



# wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 10:49 PM JST

PDB ID : 9K5B / pdb\_00009k5b  
EMDB ID : EMD-62087  
Title : Structure of substrate-engaged single-cap human proteasome in state ED0  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 3.80 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:

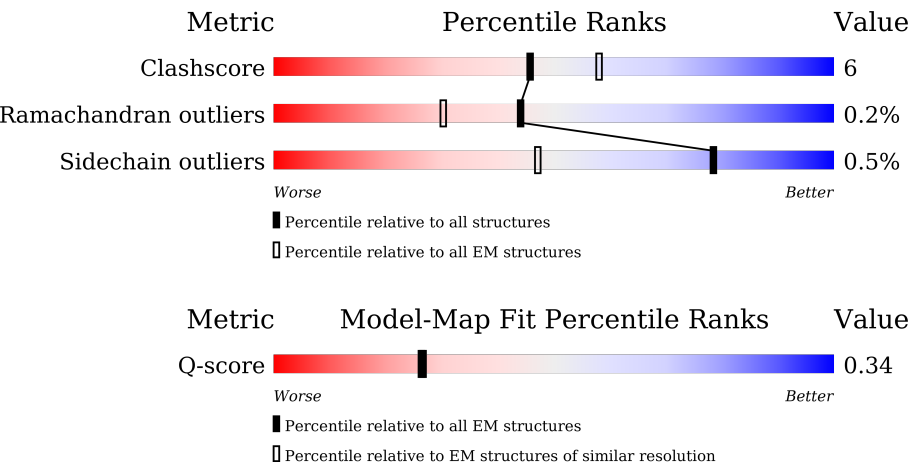
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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	<div><div>50%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>80%15%5%</div></div>
2	B	440	<div><div>29%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>76%18%7%</div></div>
3	C	398	<div><div>11%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%23%..</div></div>
4	D	418	<div><div>6%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>68%22%•9%</div></div>











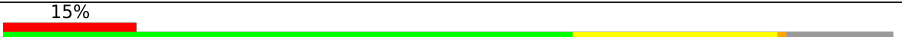


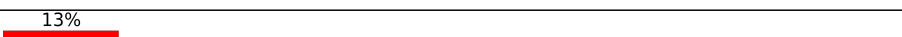
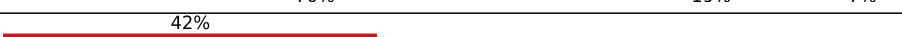
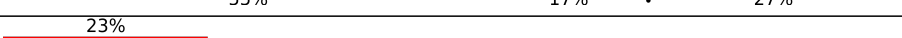
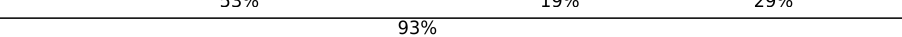
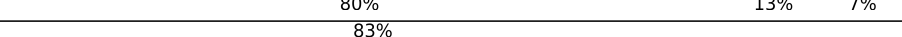
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	v	36	

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106328 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

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

- Molecule 17 is a protein called Proteasome subunit beta type-2.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1650	1044	283	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

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

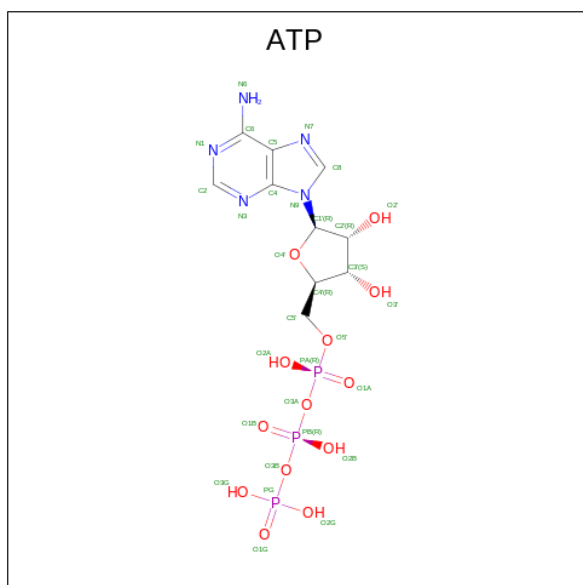
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

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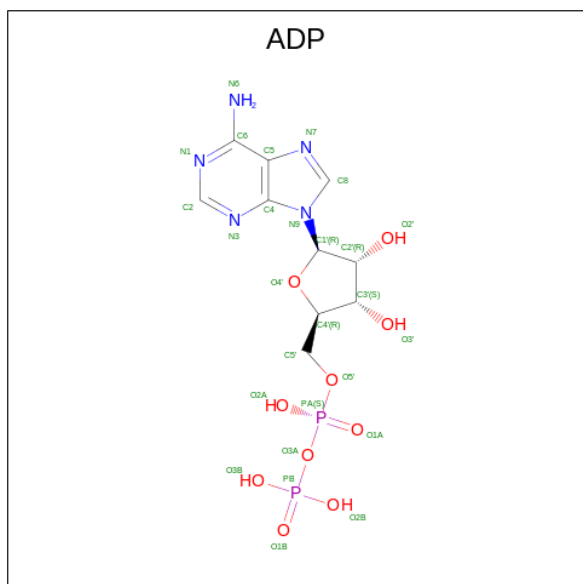
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Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: 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	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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).



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

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

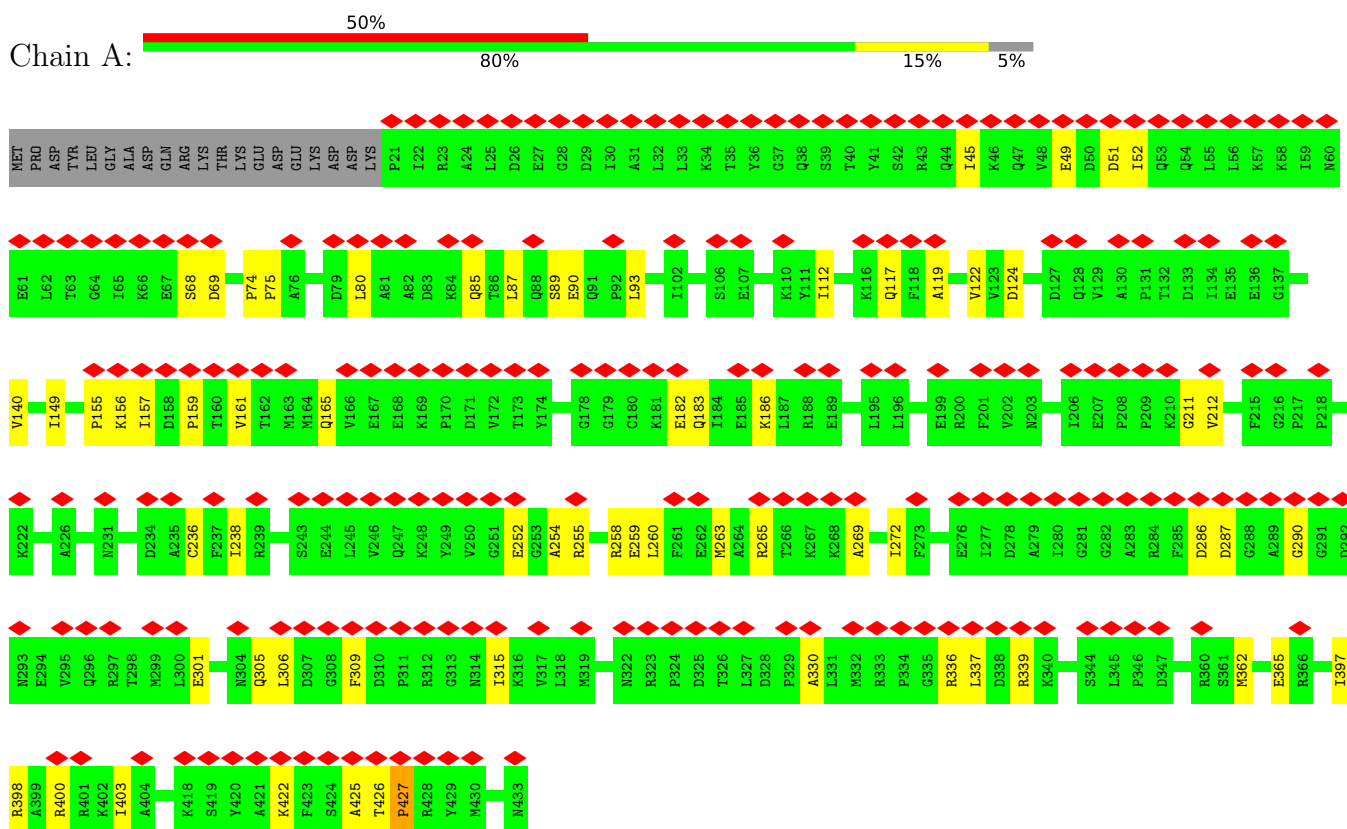
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

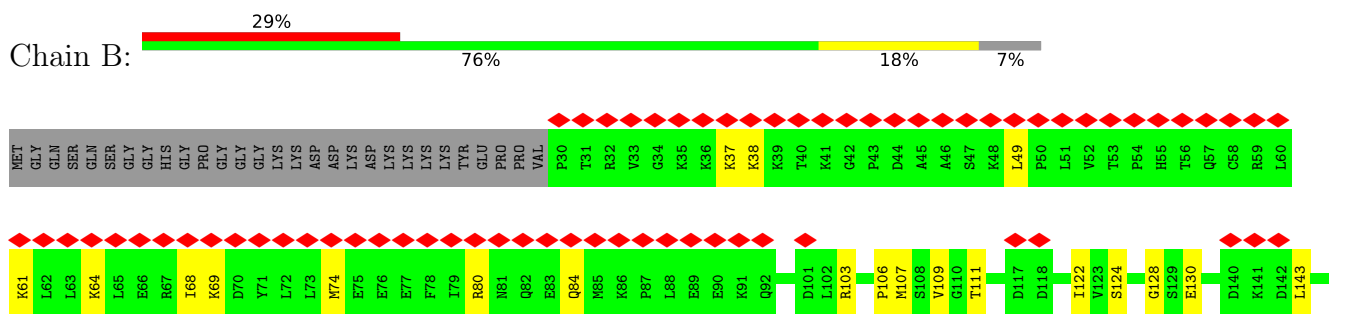
### 3 Residue-property plots

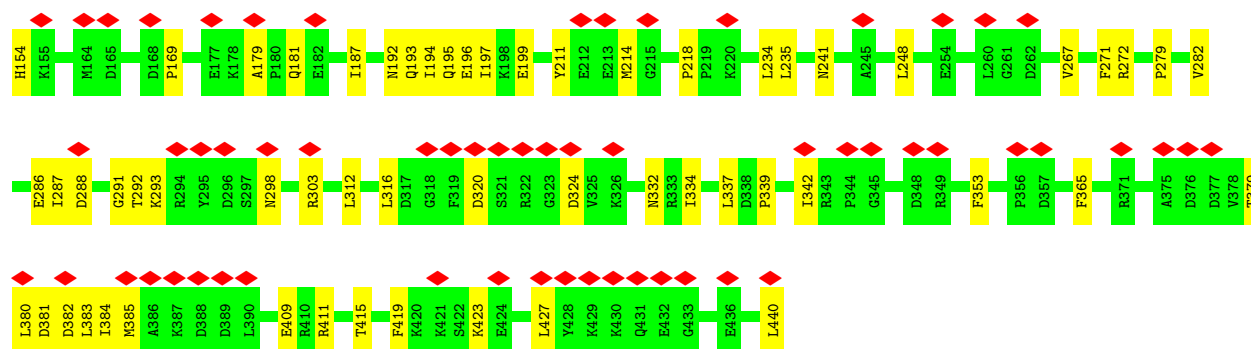
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 proteasome regulatory subunit 7

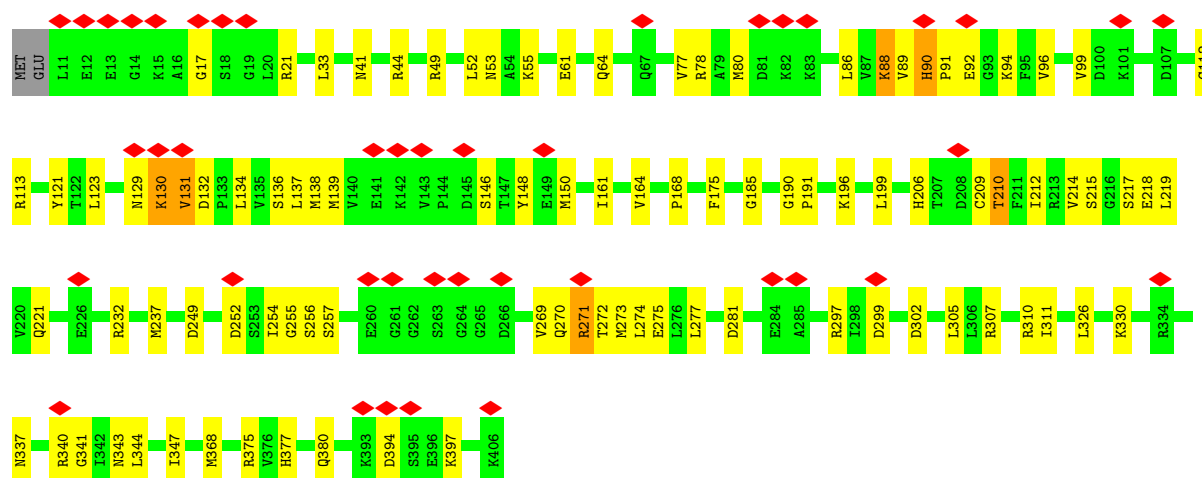


#### • Molecule 2: 26S proteasome regulatory subunit 4

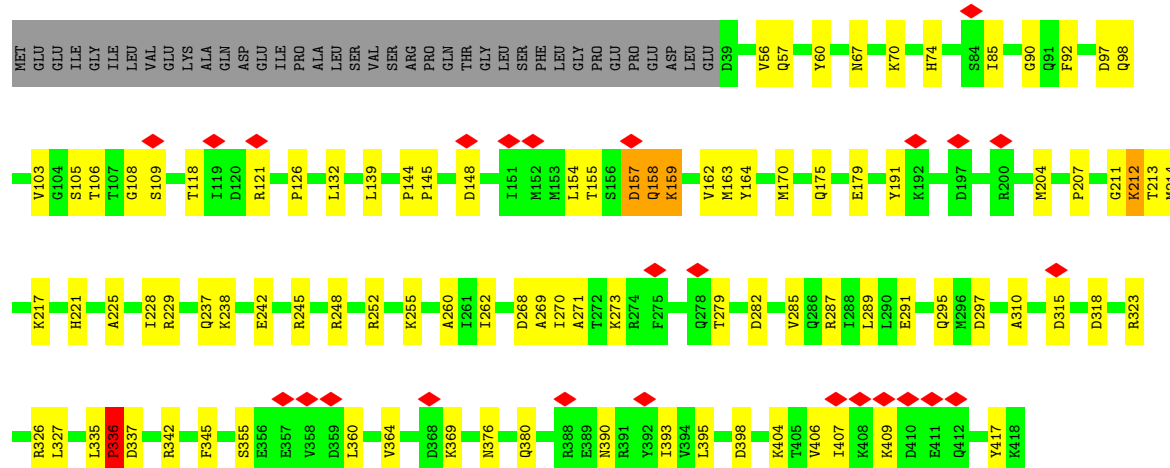




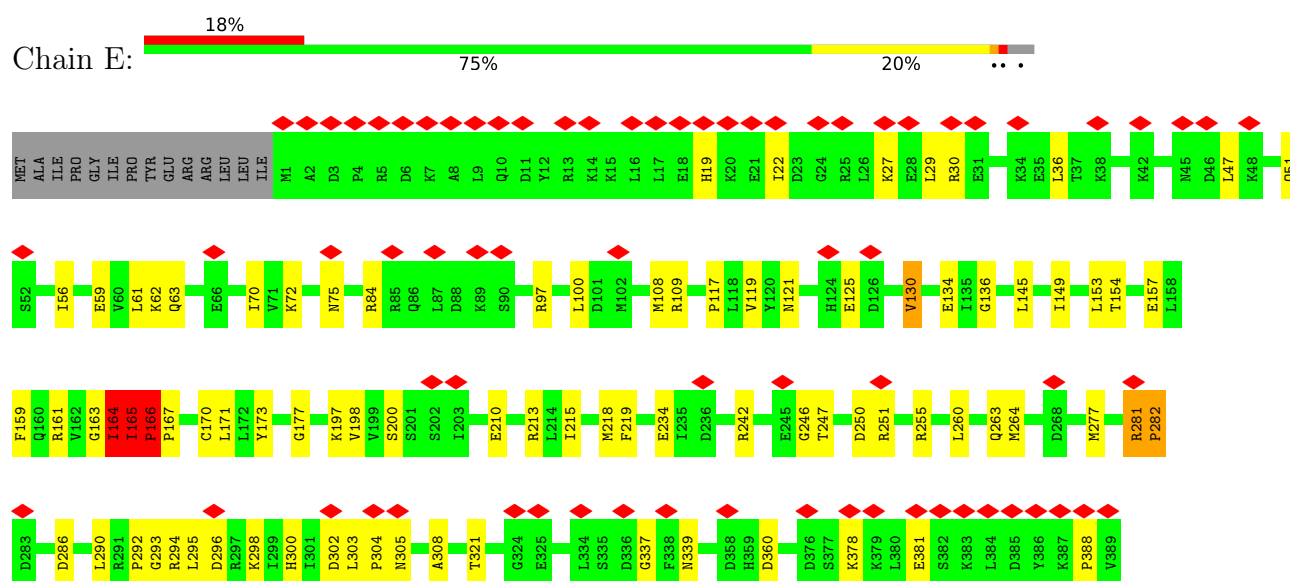
• Molecule 3: 26S proteasome regulatory subunit 8



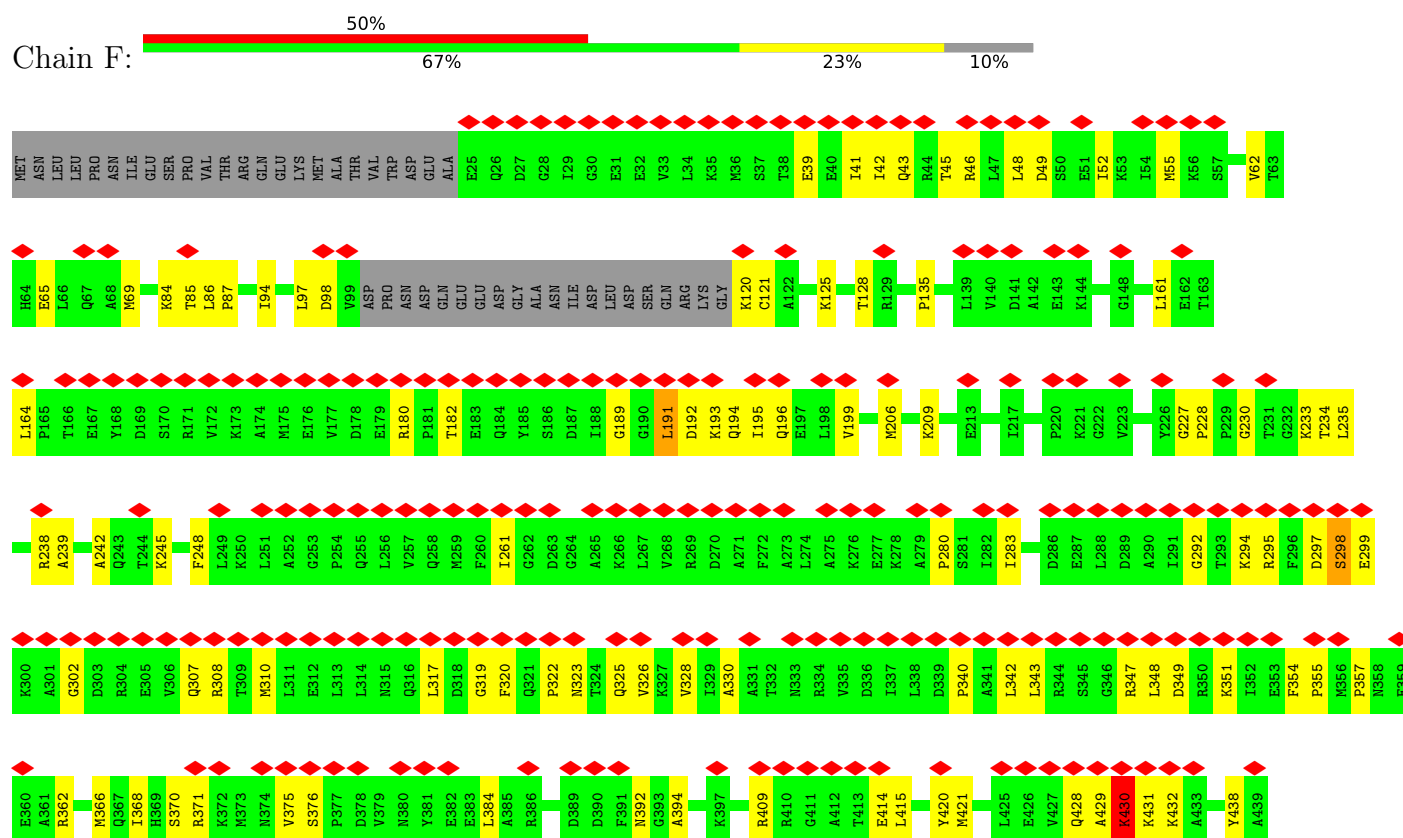
• Molecule 4: 26S proteasome regulatory subunit 6B



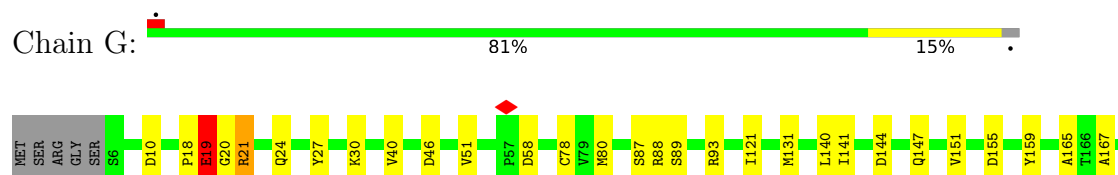
• Molecule 5: Proteasome 26S subunit, ATPase 6



• Molecule 6: 26S proteasome regulatory subunit 6A

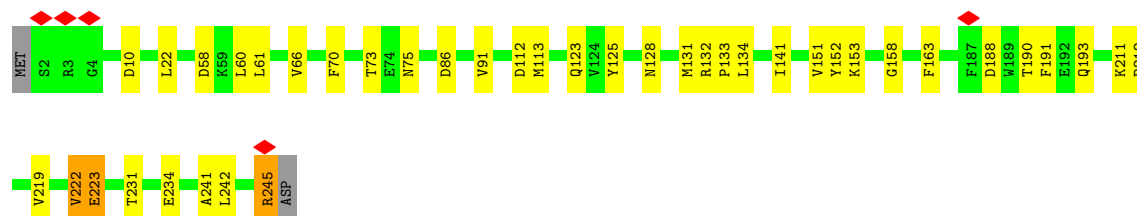
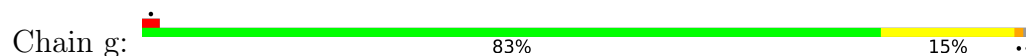


• Molecule 7: Proteasome subunit alpha type-6

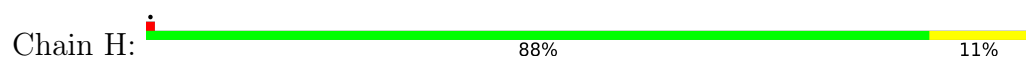




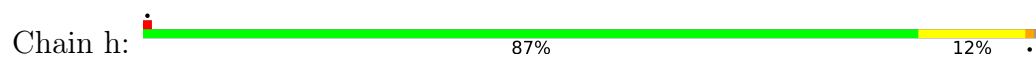
- Molecule 7: Proteasome subunit alpha type-6



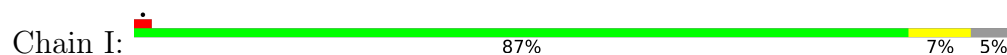
- Molecule 8: Proteasome subunit alpha type-2



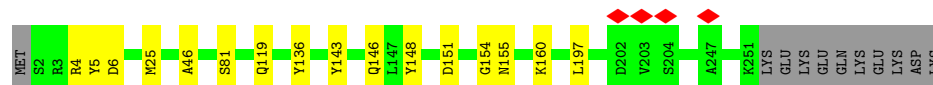
- Molecule 8: Proteasome subunit alpha type-2



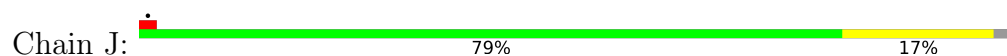
- Molecule 9: Proteasome subunit alpha type-4



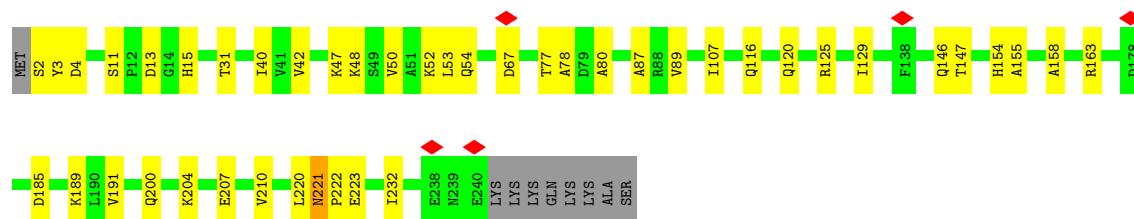
- Molecule 9: Proteasome subunit alpha type-4



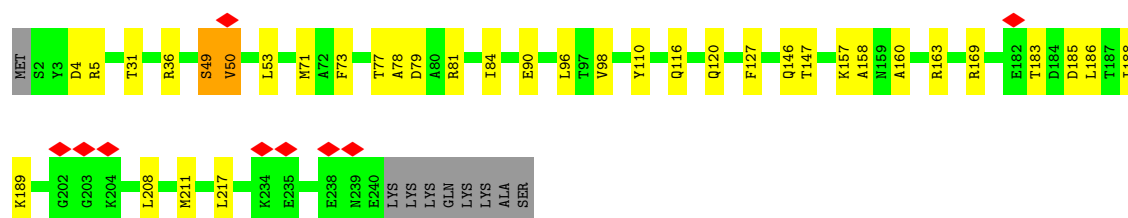
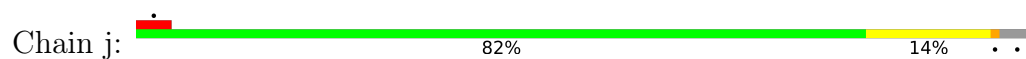
- Molecule 10: Proteasome subunit alpha type-7







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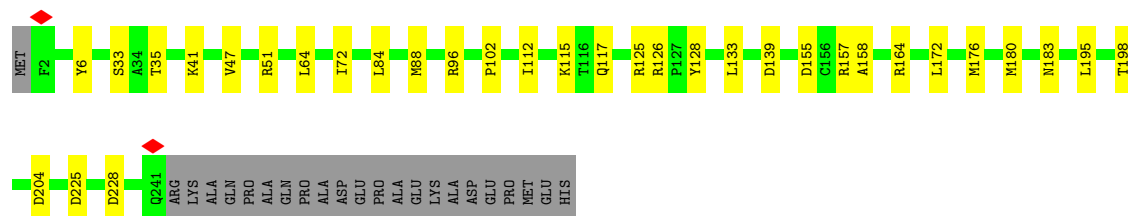
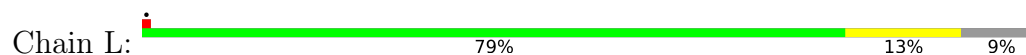
- Molecule 11: Proteasome subunit alpha type-5



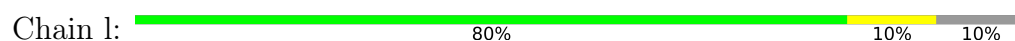
- Molecule 11: Proteasome subunit alpha type-5

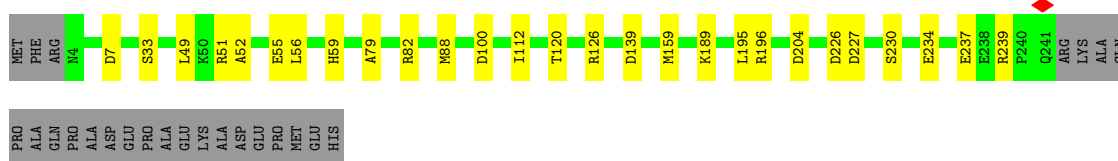


- Molecule 12: Proteasome subunit alpha type-1



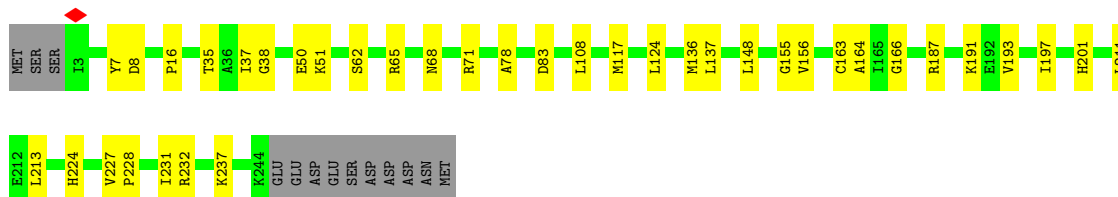
- Molecule 12: Proteasome subunit alpha type-1





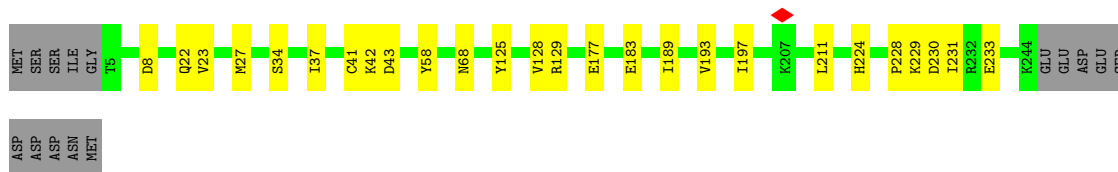
• Molecule 13: Proteasome subunit alpha type-3

Chain M: 80% 15% 5%



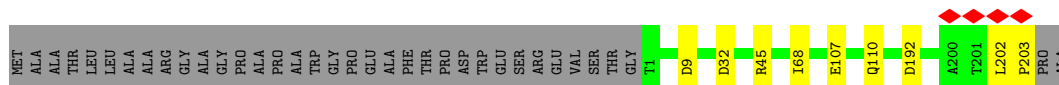
• Molecule 13: Proteasome subunit alpha type-3

Chain m: 84% 10% 6%



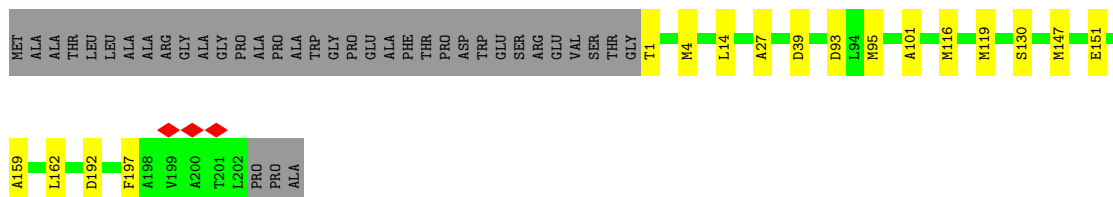
• Molecule 14: Proteasome subunit beta type-6

Chain N: 81% 15%



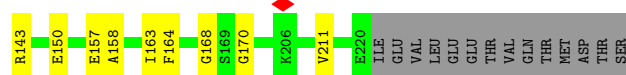
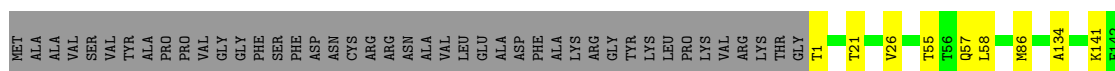
• Molecule 14: Proteasome subunit beta type-6

Chain n: 77% 7% 15%

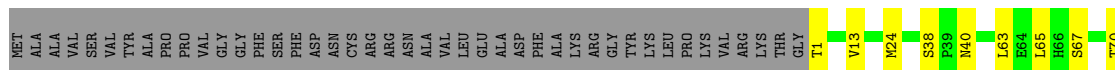


• Molecule 15: Proteasome subunit beta type-7

Chain O: 73% 6% 21%



• Molecule 15: Proteasome subunit beta type-7



• Molecule 16: Proteasome subunit beta type-3



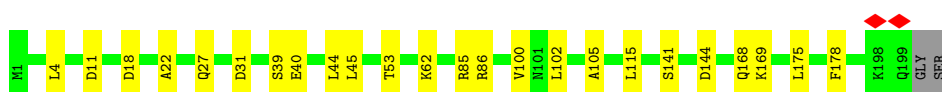
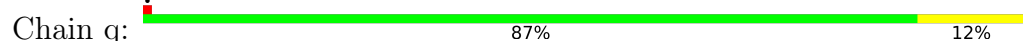
• Molecule 16: Proteasome subunit beta type-3



• Molecule 17: Proteasome subunit beta type-2

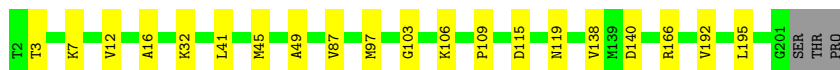
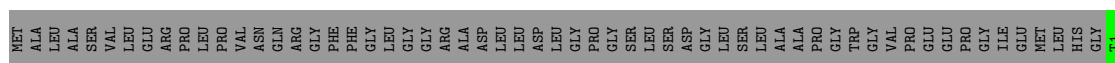


• Molecule 17: Proteasome subunit beta type-2



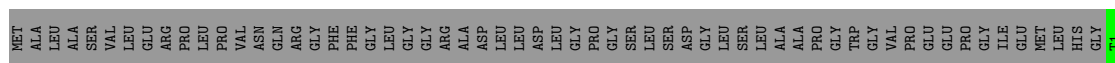
• Molecule 18: Proteasome subunit beta type-5






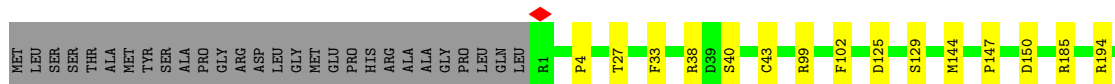
• Molecule 18: Proteasome subunit beta type-5

Chain r:  70% 7% 24%



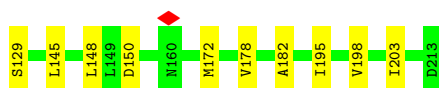
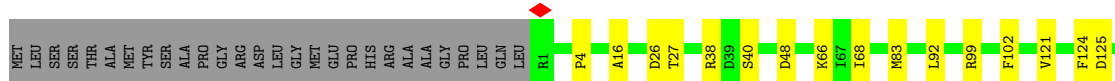
• Molecule 19: Proteasome subunit beta type-1

Chain S:  80% 8% 12%



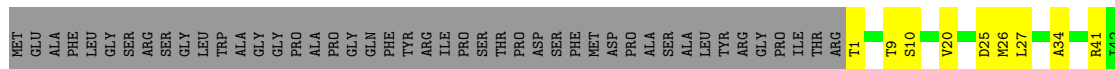
• Molecule 19: Proteasome subunit beta type-1

Chain s:  78% 11% 12%



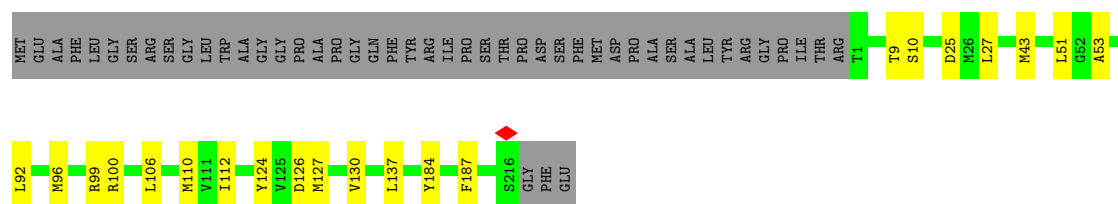
• Molecule 20: Proteasome subunit beta type-4

Chain T:  68% 14% 18%




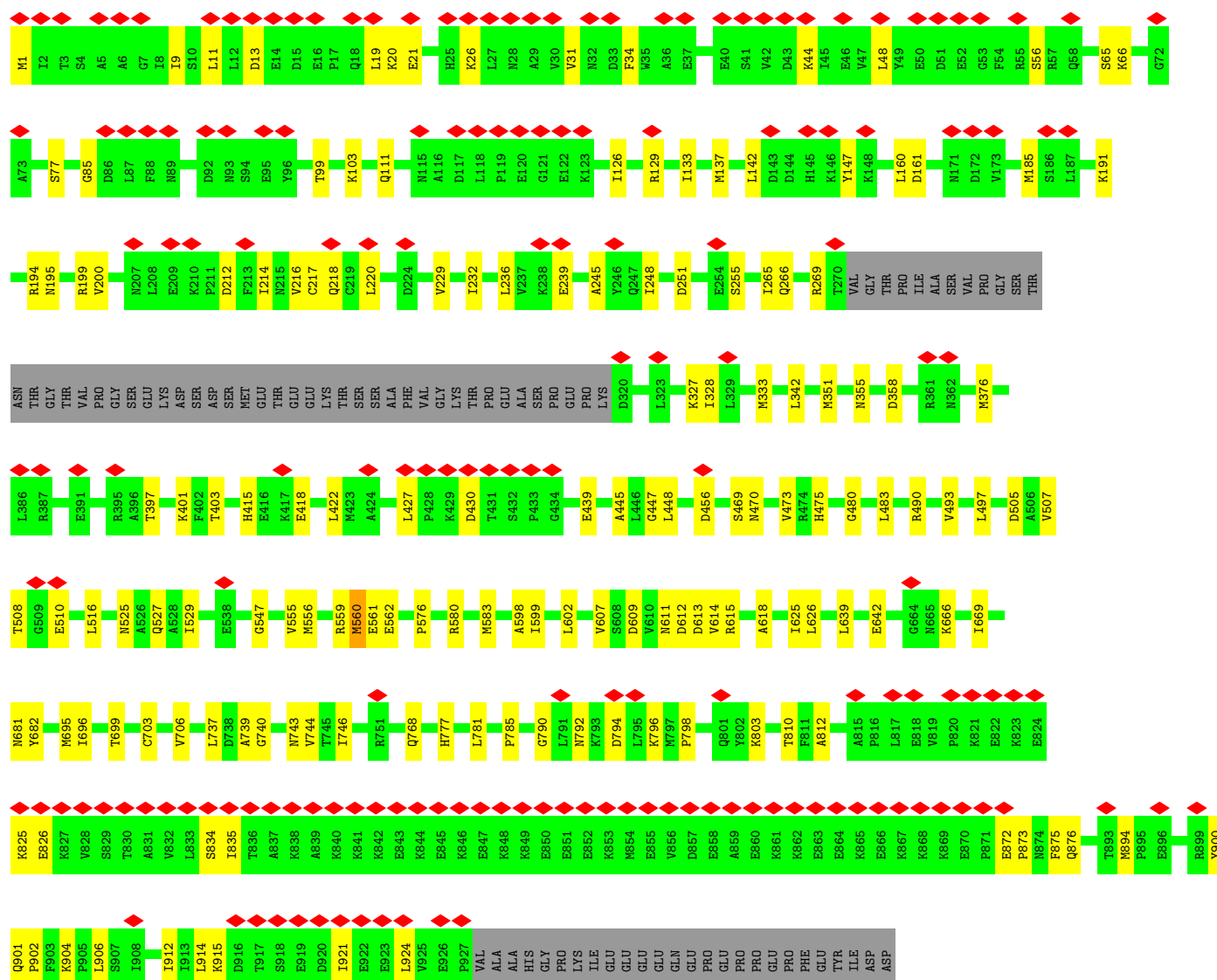
• Molecule 20: Proteasome subunit beta type-4

Chain t:  74% 8% 18%



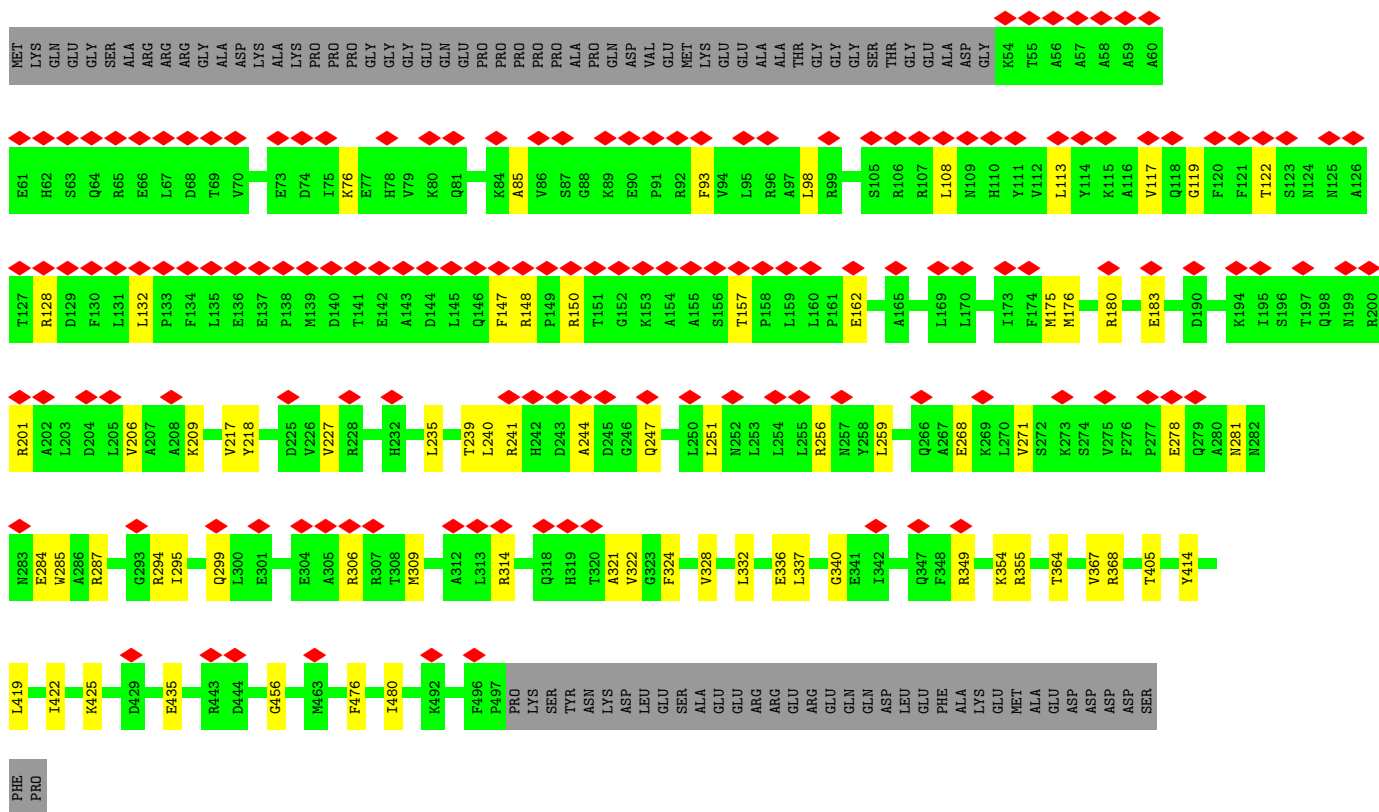
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:  19% 75% 17% 8%

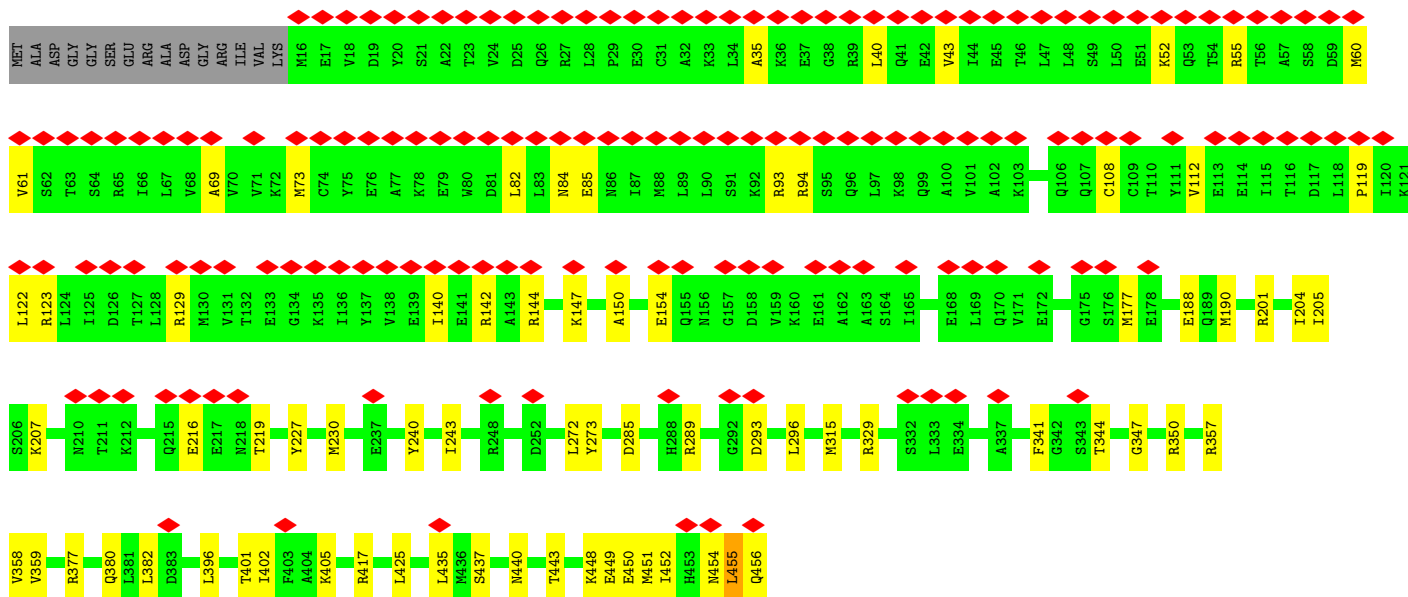
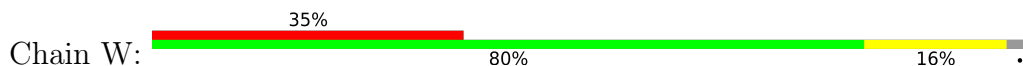


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

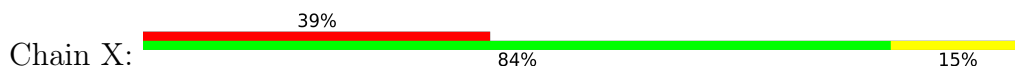
Chain V:  28% 70% 13% 17%

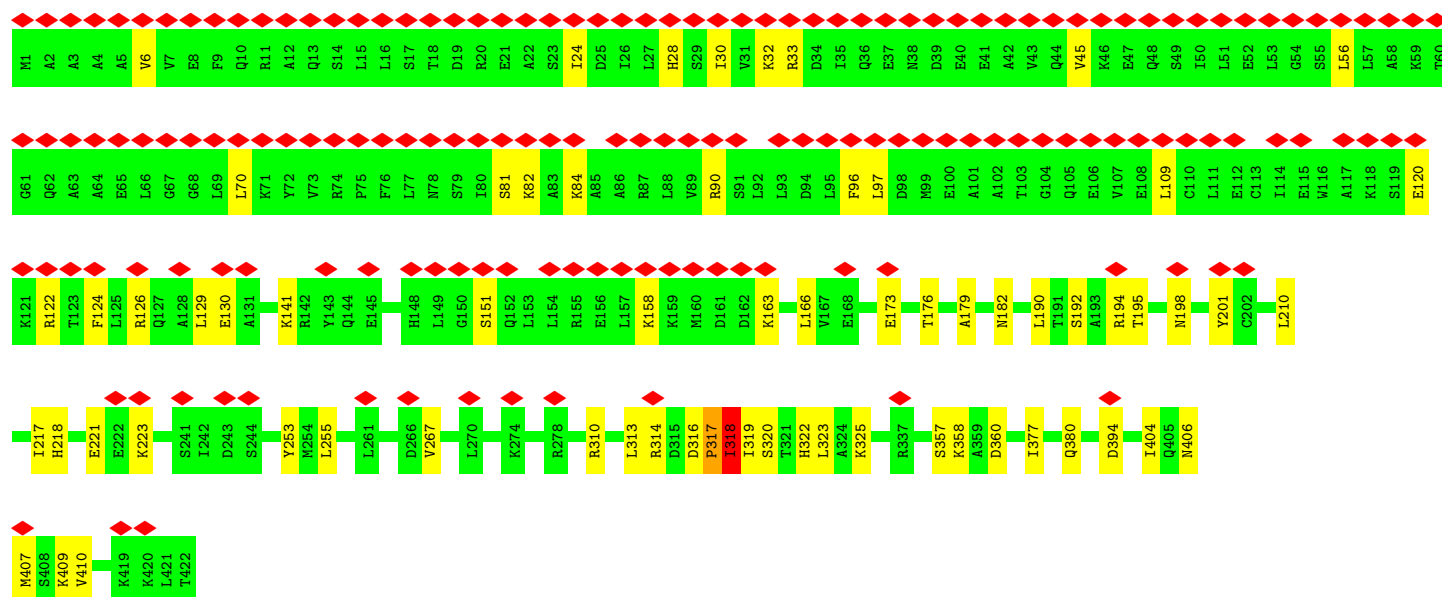


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

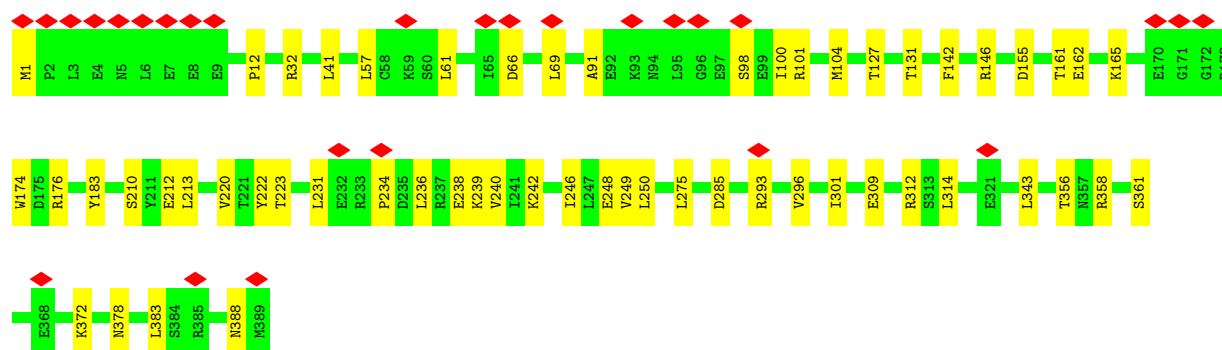
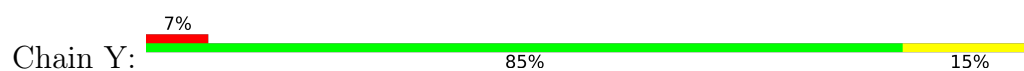


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

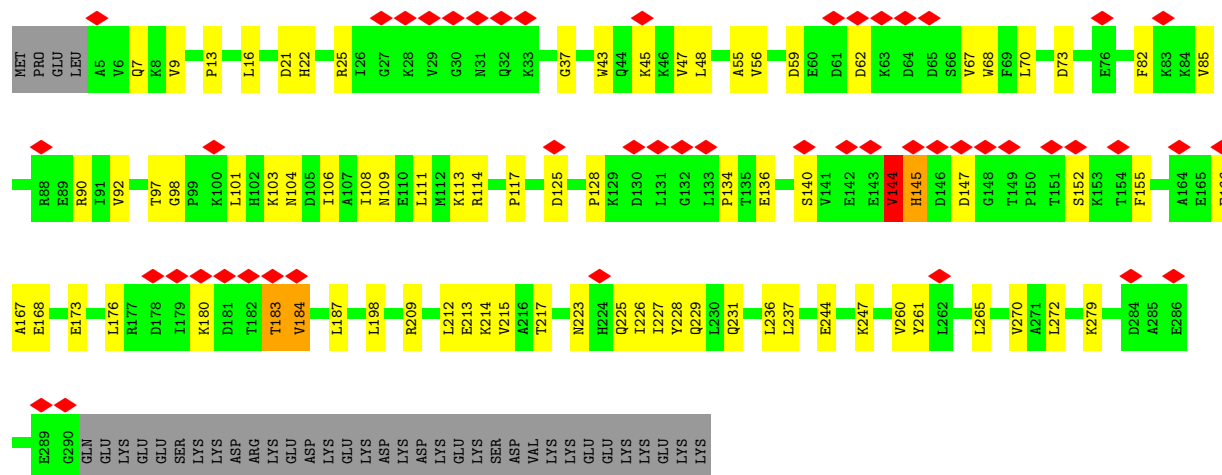


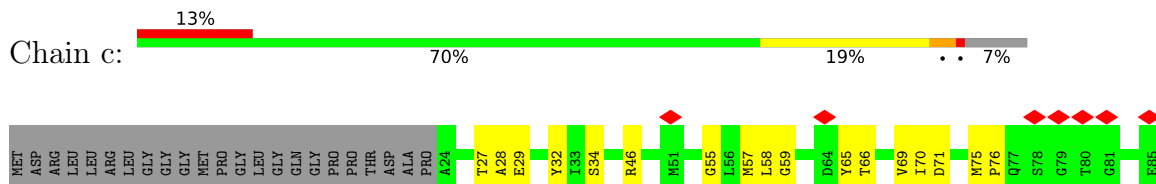


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

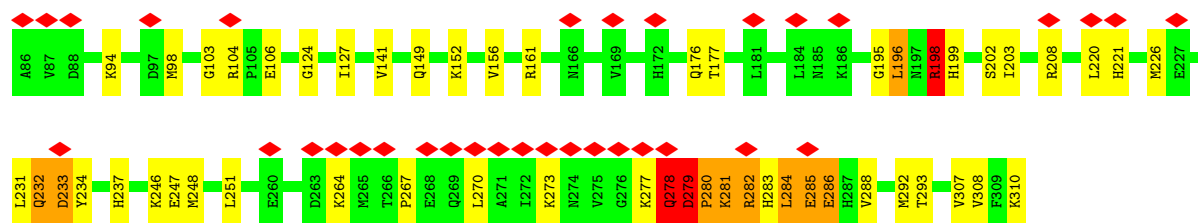


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

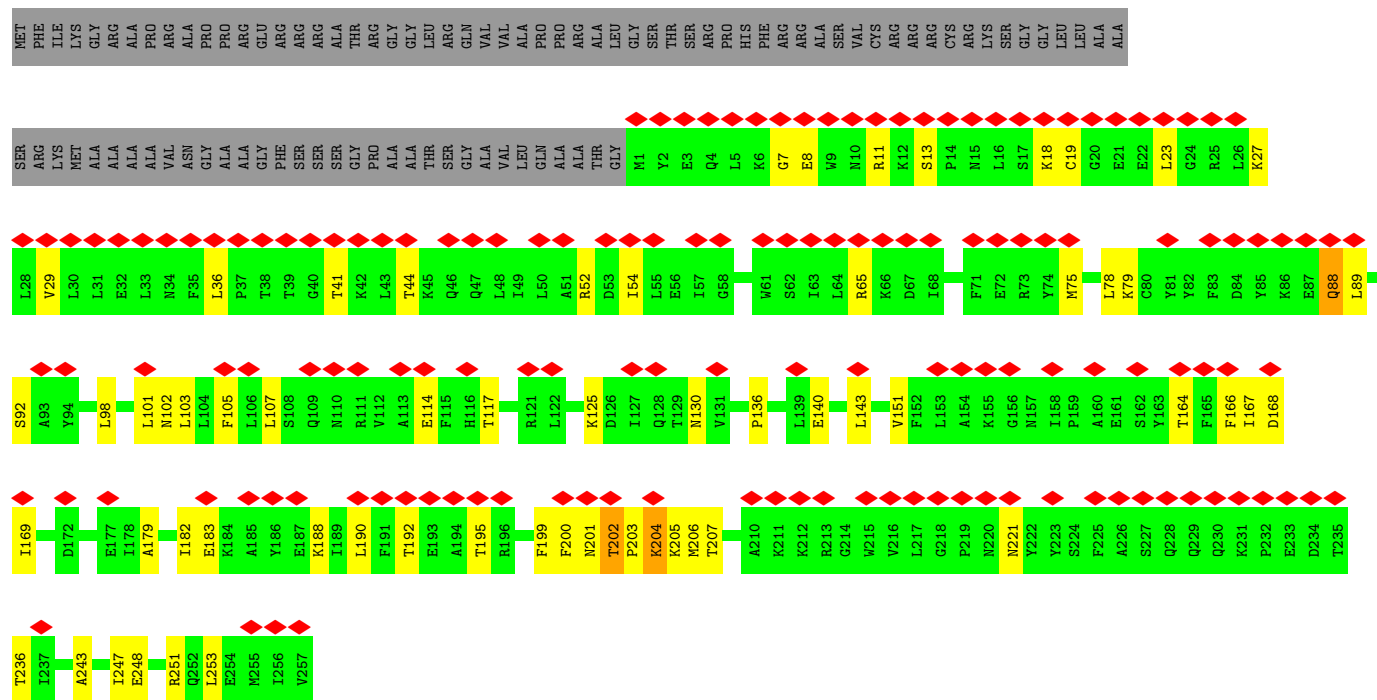
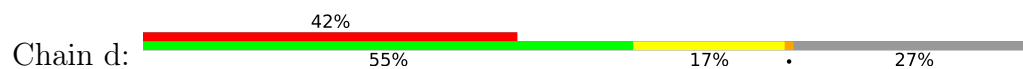




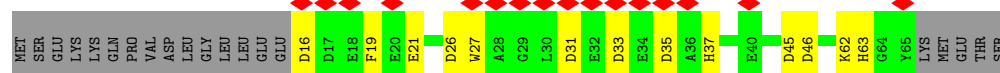




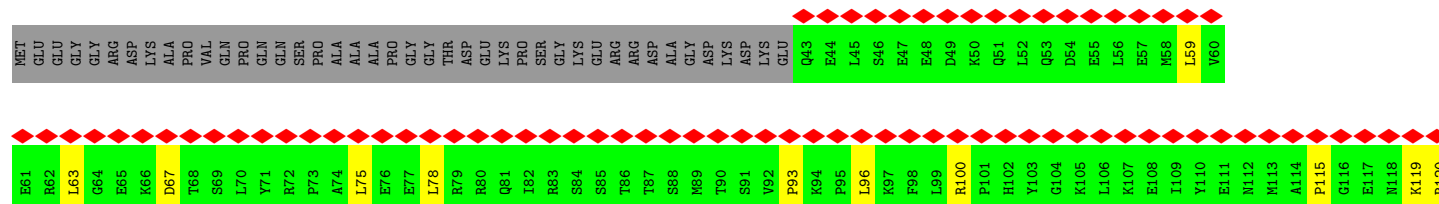
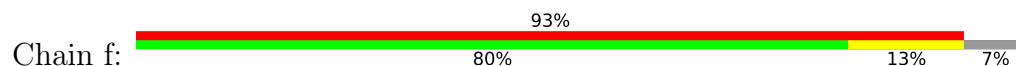
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1

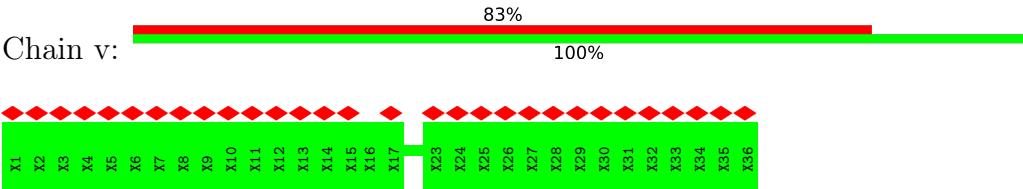


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



R901	P841	V781	V721	A661	A601	T541	S481	D421	S361	H301	P241	R181	F121
K902	V842	H782	S722	M662	G602	I542	I482	V422	G362	G302	E242	E182	A122
N903	S843	S783	S723	G663	S603	M543	F483	D423	S363	V303	P243	P183	A123
P904	V844	D784	M724	E664	G604	E544	G484	G424	Q364	F304	E244	L184	D124
N905	R845	R785	S725	E665	M605	K545	L485	G425	V365	E306	S246	T186	I125
Y906	V846	R786	T726	L666	V606	S546	G486	L426	D366	E307	S247	L187	I126
D907	G847	L787	F727	G667	L607	E547	L487	T427	S367	S308	A248	V188	S127
L908	Q848	M788	A728	T668	K608	T548	A488	Q428	A368	E309	L249	K189	V128
	A849	S789	M729	E669	V609	E549	Y489	I429	R369	E310	R250	E190	A130
	V850	Q790	G730	M670	Q610	L550	A490	D430	M370	D310	C251	I191	M131
	D851	V791	M731	A671	Q611	K551	G491	K431	N371	V311	C252	V192	T132
	V852	A792	V732	L672	L612	D552	S492	Y432	L372	E312	L253	P193	M133
	M853	V793	G733	R673	L613	T553	M493	L433	A373	E313	G254	Y194	G134
	C854	A794	S734	T674	H614	Y554	R494	Y434	S374	Y314	V255	N195	G135
	Q855	G795	G735	F675	L615	A555	E495	S435	S375	E315	V256	M196	E136
	A856	L796	T736	G676	C616	R556	D496	S436	F376	D316	F257	A197	R137
	G857	H797	M737	H677	S617	M557	Y497	E437	V377	L317	K258	H198	E138
	K858	L798	M738	L678	E618	L558	L498	D438	N378	T318	F259	N199	C139
	P859	V799	A739	L679	H619	P559	T499	Y439	G379	E319	S260	A200	L140
	K860	L800	R740	R680	F620	L560	L500	I440	F380	I320	R261	E201	K141
	T861	Y801	L741	Y681	D621	G561	L501	K441	V381	M521	R262	H202	Y142
	I862	S802	A742	G682	SER	L562	L502	S442	N382	S322	P263	E203	R143
	T863	F803	A743	E683	LYS	G563	P503	G443	A383	N323	E264	A204	L144
	C864	L804	M744	P684	LYS	L564	V504	A444	A384	Q324	G265	C205	V145
	F865	D805	L745	T685	GLU	N565	M505	L445	F385	Q325	L266	D206	G146
	Q866	V806	R746	L686	GLU	H566	G506	L446	G386	L326	R267	L207	S147
	T867	R807	Q747	R687	ASP	L567	D507	A447	Q387	N327	L268	L208	Q148
	H868	M808	L748	R688	ASP	G568	S508	G448	D388	S328	A269	M209	E149
	T869	I809	A749	A689	LYS	K569	K509	G449	K389	N329	L270	E210	E150
	T870	I810	Q750	V690	LYS	G570	S510	I450	L390	F330	M271	I211	L151
	P871	L811	Y751	P691	GLU	E571	S511	V451	L391	L331	L272	E212	A152
	V872	Q812	H752	L692	LYS	A572	M512	M452	T392	A332	L273	Q213	S153
	L873	R813	A753	A693	LYS	I573	E513	S453	D393	L333	D274	V214	W154
	L874	S814	K754	L694	ASP	E574	V514	G454	D394	A334	M275	D215	G155
	A875	H815	D755	A695	LYS	A575	A515	V455	G395	R335	E276	M216	H156
	H876	Y816	P756	L696	LYS	I576	G516	R456	N396	E336	L277	E217	E157
	G877	H817	M757	L697	GLU	L577	V517	M457	K397	L337	L278	E218	Y158
	E878	L818	N758	S698	ALA	A578	T518	E458	K398	D338	V279	K219	V159
	R879	Y819	L759	V699	PRD	A579	A519	C459	L399	I339	E279	D220	R160
	A880	Q820	F760	S700	D645	L580	L520	D460	Y400	M340	R280	I221	H161
	E881	L821	M761	W701	M646	L581	A521	P461	K401	E341	I281	D222	L162
	L882	V822	V762	P702	G647	V582	C522	A462	M402	P342	F282	E223	A163
	A883	A823	R763	R703	A648	V583	G523	L463	K403	K343	T283	N224	G164
	T884	A824	L764	L704	H649	S584	M524	A464	D404	V344	S284	A225	E165
	E885	M825	A765	W705	Q650	E585	I525	L465	H405	F345	C285	Y226	V166
	S886	Q826	Q766	L706	G651	P586	A526	L466	G406	D346	K286	E227	A167
	F887	P827	G767	L707	V652	F587	V527	S467	M407	D347	D287	K228	K168
	L888	R828	L768	D708	A653	R588	G528	D468	L408	I348	V288	V229	E169
	P889	M829	T769	T709	V654	S589	S529	Y469	S409	Y349	V289	C230	W170
	V890	L830	H770	L710	L655	F590	C530	V470	A410	K350	V290	L231	Q171
	T891	S831	L771	S711	G656	A591	N531	L471	A411	T351	Q291	Y232	E172
	R892	T832	G772	K712	L657	N592	G532	H472	A412	H352	K292	L233	L173
	L893	F833	K773	F713	A658	T593	D533	M473	S413	E354	Q293	T234	D174
	L894	S714	G774	S714	L659	L594	V534	S474	L414	N355	M294	S235	D175
	E895	H715	T775	V595	V659	V595	T535	M475	G415	N356	A295	C236	A176
	Q896	D716	L776	D596	P596	D596	S536	T476	M416	N357	F296	V237	E177
	F897	A717	T777	V597	C597	V597	T537	M477	I417	R357	M297	N238	K178
	V898	D718	L778	C598	V598	V598	I538	R478	L418	F358	L298	Y239	W179
	T899	P719	C779	A599	L539	L539	L539	L479	L419	G359	G299	V240	Q180
	L900	E720	P780	Y600	Q540	Q540	Q540	G480	M420	G360	R300		

● Molecule 33: Substrate



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42969	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00565	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	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, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.23	0/3283	0.55	0/4433
2	B	0.20	0/3254	0.51	0/4388
3	C	0.28	0/3146	0.58	2/4226 (0.0%)
4	D	0.24	0/3090	0.55	0/4168
5	E	0.28	0/3145	0.63	2/4233 (0.0%)
6	F	0.25	0/3137	0.58	2/4223 (0.0%)
7	G	0.26	0/1901	0.50	2/2572 (0.1%)
7	g	0.24	0/1913	0.46	0/2589
8	H	0.24	0/1840	0.46	0/2495
8	h	0.24	0/1844	0.44	0/2497
9	I	0.27	0/1963	0.52	0/2650
9	i	0.22	0/1985	0.44	0/2677
10	J	0.24	0/1887	0.46	0/2553
10	j	0.24	0/1887	0.51	1/2549 (0.0%)
11	K	0.22	0/1841	0.41	0/2486
11	k	0.21	0/1809	0.41	0/2444
12	L	0.23	0/1911	0.42	0/2584
12	l	0.22	0/1896	0.44	0/2565
13	M	0.24	0/1925	0.43	0/2592
13	m	0.22	0/1916	0.42	0/2580
14	N	0.23	0/1548	0.37	0/2097
14	n	0.23	0/1536	0.40	0/2080
15	O	0.23	0/1672	0.42	0/2267
15	o	0.22	0/1686	0.41	0/2282
16	P	0.23	0/1616	0.46	0/2180
16	p	0.24	0/1620	0.48	0/2184
17	Q	0.24	0/1621	0.42	0/2194
17	q	0.24	0/1611	0.42	0/2182
18	R	0.24	0/1590	0.41	0/2147
18	r	0.23	0/1580	0.42	0/2135
19	S	0.25	0/1671	0.48	0/2252
19	s	0.24	0/1680	0.46	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.25	0/1716	0.43	0/2323
20	t	0.23	0/1720	0.40	0/2328
21	U	0.20	0/6984	0.51	1/9435 (0.0%)
22	V	0.18	0/3681	0.43	0/4969
23	W	0.20	0/3644	0.48	1/4901 (0.0%)
24	X	0.21	0/3381	0.48	1/4558 (0.0%)
25	Y	0.19	0/3261	0.46	0/4393
26	Z	0.28	0/2324	0.67	2/3150 (0.1%)
27	a	0.24	0/3053	0.59	0/4133
28	b	0.21	0/1478	0.59	0/2001
29	c	0.34	1/2302 (0.0%)	0.70	1/3110 (0.0%)
30	d	0.26	0/2162	0.65	3/2919 (0.1%)
31	e	0.24	0/437	0.46	0/595
32	f	0.19	0/6640	0.45	0/8988
All	All	0.23	1/107787 (0.0%)	0.50	18/145571 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	284	LEU	N-CA	5.13	1.49	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	317	PRO	N-CA-C	-9.25	101.16	113.65
7	G	210	PHE	CA-C-N	8.57	138.97	121.48
7	G	210	PHE	C-N-CA	8.57	138.97	121.48
6	F	322	PRO	CA-N-CD	-7.76	101.13	112.00
30	d	88	GLN	N-CA-C	-7.56	104.46	112.93

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	46	0
2	B	3207	0	3278	61	0
3	C	3105	0	3219	66	0
4	D	3040	0	3076	69	0
5	E	3097	0	3174	65	0
6	F	3098	0	3187	76	0
7	G	1867	0	1867	30	0
7	g	1879	0	1872	26	0
8	H	1801	0	1773	19	0
8	h	1805	0	1798	21	0
9	I	1933	0	1923	19	0
9	i	1955	0	1955	12	0
10	J	1861	0	1846	38	0
10	j	1861	0	1865	24	0
11	K	1813	0	1796	12	0
11	k	1782	0	1766	12	0
12	L	1876	0	1856	20	0
12	l	1861	0	1839	18	0
13	M	1890	0	1880	27	0
13	m	1881	0	1868	16	0
14	N	1521	0	1494	6	0
14	n	1510	0	1483	11	0
15	O	1645	0	1648	11	0
15	o	1659	0	1681	16	0
16	P	1587	0	1598	13	0
16	p	1591	0	1609	19	0
17	Q	1588	0	1584	12	0
17	q	1578	0	1569	16	0
18	R	1559	0	1523	13	0
18	r	1549	0	1506	12	0
19	S	1641	0	1639	13	0
19	s	1650	0	1645	19	0
20	T	1683	0	1662	21	0
20	t	1687	0	1666	11	0
21	U	6867	0	6929	104	0
22	V	3612	0	3682	48	0
23	W	3596	0	3713	49	0
24	X	3335	0	3435	45	0
25	Y	3202	0	3204	39	0
26	Z	2281	0	2312	66	0
27	a	2995	0	3012	54	0
28	b	1458	0	1505	38	0
29	c	2260	0	2276	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	39	0
31	e	425	0	328	14	0
32	f	6529	0	6541	69	0
33	v	180	0	45	0	0
34	A	31	0	12	0	0
34	B	31	0	12	1	0
34	C	31	0	12	1	0
34	D	31	0	12	2	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
36	E	27	0	12	1	0
36	F	27	0	12	2	0
37	c	1	0	0	0	0
All	All	106328	0	106606	1319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1319 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:221:ASN:HD21	10:J:223:GLU:HB2	1.11	1.08
5:E:164:ILE:HG13	5:E:166:PRO:HD3	1.48	0.94
29:c:231:LEU:C	29:c:233:ASP:H	1.79	0.87
30:d:203:PRO:HD2	30:d:206:MET:HE1	1.58	0.86
10:J:221:ASN:ND2	10:J:223:GLU:HB2	1.91	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	359 (87%)	51 (12%)	1 (0%)	43	73
2	B	409/440 (93%)	374 (91%)	35 (9%)	0	100	100
3	C	394/398 (99%)	352 (89%)	40 (10%)	2 (0%)	24	57
4	D	378/418 (90%)	332 (88%)	44 (12%)	2 (0%)	24	57
5	E	387/403 (96%)	342 (88%)	40 (10%)	5 (1%)	9	38
6	F	391/439 (89%)	349 (89%)	39 (10%)	3 (1%)	16	48
7	G	238/246 (97%)	222 (93%)	15 (6%)	1 (0%)	30	62
7	g	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	62
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	246/261 (94%)	234 (95%)	10 (4%)	2 (1%)	16	48
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
10	j	237/248 (96%)	222 (94%)	14 (6%)	1 (0%)	30	62
11	K	236/241 (98%)	221 (94%)	15 (6%)	0	100	100
11	k	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
12	L	238/263 (90%)	227 (95%)	11 (5%)	0	100	100
12	l	236/263 (90%)	224 (95%)	12 (5%)	0	100	100
13	M	240/255 (94%)	231 (96%)	9 (4%)	0	100	100
13	m	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	N	201/239 (84%)	193 (96%)	8 (4%)	0	100	100
14	n	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
15	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
15	o	218/277 (79%)	205 (94%)	13 (6%)	0	100	100
16	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	197/201 (98%)	188 (95%)	9 (5%)	0	100	100
17	q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	R	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
18	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	S	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
19	s	211/241 (88%)	199 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	U	874/953 (92%)	811 (93%)	63 (7%)	0	100	100
22	V	442/534 (83%)	428 (97%)	14 (3%)	0	100	100
23	W	439/456 (96%)	431 (98%)	8 (2%)	0	100	100
24	X	420/422 (100%)	397 (94%)	22 (5%)	1 (0%)	43	73
25	Y	387/389 (100%)	363 (94%)	24 (6%)	0	100	100
26	Z	284/324 (88%)	251 (88%)	29 (10%)	4 (1%)	9	37
27	a	371/376 (99%)	339 (91%)	30 (8%)	2 (0%)	24	57
28	b	189/377 (50%)	170 (90%)	19 (10%)	0	100	100
29	c	285/310 (92%)	243 (85%)	38 (13%)	4 (1%)	9	37
30	d	255/350 (73%)	217 (85%)	37 (14%)	1 (0%)	30	62
31	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
32	f	840/908 (92%)	810 (96%)	30 (4%)	0	100	100
All	All	13415/14876 (90%)	12531 (93%)	854 (6%)	30 (0%)	44	73

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	157	ASP
4	D	336	PRO
5	E	164	ILE
5	E	166	PRO
24	X	318	ILE

### 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	A	348/372 (94%)	347 (100%)	1 (0%)	86	84
2	B	357/385 (93%)	357 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	340/346 (98%)	334 (98%)	6 (2%)	51	67
4	D	333/366 (91%)	328 (98%)	5 (2%)	57	69
5	E	341/353 (97%)	335 (98%)	6 (2%)	51	67
6	F	340/379 (90%)	337 (99%)	3 (1%)	70	74
7	G	202/210 (96%)	200 (99%)	2 (1%)	68	74
7	g	201/210 (96%)	199 (99%)	2 (1%)	68	74
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	73
9	I	202/221 (91%)	201 (100%)	1 (0%)	81	81
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	196 (100%)	1 (0%)	81	81
10	j	196/211 (93%)	195 (100%)	1 (0%)	81	81
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	200 (100%)	1 (0%)	81	81
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	197 (100%)	1 (0%)	81	81
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	752 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	87
24	X	362/362 (100%)	359 (99%)	3 (1%)	73	76
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	255 (99%)	2 (1%)	73	76
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	84
28	b	167/312 (54%)	166 (99%)	1 (1%)	78	79
29	c	252/268 (94%)	240 (95%)	12 (5%)	23	47
30	d	231/294 (79%)	227 (98%)	4 (2%)	53	67
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	89
All	All	11449/12614 (91%)	11392 (100%)	57 (0%)	78	81

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	319	ILE
12	l	33	SER
29	c	196	LEU
10	j	49	SER
32	f	828	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	283	ASN
16	p	169	GLN
26	Z	229	GLN
16	p	157	ASN
9	i	95	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 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	B	501	35	29,33,33	0.31	0	44,52,52	0.49	0
34	ATP	C	501	35	29,33,33	0.32	0	44,52,52	0.50	0
34	ATP	A	501	35	29,33,33	0.29	0	44,52,52	0.54	1 (2%)
34	ATP	D	501	35	29,33,33	0.33	0	44,52,52	0.50	0
36	ADP	F	501	-	27,29,29	1.38	4 (14%)	42,45,45	2.02	8 (19%)
36	ADP	E	401	-	27,29,29	1.37	4 (14%)	42,45,45	2.06	9 (21%)

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	B	501	35	-	5/22/38/38	0/3/3/3
34	ATP	C	501	35	-	1/22/38/38	0/3/3/3
34	ATP	A	501	35	-	4/22/38/38	0/3/3/3
34	ATP	D	501	35	-	3/22/38/38	0/3/3/3
36	ADP	F	501	-	-	2/16/32/32	0/3/3/3
36	ADP	E	401	-	-	2/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	501	ADP	C5-C4	4.70	1.47	1.39
36	E	401	ADP	C5-C4	4.41	1.47	1.39
36	E	401	ADP	C5-N7	-2.64	1.34	1.39
36	F	501	ADP	C5-C6	2.64	1.48	1.41
36	E	401	ADP	C5-C6	2.58	1.48	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	501	ADP	C5-C4-N3	-6.91	117.73	126.75
36	E	401	ADP	C5-C4-N3	-6.85	117.82	126.75
36	F	501	ADP	N3-C4-N9	5.52	136.18	127.08
36	E	401	ADP	N3-C4-N9	5.27	135.76	127.08
36	F	501	ADP	C2-N3-C4	4.00	121.21	111.75

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C5'-O5'-PA-O2A
34	A	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	C5'-O5'-PA-O1A
34	B	501	ATP	C5'-O5'-PA-O2A

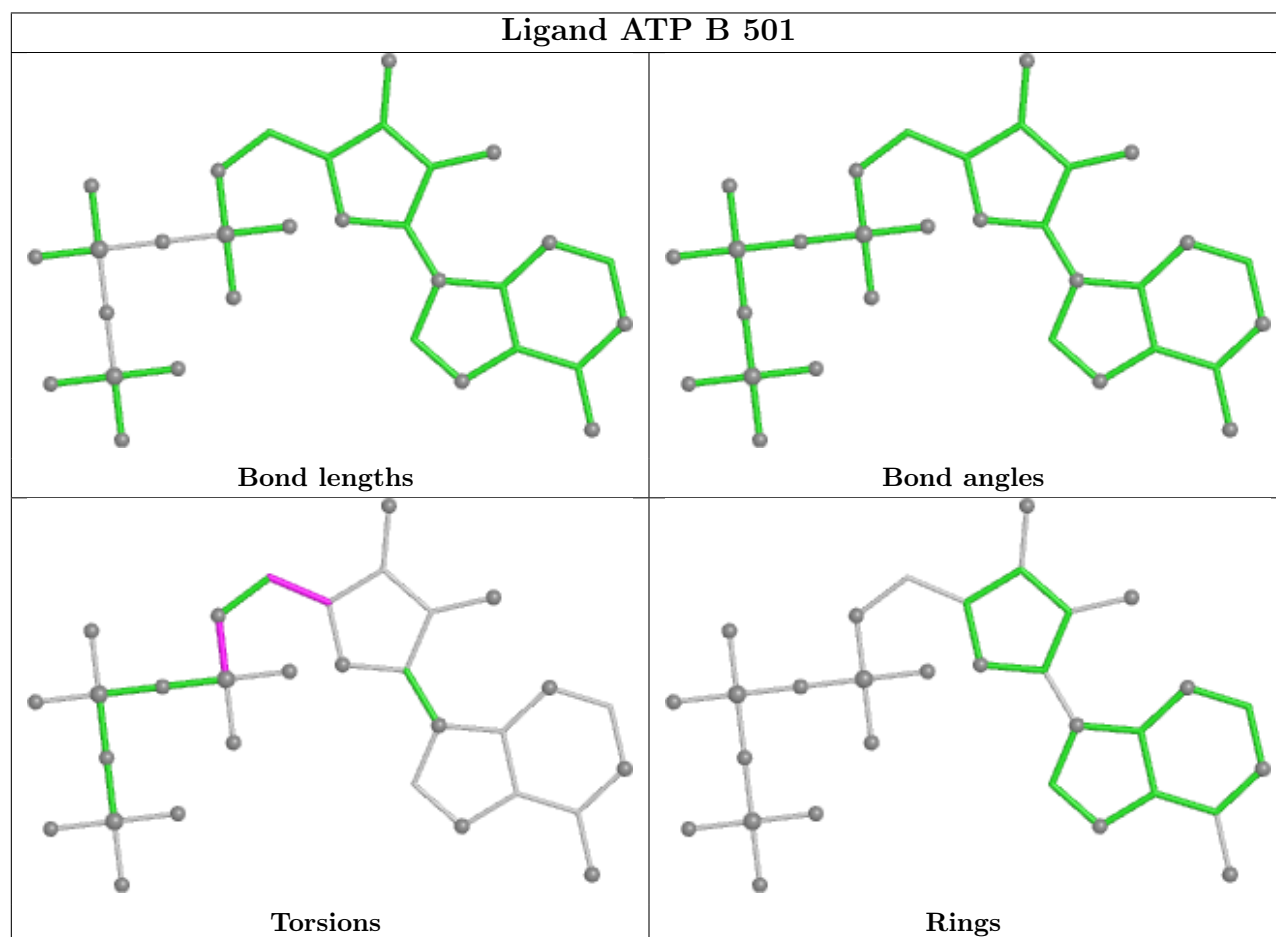
There are no ring outliers.

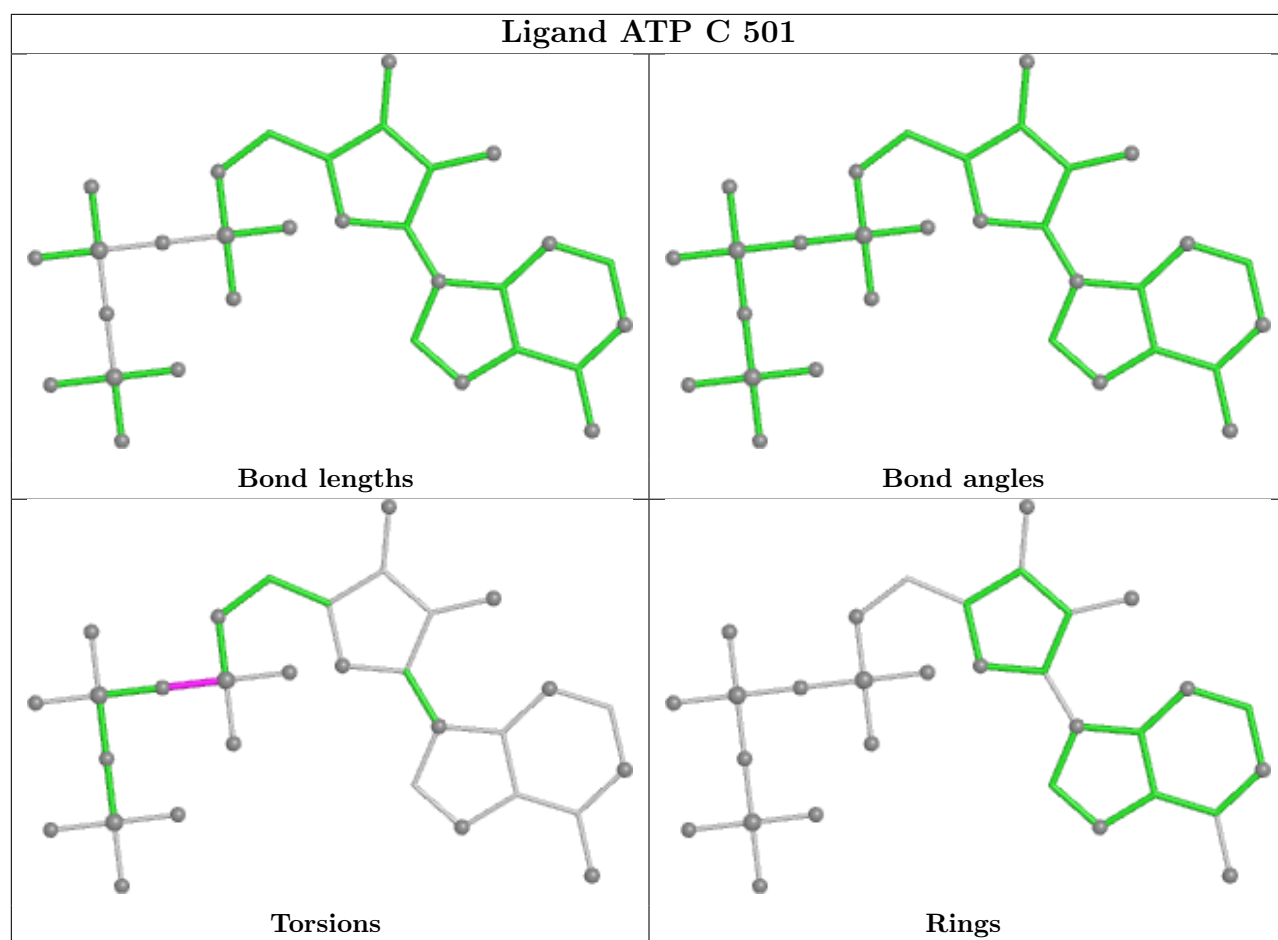
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	501	ATP	1	0
34	C	501	ATP	1	0
34	D	501	ATP	2	0
36	F	501	ADP	2	0
36	E	401	ADP	1	0

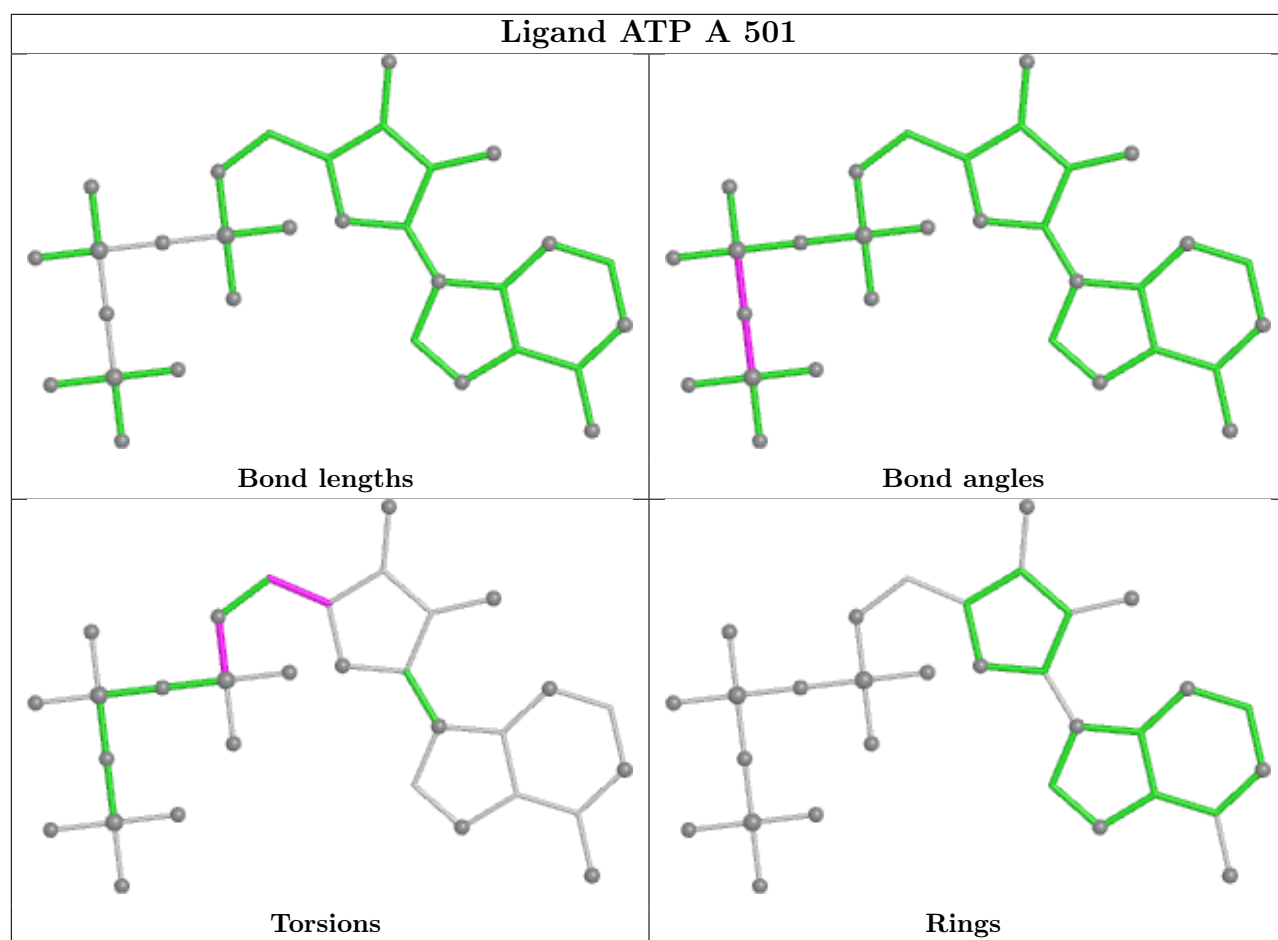
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

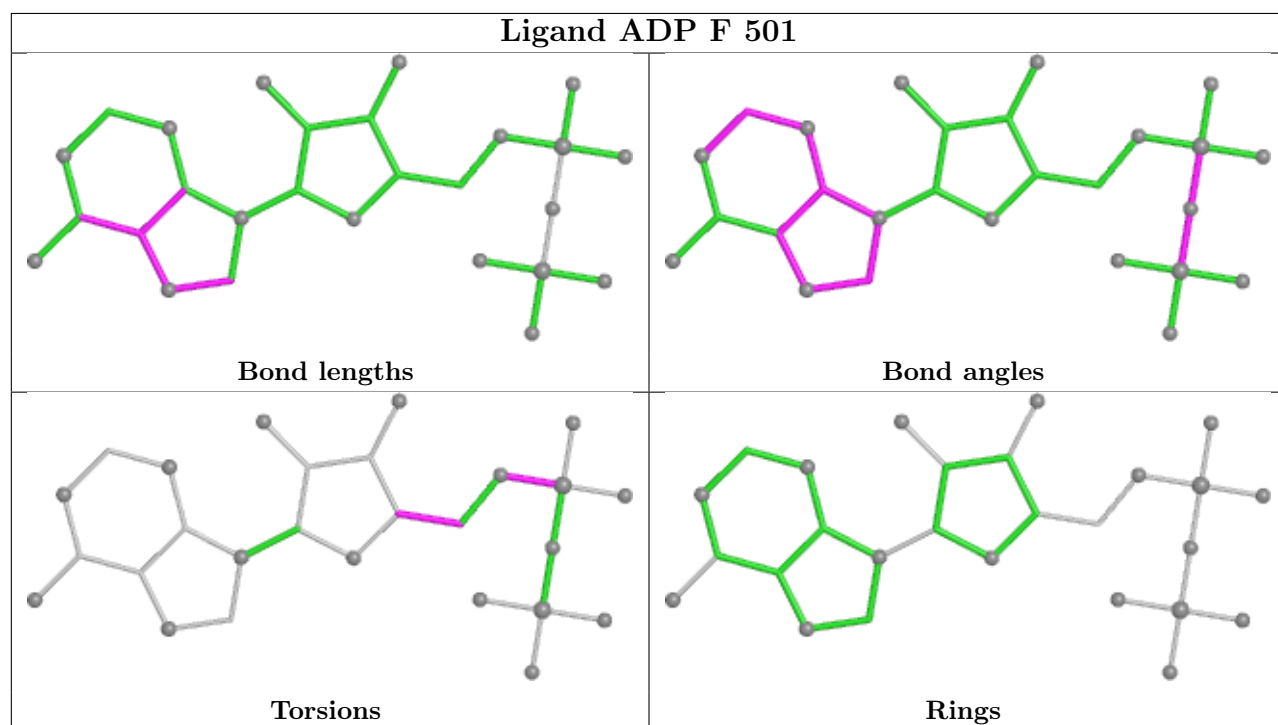
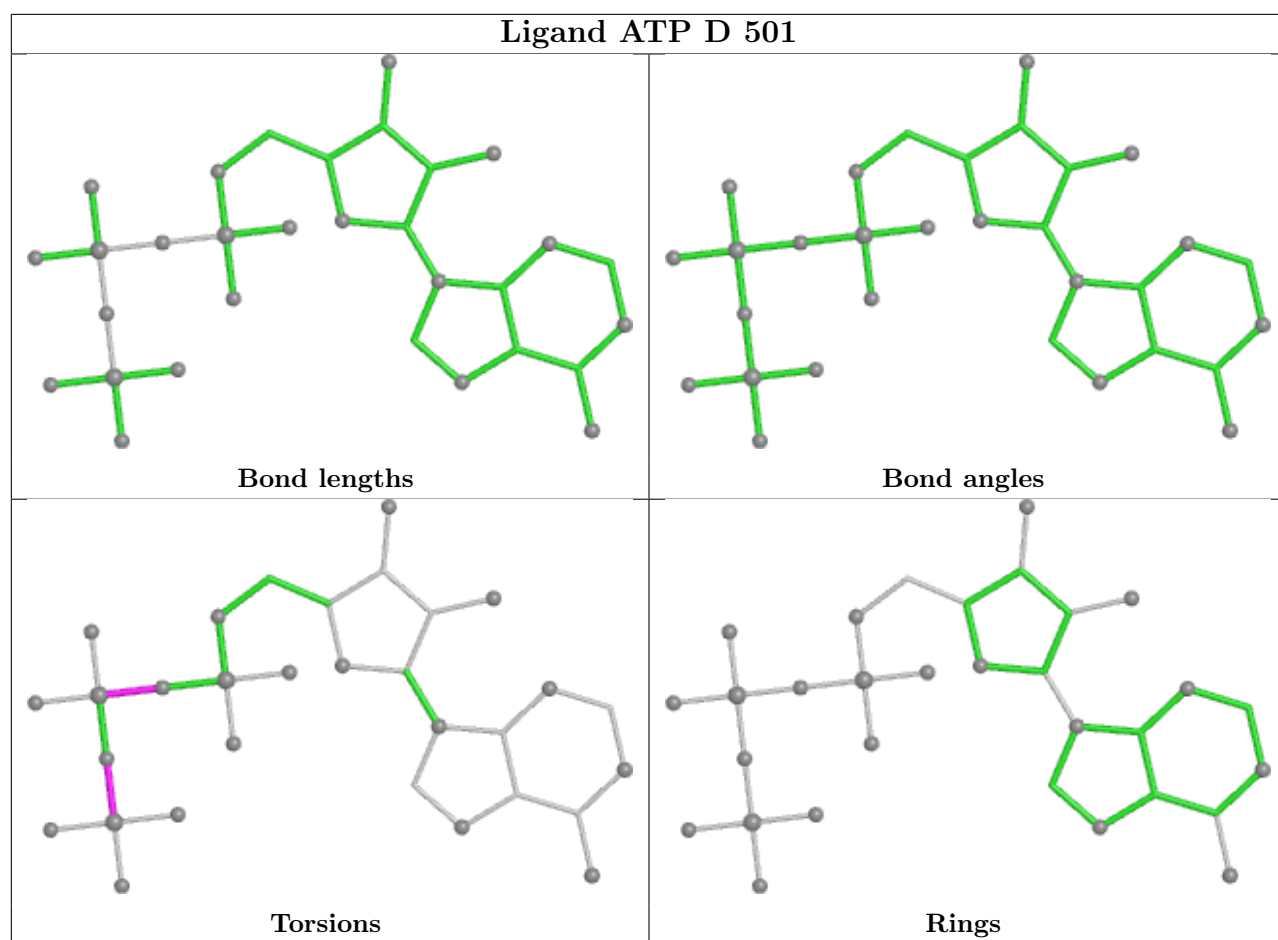
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

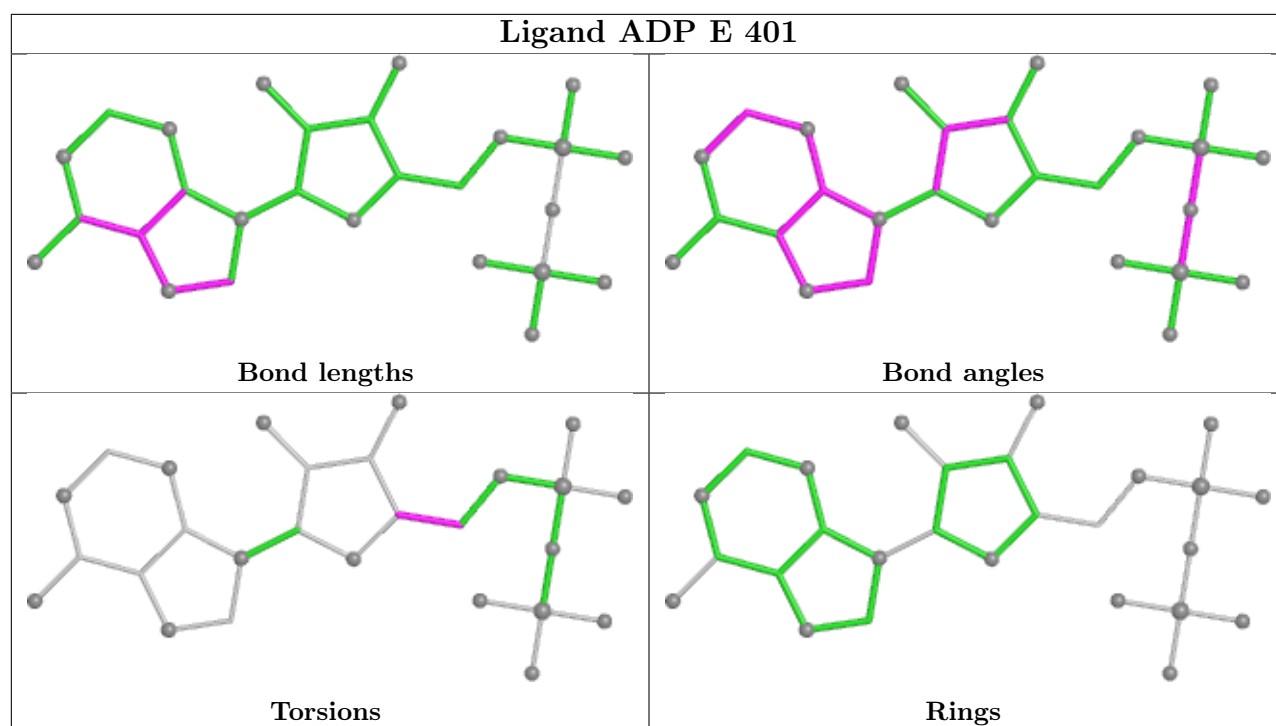












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

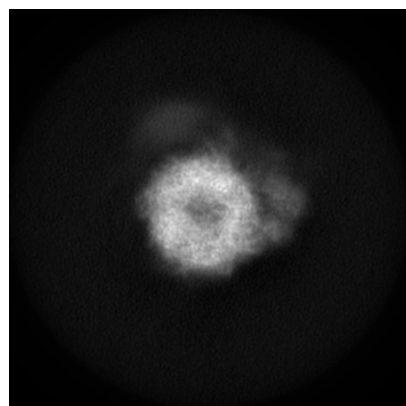
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62087. These allow visual inspection of the internal detail of the map and identification of artifacts.

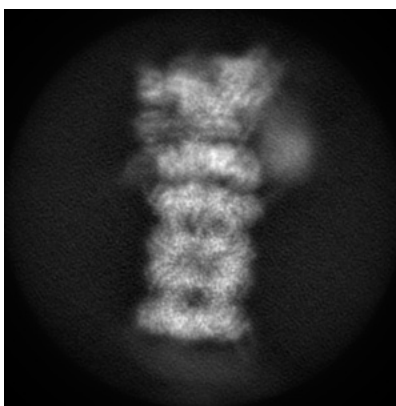
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

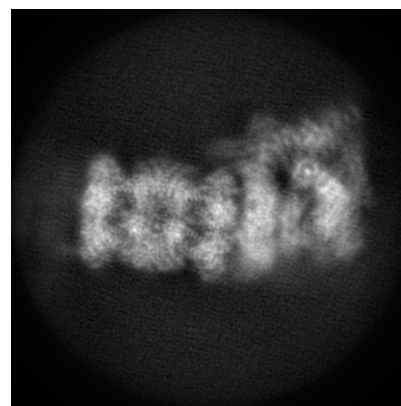
#### 6.1.1 Primary map



X

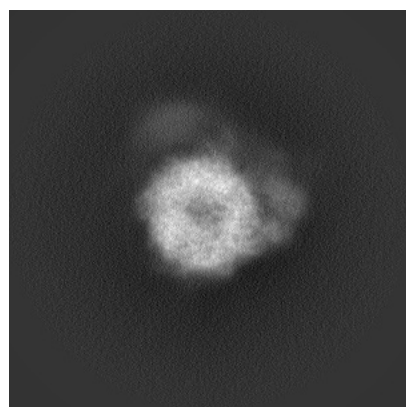


Y

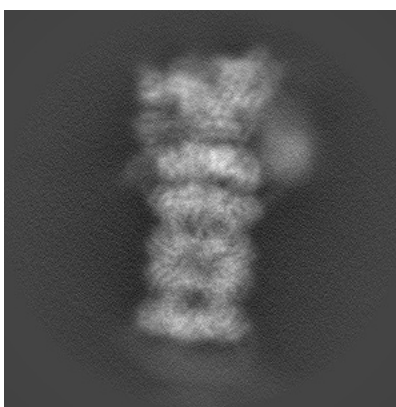


Z

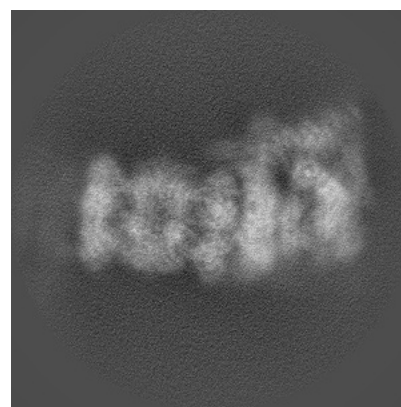
#### 6.1.2 Raw map



X



Y

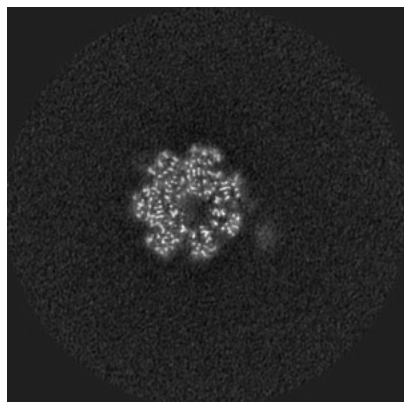


Z

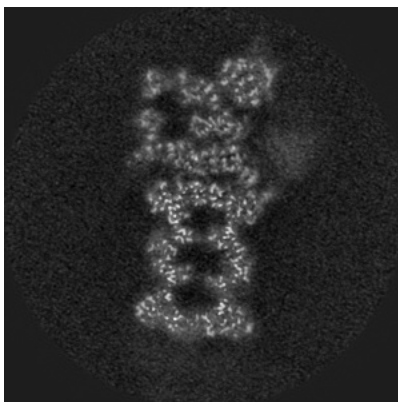
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

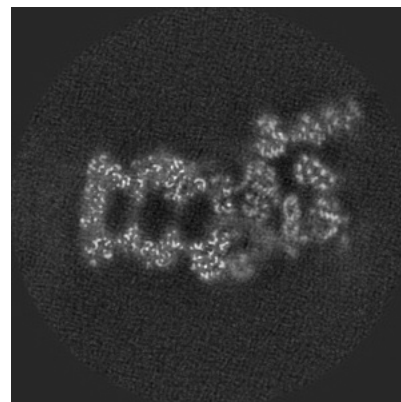
### 6.2.1 Primary map



X Index: 300

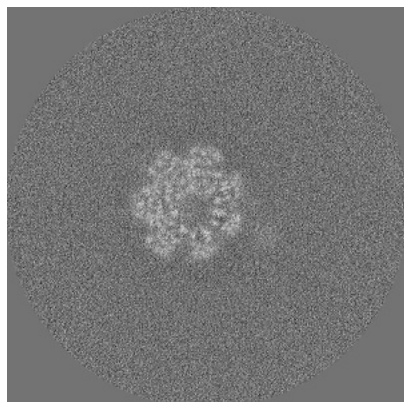


Y Index: 300

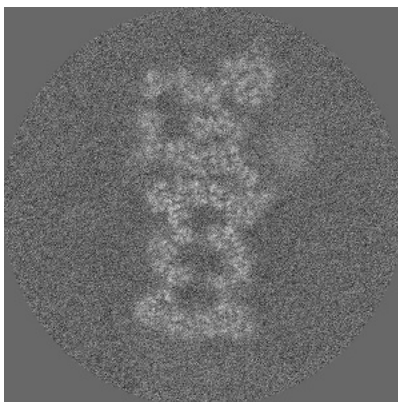


Z Index: 300

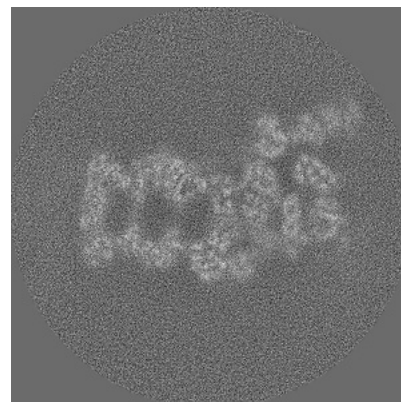
### 6.2.2 Raw map



X Index: 300



Y Index: 300

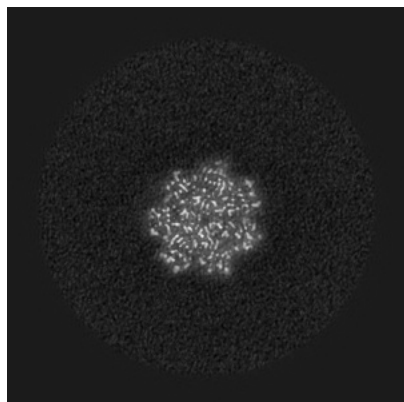


Z Index: 300

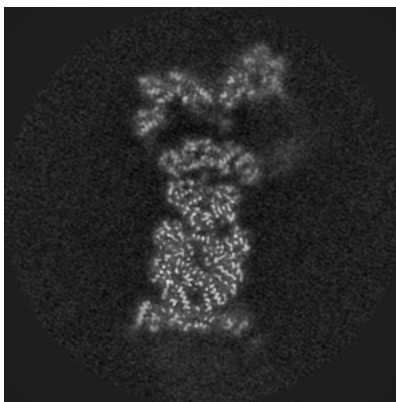
The images above show central slices of the map in three orthogonal directions.

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

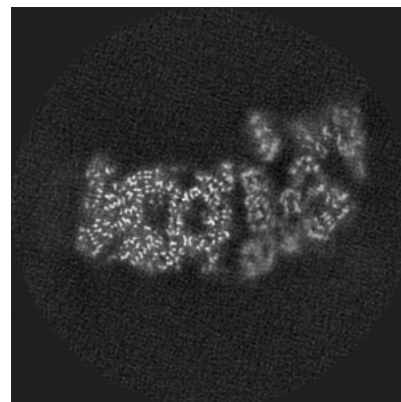
### 6.3.1 Primary map



X Index: 134

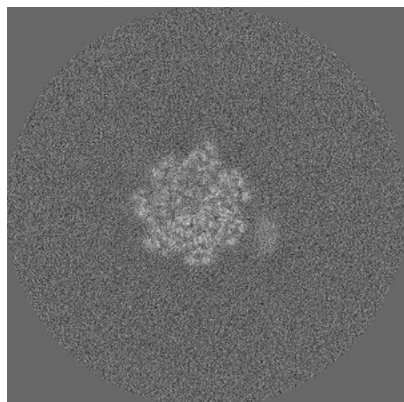


Y Index: 330

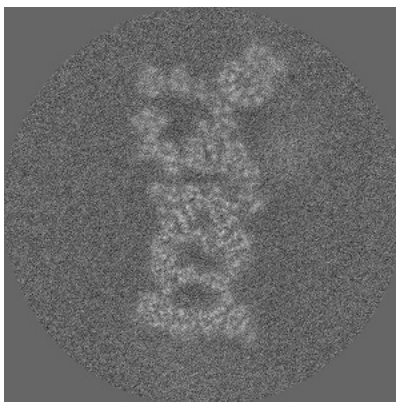


Z Index: 328

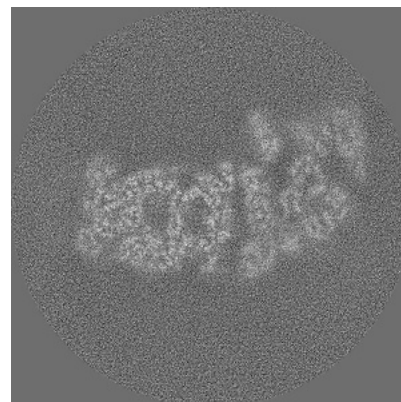
### 6.3.2 Raw map



X Index: 311



Y Index: 313



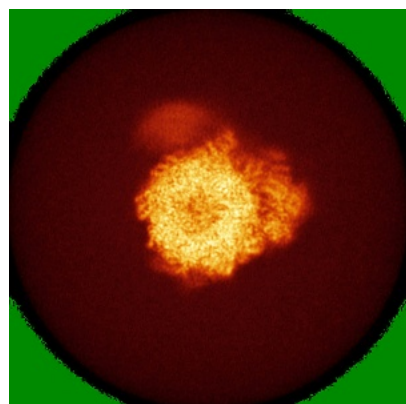
Z Index: 327

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

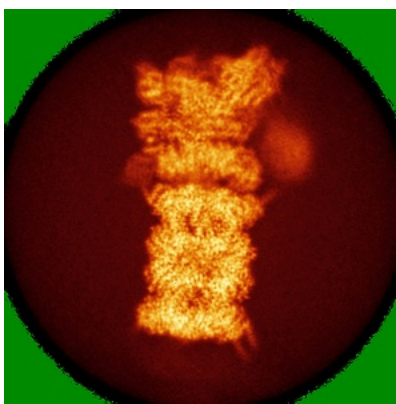


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

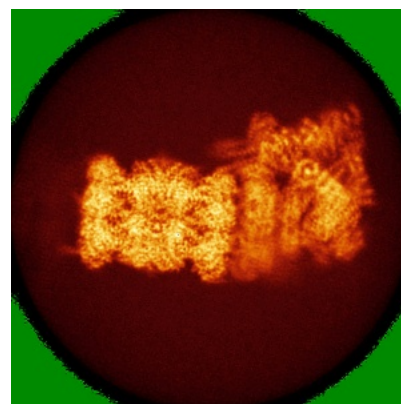
### 6.4.1 Primary map



X

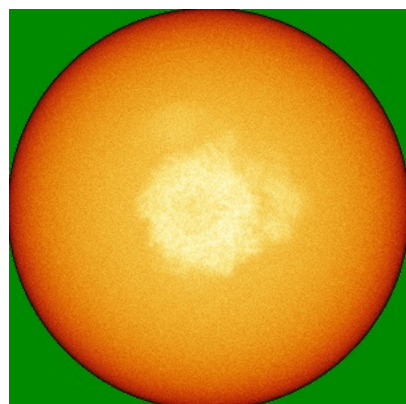


Y

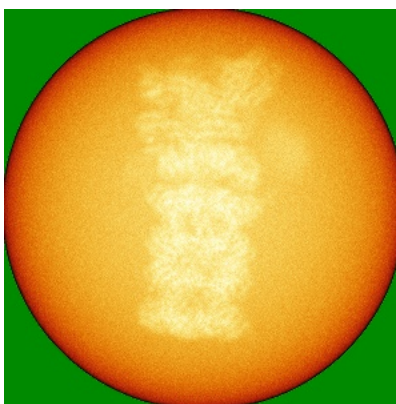


Z

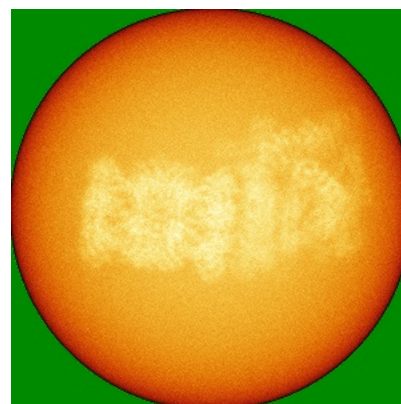
### 6.4.2 Raw map



X



Y

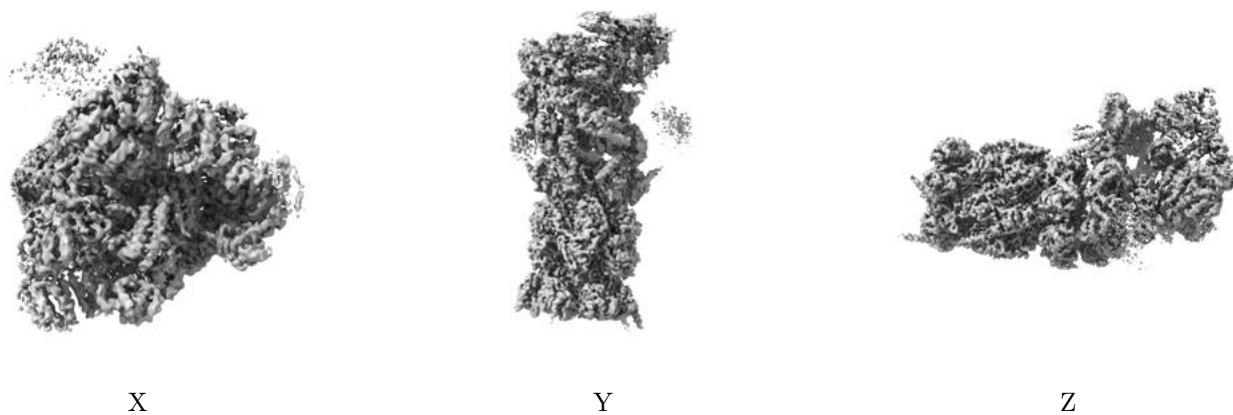


Z

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.

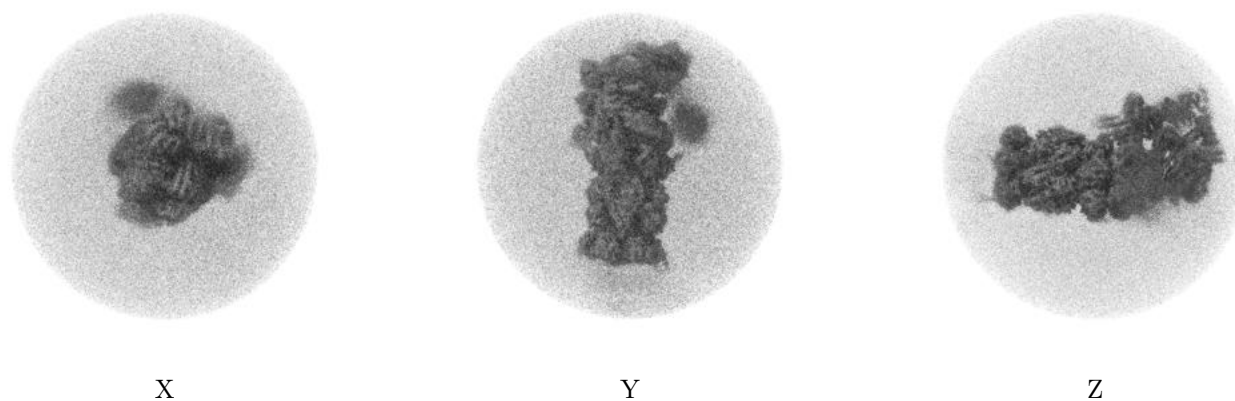
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00565. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

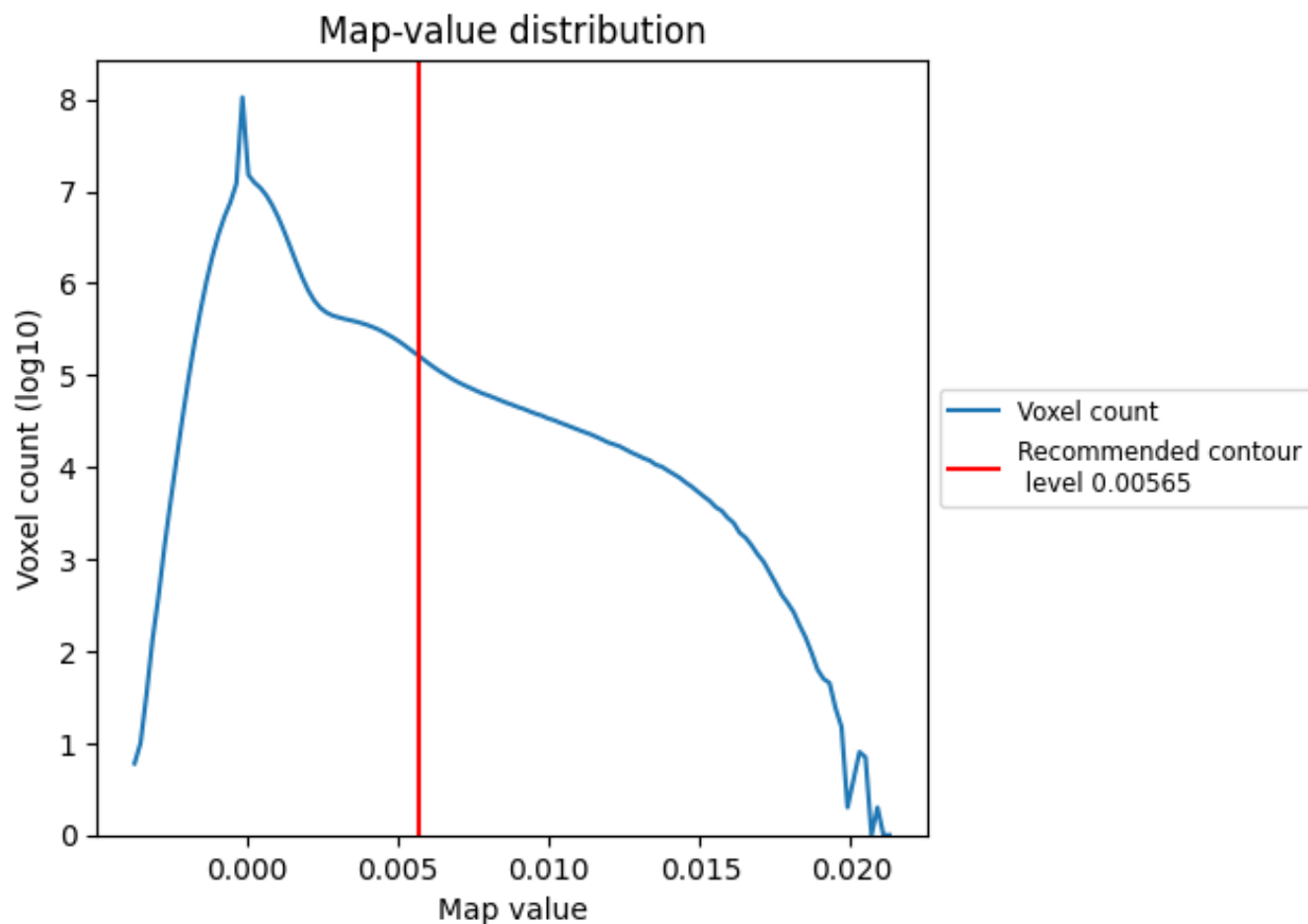
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

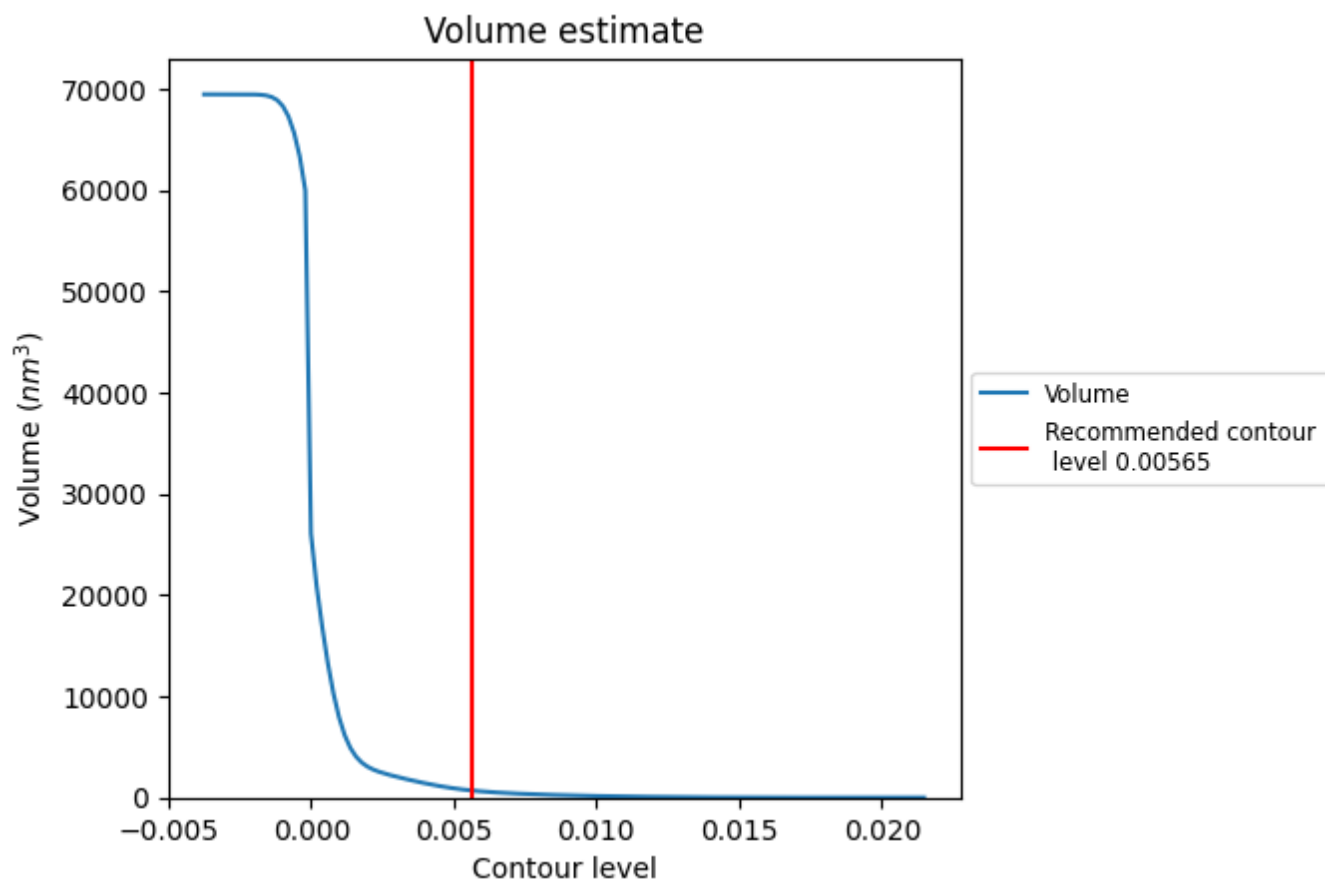
This section contains the results of statistical analysis of the map.

### 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.

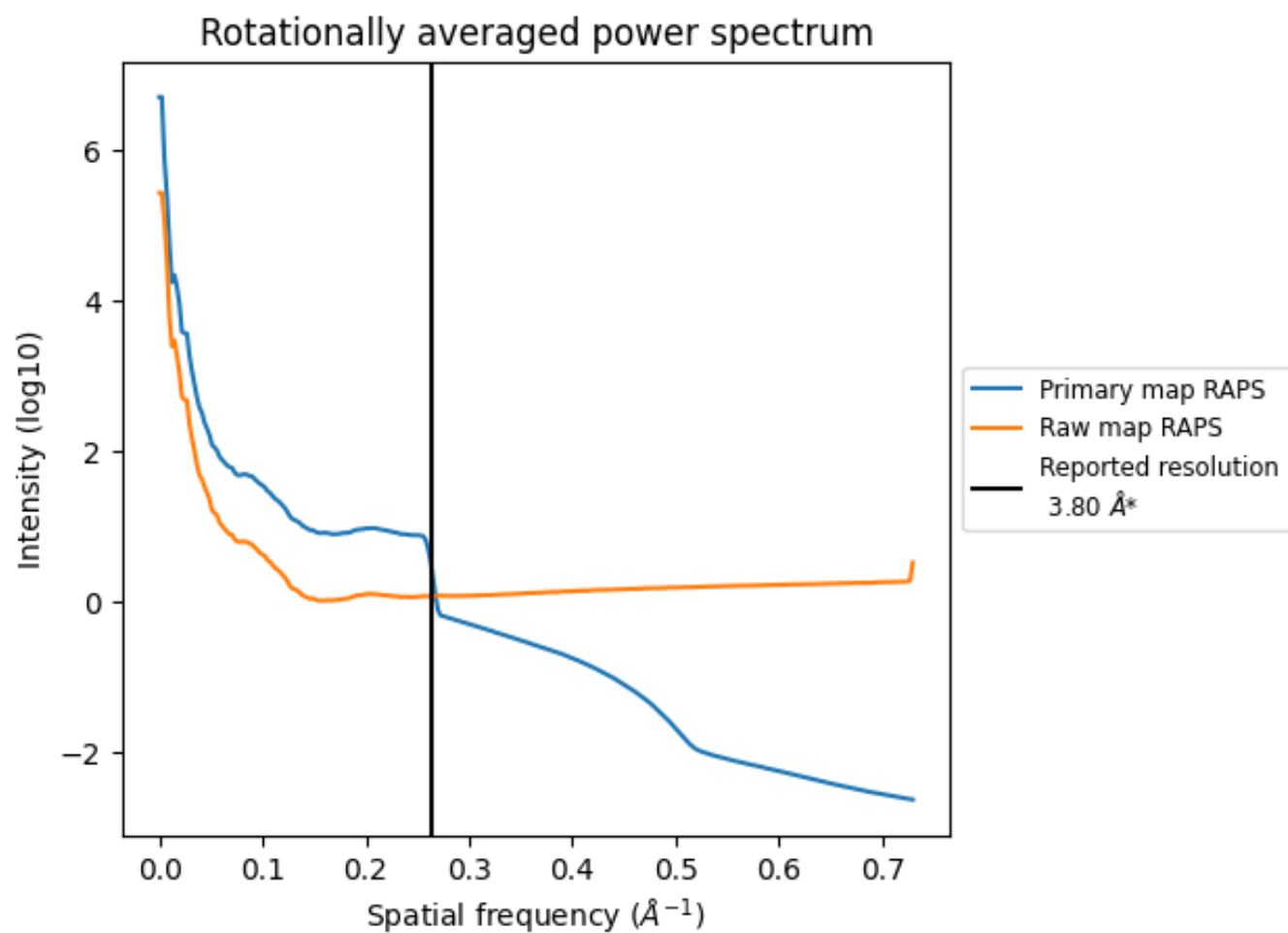
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 692 nm<sup>3</sup>; this corresponds to an approximate mass of 625 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 ⓘ

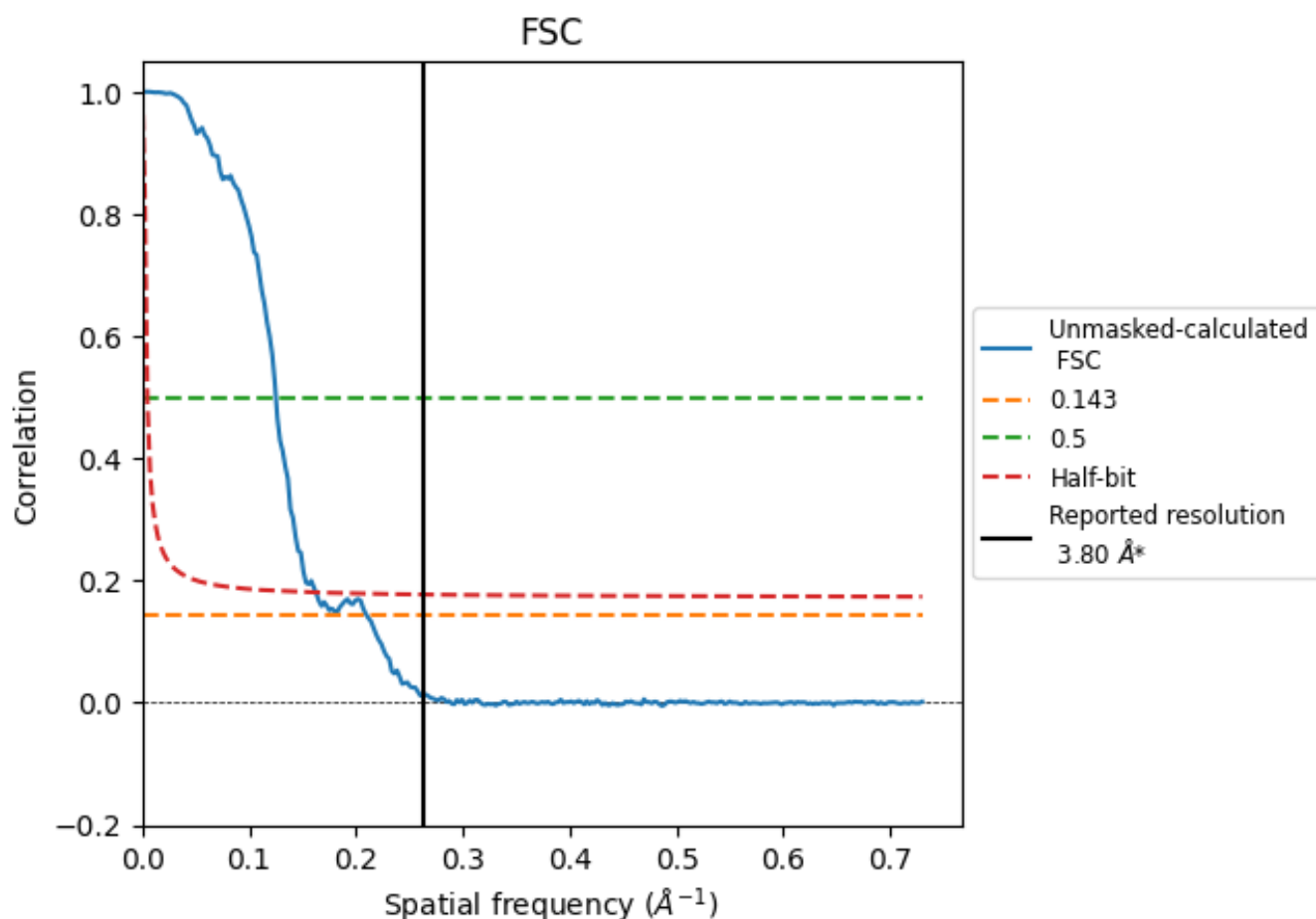


\*Reported resolution corresponds to spatial frequency of  $0.263 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

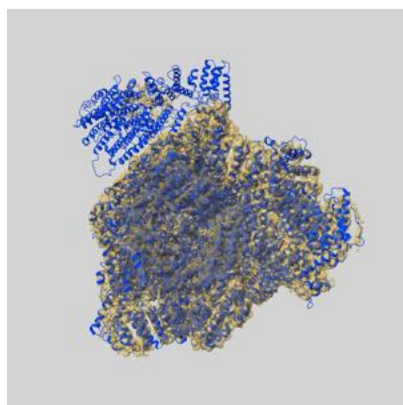
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.76	7.99	6.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.76 differs from the reported value 3.8 by more than 10 %

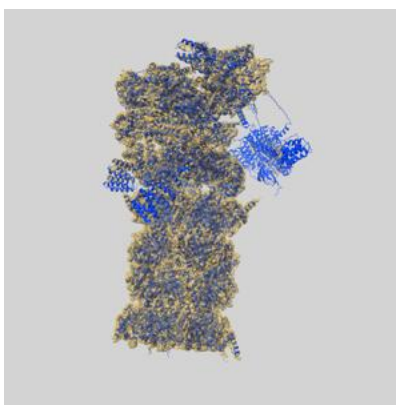
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62087 and PDB model 9K5B. Per-residue inclusion information can be found in section [3](#) on page [13](#).

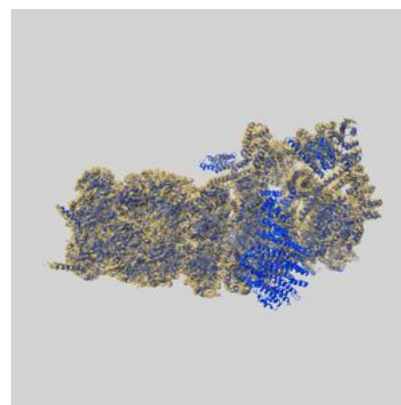
### 9.1 Map-model overlay [i](#)



X



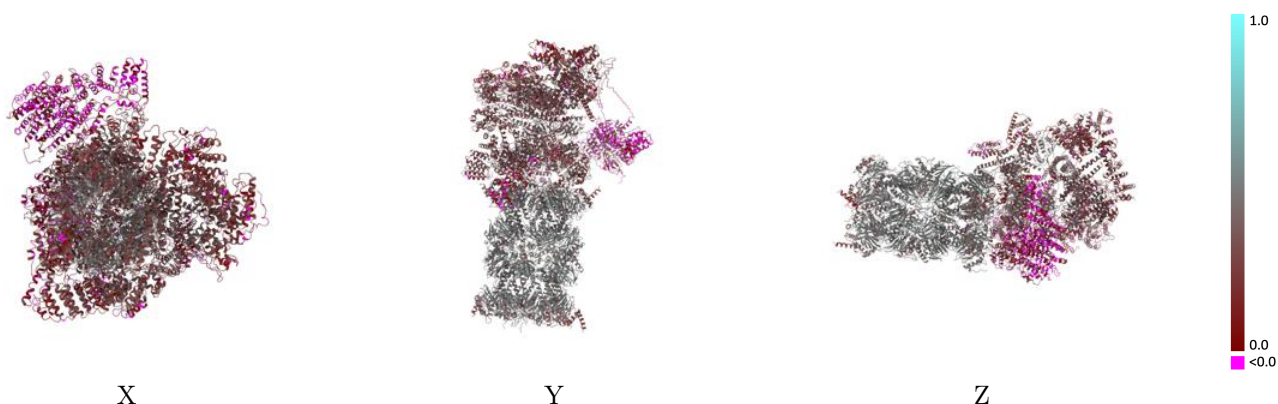
Y



Z

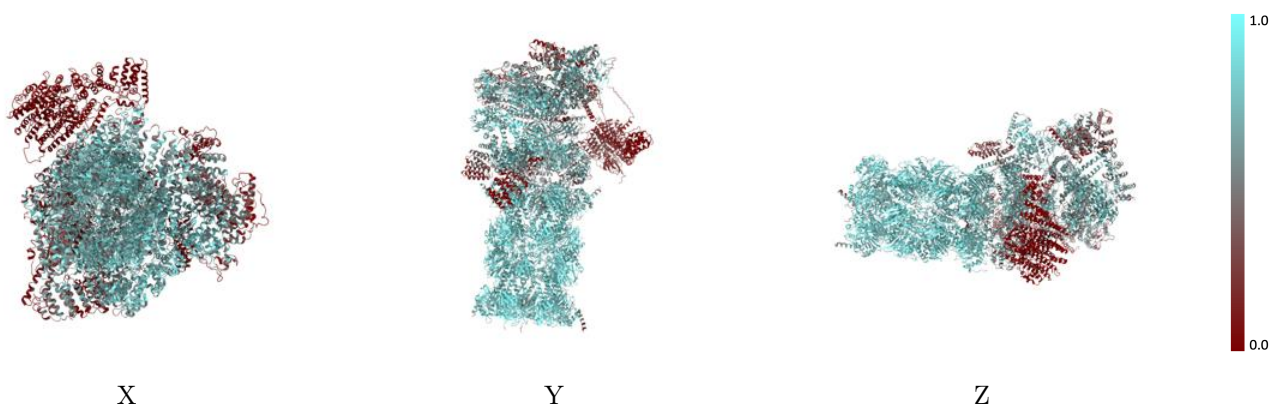
The images above show the 3D surface view of the map at the recommended contour level 0.00565 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



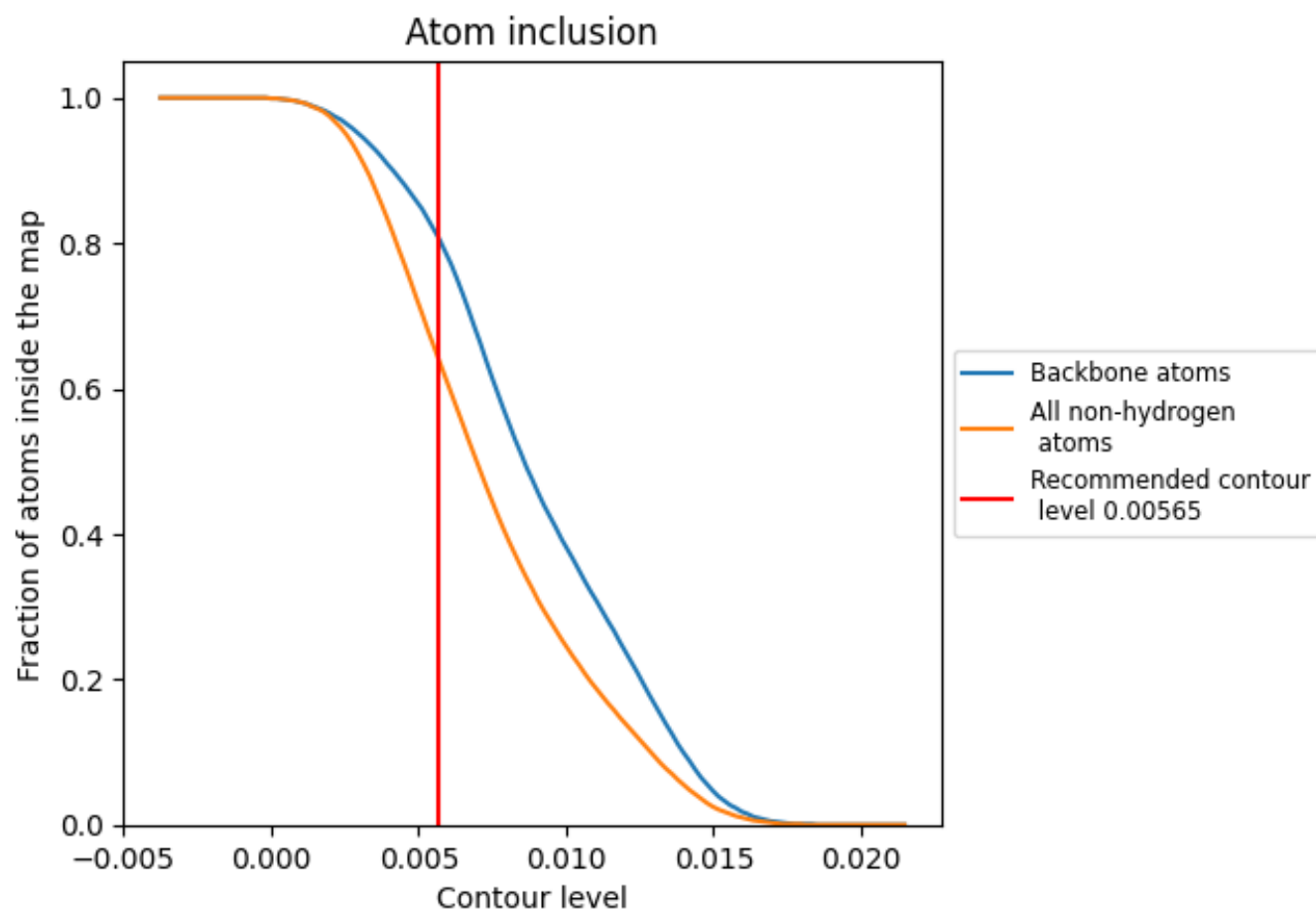
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00565).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 81% 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 (0.00565) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.3400
A	 0.3650	 0.1860
B	 0.4860	 0.2690
C	 0.6580	 0.3450
D	 0.6710	 0.3480
E	 0.5930	 0.3110
F	 0.3640	 0.1700
G	 0.8230	 0.4450
H	 0.8360	 0.4500
I	 0.7990	 0.4280
J	 0.7800	 0.4170
K	 0.7830	 0.4330
L	 0.8390	 0.4480
M	 0.8300	 0.4400
N	 0.8590	 0.4640
O	 0.8710	 0.4620
P	 0.8810	 0.4670
Q	 0.8610	 0.4640
R	 0.8910	 0.4700
S	 0.8590	 0.4650
T	 0.8750	 0.4720
U	 0.5810	 0.2780
V	 0.5070	 0.2810
W	 0.4910	 0.2770
X	 0.4650	 0.2620
Y	 0.7230	 0.3240
Z	 0.6200	 0.3000
a	 0.5760	 0.2510
b	 0.4410	 0.2270
c	 0.6300	 0.3170
d	 0.3540	 0.2090
e	 0.5440	 0.2900
f	 0.0080	 0.0560
g	 0.8430	 0.4420
h	 0.8420	 0.4410



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Chain	Atom inclusion	Q-score
i	 0.8090	 0.4280
j	 0.7810	 0.3910
k	 0.8030	 0.4290
l	 0.8590	 0.4410
m	 0.8420	 0.4370
n	 0.8710	 0.4700
o	 0.8640	 0.4600
p	 0.8790	 0.4640
q	 0.8760	 0.4680
r	 0.8930	 0.4720
s	 0.8510	 0.4620
t	 0.8810	 0.4710
v	 0.1940	 0.2210