



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 07:21 AM JST

PDB ID : 7W38  
EMDB ID : EMD-32273  
Title : Structure of USP14-bound human 26S proteasome in state EA2.0\_UBL  
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.  
Deposited on : 2021-11-25  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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:

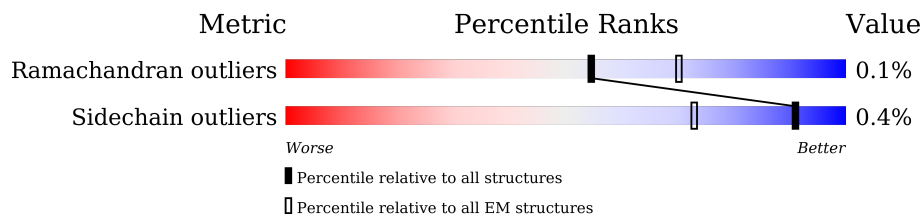
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	
5	E	403	
6	G	246	
6	g	246	
7	H	234	
7	h	234	

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Mol	Chain	Length	Quality of chain
8	I	261	
8	i	261	
9	J	248	
9	j	248	
10	K	241	
10	k	241	
11	L	269	
11	l	269	
12	M	255	
12	m	255	
13	N	239	
13	n	239	
14	O	277	
14	o	277	
15	P	205	
15	p	205	
16	Q	201	
16	q	201	
17	R	263	
17	r	263	
18	S	241	
18	s	241	
19	T	264	
19	t	264	
20	U	953	

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Mol	Chain	Length	Quality of chain
21	V	534	6% 87% 12%
22	W	456	96%
23	X	422	89% 10%
24	Y	389	96%
25	Z	324	88% 12%
26	a	376	98%
27	b	377	50% 49%
28	d	350	16% 73% 27%
29	f	908	17% 97%
30	x	494	13% 15% 85%
31	c	310	92% 7%
32	F	439	6% 94% 5%
33	u	76	100%
34	e	70	6% 71% 29%

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 106178 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 protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	413	3240	2042	567	613	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	388	3042	1915	519	593	15	0	0

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	379	2968	1867	534	551	16	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	375	2860	1796	512	536	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	244	1889	1198	316	362	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
7	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
8	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
9	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
10	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 11 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
11	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	240	1876	1191	321	353	11	0	0
12	m	240	1881	1193	321	356	11	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	202	1514	949	258	295	12	0	0
13	n	202	1510	947	258	293	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	220	1649	1038	279	320	12	0	0
14	o	220	1659	1044	283	320	12	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	204	1587	1010	264	294	19	0	0
15	p	204	1591	1013	265	294	19	0	0

- Molecule 16 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	199	1588	1017	270	292	9	0	0
16	q	199	1588	1017	270	292	9	0	0

- Molecule 17 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
17	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 18 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
18	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 19 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
19	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	764	Total	C	N	O	S	0	0
			5945	3772	1021	1108	44		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	446	Total	C	N	O	S	0	0
			3635	2302	622	687	24		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.



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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 30 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	x	76	588	378	96	108	6	0	0

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 32 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	F	415	3251	2038	561	634	18	0	0

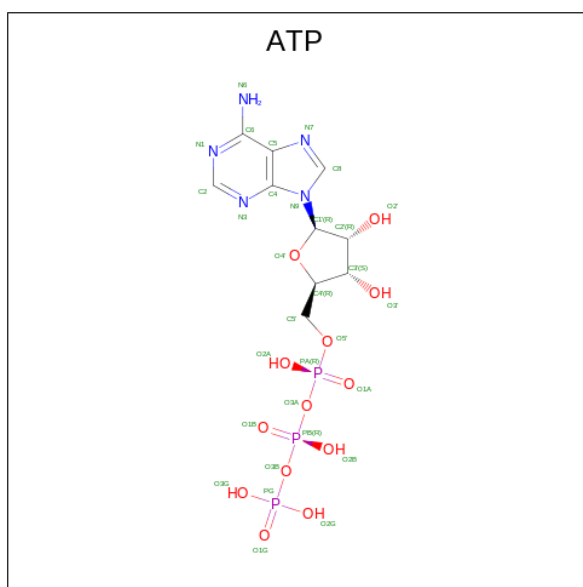
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	u	76	601	378	105	117	1	0	0

- Molecule 34 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	e	50	425	260	65	100	0	0

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

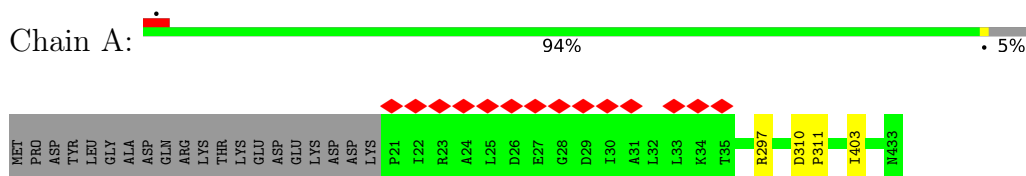
- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



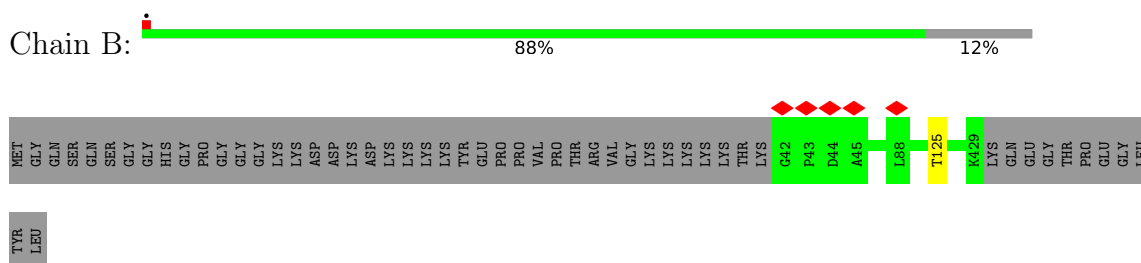
### 3 Residue-property plots [i](#)

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

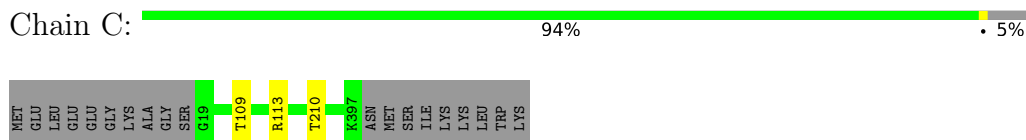
- Molecule 1: 26S protease regulatory subunit 7



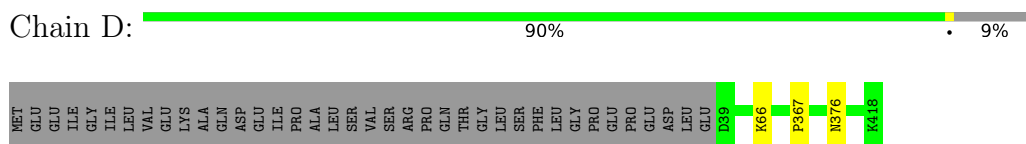
- Molecule 2: 26S protease regulatory subunit 4



- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8

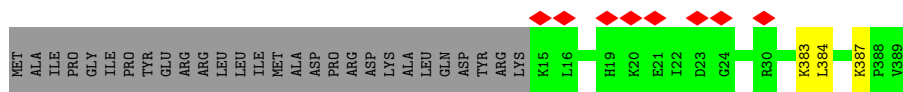


- Molecule 4: 26S protease regulatory subunit 6B

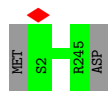


- Molecule 5: 26S proteasome regulatory subunit 10B

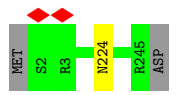




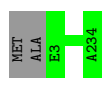
• Molecule 6: Proteasome subunit alpha type-6



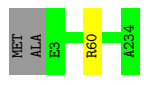
• Molecule 6: Proteasome subunit alpha type-6



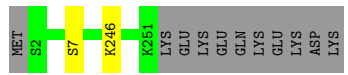
• Molecule 7: Proteasome subunit alpha type-2



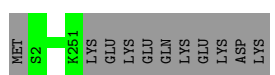
• Molecule 7: Proteasome subunit alpha type-2



• Molecule 8: Proteasome subunit alpha type-4

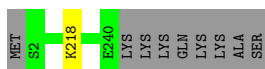


• Molecule 8: Proteasome subunit alpha type-4



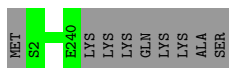
• Molecule 9: Proteasome subunit alpha type-7





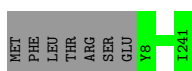
- Molecule 9: Proteasome subunit alpha type-7

Chain j: 96%



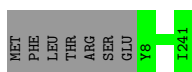
- Molecule 10: Proteasome subunit alpha type-5

Chain K: 97%



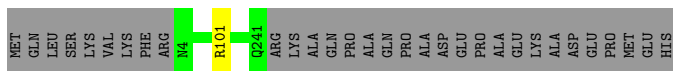
- Molecule 10: Proteasome subunit alpha type-5

Chain k: 97%



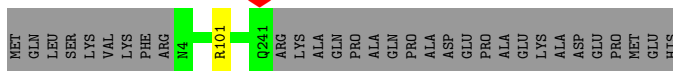
- Molecule 11: Isoform Long of Proteasome subunit alpha type-1

Chain L: 88% 12%



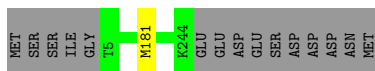
- Molecule 11: Isoform Long of Proteasome subunit alpha type-1

Chain l: 88% 12%



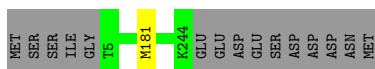
- Molecule 12: Proteasome subunit alpha type-3

Chain M: 94% 6%

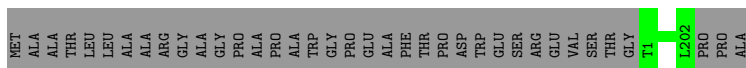
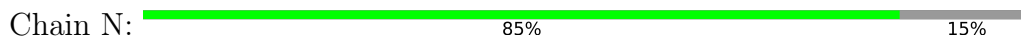


- Molecule 12: Proteasome subunit alpha type-3

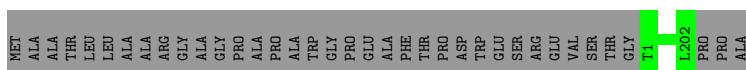
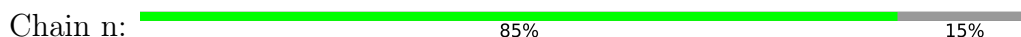
Chain m: 94% 6%



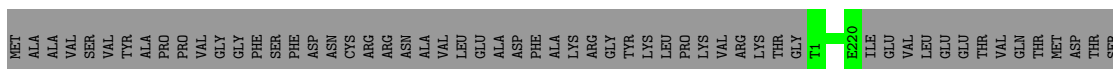
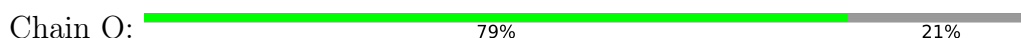
- Molecule 13: Proteasome subunit beta type-6



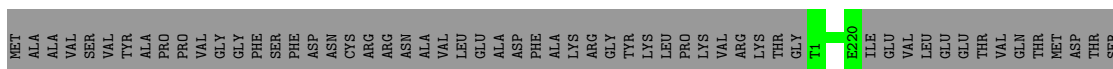
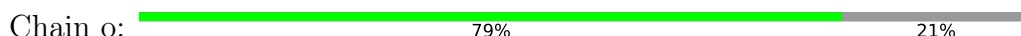
- Molecule 13: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-7



- Molecule 15: Proteasome subunit beta type-3



- Molecule 15: Proteasome subunit beta type-3



- Molecule 16: Proteasome subunit beta type-2

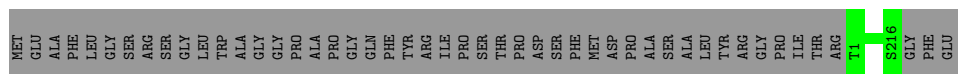






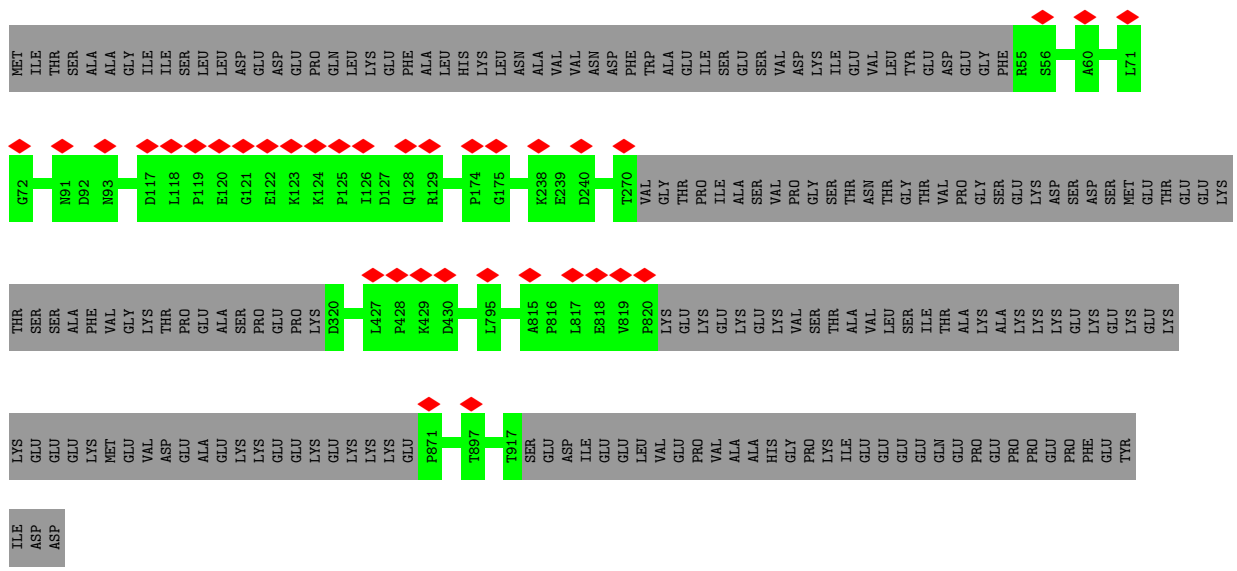
• Molecule 19: Proteasome subunit beta type-4

Chain t: 82% 18%



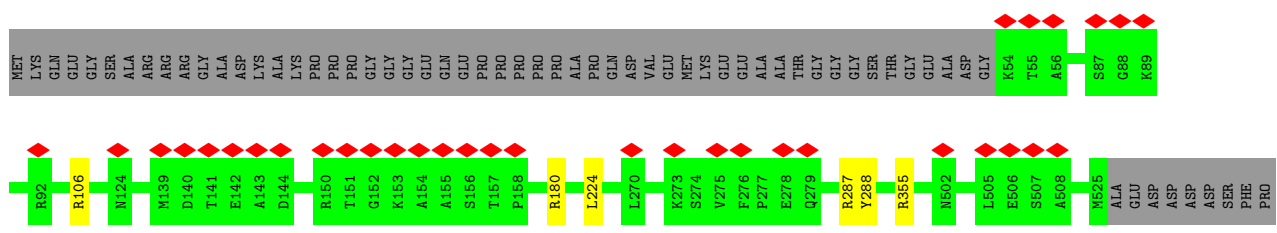
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 80% 20%



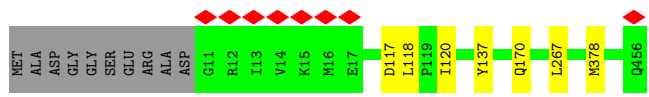
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 6% 87% 12%



• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 96%



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11

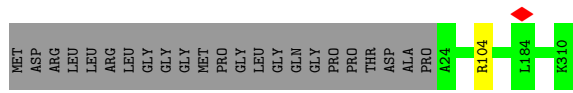
Chain X: 89% 10%



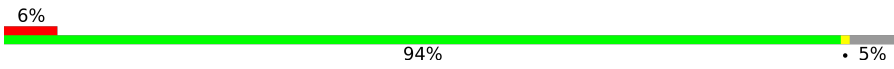


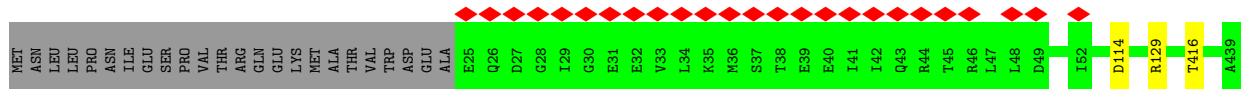
- Molecule 31: 26S proteasome non-ATPase regulatory subunit 14

Chain c:  92% 7%



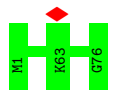
- Molecule 32: 26S protease regulatory subunit 6A

Chain F:  6% 94% 5%



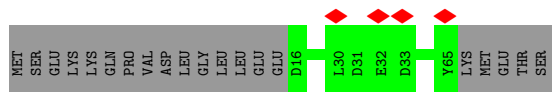
- Molecule 33: Ubiquitin

Chain u:  100%



- Molecule 34: 26S proteasome complex subunit DSS1

Chain e:  6% 71% 29%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284997	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/3294	0.57	0/4447
2	B	0.27	0/3086	0.57	0/4164
3	C	0.27	0/3007	0.58	0/4045
4	D	0.28	0/3089	0.59	0/4168
5	E	0.27	0/2904	0.58	0/3924
6	G	0.29	0/1923	0.52	0/2601
6	g	0.28	0/1914	0.53	0/2590
7	H	0.29	0/1844	0.51	0/2499
7	h	0.28	0/1844	0.50	0/2497
8	I	0.28	0/1991	0.53	0/2685
8	i	0.29	0/1985	0.53	0/2677
9	J	0.28	0/1906	0.56	0/2573
9	j	0.27	0/1887	0.54	0/2549
10	K	0.27	0/1804	0.49	0/2436
10	k	0.27	0/1809	0.50	0/2444
11	L	0.27	0/1901	0.52	0/2570
11	l	0.26	0/1896	0.54	0/2565
12	M	0.28	0/1911	0.51	0/2573
12	m	0.28	0/1916	0.49	0/2580
13	N	0.28	0/1540	0.51	0/2085
13	n	0.28	0/1536	0.51	0/2080
14	O	0.27	0/1676	0.54	0/2271
14	o	0.27	0/1686	0.53	0/2282
15	P	0.27	0/1616	0.53	0/2180
15	p	0.27	0/1620	0.53	0/2184
16	Q	0.28	0/1621	0.50	0/2194
16	q	0.28	0/1621	0.52	0/2194
17	R	0.28	0/1590	0.54	0/2147
17	r	0.28	0/1590	0.53	0/2147
18	S	0.28	0/1671	0.54	0/2252
18	s	0.28	0/1684	0.55	0/2268
19	T	0.28	0/1716	0.54	0/2323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	t	0.28	0/1720	0.52	0/2328
20	U	0.26	0/6052	0.55	0/8190
21	V	0.26	0/3824	0.55	0/5170
22	W	0.29	0/3683	0.62	2/4952 (0.0%)
23	X	0.26	0/3053	0.55	0/4115
24	Y	0.29	0/3173	0.62	0/4273
25	Z	0.28	0/2324	0.58	0/3150
26	a	0.26	0/3053	0.59	2/4133 (0.0%)
27	b	0.27	0/1478	0.60	0/2001
28	d	0.28	0/2162	0.58	0/2919
29	f	0.28	0/6980	0.61	1/9433 (0.0%)
30	x	0.26	0/599	0.53	0/805
31	c	0.28	0/2302	0.59	0/3110
32	F	0.28	0/3292	0.57	0/4435
33	u	0.26	0/607	0.54	0/816
34	e	0.28	0/437	0.53	0/595
All	All	0.28	0/107817	0.56	5/145619 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	267	LEU	CA-CB-CG	5.55	128.07	115.30
29	f	670	MET	CA-CB-CG	5.51	122.67	113.30
22	W	378	MET	CA-CB-CG	5.44	122.55	113.30
26	a	333	MET	CG-SD-CE	5.19	108.50	100.20
26	a	187	ASP	CB-CG-OD1	5.03	122.83	118.30

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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	365 (89%)	45 (11%)	1 (0%)	47	79
2	B	386/440 (88%)	363 (94%)	23 (6%)	0	100	100
3	C	377/398 (95%)	341 (90%)	36 (10%)	0	100	100
4	D	378/418 (90%)	346 (92%)	31 (8%)	1 (0%)	41	73
5	E	373/403 (93%)	343 (92%)	30 (8%)	0	100	100
6	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
6	g	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
7	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
7	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	I	249/261 (95%)	243 (98%)	6 (2%)	0	100	100
8	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
9	J	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
9	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	K	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
10	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
11	L	236/269 (88%)	232 (98%)	4 (2%)	0	100	100
11	l	236/269 (88%)	229 (97%)	7 (3%)	0	100	100
12	M	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
12	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
13	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
13	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
14	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
15	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
16	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
17	R	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
17	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
18	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
19	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	U	758/953 (80%)	713 (94%)	45 (6%)	0	100	100
21	V	470/534 (88%)	444 (94%)	23 (5%)	3 (1%)	25	59
22	W	444/456 (97%)	416 (94%)	27 (6%)	1 (0%)	47	79
23	X	378/422 (90%)	359 (95%)	19 (5%)	0	100	100
24	Y	376/389 (97%)	349 (93%)	25 (7%)	2 (0%)	29	64
25	Z	284/324 (88%)	261 (92%)	23 (8%)	0	100	100
26	a	371/376 (99%)	342 (92%)	29 (8%)	0	100	100
27	b	189/377 (50%)	174 (92%)	14 (7%)	1 (0%)	29	64
28	d	255/350 (73%)	222 (87%)	33 (13%)	0	100	100
29	f	887/908 (98%)	790 (89%)	97 (11%)	0	100	100
30	x	74/494 (15%)	72 (97%)	2 (3%)	0	100	100
31	c	285/310 (92%)	263 (92%)	22 (8%)	0	100	100
32	F	413/439 (94%)	383 (93%)	29 (7%)	1 (0%)	47	79
33	u	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
34	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
All	All	13440/15458 (87%)	12665 (94%)	765 (6%)	10 (0%)	54	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
21	V	287	ARG
21	V	288	TYR
22	W	137	TYR
32	F	114	ASP

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/372 (95%)	349 (99%)	3 (1%)	78	91
2	B	341/385 (89%)	340 (100%)	1 (0%)	92	96
3	C	325/346 (94%)	322 (99%)	3 (1%)	78	91
4	D	333/366 (91%)	331 (99%)	2 (1%)	86	94
5	E	298/353 (84%)	295 (99%)	3 (1%)	76	90
6	G	205/210 (98%)	205 (100%)	0	100	100
6	g	202/210 (96%)	201 (100%)	1 (0%)	88	94
7	H	188/191 (98%)	188 (100%)	0	100	100
7	h	188/191 (98%)	187 (100%)	1 (0%)	88	94
8	I	207/221 (94%)	204 (99%)	3 (1%)	67	86
8	i	206/221 (93%)	206 (100%)	0	100	100
9	J	201/211 (95%)	200 (100%)	1 (0%)	88	94
9	j	196/211 (93%)	196 (100%)	0	100	100
10	K	193/203 (95%)	193 (100%)	0	100	100
10	k	195/203 (96%)	195 (100%)	0	100	100
11	L	202/230 (88%)	201 (100%)	1 (0%)	88	94
11	l	201/230 (87%)	200 (100%)	1 (0%)	88	94
12	M	196/212 (92%)	195 (100%)	1 (0%)	88	94
12	m	198/212 (93%)	197 (100%)	1 (0%)	88	94
13	N	157/181 (87%)	157 (100%)	0	100	100
13	n	156/181 (86%)	156 (100%)	0	100	100
14	O	179/228 (78%)	179 (100%)	0	100	100
14	o	181/228 (79%)	181 (100%)	0	100	100
15	P	172/174 (99%)	172 (100%)	0	100	100
15	p	173/174 (99%)	173 (100%)	0	100	100
16	Q	168/171 (98%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	q	168/171 (98%)	168 (100%)	0	100	100
17	R	156/202 (77%)	155 (99%)	1 (1%)	86	94
17	r	156/202 (77%)	156 (100%)	0	100	100
18	S	175/199 (88%)	175 (100%)	0	100	100
18	s	178/199 (89%)	178 (100%)	0	100	100
19	T	178/215 (83%)	178 (100%)	0	100	100
19	t	179/215 (83%)	179 (100%)	0	100	100
20	U	649/816 (80%)	649 (100%)	0	100	100
21	V	391/460 (85%)	388 (99%)	3 (1%)	81	92
22	W	410/416 (99%)	406 (99%)	4 (1%)	76	90
23	X	327/362 (90%)	324 (99%)	3 (1%)	78	91
24	Y	334/344 (97%)	331 (99%)	3 (1%)	78	91
25	Z	257/295 (87%)	255 (99%)	2 (1%)	81	92
26	a	333/336 (99%)	332 (100%)	1 (0%)	92	96
27	b	167/312 (54%)	167 (100%)	0	100	100
28	d	231/294 (79%)	231 (100%)	0	100	100
29	f	745/763 (98%)	736 (99%)	9 (1%)	71	88
30	x	64/439 (15%)	64 (100%)	0	100	100
31	c	252/268 (94%)	251 (100%)	1 (0%)	91	96
32	F	357/379 (94%)	355 (99%)	2 (1%)	86	94
33	u	68/68 (100%)	68 (100%)	0	100	100
34	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11432/13133 (87%)	11381 (100%)	51 (0%)	91	96

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	420	LYS
29	f	8	LYS
32	F	129	ARG
24	Y	46	ARG
25	Z	202	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
29	f	457	ASN
7	h	166	ASN
10	k	99	HIS
7	h	169	ASN
27	b	161	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 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
35	ATP	E	501	36	26,33,33	0.61	0	31,52,52	0.86	2 (6%)
37	ADP	C	501	36	24,29,29	0.96	1 (4%)	29,45,45	1.55	4 (13%)
35	ATP	D	501	36	26,33,33	0.66	0	31,52,52	0.74	1 (3%)
35	ATP	A	501	36	26,33,33	0.97	2 (7%)	31,52,52	1.42	5 (16%)
35	ATP	B	501	36	26,33,33	0.90	1 (3%)	31,52,52	1.56	6 (19%)
37	ADP	F	501	36	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	E	501	36	-	6/18/38/38	0/3/3/3
37	ADP	C	501	36	-	2/12/32/32	0/3/3/3
35	ATP	D	501	36	-	4/18/38/38	0/3/3/3
35	ATP	A	501	36	-	3/18/38/38	0/3/3/3
35	ATP	B	501	36	-	1/18/38/38	0/3/3/3
37	ADP	F	501	36	-	6/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	C5-C4	2.44	1.47	1.40
37	C	501	ADP	C5-C4	2.42	1.47	1.40
35	A	501	ATP	C5-C4	2.40	1.47	1.40
37	F	501	ADP	C5-C4	2.37	1.47	1.40
35	A	501	ATP	C2-N3	2.00	1.35	1.32

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	PA-O3A-PB	-4.07	118.86	132.83
37	F	501	ADP	C3'-C2'-C1'	3.70	106.55	100.98
37	F	501	ADP	PA-O3A-PB	-3.63	120.36	132.83
37	C	501	ADP	C3'-C2'-C1'	3.57	106.35	100.98
35	B	501	ATP	C3'-C2'-C1'	3.55	106.33	100.98

There are no chirality outliers.

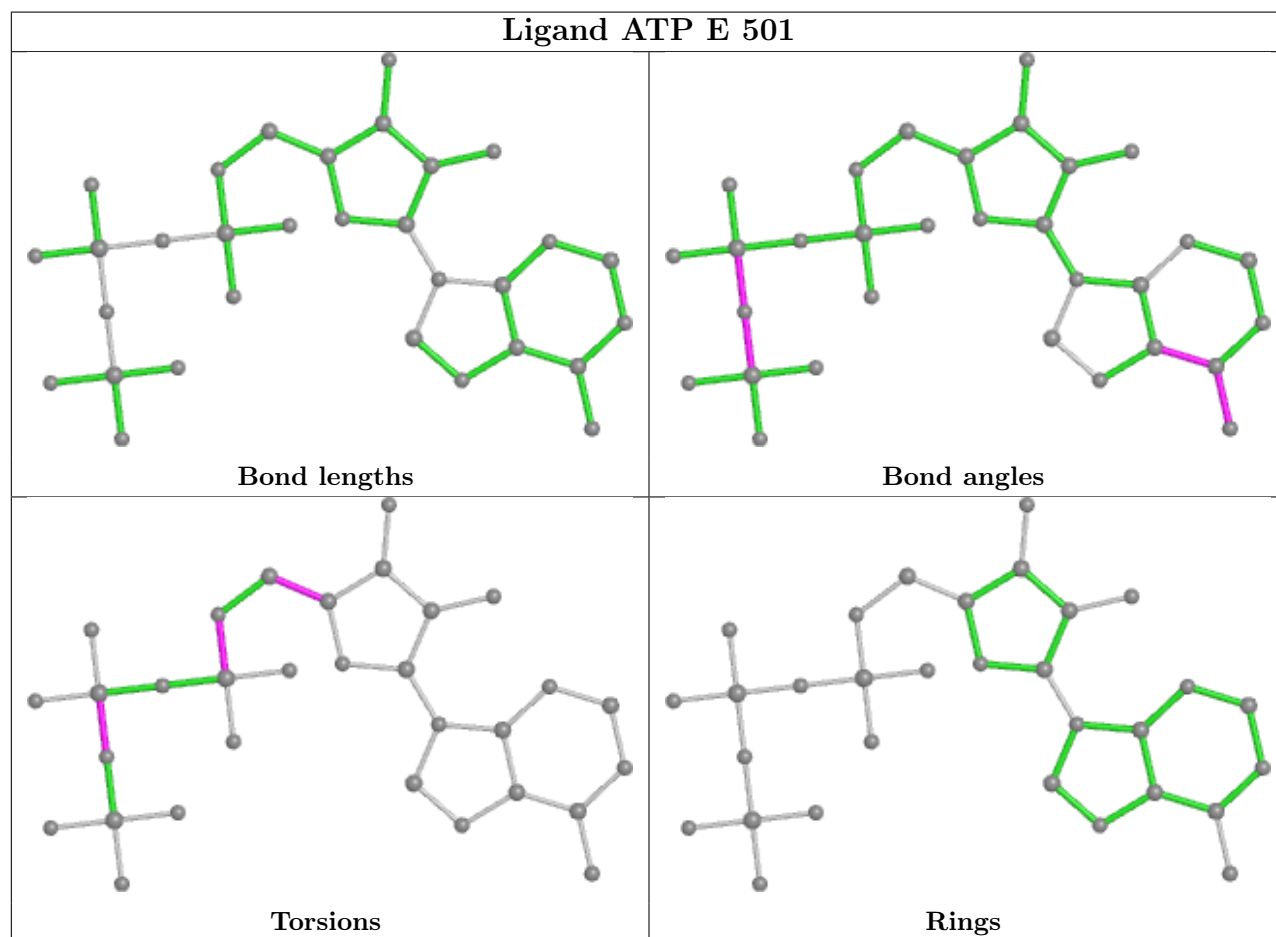
5 of 22 torsion outliers are listed below:

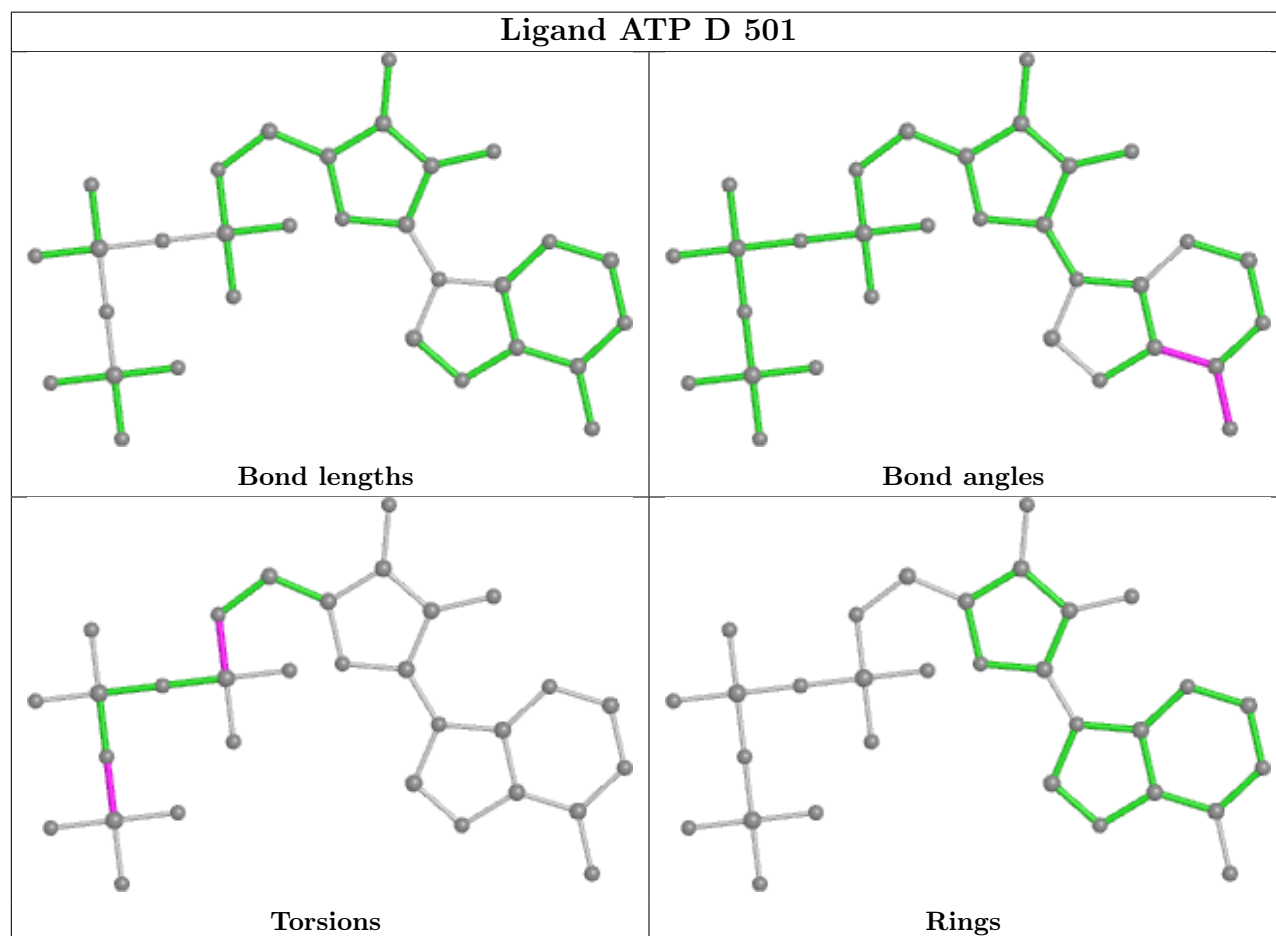
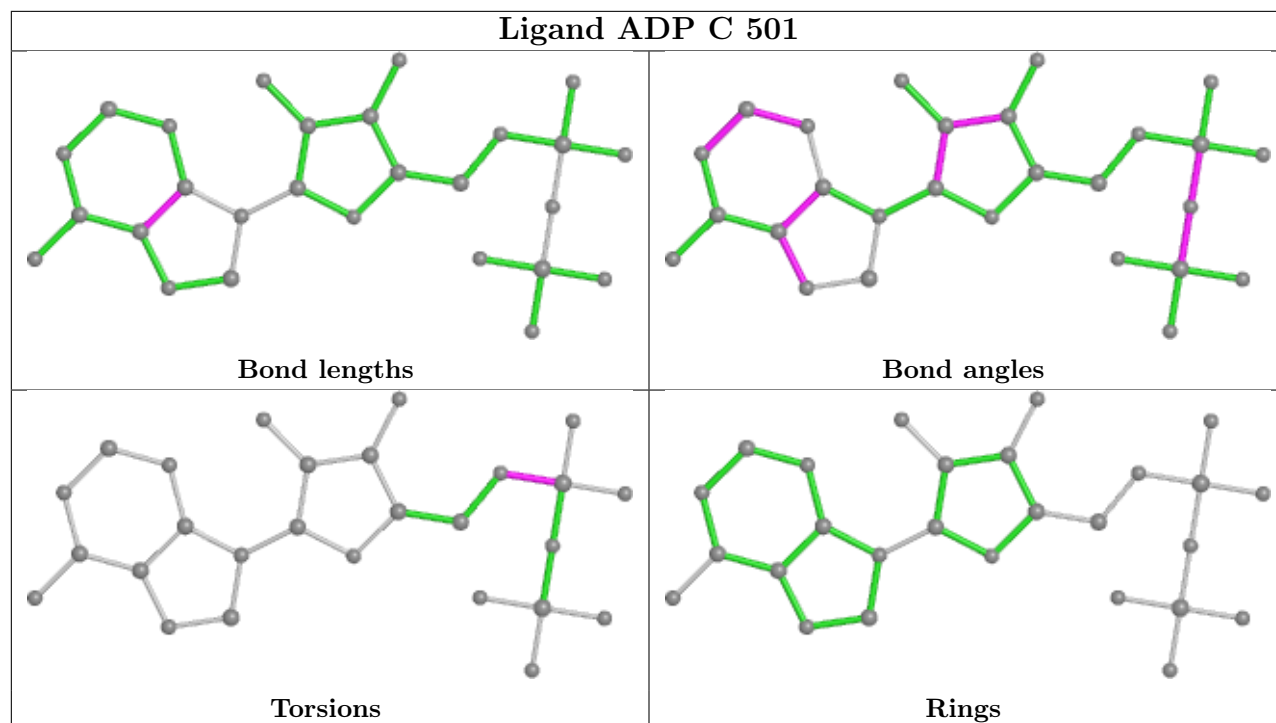
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	PB-O3B-PG-O2G
35	E	501	ATP	C5'-O5'-PA-O1A
37	C	501	ADP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

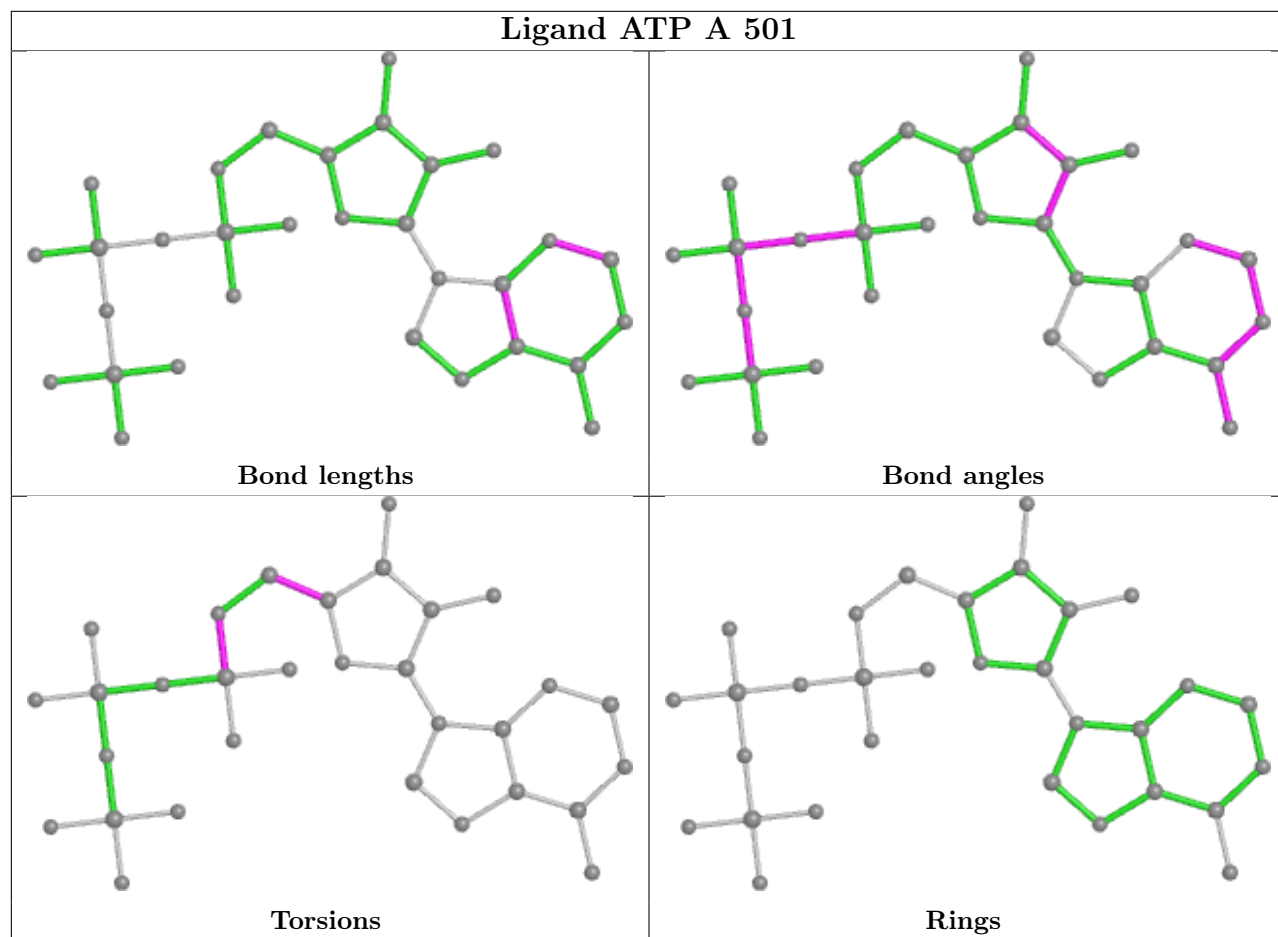
No monomer is involved in short contacts.

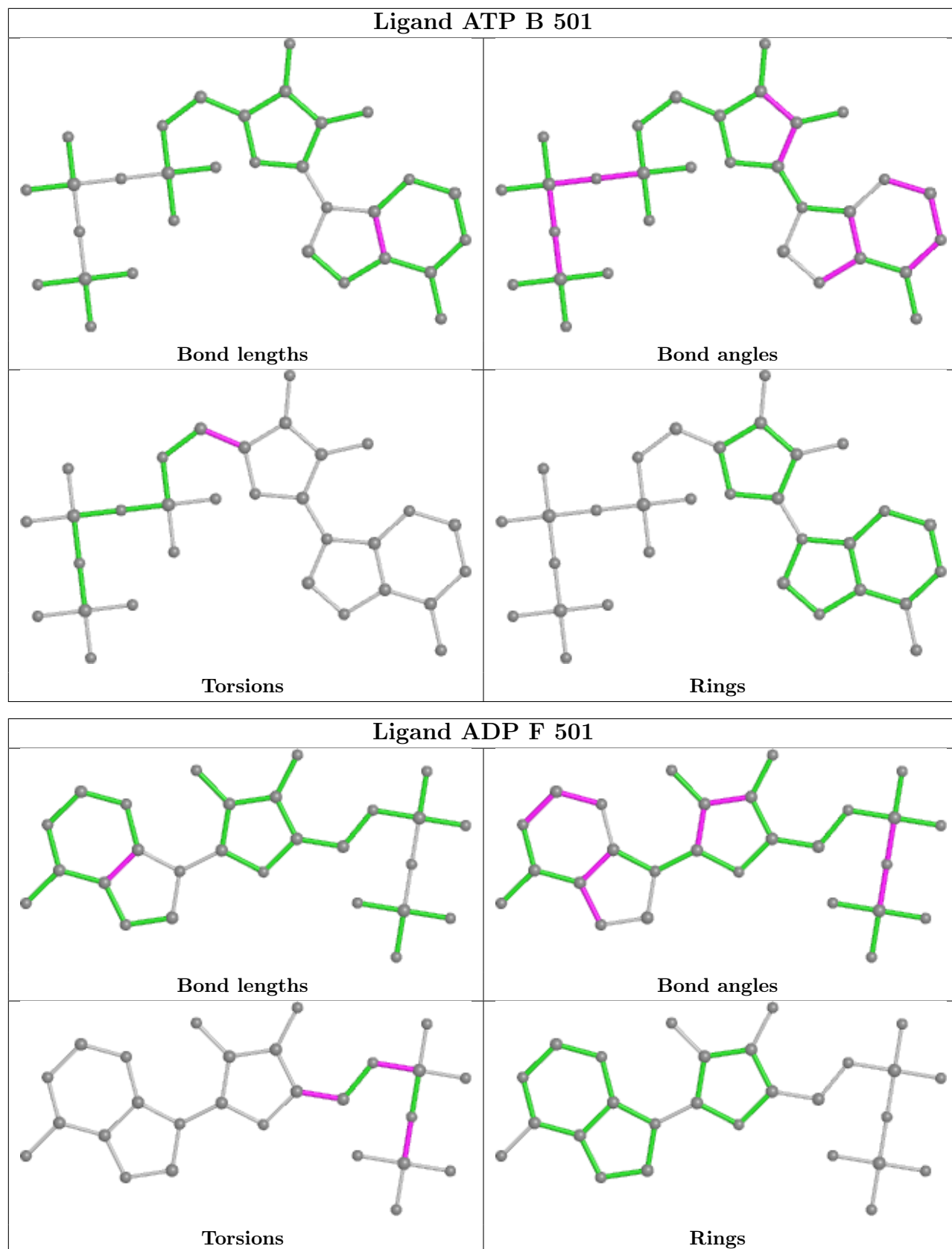
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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.

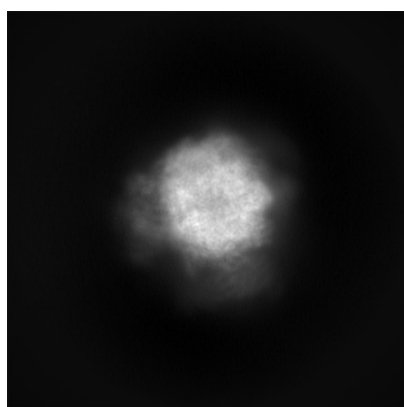
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32273. These allow visual inspection of the internal detail of the map and identification of artifacts.

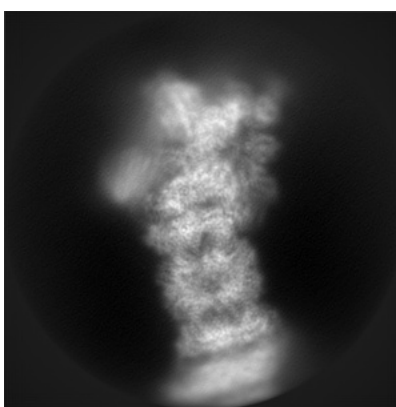
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

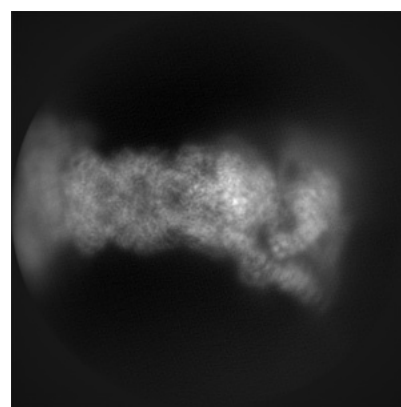
#### 6.1.1 Primary map



X



Y

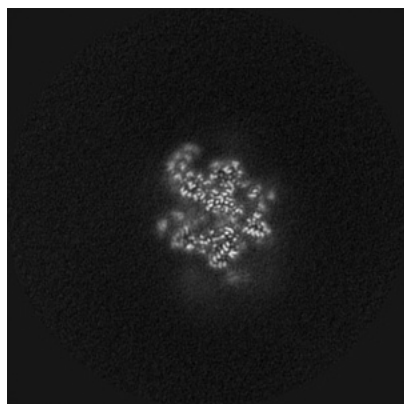


Z

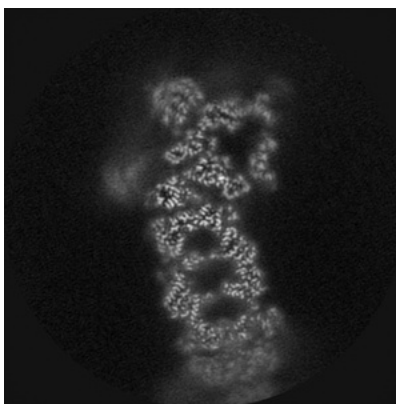
The images above show the map projected in three orthogonal directions.

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

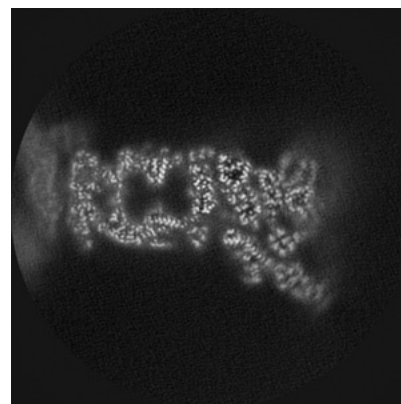
#### 6.2.1 Primary map



X Index: 320



Y Index: 320

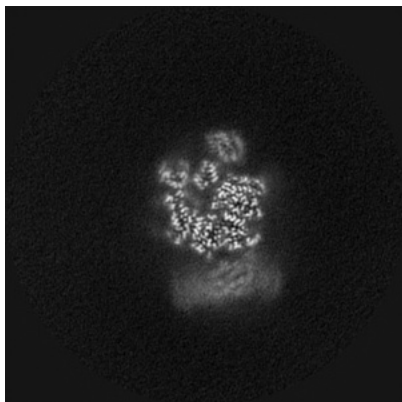


Z Index: 320

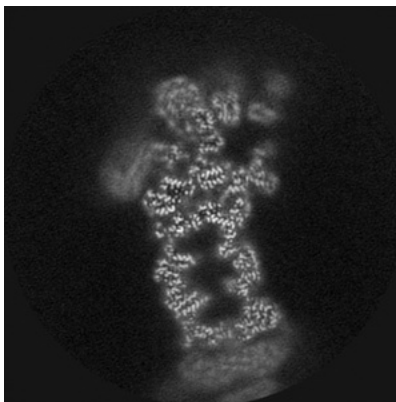
The images above show central slices of the map in three orthogonal directions.

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

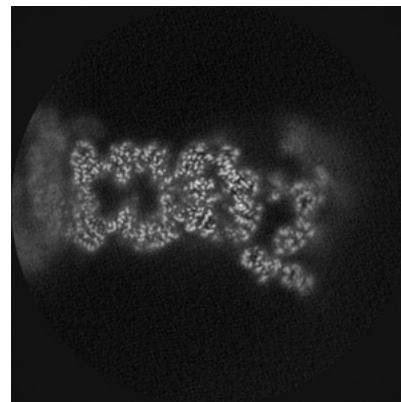
### 6.3.1 Primary map



X Index: 349



Y Index: 335



Z Index: 348

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

## 6.4 Orthogonal surface views [i](#)

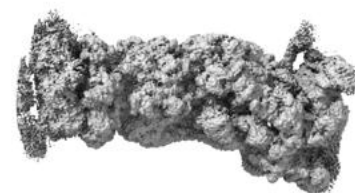
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

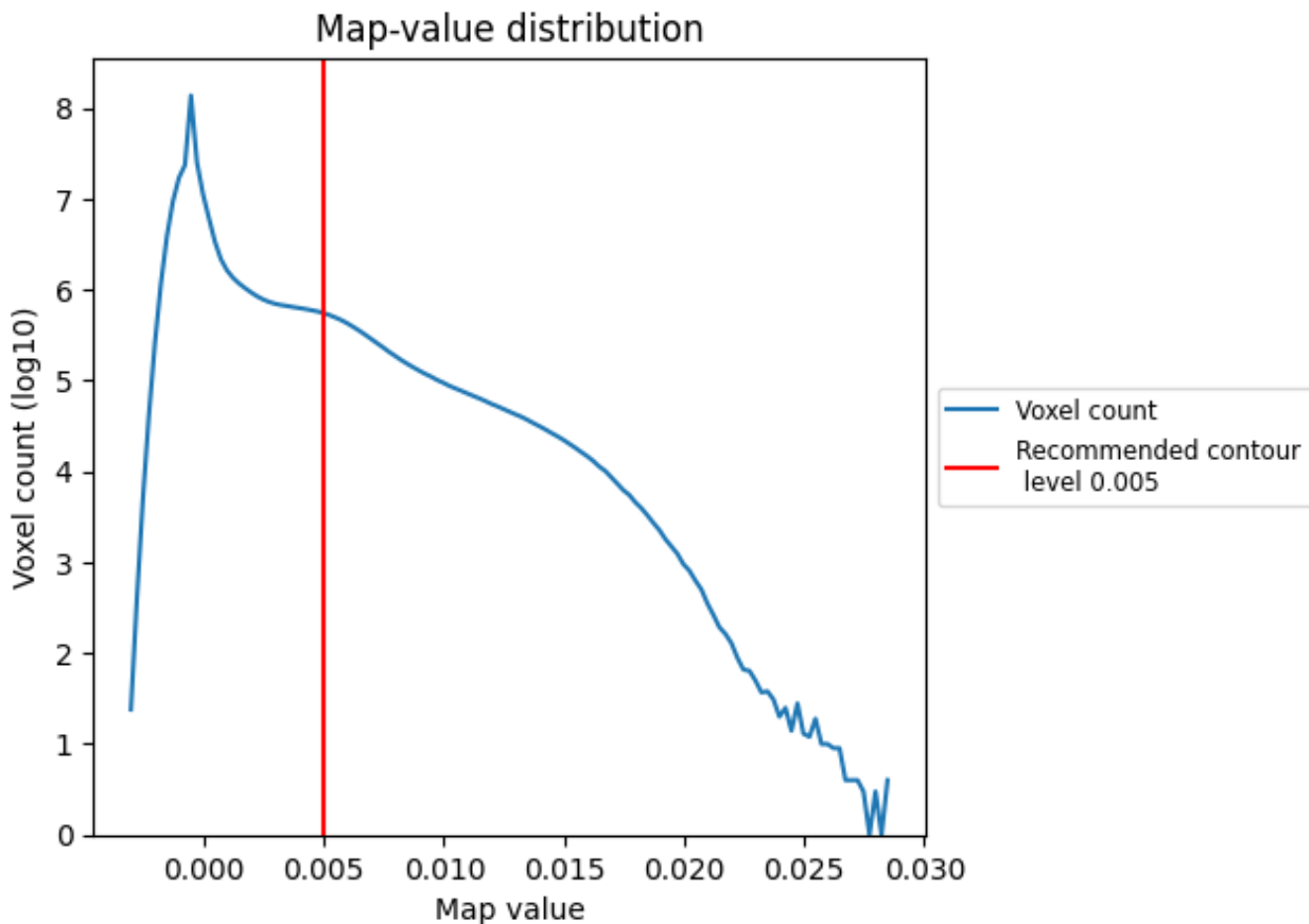
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

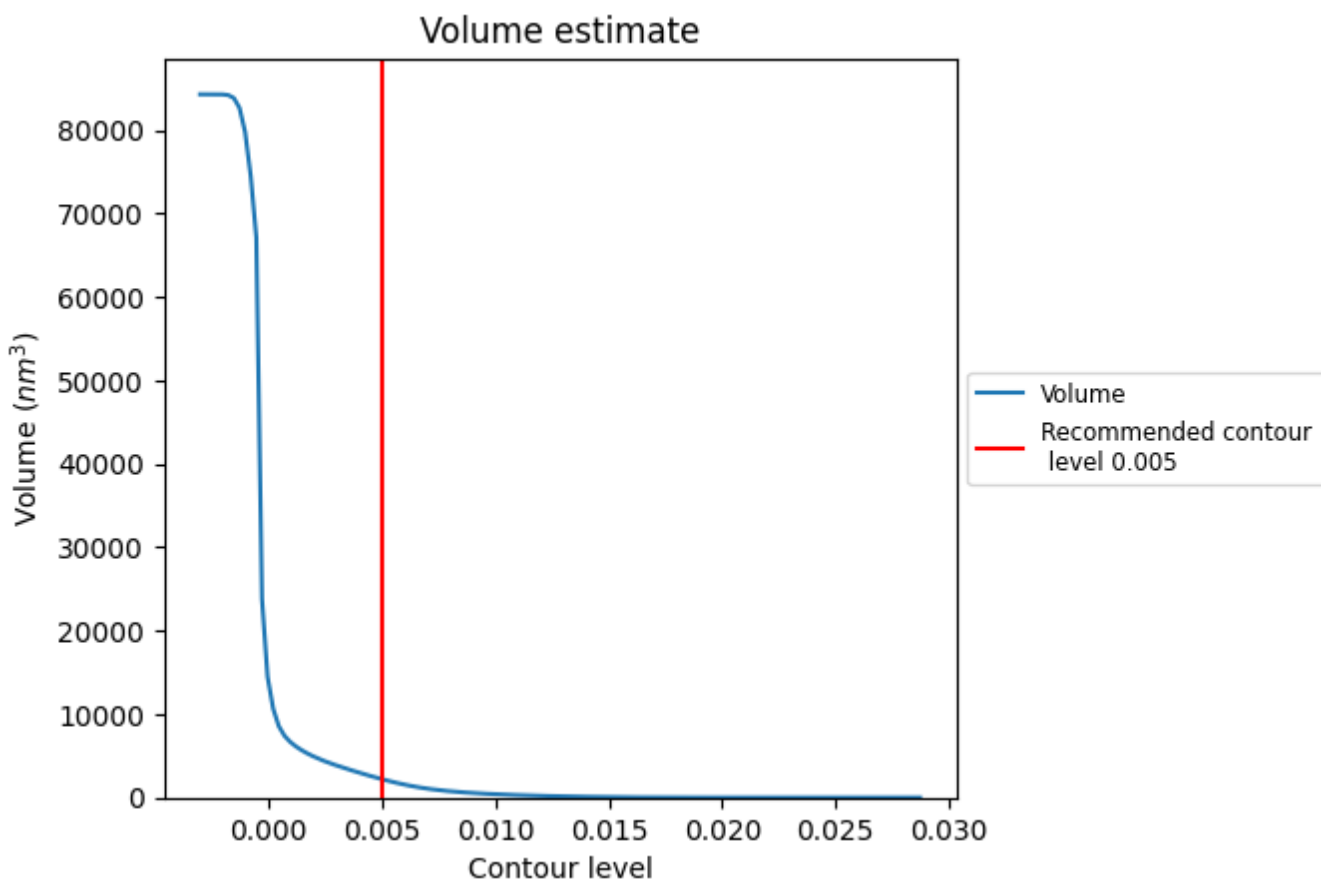
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

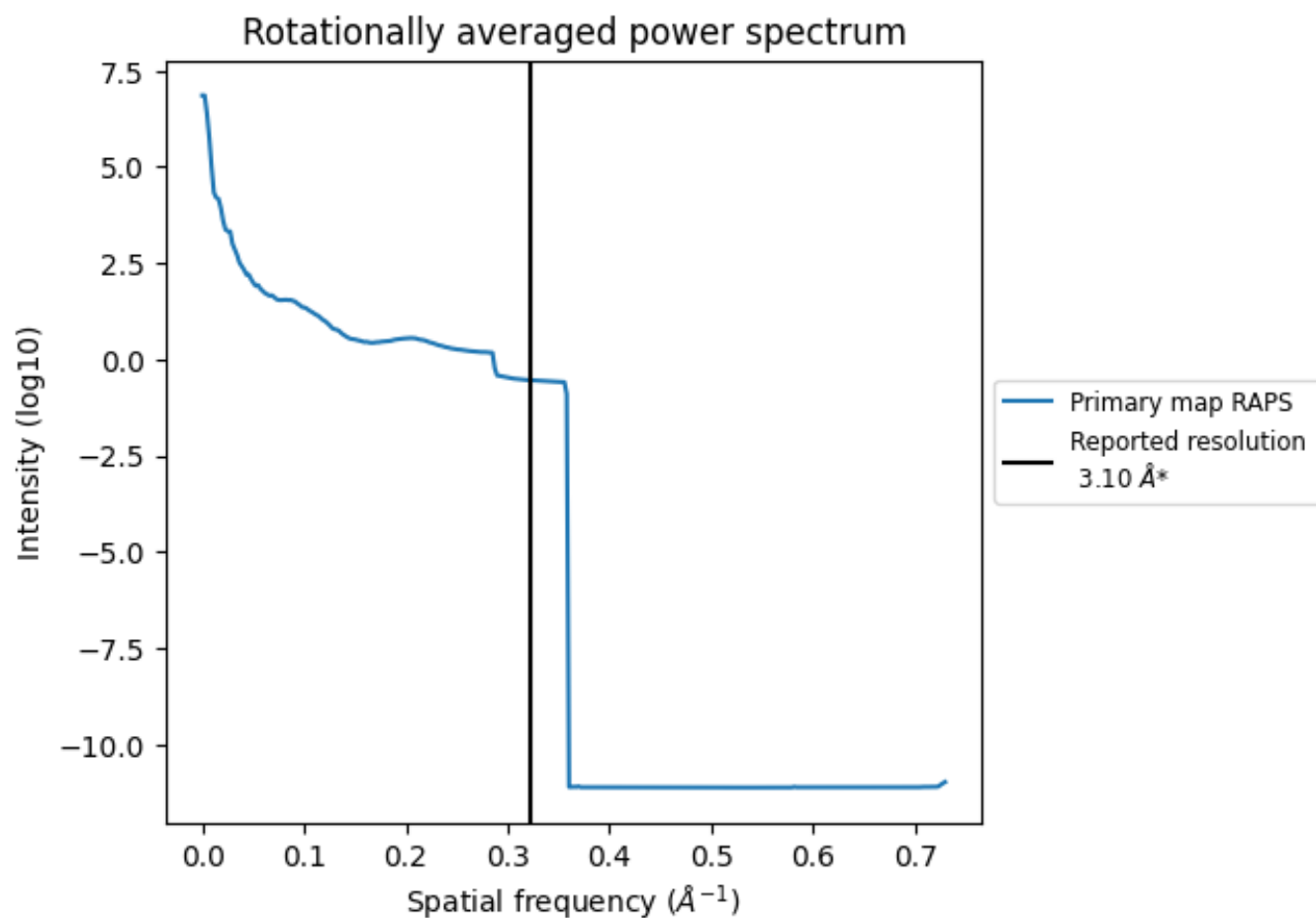


The volume at the recommended contour level is  $2193 \text{ nm}^3$ ; this corresponds to an approximate mass of 1981 kDa.

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

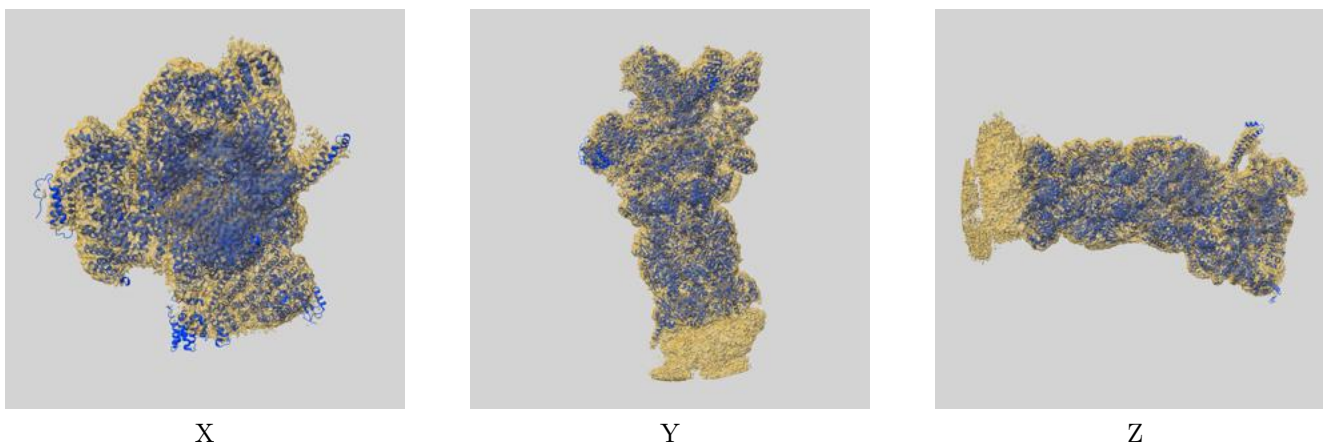
## 8 Fourier-Shell correlation

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

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

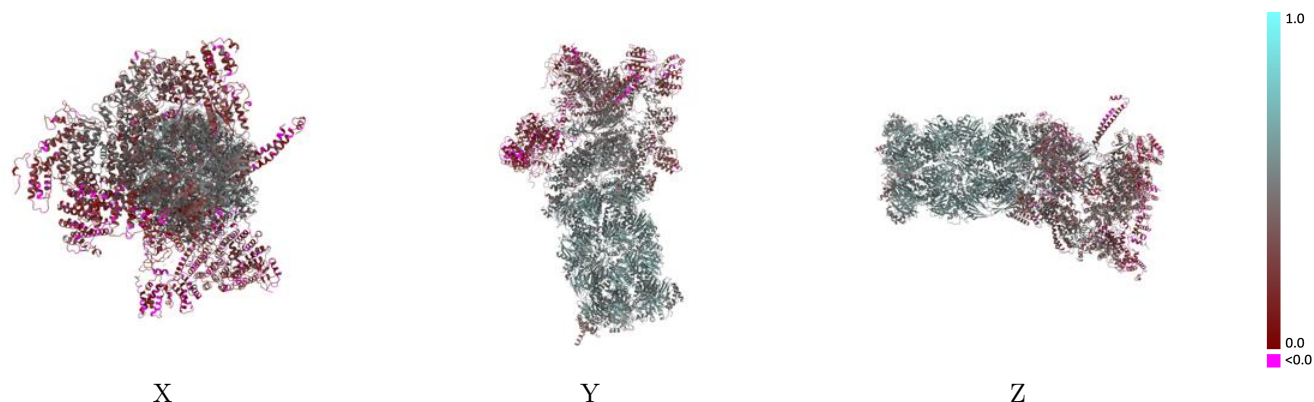
This section contains information regarding the fit between EMDB map EMD-32273 and PDB model 7W38. Per-residue inclusion information can be found in section 3 on page 13.

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



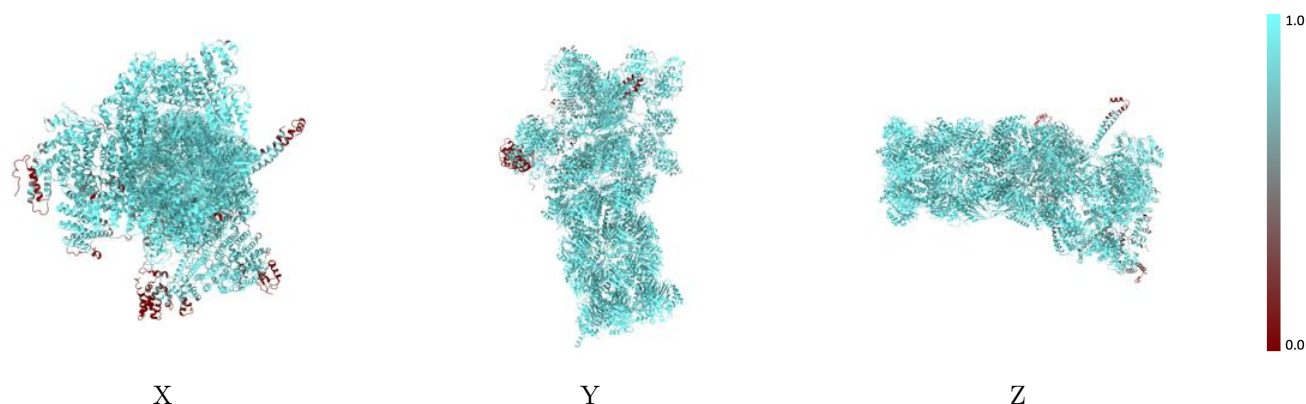
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



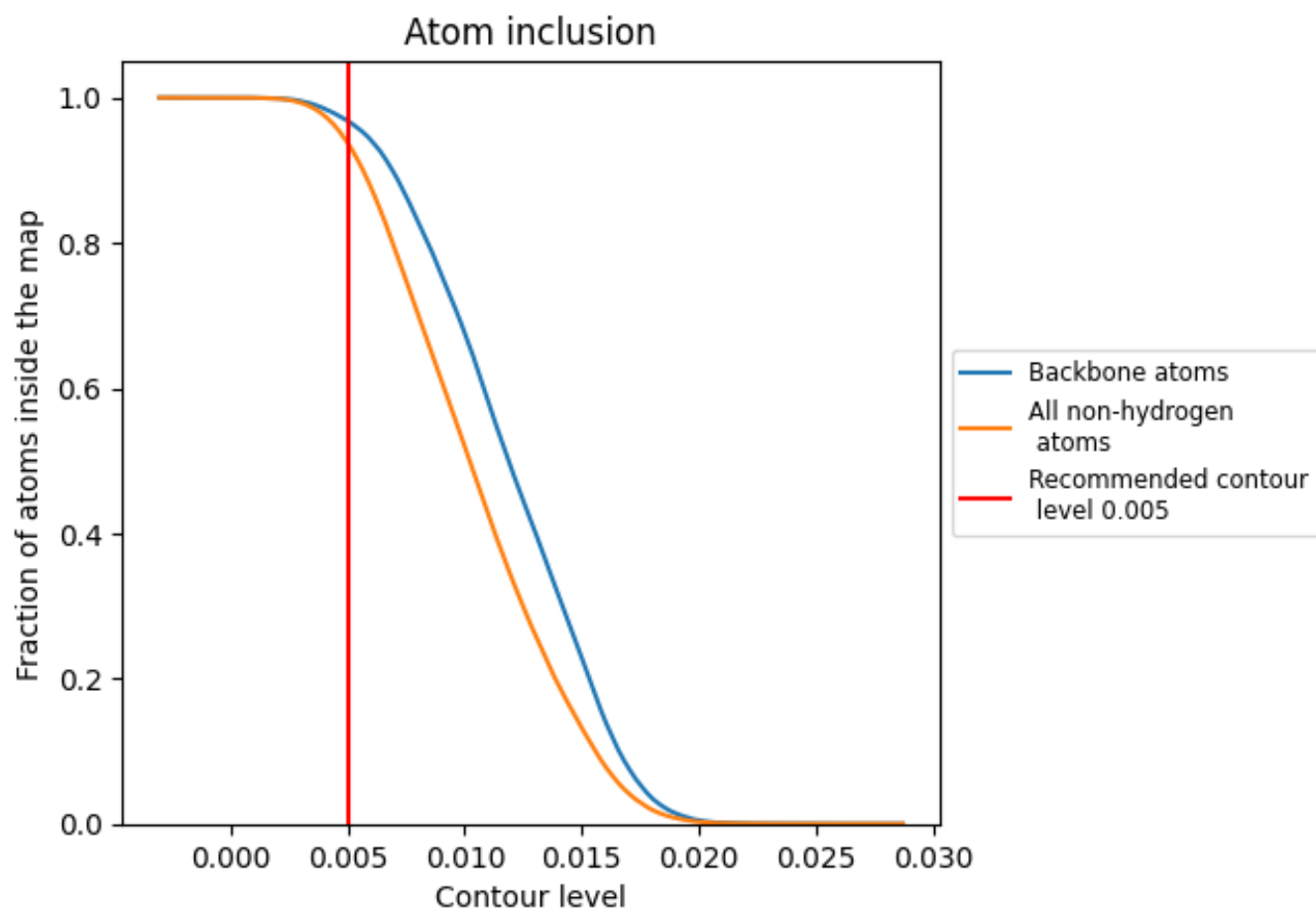
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9379	 0.4200
A	 0.9345	 0.4190
B	 0.9709	 0.4200
C	 0.9765	 0.4370
D	 0.9807	 0.4350
E	 0.9693	 0.4410
F	 0.9098	 0.4180
G	 0.9860	 0.5260
H	 0.9892	 0.5300
I	 0.9870	 0.5190
J	 0.9787	 0.4880
K	 0.9858	 0.5320
L	 0.9907	 0.5430
M	 0.9875	 0.5290
N	 0.9939	 0.5620
O	 0.9945	 0.5490
P	 0.9968	 0.5570
Q	 0.9955	 0.5510
R	 0.9973	 0.5500
S	 0.9913	 0.5510
T	 0.9896	 0.5610
U	 0.8992	 0.2490
V	 0.8725	 0.2530
W	 0.9074	 0.3040
X	 0.9547	 0.3590
Y	 0.9518	 0.3740
Z	 0.9458	 0.3600
a	 0.9071	 0.2760
b	 0.9146	 0.2090
c	 0.9633	 0.4000
d	 0.6638	 0.1910
e	 0.8926	 0.2990
f	 0.7742	 0.1590
g	 0.9756	 0.5260
h	 0.9904	 0.5320



*Continued on next page...*

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Chain	Atom inclusion	Q-score
i	 0.9703	 0.5040
j	 0.9752	 0.4660
k	 0.9785	 0.5160
l	 0.9884	 0.5330
m	 0.9810	 0.5240
n	 0.9946	 0.5690
o	 0.9914	 0.5590
p	 0.9955	 0.5590
q	 0.9968	 0.5540
r	 0.9967	 0.5620
s	 0.9926	 0.5560
t	 0.9909	 0.5630
u	 0.8953	 0.3760
x	 0.1458	 0.1300