



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 02:11 PM JST

PDB ID : 9K4O / pdb_00009k4o
EMDB ID : EMD-62065
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EA2.2
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 6.00 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:

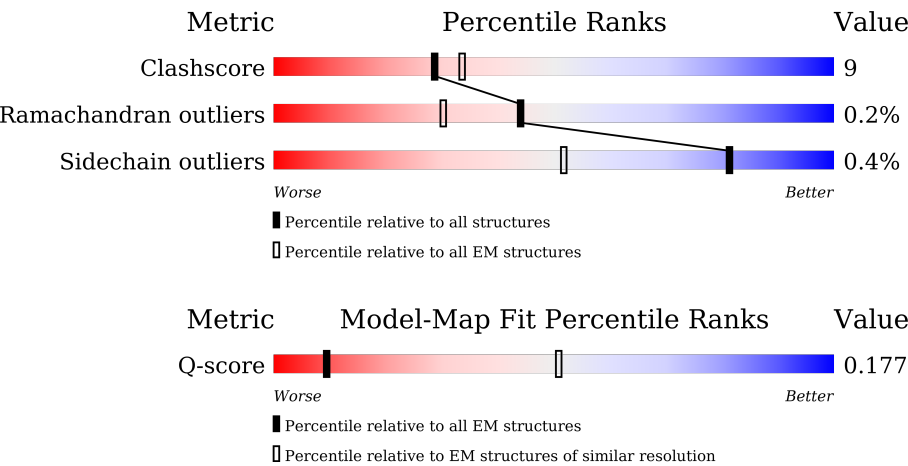
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 6.00 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	525 (5.50 - 6.50)

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>34%</div><div><div></div><div>65%</div><div>26%</div><div>9%</div></div></div>
2	B	440	<div><div>34%</div><div><div></div><div>62%</div><div>25%</div><div>13%</div></div></div>
3	C	398	<div><div>39%</div><div><div></div><div>66%</div><div>24%</div><div>• 9%</div></div></div>
4	D	418	<div><div>28%</div><div><div></div><div>67%</div><div>23%</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	
33	x	76	
33	y	76	
34	v	10	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 107132 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	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- 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
			3039	1923	524	579	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	415	Total	C	N	O	S	0	0
			3251	2038	561	634	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	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

- 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		

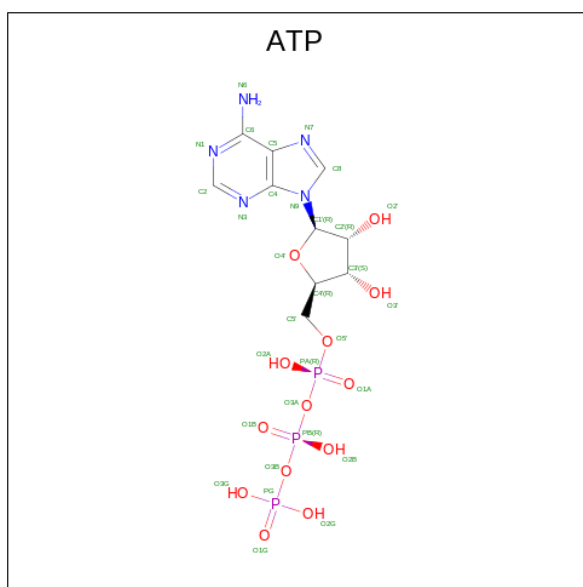
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	x	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	y	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	10	Total	C	N	O	0	0
			53	32	11	10		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

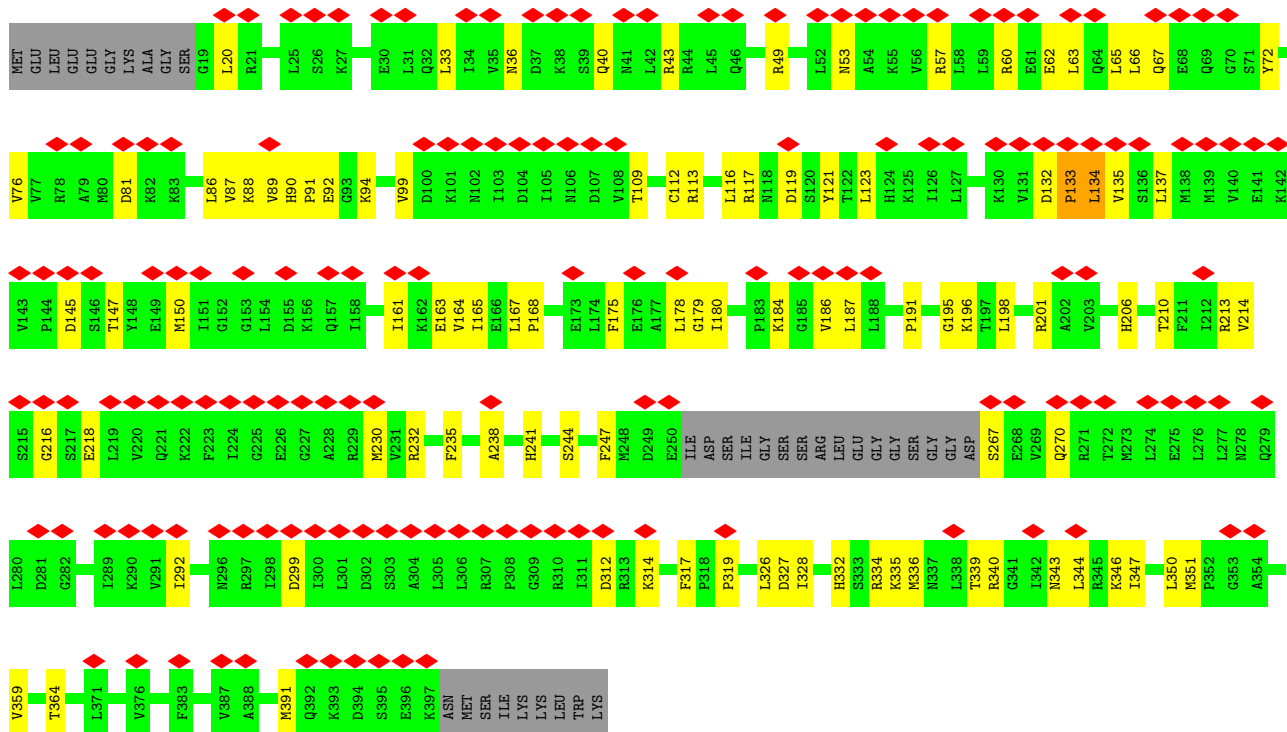
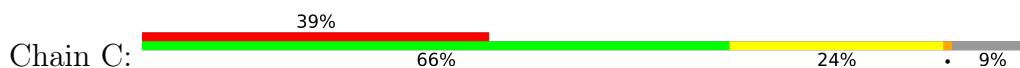


Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total 27	C 10	N 5	O 10	P 2	0
37	F	1	Total 27	C 10	N 5	O 10	P 2	0

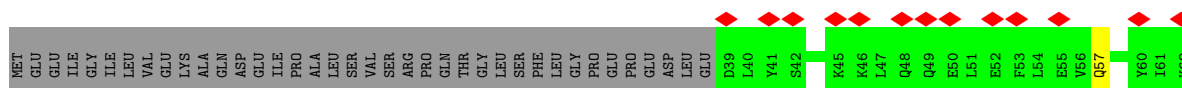
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

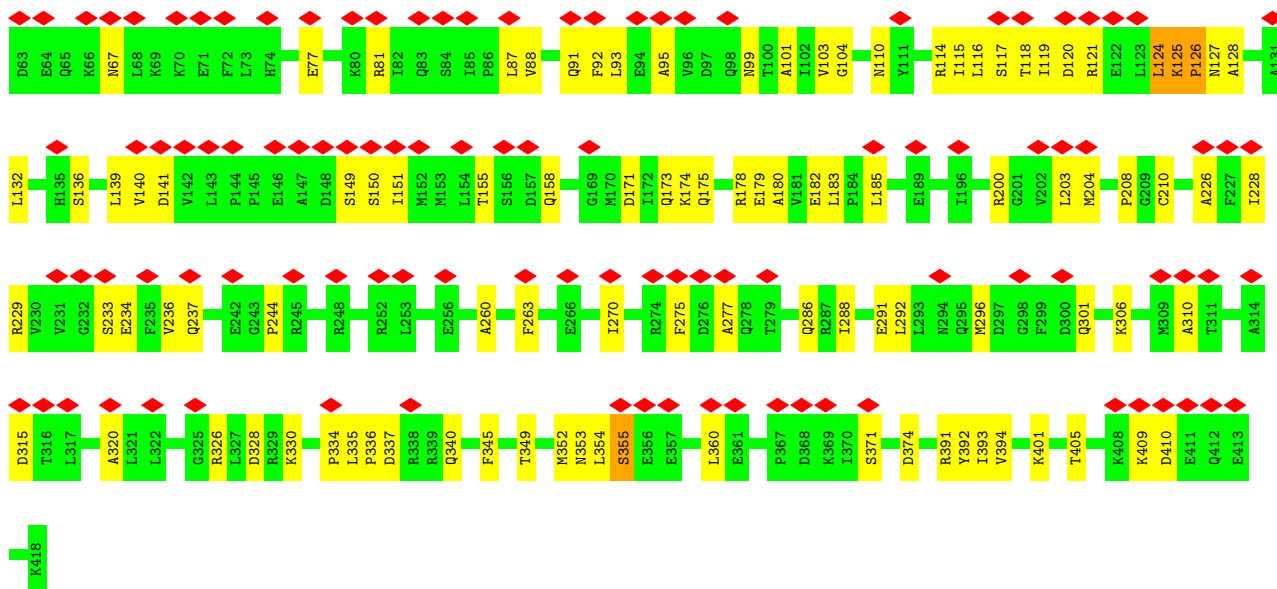
Mol	Chain	Residues	Atoms	AltConf
38	c	1	Total Zn 1 1	0

- Molecule 3: 26S proteasome regulatory subunit 8

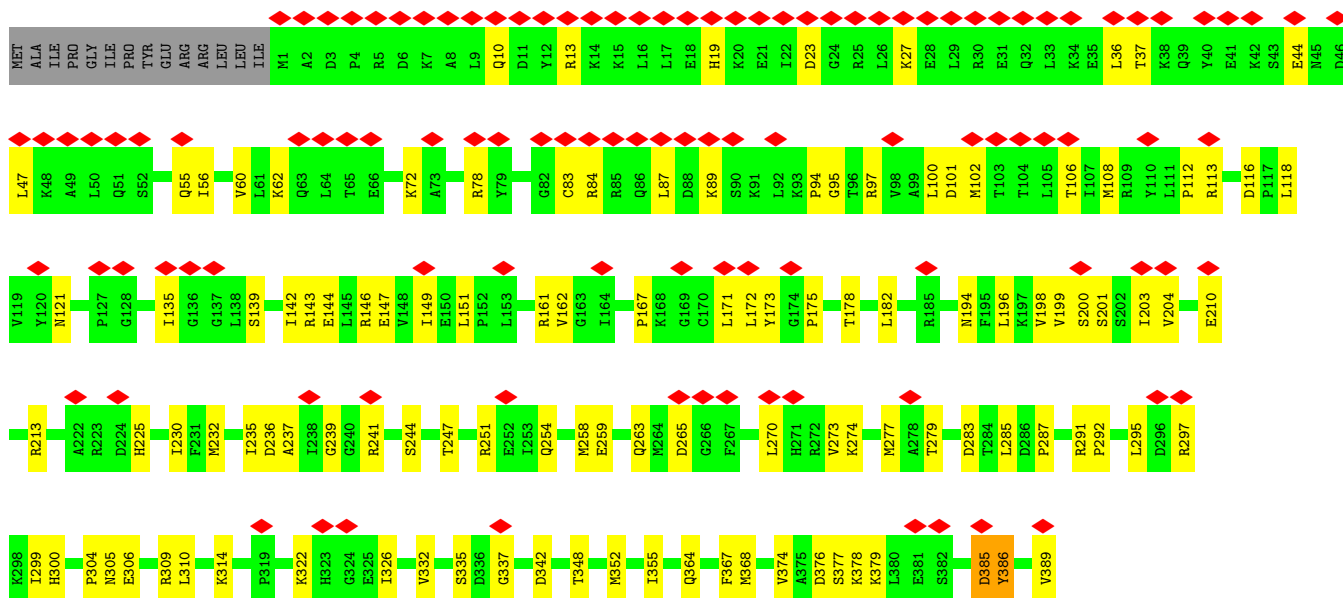


- Molecule 4: 26S proteasome regulatory subunit 6B

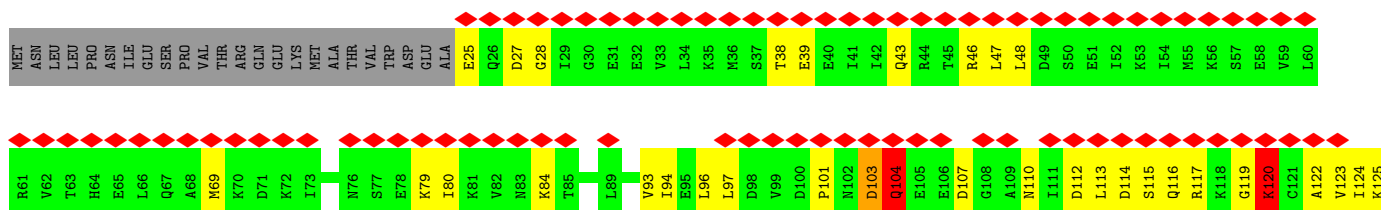


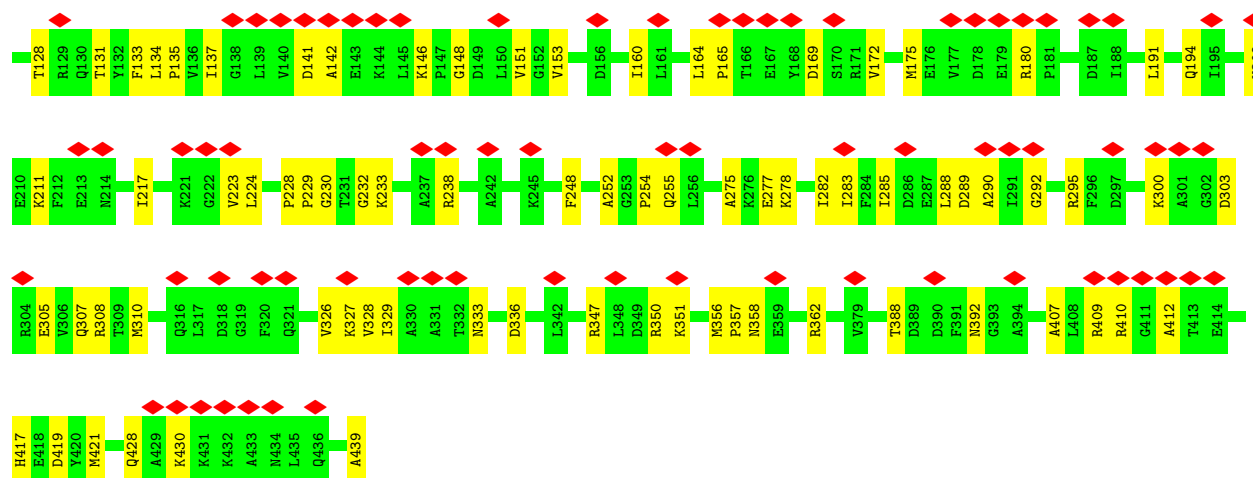


• Molecule 5: Proteasome 26S subunit, ATPase 6

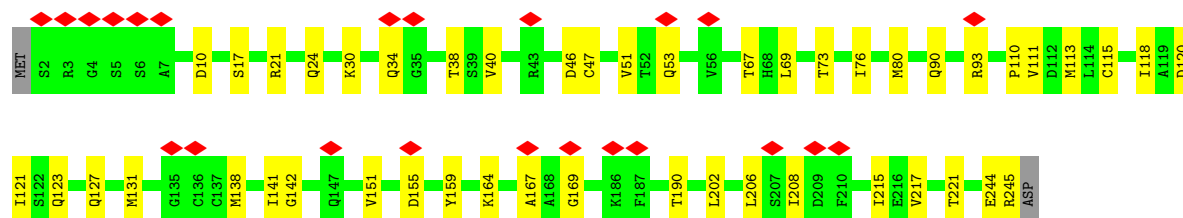
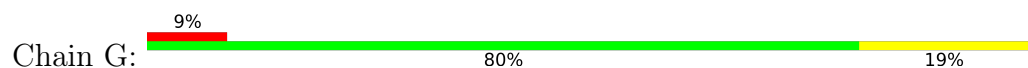


• Molecule 6: 26S proteasome regulatory subunit 6A

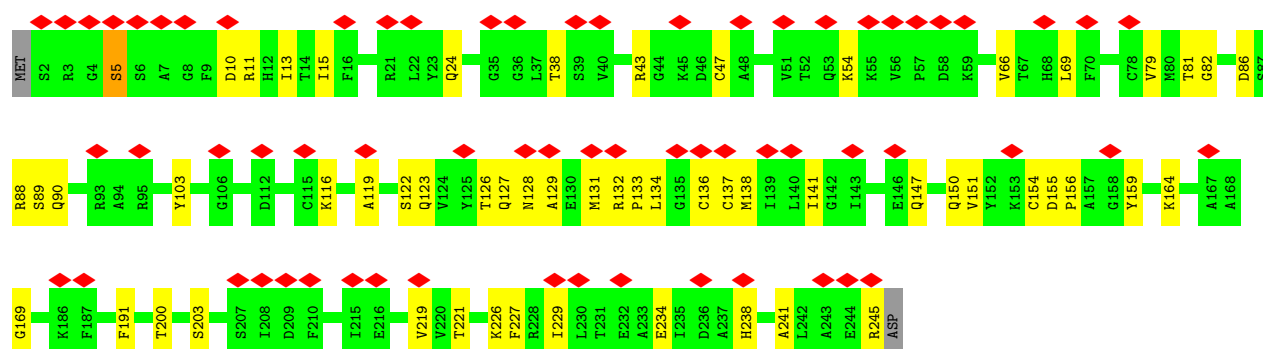
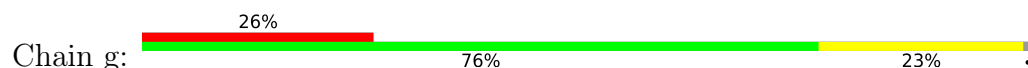




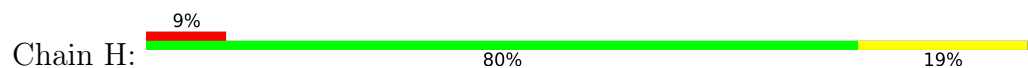
• Molecule 7: Proteasome subunit alpha type-6

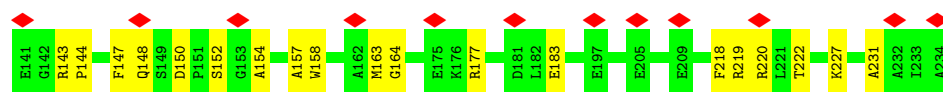


• Molecule 7: Proteasome subunit alpha type-6

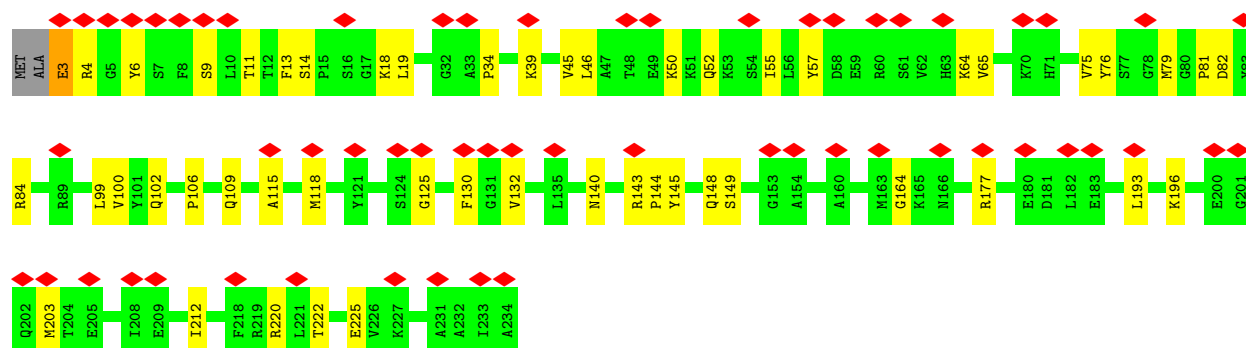
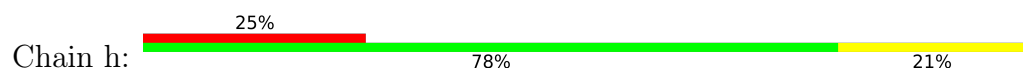


• Molecule 8: Proteasome subunit alpha type-2

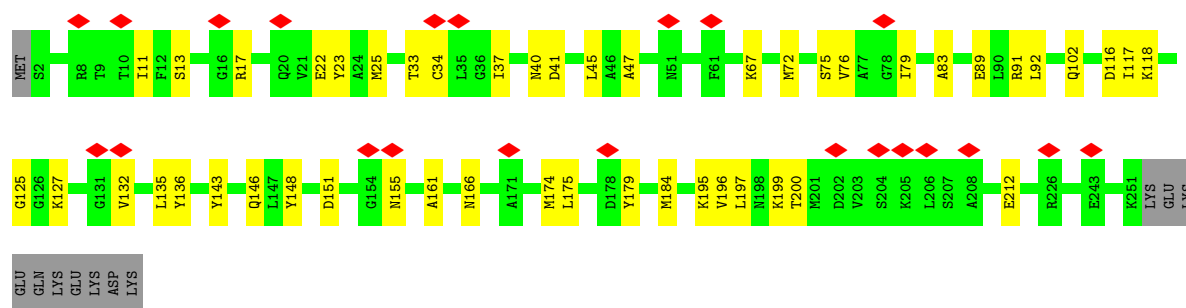
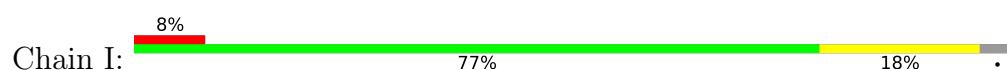




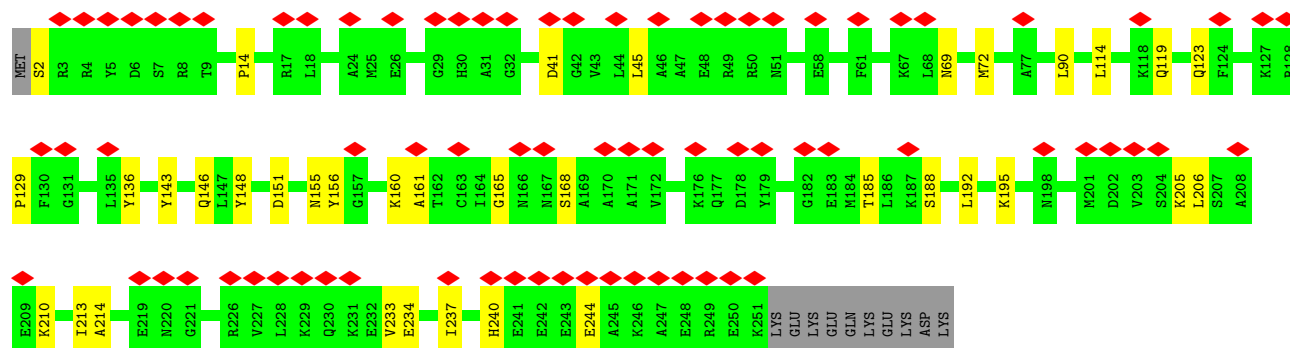
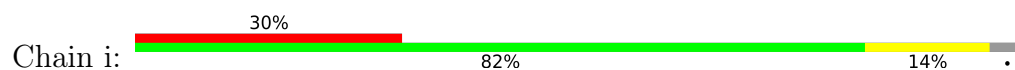
• Molecule 8: Proteasome subunit alpha type-2



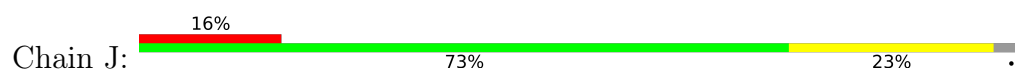
• Molecule 9: Proteasome subunit alpha type-4

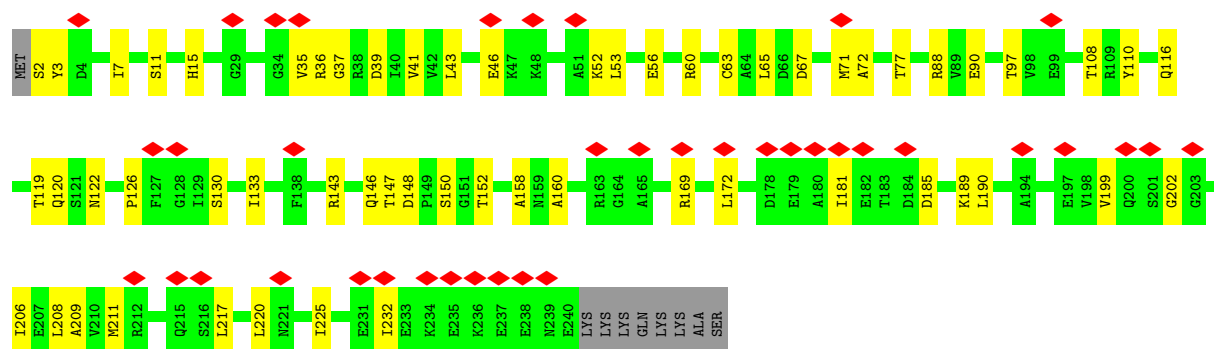


• Molecule 9: Proteasome subunit alpha type-4

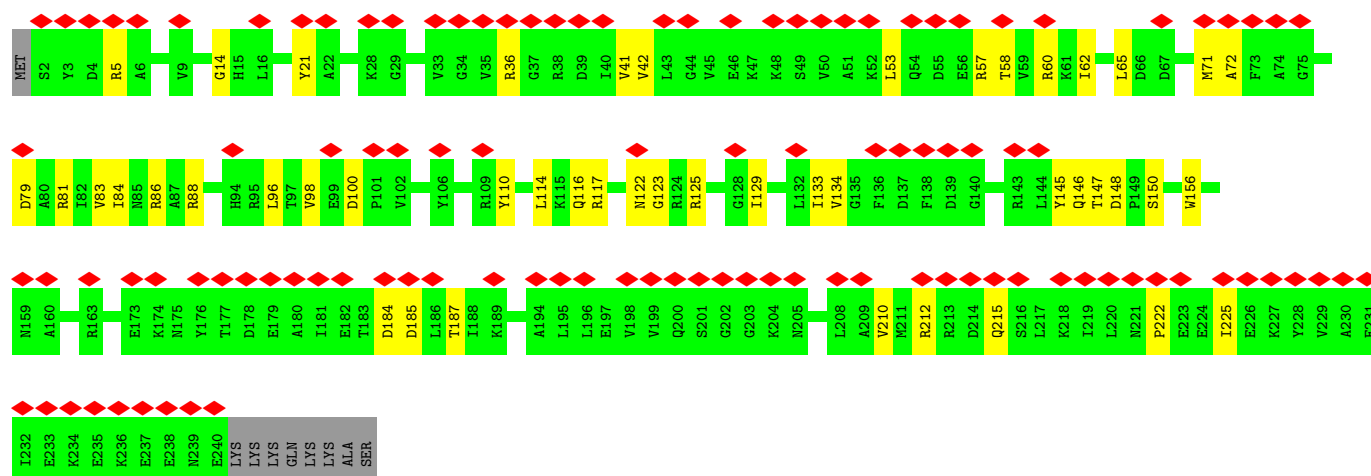
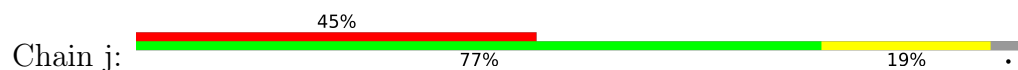


• Molecule 10: Proteasome subunit alpha type-7

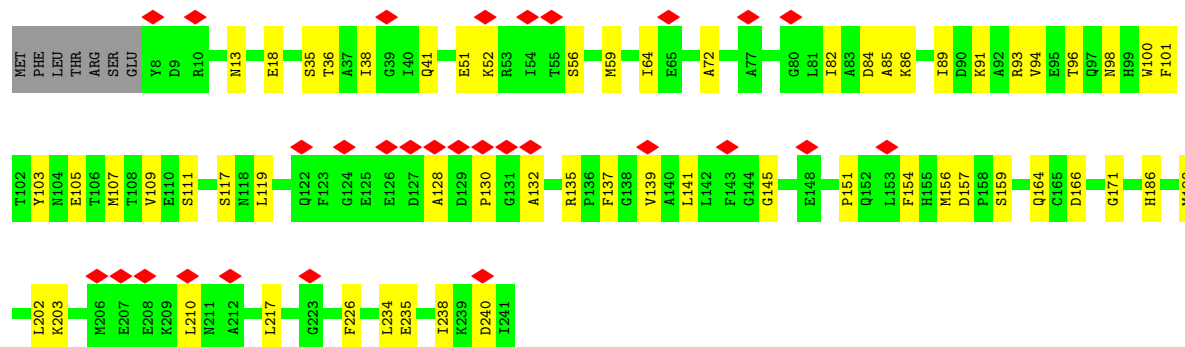
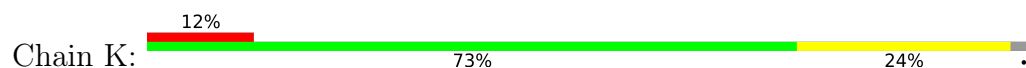




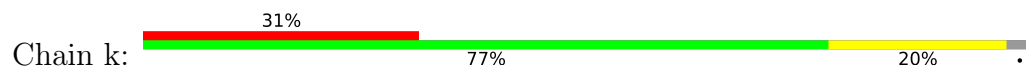
• Molecule 10: Proteasome subunit alpha type-7

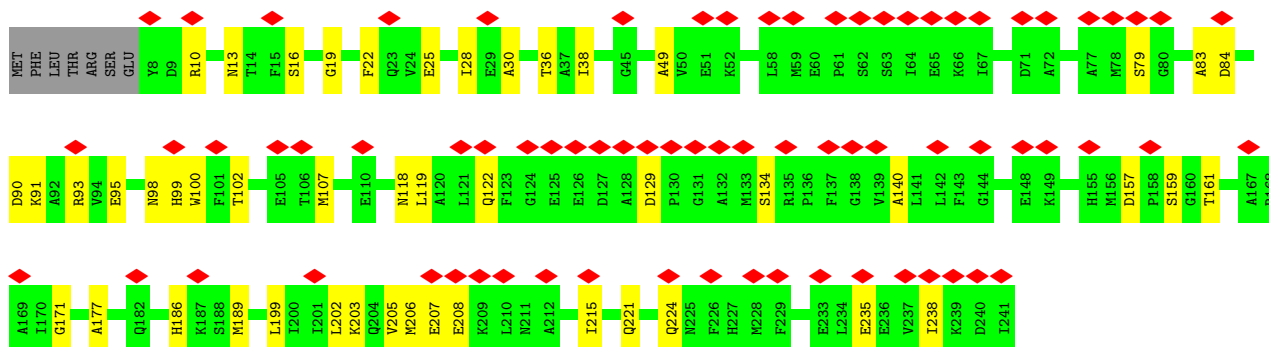


• Molecule 11: Proteasome subunit alpha type-5

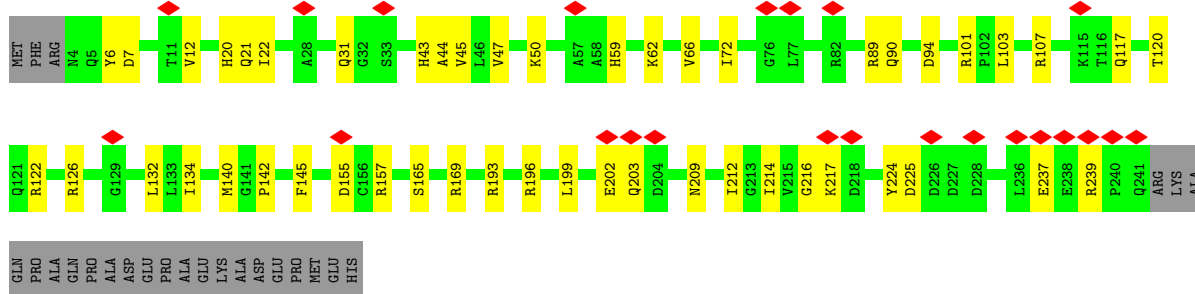


• Molecule 11: Proteasome subunit alpha type-5

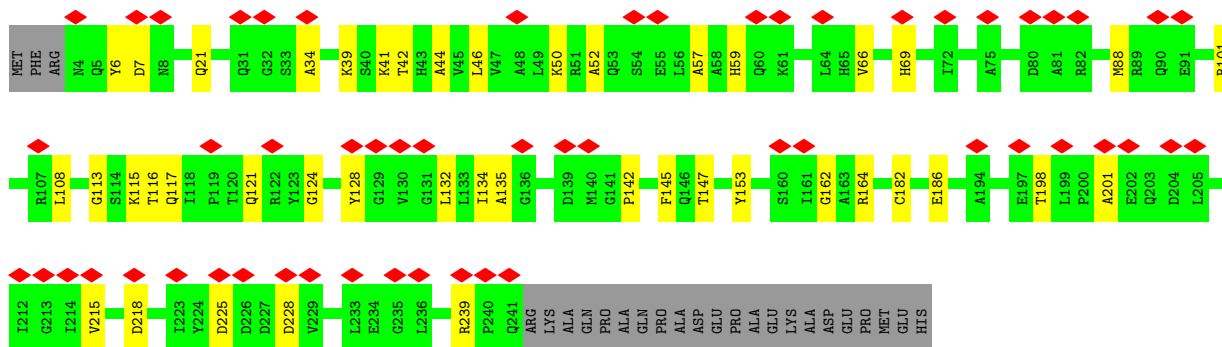
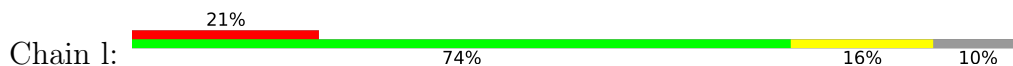




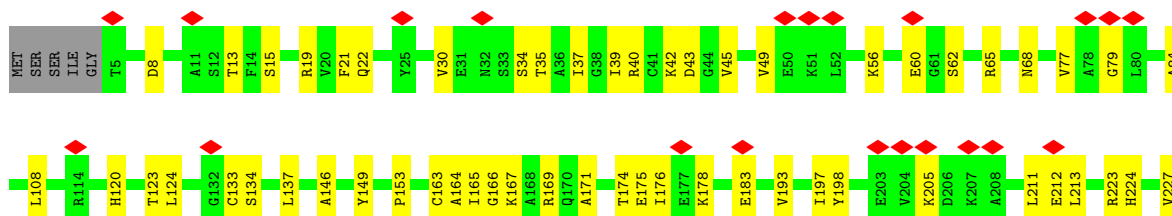
- Molecule 12: Proteasome subunit alpha type-1

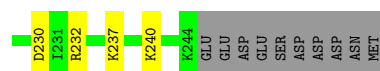


- Molecule 12: Proteasome subunit alpha type-1

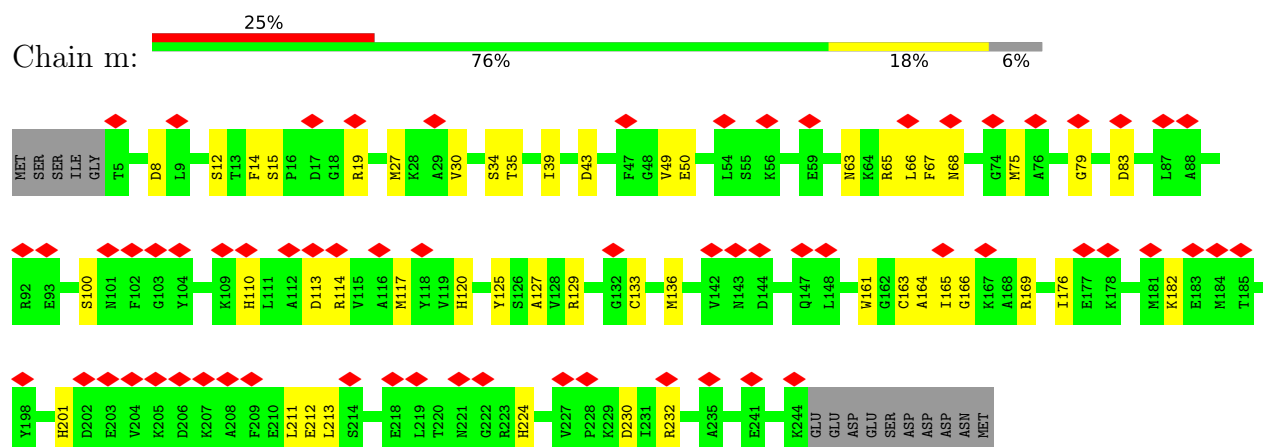


- Molecule 13: Proteasome subunit alpha type-3

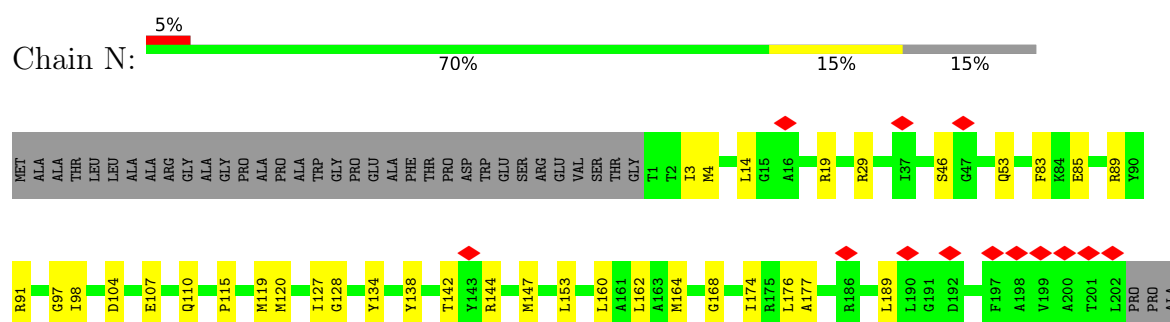




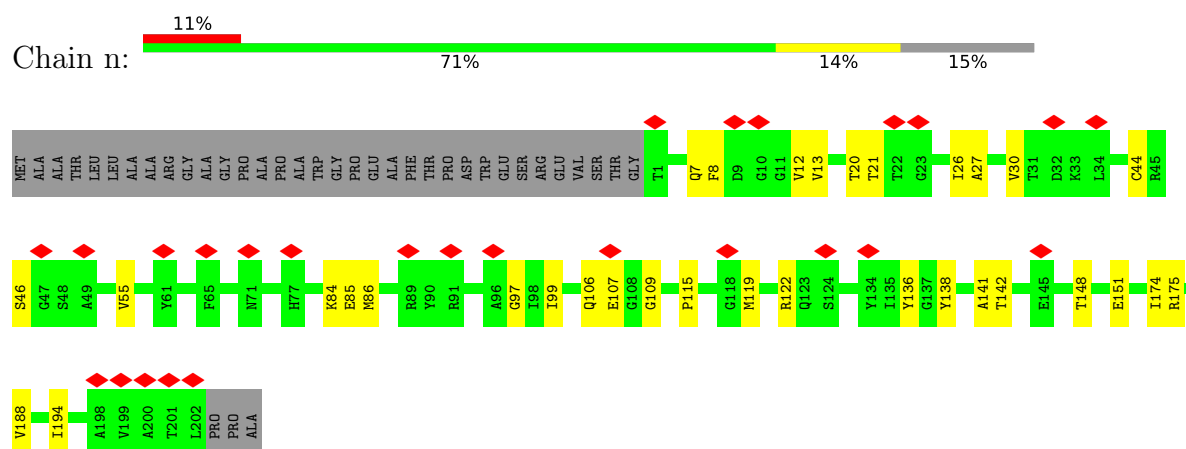
• Molecule 13: Proteasome subunit alpha type-3



• Molecule 14: Proteasome subunit beta type-6

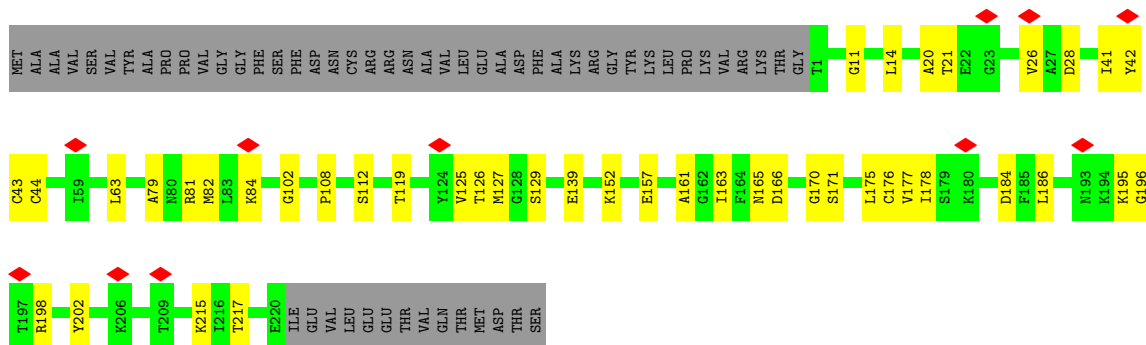


• Molecule 14: Proteasome subunit beta type-6

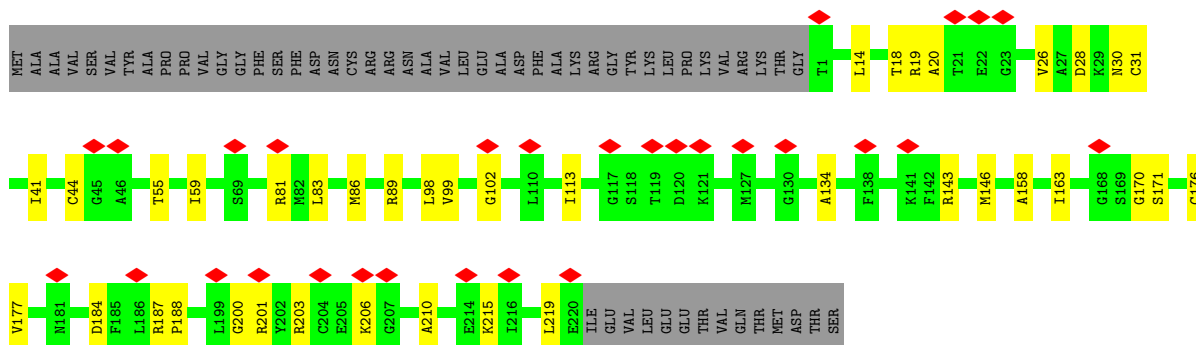


• Molecule 15: Proteasome subunit beta type-7

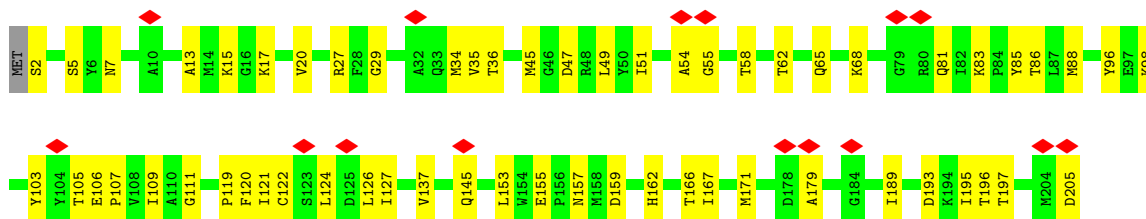




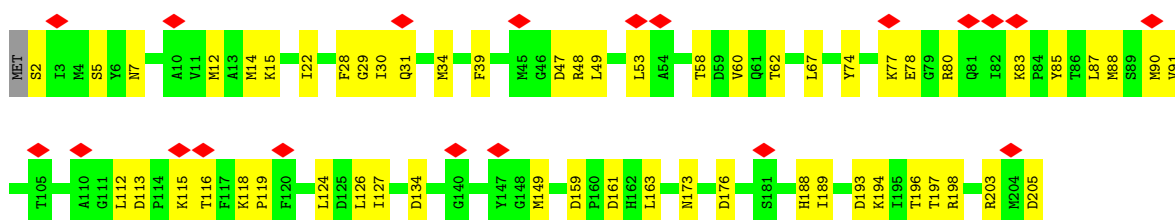
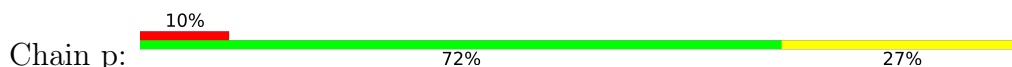
- Molecule 15: Proteasome subunit beta type-7



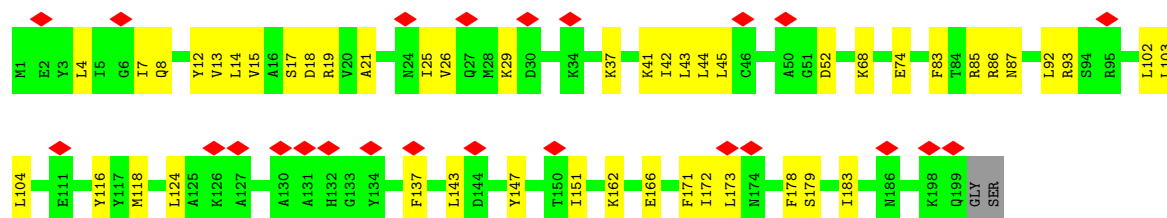
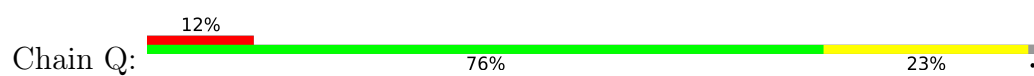
- Molecule 16: Proteasome subunit beta type-3



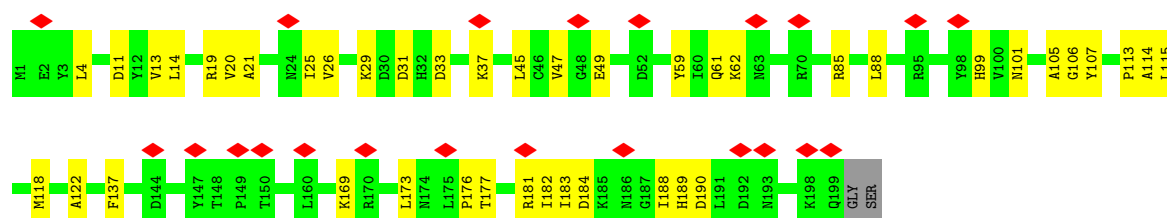
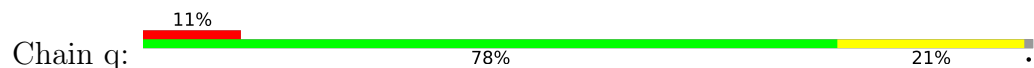
- Molecule 16: Proteasome subunit beta type-3



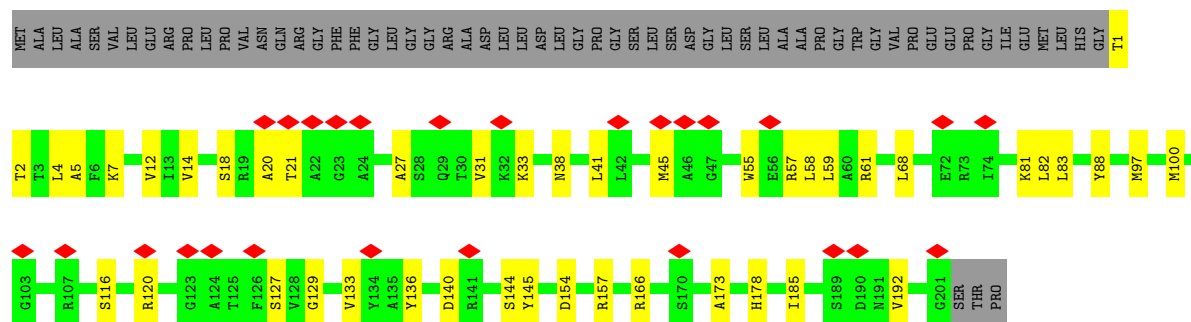
- Molecule 17: Proteasome subunit beta type-2



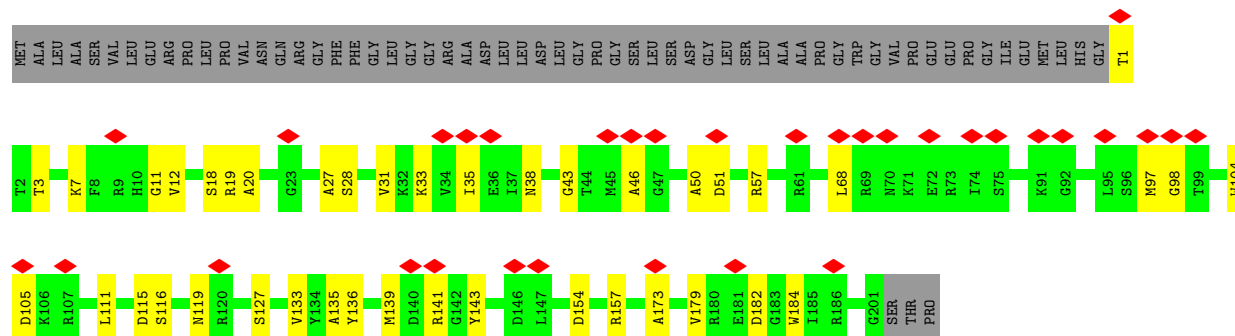
• Molecule 17: Proteasome subunit beta type-2



• Molecule 18: Proteasome subunit beta type-5

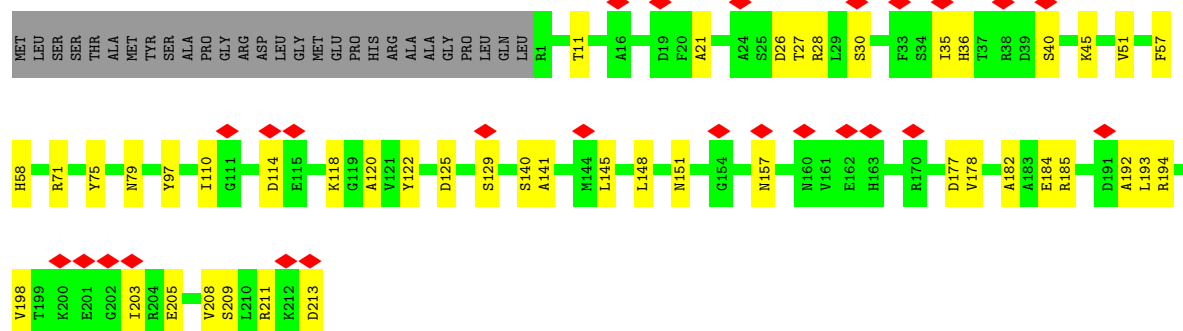


• Molecule 18: Proteasome subunit beta type-5



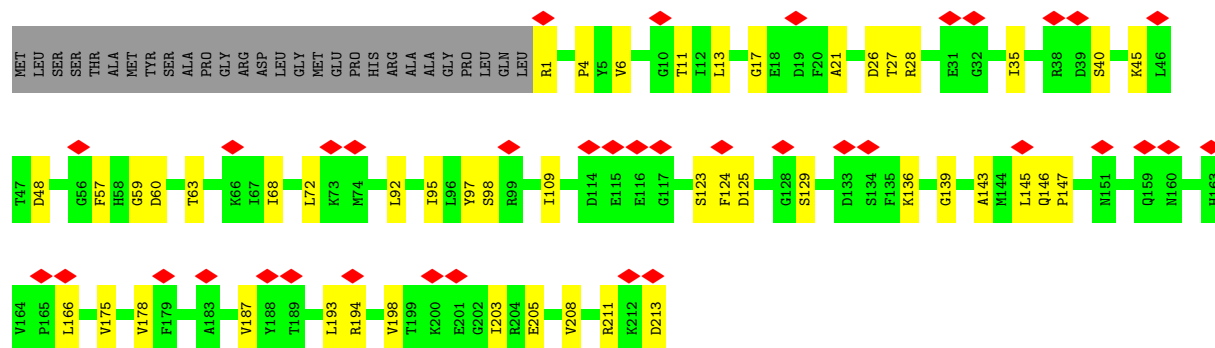
• Molecule 19: Proteasome subunit beta type-1

Chain S: 



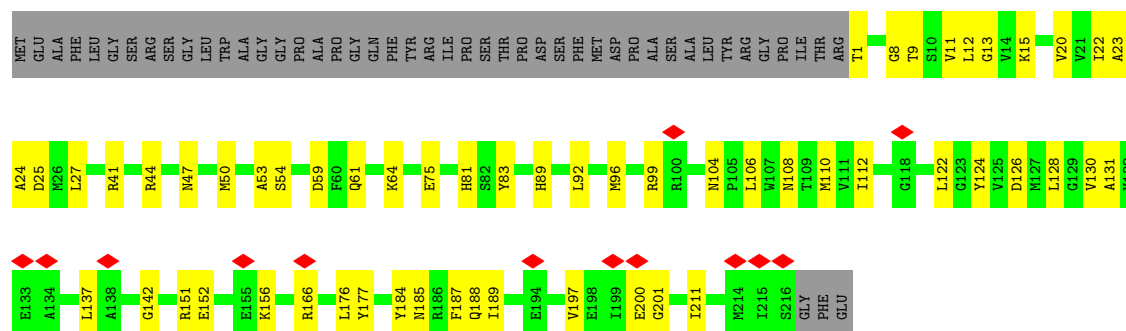
• Molecule 19: Proteasome subunit beta type-1

Chain s: 



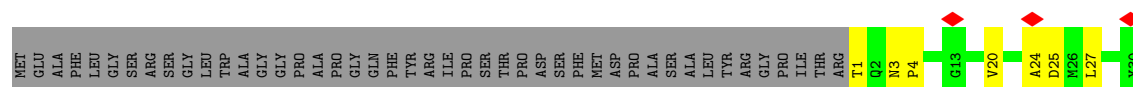
• Molecule 20: Proteasome subunit beta type-4

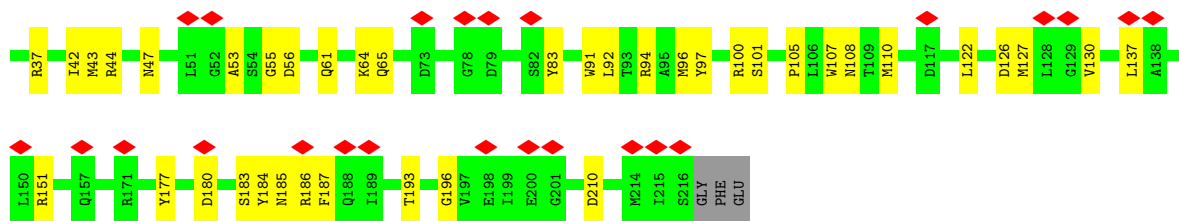
Chain T: 



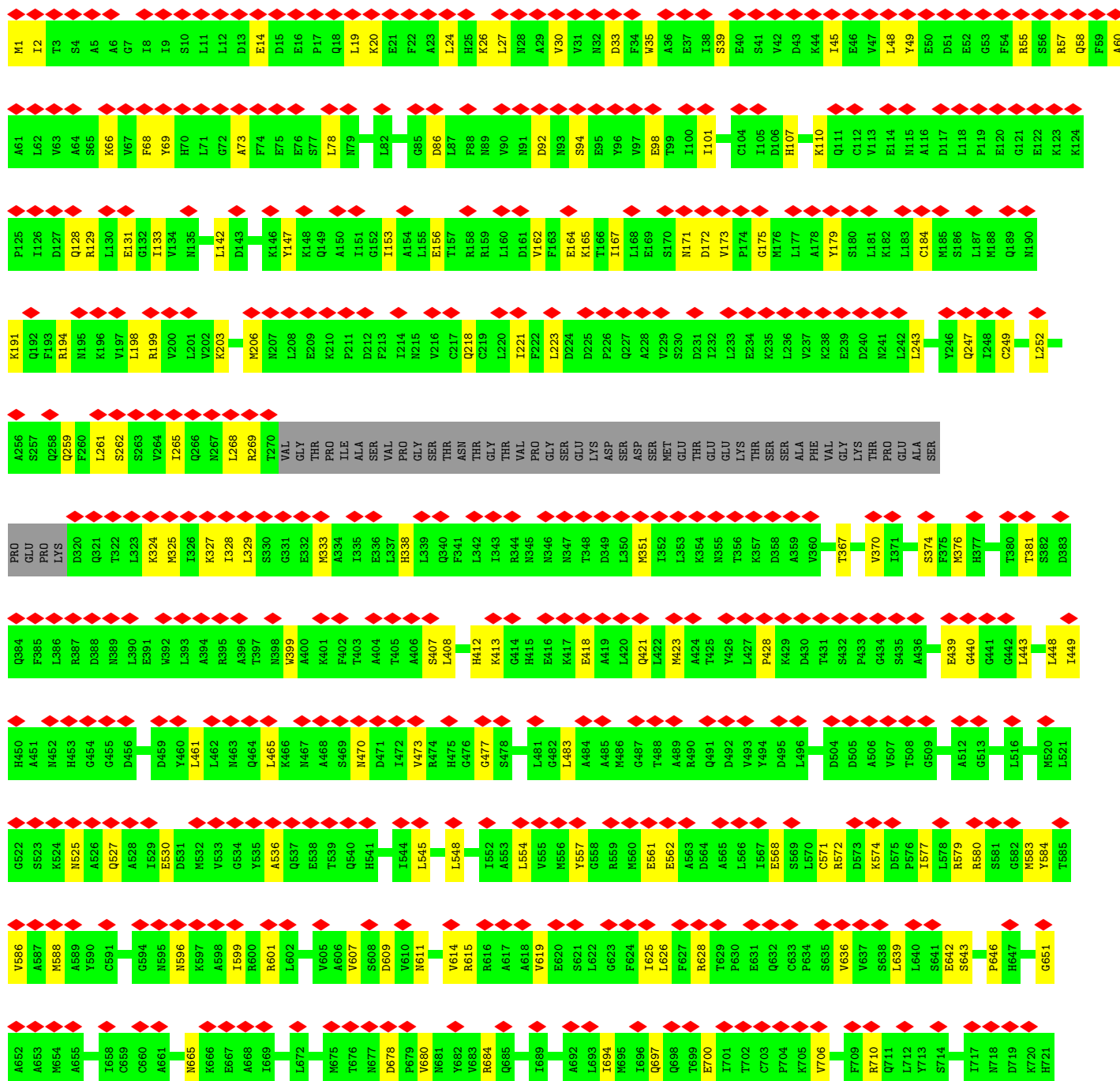
• Molecule 20: Proteasome subunit beta type-4

Chain t: 

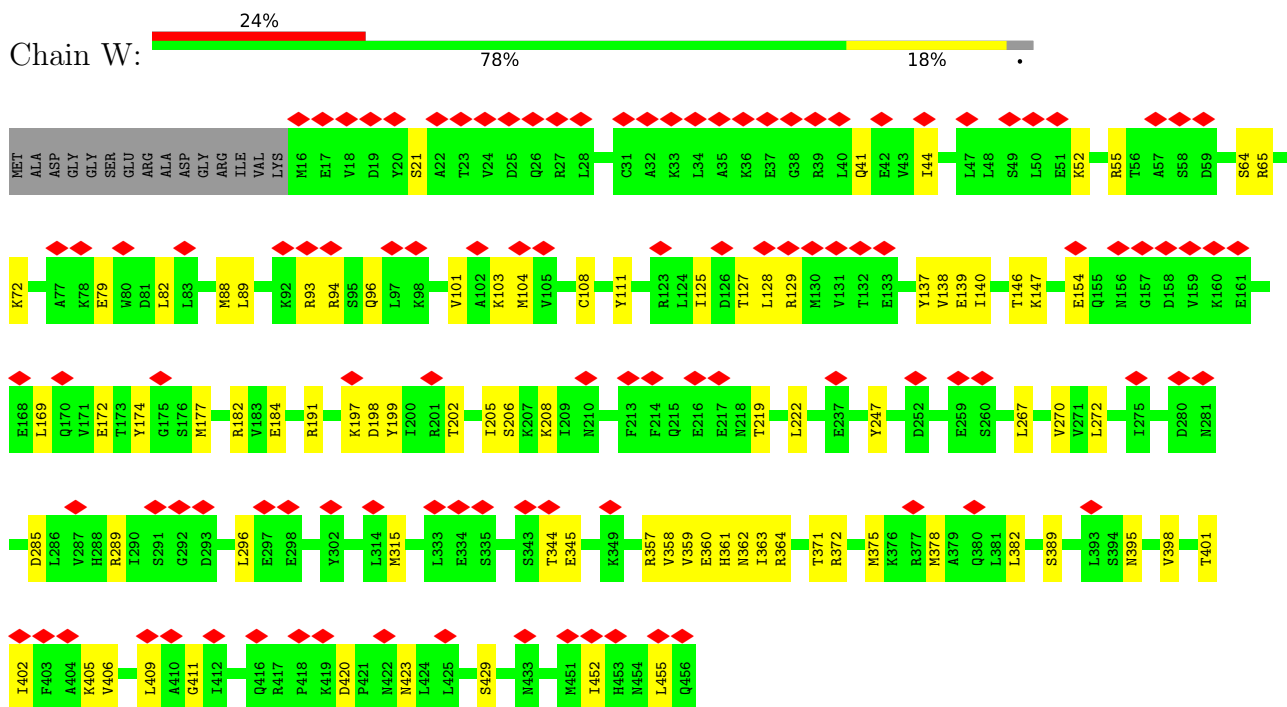




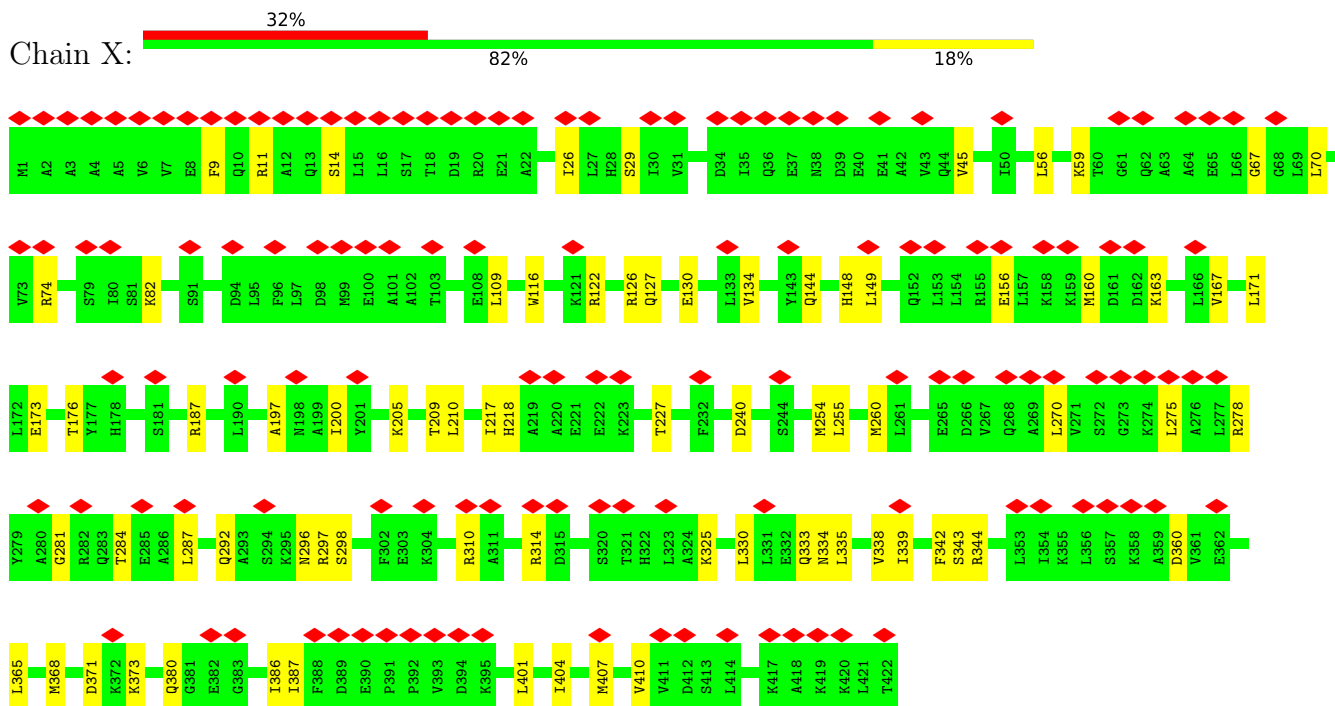
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



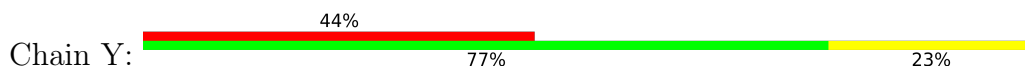
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

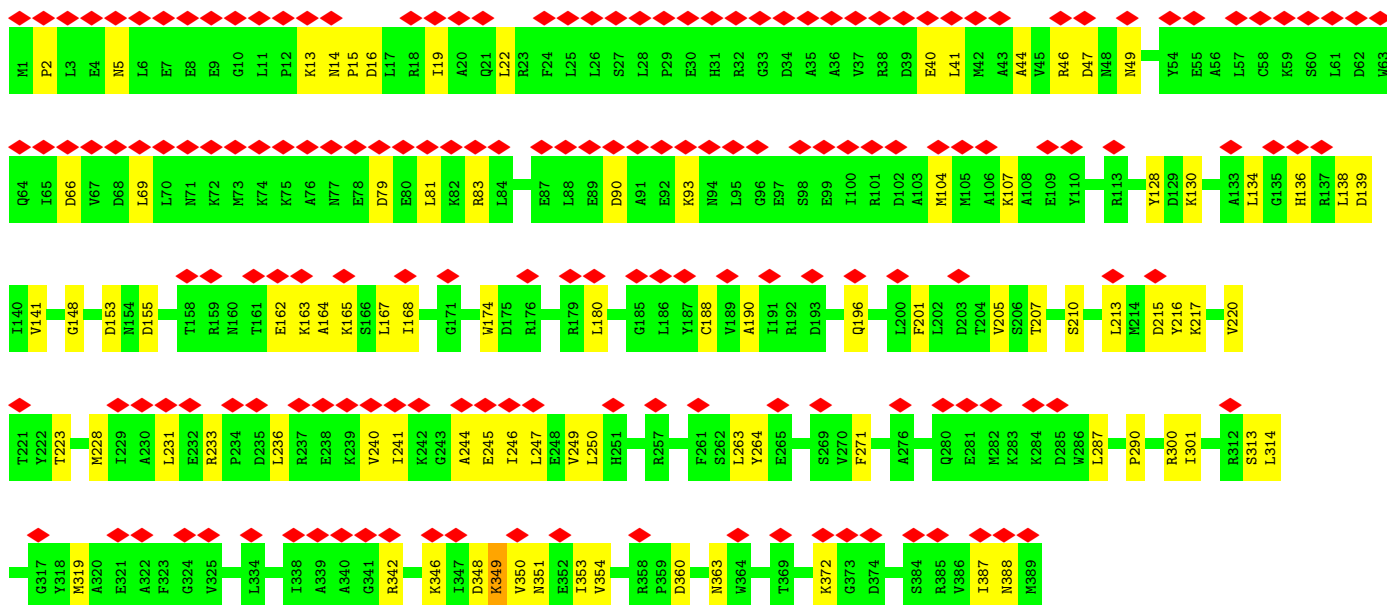


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



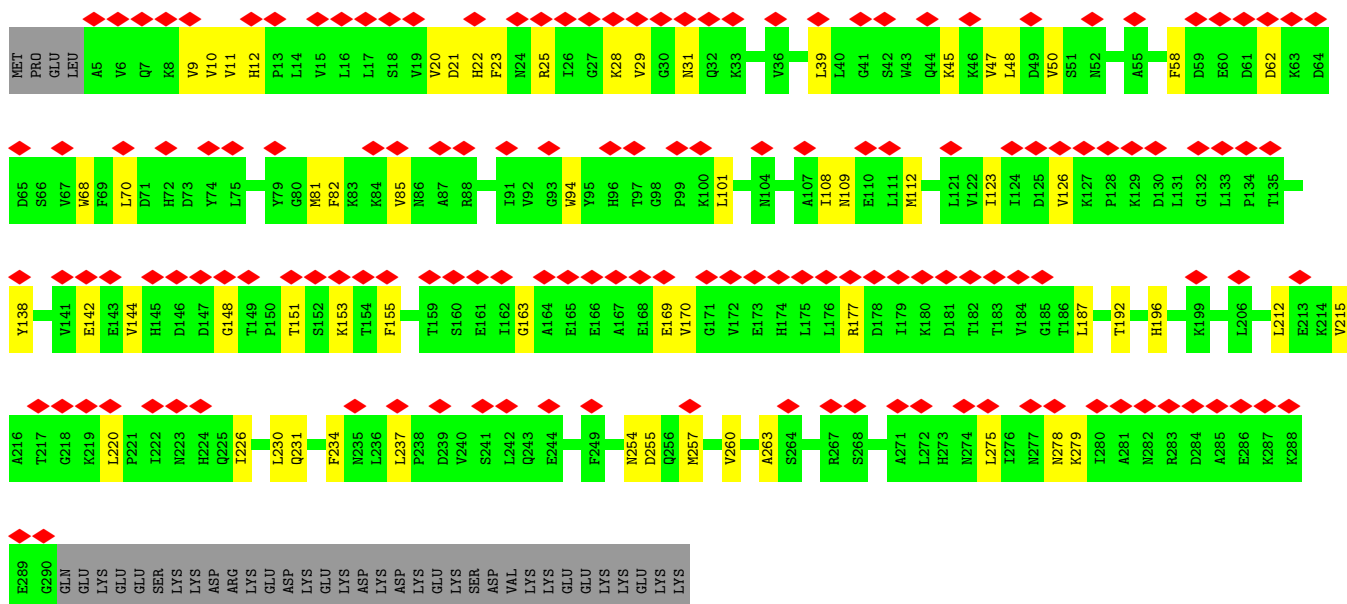
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6





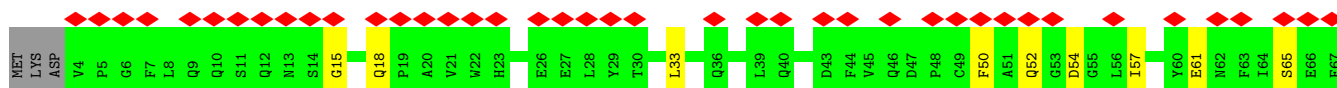
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

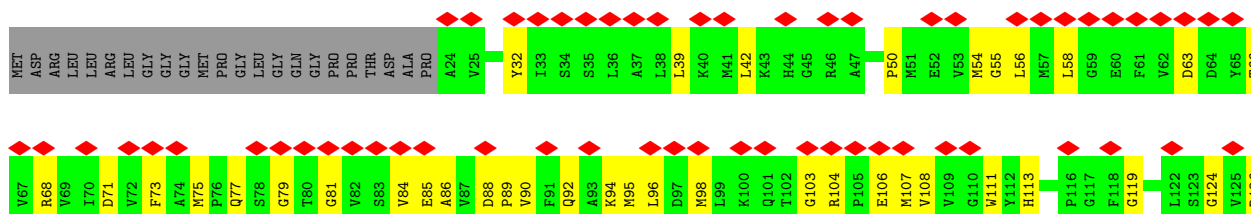
Chain Z:

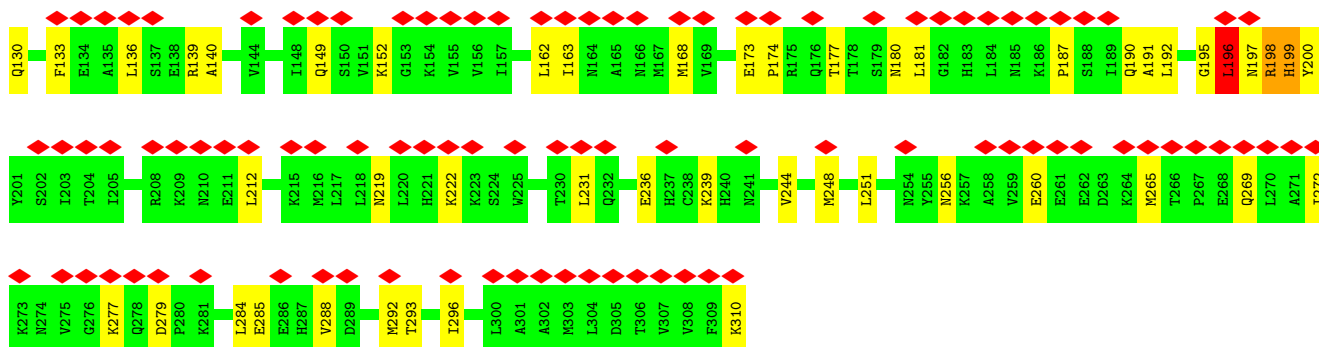


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

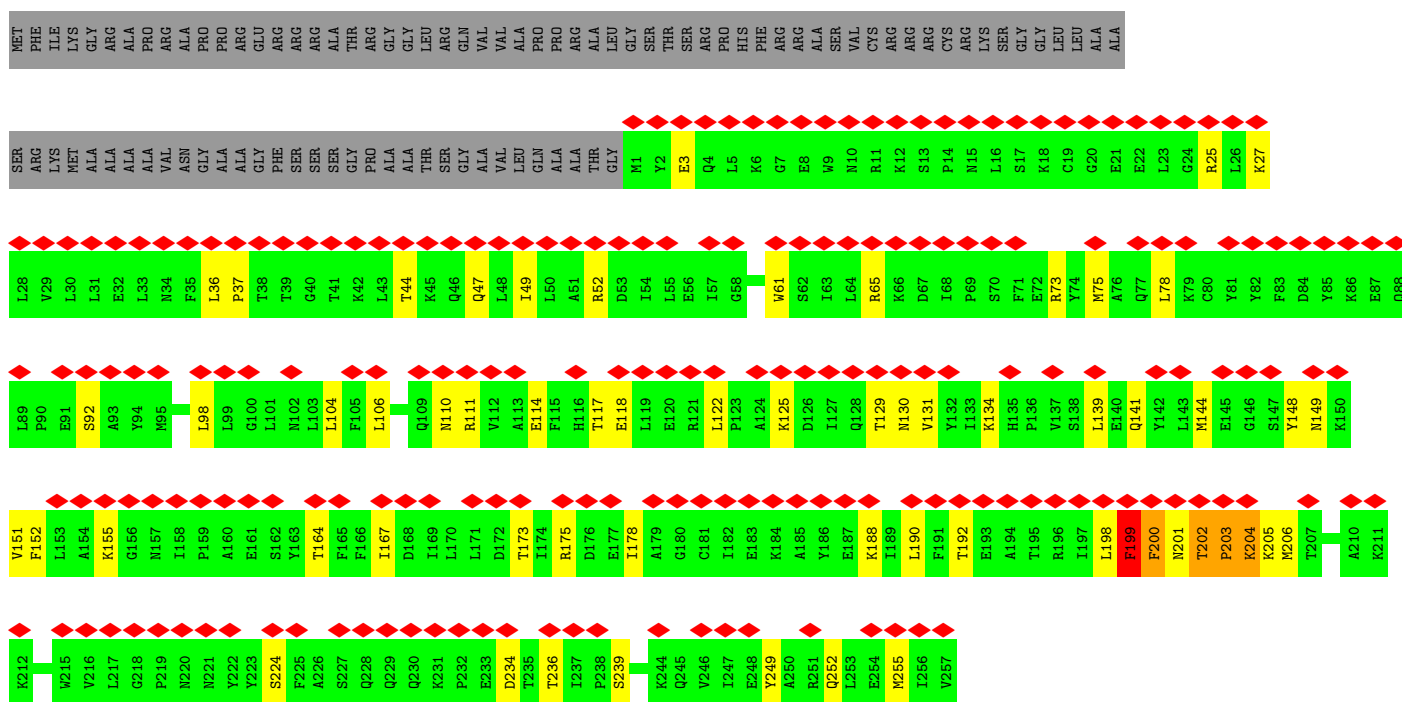
Chain a:



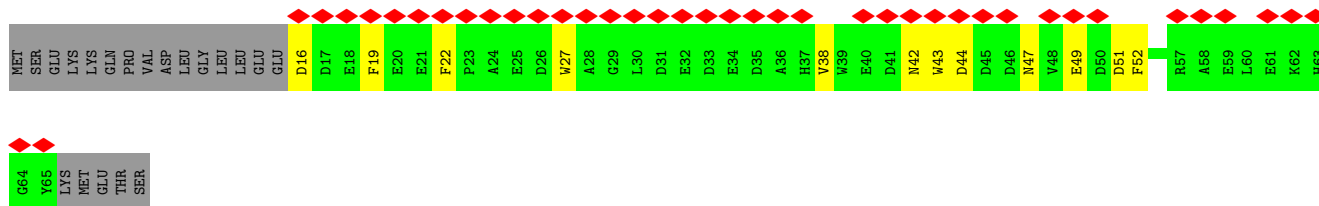




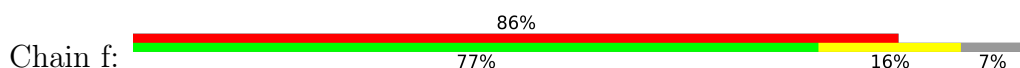
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1



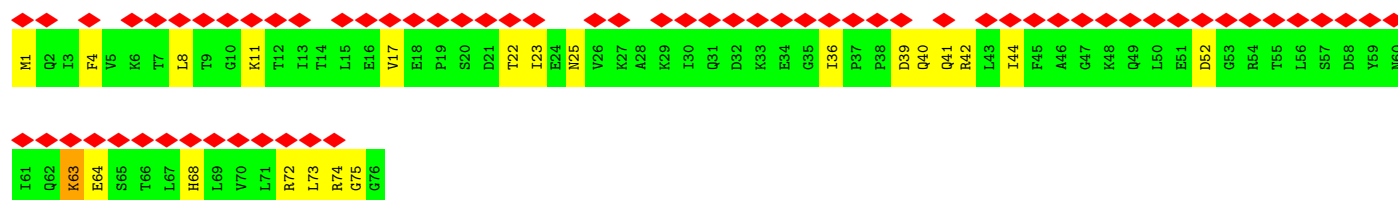
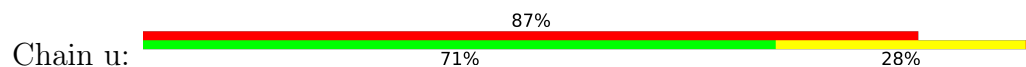
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



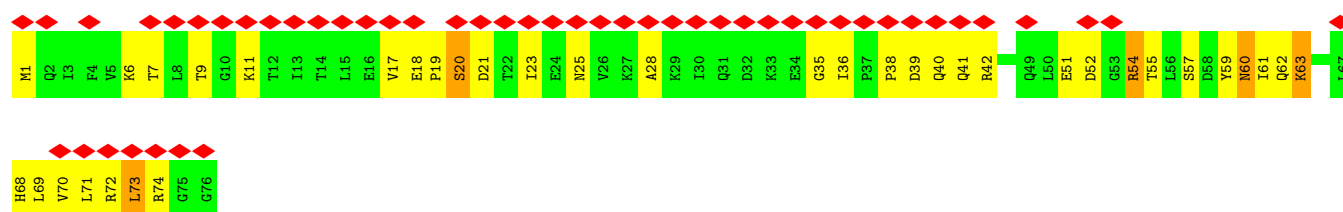
L787	F727	I666	V606	S546	L485	G425	V365	L305	P241	R181	F121	E61	MET
M788	A728	G667	L607	E647	G486	L426	D366	E306	E242	E182	A122	R62	GLU
S789	M729	A668	K608	T648	L487	T427	S367	L307	P243	P183	A123	L63	GLY
Q790	G730	E669	V609	E649	A488	Q428	A368	S308	E244	L184	D124	G64	GLY
V791	M731	M670	Q610	E509	A489	I429	R369	E309	N245	L185	I125	E65	ARG
A792	V732	A671	Q611	K651	A490	D430	M370	D310	S246	T186	I126	K66	ASP
V793	G733	L672	L612	D552	G491	K431	N371	V311	A247	L187	S127	D67	LYS
A794	S734	R673	L613	T653	S492	Y432	L372	E312	L248	V188	L128	T68	ALA
L796	G735	T674	H614	Y554	N493	L433	A373	E313	L249	K189	L129	S69	PRO
L797	T736	F675	I615	A555	R494	Y434	S374	E314	R250	E190	A130	T69	VAL
L798	N737	G676	C616	R556	E495	S435	S375	E315	C251	I191	M131	S71	GLN
V799	N738	H677	S617	W557	D496	S436	F376	D316	C252	V192	T132	R72	GLN
L800	A739	L678	E618	P559	V497	E437	V377	D317	L253	F193	M133	F73	SER
V801	R740	L679	H619	P559	L498	E437	V377	D317	A252	Y194	S134	A74	PRO
S802	L741	R680	F620	G561	T499	D438	N378	T318	K257	H195	G135	L75	ALA
F803	A743	G681	D621	L562	L500	Y439	G379	E319	K258	M196	E136	E76	ALA
L804	M744	G683	LYS	L563	L501	K441	F380	I320	P262	A197	R137	E77	PRO
D805	L745	L564	GLU	G563	L502	S442	V381	M321	P263	H198	E137	L78	GLY
V806	P746	N665	LYS	N665	P503	G443	A383	N323	E264	H199	C139	R79	THR
R807	R746	H666	GLU	H566	V504	A444	F385	V324	A265	A200	L140	R80	ASP
N808	Q747	G668	GLU	G568	G506	L446	G386	L326	L266	E201	K141	R80	GLU
I809	L748	K569	LYS	K569	D507	A447	Q387	N327	R267	H202	Y142	Q81	LYS
I810	A749	G570	LYS	G570	S508	C448	T392	N327	L268	E203	R143	R83	SER
L811	Q750	E571	LYS	E571	K509	G449	D389	N329	L270	C205	L144	S84	LYS
G812	Y751	A572	GLU	A572	S510	I450	L390	F330	M271	D206	G146	S85	GLU
K813	H752	I573	LYS	I573	S511	V451	L391	F330	L272	L207	S147	T86	ARG
A814	A753	E574	ASP	E574	M512	G452	T392	A332	L273	L207	Q148	T87	ASP
H815	K754	A575	LYS	A575	E513	S453	D389	A332	Q148	L208	E148	S88	ALA
Y816	D755	I576	ASP	I576	V514	G454	K401	A334	E149	M209	E149	H89	GLY
V817	P756	L577	LYS	L577	A515	V455	N402	A334	E150	E210	L151	T90	ASP
L818	N757	A578	GLU	A578	A516	R456	K403	R335	E276	I211	L151	S91	LYS
Y819	L759	A579	LYS	A579	V517	M457	K403	E336	L277	E212	A152	V92	ASP
G820	M760	L580	PRO	L580	T518	E458	H405	D338	E279	Q213	S153	P93	LYS
L821	V762	E581	ALA	E581	A519	C459	H405	I339	E281	V214	W154	K94	GLU
A824	R763	V582	A644	V582	L520	D460	H405	M340	D280	D215	G155	P95	Q43
S825	L764	S583	D645	S583	A521	P461	G406	K340	K286	R100	G156	L96	E44
Q826	A765	E584	M646	E584	C522	A462	G407	E341	D287	P101	E157	K97	L45
R827	Q766	E585	G847	E585	C523	L463	K401	P342	F282	H102	E157	E98	S46
Q828	L767	E586	H649	E586	M524	L464	N402	P342	T283	Y103	Y158	R97	E47
V829	G767	F587	Q650	F587	I525	L465	K403	K343	E284	G104	V159	L99	E48
L830	T768	R588	Q651	R588	A526	L466	H405	V344	C285	D220	R160	P100	D49
V831	T769	S589	V652	S589	V627	S467	G407	P344	K286	I221	H161	P101	K50
T832	H770	F590	A653	F590	G528	D468	M407	D346	D287	D222	H161	H102	Q51
F833	L771	A591	E654	A591	C530	Y469	L408	D347	V288	E223	A163	Y103	L52
S834	G772	E592	L655	E592	M531	V470	S409	I348	V290	M224	G164	G104	Q53
D834	K773	T593	G532	T593	N631	L471	S409	Y349	Q291	A225	E165	K105	D54
E835	S774	L594	D533	L594	G532	H471	A411	K350	Q291	Y226	V166	L106	E55
S836	T775	V595	D533	V595	H472	L472	A411	T351	K292	A227	A167	K107	L56
L837	L776	D596	L659	D596	A412	M473	A412	H352	Q293	K168	E167	E108	E57
R838	T777	V597	T541	V597	S413	S474	S413	L353	M294	E169	E169	M58	S57
V839	L778	E599	I642	E599	L414	M475	L414	E354	A295	W170	E170	Y109	L59
L840	R779	A599	I643	A599	G415	M476	G415	N355	F296	Q171	Q171	E111	L59
P841	C779	M599	I644	M599	M416	M477	M416	R357	M297	E172	E172	N112	E111
V842	T780	Q640	Q540	Q640	L417	L478	I417	R357	L298	L173	L173	M113	M112
S843	E720	T541	T541	T541	L418	L479	L418	F358	T234	D174	D174	M114	M113
V844	E721	I642	I642	I642	L419	G480	L419	G359	R300	D175	D175	P115	P115
R845	S722	M543	E544	M543	G480	A481	G481	H301	C236	E176	E176	G116	G116
Q846	Y723	E544	E544	E544	A481	M478	M478	G302	V237	E177	E177	N117	N117
V846	N724	E544	E544	E544	A481	M478	M478	G302	V237	E177	E177	N117	N117
S846	E725	E544	E544	E544	A481	M478	M478	G302	V237	E177	E177	N117	N117
V846	Q786	N605	N605	N605	K545	F483	F483	G363	V239	V179	Q180	K119	K119



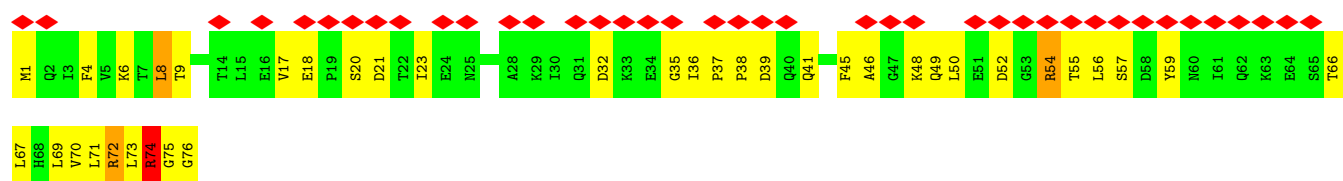
• Molecule 33: Ubiquitin



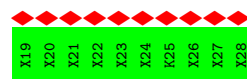
• Molecule 33: Ubiquitin



• 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	5500	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	0.012	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0044	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/3148	0.55	0/4250
2	B	0.19	0/3061	0.53	0/4129
3	C	0.20	0/2902	0.50	0/3904
4	D	0.23	0/3089	0.52	0/4168
5	E	0.19	0/3145	0.47	0/4233
6	F	0.21	0/3292	0.46	0/4435
7	G	0.19	0/1923	0.46	0/2601
7	g	0.18	0/1914	0.43	0/2590
8	H	0.16	0/1844	0.44	0/2499
8	h	0.16	0/1844	0.43	0/2497
9	I	0.16	0/1991	0.43	0/2685
9	i	0.15	0/1985	0.40	0/2677
10	J	0.18	0/1906	0.42	0/2573
10	j	0.15	0/1887	0.42	0/2549
11	K	0.18	0/1804	0.42	0/2436
11	k	0.17	0/1809	0.47	0/2444
12	L	0.15	0/1901	0.37	0/2570
12	l	0.15	0/1896	0.40	0/2565
13	M	0.16	0/1911	0.42	0/2573
13	m	0.13	0/1916	0.36	0/2580
14	N	0.15	0/1540	0.38	0/2085
14	n	0.16	0/1536	0.39	0/2080
15	O	0.16	0/1676	0.41	1/2271 (0.0%)
15	o	0.14	0/1686	0.44	0/2282
16	P	0.19	0/1616	0.53	2/2180 (0.1%)
16	p	0.16	0/1620	0.44	0/2184
17	Q	0.14	0/1621	0.36	0/2194
17	q	0.14	0/1621	0.37	0/2194
18	R	0.15	0/1590	0.41	0/2147
18	r	0.15	0/1590	0.41	0/2147
19	S	0.15	0/1671	0.39	0/2252
19	s	0.16	0/1684	0.43	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.39	0/2323
20	t	0.15	0/1720	0.41	0/2328
21	U	0.18	0/6488	0.49	0/8782
22	V	0.16	0/3681	0.42	0/4969
23	W	0.16	0/3644	0.44	0/4901
24	X	0.17	0/3381	0.47	0/4558
25	Y	0.19	0/3261	0.50	0/4393
26	Z	0.19	0/2324	0.55	0/3150
27	a	0.18	0/3053	0.51	0/4133
28	b	0.20	0/1478	0.52	0/2001
29	c	0.26	0/2302	0.58	0/3110
30	d	0.25	0/2162	0.58	2/2919 (0.1%)
31	e	0.20	0/437	0.60	1/595 (0.2%)
32	f	0.20	0/6640	0.51	1/8988 (0.0%)
33	u	0.27	0/607	0.66	2/816 (0.2%)
33	x	0.60	0/607	1.01	0/816
33	y	0.51	0/607	0.98	0/816
34	v	0.03	0/8	0.06	0/8
All	All	0.19	0/108735	0.48	9/146848 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	115	PRO	CA-N-CD	-9.51	98.69	112.00
33	u	75	GLY	CA-C-N	-8.36	106.64	121.70
33	u	75	GLY	C-N-CA	-8.36	106.64	121.70
31	e	38	VAL	N-CA-C	-6.17	106.73	112.83
30	d	204	LYS	N-CA-C	-5.99	105.63	113.17

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	3096	0	3139	84	0
2	B	3018	0	3081	78	0
3	C	2864	0	2971	63	0
4	D	3039	0	3075	77	0
5	E	3097	0	3173	83	0
6	F	3251	0	3318	87	0
7	G	1889	0	1885	32	0
7	g	1880	0	1875	39	0
8	H	1805	0	1784	31	0
8	h	1805	0	1798	36	0
9	I	1958	0	1960	31	0
9	i	1955	0	1955	25	0
10	J	1880	0	1892	41	0
10	j	1861	0	1865	34	0
11	K	1777	0	1762	39	0
11	k	1782	0	1766	32	0
12	L	1866	0	1852	35	0
12	l	1861	0	1839	28	0
13	M	1876	0	1861	40	0
13	m	1881	0	1868	34	0
14	N	1514	0	1487	21	0
14	n	1510	0	1483	21	0
15	O	1649	0	1659	28	0
15	o	1659	0	1681	27	0
16	P	1587	0	1598	39	0
16	p	1591	0	1609	41	0
17	Q	1588	0	1584	35	0
17	q	1588	0	1584	31	0
18	R	1559	0	1523	29	0
18	r	1559	0	1523	31	0
19	S	1641	0	1639	36	0
19	s	1654	0	1656	36	0
20	T	1683	0	1662	39	0
20	t	1687	0	1666	32	0
21	U	6373	0	6411	129	0
22	V	3612	0	3682	69	0
23	W	3596	0	3713	50	0
24	X	3335	0	3435	57	0
25	Y	3202	0	3204	55	0
26	Z	2281	0	2312	51	0
27	a	2995	0	3012	52	0
28	b	1458	0	1505	25	0
29	c	2260	0	2276	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	45	0
31	e	425	0	328	14	0
32	f	6529	0	6541	90	0
33	u	601	0	627	31	0
33	x	601	0	627	90	0
33	y	601	0	629	114	0
34	v	53	0	21	0	0
35	A	31	0	12	3	0
35	B	31	0	12	2	0
35	D	31	0	12	2	0
35	E	31	0	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	3	0
38	c	1	0	0	0	0
All	All	107132	0	107614	2026	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 9.

The worst 5 of 2026 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)
33:x:63:LYS:NZ	33:y:76:GLY:C	1.67	1.53
33:u:4:PHE:CE2	33:u:64:GLU:HG2	1.58	1.37
33:x:60:ASN:HA	33:y:8:LEU:CD1	1.54	1.37
33:x:60:ASN:HB3	33:y:8:LEU:CB	1.56	1.34
33:x:60:ASN:CA	33:y:8:LEU:HD12	1.55	1.34

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	392/433 (90%)	347 (88%)	43 (11%)	2 (0%)	24	63
2	B	382/440 (87%)	346 (91%)	36 (9%)	0	100	100
3	C	359/398 (90%)	333 (93%)	24 (7%)	2 (1%)	21	59
4	D	378/418 (90%)	338 (89%)	38 (10%)	2 (0%)	24	63
5	E	387/403 (96%)	351 (91%)	35 (9%)	1 (0%)	36	72
6	F	413/439 (94%)	376 (91%)	34 (8%)	3 (1%)	18	56
7	G	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	67
7	g	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	30	67
8	H	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	249/261 (95%)	241 (97%)	8 (3%)	0	100	100
9	i	248/261 (95%)	244 (98%)	4 (2%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	232/241 (96%)	218 (94%)	12 (5%)	2 (1%)	14	50
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	236/263 (90%)	231 (98%)	5 (2%)	0	100	100
12	l	236/263 (90%)	226 (96%)	10 (4%)	0	100	100
13	M	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
13	m	238/255 (93%)	232 (98%)	6 (2%)	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%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	R	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	200 (95%)	11 (5%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	201 (94%)	13 (6%)	0	100	100
21	U	812/953 (85%)	756 (93%)	56 (7%)	0	100	100
22	V	442/534 (83%)	428 (97%)	13 (3%)	1 (0%)	43	77
23	W	439/456 (96%)	430 (98%)	9 (2%)	0	100	100
24	X	420/422 (100%)	399 (95%)	21 (5%)	0	100	100
25	Y	387/389 (100%)	362 (94%)	24 (6%)	1 (0%)	36	72
26	Z	284/324 (88%)	254 (89%)	30 (11%)	0	100	100
27	a	371/376 (99%)	347 (94%)	24 (6%)	0	100	100
28	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
29	c	285/310 (92%)	258 (90%)	25 (9%)	2 (1%)	18	56
30	d	255/350 (73%)	218 (86%)	33 (13%)	4 (2%)	7	37
31	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
32	f	840/908 (92%)	804 (96%)	35 (4%)	1 (0%)	48	83
33	u	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
33	x	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	2	17
33	y	74/76 (97%)	57 (77%)	15 (20%)	2 (3%)	4	25
34	v	1/10 (10%)	0	1 (100%)	0	100	100
All	All	13515/15114 (89%)	12708 (94%)	779 (6%)	28 (0%)	44	77

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	134	LEU
4	D	126	PRO
30	d	199	PHE

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Mol	Chain	Res	Type
30	d	200	PHE
30	d	203	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	337/372 (91%)	335 (99%)	2 (1%)	78	82
2	B	339/385 (88%)	338 (100%)	1 (0%)	86	85
3	C	314/346 (91%)	311 (99%)	3 (1%)	68	78
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	75
5	E	341/353 (97%)	340 (100%)	1 (0%)	86	85
6	F	357/379 (94%)	354 (99%)	3 (1%)	73	80
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	83
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	76
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
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%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	696 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	86
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	82
26	Z	257/295 (87%)	257 (100%)	0	100	100
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	66
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	85
33	u	68/68 (100%)	67 (98%)	1 (2%)	57	72
33	x	68/68 (100%)	59 (87%)	9 (13%)	4	15
33	y	68/68 (100%)	63 (93%)	5 (7%)	13	33
34	v	1/1 (100%)	1 (100%)	0	100	100
All	All	11573/12819 (90%)	11530 (100%)	43 (0%)	81	84

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	u	63	LYS
33	x	72	ARG
33	x	20	SER
33	x	60	ASN
33	x	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
21	U	267	ASN
15	o	153	ASN
23	W	53	GLN
15	o	116	HIS
20	t	65	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ATP	A	501	36	29,33,33	0.31	0	44,52,52	0.50	1 (2%)
37	ADP	C	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.05	9 (21%)
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.49	1 (2%)
35	ATP	E	401	36	29,33,33	0.29	0	44,52,52	0.45	1 (2%)
37	ADP	F	501	36	27,29,29	1.36	4 (14%)	42,45,45	1.94	10 (23%)
35	ATP	B	501	36	29,33,33	0.29	0	44,52,52	0.45	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
35	ATP	A	501	36	-	2/22/38/38	0/3/3/3
37	ADP	C	501	-	-	2/16/32/32	0/3/3/3
35	ATP	D	501	36	-	4/22/38/38	0/3/3/3
35	ATP	E	401	36	-	2/22/38/38	0/3/3/3
37	ADP	F	501	36	-	6/16/32/32	0/3/3/3
35	ATP	B	501	36	-	5/22/38/38	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)
37	C	501	ADP	C5-C4	4.56	1.47	1.39
37	F	501	ADP	C5-C4	4.54	1.47	1.39
37	F	501	ADP	C5-C6	2.63	1.48	1.41
37	C	501	ADP	C5-C6	2.54	1.48	1.41
37	C	501	ADP	C5-N7	-2.40	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.73	117.97	126.75
37	F	501	ADP	C5-C4-N3	-6.25	118.59	126.75
37	C	501	ADP	N3-C4-N9	5.47	136.10	127.08
37	F	501	ADP	N3-C4-N9	4.86	135.09	127.08
37	C	501	ADP	C2-N3-C4	3.99	121.18	111.75

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

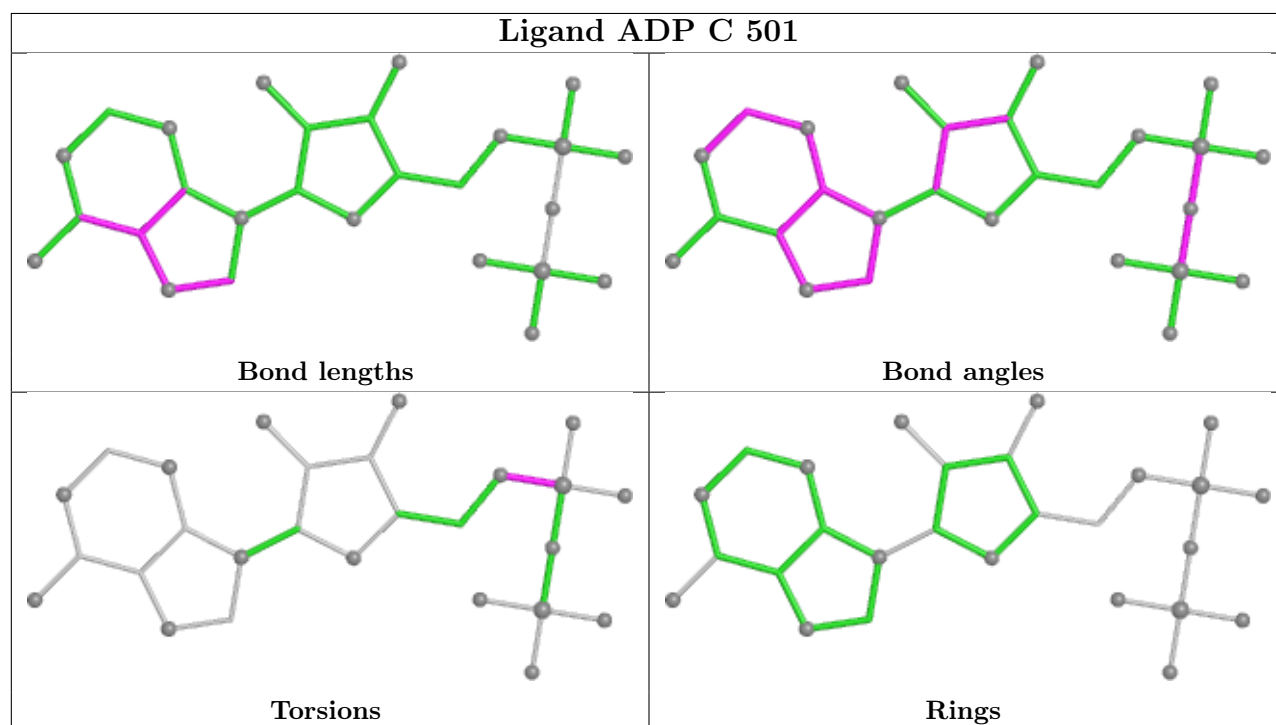
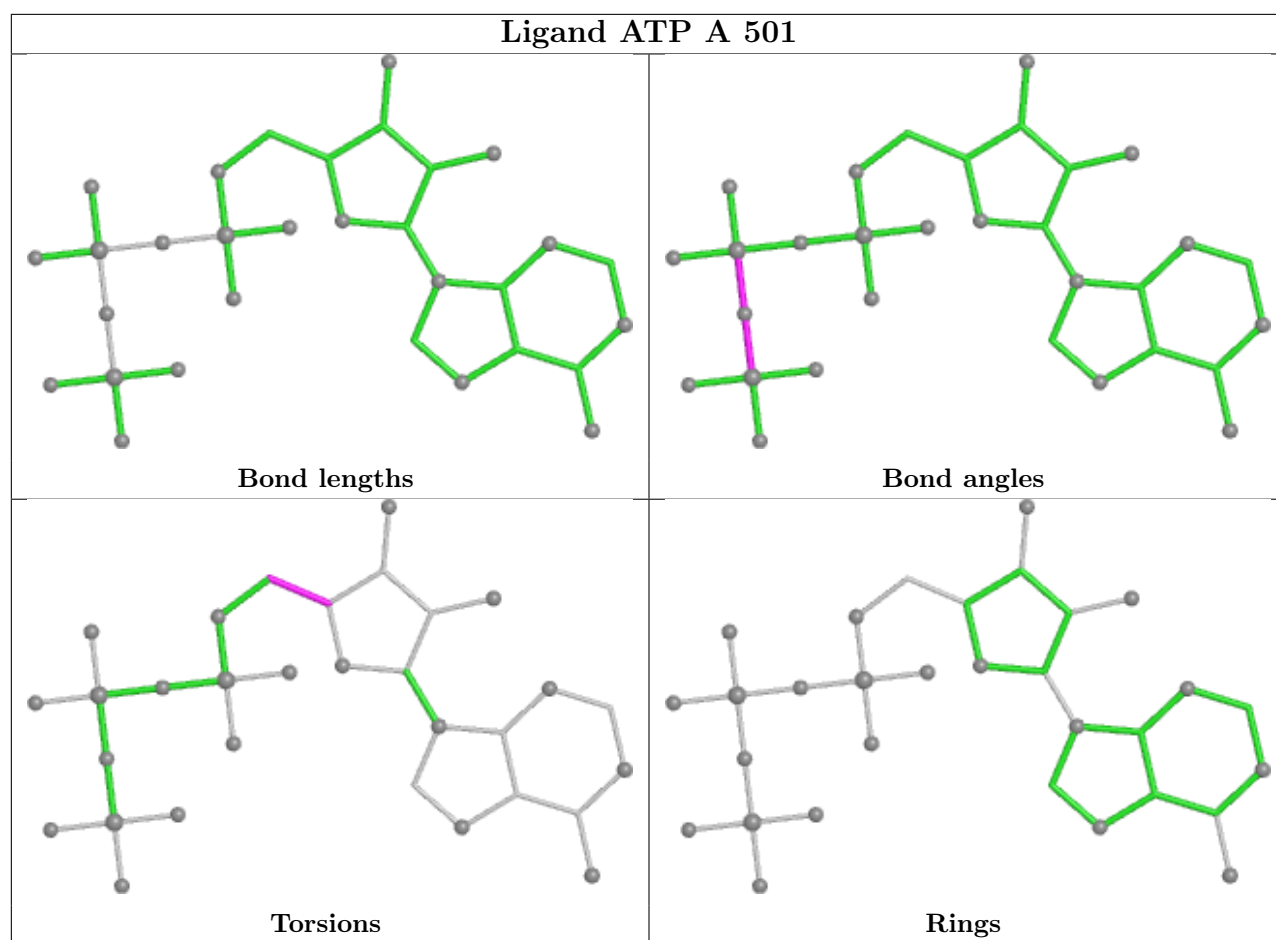
Mol	Chain	Res	Type	Atoms
35	B	501	ATP	PB-O3B-PG-O3G
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	O4'-C4'-C5'-O5'

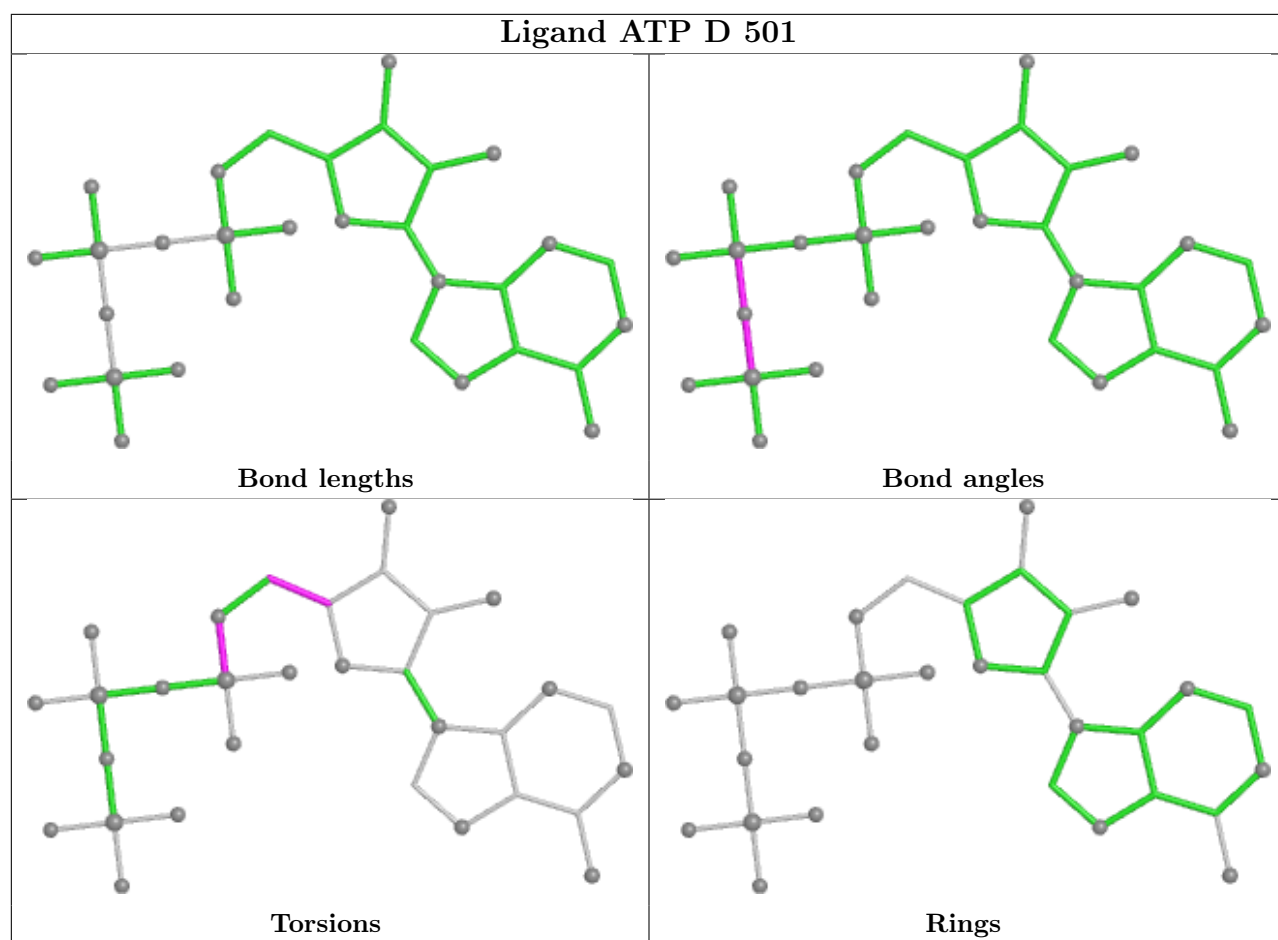
There are no ring outliers.

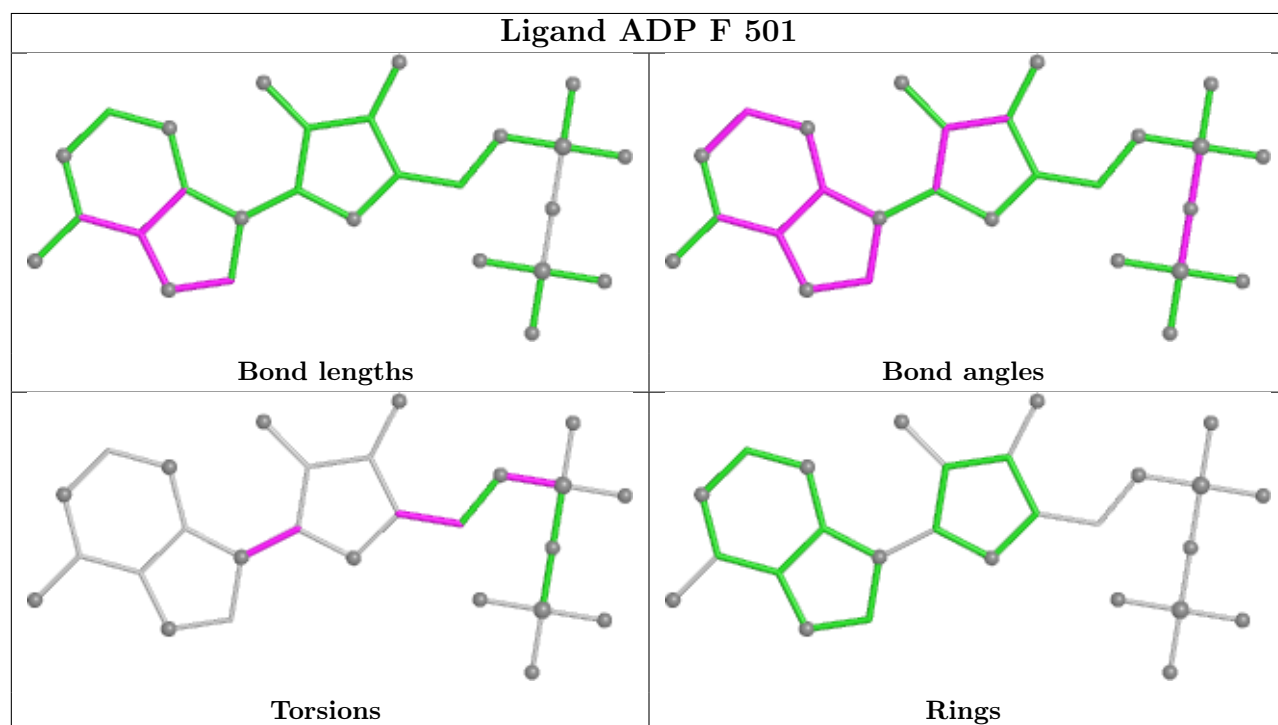
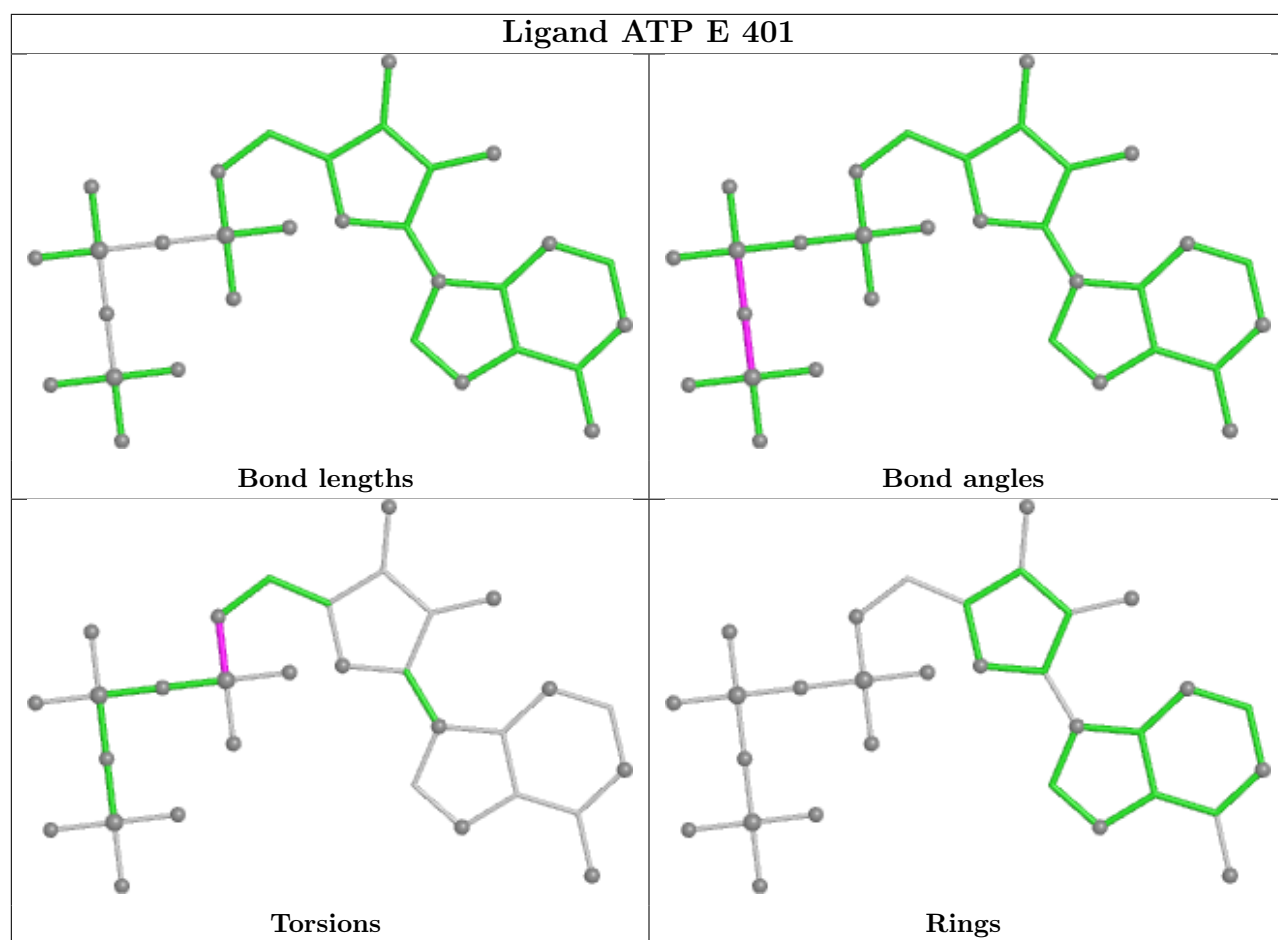
6 monomers are involved in 12 short contacts:

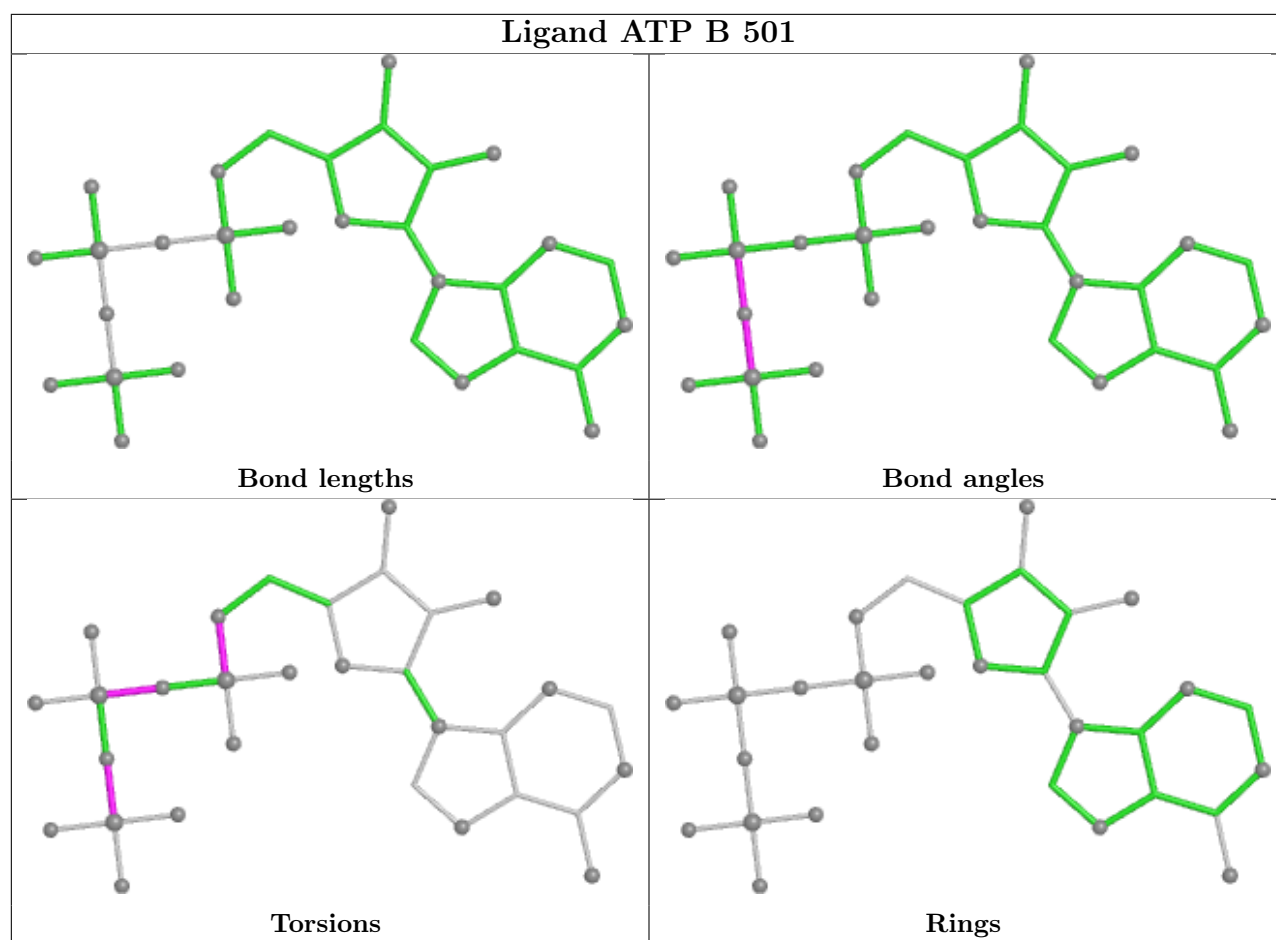
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	3	0
37	C	501	ADP	1	0
35	D	501	ATP	2	0
35	E	401	ATP	1	0
37	F	501	ADP	3	0
35	B	501	ATP	2	0

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.

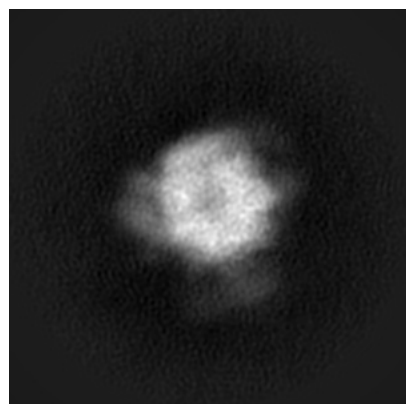
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62065. These allow visual inspection of the internal detail of the map and identification of artifacts.

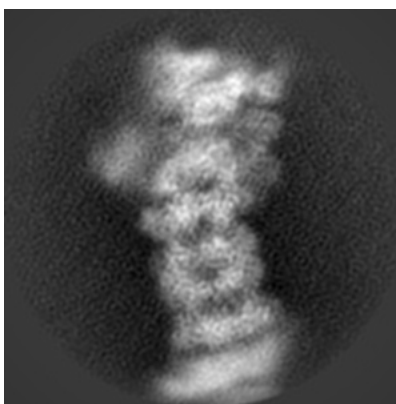
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

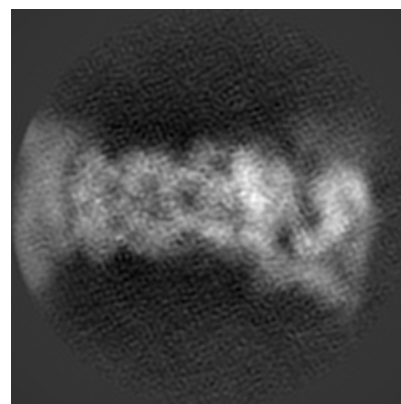
6.1.1 Primary map



X

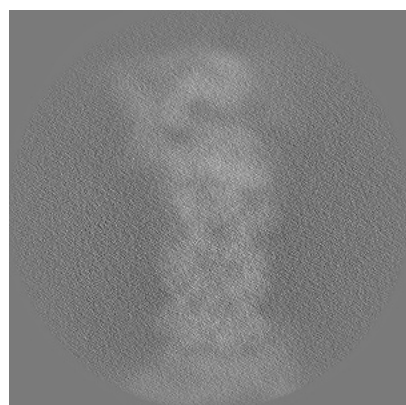


Y

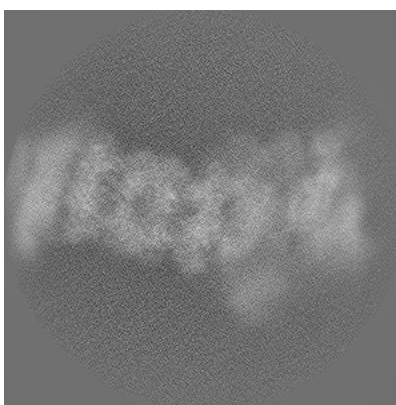


Z

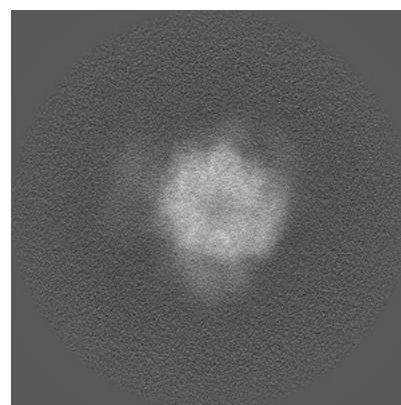
6.1.2 Raw map



X



Y

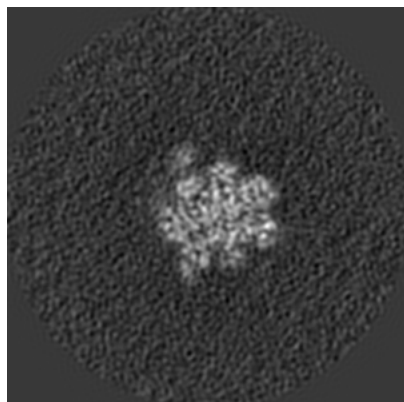


Z

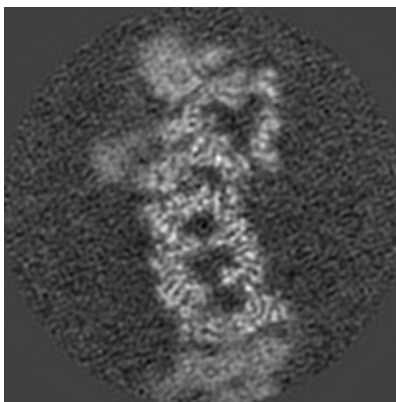
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

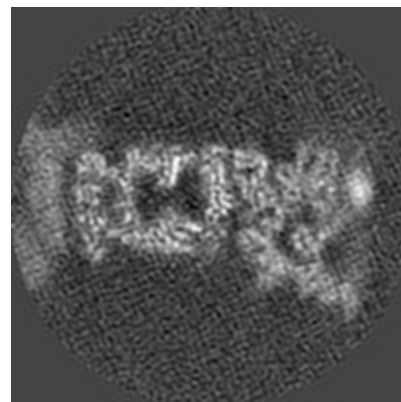
6.2.1 Primary map



X Index: 300

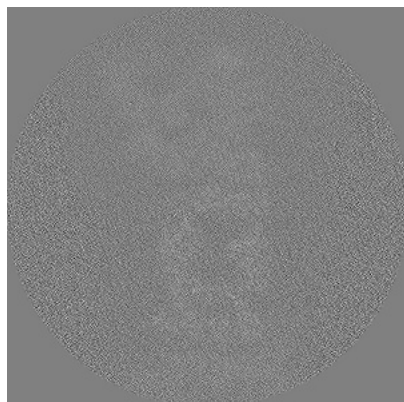


Y Index: 300

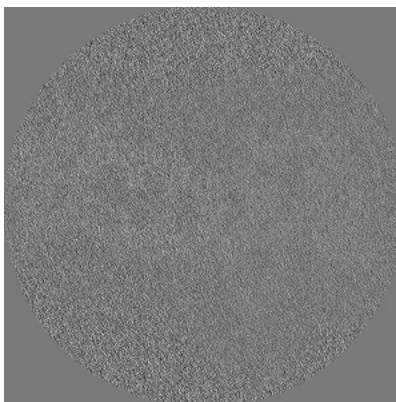


Z Index: 300

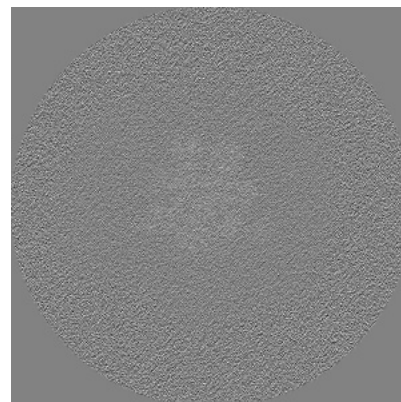
6.2.2 Raw map



X Index: 300



Y Index: 300

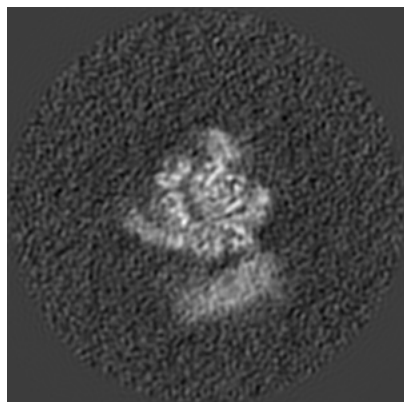


Z Index: 300

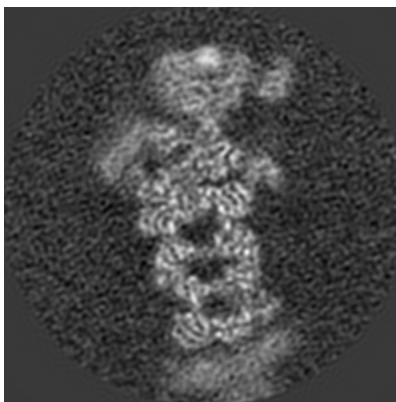
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

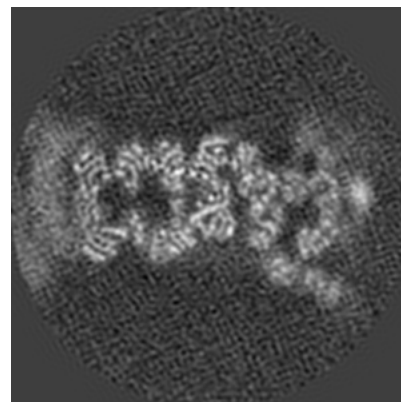
6.3.1 Primary map



X Index: 364

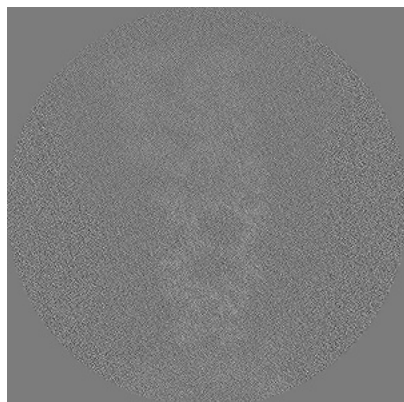


Y Index: 329

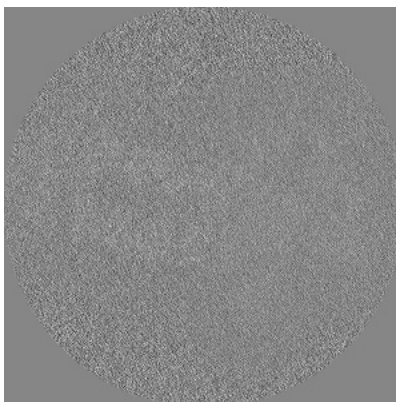


Z Index: 319

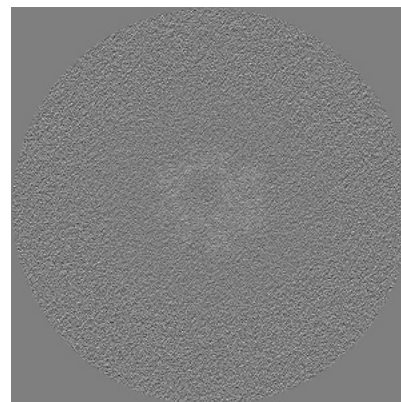
6.3.2 Raw map



X Index: 287



Y Index: 308

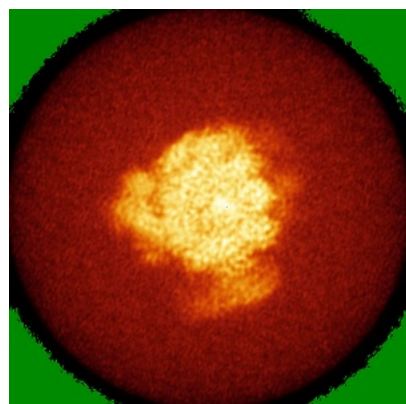


Z Index: 256

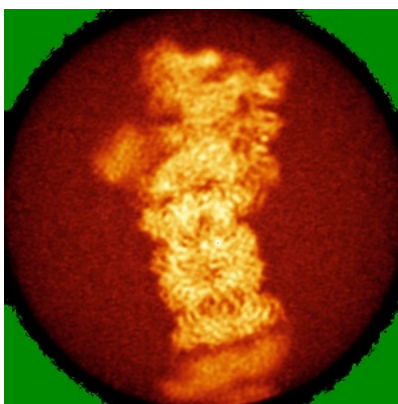
The images above show the largest variance slices of the map in three orthogonal directions.

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

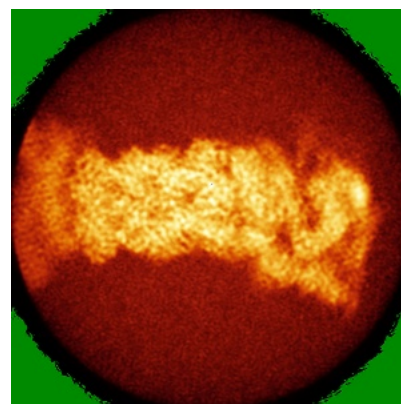
6.4.1 Primary map



X

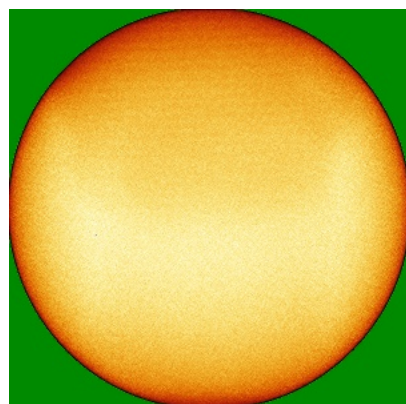


Y

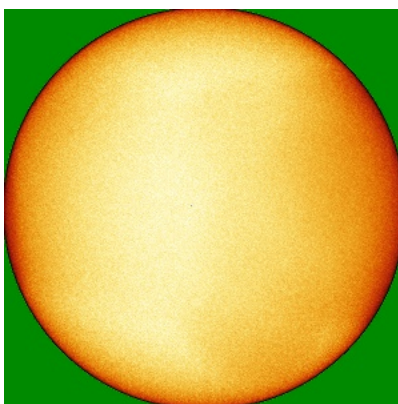


Z

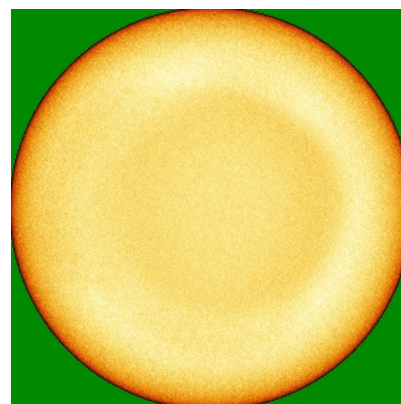
6.4.2 Raw map



X



Y

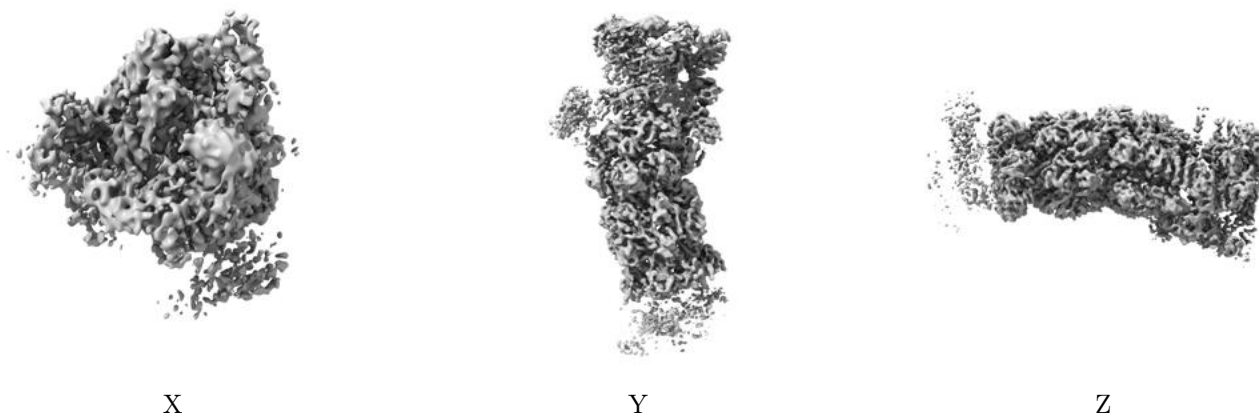


Z

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.

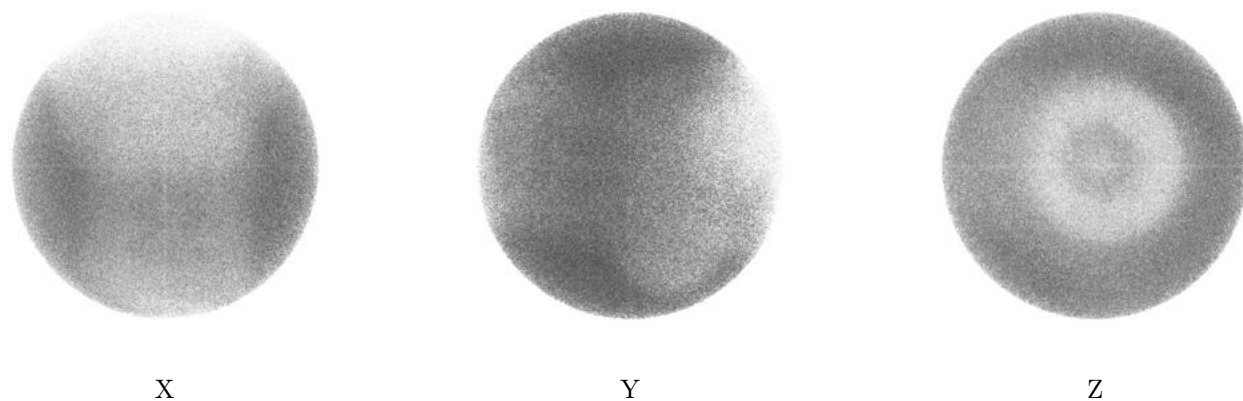
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0044. 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.

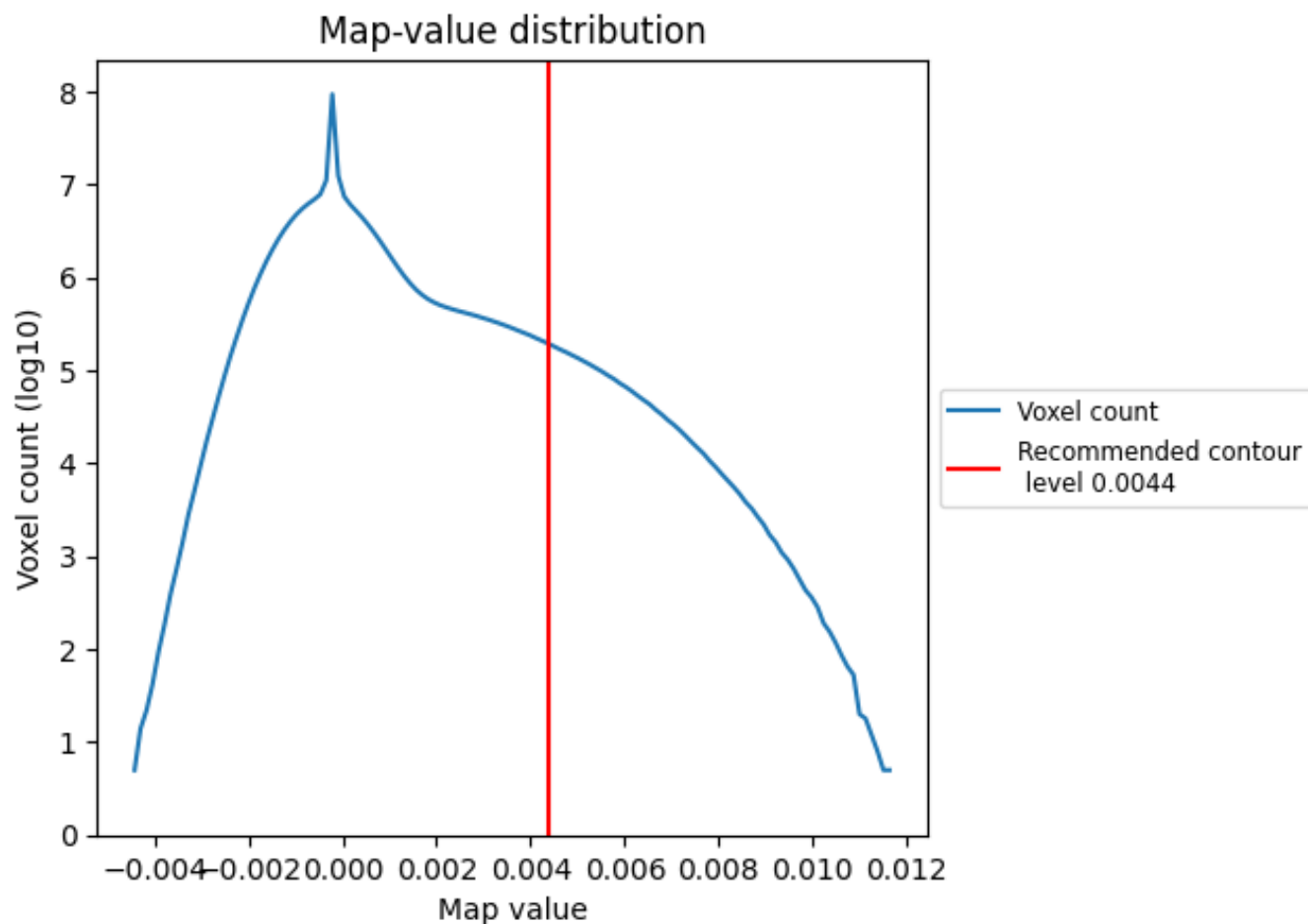
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

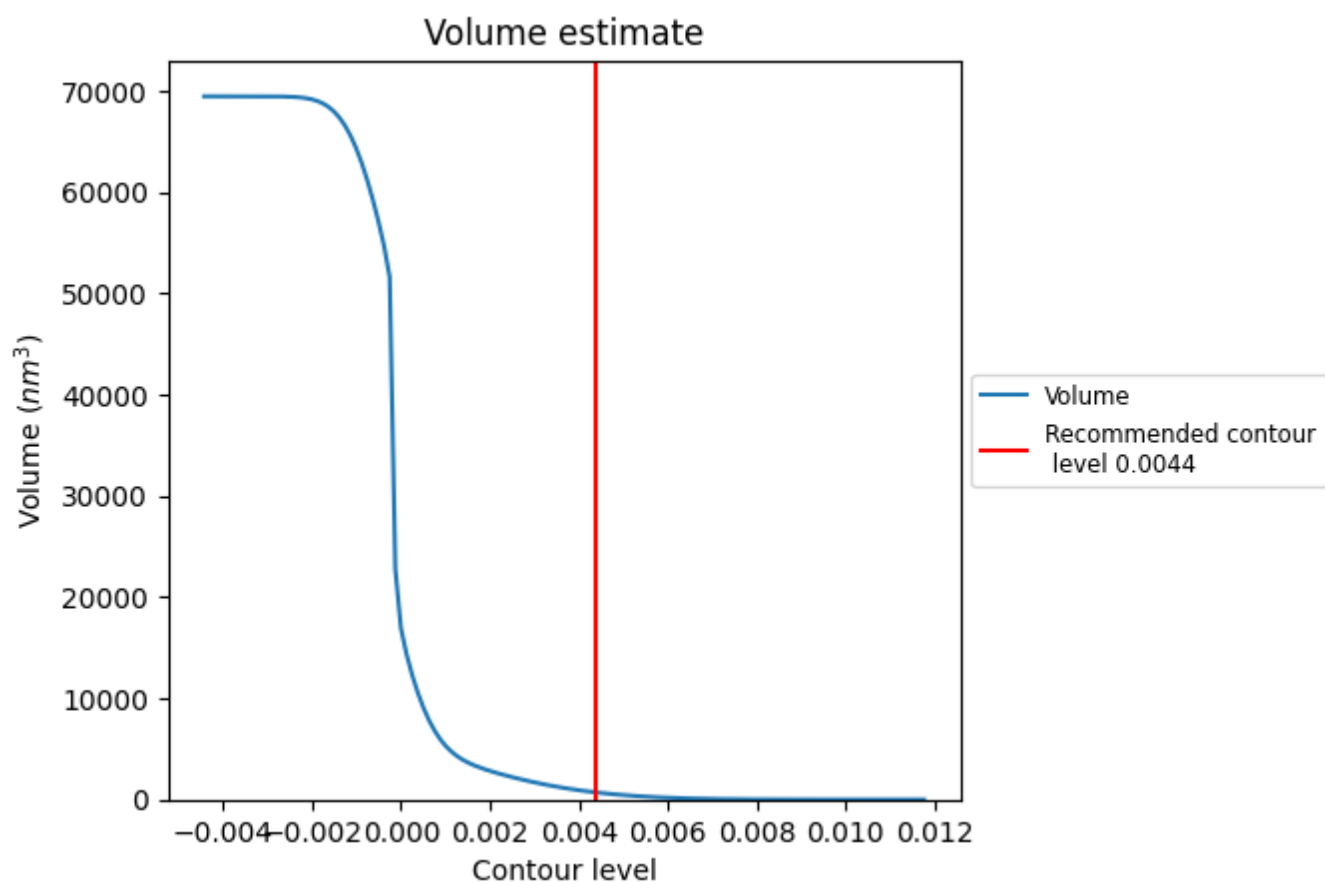
This section contains the results of statistical analysis of the map.

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.

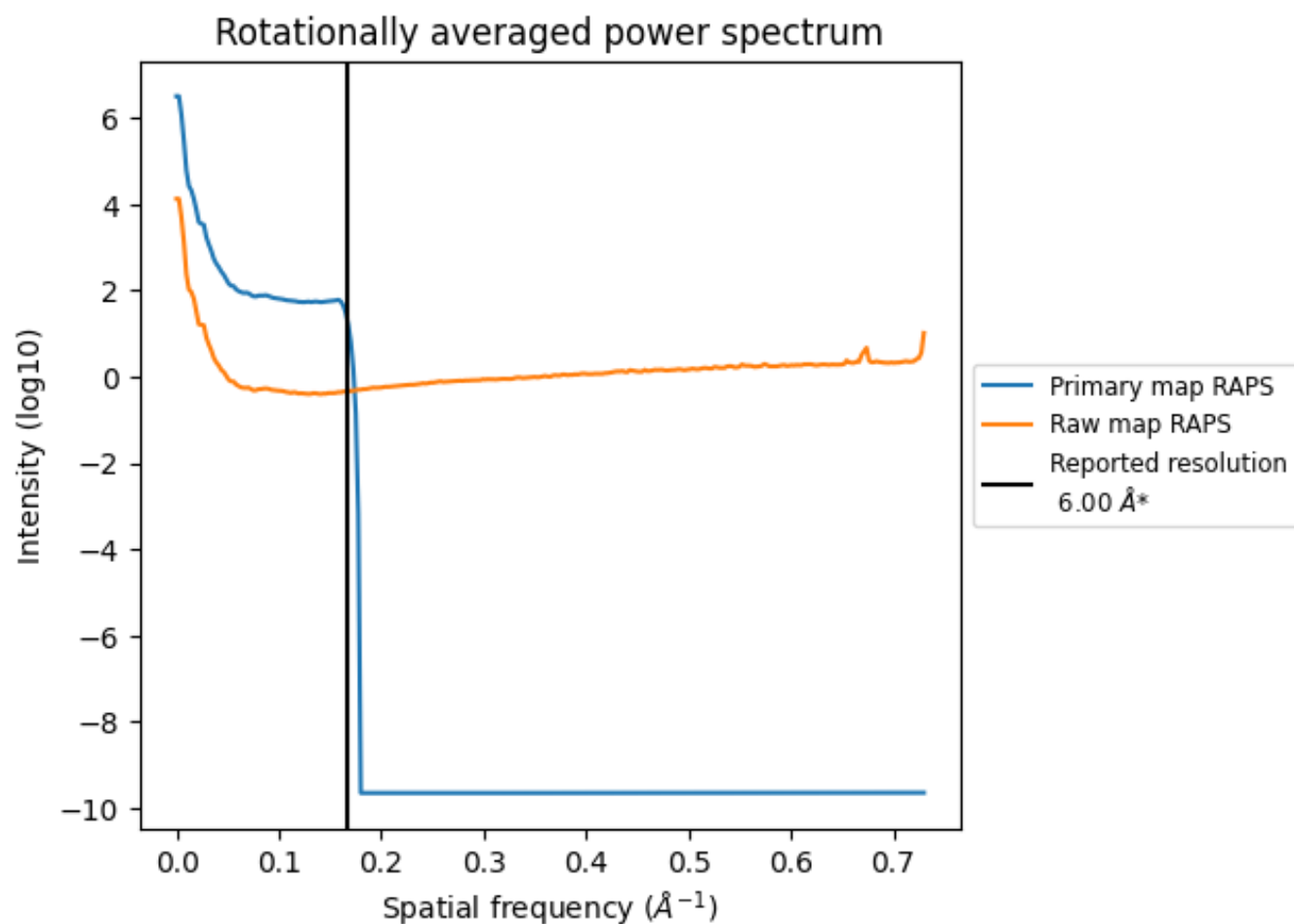
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 631 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 ⓘ

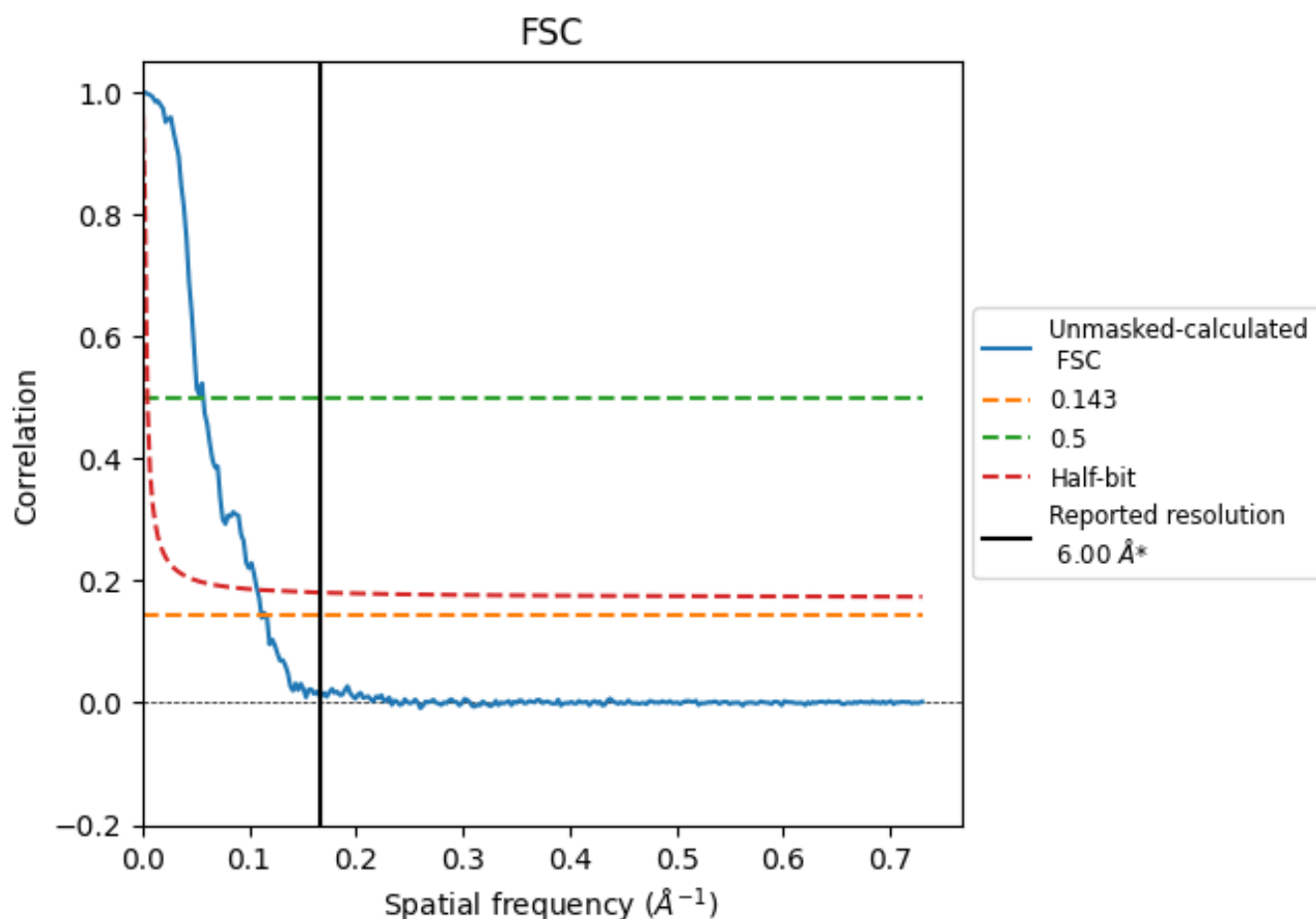


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

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 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

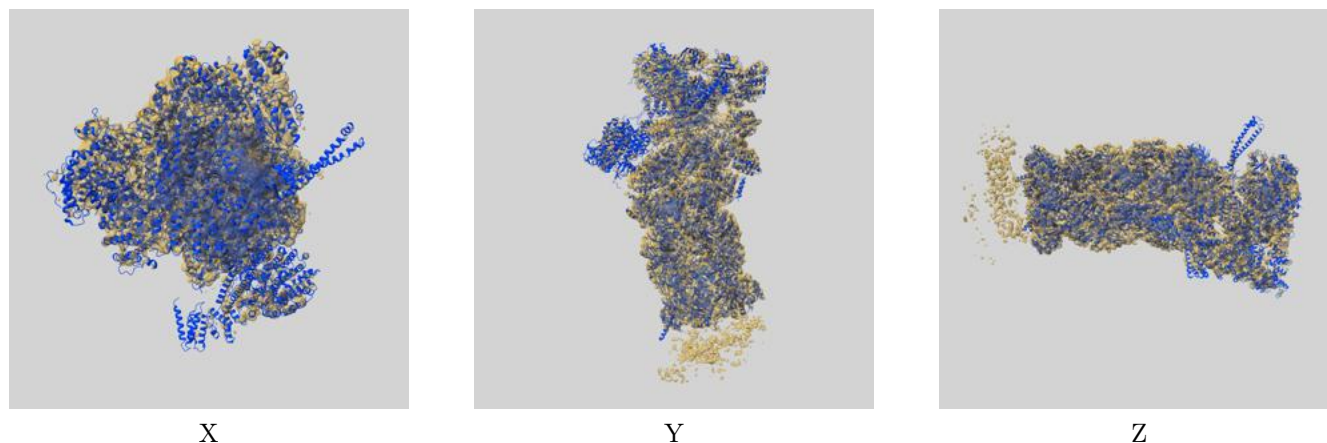
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.96	17.51	9.30

*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 8.96 differs from the reported value 6.0 by more than 10 %

9 Map-model fit [i](#)

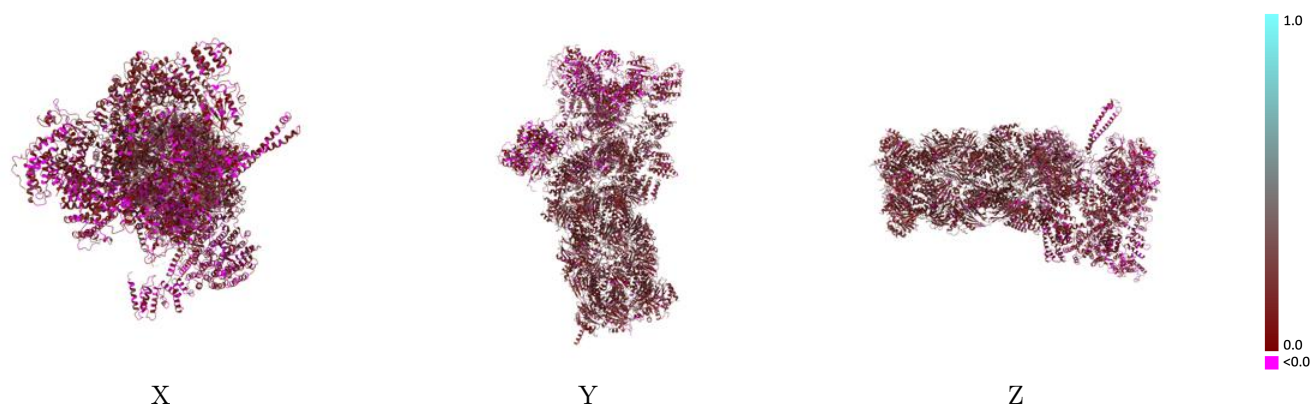
This section contains information regarding the fit between EMDB map EMD-62065 and PDB model 9K4O. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



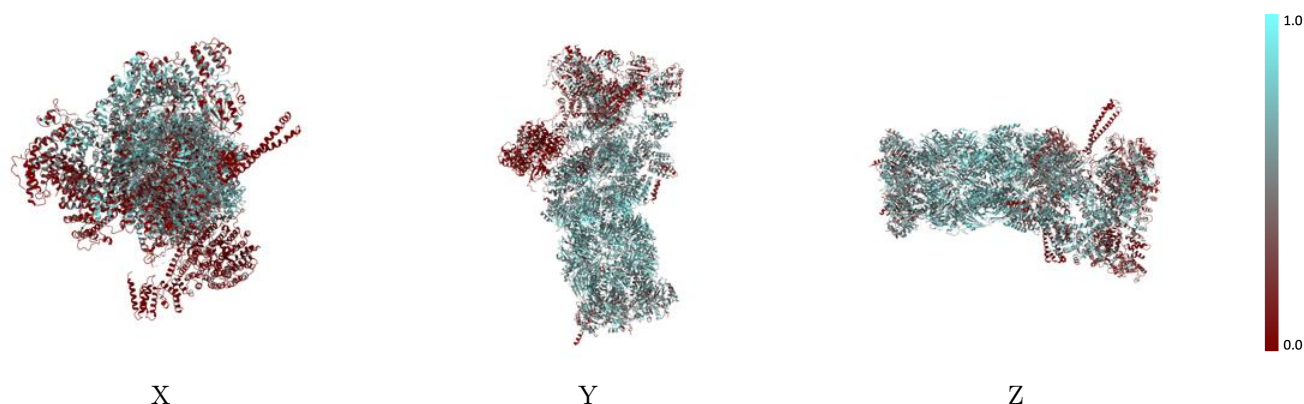
The images above show the 3D surface view of the map at the recommended contour level 0.0044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



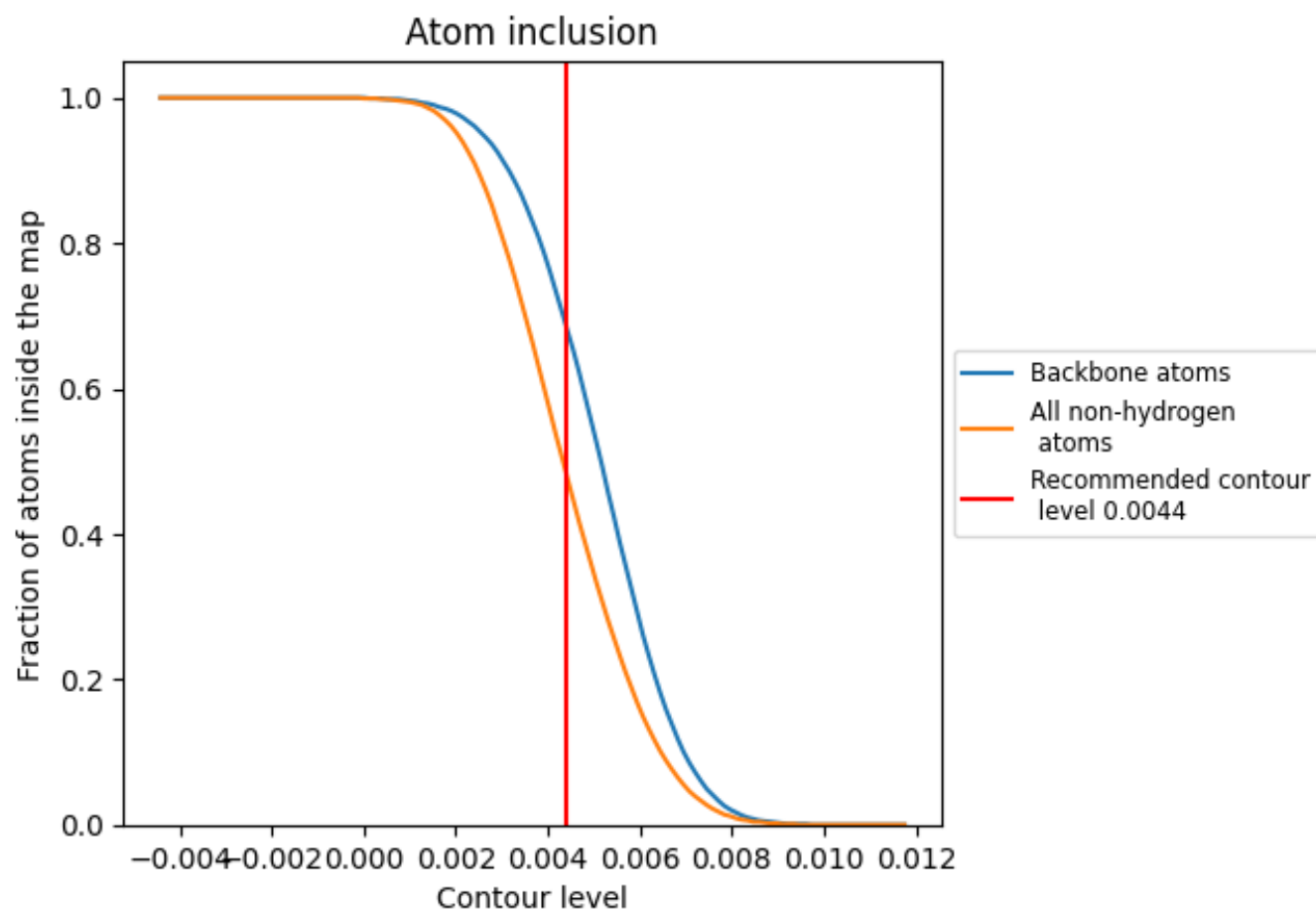
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 48% 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 (0.0044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.1770
A	0.4780	0.1810
B	0.4770	0.1800
C	0.4700	0.1770
D	0.5060	0.1740
E	0.5160	0.1840
F	0.4660	0.1780
G	0.6570	0.2190
H	0.6730	0.2180
I	0.6590	0.2180
J	0.5980	0.2010
K	0.6370	0.2200
L	0.6840	0.2200
M	0.6560	0.2110
N	0.6940	0.2200
O	0.6870	0.2330
P	0.6870	0.2130
Q	0.6340	0.2140
R	0.6500	0.2150
S	0.6430	0.2110
T	0.6940	0.2250
U	0.3070	0.1060
V	0.2820	0.1470
W	0.5430	0.1770
X	0.5100	0.1680
Y	0.4620	0.1330
Z	0.3970	0.1460
a	0.4500	0.1520
b	0.3060	0.1300
c	0.3970	0.1440
d	0.2160	0.1150
e	0.1770	0.1180
f	0.0790	0.0970
g	0.4980	0.2060
h	0.5190	0.2070



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Chain	Atom inclusion	Q-score
i	 0.4870	 0.2160
j	 0.4240	 0.2000
k	 0.4850	 0.2140
l	 0.5470	 0.2180
m	 0.5210	 0.1990
n	 0.6180	 0.2160
o	 0.6130	 0.2240
p	 0.6270	 0.2070
q	 0.6290	 0.2180
r	 0.6390	 0.2140
s	 0.6020	 0.2260
t	 0.6380	 0.2230
u	 0.1640	 0.1100
v	 0.0570	 0.0500
x	 0.3380	 0.0200
y	 0.4460	 0.0340