



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:19 AM UTC

PDB ID : 9BRD / pdb_00009brd
EMDB ID : EMD-44353
Title : Synaptic Vesicle V-ATPase with synaptophysin and SidK, State 3
Authors : Coupland, C.E.; Rubinstein, J.L.
Deposited on : 2024-05-11
Resolution : 3.50 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

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 72445 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	600	4651	2949	786	889	27	0	0
1	B	600	4651	2949	786	889	27	0	0
1	C	600	4651	2949	786	889	27	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	459	3595	2282	613	680	20	0	0
2	E	459	3595	2282	613	680	20	0	0
2	F	459	3595	2282	613	680	20	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	375	2155	1347	400	408	0	0

- Molecule 4 is a protein called ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	214	1726	1095	311	315	5	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	225	Total	C	N	O	S	0	0
			1778	1119	315	336	8		
5	J	223	Total	C	N	O	S	0	0
			1779	1120	315	334	10		
5	K	224	Total	C	N	O	S	0	0
			1657	1041	299	309	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			864	544	156	162	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	114	Total	C	N	O	S	0	0
			845	506	178	157	4		
7	N	114	Total	C	N	O	S	0	0
			916	548	190	173	5		
7	O	113	Total	C	N	O	S	0	0
			715	427	147	138	3		

- Molecule 8 is a protein called V-type proton ATPase subunit S1.

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

- Molecule 9 is a protein called Type IV secretion protein Dot.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	264	Total	C	N	O	S	0	0
			2130	1352	358	410	10		
9	R	267	Total	C	N	O	S	0	0
			2155	1369	362	413	11		
9	S	263	Total	C	N	O	S	0	0
			2126	1350	357	409	10		

- Molecule 10 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	T	430	2136	1276	430	430	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	428	PHE	ILE	conflict	UNP A0A8I5ZQ24

- Molecule 11 is a protein called Synaptophysin.

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

- Molecule 12 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	a	770	6212	4052	1046	1074	40	0	0

- Molecule 13 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

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

- Molecule 14 is a protein called V-type proton ATPase subunit.

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

- Molecule 15 is a protein called V-type proton ATPase subunit e 2.

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

- Molecule 16 is a protein called Rnasek protein.

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

- Molecule 17 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

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

- Molecule 18 is a protein called Renin receptor.

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

- Molecule 19 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



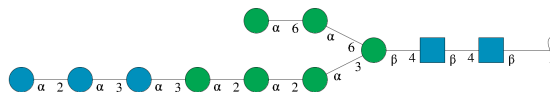
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	V	2	28	16	2	10	0	0
19	W	2	28	16	2	10	0	0

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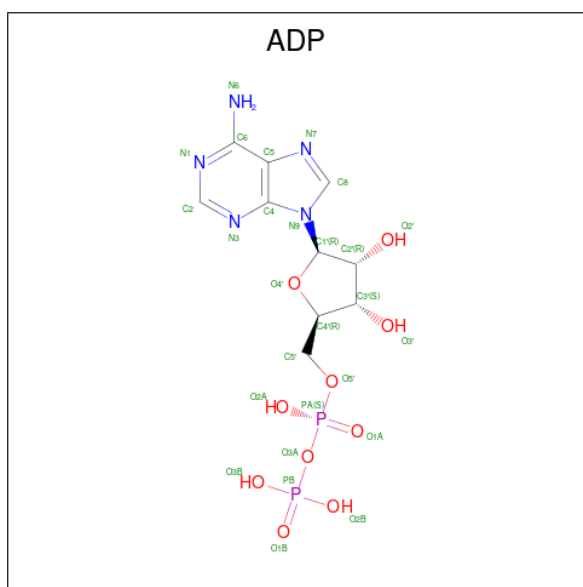
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	X	2	28	16	2	10	0	0
19	Y	2	28	16	2	10	0	0
19	Z	2	28	16	2	10	0	0
19	c	2	28	16	2	10	0	0
19	q	2	28	16	2	10	0	0
19	r	2	28	16	2	10	0	0

- Molecule 20 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranos e-(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-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ace tamido-2-deoxy-beta-D-glucopyranose.



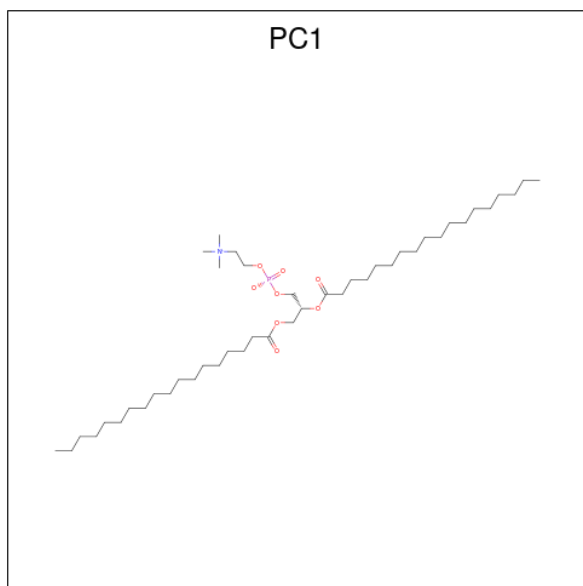
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	s	11	127	70	2	55	0	0

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 22 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



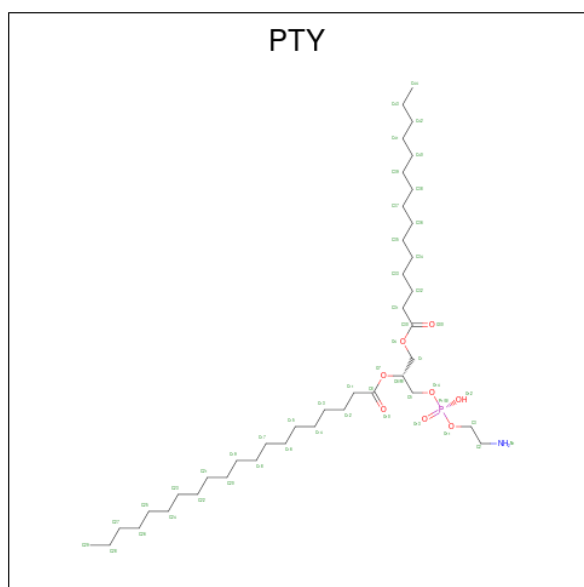
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	P	1	54	44	1	8	1	0
22	P	1	54	44	1	8	1	0

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

- Molecule 23 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



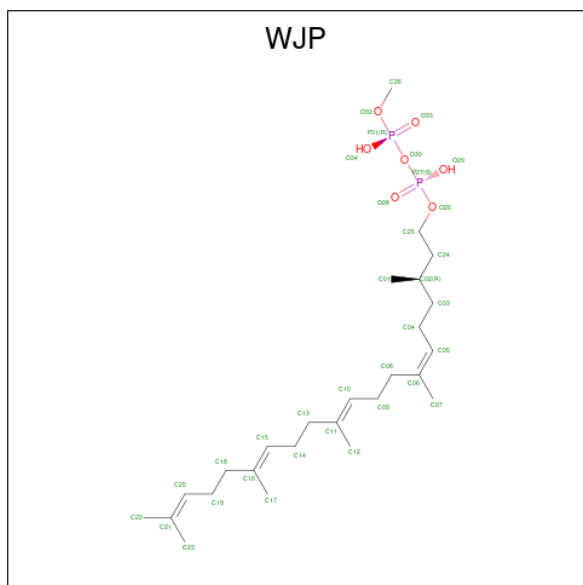
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	p	1	Total	C	N	O	P	0
			50	40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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	p	1	50	40	1	8	1	0

- Molecule 24 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylcosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$).



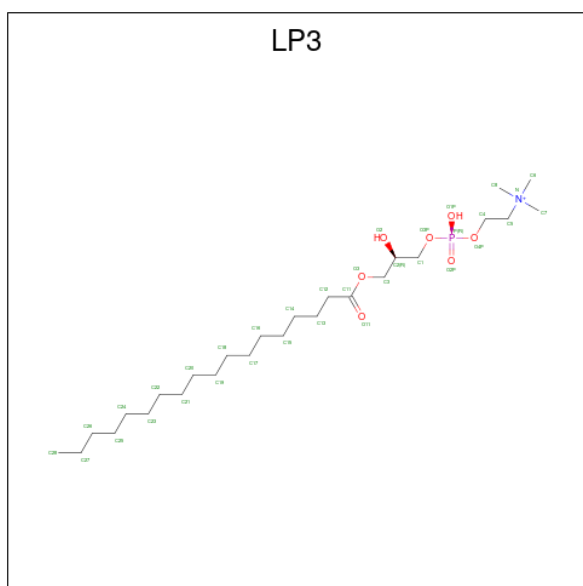
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
24	a	1	34	25	7	2	0

- Molecule 25 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



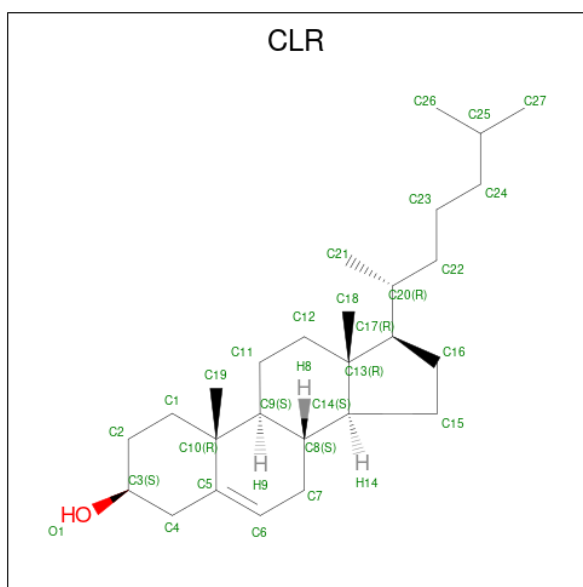
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
25	a	1	14	8	1	5	0

- Molecule 26 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: $C_{26}H_{55}NO_7P$).



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

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



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

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

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198766	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	1.587	Depositor
Minimum map value	-0.952	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.185	Depositor
Map size (\AA)	527.36, 527.36, 527.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3733333, 1.3733333, 1.3733333	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/4746	0.28	0/6425
1	B	0.14	0/4746	0.28	0/6425
1	C	0.14	0/4746	0.28	0/6425
2	D	0.15	0/3666	0.29	0/4967
2	E	0.15	0/3666	0.28	0/4967
2	F	0.16	0/3666	0.28	0/4967
3	G	0.12	0/2177	0.28	0/3017
4	H	0.12	0/1744	0.26	0/2332
5	I	0.12	0/1794	0.25	0/2408
5	J	0.13	0/1796	0.28	0/2408
5	K	0.13	0/1671	0.27	0/2255
6	L	0.11	0/877	0.29	0/1183
7	M	0.13	0/850	0.28	0/1140
7	N	0.11	0/921	0.23	0/1226
7	O	0.12	0/718	0.26	0/981
8	P	0.19	0/1707	0.36	0/2324
9	Q	0.11	0/2164	0.25	0/2915
9	R	0.12	0/2189	0.26	0/2947
9	S	0.12	0/2160	0.25	0/2910
10	T	0.08	0/2134	0.20	0/2976
11	U	0.10	0/1158	0.26	0/1601
12	a	0.18	0/6367	0.35	1/8613 (0.0%)
13	b	0.19	0/1537	0.30	0/2088
14	d	0.14	0/2899	0.27	0/3927
15	e	0.16	0/669	0.28	0/920
16	f	0.12	0/682	0.23	0/926
17	g	0.19	0/1083	0.30	0/1466
17	h	0.18	0/1083	0.29	0/1466
17	i	0.18	0/1083	0.30	0/1466
17	j	0.18	0/1083	0.31	0/1466
17	k	0.18	0/1083	0.27	0/1466
17	l	0.18	0/1083	0.28	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.17	0/1083	0.28	0/1466
17	n	0.19	0/1083	0.29	0/1466
17	o	0.19	0/1083	0.31	0/1466
18	p	0.18	0/445	0.29	0/609
All	All	0.15	0/71642	0.28	1/97076 (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
12	a	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	829	GLU	N-CA-C	-5.12	106.28	112.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	a	298	ARG	Sidechain

4.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4651	0	4644	78	0
1	B	4651	0	4644	63	0
1	C	4651	0	4644	60	0
2	D	3595	0	3602	59	0
2	E	3595	0	3602	45	0
2	F	3595	0	3602	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2155	0	1372	22	0
4	H	1726	0	1835	21	0
5	I	1778	0	1811	18	0
5	J	1779	0	1823	30	0
5	K	1657	0	1605	21	0
6	L	864	0	874	18	0
7	M	845	0	780	13	0
7	N	916	0	917	12	0
7	O	715	0	562	5	0
8	P	1652	0	1579	32	0
9	Q	2130	0	2168	27	0
9	R	2155	0	2201	29	0
9	S	2126	0	2165	14	0
10	T	2136	0	948	0	0
11	U	1150	0	644	7	0
12	a	6212	0	6186	136	0
13	b	1503	0	1551	30	0
14	d	2833	0	2770	37	0
15	e	644	0	659	19	0
16	f	666	0	663	5	0
17	g	1068	0	1136	37	0
17	h	1068	0	1136	13	0
17	i	1068	0	1136	24	0
17	j	1068	0	1136	21	0
17	k	1068	0	1136	11	0
17	l	1068	0	1136	13	0
17	m	1068	0	1136	11	0
17	n	1068	0	1136	21	0
17	o	1068	0	1136	23	0
18	p	432	0	428	16	0
19	V	28	0	25	2	0
19	W	28	0	25	1	0
19	X	28	0	25	2	0
19	Y	28	0	25	1	0
19	Z	28	0	25	0	0
19	c	28	0	25	1	0
19	q	28	0	25	3	0
19	r	28	0	25	1	0
20	s	127	0	106	3	0
21	A	27	0	12	2	0
22	P	108	0	176	4	0
22	a	54	0	88	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	54	0	88	0	0
22	l	54	0	88	0	0
23	a	150	0	237	2	0
23	b	100	0	158	1	0
23	p	200	0	316	6	0
24	a	34	0	0	1	0
25	a	14	0	13	3	0
26	a	35	0	54	0	0
27	b	28	0	46	1	0
27	h	56	0	92	3	0
27	i	112	0	184	8	0
27	j	112	0	184	7	0
27	k	84	0	138	2	0
27	l	140	0	230	1	0
27	m	84	0	138	1	0
27	n	140	0	230	7	0
27	o	84	0	138	8	0
All	All	72445	0	71419	947	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 7.

The worst 5 of 947 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)
5:I:75:LEU:HD11	7:M:73:VAL:HG11	1.47	0.97
17:g:72:VAL:HG21	17:g:99:VAL:HG21	1.47	0.95
2:D:55:GLY:O	2:D:102:THR:OG1	1.90	0.89
12:a:477:SER:OG	12:a:520:ASP:OD1	1.94	0.86
5:J:54:MET:HE1	7:N:47:TYR:CE2	2.12	0.85

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

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
19	NAG	V	1	19	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
19	NAG	V	2	19	14,14,15	0.71	0	17,19,21	0.86	0
19	NAG	W	1	19,8	14,14,15	0.70	0	17,19,21	1.21	1 (5%)
19	NAG	W	2	19	14,14,15	0.80	0	17,19,21	0.99	1 (5%)
19	NAG	X	1	19,8	14,14,15	0.59	0	17,19,21	1.16	2 (11%)
19	NAG	X	2	19	14,14,15	0.81	0	17,19,21	0.77	0
19	NAG	Y	1	19,8	14,14,15	0.83	0	17,19,21	1.58	4 (23%)
19	NAG	Y	2	19	14,14,15	0.70	0	17,19,21	1.06	1 (5%)
19	NAG	Z	1	19,8	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
19	NAG	Z	2	19	14,14,15	0.71	0	17,19,21	1.36	2 (11%)
19	NAG	c	1	19	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
19	NAG	c	2	19	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
19	NAG	q	1	19,8	14,14,15	0.77	0	17,19,21	0.80	0
19	NAG	q	2	19	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
19	NAG	r	1	19	14,14,15	0.74	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	NAG	r	2	19	14,14,15	0.70	0	17,19,21	0.82	0
20	NAG	s	1	20	14,14,15	0.77	0	17,19,21	0.81	0
20	MAN	s	10	20	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
20	MAN	s	11	20	11,11,12	0.74	0	15,15,17	0.93	1 (6%)
20	NAG	s	2	20	14,14,15	0.74	0	17,19,21	0.82	1 (5%)
20	BMA	s	3	20	11,11,12	0.78	0	15,15,17	2.16	3 (20%)
20	MAN	s	4	20	11,11,12	0.68	0	15,15,17	1.35	1 (6%)
20	MAN	s	5	20	11,11,12	0.72	0	15,15,17	1.25	1 (6%)
20	MAN	s	6	20	11,11,12	0.84	1 (9%)	15,15,17	0.93	0
20	GLC	s	7	20	11,11,12	0.65	0	15,15,17	0.49	0
20	GLC	s	8	20	11,11,12	0.61	0	15,15,17	0.81	0
20	GLC	s	9	20	11,11,12	0.60	0	15,15,17	0.68	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
19	NAG	V	1	19	-	2/6/23/26	0/1/1/1
19	NAG	V	2	19	-	0/6/23/26	0/1/1/1
19	NAG	W	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	W	2	19	-	0/6/23/26	0/1/1/1
19	NAG	X	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	X	2	19	-	0/6/23/26	0/1/1/1
19	NAG	Y	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	Y	2	19	-	1/6/23/26	0/1/1/1
19	NAG	Z	1	19,8	-	2/6/23/26	0/1/1/1
19	NAG	Z	2	19	-	1/6/23/26	0/1/1/1
19	NAG	c	1	19	-	2/6/23/26	0/1/1/1
19	NAG	c	2	19	-	2/6/23/26	0/1/1/1
19	NAG	q	1	19,8	-	1/6/23/26	0/1/1/1
19	NAG	q	2	19	-	2/6/23/26	0/1/1/1
19	NAG	r	1	19	-	2/6/23/26	0/1/1/1
19	NAG	r	2	19	-	0/6/23/26	0/1/1/1
20	NAG	s	1	20	-	0/6/23/26	0/1/1/1
20	MAN	s	10	20	-	0/2/19/22	0/1/1/1
20	MAN	s	11	20	-	0/2/19/22	0/1/1/1
20	NAG	s	2	20	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BMA	s	3	20	-	1/2/19/22	0/1/1/1
20	MAN	s	4	20	-	2/2/19/22	0/1/1/1
20	MAN	s	5	20	-	2/2/19/22	0/1/1/1
20	MAN	s	6	20	-	0/2/19/22	0/1/1/1
20	GLC	s	7	20	-	1/2/19/22	0/1/1/1
20	GLC	s	8	20	-	0/2/19/22	0/1/1/1
20	GLC	s	9	20	-	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)
20	s	6	MAN	O5-C1	-2.19	1.40	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	s	3	BMA	C1-O5-C5	6.32	120.66	112.19
19	c	1	NAG	C2-N2-C7	4.17	128.49	122.90
20	s	4	MAN	C1-O5-C5	4.13	117.72	112.19
19	Y	1	NAG	C1-O5-C5	3.85	117.34	112.19
19	Z	1	NAG	C2-N2-C7	3.77	127.95	122.90

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	V	1	NAG	C1-C2-N2-C7
19	Y	2	NAG	C1-C2-N2-C7
19	Z	2	NAG	C3-C2-N2-C7
19	q	1	NAG	C1-C2-N2-C7
19	r	1	NAG	C1-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 14 short contacts:

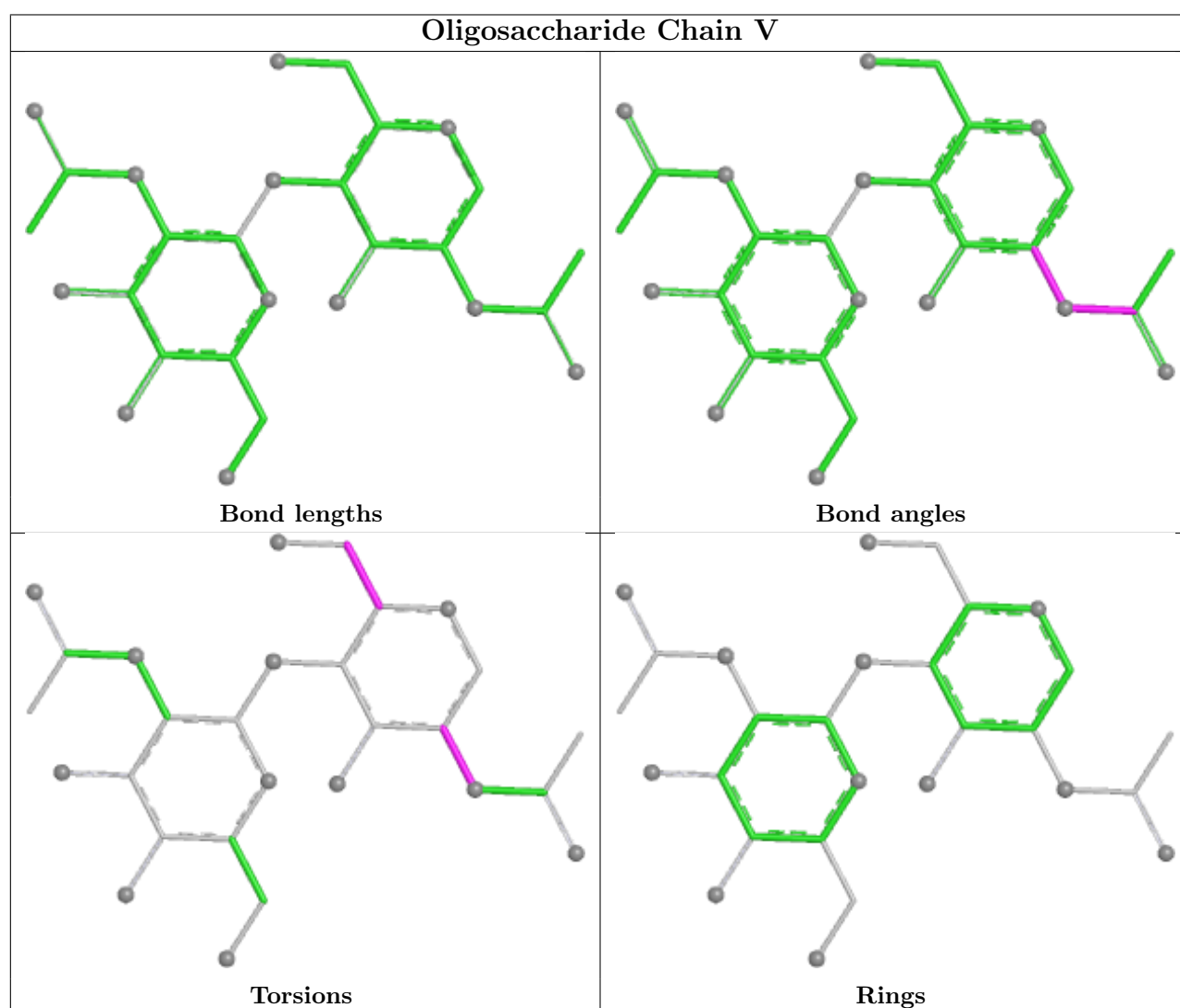
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	r	2	NAG	1	0
19	W	1	NAG	1	0
19	r	1	NAG	1	0
19	X	2	NAG	2	0

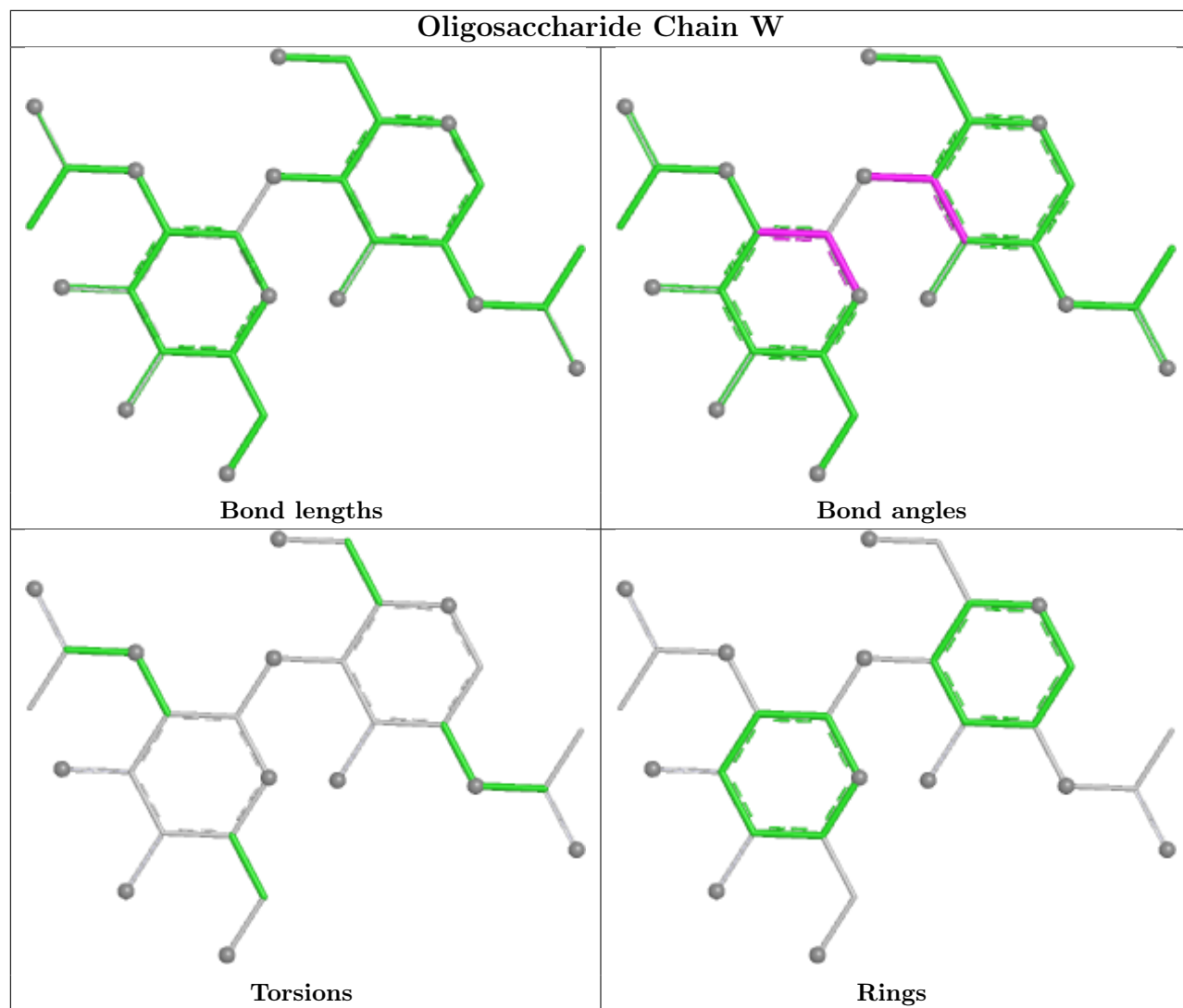
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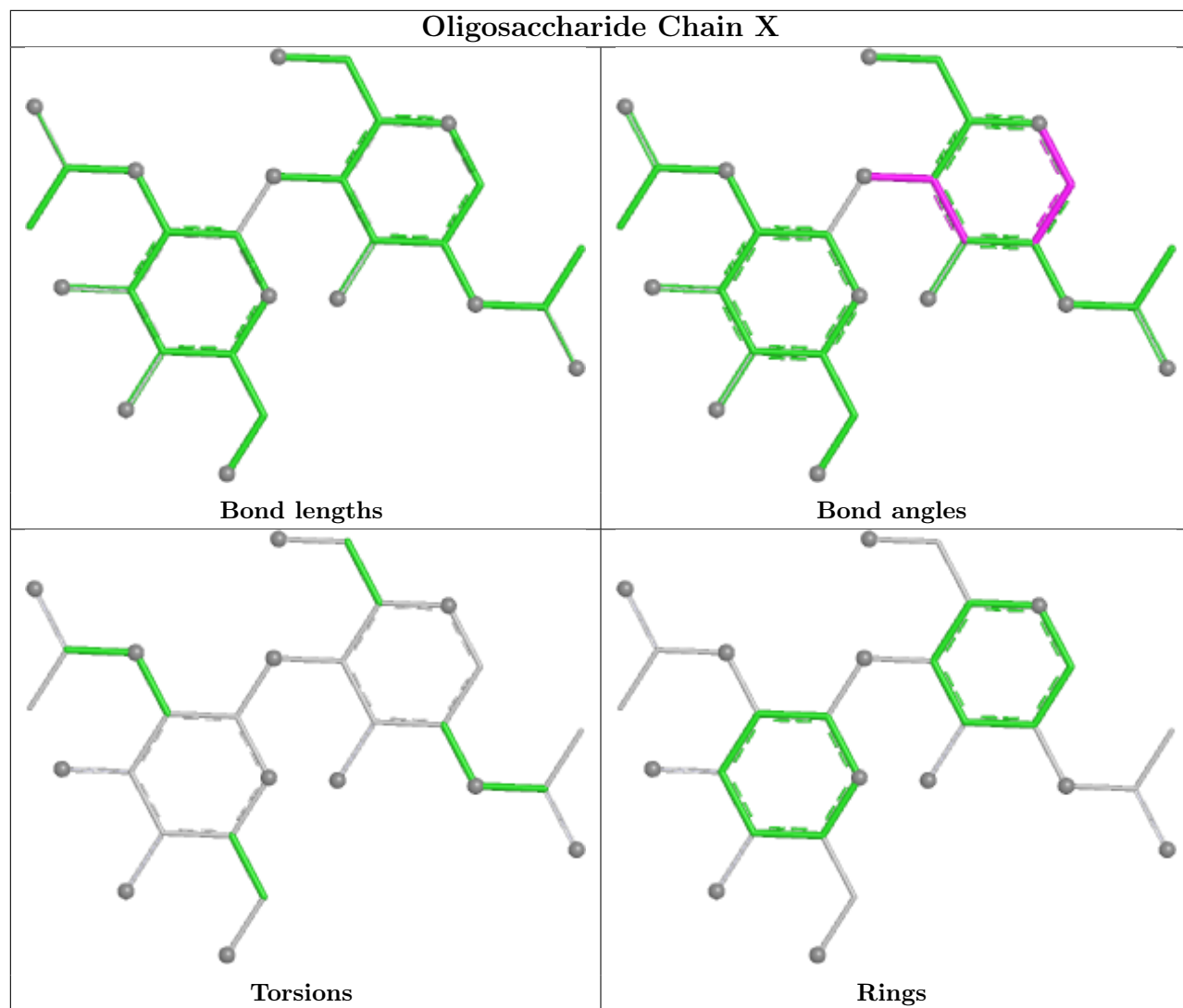
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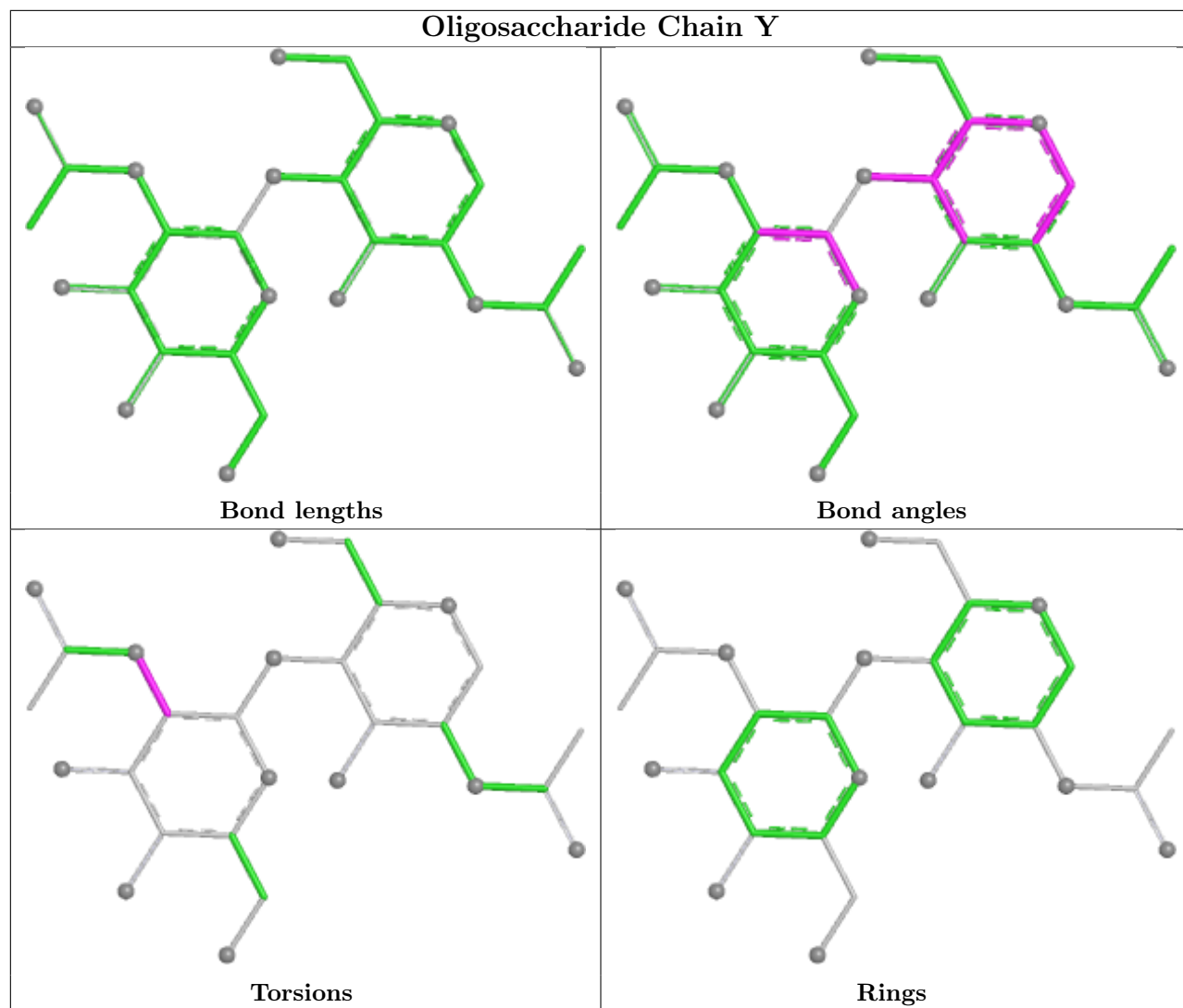
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	q	1	NAG	3	0
20	s	1	NAG	3	0
19	c	1	NAG	1	0
19	Y	2	NAG	1	0
19	q	2	NAG	1	0
19	Y	1	NAG	1	0
19	V	1	NAG	2	0

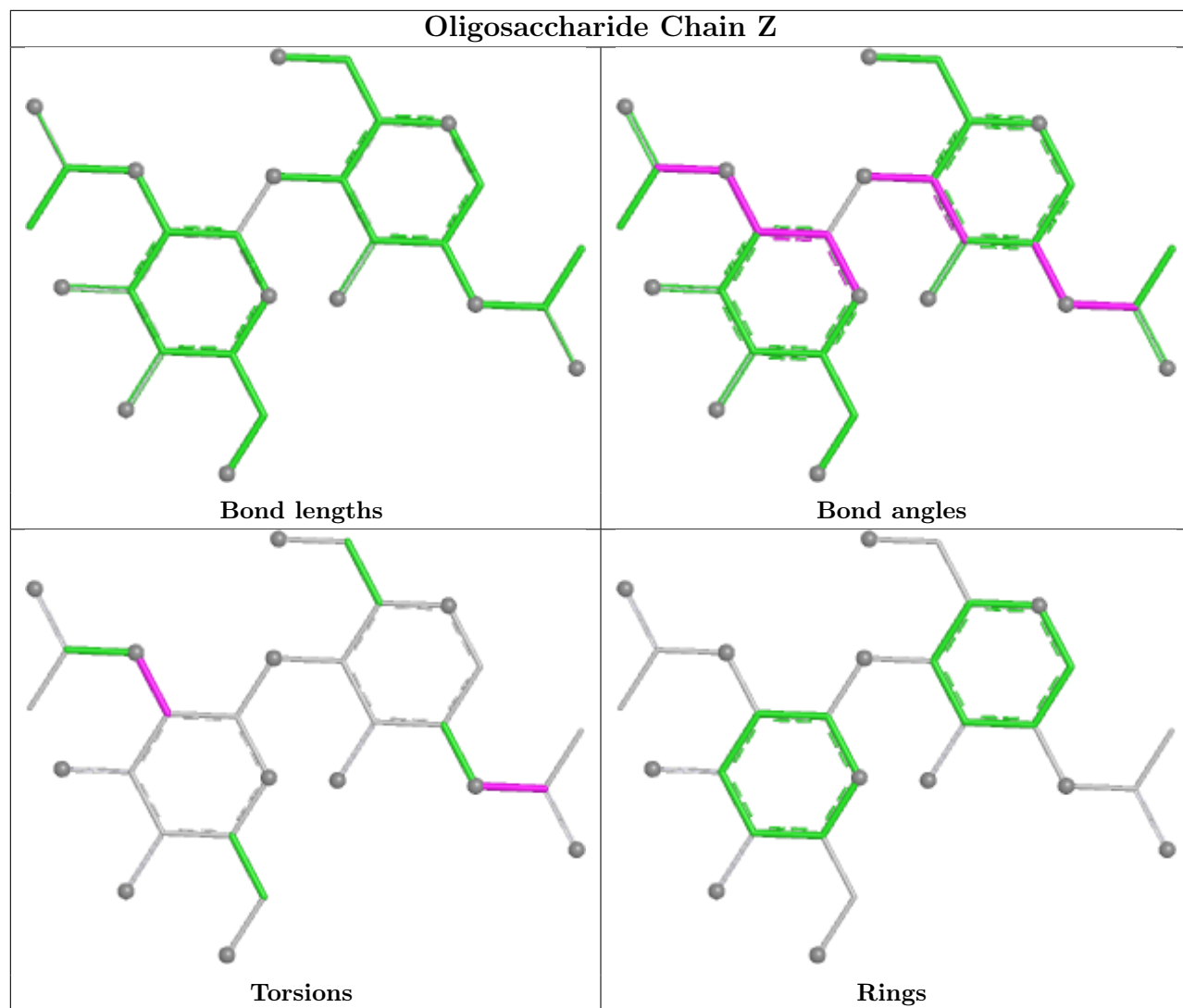
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

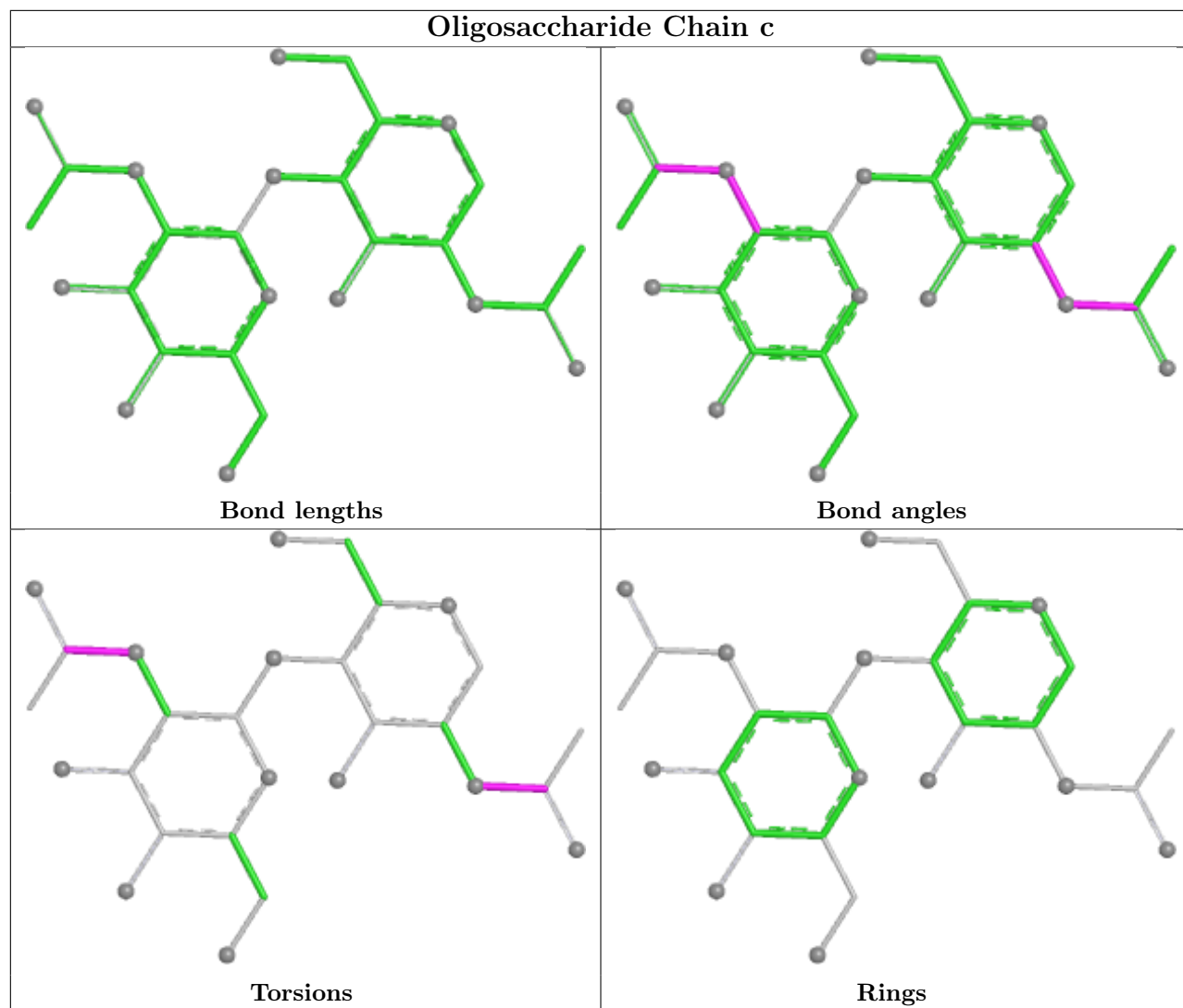


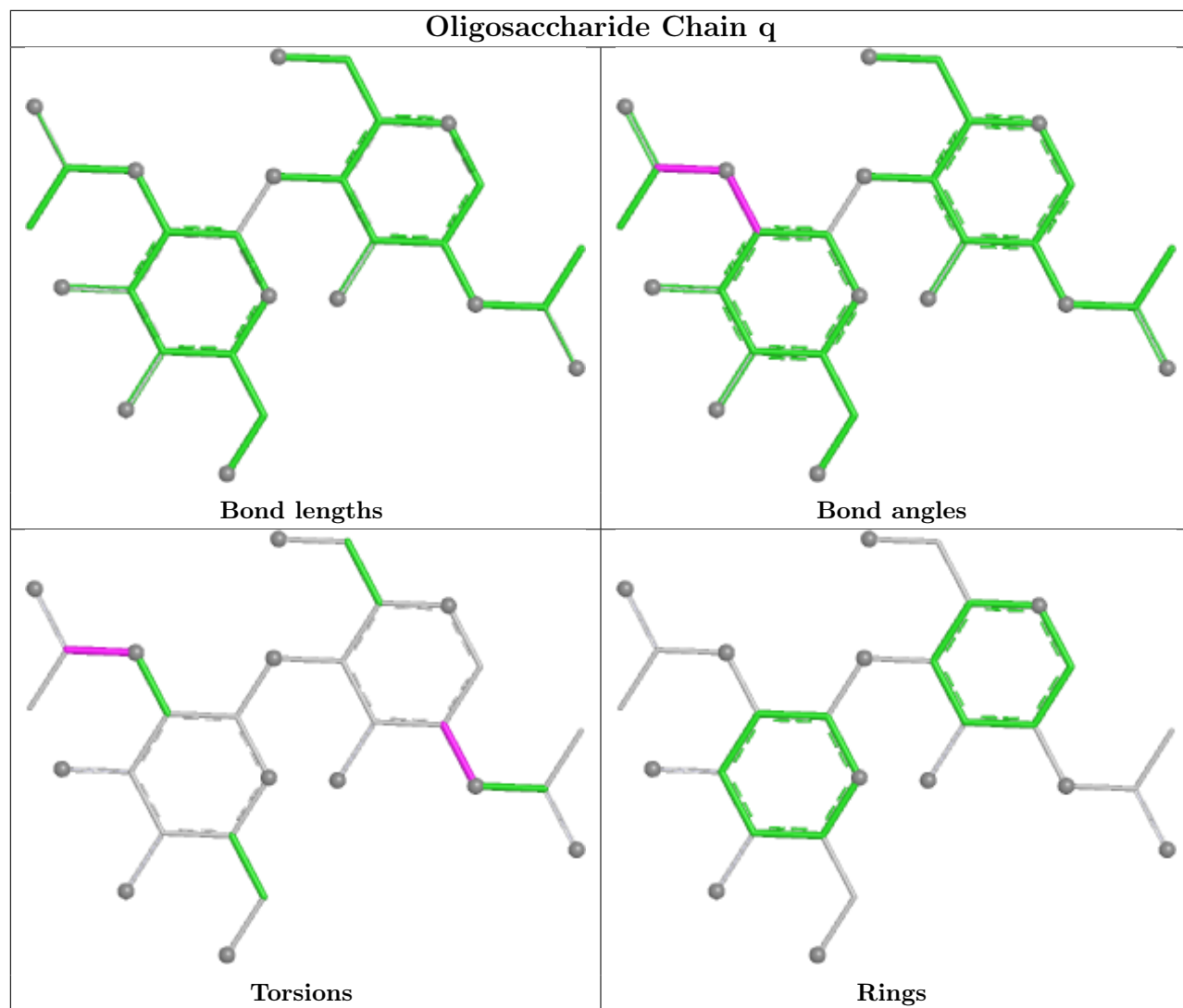


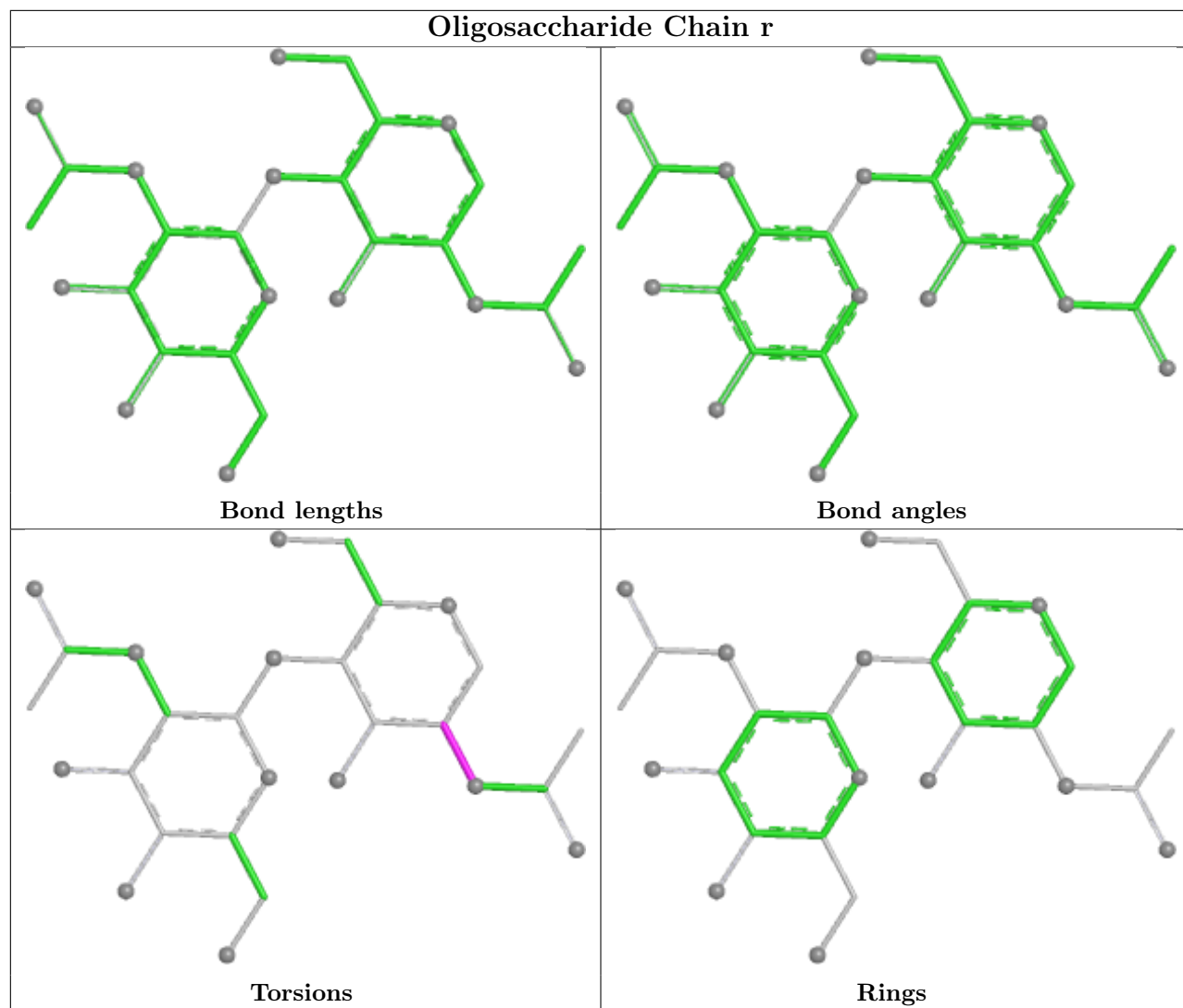


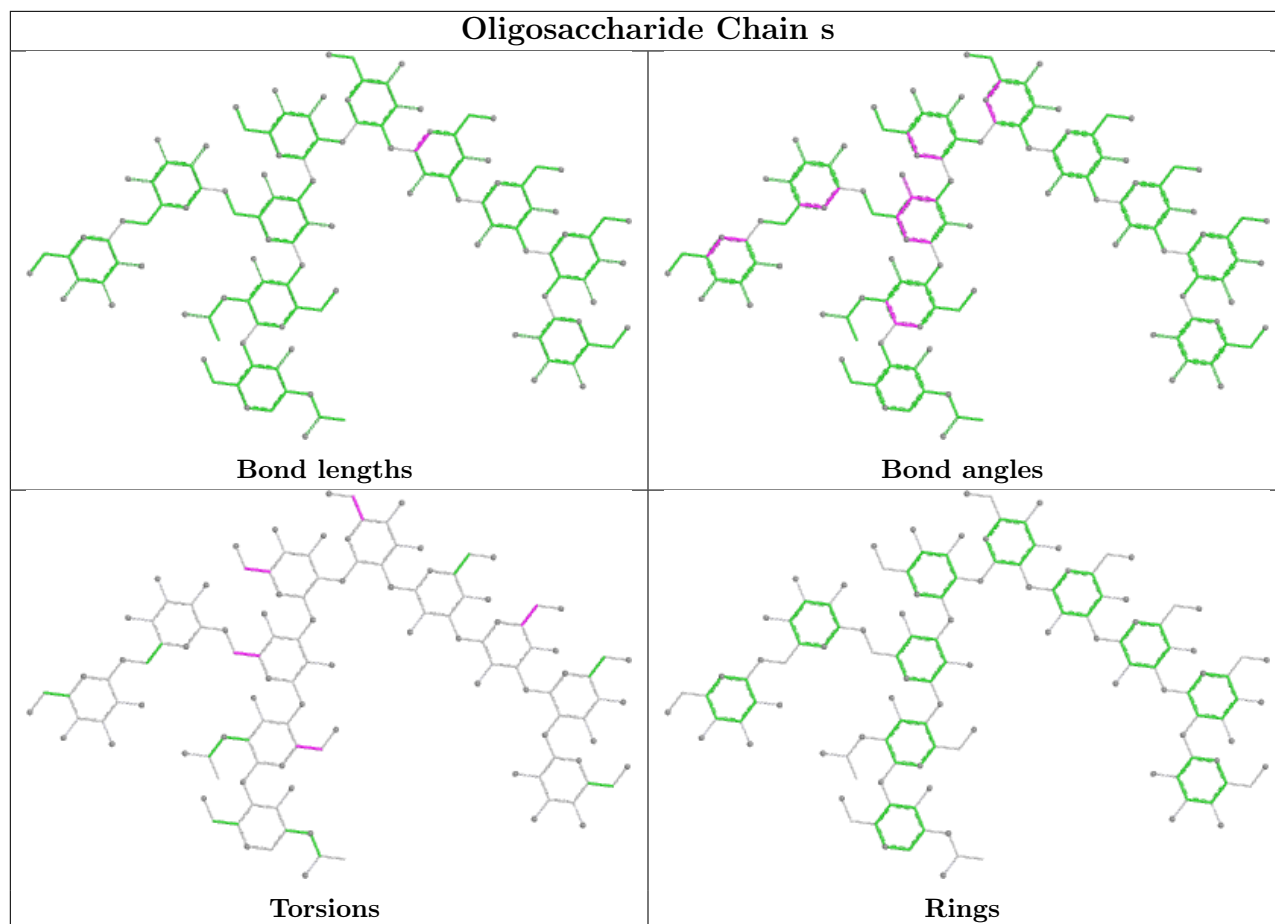












4.6 Ligand geometry [i](#)

48 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
22	PC1	a	901	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
27	CLR	j	203	-	31,31,31	0.44	0	48,48,48	0.75	1 (2%)
27	CLR	h	201	-	31,31,31	0.39	0	48,48,48	0.75	0
27	CLR	i	202	-	31,31,31	0.40	0	48,48,48	0.77	0
27	CLR	m	202	-	31,31,31	0.36	0	48,48,48	0.67	0
25	NAG	a	906	12	14,14,15	0.77	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	ADP	A	701	-	28,29,29	1.39	5 (17%)	43,45,45	1.84	11 (25%)
22	PC1	b	301	-	53,53,53	0.51	0	59,61,61	0.49	1 (1%)
27	CLR	o	201	-	31,31,31	0.40	0	48,48,48	0.88	1 (2%)
23	PTY	p	404	-	49,49,49	0.46	0	52,54,54	0.39	0
27	CLR	i	204	-	31,31,31	0.38	0	48,48,48	0.62	0
27	CLR	k	202	-	31,31,31	0.36	0	48,48,48	0.49	0
27	CLR	l	204	-	31,31,31	0.39	0	48,48,48	0.72	0
27	CLR	j	201	-	31,31,31	0.39	0	48,48,48	0.66	0
27	CLR	k	203	-	31,31,31	0.37	0	48,48,48	0.56	0
27	CLR	j	204	-	31,31,31	0.38	0	48,48,48	0.72	0
27	CLR	n	204	-	31,31,31	0.37	0	48,48,48	0.77	0
22	PC1	l	201	-	53,53,53	0.50	0	59,61,61	0.51	1 (1%)
23	PTY	a	903	-	49,49,49	0.47	0	52,54,54	0.40	0
27	CLR	i	201	-	31,31,31	0.38	0	48,48,48	0.77	1 (2%)
27	CLR	m	203	-	31,31,31	0.41	0	48,48,48	0.79	1 (2%)
27	CLR	o	202	-	31,31,31	0.45	0	48,48,48	1.00	3 (6%)
23	PTY	b	302	-	49,49,49	0.48	0	52,54,54	0.41	0
27	CLR	l	202	-	31,31,31	0.36	0	48,48,48	0.75	0
27	CLR	n	205	-	31,31,31	0.37	0	48,48,48	0.58	0
23	PTY	p	403	-	49,49,49	0.46	0	52,54,54	0.45	0
27	CLR	n	202	-	31,31,31	0.39	0	48,48,48	0.68	0
27	CLR	n	203	-	31,31,31	0.36	0	48,48,48	0.67	0
27	CLR	o	203	-	31,31,31	0.36	0	48,48,48	0.68	0
23	PTY	a	902	-	49,49,49	0.47	0	52,54,54	0.37	0
27	CLR	j	202	-	31,31,31	0.42	0	48,48,48	0.89	3 (6%)
27	CLR	h	202	-	31,31,31	0.38	0	48,48,48	0.98	4 (8%)
23	PTY	p	401	-	49,49,49	0.47	0	52,54,54	0.43	0
22	PC1	P	502	-	53,53,53	0.50	0	59,61,61	0.47	1 (1%)
27	CLR	k	201	-	31,31,31	0.36	0	48,48,48	0.66	0
27	CLR	b	304	-	31,31,31	0.40	0	48,48,48	0.61	0
22	PC1	P	501	-	53,53,53	0.50	0	59,61,61	0.53	1 (1%)
23	PTY	b	303	-	49,49,49	0.48	0	52,54,54	0.39	0
27	CLR	l	203	-	31,31,31	0.36	0	48,48,48	0.62	0
24	WJP	a	905	-	32,33,34	1.81	7 (21%)	39,43,44	6.61	7 (17%)
27	CLR	m	201	-	31,31,31	0.41	0	48,48,48	0.67	0
26	LP3	a	907	-	34,34,34	0.52	0	39,41,41	0.56	0
27	CLR	i	203	-	31,31,31	0.47	0	48,48,48	0.85	1 (2%)
27	CLR	n	201	-	31,31,31	0.36	0	48,48,48	0.83	2 (4%)
23	PTY	p	402	-	49,49,49	0.47	0	52,54,54	0.42	0
27	CLR	l	205	-	31,31,31	0.35	0	48,48,48	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLR	l	206	-	31,31,31	0.39	0	48,48,48	0.55	0
23	PTY	a	904	-	49,49,49	0.47	0	52,54,54	0.37	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
22	PC1	a	901	-	-	21/57/57/57	-
27	CLR	j	203	-	-	6/10/68/68	0/4/4/4
27	CLR	h	201	-	-	3/10/68/68	0/4/4/4
27	CLR	i	202	-	-	4/10/68/68	0/4/4/4
27	CLR	m	202	-	-	1/10/68/68	0/4/4/4
25	NAG	a	906	12	-	2/6/23/26	0/1/1/1
21	ADP	A	701	-	-	3/16/32/32	0/3/3/3
22	PC1	b	301	-	-	23/57/57/57	-
27	CLR	o	201	-	-	6/10/68/68	0/4/4/4
23	PTY	p	404	-	-	23/53/53/53	-
27	CLR	i	204	-	-	6/10/68/68	0/4/4/4
27	CLR	k	202	-	-	2/10/68/68	0/4/4/4
27	CLR	l	204	-	-	2/10/68/68	0/4/4/4
27	CLR	j	201	-	-	4/10/68/68	0/4/4/4
27	CLR	k	203	-	-	2/10/68/68	0/4/4/4
27	CLR	j	204	-	-	4/10/68/68	0/4/4/4
27	CLR	n	204	-	-	3/10/68/68	0/4/4/4
22	PC1	l	201	-	-	21/57/57/57	-
23	PTY	a	903	-	-	19/53/53/53	-
27	CLR	i	201	-	-	3/10/68/68	0/4/4/4
27	CLR	m	203	-	-	5/10/68/68	0/4/4/4
27	CLR	o	202	-	-	6/10/68/68	0/4/4/4
23	PTY	b	302	-	-	22/53/53/53	-
27	CLR	l	202	-	-	4/10/68/68	0/4/4/4
27	CLR	n	205	-	-	4/10/68/68	0/4/4/4
23	PTY	p	403	-	-	24/53/53/53	-
27	CLR	n	202	-	-	1/10/68/68	0/4/4/4
27	CLR	n	203	-	-	2/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLR	o	203	-	-	3/10/68/68	0/4/4/4
23	PTY	a	902	-	-	19/53/53/53	-
27	CLR	j	202	-	-	7/10/68/68	0/4/4/4
27	CLR	h	202	-	-	7/10/68/68	0/4/4/4
23	PTY	p	401	-	-	17/53/53/53	-
22	PC1	P	502	-	-	20/57/57/57	-
27	CLR	k	201	-	-	3/10/68/68	0/4/4/4
27	CLR	b	304	-	-	4/10/68/68	0/4/4/4
22	PC1	P	501	-	-	24/57/57/57	-
23	PTY	b	303	-	-	23/53/53/53	-
27	CLR	l	203	-	-	4/10/68/68	0/4/4/4
24	WJP	a	905	-	-	16/37/37/40	-
27	CLR	m	201	-	-	4/10/68/68	0/4/4/4
26	LP3	a	907	-	-	14/36/36/36	-
27	CLR	i	203	-	-	5/10/68/68	0/4/4/4
27	CLR	n	201	-	-	1/10/68/68	0/4/4/4
23	PTY	p	402	-	-	24/53/53/53	-
27	CLR	l	205	-	-	6/10/68/68	0/4/4/4
27	CLR	l	206	-	-	4/10/68/68	0/4/4/4
23	PTY	a	904	-	-	20/53/53/53	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	905	WJP	P27-O30	4.82	1.64	1.59
21	A	701	ADP	C5-C4	4.43	1.47	1.39
24	a	905	WJP	C18-C16	3.76	1.59	1.51
24	a	905	WJP	C07-C06	3.11	1.58	1.50
24	a	905	WJP	P31-O32	3.07	1.66	1.54

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	905	WJP	C08-C06-C05	20.90	168.09	121.17
24	a	905	WJP	C17-C16-C18	-20.34	79.92	115.23
24	a	905	WJP	C17-C16-C15	17.18	167.76	123.63
24	a	905	WJP	C07-C06-C08	-15.66	88.04	115.23
24	a	905	WJP	C18-C16-C15	-14.70	88.18	121.17

There are no chirality outliers.

5 of 451 torsion outliers are listed below:

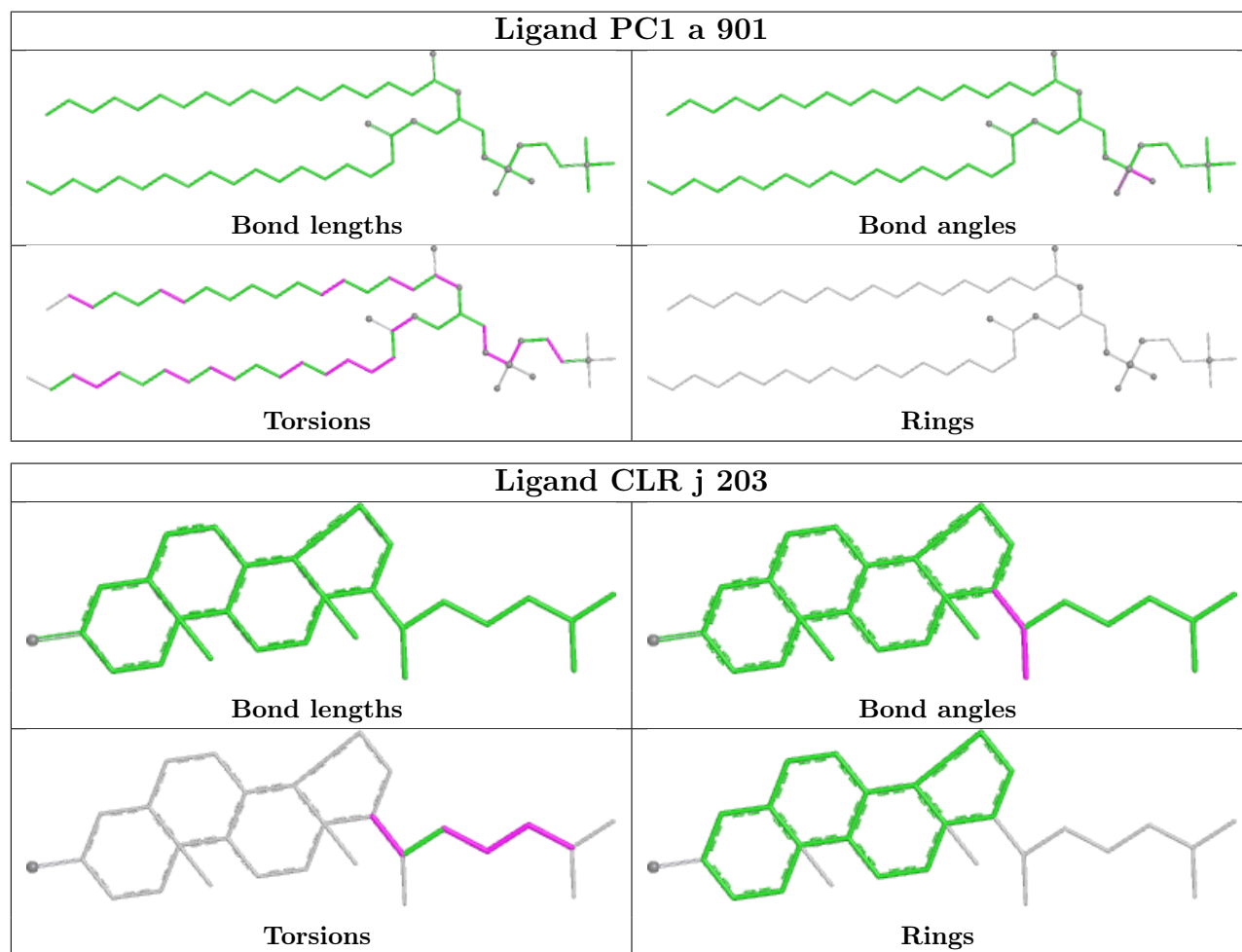
Mol	Chain	Res	Type	Atoms
21	A	701	ADP	C5'-O5'-PA-O1A
21	A	701	ADP	C5'-O5'-PA-O2A
21	A	701	ADP	C5'-O5'-PA-O3A
22	P	501	PC1	C11-O13-P-O11
22	P	501	PC1	C1-O11-P-O13

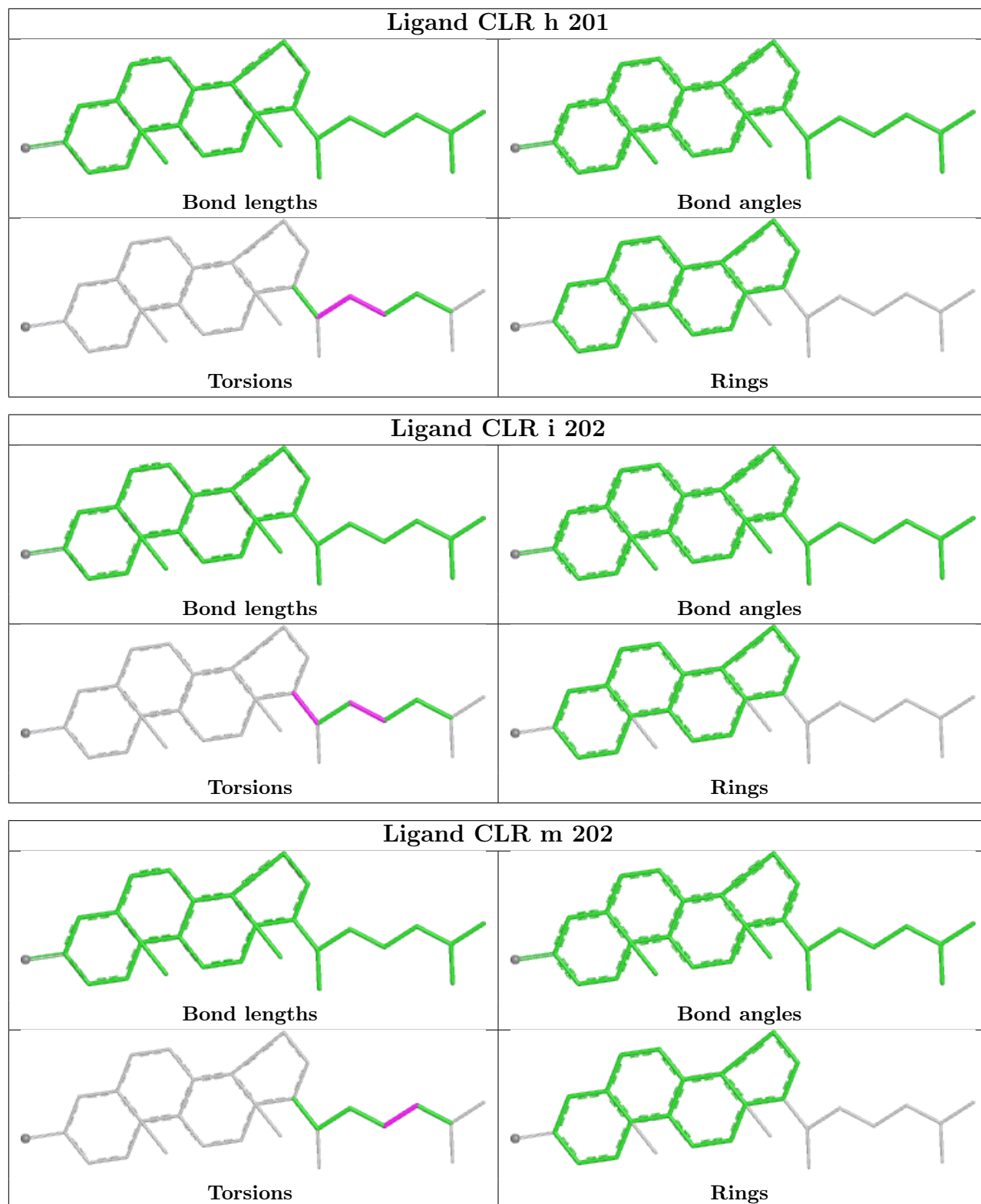
There are no ring outliers.

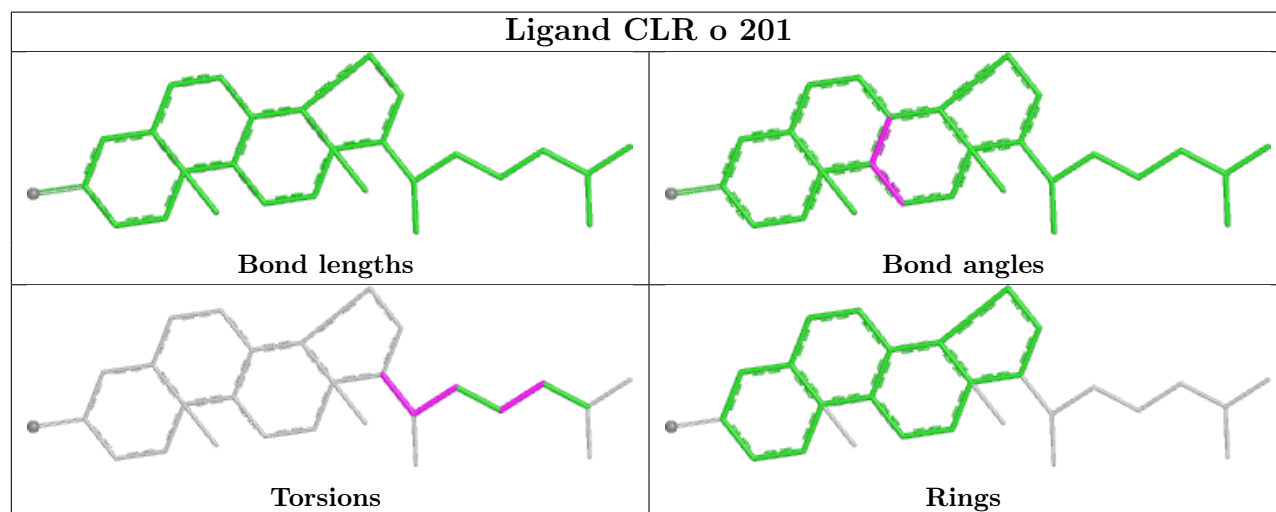
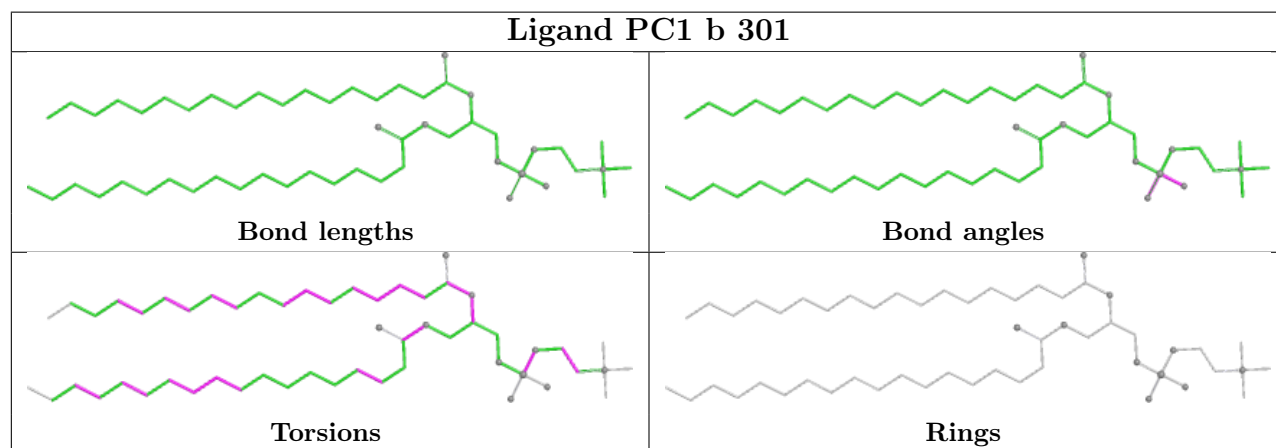
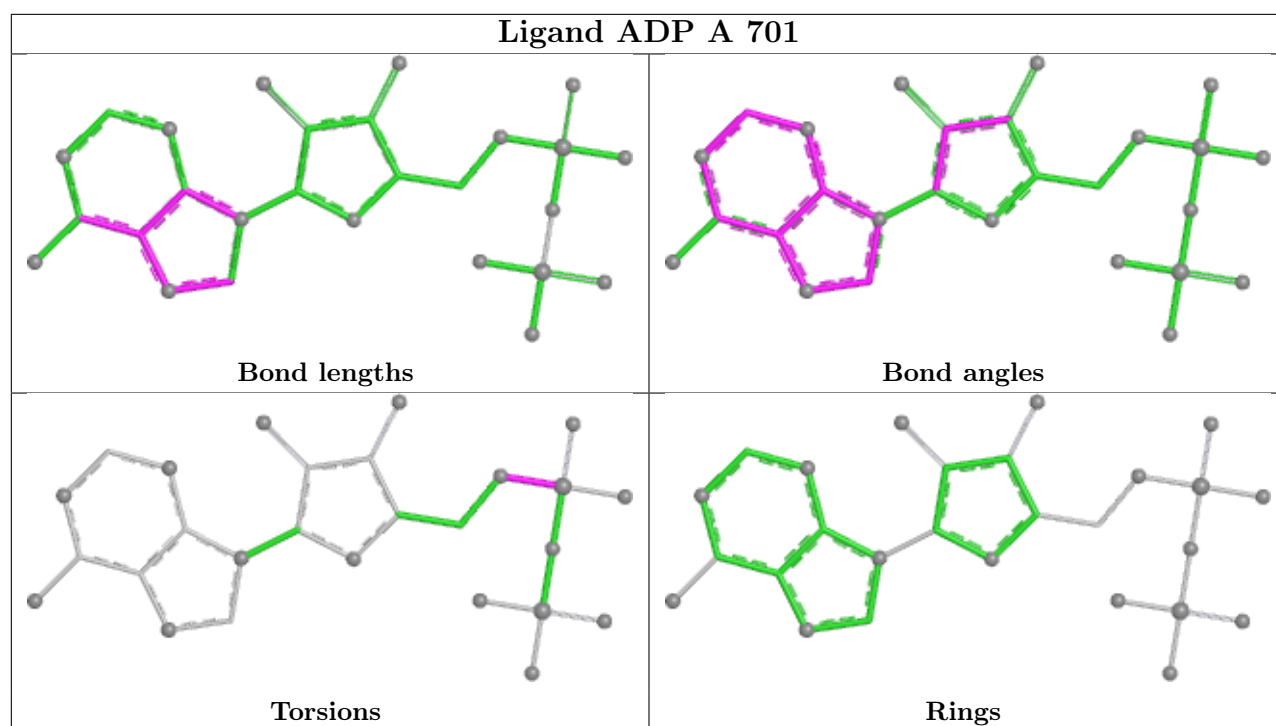
30 monomers are involved in 55 short contacts:

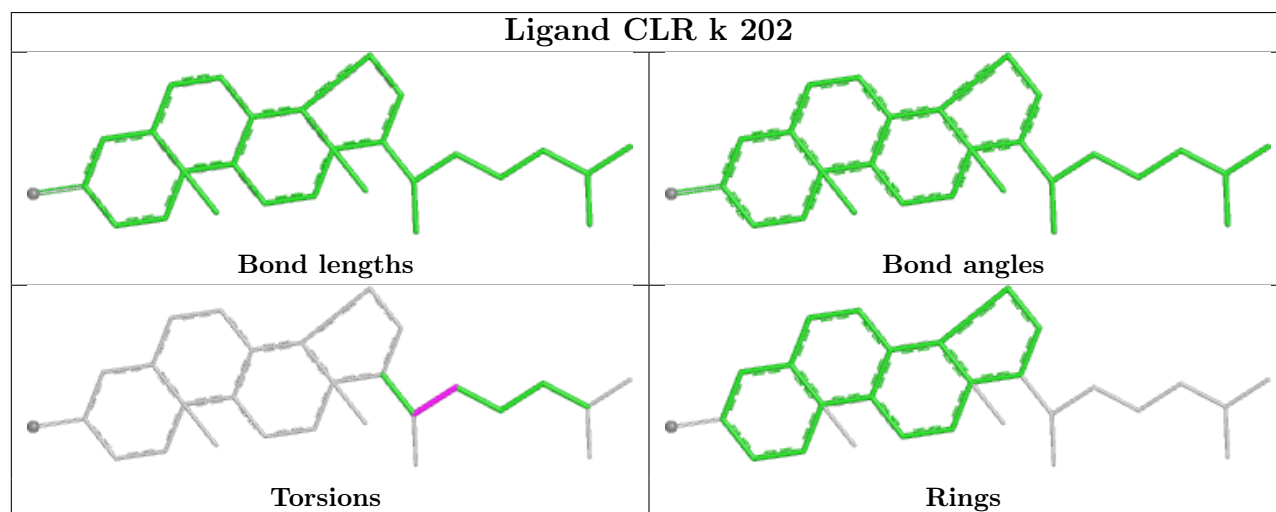
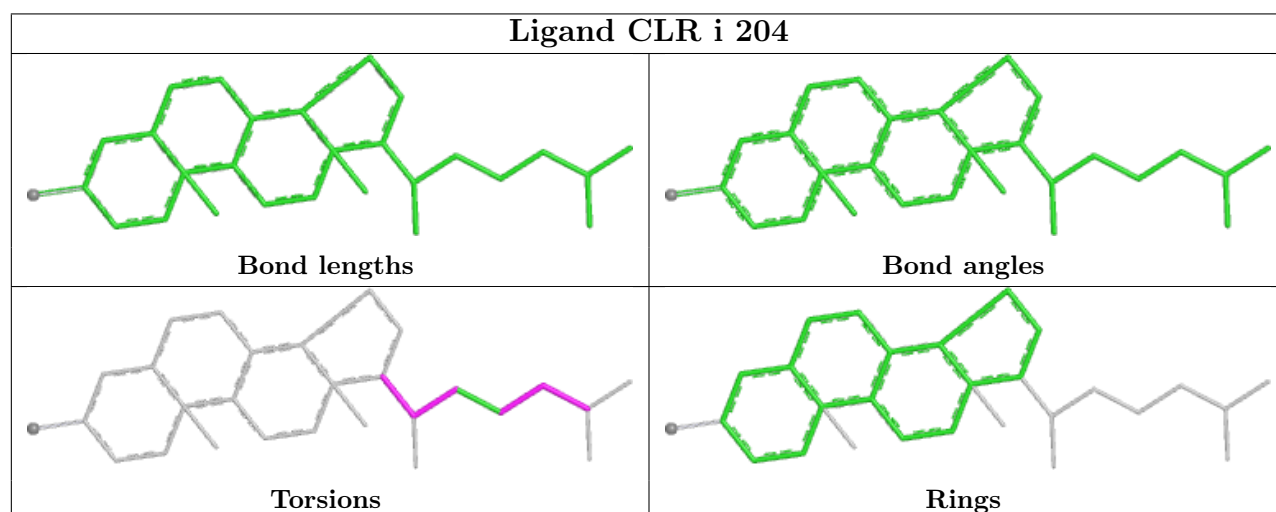
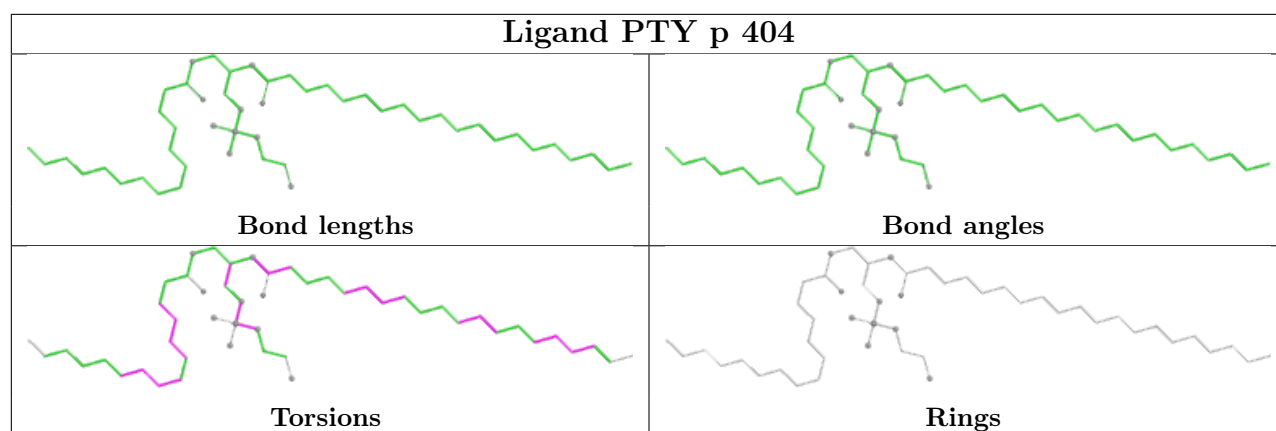
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	901	PC1	1	0
27	j	203	CLR	5	0
27	h	201	CLR	3	0
27	m	202	CLR	1	0
25	a	906	NAG	3	0
21	A	701	ADP	2	0
27	o	201	CLR	3	0
27	i	204	CLR	1	0
27	j	201	CLR	1	0
27	j	204	CLR	1	0
27	n	204	CLR	2	0
23	a	903	PTY	1	0
27	o	202	CLR	4	0
23	b	302	PTY	1	0
27	n	205	CLR	2	0
23	p	403	PTY	2	0
27	n	202	CLR	2	0
27	o	203	CLR	2	0
27	j	202	CLR	2	0
27	h	202	CLR	1	0
23	p	401	PTY	4	0
22	P	502	PC1	2	0
27	k	201	CLR	2	0
27	b	304	CLR	1	0
22	P	501	PC1	2	0
27	l	203	CLR	1	0
24	a	905	WJP	1	0
27	i	203	CLR	7	0
27	n	201	CLR	3	0
23	a	904	PTY	1	0

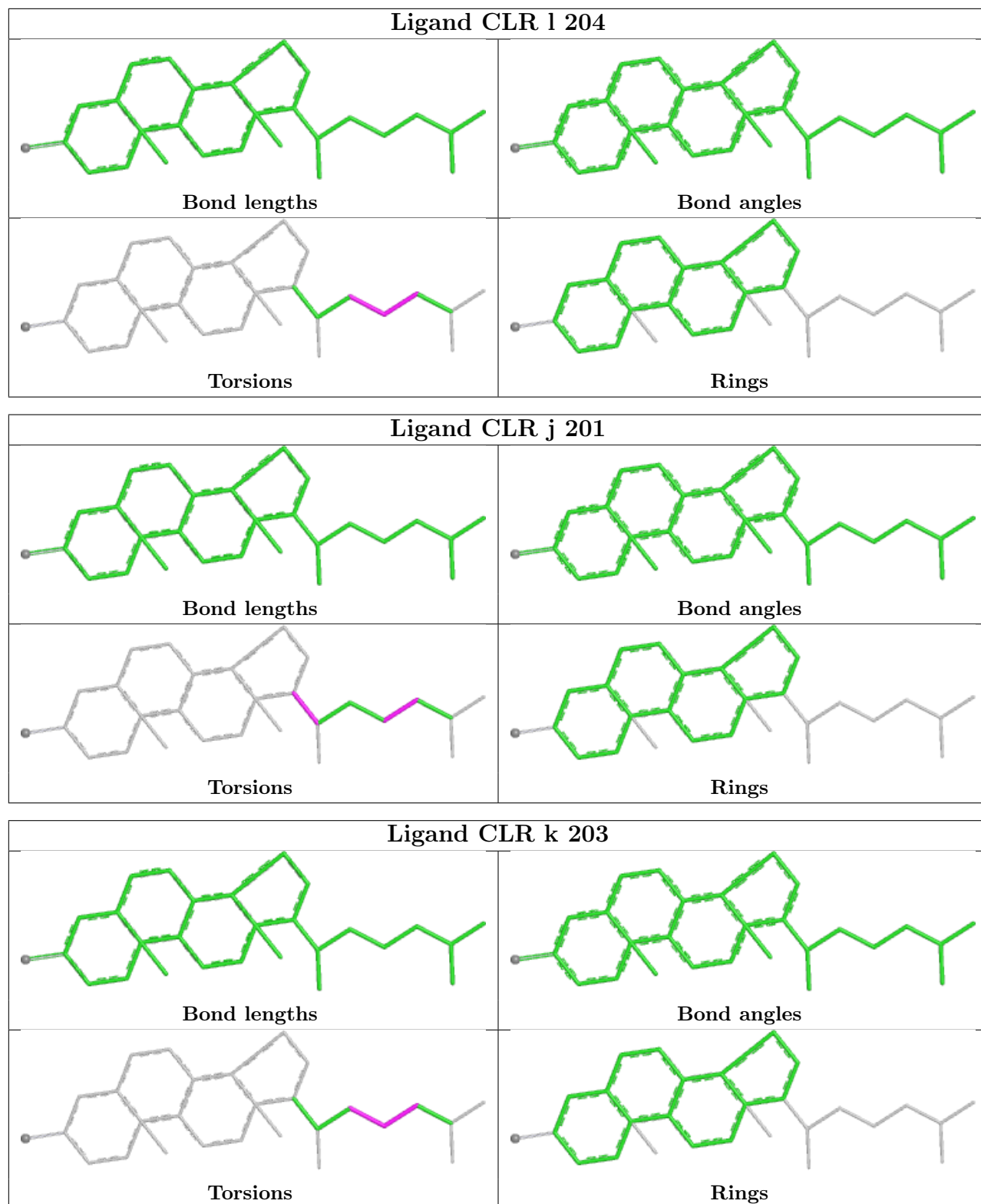
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

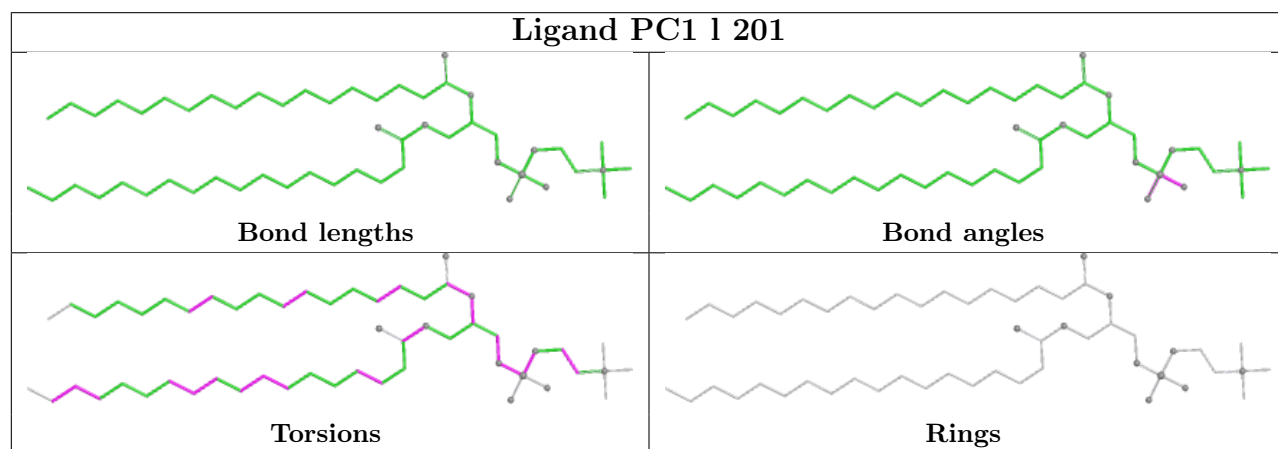
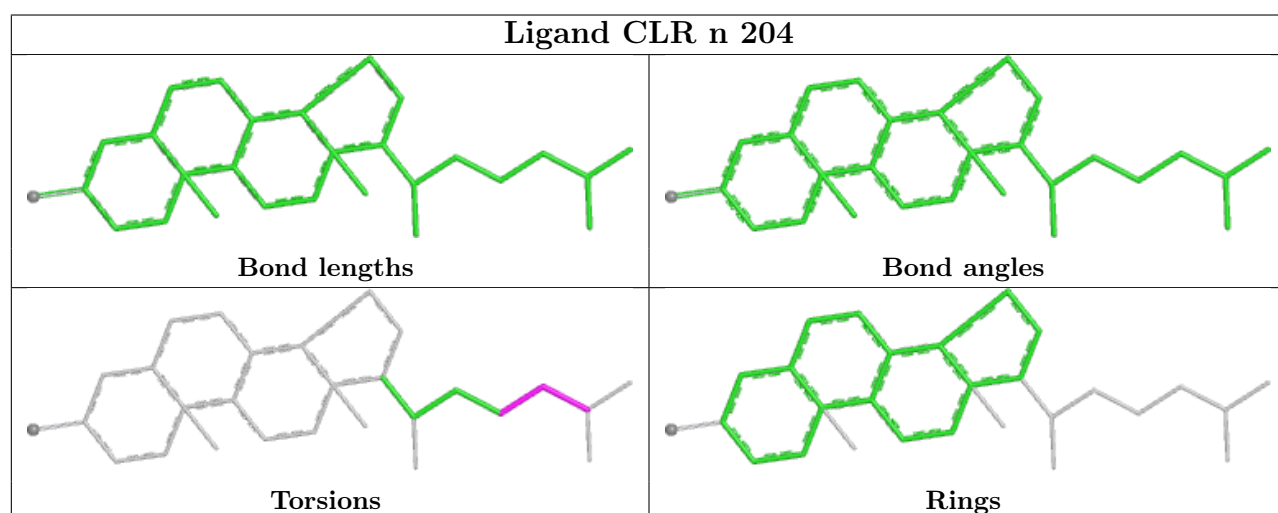
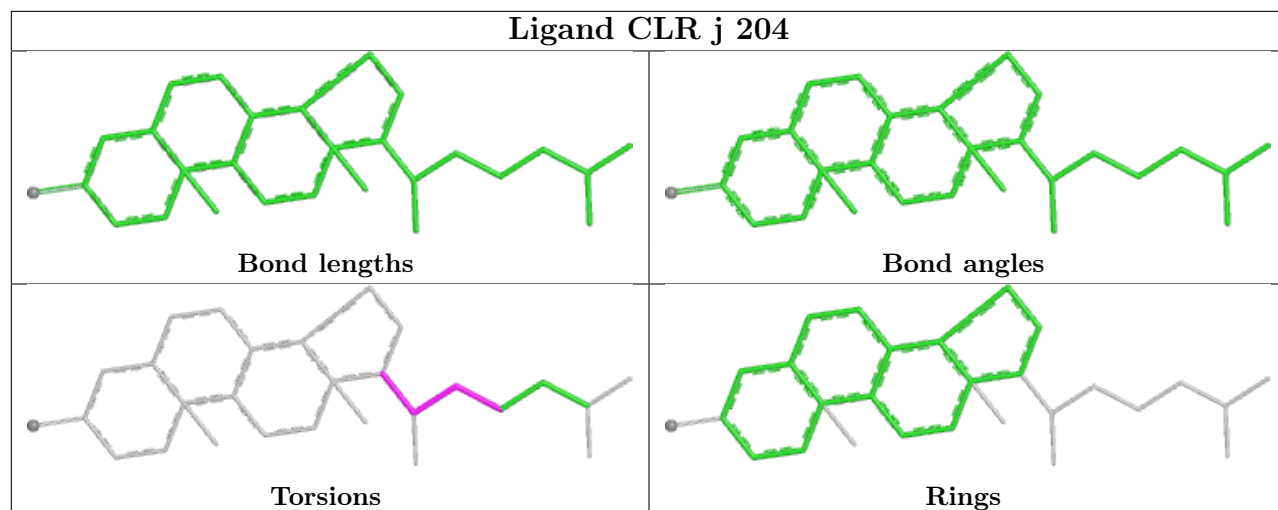


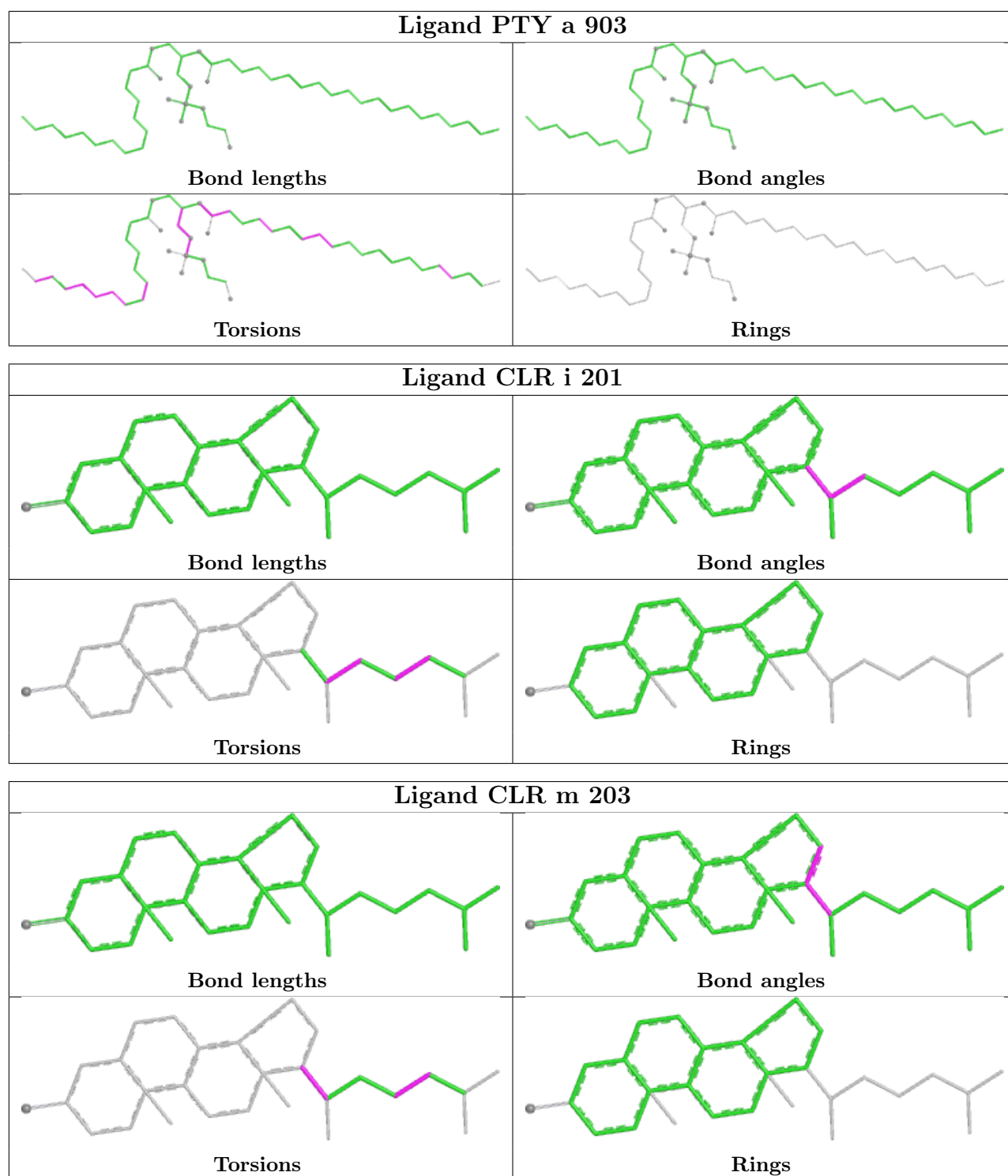


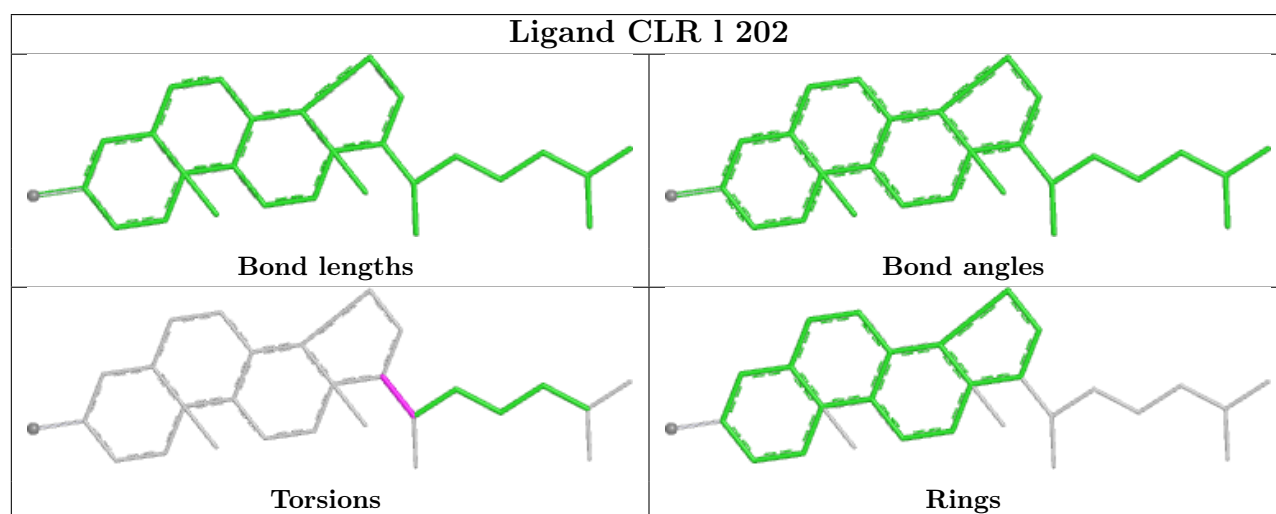
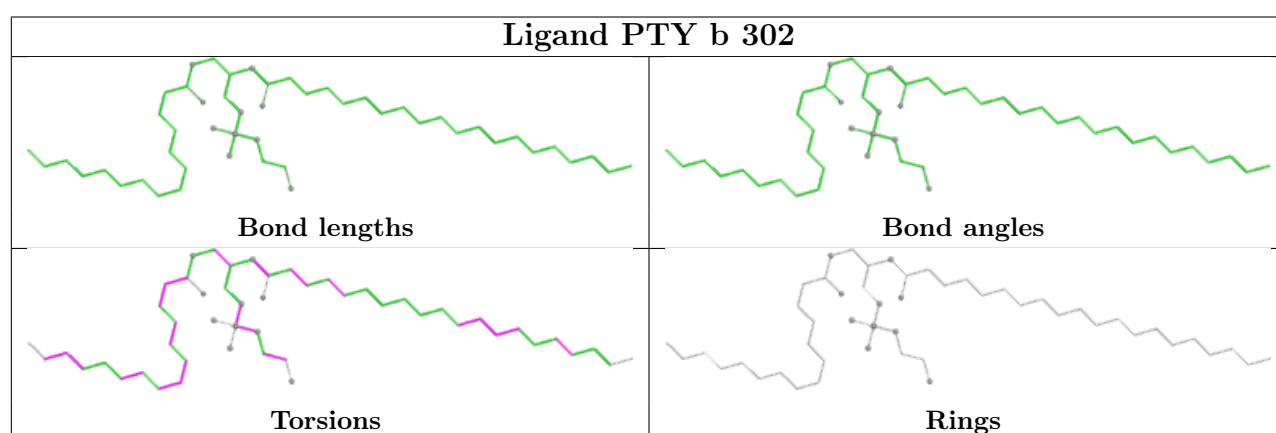
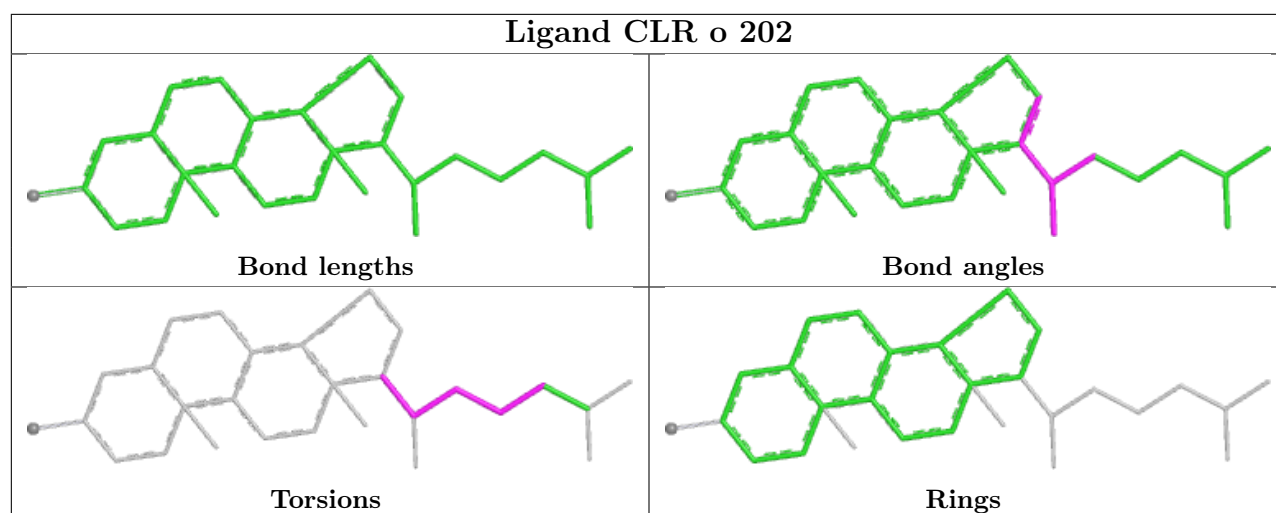


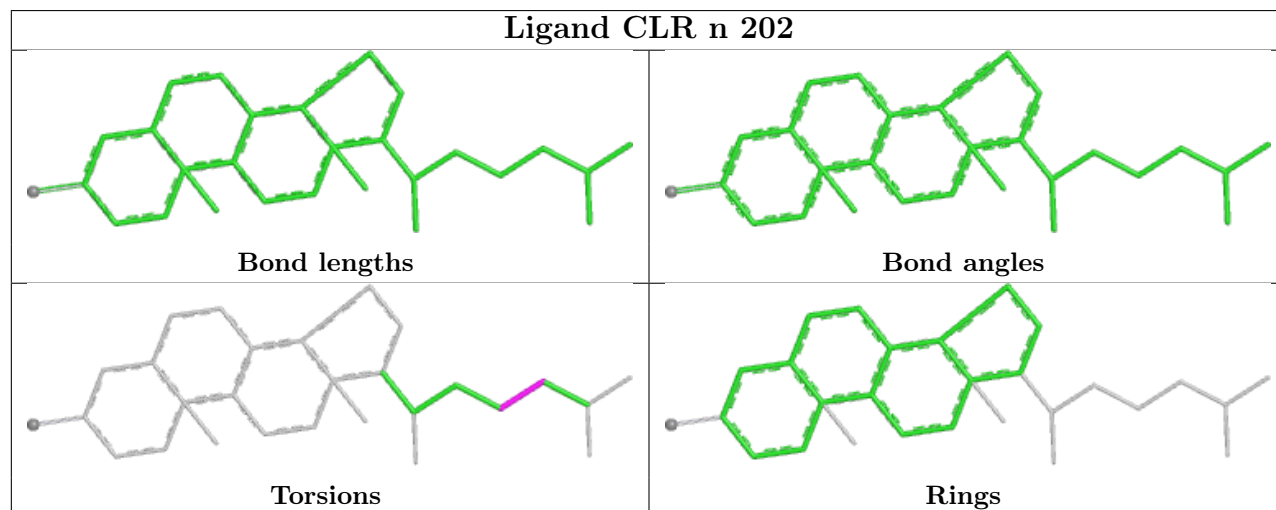
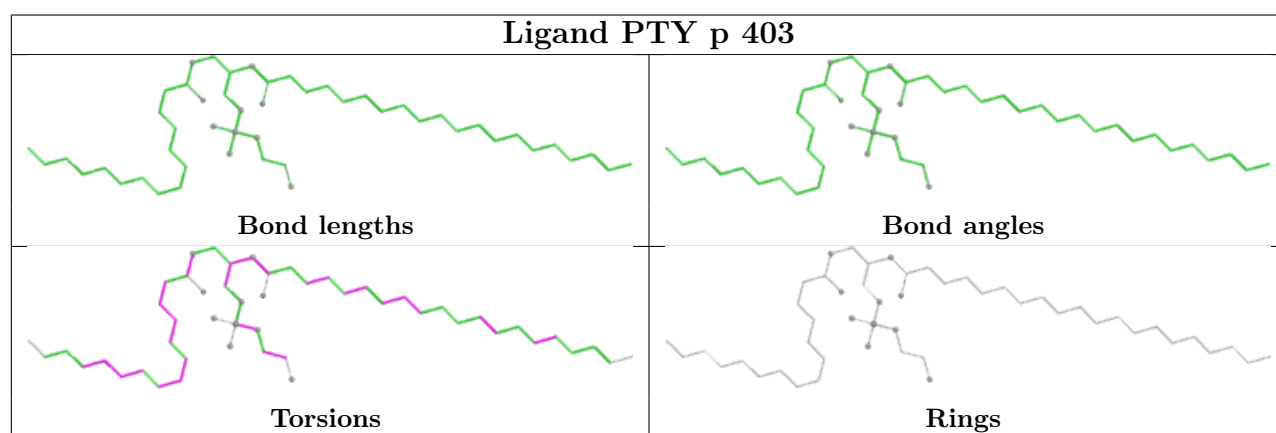
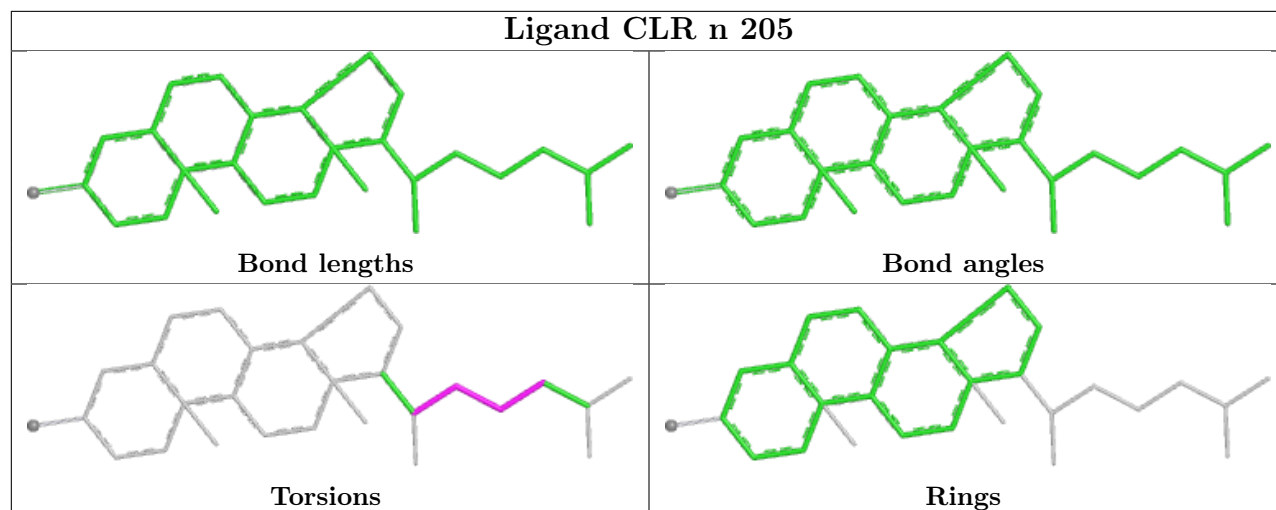


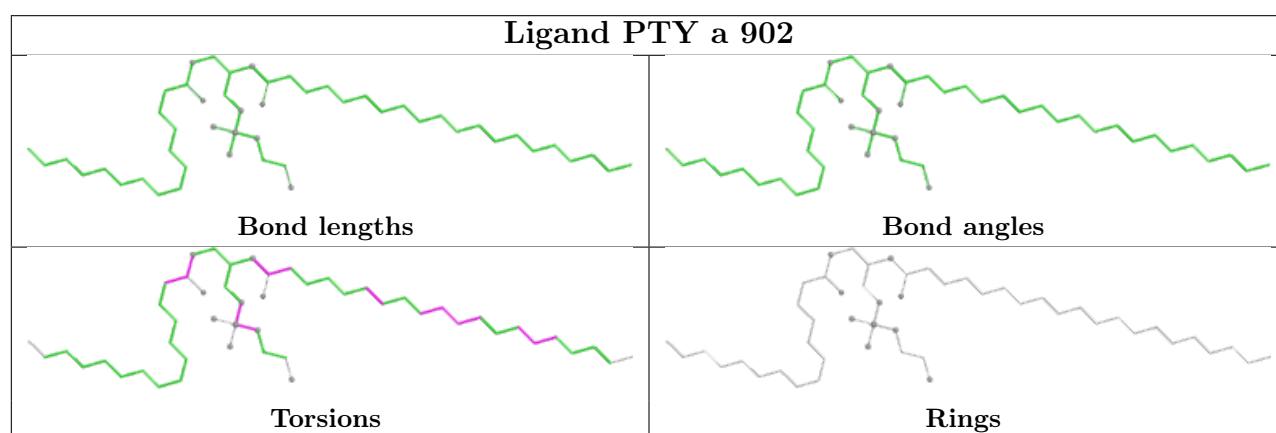
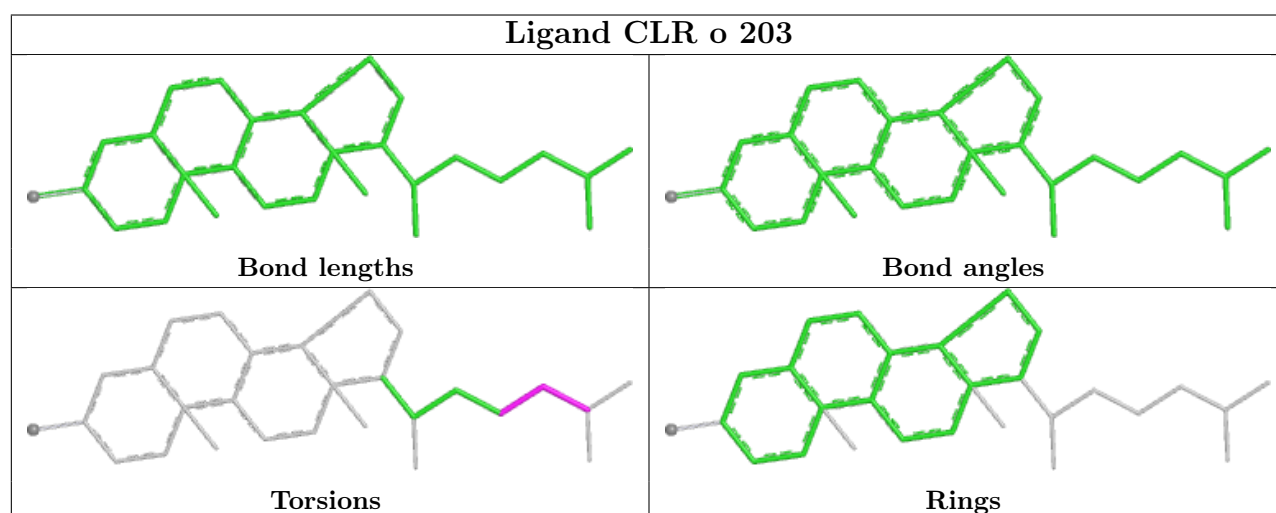
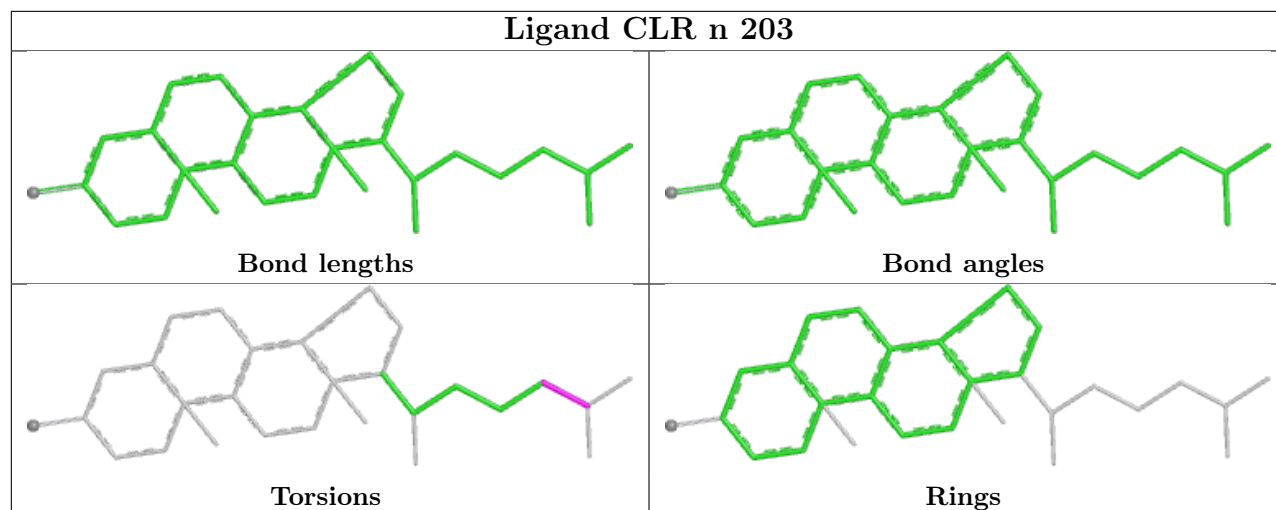


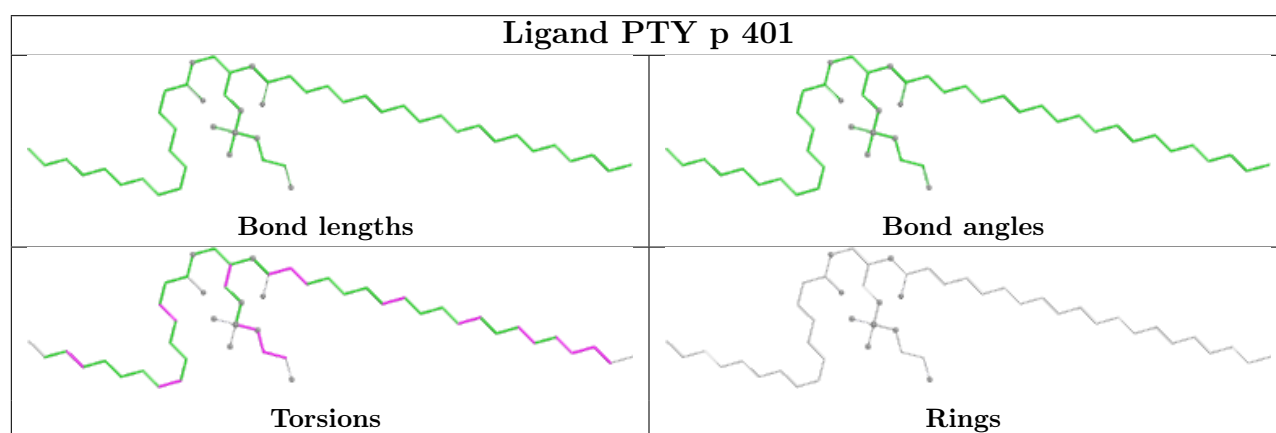
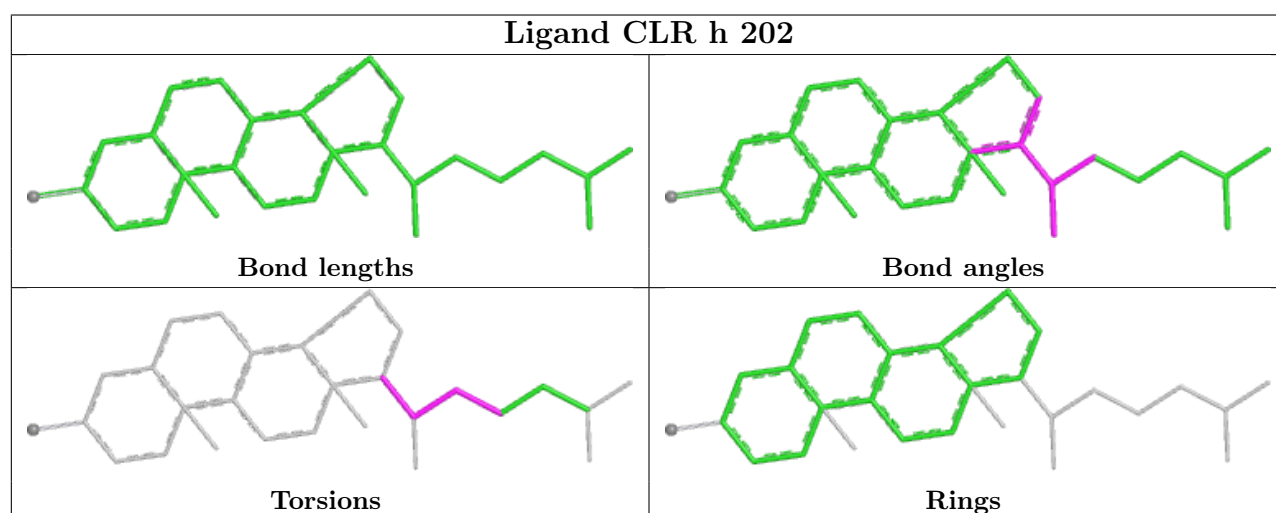
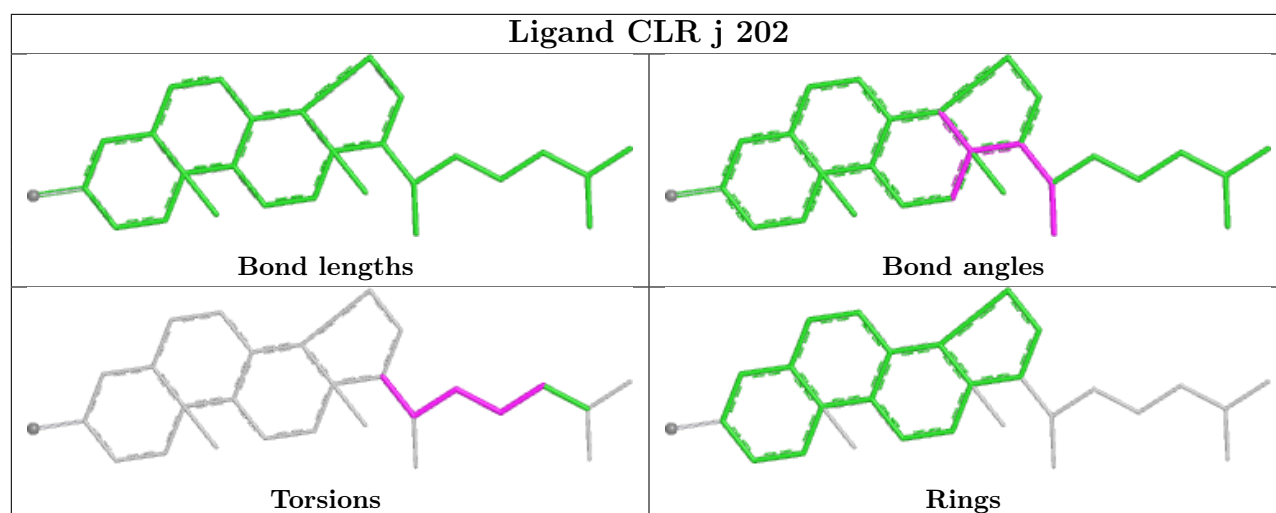


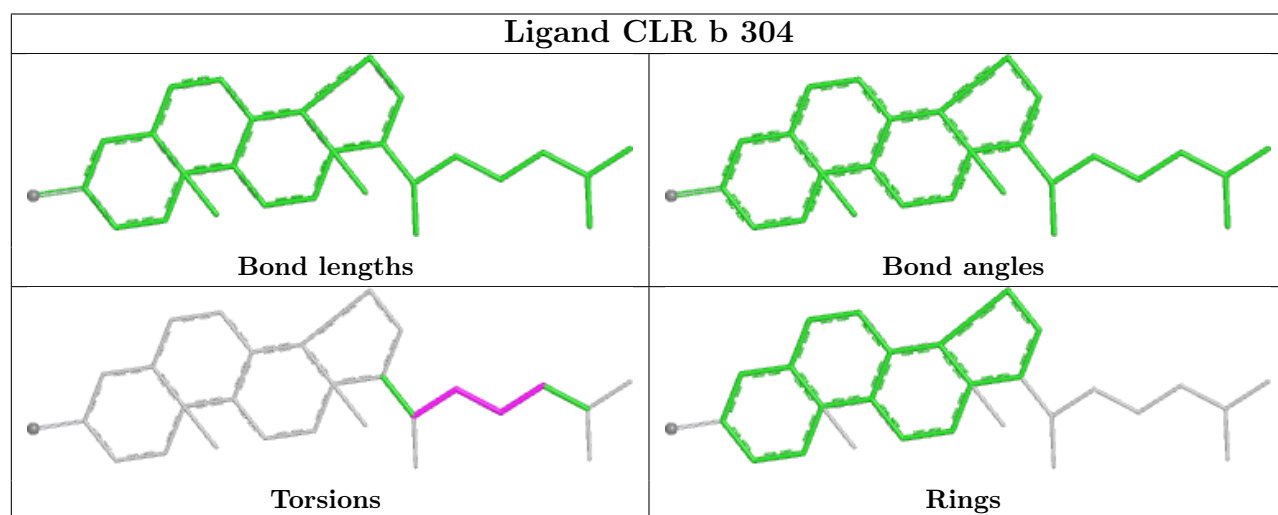
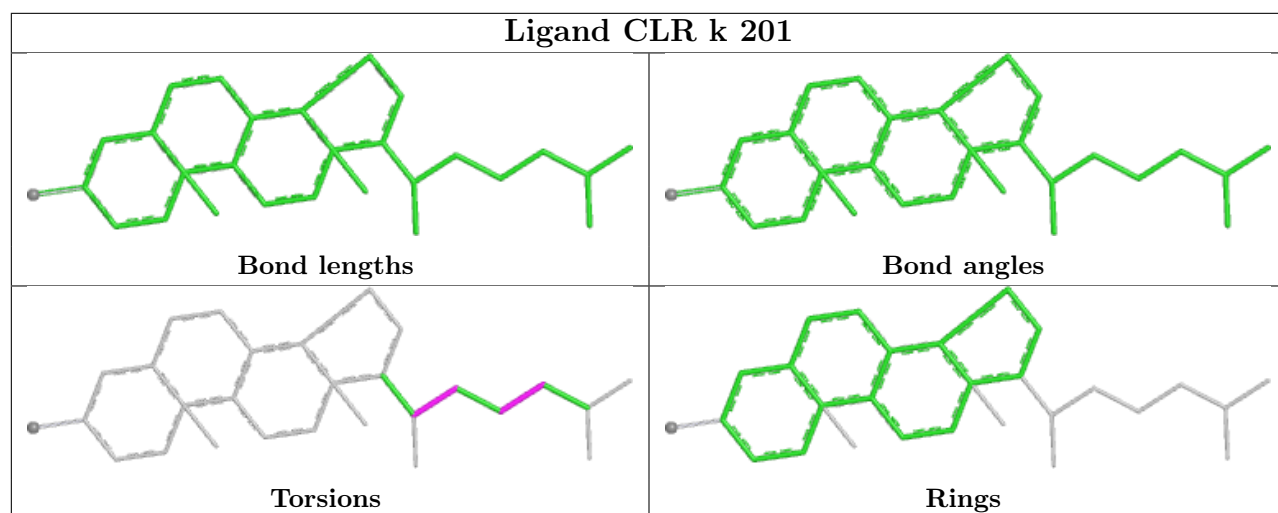
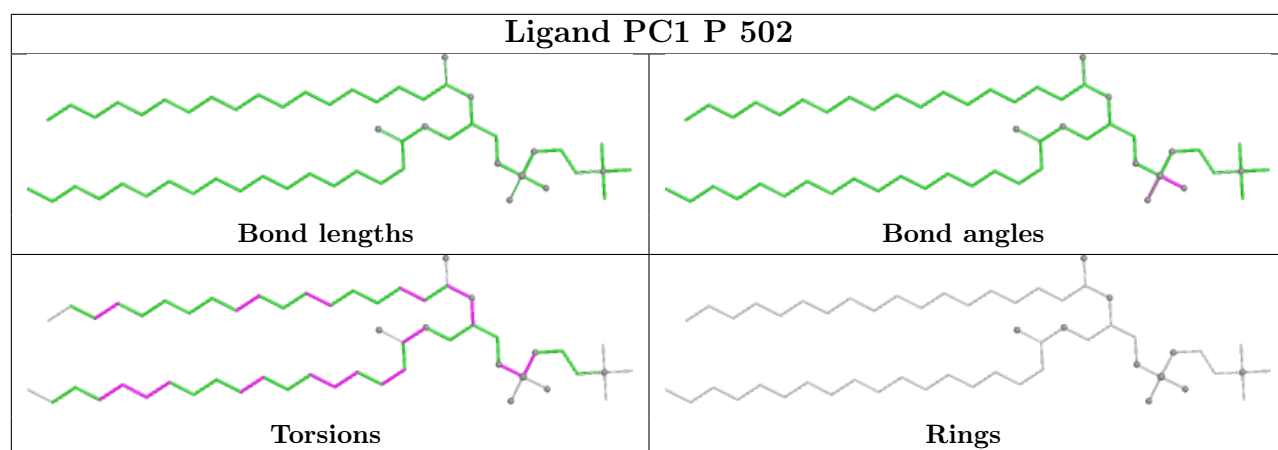


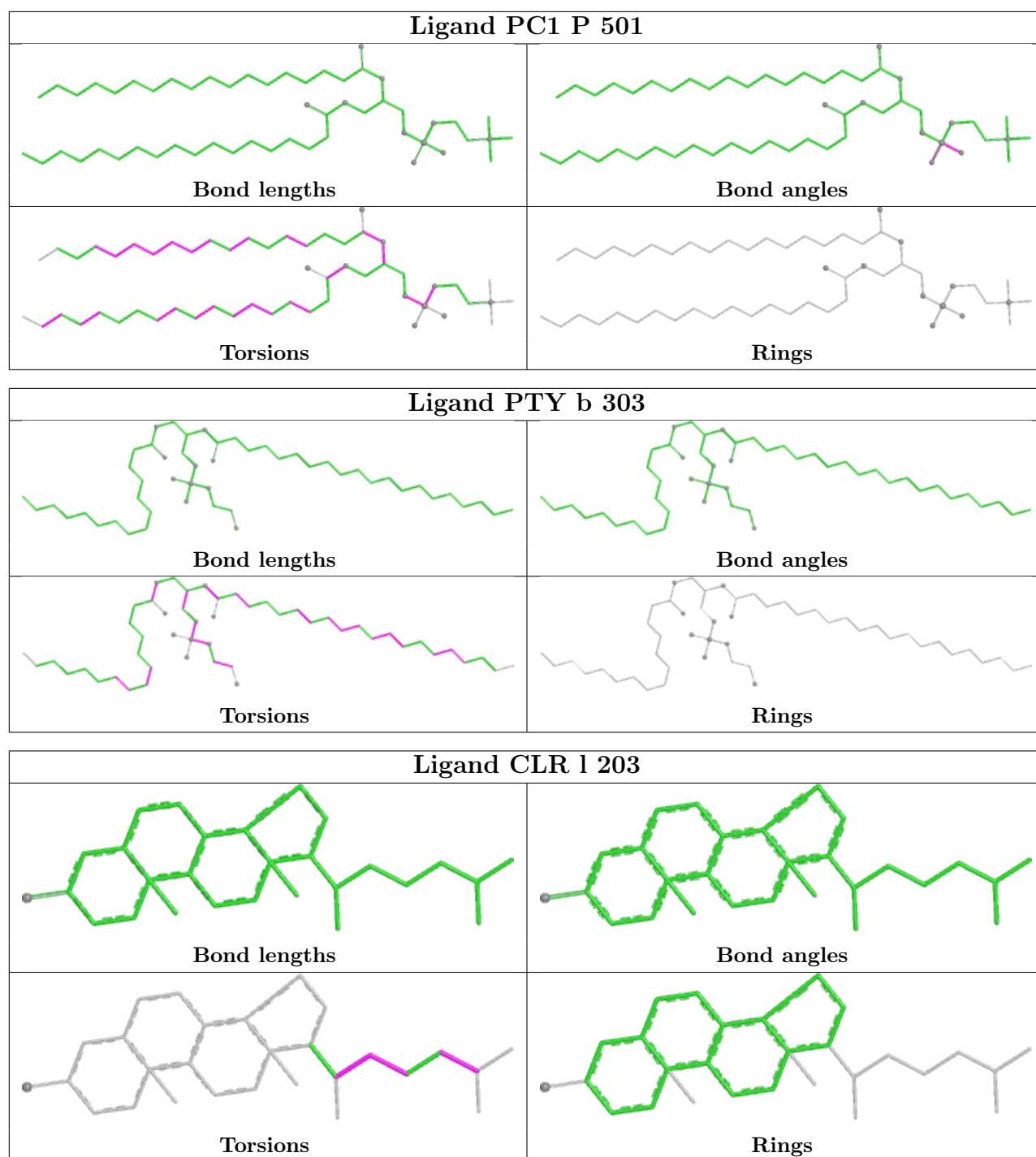


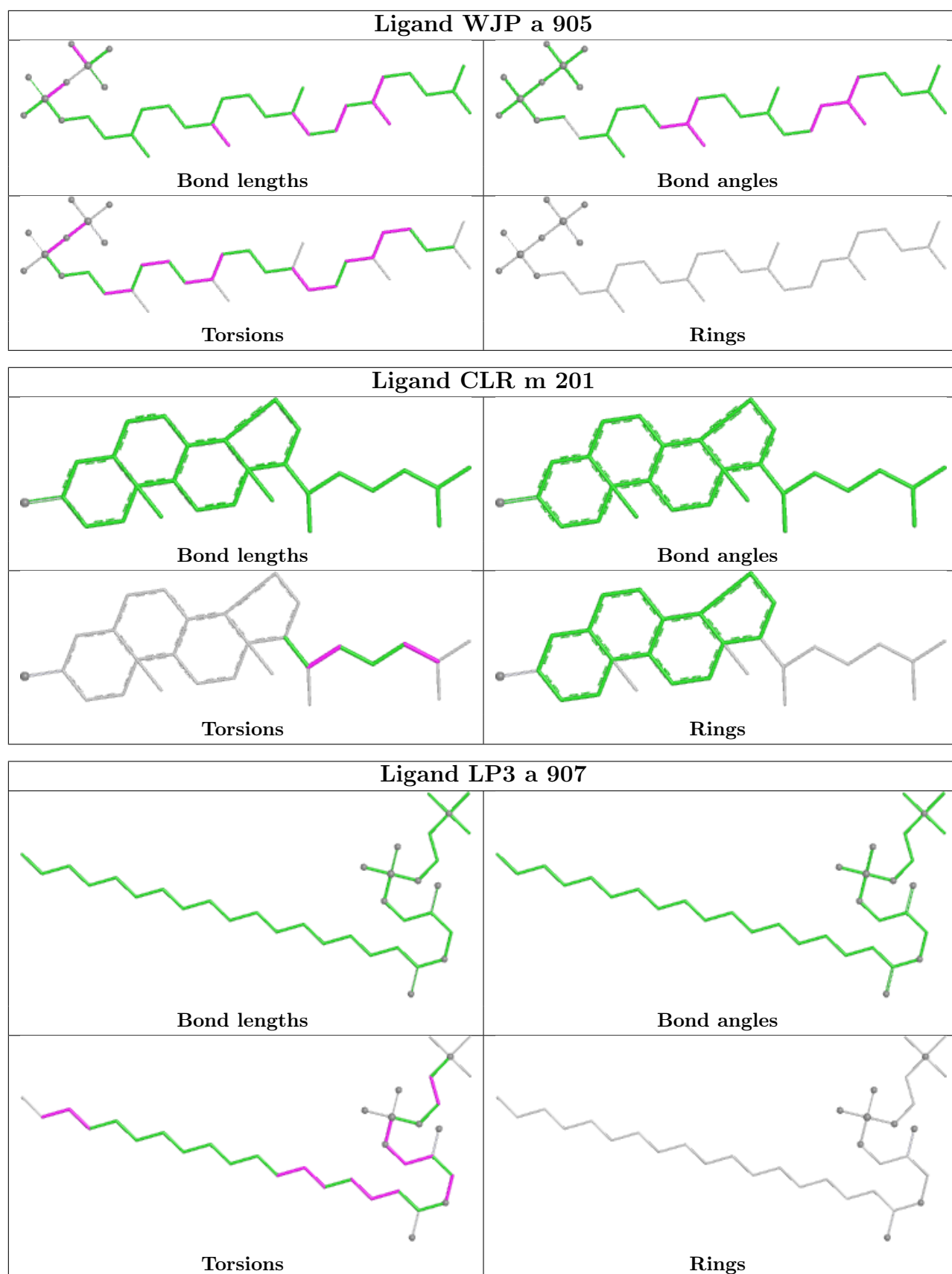


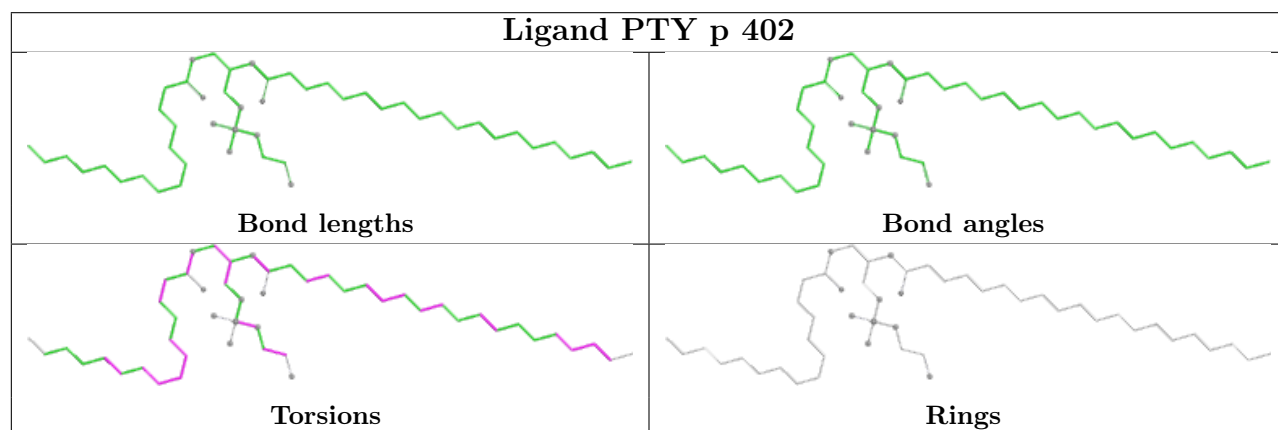
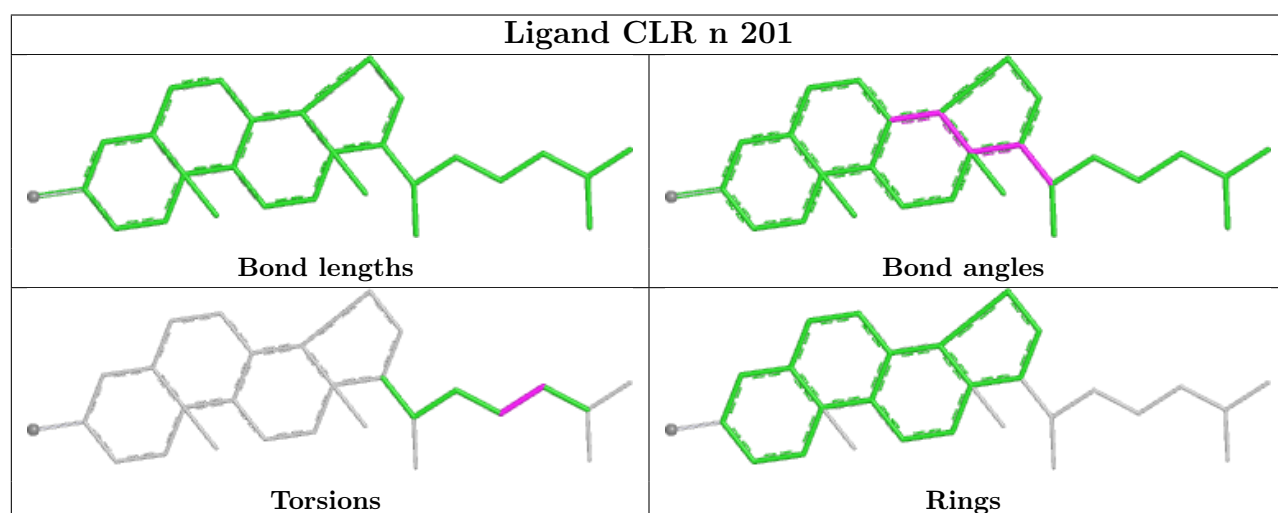
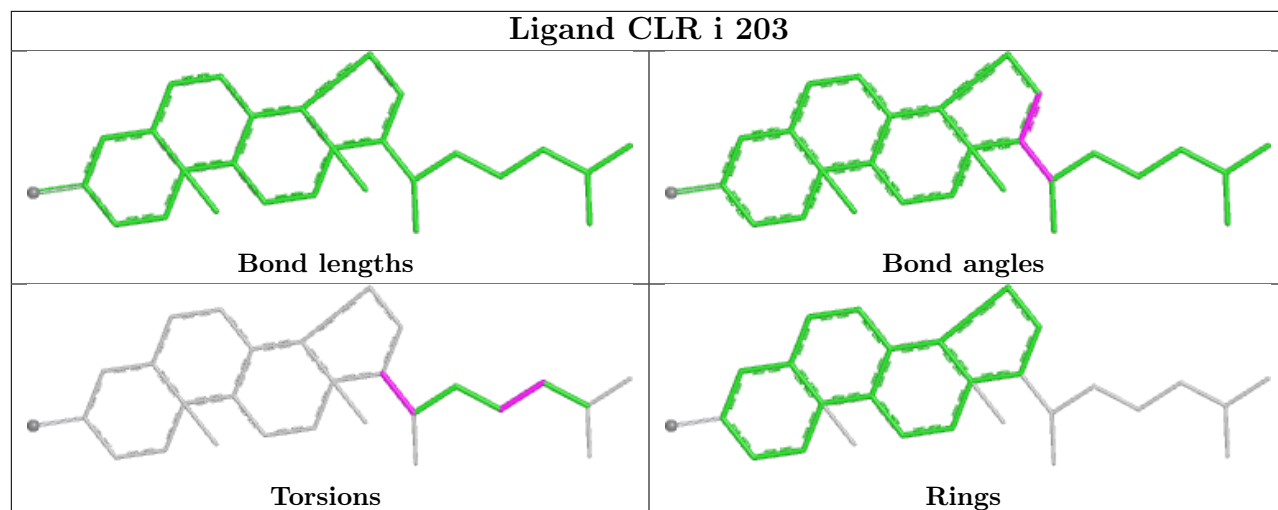


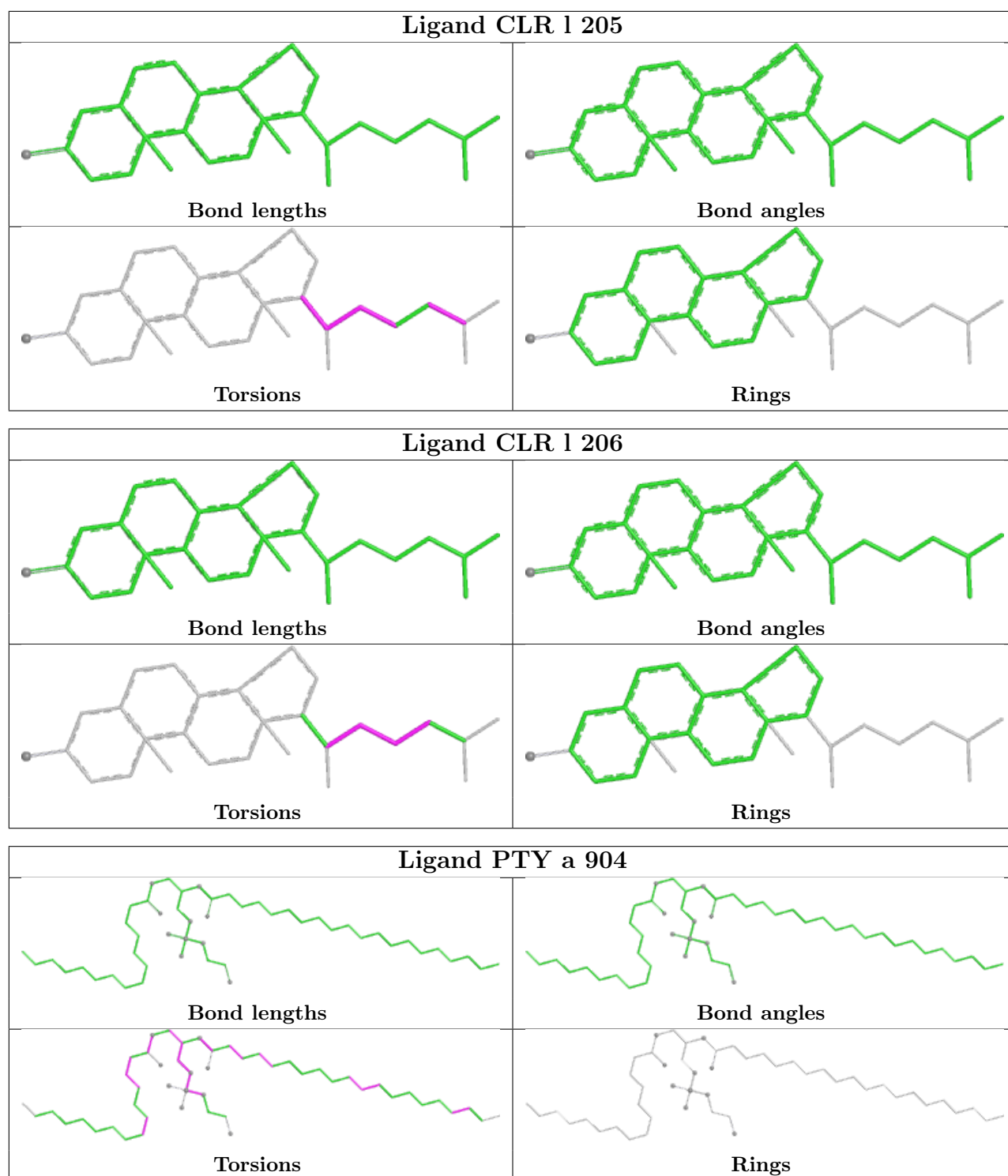












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44353. These allow visual inspection of the internal detail of the map and identification of artifacts.

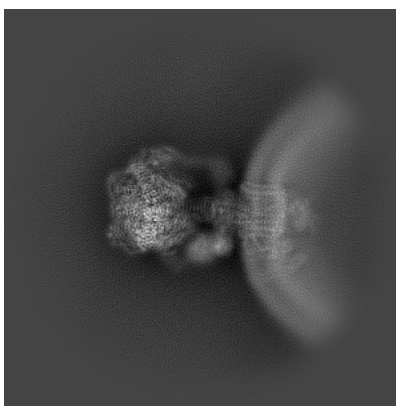
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

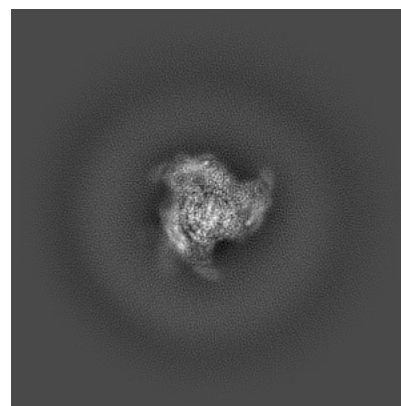
5.1.1 Primary map



X

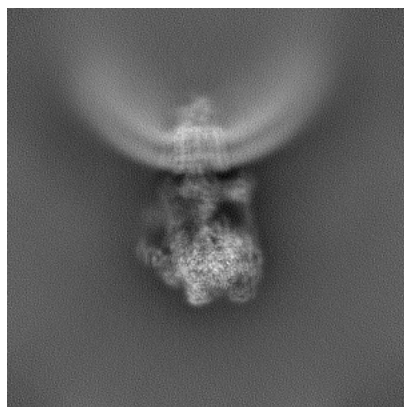


Y

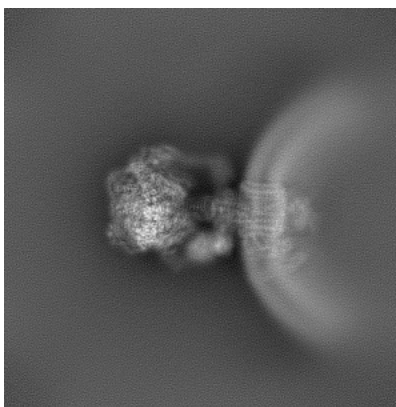


Z

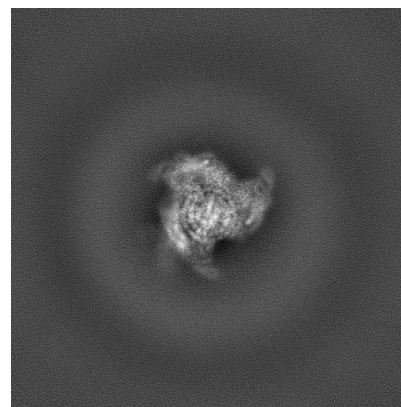
5.1.2 Raw map



X



Y



Z

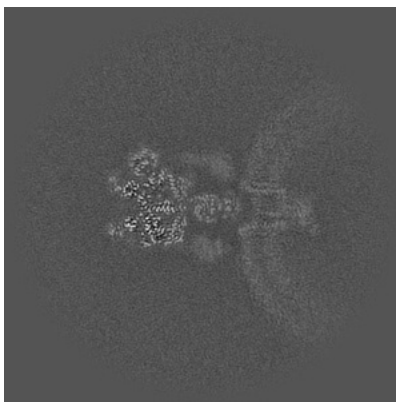
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

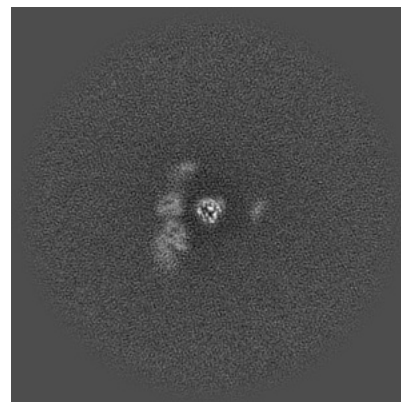
5.2.1 Primary map



X Index: 192

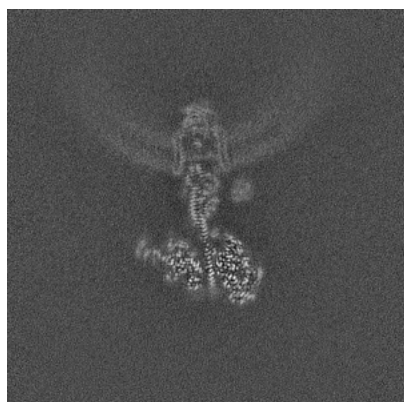


Y Index: 192

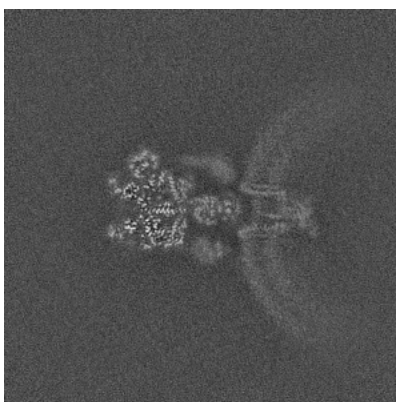


Z Index: 192

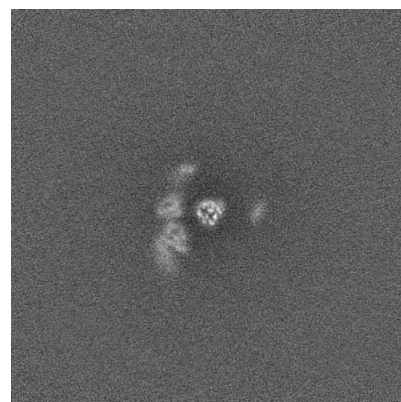
5.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

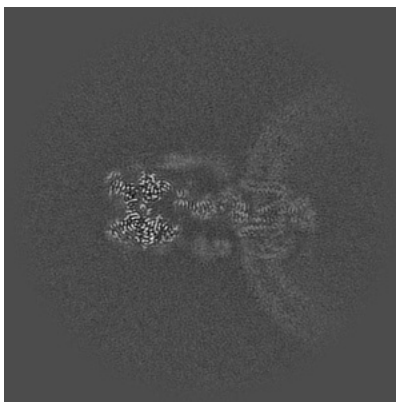
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

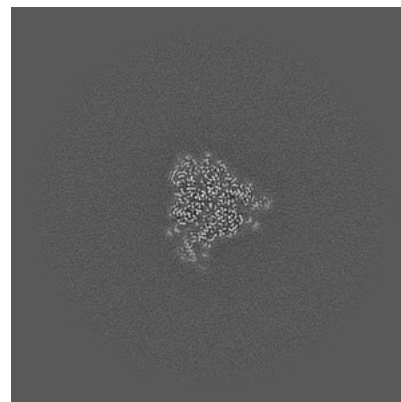
5.3.1 Primary map



X Index: 191



Y Index: 185

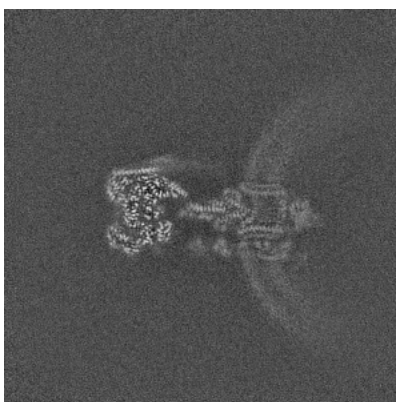


Z Index: 136

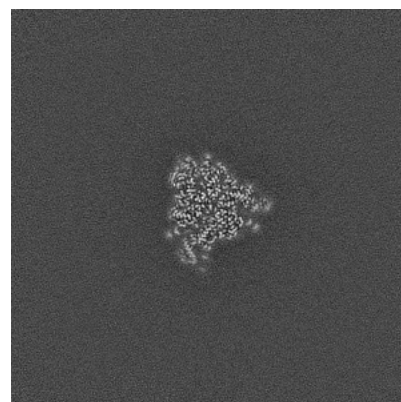
5.3.2 Raw map



X Index: 191



Y Index: 179

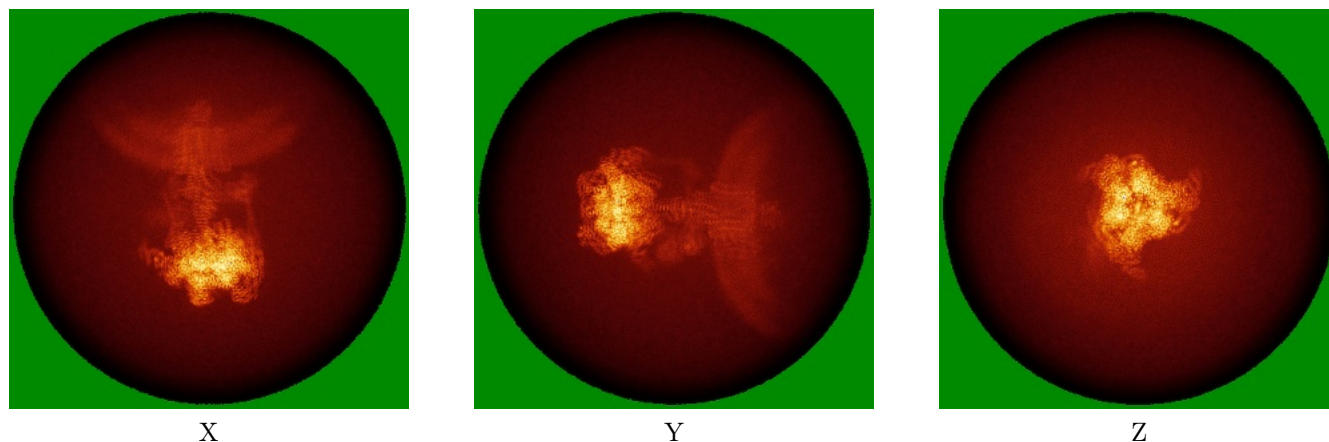


Z Index: 136

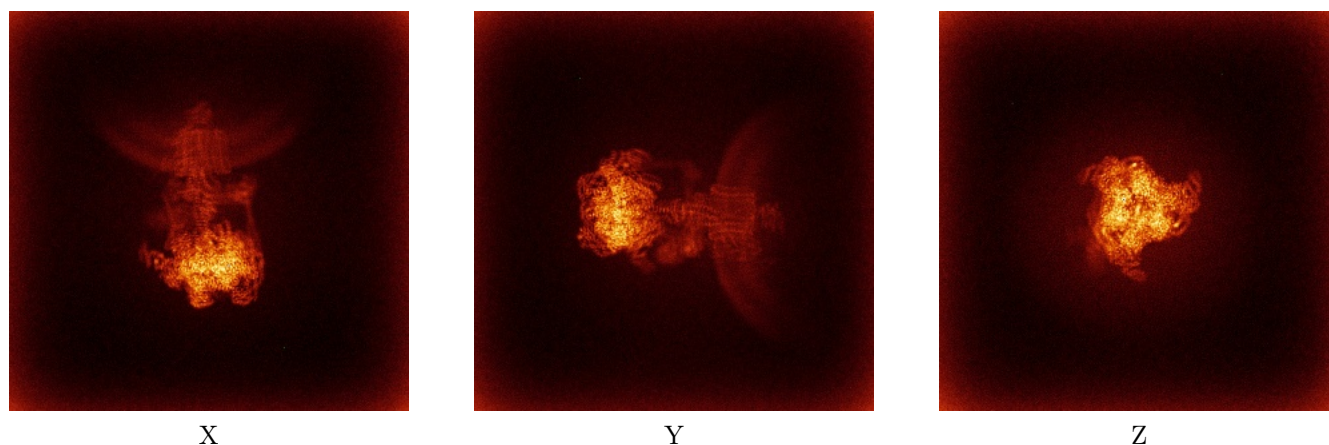
The images above show the largest variance slices of the map in three orthogonal directions.

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

5.4.1 Primary map



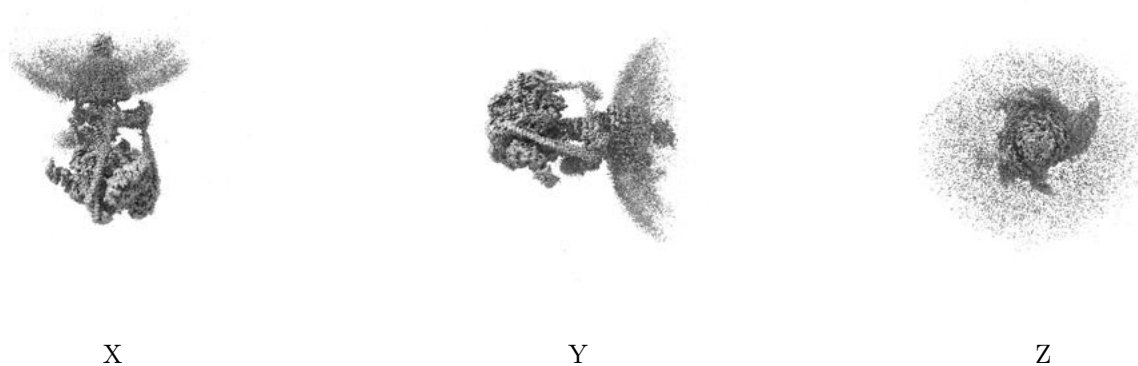
5.4.2 Raw map



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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

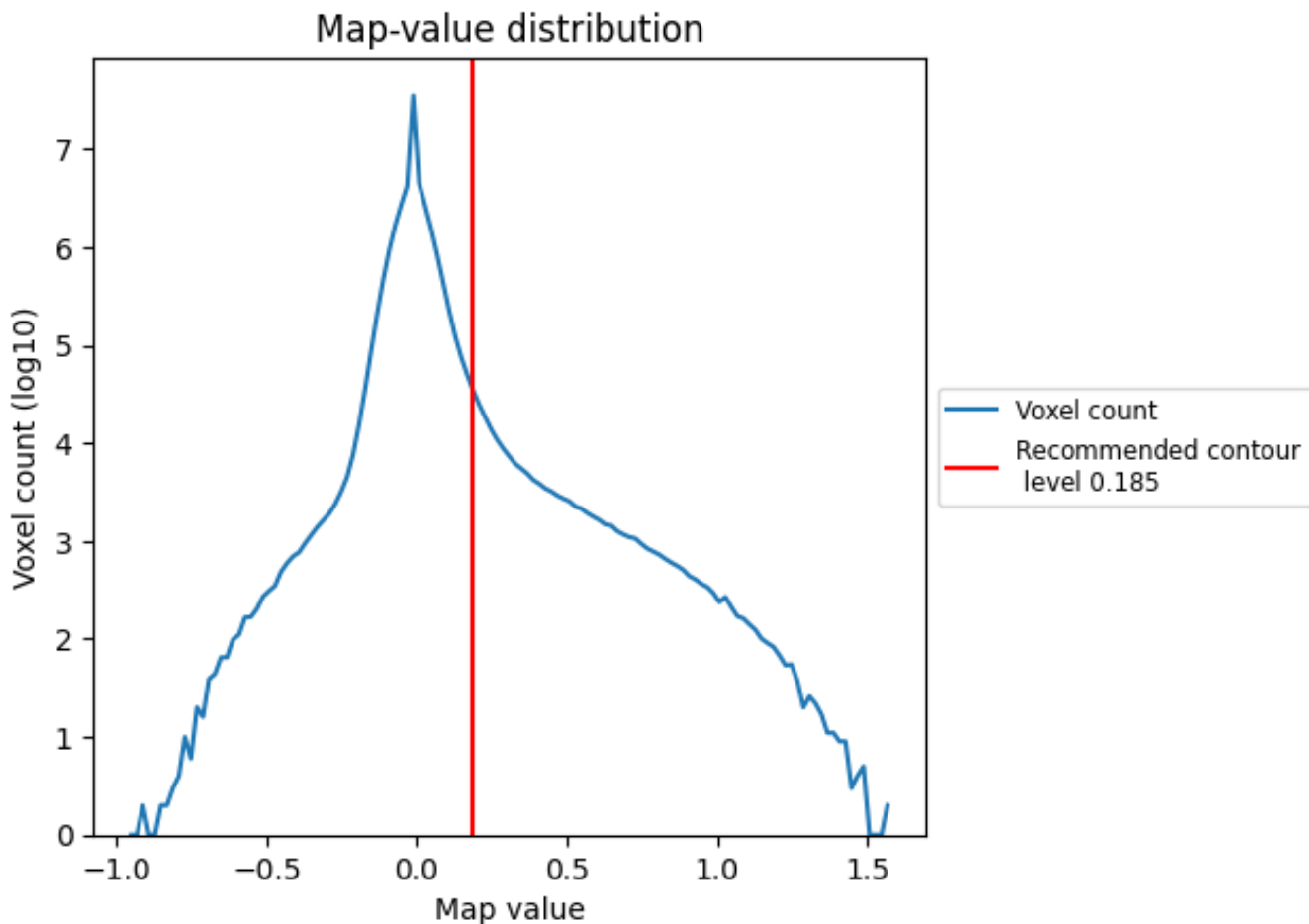
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

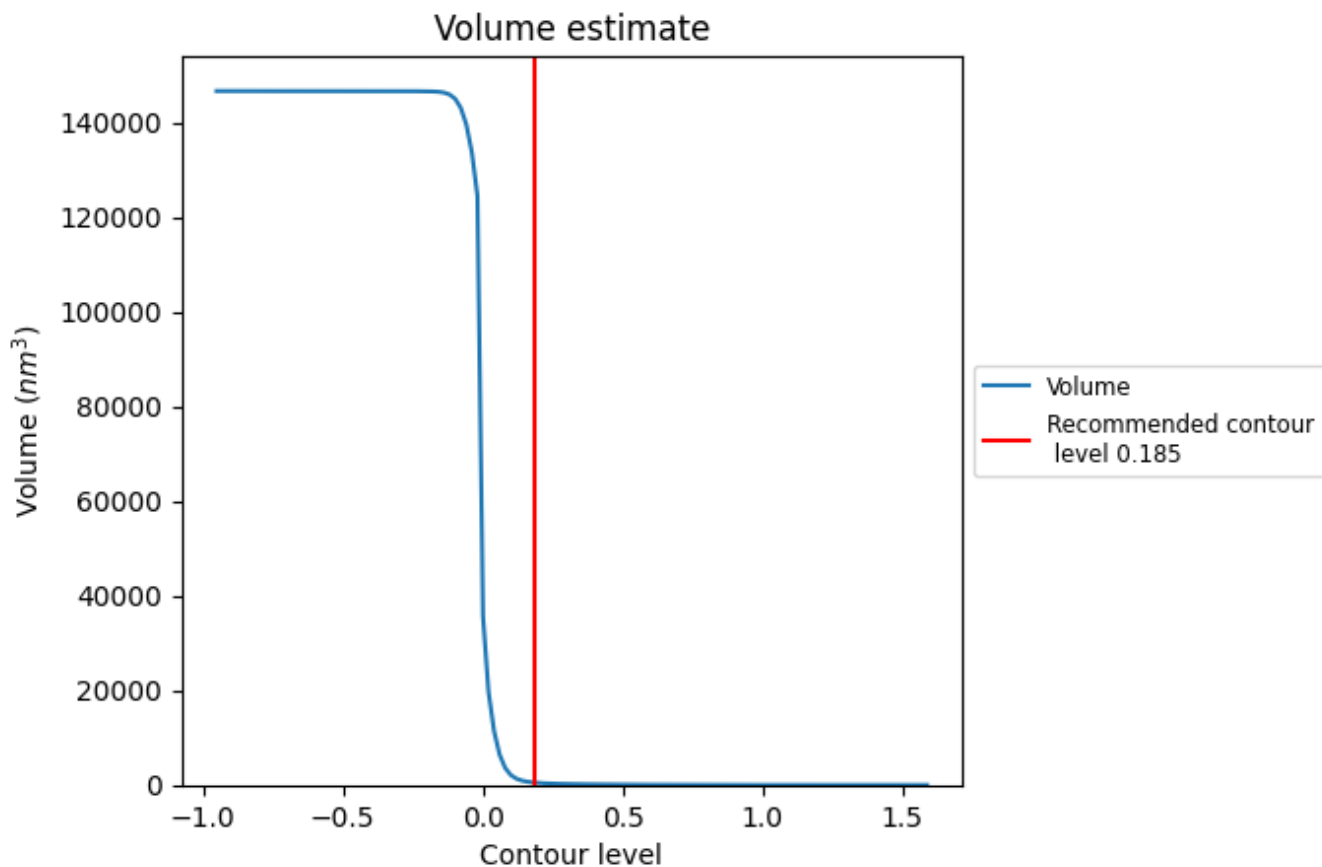
This section contains the results of statistical analysis of the map.

6.1 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.

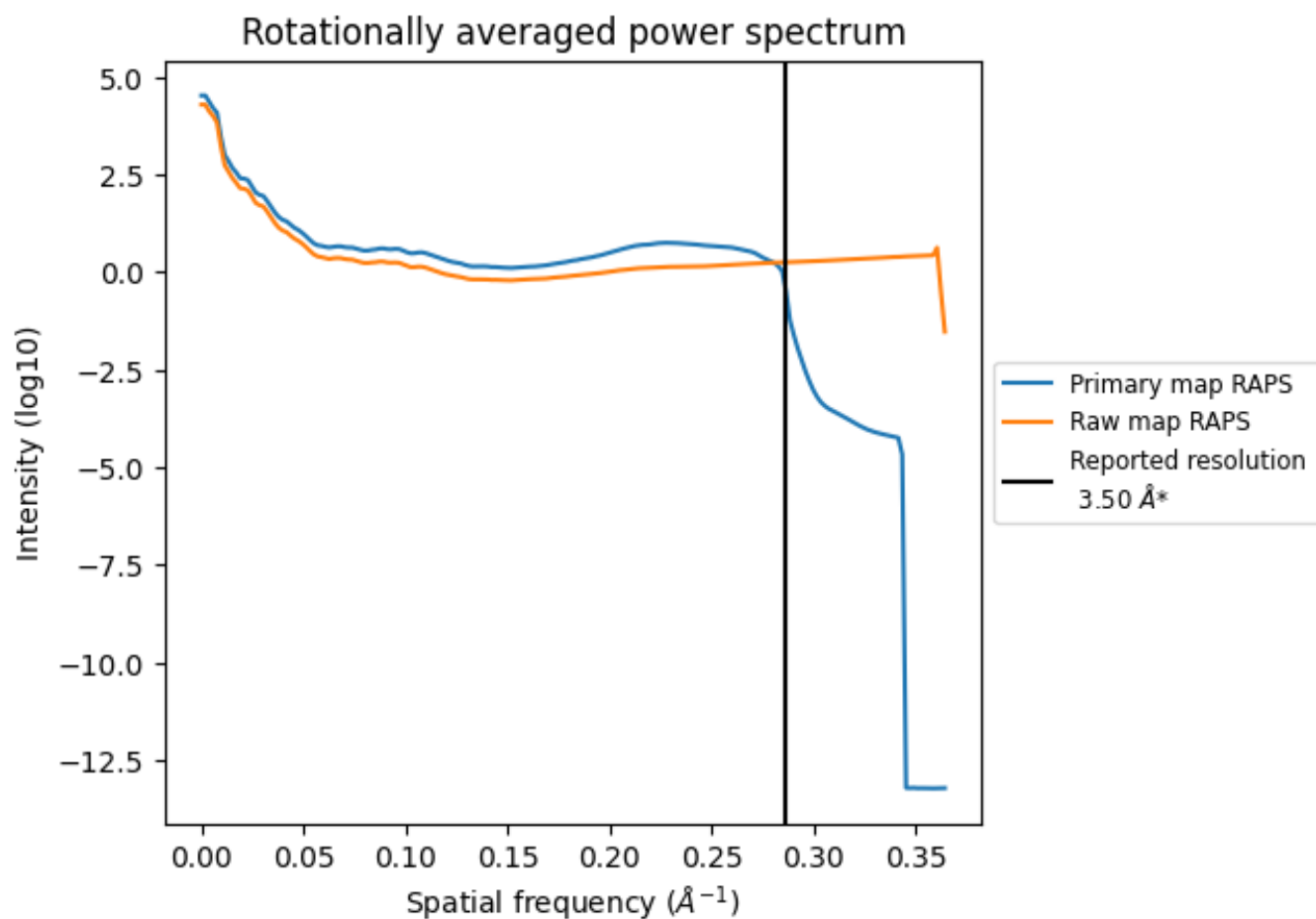
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 499 nm^3 ; this corresponds to an approximate mass of 450 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.

6.3 Rotationally averaged power spectrum [i](#)

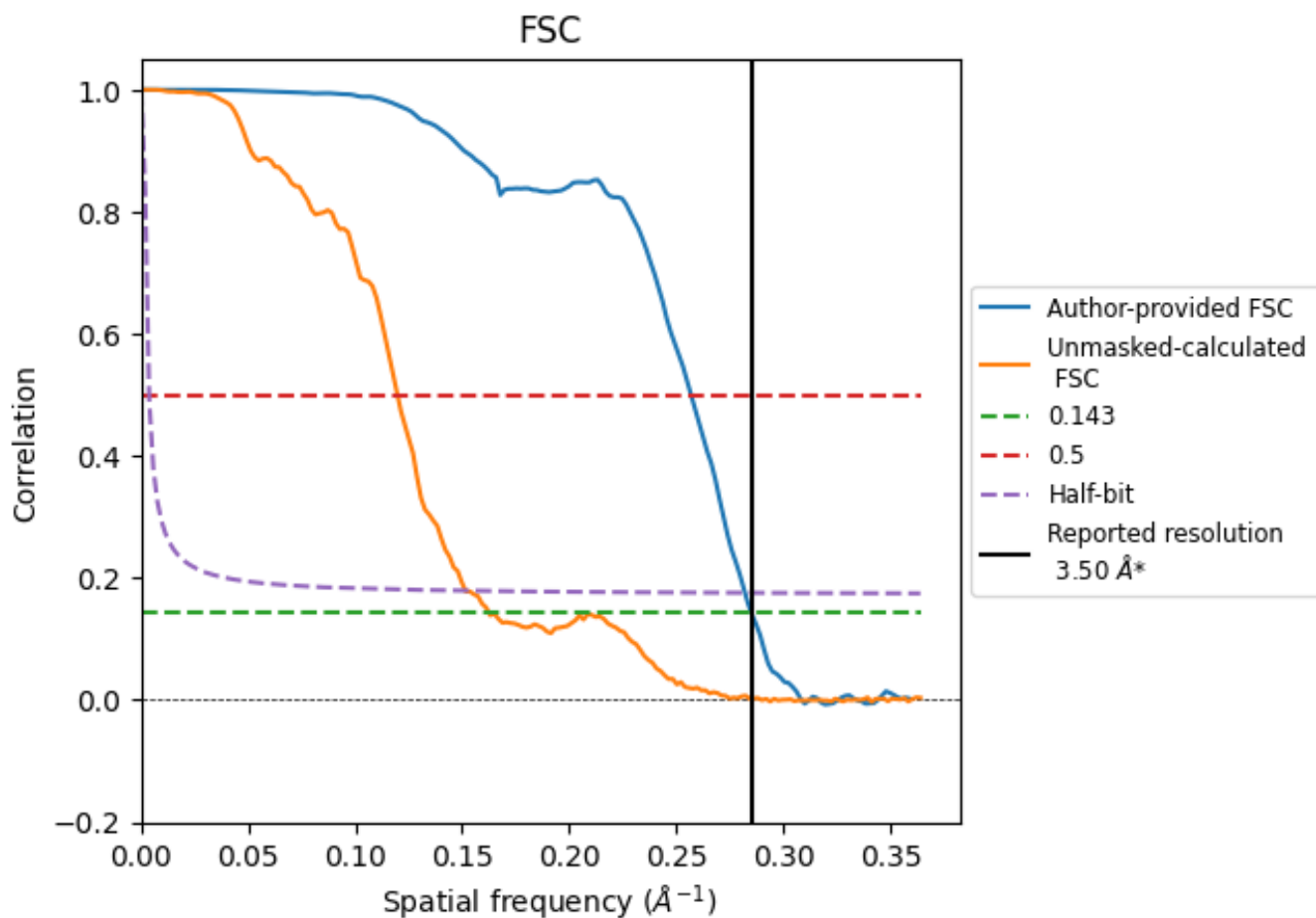


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286\AA^{-1}

7.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.89	3.54
Unmasked-calculated*	6.16	8.36	6.60

*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 6.16 differs from the reported value 3.5 by more than 10 %

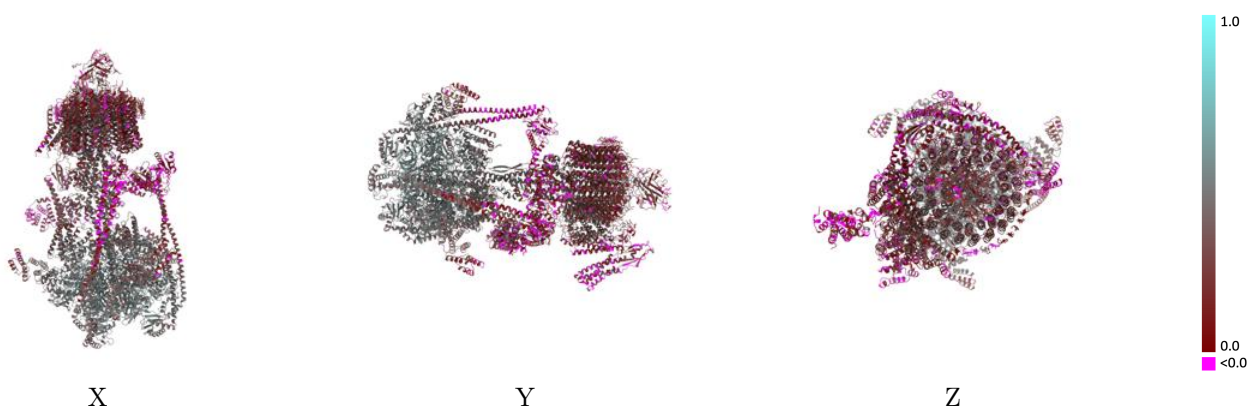
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44353 and PDB model 9BRD. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)

This section was not generated.

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

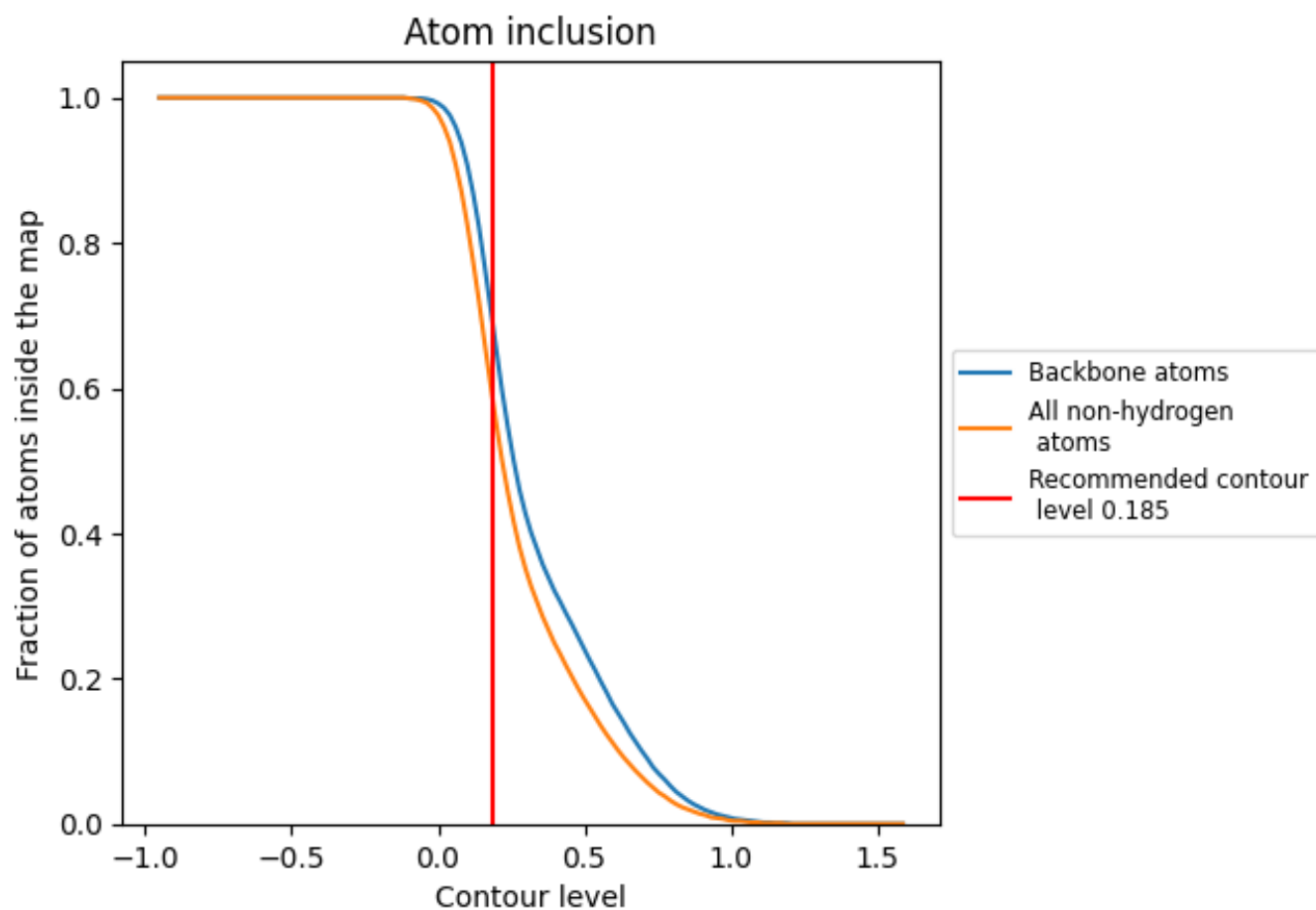


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.185) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5880	 0.3510
A	 0.8430	 0.4940
B	 0.8120	 0.4820
C	 0.8080	 0.4710
D	 0.8530	 0.5110
E	 0.8690	 0.5140
F	 0.8690	 0.5120
G	 0.2150	 0.0830
H	 0.7390	 0.4320
I	 0.7180	 0.4000
J	 0.7200	 0.3680
K	 0.6980	 0.3660
L	 0.6570	 0.3720
M	 0.6310	 0.3150
N	 0.6620	 0.3080
O	 0.5510	 0.2490
P	 0.4210	 0.2740
Q	 0.7020	 0.3570
R	 0.7140	 0.3500
S	 0.7480	 0.3820
T	 0.2470	 0.1220
U	 0.0570	 0.0590
V	 0.1430	 0.0320
W	 0.0710	 0.0100
X	 0.2500	 0.1750
Y	 0.3930	 0.3350
Z	 0.2140	 0.2230
a	 0.3280	 0.2100
b	 0.4910	 0.3580
c	 0.3210	 0.1100
d	 0.5210	 0.3490
e	 0.2770	 0.2280
f	 0.2080	 0.1400
g	 0.5340	 0.3640
h	 0.3820	 0.3030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.2390	 0.2180
j	 0.2220	 0.2160
k	 0.2700	 0.2060
l	 0.2890	 0.2180
m	 0.2850	 0.2180
n	 0.3060	 0.2520
o	 0.4130	 0.3080
p	 0.2610	 0.2900
q	 0.1070	 0.0340
r	 0.1790	 0.0680
s	 0.3460	 0.2230