



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:24 PM UTC

PDB ID : 9B8O / pdb_00009b8o
EMDB ID : EMD-44350
Title : Synaptic Vesicle V-ATPase with synaptophysin and SidK, State 3, Vo
Authors : Coupland, C.E.; Rubinstein, J.L.
Deposited on : 2024-03-31
Resolution : 3.20 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

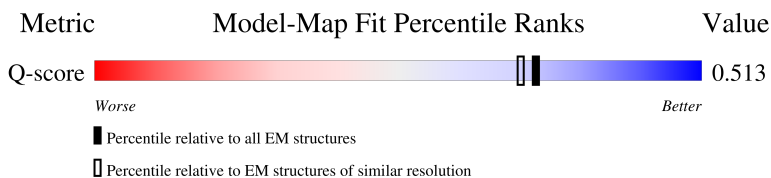
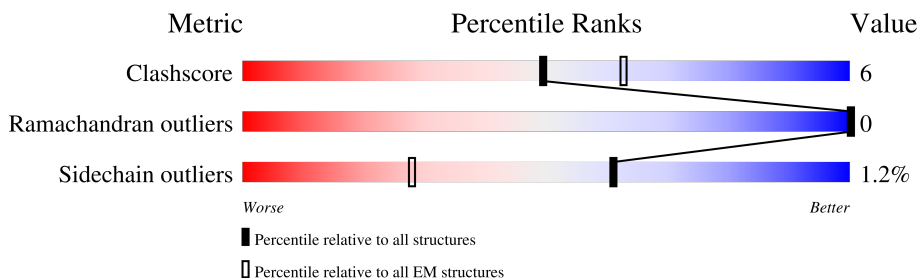
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



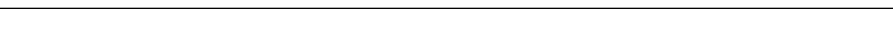
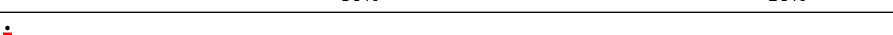
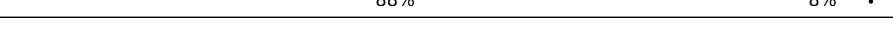
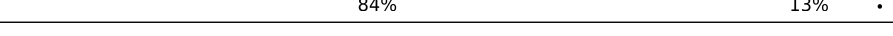
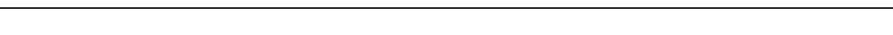
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	H	247	 23% 77%
2	P	463	 37% 7% 56%
3	U	307	 45% 69% 30%
4	a	826	 43% 8% 49%

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Mol	Chain	Length	Quality of chain
5	b	205	 84% 14% ..
6	d	351	 90% 9%
7	e	81	 84% 15% .
8	f	86	 88% 12%
9	g	155	 78% 19% .
9	h	155	 85% 12% .
9	i	155	 81% 16% .
9	j	155	 80% 16% ..
9	k	155	 88% 8% .
9	l	155	 84% 13% .
9	m	155	 86% 11% .
9	n	155	 86% 10% .
9	o	155	 80% 16% ..
10	p	350	 12% 85% .
11	L	119	 8% 92%
12	A	2	 50% 50%
12	B	2	 50% 100%
12	C	2	 100%
12	D	2	 50% 100%
12	E	2	 50% 50%
12	F	2	 50% 50%
12	G	2	 50% 50%
12	I	2	 50% 100%
13	Z	11	 9% 27% 64% 9%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 24407 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 ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	H	57	Total	C	N	O	0	0
			431	270	74	87		

- Molecule 2 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	204	Total	C	N	O	S	0	0
			1652	1087	259	297	9		

- Molecule 3 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	U	214	Total	C	N	O	0	0
			1150	702	221	227		

- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	422	Total	C	N	O	S	0	0
			3408	2286	539	560	23		

- Molecule 5 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 6 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 7 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	80	Total	C	N	O	S	0	0
			644	443	100	98	3		

- Molecule 8 is a protein called Rnasek protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	86	Total	C	N	O	S	0	0
			666	440	103	116	7		

- Molecule 9 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
9	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 10 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	52	Total	C	N	O	S	0	0
			432	290	63	76	3		

- Molecule 11 is a protein called V-type proton ATPase subunit F.

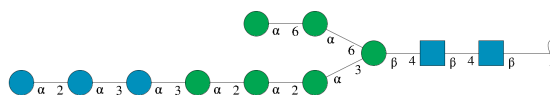
Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	10	Total	C	N	O	0	0
			82	48	19	15		

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	A	2	Total	C	N	O	0	0
			28	16	2	10		
12	B	2	Total	C	N	O	0	0
			28	16	2	10		
12	C	2	Total	C	N	O	0	0
			28	16	2	10		
12	D	2	Total	C	N	O	0	0
			28	16	2	10		
12	E	2	Total	C	N	O	0	0
			28	16	2	10		
12	F	2	Total	C	N	O	0	0
			28	16	2	10		
12	G	2	Total	C	N	O	0	0
			28	16	2	10		
12	I	2	Total	C	N	O	0	0
			28	16	2	10		

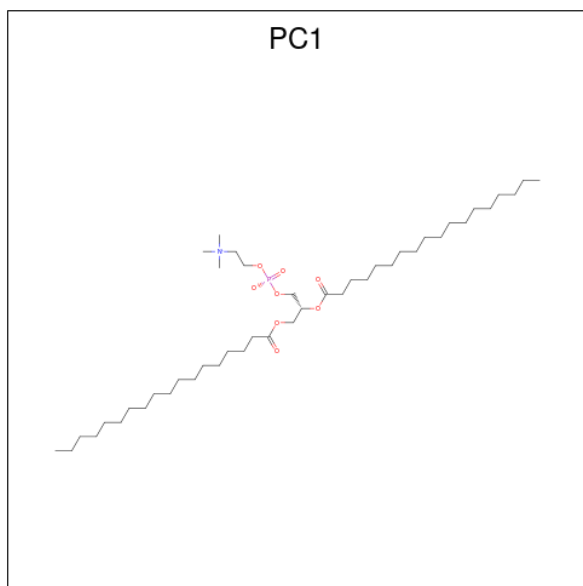
- Molecule 13 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	11	Total	C	N	O	0	0
			127	70	2	55		

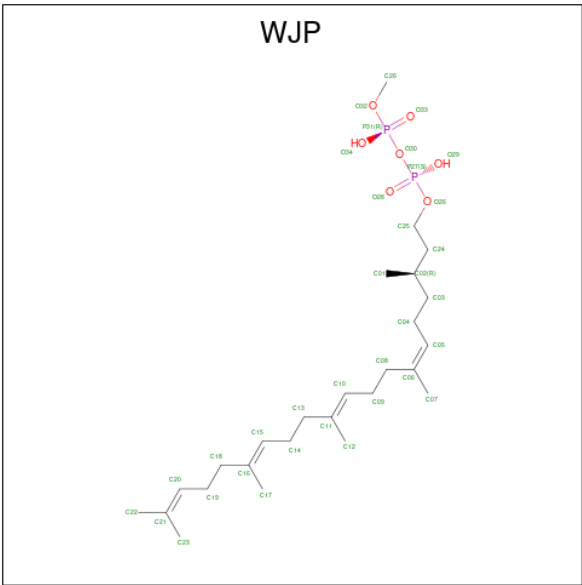
- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: $C_{44}H_{88}NO_8P$).



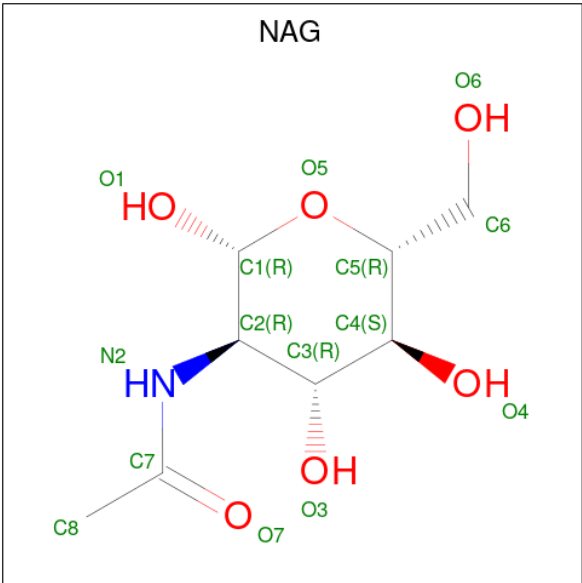
Mol	Chain	Residues	Atoms					AltConf
14	P	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	l	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 15 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$).



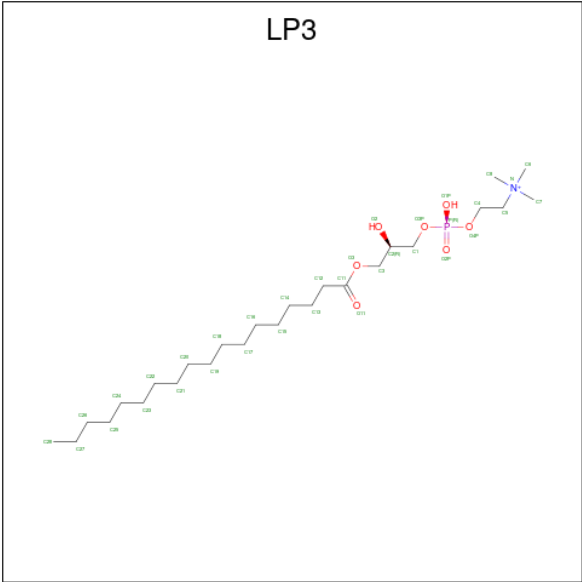
Mol	Chain	Residues	Atoms				AltConf
15	a	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



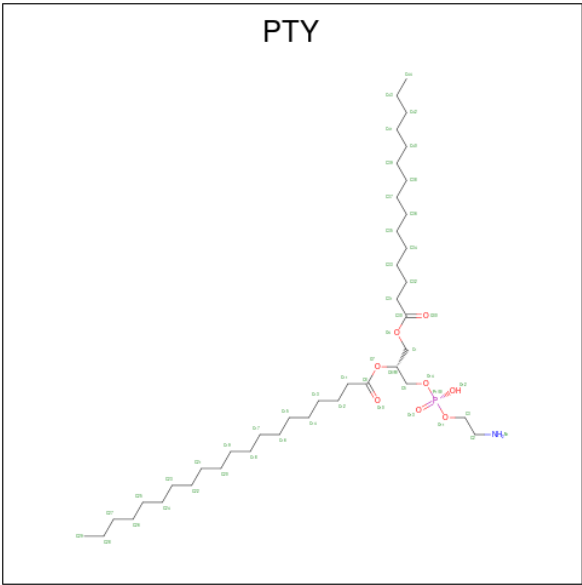
Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 17 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (CCD ID: LP3) (formula: C₂₆H₅₅NO₇P).



Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	N	O	P	0
			35	26	1	7	1	

- Molecule 18 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



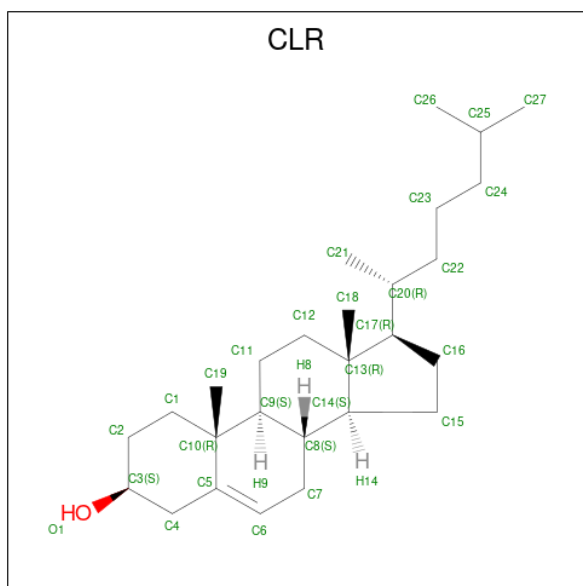
Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	b	1	Total	C	N	O	P	0
			50	40	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	e	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	j	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	p	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 19 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	C	O	0
			28	27	1	
19	h	1	Total	C	O	0
			28	27	1	
19	h	1	Total	C	O	0
			28	27	1	
19	i	1	Total	C	O	0
			28	27	1	
19	i	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
19	i	1	Total	C	O	0
			28	27	1	
19	i	1	Total	C	O	0
			28	27	1	
19	j	1	Total	C	O	0
			28	27	1	
19	j	1	Total	C	O	0
			28	27	1	
19	j	1	Total	C	O	0
			28	27	1	
19	j	1	Total	C	O	0
			28	27	1	
19	k	1	Total	C	O	0
			28	27	1	
19	k	1	Total	C	O	0
			28	27	1	
19	k	1	Total	C	O	0
			28	27	1	
19	k	1	Total	C	O	0
			28	27	1	
19	l	1	Total	C	O	0
			28	27	1	
19	l	1	Total	C	O	0
			28	27	1	
19	l	1	Total	C	O	0
			28	27	1	
19	m	1	Total	C	O	0
			28	27	1	
19	m	1	Total	C	O	0
			28	27	1	
19	m	1	Total	C	O	0
			28	27	1	
19	m	1	Total	C	O	0
			28	27	1	
19	m	1	Total	C	O	0
			28	27	1	
19	n	1	Total	C	O	0
			28	27	1	
19	n	1	Total	C	O	0
			28	27	1	
19	n	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
19	n	1	Total	C	O	0
			28	27	1	
19	o	1	Total	C	O	0
			28	27	1	
19	o	1	Total	C	O	0
			28	27	1	
19	o	1	Total	C	O	0
			28	27	1	



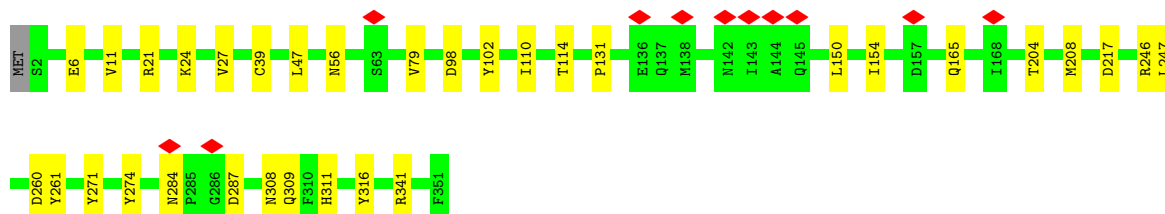
- Molecule 5: ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a

Chain b:  84% 14% ..



- Molecule 6: V-type proton ATPase subunit

Chain d:  90% 9%



- Molecule 7: V-type proton ATPase subunit e 2

Chain e:  84% 15% .



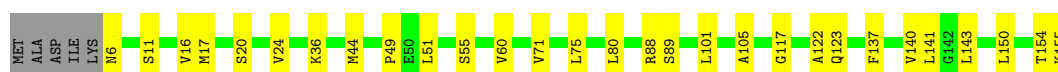
- Molecule 8: Rnasek protein

Chain f:  88% 12%



- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

Chain g:  78% 19% .



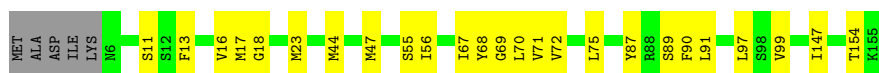
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h:  85% 12% .

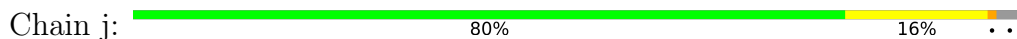


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

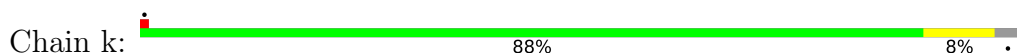
Chain i:  81% 16% .



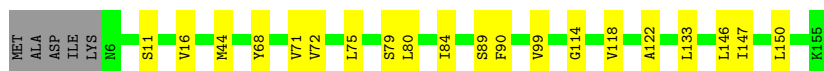
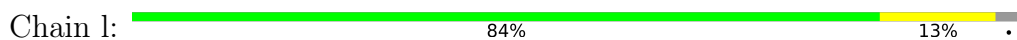
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



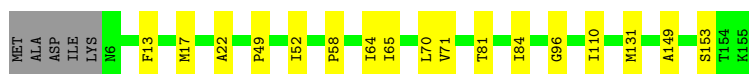
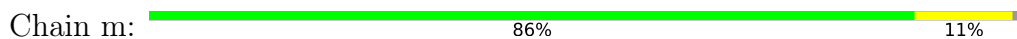
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



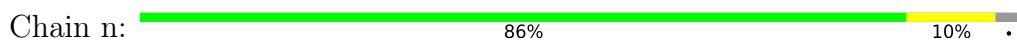
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



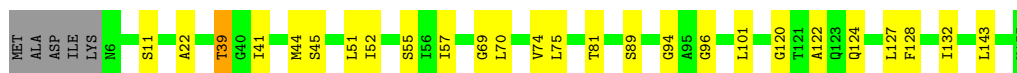
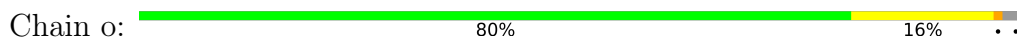
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



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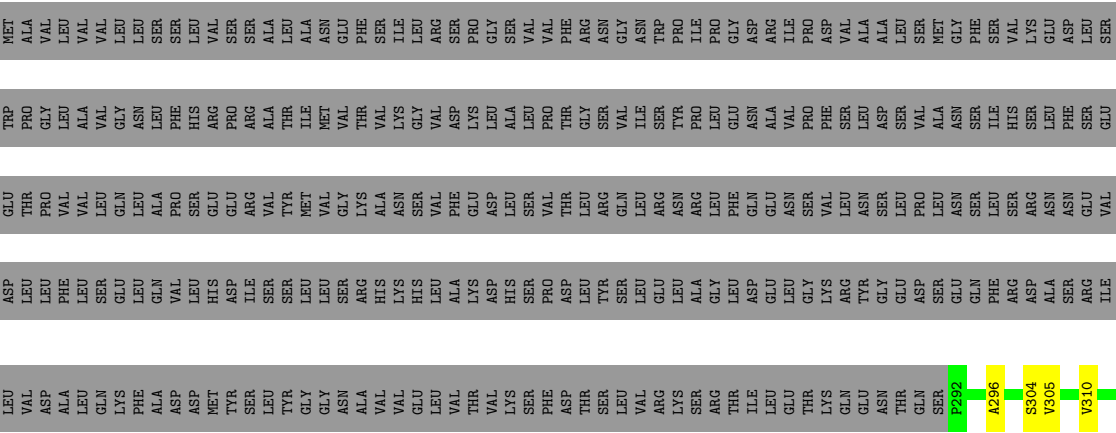


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

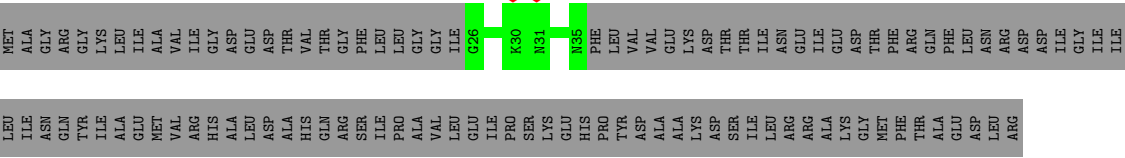


- Molecule 10: Renin receptor





● Molecule 11: V-type proton ATPase subunit F



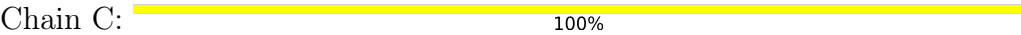
● Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1	MAG2	BM43	MAN4	MAN5	MAN6	GLC7	GLC8	GLC9	MAN10	MAN11
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198533	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 ($e^-/\text{\AA}^2$)	37.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-1.189	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	309.0, 309.0, 309.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CLR, PC1, MAN, LP3, GLC, PTY, WJP, BMA

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	H	0.15	0/434	0.32	0/581
2	P	0.17	0/1707	0.35	0/2324
3	U	0.11	0/1158	0.29	0/1601
4	a	0.14	0/3517	0.28	0/4771
5	b	0.18	0/1537	0.29	0/2088
6	d	0.13	0/2899	0.24	0/3927
7	e	0.14	0/669	0.25	0/920
8	f	0.12	0/682	0.23	0/926
9	g	0.19	0/1083	0.34	0/1466
9	h	0.18	0/1083	0.32	0/1466
9	i	0.19	0/1083	0.32	0/1466
9	j	0.19	0/1083	0.33	0/1466
9	k	0.18	0/1083	0.30	0/1466
9	l	0.18	0/1083	0.32	0/1466
9	m	0.18	0/1083	0.29	0/1466
9	n	0.18	0/1083	0.32	0/1466
9	o	0.19	0/1083	0.32	0/1466
10	p	0.15	0/445	0.26	0/609
11	L	0.08	0/83	0.26	0/110
All	All	0.16	0/22878	0.30	0/31051

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	H	431	0	428	1	0
2	P	1652	0	1579	30	0
3	U	1150	0	644	3	0
4	a	3408	0	3428	47	0
5	b	1503	0	1551	23	0
6	d	2833	0	2770	19	0
7	e	644	0	659	10	0
8	f	666	0	663	6	0
9	g	1068	0	1136	25	0
9	h	1068	0	1136	13	0
9	i	1068	0	1136	22	0
9	j	1068	0	1136	23	0
9	k	1068	0	1136	10	0
9	l	1068	0	1136	15	0
9	m	1068	0	1136	11	0
9	n	1068	0	1136	12	0
9	o	1068	0	1136	16	0
10	p	432	0	428	7	0
11	L	82	0	77	0	0
12	A	28	0	25	2	0
12	B	28	0	25	0	0
12	C	28	0	25	1	0
12	D	28	0	25	2	0
12	E	28	0	25	2	0
12	F	28	0	25	1	0
12	G	28	0	25	1	0
12	I	28	0	25	1	0
13	Z	127	0	106	4	0
14	P	54	0	88	3	0
14	a	54	0	88	0	0
14	b	108	0	176	2	0
14	l	54	0	88	0	0
15	a	34	0	0	2	0
16	a	14	0	13	0	0
17	a	35	0	54	0	0
18	a	100	0	158	1	0
18	b	100	0	158	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	e	50	0	79	1	0
18	j	50	0	79	0	0
18	p	150	0	237	2	0
19	b	28	0	46	1	0
19	h	56	0	92	4	0
19	i	112	0	184	12	0
19	j	112	0	184	6	0
19	k	112	0	184	3	0
19	l	84	0	138	6	0
19	m	140	0	230	4	0
19	n	112	0	184	10	0
19	o	84	0	138	5	0
All	All	24407	0	25355	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 284 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)
9:n:51:LEU:O	9:n:55:SER:OG	1.97	0.81
9:h:17:MET:O	9:h:21:SER:OG	2.00	0.79
6:d:217:ASP:OD2	6:d:274:TYR:OH	2.00	0.79
9:j:71:VAL:HG11	19:j:204:CLR:H182	1.68	0.76
9:i:23:MET:HE3	9:i:23:MET:O	1.86	0.74

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	H	53/247 (22%)	51 (96%)	2 (4%)	0	100	100
2	P	202/463 (44%)	188 (93%)	14 (7%)	0	100	100
3	U	212/307 (69%)	208 (98%)	4 (2%)	0	100	100
4	a	418/826 (51%)	394 (94%)	24 (6%)	0	100	100
5	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
6	d	348/351 (99%)	337 (97%)	11 (3%)	0	100	100
7	e	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	f	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
9	g	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
9	h	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
9	i	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
9	j	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
9	k	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
9	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
9	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	n	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
9	o	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
10	p	50/350 (14%)	50 (100%)	0	0	100	100
11	L	8/119 (7%)	7 (88%)	1 (12%)	0	100	100
All	All	2986/4430 (67%)	2879 (96%)	107 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	H	43/212 (20%)	43 (100%)	0	100	100
2	P	182/395 (46%)	179 (98%)	3 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	U	24/241 (10%)	24 (100%)	0	100	100
4	a	367/732 (50%)	358 (98%)	9 (2%)	42	69
5	b	156/158 (99%)	152 (97%)	4 (3%)	40	69
6	d	305/306 (100%)	304 (100%)	1 (0%)	86	88
7	e	67/68 (98%)	67 (100%)	0	100	100
8	f	72/72 (100%)	70 (97%)	2 (3%)	38	68
9	g	109/113 (96%)	107 (98%)	2 (2%)	51	74
9	h	109/113 (96%)	108 (99%)	1 (1%)	70	81
9	i	109/113 (96%)	109 (100%)	0	100	100
9	j	109/113 (96%)	107 (98%)	2 (2%)	51	74
9	k	109/113 (96%)	109 (100%)	0	100	100
9	l	109/113 (96%)	108 (99%)	1 (1%)	70	81
9	m	109/113 (96%)	109 (100%)	0	100	100
9	n	109/113 (96%)	109 (100%)	0	100	100
9	o	109/113 (96%)	107 (98%)	2 (2%)	51	74
10	p	47/313 (15%)	46 (98%)	1 (2%)	47	71
11	L	9/100 (9%)	9 (100%)	0	100	100
All	All	2253/3614 (62%)	2225 (99%)	28 (1%)	61	79

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	154	CYS
10	p	304	SER
8	f	17	VAL
9	l	133	LEU
6	d	6	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
6	d	84	HIS
9	o	123	GLN
6	d	324	GLN
10	p	330	ASN

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Mol	Chain	Res	Type
9	k	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

27 monosaccharides are modelled in this entry.

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	$\# Z > 2$
12	NAG	A	1	12	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
12	NAG	A	2	12	14,14,15	0.69	0	17,19,21	0.86	0
12	NAG	B	1	12,2	14,14,15	0.76	0	17,19,21	1.26	3 (17%)
12	NAG	B	2	12	14,14,15	0.79	0	17,19,21	1.04	1 (5%)
12	NAG	C	1	12,2	14,14,15	0.79	0	17,19,21	1.17	2 (11%)
12	NAG	C	2	12	14,14,15	0.75	0	17,19,21	0.79	0
12	NAG	D	1	12,2	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
12	NAG	D	2	12	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
12	NAG	E	1	12,2	14,14,15	0.76	0	17,19,21	1.42	2 (11%)
12	NAG	E	2	12	14,14,15	0.69	0	17,19,21	1.28	1 (5%)
12	NAG	F	1	12	14,14,15	0.72	0	17,19,21	1.35	1 (5%)
12	NAG	F	2	12	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
12	NAG	G	1	12,2	14,14,15	0.75	0	17,19,21	0.88	0
12	NAG	G	2	12	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
12	NAG	I	1	12	14,14,15	0.75	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	I	2	12	14,14,15	0.69	0	17,19,21	0.81	0
13	NAG	Z	1	13	14,14,15	0.77	0	17,19,21	0.79	0
13	MAN	Z	10	13	11,11,12	0.71	0	15,15,17	1.06	1 (6%)
13	MAN	Z	11	13	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
13	NAG	Z	2	13	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
13	BMA	Z	3	13	11,11,12	0.80	0	15,15,17	2.30	3 (20%)
13	MAN	Z	4	13	11,11,12	0.65	0	15,15,17	1.34	1 (6%)
13	MAN	Z	5	13	11,11,12	0.72	0	15,15,17	1.26	1 (6%)
13	MAN	Z	6	13	11,11,12	0.82	1 (9%)	15,15,17	0.97	1 (6%)
13	GLC	Z	7	13	11,11,12	0.65	0	15,15,17	0.52	0
13	GLC	Z	8	13	11,11,12	0.59	0	15,15,17	0.70	0
13	GLC	Z	9	13	11,11,12	0.59	0	15,15,17	0.71	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
12	NAG	A	1	12	-	2/6/23/26	0/1/1/1
12	NAG	A	2	12	-	0/6/23/26	0/1/1/1
12	NAG	B	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	2	12	-	0/6/23/26	0/1/1/1
12	NAG	C	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	C	2	12	-	0/6/23/26	0/1/1/1
12	NAG	D	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	2	12	-	1/6/23/26	0/1/1/1
12	NAG	E	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	E	2	12	-	1/6/23/26	0/1/1/1
12	NAG	F	1	12	-	2/6/23/26	0/1/1/1
12	NAG	F	2	12	-	2/6/23/26	0/1/1/1
12	NAG	G	1	12,2	-	1/6/23/26	0/1/1/1
12	NAG	G	2	12	-	2/6/23/26	0/1/1/1
12	NAG	I	1	12	-	2/6/23/26	0/1/1/1
12	NAG	I	2	12	-	0/6/23/26	0/1/1/1
13	NAG	Z	1	13	-	0/6/23/26	0/1/1/1
13	MAN	Z	10	13	-	0/2/19/22	0/1/1/1
13	MAN	Z	11	13	-	0/2/19/22	0/1/1/1
13	NAG	Z	2	13	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	Z	3	13	-	1/2/19/22	0/1/1/1
13	MAN	Z	4	13	-	2/2/19/22	0/1/1/1
13	MAN	Z	5	13	-	2/2/19/22	0/1/1/1
13	MAN	Z	6	13	-	0/2/19/22	0/1/1/1
13	GLC	Z	7	13	-	1/2/19/22	0/1/1/1
13	GLC	Z	8	13	-	0/2/19/22	0/1/1/1
13	GLC	Z	9	13	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	6	MAN	O5-C1	-2.14	1.40	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	3	BMA	C1-O5-C5	6.81	121.32	112.19
13	Z	4	MAN	C1-O5-C5	4.18	117.79	112.19
12	F	1	NAG	C2-N2-C7	4.00	128.26	122.90
12	E	1	NAG	C2-N2-C7	3.93	128.17	122.90
12	E	2	NAG	C2-N2-C7	3.53	127.63	122.90

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1	NAG	C1-C2-N2-C7
12	D	2	NAG	C3-C2-N2-C7
12	E	2	NAG	C3-C2-N2-C7
12	G	1	NAG	C1-C2-N2-C7
12	I	1	NAG	C1-C2-N2-C7

There are no ring outliers.

13 monomers are involved in 14 short contacts:

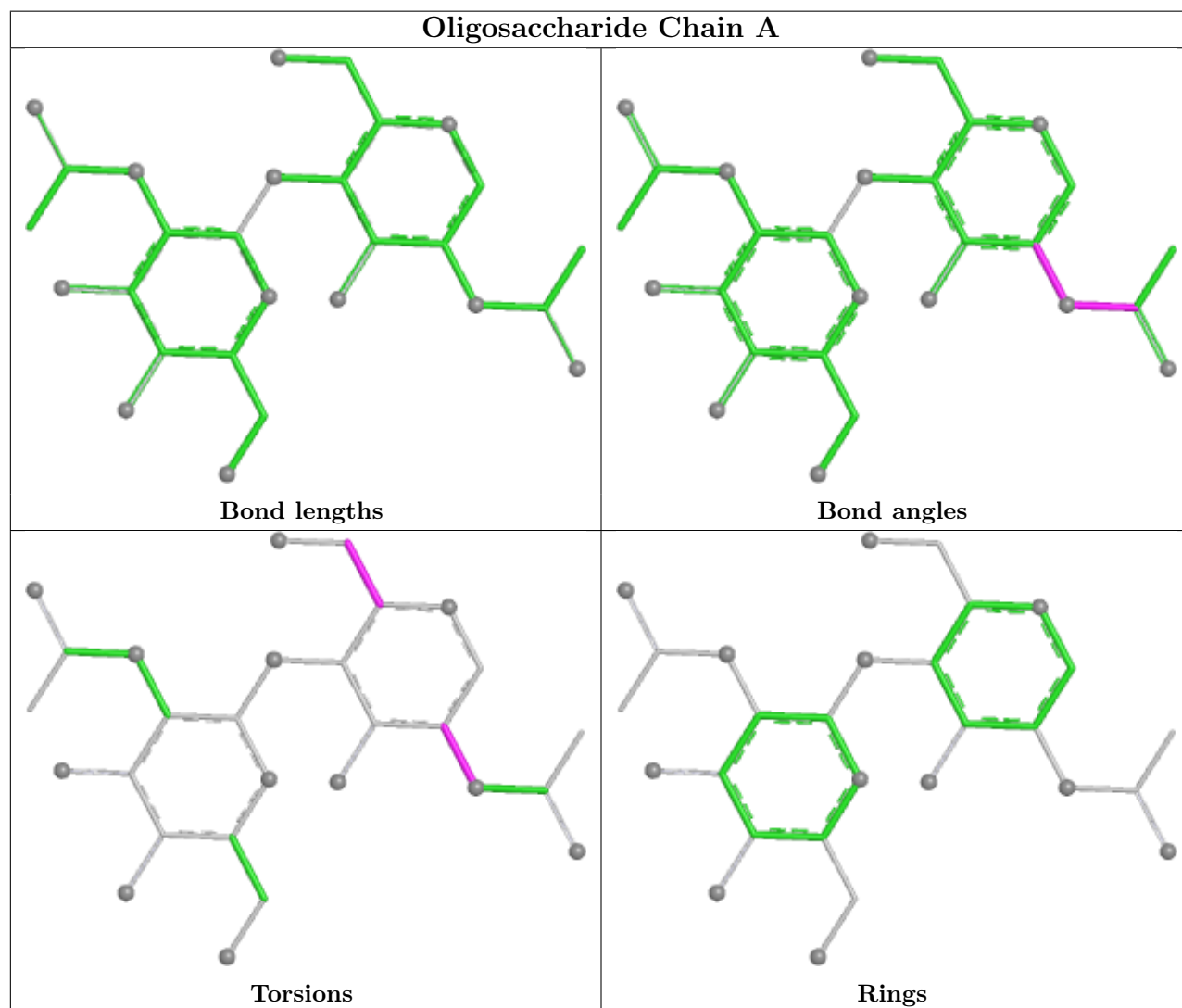
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	2	NAG	1	0
12	C	2	NAG	1	0
12	E	1	NAG	2	0
12	F	1	NAG	1	0

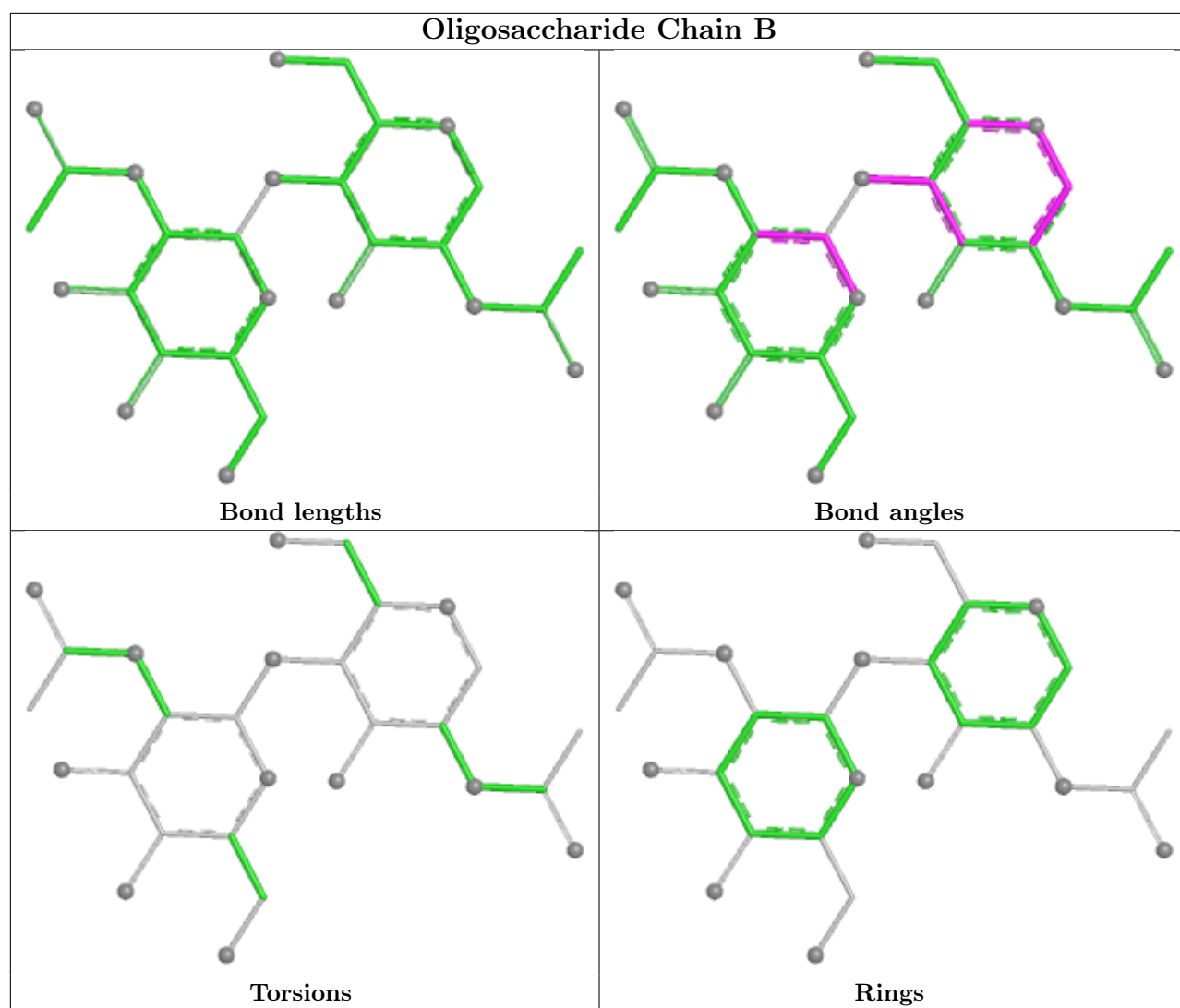
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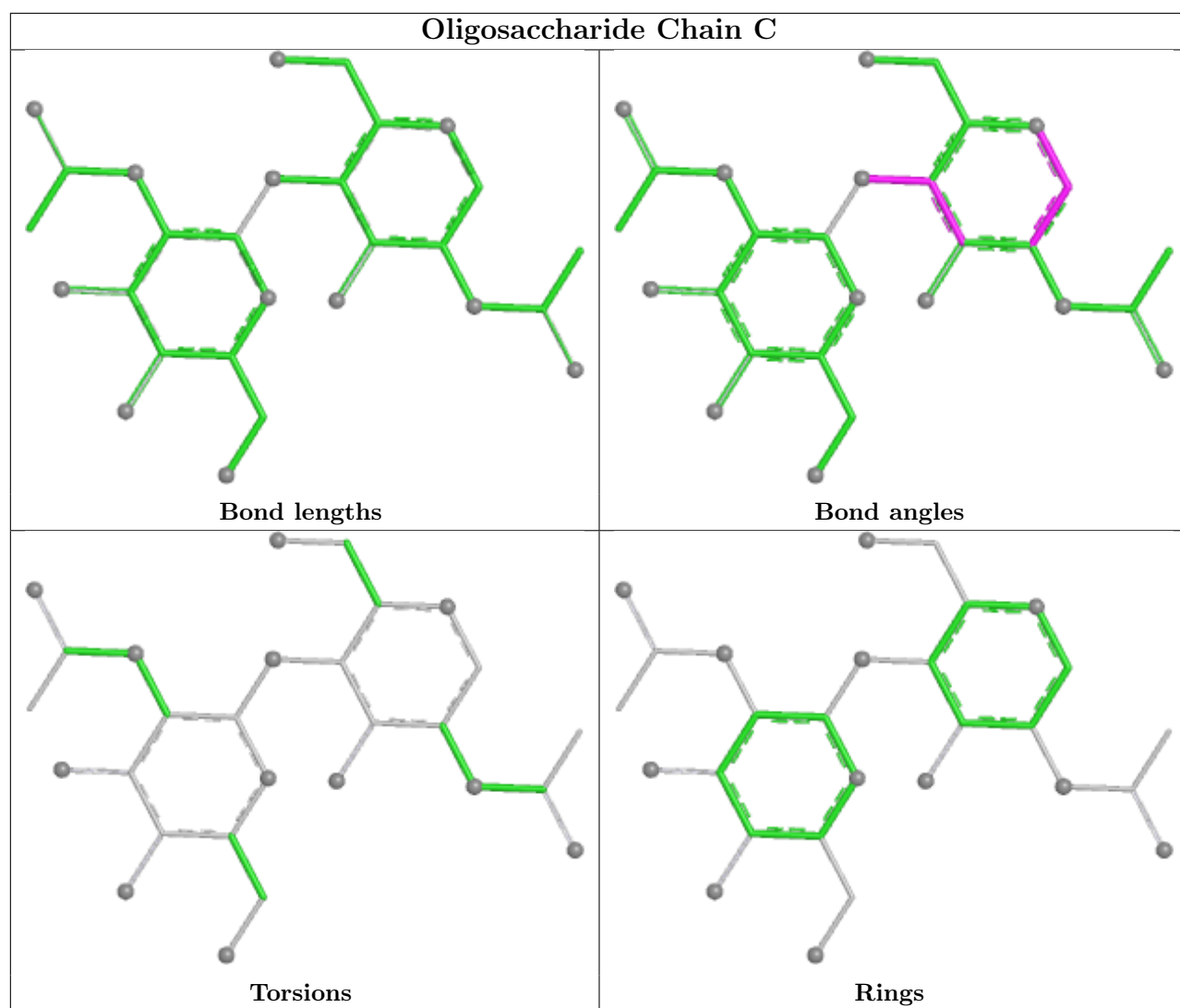
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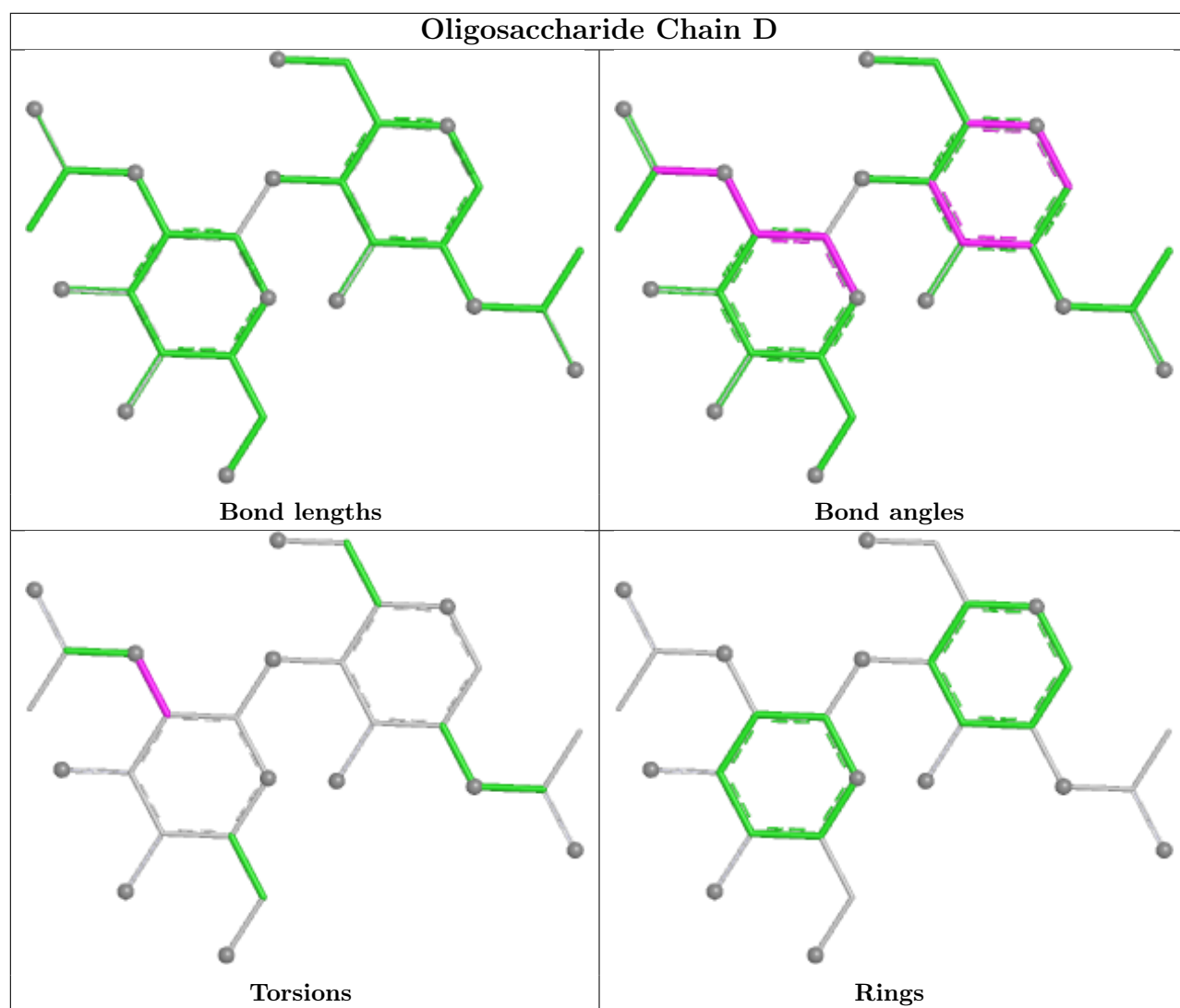
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	1	NAG	3	0
12	D	1	NAG	2	0
12	I	2	NAG	1	0
12	G	1	NAG	1	0
13	Z	2	NAG	1	0
12	G	2	NAG	1	0
12	D	2	NAG	2	0
12	I	1	NAG	1	0
12	A	1	NAG	2	0

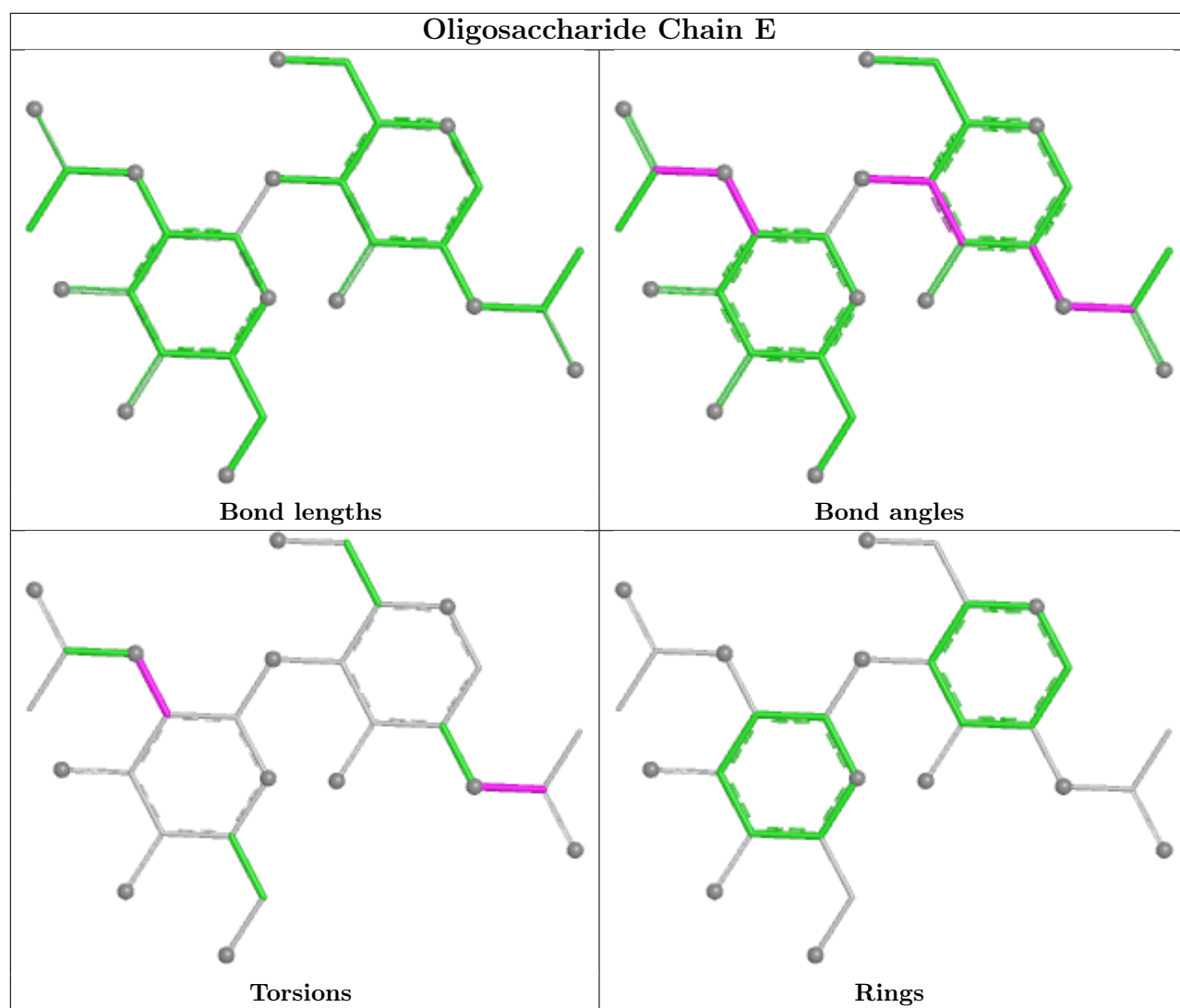
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

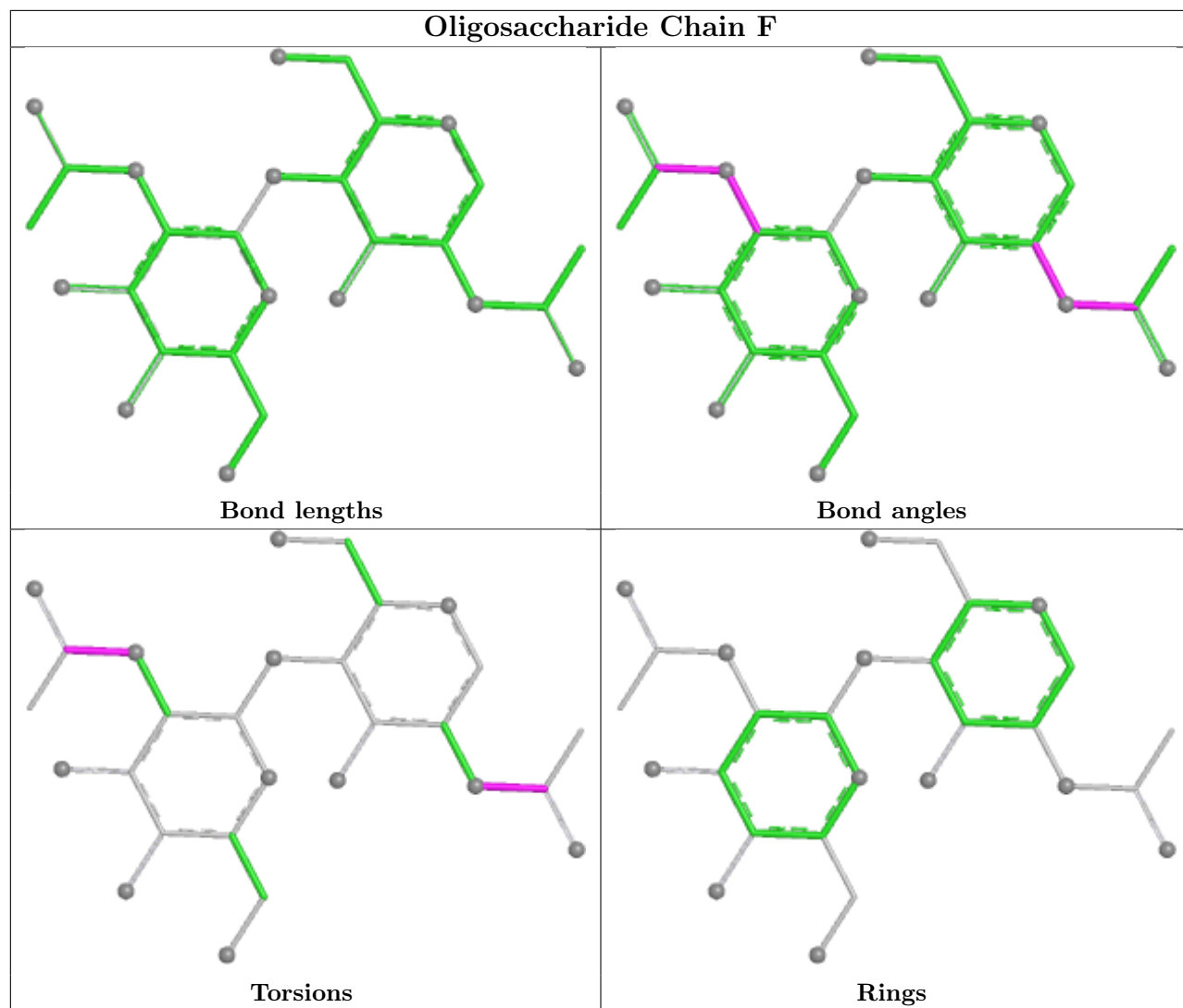


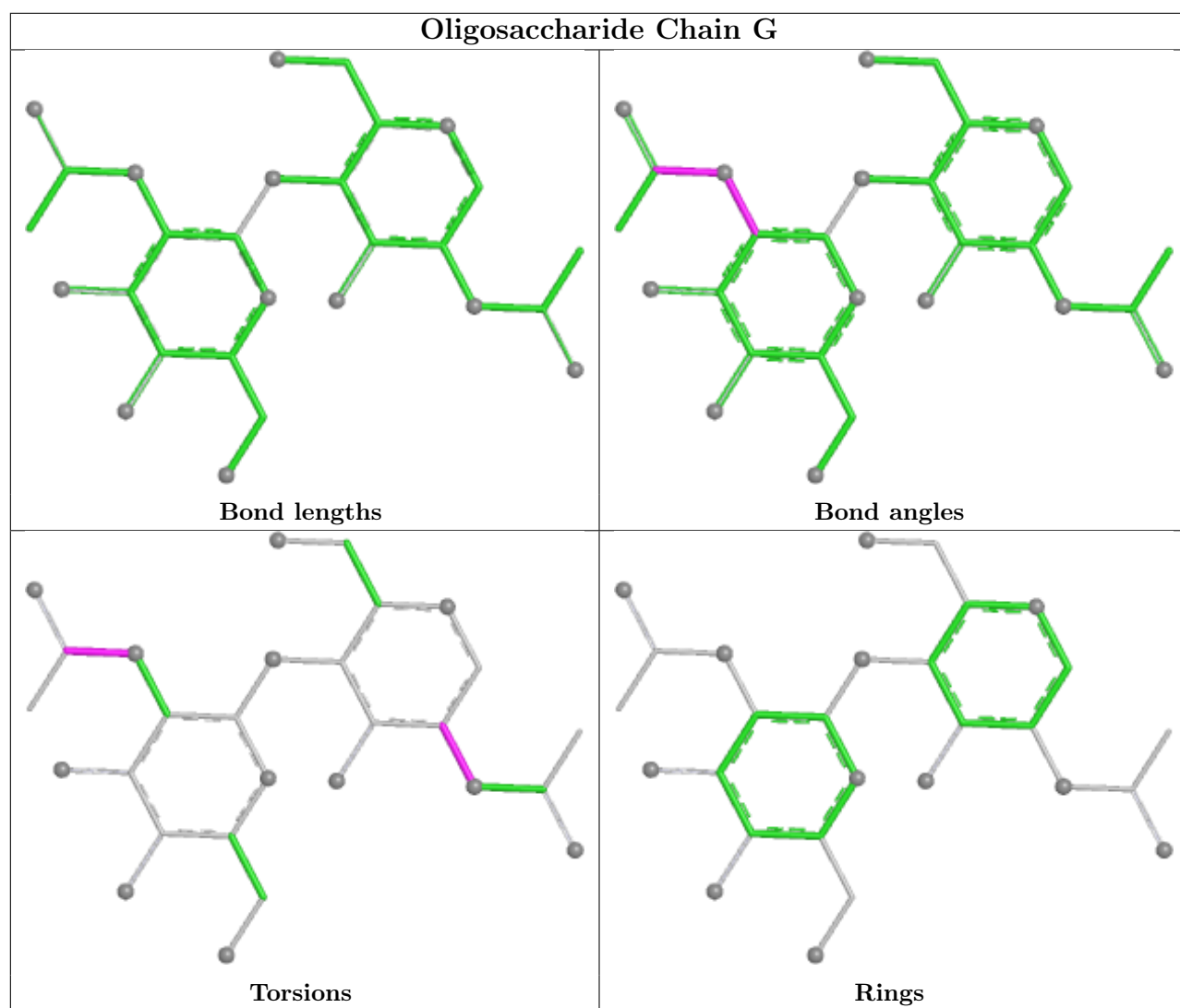


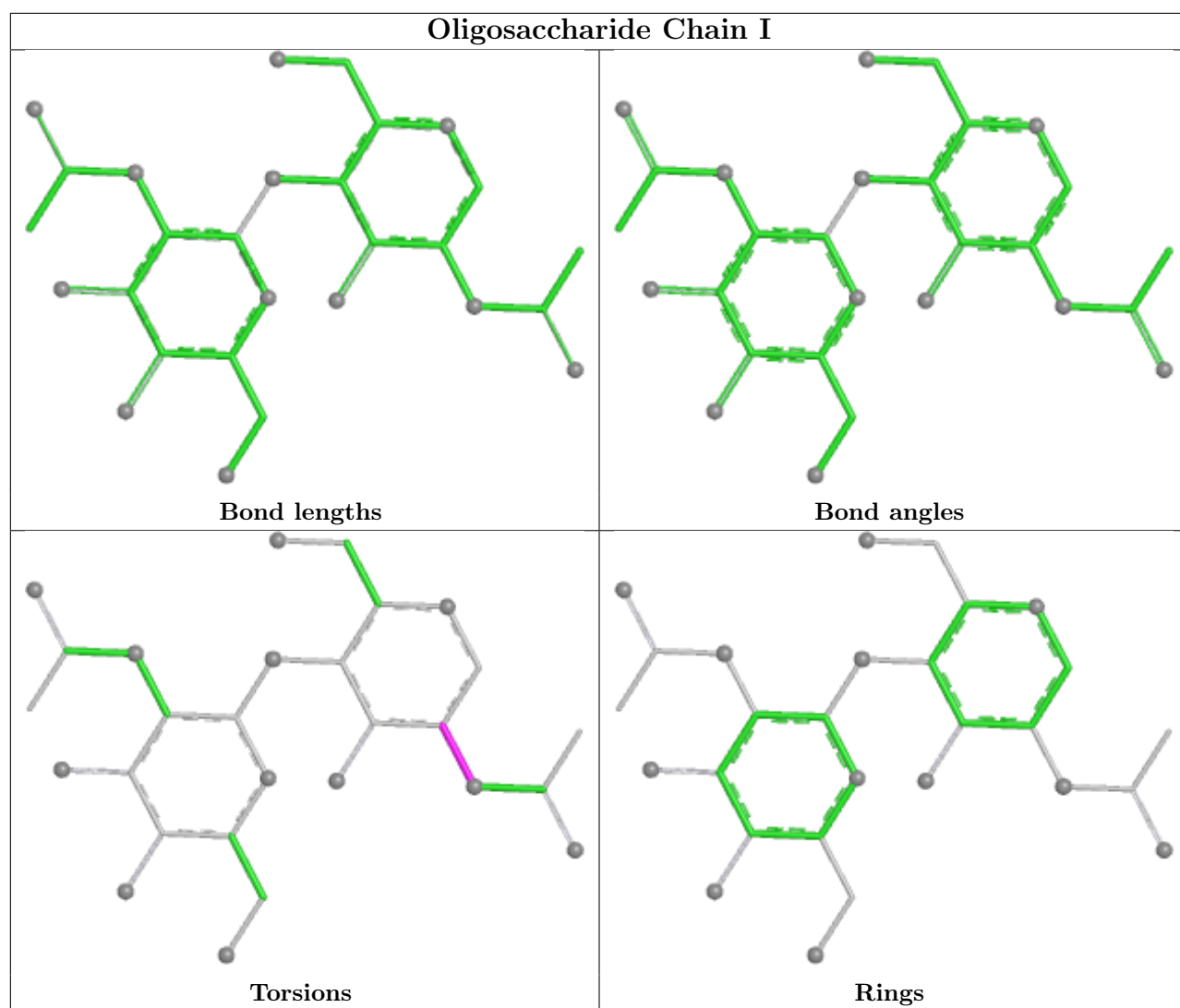


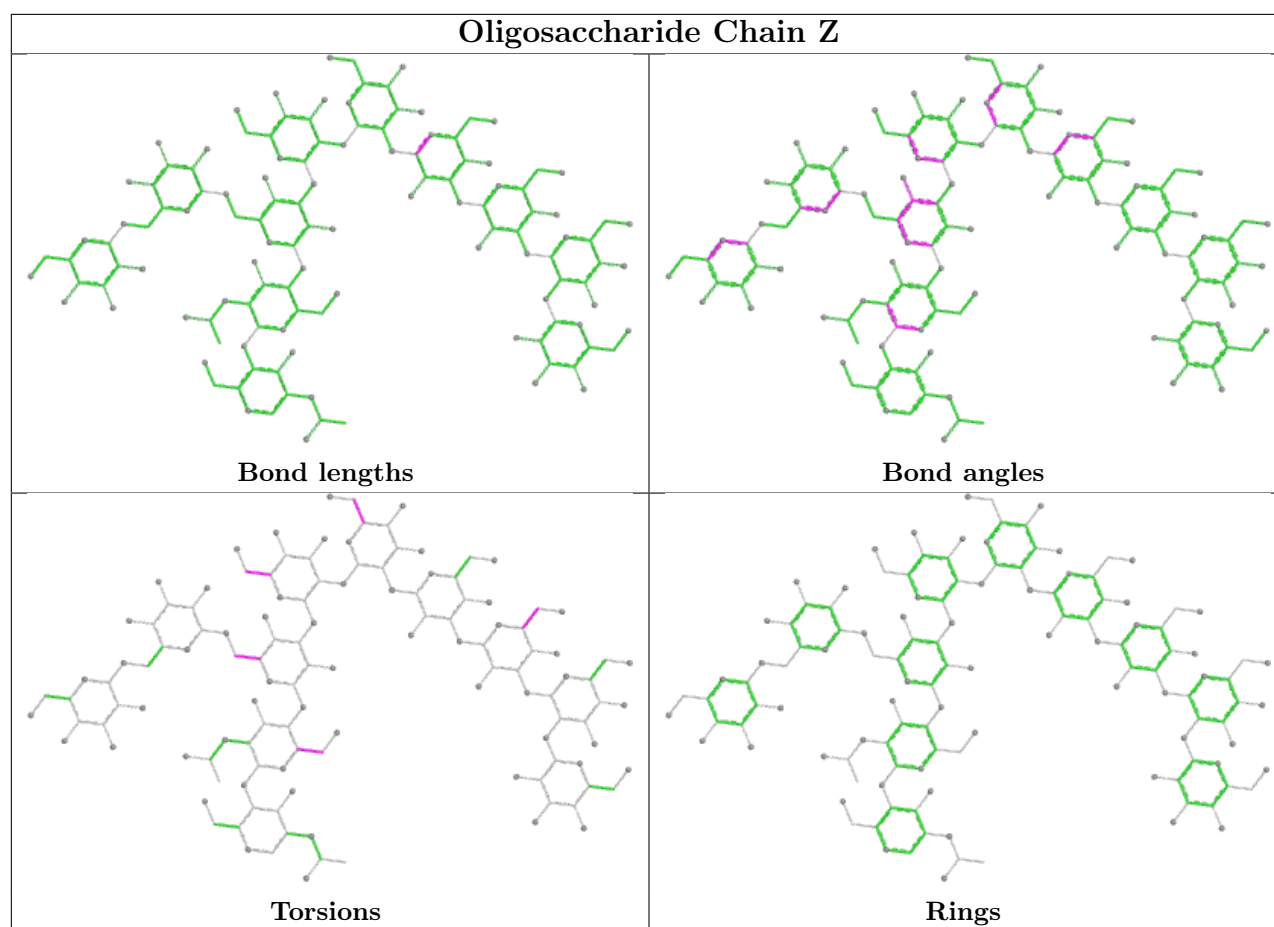












5.6 Ligand geometry [i](#)

47 ligands are modelled in this entry.

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	$\# Z > 2$
19	CLR	i	203	-	31,31,31	0.59	0	48,48,48	1.26	4 (8%)
19	CLR	l	202	-	31,31,31	0.43	0	48,48,48	1.11	5 (10%)
19	CLR	k	203	-	31,31,31	0.40	0	48,48,48	0.85	1 (2%)
19	CLR	o	203	-	31,31,31	0.40	0	48,48,48	1.21	3 (6%)
18	PTY	e	101	-	49,49,49	0.47	0	52,54,54	0.43	0
18	PTY	b	304	-	49,49,49	0.47	0	52,54,54	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLR	k	201	-	31,31,31	0.46	0	48,48,48	1.10	3 (6%)
19	CLR	o	202	-	31,31,31	0.47	0	48,48,48	1.10	4 (8%)
14	PC1	b	302	-	53,53,53	0.50	0	59,61,61	0.55	1 (1%)
19	CLR	b	305	-	31,31,31	0.39	0	48,48,48	0.65	0
14	PC1	P	501	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
18	PTY	p	402	-	49,49,49	0.47	0	52,54,54	0.43	0
19	CLR	m	203	-	31,31,31	0.38	0	48,48,48	0.80	0
19	CLR	m	202	-	31,31,31	0.48	0	48,48,48	1.10	3 (6%)
19	CLR	j	202	-	31,31,31	0.41	0	48,48,48	0.66	0
18	PTY	a	905	-	49,49,49	0.47	0	52,54,54	0.38	0
19	CLR	i	202	-	31,31,31	0.40	0	48,48,48	0.75	1 (2%)
19	CLR	h	202	-	31,31,31	0.40	0	48,48,48	1.02	3 (6%)
19	CLR	o	201	-	31,31,31	0.45	0	48,48,48	1.26	4 (8%)
15	WJP	a	901	-	32,33,34	1.85	8 (25%)	39,43,44	6.64	8 (20%)
19	CLR	n	201	-	31,31,31	0.36	0	48,48,48	0.83	2 (4%)
18	PTY	j	201	-	49,49,49	0.48	0	52,54,54	0.41	0
19	CLR	m	201	-	31,31,31	0.46	0	48,48,48	1.33	5 (10%)
19	CLR	i	204	-	31,31,31	0.39	0	48,48,48	0.74	1 (2%)
18	PTY	p	401	-	49,49,49	0.49	0	52,54,54	0.47	0
19	CLR	k	204	-	31,31,31	0.46	0	48,48,48	1.08	3 (6%)
19	CLR	h	201	-	31,31,31	0.42	0	48,48,48	1.34	3 (6%)
18	PTY	p	403	-	49,49,49	0.46	0	52,54,54	0.38	0
19	CLR	l	204	-	31,31,31	0.40	0	48,48,48	0.67	0
19	CLR	i	201	-	31,31,31	0.43	0	48,48,48	1.18	2 (4%)
19	CLR	j	204	-	31,31,31	0.44	0	48,48,48	0.80	2 (4%)
14	PC1	l	201	-	53,53,53	0.50	0	59,61,61	0.51	1 (1%)
18	PTY	a	906	-	49,49,49	0.47	0	52,54,54	0.38	0
19	CLR	n	203	-	31,31,31	0.46	0	48,48,48	1.19	3 (6%)
17	LP3	a	903	-	34,34,34	0.52	0	39,41,41	0.54	0
19	CLR	m	204	-	31,31,31	0.42	0	48,48,48	0.87	2 (4%)
19	CLR	n	204	-	31,31,31	0.38	0	48,48,48	0.96	2 (4%)
19	CLR	j	203	-	31,31,31	0.42	0	48,48,48	0.94	4 (8%)
14	PC1	a	904	-	53,53,53	0.50	0	59,61,61	0.47	1 (1%)
19	CLR	n	202	-	31,31,31	0.41	0	48,48,48	0.87	0
18	PTY	b	303	-	49,49,49	0.48	0	52,54,54	0.41	0
19	CLR	l	203	-	31,31,31	0.43	0	48,48,48	1.00	2 (4%)
19	CLR	j	205	-	31,31,31	0.39	0	48,48,48	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLR	m	205	-	31,31,31	0.40	0	48,48,48	1.11	4 (8%)
16	NAG	a	902	4	14,14,15	0.72	0	17,19,21	1.46	2 (11%)
14	PC1	b	301	-	53,53,53	0.51	0	59,61,61	0.49	1 (1%)
19	CLR	k	202	-	31,31,31	0.41	0	48,48,48	0.99	2 (4%)

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
19	CLR	i	203	-	-	6/10/68/68	0/4/4/4
19	CLR	l	202	-	-	9/10/68/68	0/4/4/4
19	CLR	k	203	-	-	2/10/68/68	0/4/4/4
19	CLR	o	203	-	-	6/10/68/68	0/4/4/4
18	PTY	e	101	-	-	21/53/53/53	-
18	PTY	b	304	-	-	23/53/53/53	-
19	CLR	k	201	-	-	5/10/68/68	0/4/4/4
19	CLR	o	202	-	-	8/10/68/68	0/4/4/4
14	PC1	b	302	-	-	20/57/57/57	-
19	CLR	b	305	-	-	10/10/68/68	0/4/4/4
14	PC1	P	501	-	-	19/57/57/57	-
18	PTY	p	402	-	-	24/53/53/53	-
19	CLR	m	203	-	-	5/10/68/68	0/4/4/4
19	CLR	m	202	-	-	5/10/68/68	0/4/4/4
19	CLR	j	202	-	-	4/10/68/68	0/4/4/4
18	PTY	a	905	-	-	19/53/53/53	-
19	CLR	i	202	-	-	5/10/68/68	0/4/4/4
19	CLR	h	202	-	-	7/10/68/68	0/4/4/4
19	CLR	o	201	-	-	8/10/68/68	0/4/4/4
15	WJP	a	901	-	-	11/37/37/40	-
19	CLR	n	201	-	-	3/10/68/68	0/4/4/4
18	PTY	j	201	-	-	23/53/53/53	-
19	CLR	m	201	-	-	4/10/68/68	0/4/4/4
19	CLR	i	204	-	-	9/10/68/68	0/4/4/4
18	PTY	p	401	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLR	k	204	-	-	7/10/68/68	0/4/4/4
19	CLR	h	201	-	-	6/10/68/68	0/4/4/4
18	PTY	p	403	-	-	27/53/53/53	-
19	CLR	l	204	-	-	9/10/68/68	0/4/4/4
19	CLR	i	201	-	-	10/10/68/68	0/4/4/4
19	CLR	j	204	-	-	8/10/68/68	0/4/4/4
14	PC1	l	201	-	-	21/57/57/57	-
18	PTY	a	906	-	-	18/53/53/53	-
19	CLR	n	203	-	-	8/10/68/68	0/4/4/4
17	LP3	a	903	-	-	14/36/36/36	-
19	CLR	m	204	-	-	5/10/68/68	0/4/4/4
19	CLR	n	204	-	-	9/10/68/68	0/4/4/4
19	CLR	j	203	-	-	7/10/68/68	0/4/4/4
14	PC1	a	904	-	-	22/57/57/57	-
19	CLR	n	202	-	-	3/10/68/68	0/4/4/4
18	PTY	b	303	-	-	24/53/53/53	-
19	CLR	l	203	-	-	3/10/68/68	0/4/4/4
19	CLR	j	205	-	-	4/10/68/68	0/4/4/4
19	CLR	m	205	-	-	5/10/68/68	0/4/4/4
16	NAG	a	902	4	-	2/6/23/26	0/1/1/1
14	PC1	b	301	-	-	25/57/57/57	-
19	CLR	k	202	-	-	7/10/68/68	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	901	WJP	P27-O30	5.01	1.64	1.59
15	a	901	WJP	C18-C16	3.50	1.58	1.51
15	a	901	WJP	C07-C06	3.18	1.58	1.50
15	a	901	WJP	P31-O32	3.11	1.66	1.54
15	a	901	WJP	C17-C16	2.96	1.57	1.50

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	901	WJP	C08-C06-C05	20.56	167.33	121.17
15	a	901	WJP	C17-C16-C18	-19.86	80.75	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	901	WJP	C18-C16-C15	-17.24	82.46	121.17
15	a	901	WJP	C17-C16-C15	15.39	163.16	123.63
15	a	901	WJP	C07-C06-C08	-15.17	88.89	115.23

There are no chirality outliers.

5 of 522 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	P	501	PC1	C11-O13-P-O12
14	P	501	PC1	C11-O13-P-O11
14	P	501	PC1	C1-O11-P-O14
14	P	501	PC1	O22-C21-O21-C2
14	a	904	PC1	C11-O13-P-O11

There are no ring outliers.

32 monomers are involved in 57 short contacts:

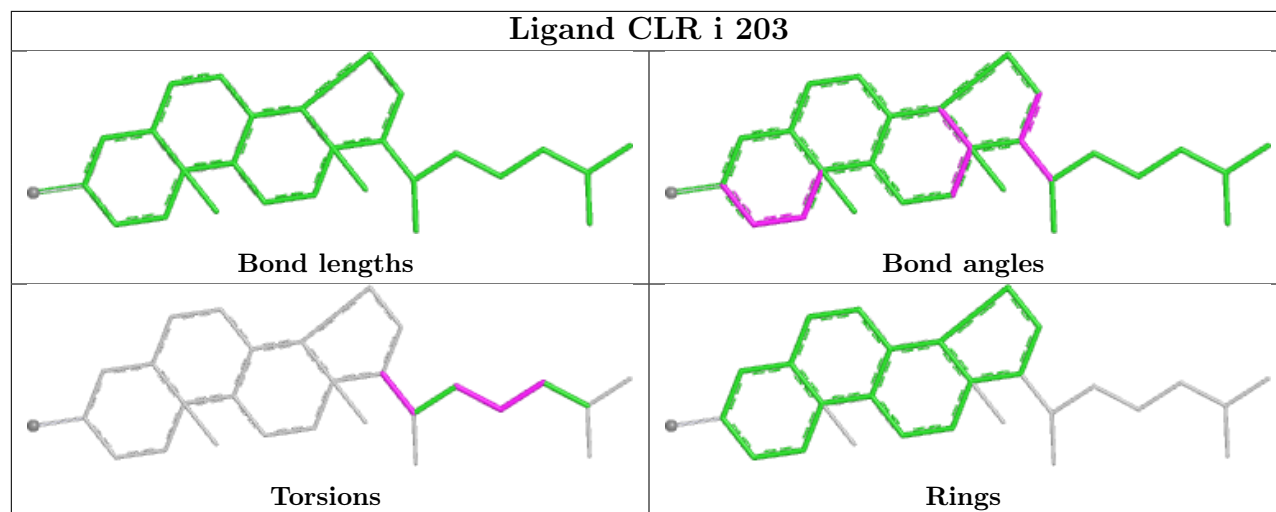
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	i	203	CLR	5	0
19	k	203	CLR	1	0
19	o	203	CLR	1	0
18	e	101	PTY	1	0
19	o	202	CLR	4	0
14	b	302	PC1	1	0
19	b	305	CLR	1	0
14	P	501	PC1	3	0
19	m	203	CLR	1	0
19	j	202	CLR	2	0
19	i	202	CLR	2	0
19	h	202	CLR	2	0
19	o	201	CLR	1	0
15	a	901	WJP	2	0
19	n	201	CLR	3	0
19	m	201	CLR	3	0
19	i	204	CLR	3	0
18	p	401	PTY	2	0
19	k	204	CLR	1	0
19	h	201	CLR	3	0
19	l	204	CLR	2	0
19	i	201	CLR	3	0
19	j	204	CLR	2	0

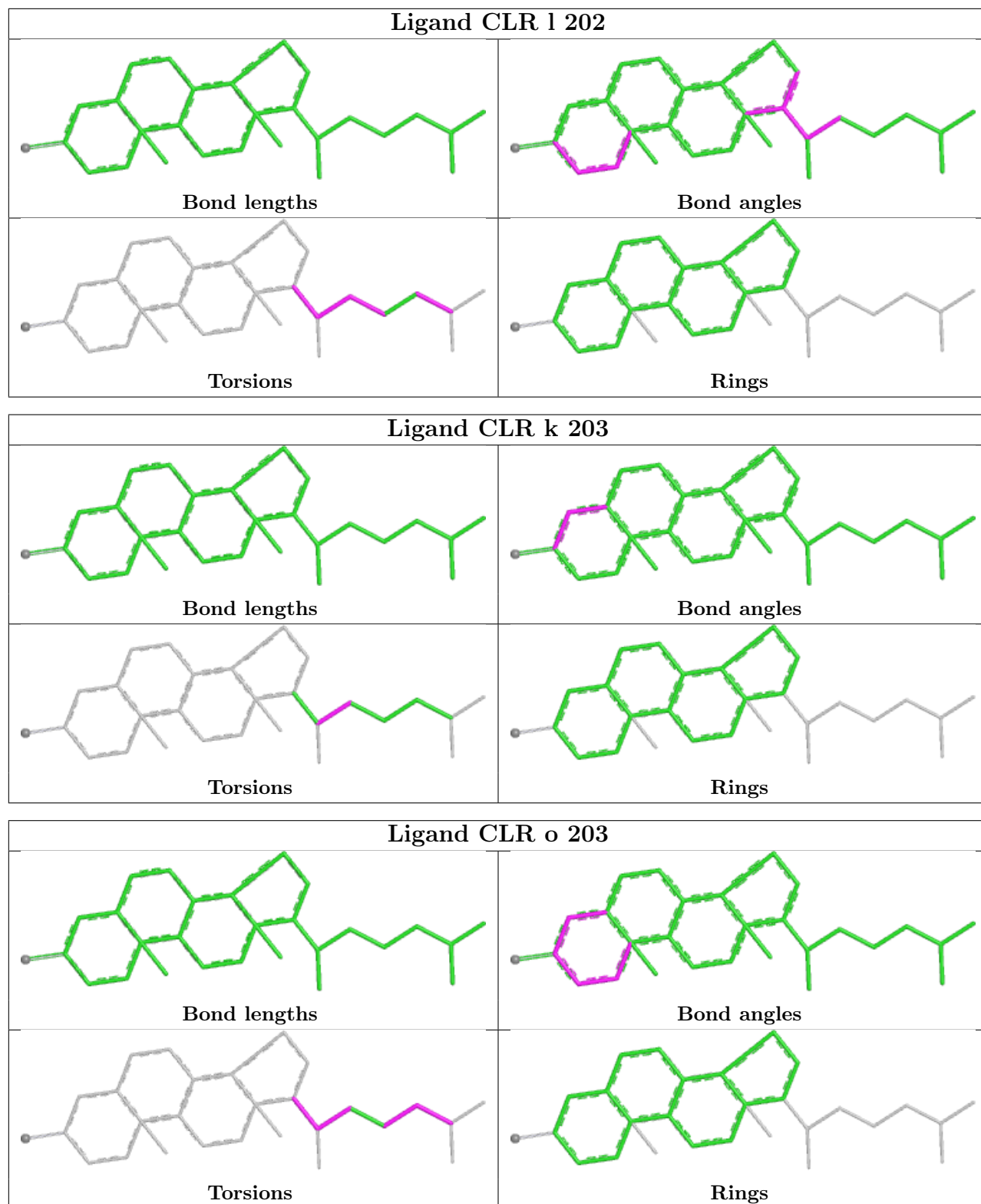
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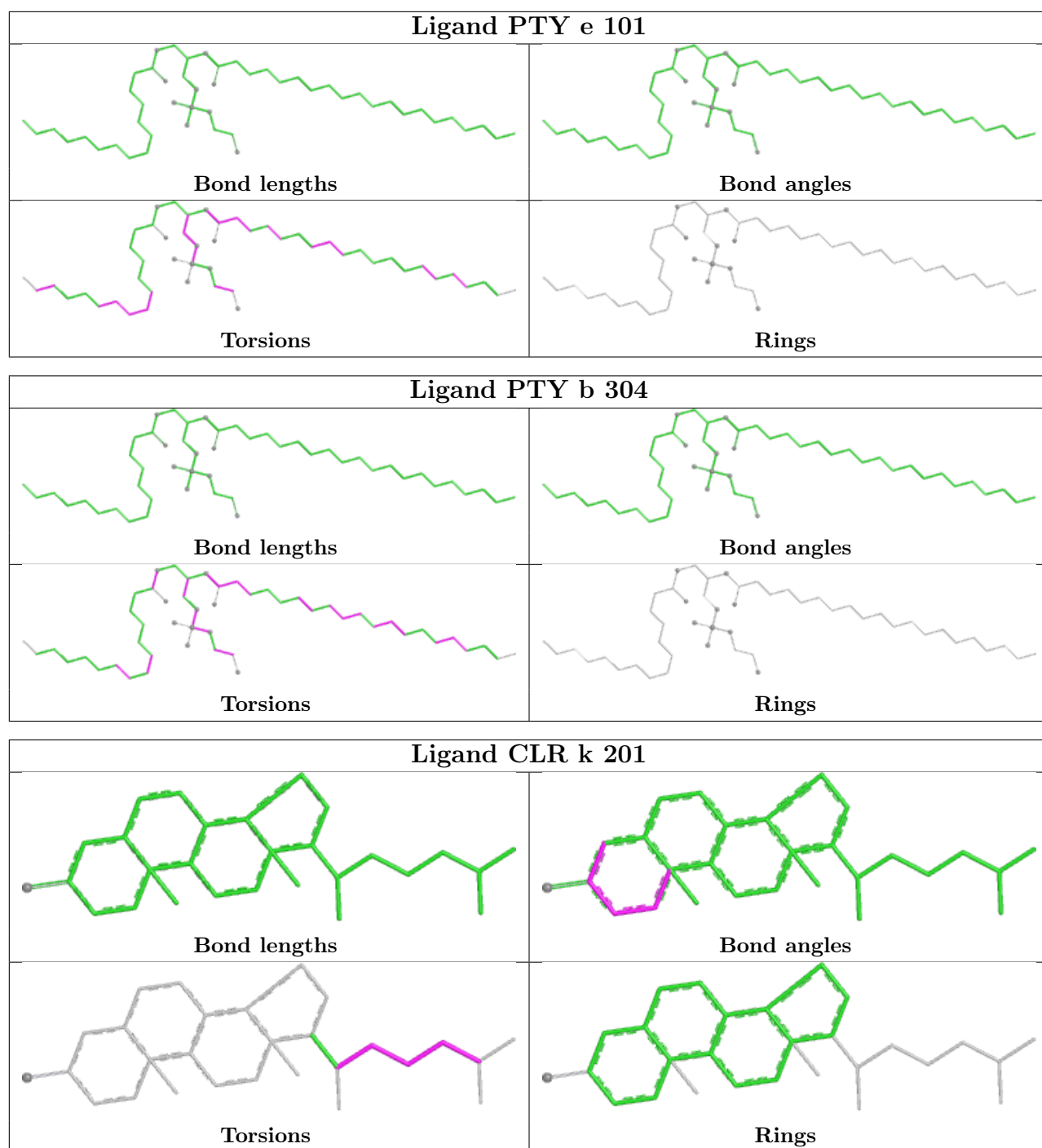
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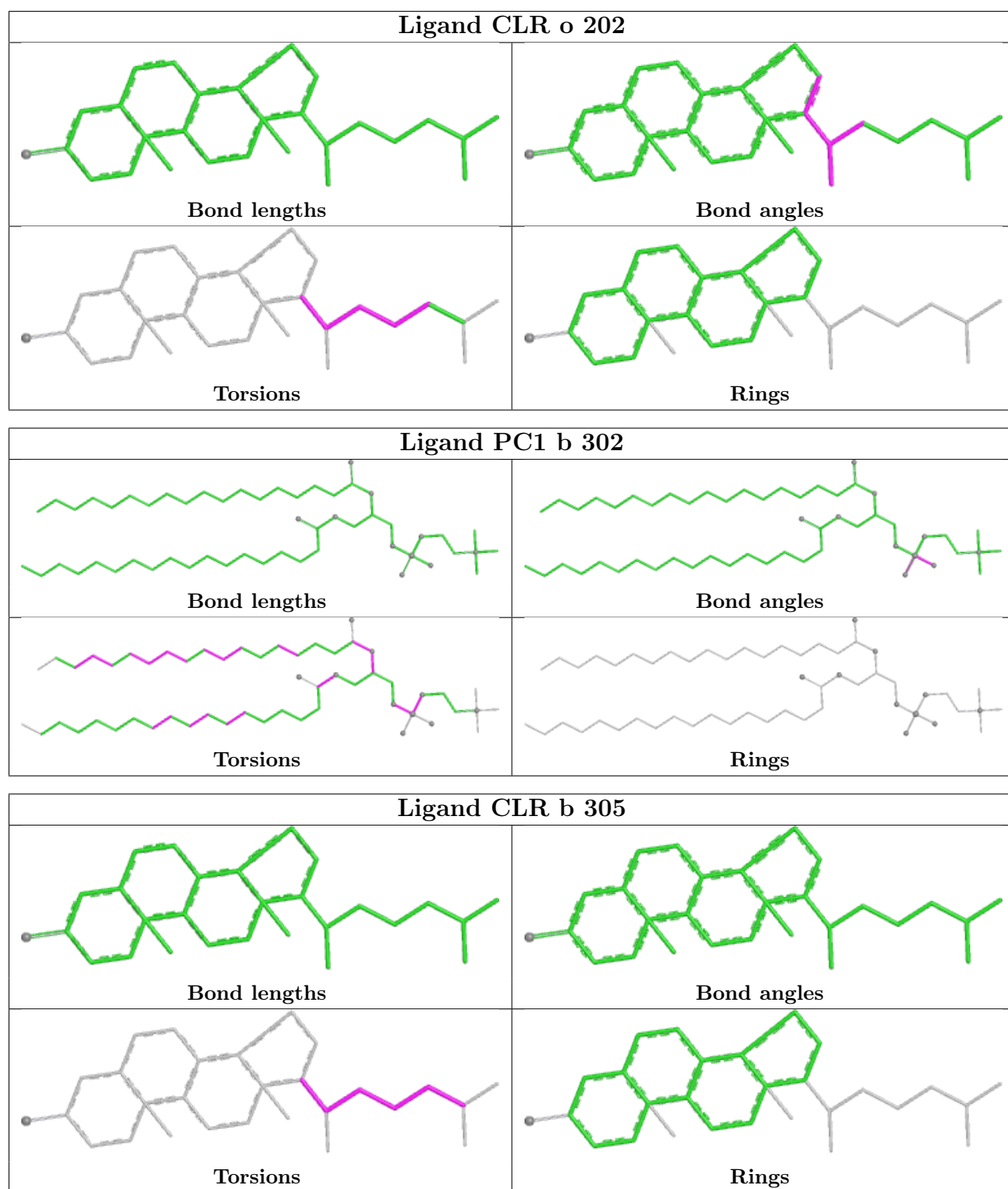
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	906	PTY	1	0
19	n	204	CLR	6	0
19	j	203	CLR	2	0
19	n	202	CLR	2	0
18	b	303	PTY	1	0
19	l	203	CLR	4	0
19	j	205	CLR	1	0
14	b	301	PC1	1	0
19	k	202	CLR	2	0

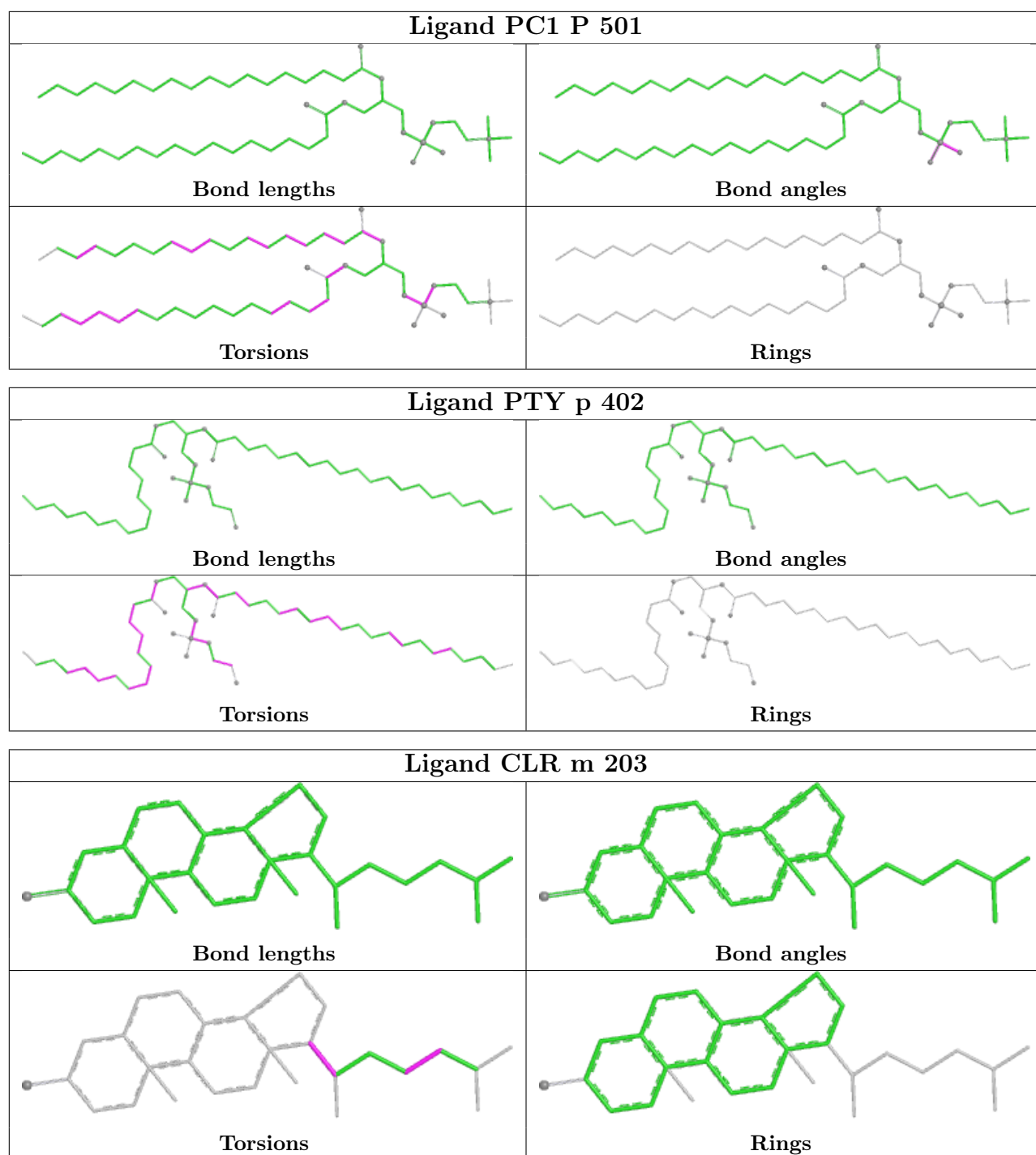
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

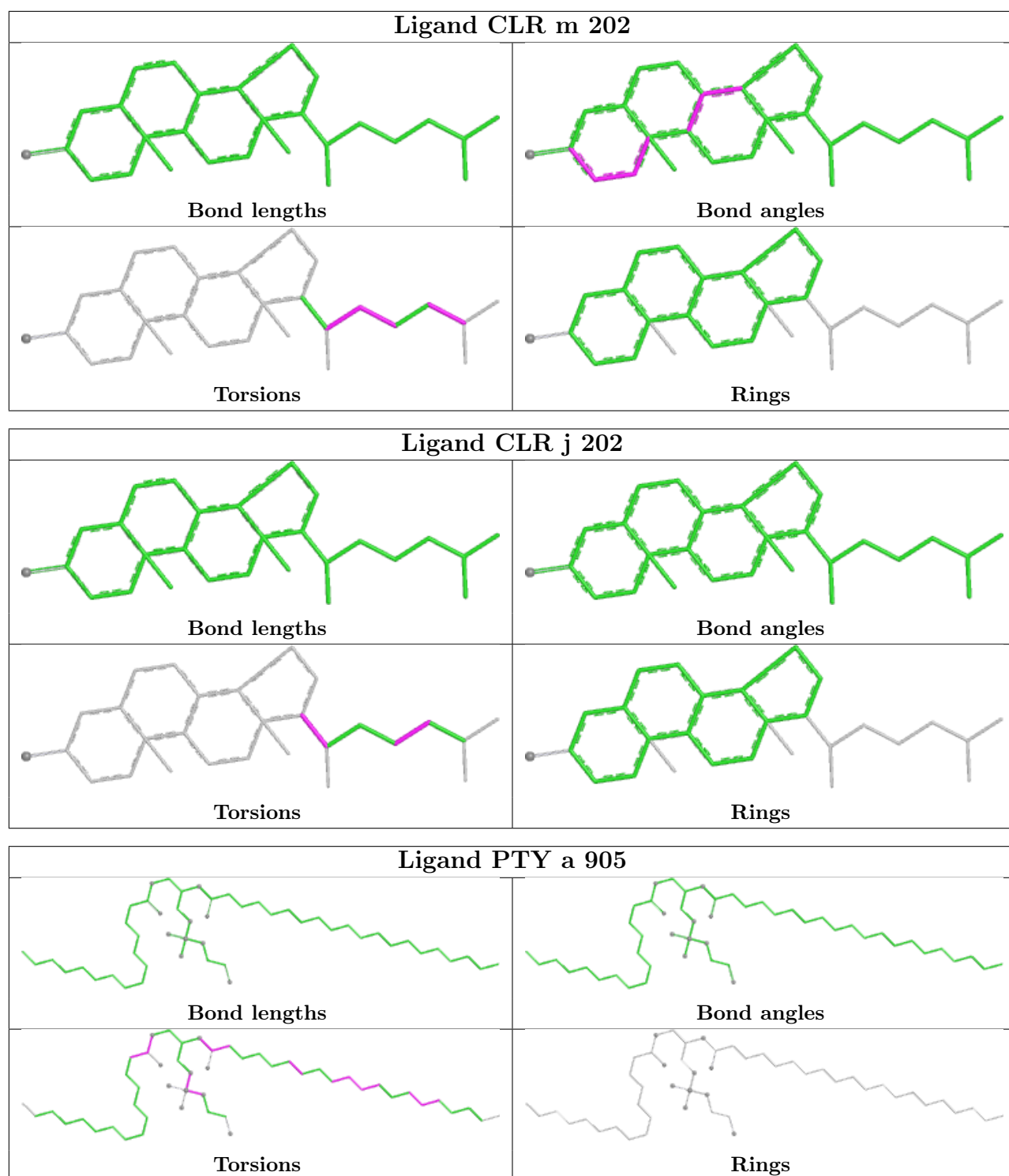


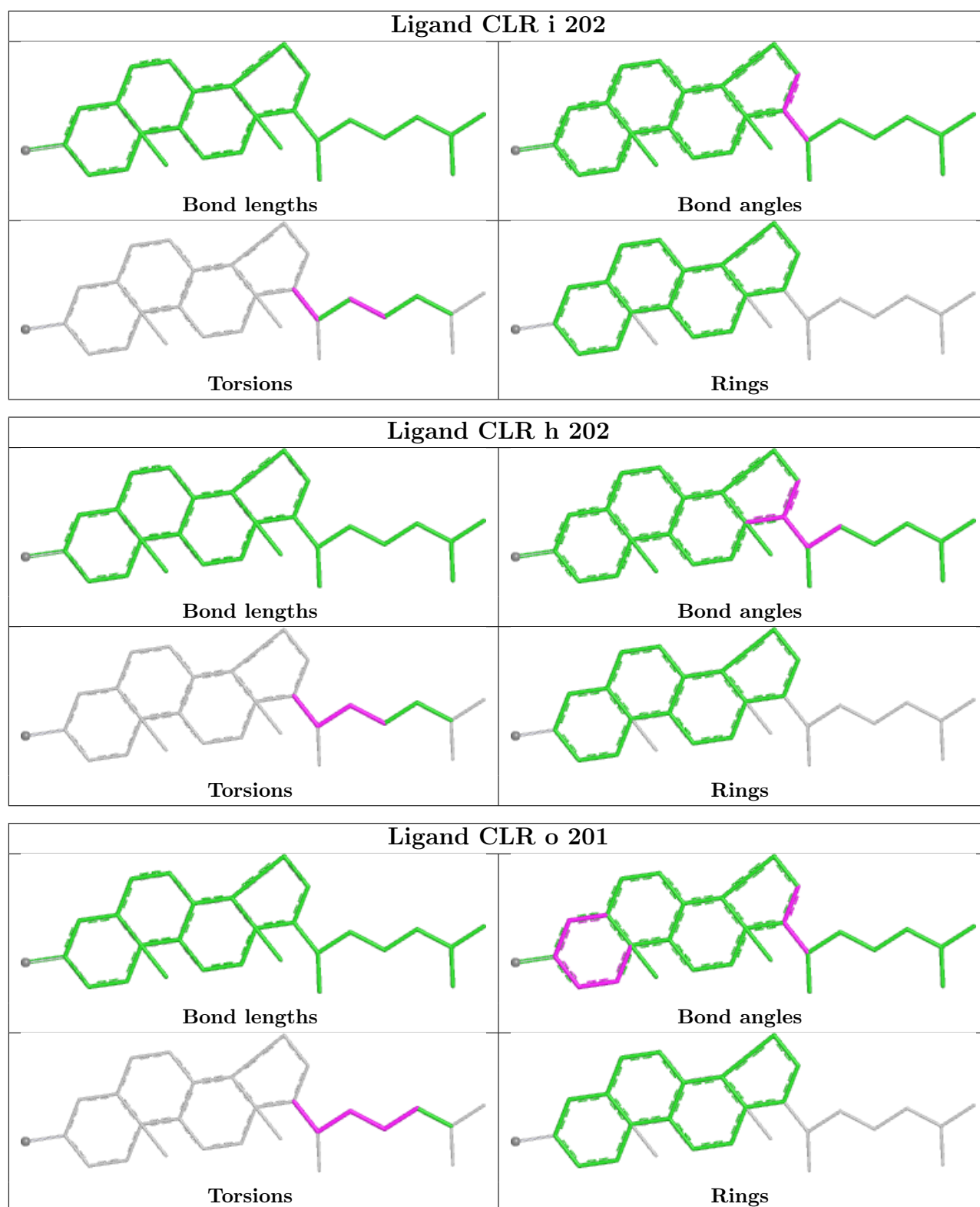


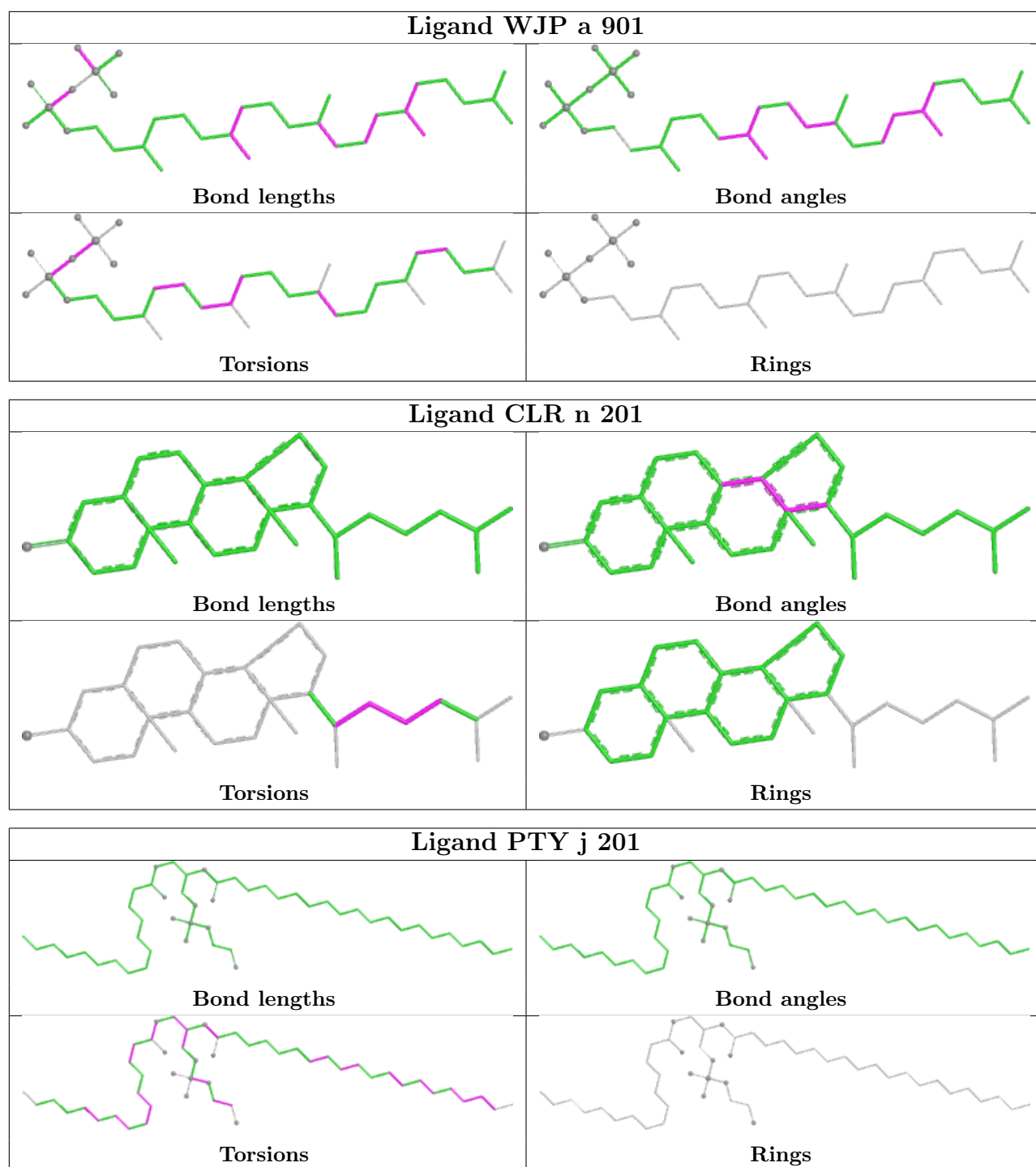


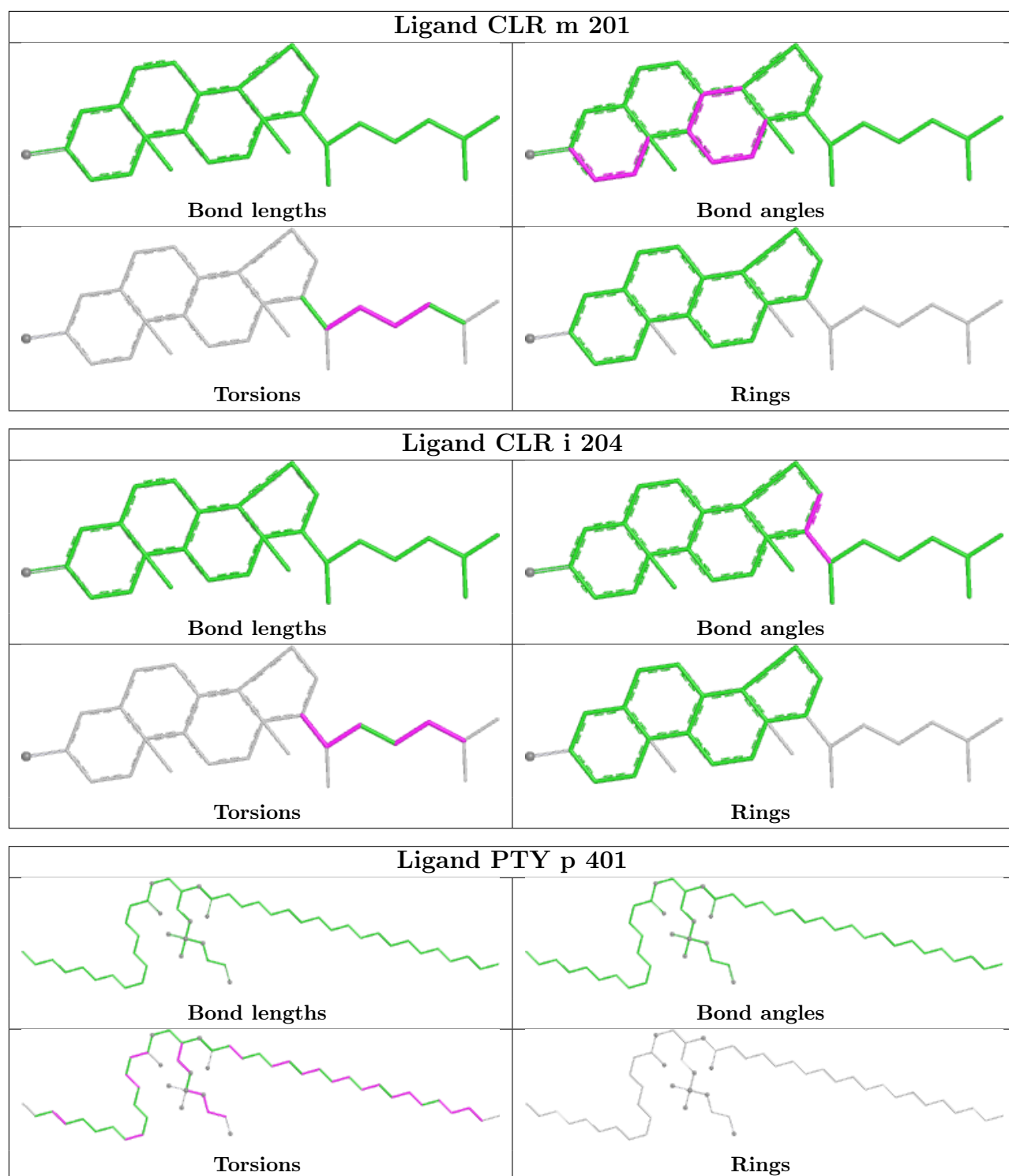


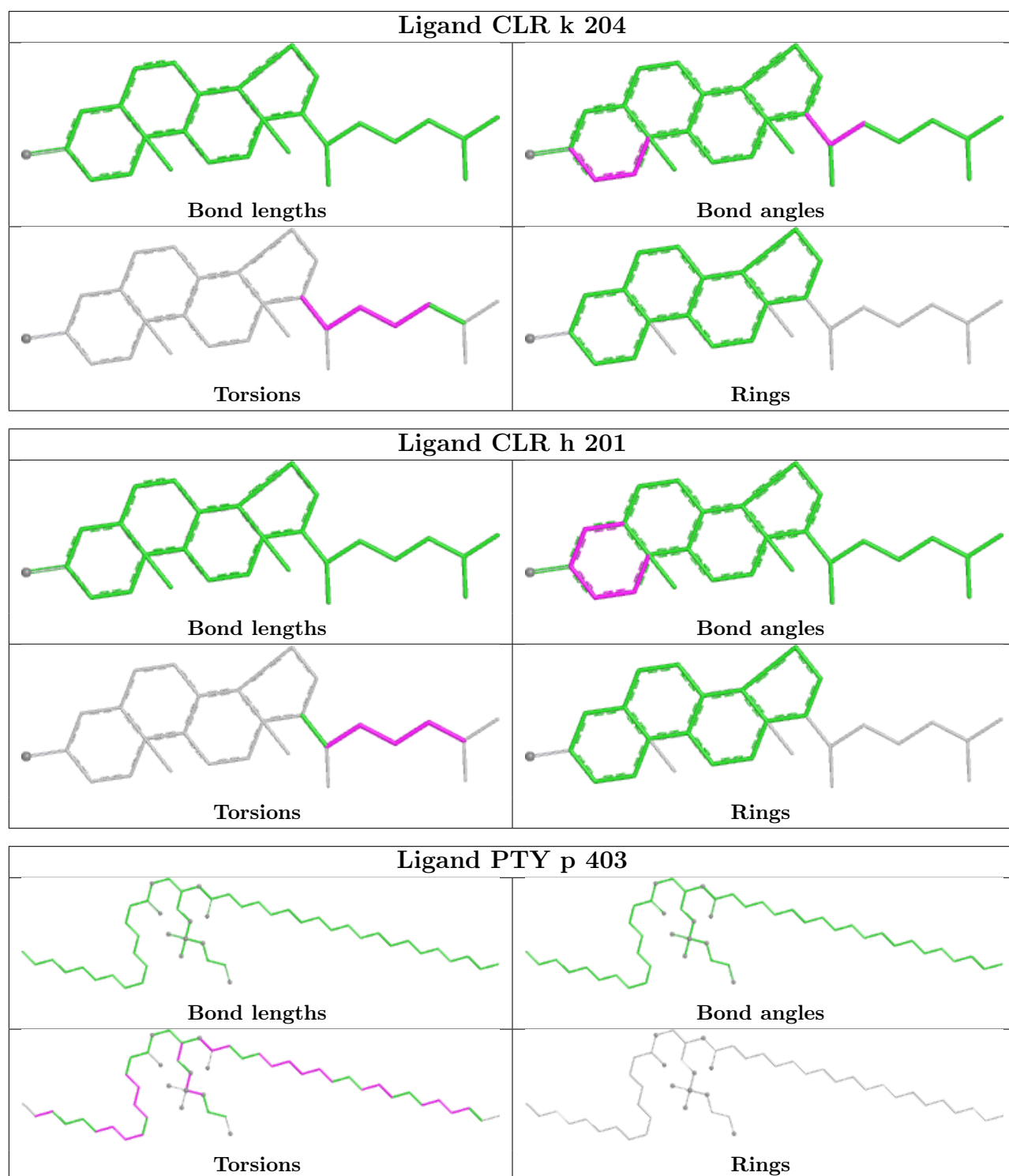


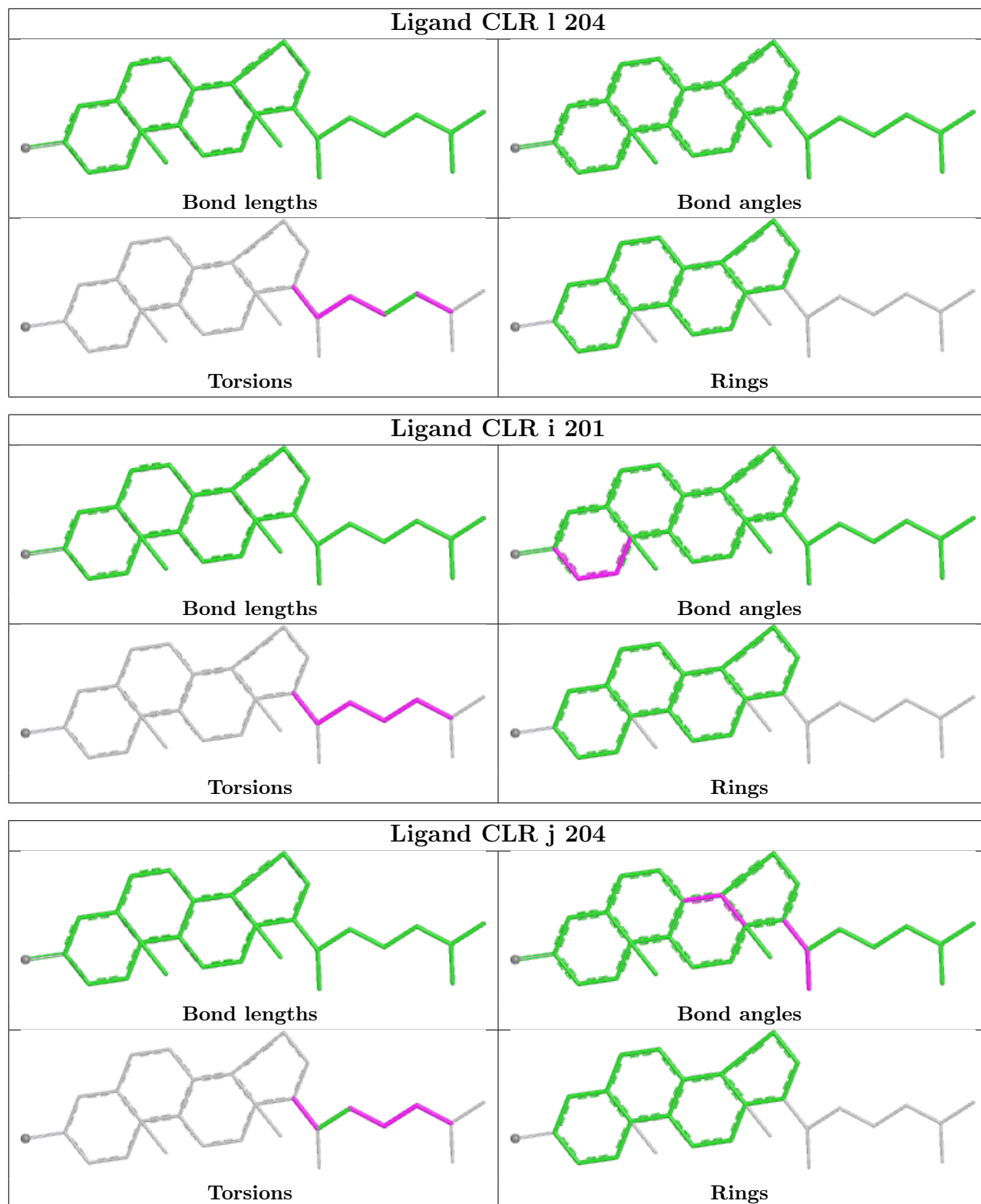


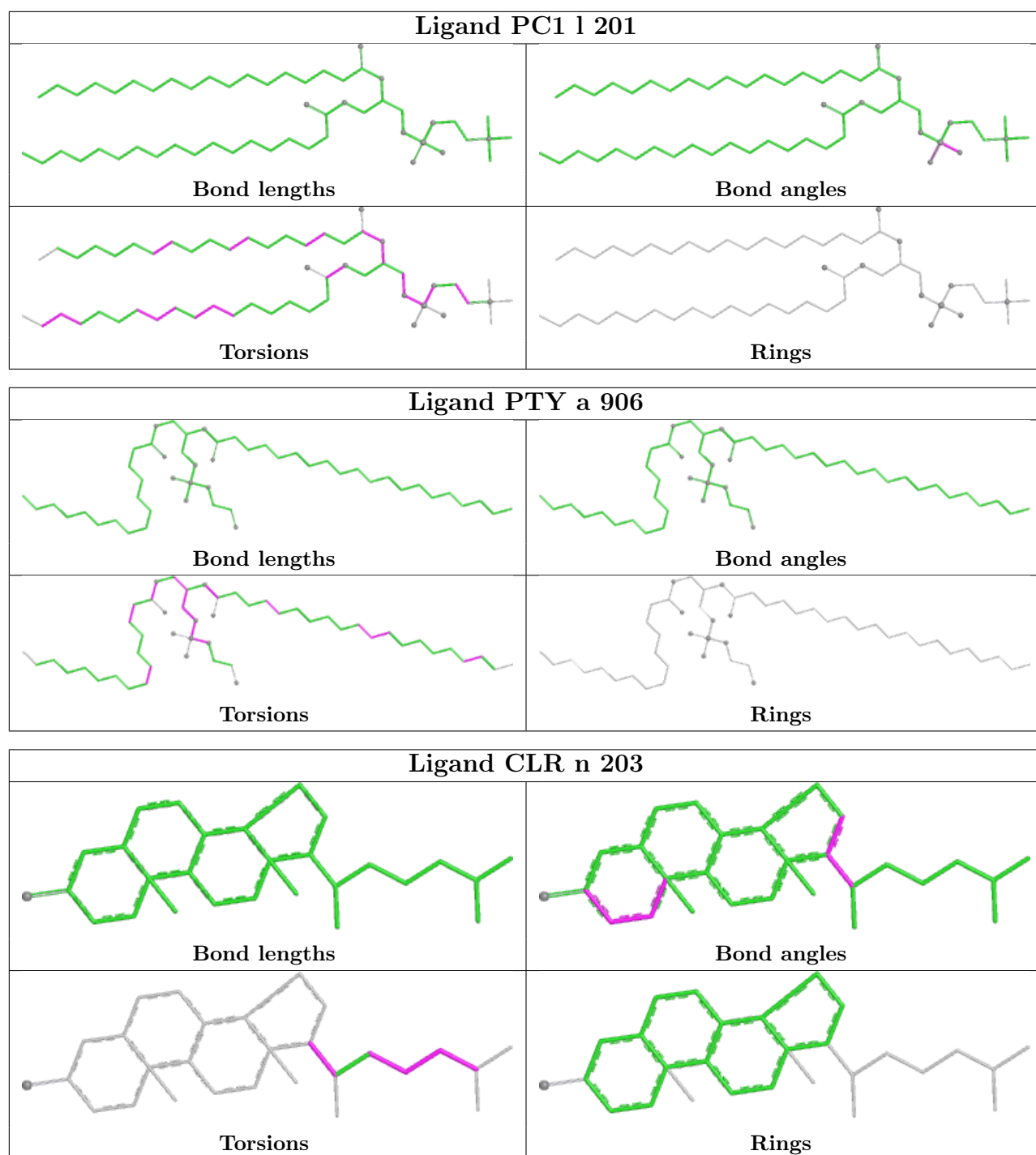


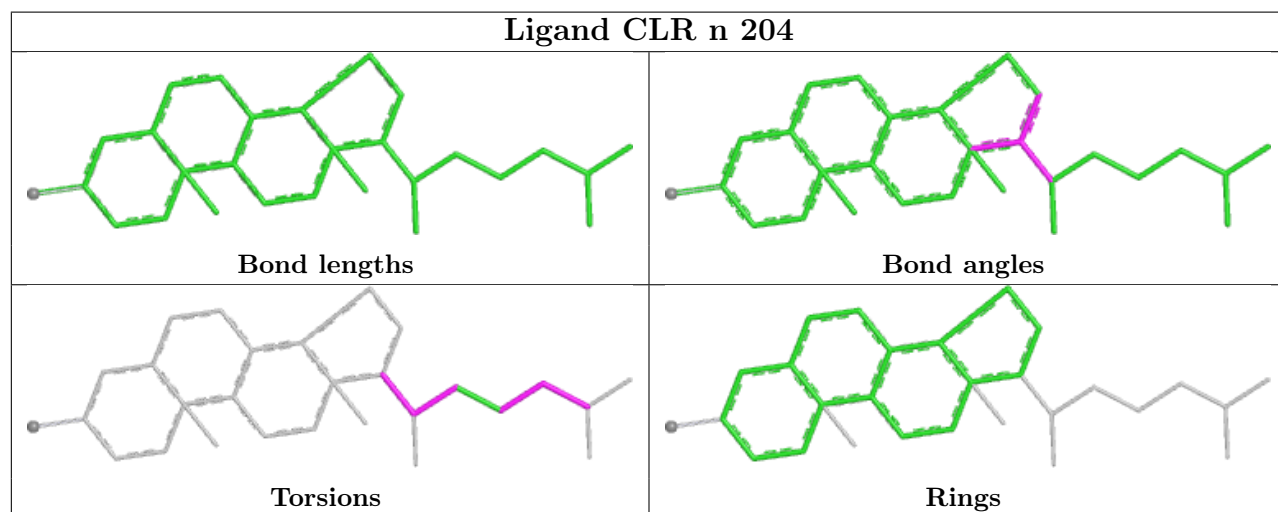
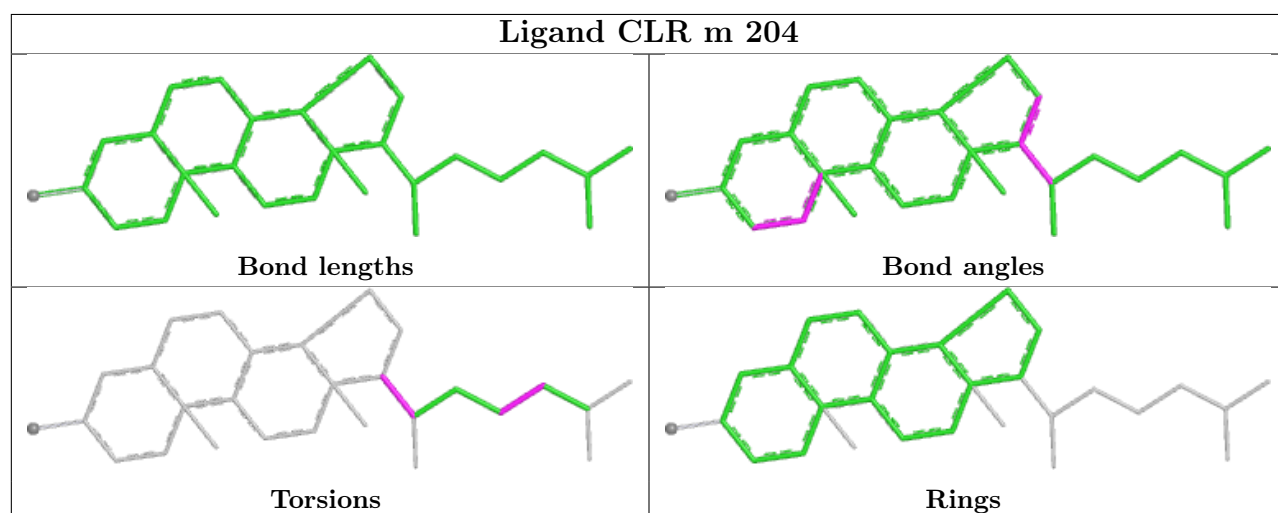
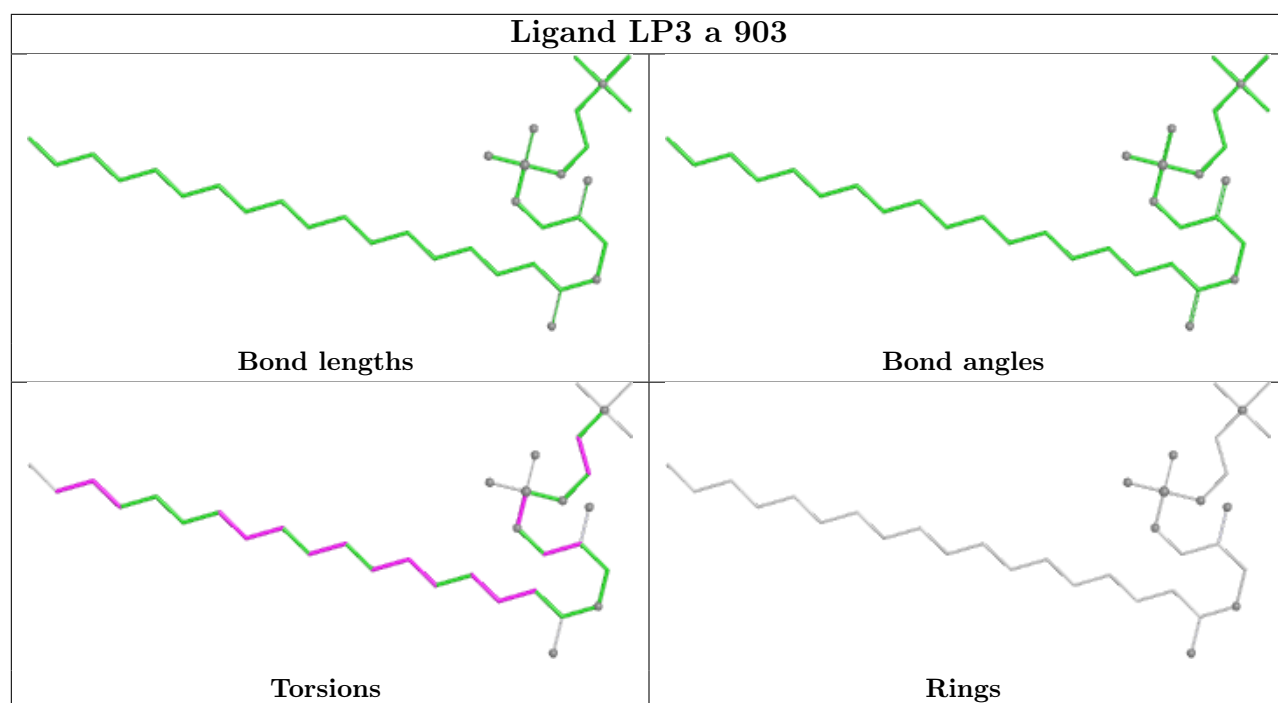


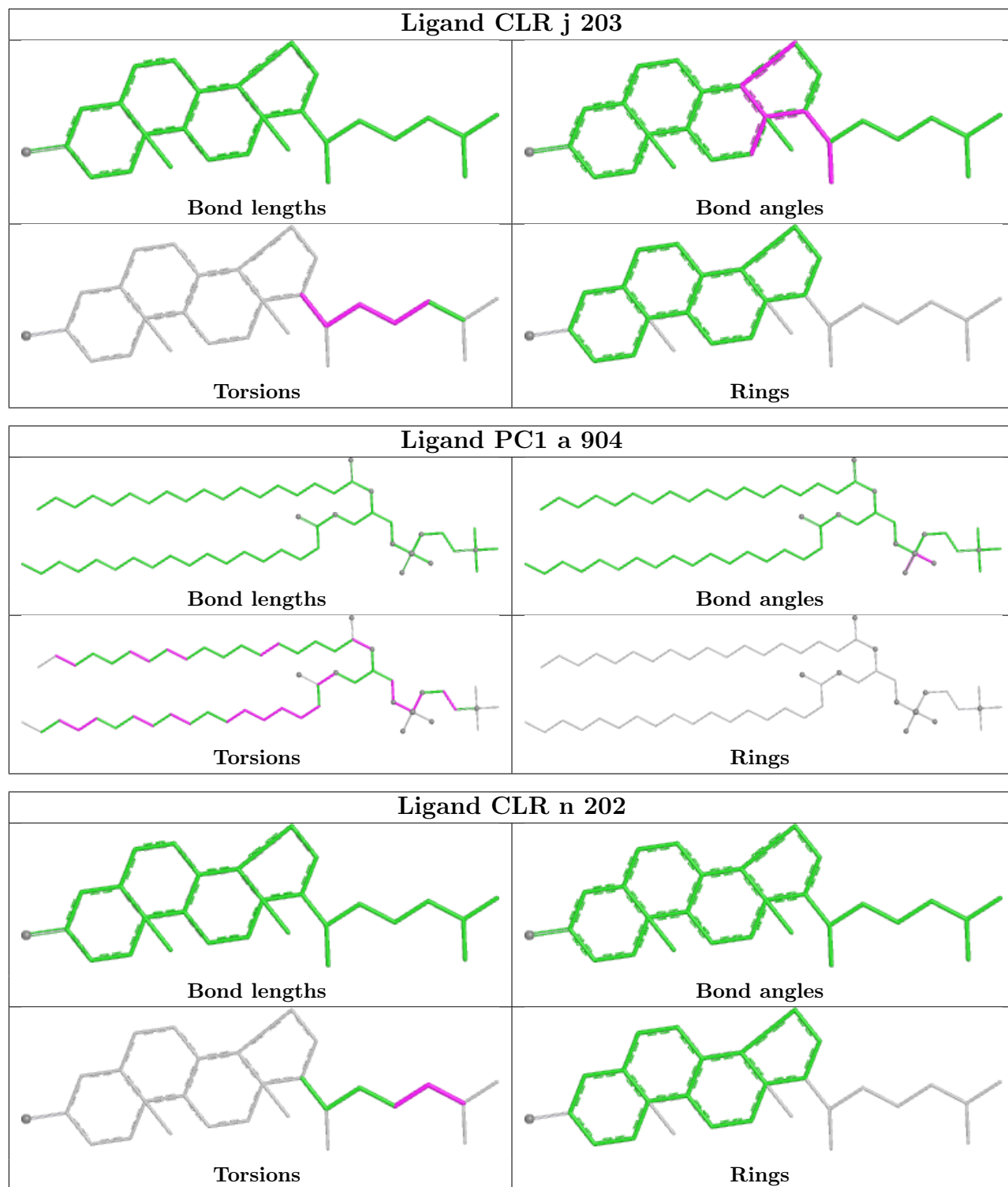


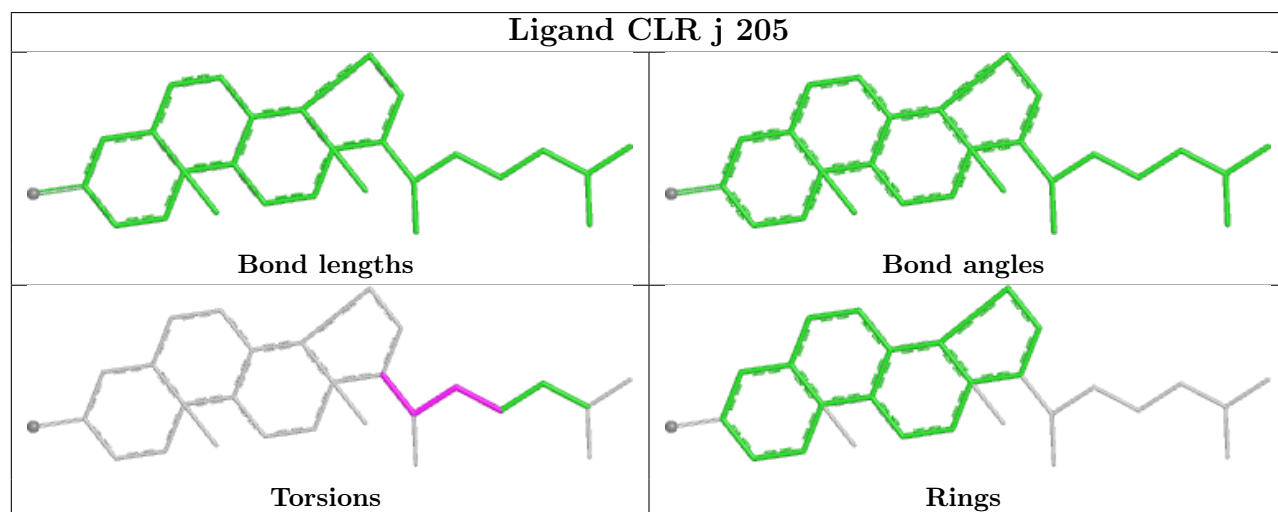
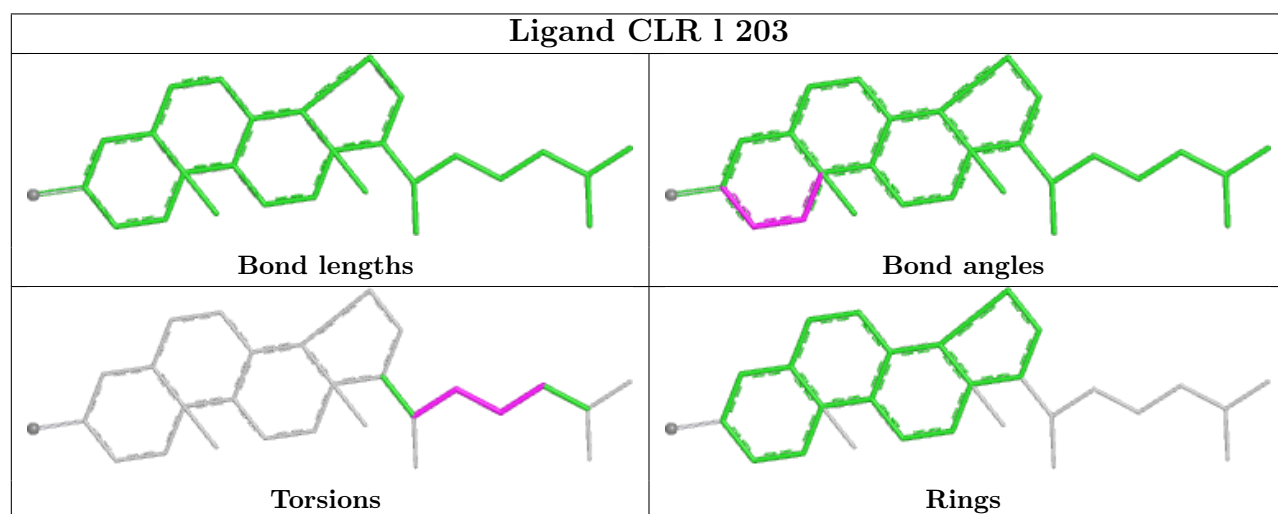
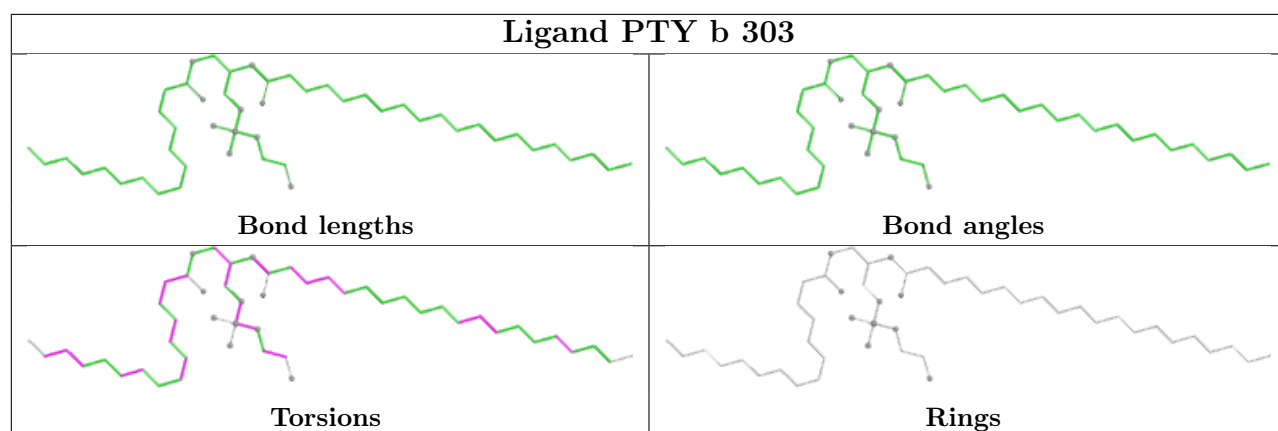


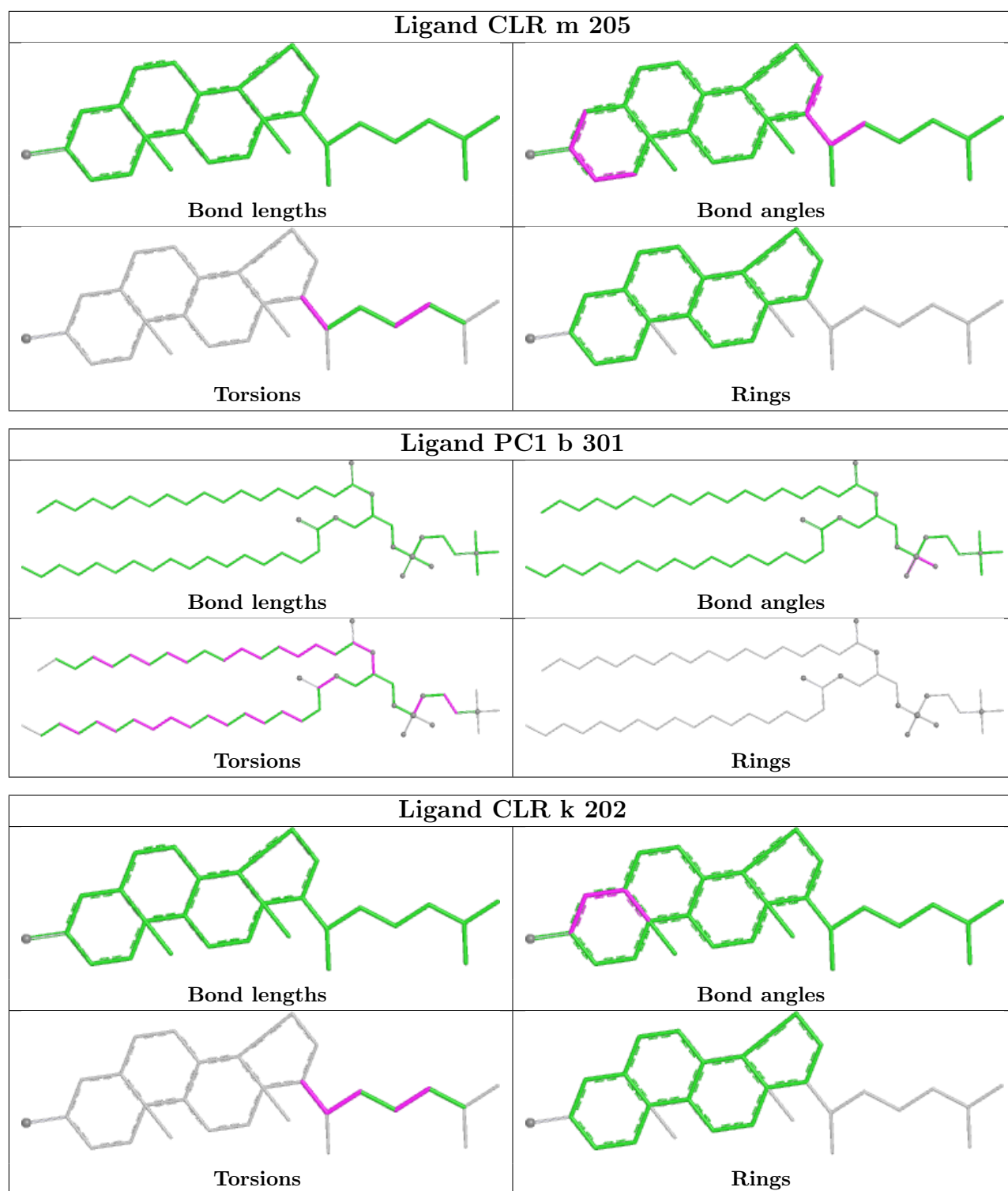












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

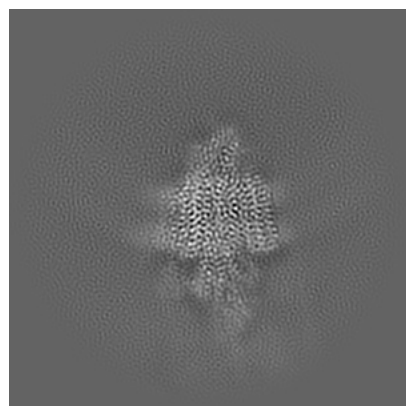
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44350. These allow visual inspection of the internal detail of the map and identification of artifacts.

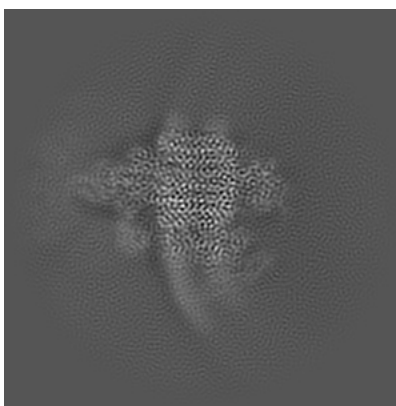
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

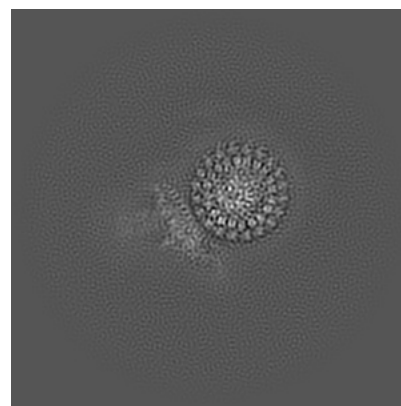
6.1.1 Primary map



X

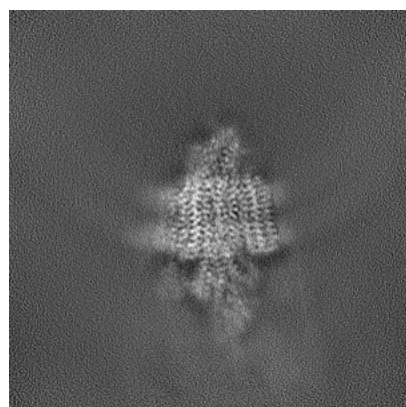


Y

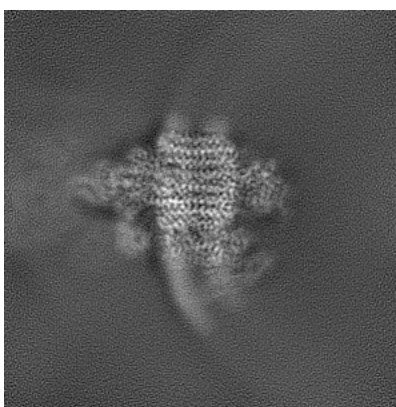


Z

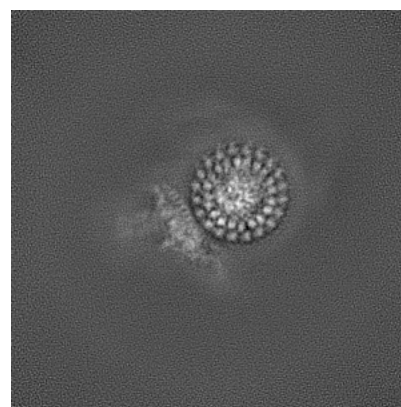
6.1.2 Raw map



X



Y

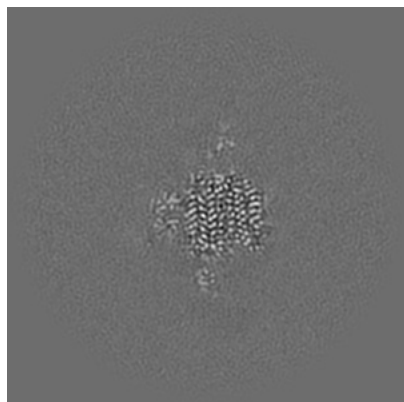


Z

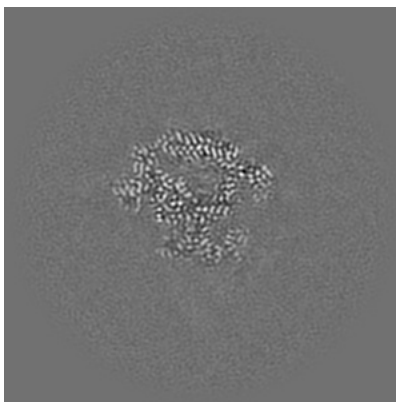
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

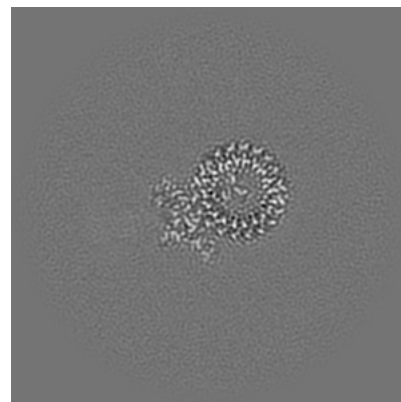
6.2.1 Primary map



X Index: 150

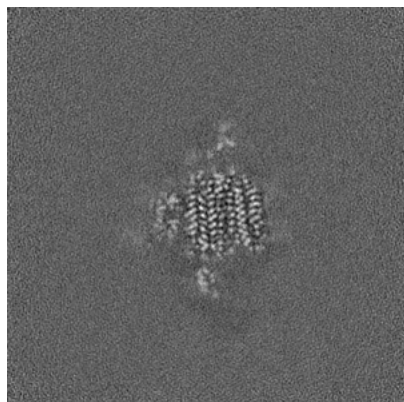


Y Index: 150

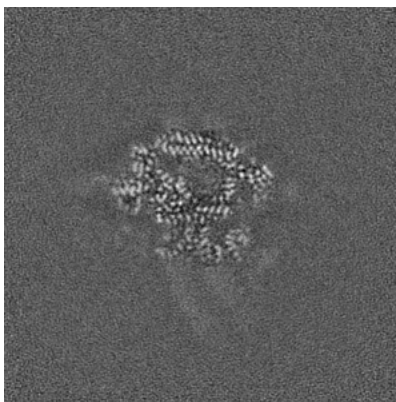


Z Index: 150

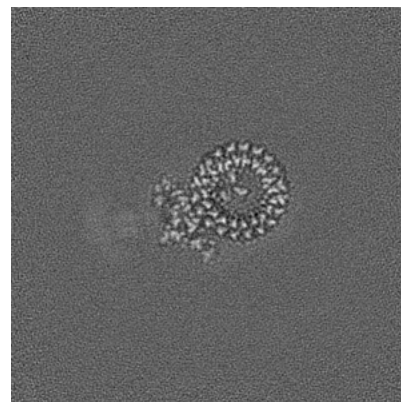
6.2.2 Raw map



X Index: 150



Y Index: 150

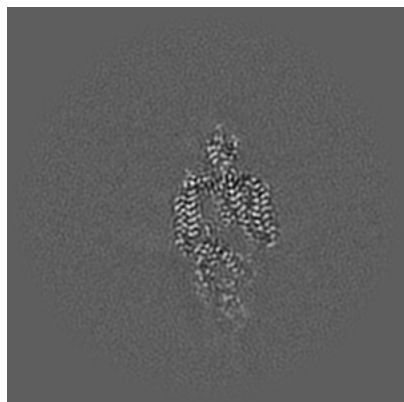


Z Index: 150

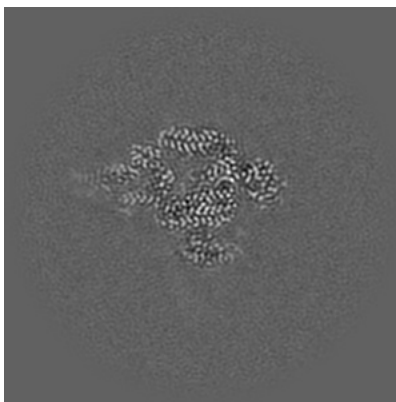
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

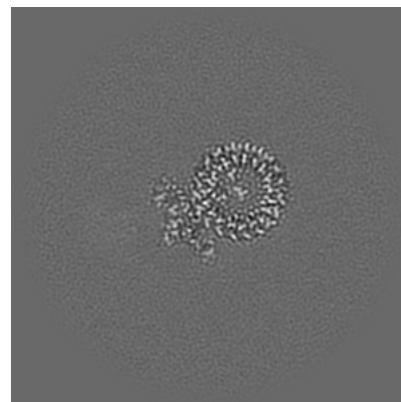
6.3.1 Primary map



X Index: 167

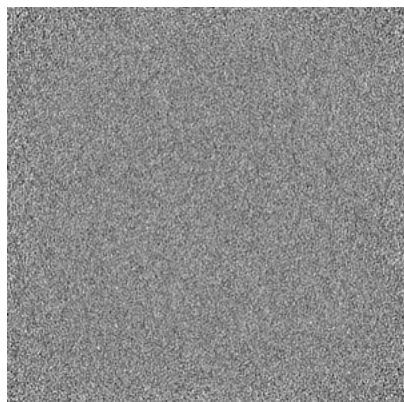


Y Index: 158

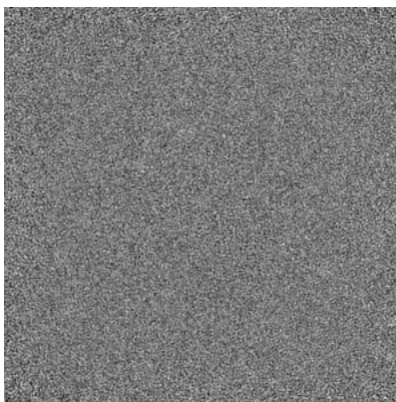


Z Index: 149

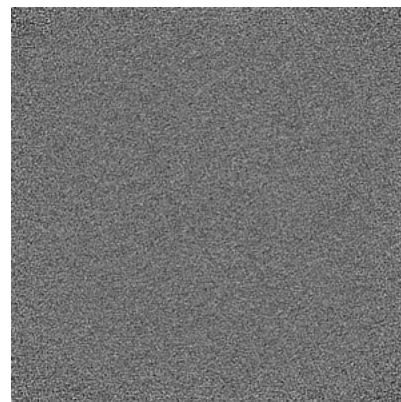
6.3.2 Raw map



X Index: 0



Y Index: 0

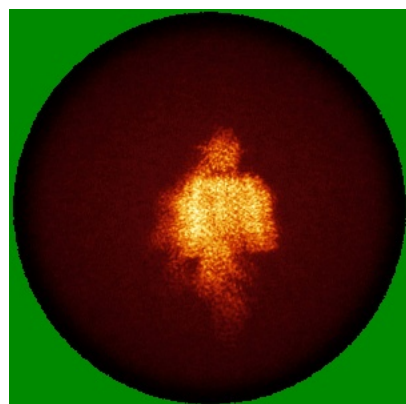


Z Index: 0

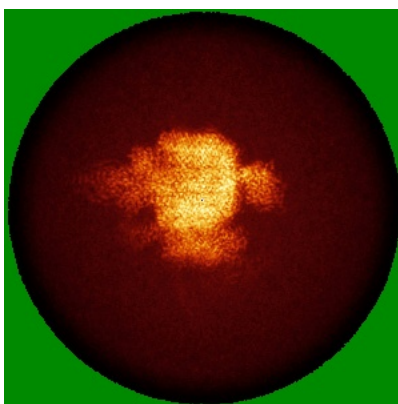
The images above show the largest variance slices of the map in three orthogonal directions.

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

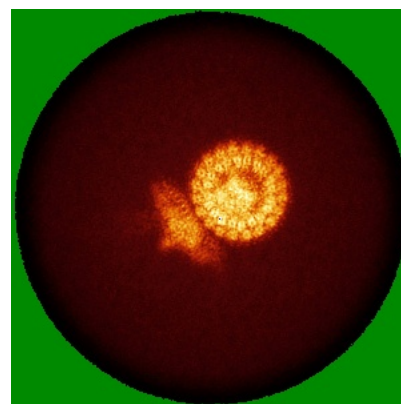
6.4.1 Primary map



X

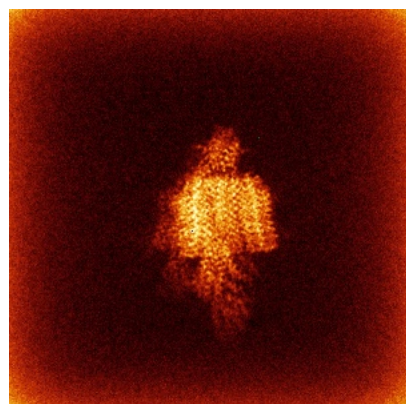


Y

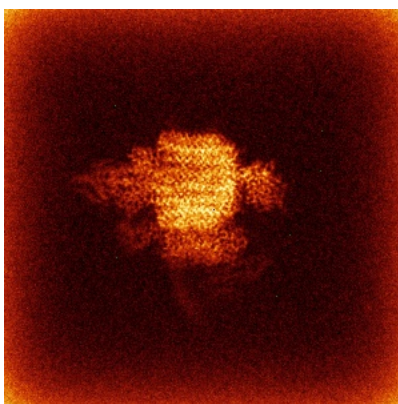


Z

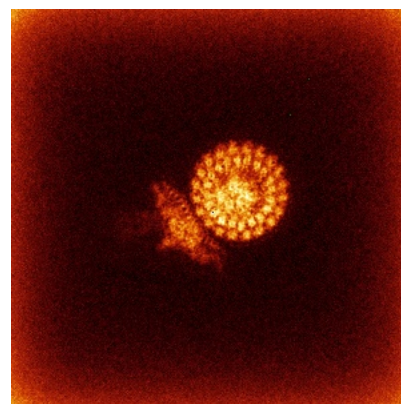
6.4.2 Raw map



X



Y

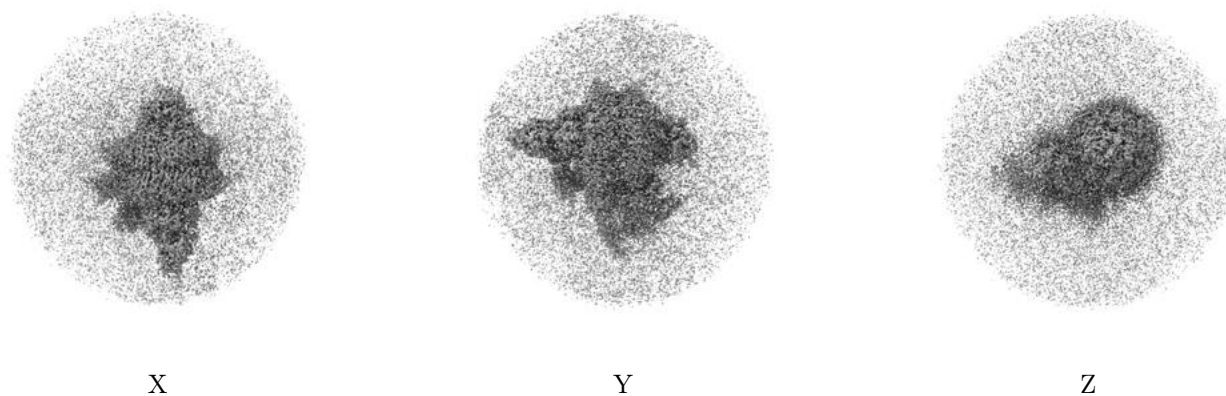


Z

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.

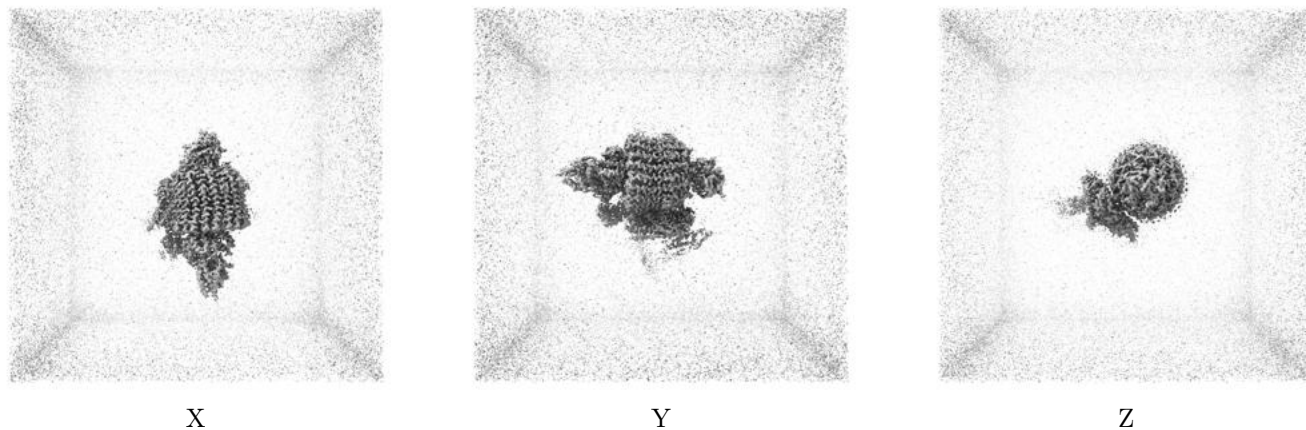
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.108. 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.

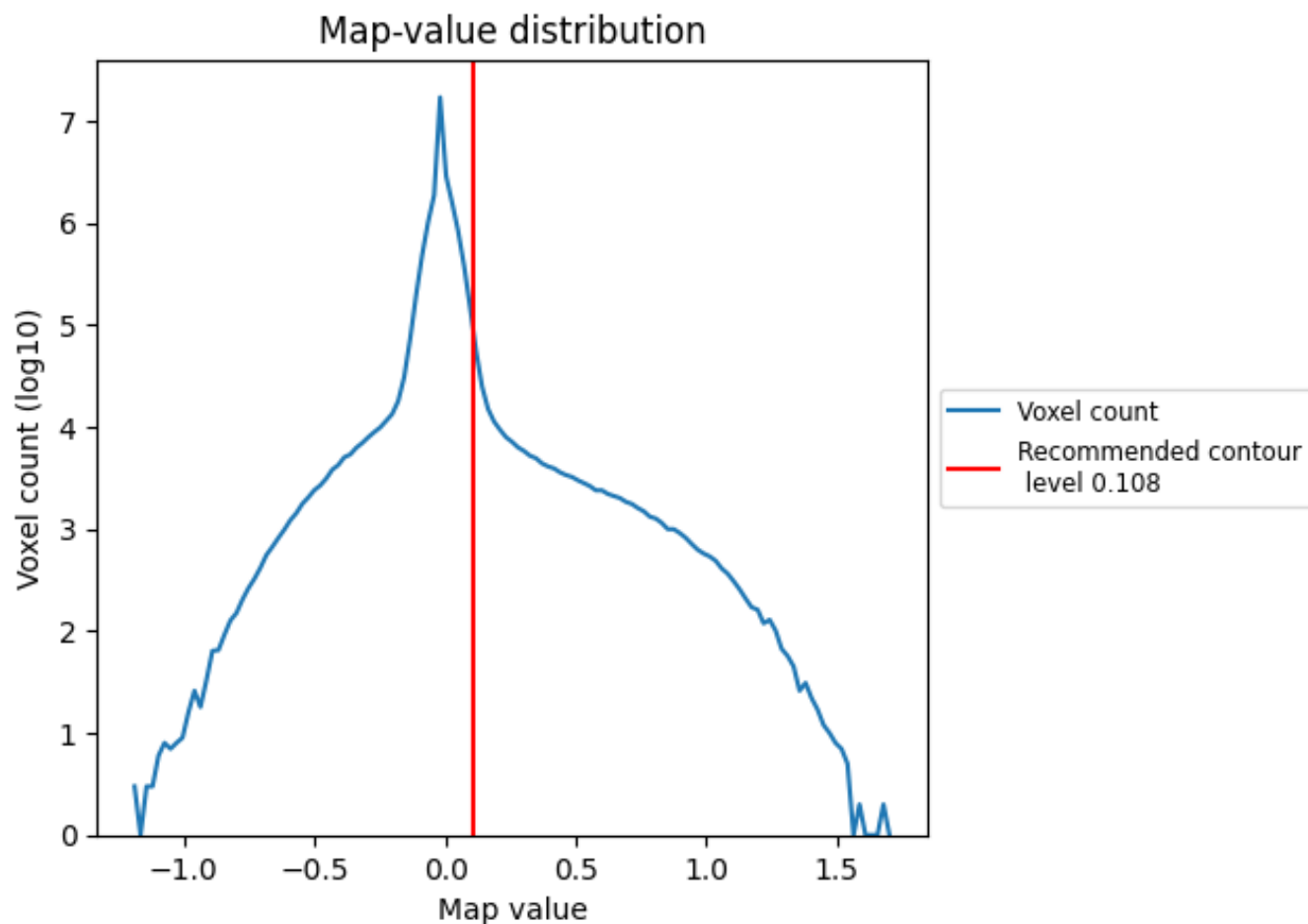
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

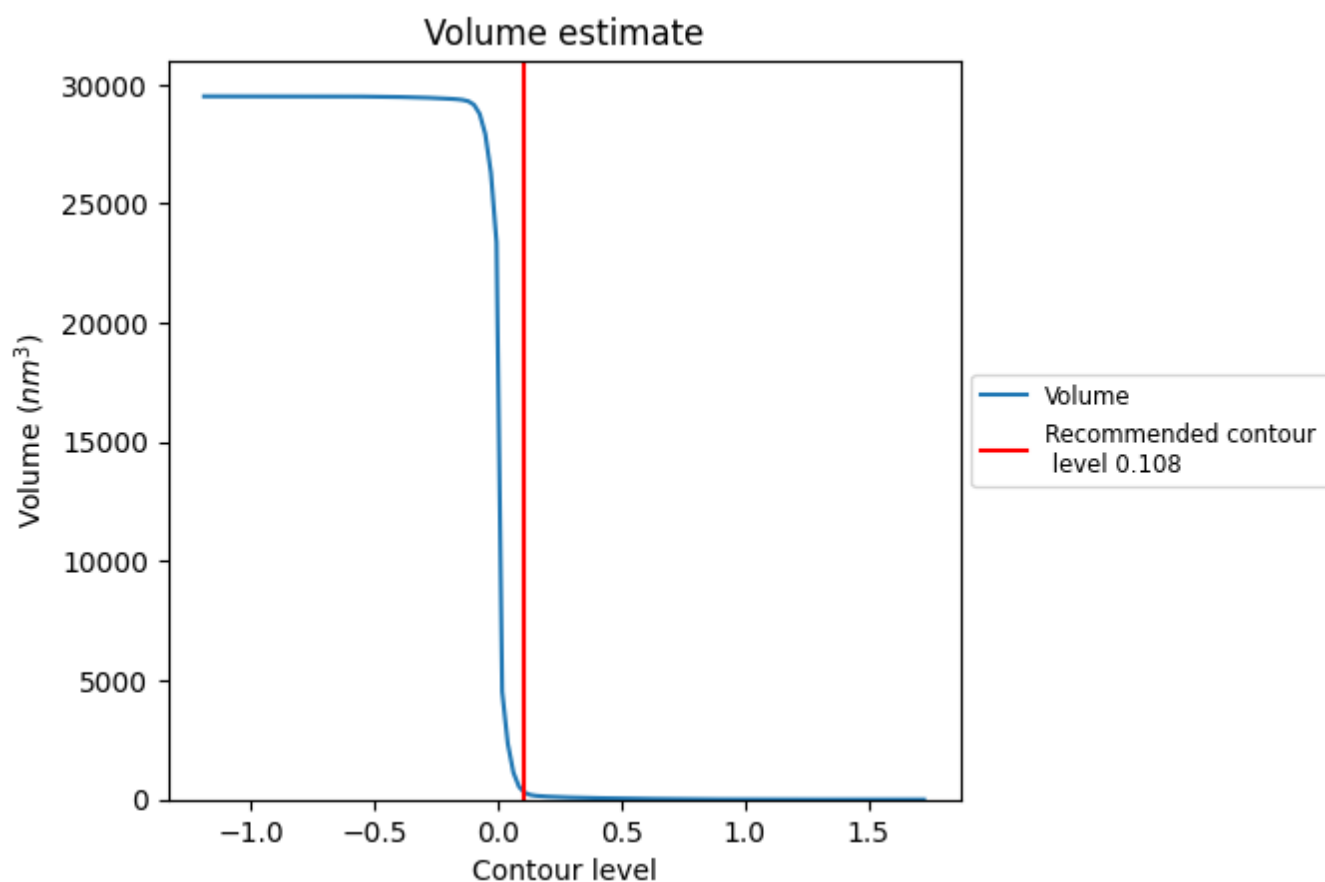
This section contains the results of statistical analysis of the map.

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.

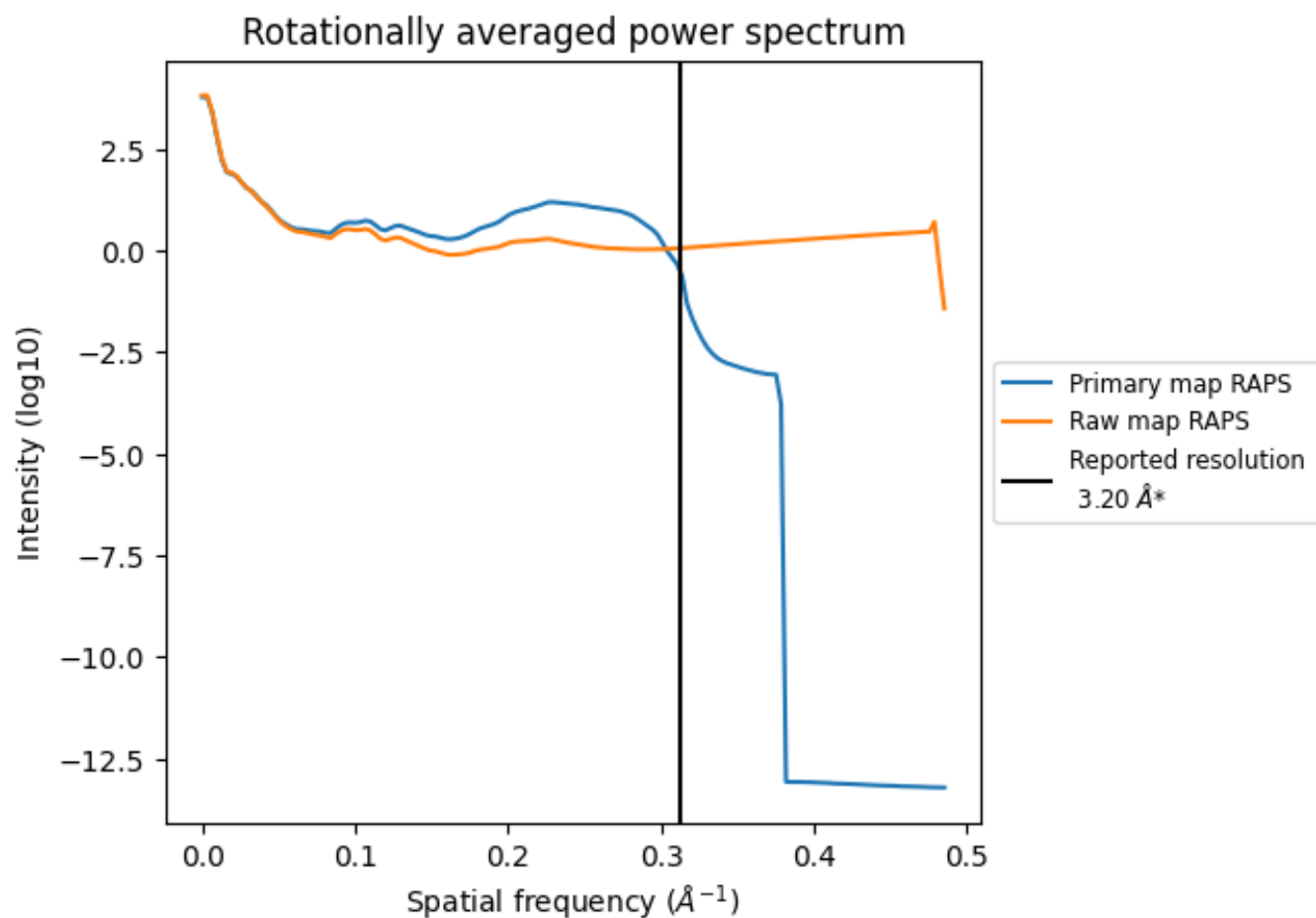
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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 ⓘ

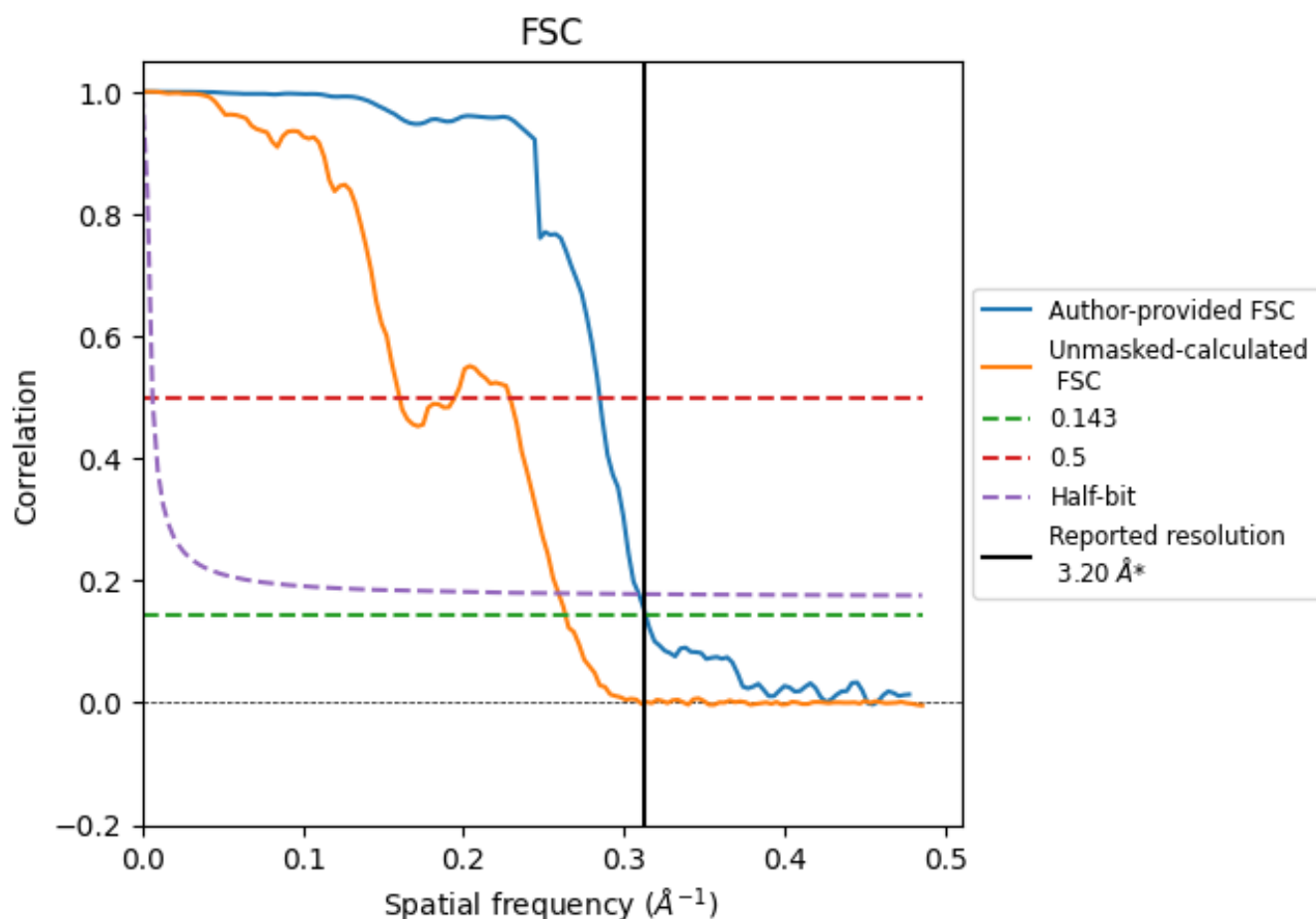


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

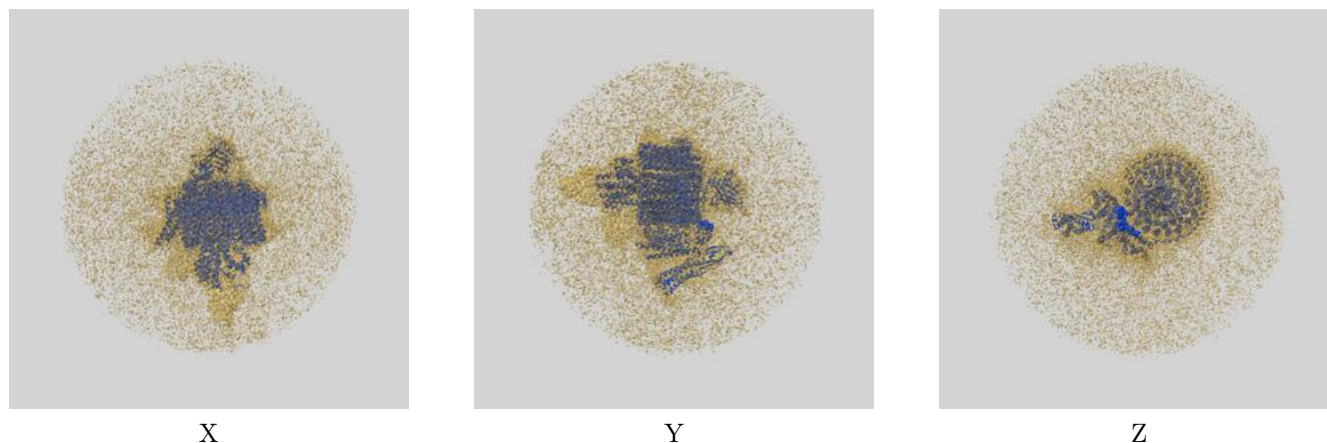
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.51	3.24
Unmasked-calculated*	3.80	6.25	3.86

*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 3.80 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

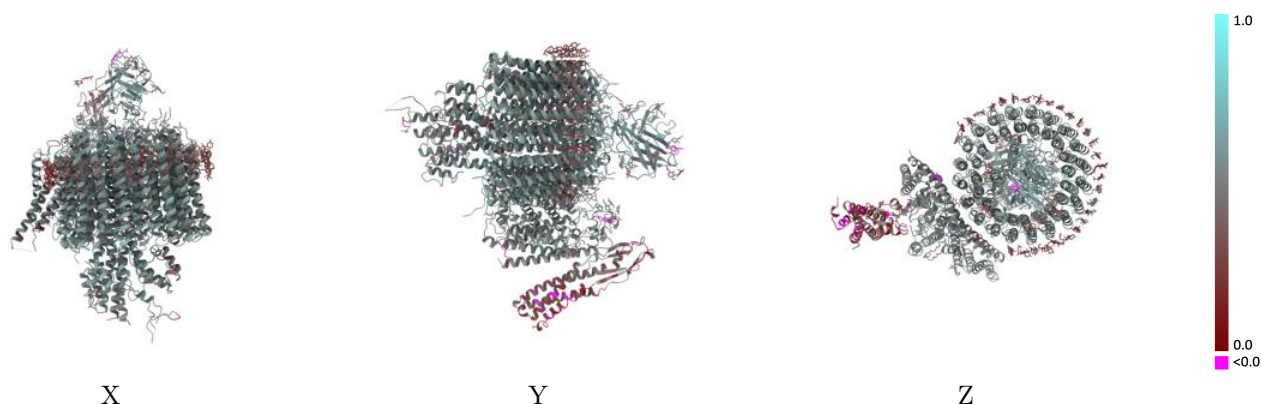
This section contains information regarding the fit between EMDB map EMD-44350 and PDB model 9B8O. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



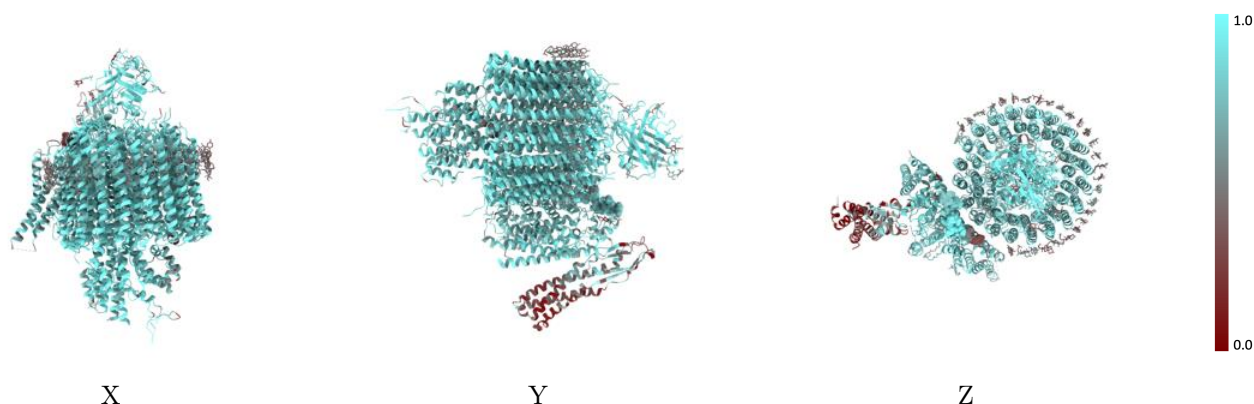
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



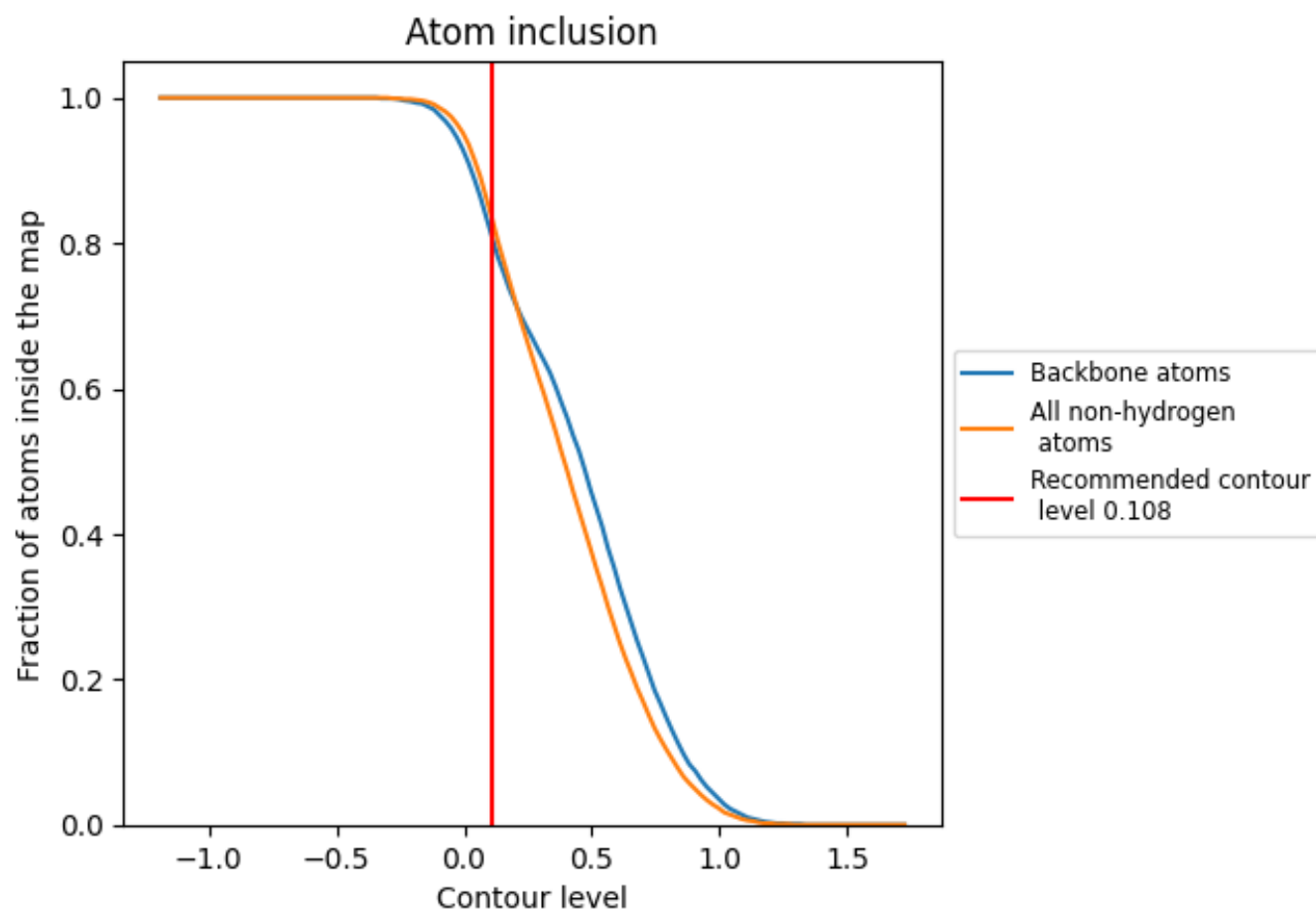
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.108).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 84% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5130
A	 0.5360	 0.2170
B	 0.5360	 0.2010
C	 0.6430	 0.3900
D	 0.4640	 0.2620
E	 0.7500	 0.4200
F	 0.6070	 0.2740
G	 0.5000	 0.2300
H	 0.8640	 0.5080
I	 0.4640	 0.2340
L	 0.6620	 0.3670
P	 0.9210	 0.5570
U	 0.4130	 0.2630
Z	 0.7870	 0.4510
a	 0.8570	 0.5280
b	 0.8990	 0.5570
d	 0.8480	 0.5240
e	 0.8670	 0.5310
f	 0.8010	 0.4880
g	 0.8930	 0.5480
h	 0.8870	 0.5360
i	 0.8460	 0.5190
j	 0.8320	 0.5200
k	 0.8280	 0.5190
l	 0.8520	 0.5230
m	 0.8490	 0.5190
n	 0.8350	 0.5120
o	 0.8600	 0.5280
p	 0.8700	 0.5240

