



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 01:05 PM JST

PDB ID : 9K4U / pdb_00009k4u
EMDB ID : EMD-62070
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EC1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.40 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

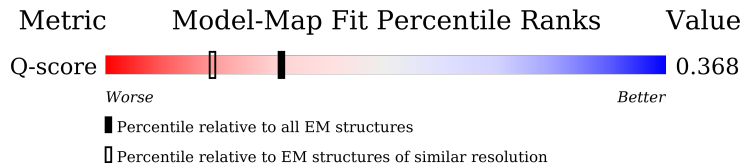
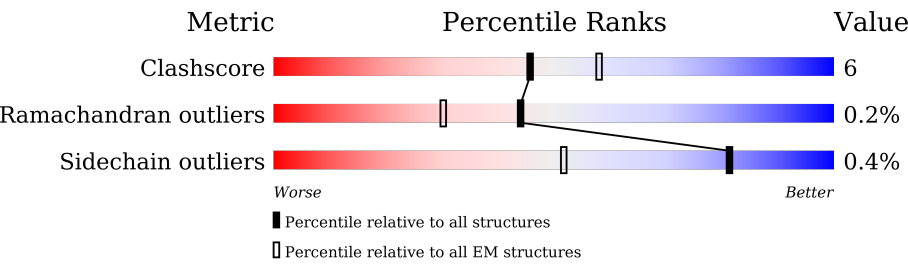
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 ≥ 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>36%</div><div><div></div><div>72%</div><div>20%</div><div>• 7%</div></div></div>
2	B	440	<div><div>56%</div><div><div></div><div>68%</div><div>22%</div><div>• 9%</div></div></div>
3	C	398	<div><div>22%</div><div><div></div><div>81%</div><div>18%</div><div>•</div></div></div>
4	D	418	<div><div>8%</div><div><div></div><div>73%</div><div>17%</div><div>• 9%</div></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	u	76	
34	v	24	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106690 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	402	Total	C	N	O	S	0	0
			3135	1973	551	594	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			3122	1967	529	611	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	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	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
			1805	1152	305	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	250	Total	C	N	O	S	1	0
			1958	1236	336	376	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
			1880	1179	333	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	234	Total	C	N	O	S	0	0
			1777	1117	295	354	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	238	Total	C	N	O	S	0	0
			1866	1169	336	350	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	240	Total	C	N	O	S	0	0
			1876	1191	321	353	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	202	Total	C	N	O	S	0	0
			1514	949	258	295	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
			1649	1038	279	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
			1588	1017	270	292	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
			1559	982	274	294	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
			1654	1047	284	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		

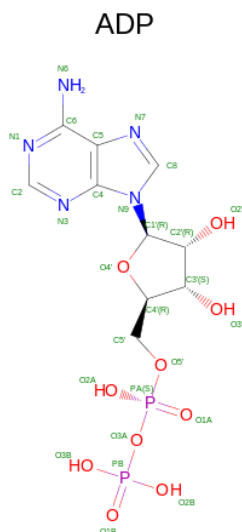
- Molecule 33 is a protein called Ubiquitin.

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

- Molecule 34 is a protein called Substrate.

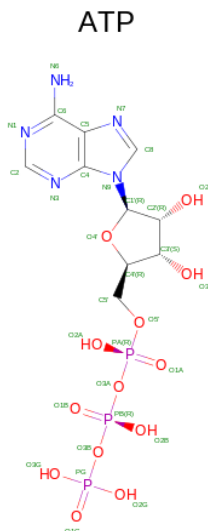
Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	

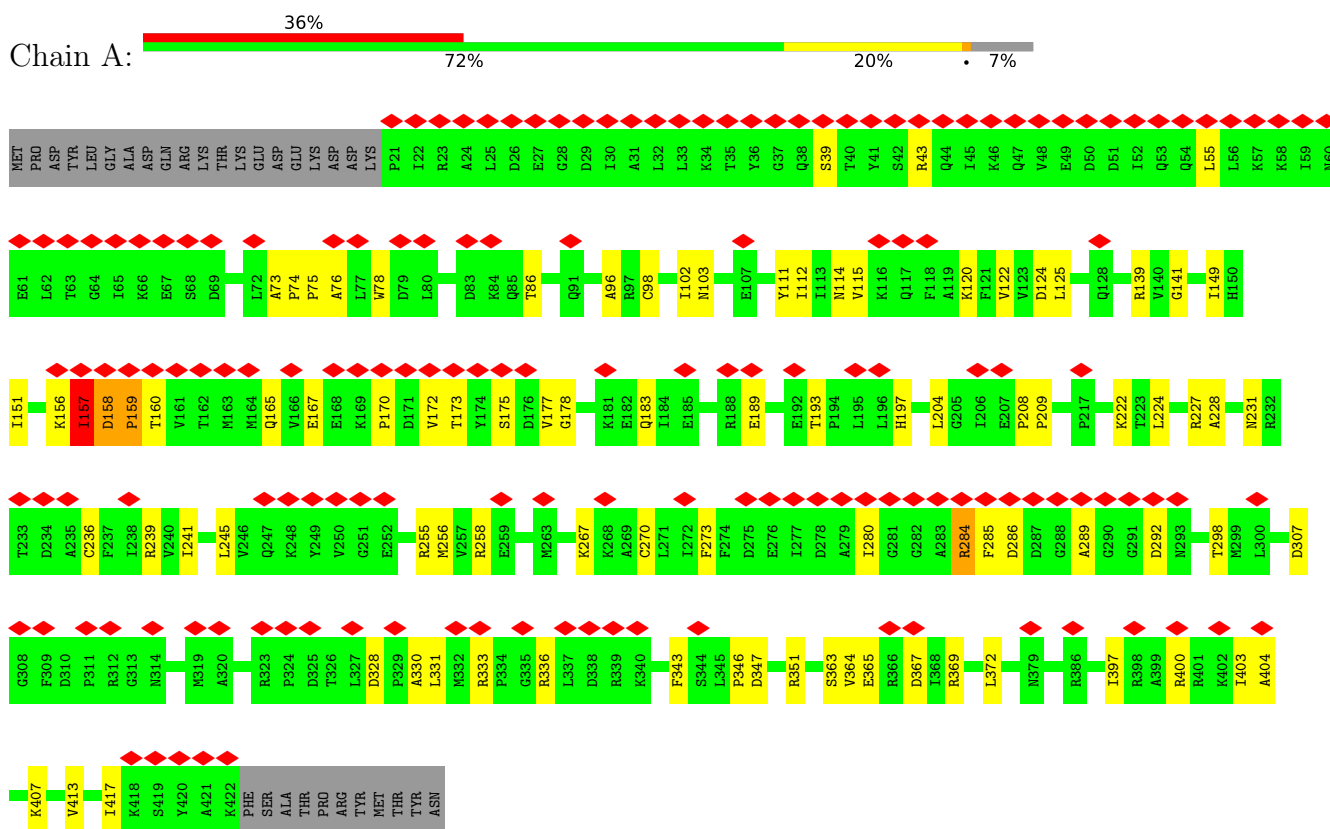
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

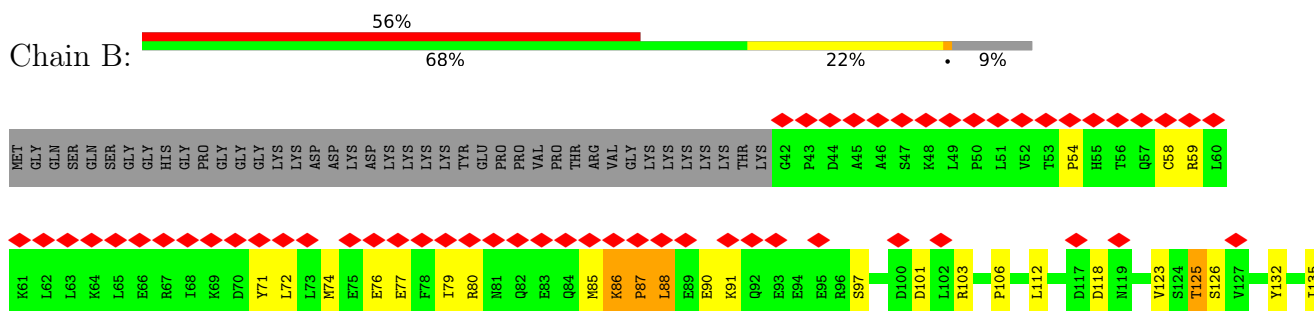
3 Residue-property plots

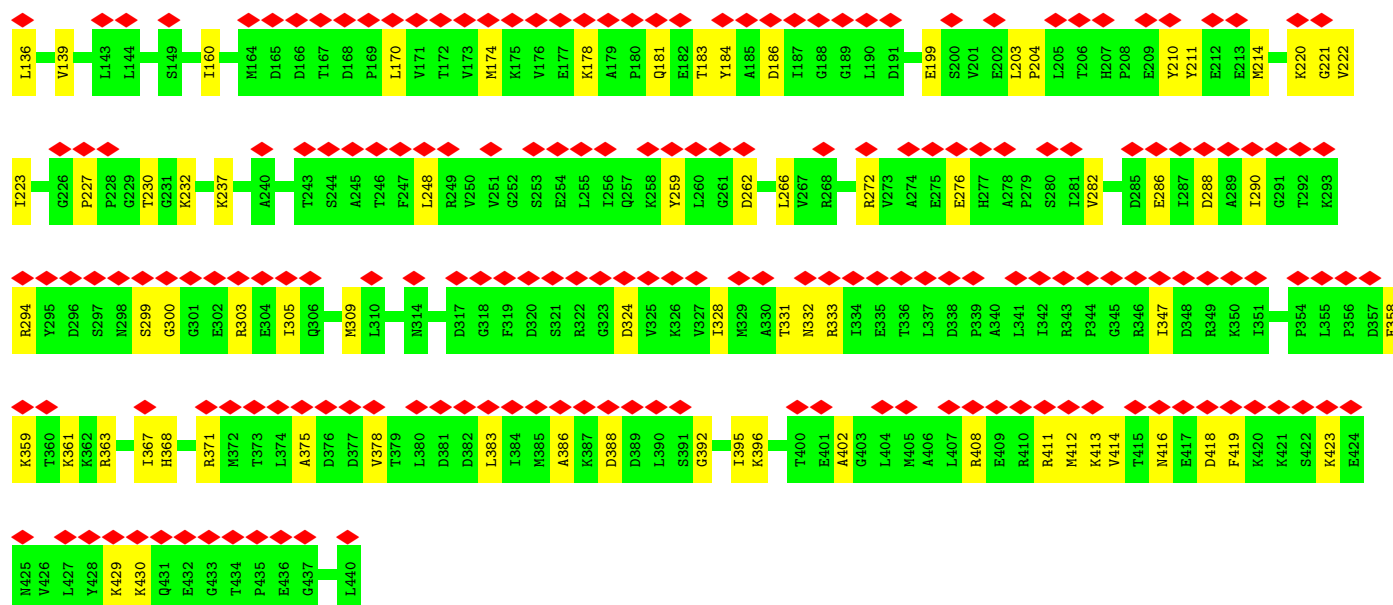
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

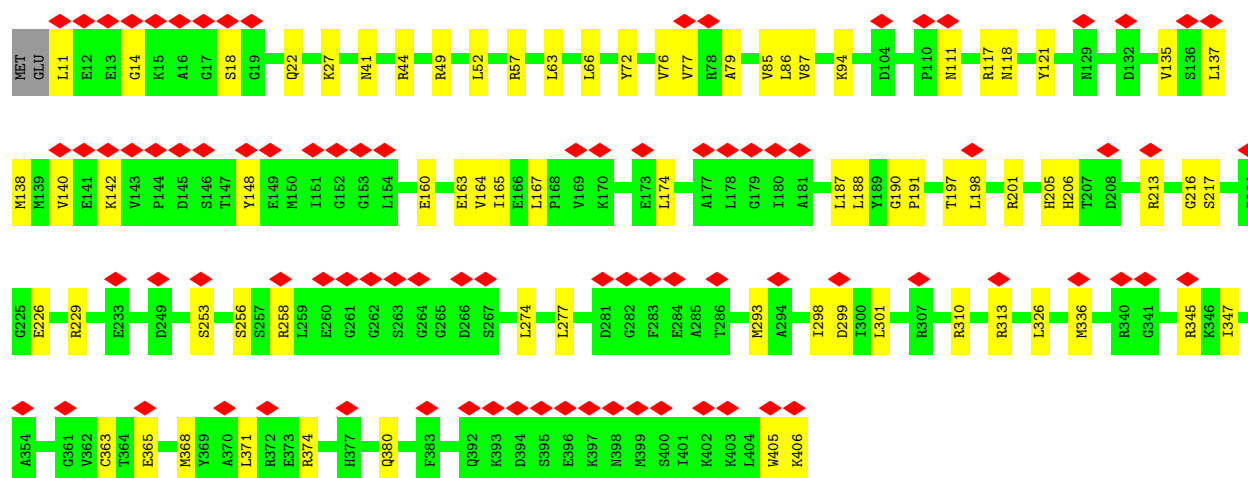
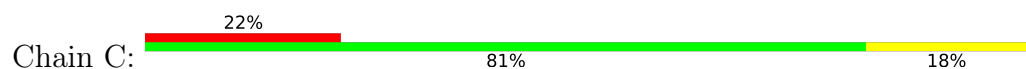


• Molecule 2: 26S proteasome regulatory subunit 4

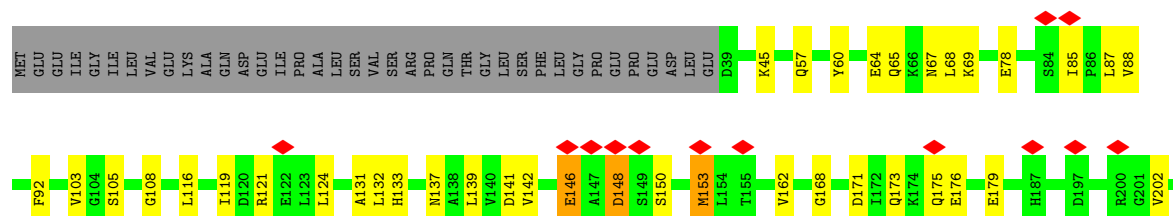


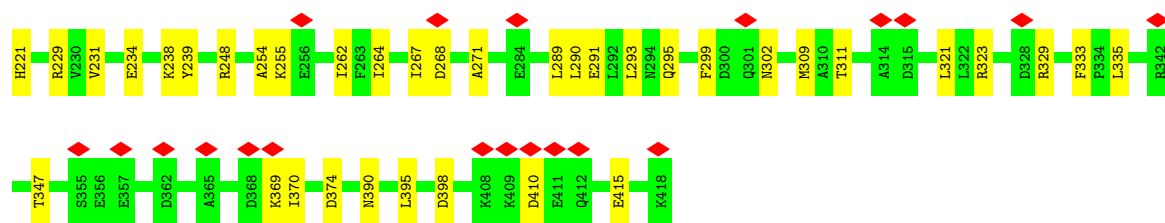


• Molecule 3: 26S proteasome regulatory subunit 8

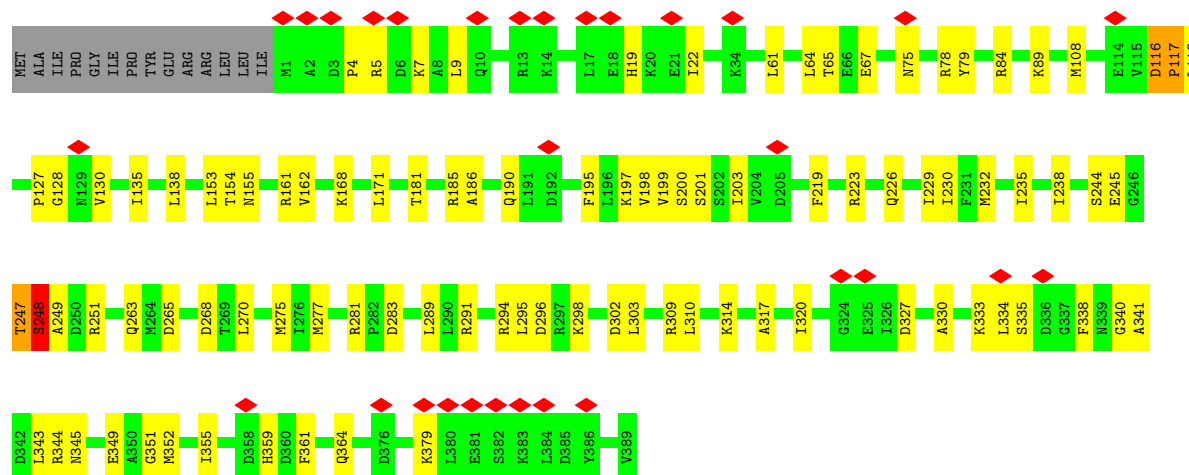
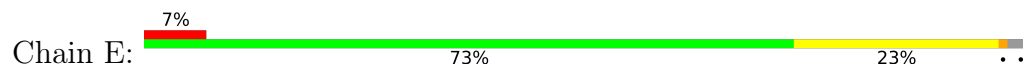


• Molecule 4: 26S proteasome regulatory subunit 6B

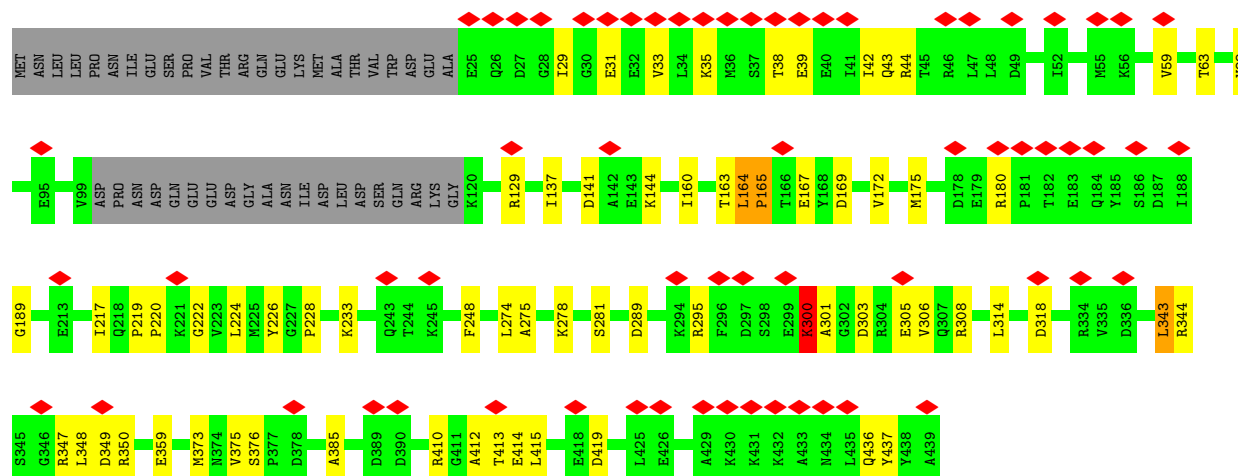
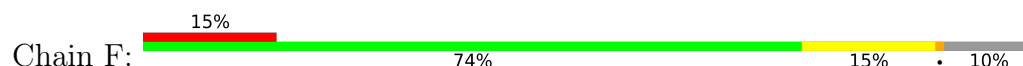




• Molecule 5: Proteasome 26S subunit, ATPase 6



• Molecule 6: 26S proteasome regulatory subunit 6A

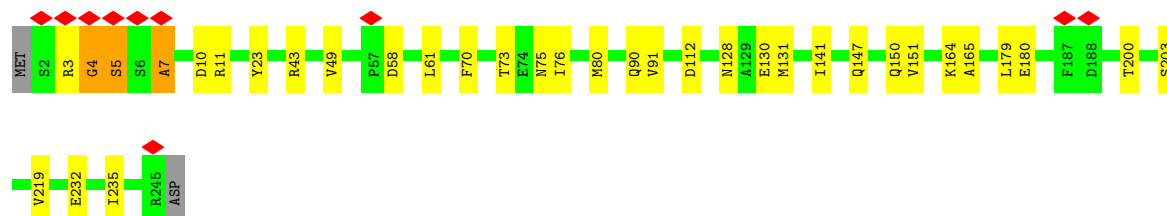
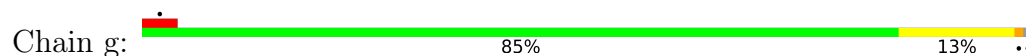


• Molecule 7: Proteasome subunit alpha type-6

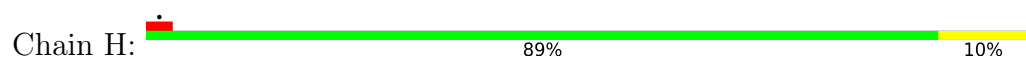




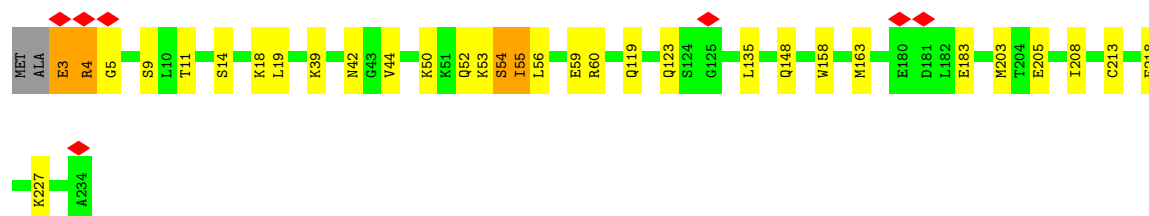
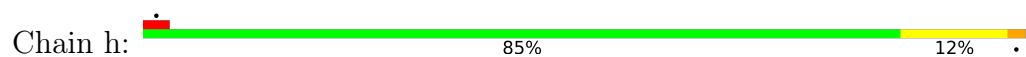
• Molecule 7: Proteasome subunit alpha type-6



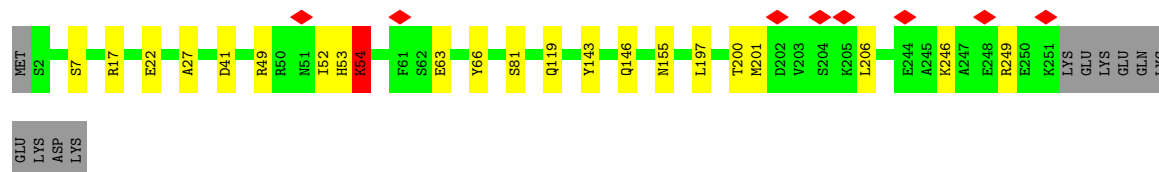
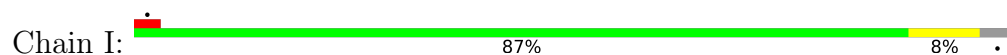
• Molecule 8: Proteasome subunit alpha type-2



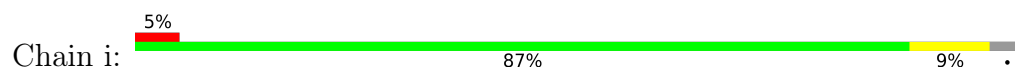
• Molecule 8: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-4

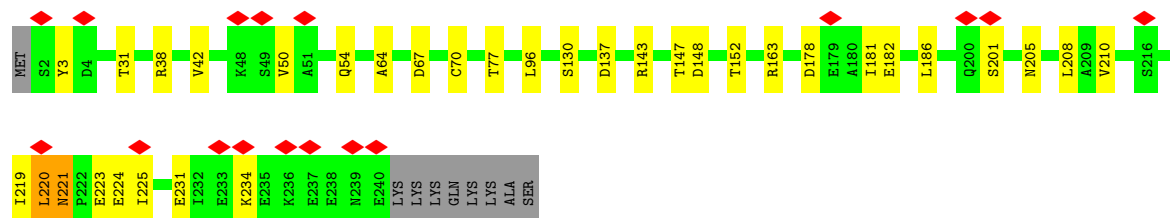
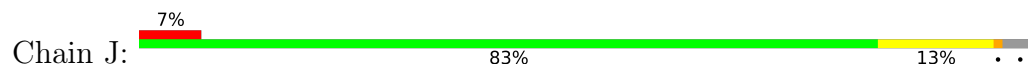


• Molecule 9: Proteasome subunit alpha type-4

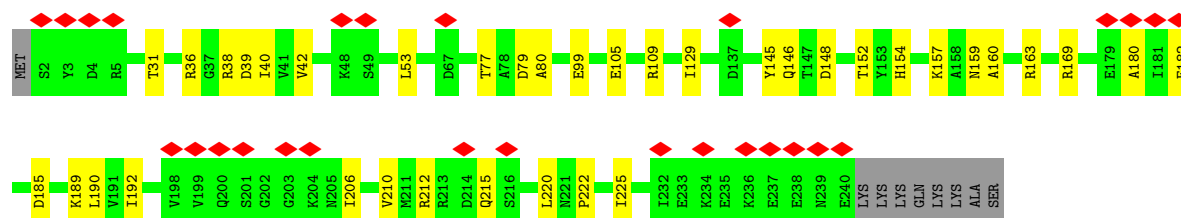
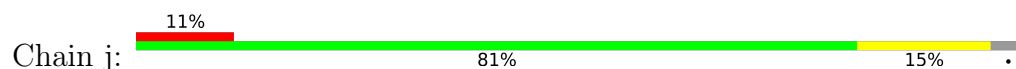




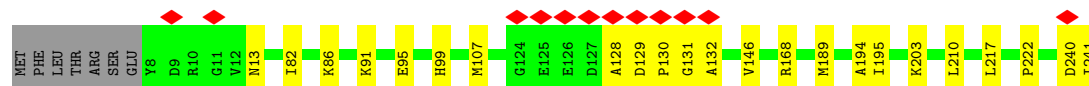
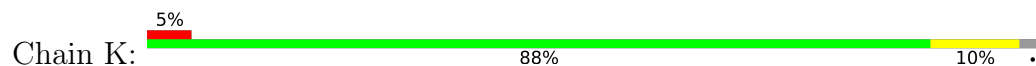
- Molecule 10: Proteasome subunit alpha type-7



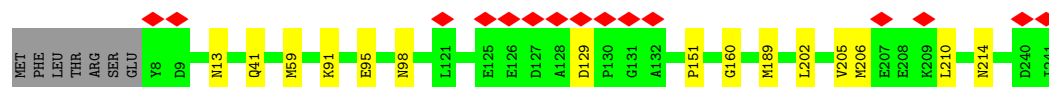
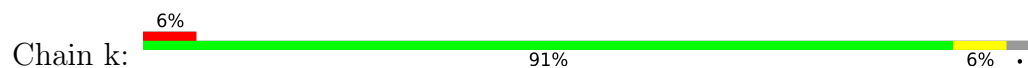
- Molecule 10: Proteasome subunit alpha type-7



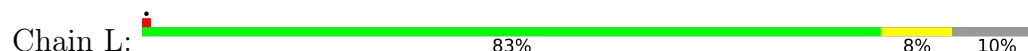
- Molecule 11: Proteasome subunit alpha type-5

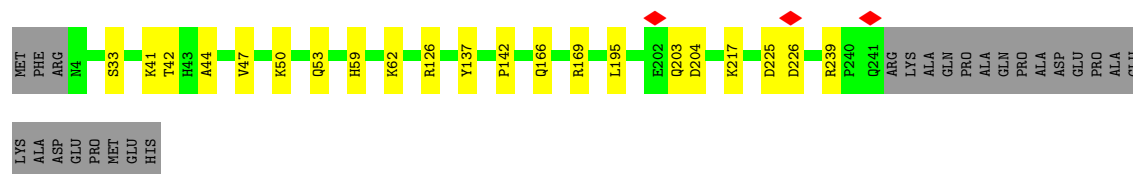


- Molecule 11: Proteasome subunit alpha type-5

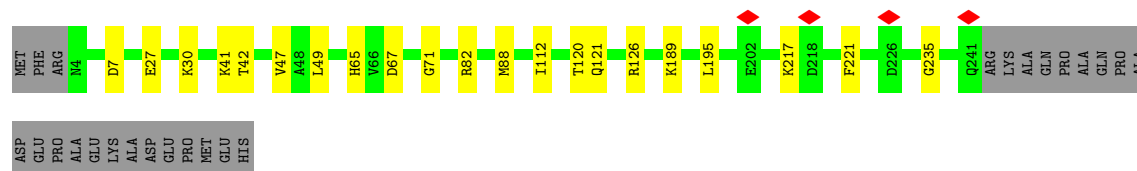
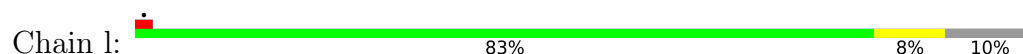


- Molecule 12: Proteasome subunit alpha type-1

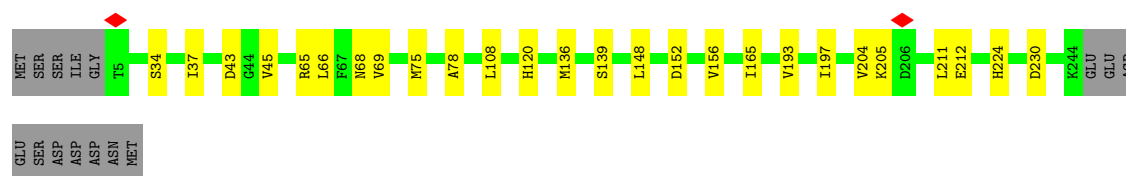
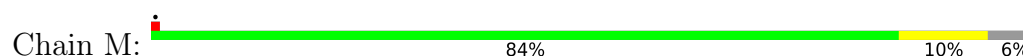




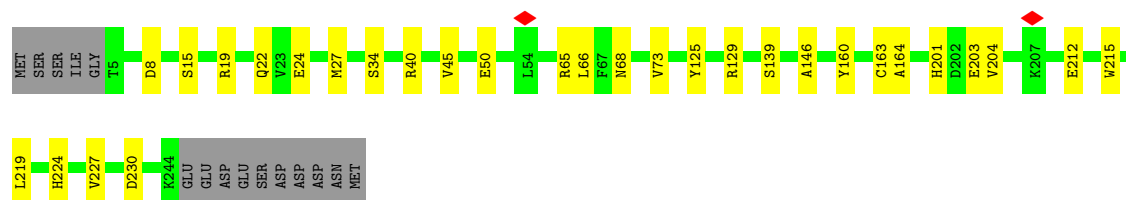
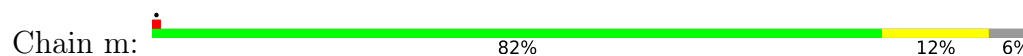
• Molecule 12: Proteasome subunit alpha type-1



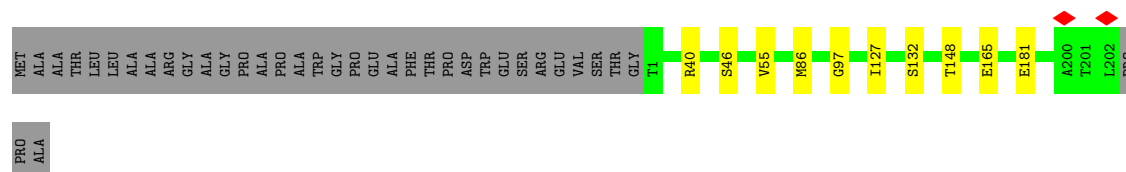
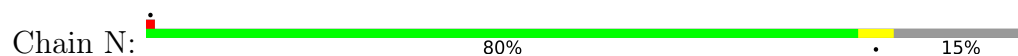
• Molecule 13: Proteasome subunit alpha type-3



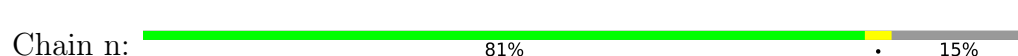
• Molecule 13: Proteasome subunit alpha type-3

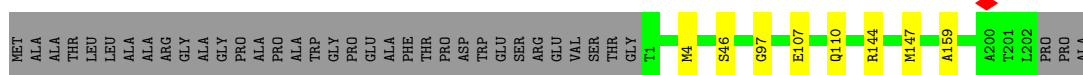


• Molecule 14: Proteasome subunit beta type-6

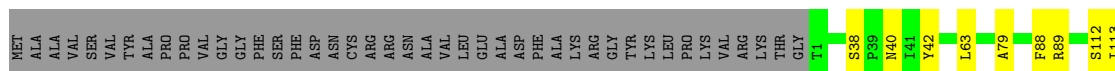


• Molecule 14: Proteasome subunit beta type-6

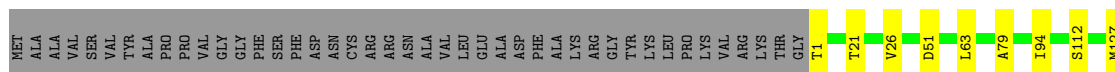




• Molecule 15: Proteasome subunit beta type-7



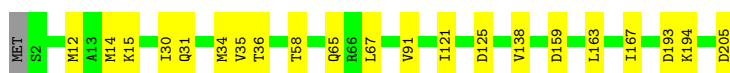
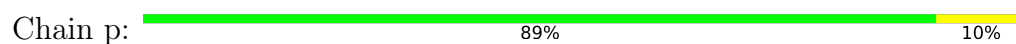
• Molecule 15: Proteasome subunit beta type-7



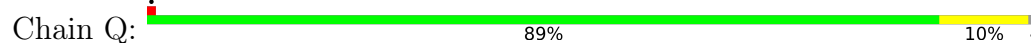
• Molecule 16: Proteasome subunit beta type-3



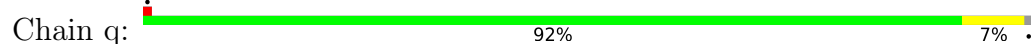
• Molecule 16: Proteasome subunit beta type-3



• Molecule 17: Proteasome subunit beta type-2



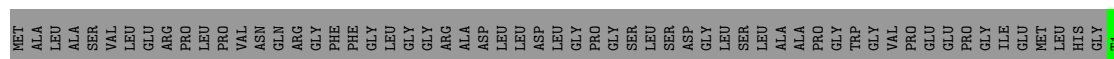
• Molecule 17: Proteasome subunit beta type-2





- Molecule 18: Proteasome subunit beta type-5

Chain R: 70% 6% 24%



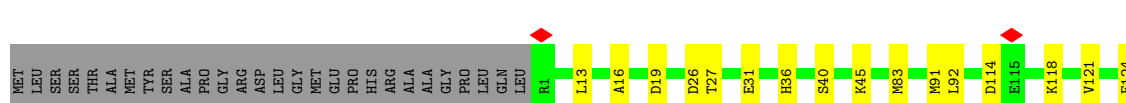
- Molecule 18: Proteasome subunit beta type-5

Chain r: 68% 8% 24%



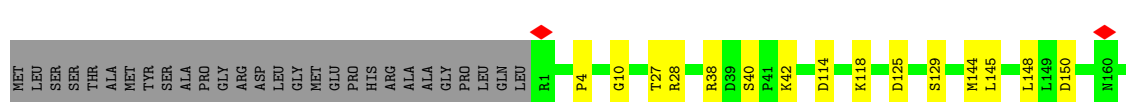
- Molecule 19: Proteasome subunit beta type-1

Chain S: 78% 10% 12%



- Molecule 19: Proteasome subunit beta type-1

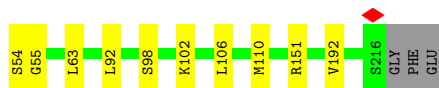
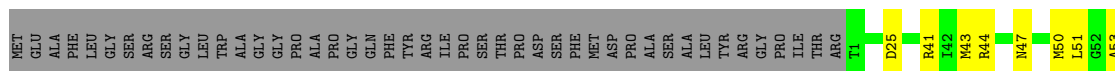
Chain s: 78% 10% 12%



- Molecule 20: Proteasome subunit beta type-4

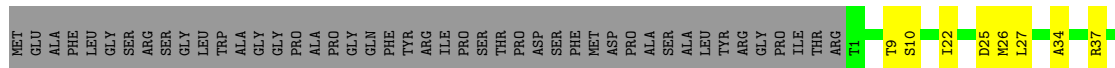
Chain T: 75% 7% 18%





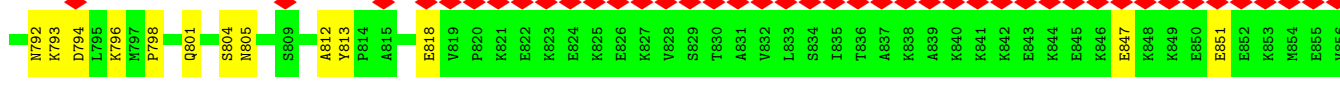
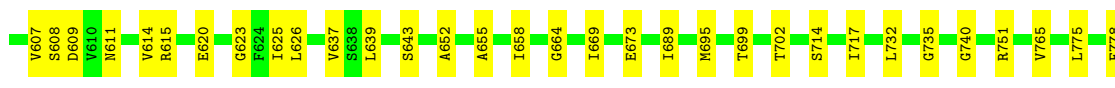
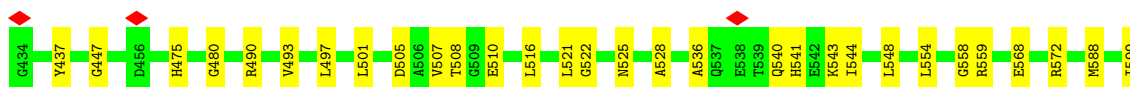
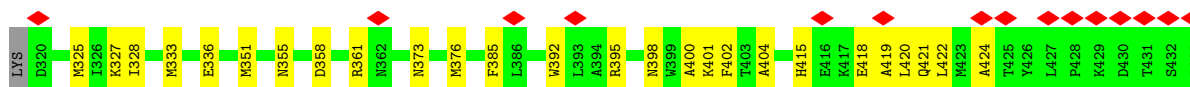
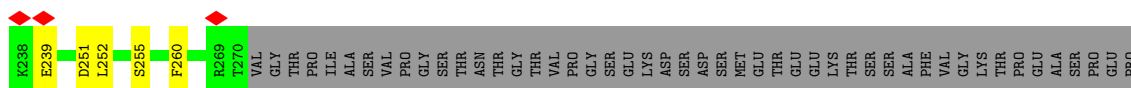
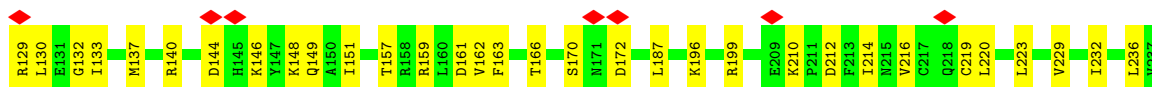
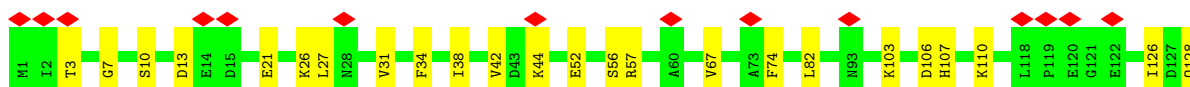
• Molecule 20: Proteasome subunit beta type-4

Chain t: 74% 8% 18%



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

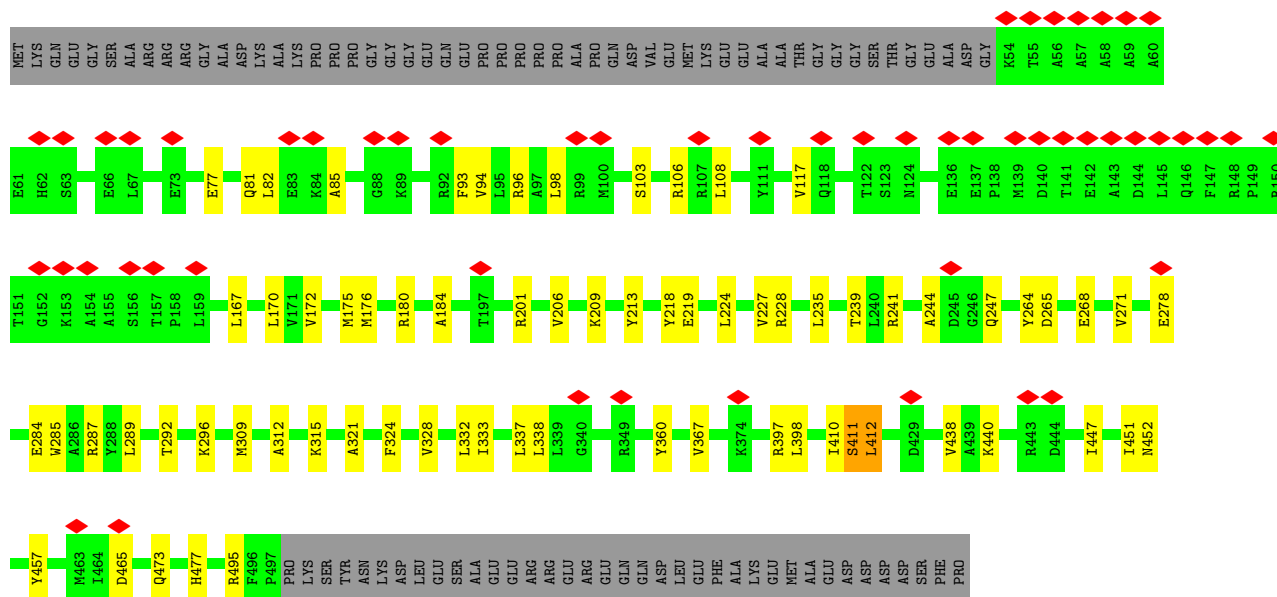
Chain U: 11% 73% 19% 8%



GLU
GLU
GLU
GLU
GLN
GLU
PRO
GLU
PRO
PHE
GLU
TYR
ASP
ASP

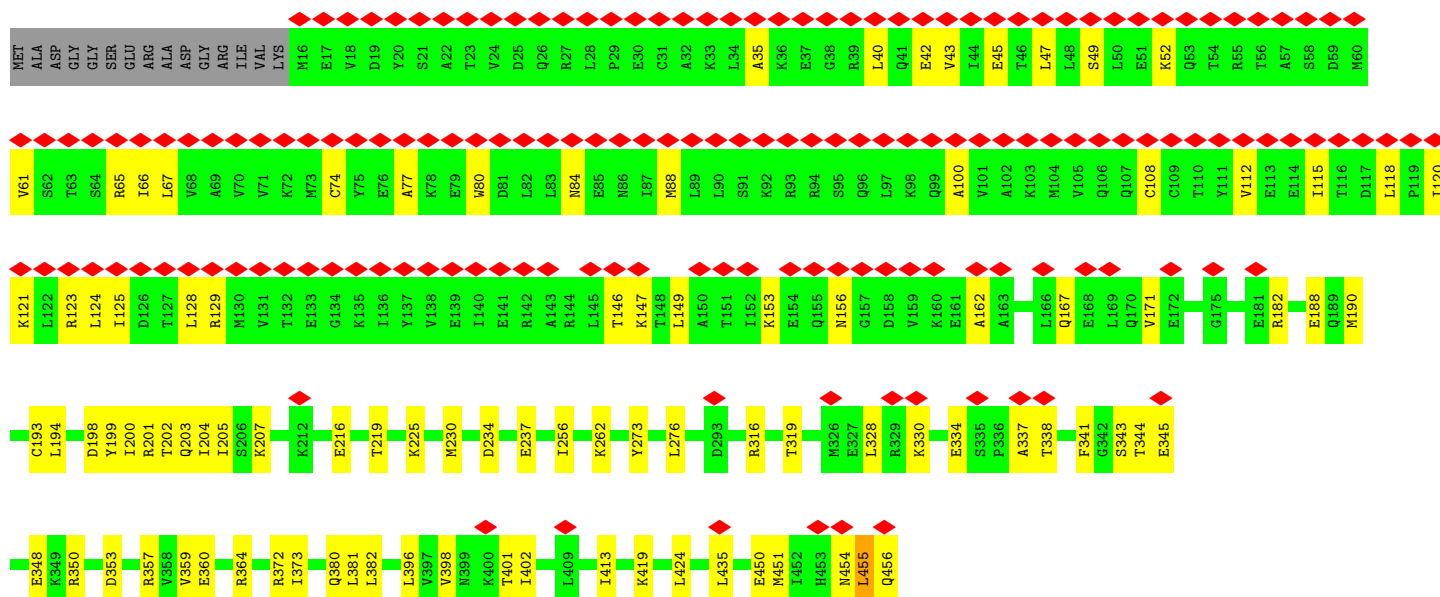
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 10% 70% 13% 17%



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

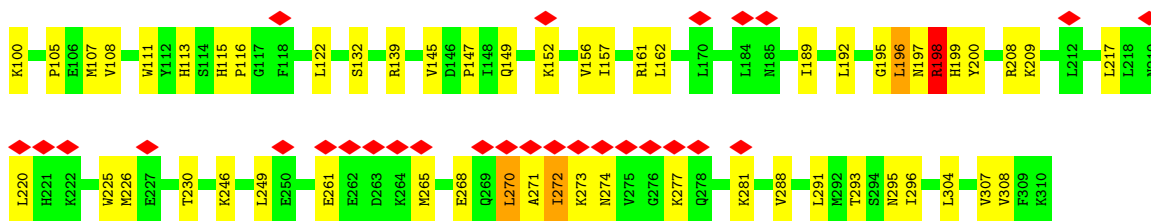
Chain W: 36% 75% 21%



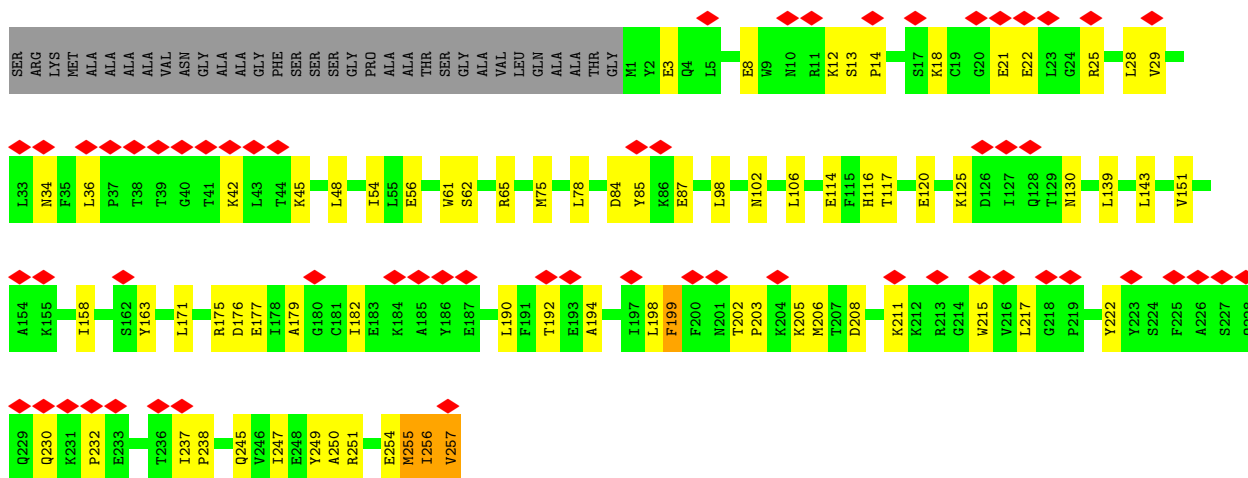
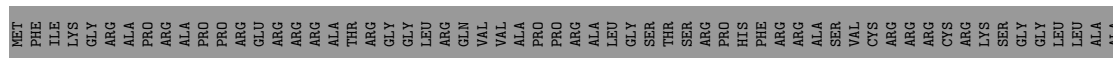
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 60% 78% 19%

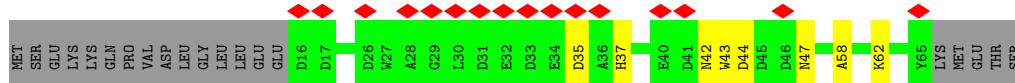




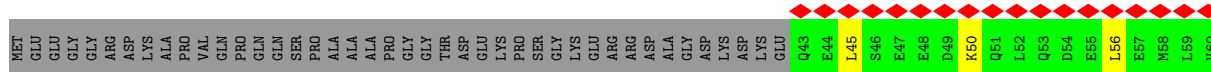
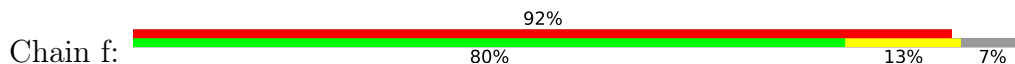
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1

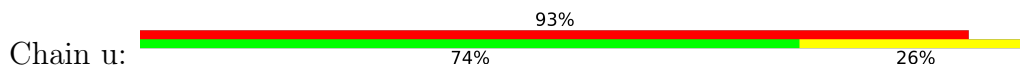


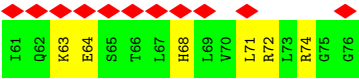
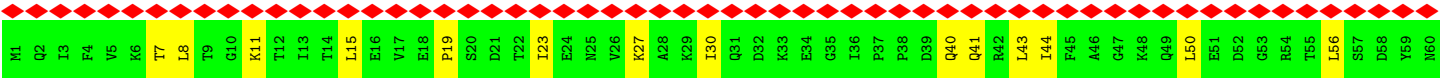
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



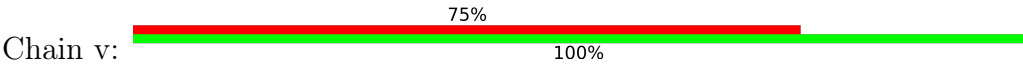
R181	P241	H301	S361	D421	S481	T541	A601	M662	S722	H782	V842
E182	E242	G302	G362	V422	I482	I542	G602	G663	V723	S783	S843
P183	P243	V303	S363	D423	F483	M543	S603	E664	M724	D784	V844
L184	E244	F304	Q364	G424	G484	E544	G604	E665	S725	R785	R845
L185	N245	L305	V365	G425	L485	K545	M605	I666	I726	R786	V846
T186	S246	E306	D366	L426	G486	S546	V606	G667	F727	L787	G847
L187	A247	L307	S367	T427	L487	E547	L607	A668	A728	M788	Q848
V188	L248	S308	A368	Q428	A488	T548	Q610	E669	A729	S789	A849
K189	L249	E309	R369	I429	Y489	E549	D611	M670	G730	S790	V850
E190	R250	D310	M370	D430	A490	L550	L612	A671	M731	Q791	D851
I191	C251	V311	N371	K431	G491	K551	L613	L672	V732	A792	V852
V192	A252	E312	L372	Y432	S492	D552	H614	R673	G733	V793	V853
P193	L253	E313	A373	L433	M493	T553	H615	T674	S734	A794	G854
Y194	G254	Y314	S374	Y434	R494	Y554	I616	F675	G735	L796	A856
N195	V255	E315	S375	S435	E495	A555	C616	G676	T736	L797	G857
M196	F256	D316	F376	S436	D496	R556	S617	H677	N737	T798	R858
A197	R257	L317	V377	E437	V497	M557	H618	L678	M738	V799	P859
H198	K258	T318	N378	D438	L498	L558	H619	L679	A739	L800	K860
N199	F259	E319	G379	Y439	T499	P559	F620	R680	R740	L801	T861
A200	S260	I320	G380	I440	L500	L560	S621	Y681	L741	V801	L862
E201	R261	M321	V381	K441	L501	G561	LYS	G682	A742	S802	T863
H202	F262	S322	N382	S442	L502	L562	GLU	E563	A743	F803	G864
E203	P263	N323	A383	G443	P503	G563	LYS	G684	M744	L804	F865
A204	E264	V324	A384	A444	V504	L564	GLU	T685	L745	D805	G866
C205	A265	Q325	F385	L445	M505	N565	ASP	L686	R746	Y806	T867
D206	L266	L326	G386	L446	G506	H566	ASP	R687	Q747	R807	H868
L207	R267	N327	Q387	A447	D507	L567	ASP	R688	L748	R808	T869
M208	L268	S328	D388	C448	S508	G568	LYS	A689	A749	I809	T870
M209	A269	N329	K389	G449	K509	K569	LYS	V690	Q750	I810	P871
E210	L270	F330	L390	I450	S510	G570	GLU	P691	Y751	L811	V872
I211	M271	L331	L391	V451	S511	E571	LYS	L692	H752	G812	L873
E212	L272	A332	T392	M452	M512	A572	ASP	A693	A753	R813	L874
Q213	N273	L333	D393	S453	E513	I573	ASP	L694	K754	S814	A875
V214	D274	A334	D394	G454	V514	E574	LYS	A695	D755	H815	H876
D215	M275	R335	G395	V455	A515	A575	LYS	L696	P756	Y816	G877
M216	E276	E336	N396	R456	G516	I576	GLU	T697	N757	H817	E878
L217	L277	L337	K397	M457	V517	L577	ALA	S698	M758	L818	R879
E218	V278	D338	W398	E458	T518	A578	A644	V699	L759	Y819	A880
K219	E279	I339	L399	C459	A519	A579	D645	S700	F760	G820	E881
D220	D280	M340	K400	D460	L520	L580	M646	T701	M761	L821	L882
I221	I281	E341	K401	P461	A521	E581	G647	F702	V762	V822	T884
E223	F282	P342	N402	A462	C522	V582	A648	R703	R763	A824	E885
N224	S283	K343	K403	L463	G523	S583	H649	L704	L764	M825	Q826
A225	D284	V344	D404	A464	M524	S584	Q650	M705	A765	K826	R827
A226	C285	P345	H405	L465	I525	E585	G651	L706	Q766	Q827	L888
Y226	K286	D346	G406	L466	A526	P586	V652	L707	G767	F827	P889
A227	D287	D347	M407	S467	V527	F587	A653	D708	L768	R828	V890
K228	V288	E348	L408	D468	G528	R588	V654	T709	T769	M829	T891
V229	V289	Y349	S409	Y469	S529	S589	L655	L710	H770	L830	P892
C230	V290	A410	A410	V470	C530	F590	Q656	S711	L771	R831	L894
L231	Q291	T351	A411	L471	N531	I591	L657	K712	G772	T832	E895
E232	K292	H352	A412	H472	G532	N592	A658	F713	K773	F833	G896
L233	Q293	L353	S413	M473	D533	T593	L659	S714	G774	D834	F897
T234	M294	E354	L414	S474	V534	L594	T660	H715	L775	E835	V898
S235	A295	N355	G415	M475	T535	V595	A661	D716	L776	R836	L900
C236	F296	N356	M416	T476	S536	D596		A717	T777	L837	P841
V237	M297	R357	I417	M477	T537	V597		D718	L778	R838	
L238	F298	F358	L418	R478	C598	V597		P719	C779	P839	
Y239	G299	G359	L419	L479	A599	C598		E720	P780	L840	
V240	R300	G360	W420	G480	Q540	Y600		V721	Y781		

● Molecule 33: Ubiquitin





● Molecule 34: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68506	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	0.022	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00603	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/3185	0.52	2/4299 (0.0%)
2	B	0.20	0/3168	0.57	4/4276 (0.1%)
3	C	0.22	0/3146	0.53	0/4226
4	D	0.25	0/3090	0.61	3/4168 (0.1%)
5	E	0.25	0/3145	0.57	4/4233 (0.1%)
6	F	0.24	0/3137	0.54	0/4223
7	G	0.26	0/1923	0.47	0/2601
7	g	0.28	0/1914	0.48	0/2590
8	H	0.27	0/1844	0.49	0/2499
8	h	0.26	0/1844	0.44	0/2497
9	I	0.27	0/1991	0.53	1/2685 (0.0%)
9	i	0.24	0/1985	0.47	1/2677 (0.0%)
10	J	0.26	0/1906	0.51	0/2573
10	j	0.23	0/1887	0.48	0/2549
11	K	0.26	0/1804	0.44	0/2436
11	k	0.23	0/1809	0.43	0/2444
12	L	0.24	0/1901	0.42	0/2570
12	l	0.25	0/1896	0.45	0/2565
13	M	0.23	0/1911	0.40	0/2573
13	m	0.24	0/1916	0.42	0/2580
14	N	0.26	0/1540	0.41	0/2085
14	n	0.26	0/1536	0.39	0/2080
15	O	0.27	0/1676	0.44	0/2271
15	o	0.26	0/1686	0.43	0/2282
16	P	0.27	0/1616	0.50	0/2180
16	p	0.26	0/1620	0.45	0/2184
17	Q	0.27	0/1621	0.40	0/2194
17	q	0.27	0/1621	0.42	0/2194
18	R	0.28	0/1590	0.45	0/2147
18	r	0.29	0/1590	0.45	0/2147
19	S	0.27	0/1671	0.46	0/2252
19	s	0.27	0/1684	0.49	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.26	0/1716	0.42	0/2323
20	t	0.27	0/1720	0.43	0/2328
21	U	0.24	0/6984	0.54	0/9435
22	V	0.20	0/3681	0.45	0/4969
23	W	0.21	0/3644	0.50	0/4901
24	X	0.27	0/3381	0.56	1/4558 (0.0%)
25	Y	0.23	0/3261	0.53	1/4393 (0.0%)
26	Z	0.25	0/2324	0.62	3/3150 (0.1%)
27	a	0.22	0/3053	0.57	0/4133
28	b	0.19	0/1478	0.51	0/2001
29	c	0.28	0/2302	0.63	0/3110
30	d	0.26	0/2162	0.59	0/2919
31	e	0.25	0/437	0.69	0/595
32	f	0.19	0/6640	0.49	0/8988
33	u	0.18	0/607	0.44	0/816
All	All	0.24	0/108243	0.50	20/146167 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	317	PRO	N-CA-C	-9.30	99.93	112.48
5	E	116	ASP	CA-C-N	8.87	130.93	119.84
5	E	116	ASP	C-N-CA	8.87	130.93	119.84
2	B	86	LYS	CA-C-N	8.84	130.89	119.84
2	B	86	LYS	C-N-CA	8.84	130.89	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3135	0	3175	73	0
2	B	3122	0	3174	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3105	0	3219	51	0
4	D	3040	0	3076	62	0
5	E	3097	0	3173	68	0
6	F	3098	0	3187	55	0
7	G	1889	0	1885	12	0
7	g	1880	0	1875	24	0
8	H	1805	0	1784	16	0
8	h	1805	0	1798	20	0
9	I	1958	0	1960	13	0
9	i	1955	0	1955	14	0
10	J	1880	0	1892	25	0
10	j	1861	0	1865	25	0
11	K	1777	0	1762	14	0
11	k	1782	0	1766	11	0
12	L	1866	0	1852	14	0
12	l	1861	0	1839	15	0
13	M	1876	0	1861	15	0
13	m	1881	0	1868	21	0
14	N	1514	0	1487	5	0
14	n	1510	0	1483	4	0
15	O	1649	0	1659	11	0
15	o	1659	0	1681	8	0
16	P	1587	0	1598	13	0
16	p	1591	0	1609	18	0
17	Q	1588	0	1584	16	0
17	q	1588	0	1584	11	0
18	R	1559	0	1523	11	0
18	r	1559	0	1523	14	0
19	S	1641	0	1639	15	0
19	s	1654	0	1656	14	0
20	T	1683	0	1662	10	0
20	t	1687	0	1666	13	0
21	U	6867	0	6929	120	0
22	V	3612	0	3682	46	0
23	W	3596	0	3713	61	0
24	X	3335	0	3435	82	0
25	Y	3202	0	3204	61	0
26	Z	2281	0	2312	52	0
27	a	2995	0	3012	46	0
28	b	1458	0	1505	29	0
29	c	2260	0	2276	59	0
30	d	2116	0	2146	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	e	425	0	328	5	0
32	f	6529	0	6541	72	0
33	u	601	0	629	13	0
34	v	120	0	32	0	0
35	A	27	0	12	2	0
35	F	27	0	12	1	0
36	C	31	0	12	3	0
36	D	31	0	12	1	0
36	E	31	0	12	3	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
38	c	1	0	0	0	0
All	All	106690	0	107124	1327	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 1327 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)
24:X:142:ARG:HG2	24:X:145:GLU:OE2	1.43	1.16
25:Y:236:LEU:HD12	25:Y:239:LYS:HZ1	1.22	1.02
24:X:317:PRO:HD2	24:X:319:ILE:HG12	1.42	1.00
24:X:183:LEU:HB3	24:X:184:PRO:HD3	1.43	0.98
23:W:451:MET:HE3	23:W:455:LEU:HD11	1.45	0.96

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	400/433 (92%)	351 (88%)	46 (12%)	3 (1%)	16	44
2	B	397/440 (90%)	359 (90%)	36 (9%)	2 (0%)	24	54
3	C	394/398 (99%)	339 (86%)	55 (14%)	0	100	100
4	D	378/418 (90%)	327 (86%)	49 (13%)	2 (0%)	24	54
5	E	387/403 (96%)	340 (88%)	43 (11%)	4 (1%)	12	40
6	F	391/439 (89%)	345 (88%)	44 (11%)	2 (0%)	24	54
7	G	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
7	g	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	10	35
8	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
8	h	230/234 (98%)	219 (95%)	9 (4%)	2 (1%)	14	42
9	I	249/261 (95%)	240 (96%)	7 (3%)	2 (1%)	16	44
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	j	237/248 (96%)	220 (93%)	17 (7%)	0	100	100
11	K	232/241 (96%)	219 (94%)	11 (5%)	2 (1%)	14	42
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
12	l	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
13	M	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
14	N	200/239 (84%)	194 (97%)	6 (3%)	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%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	203 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
20	t	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
21	U	874/953 (92%)	800 (92%)	73 (8%)	1 (0%)	48	78
22	V	442/534 (83%)	419 (95%)	23 (5%)	0	100	100
23	W	439/456 (96%)	425 (97%)	14 (3%)	0	100	100
24	X	420/422 (100%)	393 (94%)	24 (6%)	3 (1%)	18	47
25	Y	387/389 (100%)	363 (94%)	24 (6%)	0	100	100
26	Z	284/324 (88%)	252 (89%)	32 (11%)	0	100	100
27	a	371/376 (99%)	335 (90%)	35 (9%)	1 (0%)	36	65
28	b	189/377 (50%)	169 (89%)	20 (11%)	0	100	100
29	c	285/310 (92%)	236 (83%)	47 (16%)	2 (1%)	18	47
30	d	255/350 (73%)	215 (84%)	40 (16%)	0	100	100
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	802 (96%)	38 (4%)	0	100	100
33	u	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	13464/14952 (90%)	12535 (93%)	900 (7%)	29 (0%)	44	71

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
2	B	87	PRO
5	E	117	PRO
5	E	247	THR
5	E	248	SER

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	338/372 (91%)	335 (99%)	3 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	349/385 (91%)	347 (99%)	2 (1%)	78	80
3	C	340/346 (98%)	340 (100%)	0	100	100
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	80
5	E	341/353 (97%)	339 (99%)	2 (1%)	78	80
6	F	340/379 (90%)	336 (99%)	4 (1%)	63	72
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	202 (100%)	0	100	100
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	185 (98%)	3 (2%)	55	68
9	I	207/221 (94%)	204 (99%)	3 (1%)	59	70
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	198 (98%)	3 (2%)	57	69
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (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%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	156 (99%)	1 (1%)	78	80
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (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	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	751 (100%)	1 (0%)	88	89
22	V	390/460 (85%)	388 (100%)	2 (0%)	81	81
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	85
24	X	362/362 (100%)	354 (98%)	8 (2%)	45	63
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	83
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	247 (98%)	5 (2%)	48	65
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
33	u	68/68 (100%)	68 (100%)	0	100	100
All	All	11512/12682 (91%)	11466 (100%)	46 (0%)	81	83

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	313	LEU
29	c	198	ARG
24	X	314	ARG
26	Z	144	VAL
29	c	272	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	292	GLN
28	b	161	ASN
17	q	110	HIS
24	X	406	ASN
26	Z	145	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
36	ATP	D	501	37	29,33,33	0.37	0	44,52,52	0.52	1 (2%)
35	ADP	A	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.98	10 (23%)
36	ATP	E	401	-	29,33,33	0.36	0	44,52,52	0.60	0
35	ADP	F	501	-	27,29,29	1.39	4 (14%)	42,45,45	2.07	9 (21%)
36	ATP	C	501	37	29,33,33	0.34	0	44,52,52	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	D	501	37	-	5/22/38/38	0/3/3/3
35	ADP	A	501	-	-	2/16/32/32	0/3/3/3
36	ATP	E	401	-	-	9/22/38/38	0/3/3/3
35	ADP	F	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	C	501	37	-	3/22/38/38	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)
35	A	501	ADP	C5-C4	4.54	1.47	1.39
35	F	501	ADP	C5-C4	4.53	1.47	1.39
35	F	501	ADP	C5-N7	-2.72	1.33	1.39
35	A	501	ADP	C5-C6	2.59	1.48	1.41
35	F	501	ADP	C5-C6	2.53	1.48	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	501	ADP	C5-C4-N3	-7.02	117.59	126.75
35	A	501	ADP	C5-C4-N3	-6.06	118.85	126.75
35	F	501	ADP	N3-C4-N9	5.61	136.33	127.08
35	A	501	ADP	N3-C4-N9	4.80	134.99	127.08
35	F	501	ADP	C2-N3-C4	4.01	121.21	111.75

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	F	501	ADP	PA-O3A-PB-O3B
35	F	501	ADP	C5'-O5'-PA-O1A
35	F	501	ADP	C5'-O5'-PA-O2A
35	F	501	ADP	C5'-O5'-PA-O3A
36	C	501	ATP	PB-O3B-PG-O3G

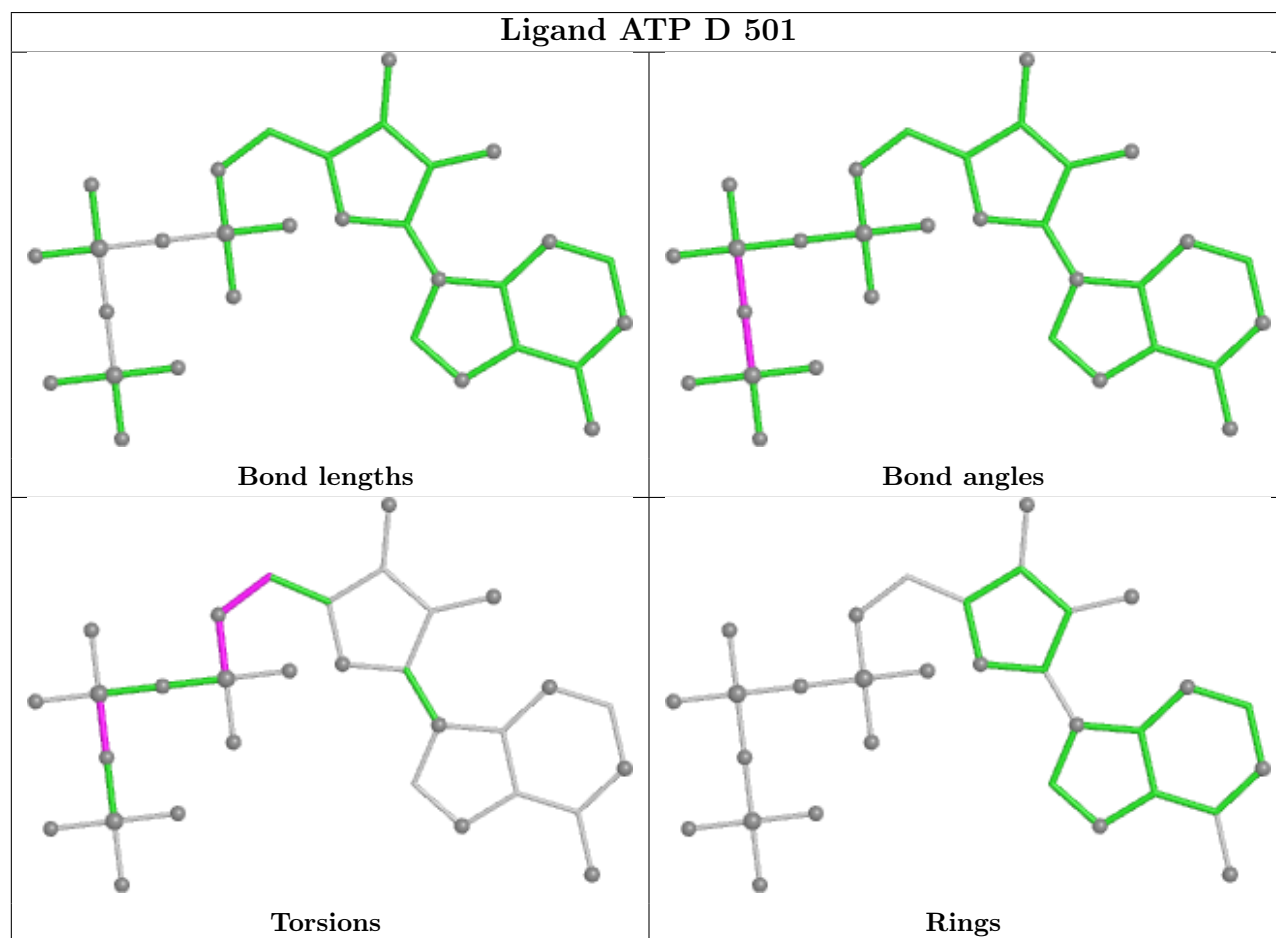
There are no ring outliers.

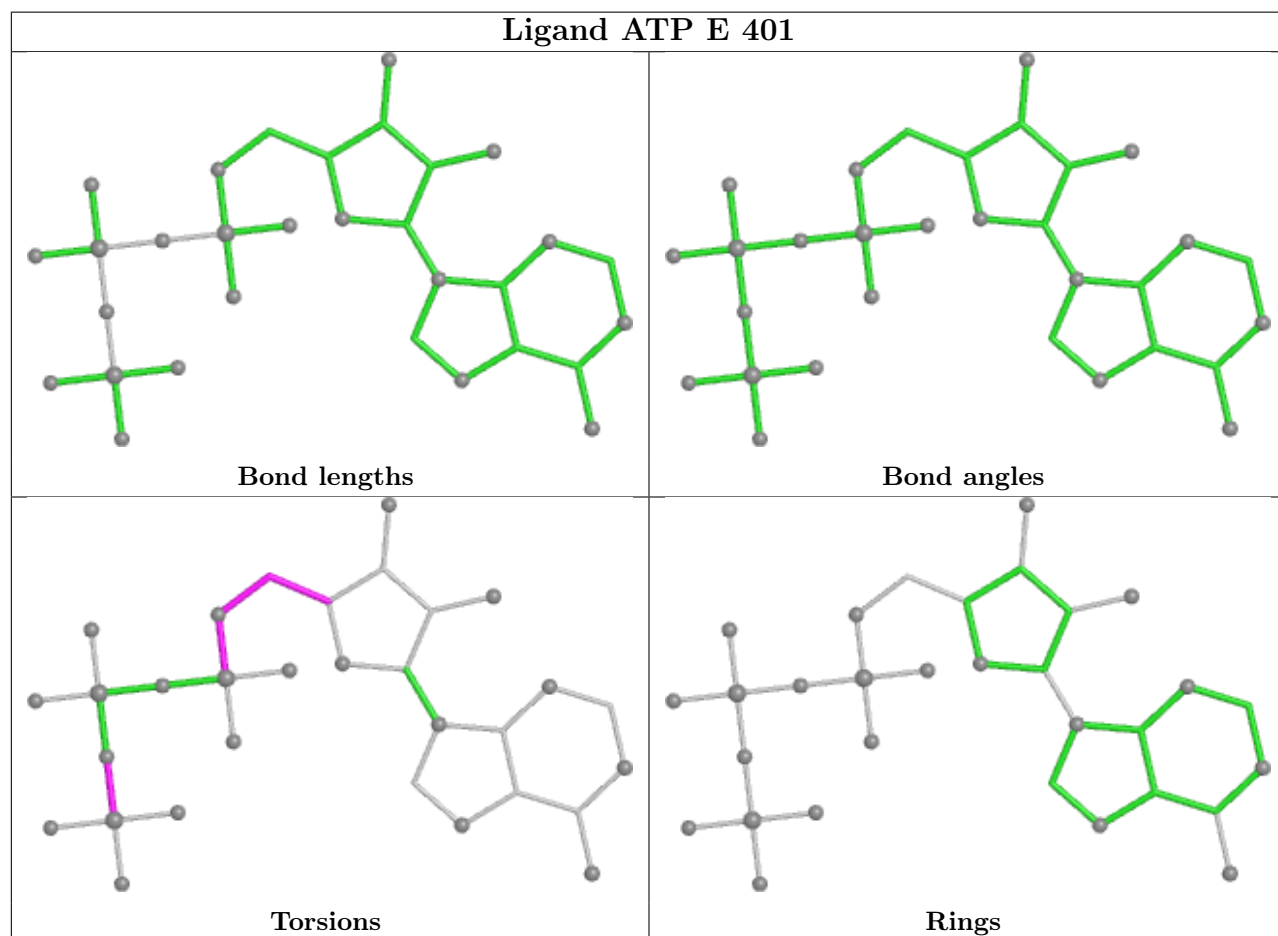
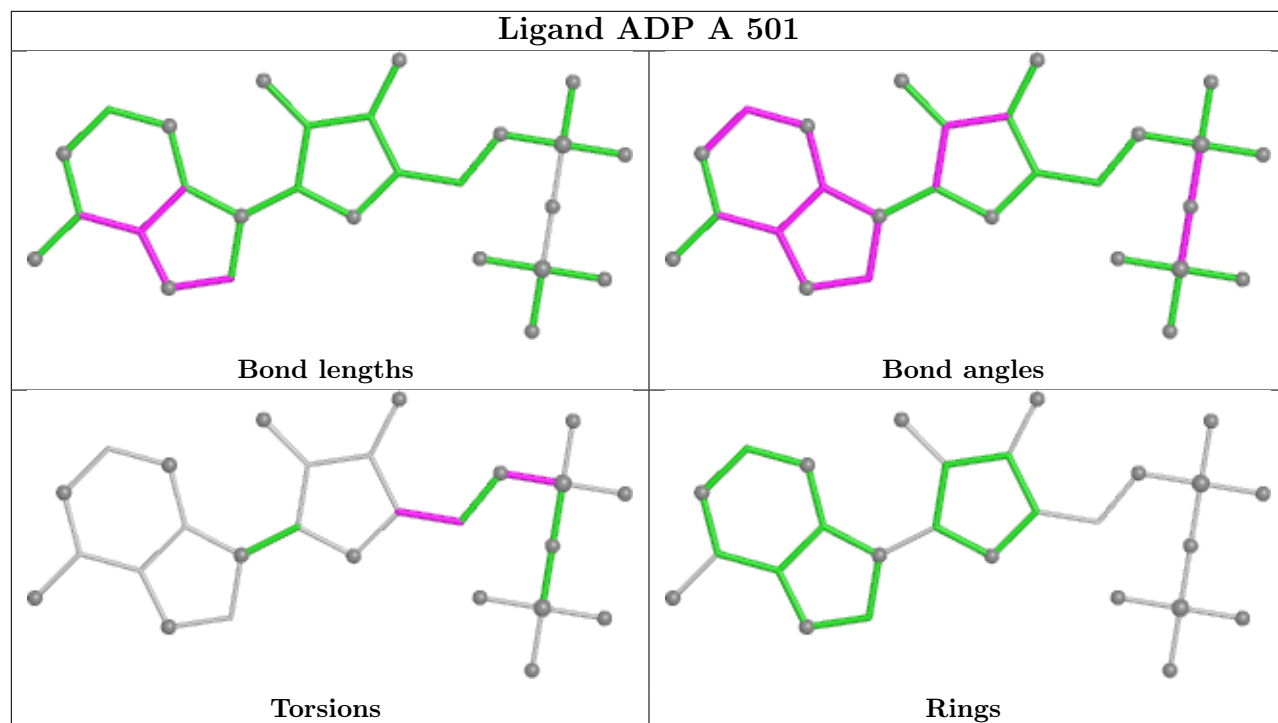
5 monomers are involved in 10 short contacts:

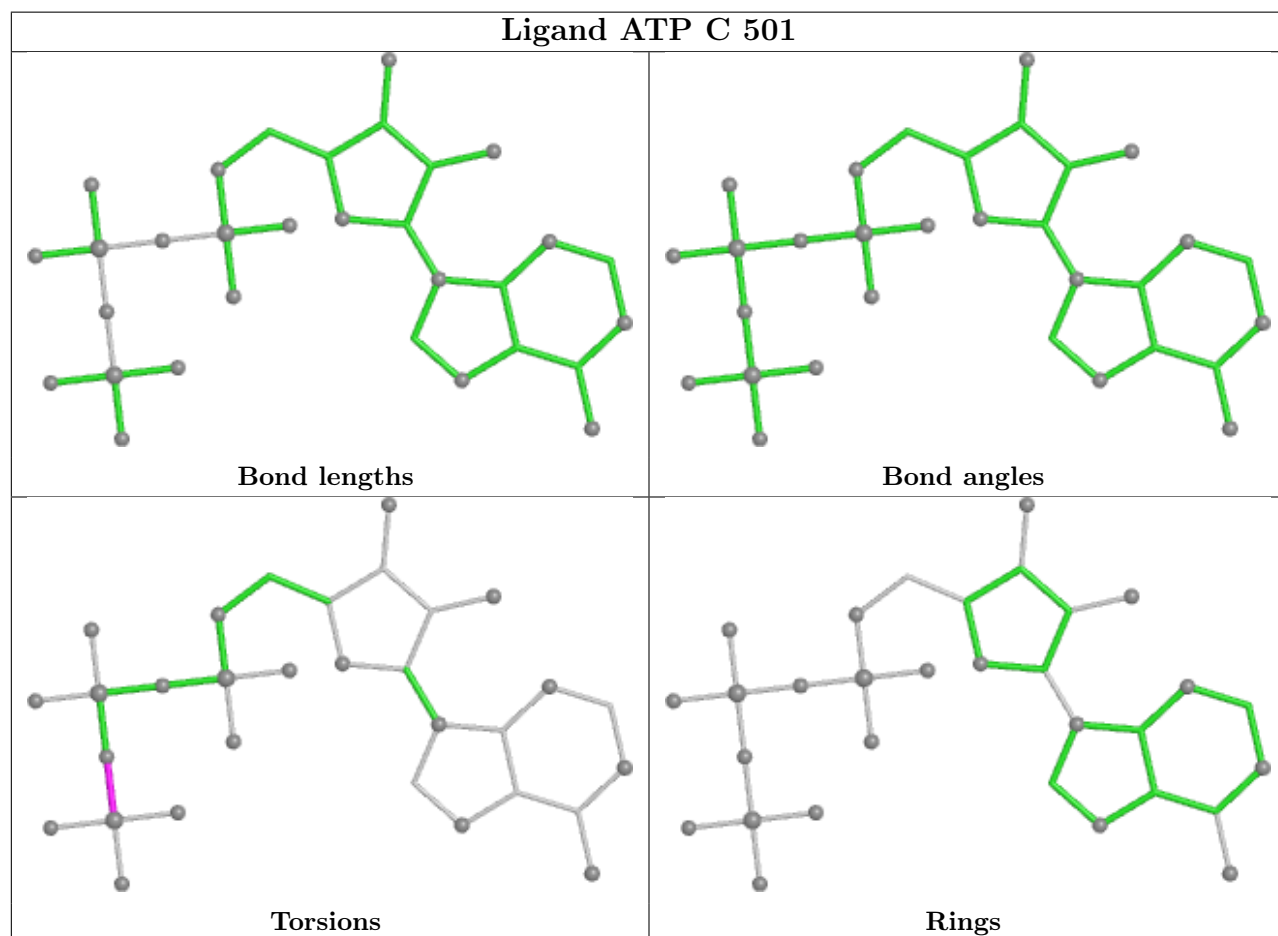
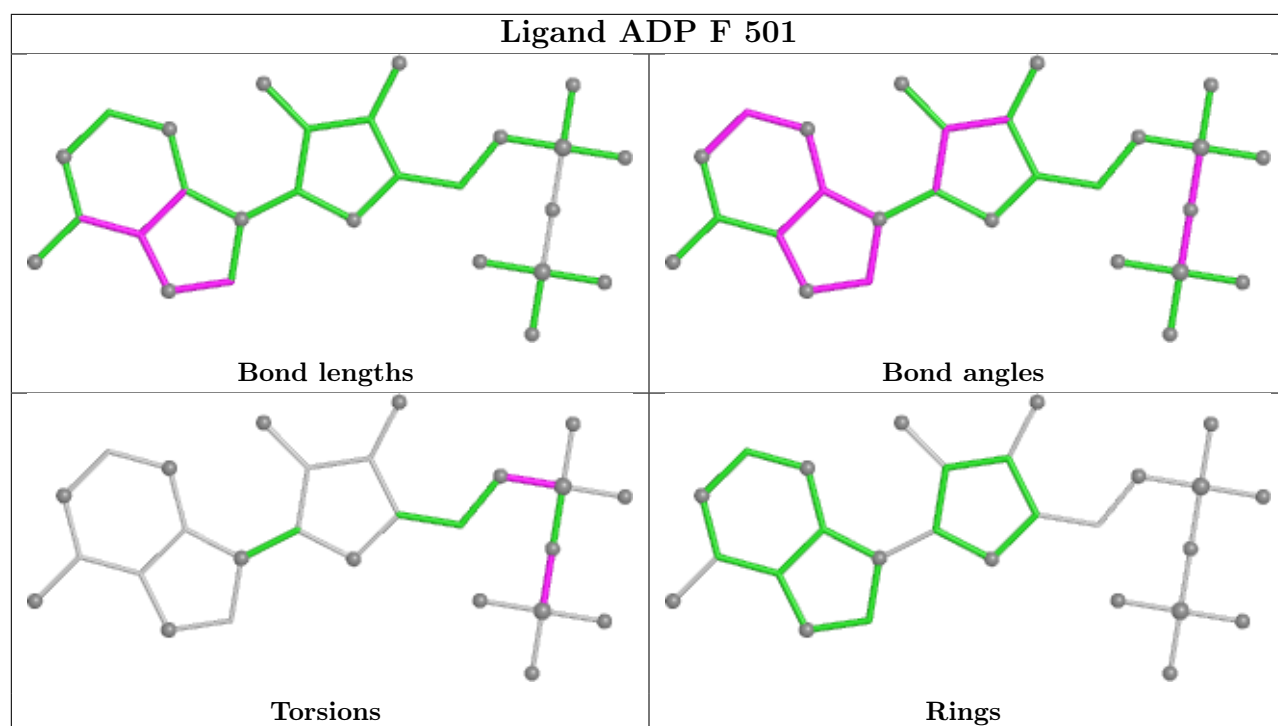
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	D	501	ATP	1	0
35	A	501	ADP	2	0
36	E	401	ATP	3	0
35	F	501	ADP	1	0
36	C	501	ATP	3	0

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.

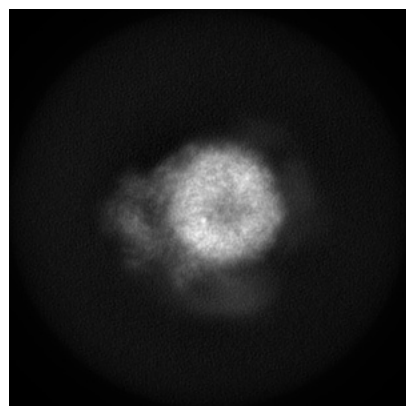
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62070. 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](#)

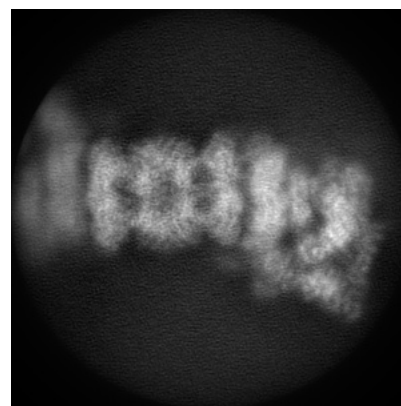
6.1.1 Primary map



X

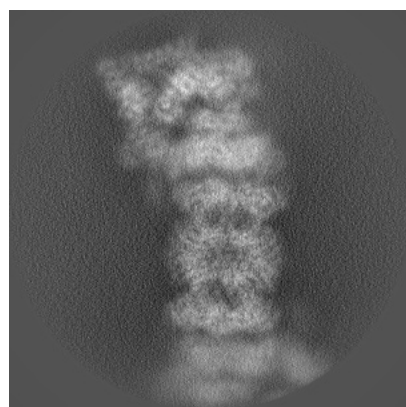


Y

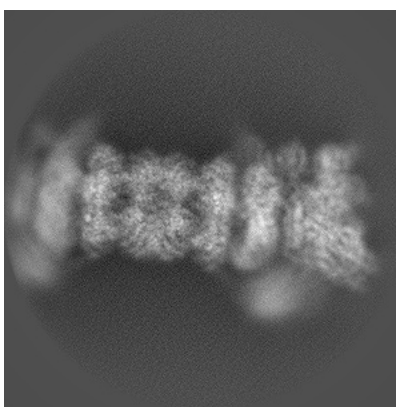


Z

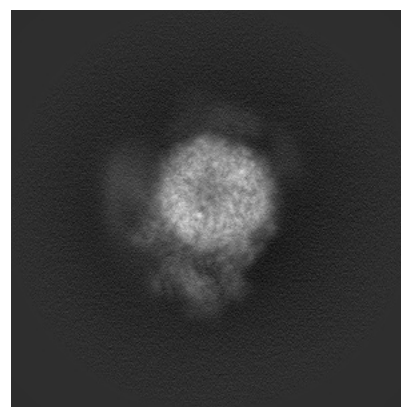
6.1.2 Raw map



X



Y

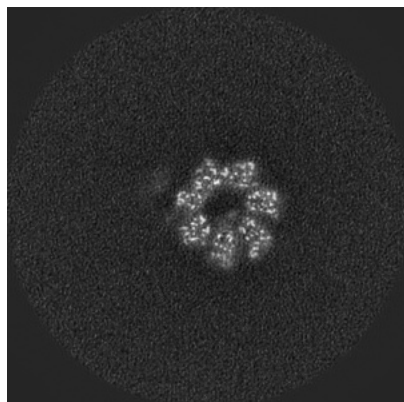


Z

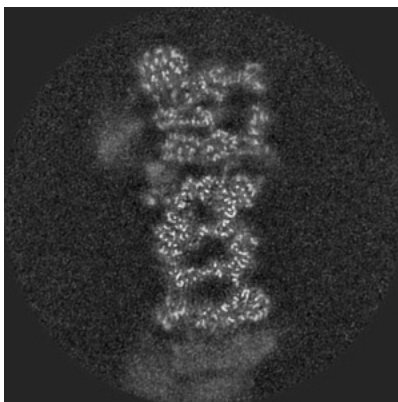
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

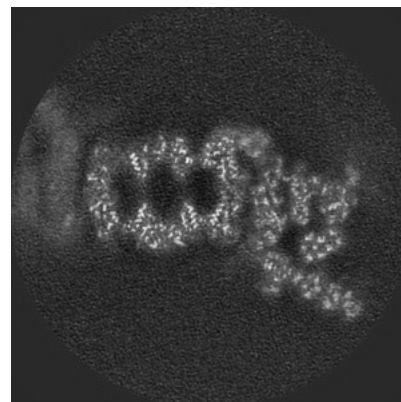
6.2.1 Primary map



X Index: 300

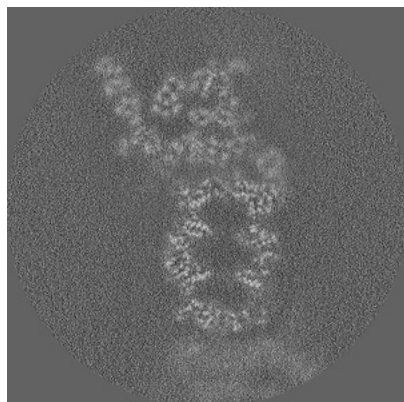


Y Index: 300

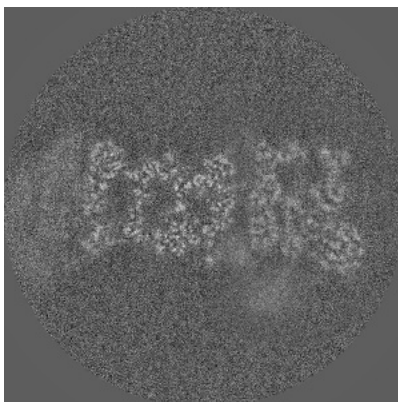


Z Index: 300

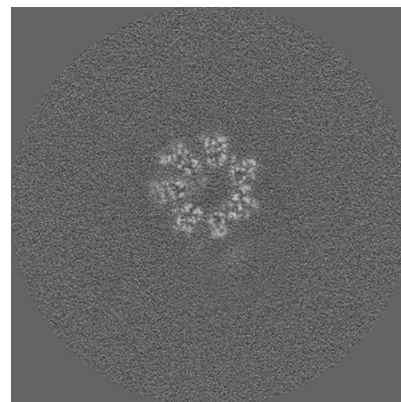
6.2.2 Raw map



X Index: 300



Y Index: 300

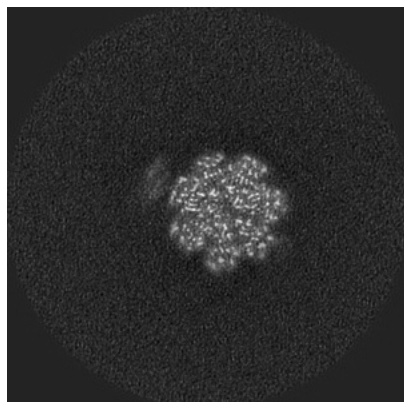


Z Index: 300

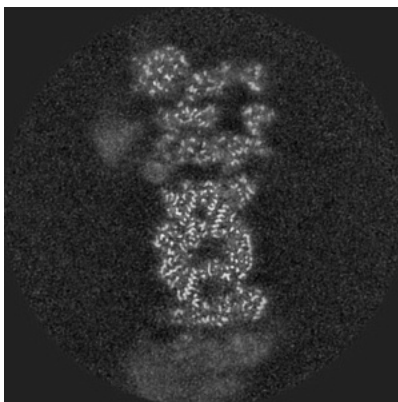
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

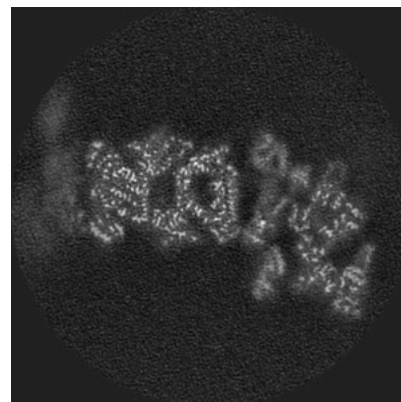
6.3.1 Primary map



X Index: 317

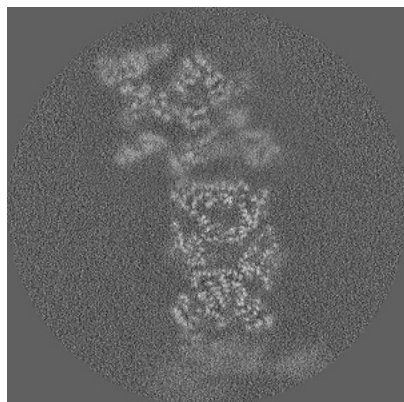


Y Index: 290

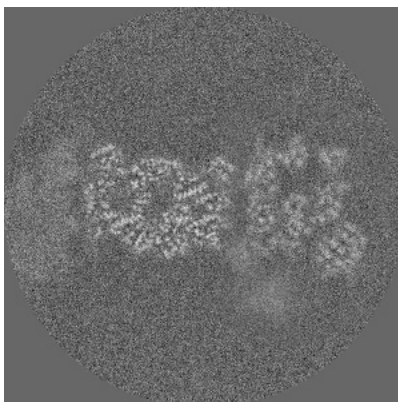


Z Index: 270

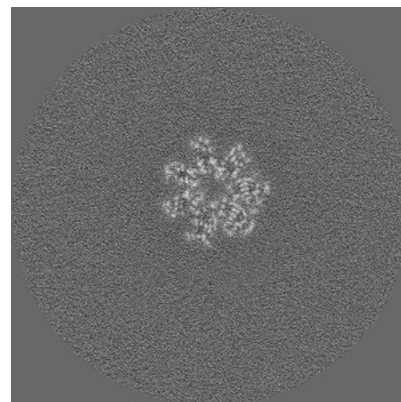
6.3.2 Raw map



X Index: 269



Y Index: 290

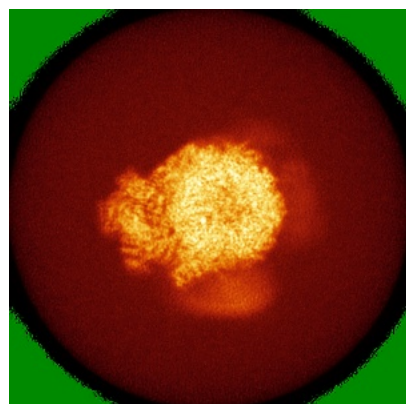


Z Index: 263

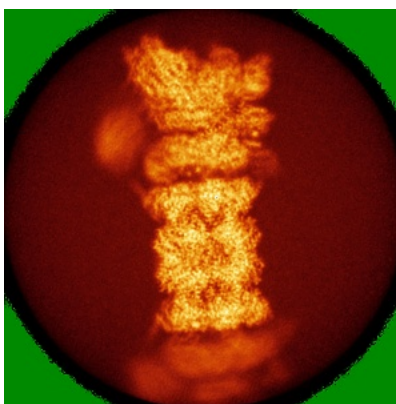
The images above show the largest variance slices of the map in three orthogonal directions.

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

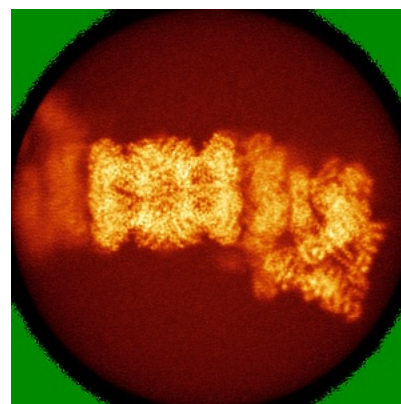
6.4.1 Primary map



X

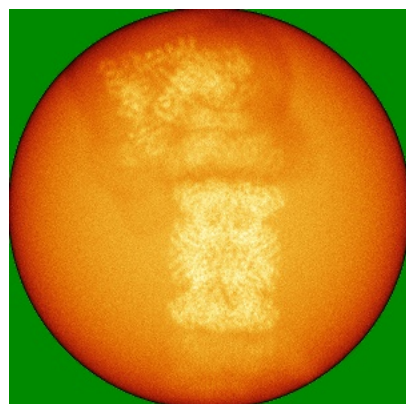


Y

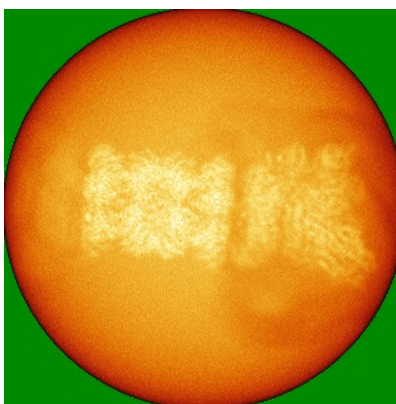


Z

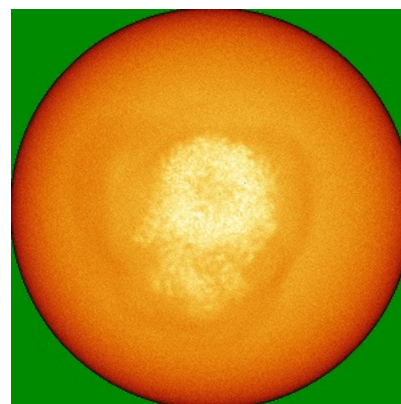
6.4.2 Raw map



X



Y

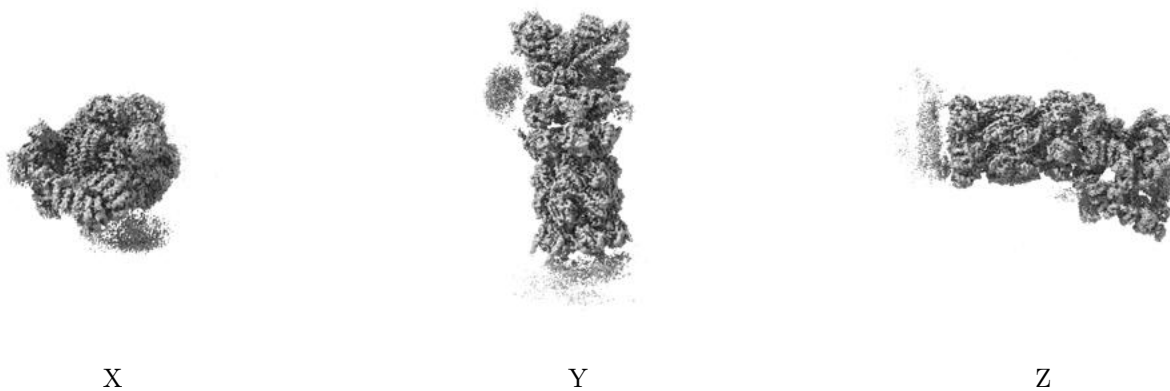


Z

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.

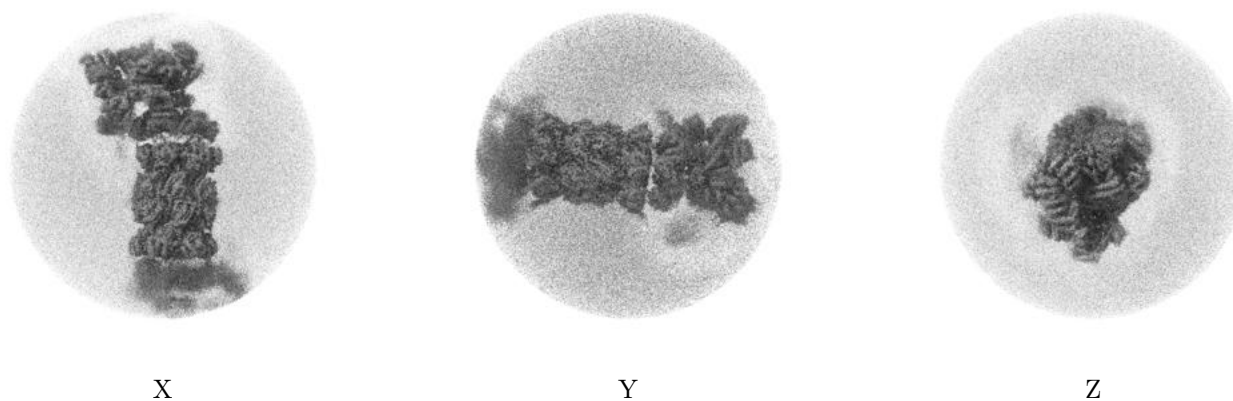
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00603. 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.

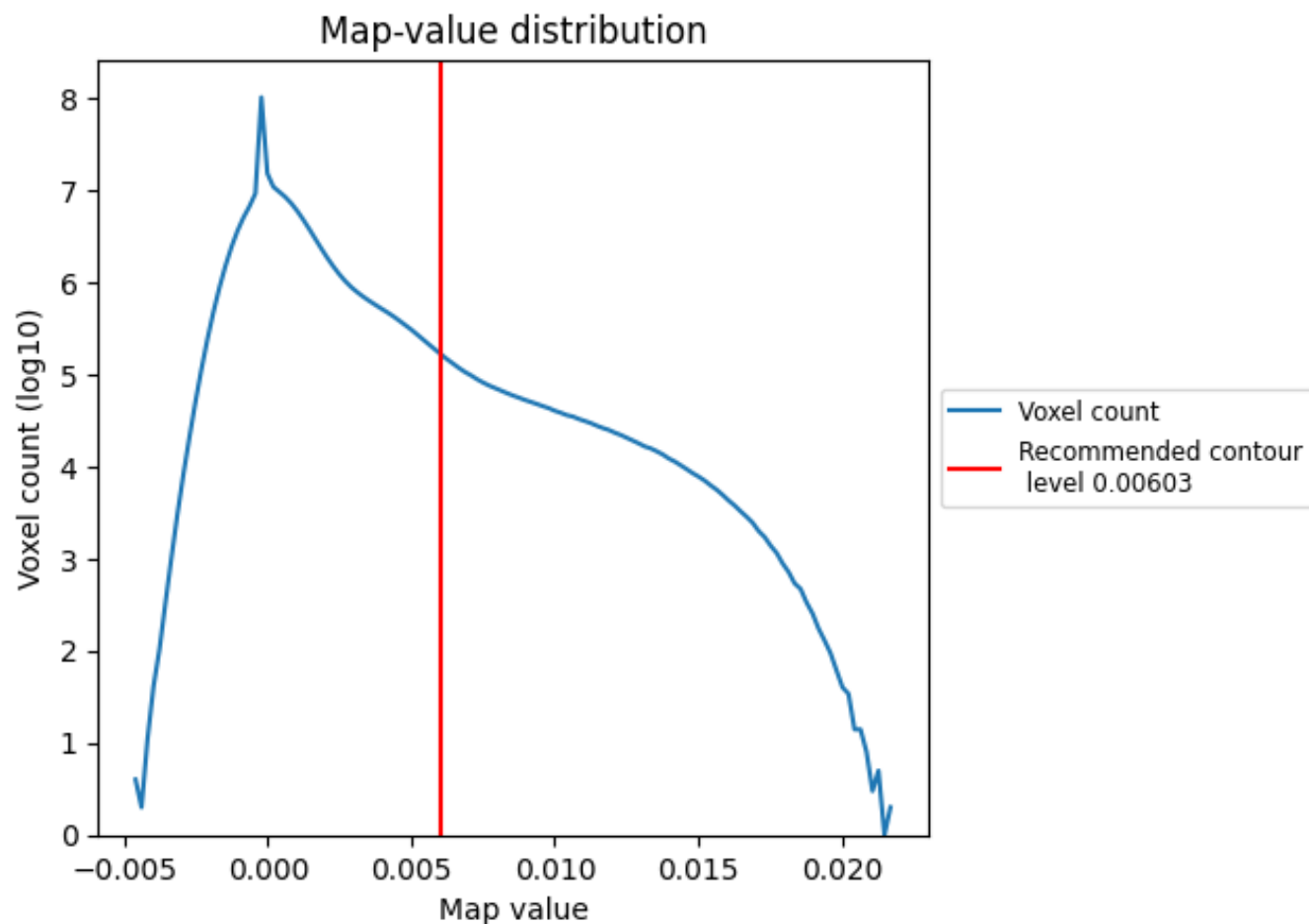
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

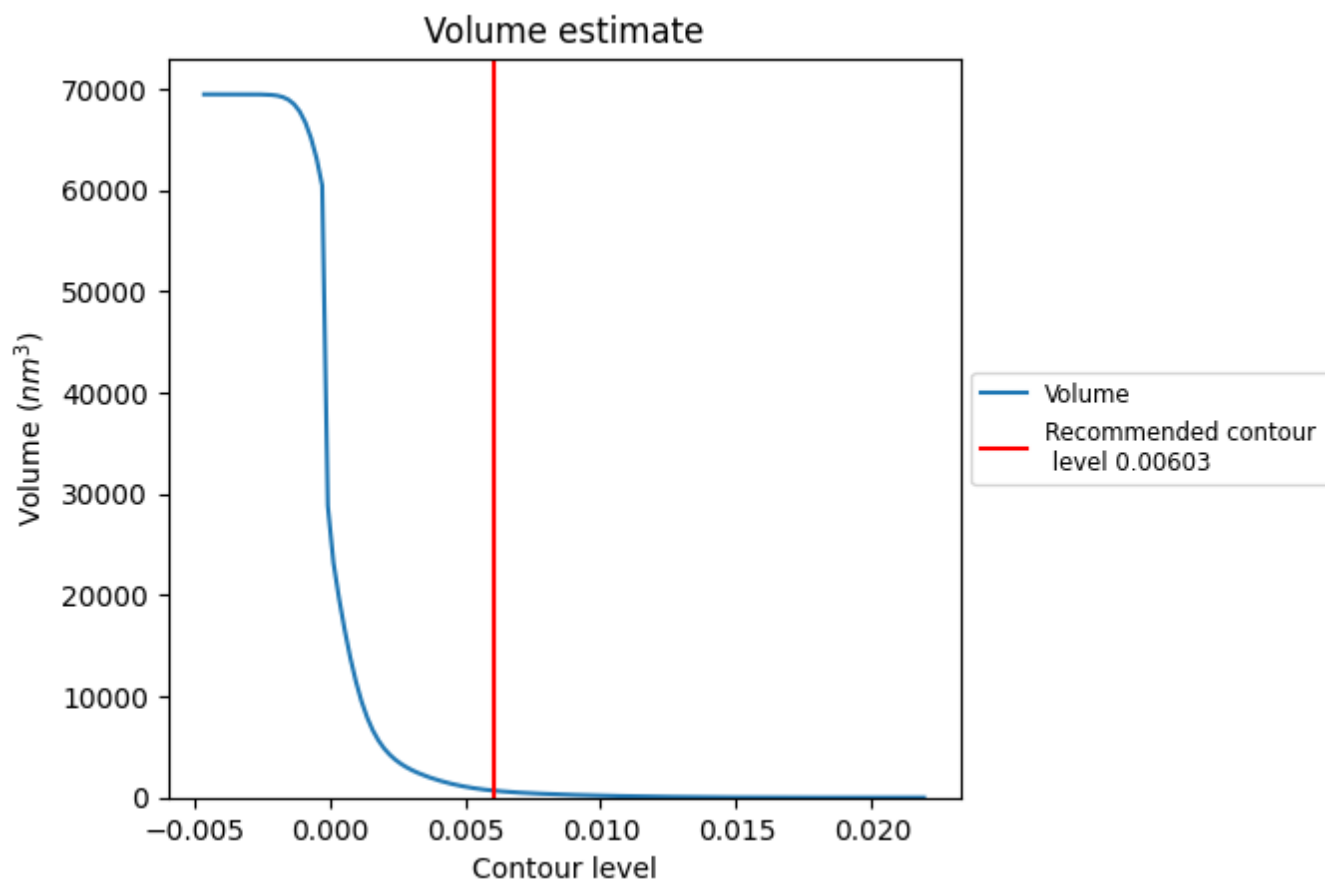
This section contains the results of statistical analysis of the map.

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.

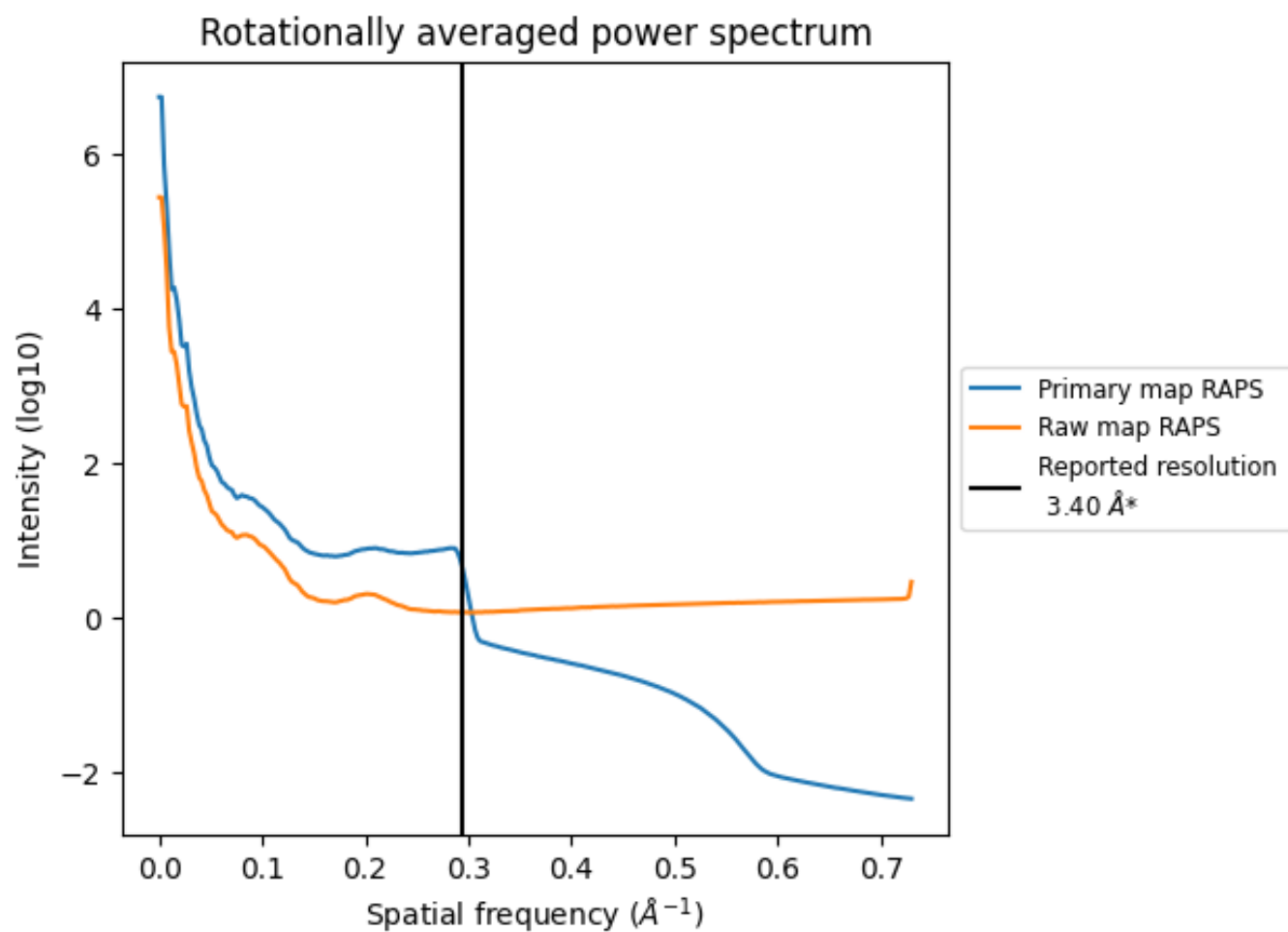
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 693 nm³; this corresponds to an approximate mass of 626 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 ⓘ

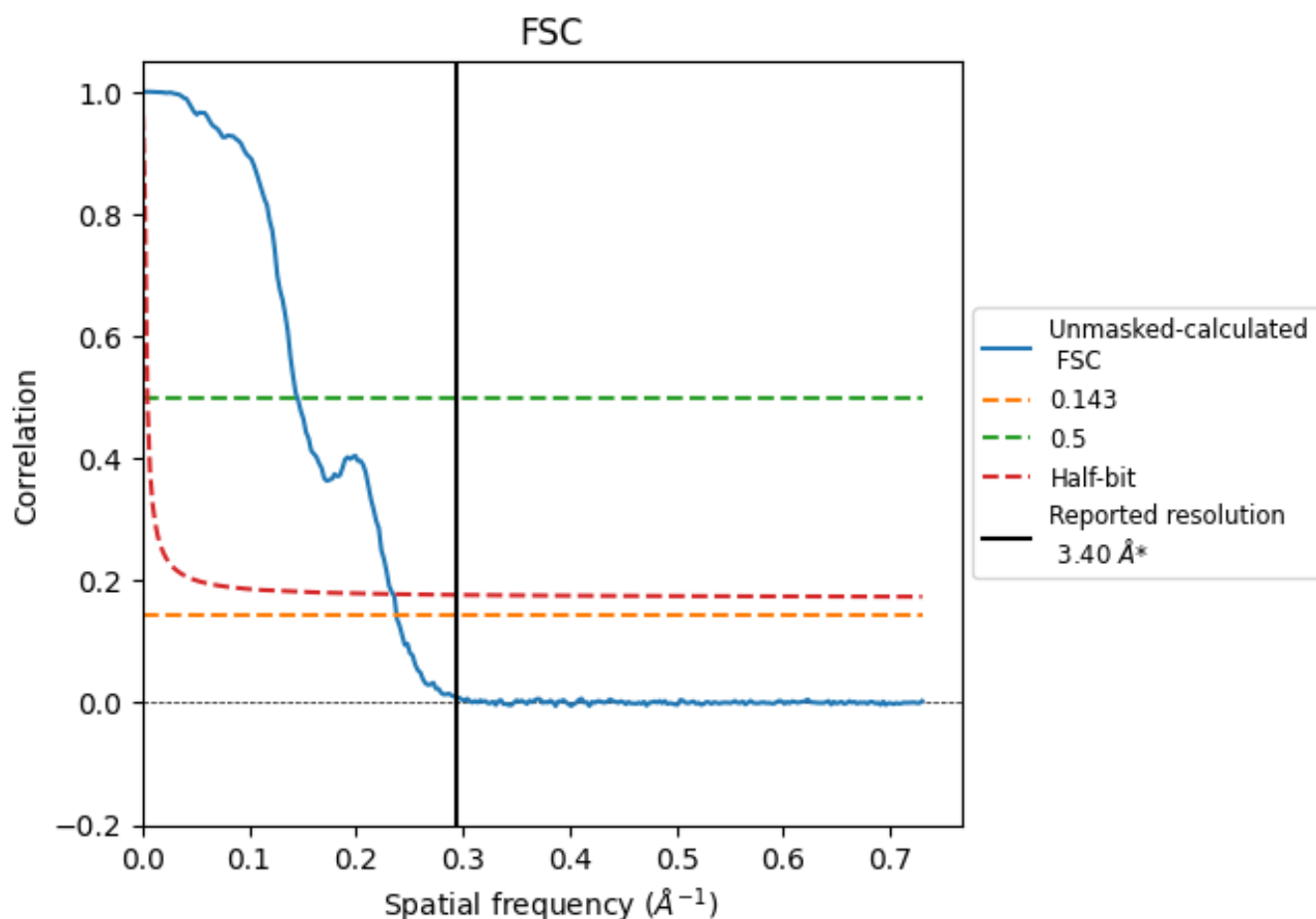


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

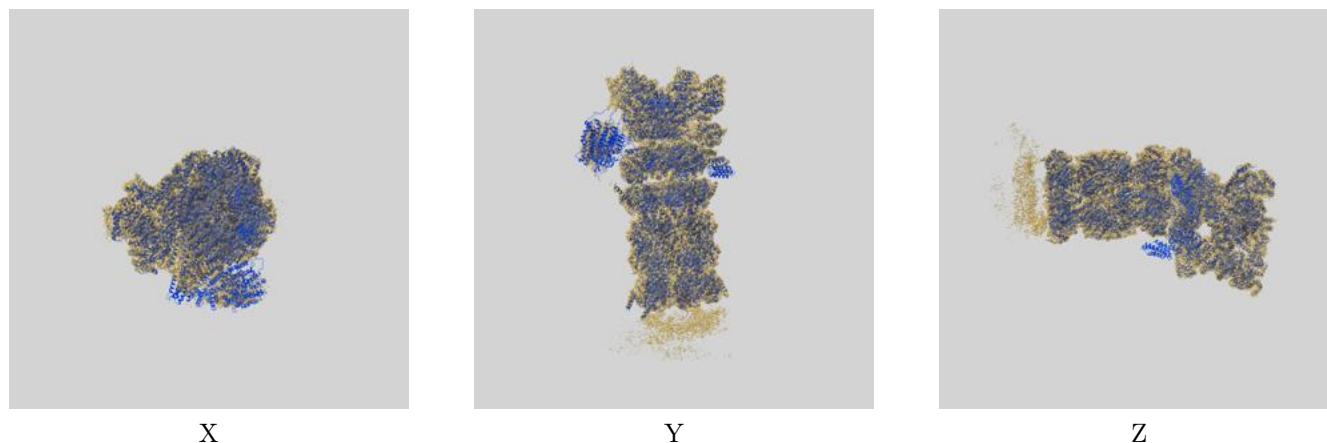
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	6.90	4.26

*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 4.20 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

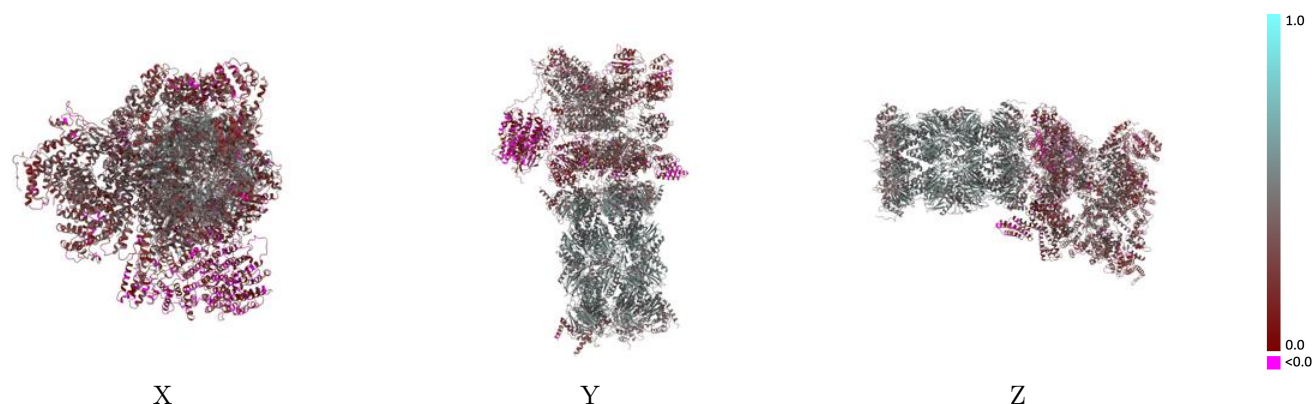
This section contains information regarding the fit between EMDB map EMD-62070 and PDB model 9K4U. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



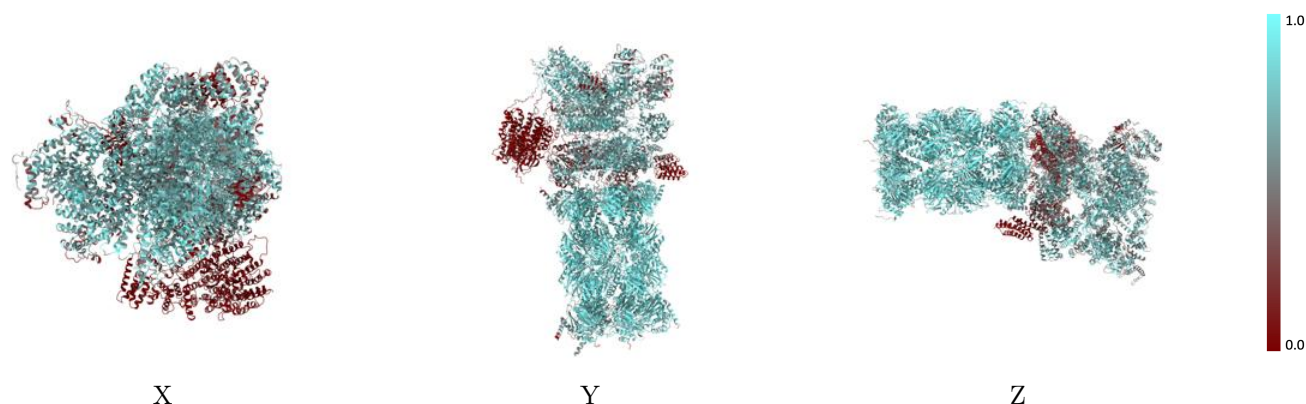
The images above show the 3D surface view of the map at the recommended contour level 0.00603 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



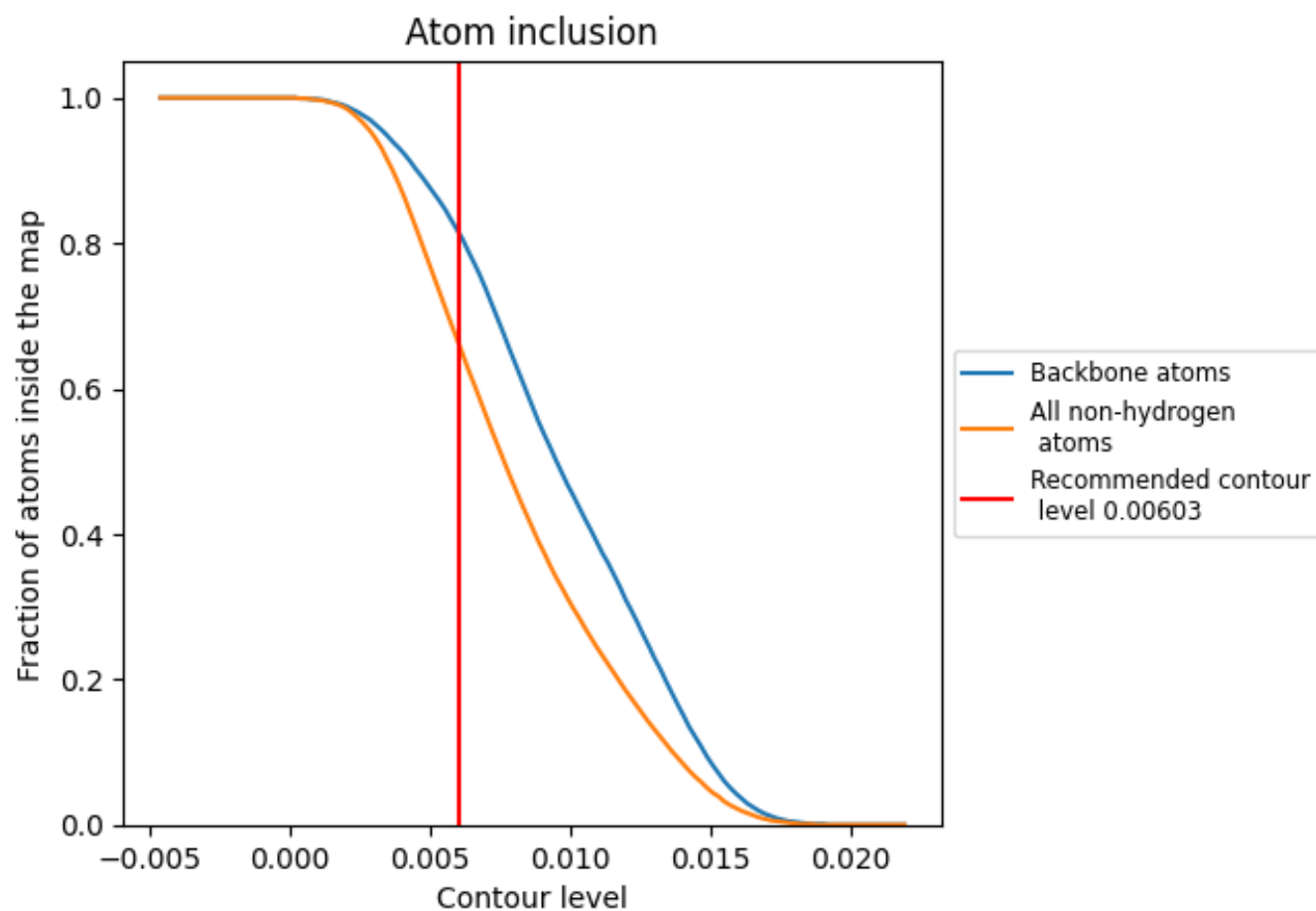
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00603).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 66% 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 (0.00603) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6610	 0.3680
A	 0.4530	 0.2370
B	 0.3200	 0.1890
C	 0.5850	 0.3170
D	 0.6790	 0.3630
E	 0.6900	 0.3620
F	 0.6220	 0.3120
G	 0.8240	 0.4720
H	 0.8410	 0.4740
I	 0.7760	 0.4470
J	 0.7390	 0.4160
K	 0.7890	 0.4580
L	 0.8620	 0.4800
M	 0.8500	 0.4750
N	 0.8830	 0.5120
O	 0.8730	 0.5010
P	 0.8840	 0.5030
Q	 0.8750	 0.5060
R	 0.8880	 0.5070
S	 0.8490	 0.5020
T	 0.8870	 0.5080
U	 0.6720	 0.3220
V	 0.6780	 0.3240
W	 0.4890	 0.2810
X	 0.3340	 0.2500
Y	 0.6800	 0.3100
Z	 0.6630	 0.3400
a	 0.6220	 0.2620
b	 0.5820	 0.2670
c	 0.6890	 0.3600
d	 0.5510	 0.2480
e	 0.5490	 0.3050
f	 0.0510	 0.0970
g	 0.7930	 0.4590
h	 0.8010	 0.4670



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Chain	Atom inclusion	Q-score
i	 0.7530	 0.4430
j	 0.6960	 0.4000
k	 0.7420	 0.4520
l	 0.8240	 0.4770
m	 0.8190	 0.4660
n	 0.8770	 0.5150
o	 0.8660	 0.4980
p	 0.8830	 0.5080
q	 0.8650	 0.4970
r	 0.8890	 0.5120
s	 0.8550	 0.5010
t	 0.8770	 0.5090
u	 0.1120	 0.2650
v	 0.2500	 0.3590