



## wwPDB EM Validation Summary Report ⓘ

Apr 28, 2025 – 04:50 PM EDT

PDB ID : 9NKF / pdb\_00009nkf  
EMDB ID : EMD-49507  
Title : Structure of human substrate-free 26S proteasome in the presence of ATPgS and MG-132, SA-like state (composite map)  
Authors : Peddada, N.; Beutler, B.  
Deposited on : 2025-02-28  
Resolution : 2.90 Å (reported)  
Based on initial model : 6MSB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

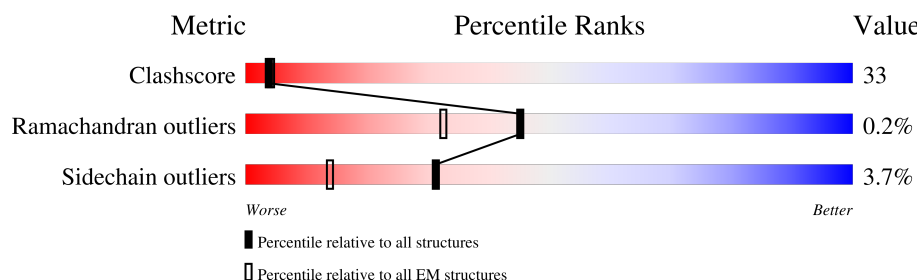
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.









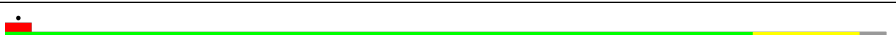
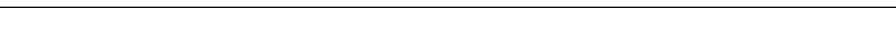
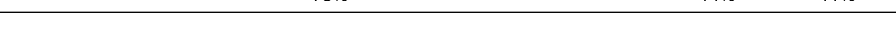
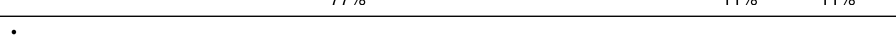
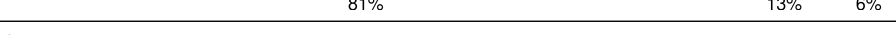
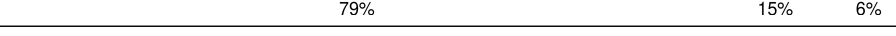













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	
5	E	403	
6	G	246	
6	g	246	
7	H	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	h	234	
8	I	261	
8	i	261	
9	J	248	
9	j	248	
10	K	241	
10	k	241	
11	L	263	
11	l	263	
12	M	255	
12	m	255	
13	N	239	
13	n	239	
14	O	277	
14	o	277	
15	P	205	
15	p	205	
16	Q	201	
16	q	201	
17	R	263	
17	r	263	
18	S	241	
18	s	241	
19	T	264	
19	t	264	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
20	V	534	
21	W	456	
22	X	422	
23	Y	389	
24	Z	324	
25	a	376	
26	b	377	
27	c	310	
28	d	350	
29	e	70	
30	f	908	
31	F	439	
32	U	953	

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 145524 atoms, of which 44186 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	366	Total	C	N	O	S	0	0
			2863	1805	503	537	18		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2968	1867	534	551	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 26S proteasome regulatory subunit 10B.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	240	Total	C	H	N	O	S	0	0
			3402	1108	1660	304	318	12		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf	Trace
6	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		
7	h	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	247	Total	C	H	N	O	S	0	0
			3543	1150	1741	322	320	10		
8	i	247	Total	C	H	N	O	S	0	0
			3503	1143	1717	320	313	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		
9	j	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	233	Total	C	H	N	O	S	0	0
			3255	1057	1592	287	308	11		
10	k	233	Total	C	H	N	O	S	0	0
			3249	1056	1589	287	306	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	233	Total	C	H	N	O	S	0	0
			3359	1090	1649	318	293	9		
11	l	233	Total	C	H	N	O	S	0	0
			3352	1089	1645	315	293	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		
12	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	202	Total	C	H	N	O	S	0	0
			2891	928	1422	257	272	12		
13	n	202	Total	C	H	N	O	S	0	0
			2881	926	1416	256	271	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	220	Total	C	H	N	O	S	0	0
			3139	1005	1559	272	294	9		
14	o	220	Total	C	H	N	O	S	0	0
			3131	1003	1555	272	292	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	204	Total	C	H	N	O	S	0	0
			3096	992	1550	262	273	19		
15	p	204	Total	C	H	N	O	S	0	0
			3081	989	1543	263	268	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	196	Total	C	H	N	O	S	0	0
			2986	974	1477	259	268	8		
16	q	196	Total	C	H	N	O	S	0	0
			2981	973	1475	259	266	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	200	Total	C	H	N	O	S	0	0
			2953	957	1449	271	267	9		
17	r	200	Total	C	H	N	O	S	0	0
			2938	954	1438	270	267	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	212	Total	C	H	N	O	S	0	0
			3163	1016	1579	279	279	10		
18	s	212	Total	C	H	N	O	S	0	0
			3168	1017	1581	279	281	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	212	Total	C	H	N	O	S	0	0
			3102	1003	1526	280	282	11		
19	t	212	Total	C	H	N	O	S	0	0
			3079	998	1511	279	280	11		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	334	Total	C	N	O	S	0	0
			2664	1696	448	508	12		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 6.



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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

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

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

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

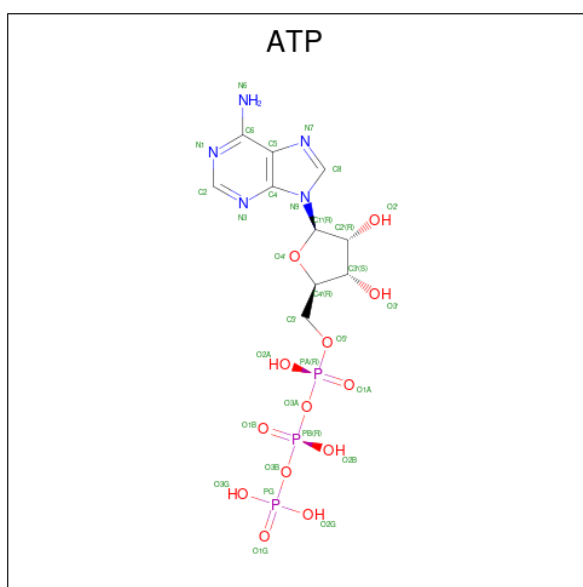
- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	808	Total	C	N	O	S	0	0
			6304	4003	1074	1183	44		

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

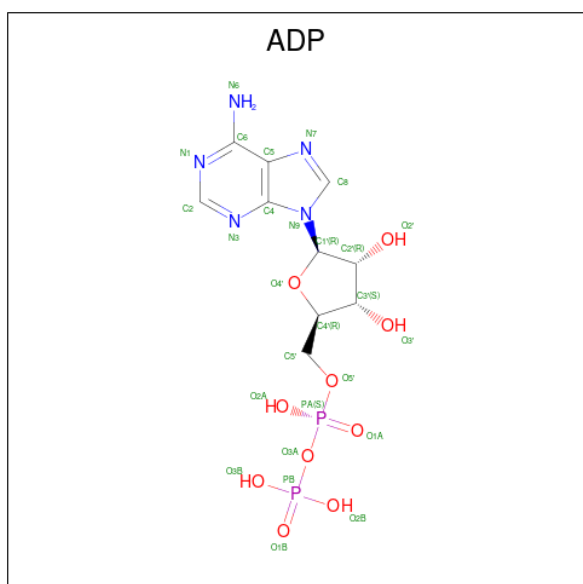


Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

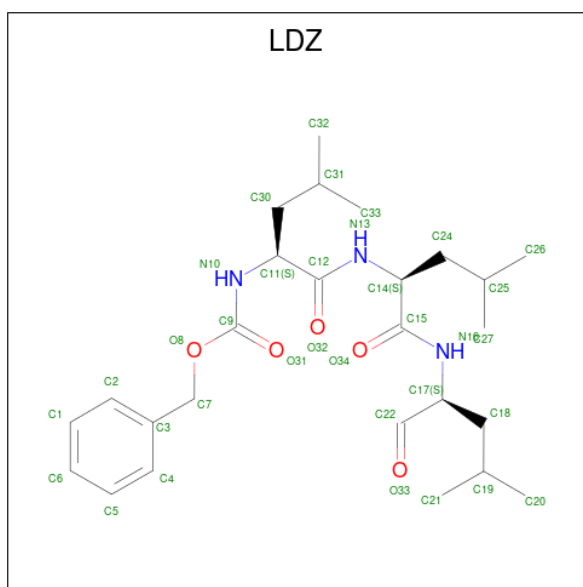
Mol	Chain	Residues	Atoms		AltConf
34	A	2	Total	Mg	0
			2	2	
34	B	1	Total	Mg	0
			1	1	
34	E	2	Total	Mg	0
			2	2	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C<sub>26</sub>H<sub>41</sub>N<sub>3</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

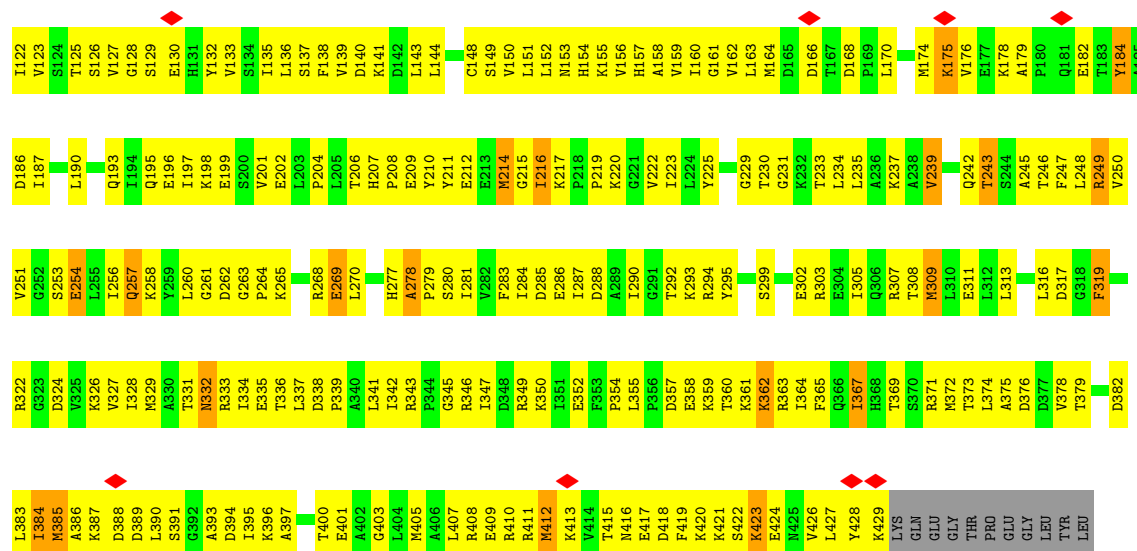


Mol	Chain	Residues	Atoms					AltConf
36	N	1	Total	C	H	N	O	0
			75	26	41	3	5	
36	O	1	Total	C	H	N	O	0
			75	26	41	3	5	
36	R	1	Total	C	H	N	O	0
			75	26	41	3	5	
36	n	1	Total	C	H	N	O	0
			75	26	41	3	5	
36	o	1	Total	C	H	N	O	0
			75	26	41	3	5	
36	r	1	Total	C	H	N	O	0
			75	26	41	3	5	

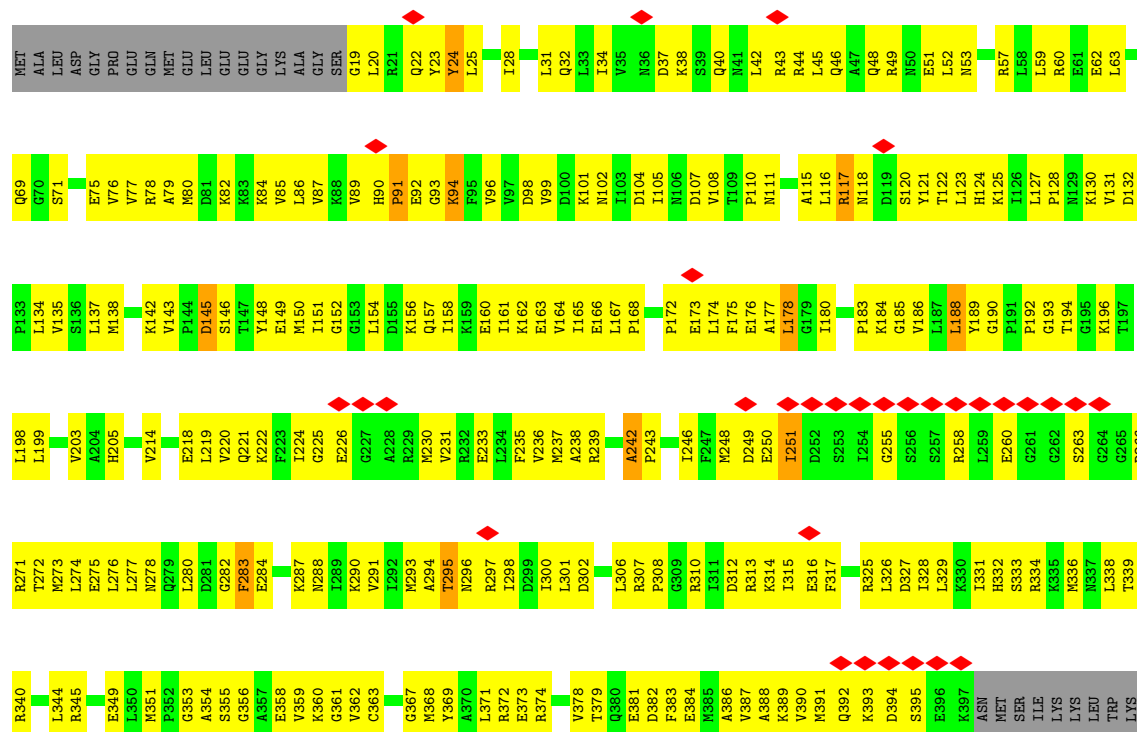
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

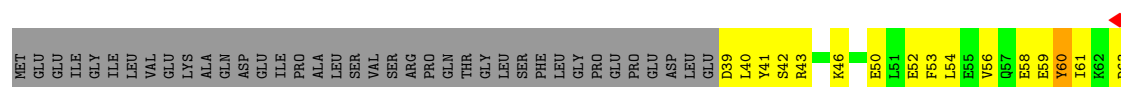


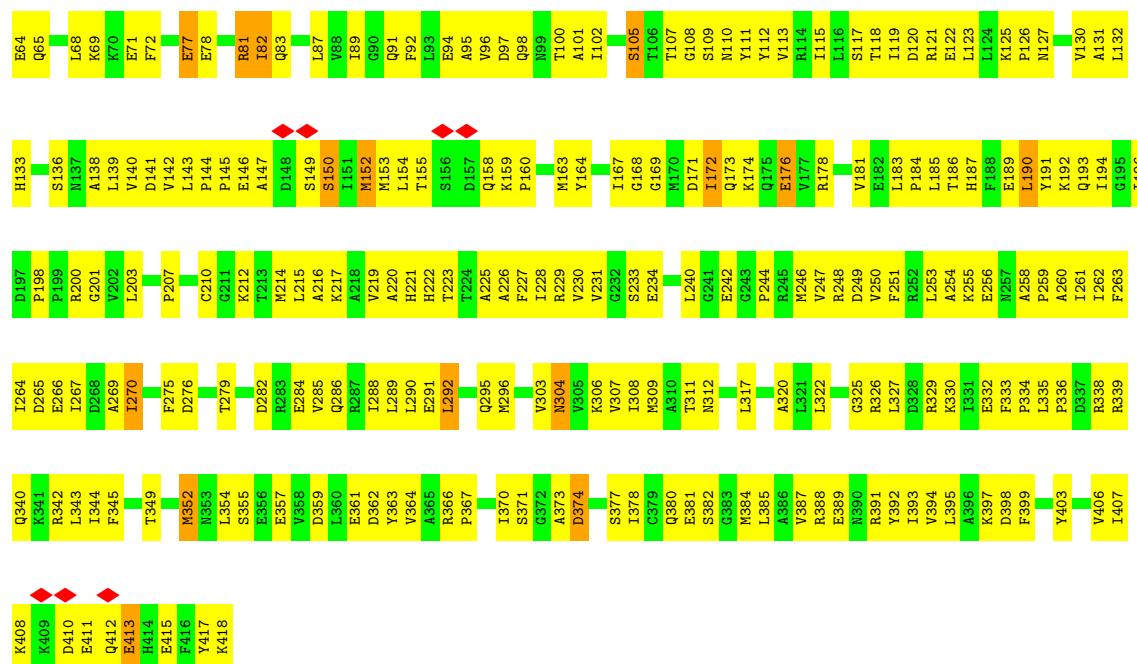


• Molecule 3: 26S protease regulatory subunit 8

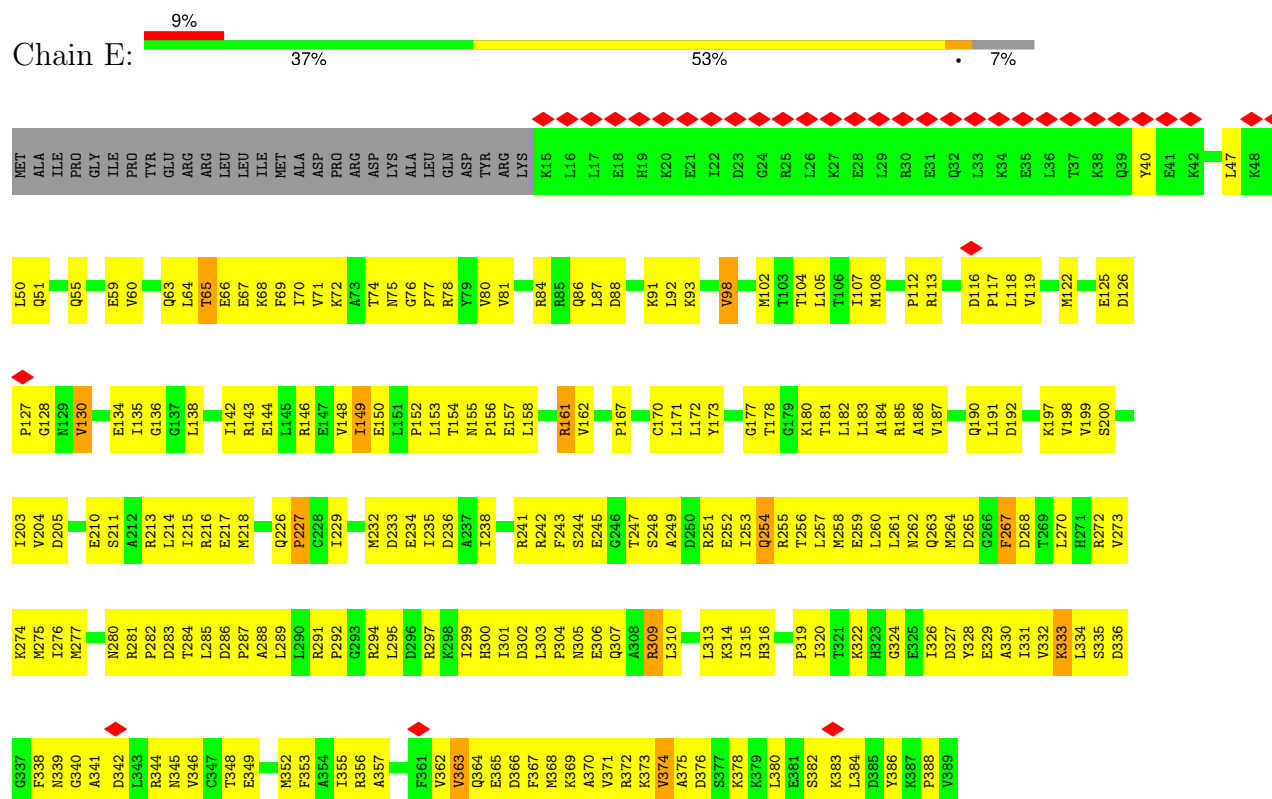


• Molecule 4: 26S proteasome regulatory subunit 6B

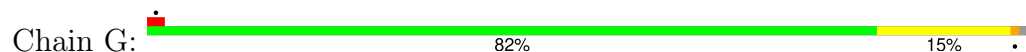




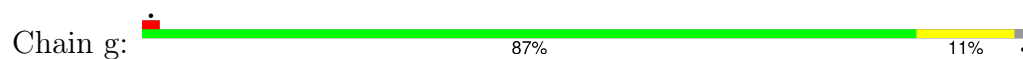
• Molecule 5: 26S proteasome regulatory subunit 10B



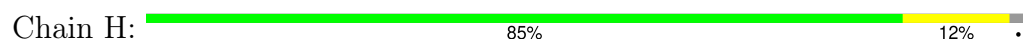
• Molecule 6: Proteasome subunit alpha type-6



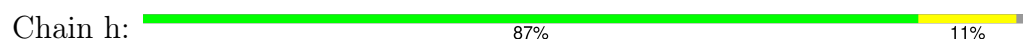
- Molecule 6: Proteasome subunit alpha type-6



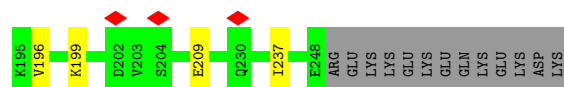
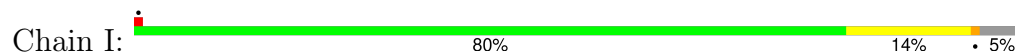
- Molecule 7: Proteasome subunit alpha type-2



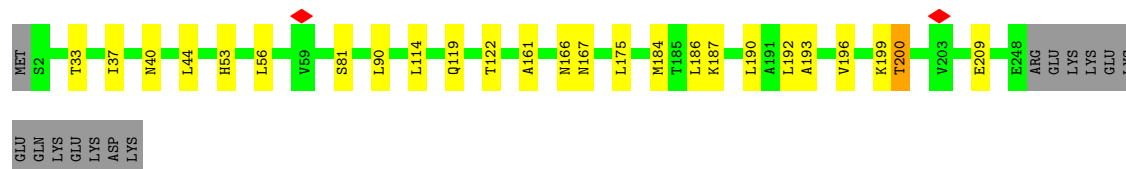
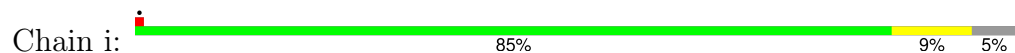
- Molecule 7: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-4




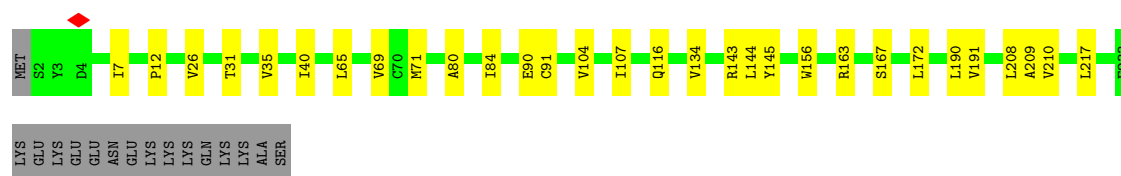
- Molecule 8: Proteasome subunit alpha type-4






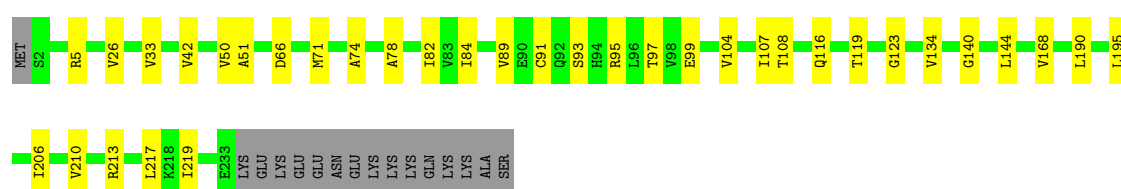
- Molecule 9: Proteasome subunit alpha type-7

Chain J:  81% 12% 6%




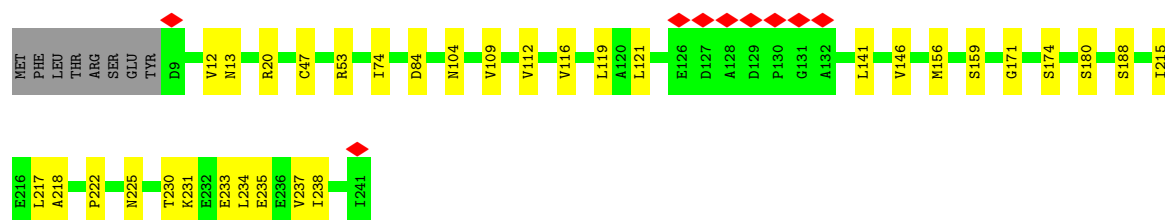
- Molecule 9: Proteasome subunit alpha type-7

Chain j:  79% 14% 6%




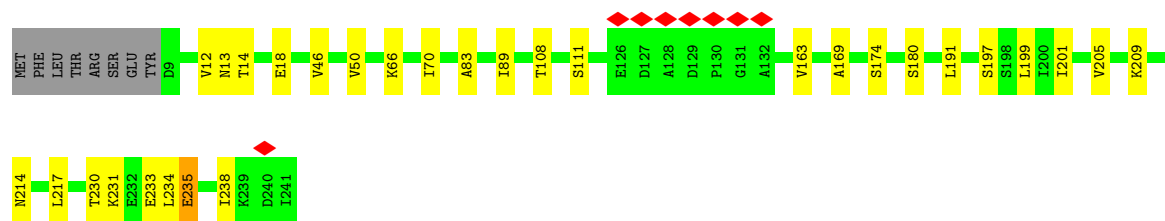
- Molecule 10: Proteasome subunit alpha type-5

Chain K:  83% 14% 3%



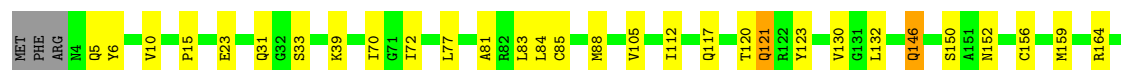
- Molecule 10: Proteasome subunit alpha type-5

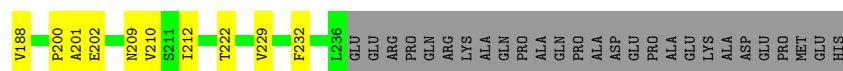
Chain k:  84% 12% 4%



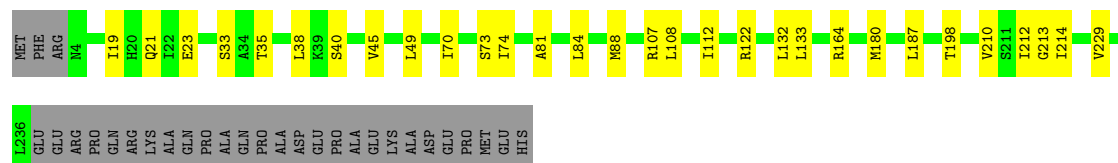
- Molecule 11: Proteasome subunit alpha type-1

Chain L:  73% 14% 11%

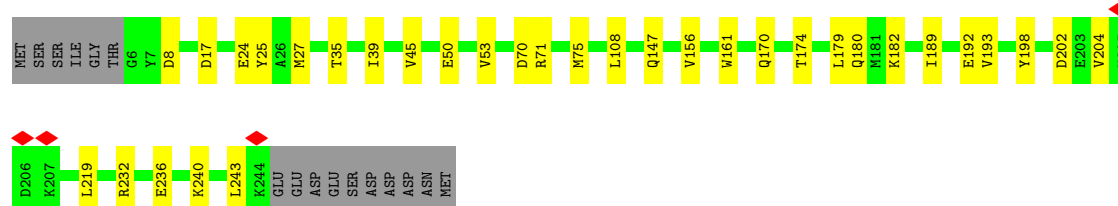
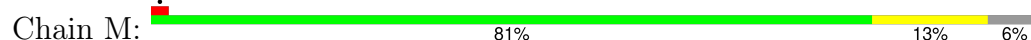




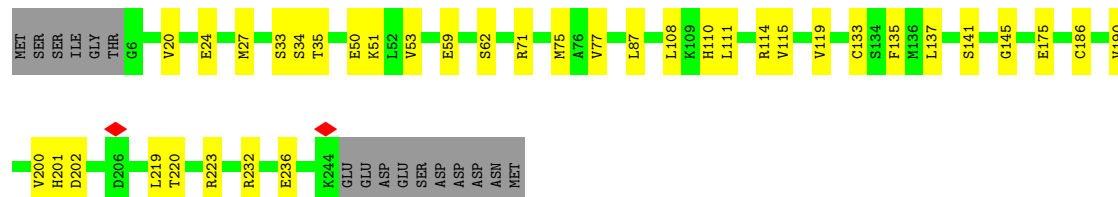
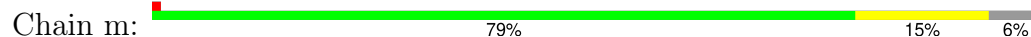
- Molecule 11: Proteasome subunit alpha type-1



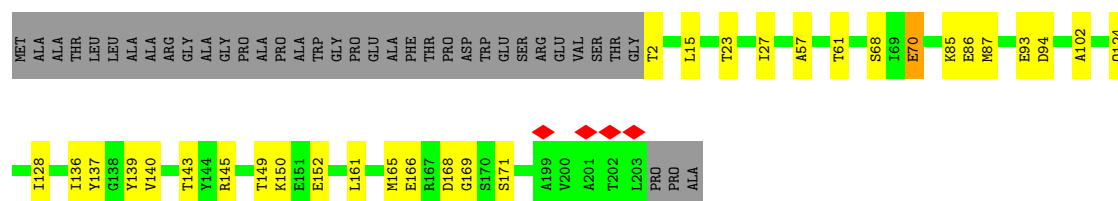
- Molecule 12: Proteasome subunit alpha type-3



- Molecule 12: Proteasome subunit alpha type-3

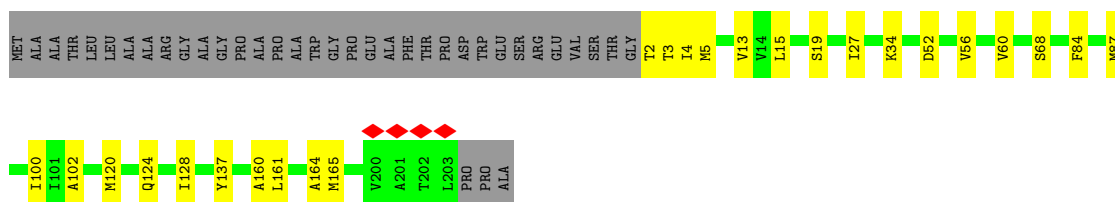


- Molecule 13: Proteasome subunit beta type-6

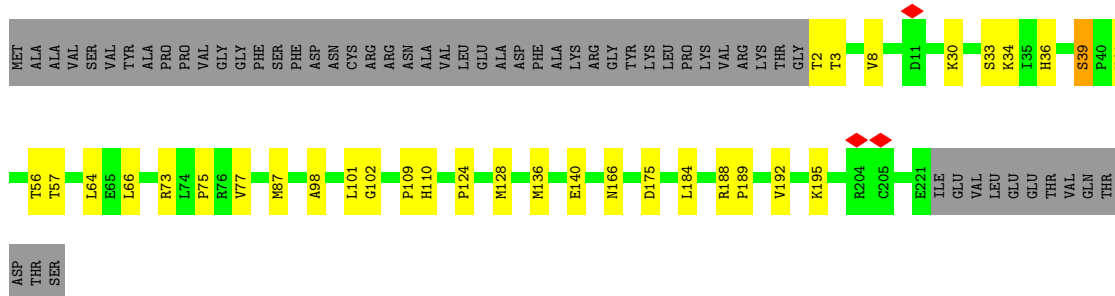


- Molecule 13: Proteasome subunit beta type-6

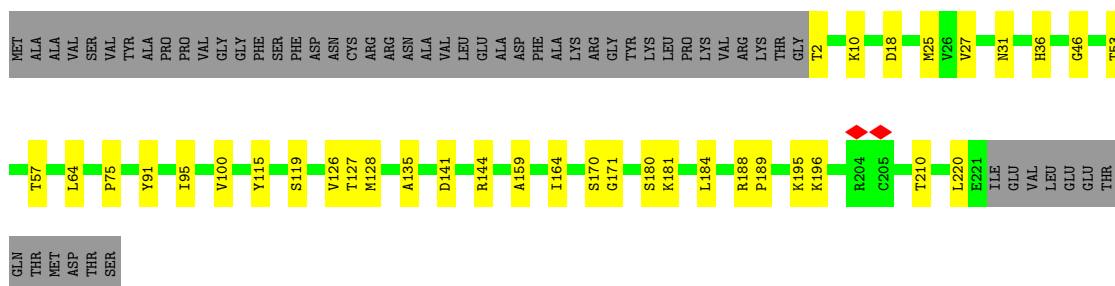




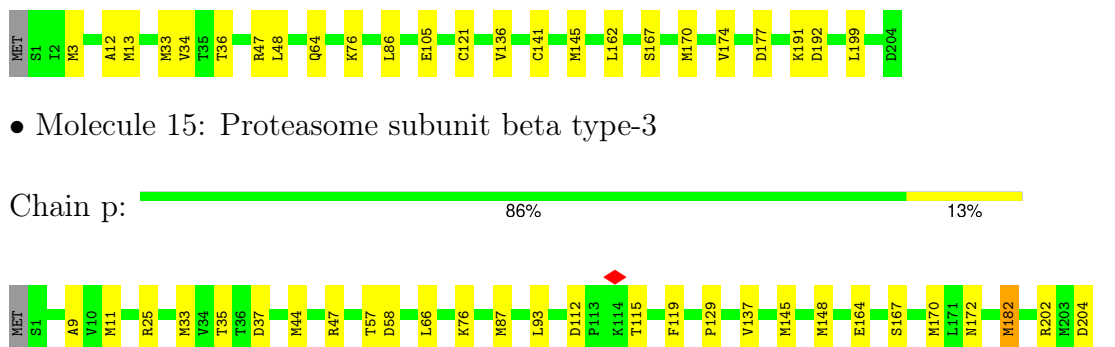
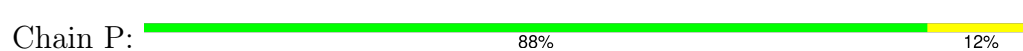
• Molecule 14: Proteasome subunit beta type-7




• Molecule 14: Proteasome subunit beta type-7



• Molecule 15: Proteasome subunit beta type-3




• Molecule 16: Proteasome subunit beta type-2

Chain Q:  84% 13%



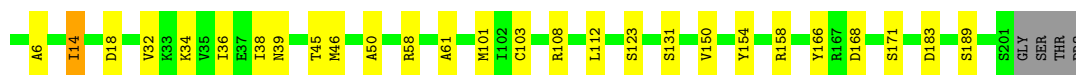
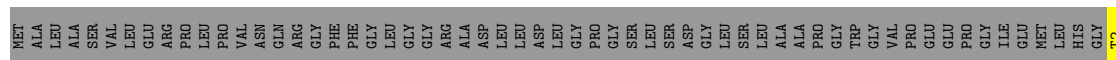
- Molecule 16: Proteasome subunit beta type-2

Chain q:  84% 13%



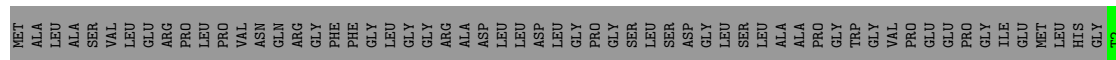
- Molecule 17: Proteasome subunit beta type-5

Chain R:  65% 10% 24%




- Molecule 17: Proteasome subunit beta type-5

Chain r:  65% 10% 24%




THR  
PRO

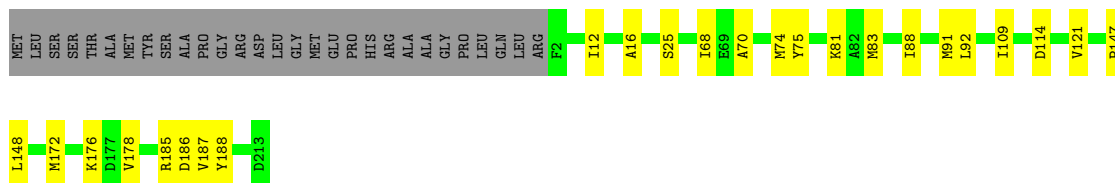
- Molecule 18: Proteasome subunit beta type-1

Chain S:  81% 7% 12%

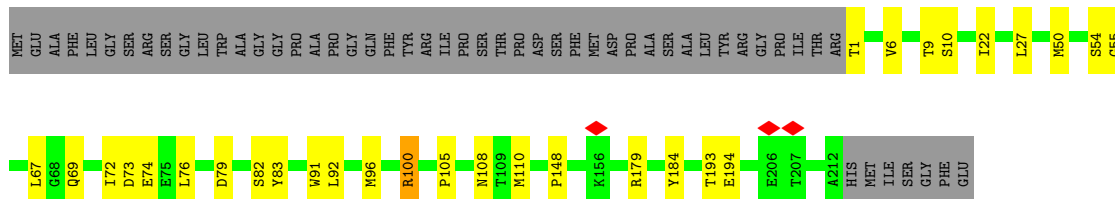


- Molecule 18: Proteasome subunit beta type-1

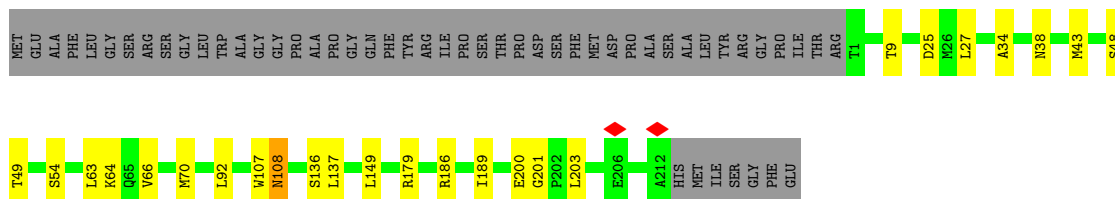
Chain s:  78% 10% 12%



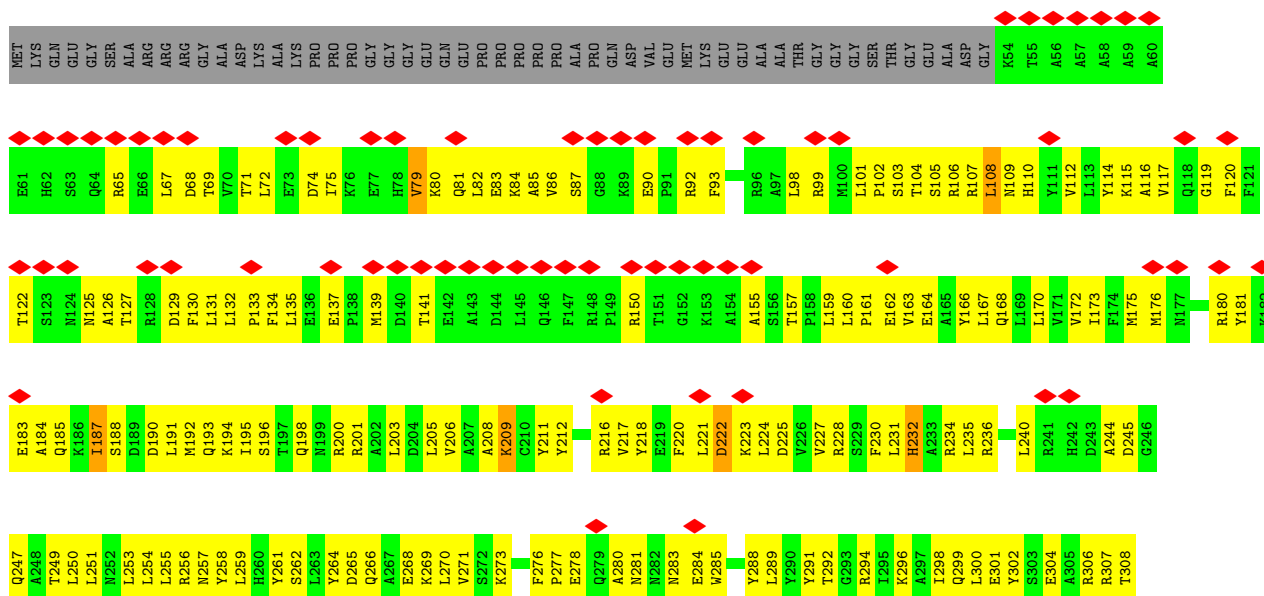
- Molecule 19: Proteasome subunit beta type-4

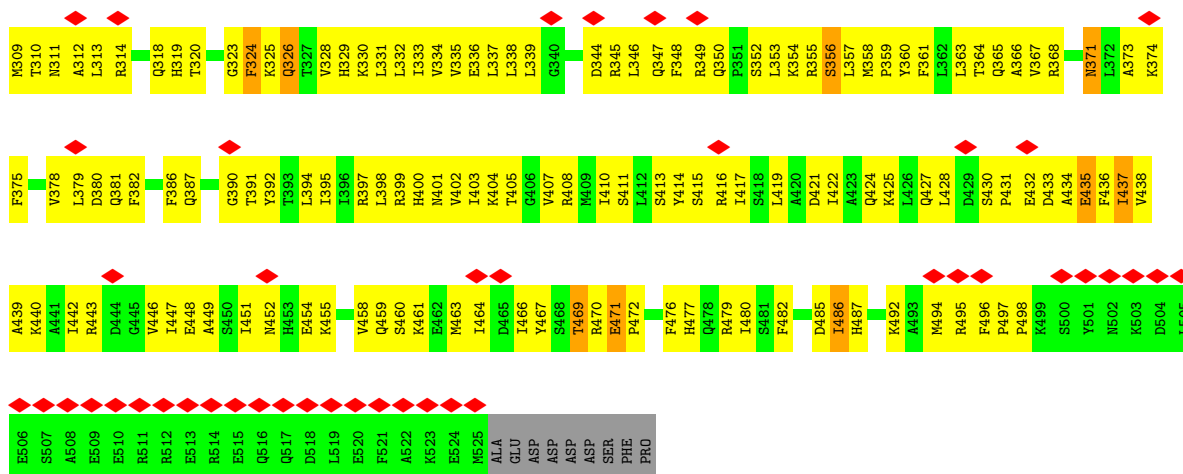


- Molecule 19: Proteasome subunit beta type-4

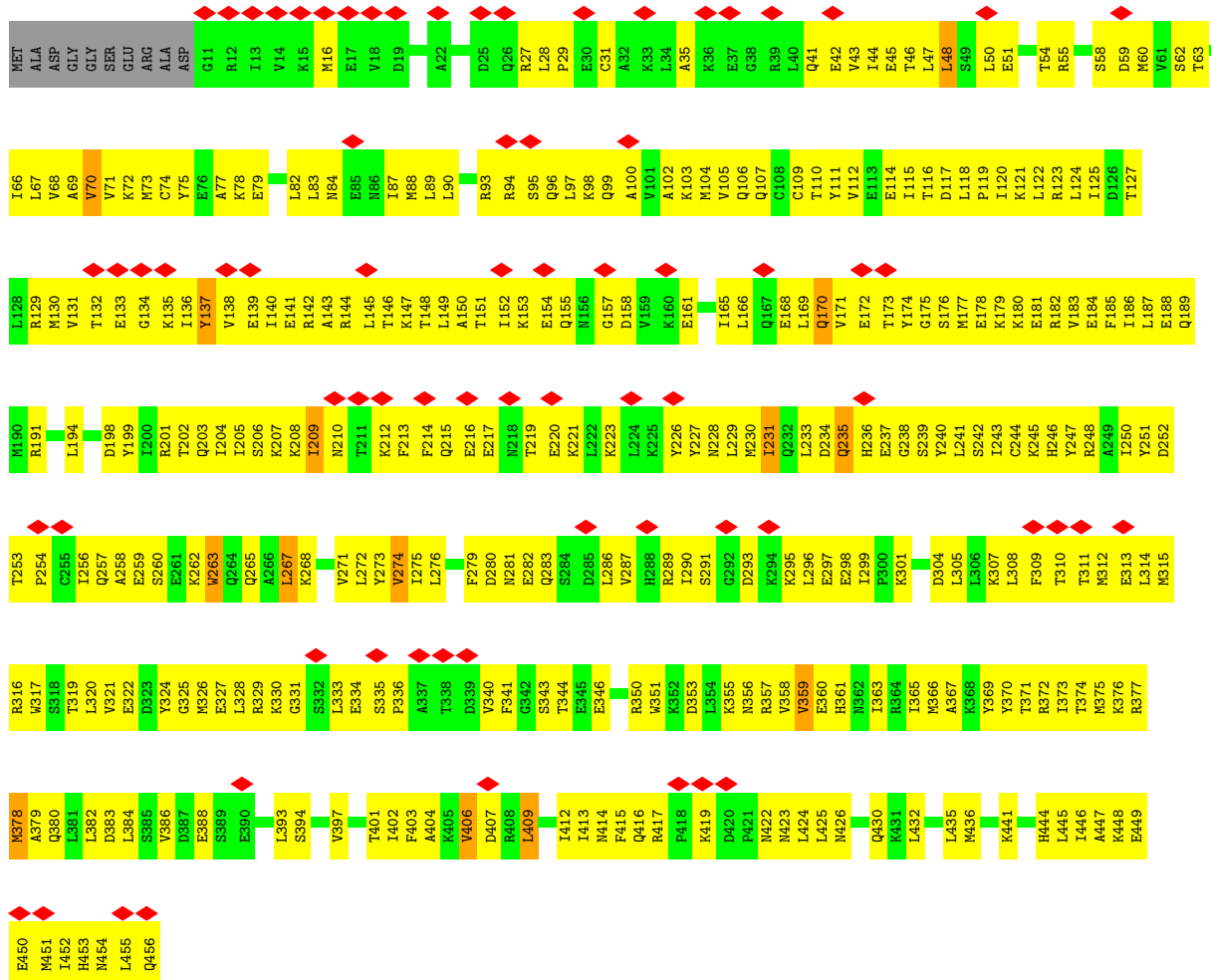


- Molecule 20: 26S proteasome non-ATPase regulatory subunit 3

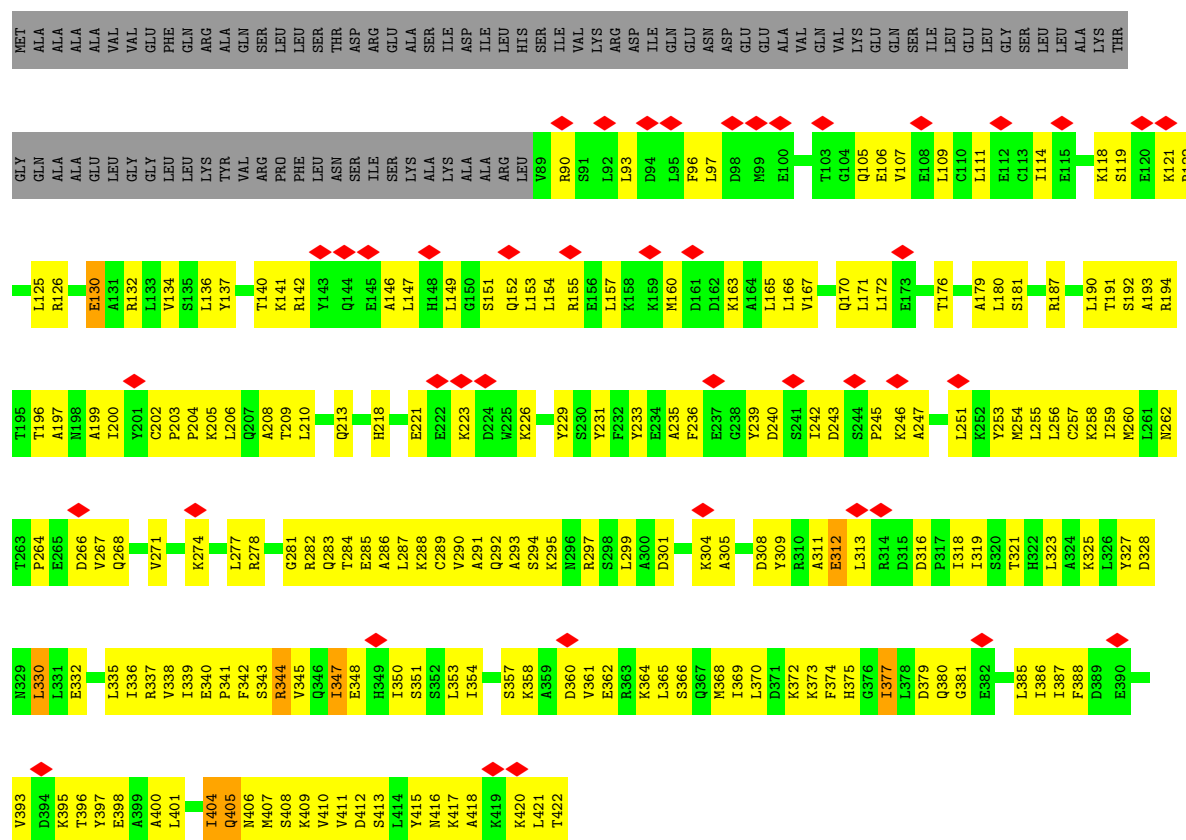




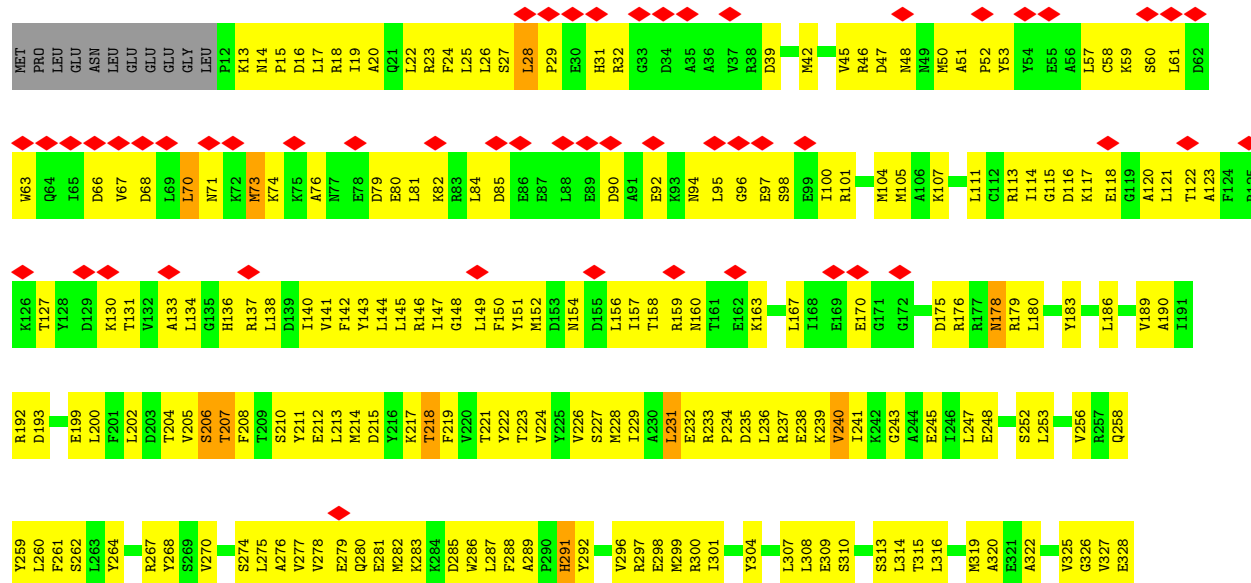
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 12

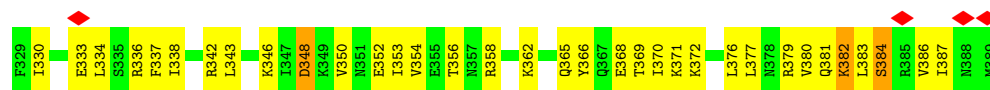


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 11

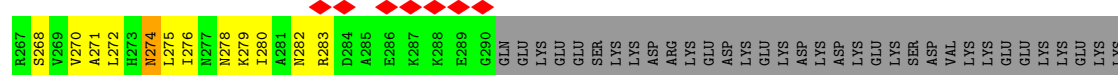
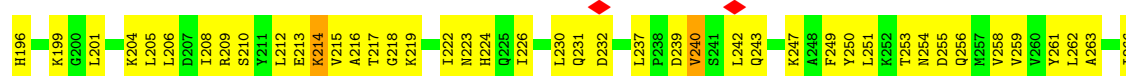
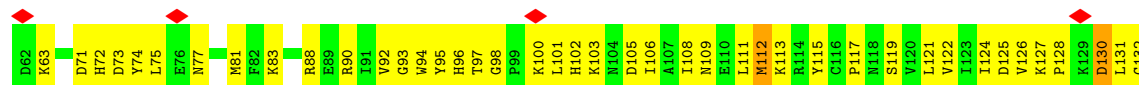
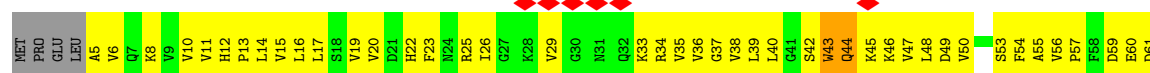


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 6

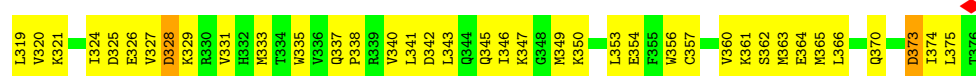
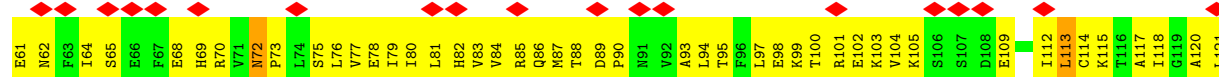
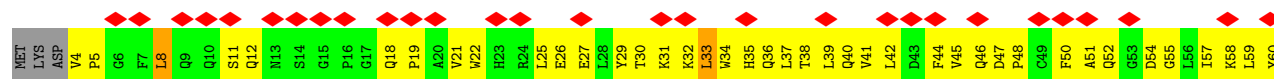




• Molecule 24: 26S proteasome non-ATPase regulatory subunit 7

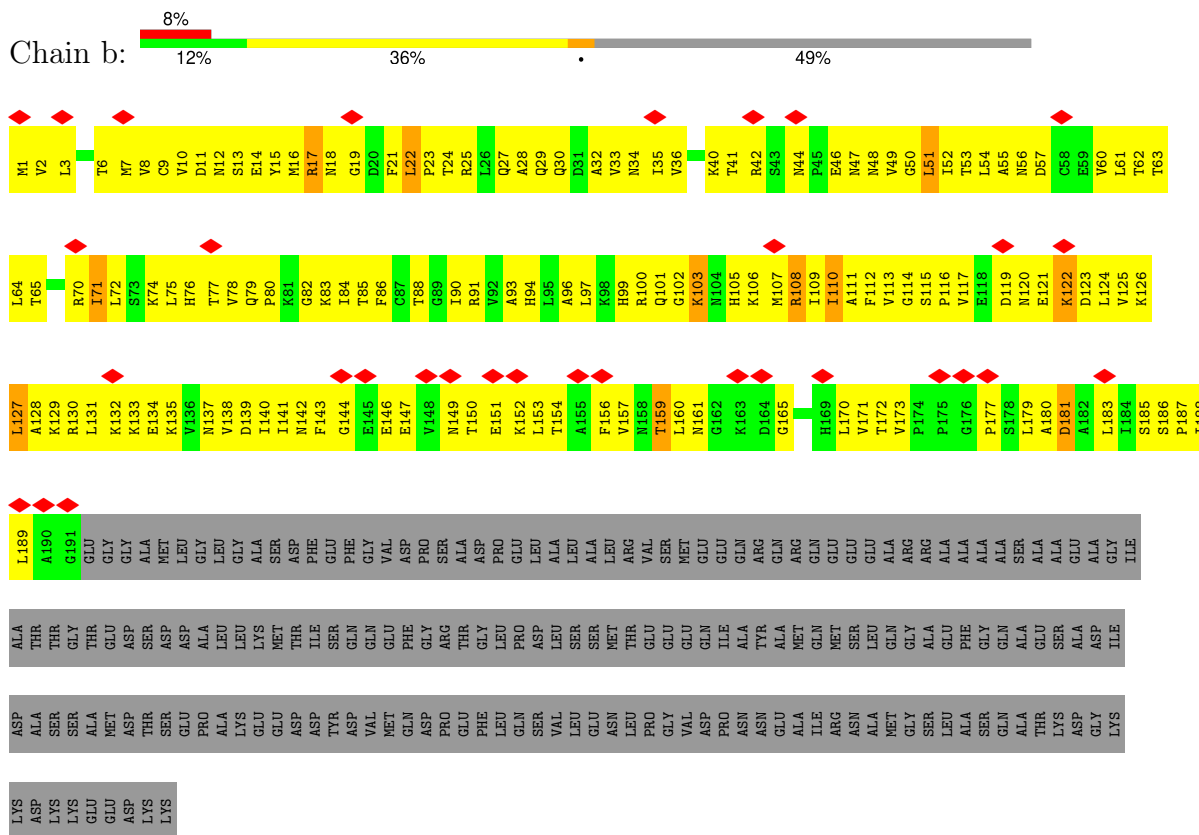


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 13

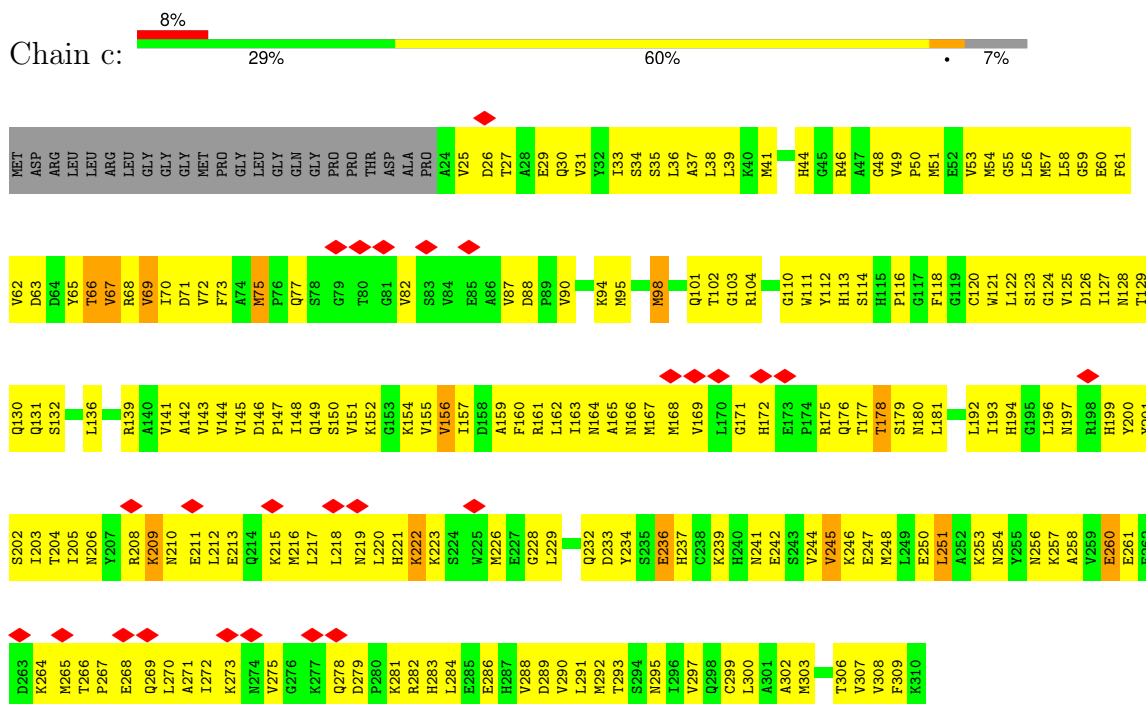




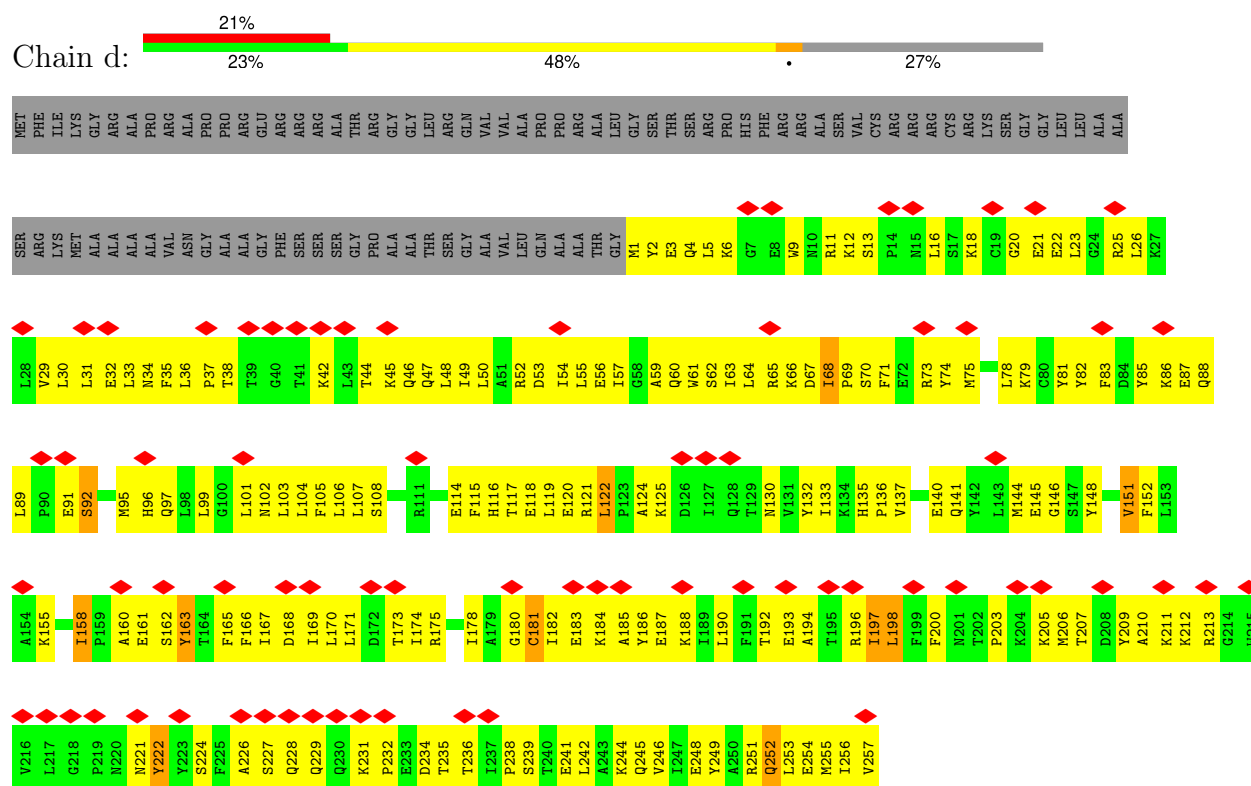
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 4



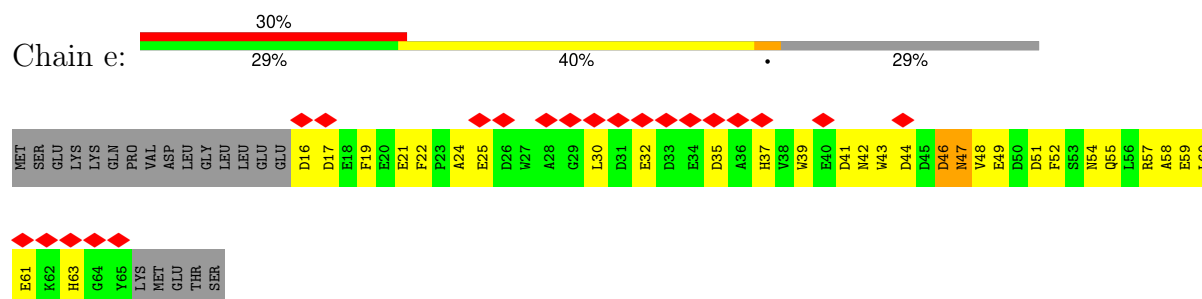
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 14



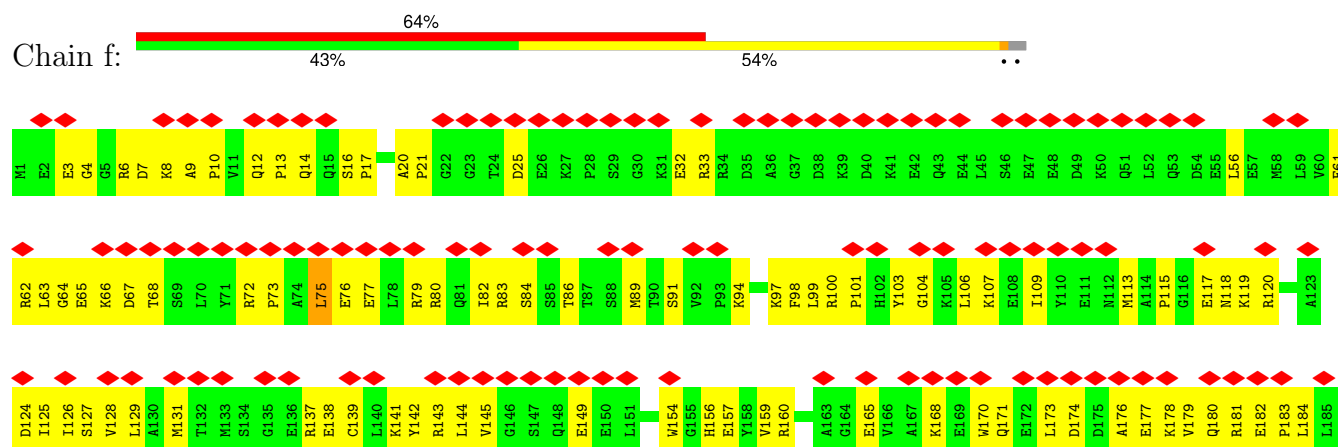
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 29: 26S proteasome complex subunit SEM1

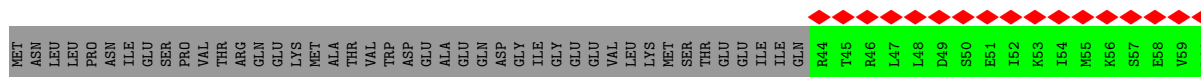


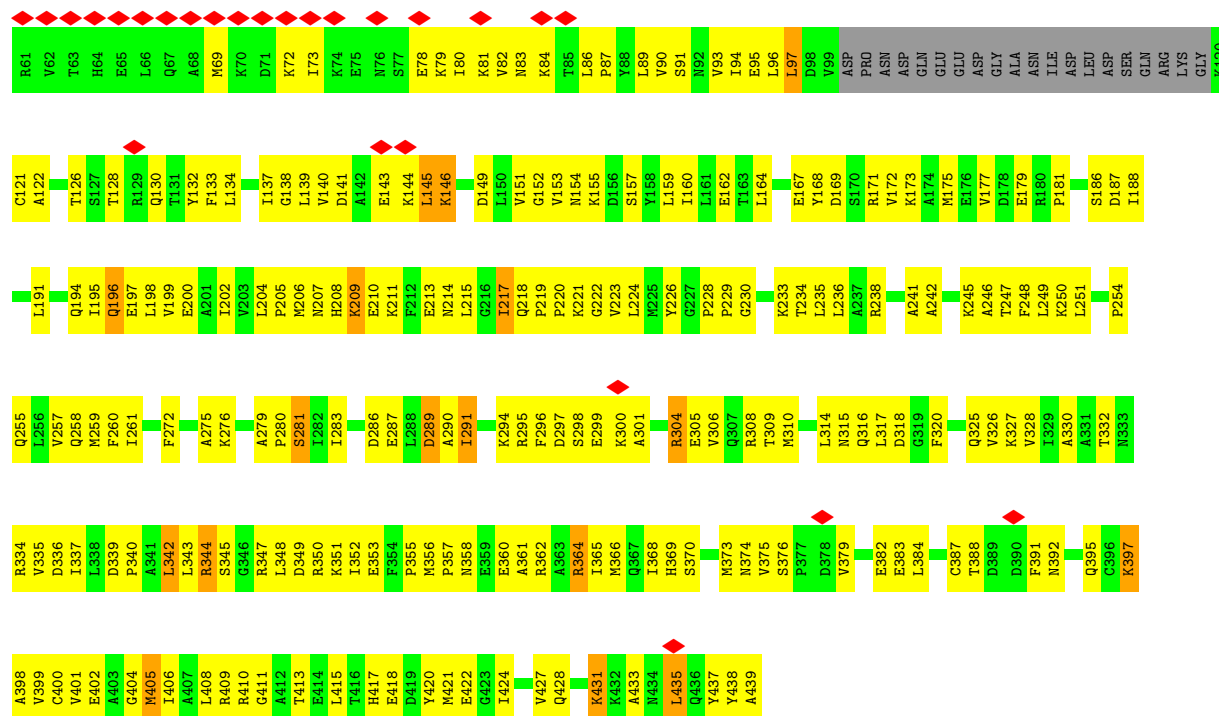
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 2



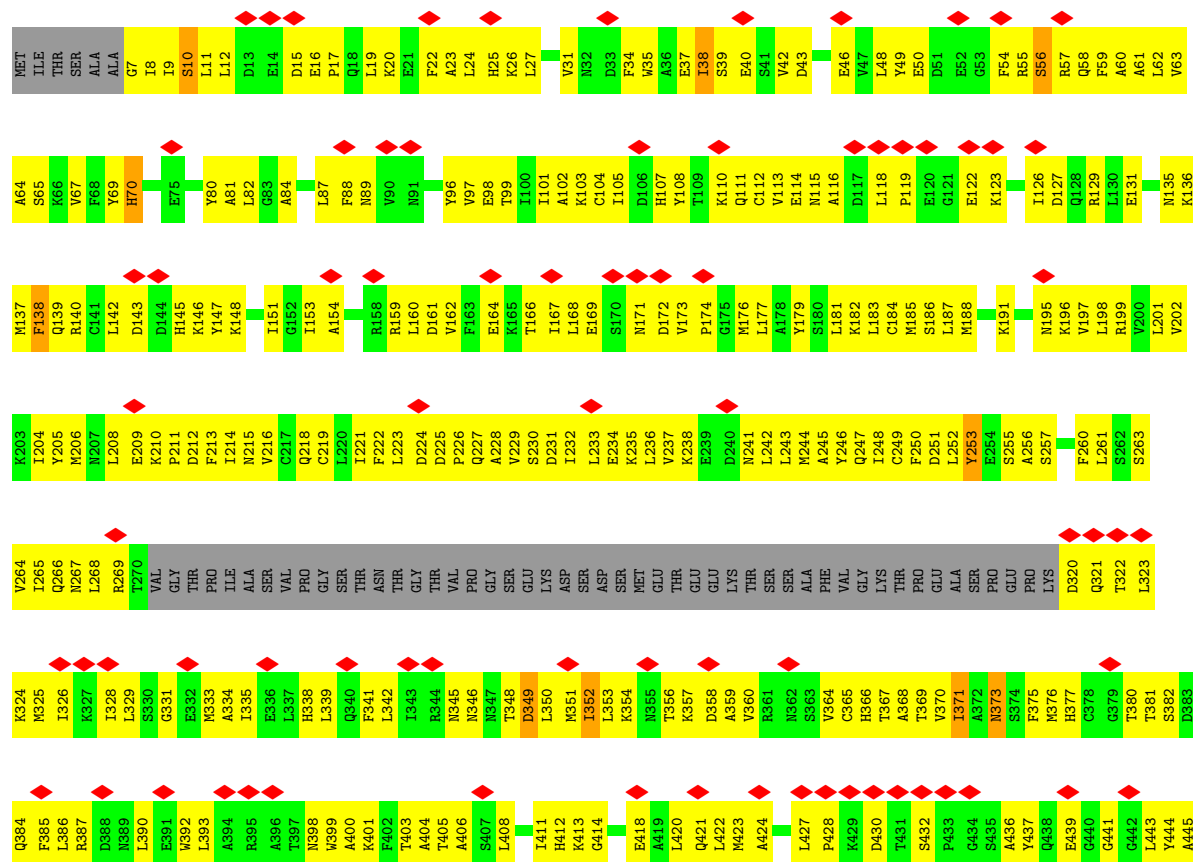


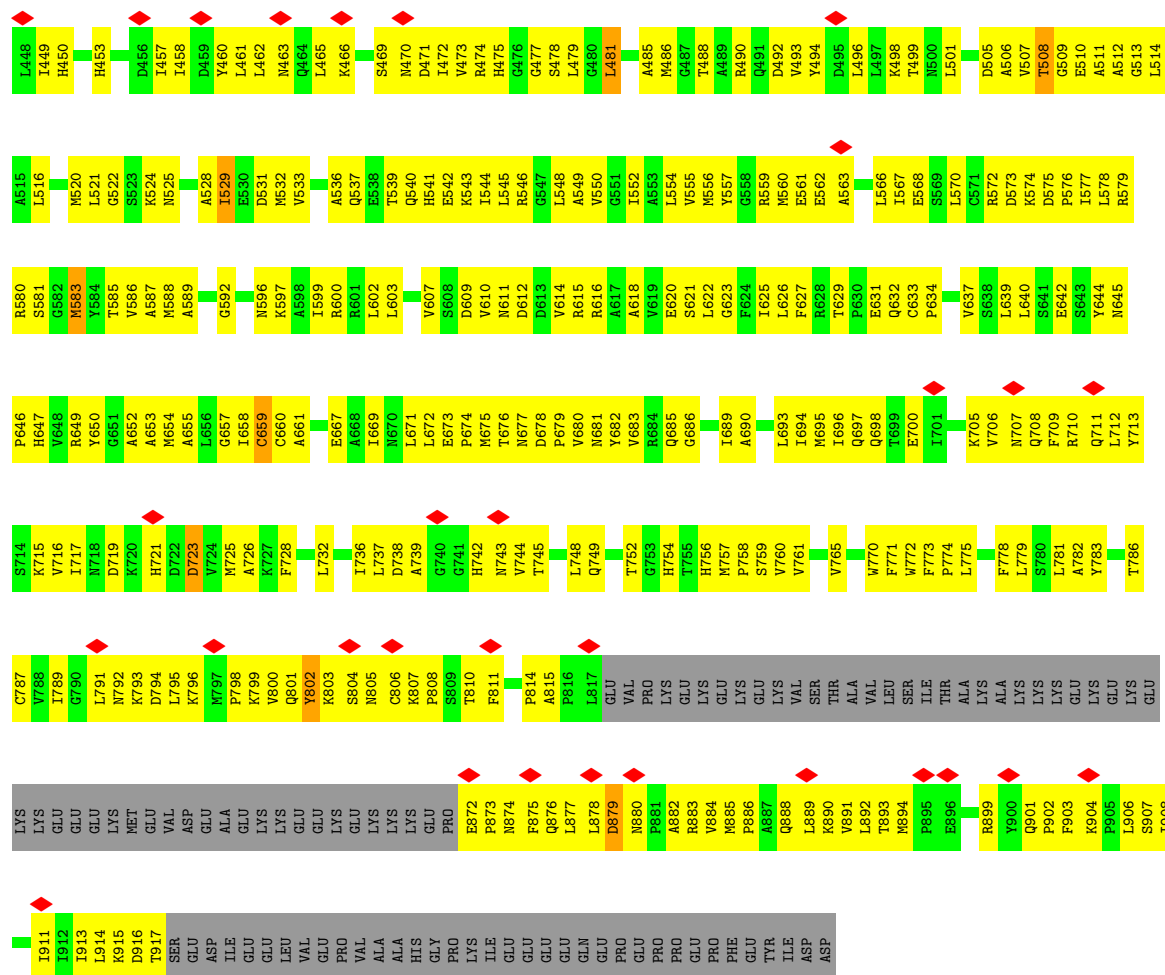
• Molecule 31: 26S proteasome regulatory subunit 6A





• Molecule 32: 26S proteasome non-ATPase regulatory subunit 1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.990	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	691.656, 689.508, 691.656	wwPDB
Map dimensions	644, 642, 644	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.19	0/2914	0.36	0/3937
2	B	0.18	0/3086	0.37	0/4164
3	C	0.19	0/3007	0.36	0/4045
4	D	0.19	0/3089	0.32	0/4168
5	E	0.19	0/2904	0.34	0/3924
6	G	0.17	0/1771	0.30	0/2403
6	g	0.16	0/1790	0.27	0/2429
7	H	0.17	0/1701	0.29	0/2318
7	h	0.17	0/1701	0.28	0/2318
8	I	0.19	0/1831	0.31	0/2487
8	i	0.16	0/1815	0.27	0/2466
9	J	0.17	0/1657	0.28	0/2261
9	j	0.16	0/1657	0.29	0/2261
10	K	0.17	0/1689	0.28	0/2294
10	k	0.15	0/1686	0.24	0/2290
11	L	0.18	0/1744	0.29	0/2371
11	l	0.16	0/1741	0.27	0/2367
12	M	0.17	0/1795	0.28	0/2434
12	m	0.16	0/1796	0.27	0/2435
13	N	0.16	0/1495	0.25	0/2026
13	n	0.16	0/1491	0.24	0/2021
14	O	0.16	0/1607	0.28	0/2185
14	o	0.17	0/1603	0.26	0/2180
15	P	0.17	0/1575	0.29	0/2128
15	p	0.18	0/1567	0.29	0/2118
16	Q	0.16	0/1541	0.25	0/2092
16	q	0.16	0/1538	0.28	0/2088
17	R	0.16	0/1535	0.25	0/2080
17	r	0.16	0/1531	0.26	0/2076
18	S	0.16	0/1614	0.27	0/2178
18	s	0.16	0/1617	0.27	0/2182
19	T	0.17	0/1606	0.26	0/2179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	t	0.17	0/1598	0.28	0/2170
20	V	0.15	0/3824	0.30	0/5170
21	W	0.15	0/3683	0.32	0/4952
22	X	0.13	0/2705	0.29	0/3648
23	Y	0.16	0/3173	0.28	0/4273
24	Z	0.18	0/2324	0.29	0/3150
25	a	0.16	0/3053	0.33	0/4133
26	b	0.15	0/1478	0.38	0/2001
27	c	0.19	0/2302	0.33	0/3110
28	d	0.15	0/2162	0.31	0/2919
29	e	0.12	0/437	0.25	0/595
30	f	0.08	0/6980	0.25	0/9433
31	F	0.19	0/2896	0.33	0/3912
32	U	0.16	0/6417	0.32	0/8684
All	All	0.16	0/102726	0.30	0/139055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2863	0	2895	357	0
2	B	3042	0	3100	418	0
3	C	2968	0	3066	334	0
4	D	3039	0	3074	353	0
5	E	2860	0	2828	338	0
6	G	1742	1660	1660	27	0
6	g	1758	1687	1687	19	0
7	H	1662	1590	1590	23	0
7	h	1662	1590	1590	18	0
8	I	1802	1741	1741	26	0
8	i	1786	1717	1717	15	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	1633	1518	1518	22	0
9	j	1633	1518	1518	20	0
10	K	1663	1592	1591	26	0
10	k	1660	1589	1589	16	0
11	L	1710	1649	1649	27	0
11	l	1707	1645	1645	22	0
12	M	1760	1680	1680	21	0
12	m	1761	1683	1683	21	0
13	N	1469	1422	1422	18	0
13	n	1465	1416	1416	17	0
14	O	1580	1559	1559	23	0
14	o	1576	1555	1555	28	0
15	P	1546	1550	1552	19	0
15	p	1538	1543	1545	24	0
16	Q	1509	1477	1477	17	0
16	q	1506	1475	1475	17	0
17	R	1504	1449	1449	23	0
17	r	1500	1438	1438	18	0
18	S	1584	1579	1579	11	0
18	s	1587	1581	1581	14	0
19	T	1576	1526	1528	20	0
19	t	1568	1511	1513	14	0
20	V	3754	0	3749	429	0
21	W	3635	0	3762	522	0
22	X	2664	0	2732	248	0
23	Y	3115	0	3120	375	0
24	Z	2281	0	2312	297	0
25	a	2995	0	3012	397	0
26	b	1458	0	1505	247	0
27	c	2260	0	2276	292	0
28	d	2116	0	2146	278	0
29	e	425	0	328	40	0
30	f	6866	0	6866	794	0
31	F	2858	0	2853	288	0
32	U	6304	0	6334	785	0
33	A	31	0	12	4	0
33	B	31	0	12	3	0
33	D	31	0	12	8	0
33	E	31	0	12	7	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	E	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	27	0	12	4	0
35	F	27	0	12	2	0
36	N	34	41	41	1	0
36	O	34	41	41	0	0
36	R	34	41	41	7	0
36	n	34	41	41	3	0
36	o	34	41	41	1	0
36	r	34	41	41	0	0
37	c	1	0	0	0	0
All	All	101338	44186	100223	6735	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 33.

The worst 5 of 6735 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)
2:B:217:LYS:HA	2:B:217:LYS:HE3	1.20	1.17
2:B:361:LYS:HD3	2:B:390:LEU:HD11	1.25	1.15
26:b:111:ALA:HB3	26:b:140:ILE:HA	1.29	1.14
2:B:342:ILE:HG23	2:B:347:ILE:HD11	1.29	1.13
3:C:248:MET:HE1	3:C:273:MET:HG3	1.14	1.13

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/433 (84%)	306 (84%)	52 (14%)	6 (2%)	8	28
2	B	386/440 (88%)	335 (87%)	50 (13%)	1 (0%)	37	66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	377/406 (93%)	329 (87%)	44 (12%)	4 (1%)	12	37
4	D	378/418 (90%)	332 (88%)	45 (12%)	1 (0%)	37	66
5	E	373/403 (93%)	331 (89%)	41 (11%)	1 (0%)	37	66
6	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
6	g	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
7	H	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
7	h	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
8	I	245/261 (94%)	239 (98%)	6 (2%)	0	100	100
8	i	245/261 (94%)	242 (99%)	3 (1%)	0	100	100
9	J	230/248 (93%)	221 (96%)	9 (4%)	0	100	100
9	j	230/248 (93%)	221 (96%)	9 (4%)	0	100	100
10	K	231/241 (96%)	225 (97%)	6 (3%)	0	100	100
10	k	231/241 (96%)	227 (98%)	4 (2%)	0	100	100
11	L	231/263 (88%)	220 (95%)	10 (4%)	1 (0%)	30	60
11	l	231/263 (88%)	224 (97%)	7 (3%)	0	100	100
12	M	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
12	m	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
13	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
13	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
14	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	P	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
15	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
16	Q	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	25	56
16	q	194/201 (96%)	186 (96%)	8 (4%)	0	100	100
17	R	198/263 (75%)	197 (100%)	1 (0%)	0	100	100
17	r	198/263 (75%)	194 (98%)	4 (2%)	0	100	100
18	S	210/241 (87%)	205 (98%)	5 (2%)	0	100	100
18	s	210/241 (87%)	209 (100%)	1 (0%)	0	100	100
19	T	210/264 (80%)	199 (95%)	11 (5%)	0	100	100
19	t	210/264 (80%)	198 (94%)	12 (6%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	V	470/534 (88%)	450 (96%)	20 (4%)	0	100	100
21	W	444/456 (97%)	409 (92%)	34 (8%)	1 (0%)	44	73
22	X	332/422 (79%)	315 (95%)	17 (5%)	0	100	100
23	Y	376/389 (97%)	355 (94%)	21 (6%)	0	100	100
24	Z	284/324 (88%)	252 (89%)	31 (11%)	1 (0%)	30	60
25	a	371/376 (99%)	327 (88%)	44 (12%)	0	100	100
26	b	189/377 (50%)	146 (77%)	40 (21%)	3 (2%)	8	28
27	c	285/310 (92%)	254 (89%)	30 (10%)	1 (0%)	30	60
28	d	255/350 (73%)	220 (86%)	35 (14%)	0	100	100
29	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
30	f	887/908 (98%)	840 (95%)	47 (5%)	0	100	100
31	F	372/439 (85%)	334 (90%)	37 (10%)	1 (0%)	37	66
32	U	802/953 (84%)	752 (94%)	49 (6%)	1 (0%)	48	77
All	All	13135/14884 (88%)	12297 (94%)	815 (6%)	23 (0%)	45	73

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	109	PRO
1	A	424	SER
3	C	91	PRO
4	D	413	GLU

### 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	310/372 (83%)	296 (96%)	14 (4%)	23	56
2	B	341/385 (89%)	312 (92%)	29 (8%)	8	27
3	C	325/352 (92%)	315 (97%)	10 (3%)	35	70

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	333/366 (91%)	316 (95%)	17 (5%)	20	51
5	E	298/353 (84%)	282 (95%)	16 (5%)	18	49
6	G	165/210 (79%)	161 (98%)	4 (2%)	44	76
6	g	168/210 (80%)	166 (99%)	2 (1%)	67	89
7	H	150/191 (78%)	148 (99%)	2 (1%)	65	88
7	h	150/191 (78%)	149 (99%)	1 (1%)	81	94
8	I	166/221 (75%)	160 (96%)	6 (4%)	30	65
8	i	160/221 (72%)	155 (97%)	5 (3%)	35	70
9	J	136/211 (64%)	134 (98%)	2 (2%)	60	85
9	j	136/211 (64%)	133 (98%)	3 (2%)	47	78
10	K	159/203 (78%)	156 (98%)	3 (2%)	52	81
10	k	158/203 (78%)	154 (98%)	4 (2%)	42	75
11	L	161/224 (72%)	155 (96%)	6 (4%)	29	64
11	l	161/224 (72%)	161 (100%)	0	100	100
12	M	162/212 (76%)	158 (98%)	4 (2%)	42	75
12	m	163/212 (77%)	159 (98%)	4 (2%)	42	75
13	N	141/181 (78%)	136 (96%)	5 (4%)	31	66
13	n	140/181 (77%)	138 (99%)	2 (1%)	62	86
14	O	158/228 (69%)	153 (97%)	5 (3%)	34	69
14	o	157/228 (69%)	156 (99%)	1 (1%)	84	95
15	P	159/174 (91%)	158 (99%)	1 (1%)	84	95
15	p	156/174 (90%)	154 (99%)	2 (1%)	65	88
16	Q	149/171 (87%)	146 (98%)	3 (2%)	50	79
16	q	148/171 (86%)	147 (99%)	1 (1%)	81	94
17	R	139/202 (69%)	135 (97%)	4 (3%)	37	72
17	r	138/202 (68%)	132 (96%)	6 (4%)	25	57
18	S	158/199 (79%)	156 (99%)	2 (1%)	65	88
18	s	159/199 (80%)	157 (99%)	2 (1%)	65	88
19	T	151/215 (70%)	150 (99%)	1 (1%)	81	94
19	t	149/215 (69%)	148 (99%)	1 (1%)	81	94
20	V	391/460 (85%)	372 (95%)	19 (5%)	21	53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	W	410/416 (99%)	390 (95%)	20 (5%)	21	53
22	X	291/362 (80%)	279 (96%)	12 (4%)	26	60
23	Y	334/344 (97%)	318 (95%)	16 (5%)	21	54
24	Z	257/295 (87%)	237 (92%)	20 (8%)	10	31
25	a	333/336 (99%)	317 (95%)	16 (5%)	21	54
26	b	167/312 (54%)	158 (95%)	9 (5%)	18	49
27	c	252/268 (94%)	232 (92%)	20 (8%)	10	30
28	d	231/294 (79%)	217 (94%)	14 (6%)	15	43
29	e	44/63 (70%)	42 (96%)	2 (4%)	23	56
30	f	745/763 (98%)	730 (98%)	15 (2%)	50	79
31	F	296/379 (78%)	271 (92%)	25 (8%)	9	28
32	U	688/816 (84%)	657 (96%)	31 (4%)	23	56
All	All	10343/12620 (82%)	9956 (96%)	387 (4%)	31	64

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	a	273	GLN
30	f	350	LYS
26	b	51	LEU
27	c	245	VAL
8	i	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
23	Y	367	GLN
32	U	777	HIS
26	b	27	GLN
32	U	685	GLN
31	F	194	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	ADP	F	501	-	24,29,29	0.83	0	29,45,45	1.21	2 (6%)
33	ATP	D	501	-	28,33,33	0.84	0	34,52,52	0.75	2 (5%)
36	LDZ	N	301	-	33,34,34	0.55	1 (3%)	42,44,44	0.80	1 (2%)
36	LDZ	O	301	-	33,34,34	0.54	1 (3%)	42,44,44	0.66	1 (2%)
33	ATP	E	402	34	28,33,33	0.73	0	34,52,52	0.73	2 (5%)
36	LDZ	o	301	-	33,34,34	0.50	1 (3%)	42,44,44	0.71	1 (2%)
36	LDZ	R	301	-	33,34,34	0.50	1 (3%)	42,44,44	0.74	1 (2%)
36	LDZ	r	301	-	33,34,34	0.52	1 (3%)	42,44,44	0.92	1 (2%)
35	ADP	C	501	-	24,29,29	0.82	0	29,45,45	1.24	2 (6%)
36	LDZ	n	301	-	33,34,34	0.52	1 (3%)	42,44,44	0.77	1 (2%)
33	ATP	A	501	34	28,33,33	0.85	1 (3%)	34,52,52	0.65	1 (2%)
33	ATP	B	501	34	28,33,33	0.67	0	34,52,52	0.90	2 (5%)

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	ADP	F	501	-	-	2/12/32/32	0/3/3/3
33	ATP	D	501	-	-	0/18/38/38	0/3/3/3
36	LDZ	N	301	-	-	11/38/39/39	0/1/1/1
36	LDZ	O	301	-	-	13/38/39/39	0/1/1/1
33	ATP	E	402	34	-	5/18/38/38	0/3/3/3
36	LDZ	o	301	-	-	5/38/39/39	0/1/1/1
36	LDZ	R	301	-	-	4/38/39/39	0/1/1/1
36	LDZ	r	301	-	-	13/38/39/39	0/1/1/1
35	ADP	C	501	-	-	3/12/32/32	0/3/3/3
36	LDZ	n	301	-	-	13/38/39/39	0/1/1/1
33	ATP	A	501	34	-	3/18/38/38	0/3/3/3
33	ATP	B	501	34	-	3/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	301	LDZ	C17-N16	-2.29	1.43	1.46
36	N	301	LDZ	C17-N16	-2.27	1.43	1.46
36	o	301	LDZ	C17-N16	-2.06	1.43	1.46
36	r	301	LDZ	C17-N16	-2.05	1.43	1.46
33	A	501	ATP	PB-O3B	-2.04	1.57	1.59

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	501	ATP	C4'-O4'-C1'	-3.90	106.35	109.92
36	r	301	LDZ	C14-N13-C12	3.87	129.96	121.65
35	C	501	ADP	N3-C2-N1	-3.74	123.60	128.67
35	F	501	ADP	N3-C2-N1	-3.63	123.75	128.67
36	N	301	LDZ	C15-C14-N13	-2.97	103.08	111.11

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	501	ATP	PB-O3B-PG-O3G
33	B	501	ATP	C4'-C5'-O5'-PA
33	E	402	ATP	C5'-O5'-PA-O2A
33	E	402	ATP	C5'-O5'-PA-O3A
35	C	501	ADP	C5'-O5'-PA-O1A

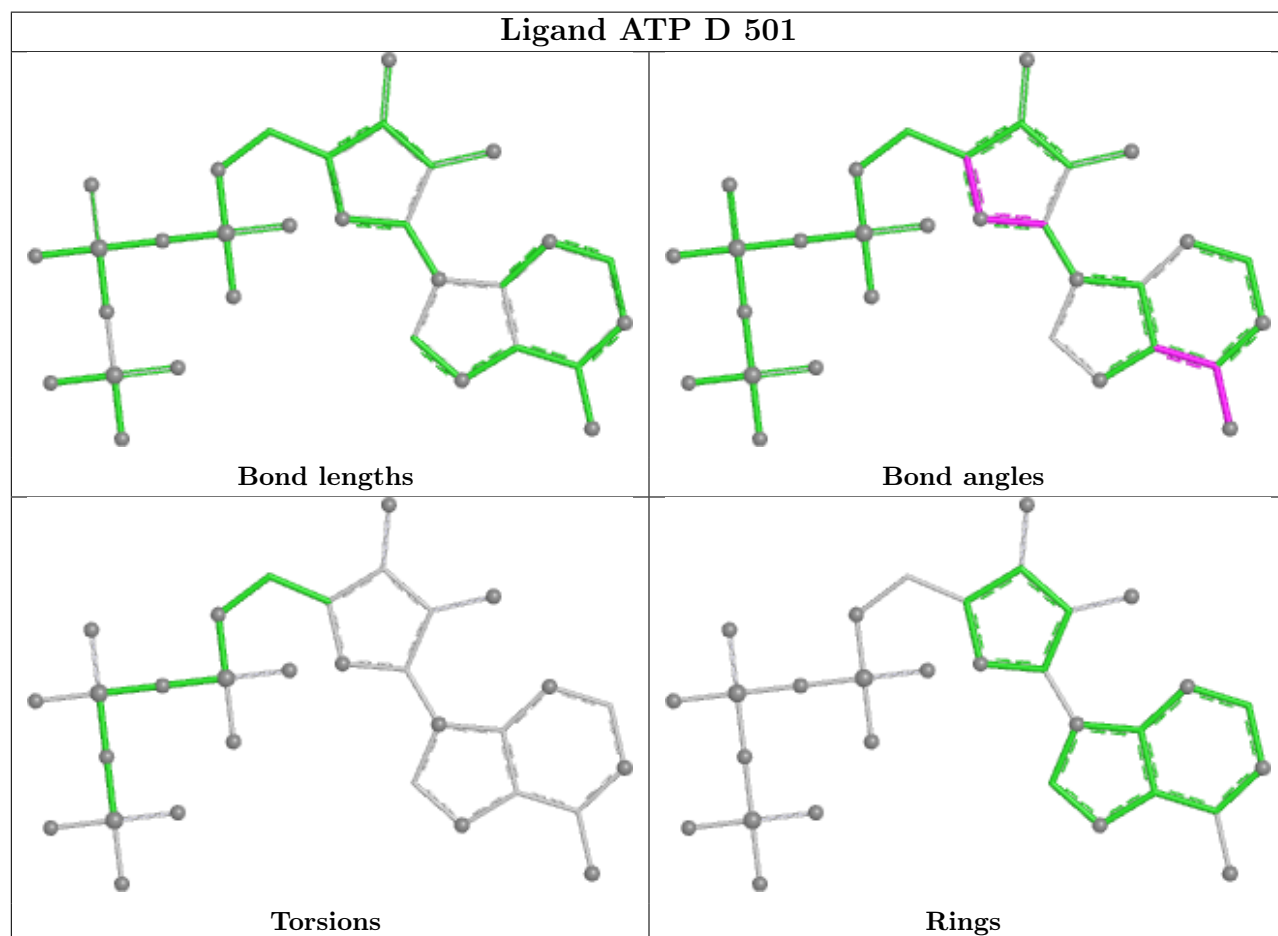
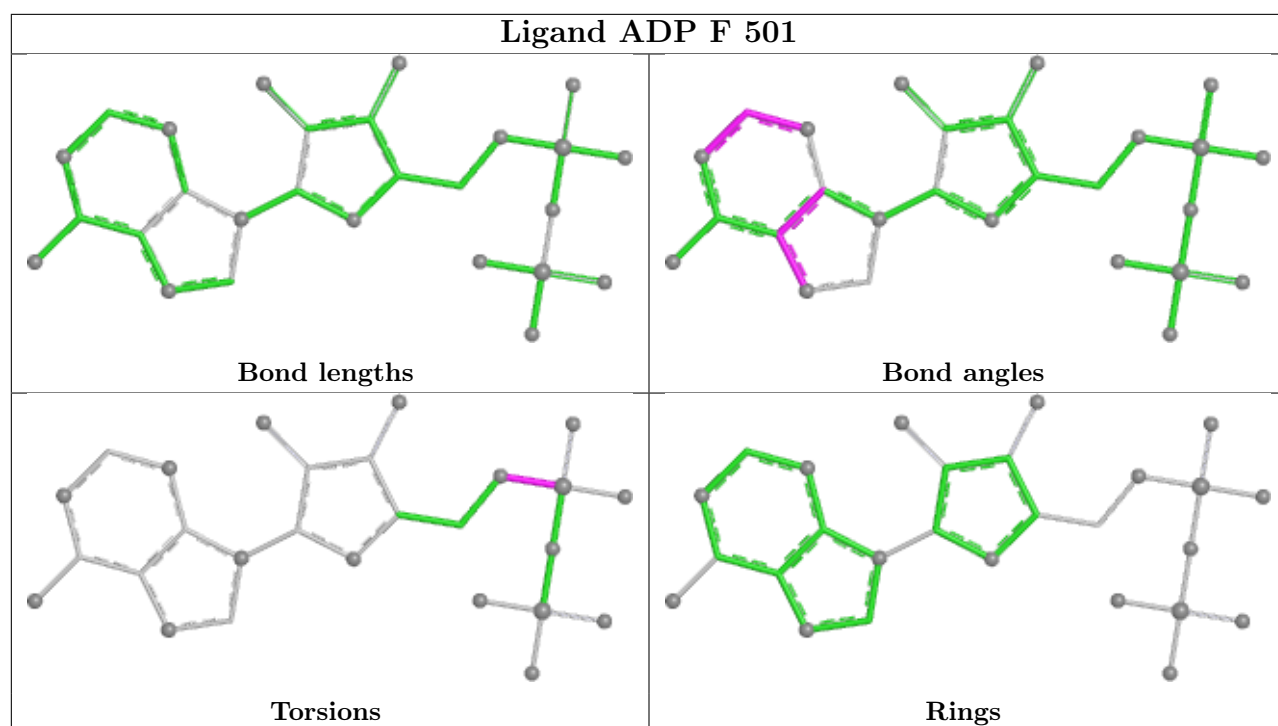


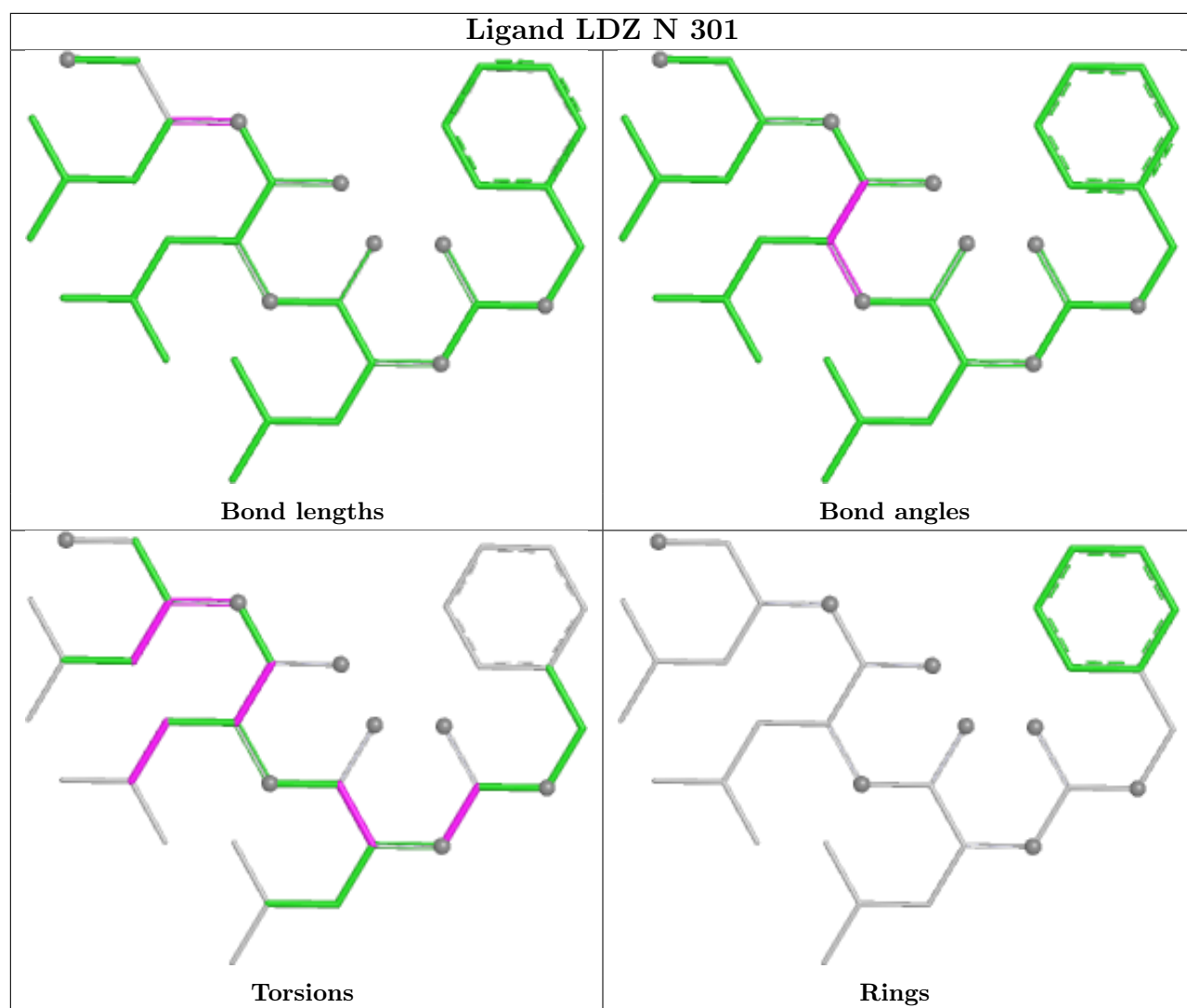
There are no ring outliers.

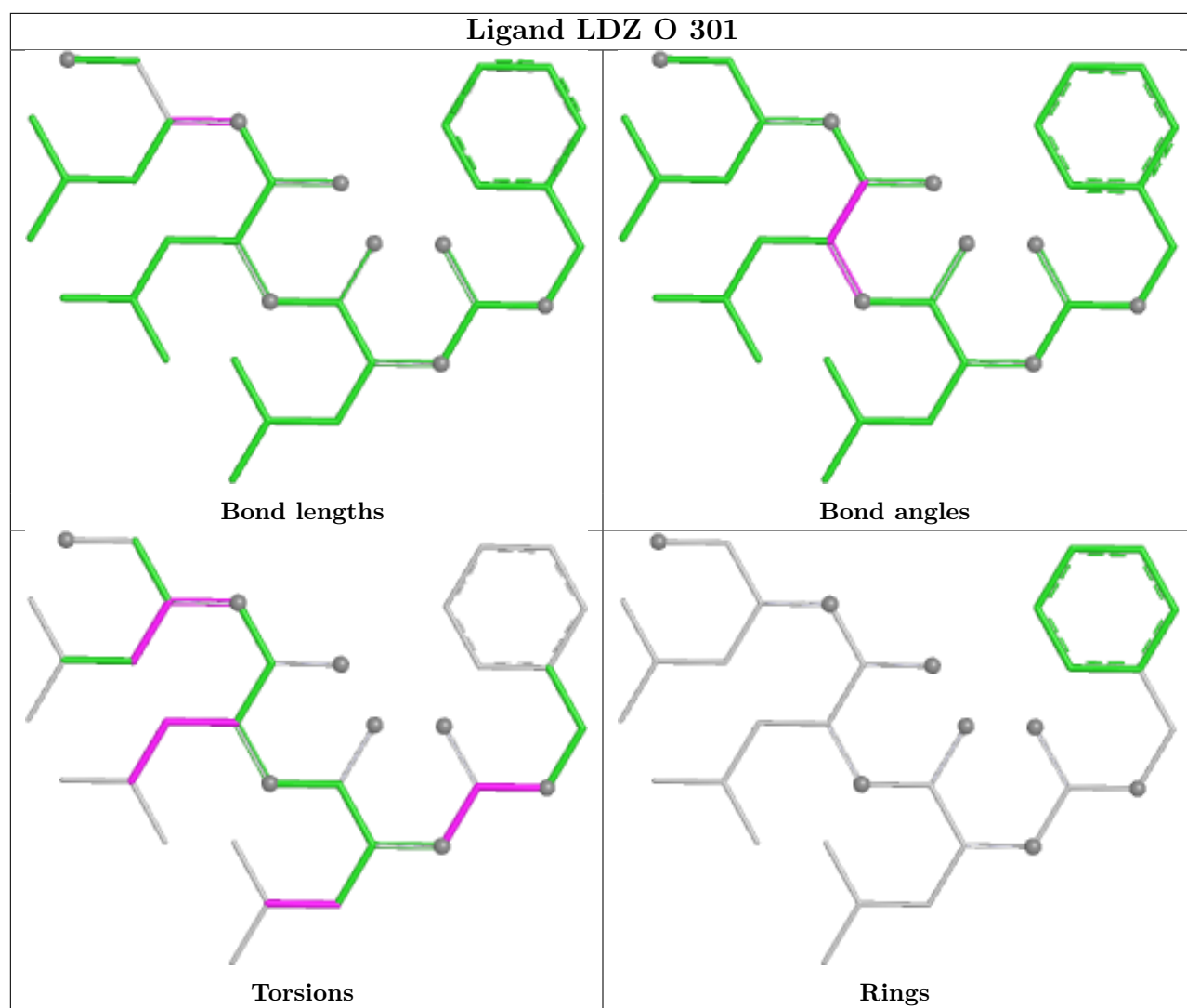
10 monomers are involved in 40 short contacts:

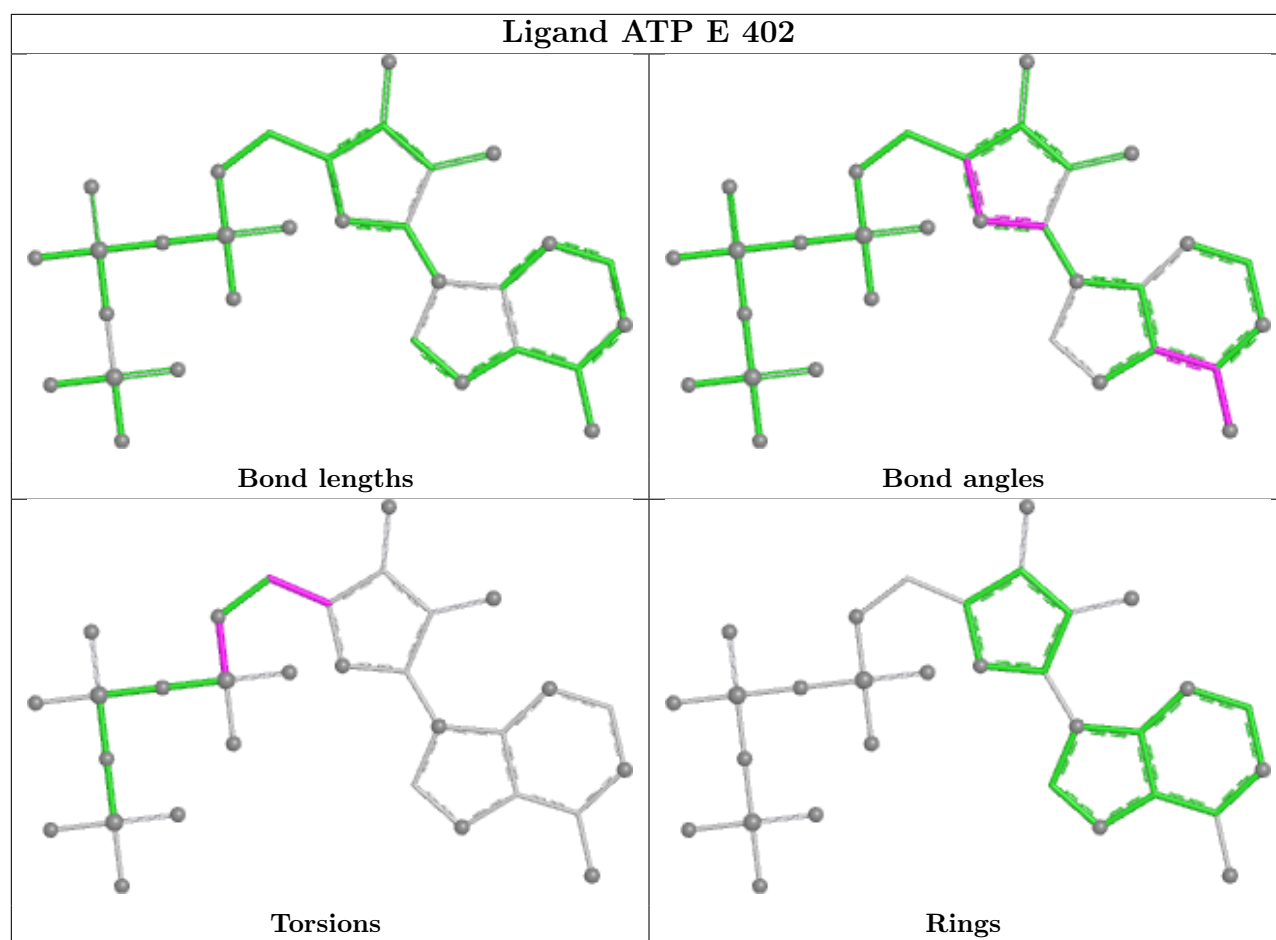
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	F	501	ADP	2	0
33	D	501	ATP	8	0
36	N	301	LDZ	1	0
33	E	402	ATP	7	0
36	o	301	LDZ	1	0
36	R	301	LDZ	7	0
35	C	501	ADP	4	0
36	n	301	LDZ	3	0
33	A	501	ATP	4	0
33	B	501	ATP	3	0

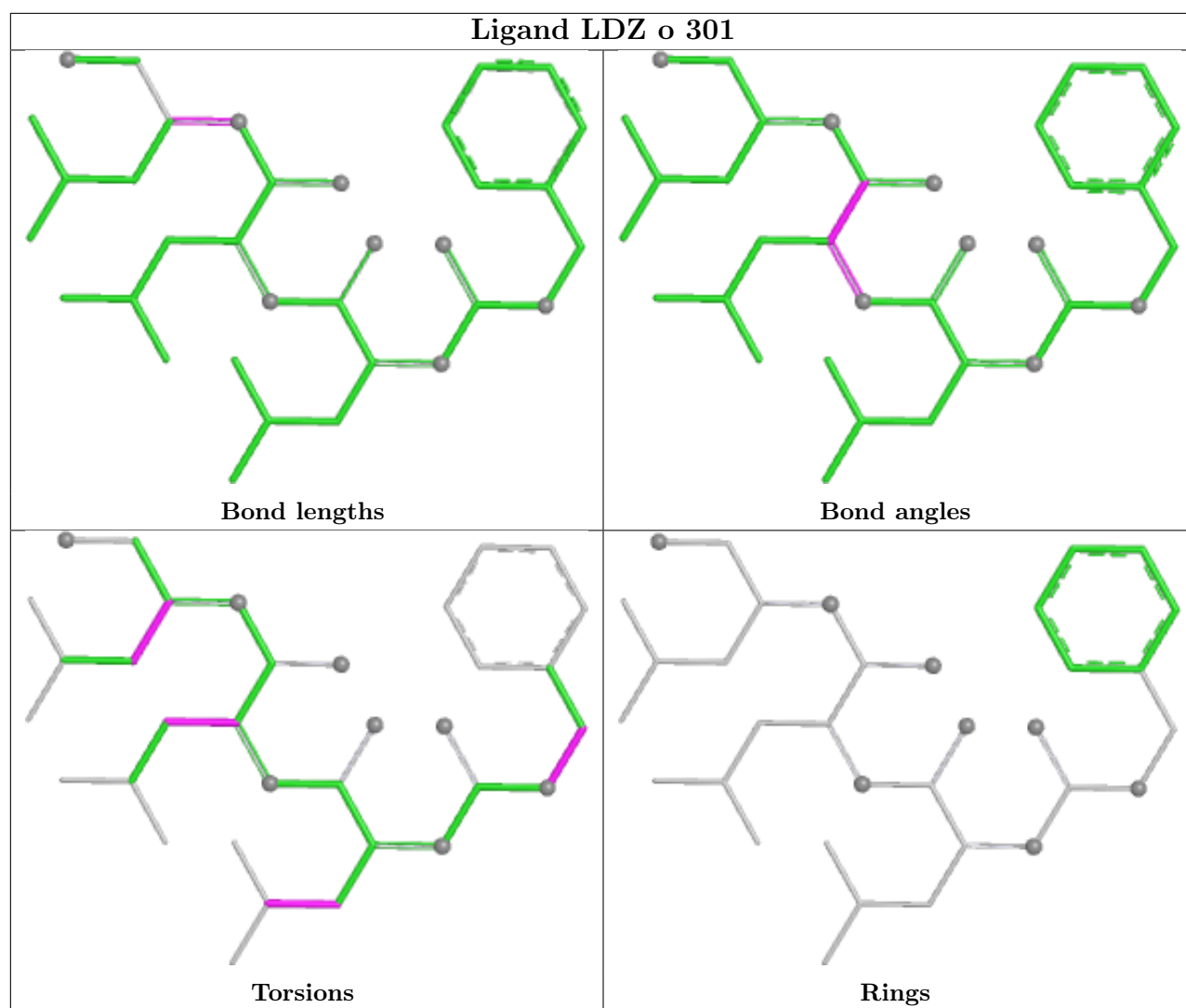
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

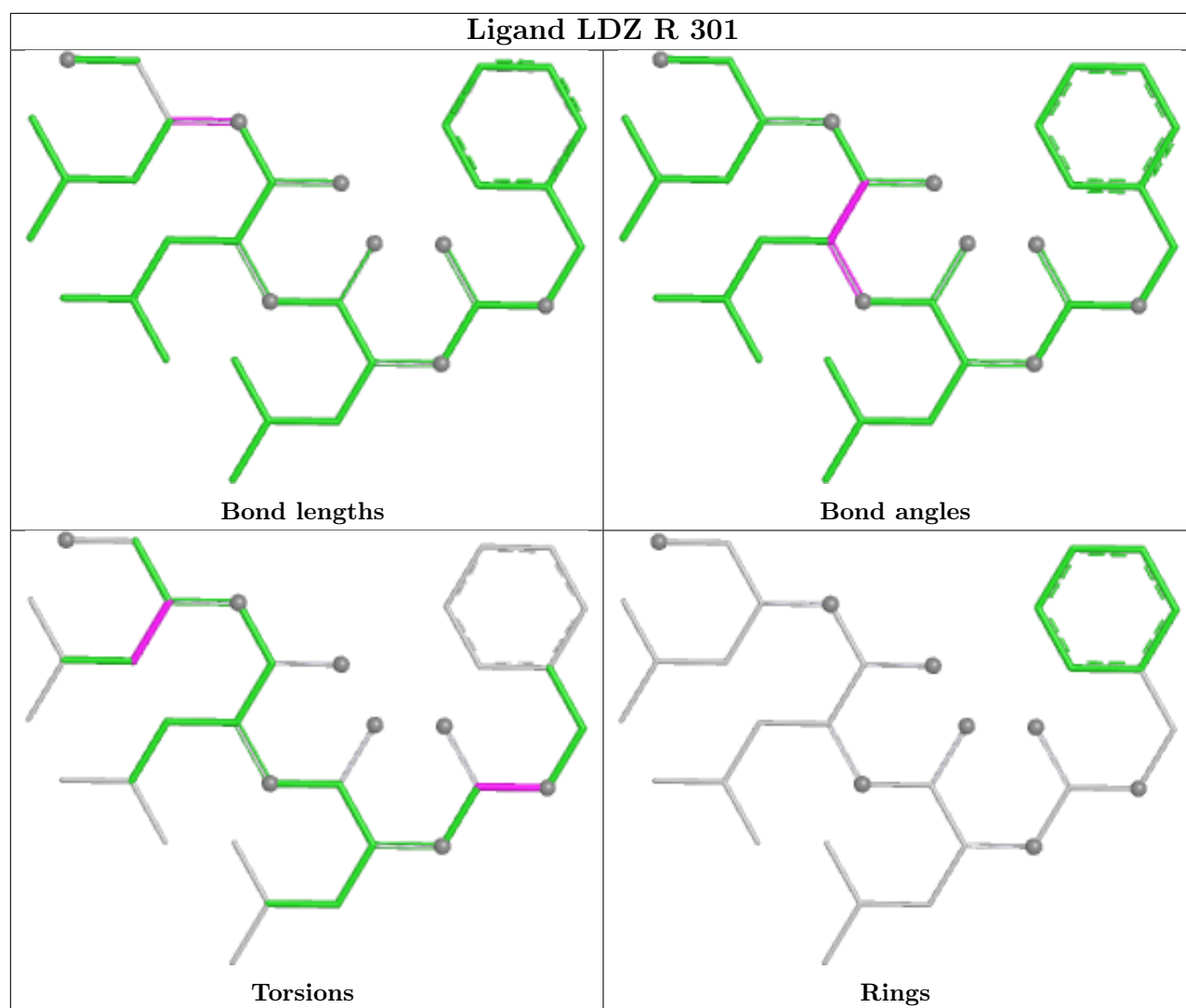


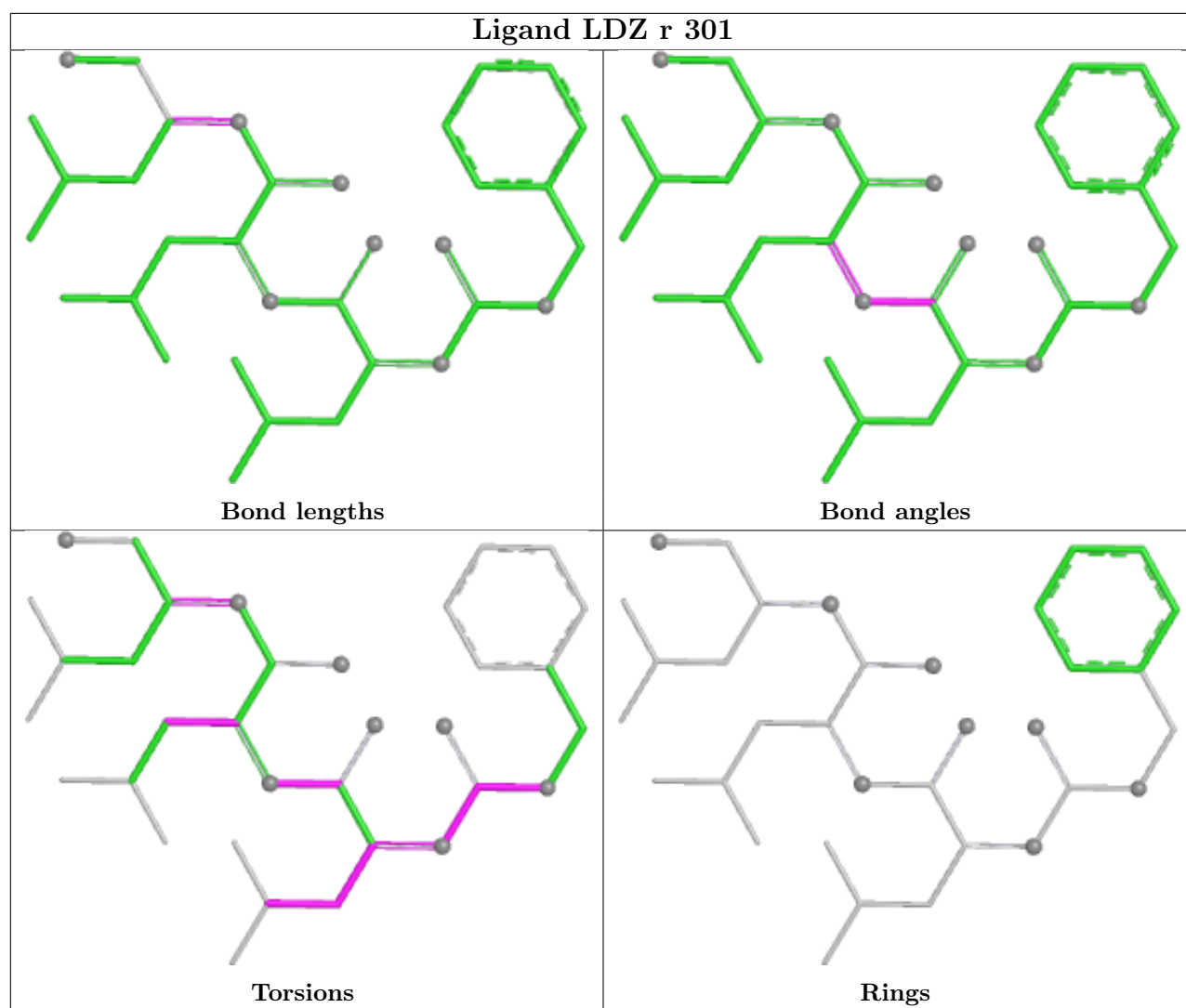




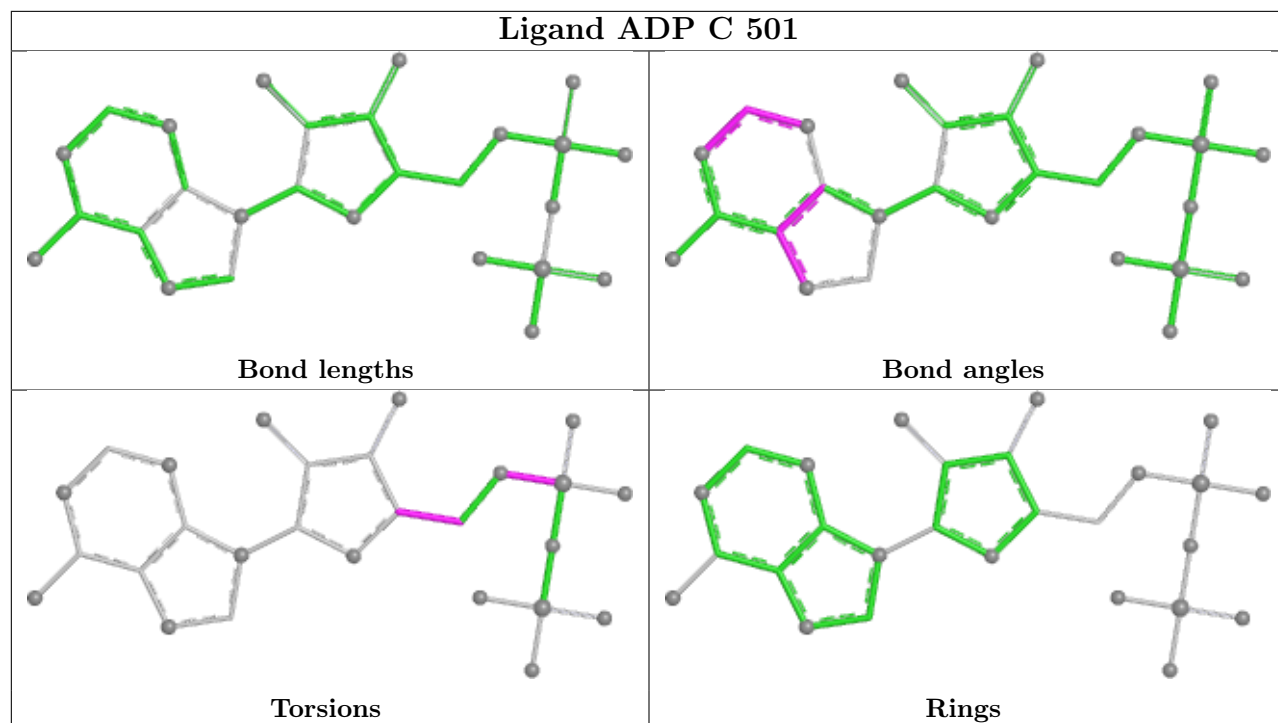


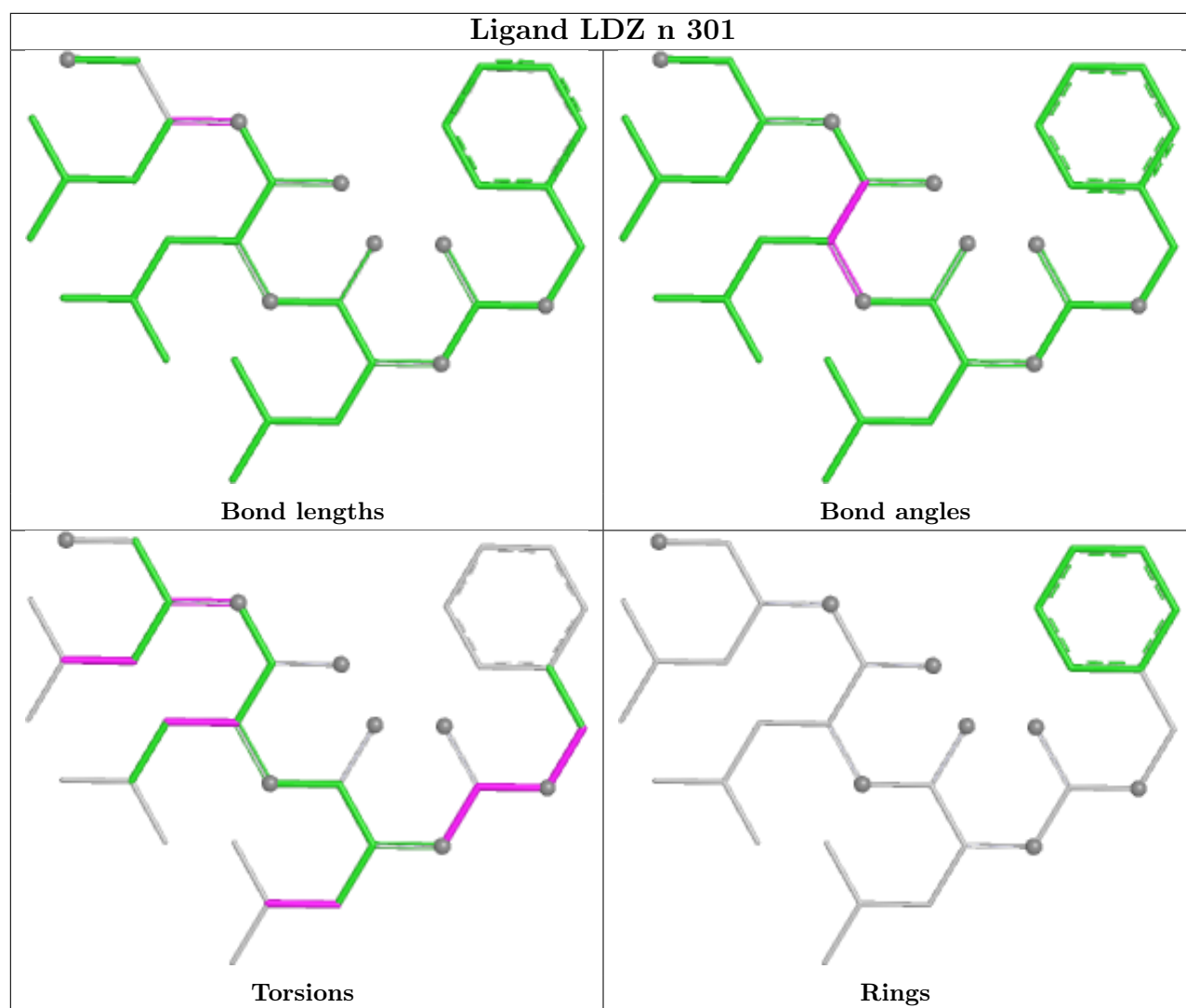


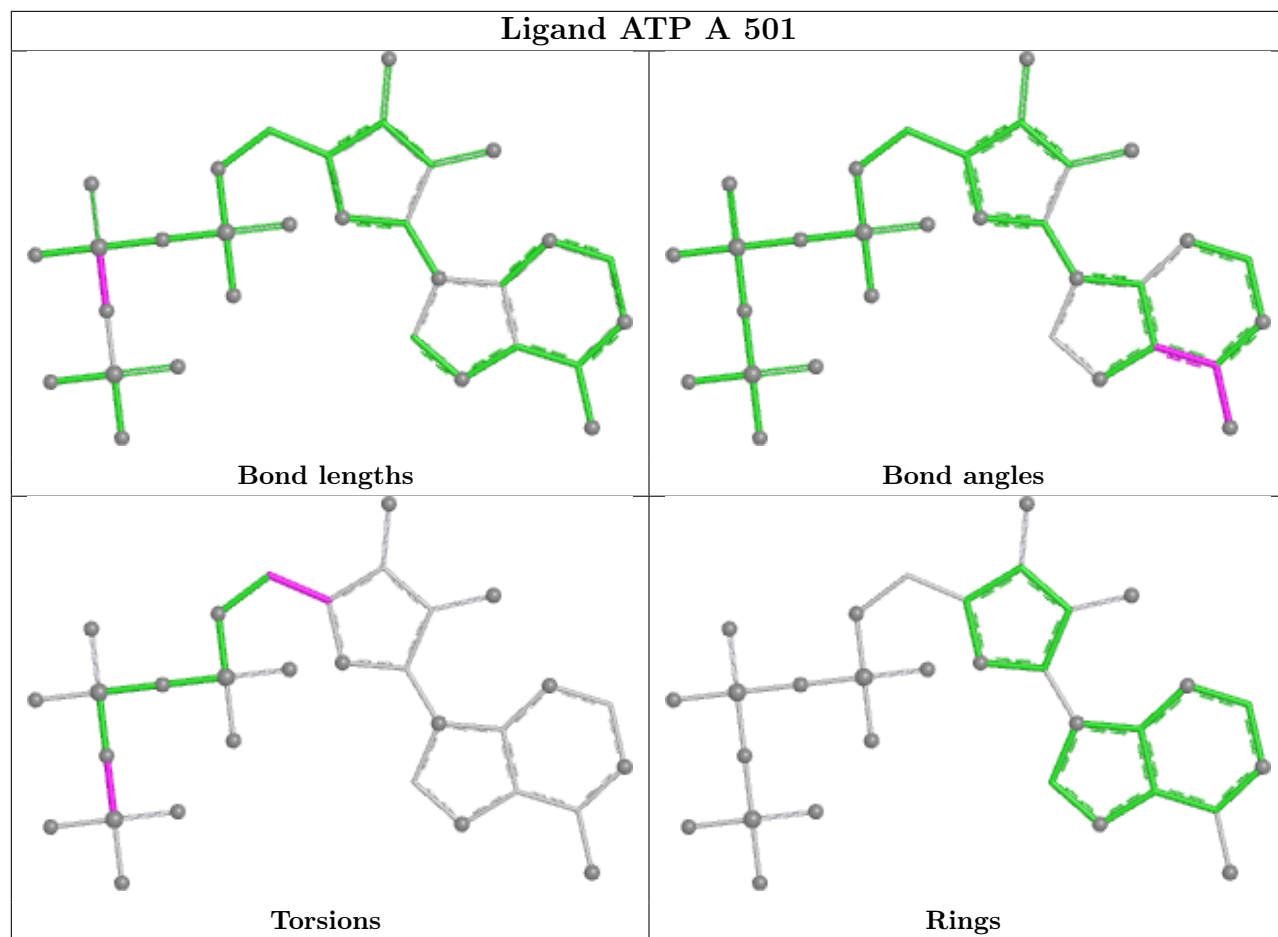


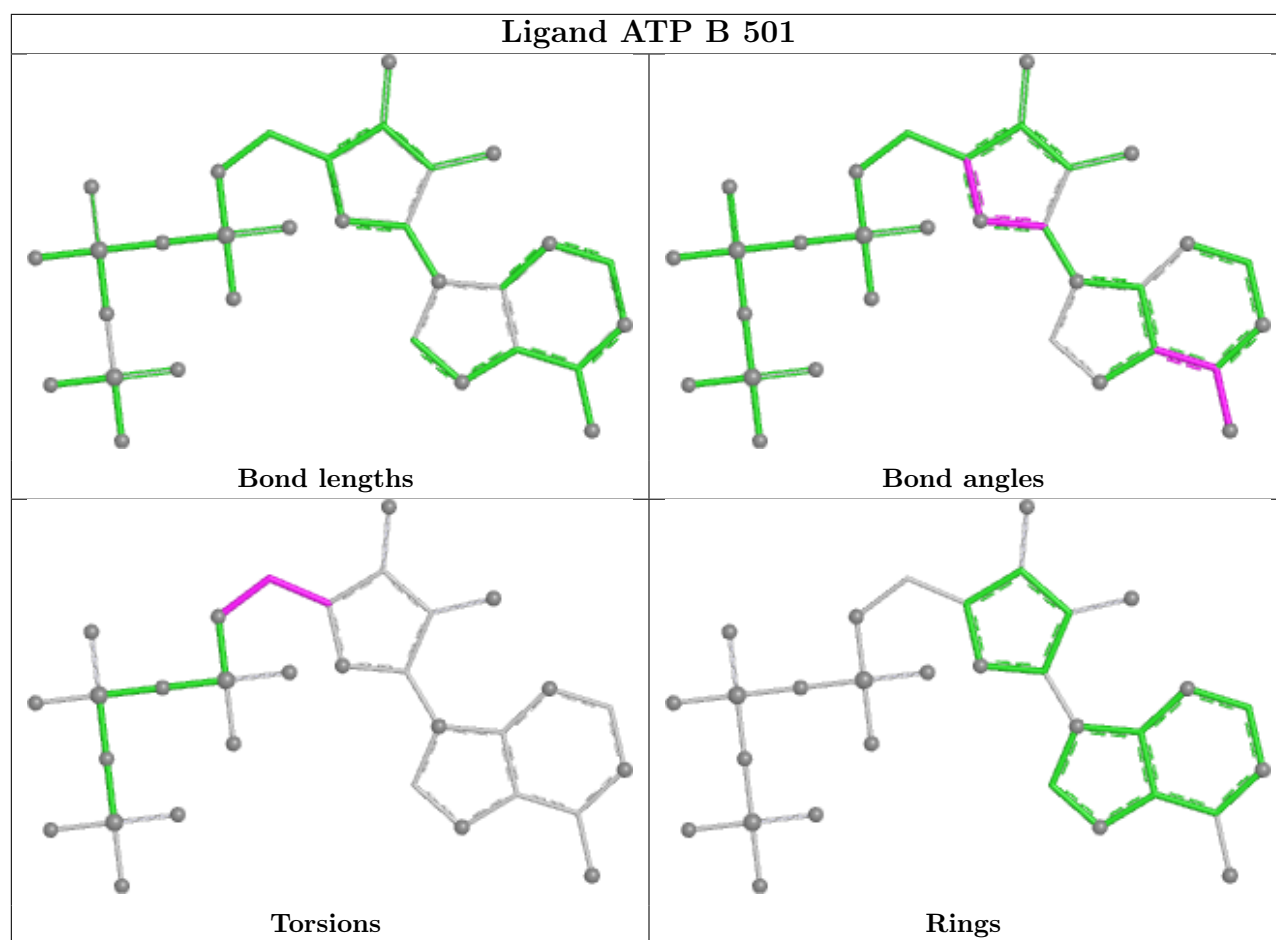












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49507. These allow visual inspection of the internal detail of the map and identification of artifacts.

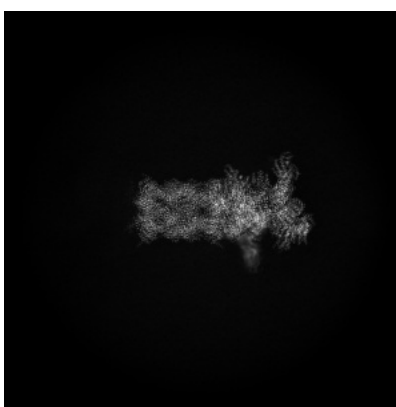
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

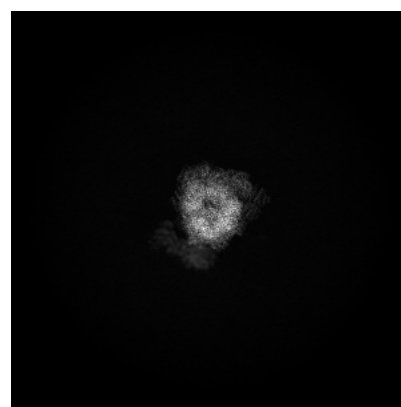
#### 6.1.1 Primary map



X



Y



Z

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

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

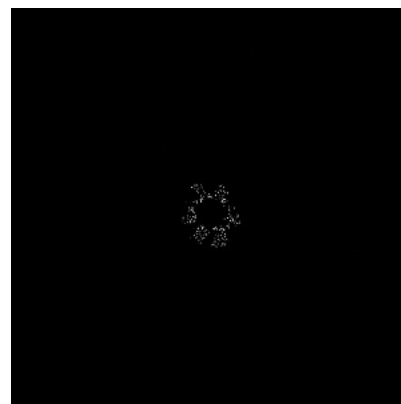
#### 6.2.1 Primary map



X Index: 322



Y Index: 321

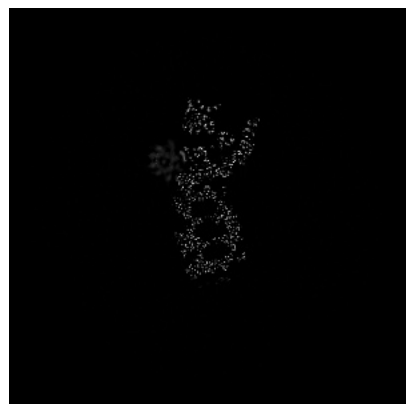


Z Index: 322

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: 309



Y Index: 300



Z Index: 454

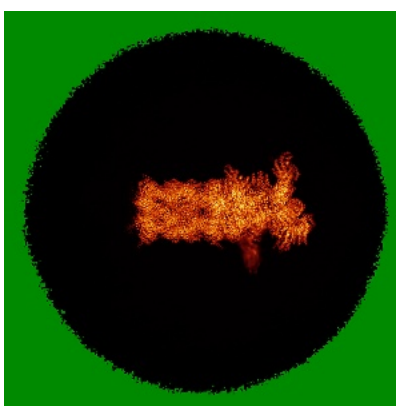
The images above show the largest variance slices of the map in three orthogonal directions.

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

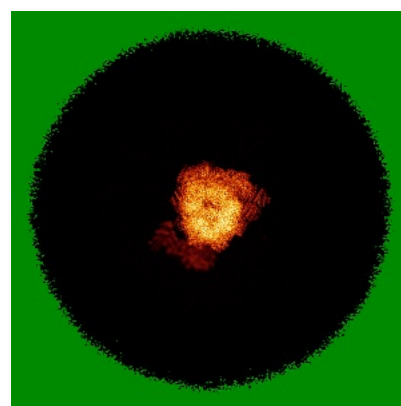
### 6.4.1 Primary map



X



Y

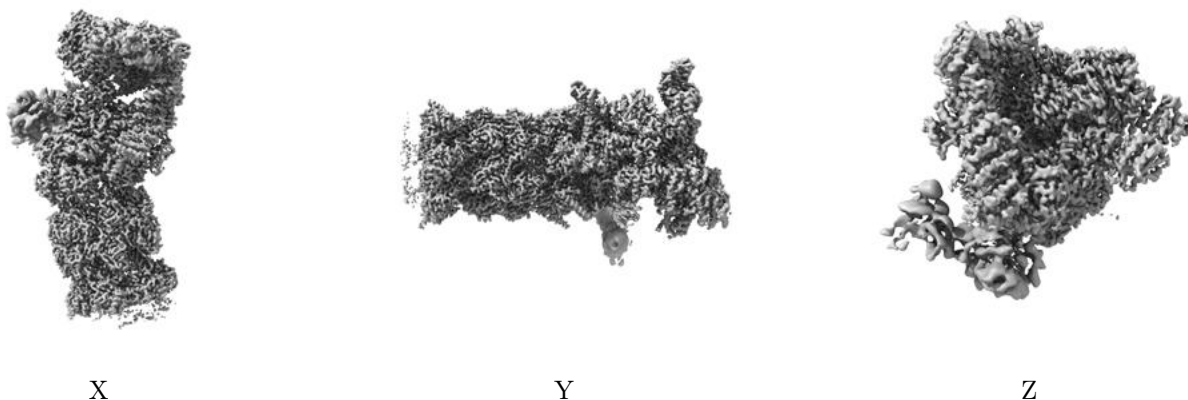


Z

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 0.165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

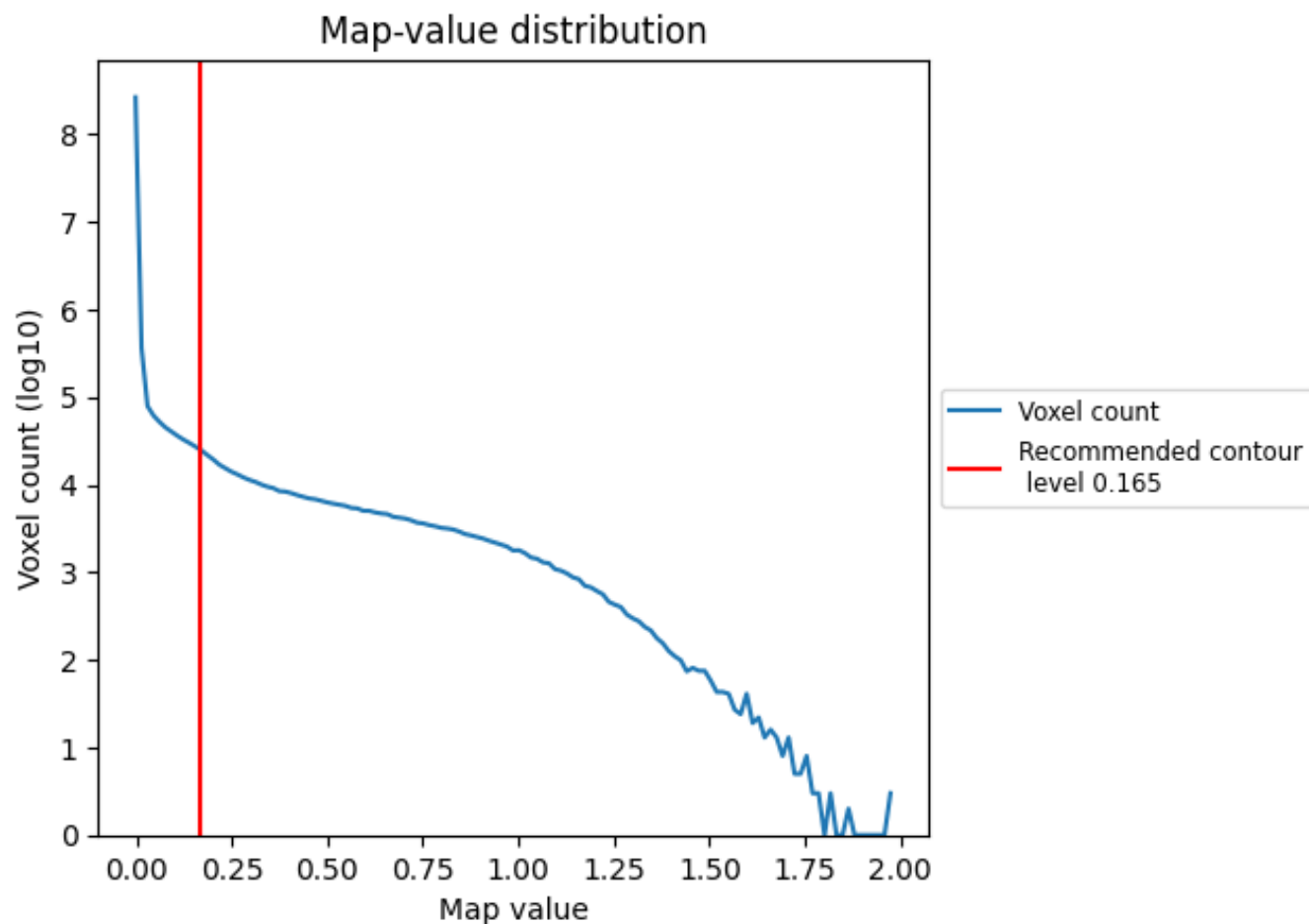
## 6.6 Mask visualisation [i](#)

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.

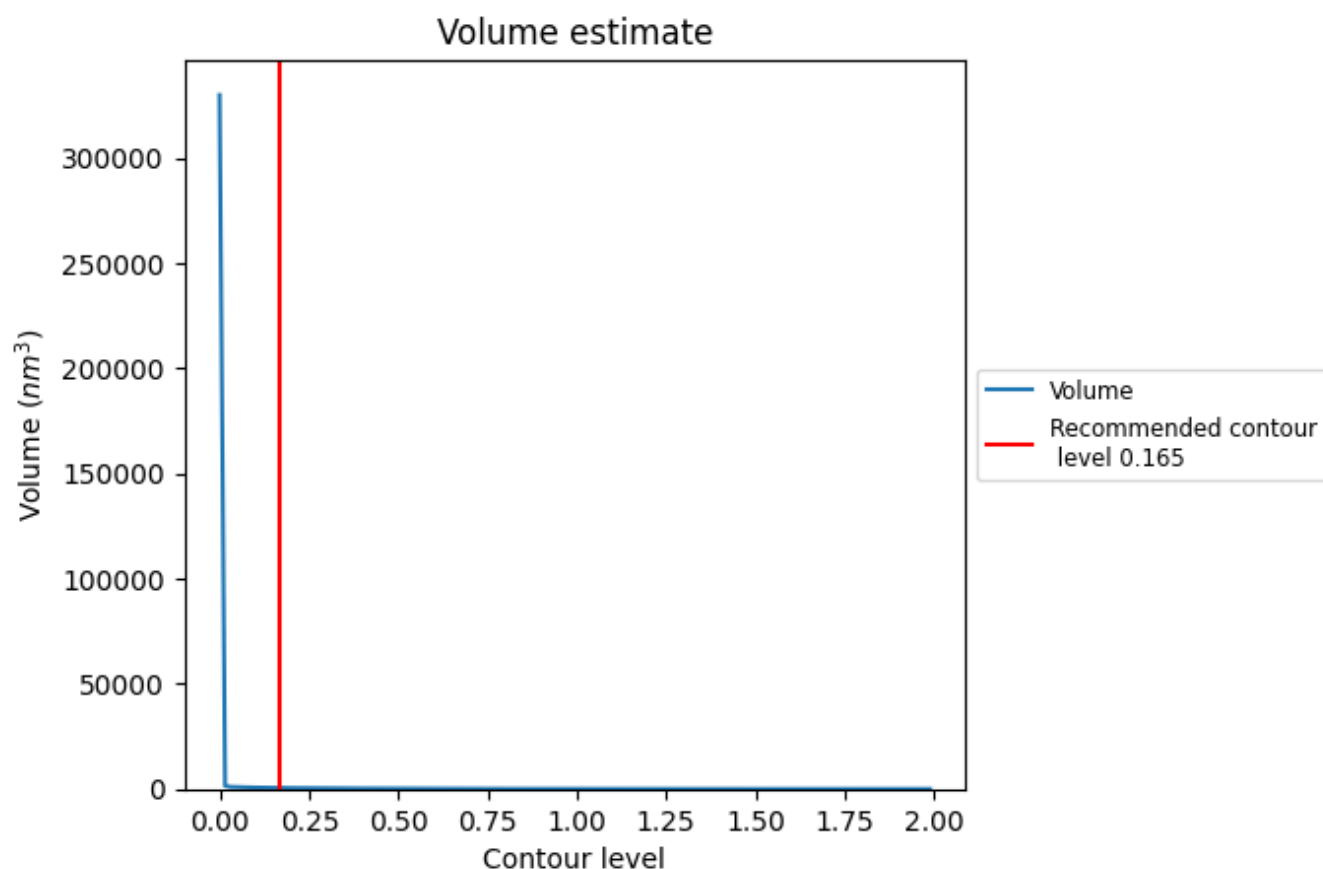
### 7.1 Map-value distribution [i](#)



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 497 nm<sup>3</sup>; this corresponds to an approximate mass of 449 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

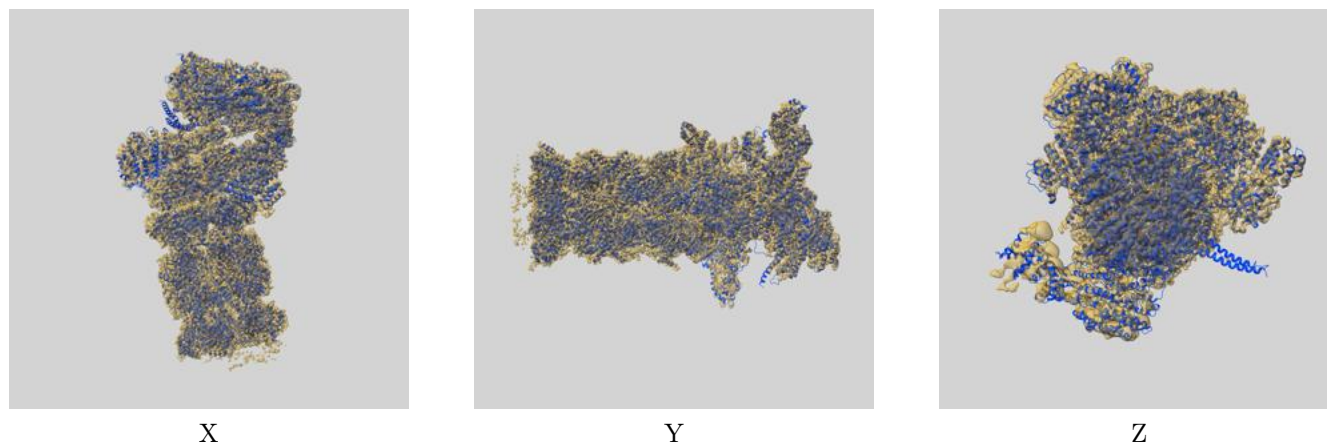
## 8 Fourier-Shell correlation

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

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

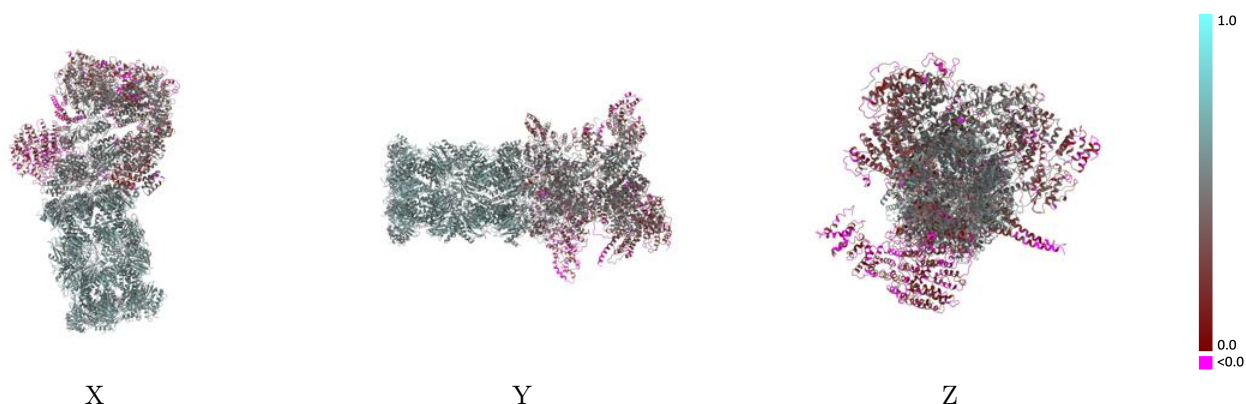
This section contains information regarding the fit between EMDB map EMD-49507 and PDB model 9NKF. Per-residue inclusion information can be found in section 3 on page 13.

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



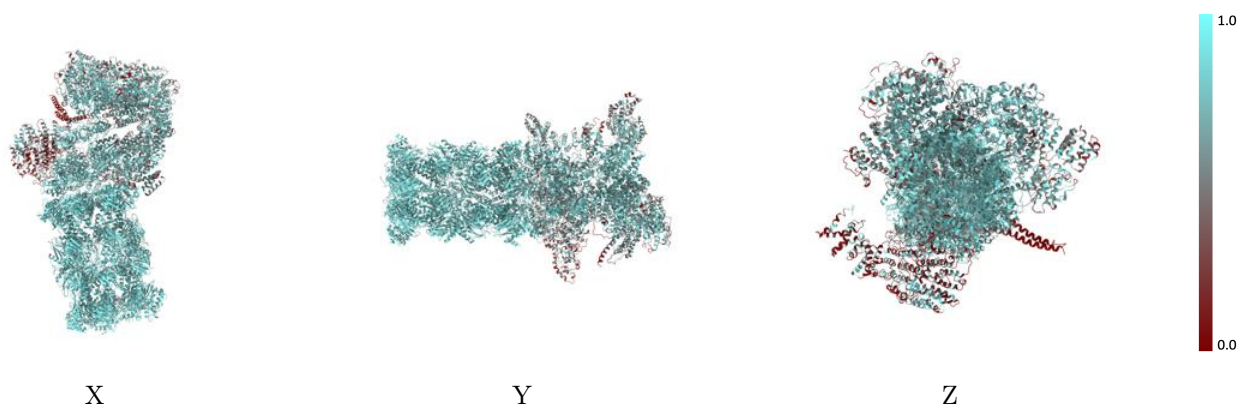
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



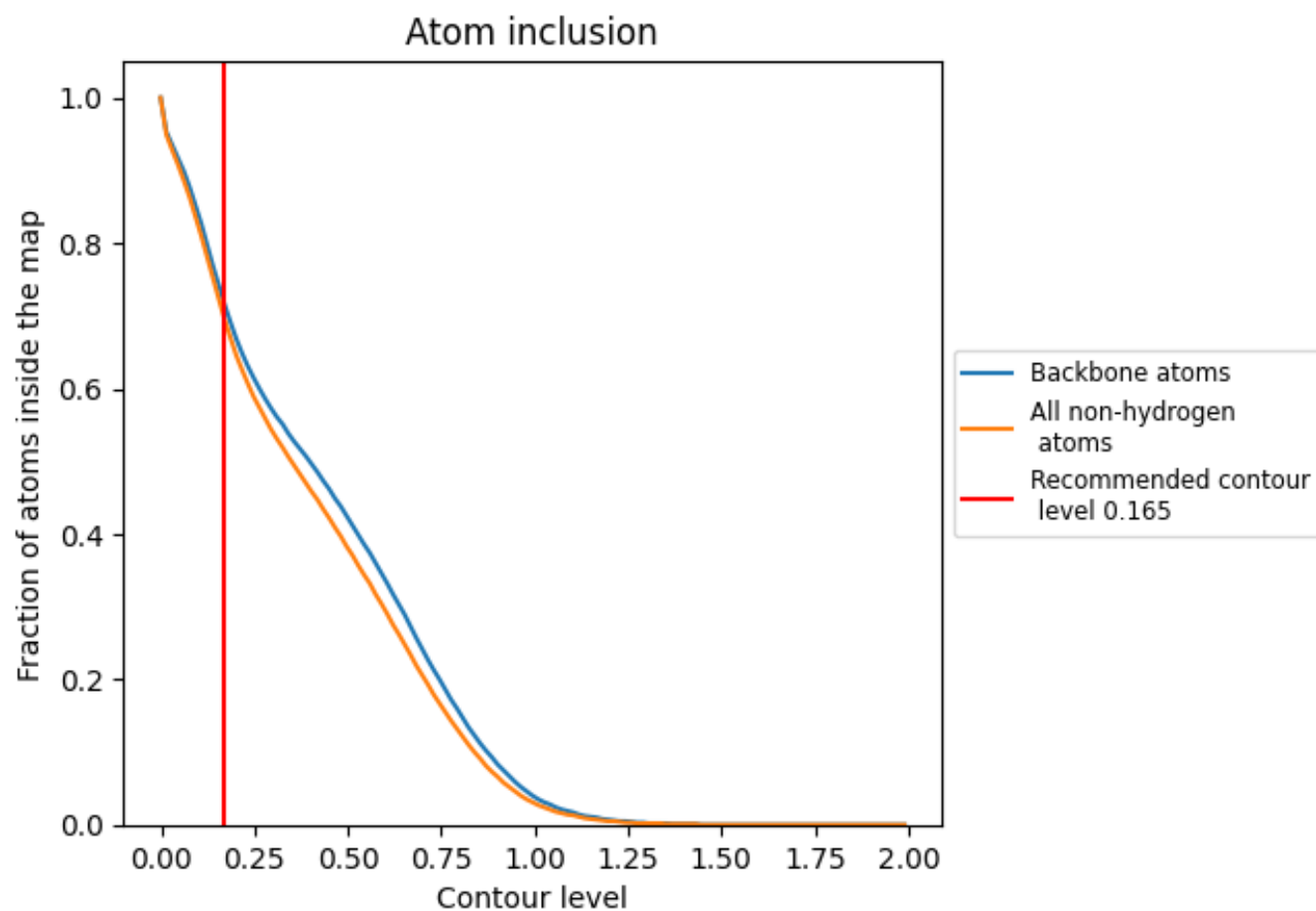
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.4450
A	 0.7920	 0.4600
B	 0.6900	 0.3920
C	 0.7200	 0.4500
D	 0.7410	 0.4630
E	 0.7280	 0.4590
F	 0.7060	 0.4510
G	 0.8350	 0.5330
H	 0.8500	 0.5530
I	 0.8230	 0.5480
J	 0.8520	 0.5590
K	 0.8200	 0.5460
L	 0.8480	 0.5620
M	 0.8290	 0.5430
N	 0.8060	 0.5640
O	 0.7820	 0.5670
P	 0.7960	 0.5650
Q	 0.8280	 0.5750
R	 0.8200	 0.5730
S	 0.8060	 0.5710
T	 0.8260	 0.5700
U	 0.6610	 0.3550
V	 0.5890	 0.3150
W	 0.6160	 0.3330
X	 0.6240	 0.3900
Y	 0.6510	 0.3810
Z	 0.7060	 0.4050
a	 0.6230	 0.3350
b	 0.5920	 0.3200
c	 0.7140	 0.4250
d	 0.5510	 0.2510
e	 0.4560	 0.2660
f	 0.3110	 0.0940
g	 0.7900	 0.5540
h	 0.8220	 0.5660



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.8200	 0.5610
j	 0.8260	 0.5590
k	 0.7850	 0.5530
l	 0.8140	 0.5700
m	 0.7960	 0.5570
n	 0.8120	 0.5720
o	 0.8120	 0.5680
p	 0.8250	 0.5740
q	 0.8260	 0.5820
r	 0.8130	 0.5650
s	 0.8150	 0.5730
t	 0.8400	 0.5750