



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 11:52 AM JST

PDB ID : 9K4Z / pdb_00009k4z
EMDB ID : EMD-62075
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state ED1.1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.30 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

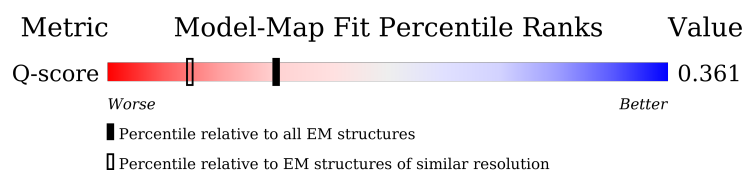
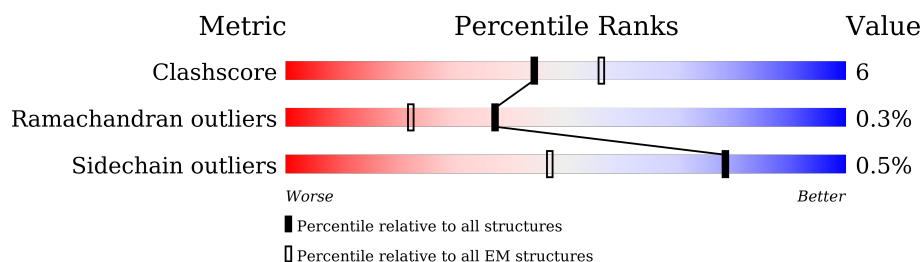
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	
2	B	440	
3	C	398	
4	D	418	









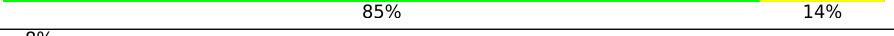
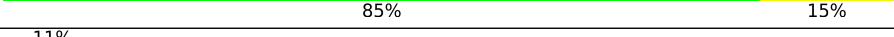
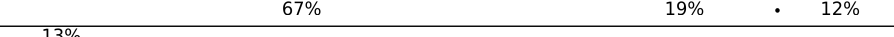


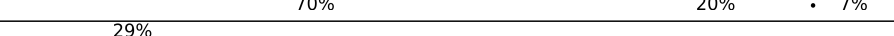



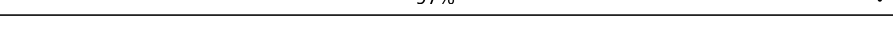
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	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 106334 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	1	0
			1893	1202	323	356	12		
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	1	0
			1591	1019	270	292	10		

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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		

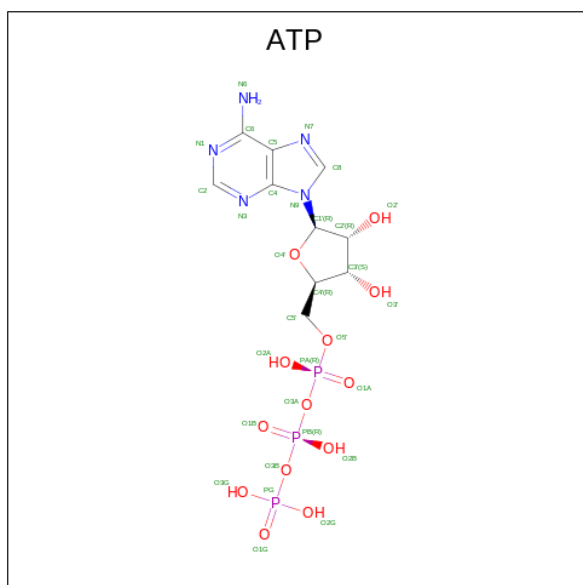
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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).



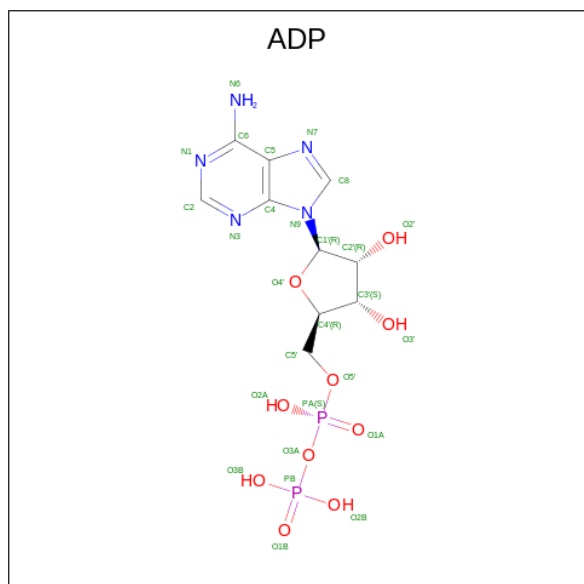
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Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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: C₁₀H₁₅N₅O₁₀P₂) (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	

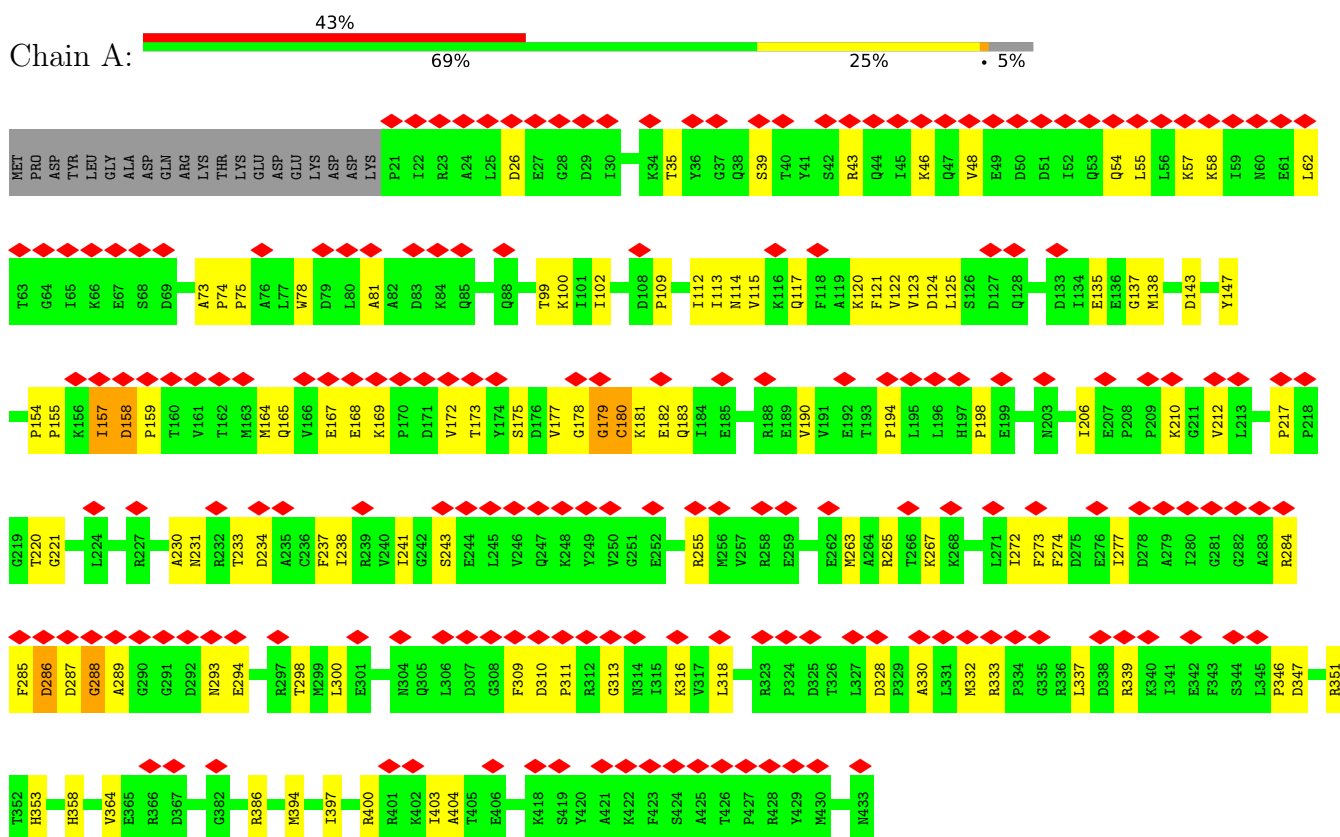
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

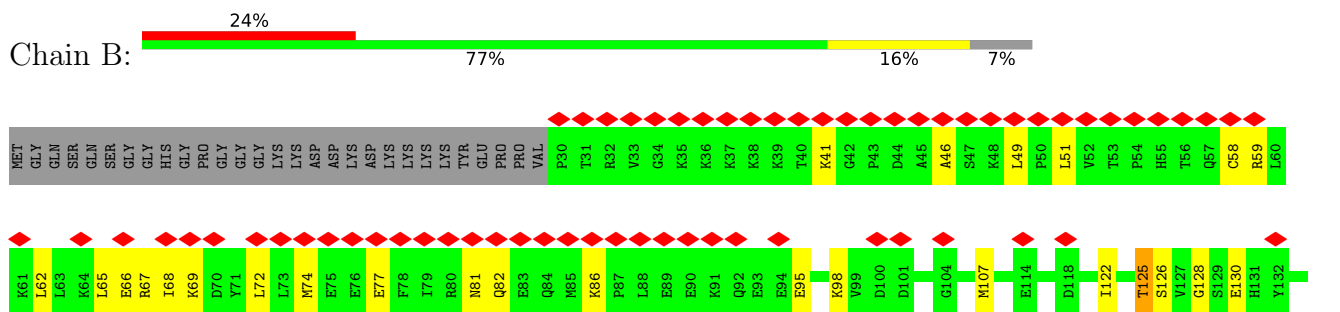
3 Residue-property plots

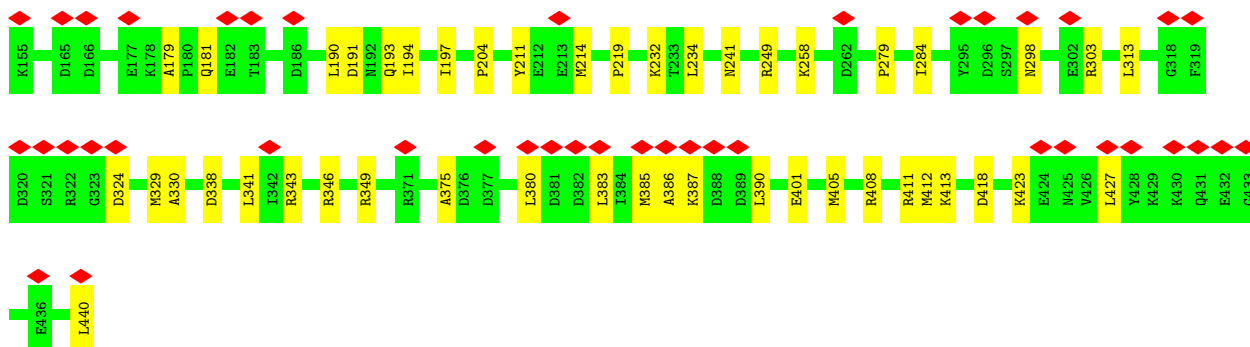
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

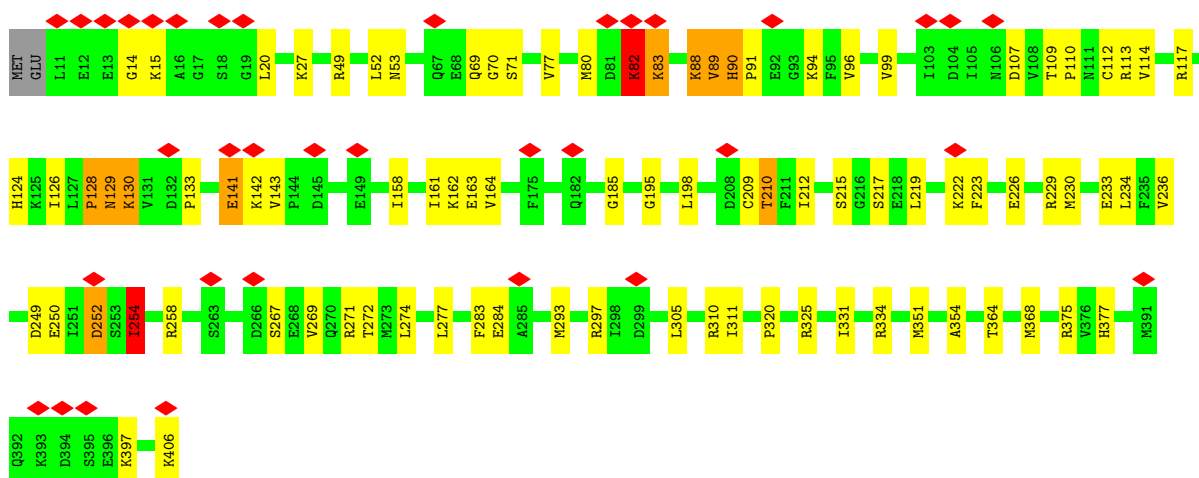
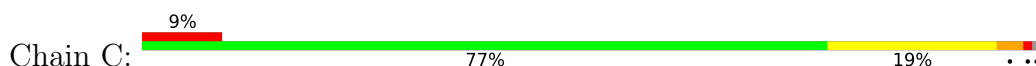


- Molecule 2: 26S proteasome regulatory subunit 4

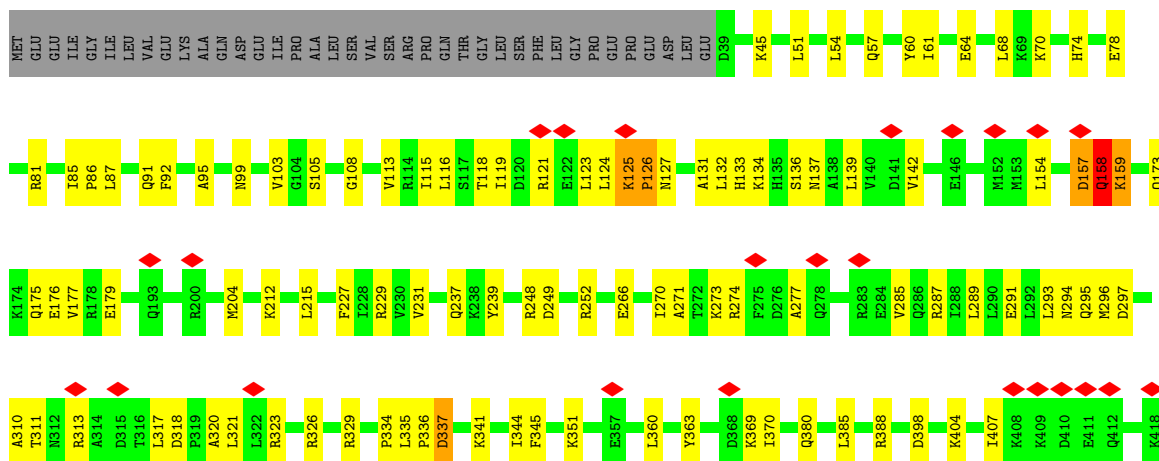




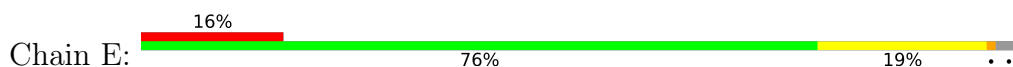
- Molecule 3: 26S proteasome regulatory subunit 8

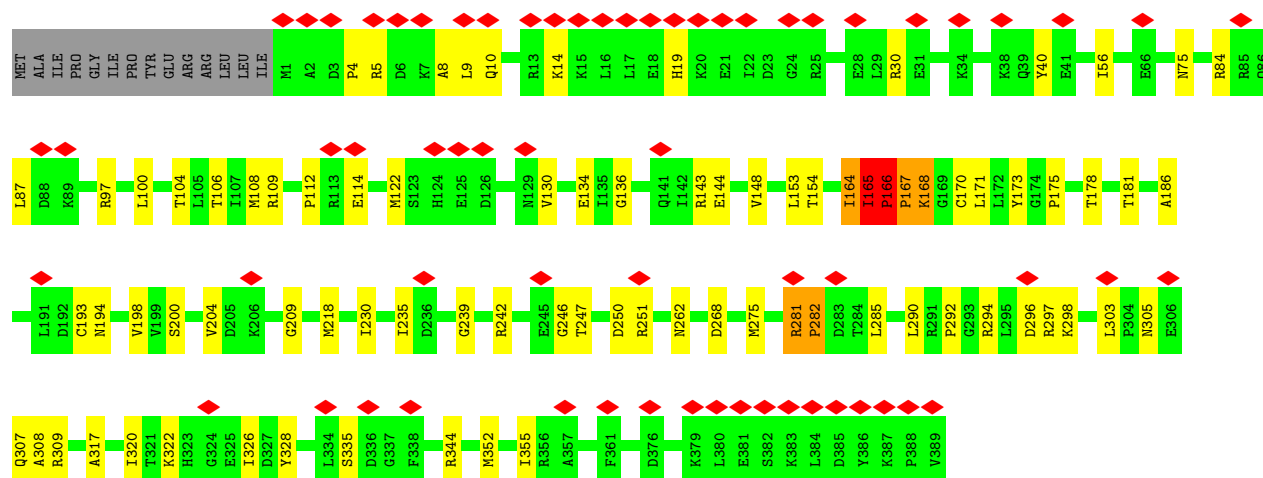


- Molecule 4: 26S proteasome regulatory subunit 6B

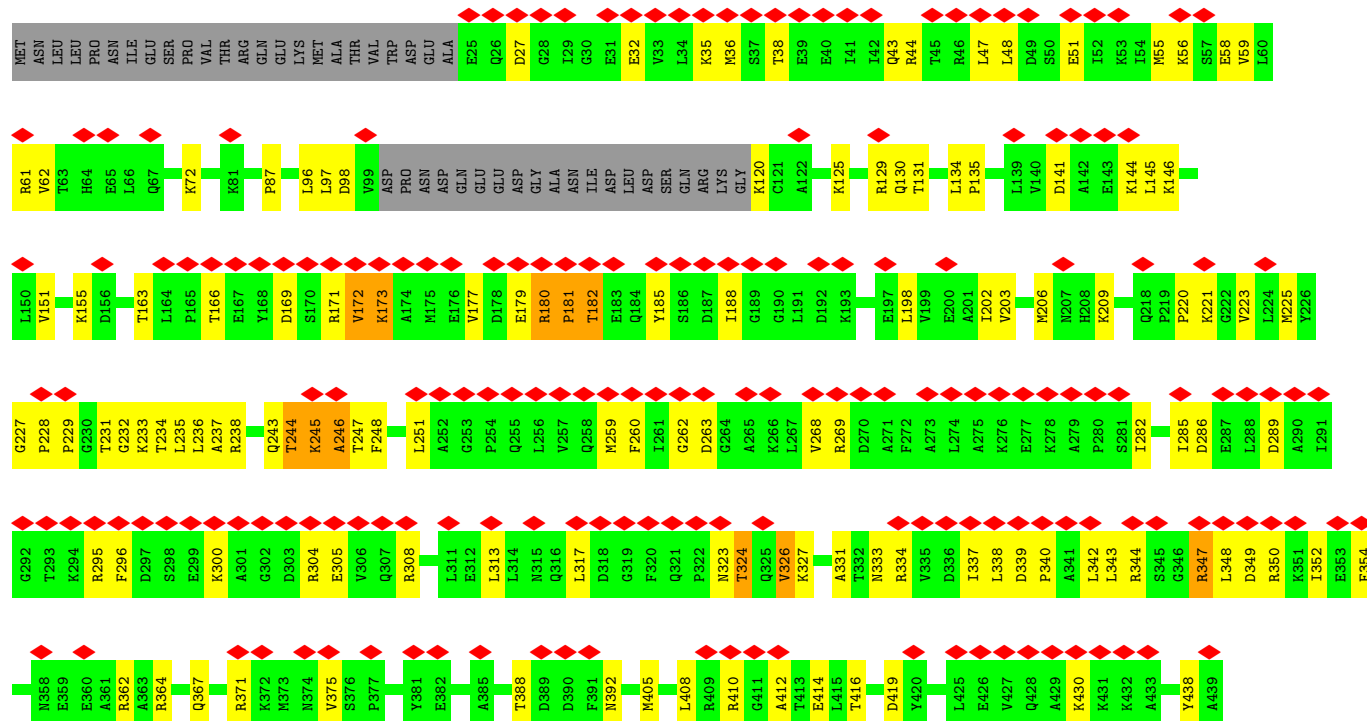
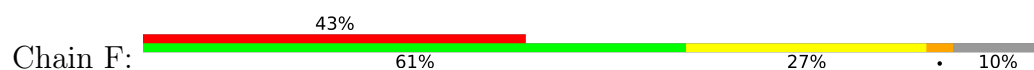


- Molecule 5: Proteasome 26S subunit, ATPase 6

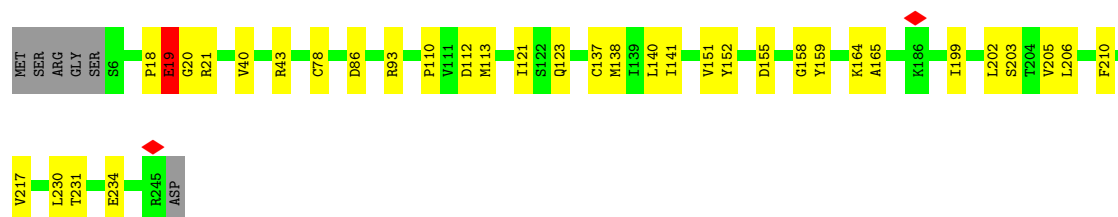
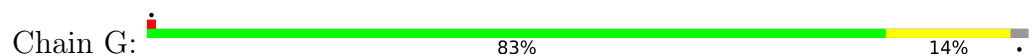




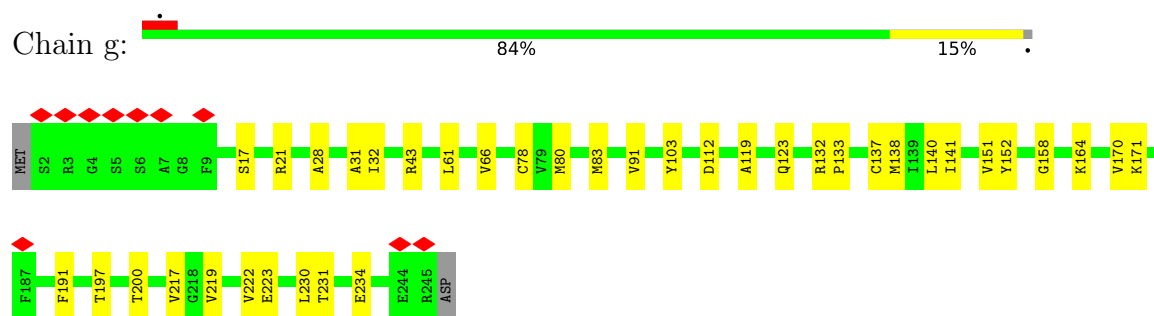
• Molecule 6: 26S proteasome regulatory subunit 6A



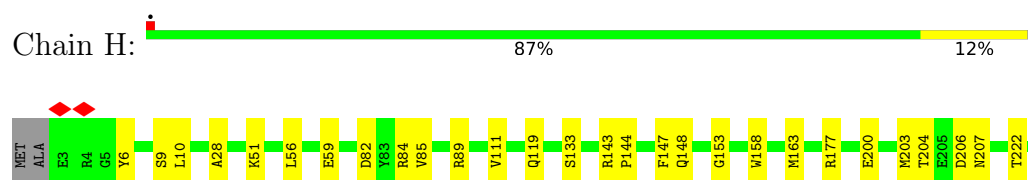
• Molecule 7: Proteasome subunit alpha type-6



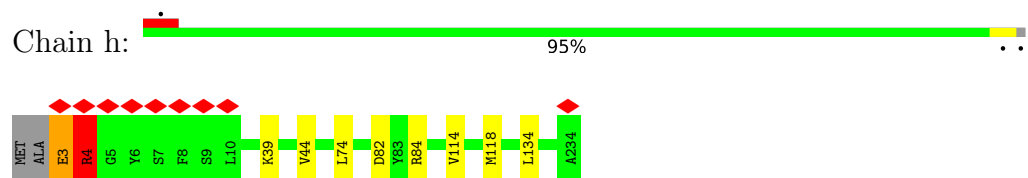
- Molecule 7: Proteasome subunit alpha type-6



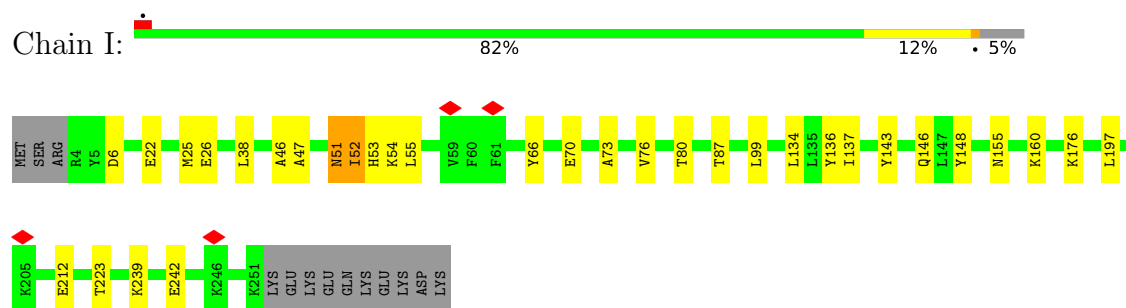
- Molecule 8: Proteasome subunit alpha type-2



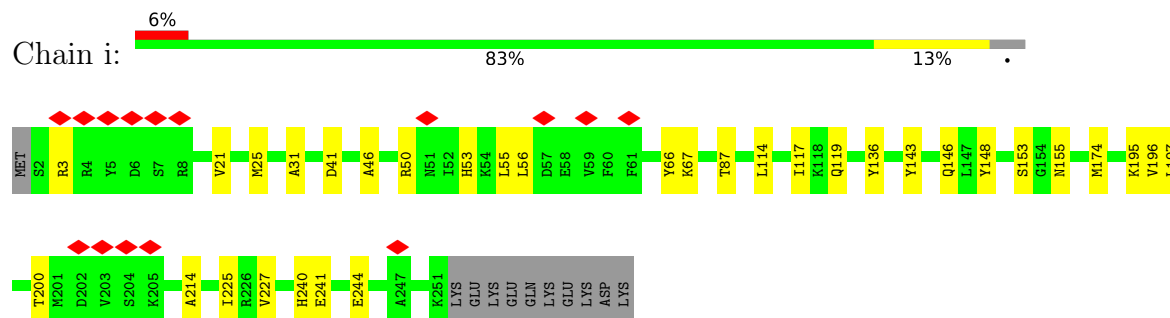
- Molecule 8: Proteasome subunit alpha type-2




- Molecule 9: Proteasome subunit alpha type-4

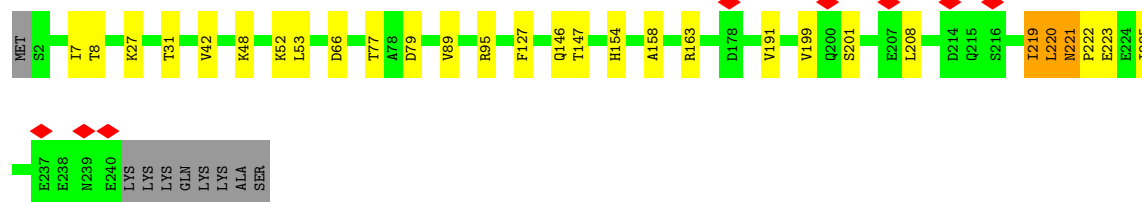


- Molecule 9: Proteasome subunit alpha type-4




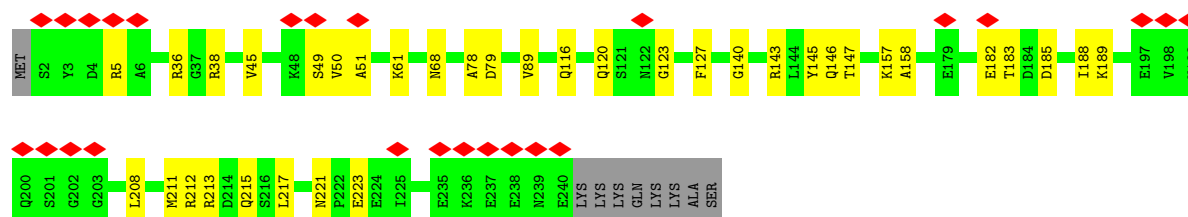
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 10% . .




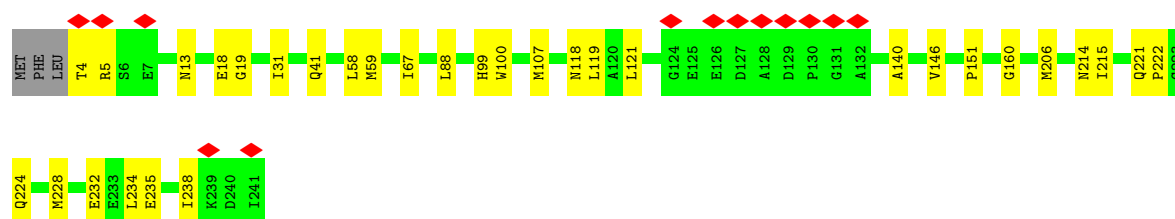
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  10% 82% 15% .




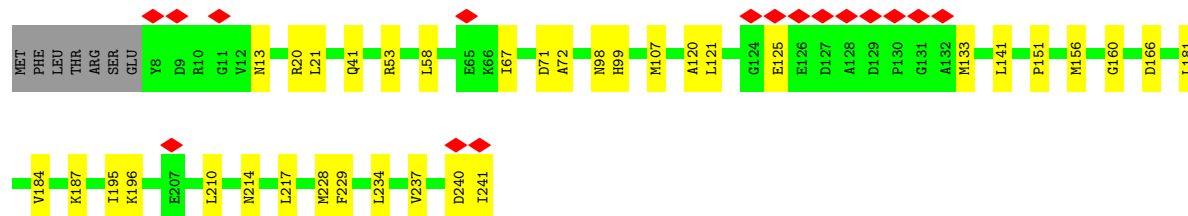
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  5% 85% 13% .




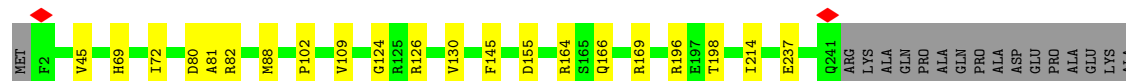
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  7% 83% 15% .



- Molecule 12: Proteasome subunit alpha type-1

Chain L:  83% 8% 9%



ASP
GLU
PRO
MET
GLU
HIS

• Molecule 12: Proteasome subunit alpha type-1

Chain l: 83% 8% 10%

MET PHE ARG N4 D7 H20 Q21 T22 E23 S33 E55 L56 K61 K62 I63 I72 R82 M88 D100 I112 T120 R126 I134 M140 K189 D218 E234 Q241 ARG LYS ALA GLN PRO ALA GLN PRO ALA ASP GLU PRO ALA GLU

LYS
ALA
ASP
GLU
PRO
MET
GLU
HIS

• Molecule 13: Proteasome subunit alpha type-3

Chain M: 83% 12% 5%

MET SER I3 Y7 P16 S34 K42 K51 L52 S62 N63 K64 R65 L66 F67 N68 H72 N105 L108 K109 H120 Y125 V128 L137 Y149 C163 A164 E183 E192 I196 E203 D206 F209 E210 L211 W215

H224 V227 R232 K244 GLU ASP GLU ASP SER ASP ASP ASN MET

• Molecule 13: Proteasome subunit alpha type-3

Chain m: 81% 13% 6%

MET SER ILE GLY T5 D8 S15 R19 Q22 V23 E24 M27 S34 T35 A36 I37 R40 C41 V46 R65 N68 A78 Y125 S126 A127 V128 R129 A146 M150 G166 R169 A172 I176 M181 I189 V193 K205

D206 K207 W215 L219 T220 R223 H224 E225 P228 I231 K244 GLU GLU ASP GLU SER ASP ASP ASN MET

• Molecule 14: Proteasome subunit beta type-6

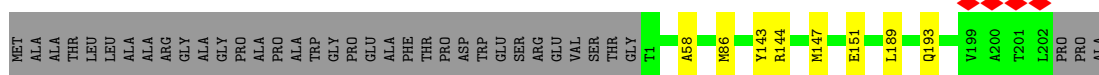
Chain N: 79% 6% 15%

MET ALA THR LEU ALA ARG GLY ALA PRO PRO TRP GLY PRO GLU PHE THR PRO ASP TRP GLU SER ARG GLU VAL SER THR GLY T1 Q7 F8 D9 D32 R45 A58 K84 E85 M86 G109 M120 I179 V184 L190

I194 P195 K196 A200 T201 L202 P203 PRO ALA

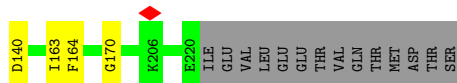
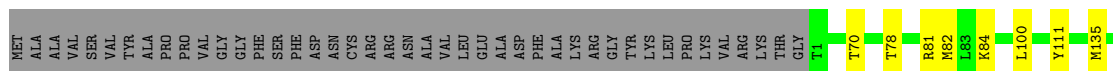
• Molecule 14: Proteasome subunit beta type-6

Chain n: 81% 15%



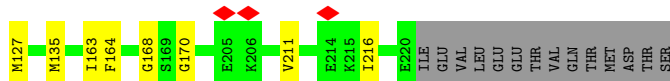
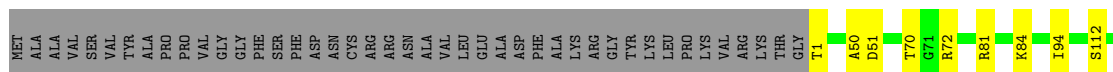
• Molecule 15: Proteasome subunit beta type-7

Chain O: 75% 21%



• Molecule 15: Proteasome subunit beta type-7

Chain o: 73% 6% 21%



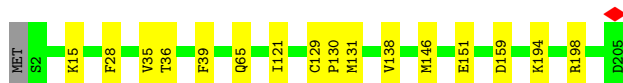
• Molecule 16: Proteasome subunit beta type-3

Chain P: 91% 8%



• Molecule 16: Proteasome subunit beta type-3

Chain p: 92% 8%



• Molecule 17: Proteasome subunit beta type-2

Chain Q: 91% 8%

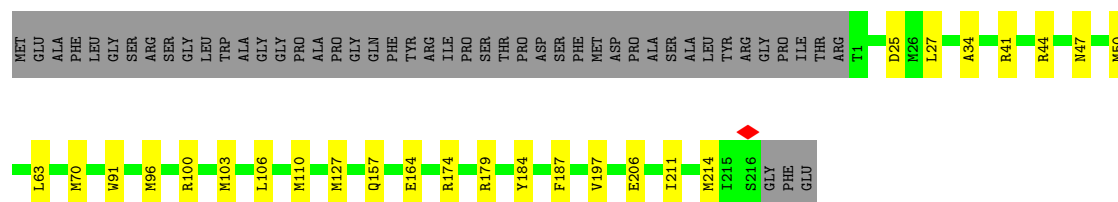


• Molecule 17: Proteasome subunit beta type-2



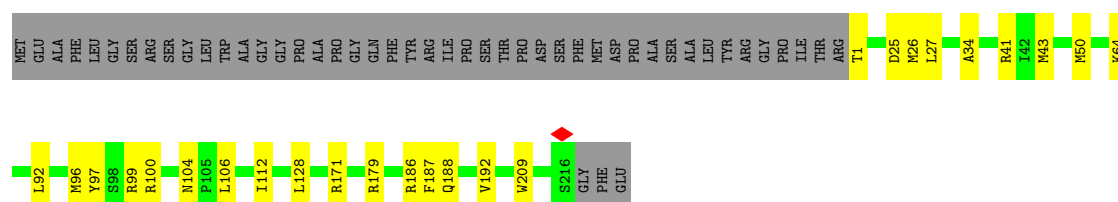
- Molecule 20: Proteasome subunit beta type-4

Chain T: 




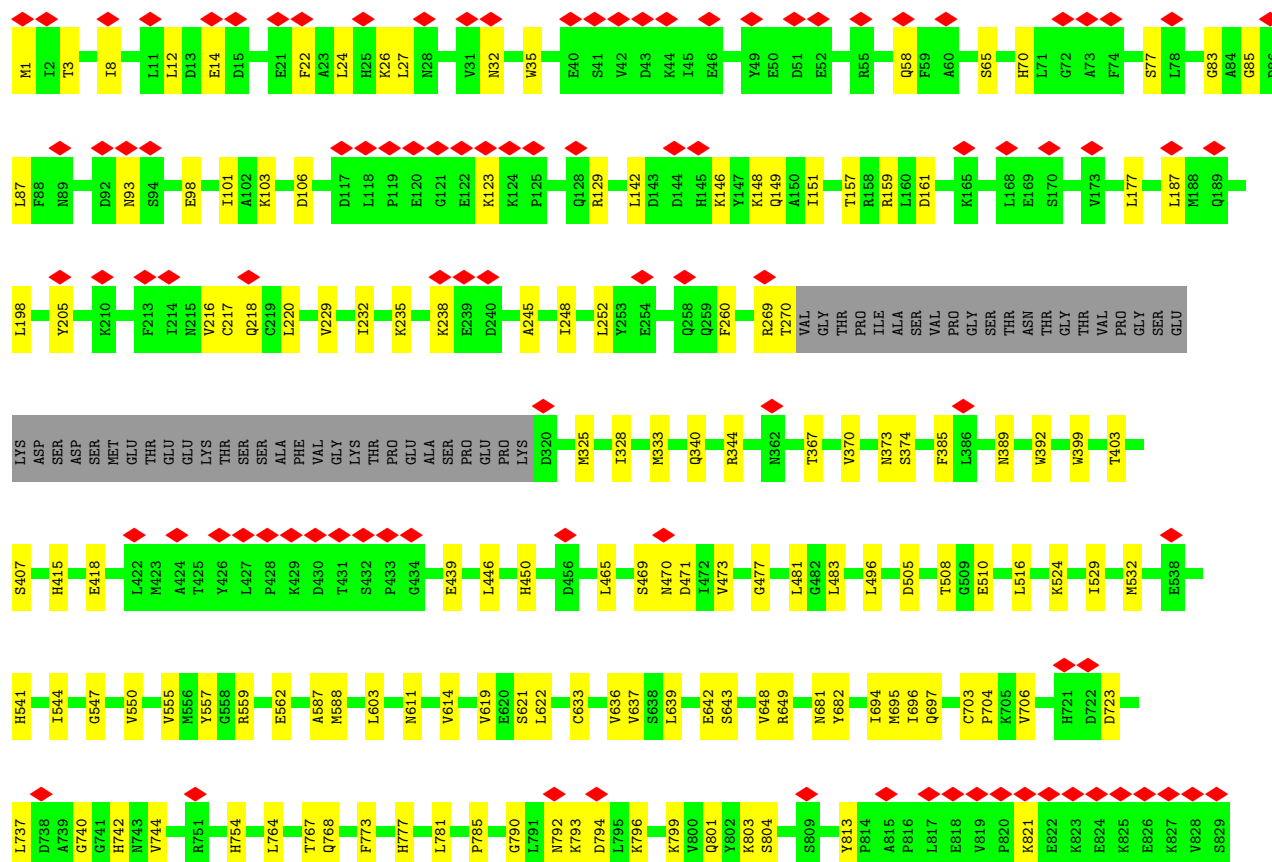
- Molecule 20: Proteasome subunit beta type-4

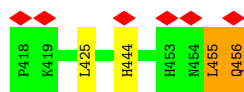
Chain t: 



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

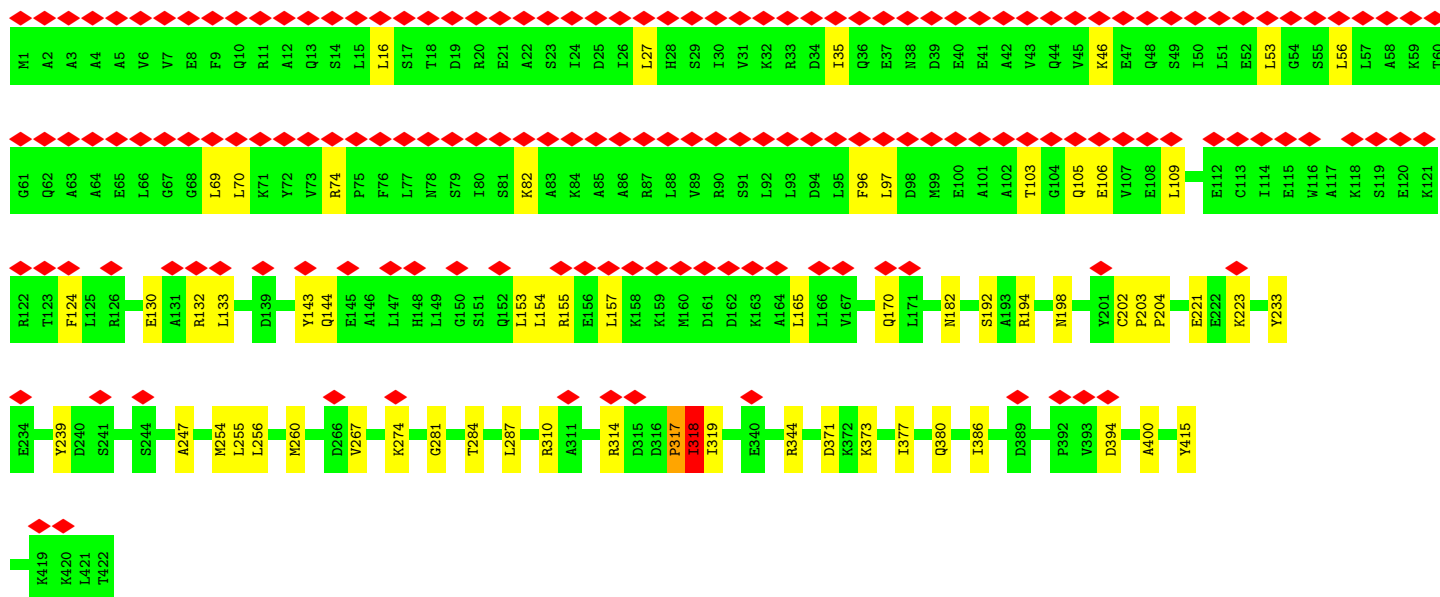
Chain U: 





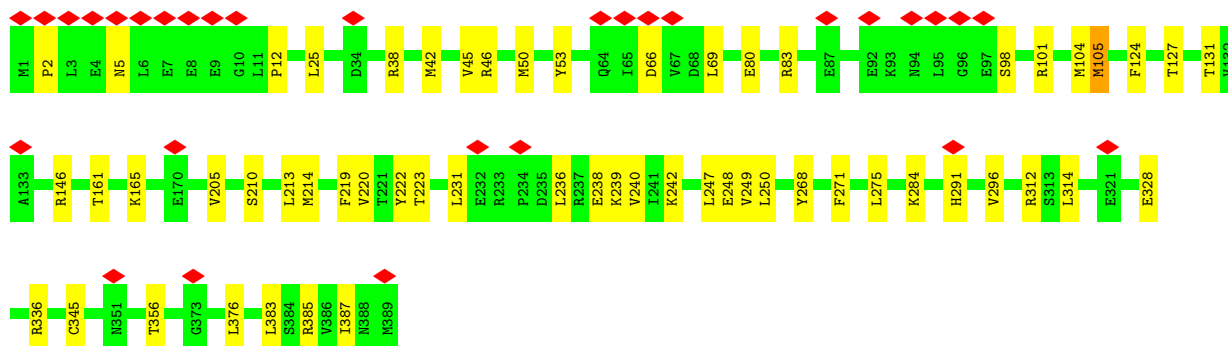
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 39% 85% 14%



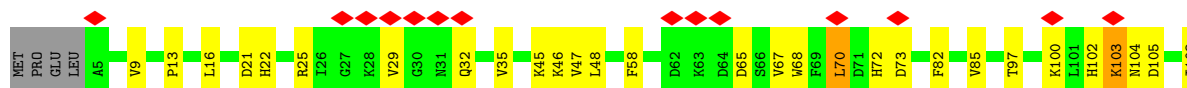
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

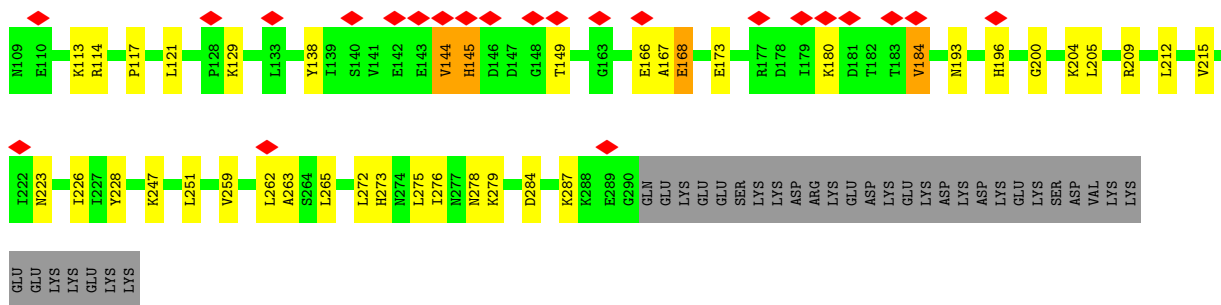
Chain Y: 8% 85% 15%



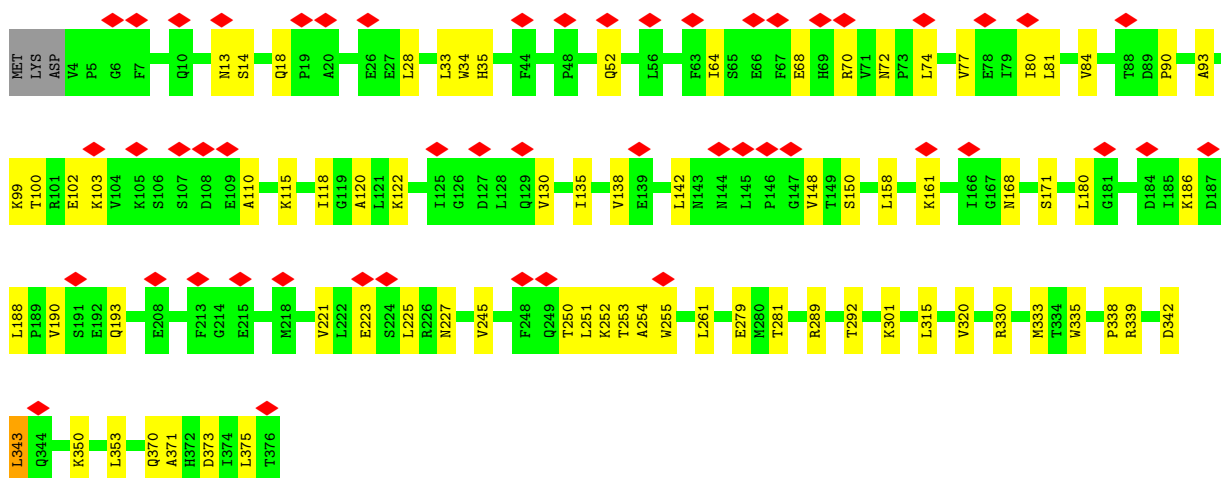
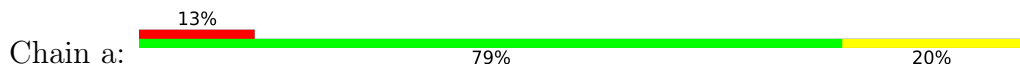
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 11% 67% 19% 12%

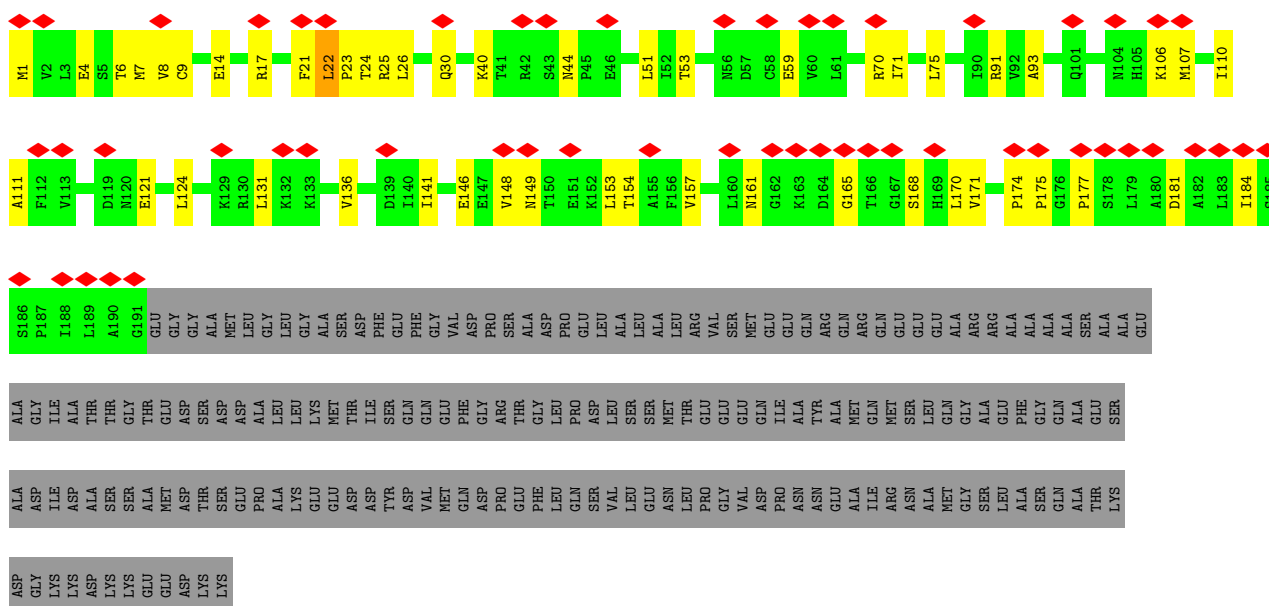
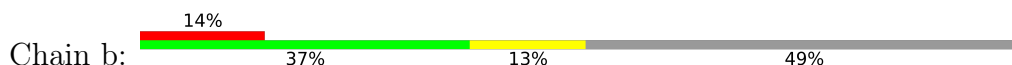




- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

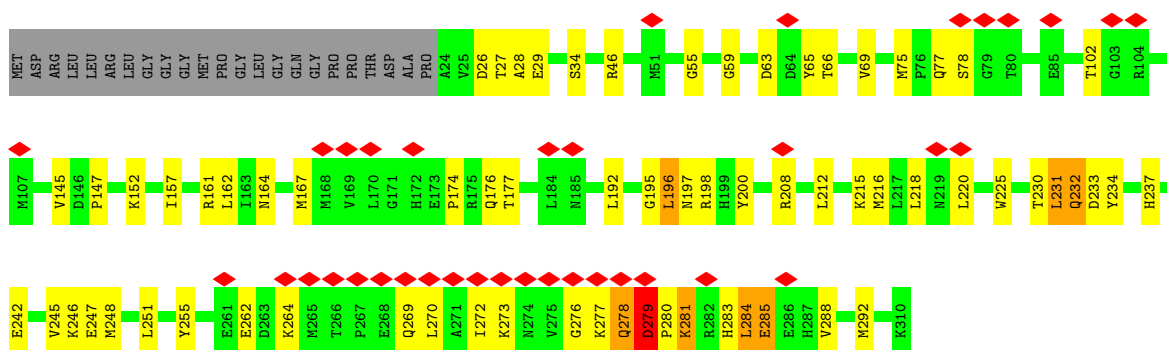


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4



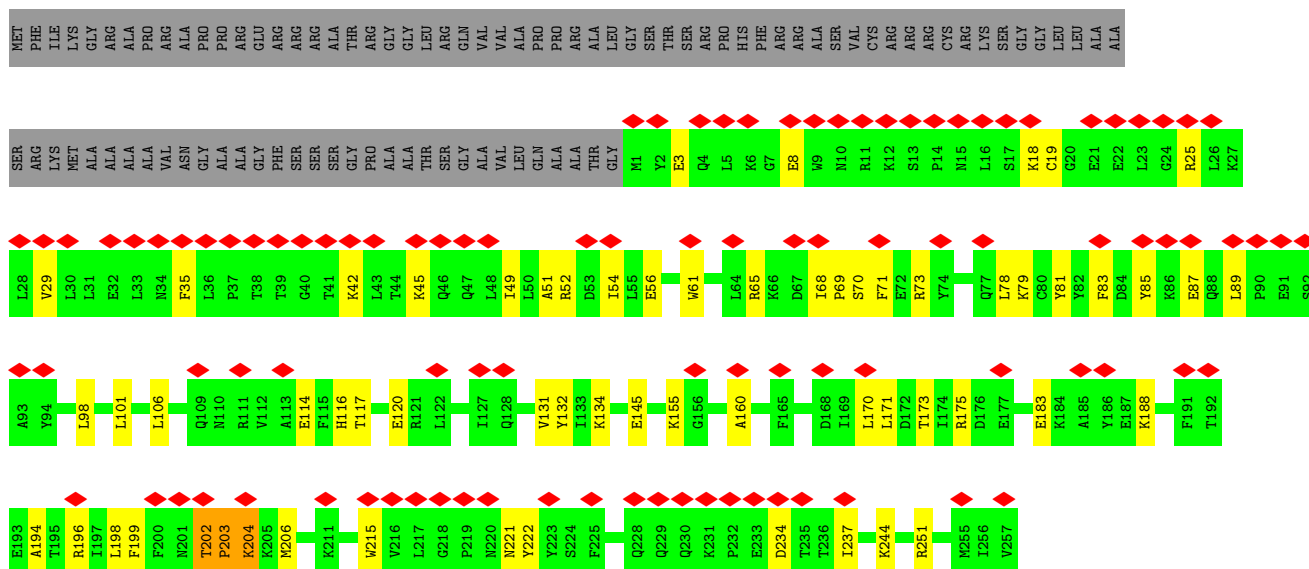
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 



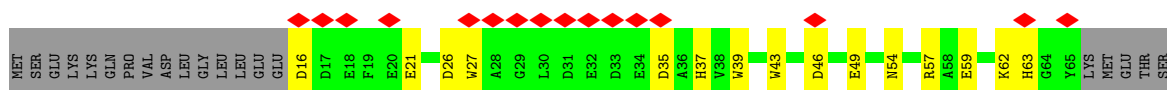
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 



- Molecule 31: 26S proteasome complex subunit SEM1

Chain e: 



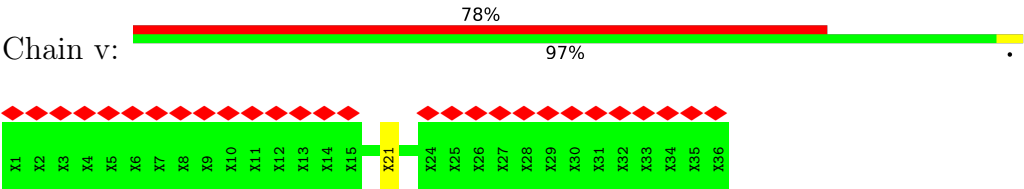
- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 



T870	P871	V872	L873	A875	H876	Q877	E878	R879	A880	E881	L882	A883	T884	E885	E886	F887	L888	P889	V890	F891	R892	I893	L894	E895	G896	F897	V898	I899	L900	R901	K902	N903	P904	N905	Y906	D907	L908																							
R807		L810	L811	G812	K813		Y816	R817	L818		L821	V822	A823	M825	Q826	P827	R828	M829	L830	V831	T832	F833	D834	E835	E836	L837	R838	P839	L840	P841	V842	S843	L844	R845	V846	G847	Q848	A849	V850	D851	V852	R853	G854	Q855	A856	G857	K858	P859	K860	T861	L796	L797	T798	G864	F865	Q866	T867	H868	T869	
R740	L741	A742	A743	M744	L745	R746	Q747	L748	A749	Q750	Y751	H752	A753	K754	D755	F756	H757	N758	L759	F760	M761	F762	R763	L764	A765	Q766		H770		K773	G774	T775	L776	T777	L778	C779	F780	Y781	H782	S783	D784	R785	Q786	L787	M788	S789	Y790	Y791		A794	G795	L796	L797	T798	F803	L804	D805	V806		
L672	A673	T674	F675	G676	H677	L678	L679	R680	V681	G682	E683	L686		V690	P691	L692	A693	L694	A695	L696	L697	S698	V699	S700	N701	F702	R703	L704	N705	L706	L707	D708	T709	L710	S711	K712	F713	S714	H715	D716	A717	D718	F719		S722		S725	L726	F727	A728	M729	L730	N731		T736	N737	N738	A739		
L612	L613	H614	L615	C616	S617	E618	F620	D621	S621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	
L550	K551	D552	T553	Y554	A555	R556	W557	L558	P559	G560	L561	L562	G563	L564	H565	H566	G567		G570	E571	A572	I573	E574	A575	L576	L577	A578	L579	E580	E581	V582	V583	S584	E585	F586	R587	S588	S589	F590	A591	G592	T593		D596	V597	C598	A599	Y600	L601	G602	S603	G604	N605	V606	L607	K608	V609	Q610	Q611	
Y489	A490	G491	S492	N493	R494	E495	D496	L497	L498	T499	L500	L501	L502	P503	Y504	M505	D507	S508	K509	S510	S511	N512	E513	V514	A515	G516	V517	T518	L519	A520	E521	C522	G523	M524	L525	S529	C530	N531	D532	D533	V534	T535	S536	T537	L538	L539	Q540	T541	I542	M543	E544	K545	S546	E547	T548	E549				
G424		T427	Q428	I429	D430	K431	Y432	L433	Y434	S435	S436		D438	Y439				G443	A444	L445	A446	C448	G449	I450	V451	N452		V455	R456	N457	E458	C459	D460	P461	A462	L463	A464	L465	L466	S467	D468	Y469	V470	L471	H472	N473	S474		R478	L479	G480	S481	I482	F483	G484	L485	G486	L487	A488	
S361	G362	S363	Q364	V365	D366	S367	A368	R369	K370	N371	L372		V377	N378	G379	F380	N382	N383	N384	F385	G386	N322	N323	V324	Q325	L326	N327	S328	N329	F330	L331	A332	L333	A334	R335	E336	L337	D338	I339	K340	E341	P342	K343	V344	P345	D346	D347	I348	Y349	K350	T351	H352	L353	E354	N355	N356	R357	F358	G359	G360
F121	A122	A123	D124	I125	I126	S127	V128	L129	A130	M131	T132	M133	S134	G135	E136	R137	E138	C139	L140	K141	Y142	R143	E144	A145	G146	S147	Q148	E149	E150	L151	A152	S153	V154	G155	H156	E157	Y158	V159	R160	H161	L162	A163	G164	E165	V166	A167	K168	E169	W170	Q171	E172	L173	D174	D175	A176	E177	K178	V179	Q180	
E61	R62	L63	G64	E65	K66	D67	T68	S69	L70	Y71	R72	P73	A74	L75	E76	E77	L78	R79	R80	Q81	I82	R83	S84	S85	T86	T87	S88	M89	T90	S91	V92	P93	P95	L96	K97	F98	L99	R100	P101	H102	Y103	G104	K105	L106	K107	E108	I109	Y110	E111	M112	M113	A114	P115	G116	E117	N118	K119	R120		

● Molecule 33: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92777	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	0.00588	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, 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	0.27	0/3283	0.62	0/4433
2	B	0.21	0/3254	0.55	0/4388
3	C	0.29	0/3146	0.64	6/4226 (0.1%)
4	D	0.27	0/3090	0.63	1/4168 (0.0%)
5	E	0.26	0/3145	0.62	1/4233 (0.0%)
6	F	0.29	0/3137	0.60	1/4223 (0.0%)
7	G	0.21	0/1901	0.48	0/2572
7	g	0.19	0/1913	0.47	0/2589
8	H	0.17	0/1840	0.46	0/2495
8	h	0.17	0/1844	0.41	0/2497
9	I	0.21	0/1963	0.48	0/2650
9	i	0.18	0/1985	0.47	0/2677
10	J	0.21	0/1887	0.50	0/2553
10	j	0.19	0/1887	0.48	0/2549
11	K	0.16	0/1841	0.40	0/2486
11	k	0.15	0/1809	0.42	1/2444 (0.0%)
12	L	0.15	0/1911	0.40	0/2584
12	l	0.14	0/1896	0.40	0/2565
13	M	0.17	0/1931	0.45	0/2600
13	m	0.15	0/1916	0.43	0/2580
14	N	0.12	0/1548	0.32	0/2097
14	n	0.14	0/1536	0.36	0/2080
15	O	0.17	0/1672	0.47	0/2267
15	o	0.17	0/1686	0.46	0/2282
16	P	0.17	0/1616	0.46	1/2180 (0.0%)
16	p	0.17	0/1620	0.48	0/2184
17	Q	0.16	0/1627	0.42	0/2202
17	q	0.16	0/1611	0.42	0/2182
18	R	0.15	0/1590	0.42	0/2147
18	r	0.14	0/1580	0.38	0/2135
19	S	0.16	0/1671	0.45	0/2252
19	s	0.16	0/1680	0.43	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.43	0/2323
20	t	0.14	0/1720	0.40	0/2328
21	U	0.21	0/6984	0.52	0/9435
22	V	0.21	0/3681	0.51	0/4969
23	W	0.22	0/3644	0.53	0/4901
24	X	0.19	0/3381	0.50	2/4558 (0.0%)
25	Y	0.19	0/3261	0.50	2/4393 (0.0%)
26	Z	0.27	0/2324	0.67	2/3150 (0.1%)
27	a	0.23	0/3053	0.62	0/4133
28	b	0.23	0/1478	0.57	0/2001
29	c	0.27	0/2302	0.69	4/3110 (0.1%)
30	d	0.27	0/2162	0.67	0/2919
31	e	0.25	0/437	0.67	0/595
32	f	0.22	0/6640	0.55	0/8988
All	All	0.21	0/107799	0.52	21/145587 (0.0%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	317	PRO	N-CA-C	-12.21	97.03	113.40
26	Z	144	VAL	N-CA-C	-7.19	103.84	110.82
3	C	82	LYS	N-CA-C	-6.89	102.16	111.87
16	P	3	ILE	N-CA-C	-6.44	107.22	113.53
3	C	143	VAL	CA-C-N	-6.21	114.37	120.52

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	81	0
2	B	3207	0	3278	55	0
3	C	3105	0	3219	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3040	0	3075	82	0
5	E	3097	0	3174	71	0
6	F	3098	0	3187	111	0
7	G	1867	0	1867	23	0
7	g	1879	0	1872	20	0
8	H	1801	0	1773	18	0
8	h	1805	0	1798	10	0
9	I	1933	0	1923	28	0
9	i	1955	0	1955	20	0
10	J	1861	0	1846	24	0
10	j	1861	0	1865	23	0
11	K	1813	0	1796	20	0
11	k	1782	0	1766	21	0
12	L	1876	0	1856	12	0
12	l	1861	0	1839	13	0
13	M	1893	0	1885	17	0
13	m	1881	0	1868	21	0
14	N	1521	0	1494	8	0
14	n	1510	0	1483	5	0
15	O	1645	0	1648	8	0
15	o	1659	0	1681	13	0
16	P	1587	0	1598	10	0
16	p	1591	0	1609	11	0
17	Q	1591	0	1589	14	0
17	q	1578	0	1569	19	0
18	R	1559	0	1523	9	0
18	r	1549	0	1506	12	0
19	S	1641	0	1639	15	0
19	s	1650	0	1645	16	0
20	T	1683	0	1662	17	0
20	t	1687	0	1666	17	0
21	U	6867	0	6929	110	0
22	V	3612	0	3682	46	0
23	W	3596	0	3713	49	0
24	X	3335	0	3435	46	0
25	Y	3202	0	3204	38	0
26	Z	2281	0	2312	54	0
27	a	2995	0	3012	47	0
28	b	1458	0	1505	35	0
29	c	2260	0	2276	67	0
30	d	2116	0	2146	49	0
31	e	425	0	328	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	f	6529	0	6541	93	0
33	v	180	0	50	1	0
34	A	31	0	12	4	0
34	B	31	0	12	1	0
34	C	31	0	12	2	0
34	D	31	0	12	1	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	3	0
36	F	27	0	12	1	0
37	c	1	0	0	0	0
All	All	106334	0	106620	1368	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 1368 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)
29:c:279:ASP:HA	29:c:283:HIS:HB3	1.13	1.07
5:E:165:ILE:H	5:E:166:PRO:HD2	1.27	0.97
29:c:279:ASP:HA	29:c:283:HIS:CB	1.94	0.96
5:E:165:ILE:C	5:E:167:PRO:HD3	1.91	0.95
30:d:204:LYS:NZ	30:d:204:LYS:HA	1.83	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	354 (86%)	51 (12%)	6 (2%)	8	32
2	B	409/440 (93%)	366 (90%)	43 (10%)	0	100	100
3	C	394/398 (99%)	342 (87%)	45 (11%)	7 (2%)	6	29
4	D	378/418 (90%)	328 (87%)	48 (13%)	2 (0%)	24	55
5	E	387/403 (96%)	348 (90%)	34 (9%)	5 (1%)	9	35
6	F	391/439 (89%)	351 (90%)	33 (8%)	7 (2%)	6	29
7	G	238/246 (97%)	225 (94%)	12 (5%)	1 (0%)	30	60
7	g	242/246 (98%)	226 (93%)	15 (6%)	1 (0%)	30	60
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	220 (96%)	9 (4%)	1 (0%)	30	60
9	I	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
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%)	223 (94%)	13 (6%)	1 (0%)	30	60
11	K	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	238/263 (90%)	227 (95%)	11 (5%)	0	100	100
12	l	236/263 (90%)	225 (95%)	11 (5%)	0	100	100
13	M	241/255 (94%)	233 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	198/201 (98%)	190 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (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%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
21	U	874/953 (92%)	804 (92%)	69 (8%)	1 (0%)	48	75
22	V	442/534 (83%)	426 (96%)	16 (4%)	0	100	100
23	W	439/456 (96%)	428 (98%)	11 (2%)	0	100	100
24	X	420/422 (100%)	402 (96%)	16 (4%)	2 (0%)	24	55
25	Y	387/389 (100%)	364 (94%)	23 (6%)	0	100	100
26	Z	284/324 (88%)	250 (88%)	31 (11%)	3 (1%)	11	39
27	a	371/376 (99%)	344 (93%)	25 (7%)	2 (0%)	24	55
28	b	189/377 (50%)	165 (87%)	23 (12%)	1 (0%)	24	55
29	c	285/310 (92%)	241 (85%)	42 (15%)	2 (1%)	18	49
30	d	255/350 (73%)	214 (84%)	38 (15%)	3 (1%)	10	37
31	e	48/70 (69%)	45 (94%)	3 (6%)	0	100	100
32	f	840/908 (92%)	813 (97%)	27 (3%)	0	100	100
All	All	13417/14876 (90%)	12567 (94%)	805 (6%)	45 (0%)	37	65

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
3	C	90	HIS
3	C	141	GLU
4	D	157	ASP
5	E	166	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/372 (94%)	346 (99%)	2 (1%)	78	81
2	B	357/385 (93%)	356 (100%)	1 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	340/346 (98%)	329 (97%)	11 (3%)	34	60
4	D	333/366 (91%)	328 (98%)	5 (2%)	57	72
5	E	341/353 (97%)	338 (99%)	3 (1%)	70	78
6	F	340/379 (90%)	334 (98%)	6 (2%)	51	70
7	G	202/210 (96%)	200 (99%)	2 (1%)	68	76
7	g	201/210 (96%)	200 (100%)	1 (0%)	81	83
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	76
9	I	202/221 (91%)	200 (99%)	2 (1%)	68	76
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	194 (98%)	3 (2%)	57	72
10	j	196/211 (93%)	196 (100%)	0	100	100
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%)	201 (100%)	0	100	100
13	M	199/212 (94%)	199 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
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	169/171 (99%)	169 (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%)	751 (100%)	1 (0%)	88	90
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	83
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	81
26	Z	257/295 (87%)	254 (99%)	3 (1%)	63	75
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	86
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	244 (97%)	8 (3%)	34	60
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	43 (98%)	1 (2%)	44	66
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	90
All	All	11451/12614 (91%)	11393 (100%)	58 (0%)	78	83

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	19	GLU
7	g	222	VAL
21	U	874	ASN
32	f	87	THR
29	c	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	456	GLN
27	a	62	ASN
11	k	41	GLN
24	X	296	ASN
25	Y	351	ASN

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	C	501	35	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
36	ADP	F	501	-	27,29,29	1.36	4 (14%)	42,45,45	1.99	10 (23%)
36	ADP	E	401	-	27,29,29	1.37	4 (14%)	42,45,45	1.95	10 (23%)
34	ATP	A	501	35	29,33,33	0.26	0	44,52,52	0.49	0
34	ATP	B	501	35	29,33,33	0.27	0	44,52,52	0.54	1 (2%)
34	ATP	D	501	35	29,33,33	0.27	0	44,52,52	0.51	1 (2%)

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	C	501	35	-	7/22/38/38	0/3/3/3
36	ADP	F	501	-	-	5/16/32/32	0/3/3/3
36	ADP	E	401	-	-	3/16/32/32	0/3/3/3
34	ATP	A	501	35	-	3/22/38/38	0/3/3/3
34	ATP	B	501	35	-	5/22/38/38	0/3/3/3
34	ATP	D	501	35	-	4/22/38/38	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)
36	E	401	ADP	C5-C4	4.59	1.47	1.39
36	F	501	ADP	C5-C4	4.57	1.47	1.39
36	F	501	ADP	C5-C6	2.70	1.48	1.41
36	E	401	ADP	C5-C6	2.68	1.48	1.41
36	E	401	ADP	C8-N7	2.37	1.36	1.31

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	501	ADP	C5-C4-N3	-6.55	118.20	126.75
36	E	401	ADP	C5-C4-N3	-6.49	118.28	126.75
36	F	501	ADP	N3-C4-N9	5.17	135.60	127.08
36	E	401	ADP	N3-C4-N9	5.03	135.37	127.08
36	E	401	ADP	C2-N3-C4	3.95	121.09	111.75

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C3'-C4'-C5'-O5'
34	C	501	ATP	C5'-O5'-PA-O1A
34	C	501	ATP	C5'-O5'-PA-O2A

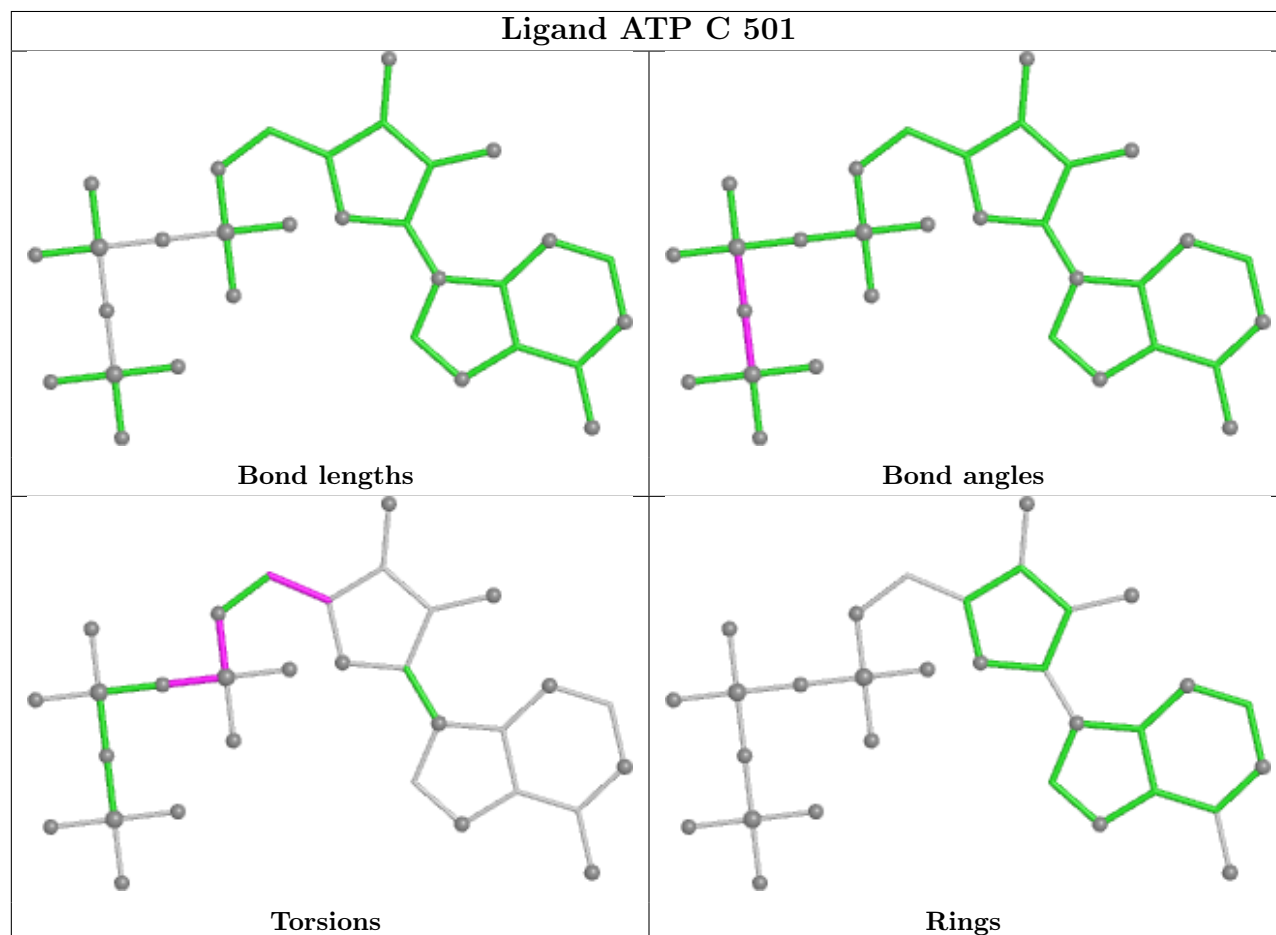
There are no ring outliers.

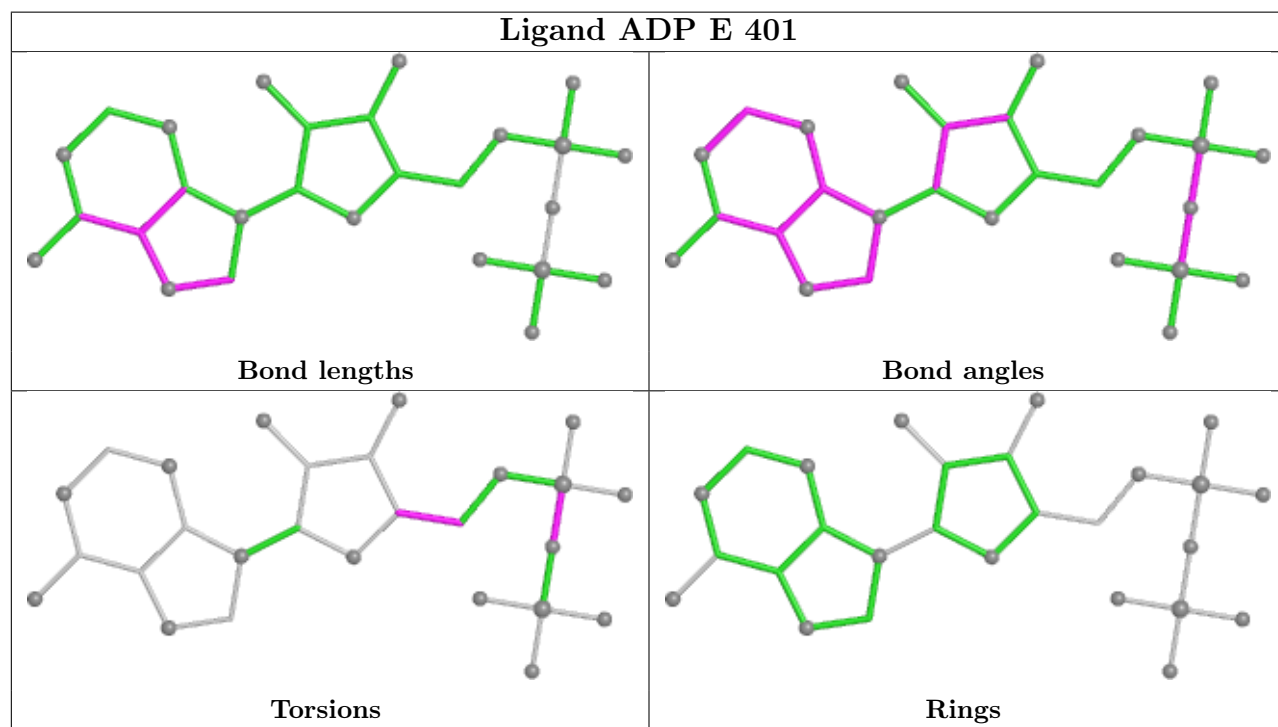
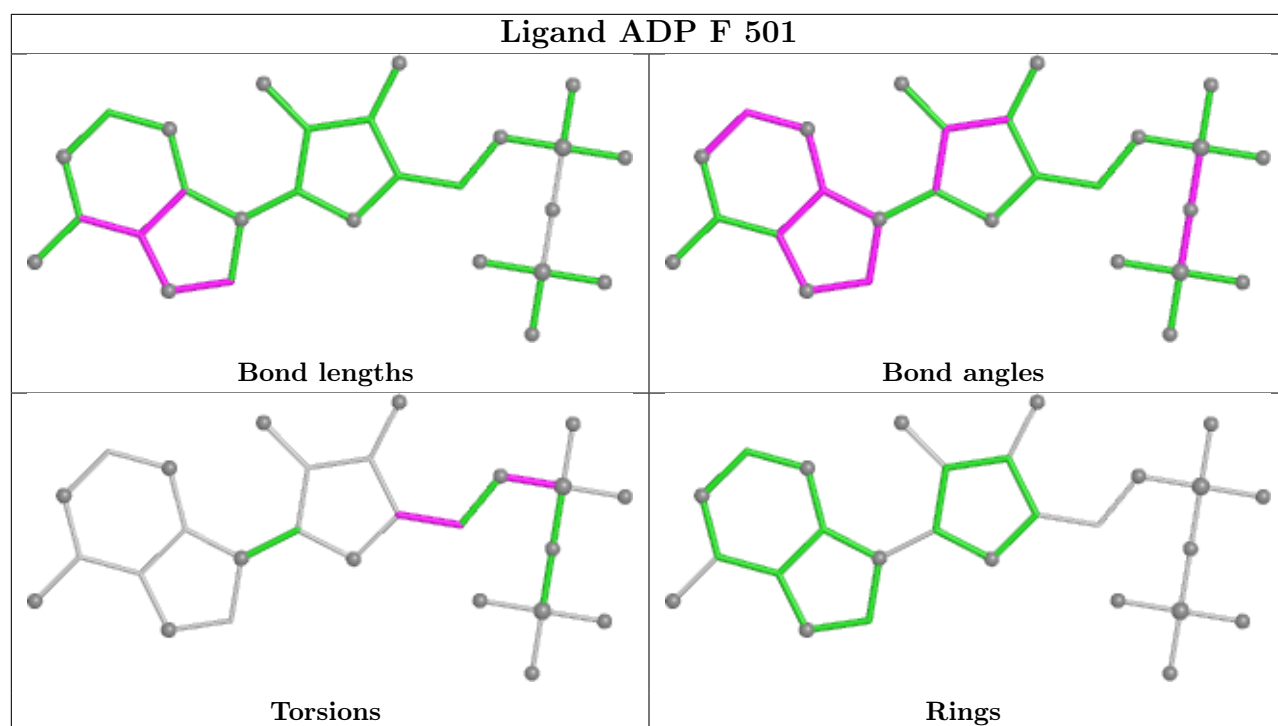
6 monomers are involved in 12 short contacts:

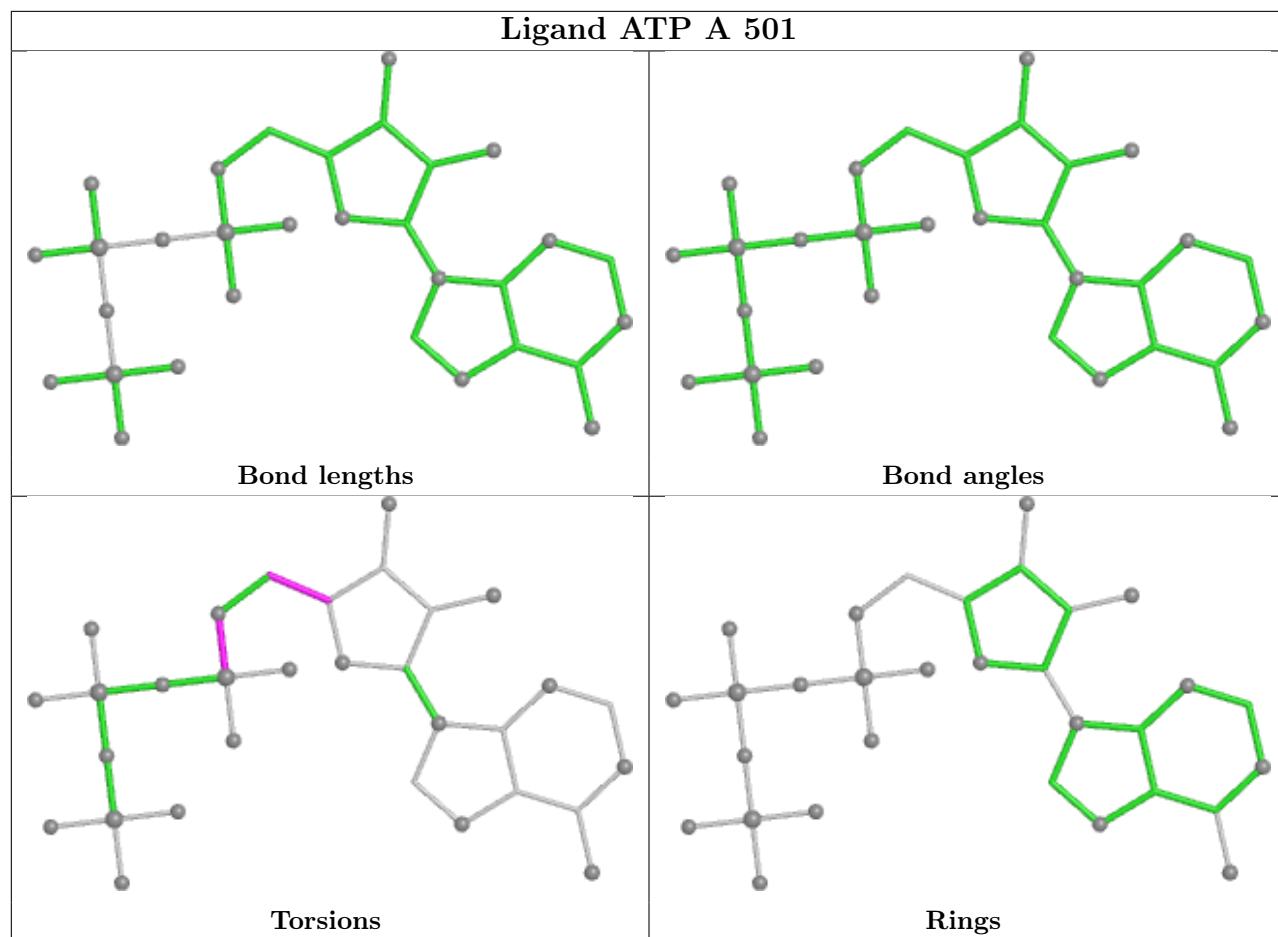
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	501	ATP	2	0
36	F	501	ADP	1	0
36	E	401	ADP	3	0
34	A	501	ATP	4	0
34	B	501	ATP	1	0
34	D	501	ATP	1	0

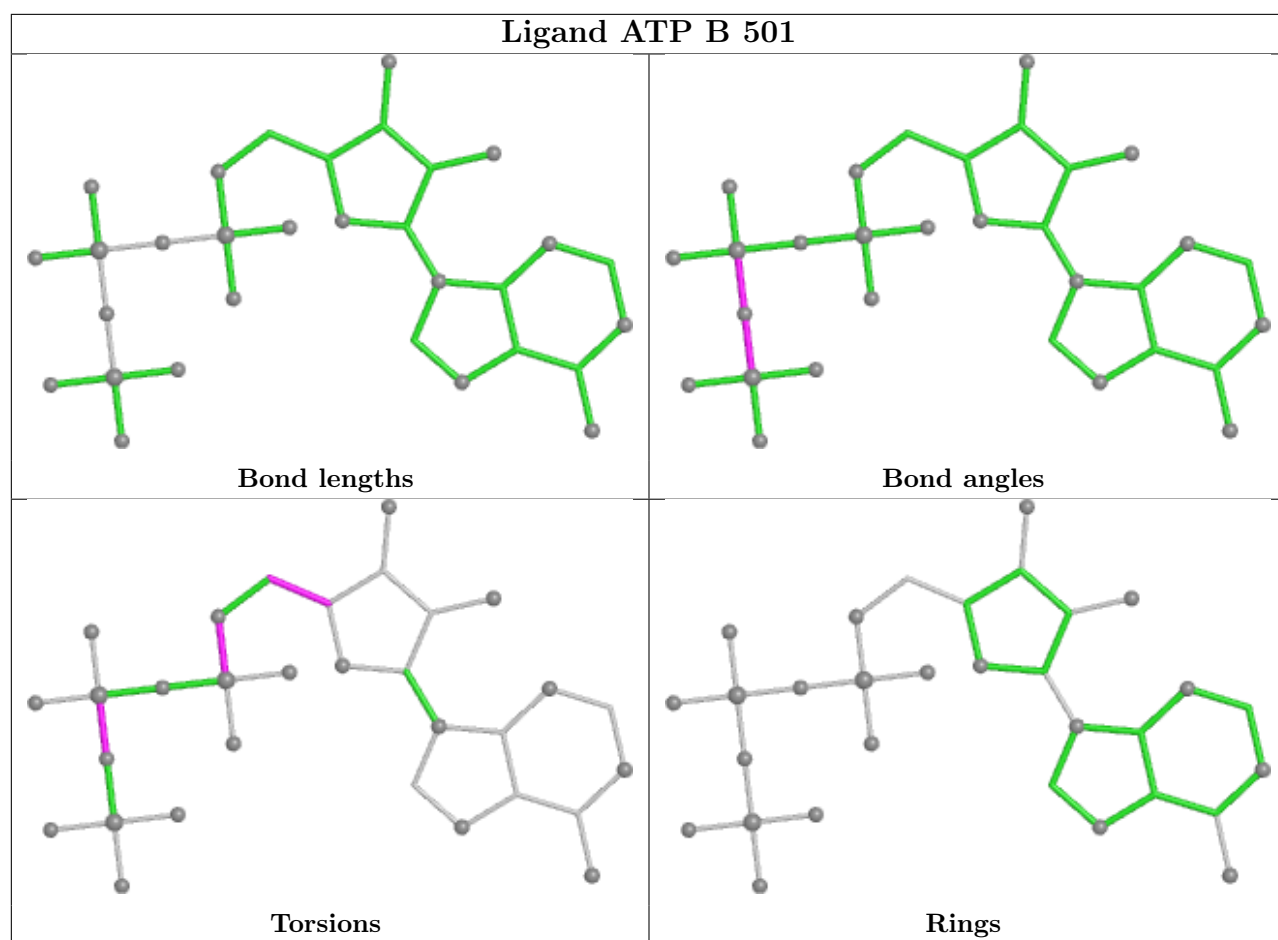
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

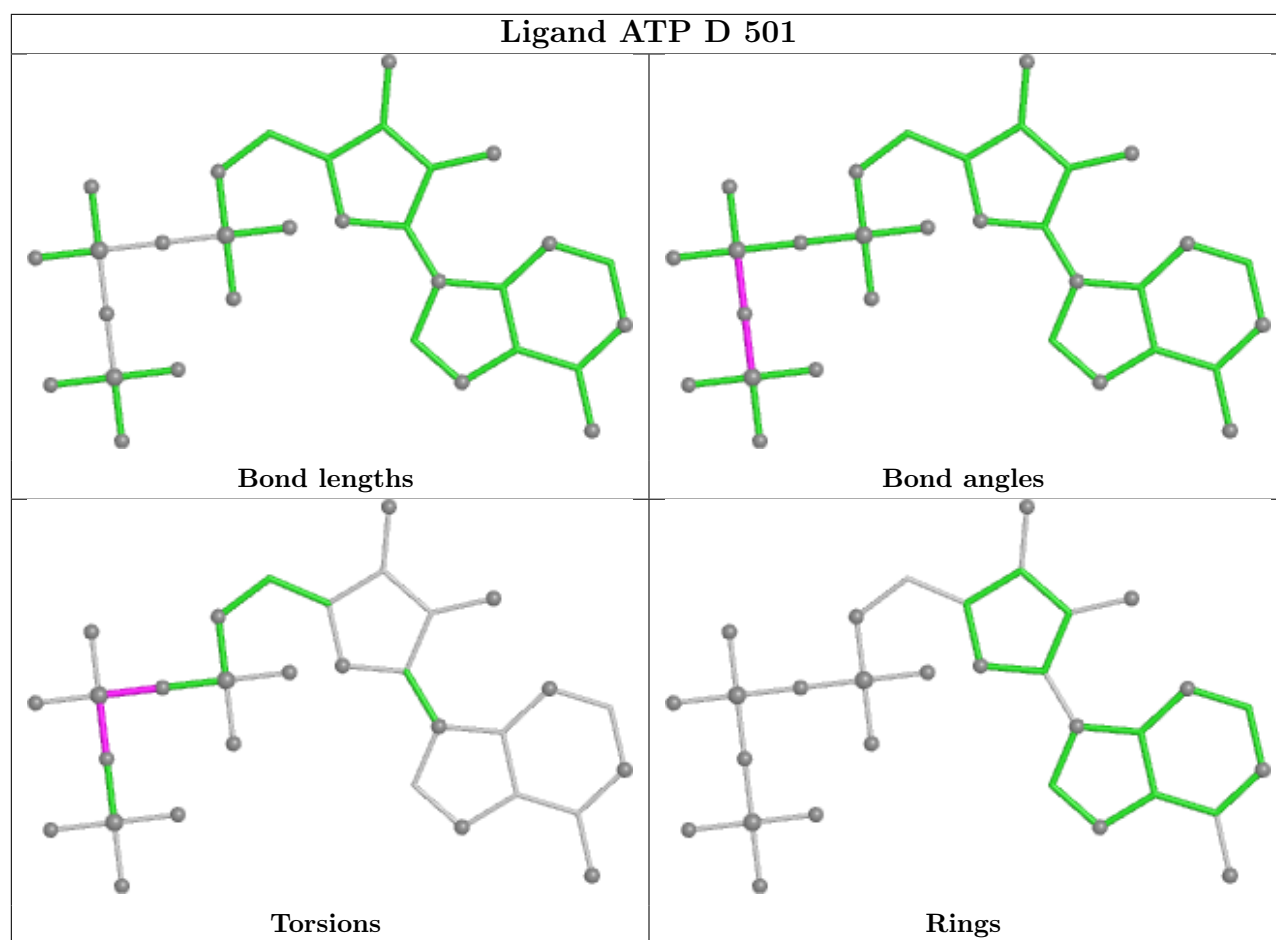
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

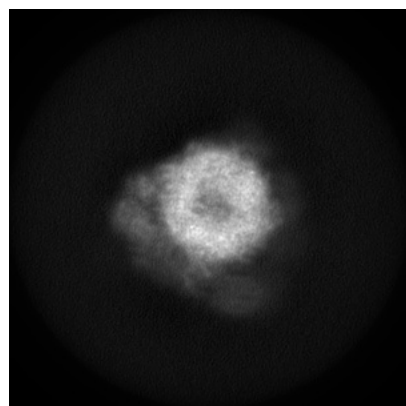
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62075. These allow visual inspection of the internal detail of the map and identification of artifacts.

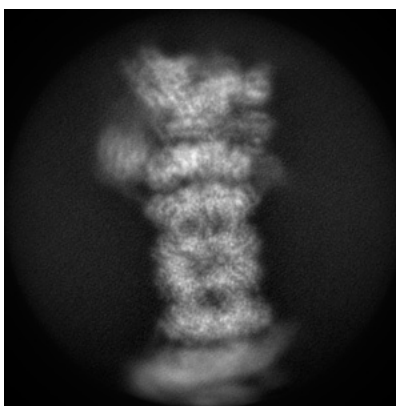
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

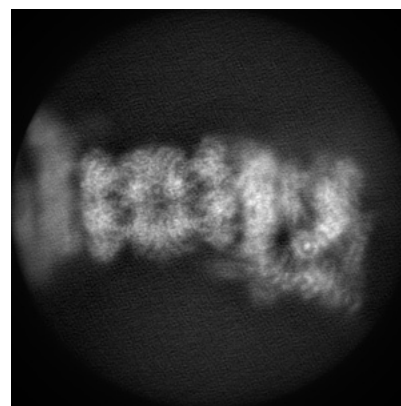
6.1.1 Primary map



X

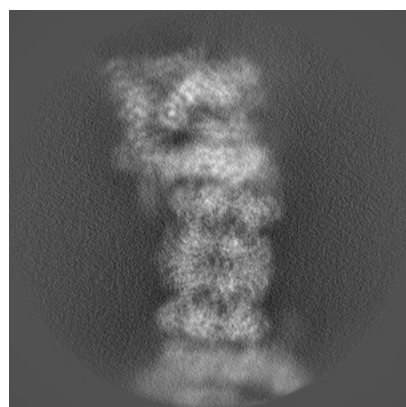


Y

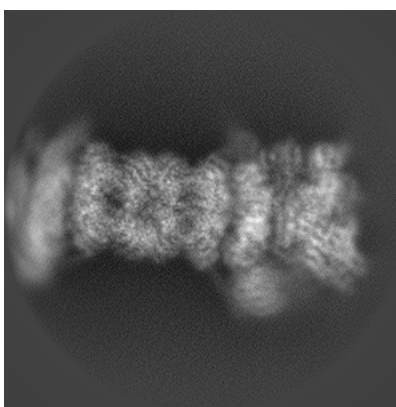


Z

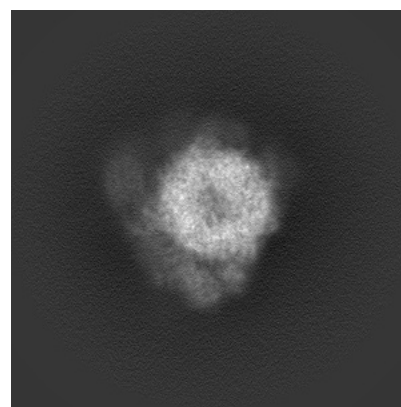
6.1.2 Raw map



X



Y

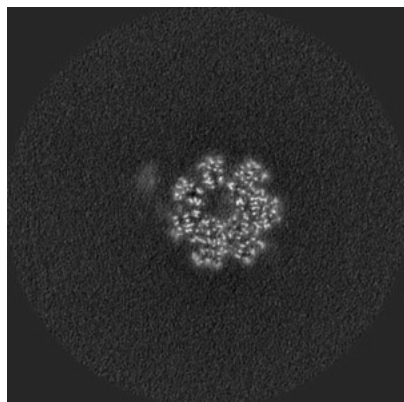


Z

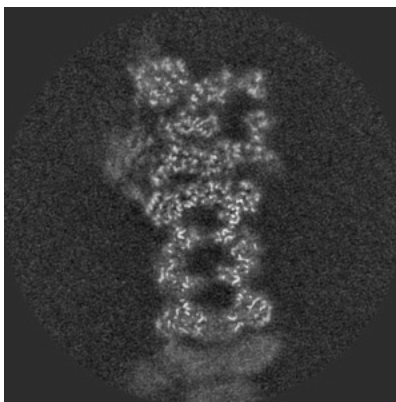
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

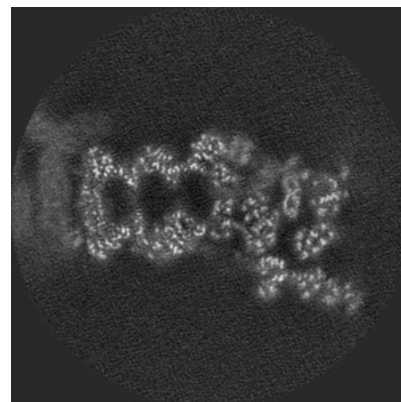
6.2.1 Primary map



X Index: 300

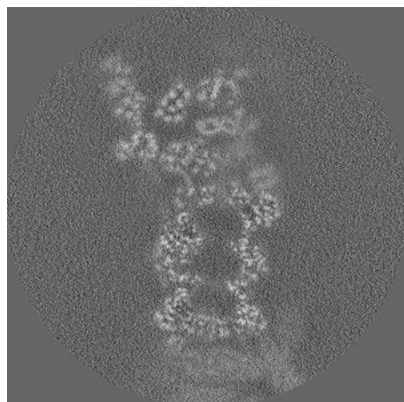


Y Index: 300

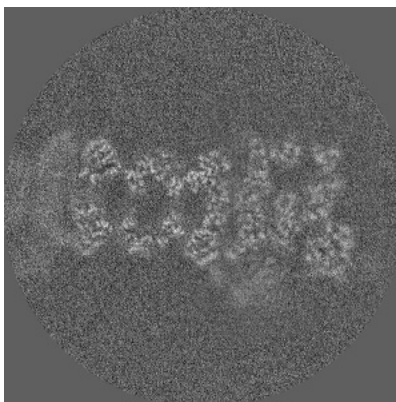


Z Index: 300

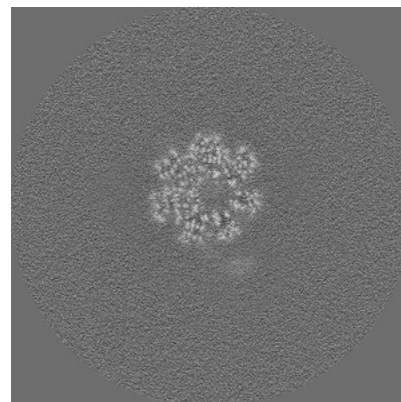
6.2.2 Raw map



X Index: 300



Y Index: 300

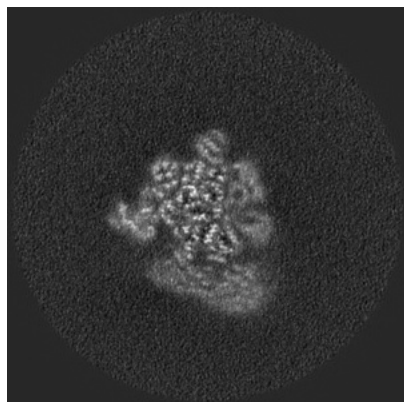


Z Index: 300

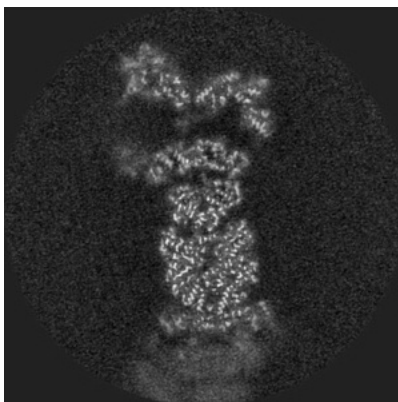
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

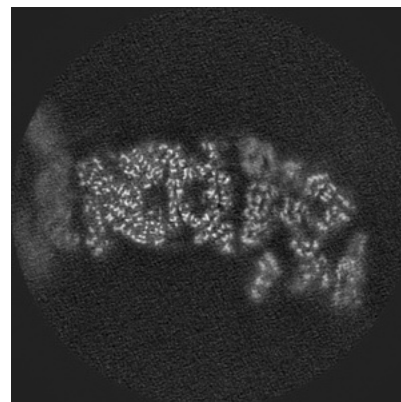
6.3.1 Primary map



X Index: 373

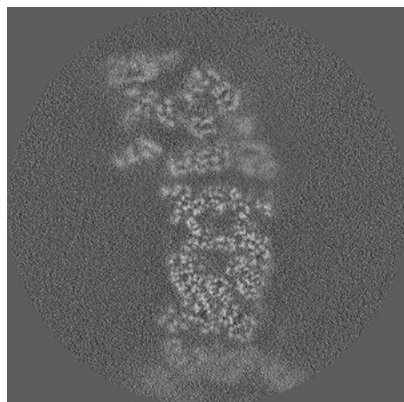


Y Index: 269

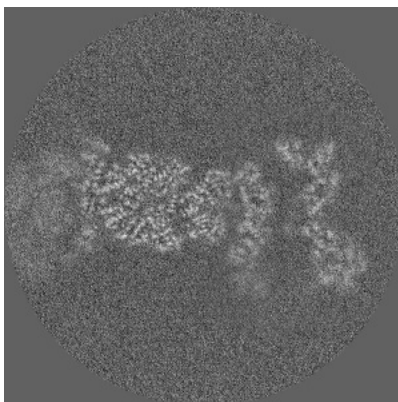


Z Index: 270

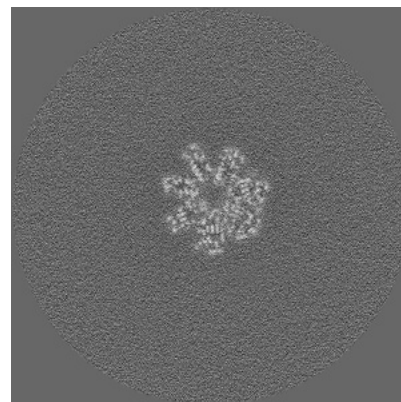
6.3.2 Raw map



X Index: 271



Y Index: 269

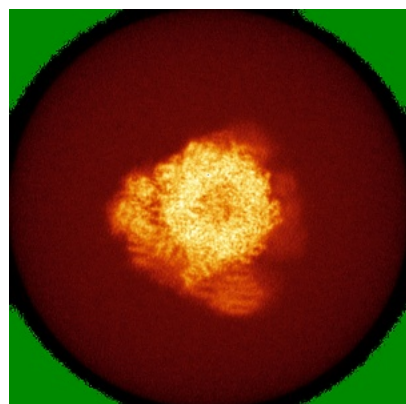


Z Index: 252

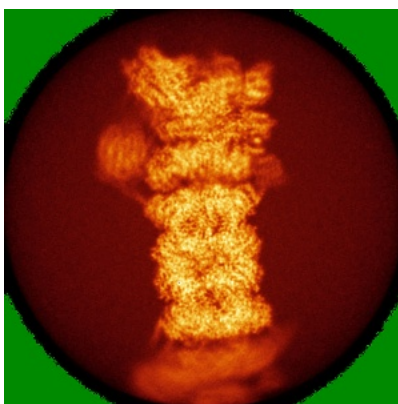
The images above show the largest variance slices of the map in three orthogonal directions.

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

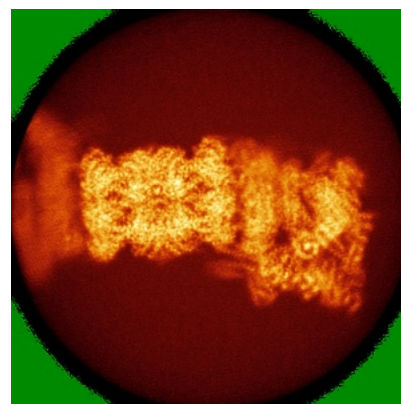
6.4.1 Primary map



X

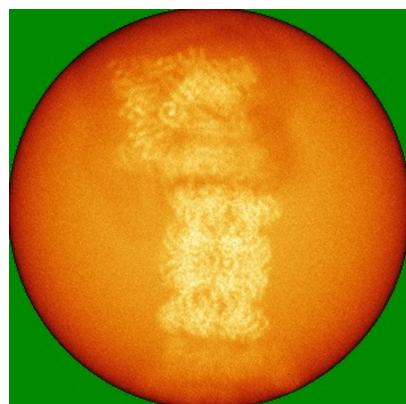


Y

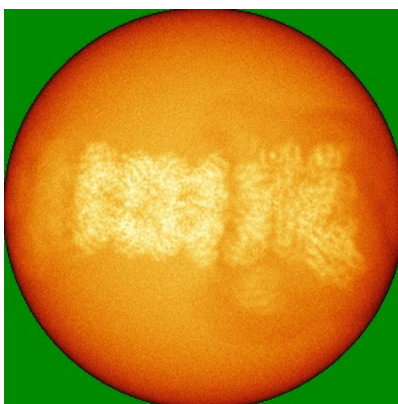


Z

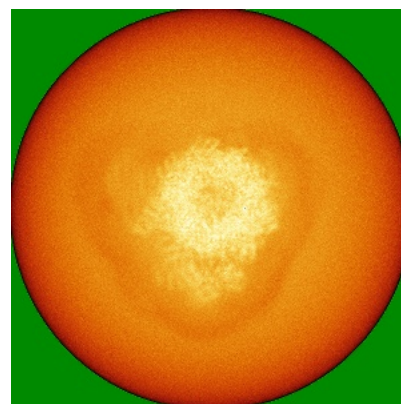
6.4.2 Raw map



X



Y

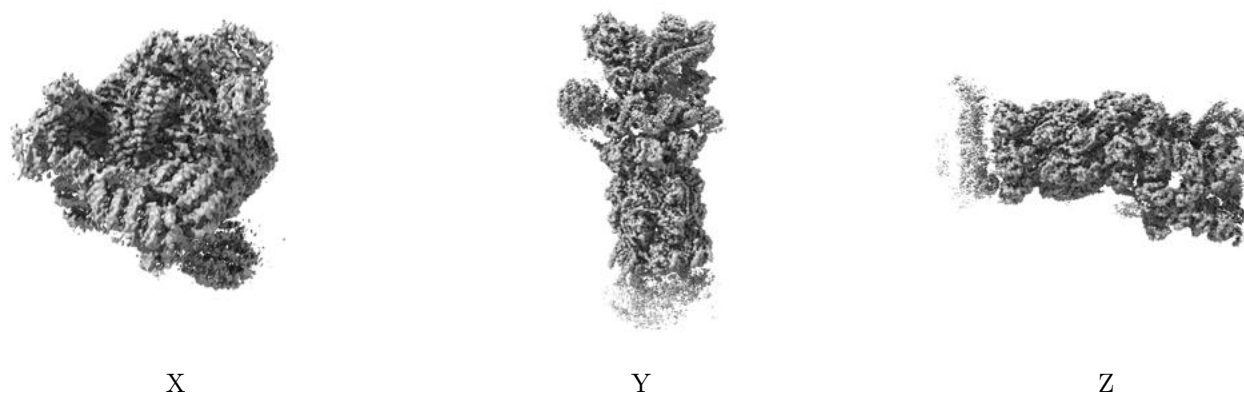


Z

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.

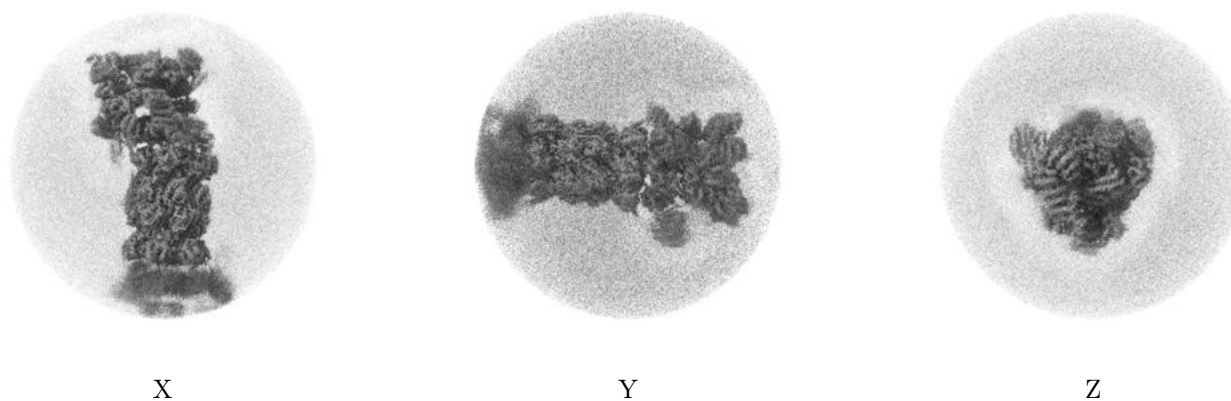
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00588. 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.

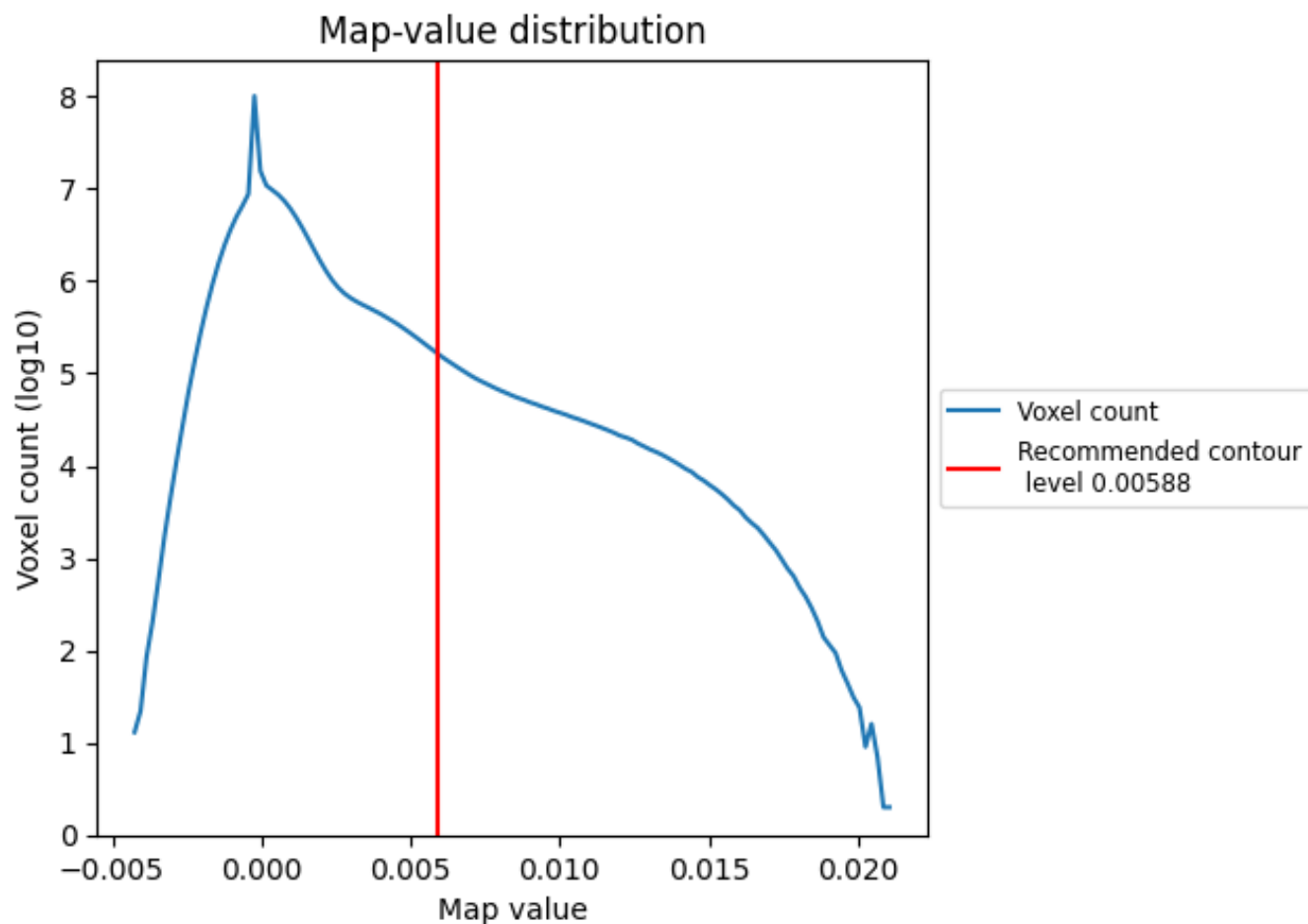
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

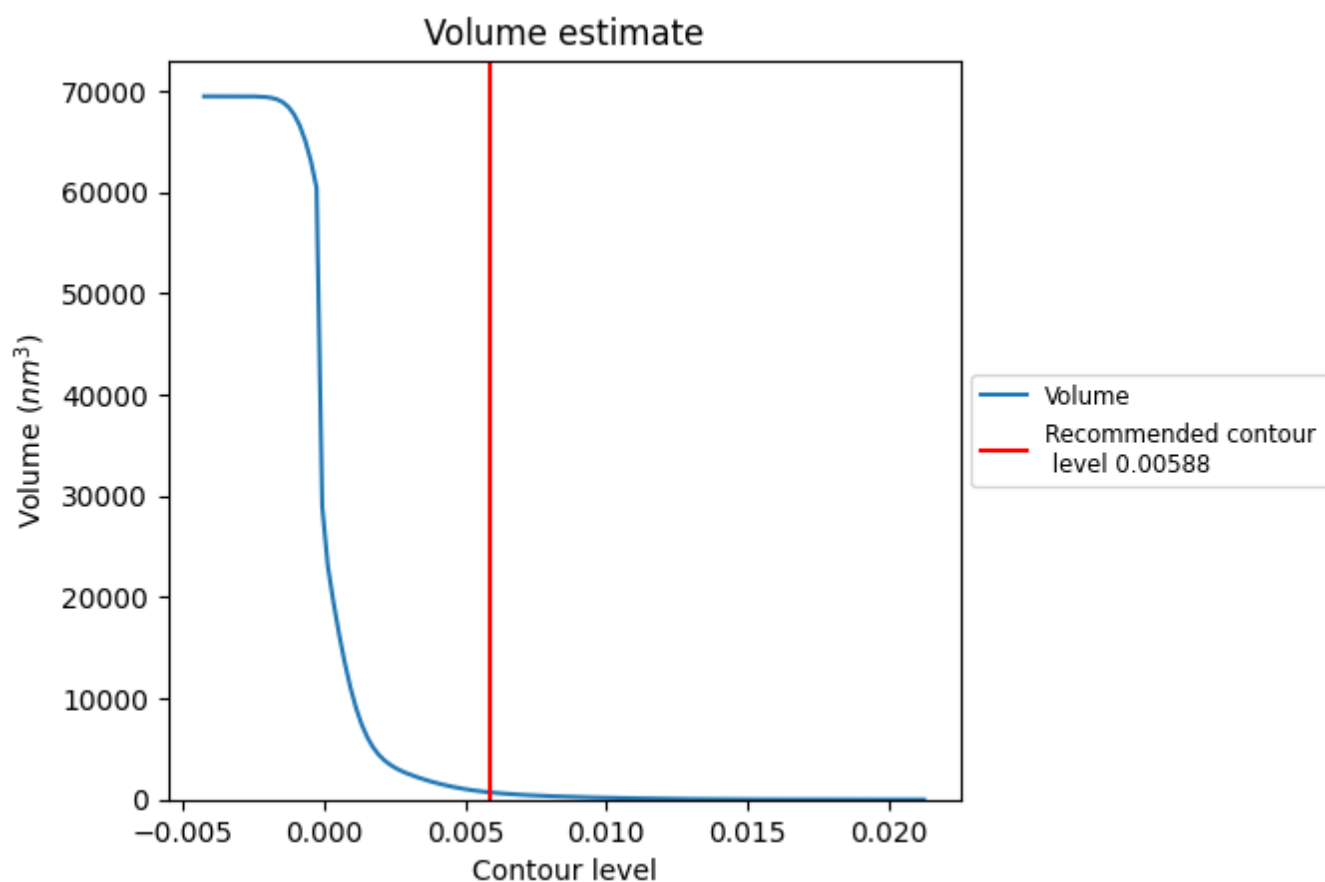
This section contains the results of statistical analysis of the map.

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.

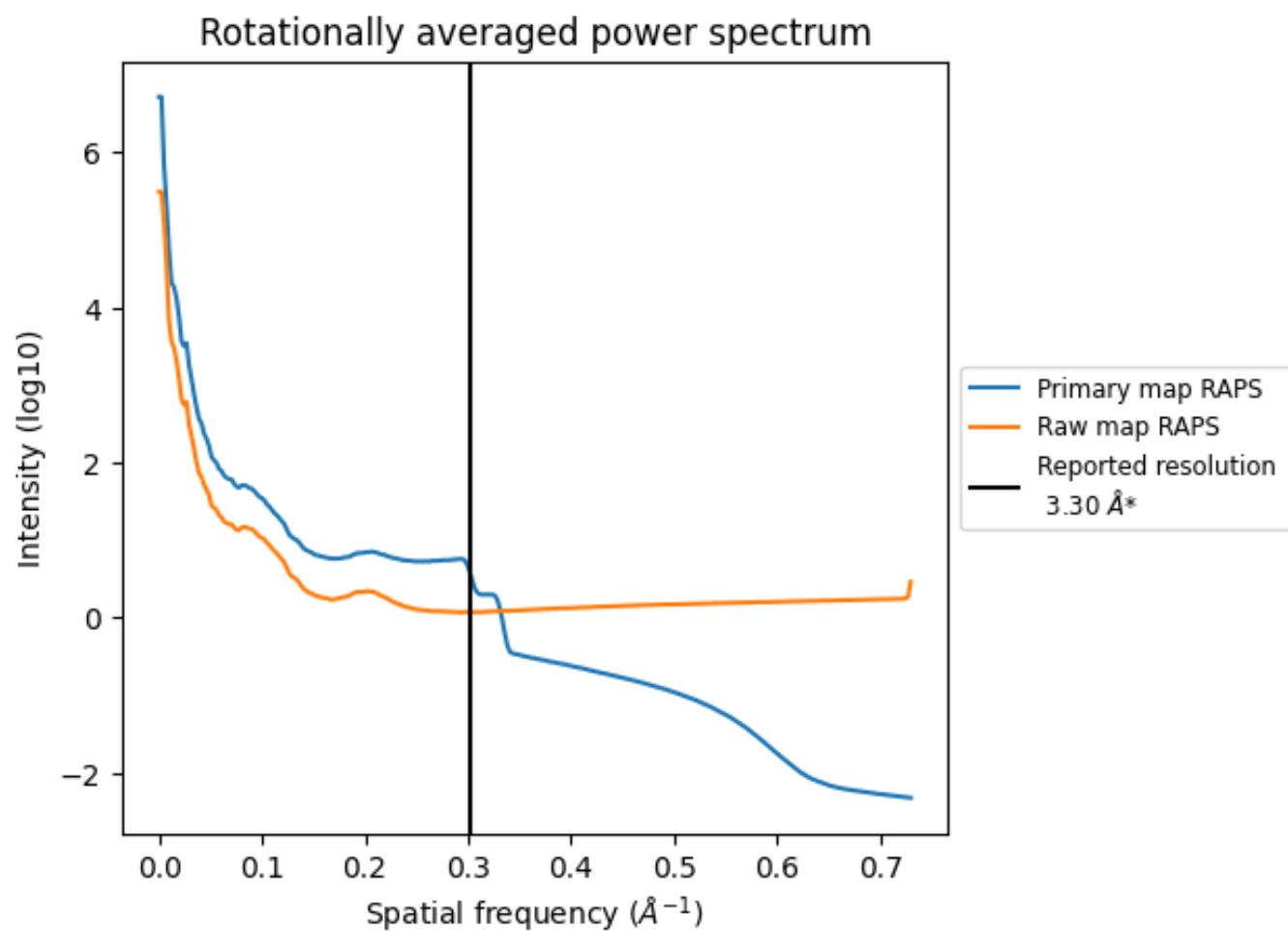
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm³; this corresponds to an approximate mass of 641 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 ⓘ

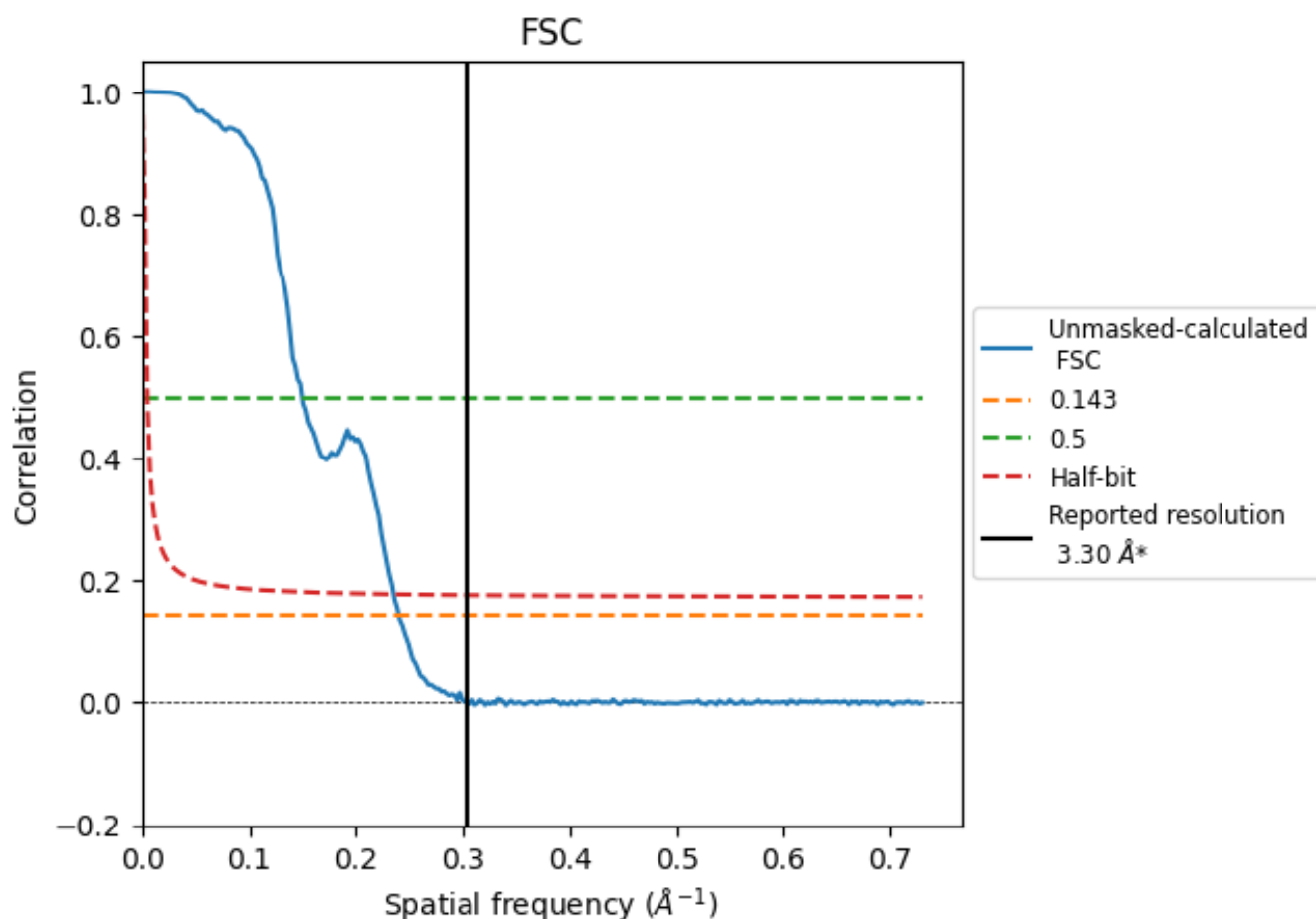


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

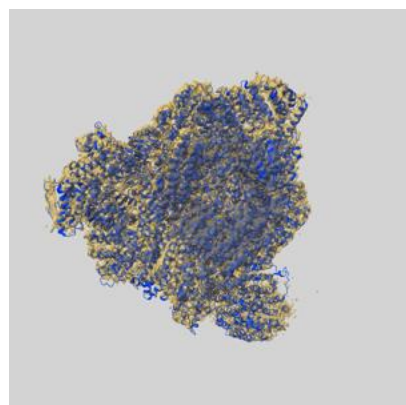
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.66	4.25

*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 4.17 differs from the reported value 3.3 by more than 10 %

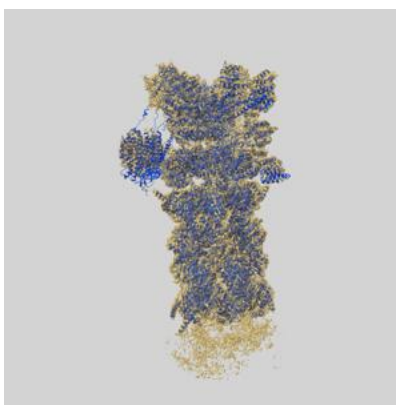
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62075 and PDB model 9K4Z. Per-residue inclusion information can be found in section [3](#) on page [13](#).

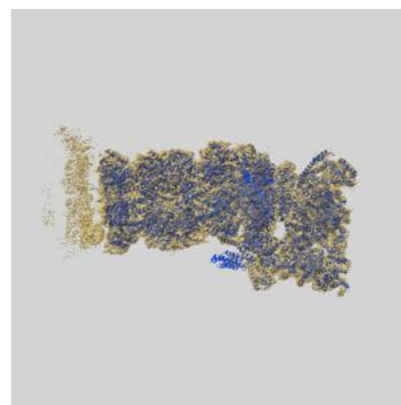
9.1 Map-model overlay [i](#)



X



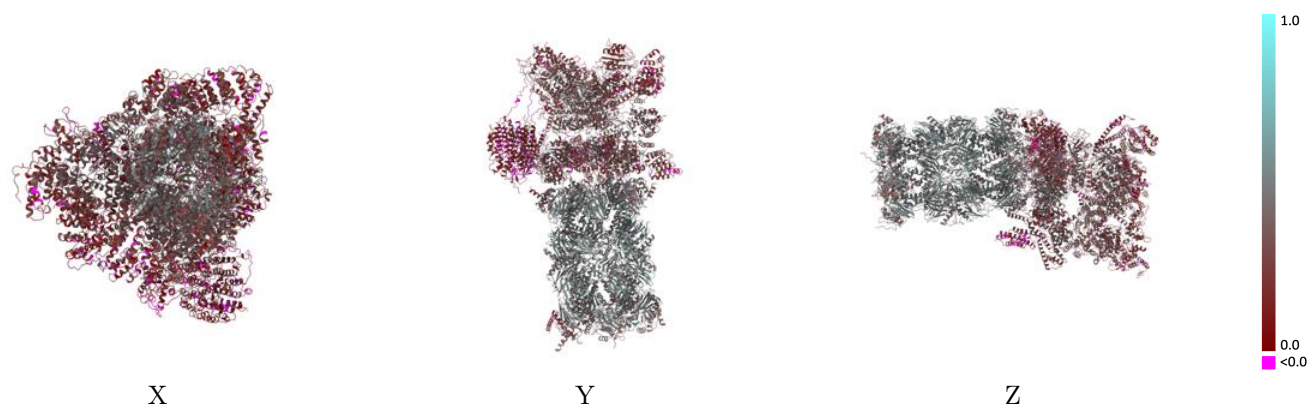
Y



Z

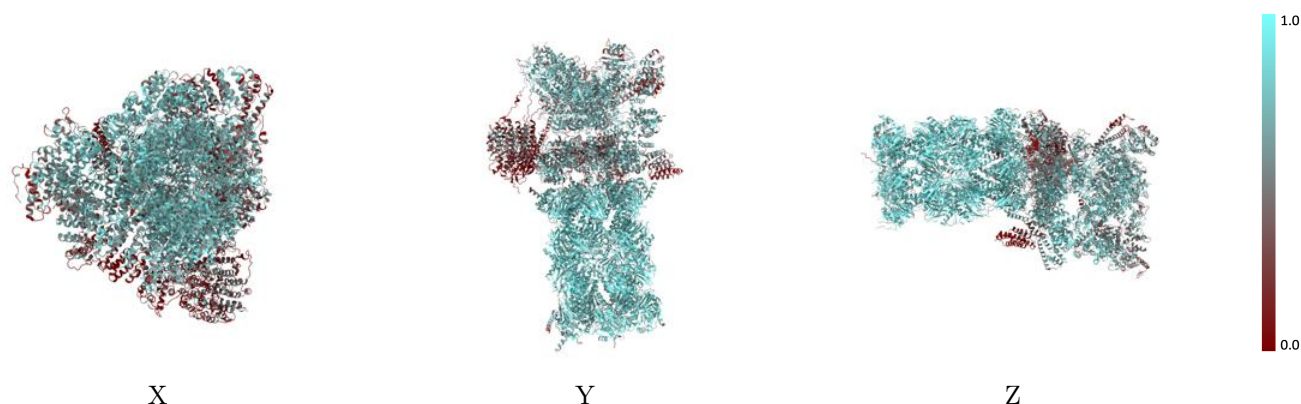
The images above show the 3D surface view of the map at the recommended contour level 0.00588 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



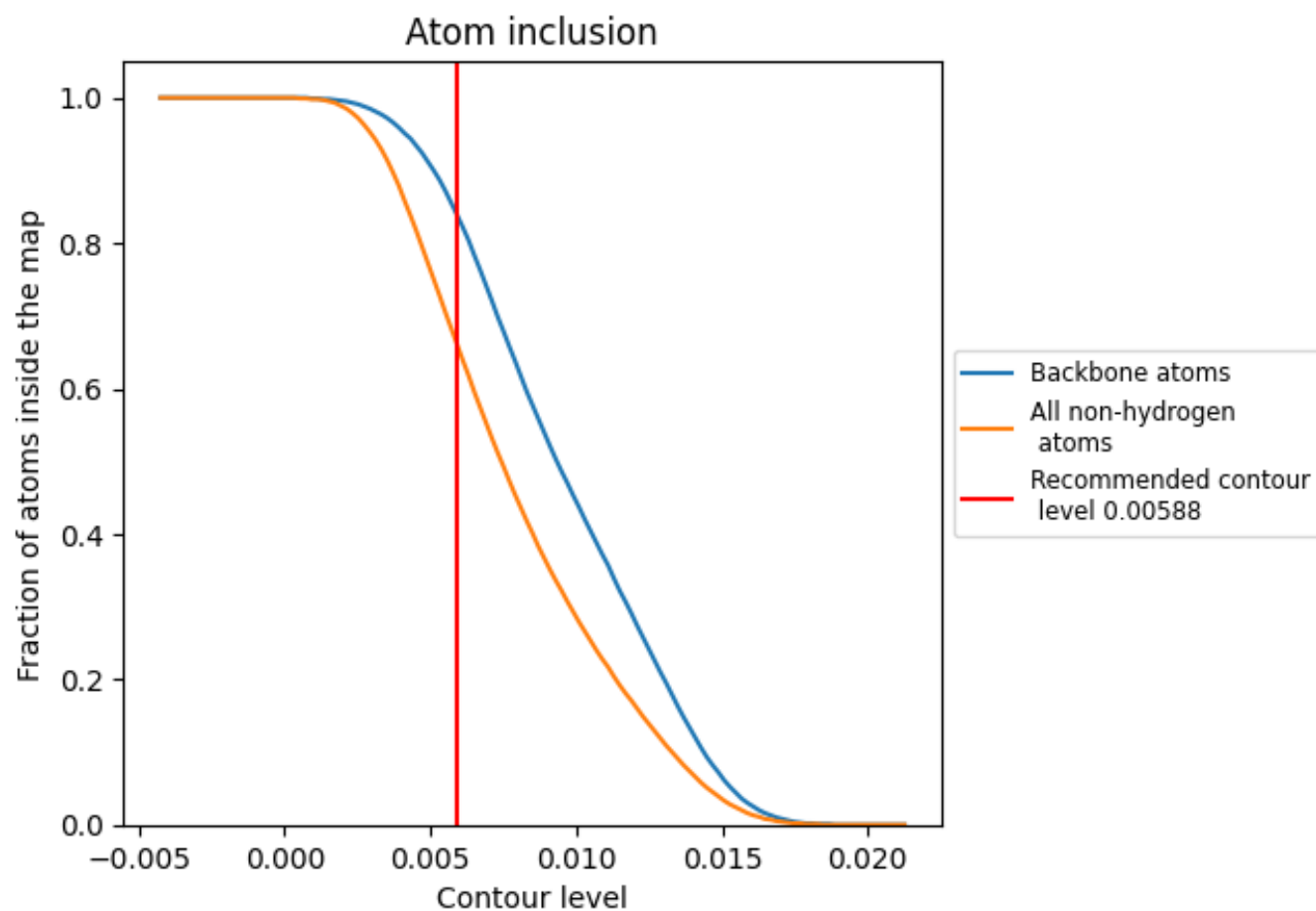
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00588).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.00588) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3610
A	 0.4460	 0.2480
B	 0.5460	 0.3270
C	 0.6780	 0.3640
D	 0.6950	 0.3830
E	 0.6030	 0.3290
F	 0.4140	 0.2250
G	 0.8210	 0.4650
H	 0.8210	 0.4700
I	 0.7970	 0.4560
J	 0.7720	 0.4360
K	 0.7660	 0.4560
L	 0.8290	 0.4720
M	 0.8120	 0.4660
N	 0.8550	 0.4990
O	 0.8690	 0.4930
P	 0.8750	 0.5010
Q	 0.8570	 0.4870
R	 0.8690	 0.4930
S	 0.8430	 0.4840
T	 0.8630	 0.5020
U	 0.6030	 0.2540
V	 0.5810	 0.2700
W	 0.5410	 0.2730
X	 0.4750	 0.2510
Y	 0.7210	 0.2970
Z	 0.6520	 0.3260
a	 0.6190	 0.2560
b	 0.5340	 0.2580
c	 0.6700	 0.3400
d	 0.4460	 0.2290
e	 0.5490	 0.2900
f	 0.1980	 0.1370
g	 0.7870	 0.4500
h	 0.7890	 0.4530



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Chain	Atom inclusion	Q-score
i	 0.7420	 0.4340
j	 0.7050	 0.3870
k	 0.7360	 0.4390
l	 0.8200	 0.4650
m	 0.8110	 0.4520
n	 0.8620	 0.4900
o	 0.8490	 0.4850
p	 0.8580	 0.4860
q	 0.8560	 0.4840
r	 0.8630	 0.4930
s	 0.8360	 0.4830
t	 0.8760	 0.4910
v	 0.2330	 0.3070