	C	501	ADP	C5'-C4'-C3'	-2.26	106.71	115.18
34	B	501	ATP	C2-N1-C6	2.24	122.59	118.75
34	B	501	ATP	C4-C5-N7	-2.22	107.08	109.40
34	B	501	ATP	O2B-PB-O1B	2.21	123.15	112.24
36	C	501	ADP	O3B-PB-O2B	2.17	115.94	107.64
34	D	501	ATP	O2A-PA-O1A	2.15	122.86	112.24
36	F	501	ADP	C4-C5-N7	-2.14	107.17	109.40
34	D	501	ATP	C2'-C3'-C4'	2.06	106.64	102.64
34	E	401	ATP	O2B-PB-O1B	2.04	122.34	112.24
36	F	501	ADP	O2A-PA-O1A	2.02	122.20	112.24

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	D	501	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	O4'-C4'-C5'-O5'

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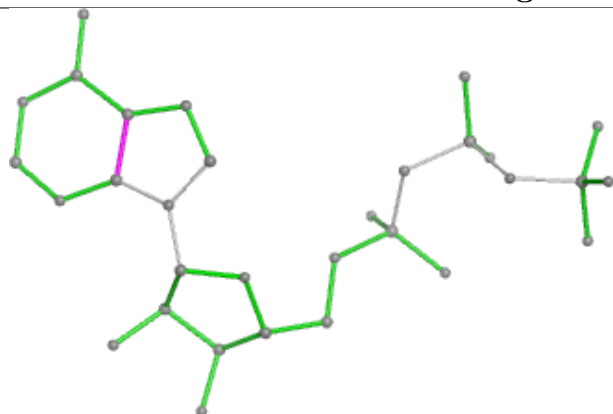
Mol	Chain	Res	Type	Atoms
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	F	501	ADP	PA-O3A-PB-O2B
34	D	501	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	O4'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'
34	D	501	ATP	C5'-O5'-PA-O1A
34	B	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C3'-C4'-C5'-O5'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

There are no ring outliers.

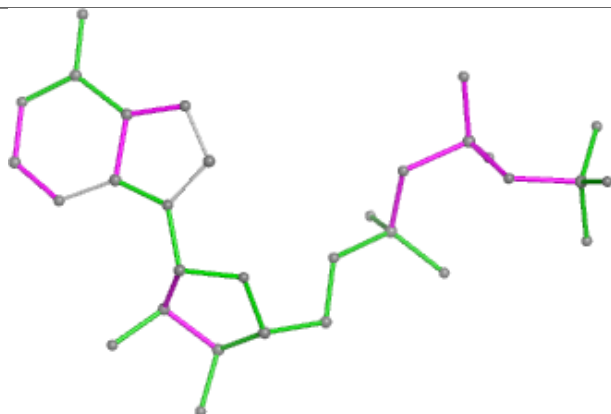
No monomer is involved in short contacts.

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

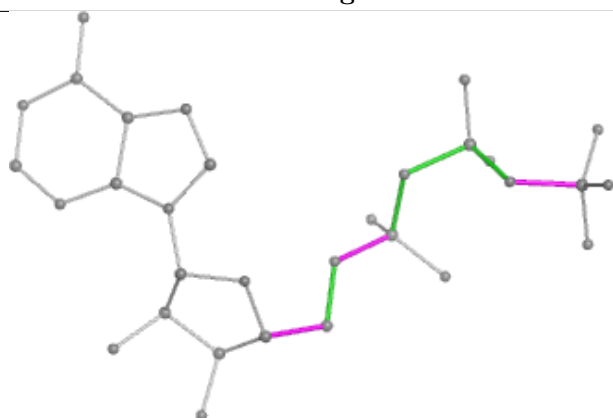
## Ligand ATP E 401



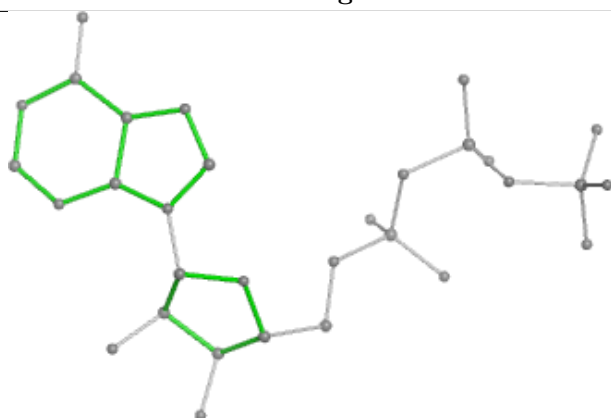
Bond lengths



Bond angles

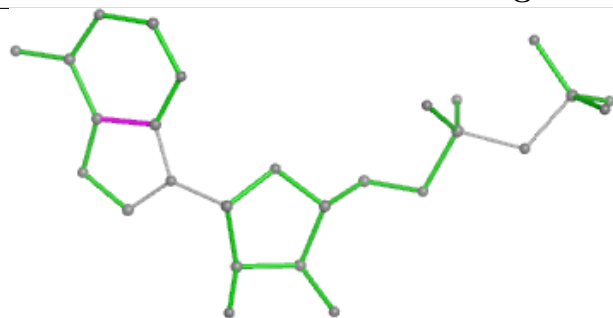


Torsions

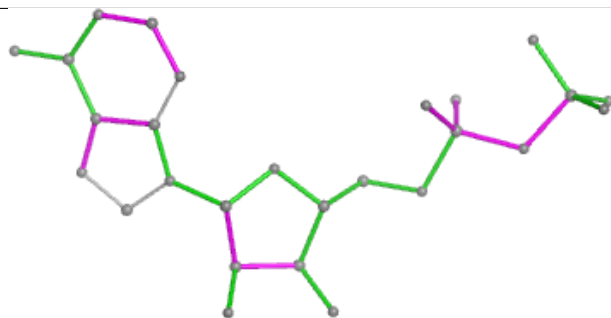


Rings

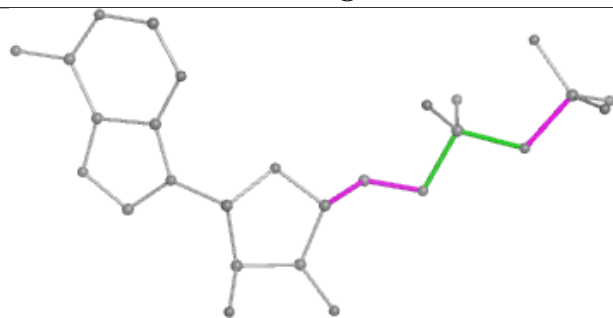
## Ligand ADP F 501



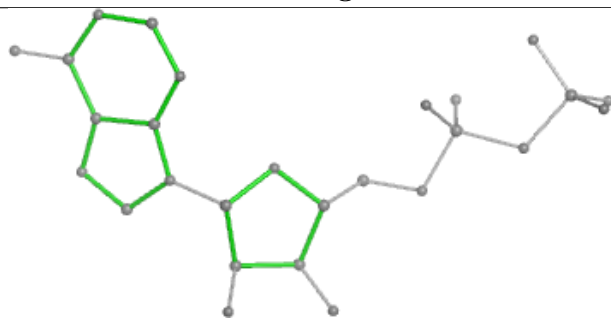
Bond lengths



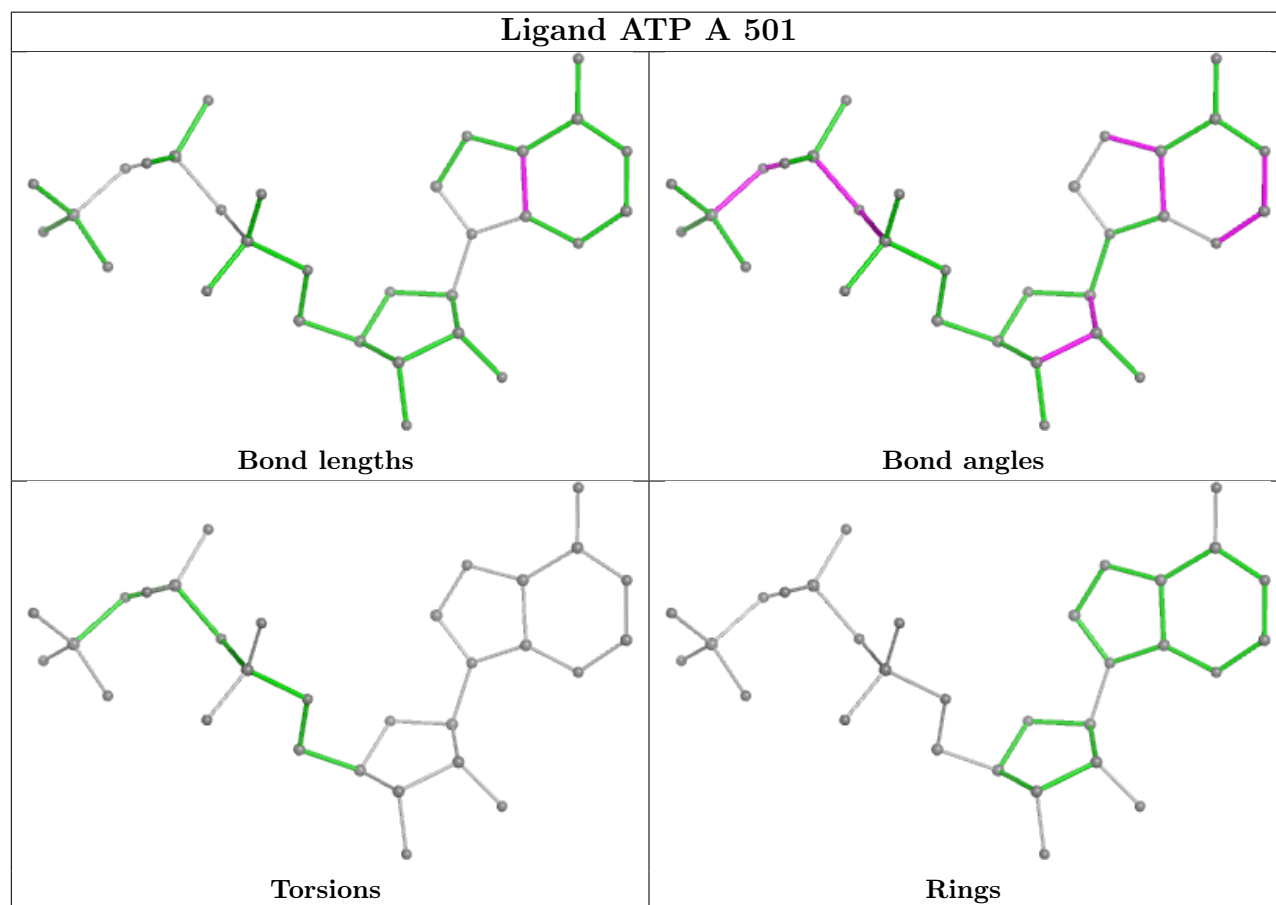
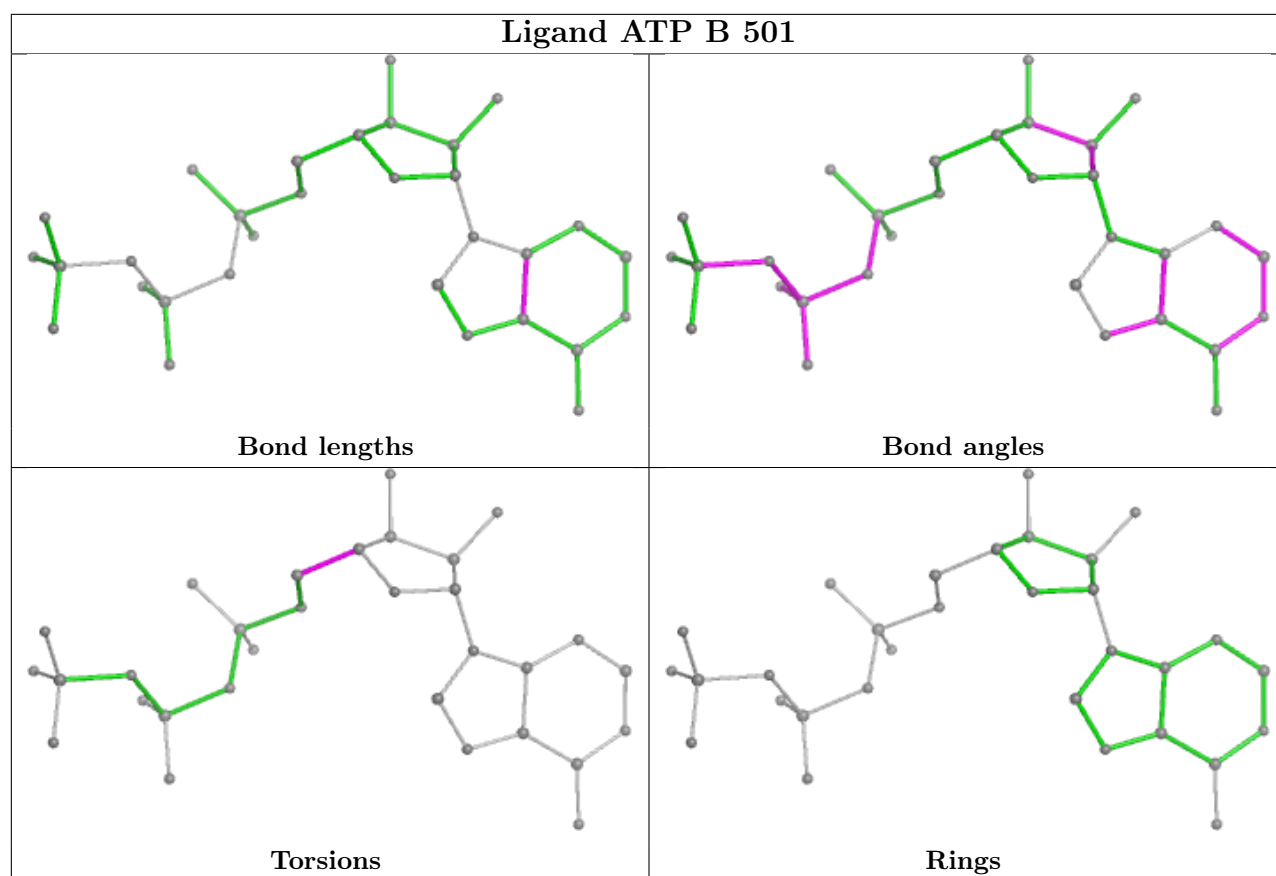
Bond angles

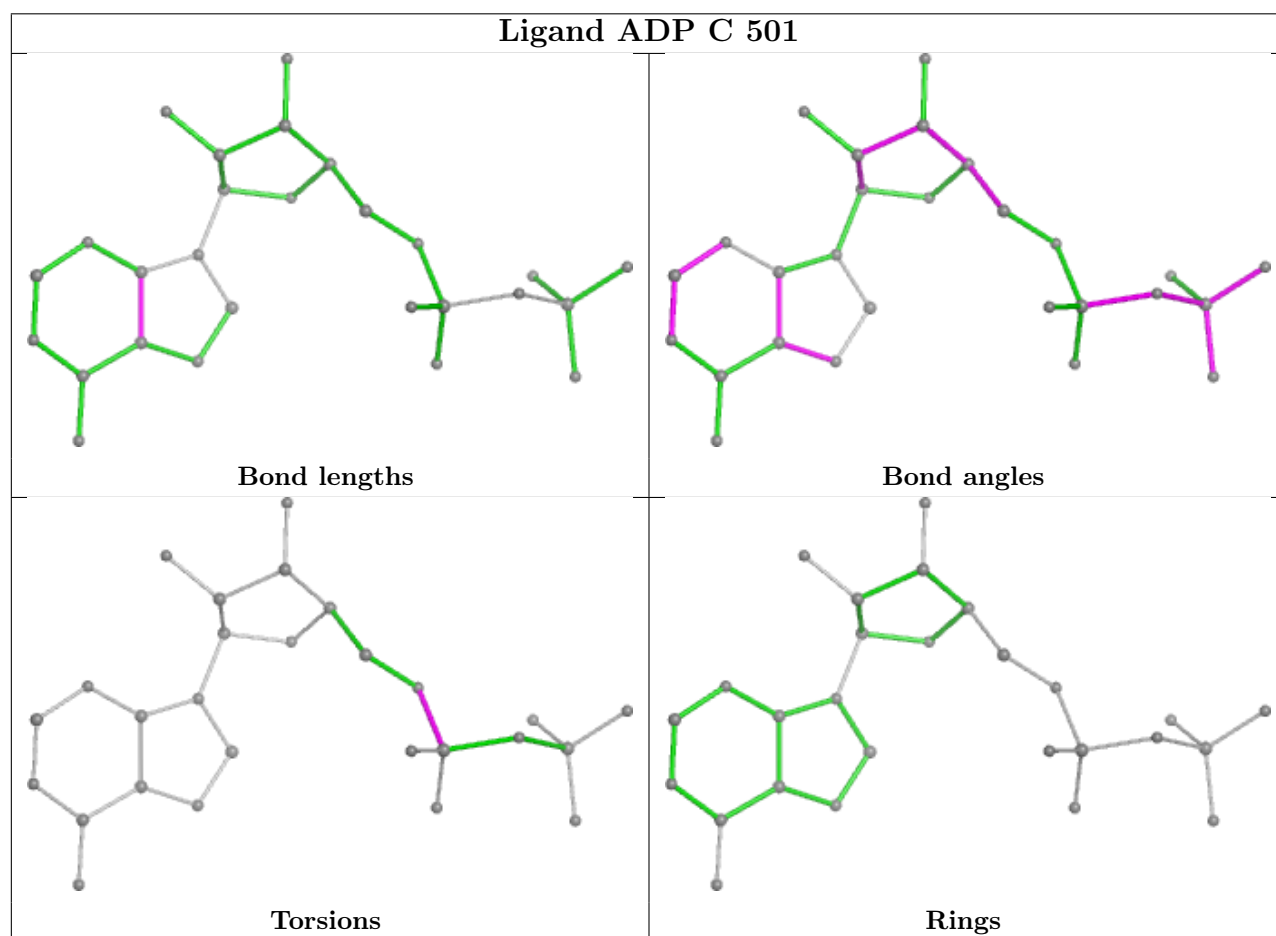
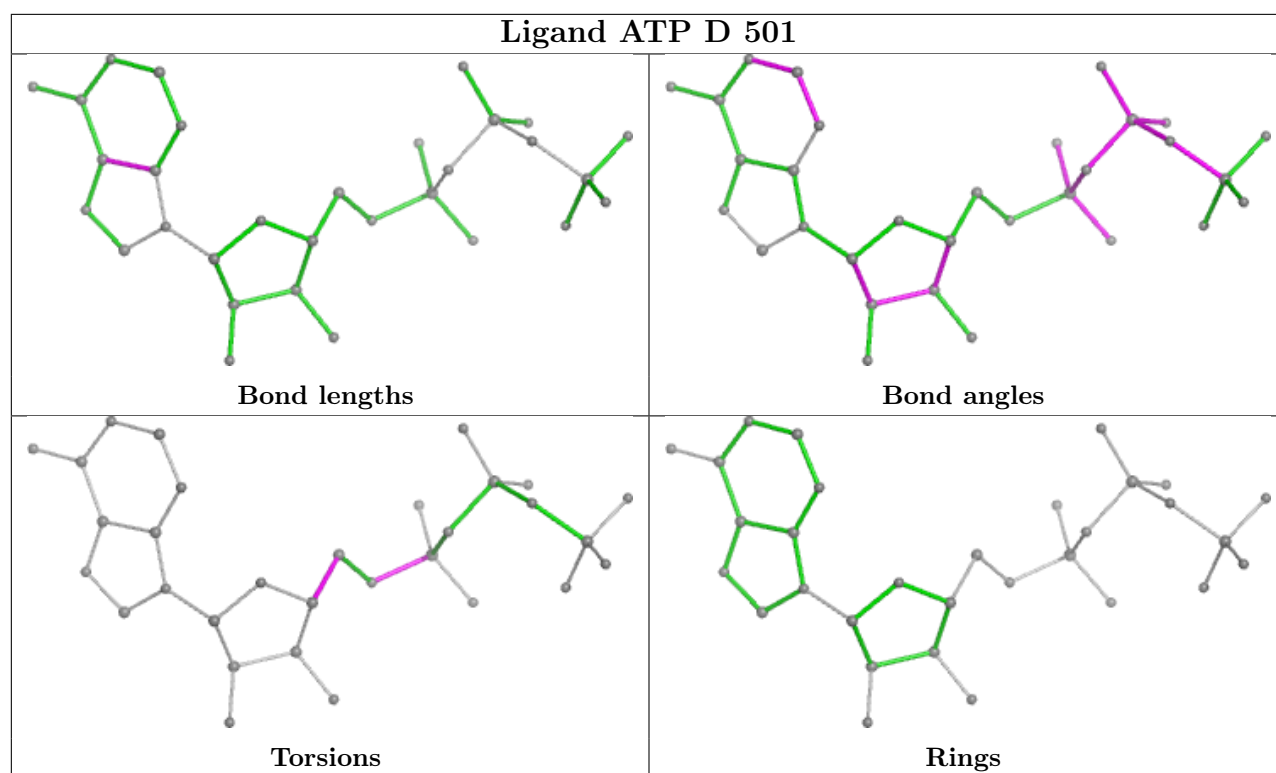


Torsions



Rings





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



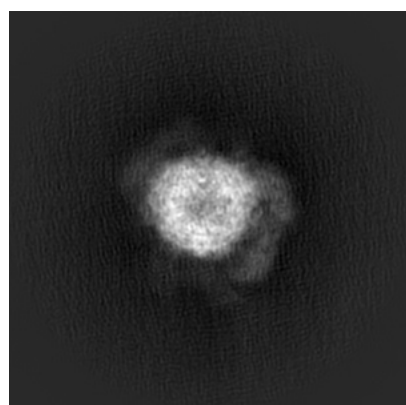
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14205. These allow visual inspection of the internal detail of the map and identification of artifacts.

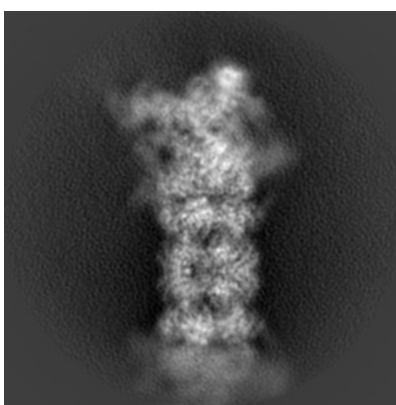
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y

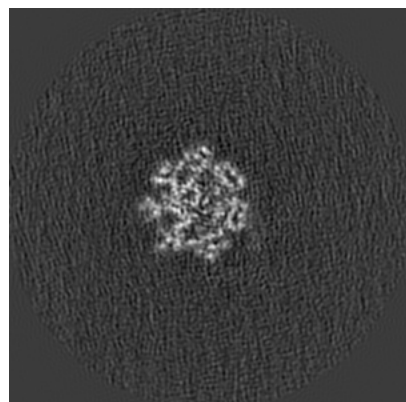


Z

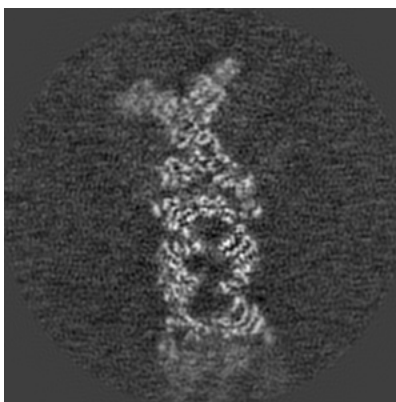
The images above show the map projected in three orthogonal directions.

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

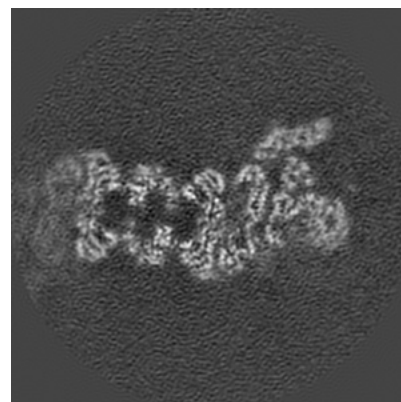
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

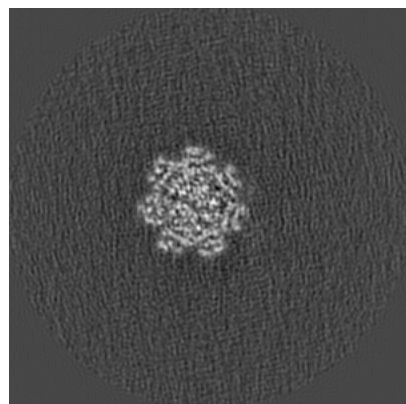


Z Index: 160

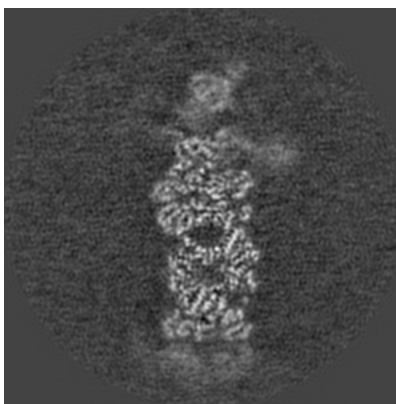
The images above show central slices of the map in three orthogonal directions.

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

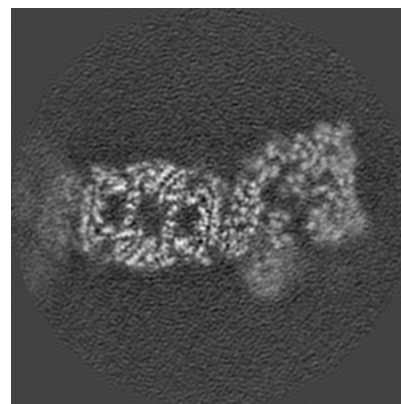
### 6.3.1 Primary map



X Index: 154



Y Index: 136

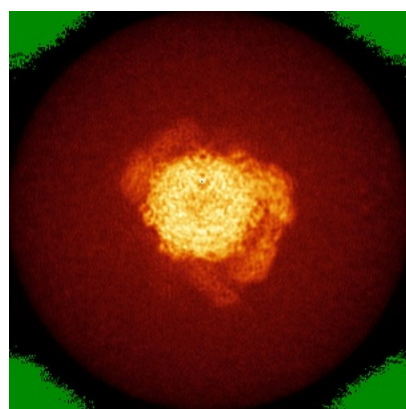


Z Index: 176

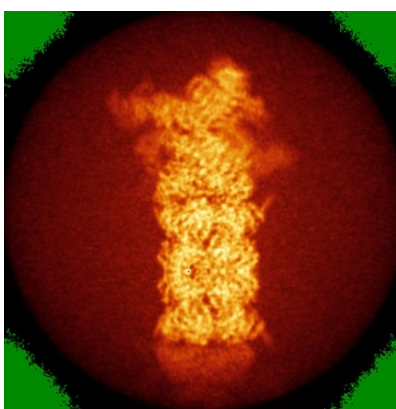
The images above show the largest variance slices of the map in three orthogonal directions.

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

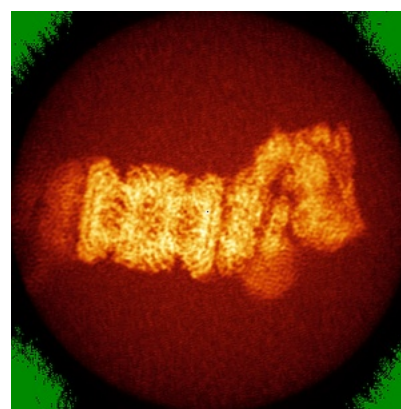
### 6.4.1 Primary map



X



Y

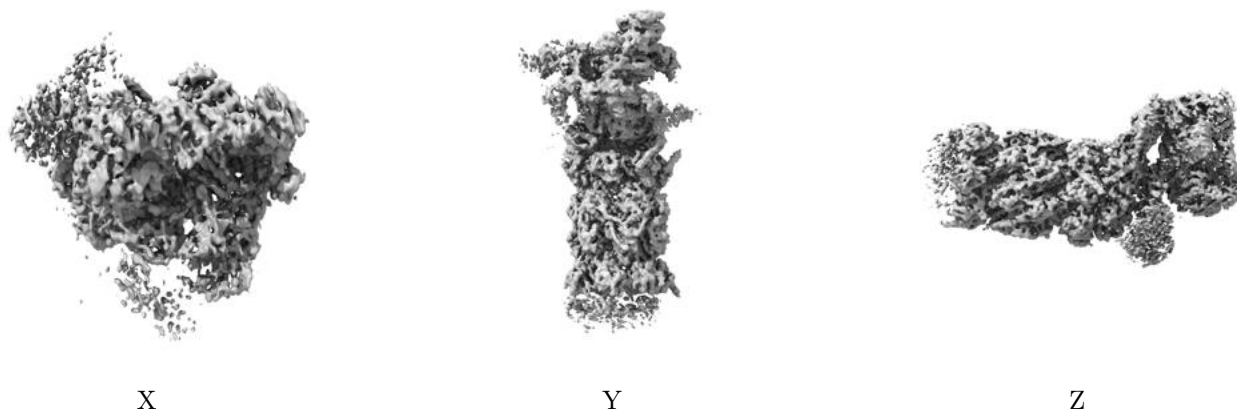


Z

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 0.0324. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

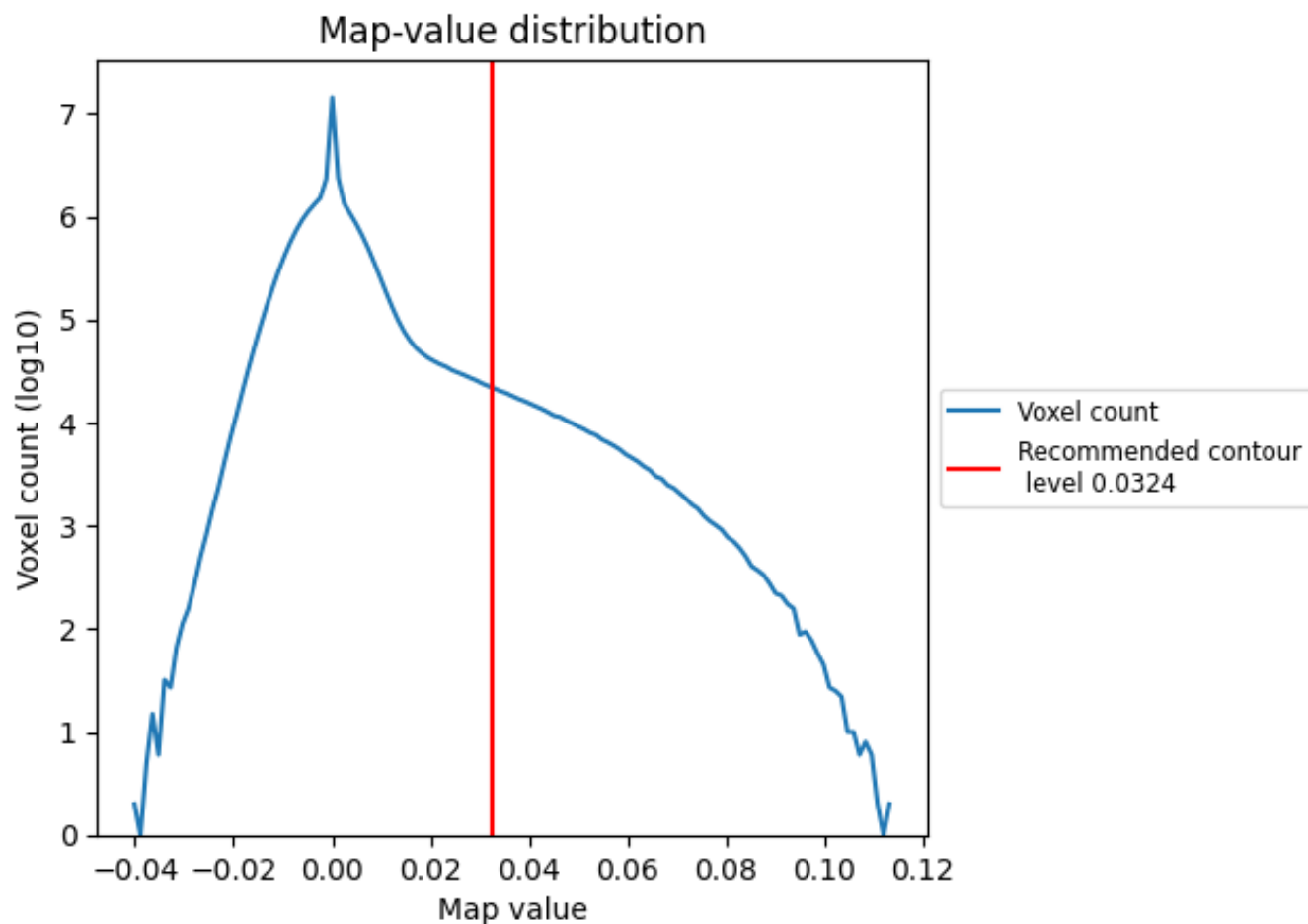
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

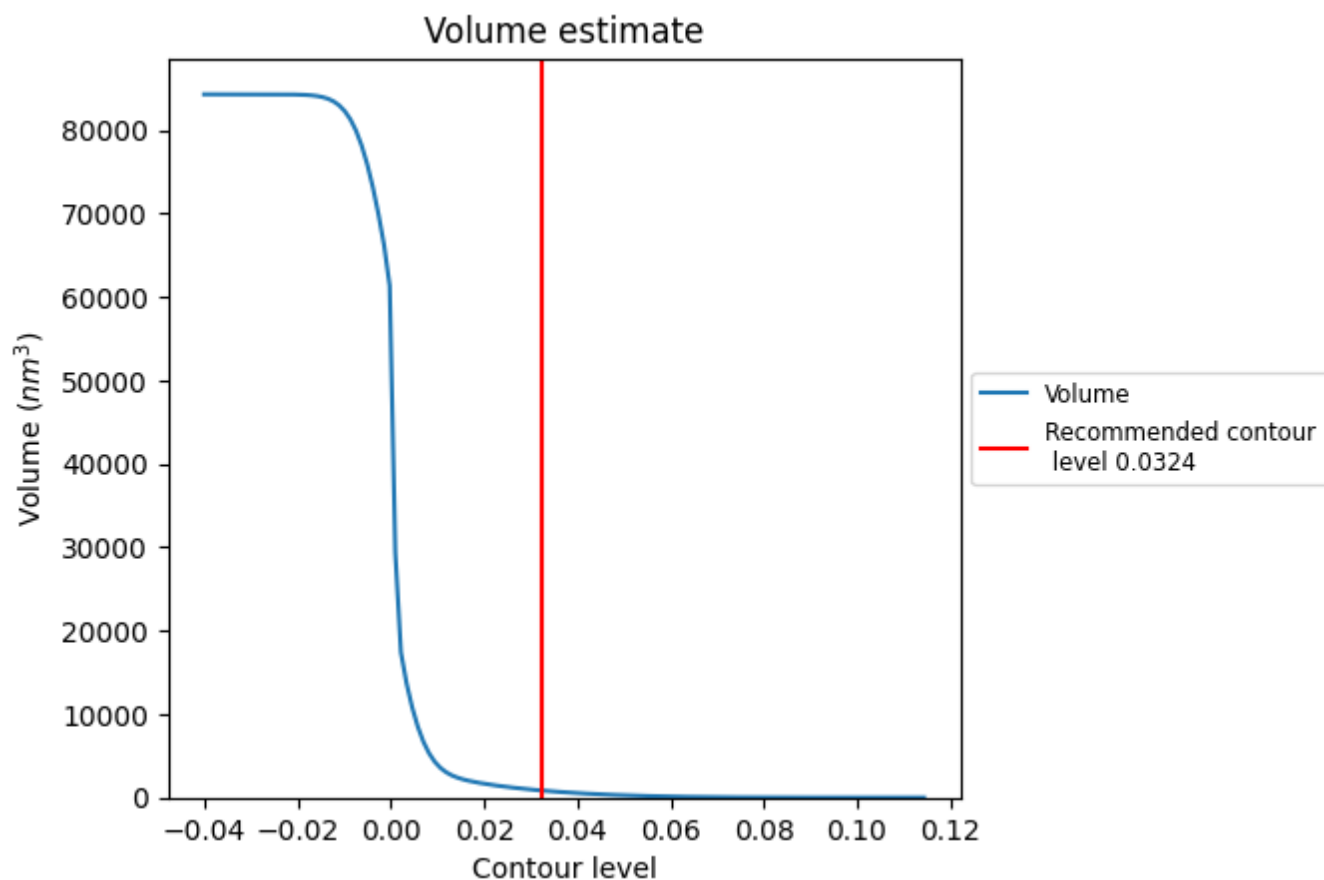
This section contains the results of statistical analysis of the map.

### 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.

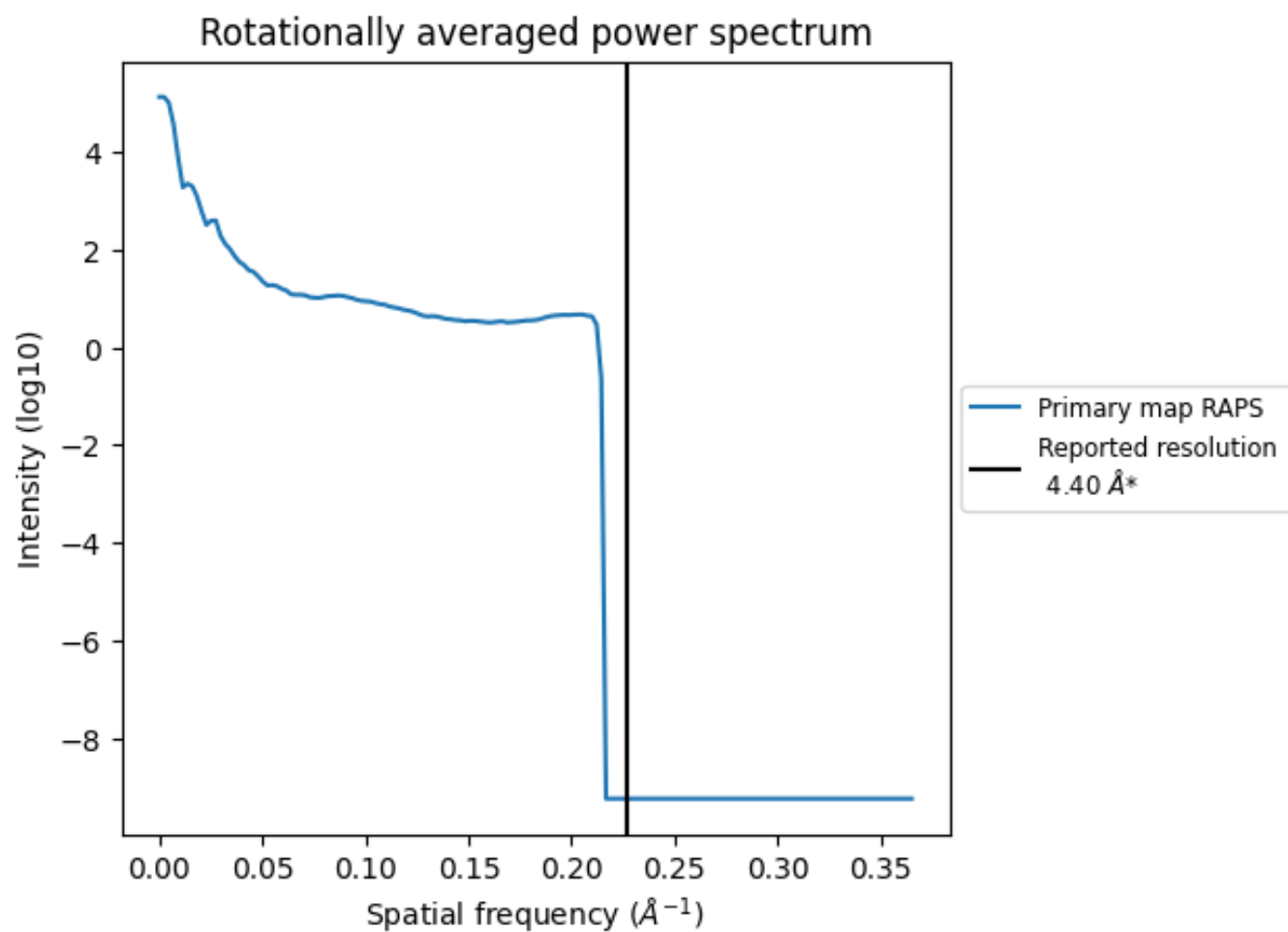
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 841 nm<sup>3</sup>; this corresponds to an approximate mass of 760 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 0.227 Å<sup>-1</sup>

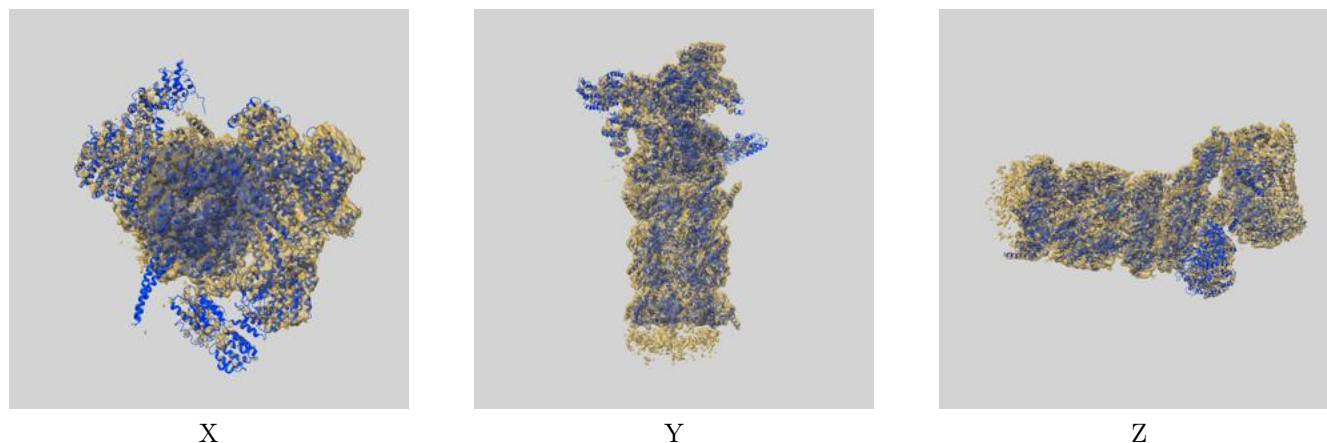
## 8 Fourier-Shell correlation ⓘ

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-14205 and PDB model 7QXX. Per-residue inclusion information can be found in section [3](#) on page [13](#).

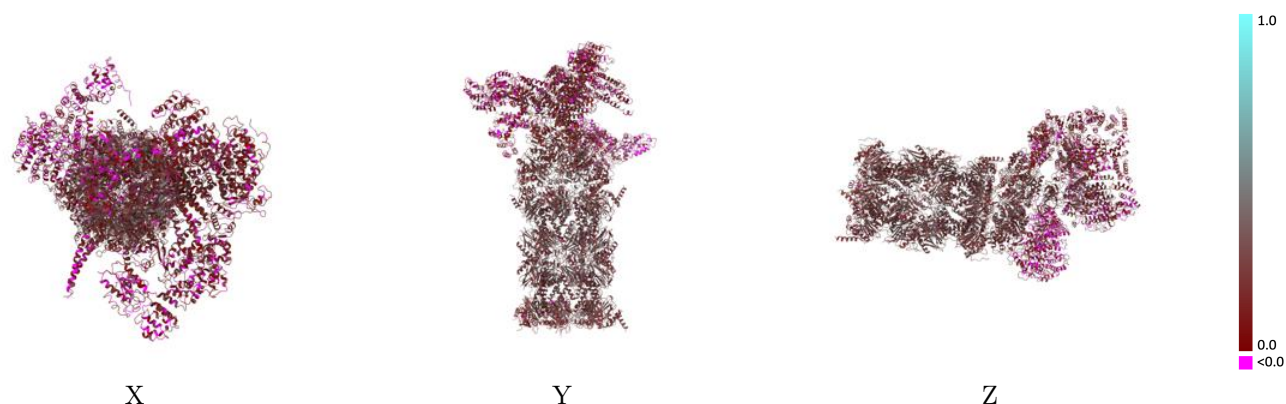
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0324 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.

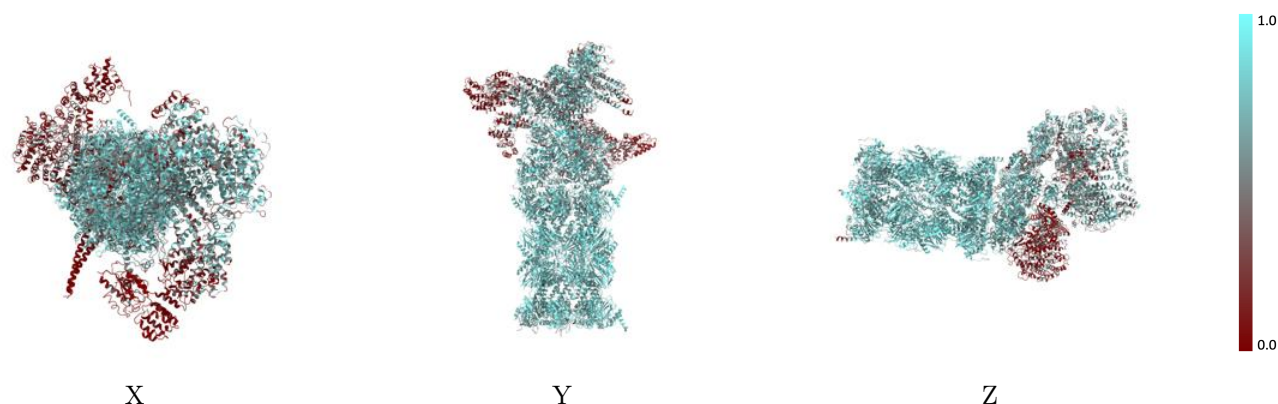


## 9.2 Q-score mapped to coordinate model [i](#)



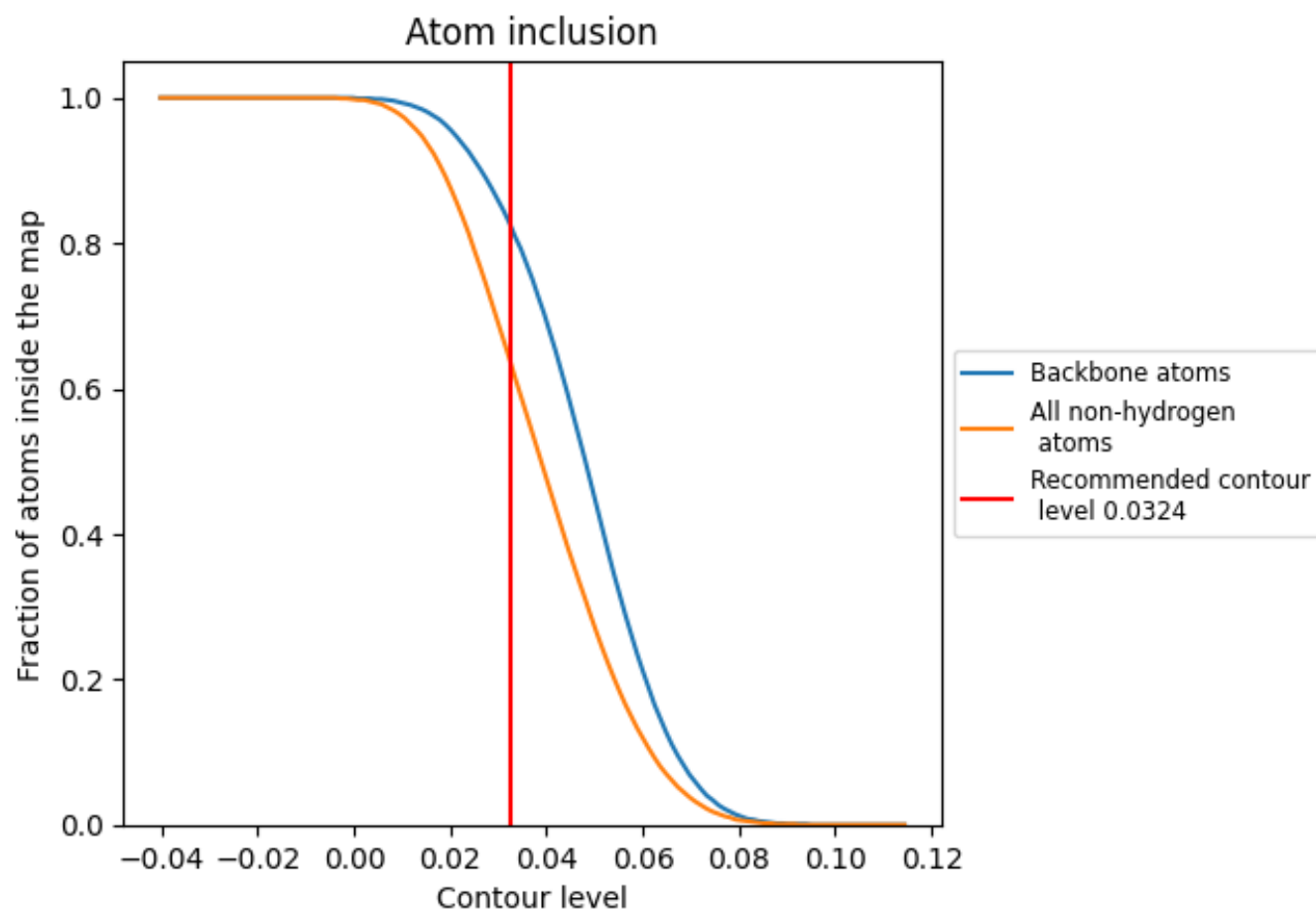
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0324).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% 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 (0.0324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.2330
A	 0.6820	 0.2560
B	 0.6580	 0.2460
C	 0.7190	 0.2610
D	 0.7020	 0.2520
E	 0.6690	 0.2520
F	 0.6680	 0.2560
G	 0.7730	 0.2900
H	 0.7890	 0.2980
I	 0.7660	 0.2880
J	 0.8040	 0.2900
K	 0.7810	 0.2900
L	 0.8000	 0.2970
M	 0.7640	 0.2770
N	 0.8240	 0.3070
O	 0.8020	 0.2970
P	 0.8070	 0.3120
Q	 0.8140	 0.3010
R	 0.8330	 0.3090
S	 0.8370	 0.3190
T	 0.8100	 0.3080
U	 0.6060	 0.1620
V	 0.5090	 0.1520
W	 0.3510	 0.1300
X	 0.5550	 0.1530
Y	 0.6720	 0.1850
Z	 0.5070	 0.1850
a	 0.2550	 0.1150
b	 0.1030	 0.1040
c	 0.6170	 0.2160
d	 0.5590	 0.1510
e	 0.4000	 0.1080
f	 0.1440	 0.0970
g	 0.7160	 0.2660
h	 0.7300	 0.2880



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Chain	Atom inclusion	Q-score
i	 0.6950	 0.2660
j	 0.7500	 0.2710
k	 0.7160	 0.2690
l	 0.7410	 0.2690
m	 0.6990	 0.2560
n	 0.7910	 0.2810
o	 0.7970	 0.3020
p	 0.7960	 0.3010
q	 0.7990	 0.3020
r	 0.8430	 0.3070
s	 0.7940	 0.3020
t	 0.7970	 0.2880