



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 11:58 PM UTC

PDB ID : 22MM / pdb_000022mm
EMDB ID : EMD-68472
Title : Structure of human 26S proteasome complexed with midnolin(1-111+337-468)
Authors : Liang, L.; Zhu, C.; Qin, L.
Deposited on : 2026-01-16
Resolution : 3.42 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

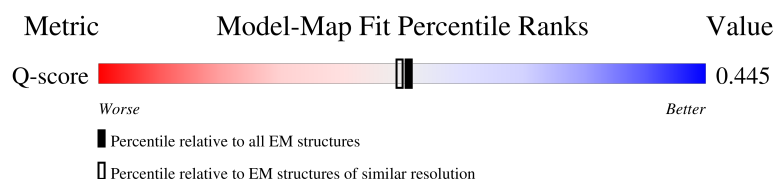
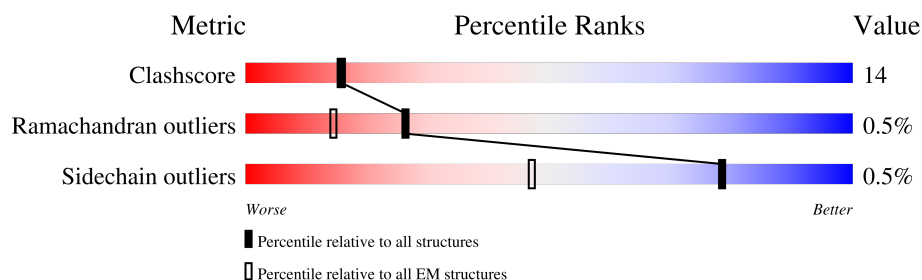
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 Å.

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







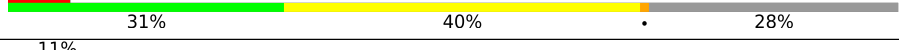
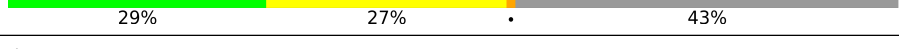
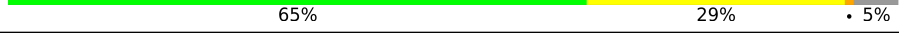
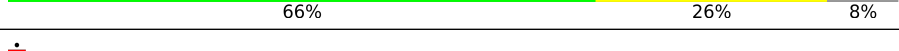
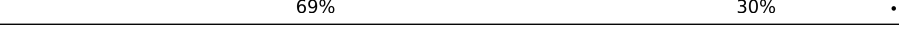
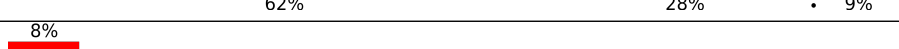


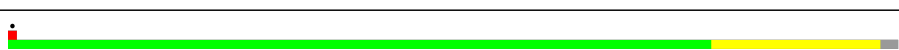

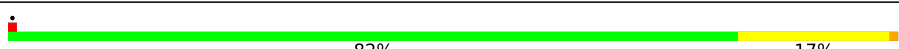





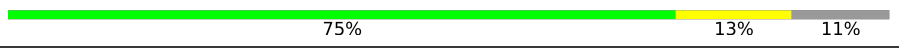
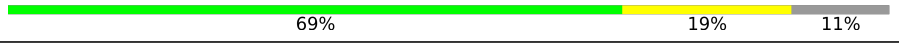



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13959 (2.92 - 3.92)

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	U	953	<div> <div>11%</div> <div>51%</div> <div>37%</div> <div>11%</div> </div>
2	V	533	<div> <div>11%</div> <div>47%</div> <div>43%</div> <div>10%</div> </div>
3	W	456	<div> <div>44%</div> <div>53%</div> <div>10%</div> </div>
4	X	422	<div> <div>57%</div> <div>32%</div> <div>10%</div> </div>


















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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	c	309	
9	d	349	
10	e	70	
11	A	433	
12	B	440	
13	C	398	
14	D	418	
15	E	403	
16	F	439	
17	G	245	
17	g	245	
18	H	233	
18	h	233	
19	I	260	
19	i	260	
20	J	248	
21	K	241	
21	k	241	
22	L	268	
22	l	268	
23	M	254	
23	m	254	

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Mol	Chain	Length	Quality of chain
24	N	238	
24	n	238	
25	O	276	
25	o	276	
26	P	204	
26	p	204	
27	Q	201	
27	q	201	
28	R	262	
28	r	262	
29	S	240	
29	s	240	
30	T	263	
30	t	263	
31	j	247	
32	f	445	
33	u	908	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 103249 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	845	Total	C	N	O	S	0	0
			6595	4186	1120	1245	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	452	Total	C	N	O	S	0	0
			3667	2314	631	697	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	253	Total	C	N	O	S	0	0
			2078	1348	340	381	9		

- Molecule 10 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	405	Total	C	N	O	S	0	0
			3162	1994	538	615	15		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 15 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	352	Total	C	N	O	S	0	0
			2786	1750	496	524	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	362	Total	C	N	O	S	0	0
			2834	1789	489	540	16		

- Molecule 17 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		
17	g	240	Total	C	N	O	S	0	0
			1830	1163	306	348	13		

- Molecule 18 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	231	Total	C	N	O	S	0	0
			1726	1097	293	331	5		
18	h	232	Total	C	N	O	S	0	0
			1727	1096	292	334	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
19	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 20 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	247	Total	C	N	O	S	0	0
			1844	1148	331	360	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	230	Total	C	N	O	S	0	0
			1746	1096	286	353	11		
21	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 22 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
22	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 23 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
23	m	240	Total	C	N	O	S	0	0
			1862	1181	317	353	11		

- Molecule 24 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		
24	n	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

- Molecule 25 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
25	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
26	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 27 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
27	q	199	Total	C	N	O	S	0	0
			1574	1009	266	290	9		

- Molecule 28 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
28	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 29 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
29	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 30 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
30	t	215	Total	C	N	O	S	0	0
			1673	1055	288	318	12		

- Molecule 31 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 32 is a protein called Midnolin,MCHERRY,fusion tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			453	266	108	76	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	469	SER	-	linker	UNP Q504T8
f	470	ARG	-	linker	UNP Q504T8
f	471	GLU	-	linker	UNP Q504T8
f	472	ASN	-	linker	UNP Q504T8
f	473	LEU	-	linker	UNP Q504T8
f	474	TYR	-	linker	UNP Q504T8
f	475	PHE	-	linker	UNP Q504T8
f	476	GLN	-	linker	UNP Q504T8
f	477	GLY	-	linker	UNP Q504T8
f	478	ALA	-	linker	UNP Q504T8

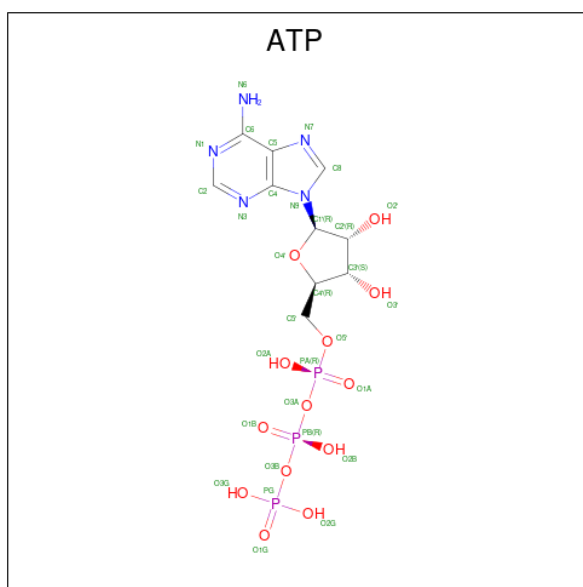
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	832	Total	C	N	O	S	0	0
			6439	4072	1090	1232	45		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

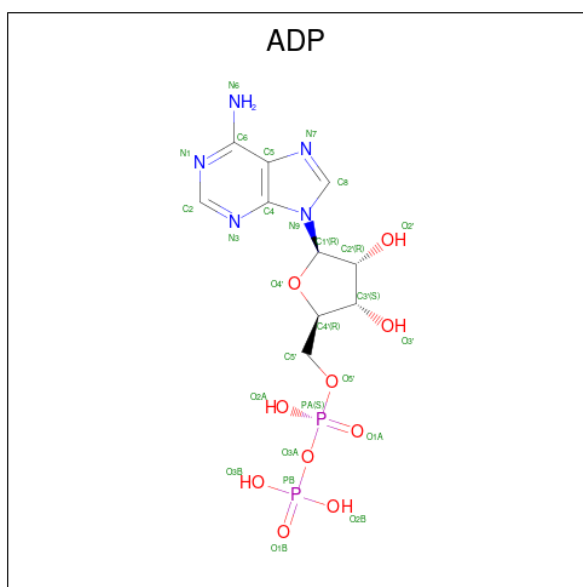


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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



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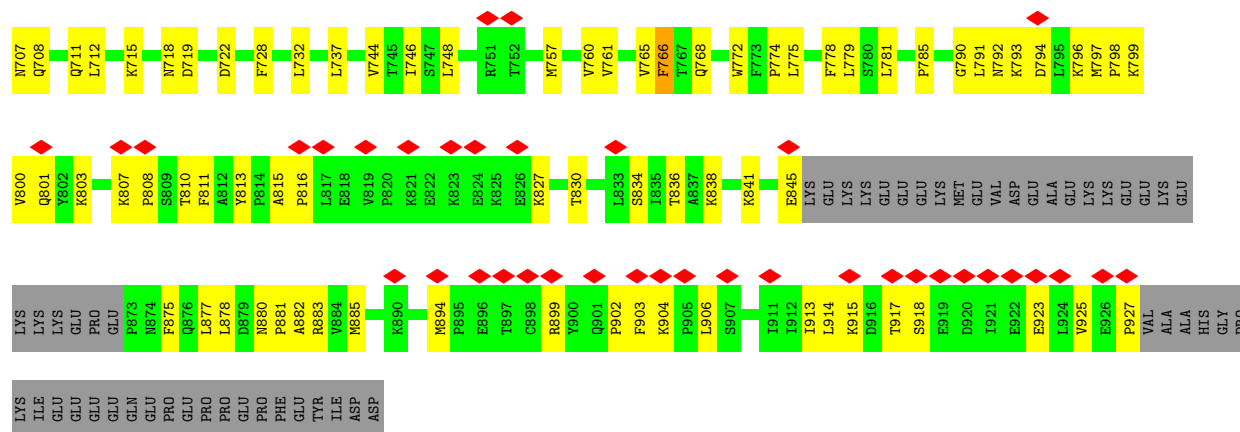
Mol	Chain	Residues	Atoms				AltConf
38	O	1	Total 34	C 26	N 3	O 5	0
38	R	1	Total 34	C 26	N 3	O 5	0
38	n	1	Total 34	C 26	N 3	O 5	0
38	o	1	Total 34	C 26	N 3	O 5	0
38	r	1	Total 34	C 26	N 3	O 5	0

3 Residue-property plots

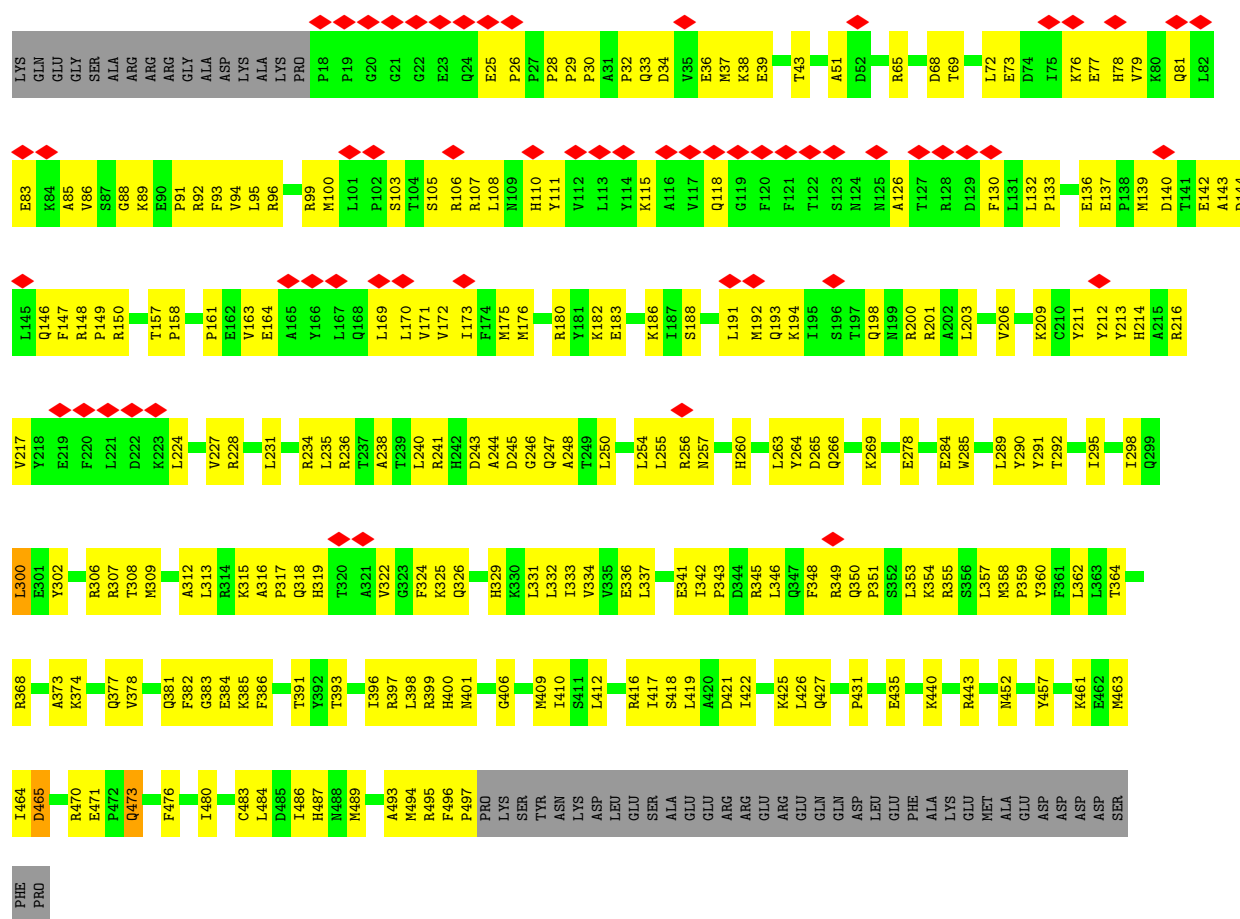
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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





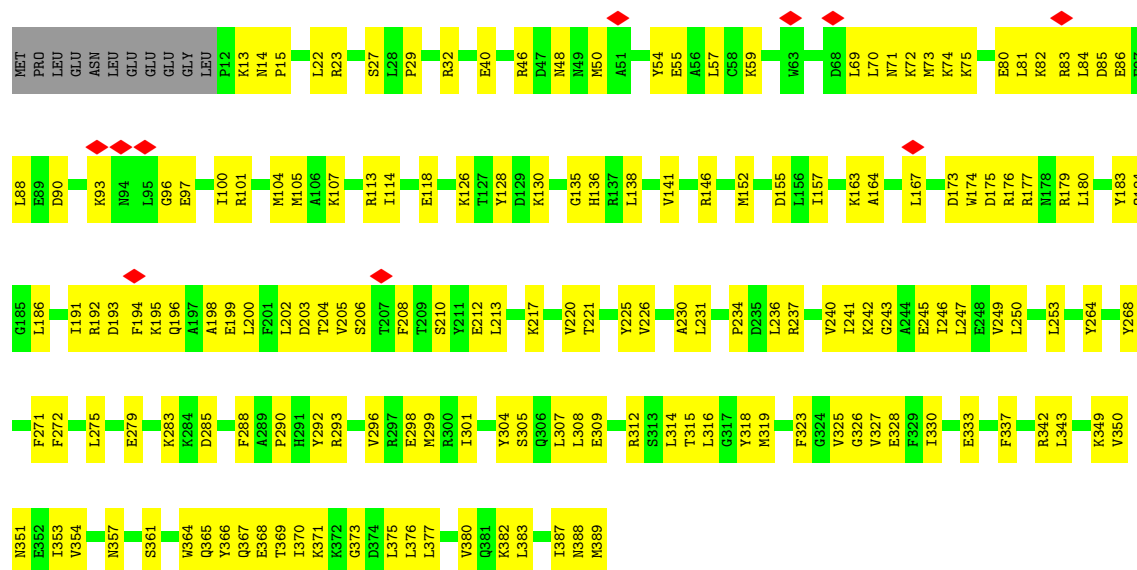
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

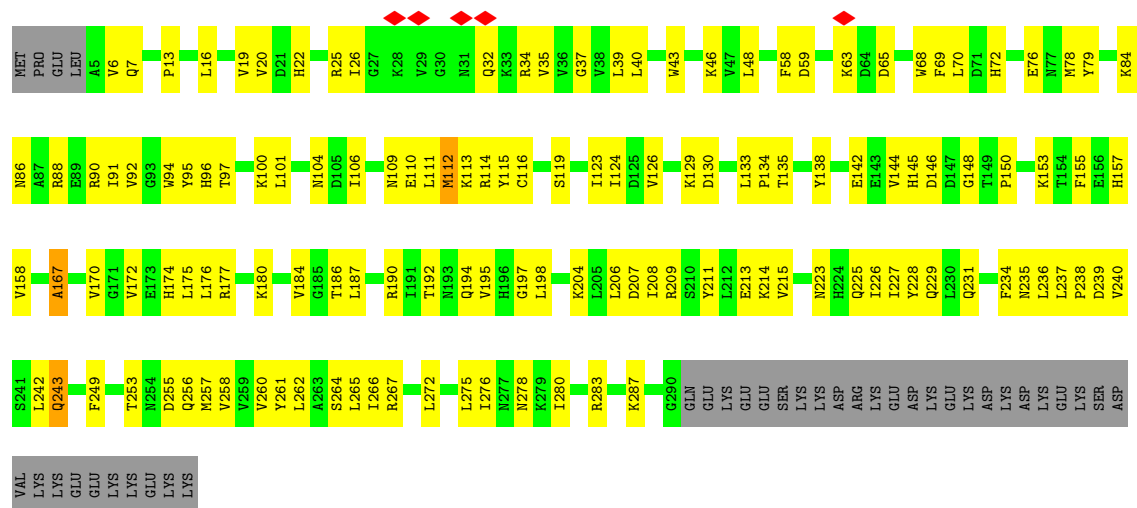






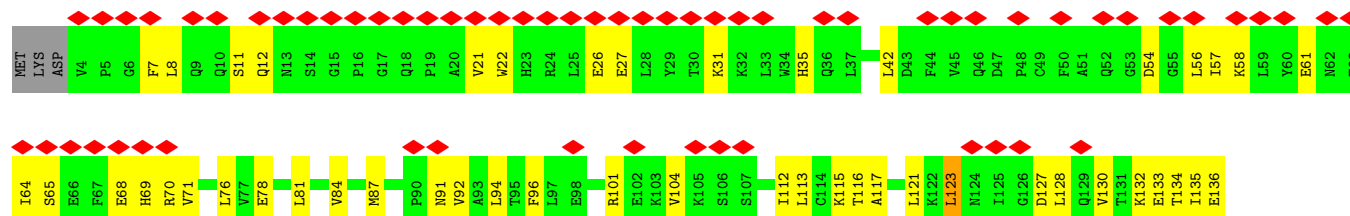
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

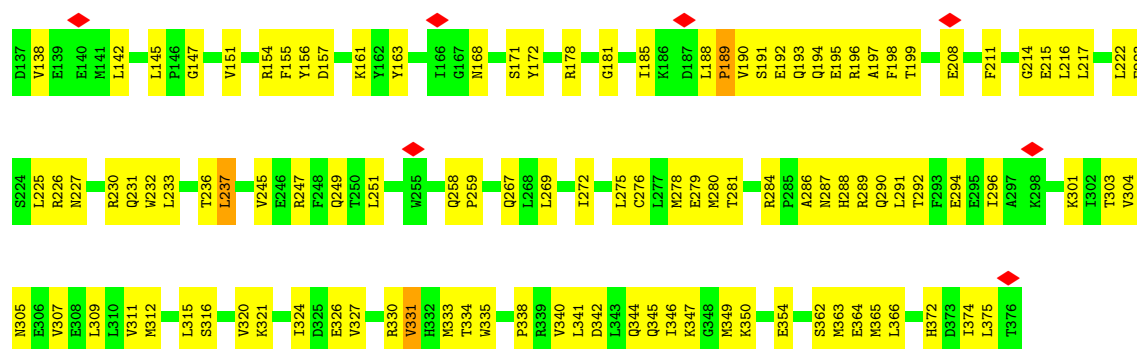
Chain Z: 47% 40% 12%



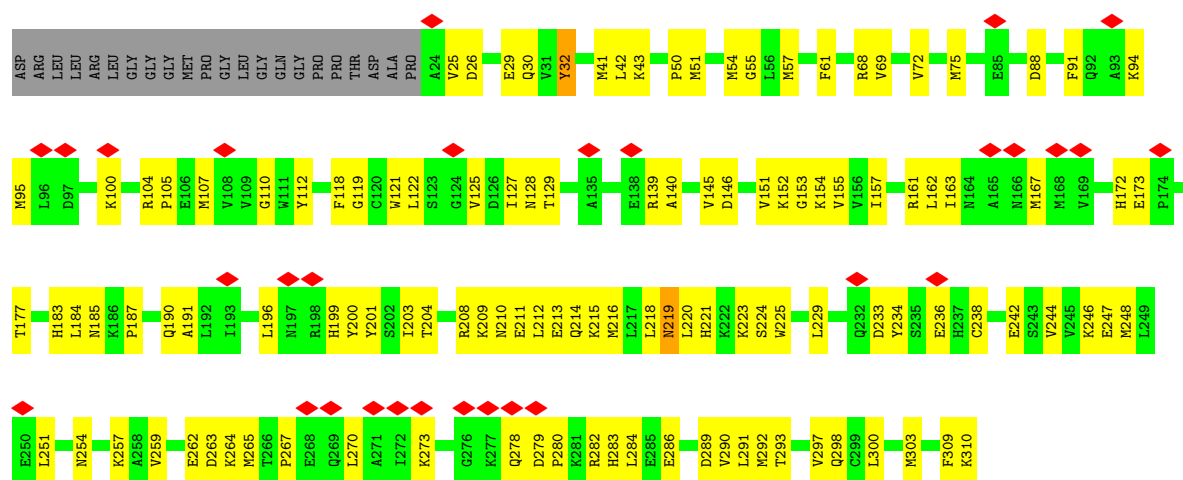
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 18% 57% 41%

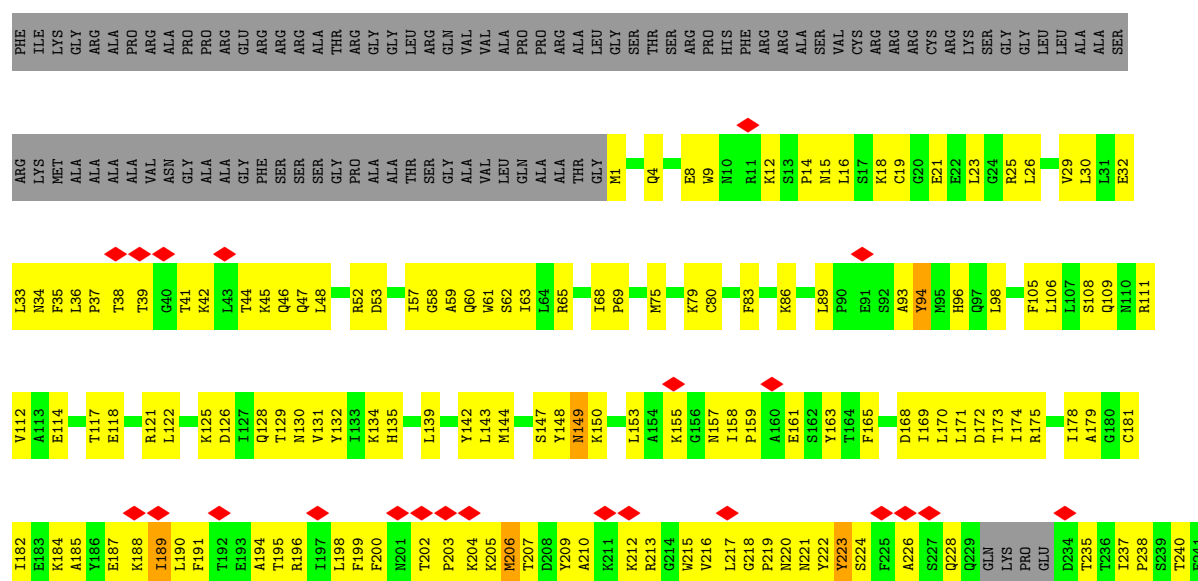




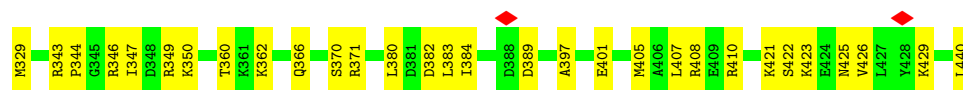
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 14



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 8

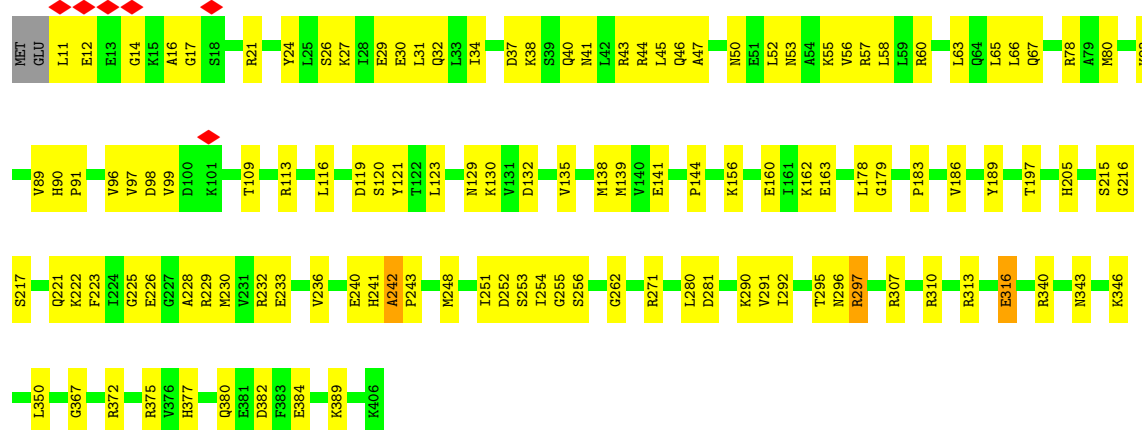






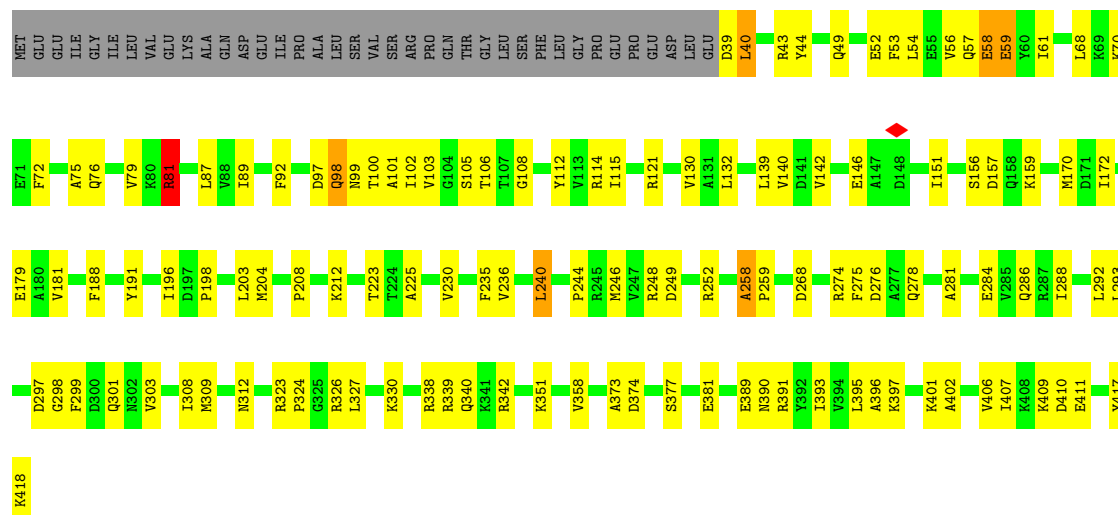
• Molecule 13: 26S proteasome regulatory subunit 8

Chain C: 69% 30%



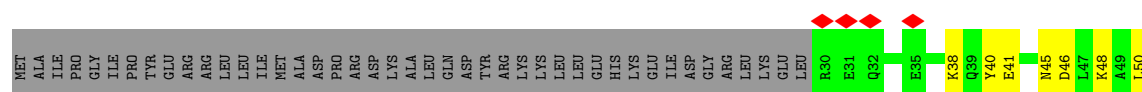
• Molecule 14: 26S proteasome regulatory subunit 6B

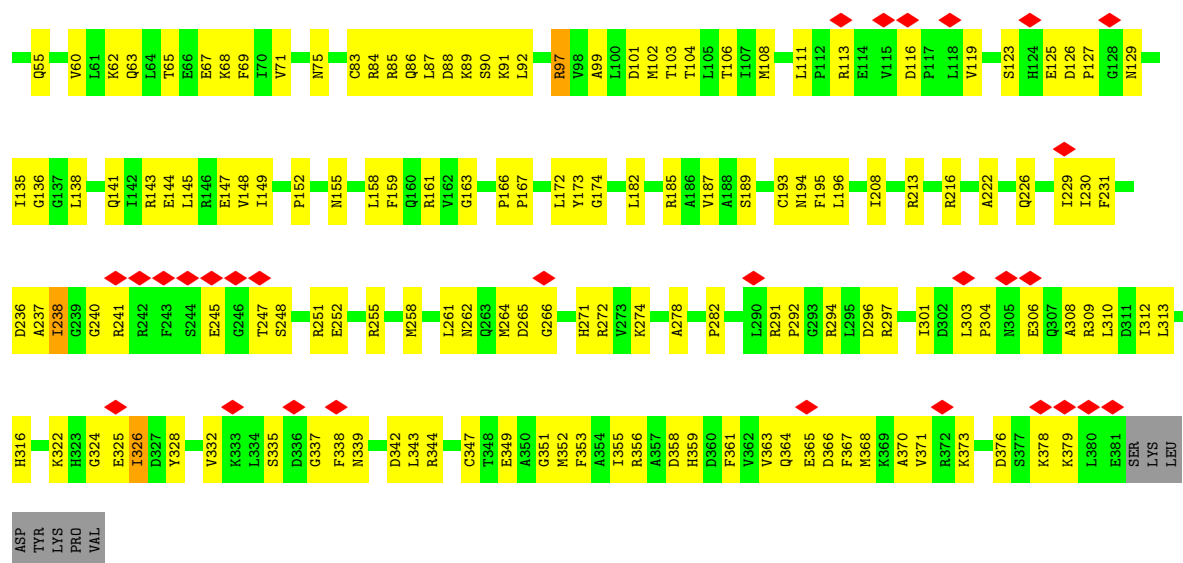
Chain D: 62% 28% 9%



• Molecule 15: Proteasome 26S subunit, ATPase 6

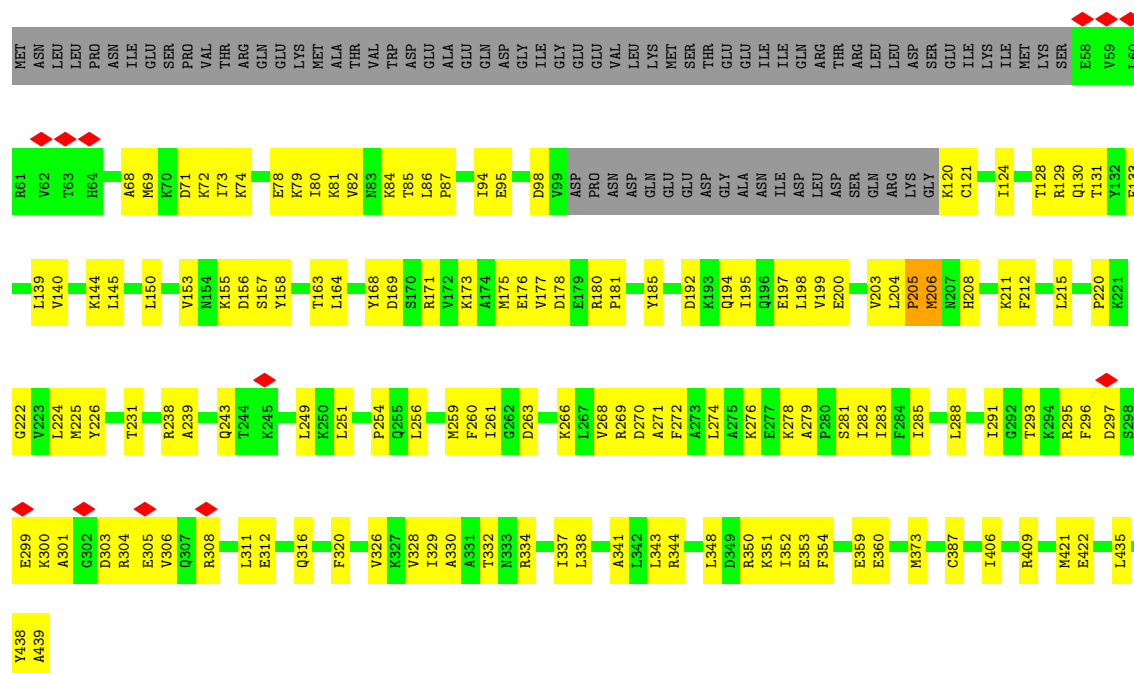
Chain E: 8% 49% 37% 13%





• Molecule 16: 26S proteasome regulatory subunit 6A

Chain F: 50% 32% 18%



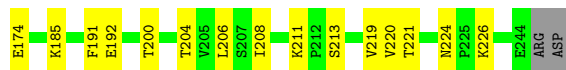
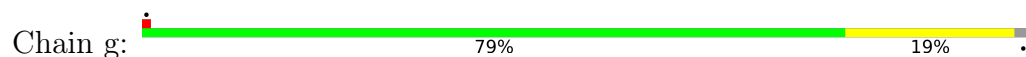
• Molecule 17: Proteasome subunit alpha type-6

Chain G: 82% 15%

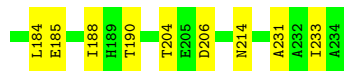
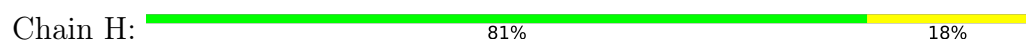




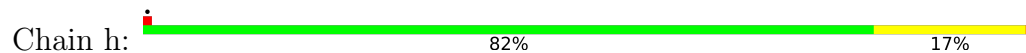
• Molecule 17: Proteasome subunit alpha type-6



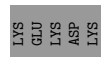
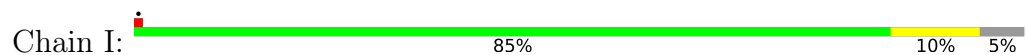
• Molecule 18: Proteasome subunit alpha type-2



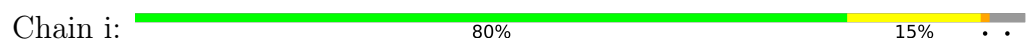
• Molecule 18: Proteasome subunit alpha type-2

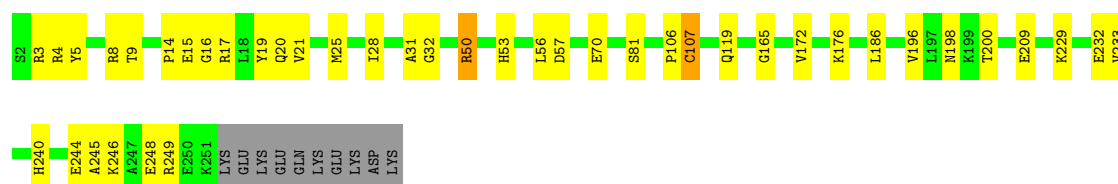


• Molecule 19: Proteasome subunit alpha type-4

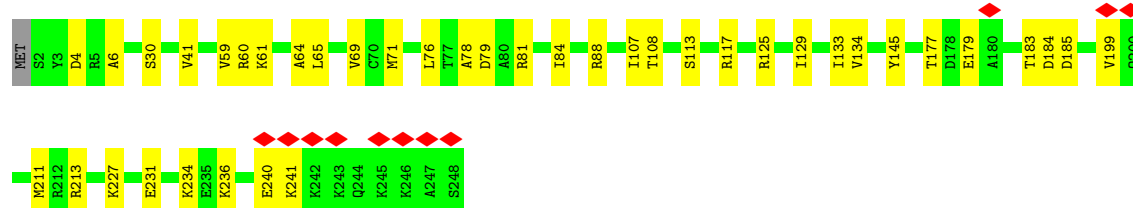
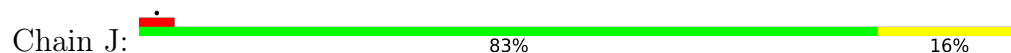


• Molecule 19: Proteasome subunit alpha type-4

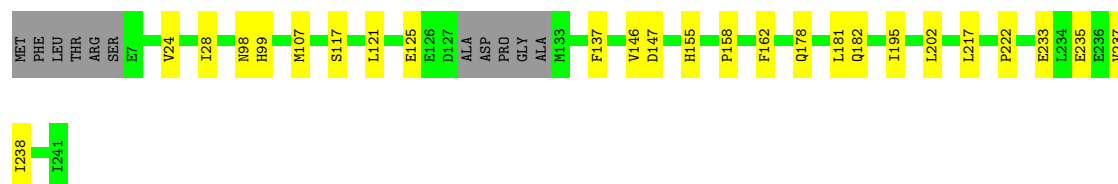
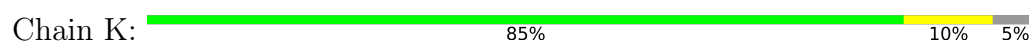




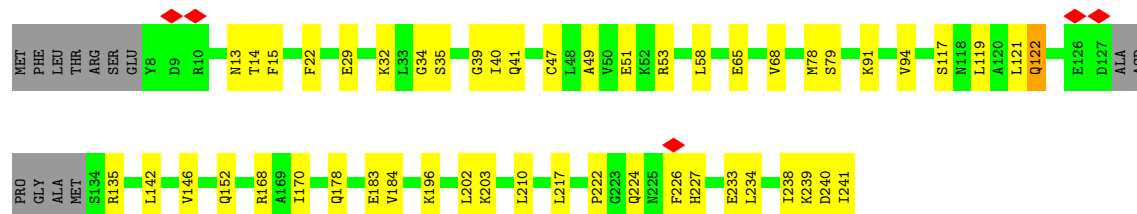
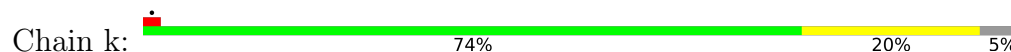
- Molecule 20: Proteasome subunit alpha type-7



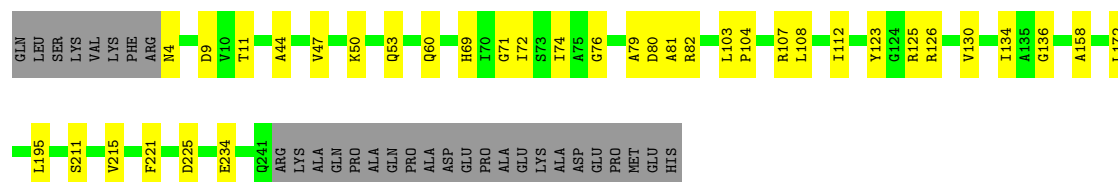
- Molecule 21: Proteasome subunit alpha type-5



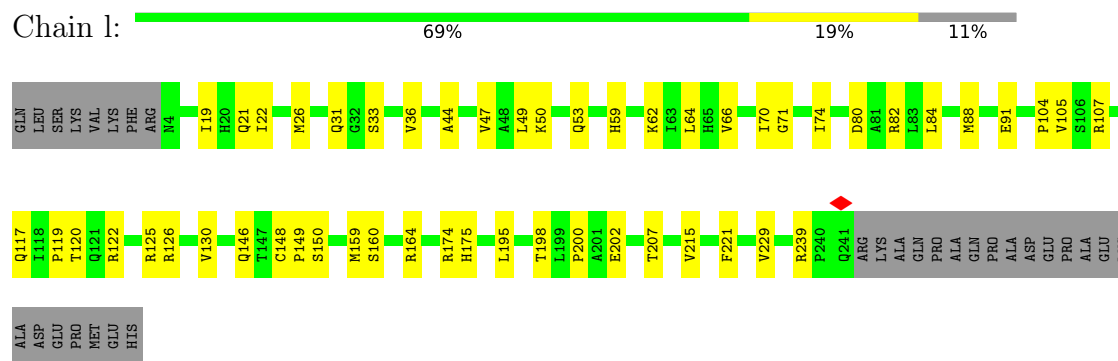
- Molecule 21: Proteasome subunit alpha type-5



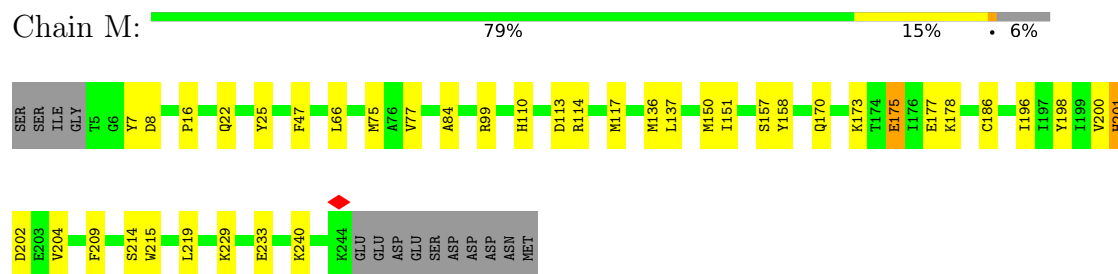
- Molecule 22: Isoform Long of Proteasome subunit alpha type-1



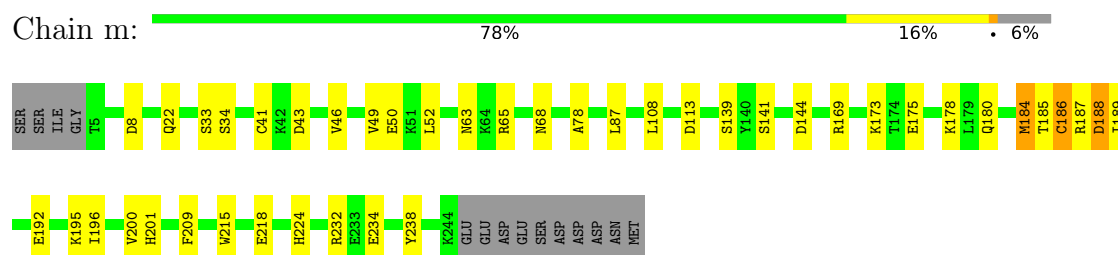
- Molecule 22: Isoform Long of Proteasome subunit alpha type-1



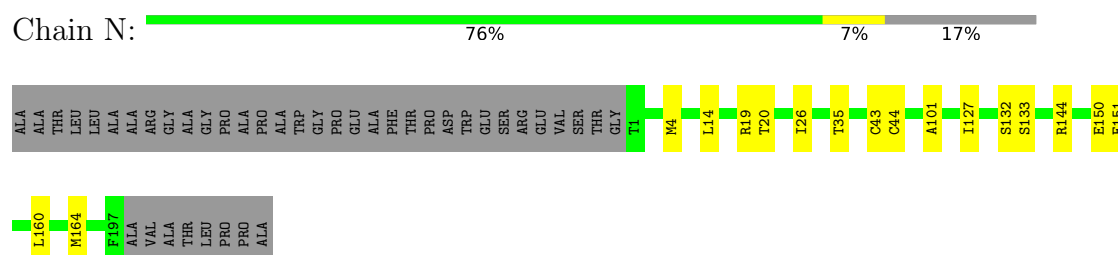
- Molecule 23: Proteasome subunit alpha type-3



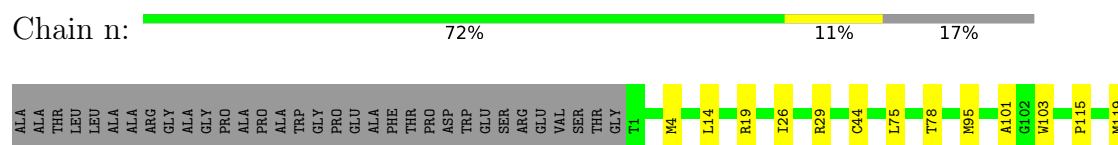
- Molecule 23: Proteasome subunit alpha type-3

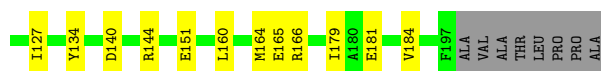


- Molecule 24: Proteasome subunit beta type-6

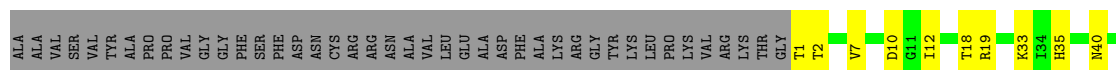


- Molecule 24: Proteasome subunit beta type-6

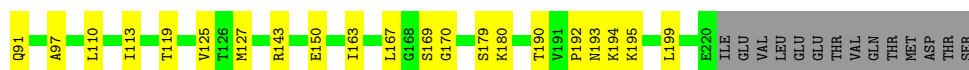
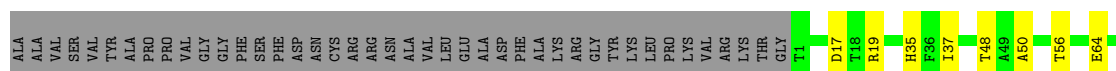




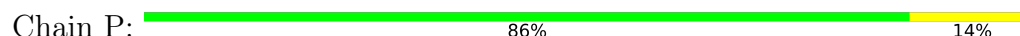
- Molecule 25: Proteasome subunit beta type-7



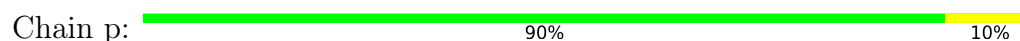
- Molecule 25: Proteasome subunit beta type-7



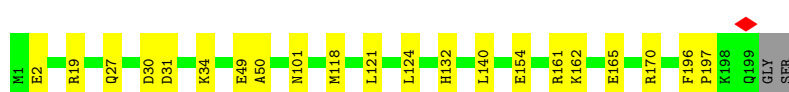
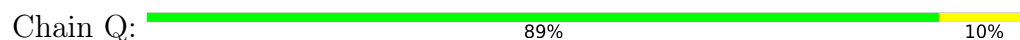
- Molecule 26: Proteasome subunit beta type-3



- Molecule 26: Proteasome subunit beta type-3



- Molecule 27: Proteasome subunit beta type-2



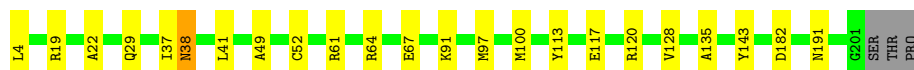
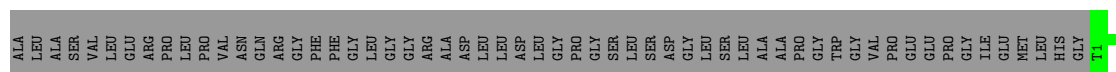
- Molecule 27: Proteasome subunit beta type-2

Chain q:  91% 8%



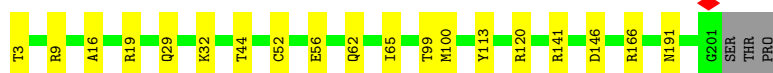
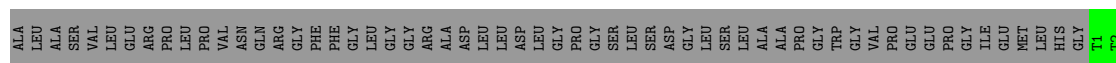
- Molecule 28: Proteasome subunit beta type-5

Chain R:  68% 8% 23%




- Molecule 28: Proteasome subunit beta type-5

Chain r:  69% 7% 23%




- Molecule 29: Proteasome subunit beta type-1

Chain S:  82% 6% 11%



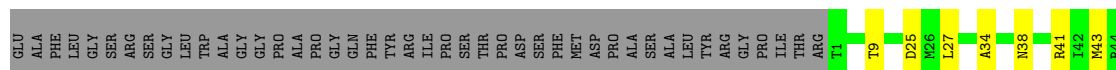
- Molecule 29: Proteasome subunit beta type-1

Chain s:  81% 8% 11%

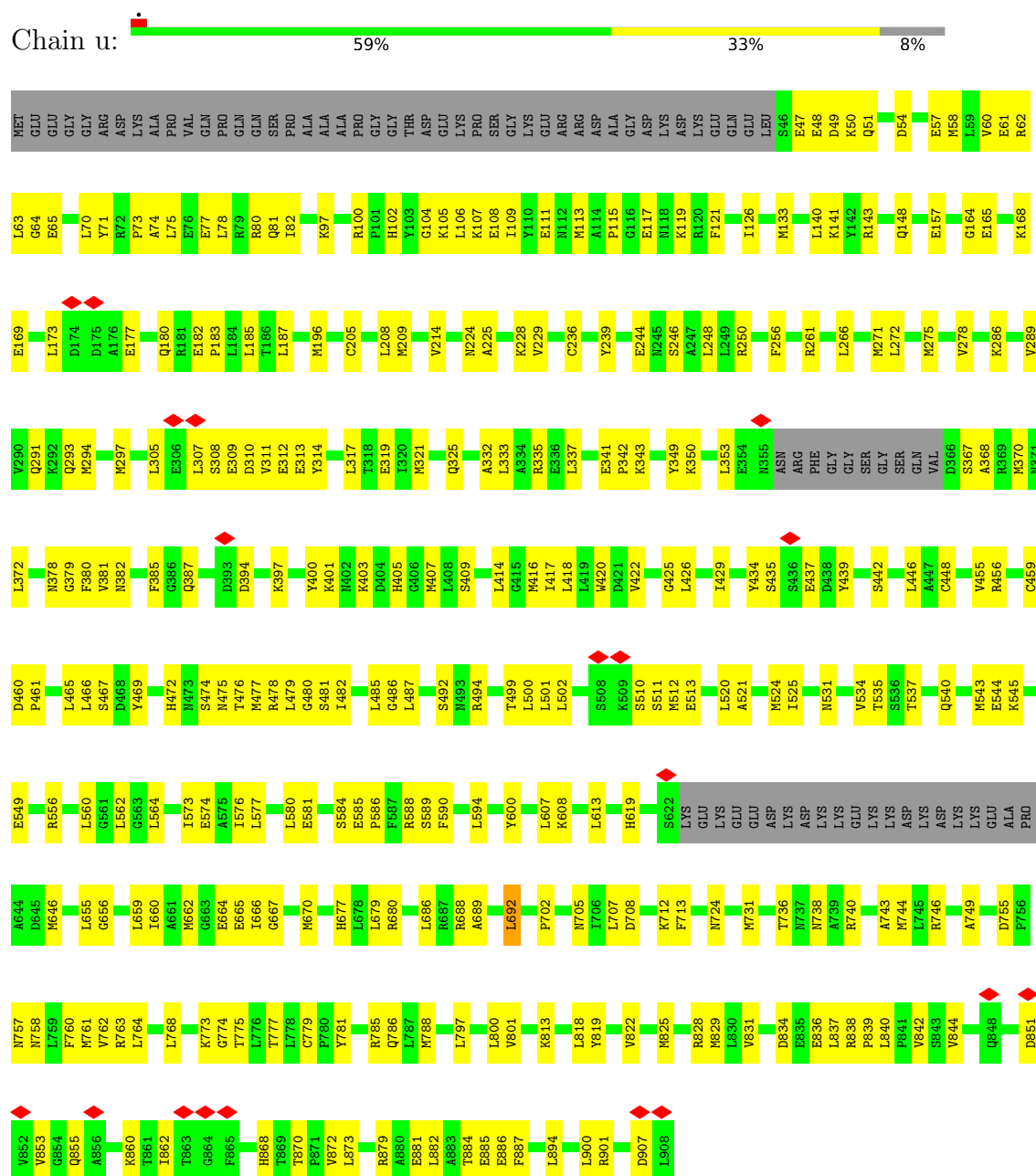


- Molecule 30: Proteasome subunit beta type-4

Chain T:  70% 12% 18%



● Molecule 33: 26S proteasome non-ATPase regulatory subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17418	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	20.957	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.550	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, MG, LDZ, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.17	0/6710	0.45	0/9074
2	V	0.21	0/3929	0.55	0/5309
3	W	0.32	0/3713	0.67	0/4988
4	X	0.18	0/3053	0.47	1/4115 (0.0%)
5	Y	0.18	0/3173	0.49	0/4273
6	Z	0.22	0/2324	0.58	1/3150 (0.0%)
7	a	0.19	0/3053	0.55	2/4133 (0.0%)
8	c	0.20	0/2302	0.57	0/3110
9	d	0.21	0/2122	0.60	0/2864
10	e	0.21	0/338	0.64	0/450
11	A	0.18	0/3283	0.47	0/4433
12	B	0.19	0/3208	0.46	0/4327
13	C	0.22	0/3146	0.50	0/4226
14	D	0.25	0/3090	0.55	3/4168 (0.1%)
15	E	0.20	0/2829	0.51	0/3812
16	F	0.21	0/2873	0.54	1/3872 (0.0%)
17	G	0.16	0/1842	0.37	0/2500
17	g	0.14	0/1863	0.34	0/2527
18	H	0.18	0/1762	0.38	0/2394
18	h	0.25	0/1764	0.44	0/2399
19	I	0.16	0/1925	0.37	0/2606
19	i	0.16	0/1942	0.41	0/2628
20	J	0.16	0/1869	0.39	0/2531
21	K	0.14	0/1772	0.31	0/2397
21	k	0.18	0/1747	0.40	1/2364 (0.0%)
22	L	0.15	0/1885	0.34	0/2552
22	l	0.15	0/1885	0.36	0/2552
23	M	0.15	0/1891	0.35	0/2552
23	m	0.25	0/1897	0.42	0/2559
24	N	0.15	0/1508	0.34	0/2040
24	n	0.14	0/1508	0.33	0/2040
25	O	0.16	0/1670	0.37	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	o	0.15	0/1670	0.41	0/2265
26	P	0.15	0/1620	0.33	0/2184
26	p	0.15	0/1620	0.32	0/2184
27	Q	0.14	0/1603	0.33	0/2174
27	q	0.14	0/1607	0.34	0/2178
28	R	0.14	0/1579	0.32	0/2134
28	r	0.14	0/1579	0.32	0/2134
29	S	0.16	0/1671	0.35	0/2253
29	s	0.15	0/1671	0.34	0/2253
30	T	0.15	0/1700	0.35	0/2305
30	t	0.15	0/1706	0.34	0/2312
31	j	0.15	0/1728	0.38	0/2358
32	f	0.24	0/455	0.72	0/600
33	u	0.18	0/6548	0.45	0/8864
All	All	0.19	0/104633	0.45	9/141408 (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
3	W	0	1
9	d	0	1
14	D	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	205	PRO	CA-N-CD	-9.74	98.36	112.00
7	a	189	PRO	CA-N-CD	-7.01	102.19	112.00
7	a	259	PRO	CA-N-CD	-6.45	102.97	112.00
14	D	58	GLU	CA-C-N	-5.92	111.66	122.38
14	D	58	GLU	C-N-CA	-5.92	111.66	122.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	D	81	ARG	Sidechain
3	W	27	ARG	Sidechain
9	d	189	ILE	Peptide

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	U	6595	0	6650	305	0
2	V	3852	0	3893	205	0
3	W	3667	0	3786	271	0
4	X	3009	0	3113	124	0
5	Y	3115	0	3120	156	0
6	Z	2281	0	2312	144	0
7	a	2995	0	3012	133	0
8	c	2260	0	2276	108	0
9	d	2078	0	2107	154	0
10	e	334	0	294	19	0
11	A	3229	0	3263	116	0
12	B	3162	0	3225	110	0
13	C	3105	0	3219	126	0
14	D	3040	0	3076	115	0
15	E	2786	0	2843	147	0
16	F	2834	0	2912	127	0
17	G	1809	0	1781	23	0
17	g	1830	0	1807	30	0
18	H	1726	0	1646	31	0
18	h	1727	0	1619	28	0
19	I	1895	0	1833	19	0
19	i	1912	0	1851	36	0
20	J	1844	0	1747	29	0
21	K	1746	0	1695	18	0
21	k	1722	0	1673	37	0
22	L	1850	0	1822	28	0
22	l	1850	0	1822	36	0
23	M	1856	0	1816	25	0
23	m	1862	0	1827	36	0
24	N	1482	0	1450	12	0
24	n	1482	0	1450	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	O	1643	0	1644	28	0
25	o	1643	0	1644	20	0
26	P	1591	0	1609	20	0
26	p	1591	0	1609	12	0
27	Q	1570	0	1547	17	0
27	q	1574	0	1558	13	0
28	R	1548	0	1499	16	0
28	r	1548	0	1499	16	0
29	S	1641	0	1618	12	0
29	s	1641	0	1618	13	0
30	T	1667	0	1628	21	0
30	t	1673	0	1639	19	0
31	j	1704	0	1517	36	0
32	f	453	0	481	30	0
33	u	6439	0	6456	245	0
34	c	1	0	0	0	0
35	A	31	0	12	0	0
35	B	31	0	12	3	0
35	C	31	0	12	0	0
35	F	31	0	12	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	D	27	0	12	0	0
37	E	27	0	12	2	0
38	N	34	0	41	3	0
38	O	34	0	41	4	0
38	R	34	0	41	3	0
38	n	34	0	41	2	0
38	o	34	0	41	1	0
38	r	34	0	41	2	0
All	All	103249	0	102824	2984	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 14.

The worst 5 of 2984 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:E:303:LEU:HD12	15:E:304:PRO:HD2	1.41	1.03
3:W:320:LEU:O	3:W:324:TYR:HB3	1.61	1.01
3:W:35:ALA:HB1	3:W:48:LEU:HD22	1.43	1.00
8:c:55:GLY:HA2	8:c:75:MET:HG2	1.49	0.95
2:V:148:ARG:HD2	2:V:149:PRO:HD3	1.47	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	839/953 (88%)	761 (91%)	75 (9%)	3 (0%)	30	59
2	V	478/533 (90%)	427 (89%)	49 (10%)	2 (0%)	30	59
3	W	448/456 (98%)	400 (89%)	42 (9%)	6 (1%)	9	33
4	X	378/422 (90%)	365 (97%)	12 (3%)	1 (0%)	36	65
5	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	24	54
6	Z	284/324 (88%)	250 (88%)	32 (11%)	2 (1%)	18	47
7	a	371/376 (99%)	329 (89%)	40 (11%)	2 (0%)	24	54
8	c	285/309 (92%)	247 (87%)	36 (13%)	2 (1%)	18	47
9	d	249/349 (71%)	200 (80%)	46 (18%)	3 (1%)	10	35
10	e	36/70 (51%)	26 (72%)	8 (22%)	2 (6%)	1	10
11	A	411/433 (95%)	371 (90%)	37 (9%)	3 (1%)	18	47
12	B	403/440 (92%)	365 (91%)	36 (9%)	2 (0%)	24	54
13	C	394/398 (99%)	361 (92%)	29 (7%)	4 (1%)	12	39
14	D	378/418 (90%)	339 (90%)	36 (10%)	3 (1%)	16	44
15	E	350/403 (87%)	309 (88%)	36 (10%)	5 (1%)	9	31
16	F	358/439 (82%)	321 (90%)	36 (10%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	G	235/245 (96%)	225 (96%)	9 (4%)	1 (0%)	30	59
17	g	238/245 (97%)	231 (97%)	7 (3%)	0	100	100
18	H	229/233 (98%)	214 (93%)	14 (6%)	1 (0%)	30	59
18	h	230/233 (99%)	222 (96%)	7 (3%)	1 (0%)	30	59
19	I	246/260 (95%)	228 (93%)	17 (7%)	1 (0%)	30	59
19	i	248/260 (95%)	235 (95%)	12 (5%)	1 (0%)	30	59
20	J	245/248 (99%)	231 (94%)	10 (4%)	4 (2%)	7	29
21	K	226/241 (94%)	220 (97%)	6 (3%)	0	100	100
21	k	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
22	L	236/268 (88%)	230 (98%)	6 (2%)	0	100	100
22	l	236/268 (88%)	227 (96%)	9 (4%)	0	100	100
23	M	238/254 (94%)	233 (98%)	4 (2%)	1 (0%)	30	59
23	m	238/254 (94%)	227 (95%)	11 (5%)	0	100	100
24	N	195/238 (82%)	188 (96%)	6 (3%)	1 (0%)	24	54
24	n	195/238 (82%)	189 (97%)	6 (3%)	0	100	100
25	O	218/276 (79%)	209 (96%)	8 (4%)	1 (0%)	24	54
25	o	218/276 (79%)	203 (93%)	15 (7%)	0	100	100
26	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
26	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
27	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
27	q	197/201 (98%)	187 (95%)	10 (5%)	0	100	100
28	R	199/262 (76%)	195 (98%)	2 (1%)	2 (1%)	12	39
28	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
29	S	211/240 (88%)	206 (98%)	4 (2%)	1 (0%)	24	54
29	s	211/240 (88%)	208 (99%)	3 (1%)	0	100	100
30	T	213/263 (81%)	207 (97%)	5 (2%)	1 (0%)	24	54
30	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
31	j	237/247 (96%)	219 (92%)	17 (7%)	1 (0%)	30	59
32	f	53/445 (12%)	48 (91%)	4 (8%)	1 (2%)	6	26
33	u	826/908 (91%)	797 (96%)	29 (4%)	0	100	100
All	All	13093/14930 (88%)	12167 (93%)	865 (7%)	61 (0%)	26	54

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	41	SER
3	W	45	GLU
3	W	375	MET
4	X	310	ARG
5	Y	361	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	722/816 (88%)	717 (99%)	5 (1%)	76	78
2	V	414/459 (90%)	412 (100%)	2 (0%)	81	80
3	W	412/416 (99%)	407 (99%)	5 (1%)	63	72
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	84
5	Y	334/344 (97%)	334 (100%)	0	100	100
6	Z	257/295 (87%)	255 (99%)	2 (1%)	73	76
7	a	333/336 (99%)	329 (99%)	4 (1%)	63	72
8	c	252/267 (94%)	251 (100%)	1 (0%)	84	82
9	d	226/293 (77%)	224 (99%)	2 (1%)	70	75
10	e	38/63 (60%)	38 (100%)	0	100	100
11	A	348/372 (94%)	347 (100%)	1 (0%)	86	84
12	B	352/385 (91%)	352 (100%)	0	100	100
13	C	340/346 (98%)	336 (99%)	4 (1%)	63	72
14	D	333/366 (91%)	328 (98%)	5 (2%)	57	69
15	E	307/353 (87%)	306 (100%)	1 (0%)	86	84
16	F	309/379 (82%)	308 (100%)	1 (0%)	86	84
17	G	191/209 (91%)	191 (100%)	0	100	100
17	g	194/209 (93%)	192 (99%)	2 (1%)	68	74
18	H	169/190 (89%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	h	167/190 (88%)	164 (98%)	3 (2%)	51	66
19	I	191/220 (87%)	191 (100%)	0	100	100
19	i	193/220 (88%)	192 (100%)	1 (0%)	81	80
20	J	179/211 (85%)	179 (100%)	0	100	100
21	K	189/203 (93%)	189 (100%)	0	100	100
21	k	186/203 (92%)	186 (100%)	0	100	100
22	L	198/229 (86%)	198 (100%)	0	100	100
22	l	198/229 (86%)	198 (100%)	0	100	100
23	M	192/211 (91%)	190 (99%)	2 (1%)	68	74
23	m	193/211 (92%)	190 (98%)	3 (2%)	55	68
24	N	154/180 (86%)	154 (100%)	0	100	100
24	n	154/180 (86%)	153 (99%)	1 (1%)	78	80
25	O	177/227 (78%)	177 (100%)	0	100	100
25	o	177/227 (78%)	176 (99%)	1 (1%)	78	80
26	P	173/173 (100%)	173 (100%)	0	100	100
26	p	173/173 (100%)	170 (98%)	3 (2%)	53	67
27	Q	164/171 (96%)	164 (100%)	0	100	100
27	q	165/171 (96%)	165 (100%)	0	100	100
28	R	153/201 (76%)	153 (100%)	0	100	100
28	r	153/201 (76%)	153 (100%)	0	100	100
29	S	174/198 (88%)	174 (100%)	0	100	100
29	s	174/198 (88%)	174 (100%)	0	100	100
30	T	175/214 (82%)	174 (99%)	1 (1%)	78	80
30	t	176/214 (82%)	175 (99%)	1 (1%)	78	80
31	j	152/210 (72%)	152 (100%)	0	100	100
32	f	45/364 (12%)	44 (98%)	1 (2%)	45	63
33	u	702/763 (92%)	700 (100%)	2 (0%)	86	84
All	All	10985/12652 (87%)	10930 (100%)	55 (0%)	78	80

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	D	81	ARG

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Mol	Chain	Res	Type
23	M	175	GLU
33	u	744	MET
26	p	115	LYS
14	D	98	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
28	R	29	GLN
23	m	97	ASN
29	S	108	ASN
19	i	109	GLN
26	p	93	ASN

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 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	ATP	C	501	36	32,33,33	0.30	0	48,52,52	0.30	0
37	ADP	E	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	8 (18%)
38	LDZ	n	301	-	33,34,34	0.50	0	42,44,44	1.40	3 (7%)
35	ATP	B	501	36	32,33,33	0.35	0	48,52,52	0.33	0
38	LDZ	o	301	-	33,34,34	0.49	0	42,44,44	0.70	0
37	ADP	D	501	36	28,29,29	1.41	4 (14%)	43,45,45	1.86	8 (18%)
38	LDZ	N	301	-	33,34,34	0.41	0	42,44,44	0.70	0
38	LDZ	O	301	-	33,34,34	0.39	0	42,44,44	1.53	3 (7%)
35	ATP	F	501	36	32,33,33	0.31	0	48,52,52	0.32	0
38	LDZ	r	301	-	33,34,34	0.44	0	42,44,44	0.80	2 (4%)
35	ATP	A	501	36	32,33,33	0.28	0	48,52,52	0.28	0
38	LDZ	R	301	-	33,34,34	0.47	0	42,44,44	0.58	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
35	ATP	C	501	36	-	4/22/38/38	0/3/3/3
37	ADP	E	401	-	-	5/16/32/32	0/3/3/3
38	LDZ	n	301	-	-	22/38/39/39	0/1/1/1
35	ATP	B	501	36	-	6/22/38/38	0/3/3/3
38	LDZ	o	301	-	-	14/38/39/39	0/1/1/1
37	ADP	D	501	36	-	0/16/32/32	0/3/3/3
38	LDZ	N	301	-	-	8/38/39/39	0/1/1/1
38	LDZ	O	301	-	-	15/38/39/39	0/1/1/1
35	ATP	F	501	36	-	6/22/38/38	0/3/3/3
38	LDZ	r	301	-	-	13/38/39/39	0/1/1/1
35	ATP	A	501	36	-	5/22/38/38	0/3/3/3
38	LDZ	R	301	-	-	14/38/39/39	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	401	ADP	C5-C4	4.76	1.47	1.39
37	D	501	ADP	C5-C4	4.70	1.47	1.39
37	E	401	ADP	C5-C6	2.69	1.48	1.41
37	D	501	ADP	C5-C6	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	501	ADP	C5-N7	-2.37	1.34	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	301	LDZ	C18-C17-N16	7.84	122.52	110.69
38	n	301	LDZ	C14-N13-C12	7.07	136.85	121.65
37	E	401	ADP	C5-C4-N3	-5.93	118.56	126.72
37	D	501	ADP	C5-C4-N3	-5.91	118.58	126.72
37	D	501	ADP	N3-C4-N9	4.76	135.26	127.17

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

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

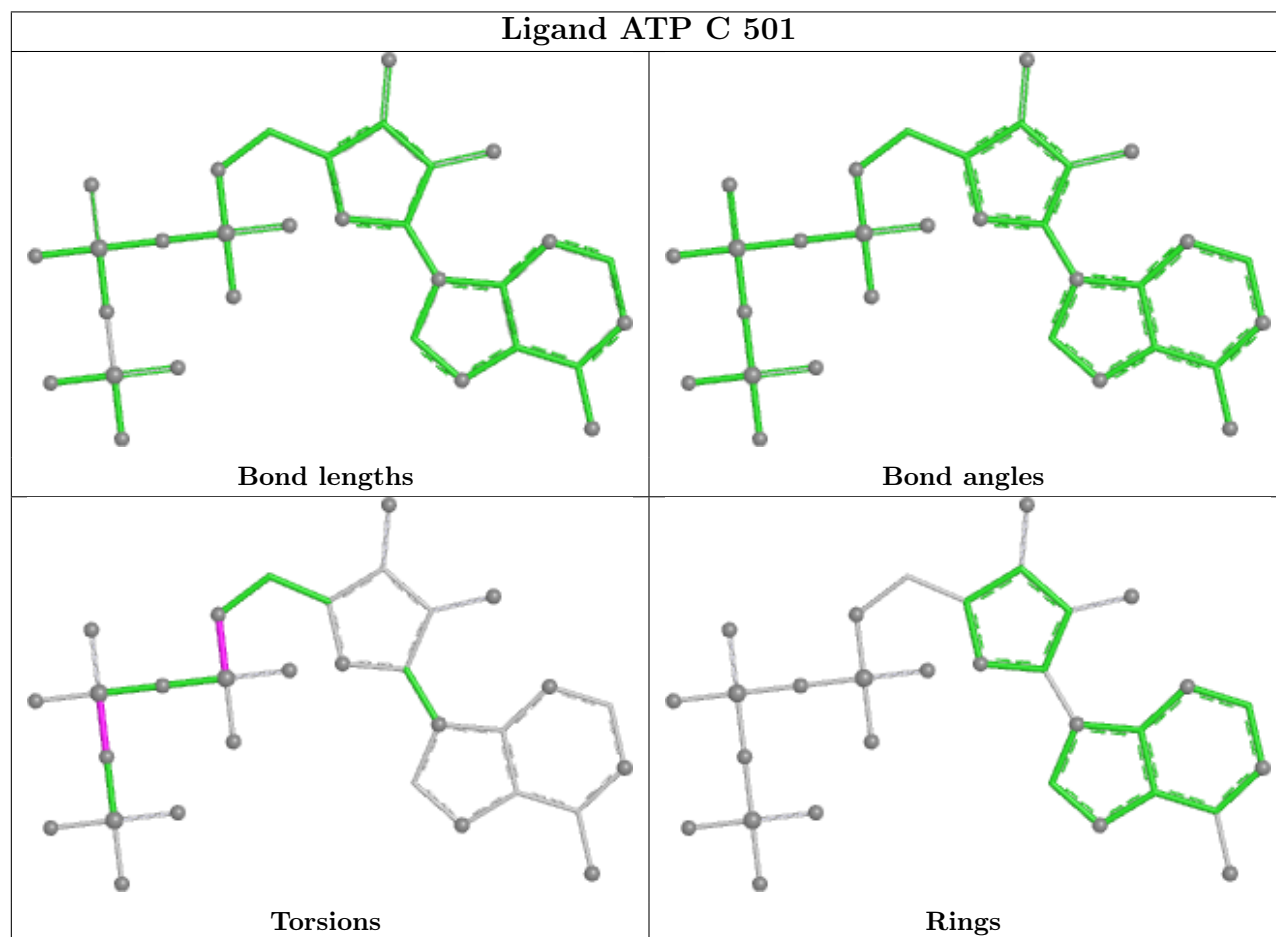
There are no ring outliers.

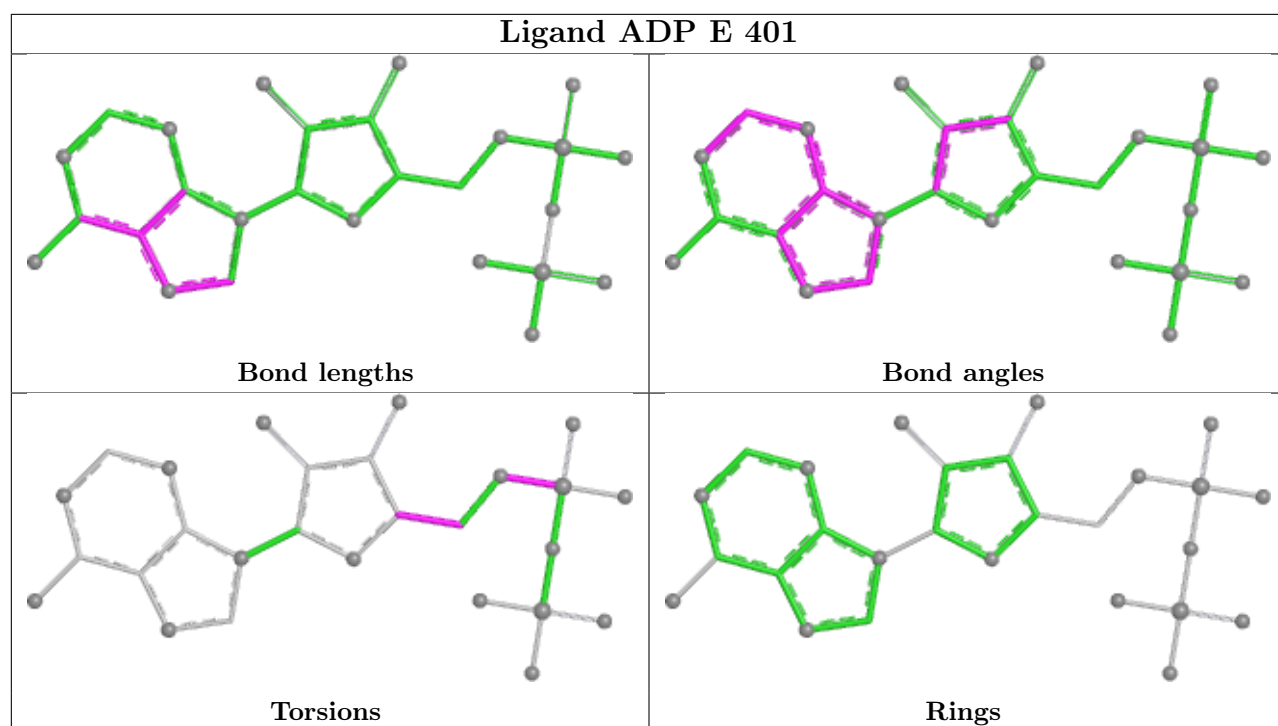
8 monomers are involved in 20 short contacts:

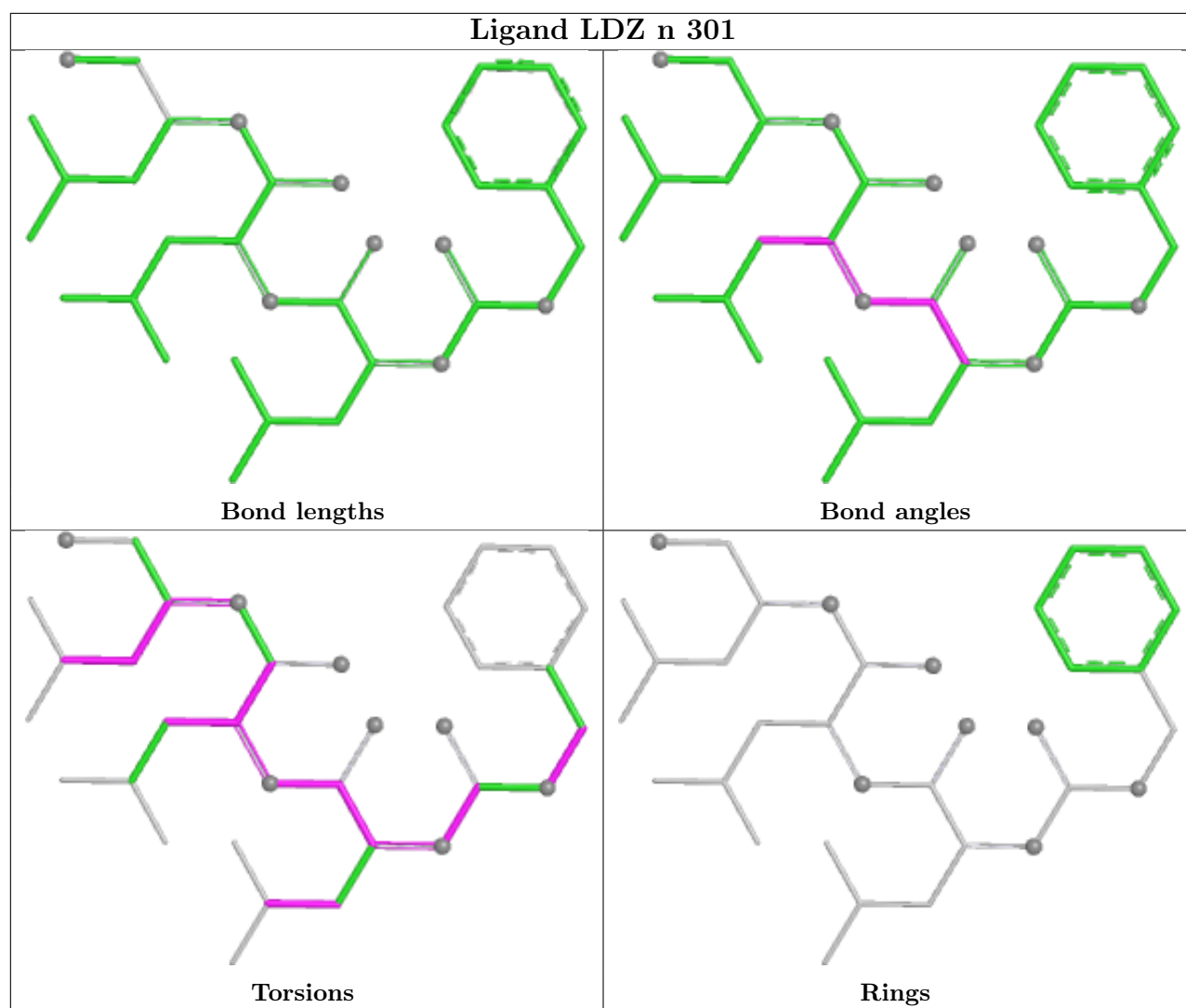
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	2	0
38	n	301	LDZ	2	0
35	B	501	ATP	3	0
38	o	301	LDZ	1	0
38	N	301	LDZ	3	0
38	O	301	LDZ	4	0
38	r	301	LDZ	2	0
38	R	301	LDZ	3	0

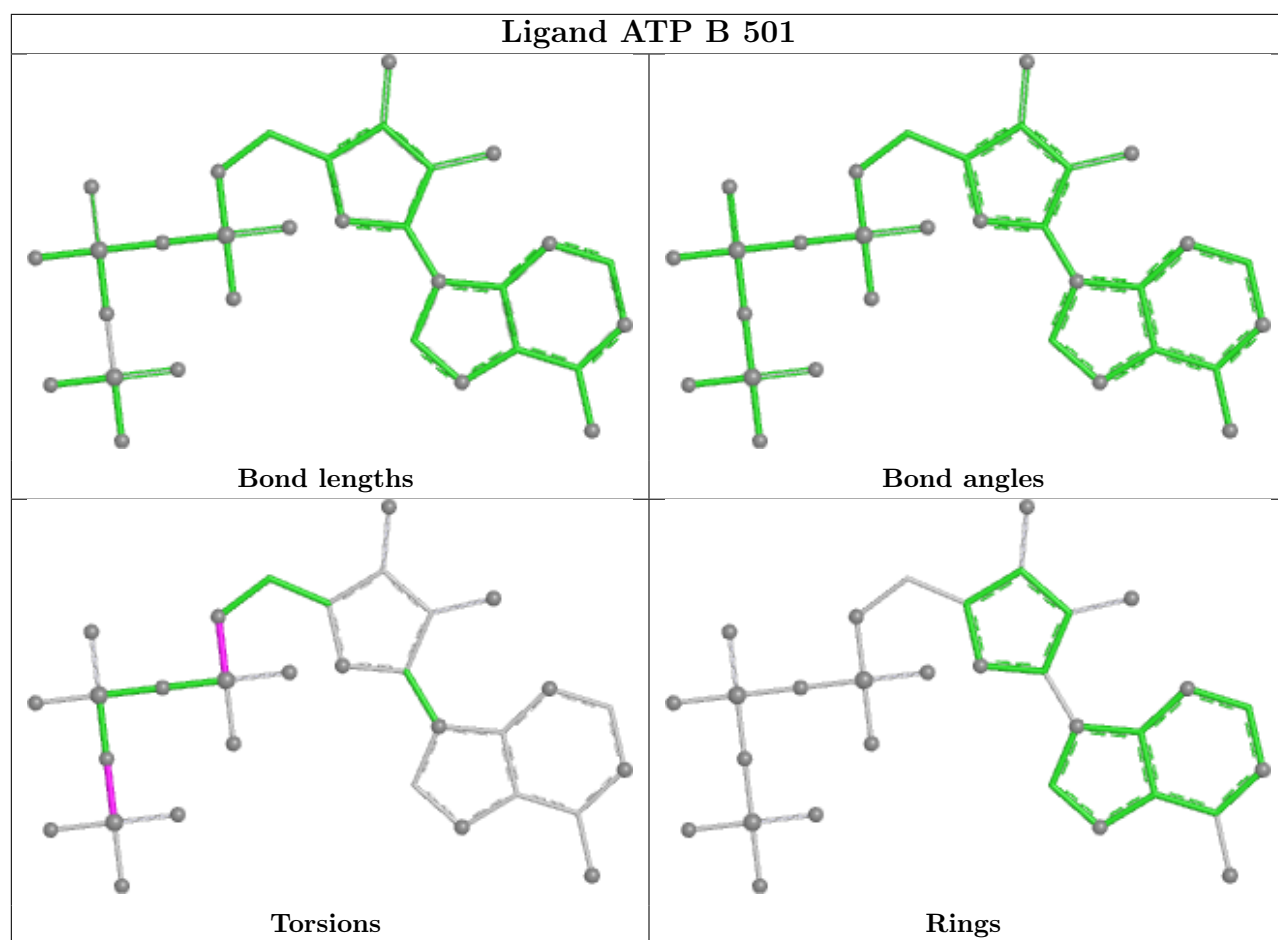
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

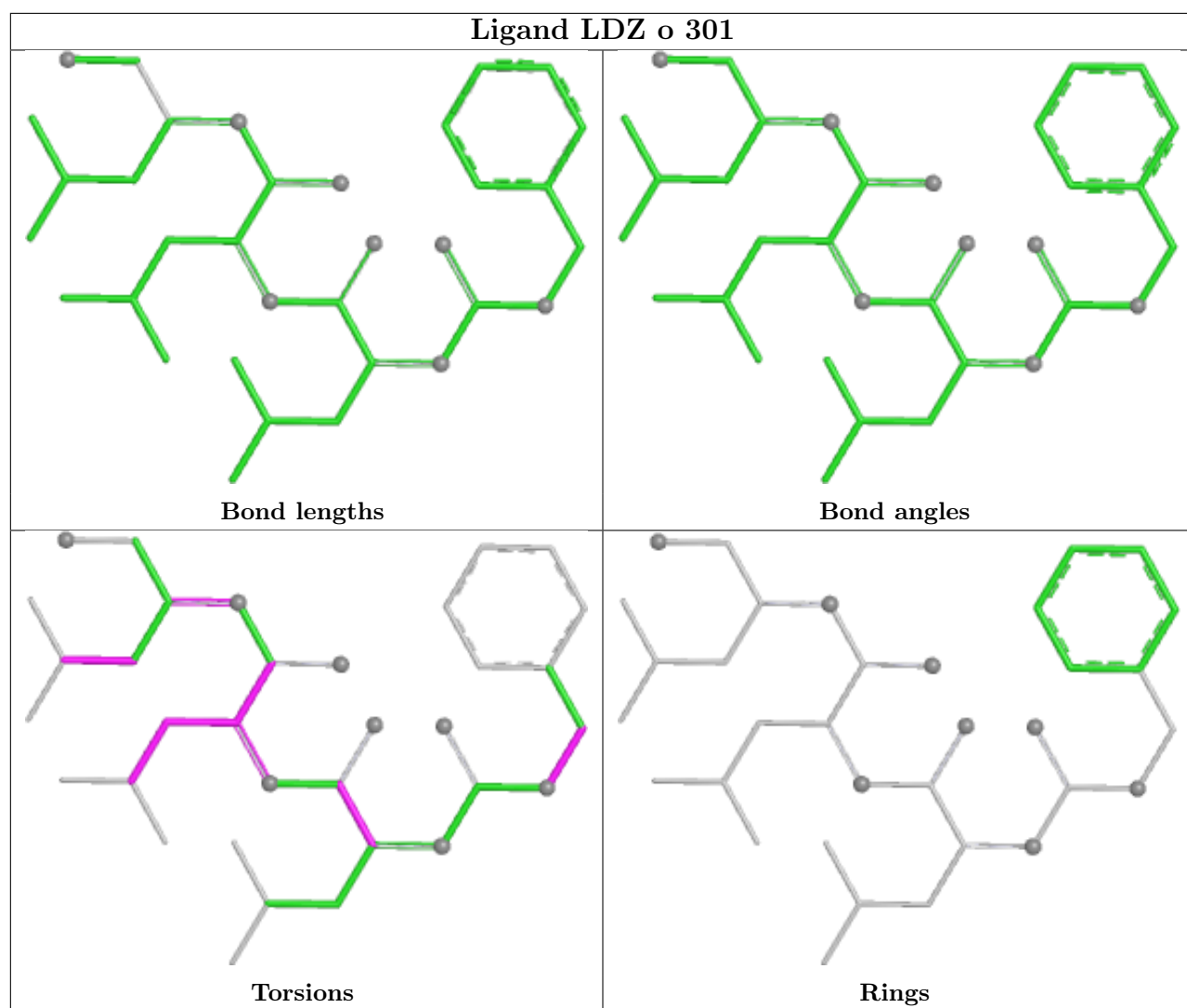
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

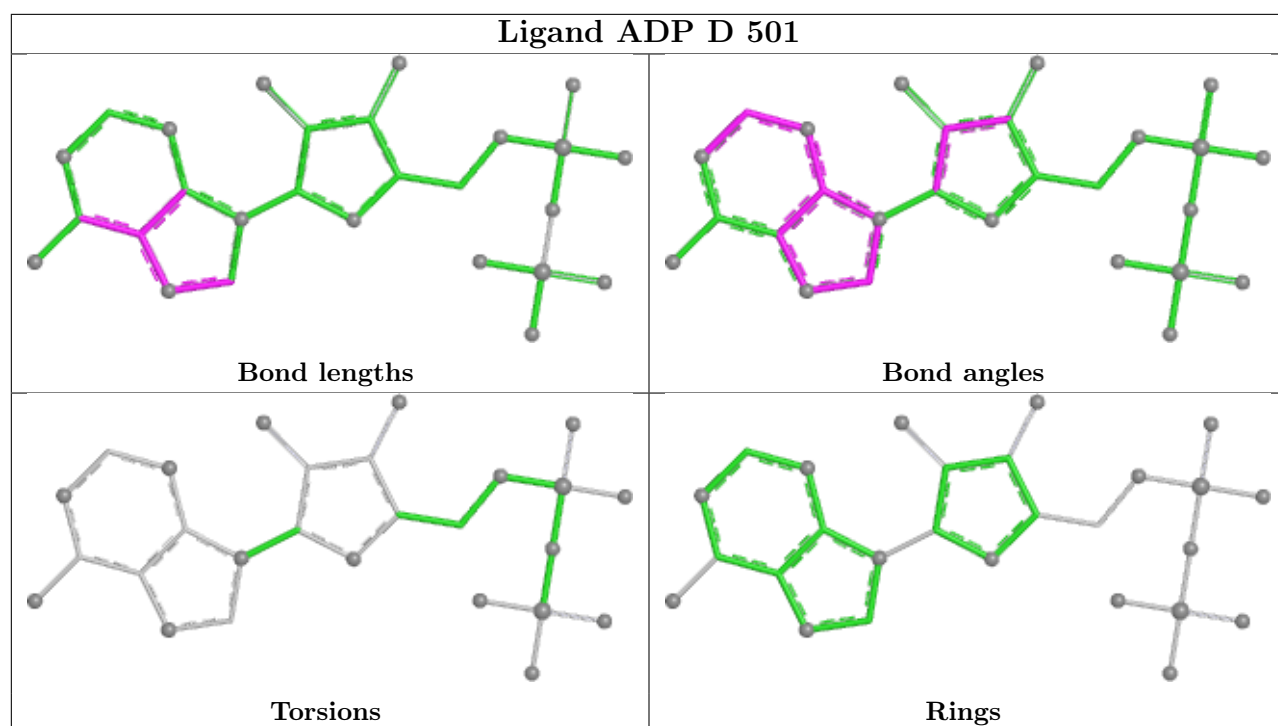


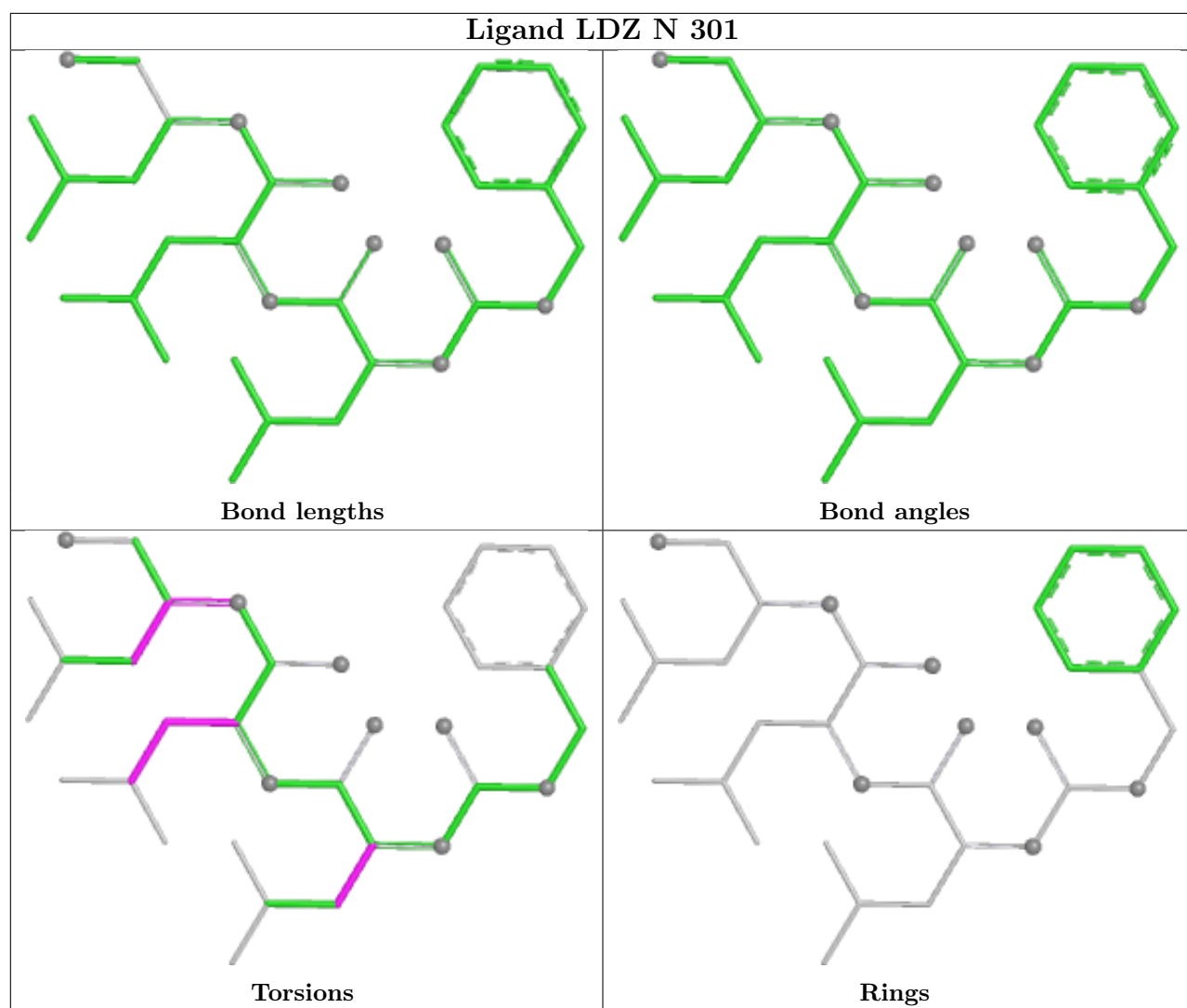


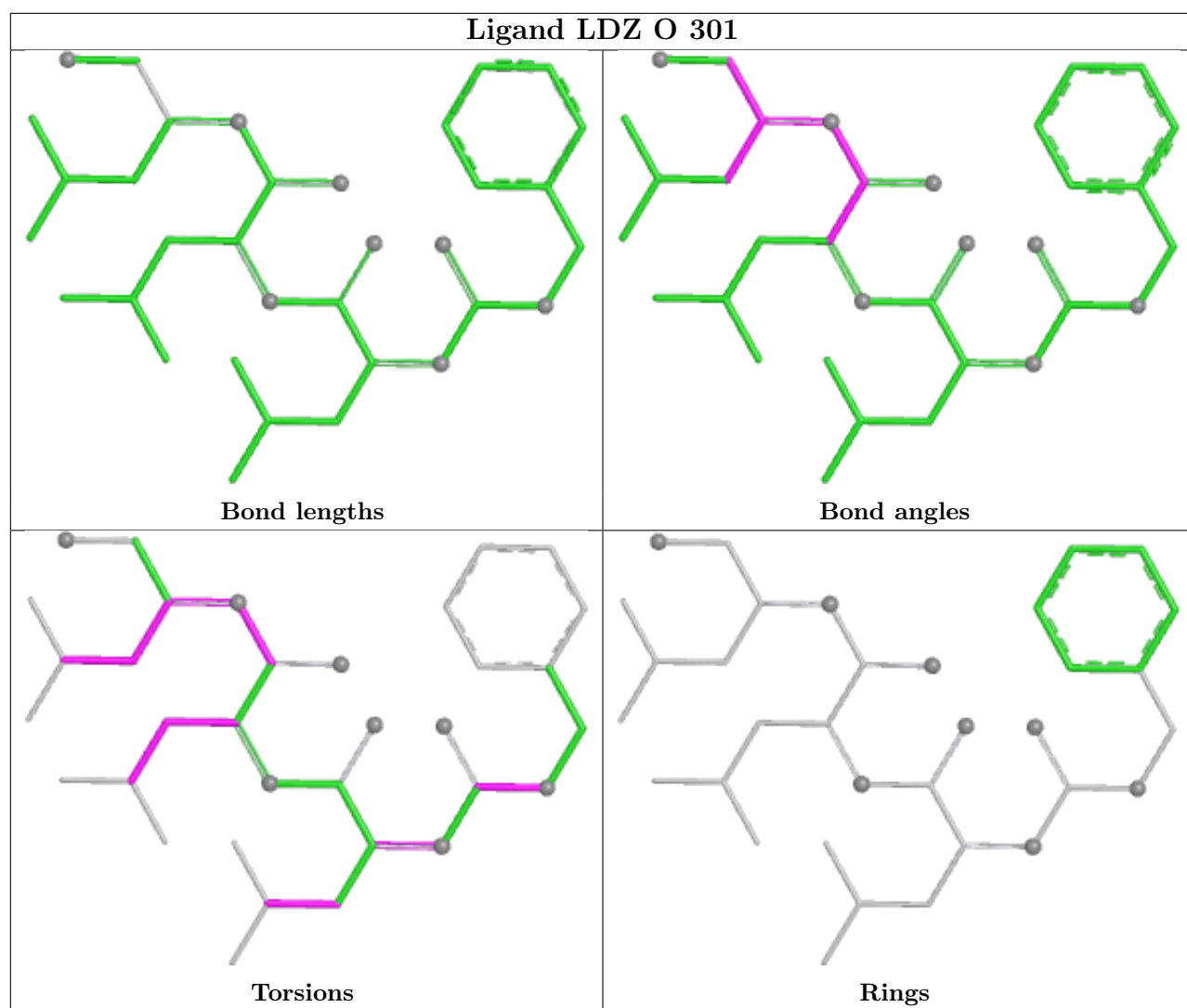


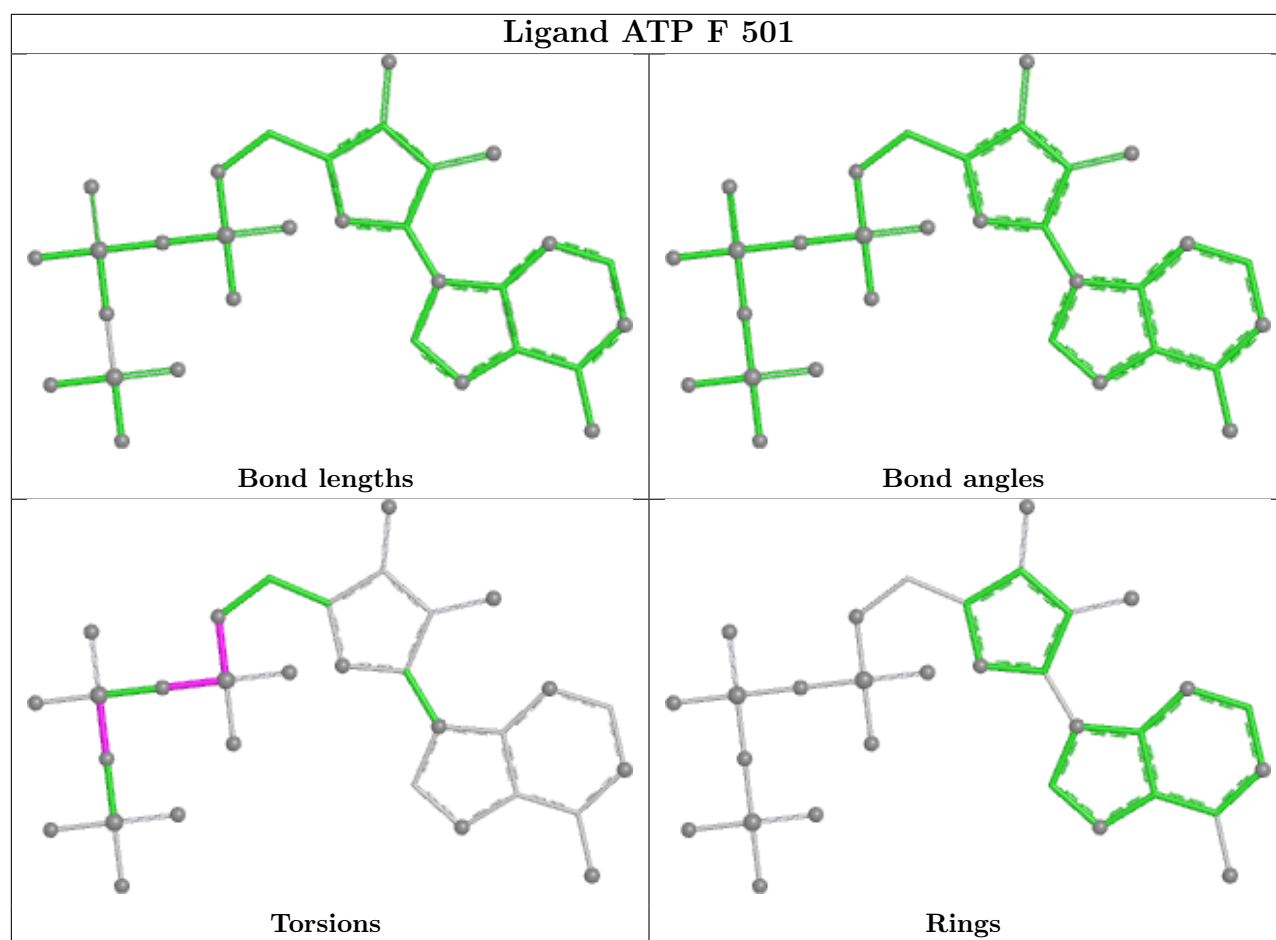


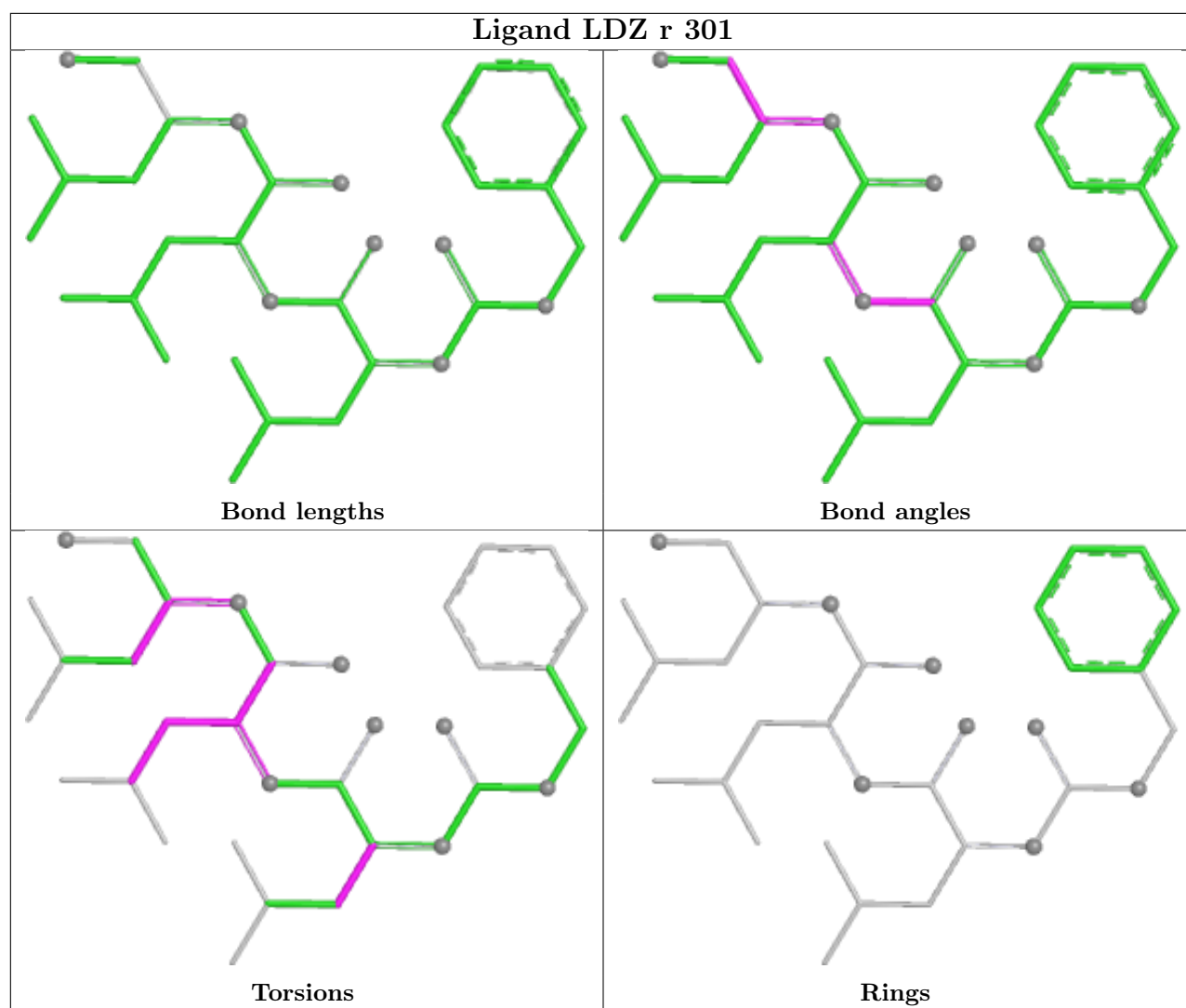


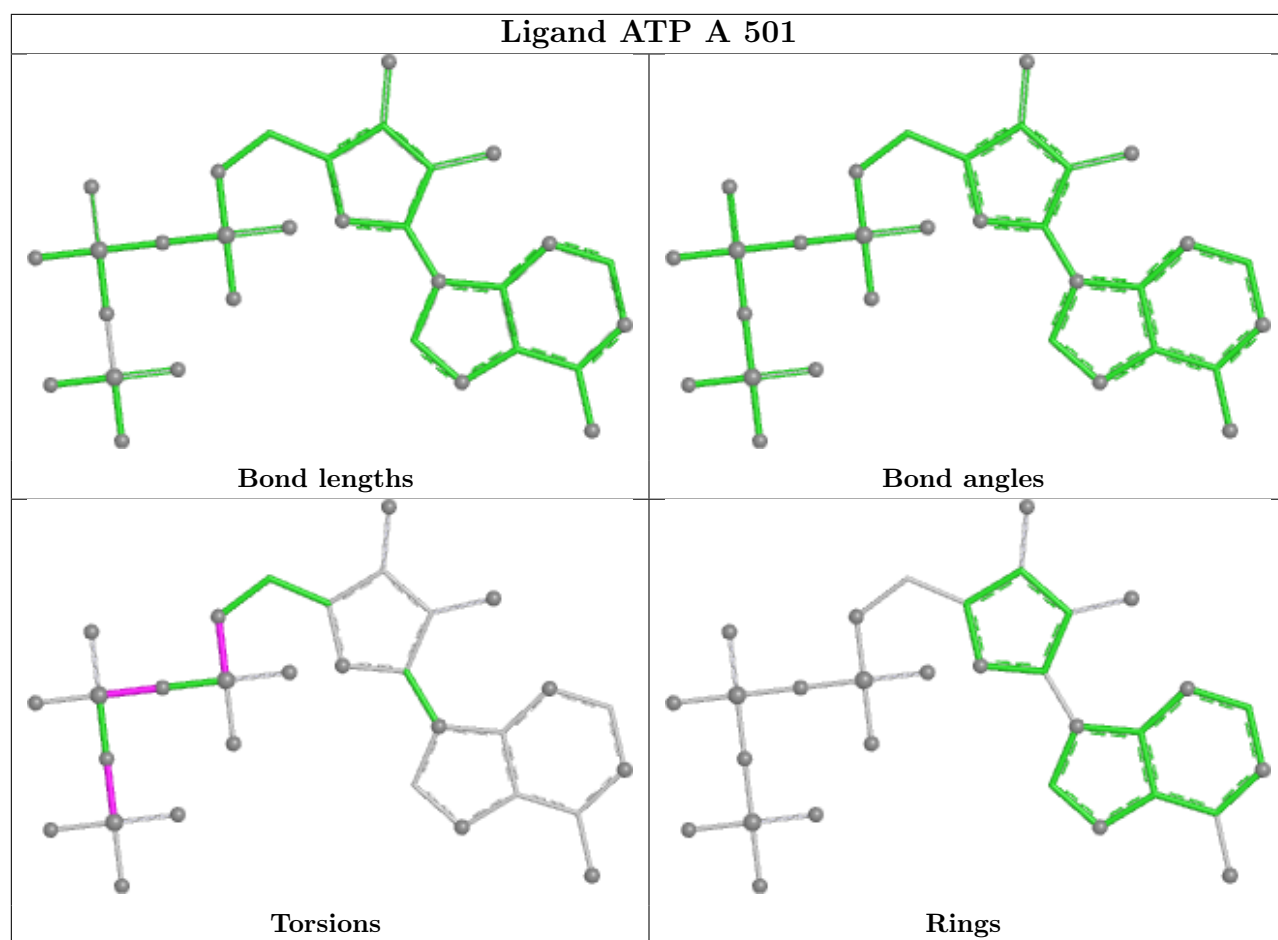


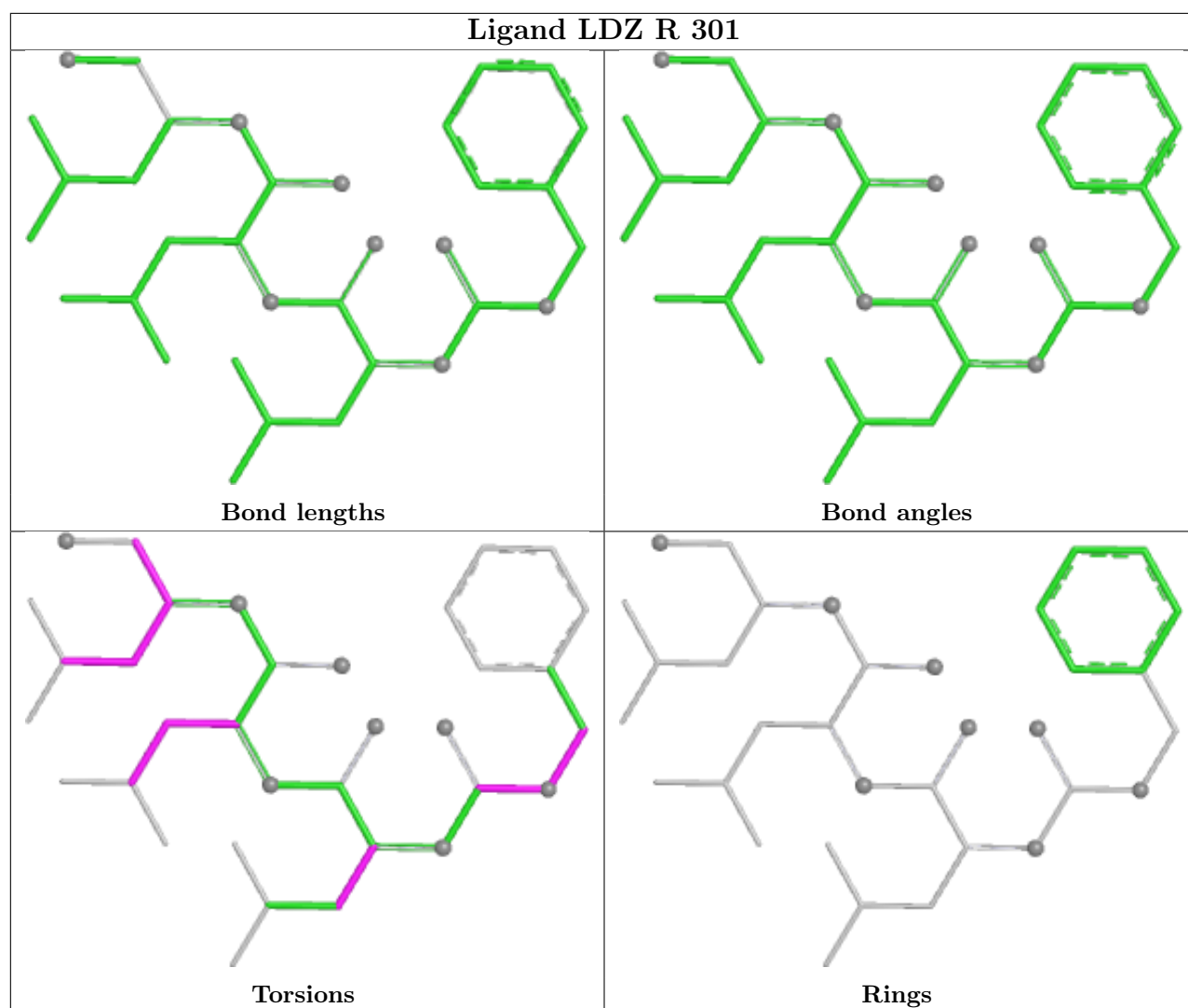












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

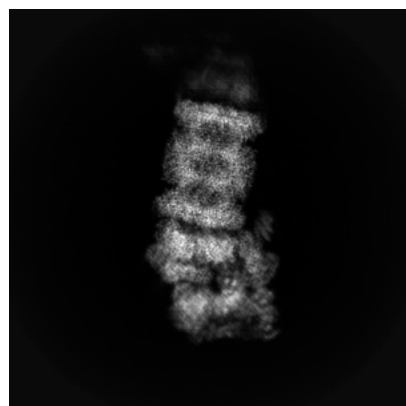
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68472. These allow visual inspection of the internal detail of the map and identification of artifacts.

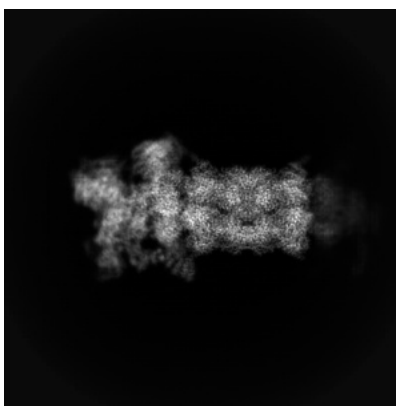
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

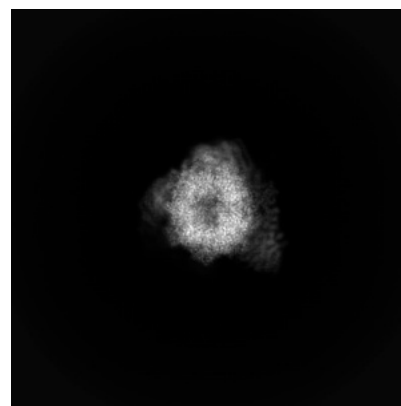
6.1.1 Primary map



X

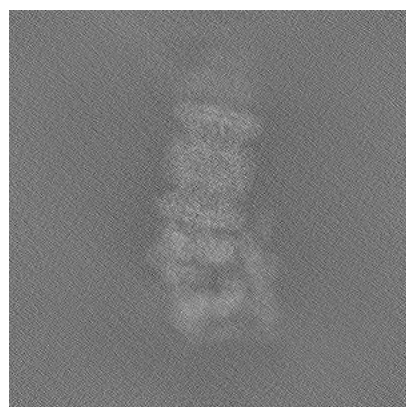


Y

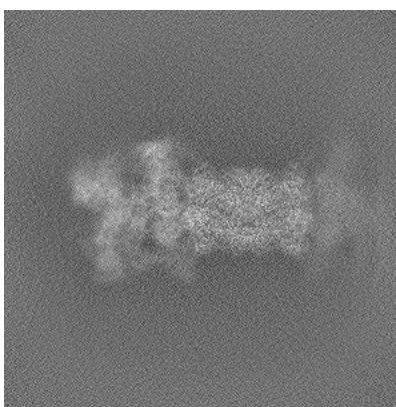


Z

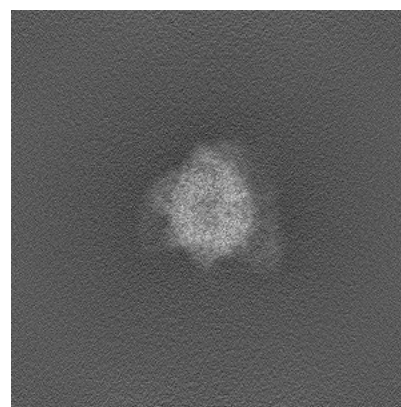
6.1.2 Raw map



X



Y

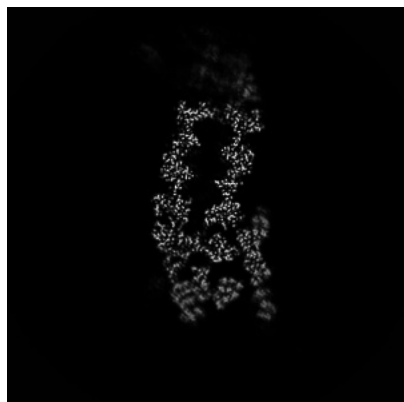


Z

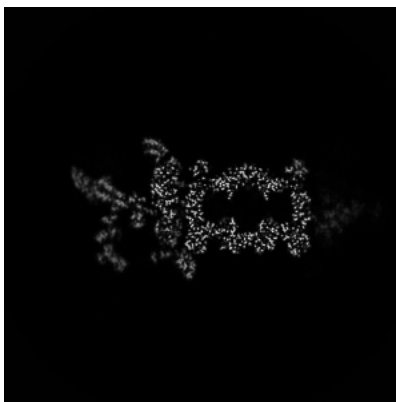
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

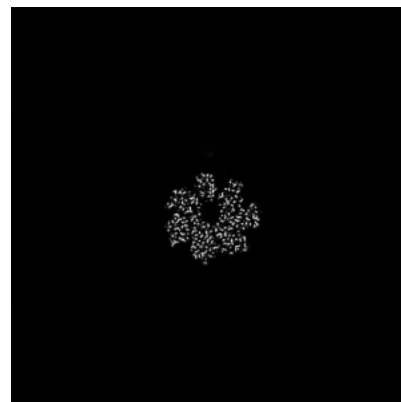
6.2.1 Primary map



X Index: 300

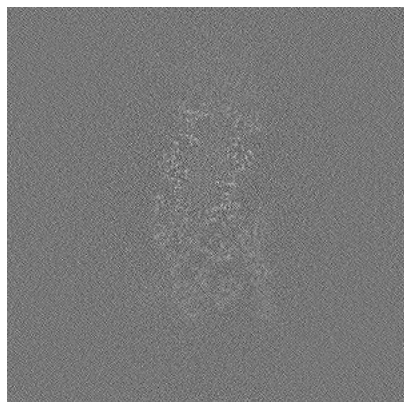


Y Index: 300

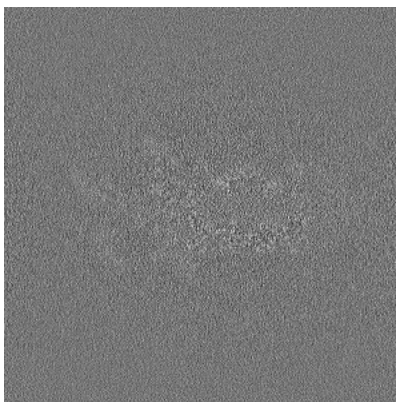


Z Index: 300

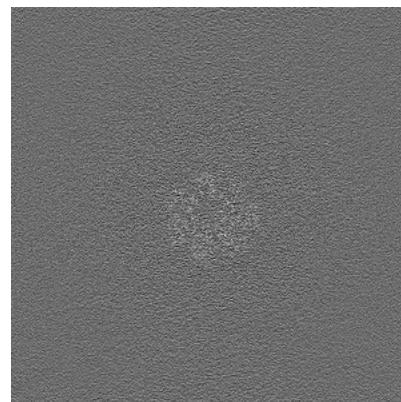
6.2.2 Raw map



X Index: 300



Y Index: 300

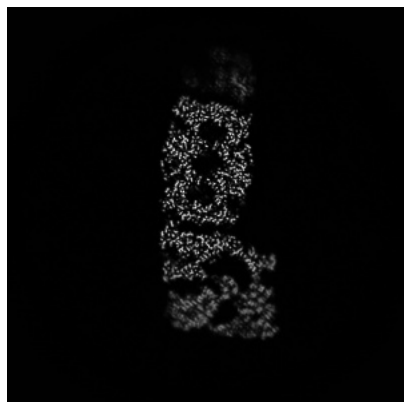


Z Index: 300

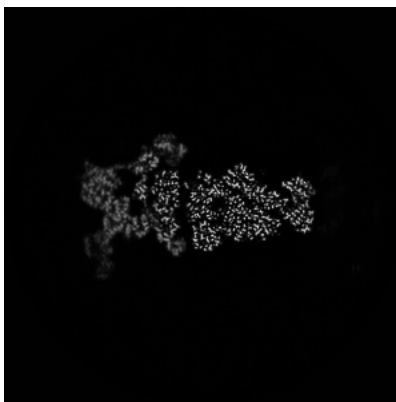
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

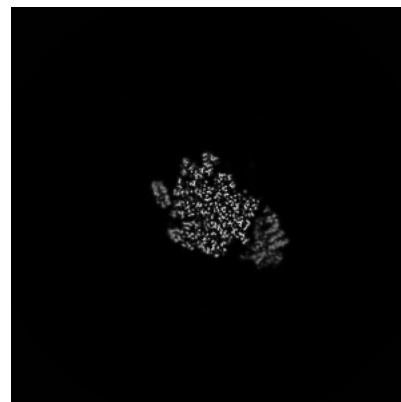
6.3.1 Primary map



X Index: 320

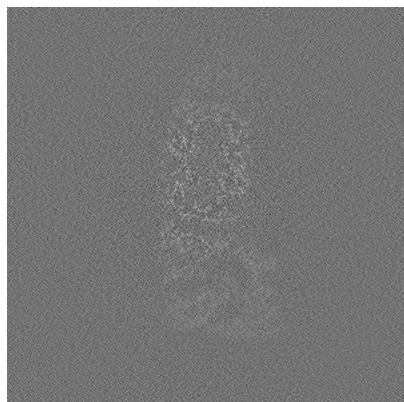


Y Index: 264

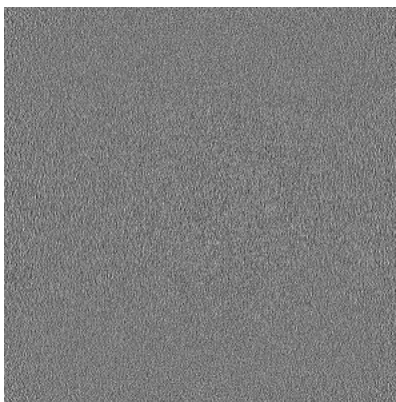


Z Index: 246

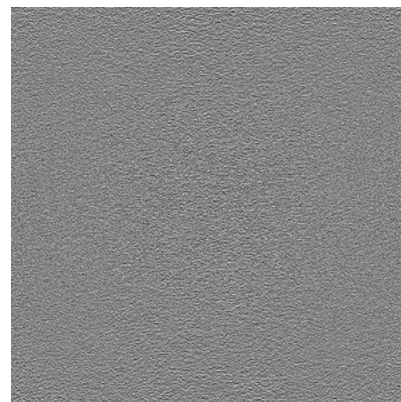
6.3.2 Raw map



X Index: 320



Y Index: 0

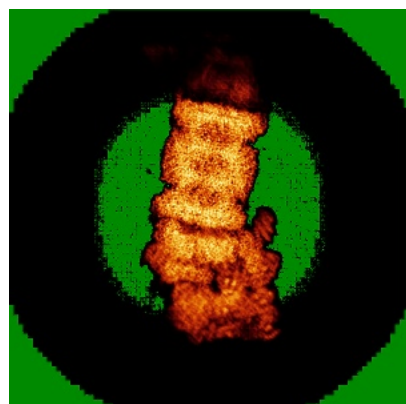


Z Index: 0

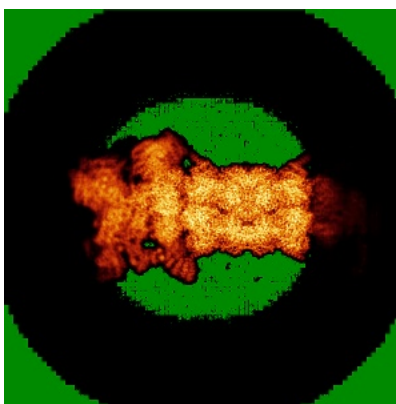
The images above show the largest variance slices of the map in three orthogonal directions.

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

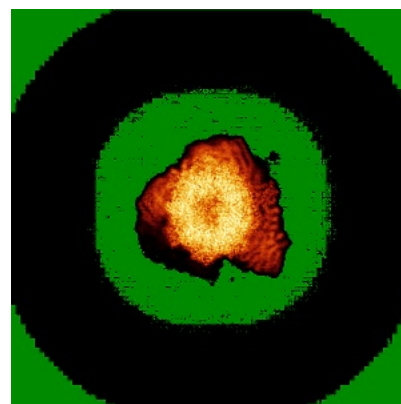
6.4.1 Primary map



X

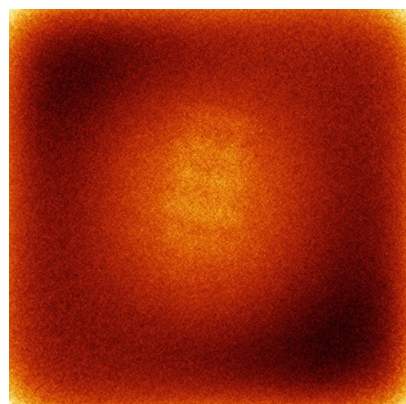


Y

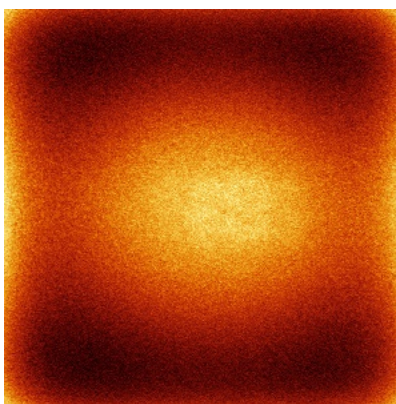


Z

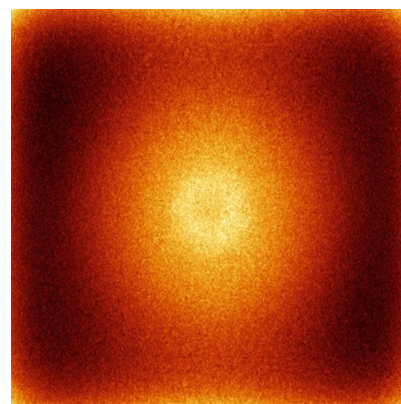
6.4.2 Raw map



X



Y

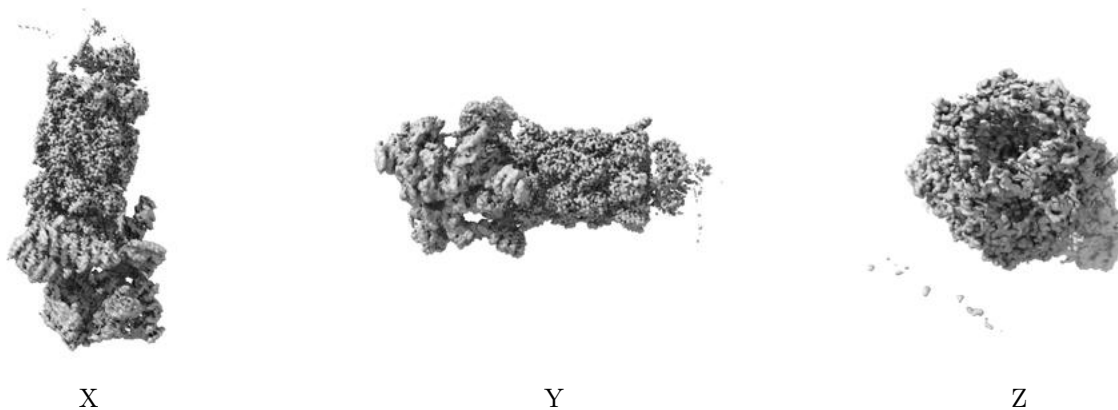


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

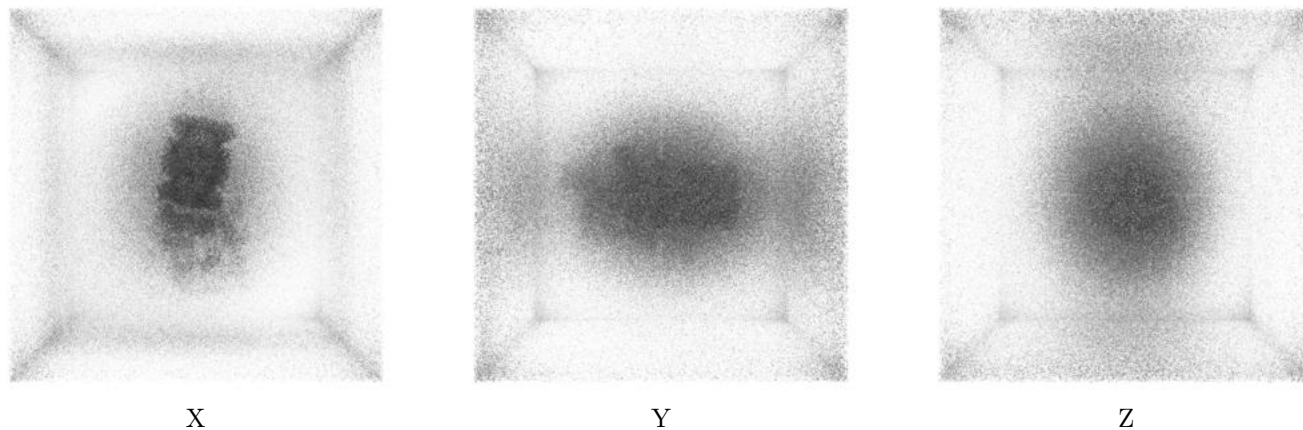
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

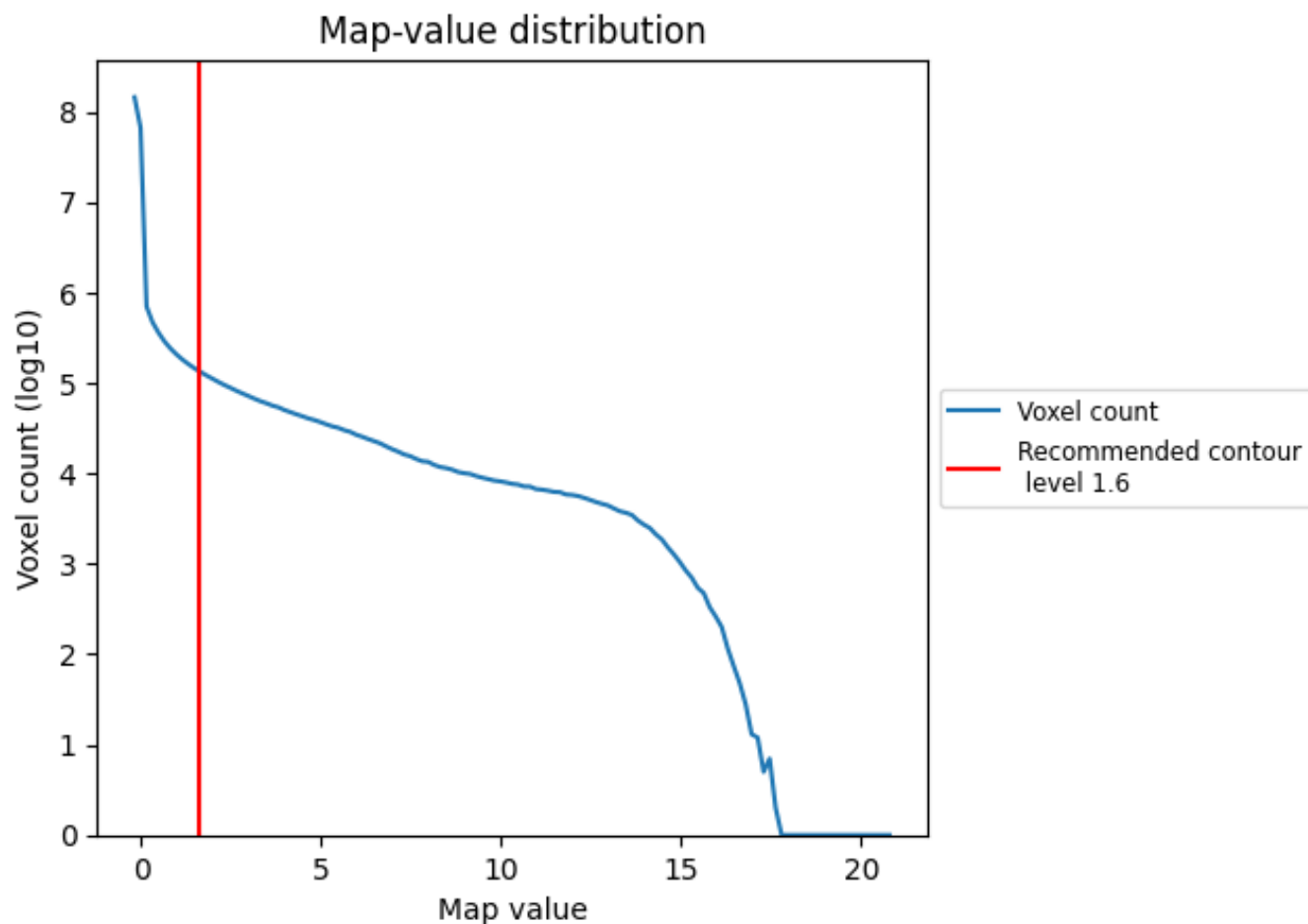
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

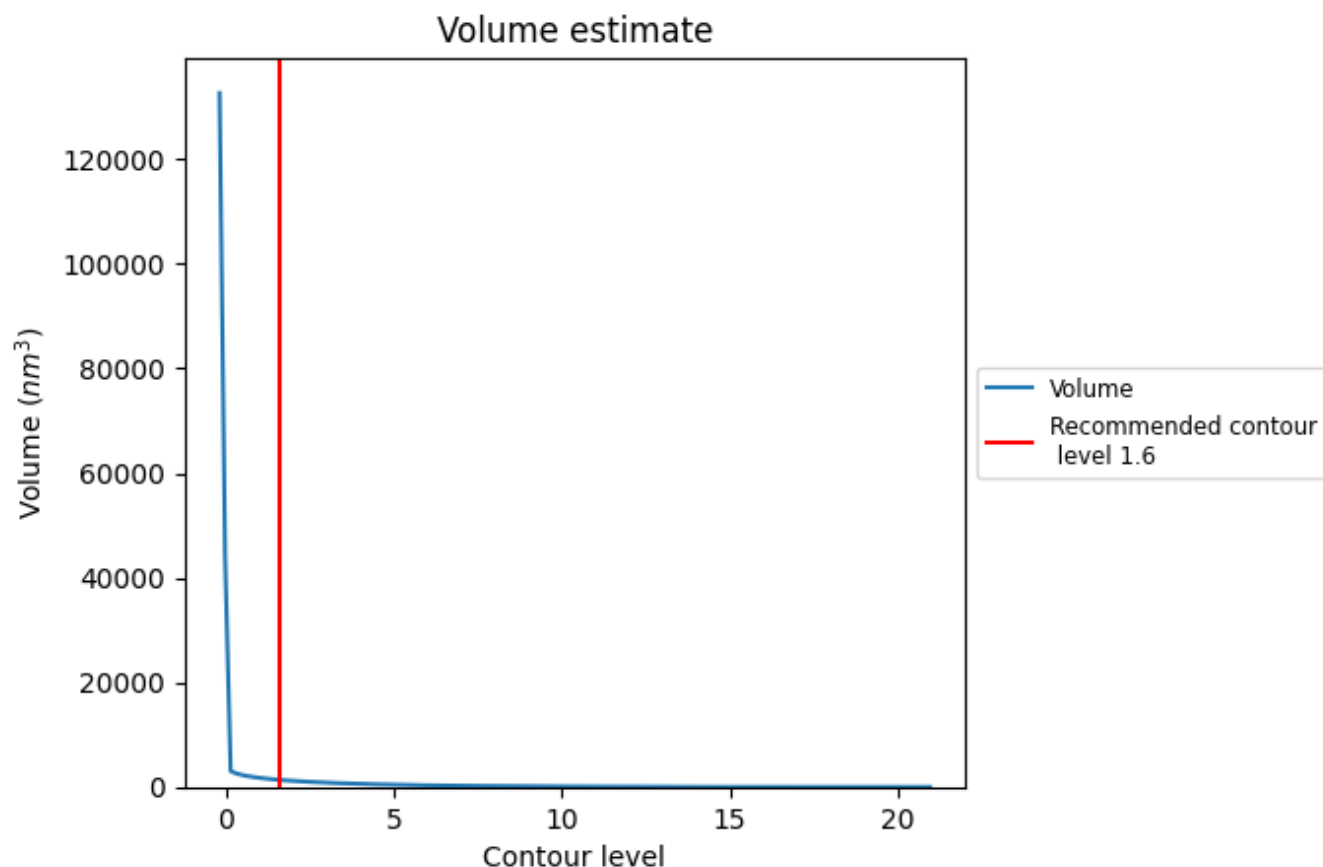
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

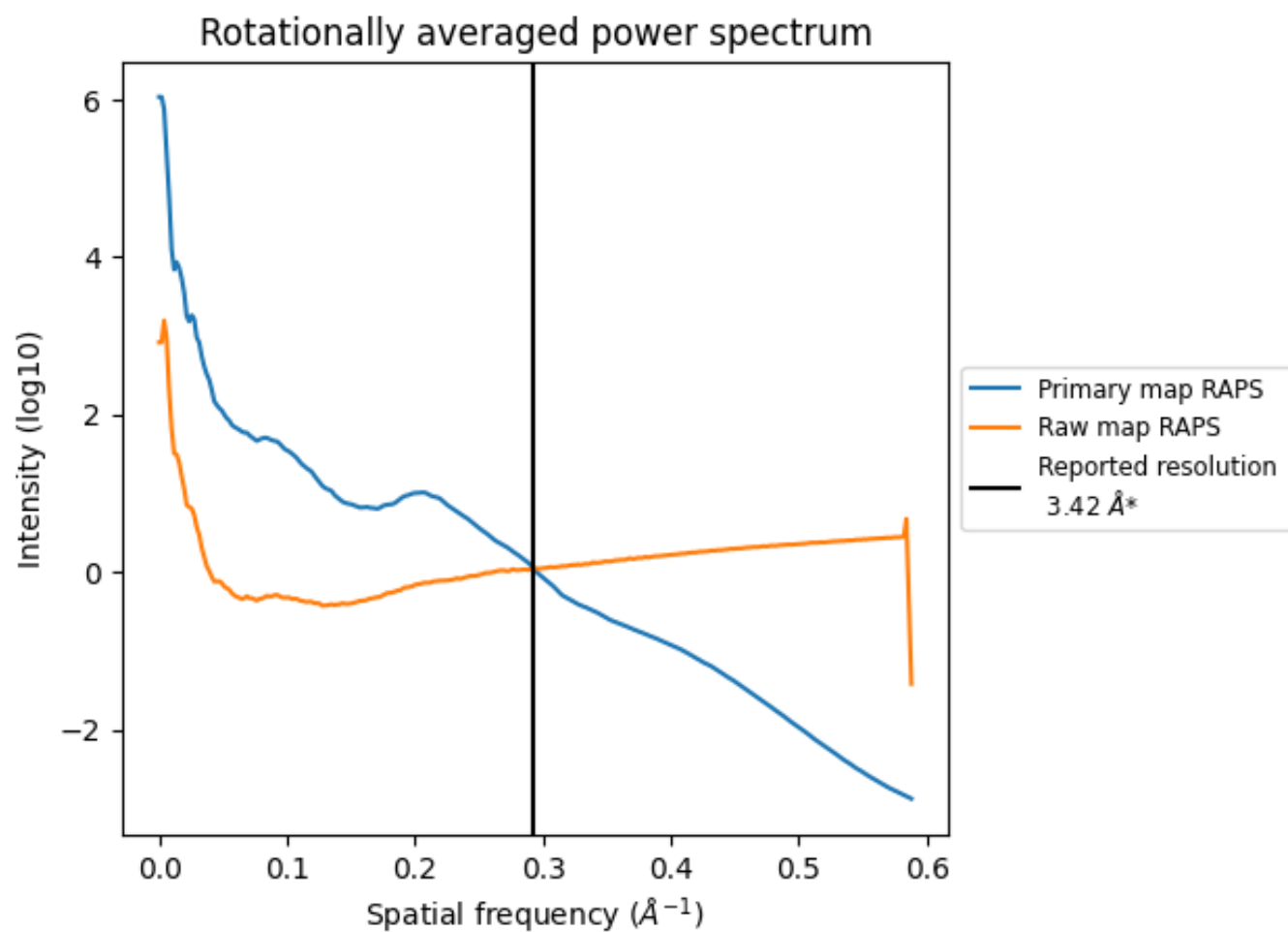
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1351 nm^3 ; this corresponds to an approximate mass of 1221 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 ⓘ

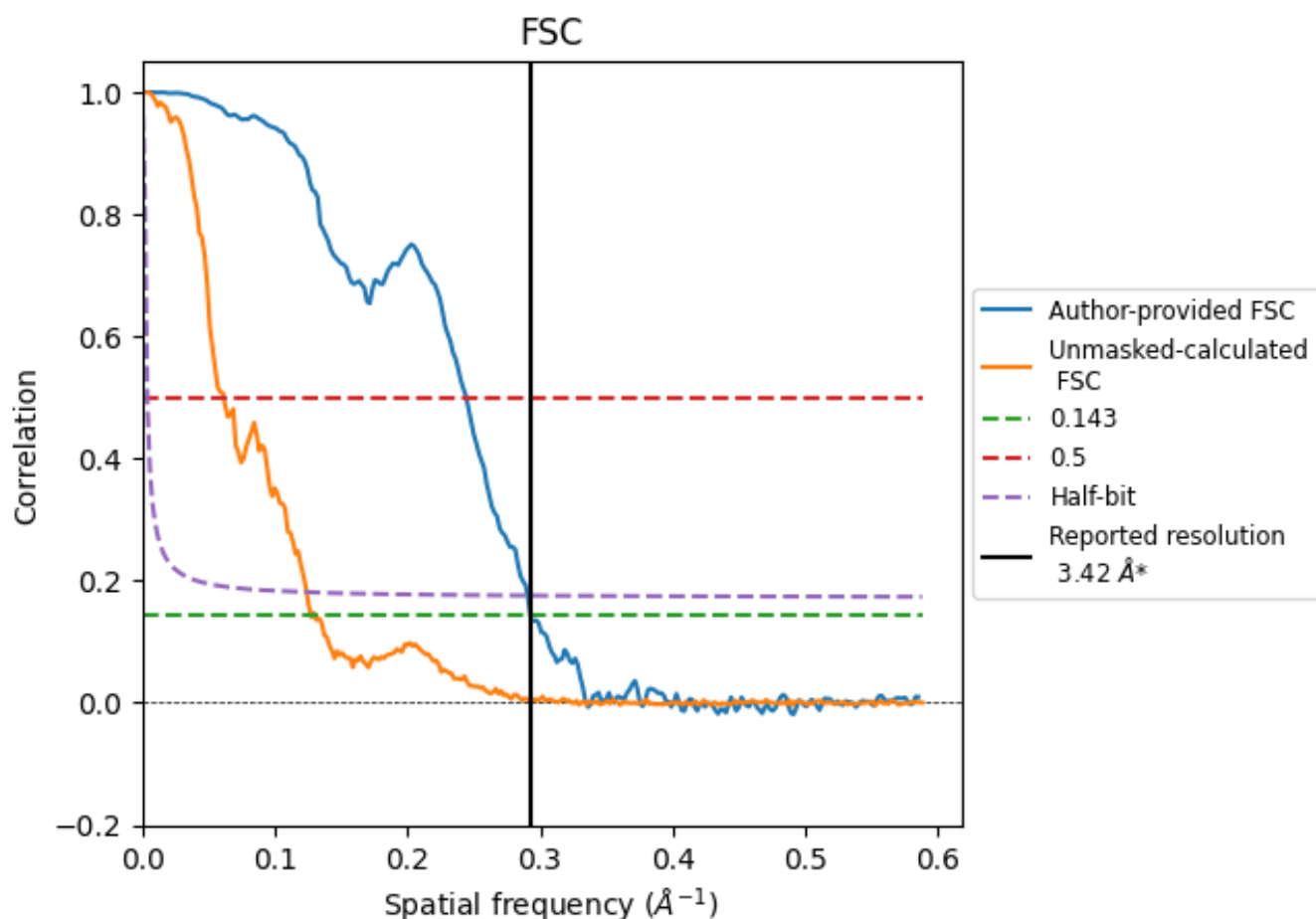


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

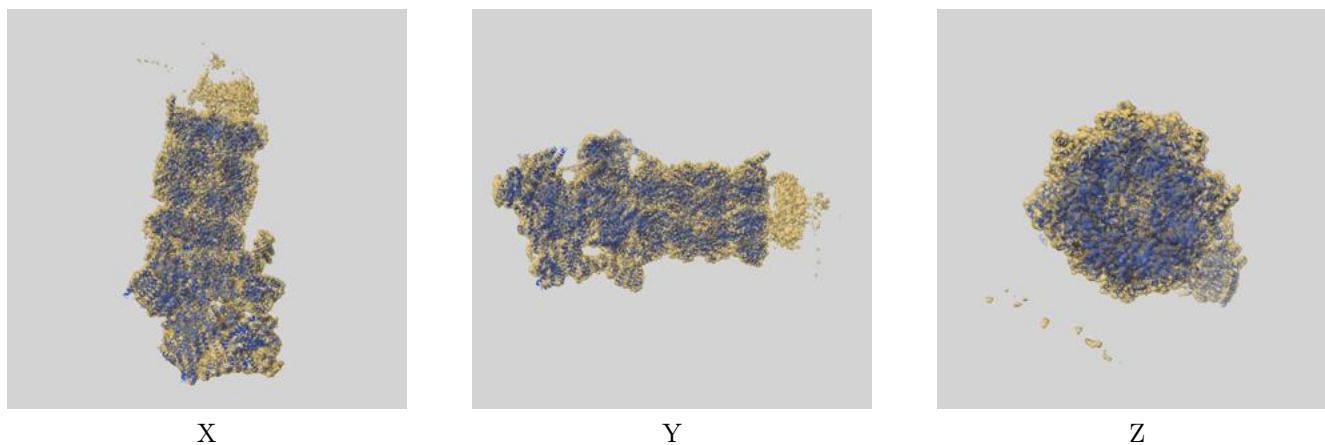
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	4.09	3.44
Unmasked-calculated*	7.86	16.29	8.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.86 differs from the reported value 3.42 by more than 10 %

9 Map-model fit [i](#)

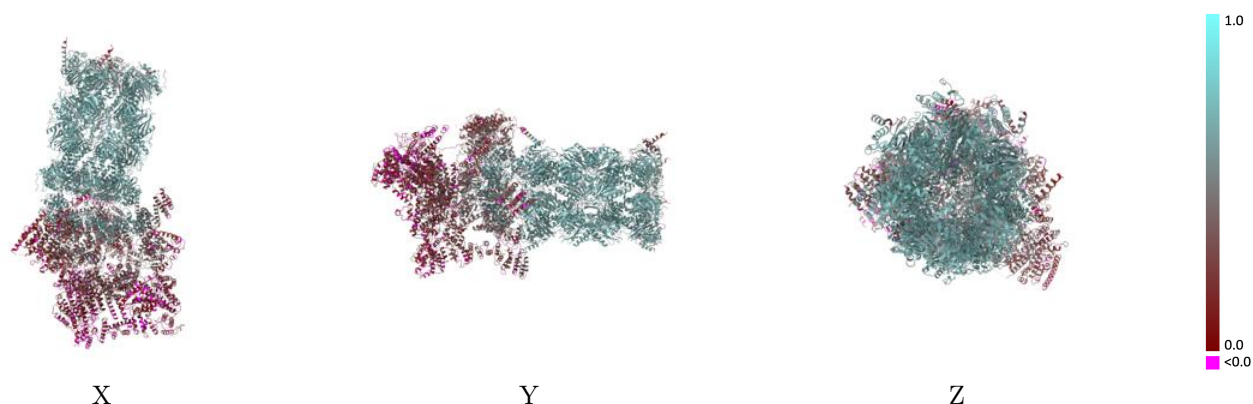
This section contains information regarding the fit between EMDB map EMD-68472 and PDB model 22MM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



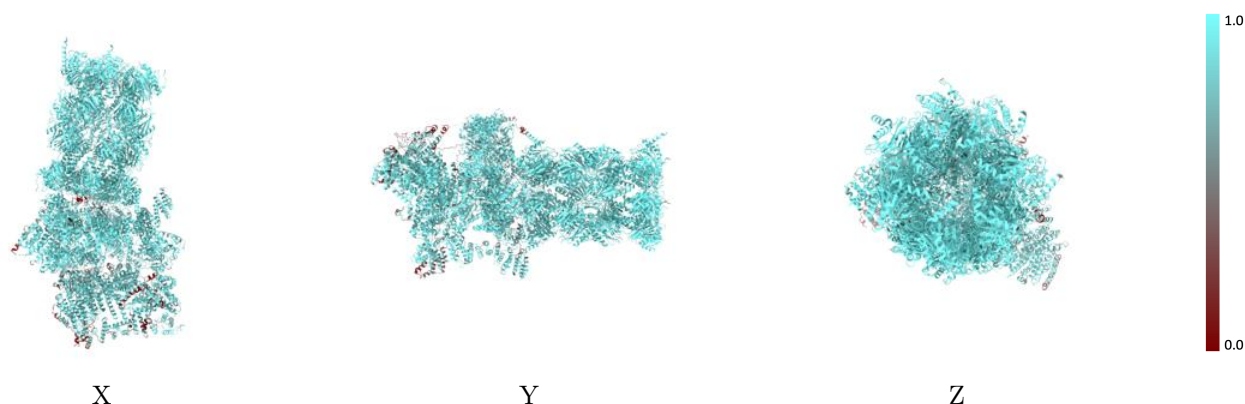
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



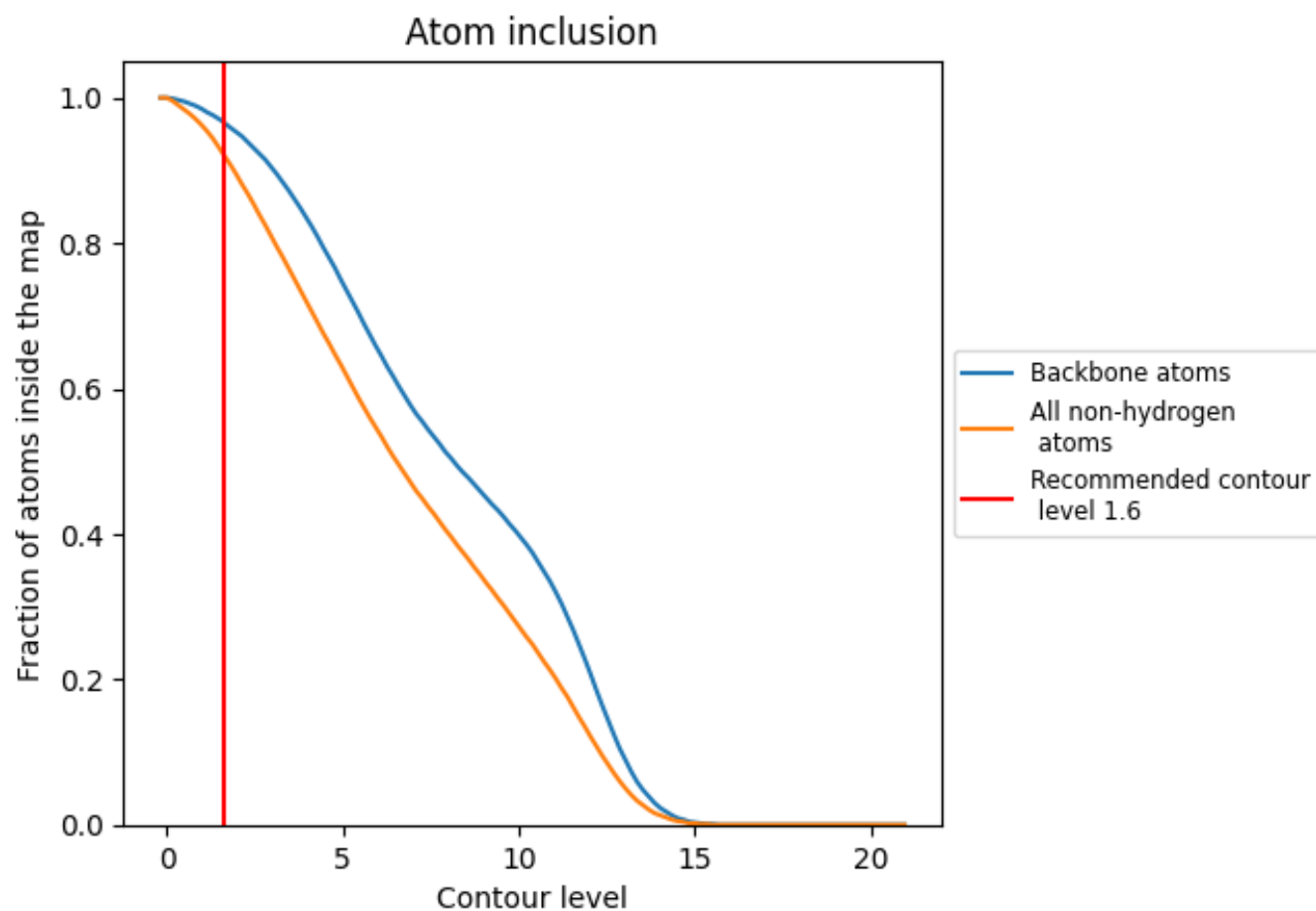
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.4450
A	 0.9360	 0.4690
B	 0.9490	 0.5070
C	 0.9520	 0.5030
D	 0.9450	 0.4750
E	 0.8290	 0.2950
F	 0.9030	 0.3670
G	 0.9900	 0.6350
H	 0.9910	 0.6450
I	 0.9750	 0.6210
J	 0.9420	 0.5940
K	 0.9890	 0.6470
L	 0.9910	 0.6510
M	 0.9840	 0.6350
N	 0.9890	 0.6630
O	 0.9860	 0.6470
P	 0.9970	 0.6600
Q	 0.9950	 0.6610
R	 0.9890	 0.6630
S	 0.9950	 0.6680
T	 0.9970	 0.6630
U	 0.8000	 0.1400
V	 0.8090	 0.1520
W	 0.8750	 0.2220
X	 0.9300	 0.3610
Y	 0.9020	 0.2930
Z	 0.9230	 0.2240
a	 0.7090	 0.1280
c	 0.8230	 0.1570
d	 0.8210	 0.1530
e	 0.7510	 0.1290
f	 0.6350	 0.2000
g	 0.9820	 0.6120
h	 0.9730	 0.6000
i	 0.9670	 0.5660



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Chain	Atom inclusion	Q-score
j	 0.9610	 0.5210
k	 0.9530	 0.5720
l	 0.9830	 0.6150
m	 0.9810	 0.6000
n	 0.9860	 0.6600
o	 0.9890	 0.6370
p	 0.9940	 0.6560
q	 0.9950	 0.6590
r	 0.9880	 0.6560
s	 0.9940	 0.6620
t	 0.9960	 0.6650
u	 0.9050	 0.2610