



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:55 PM UTC

PDB ID : 9NKJ / pdb_00009nkj
EMDB ID : EMD-49510
Title : Structure of substrates-engaged MIDN-bound human 26S proteasome,ED-MIDN state (Composite map)
Authors : Peddada, N.; Beutler, B.
Deposited on : 2025-02-28
Resolution : 3.84 Å(reported)
Based on initial model : 6MSK

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:

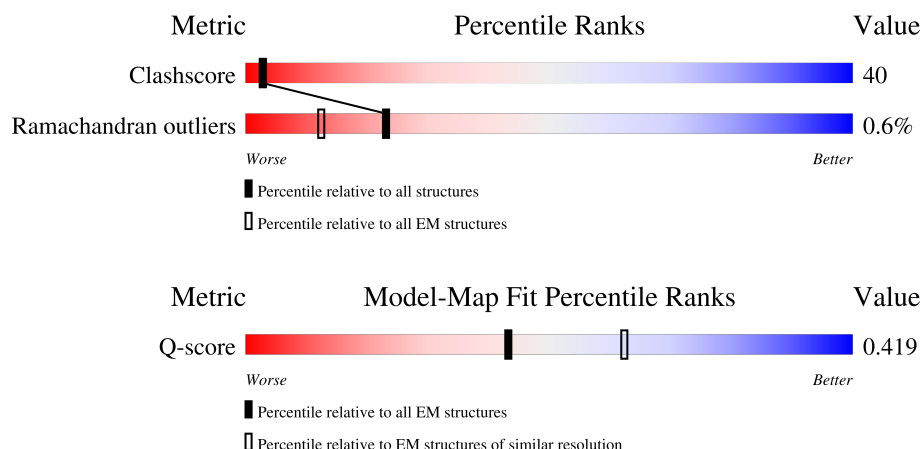
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.84 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.



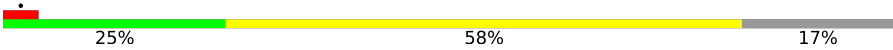
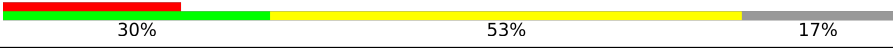
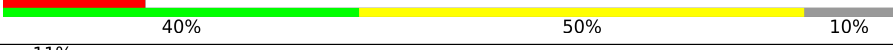
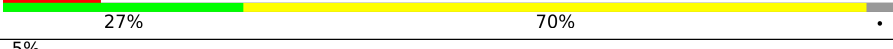
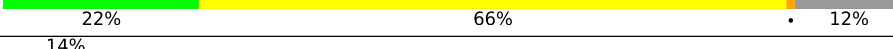
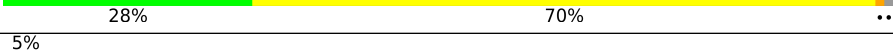
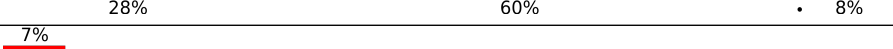
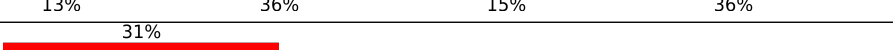
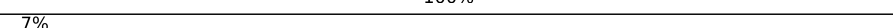
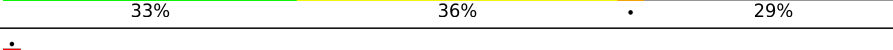
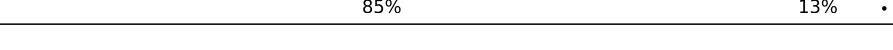
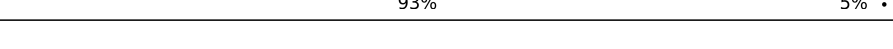
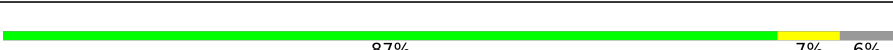
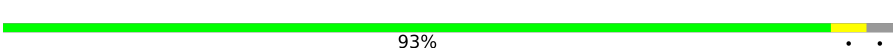
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	9033 (3.34 - 4.34)

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	 5% 34% 60% • 5%
2	B	440	 30% 60% • 8%
3	C	406	 29% 66% • 5%
4	D	418	 30% 60% • 9%
5	E	403	 21% 25% 67% • 7%

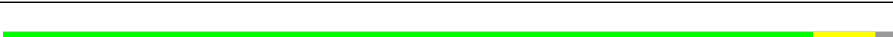
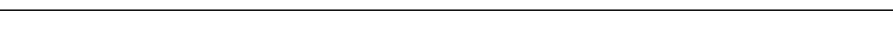
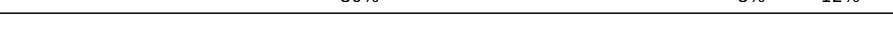
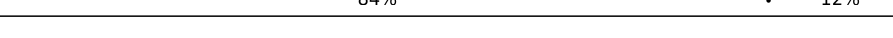
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Mol	Chain	Length	Quality of chain
6	F	439	
7	U	953	
8	V	534	
9	X	422	
10	Y	389	
11	Z	324	
12	a	376	
13	b	377	
14	c	310	
15	d	350	
16	f	908	
17	v	8	
18	W	456	
19	e	70	
20	G	246	
20	g	246	
21	H	234	
21	h	234	
22	I	261	
22	i	261	
23	J	248	
23	j	248	
24	K	241	
24	k	241	
25	L	263	

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Mol	Chain	Length	Quality of chain
25	l	263	
26	M	255	
26	m	255	
27	N	239	
27	n	239	
28	O	277	
28	o	277	
29	P	205	
29	p	205	
30	Q	201	
30	q	201	
31	R	263	
31	r	263	
32	S	241	
32	s	241	
33	T	264	
33	t	264	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ATP	A	501	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 146355 atoms, of which 44182 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3245	2044	570	613	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	403	Total	C	N	O	S	0	0
			3137	1976	534	612	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	387	Total	C	N	O	S	0	0
			3047	1920	548	562	17		

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

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

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	375	Total	C	N	O	S	0	0
			2993	1886	530	560	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	363	Total	C	N	O	S	0	0
			2834	1789	487	542	16		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	851	Total	C	N	O	S	0	0
			6640	4213	1129	1254	44		

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

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	380	Total	C	N	O	S	0	0
			3006	1917	509	568	12		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	189	Total	C	N	O	S	0	0
			1427	894	257	269	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	284	Total	C	N	O	S	0	0
			2227	1409	381	418	19		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d	224	Total	C	N	O	S	0	0
			1813	1173	298	333	9		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	889	Total	C	N	O	S	0	0
			6859	4309	1174	1330	46		

- Molecule 17 is a protein called unknown density-Substrate density.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	v	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	240	Total	C	H	N	O	S	0	0
			3394	1106	1656	304	316	12		
20	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

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

- Molecule 28 is a protein called Proteasome subunit beta type-7.

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

- Molecule 29 is a protein called Proteasome subunit beta type-3.

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

- Molecule 30 is a protein called Proteasome subunit beta type-2.

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

- Molecule 31 is a protein called Proteasome subunit beta type-5.

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

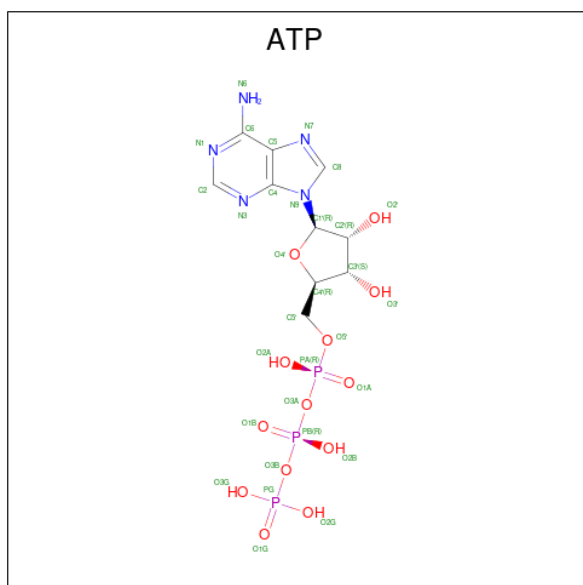
- Molecule 32 is a protein called Proteasome subunit beta type-1.

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

- Molecule 33 is a protein called Proteasome subunit beta type-4.

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

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

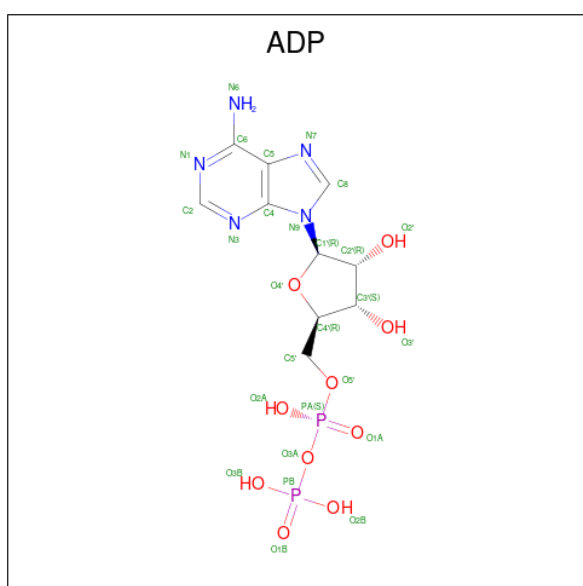


Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

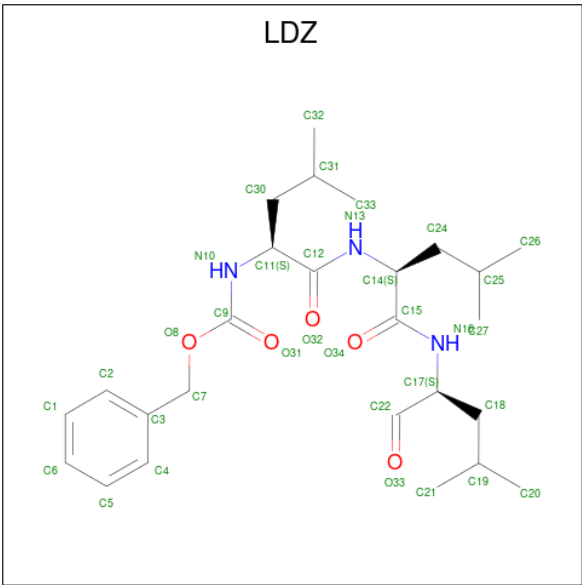


Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

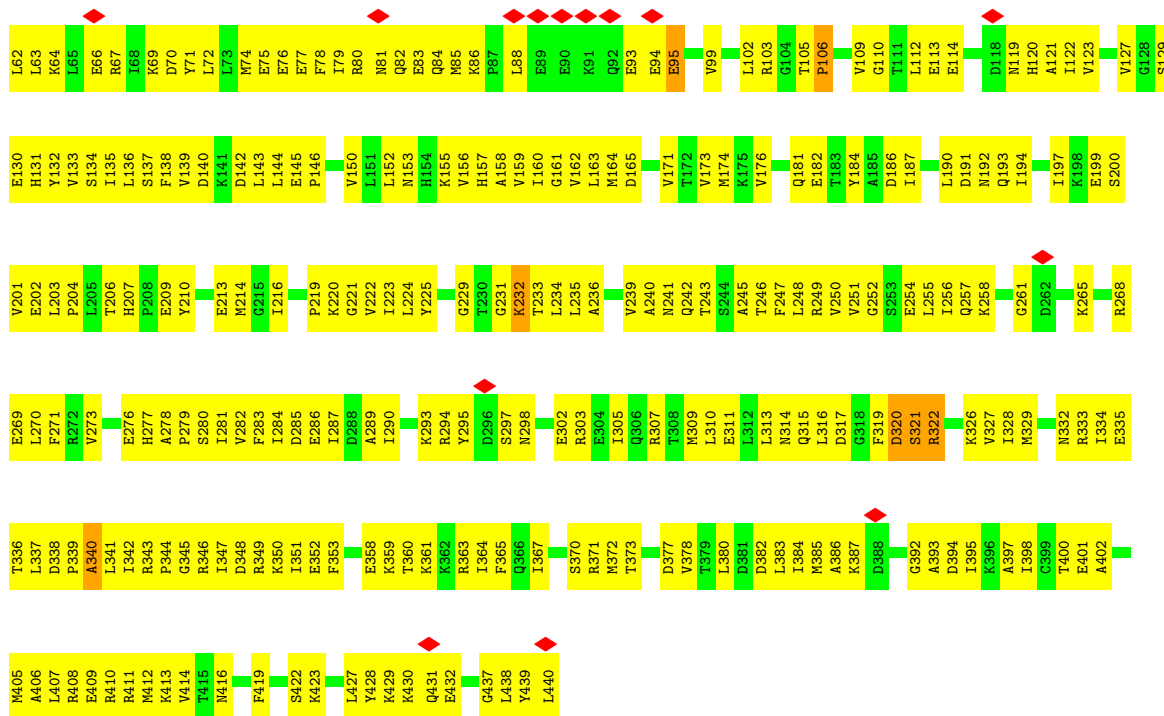
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 38 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).

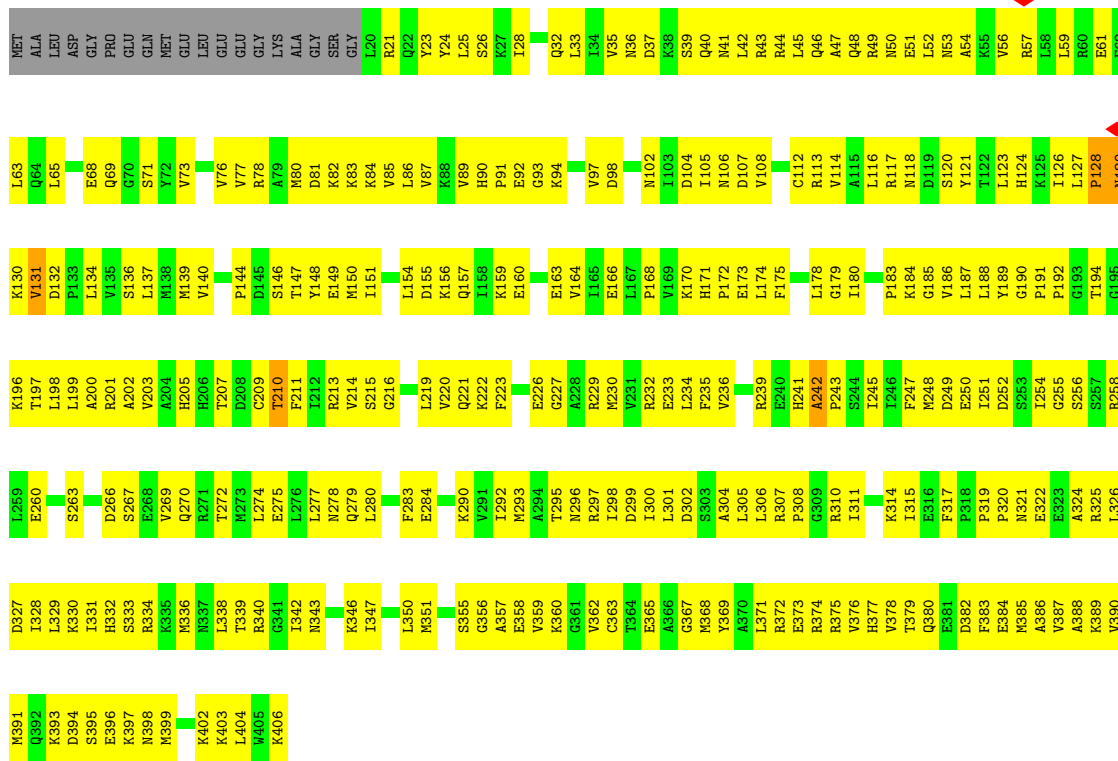


Mol	Chain	Residues	Atoms					AltConf
38	N	1	Total	C	H	N	O	0
			75	26	41	3	5	
38	O	1	Total	C	H	N	O	0
			75	26	41	3	5	
38	R	1	Total	C	H	N	O	0
			75	26	41	3	5	
38	n	1	Total	C	H	N	O	0
			75	26	41	3	5	
38	o	1	Total	C	H	N	O	0
			75	26	41	3	5	
38	r	1	Total	C	H	N	O	0
			75	26	41	3	5	



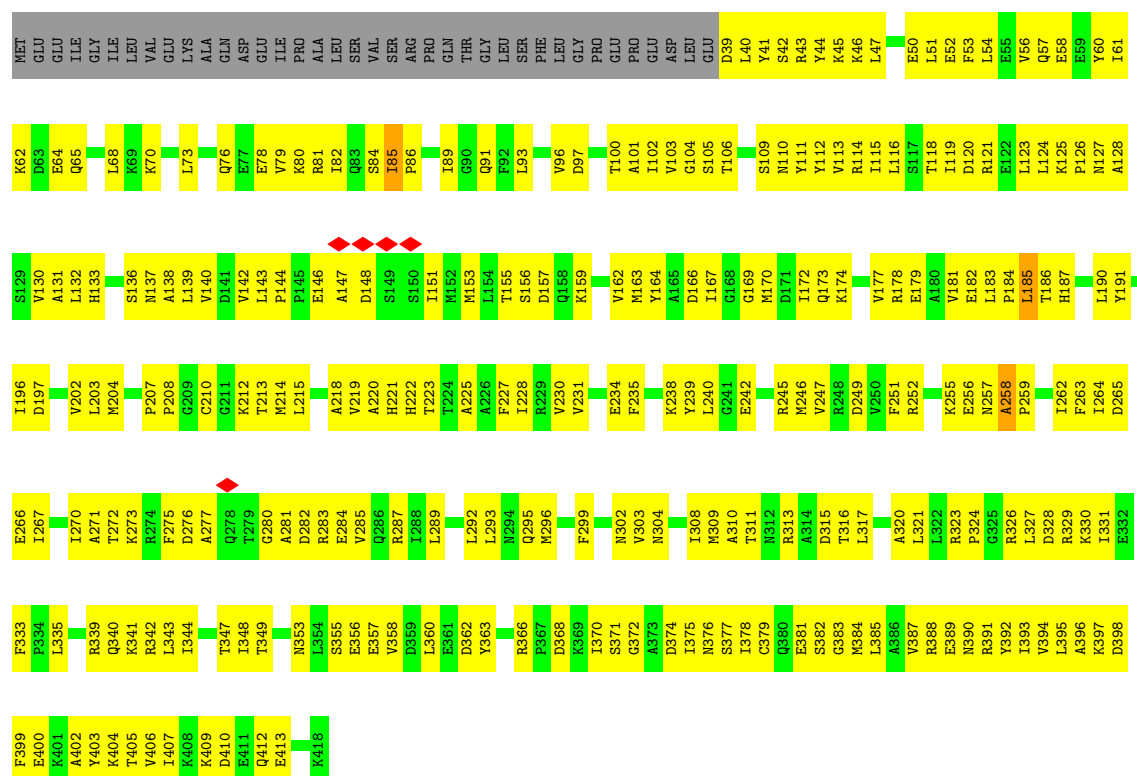
• Molecule 3: 26S protease regulatory subunit 8

Chain C: 29% 66% 5%



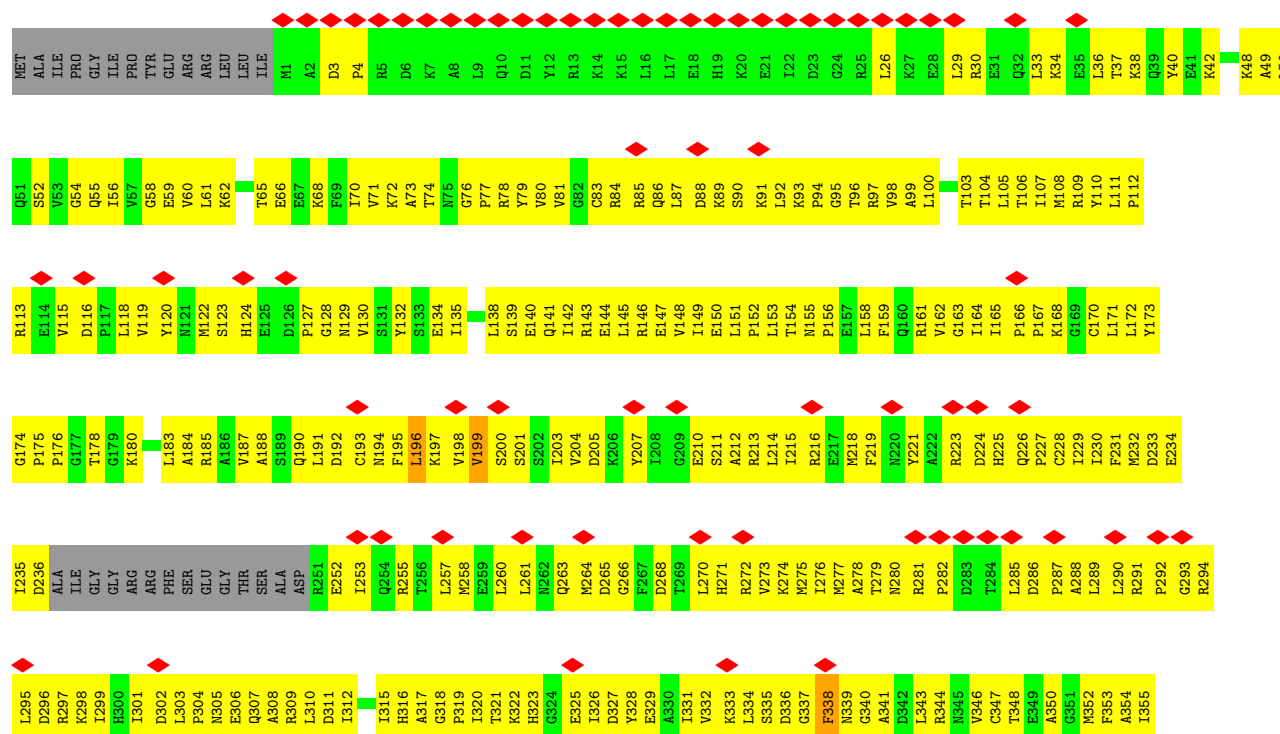
• Molecule 4: 26S proteasome regulatory subunit 6B

Chain D:  30% 60% 9%



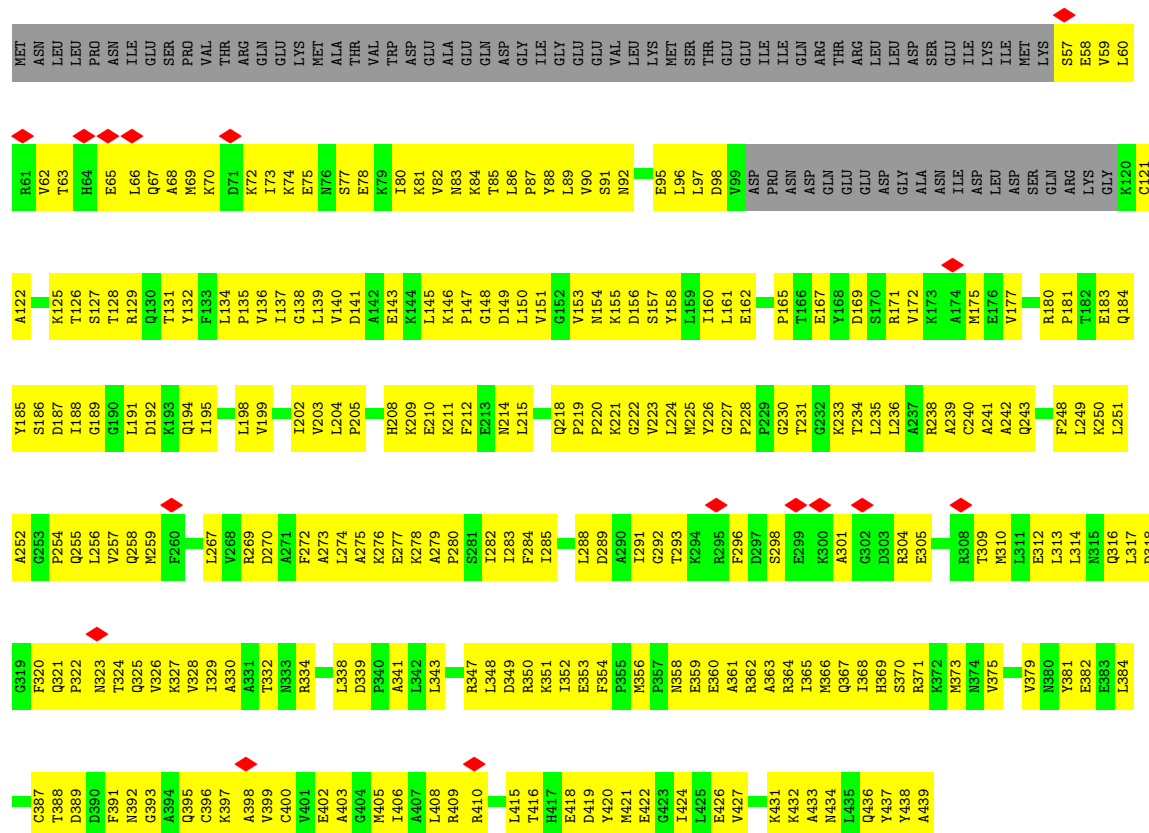
• Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:  21% 25% 67% 7%

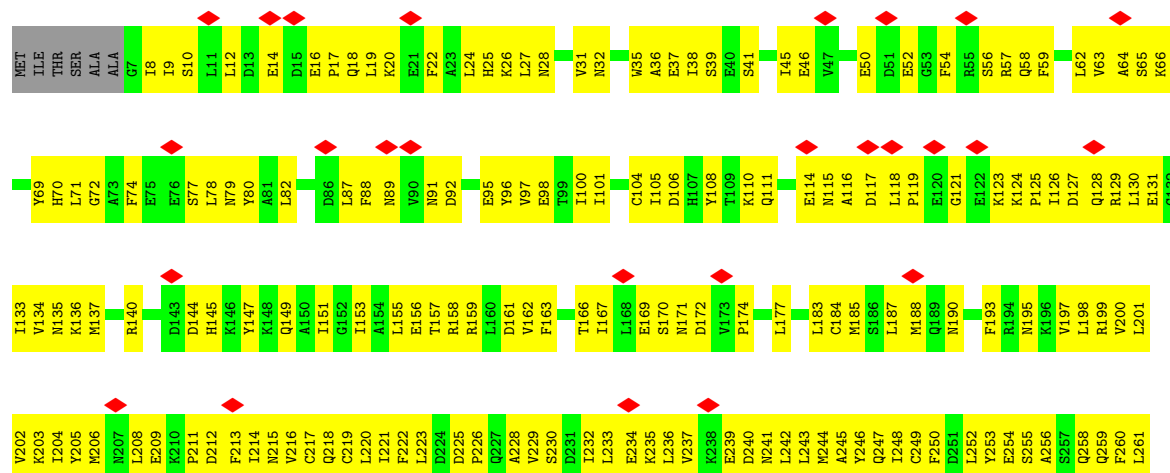


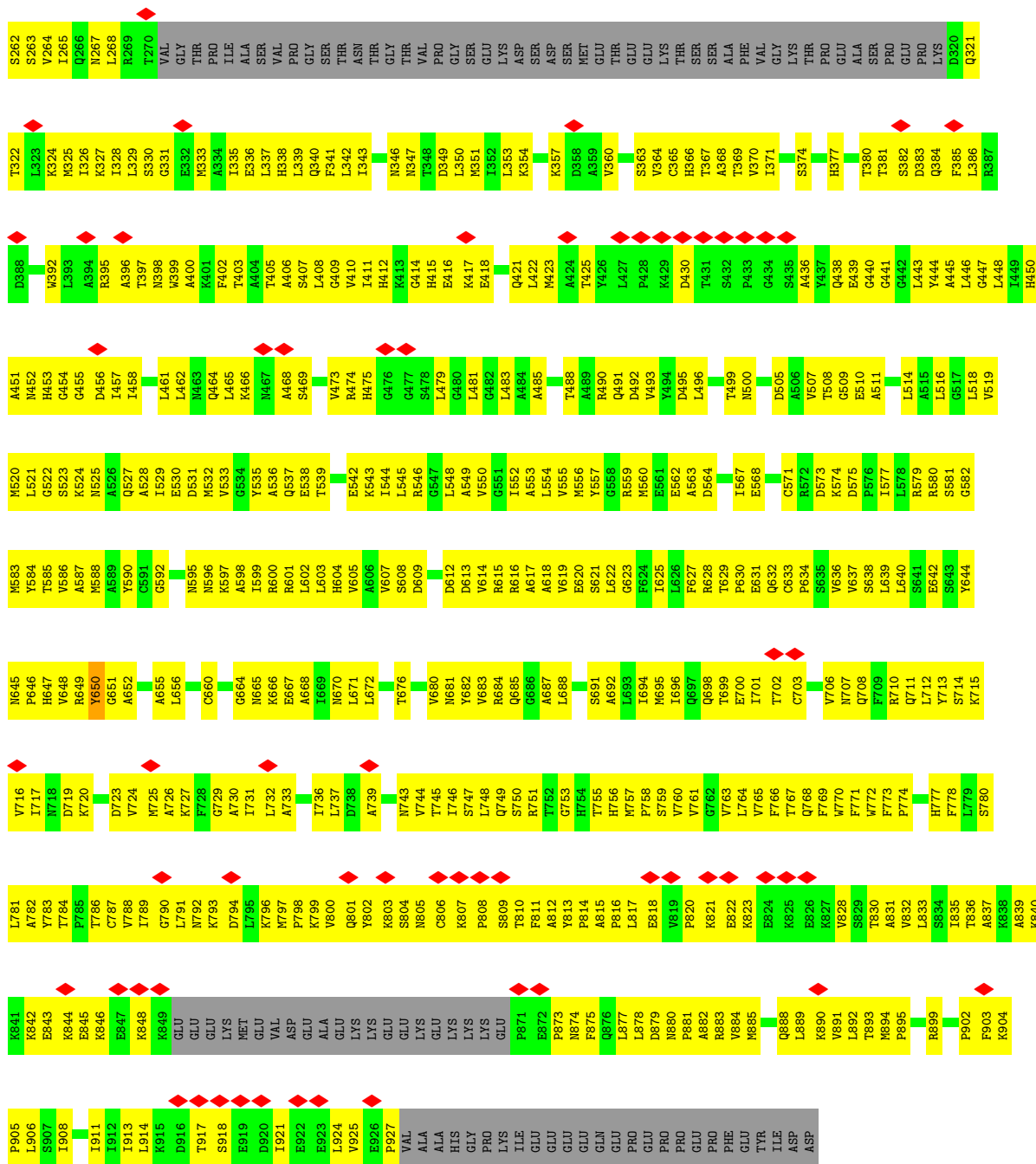


• Molecule 6: 26S proteasome regulatory subunit 6A

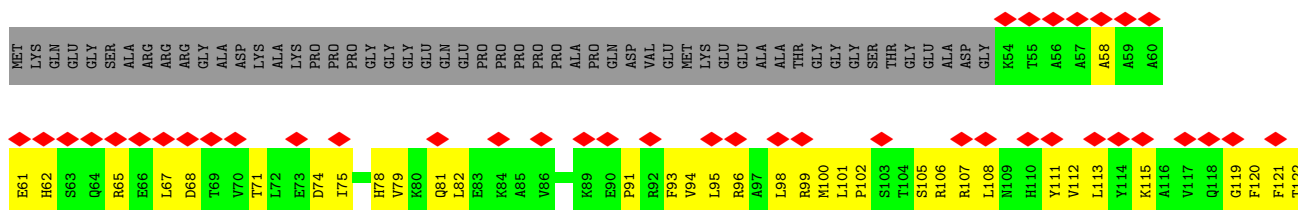


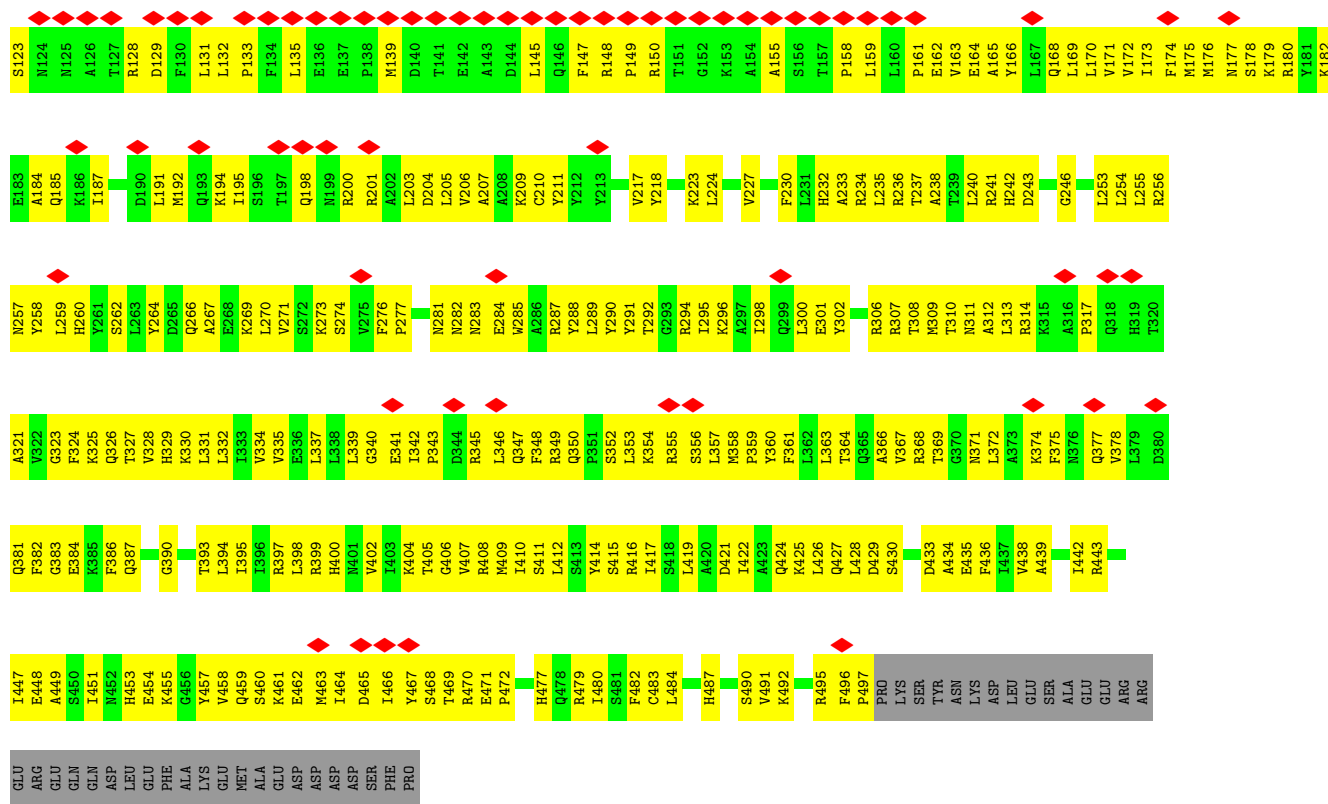
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



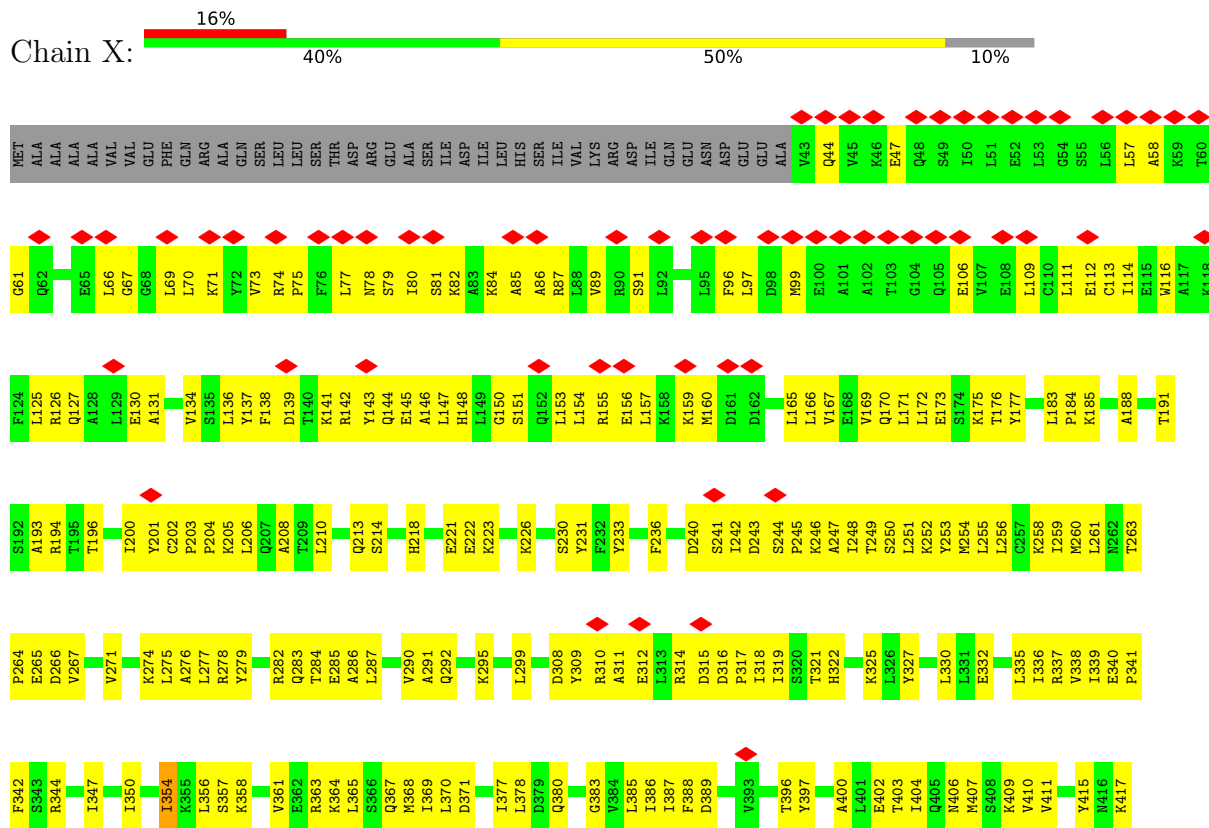


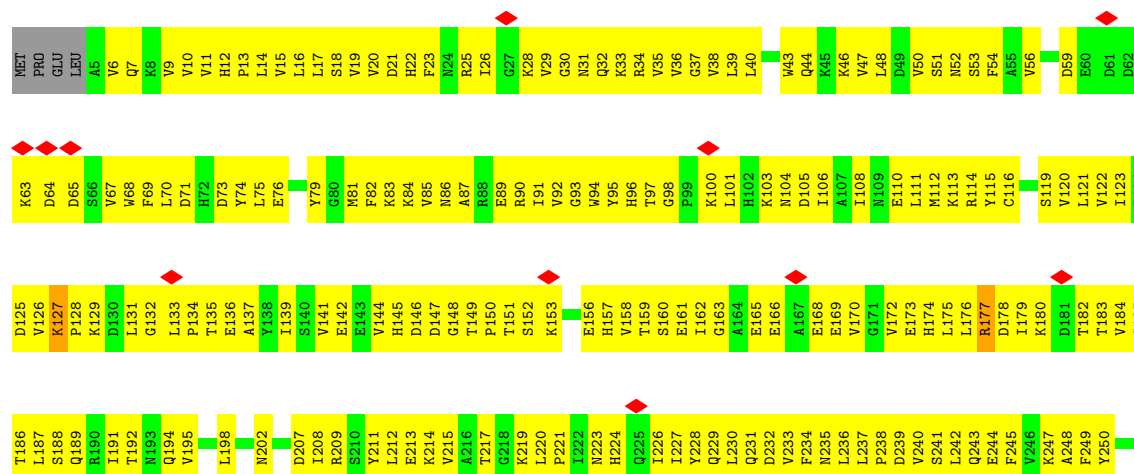
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 3



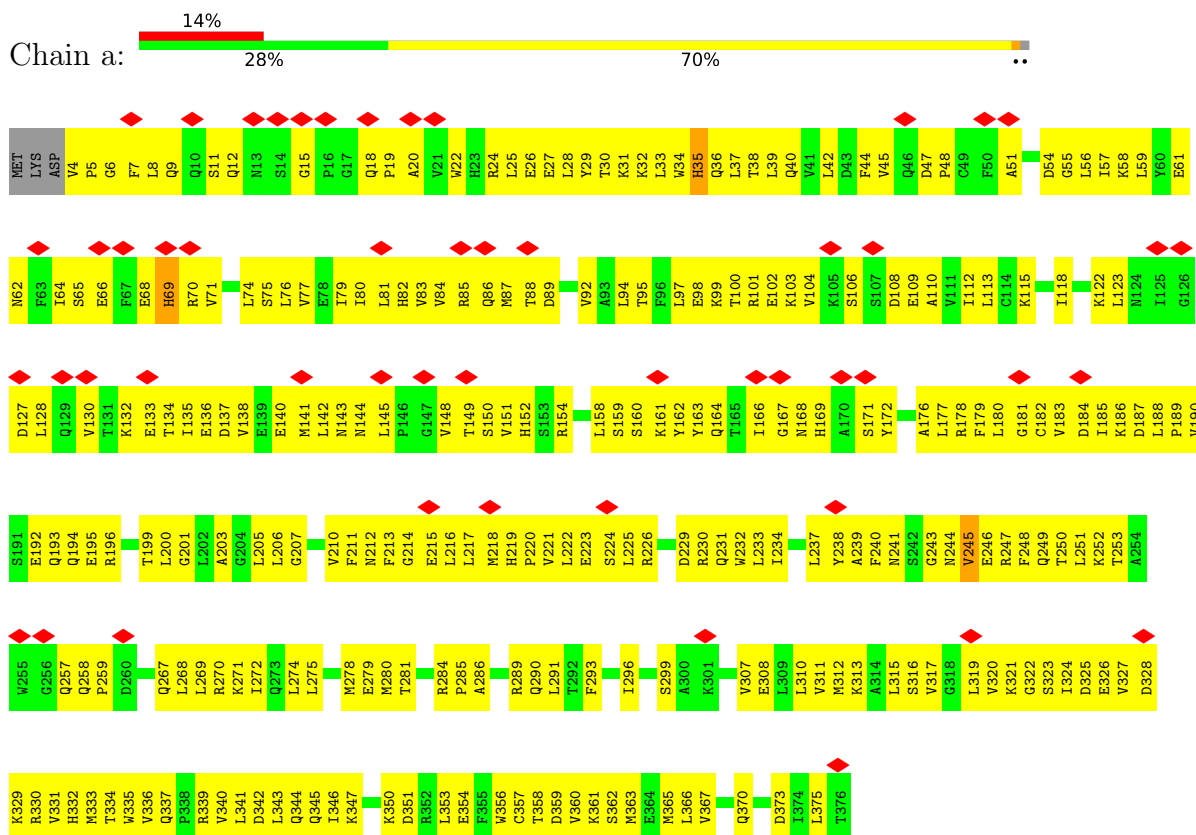


● Molecule 9: 26S proteasome non-ATPase regulatory subunit 11

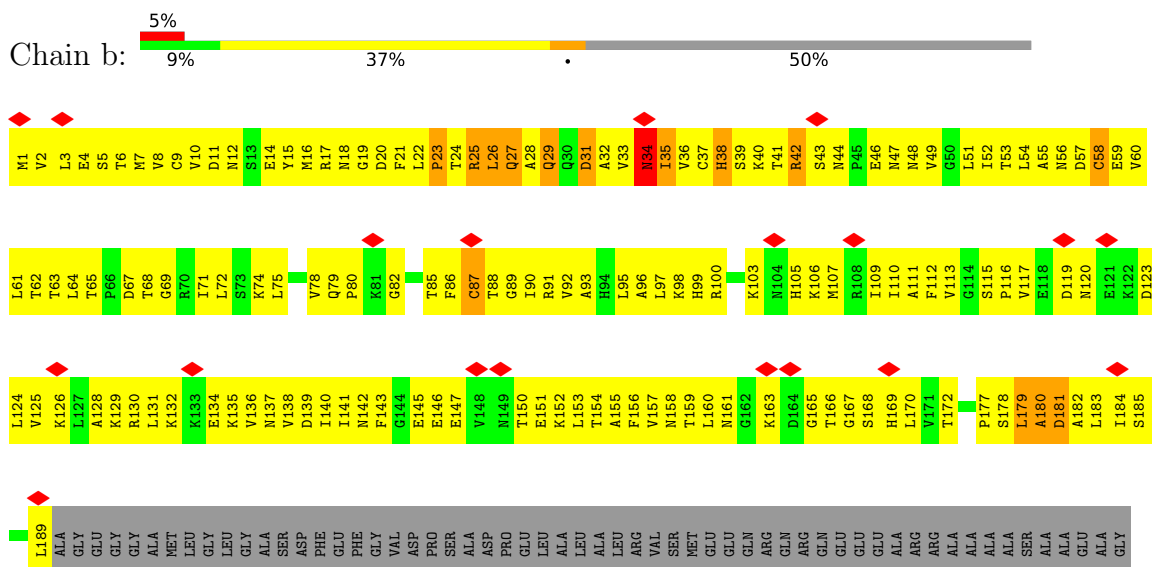




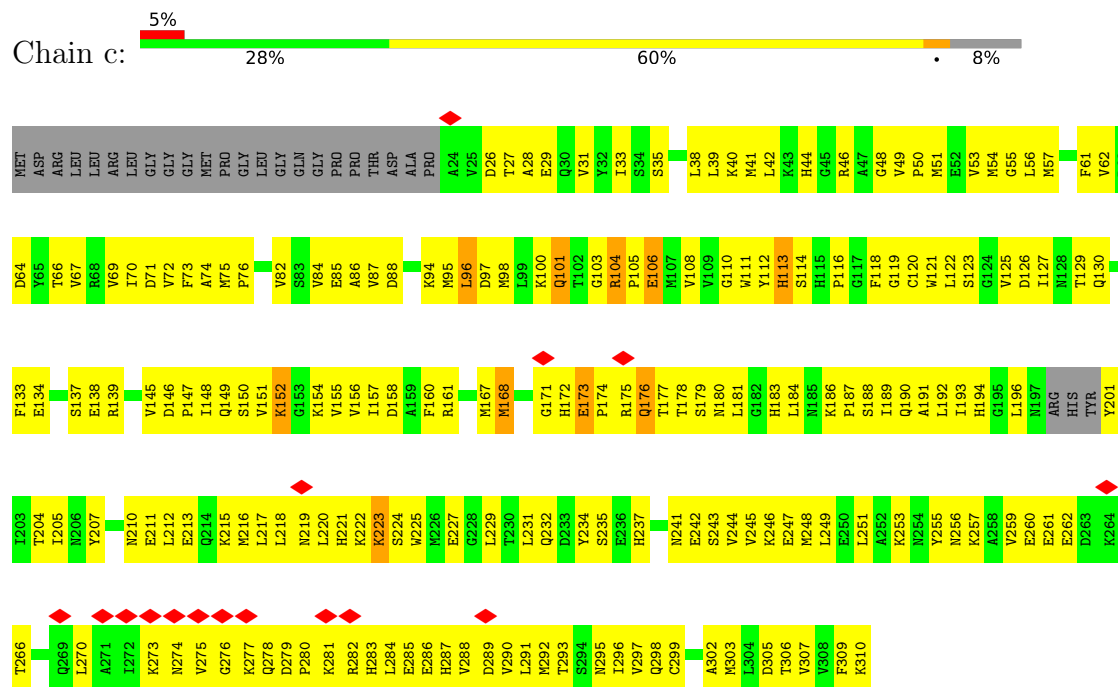
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 13



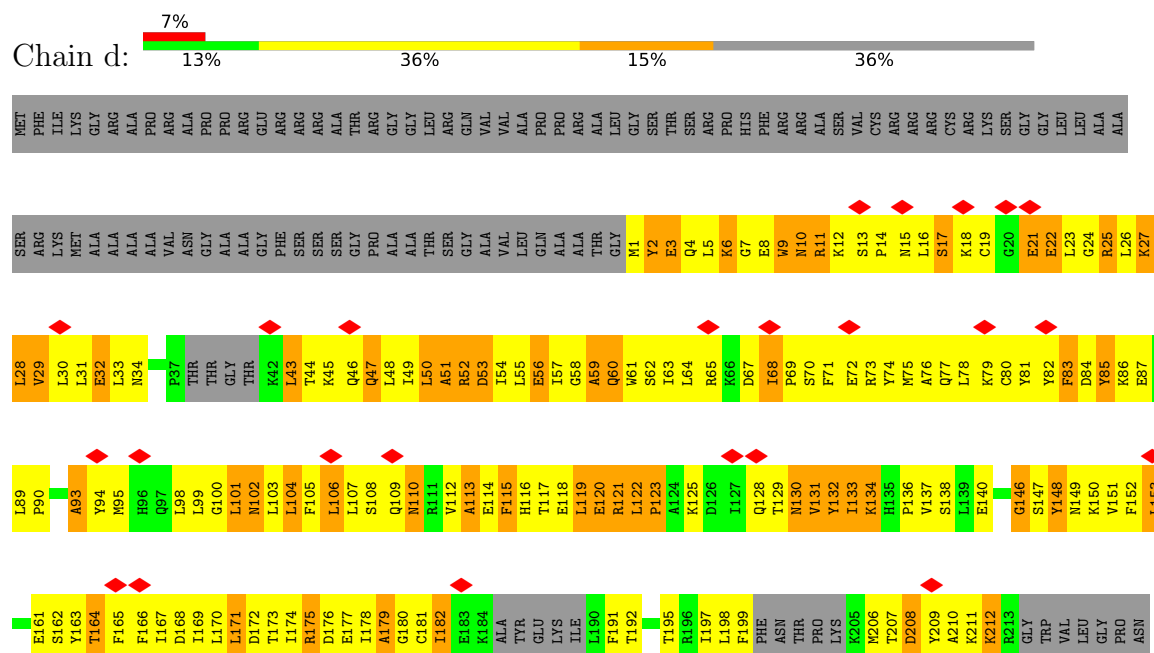
- Molecule 13: 26S proteasome non-ATPase regulatory subunit 4



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

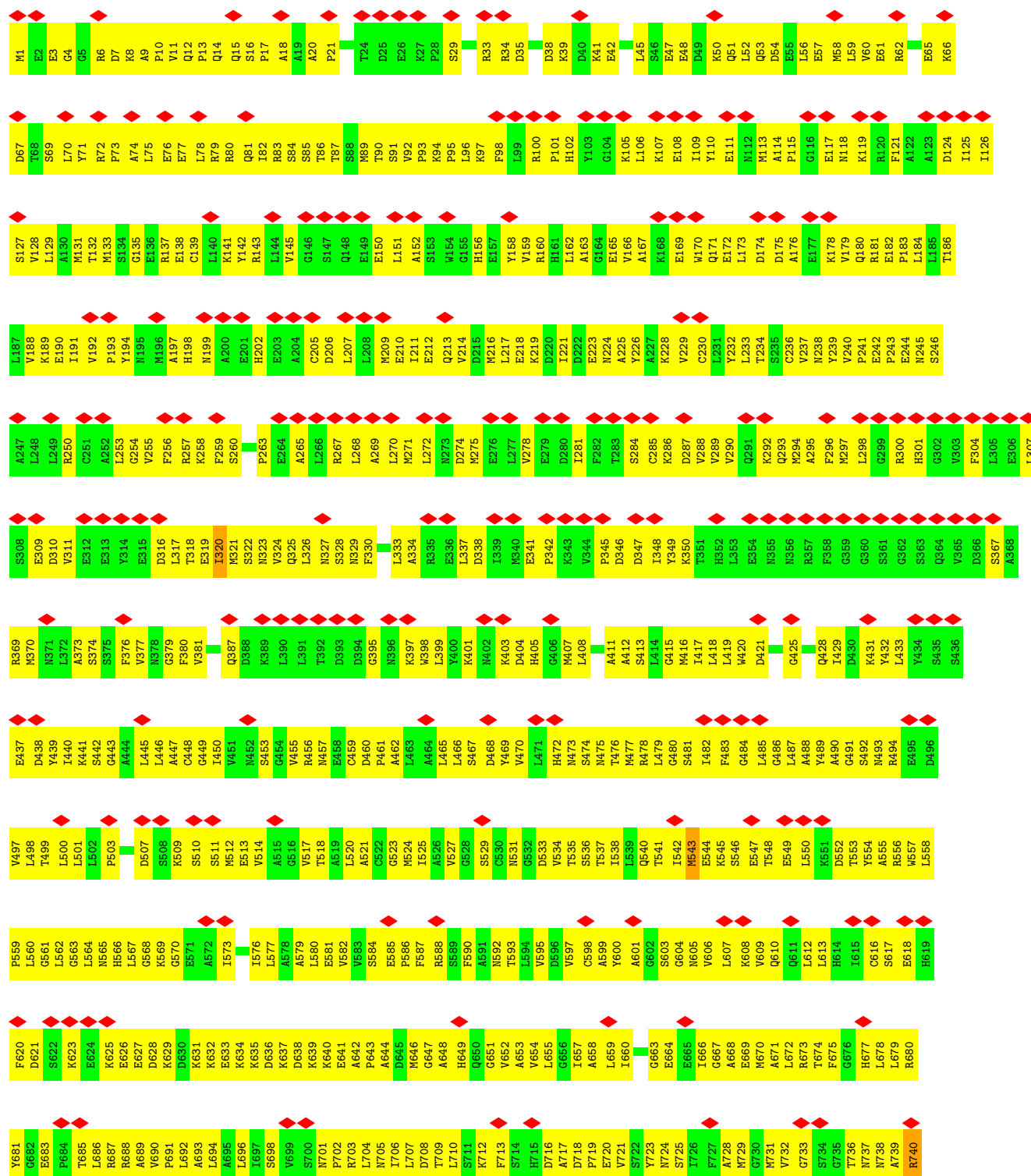


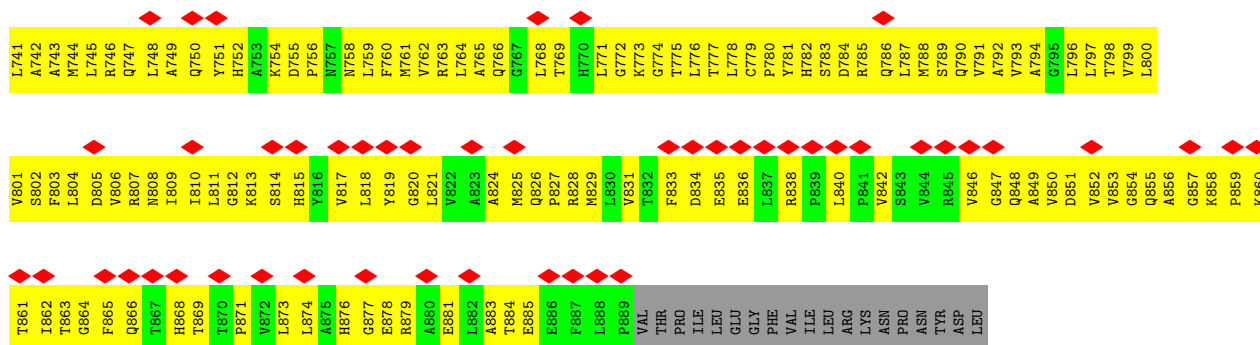
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 8



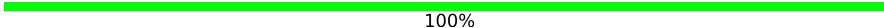


• Molecule 16: 26S proteasome non-ATPase regulatory subunit 2





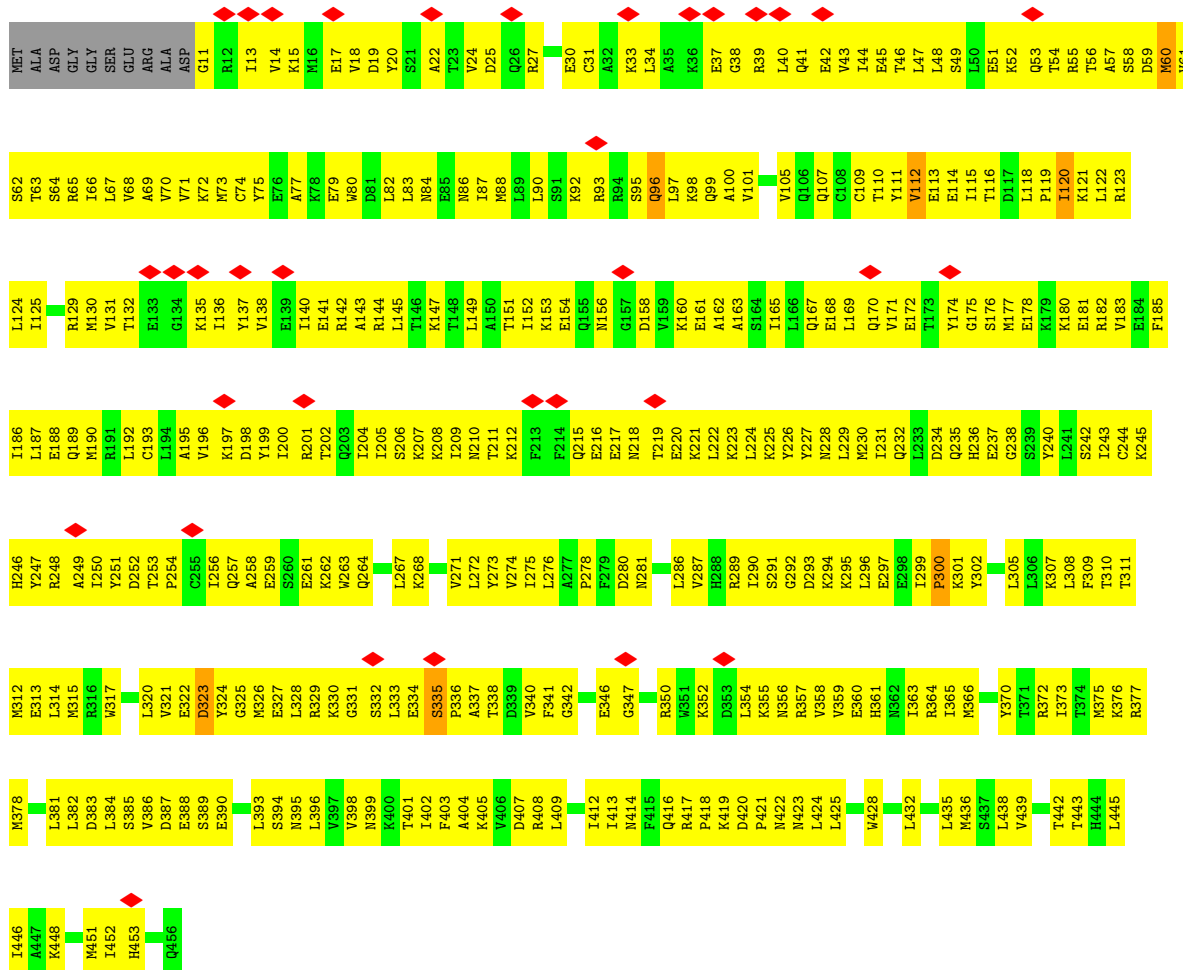
- Molecule 17: unknown density-Substrate density

Chain v:  100%

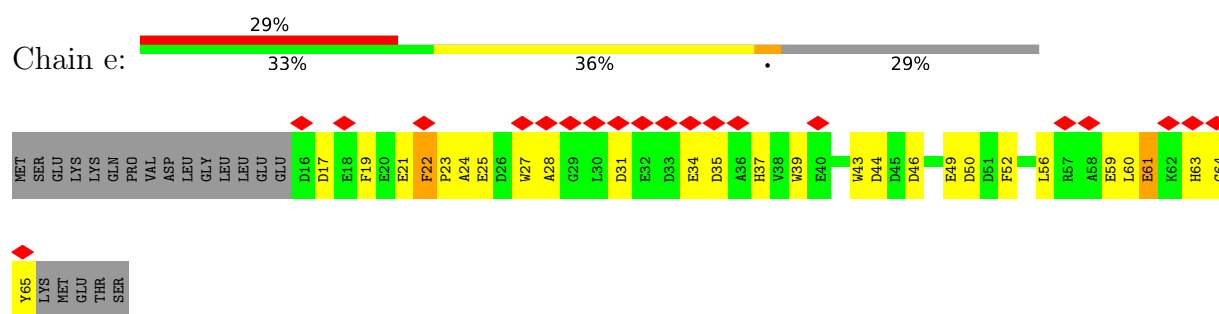
There are no outlier residues recorded for this chain.

- Molecule 18: 26S proteasome non-ATPase regulatory subunit 12

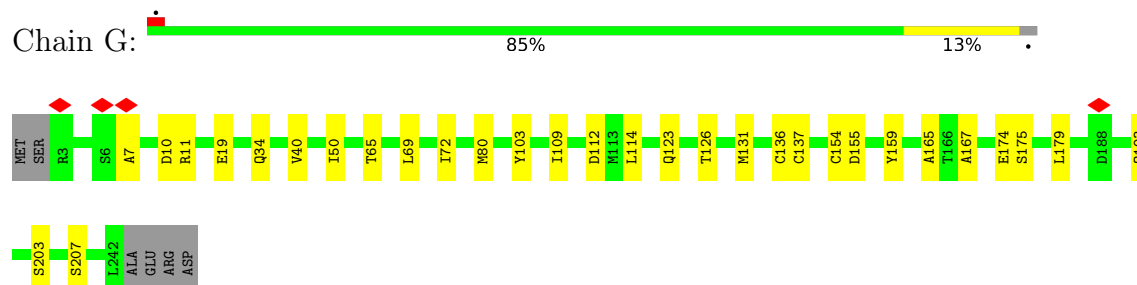
Chain W:  7% 24% 72% ..



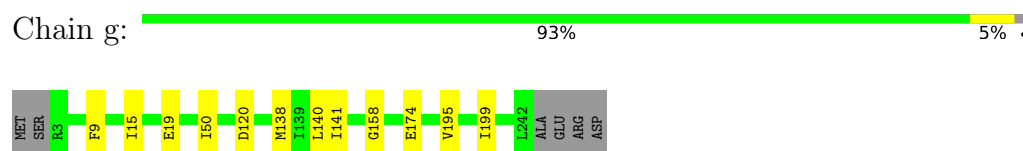
- Molecule 19: 26S proteasome complex subunit SEM1



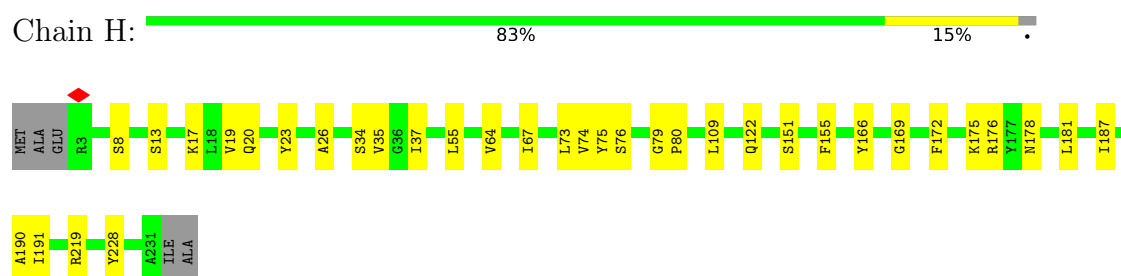
- Molecule 20: Proteasome subunit alpha type-6



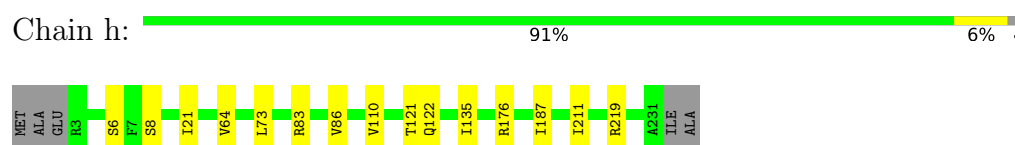
- Molecule 20: Proteasome subunit alpha type-6



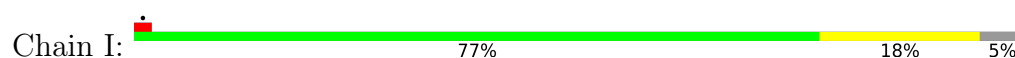
- Molecule 21: Proteasome subunit alpha type-2



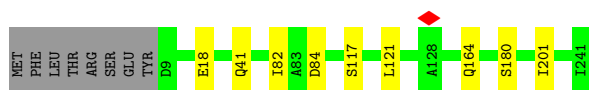
- Molecule 21: Proteasome subunit alpha type-2



- Molecule 22: Proteasome subunit alpha type-4

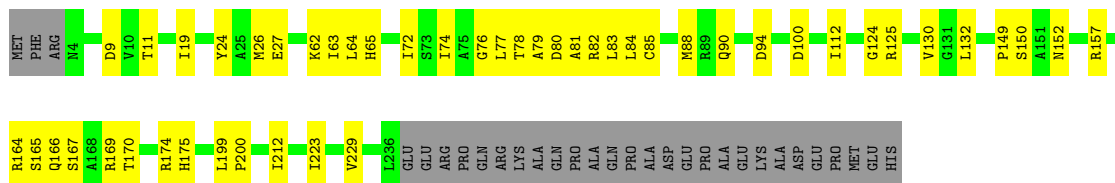






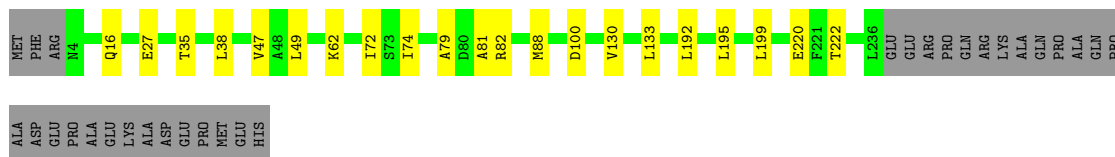
- Molecule 25: Proteasome subunit alpha type-1

Chain L: 70% 18% 11%



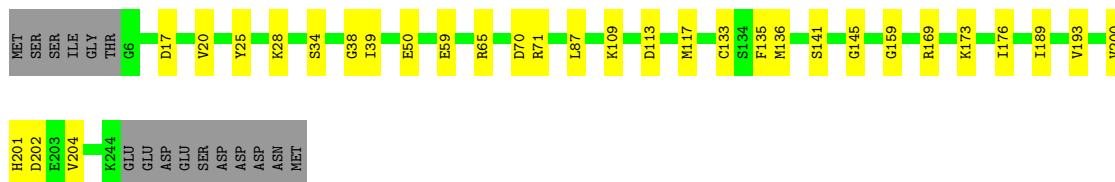
- Molecule 25: Proteasome subunit alpha type-1

Chain l: 81% 8% 11%



- Molecule 26: Proteasome subunit alpha type-3

Chain M: 82% 12% 6%



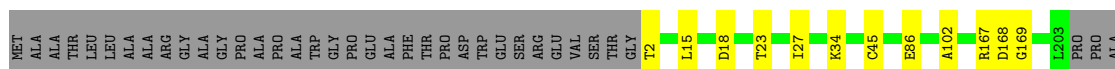
- Molecule 26: Proteasome subunit alpha type-3

Chain m: 89% 6% 5%



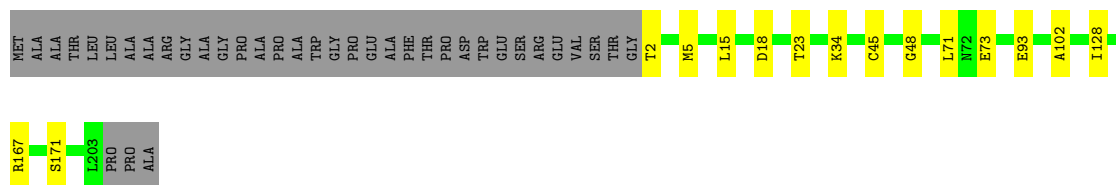
- Molecule 27: Proteasome subunit beta type-6

Chain N: 79% 5% 15%



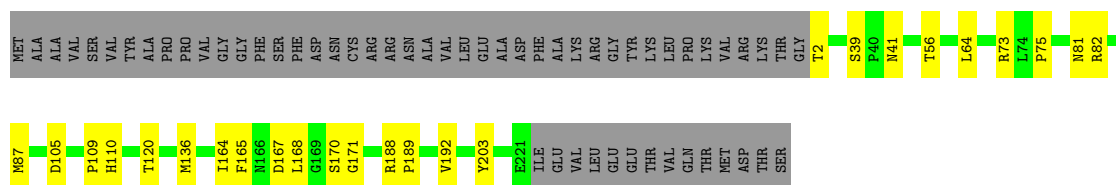
- Molecule 27: Proteasome subunit beta type-6

Chain n:  78% 6% 15%



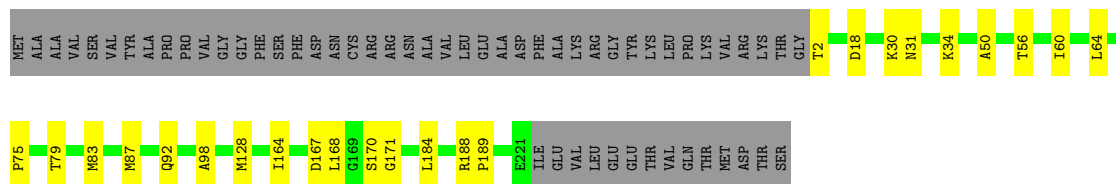
- Molecule 28: Proteasome subunit beta type-7

Chain O:  70% 9% 21%

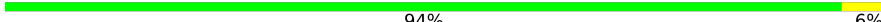


- Molecule 28: Proteasome subunit beta type-7

Chain o:  71% 9% 21%

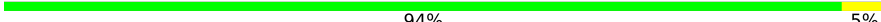


- Molecule 29: Proteasome subunit beta type-3

Chain P:  94% 6%



- Molecule 29: Proteasome subunit beta type-3

Chain p:  94% 5%



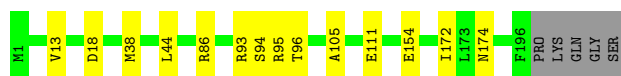
- Molecule 30: Proteasome subunit beta type-2

Chain Q:  89% 8%



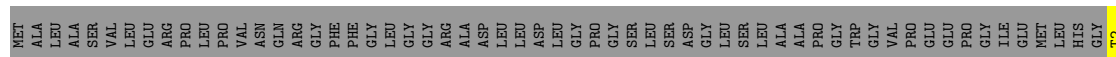
- Molecule 30: Proteasome subunit beta type-2

Chain q:  91% 7% .



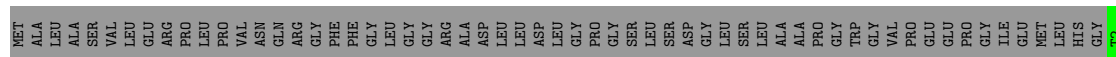
- Molecule 31: Proteasome subunit beta type-5

Chain R:  70% 6% 24%



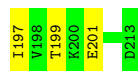
- Molecule 31: Proteasome subunit beta type-5

Chain r:  69% 7% 24%



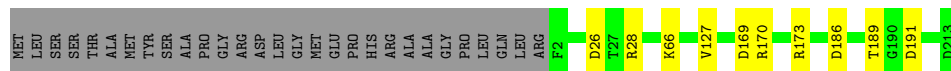
- Molecule 32: Proteasome subunit beta type-1

Chain S:  80% 8% 12%



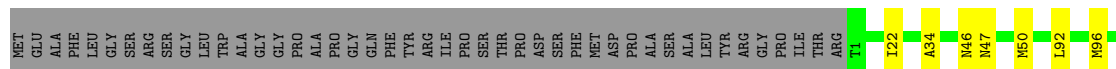
- Molecule 32: Proteasome subunit beta type-1

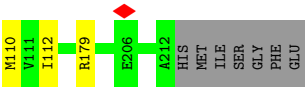
Chain s:  84% 12%



- Molecule 33: Proteasome subunit beta type-4

Chain T:  77% 20%





• Molecule 33: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39000	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)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.985	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	687.36, 687.36, 687.36	wwPDB
Map dimensions	640, 640, 640	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: ADP, ZN, ATP, MG, 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	0.26	0/3299	0.37	0/4454
2	B	0.30	0/3182	0.42	0/4294
3	C	0.29	0/3088	0.42	1/4150 (0.0%)
4	D	0.27	0/3090	0.41	0/4168
5	E	0.19	0/3038	0.39	0/4089
6	F	0.25	0/2873	0.44	0/3873
7	U	0.24	0/6755	0.39	0/9132
8	V	0.20	0/3681	0.34	0/4969
9	X	0.31	0/3050	0.51	3/4111 (0.1%)
10	Y	0.24	0/3173	0.39	0/4273
11	Z	0.29	0/2324	0.41	0/3150
12	a	0.22	0/3053	0.38	0/4133
13	b	0.47	0/1447	0.85	9/1962 (0.5%)
14	c	0.34	0/2266	0.58	2/3060 (0.1%)
15	d	0.81	0/1843	1.47	30/2480 (1.2%)
16	f	0.20	0/6972	0.40	1/9422 (0.0%)
18	W	0.24	0/3683	0.39	0/4952
19	e	0.21	0/437	0.47	0/595
20	G	0.21	0/1767	0.32	0/2398
20	g	0.16	0/1790	0.23	0/2429
21	H	0.22	0/1701	0.32	0/2318
21	h	0.17	0/1701	0.25	0/2318
22	I	0.20	0/1831	0.36	0/2487
22	i	0.16	0/1815	0.25	0/2466
23	J	0.19	0/1657	0.35	0/2261
23	j	0.16	0/1657	0.27	0/2261
24	K	0.21	0/1689	0.36	0/2294
24	k	0.16	0/1686	0.24	0/2290
25	L	0.21	0/1744	0.37	0/2371
25	l	0.17	0/1741	0.26	0/2367
26	M	0.18	0/1795	0.31	0/2434
26	m	0.16	0/1796	0.23	0/2435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
27	N	0.18	0/1495	0.23	0/2026
27	n	0.19	0/1491	0.23	0/2021
28	O	0.17	0/1607	0.26	0/2185
28	o	0.18	0/1603	0.24	0/2180
29	P	0.18	0/1575	0.25	0/2128
29	p	0.18	0/1567	0.25	0/2118
30	Q	0.17	0/1541	0.23	0/2092
30	q	0.18	0/1538	0.24	0/2088
31	R	0.17	0/1535	0.22	0/2080
31	r	0.18	0/1531	0.24	0/2076
32	S	0.18	0/1614	0.25	0/2178
32	s	0.17	0/1617	0.25	0/2182
33	T	0.19	0/1606	0.27	0/2179
33	t	0.18	0/1598	0.26	0/2170
All	All	0.25	0/103542	0.41	46/140099 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	U	0	1
9	X	0	1
13	b	0	1
14	c	0	2
15	d	0	4
All	All	0	9

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	52	ARG	N-CA-C	-10.40	100.26	113.16
15	d	85	TYR	N-CA-C	-8.02	101.49	111.75
15	d	83	PHE	N-CA-C	-7.85	103.59	113.01
15	d	6	LYS	N-CA-C	-7.50	104.02	113.02
13	b	29	GLN	N-CA-C	-7.24	102.43	111.11

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	U	650	TYR	Peptide
9	X	363	ARG	Sidechain
13	b	25	ARG	Sidechain
14	c	104	ARG	Sidechain
14	c	223	LYS	Peptide

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	3245	0	3302	462	0
2	B	3137	0	3192	476	0
3	C	3047	0	3164	440	0
4	D	3040	0	3076	401	0
5	E	2993	0	3076	508	0
6	F	2834	0	2904	420	0
7	U	6640	0	6699	905	0
8	V	3612	0	3682	429	0
9	X	3006	0	3111	279	0
10	Y	3115	0	3120	445	0
11	Z	2281	0	2312	394	0
12	a	2995	0	3012	455	0
13	b	1427	0	1468	274	0
14	c	2227	0	2246	318	0
15	d	1813	0	1834	325	0
16	f	6859	0	6859	1165	0
17	v	40	0	12	0	0
18	W	3635	0	3762	615	0
19	e	425	0	328	68	0
20	G	1738	1656	1656	25	0
20	g	1758	1687	1687	8	0
21	H	1662	1590	1590	26	0
21	h	1662	1590	1590	10	0
22	I	1802	1741	1741	41	0
22	i	1786	1717	1717	8	0
23	J	1633	1518	1518	44	0
23	j	1633	1518	1518	12	0
24	K	1663	1592	1591	26	0
24	k	1660	1589	1589	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	1710	1649	1649	44	0
25	l	1707	1645	1645	14	0
26	M	1760	1680	1680	25	0
26	m	1761	1683	1683	8	0
27	N	1469	1422	1422	11	0
27	n	1465	1416	1416	11	0
28	O	1580	1559	1559	17	0
28	o	1576	1555	1555	18	0
29	P	1546	1550	1552	8	0
29	p	1538	1543	1545	8	0
30	Q	1509	1477	1477	14	0
30	q	1506	1475	1475	11	0
31	R	1504	1449	1449	17	0
31	r	1500	1438	1438	14	0
32	S	1584	1579	1579	12	0
32	s	1587	1581	1581	7	0
33	T	1576	1526	1528	9	0
33	t	1568	1511	1513	8	0
34	A	31	0	12	11	0
34	B	31	0	12	7	0
34	C	31	0	12	6	0
34	F	31	0	12	6	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	F	1	0	0	0	0
36	D	27	0	12	6	0
37	c	1	0	0	0	0
38	N	34	41	41	2	0
38	O	34	41	41	2	0
38	R	34	41	41	7	0
38	n	34	41	41	5	0
38	o	34	41	41	3	0
38	r	34	41	41	1	0
All	All	102173	44182	101408	8138	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 40.

The worst 5 of 8138 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)
15:d:116:HIS:NE2	15:d:140:GLU:OE2	1.63	1.27
15:d:115:PHE:O	15:d:119:LEU:HD13	1.15	1.23
15:d:43:LEU:CD2	15:d:48:LEU:HD11	1.68	1.22
6:F:188:ILE:HD11	6:F:191:LEU:HG	1.20	1.17
16:f:486:GLY:HA3	16:f:521:ALA:HB1	1.25	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	335 (82%)	72 (18%)	4 (1%)	12	45
2	B	401/440 (91%)	323 (80%)	70 (18%)	8 (2%)	6	33
3	C	385/406 (95%)	315 (82%)	65 (17%)	5 (1%)	9	40
4	D	378/418 (90%)	312 (82%)	62 (16%)	4 (1%)	11	43
5	E	371/403 (92%)	297 (80%)	71 (19%)	3 (1%)	16	50
6	F	359/439 (82%)	289 (80%)	69 (19%)	1 (0%)	36	69
7	U	845/953 (89%)	738 (87%)	107 (13%)	0	100	100
8	V	442/534 (83%)	418 (95%)	24 (5%)	0	100	100
9	X	378/422 (90%)	355 (94%)	23 (6%)	0	100	100
10	Y	376/389 (97%)	328 (87%)	48 (13%)	0	100	100
11	Z	284/324 (88%)	237 (84%)	45 (16%)	2 (1%)	18	53
12	a	371/376 (99%)	326 (88%)	42 (11%)	3 (1%)	16	50
13	b	187/377 (50%)	143 (76%)	35 (19%)	9 (5%)	2	19
14	c	280/310 (90%)	219 (78%)	55 (20%)	6 (2%)	5	32
15	d	214/350 (61%)	136 (64%)	52 (24%)	26 (12%)	0	4
16	f	887/908 (98%)	730 (82%)	155 (18%)	2 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	W	444/456 (97%)	355 (80%)	79 (18%)	10 (2%)	5	31
19	e	48/70 (69%)	33 (69%)	13 (27%)	2 (4%)	2	20
20	G	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
20	g	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
21	H	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
21	h	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
22	I	245/261 (94%)	235 (96%)	10 (4%)	0	100	100
22	i	245/261 (94%)	239 (98%)	6 (2%)	0	100	100
23	J	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
23	j	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
24	K	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
24	k	231/241 (96%)	227 (98%)	4 (2%)	0	100	100
25	L	231/263 (88%)	221 (96%)	10 (4%)	0	100	100
25	l	231/263 (88%)	228 (99%)	3 (1%)	0	100	100
26	M	237/255 (93%)	230 (97%)	7 (3%)	0	100	100
26	m	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
27	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
27	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
28	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
28	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
29	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
29	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
30	Q	194/201 (96%)	186 (96%)	8 (4%)	0	100	100
30	q	194/201 (96%)	187 (96%)	7 (4%)	0	100	100
31	R	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
31	r	198/263 (75%)	197 (100%)	1 (0%)	0	100	100
32	S	210/241 (87%)	204 (97%)	6 (3%)	0	100	100
32	s	210/241 (87%)	207 (99%)	3 (1%)	0	100	100
33	T	210/264 (80%)	199 (95%)	11 (5%)	0	100	100
33	t	210/264 (80%)	200 (95%)	10 (5%)	0	100	100
All	All	13203/14884 (89%)	11845 (90%)	1273 (10%)	85 (1%)	23	55

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
2	B	106	PRO
2	B	320	ASP
2	B	321	SER
2	B	340	ALA

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
38	LDZ	o	301	-	33,34,34	0.47	0	42,44,44	0.67	2 (4%)
34	ATP	F	501	-	32,33,33	0.57	0	48,52,52	0.38	0
38	LDZ	O	301	-	33,34,34	0.53	1 (3%)	42,44,44	0.77	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LDZ	N	301	-	33,34,34	0.53	1 (3%)	42,44,44	0.66	0
36	ADP	D	501	-	28,29,29	1.36	6 (21%)	43,45,45	1.89	9 (20%)
38	LDZ	n	301	-	33,34,34	0.52	1 (3%)	42,44,44	0.68	0
34	ATP	C	501	-	32,33,33	0.81	1 (3%)	48,52,52	0.37	0
38	LDZ	R	301	-	33,34,34	0.49	0	42,44,44	0.67	0
34	ATP	B	501	-	32,33,33	0.60	1 (3%)	48,52,52	0.39	0
38	LDZ	r	301	-	33,34,34	0.54	1 (3%)	42,44,44	0.92	1 (2%)
34	ATP	A	501	35	32,33,33	0.48	0	48,52,52	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LDZ	o	301	-	-	8/38/39/39	0/1/1/1
34	ATP	F	501	-	-	5/22/38/38	0/3/3/3
38	LDZ	O	301	-	-	13/38/39/39	0/1/1/1
38	LDZ	N	301	-	-	8/38/39/39	0/1/1/1
36	ADP	D	501	-	-	7/16/32/32	0/3/3/3
38	LDZ	n	301	-	-	4/38/39/39	0/1/1/1
34	ATP	C	501	-	-	1/22/38/38	0/3/3/3
38	LDZ	R	301	-	-	10/38/39/39	0/1/1/1
34	ATP	B	501	-	-	3/22/38/38	0/3/3/3
38	LDZ	r	301	-	-	11/38/39/39	0/1/1/1
34	ATP	A	501	35	-	2/22/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ADP	C5-C4	4.24	1.46	1.39
34	C	501	ATP	PB-O3B	-3.77	1.55	1.59
36	D	501	ADP	C5-N7	-2.49	1.34	1.39
34	B	501	ATP	PA-O3A	-2.31	1.57	1.59
36	D	501	ADP	C4-N9	-2.30	1.32	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ADP	C5-C4-N3	-5.86	118.65	126.72
36	D	501	ADP	N3-C4-N9	4.80	135.32	127.17
38	r	301	LDZ	C14-N13-C12	3.86	129.94	121.65
36	D	501	ADP	C2-N3-C4	3.52	120.43	111.83
36	D	501	ADP	C4-C5-N7	-3.20	106.92	110.58

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	PB-O3B-PG-O2G
34	F	501	ATP	PB-O3B-PG-O2G
34	F	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	C4'-C5'-O5'-PA
36	D	501	ADP	PA-O3A-PB-O2B

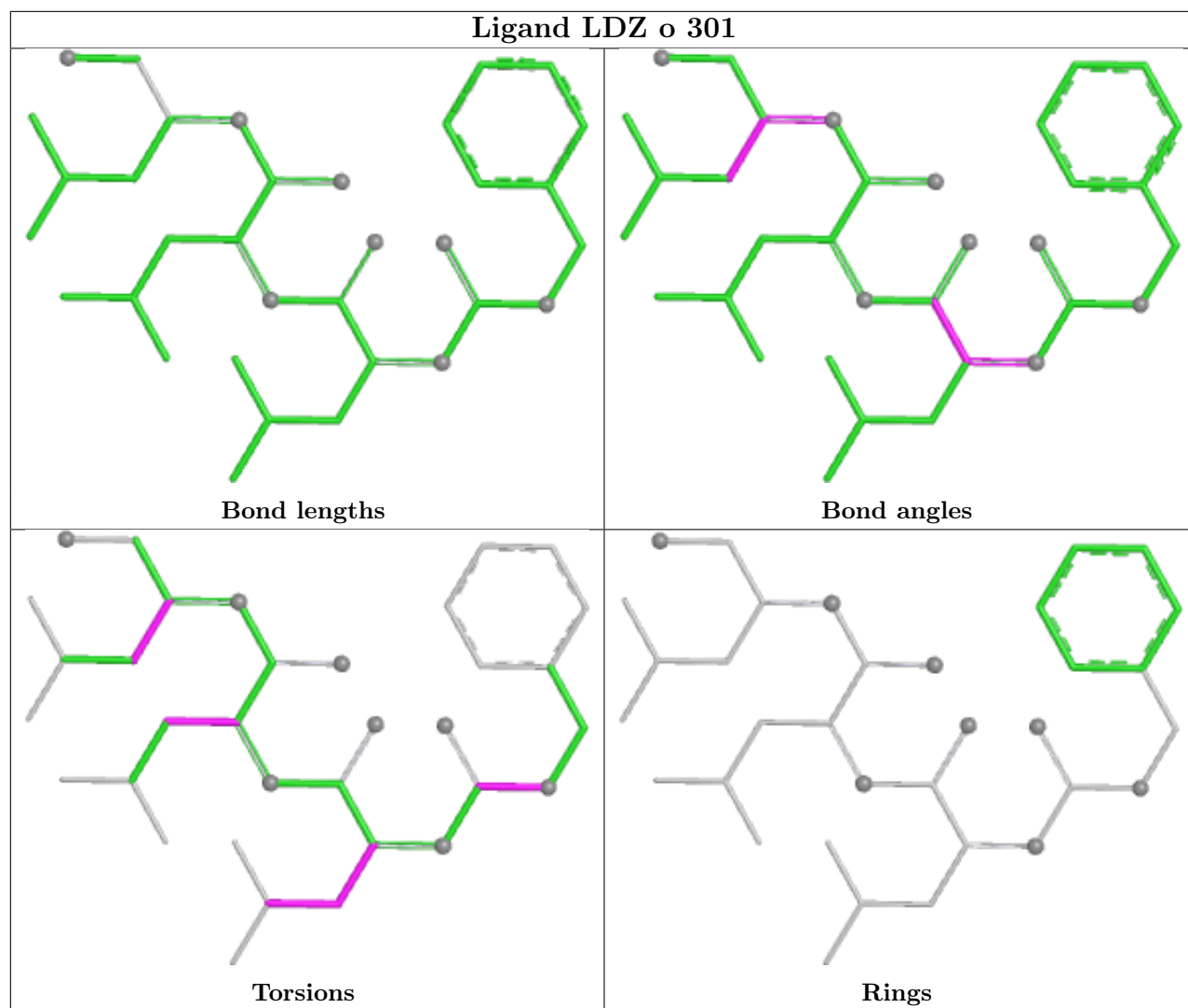
There are no ring outliers.

11 monomers are involved in 56 short contacts:

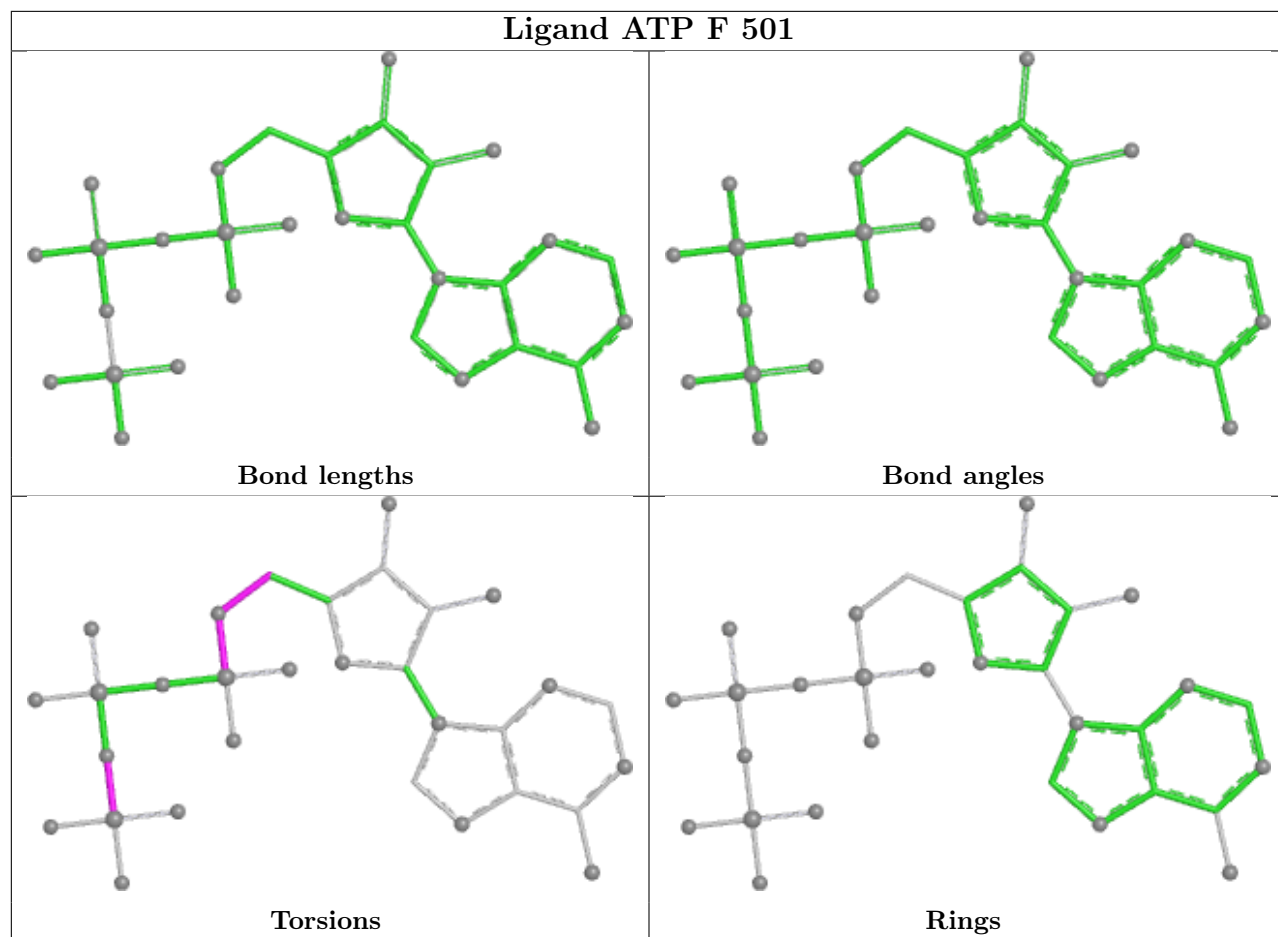
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	o	301	LDZ	3	0
34	F	501	ATP	6	0
38	O	301	LDZ	2	0
38	N	301	LDZ	2	0
36	D	501	ADP	6	0
38	n	301	LDZ	5	0
34	C	501	ATP	6	0
38	R	301	LDZ	7	0
34	B	501	ATP	7	0
38	r	301	LDZ	1	0
34	A	501	ATP	11	0

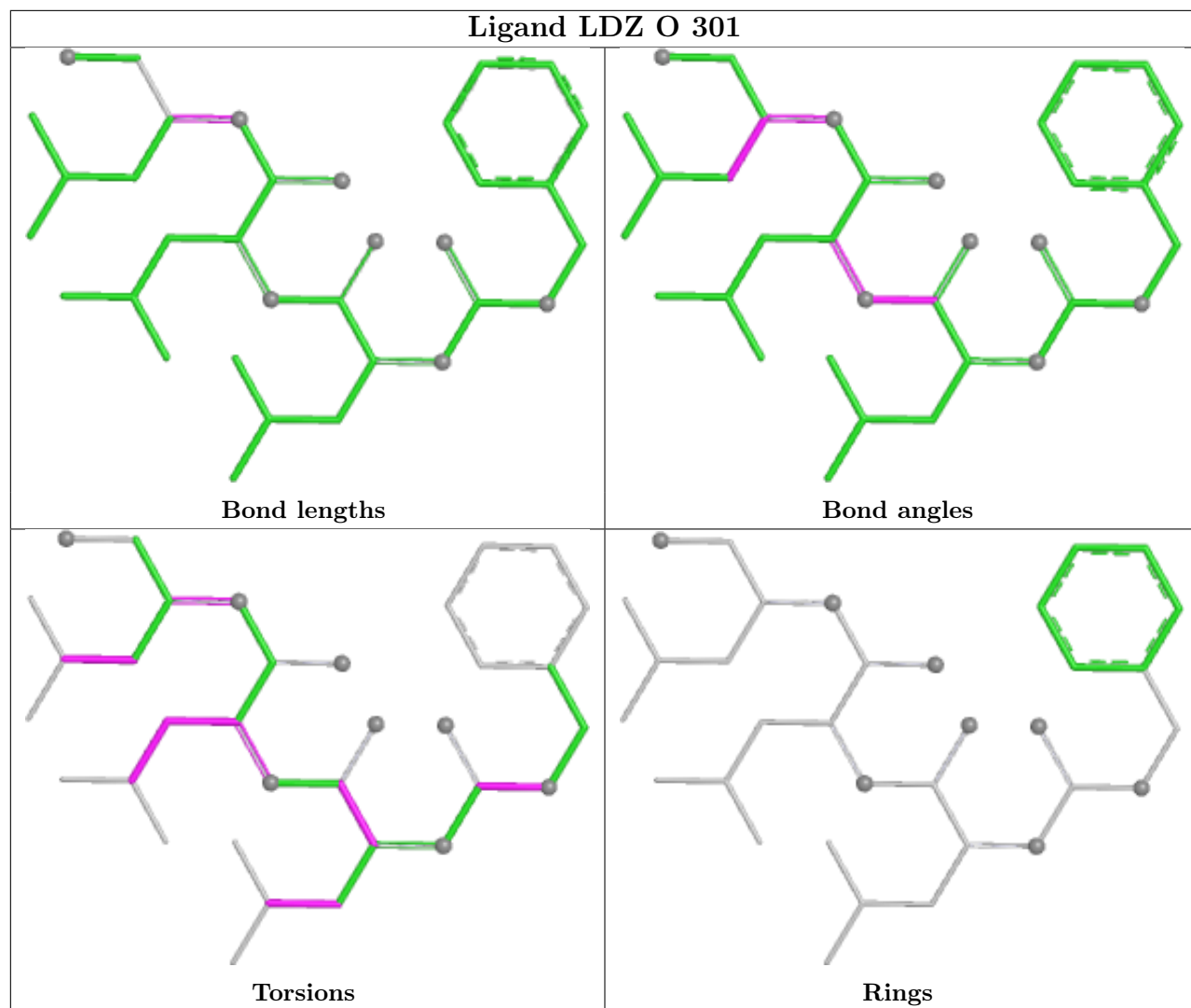
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

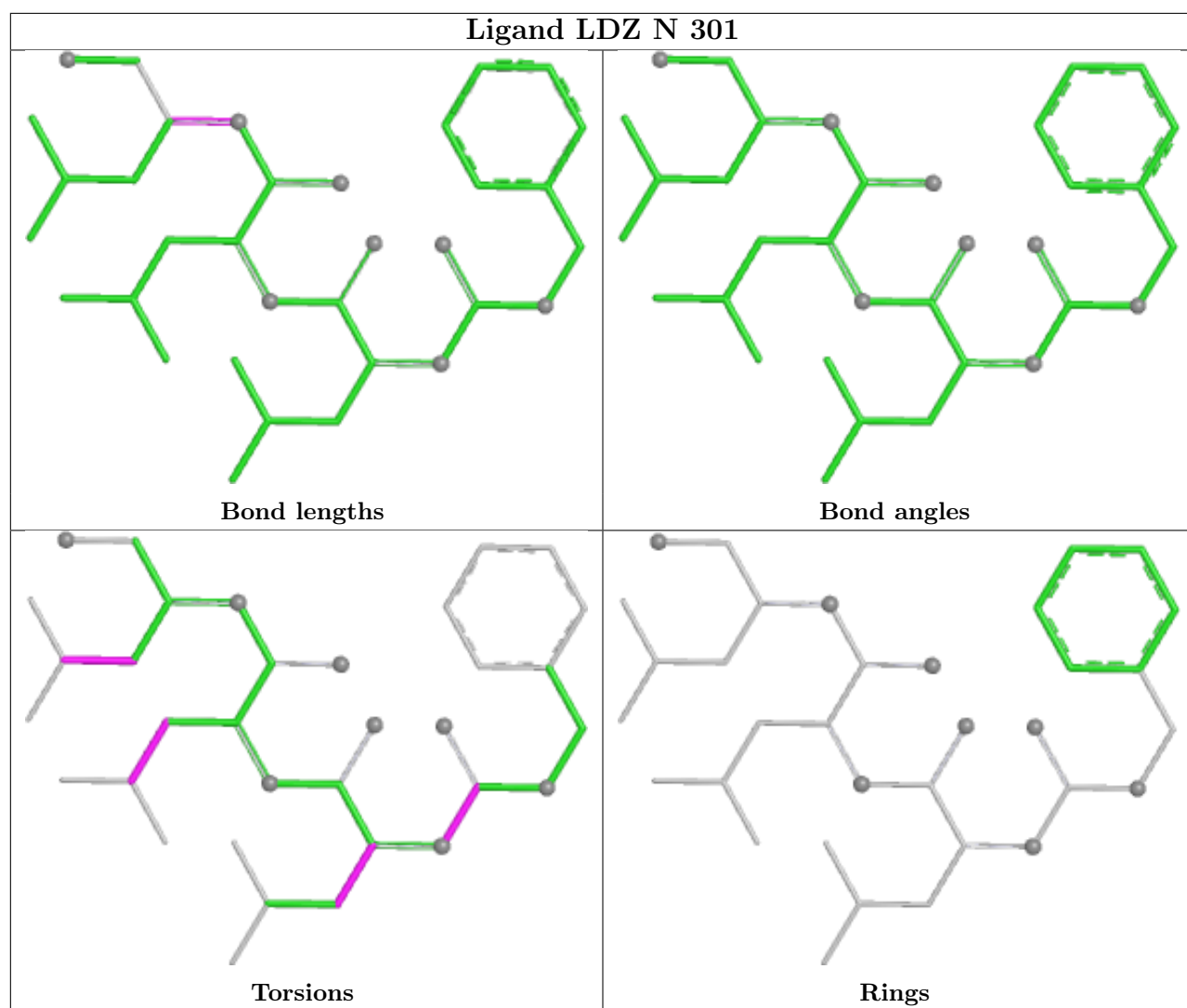
equivalents in the CSD to analyse the geometry.

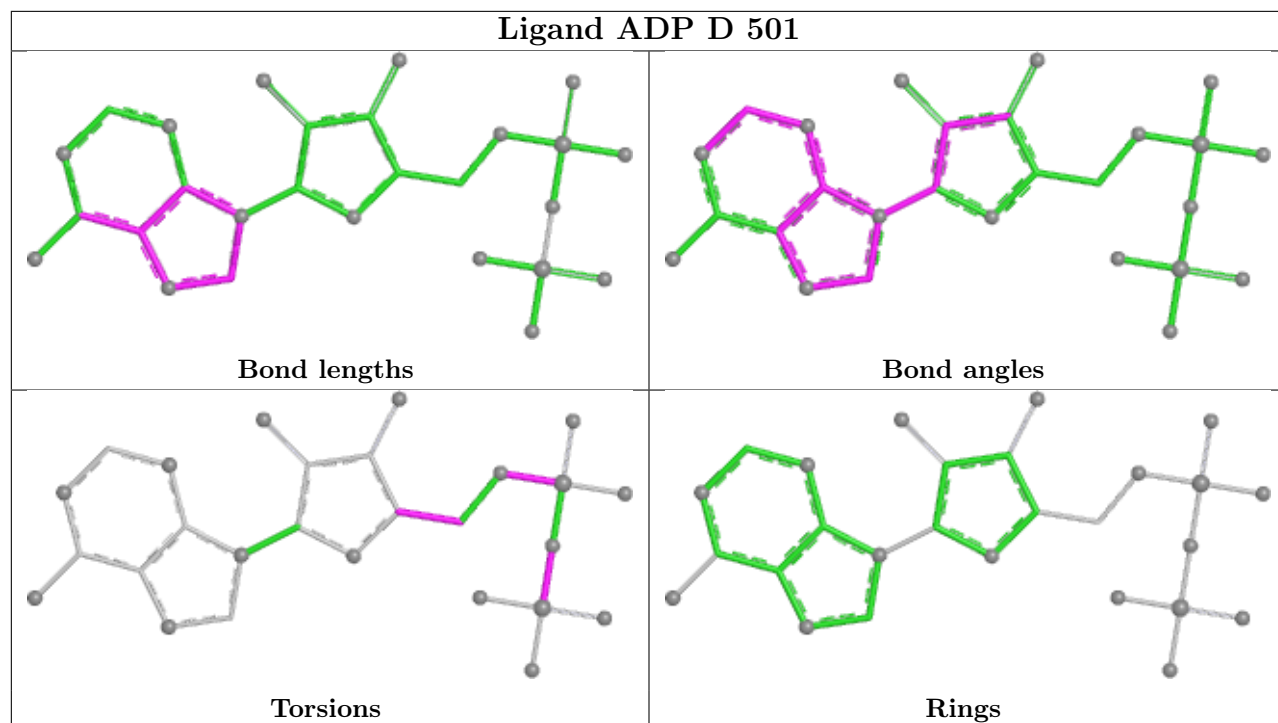


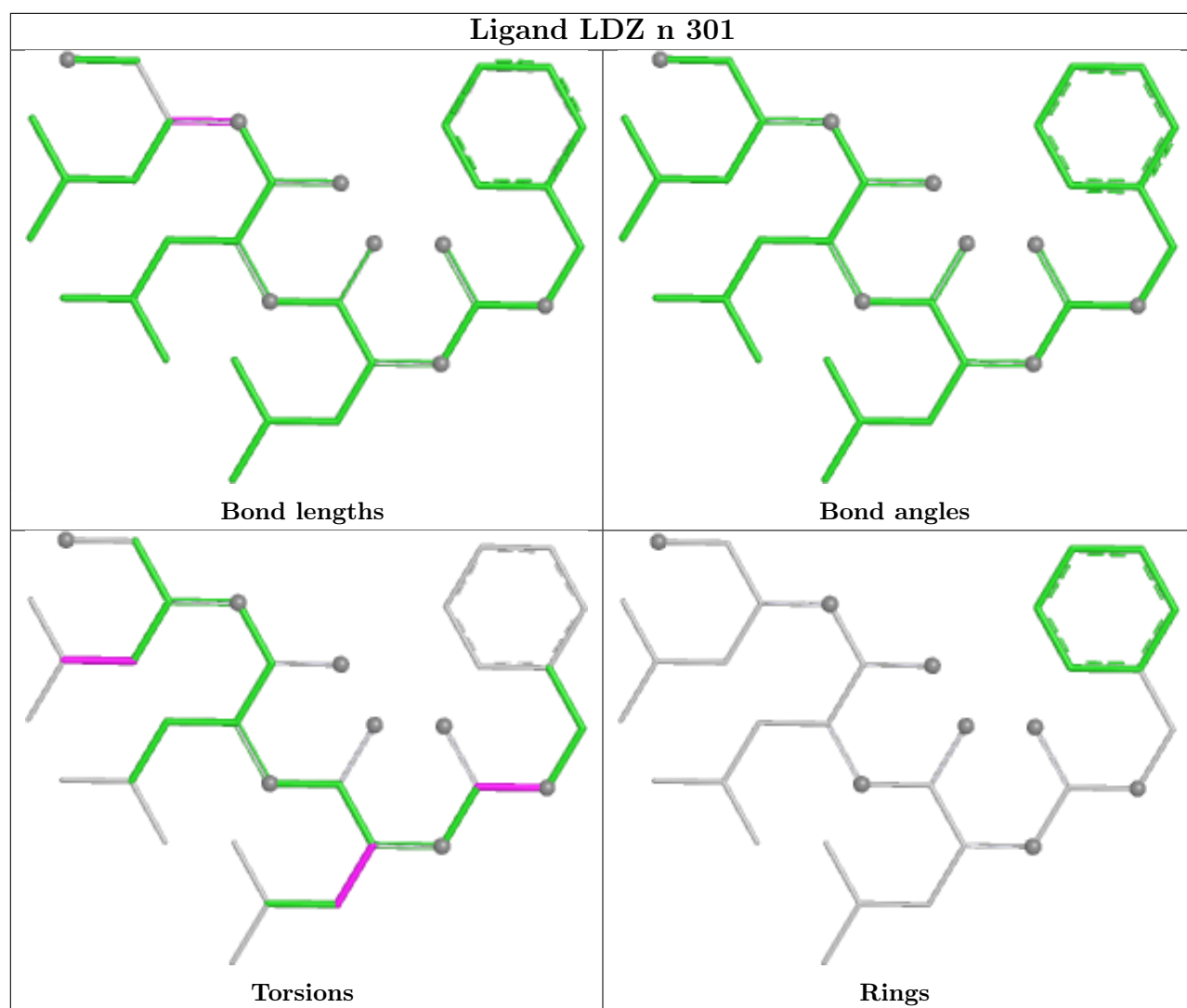
Ligand ATP F 501

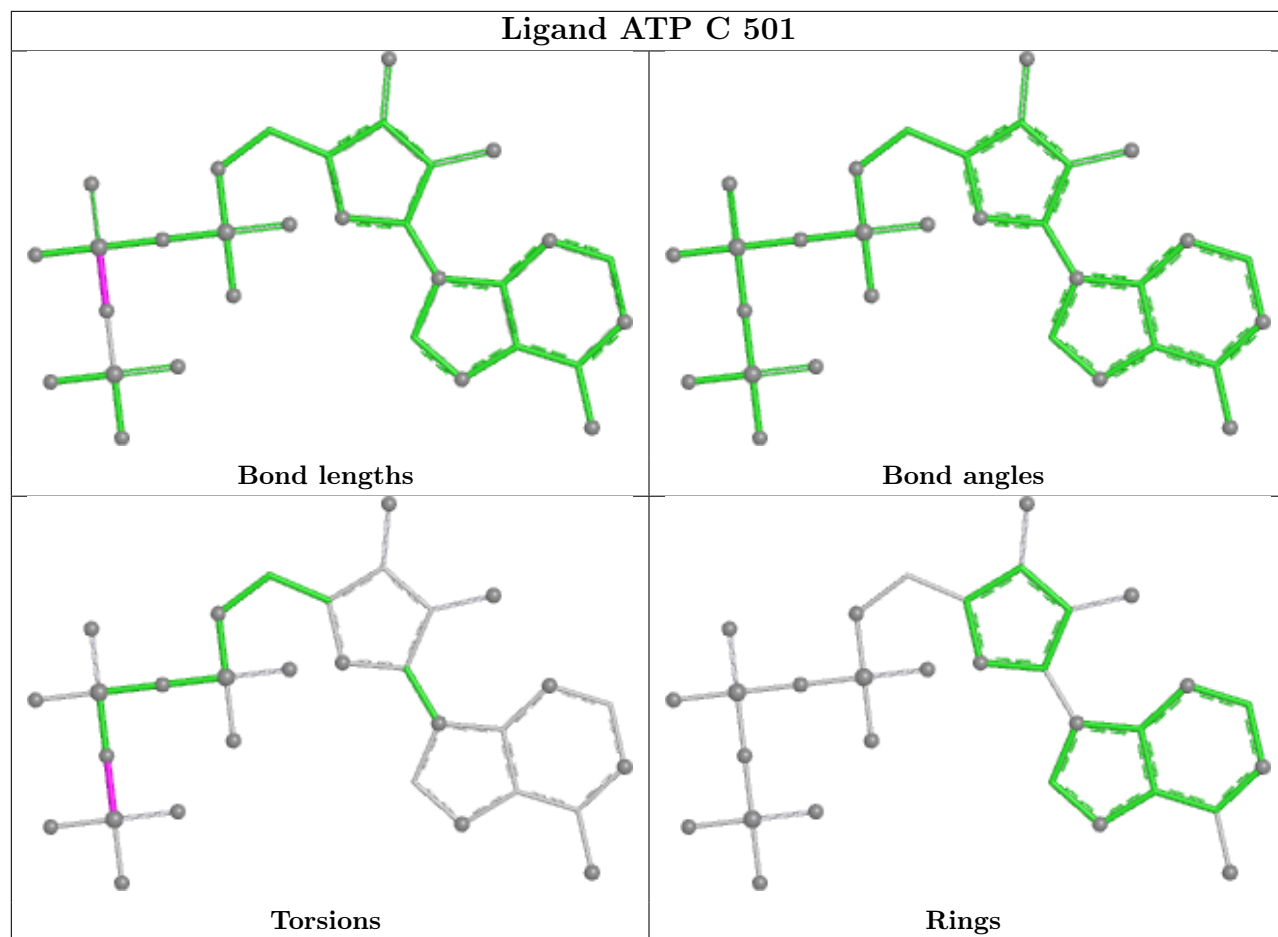


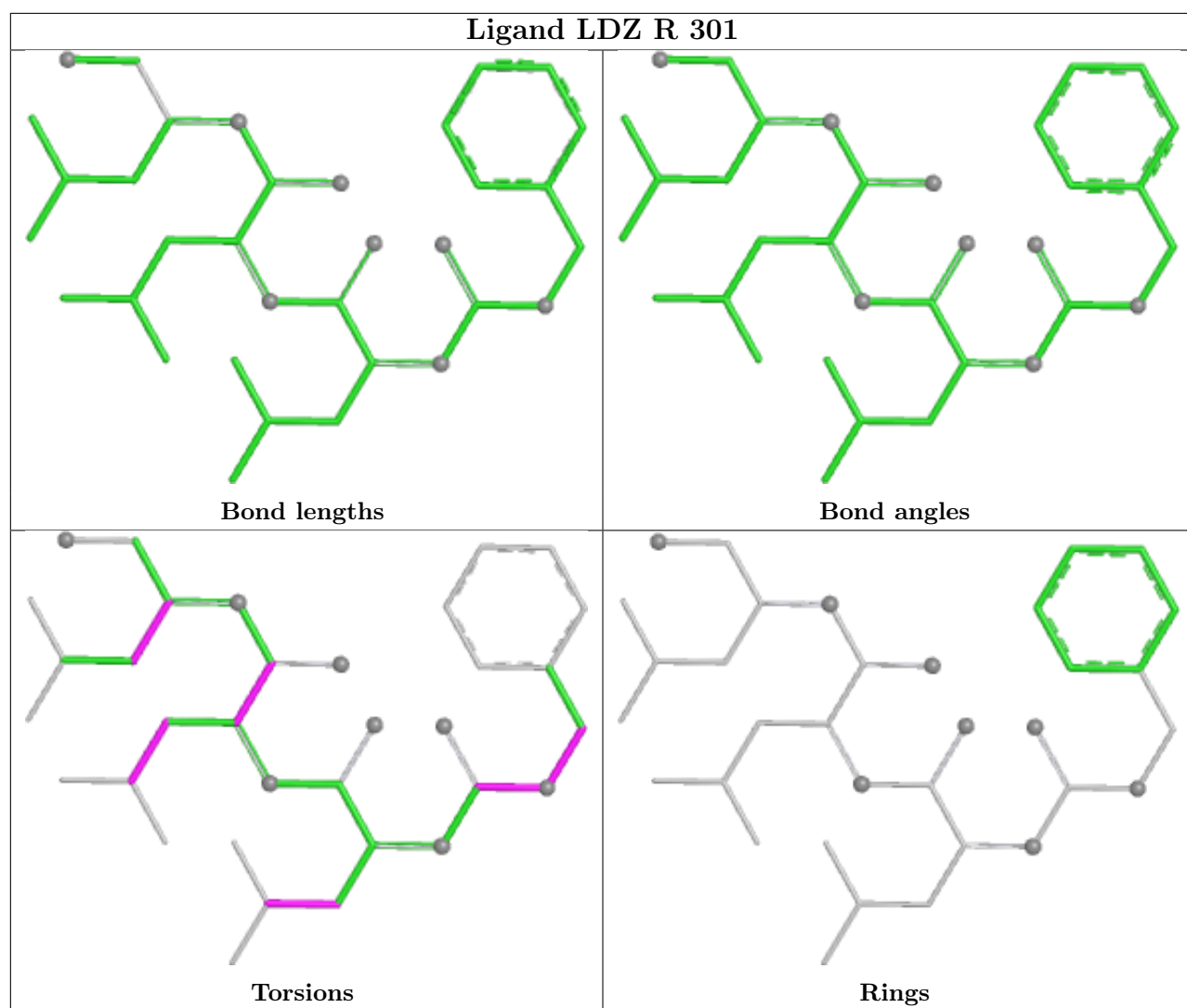


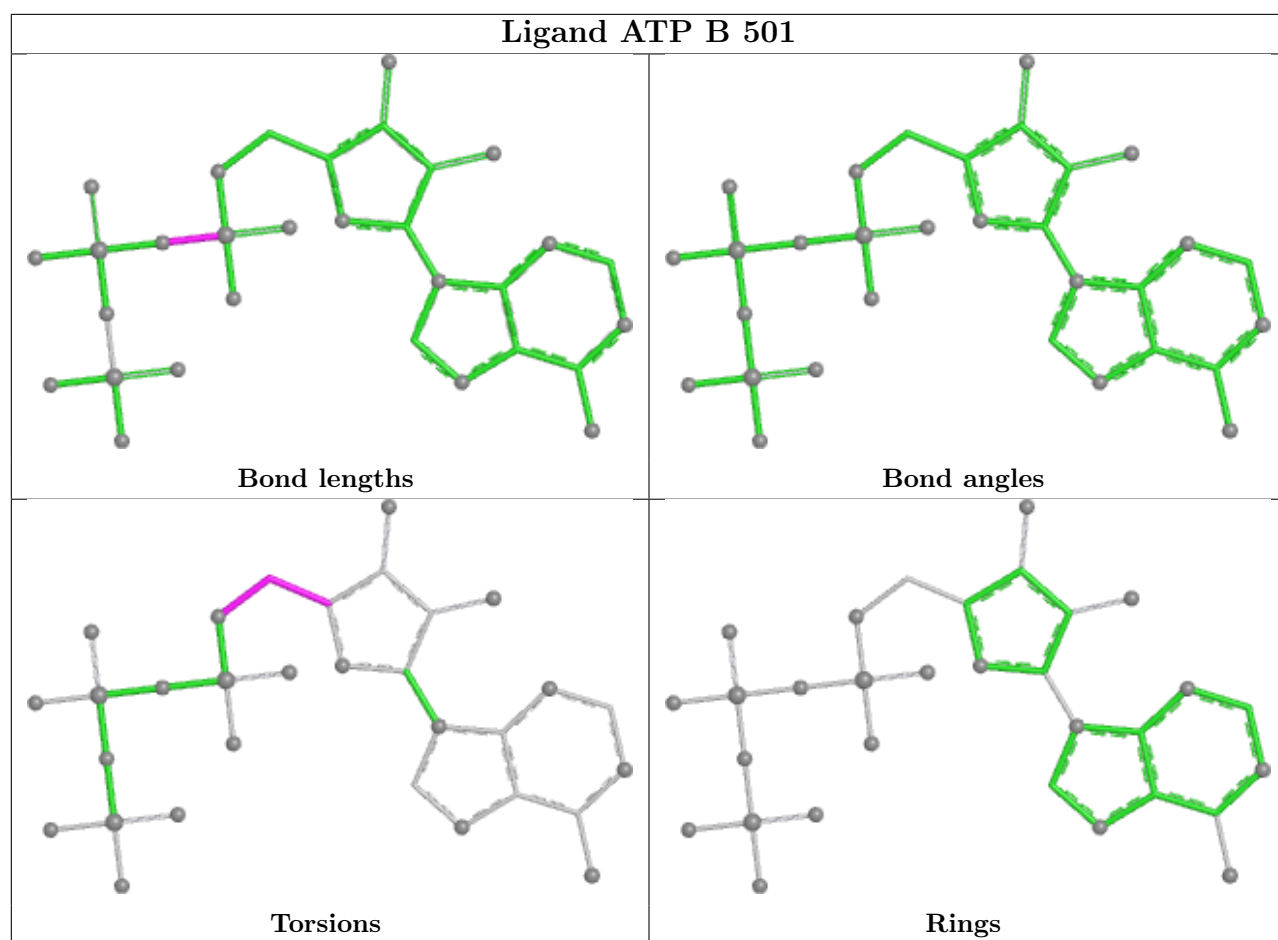


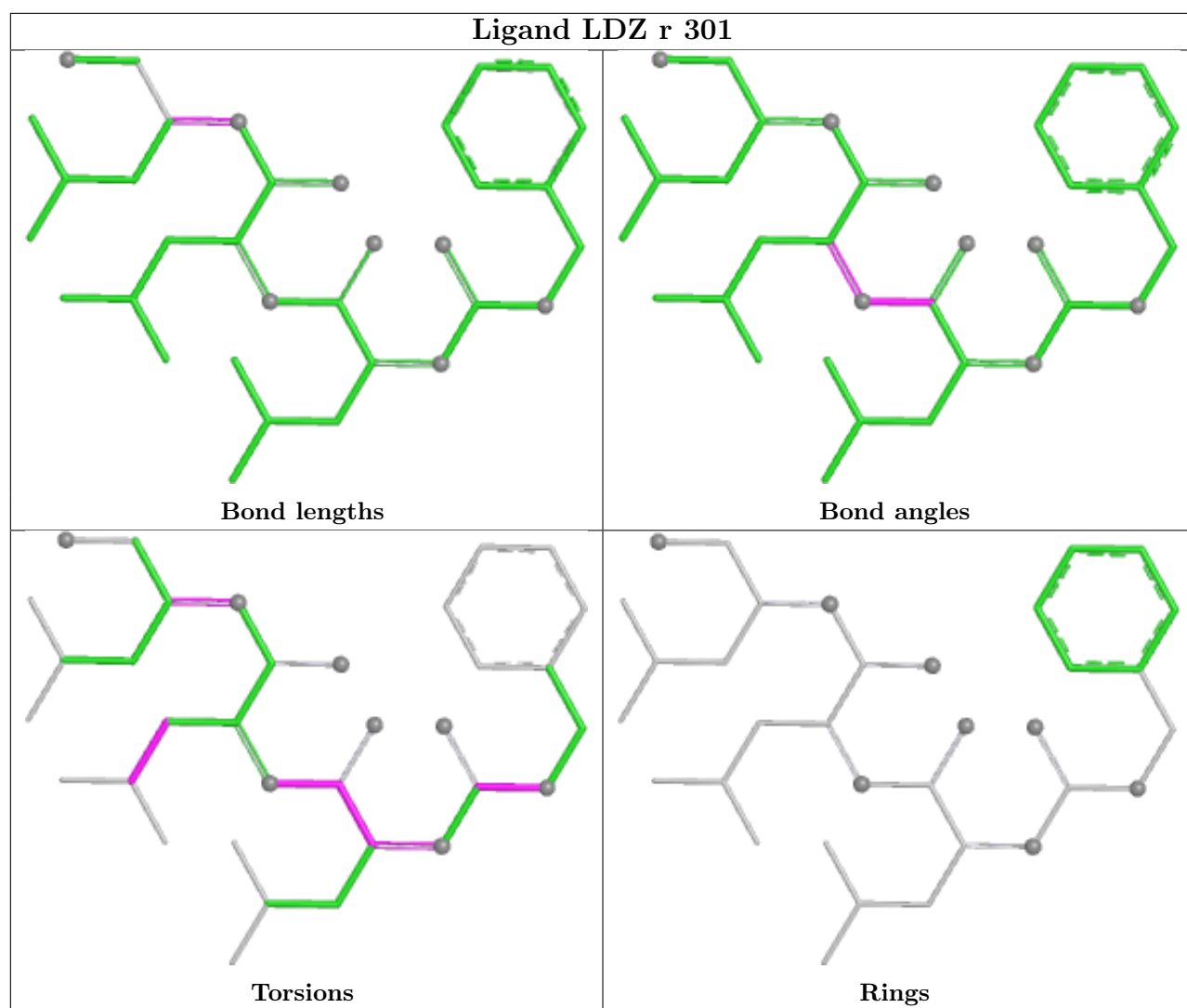


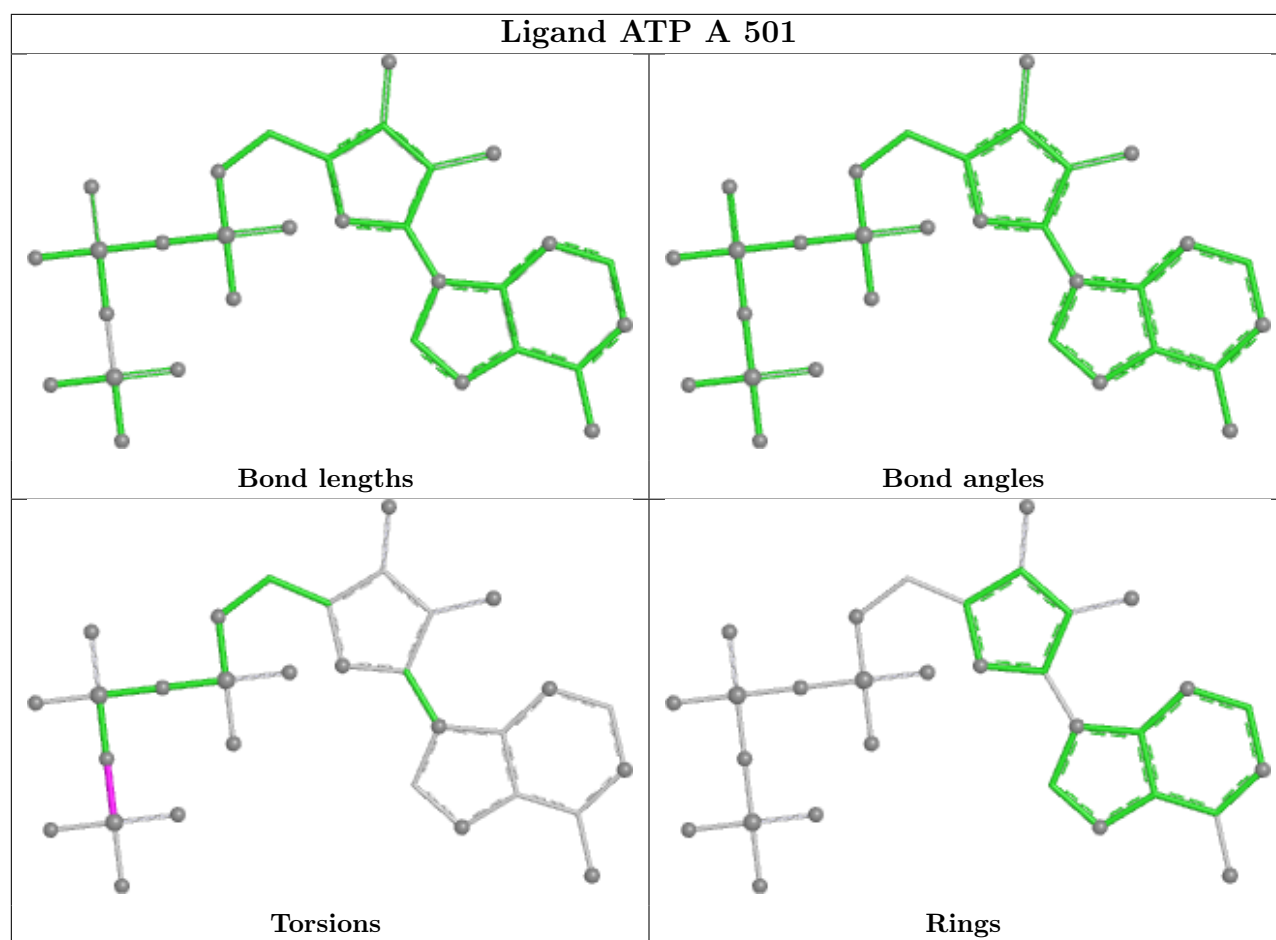












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

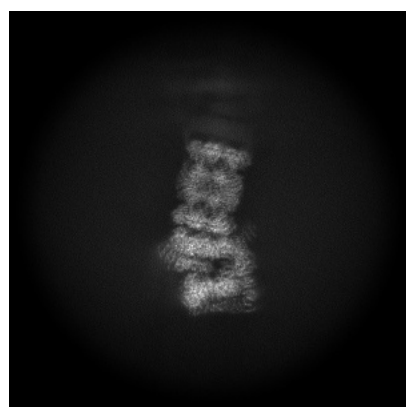
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49510. These allow visual inspection of the internal detail of the map and identification of artifacts.

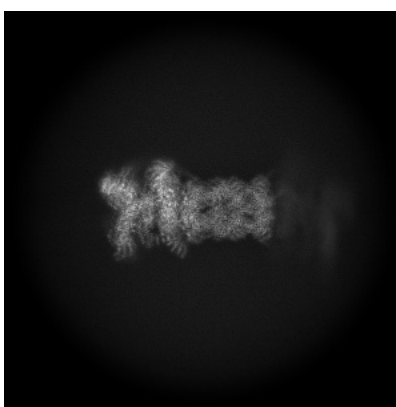
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

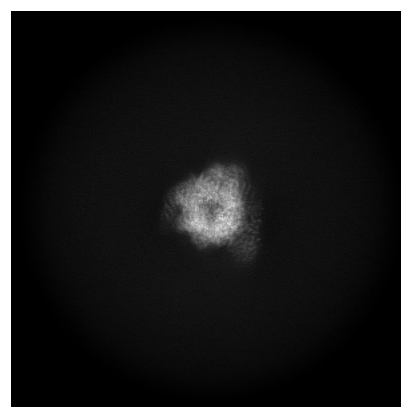
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

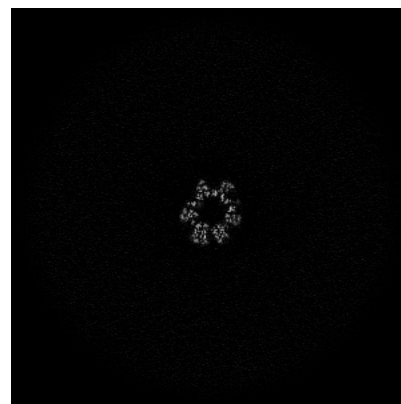
6.2.1 Primary map



X Index: 320



Y Index: 320

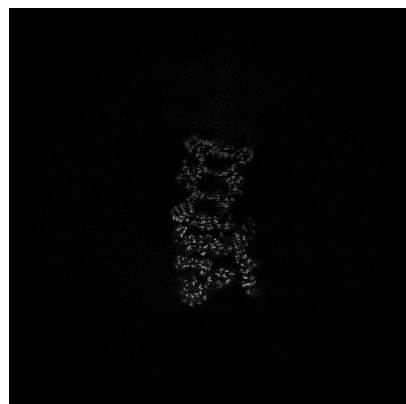


Z Index: 320

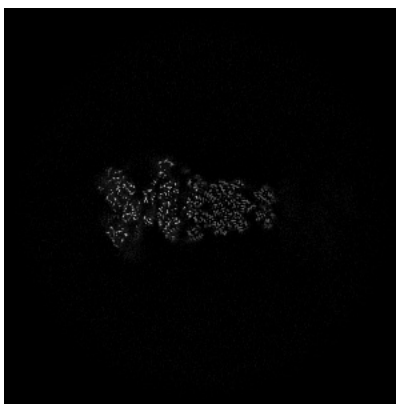
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

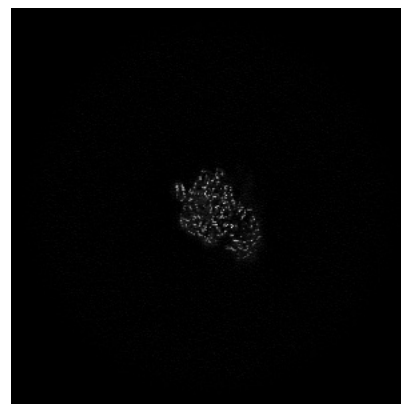
6.3.1 Primary map



X Index: 333



Y Index: 293

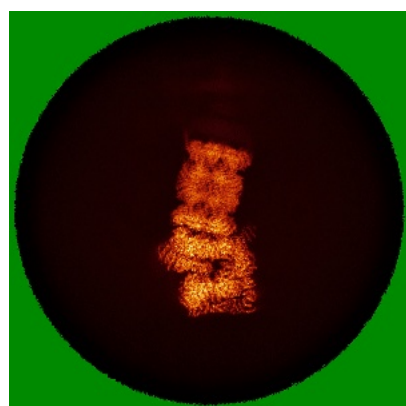


Z Index: 263

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

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

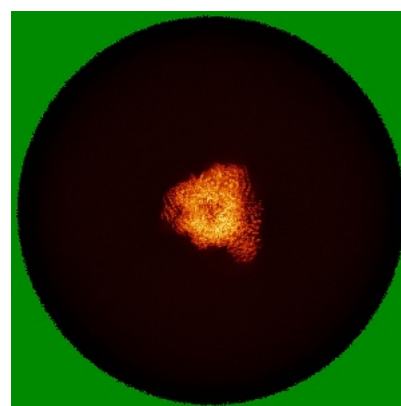
6.4.1 Primary map



X



Y

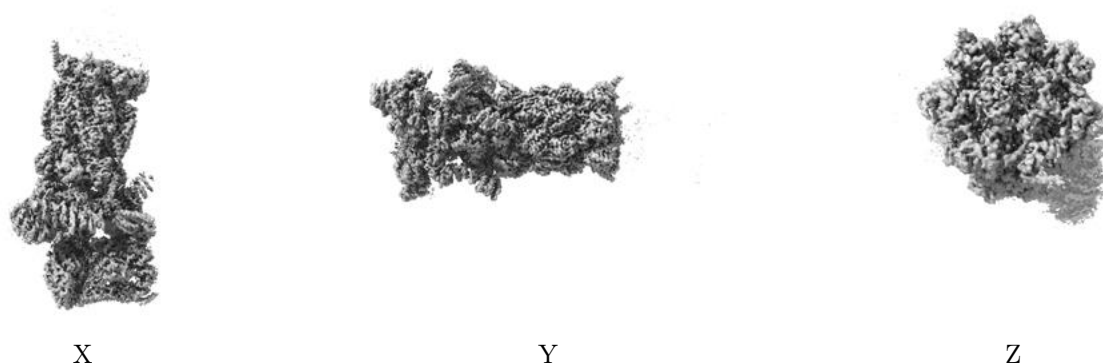


Z

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.

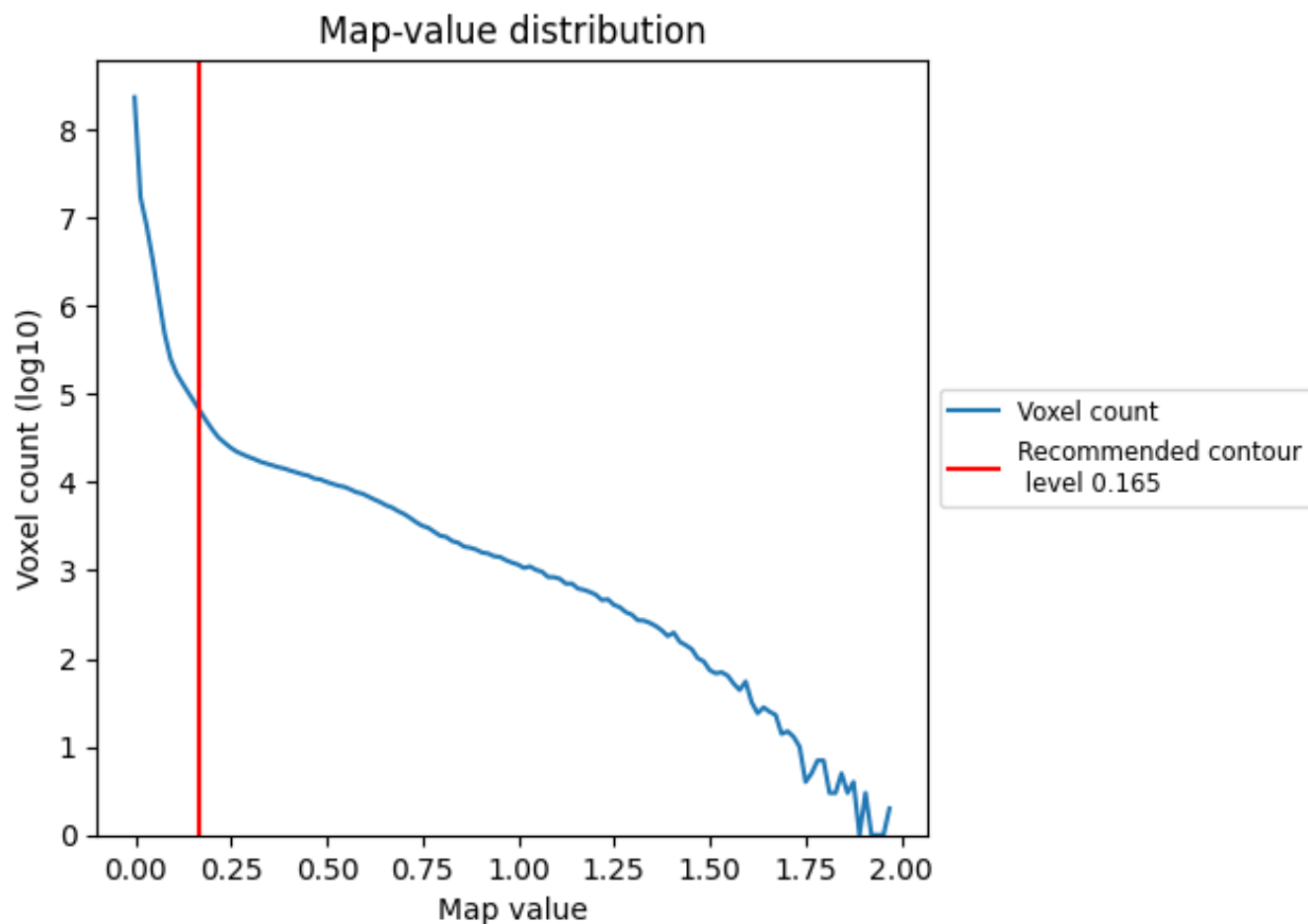
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

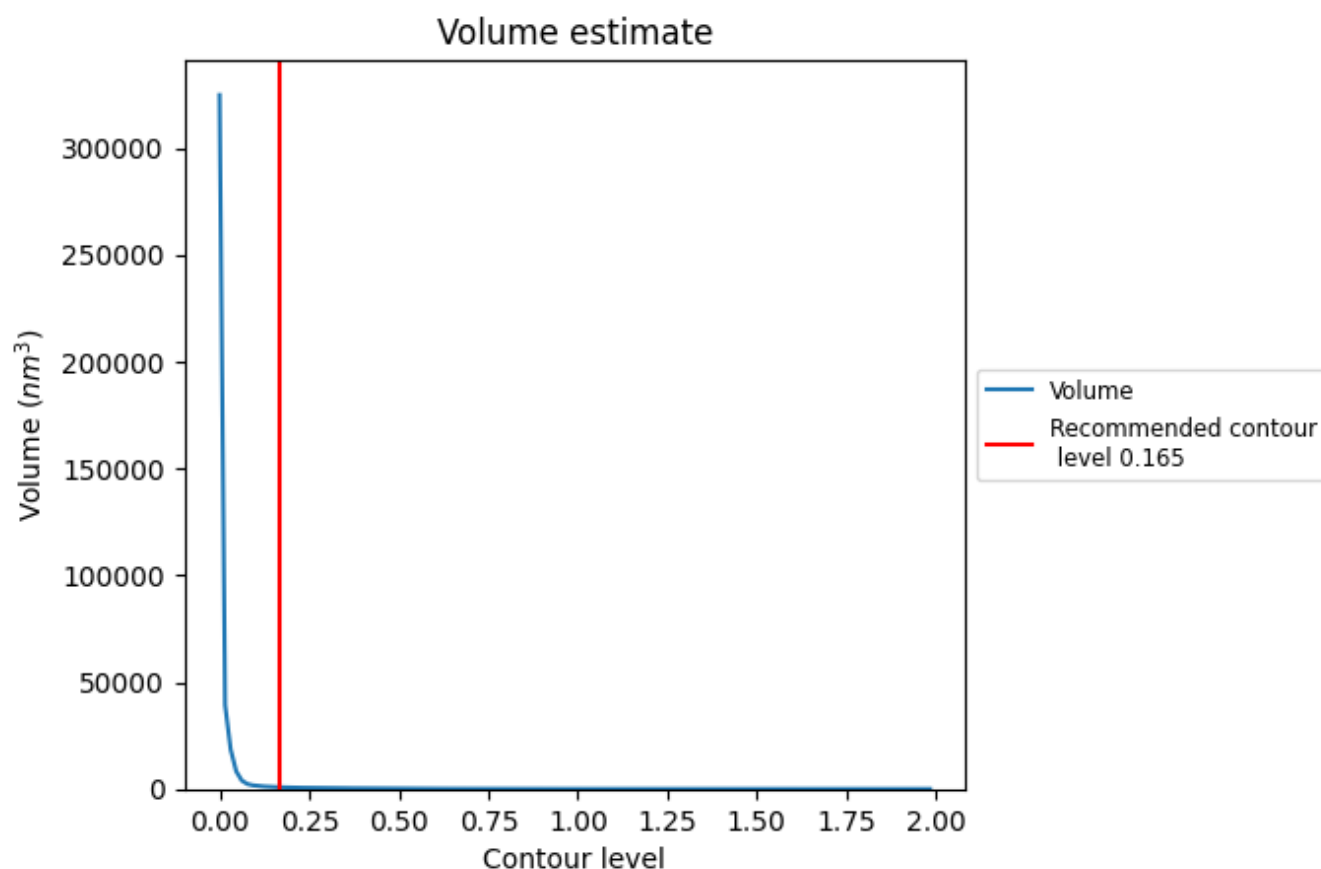
This section contains the results of statistical analysis of the map.

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.

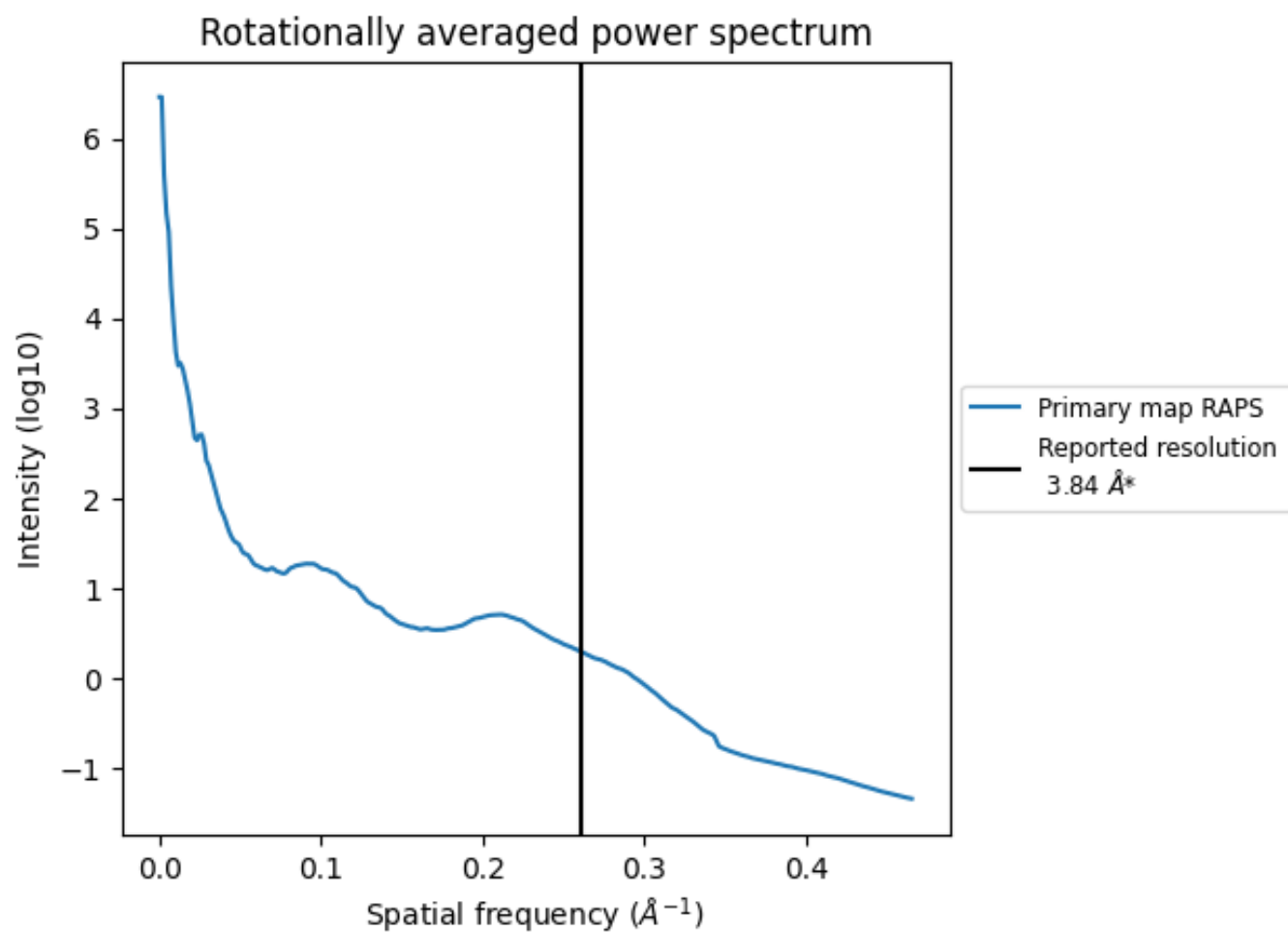
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 806 nm^3 ; this corresponds to an approximate mass of 728 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 0.260 Å⁻¹

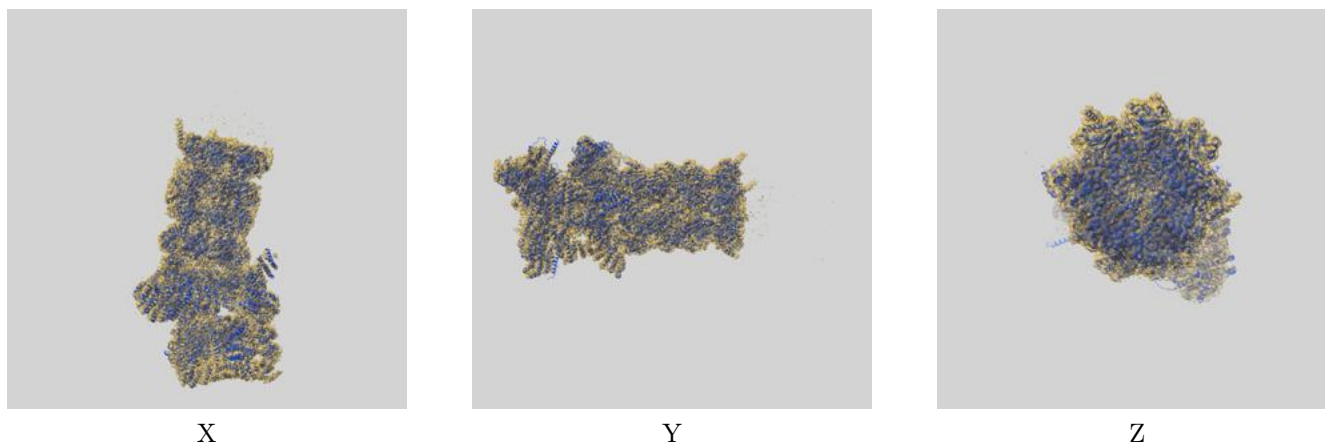
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

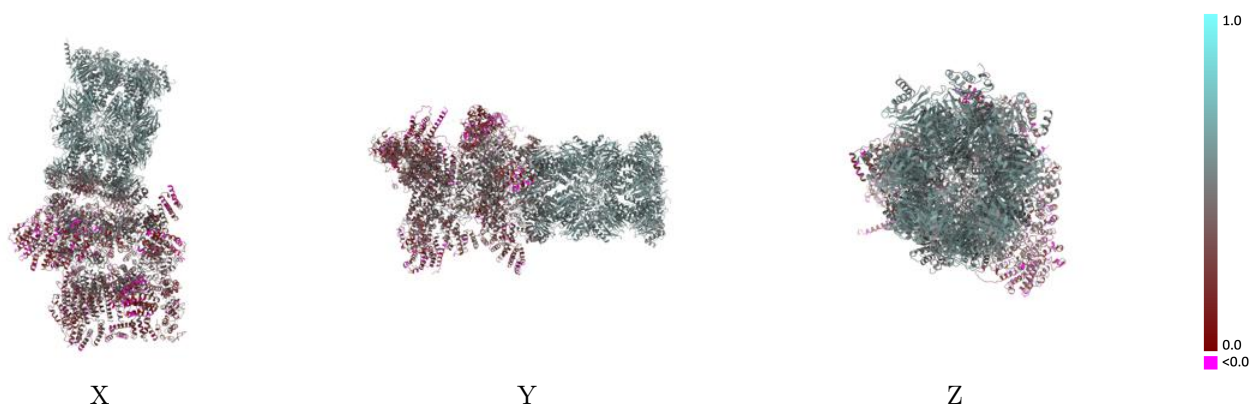
This section contains information regarding the fit between EMDB map EMD-49510 and PDB model 9NKJ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



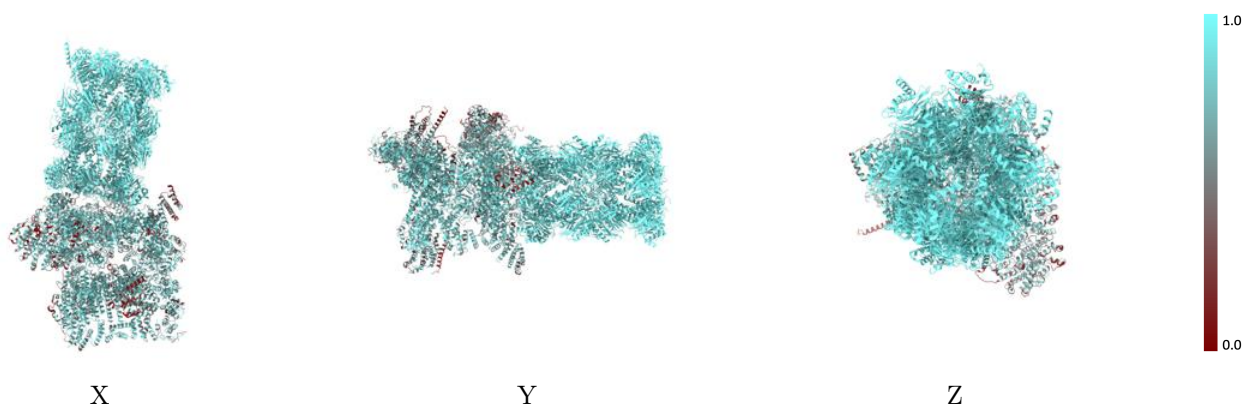
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



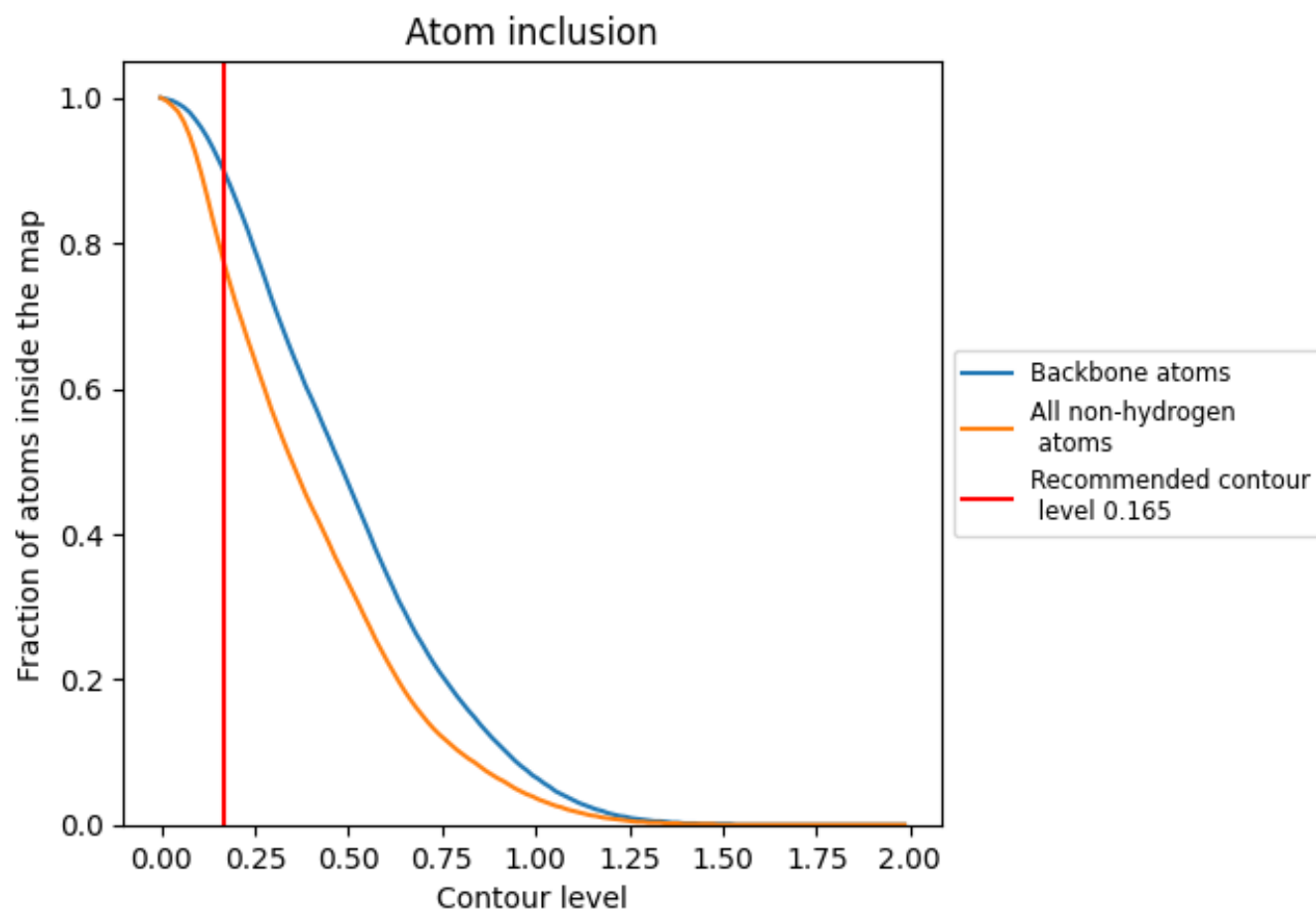
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 90% of all backbone atoms, 78% 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	 0.7780	 0.4190
A	 0.7740	 0.3840
B	 0.8010	 0.4170
C	 0.8340	 0.4330
D	 0.8240	 0.4110
E	 0.6170	 0.2560
F	 0.7720	 0.3710
G	 0.9460	 0.4870
H	 0.9520	 0.5110
I	 0.9170	 0.4810
J	 0.9000	 0.4250
K	 0.9030	 0.4600
L	 0.9710	 0.4980
M	 0.9490	 0.5090
N	 0.9700	 0.5620
O	 0.9750	 0.5660
P	 0.9710	 0.5650
Q	 0.9770	 0.5700
R	 0.9790	 0.5730
S	 0.9750	 0.5710
T	 0.9810	 0.5740
U	 0.7320	 0.2840
V	 0.5870	 0.2420
W	 0.6950	 0.3110
X	 0.6620	 0.3290
Y	 0.7190	 0.3150
Z	 0.7950	 0.3600
a	 0.7020	 0.2690
b	 0.7160	 0.3270
c	 0.7670	 0.3730
d	 0.6470	 0.3120
e	 0.5150	 0.2560
f	 0.5510	 0.2220
g	 0.9610	 0.5530
h	 0.9800	 0.5640



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Chain	Atom inclusion	Q-score
i	 0.9620	 0.5540
j	 0.9760	 0.5510
k	 0.9560	 0.5520
l	 0.9690	 0.5590
m	 0.9620	 0.5530
n	 0.9710	 0.5700
o	 0.9800	 0.5720
p	 0.9780	 0.5730
q	 0.9800	 0.5790
r	 0.9830	 0.5750
s	 0.9670	 0.5700
t	 0.9810	 0.5690
v	 0.9000	 0.5410