



## Full wwPDB EM Validation Report ⓘ

Jul 13, 2024 – 12:31 PM EDT

PDB ID : 9B8O  
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

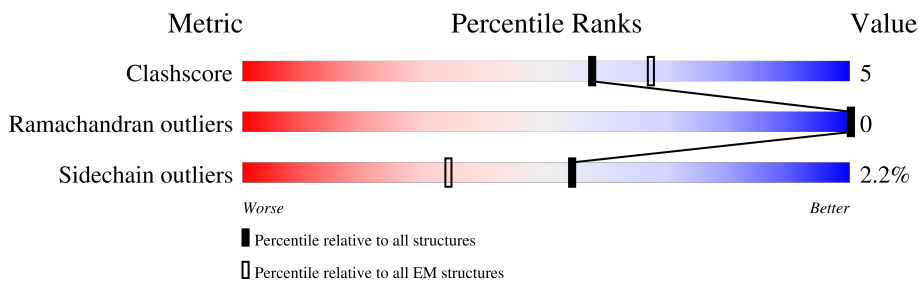
# 1 Overall quality at a glance i

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.



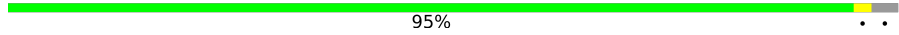
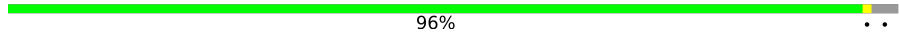
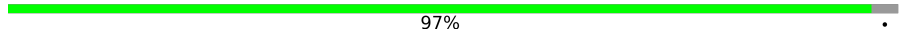
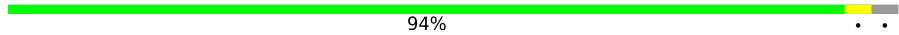
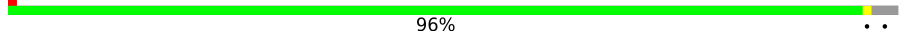
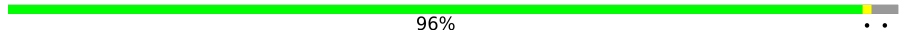
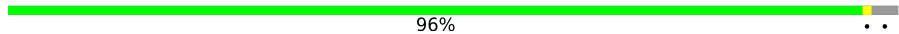
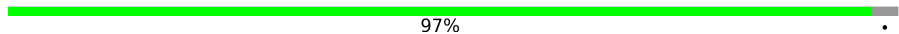
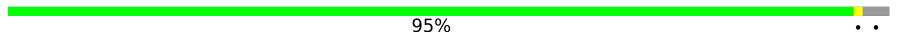




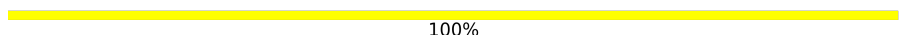






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	H	247	
2	P	463	
3	U	307	
4	a	826	
5	b	205	
6	d	351	
7	e	81	
8	f	86	

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Mol	Chain	Length	Quality of chain
9	g	155	 95%
9	h	155	 96%
9	i	155	 97%
9	j	155	 94%
9	k	155	 96%
9	l	155	 96%
9	m	155	 96%
9	n	155	 97%
9	o	155	 95%
10	p	350	 15% 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% 73%

## 2 Entry composition [i](#)

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<sup>+</sup>-transporting V1 subunit D.

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

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

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

- Molecule 3 is a protein called Synaptophysin.

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

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

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

- Molecule 5 is a protein called ATPase, H<sup>+</sup> transporting, V0 subunit B (Predicted), isoform CRA\_a.

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

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

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

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

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

- Molecule 8 is a protein called Rnasek protein.

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

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

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

- Molecule 10 is a protein called Renin receptor.

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

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

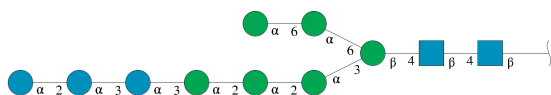
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	L	10	82	48	19	15	0	0

- 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
			Total	C	N	O		
12	A	2	28	16	2	10	0	0
12	B	2	28	16	2	10	0	0
12	C	2	28	16	2	10	0	0
12	D	2	28	16	2	10	0	0
12	E	2	28	16	2	10	0	0
12	F	2	28	16	2	10	0	0
12	G	2	28	16	2	10	0	0
12	I	2	28	16	2	10	0	0

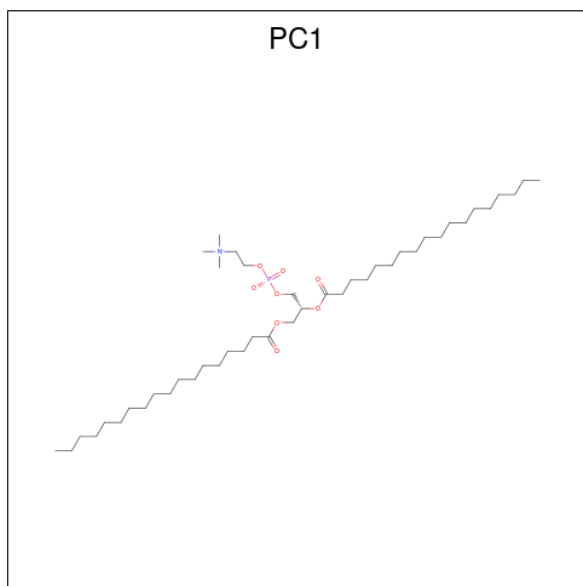
- Molecule 13 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-be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



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

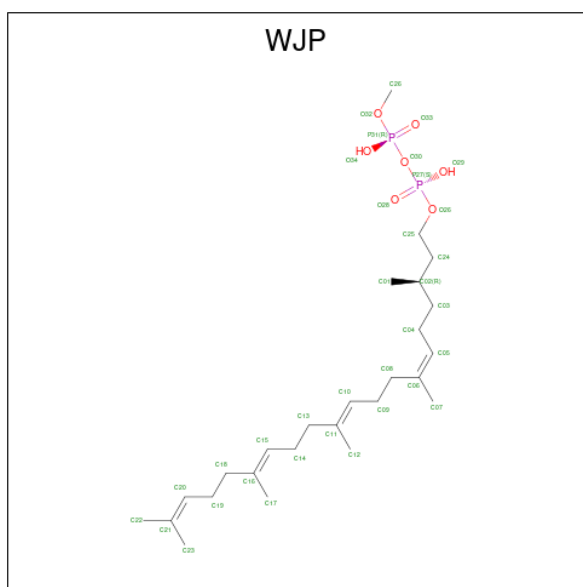
- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code:

PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



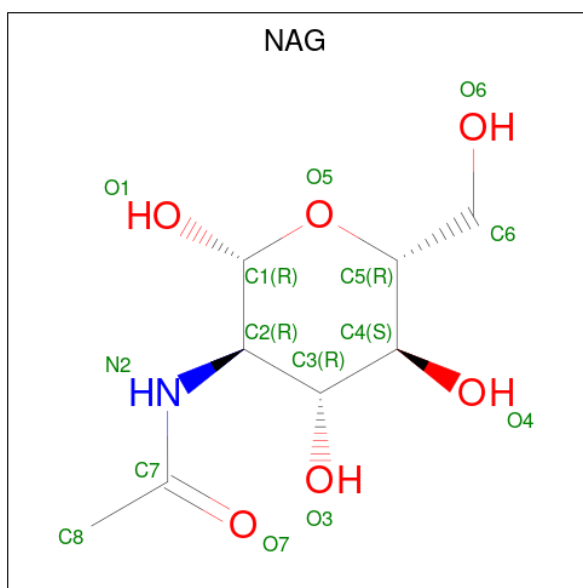
Mol	Chain	Residues	Atoms					AltConf
14	P	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	l	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 15 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylcosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (three-letter code: WJP) (formula: C<sub>26</sub>H<sub>48</sub>O<sub>7</sub>P<sub>2</sub>).



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

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

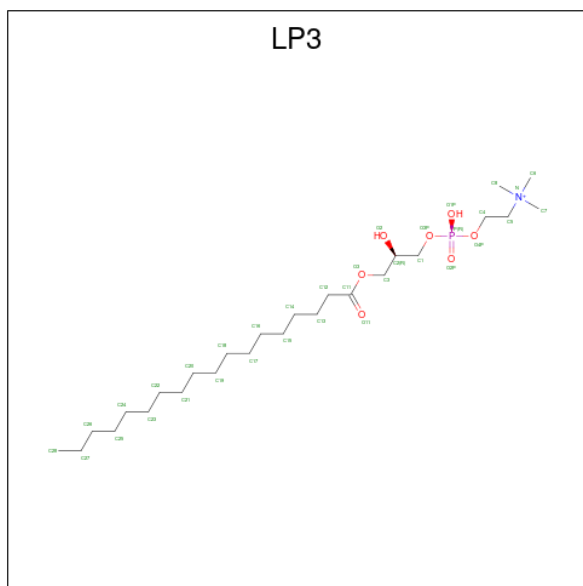


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	a	1	14	8	1	5	0

- Molecule 17 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (three-letter code: LP3) (formula:

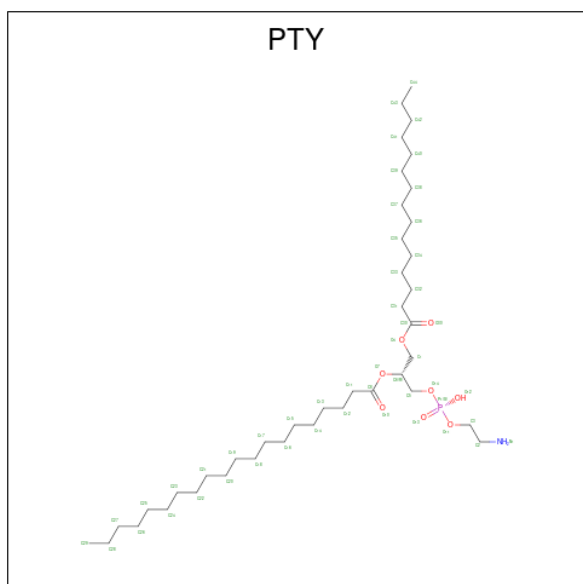


C<sub>26</sub>H<sub>55</sub>NO<sub>7</sub>P).



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

- Molecule 18 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



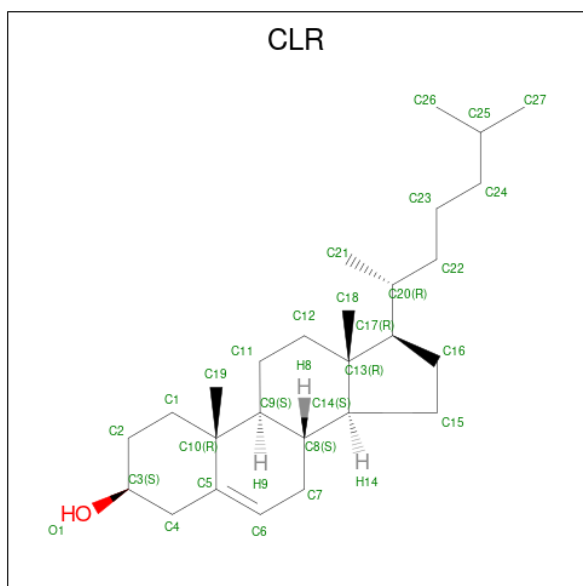
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	a	1	50	40	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
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	
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 (three-letter code: 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	

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

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

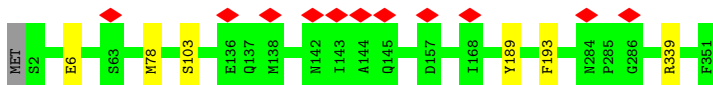






- Molecule 6: V-type proton ATPase subunit

Chain d: 98%



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

Chain e: 99%



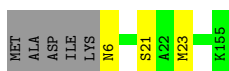
- Molecule 8: Rnasek protein

Chain f: 98%



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

Chain g: 95%



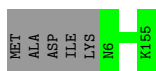
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h: 96%



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

Chain i: 97%



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

Chain j: 94%

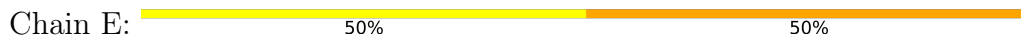








- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



## 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 ( $\text{\AA}$ )	309.0, 309.0, 309.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: BMA, PC1, NAG, LP3, WJP, MAN, GLC, PTY, CLR

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	0.27	0/434	0.49	0/581
2	P	0.28	0/1707	0.48	0/2324
3	U	0.24	0/1158	0.42	0/1601
4	a	0.27	0/3517	0.43	0/4771
5	b	0.29	0/1537	0.43	0/2088
6	d	0.26	0/2899	0.44	0/3927
7	e	0.26	0/669	0.42	0/920
8	f	0.26	0/682	0.38	0/926
9	g	0.29	0/1083	0.47	0/1466
9	h	0.28	0/1083	0.46	0/1466
9	i	0.28	0/1083	0.46	0/1466
9	j	0.29	0/1083	0.47	0/1466
9	k	0.27	0/1083	0.45	0/1466
9	l	0.27	0/1083	0.46	0/1466
9	m	0.27	0/1083	0.45	0/1466
9	n	0.28	0/1083	0.46	0/1466
9	o	0.28	0/1083	0.46	0/1466
10	p	0.27	0/445	0.41	0/609
11	L	0.23	0/83	0.50	0/110
All	All	0.27	0/22878	0.45	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 [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	H	431	0	428	1	0
2	P	1652	0	1579	23	0
3	U	1150	0	644	1	0
4	a	3408	0	3428	0	0
5	b	1503	0	1551	0	0
6	d	2833	0	2770	0	0
7	e	644	0	659	0	0
8	f	666	0	663	0	0
9	g	1068	0	1136	0	0
9	h	1068	0	1136	0	0
9	i	1068	0	1136	0	0
9	j	1068	0	1136	0	0
9	k	1068	0	1136	0	0
9	l	1068	0	1136	0	0
9	m	1068	0	1136	0	0
9	n	1068	0	1136	0	0
9	o	1068	0	1136	0	0
10	p	432	0	428	0	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	0	0
14	P	54	0	88	1	0
14	a	54	0	88	0	0
14	b	108	0	176	0	0
14	l	54	0	88	0	0
15	a	34	0	0	0	0
16	a	14	0	13	0	0
17	a	35	0	54	0	0
18	a	100	0	158	0	0
18	b	100	0	158	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	e	50	0	79	0	0
18	j	50	0	79	0	0
18	p	150	0	237	0	0
19	b	28	0	46	0	0
19	h	56	0	92	0	0
19	i	112	0	184	0	0
19	j	112	0	184	0	0
19	k	112	0	184	0	0
19	l	84	0	138	0	0
19	m	140	0	230	0	0
19	n	112	0	184	0	0
19	o	84	0	138	0	0
All	All	24407	0	25355	31	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 5.

All (31) 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)
12:D:1:NAG:O3	12:D:2:NAG:O5	2.15	0.63
2:P:344:ASN:O	2:P:346:SER:N	2.36	0.59
2:P:381:ASN:OD1	12:F:1:NAG:H82	2.04	0.56
12:I:1:NAG:O3	12:I:2:NAG:O5	2.24	0.54
2:P:410:ASP:OD1	2:P:410:ASP:N	2.41	0.53
2:P:314:THR:HG23	2:P:314:THR:O	2.09	0.53
2:P:270:VAL:CG1	2:P:279:LEU:HD11	2.39	0.52
2:P:310:LEU:HD23	2:P:311:PHE:CG	2.45	0.51
3:U:30:PHE:O	3:U:31:ALA:HB3	2.10	0.51
2:P:340:GLU:OE2	2:P:342:HIS:NE2	2.43	0.50
2:P:270:VAL:HG11	2:P:279:LEU:HD11	1.91	0.50
2:P:328:VAL:HG12	2:P:328:VAL:O	2.12	0.49
2:P:352:VAL:HG22	2:P:378:LEU:HD23	1.94	0.49
12:G:1:NAG:O3	12:G:2:NAG:O5	2.21	0.46
2:P:282:LEU:O	2:P:286:VAL:HG21	2.16	0.46
1:H:64:GLU:OE2	1:H:64:GLU:HA	2.17	0.45
2:P:403:GLU:HG2	12:C:2:NAG:H82	1.97	0.45
2:P:368:VAL:HG21	2:P:393:PHE:CD2	2.53	0.44
14:P:501:PC1:O13	14:P:501:PC1:H143	2.17	0.44
2:P:376:SER:O	2:P:376:SER:OG	2.29	0.43
2:P:279:LEU:HD21	2:P:310:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1:NAG:O3	12:A:2:NAG:O5	2.30	0.43
2:P:257:THR:O	2:P:257:THR:HG22	2.19	0.43
2:P:343:SER:HB2	12:A:1:NAG:H81	2.01	0.43
2:P:256:ASP:O	2:P:257:THR:HB	2.19	0.42
2:P:381:ASN:OD1	2:P:381:ASN:N	2.47	0.42
2:P:352:VAL:HG22	2:P:378:LEU:CD2	2.48	0.42
2:P:278:ASP:OD1	2:P:279:LEU:N	2.53	0.42
2:P:267:ASN:ND2	12:E:1:NAG:H83	2.34	0.42
2:P:267:ASN:HD22	12:E:1:NAG:H83	1.86	0.41
12:D:1:NAG:HO3	12:D:2:NAG:C1	2.30	0.41

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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%)	41 (95%)	2 (5%)	26	62
2	P	182/395 (46%)	174 (96%)	8 (4%)	28	64
3	U	24/241 (10%)	24 (100%)	0	100	100
4	a	367/732 (50%)	356 (97%)	11 (3%)	41	73
5	b	156/158 (99%)	149 (96%)	7 (4%)	27	63
6	d	305/306 (100%)	299 (98%)	6 (2%)	55	80
7	e	67/68 (98%)	67 (100%)	0	100	100
8	f	72/72 (100%)	70 (97%)	2 (3%)	43	74
9	g	109/113 (96%)	106 (97%)	3 (3%)	43	74
9	h	109/113 (96%)	108 (99%)	1 (1%)	78	91
9	i	109/113 (96%)	109 (100%)	0	100	100
9	j	109/113 (96%)	105 (96%)	4 (4%)	34	68
9	k	109/113 (96%)	108 (99%)	1 (1%)	78	91
9	l	109/113 (96%)	108 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	m	109/113 (96%)	108 (99%)	1 (1%)	78	91
9	n	109/113 (96%)	109 (100%)	0	100	100
9	o	109/113 (96%)	107 (98%)	2 (2%)	59	82
10	p	47/313 (15%)	46 (98%)	1 (2%)	53	79
11	L	9/100 (9%)	9 (100%)	0	100	100
All	All	2253/3614 (62%)	2203 (98%)	50 (2%)	54	79

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	68	SER
1	H	118	SER
2	P	274	ASP
2	P	297	ASN
2	P	321	LEU
2	P	324	ARG
2	P	334	PHE
2	P	376	SER
2	P	410	ASP
2	P	442	SER
4	a	367	THR
4	a	469	SER
4	a	489	ASN
4	a	502	GLN
4	a	504	ASN
4	a	613	PHE
4	a	645	MET
4	a	738	SER
4	a	741	ARG
4	a	805	ARG
4	a	821	PHE
5	b	30	ASP
5	b	36	ASP
5	b	70	TYR
5	b	98	GLU
5	b	112	SER
5	b	151	CYS
5	b	154	CYS
6	d	6	GLU
6	d	78	MET

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Mol	Chain	Res	Type
6	d	103	SER
6	d	189	TYR
6	d	193	PHE
6	d	339	ARG
8	f	17	VAL
8	f	66	SER
9	g	6	ASN
9	g	21	SER
9	g	23	MET
9	h	115	ASP
9	j	23	MET
9	j	45	SER
9	j	88	ARG
9	j	98	SER
9	k	47	MET
9	l	79	SER
9	m	82	ASP
9	o	39	THR
9	o	55	SER
10	p	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	0.75	0	17,19,21	1.07	1 (5%)
12	NAG	A	2	12	14,14,15	0.69	0	17,19,21	0.88	0
12	NAG	B	1	2,12	14,14,15	0.76	0	17,19,21	1.25	2 (11%)
12	NAG	B	2	12	14,14,15	0.77	0	17,19,21	1.07	1 (5%)
12	NAG	C	1	2,12	14,14,15	0.81	0	17,19,21	1.17	2 (11%)
12	NAG	C	2	12	14,14,15	0.76	0	17,19,21	0.80	0
12	NAG	D	1	2,12	14,14,15	0.72	0	17,19,21	1.13	2 (11%)
12	NAG	D	2	12	14,14,15	0.69	0	17,19,21	1.30	2 (11%)
12	NAG	E	1	2,12	14,14,15	0.78	0	17,19,21	1.39	2 (11%)
12	NAG	E	2	12	14,14,15	0.70	0	17,19,21	1.25	1 (5%)
12	NAG	F	1	12	14,14,15	0.74	0	17,19,21	1.31	1 (5%)
12	NAG	F	2	12	14,14,15	0.68	0	17,19,21	1.10	1 (5%)
12	NAG	G	1	2,12	14,14,15	0.76	0	17,19,21	0.89	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	0.76	0	17,19,21	0.77	0
12	NAG	I	2	12	14,14,15	0.69	0	17,19,21	0.84	0
13	NAG	Z	1	13	14,14,15	0.78	0	17,19,21	0.82	0
13	MAN	Z	10	13	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
13	MAN	Z	11	13	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
13	NAG	Z	2	13	14,14,15	0.75	0	17,19,21	0.90	1 (5%)
13	BMA	Z	3	13	11,11,12	0.82	0	15,15,17	2.31	3 (20%)
13	MAN	Z	4	13	11,11,12	0.68	0	15,15,17	1.36	1 (6%)
13	MAN	Z	5	13	11,11,12	0.75	0	15,15,17	1.29	1 (6%)
13	MAN	Z	6	13	11,11,12	0.85	1 (9%)	15,15,17	1.01	0
13	GLC	Z	7	13	11,11,12	0.67	0	15,15,17	0.64	0
13	GLC	Z	8	13	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
13	GLC	Z	9	13	11,11,12	0.61	0	15,15,17	0.84	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	2	12	-	0/6/23/26	0/1/1/1
12	NAG	B	1	2,12	-	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	2,12	-	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	2,12	-	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	2,12	-	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	2,12	-	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
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	-2.27	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	3	BMA	C1-O5-C5	6.74	121.32	112.19
13	Z	4	MAN	C1-O5-C5	4.13	117.79	112.19
12	F	1	NAG	C2-N2-C7	3.76	128.26	122.90
12	E	1	NAG	C2-N2-C7	3.70	128.17	122.90
13	Z	5	MAN	C1-O5-C5	3.47	116.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2	NAG	O5-C1-C2	-3.39	105.94	111.29
12	E	2	NAG	C2-N2-C7	3.32	127.63	122.90
13	Z	3	BMA	C3-C4-C5	3.30	116.13	110.24
12	G	2	NAG	C2-N2-C7	3.12	127.34	122.90
12	F	2	NAG	C2-N2-C7	3.02	127.21	122.90
12	C	1	NAG	O4-C4-C3	-2.87	103.72	110.35
13	Z	10	MAN	C1-O5-C5	2.83	116.03	112.19
12	B	2	NAG	O5-C1-C2	-2.81	106.84	111.29
12	D	2	NAG	C2-N2-C7	2.70	126.75	122.90
12	A	1	NAG	C2-N2-C7	2.69	126.73	122.90
12	B	1	NAG	O4-C4-C3	-2.46	104.66	110.35
13	Z	3	BMA	O4-C4-C3	-2.42	104.75	110.35
13	Z	11	MAN	C1-O5-C5	2.41	115.45	112.19
12	E	1	NAG	O4-C4-C3	-2.33	104.97	110.35
13	Z	8	GLC	O5-C1-C2	-2.30	107.22	110.77
12	D	1	NAG	C4-C3-C2	-2.25	107.72	111.02
12	D	1	NAG	C1-O5-C5	2.19	115.17	112.19
12	B	1	NAG	O5-C1-C2	-2.15	107.89	111.29
13	Z	2	NAG	O5-C1-C2	-2.08	108.01	111.29
12	C	1	NAG	O5-C1-C2	-2.04	108.06	111.29

There are no chirality outliers.

All (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	I	1	NAG	C3-C2-N2-C7
13	Z	2	NAG	O5-C5-C6-O6
13	Z	5	MAN	O5-C5-C6-O6
13	Z	4	MAN	O5-C5-C6-O6
13	Z	2	NAG	C4-C5-C6-O6
13	Z	5	MAN	C4-C5-C6-O6
12	E	1	NAG	C8-C7-N2-C2
12	E	1	NAG	O7-C7-N2-C2
12	F	1	NAG	C8-C7-N2-C2
12	F	1	NAG	O7-C7-N2-C2
12	F	2	NAG	C8-C7-N2-C2
12	F	2	NAG	O7-C7-N2-C2
12	G	2	NAG	C8-C7-N2-C2
12	G	2	NAG	O7-C7-N2-C2

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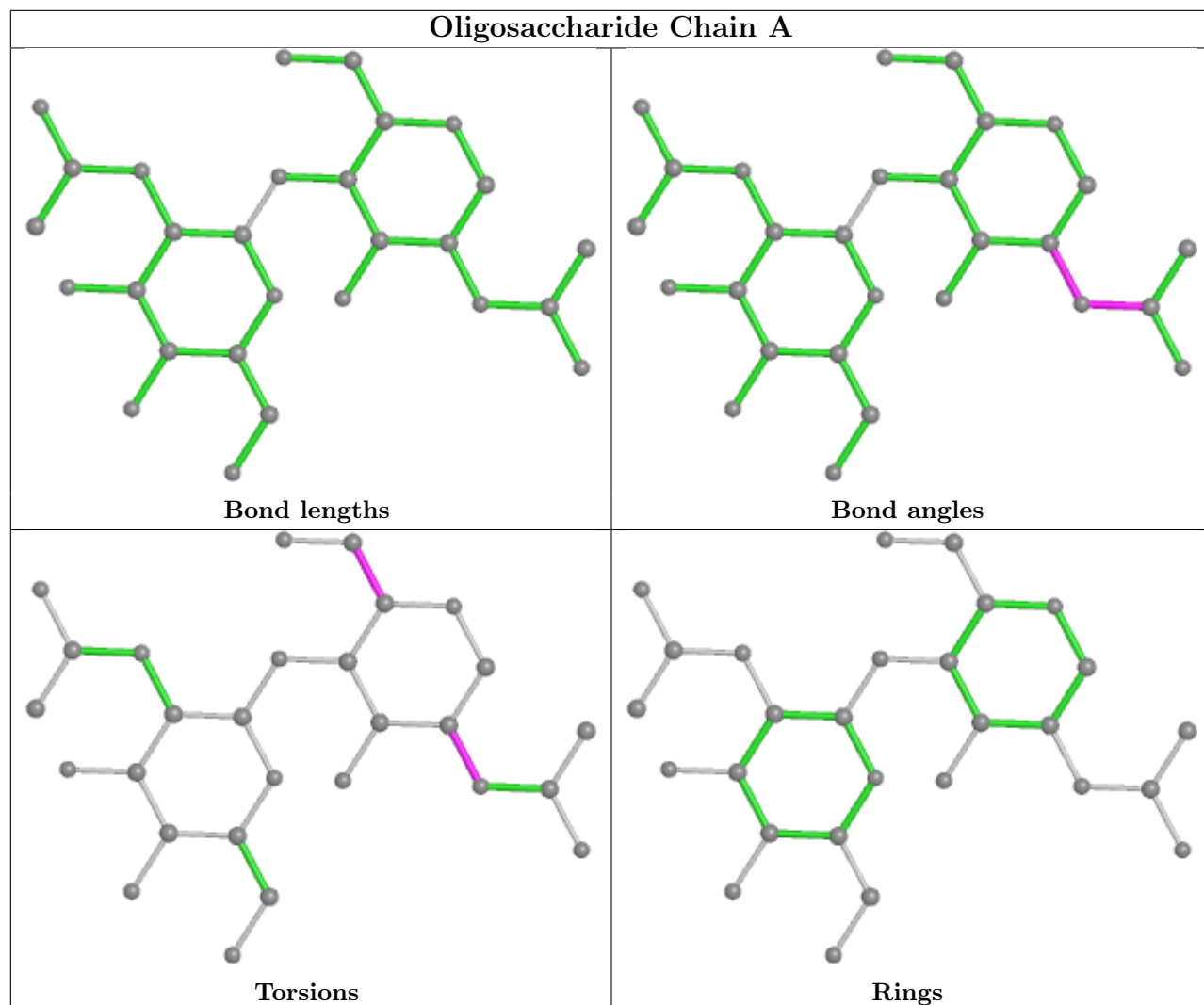
Mol	Chain	Res	Type	Atoms
13	Z	4	MAN	C4-C5-C6-O6
12	G	1	NAG	C1-C2-N2-C7
13	Z	7	GLC	O5-C5-C6-O6
12	A	1	NAG	O5-C5-C6-O6
12	I	1	NAG	C1-C2-N2-C7
13	Z	3	BMA	O5-C5-C6-O6

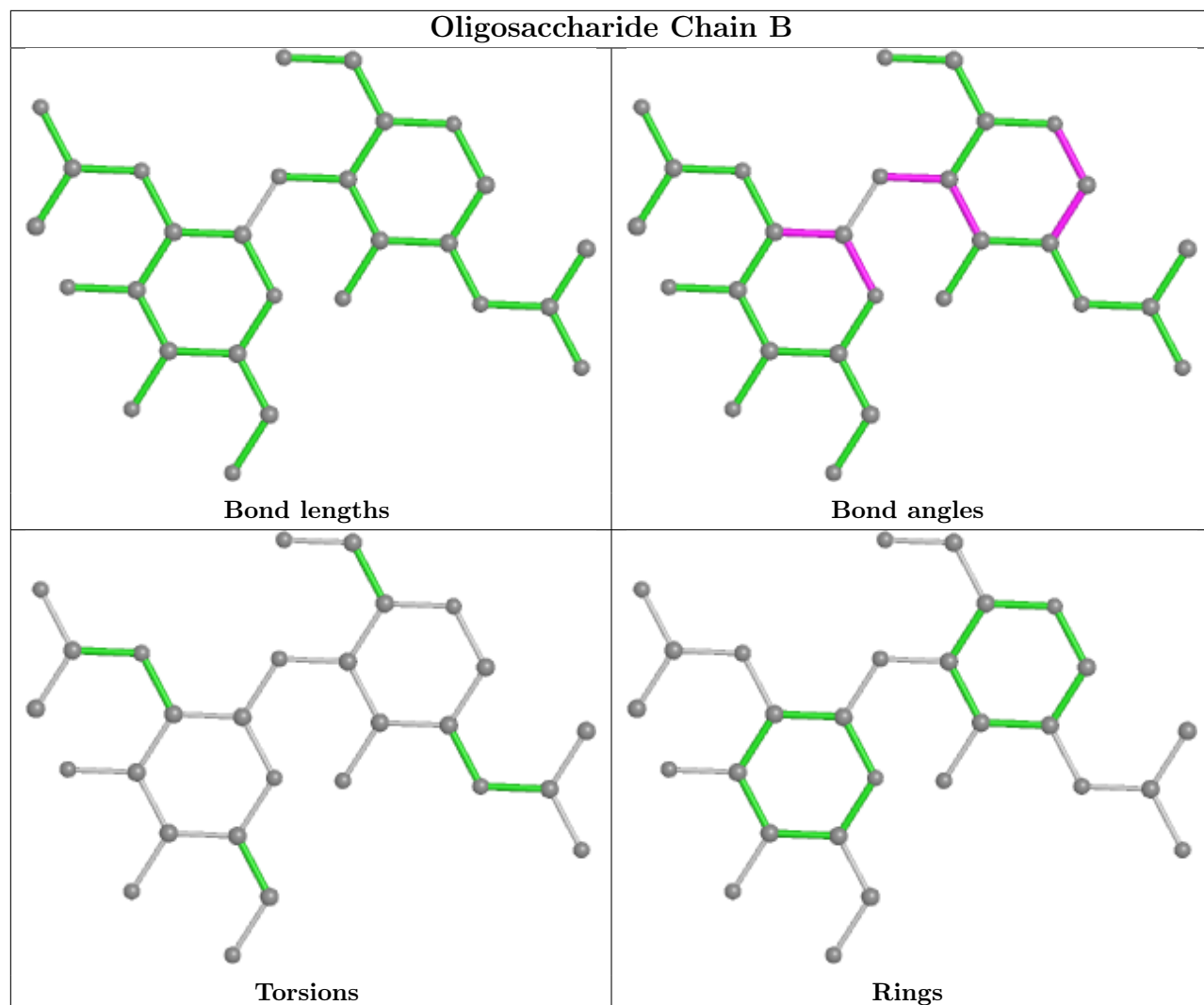
There are no ring outliers.

11 monomers are involved in 10 short contacts:

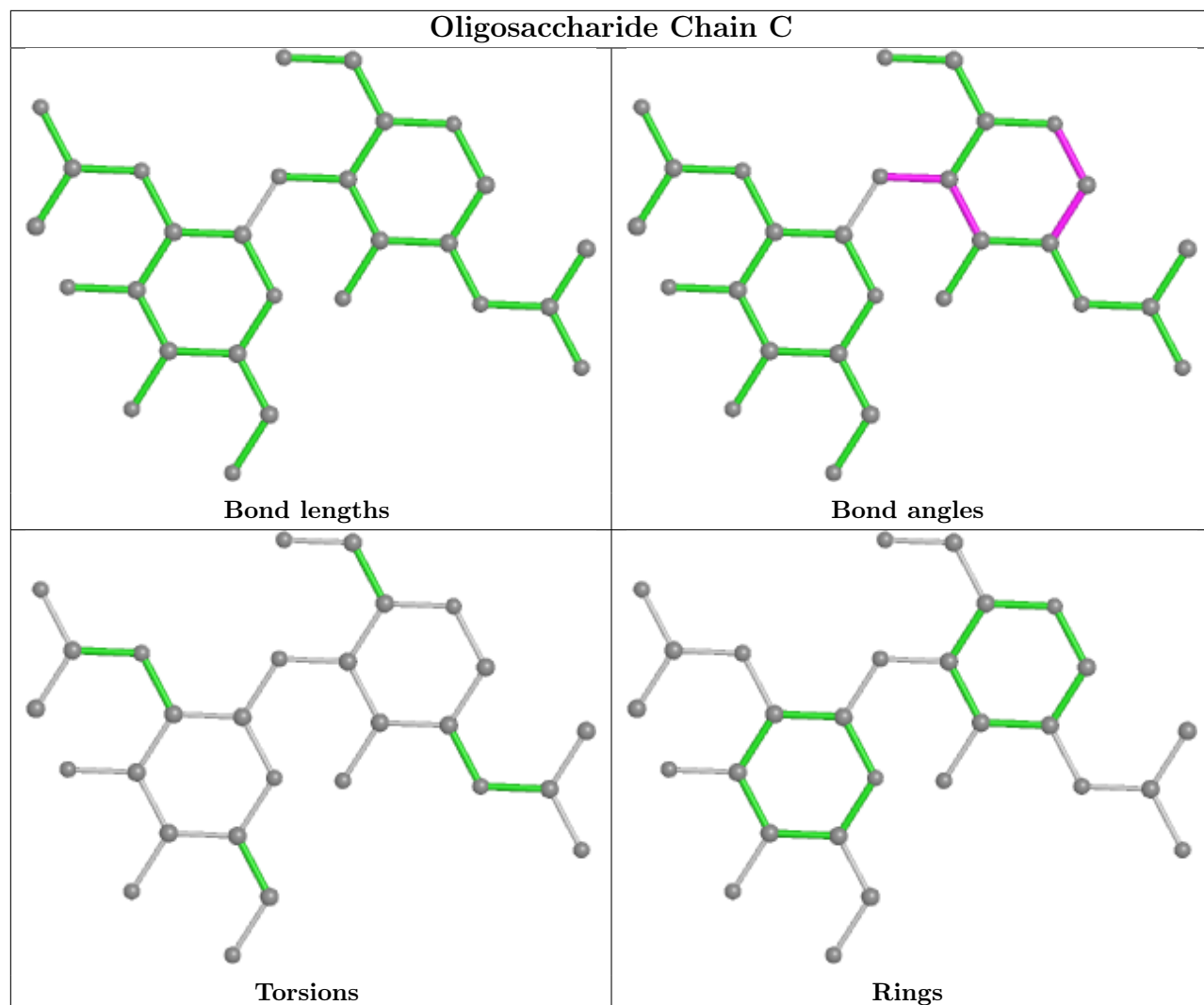
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	2	NAG	1	0
12	E	1	NAG	2	0
12	A	1	NAG	2	0
12	D	2	NAG	2	0
12	I	2	NAG	1	0
12	I	1	NAG	1	0
12	F	1	NAG	1	0
12	G	1	NAG	1	0
12	G	2	NAG	1	0
12	D	1	NAG	2	0
12	A	2	NAG	1	0

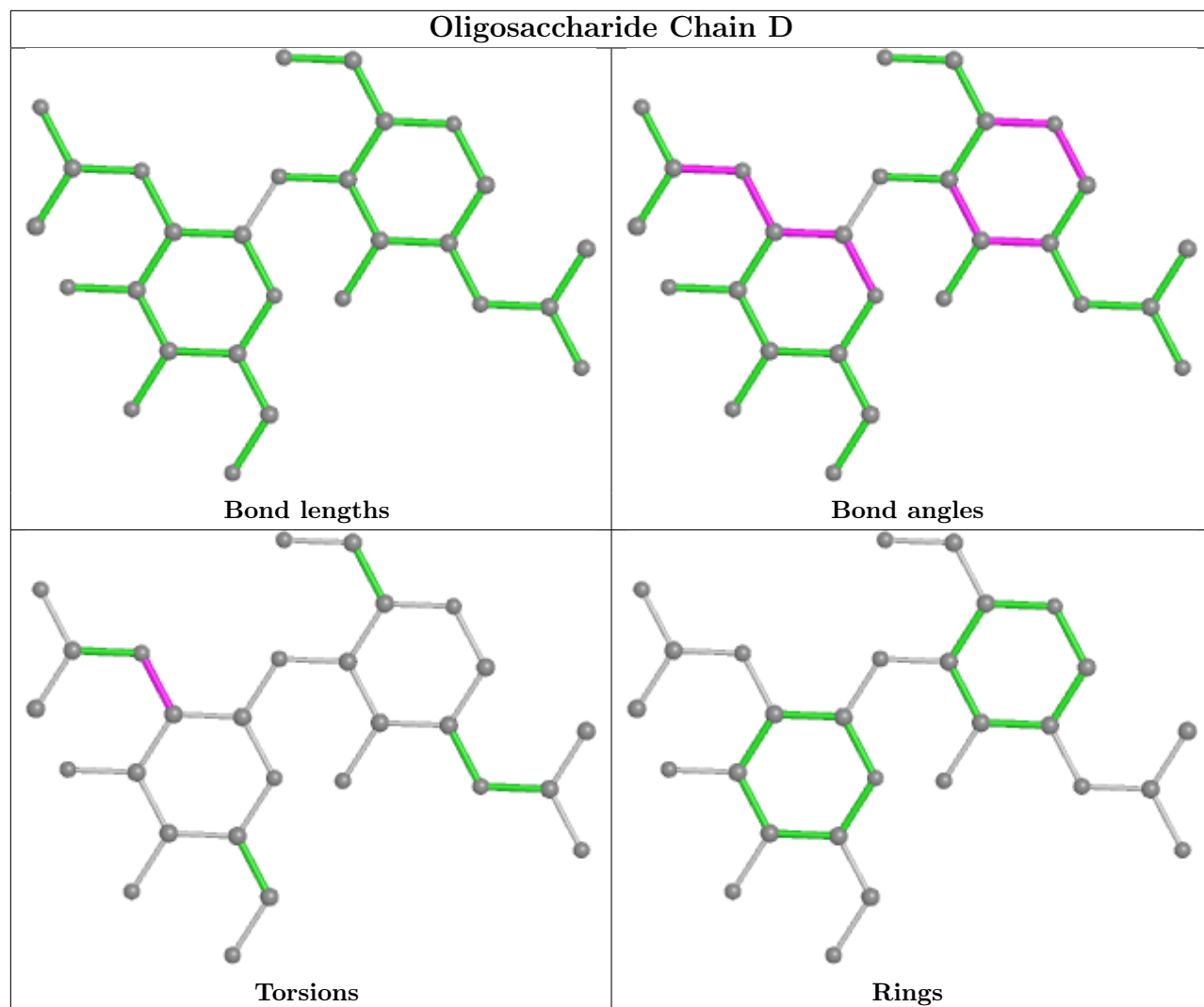
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

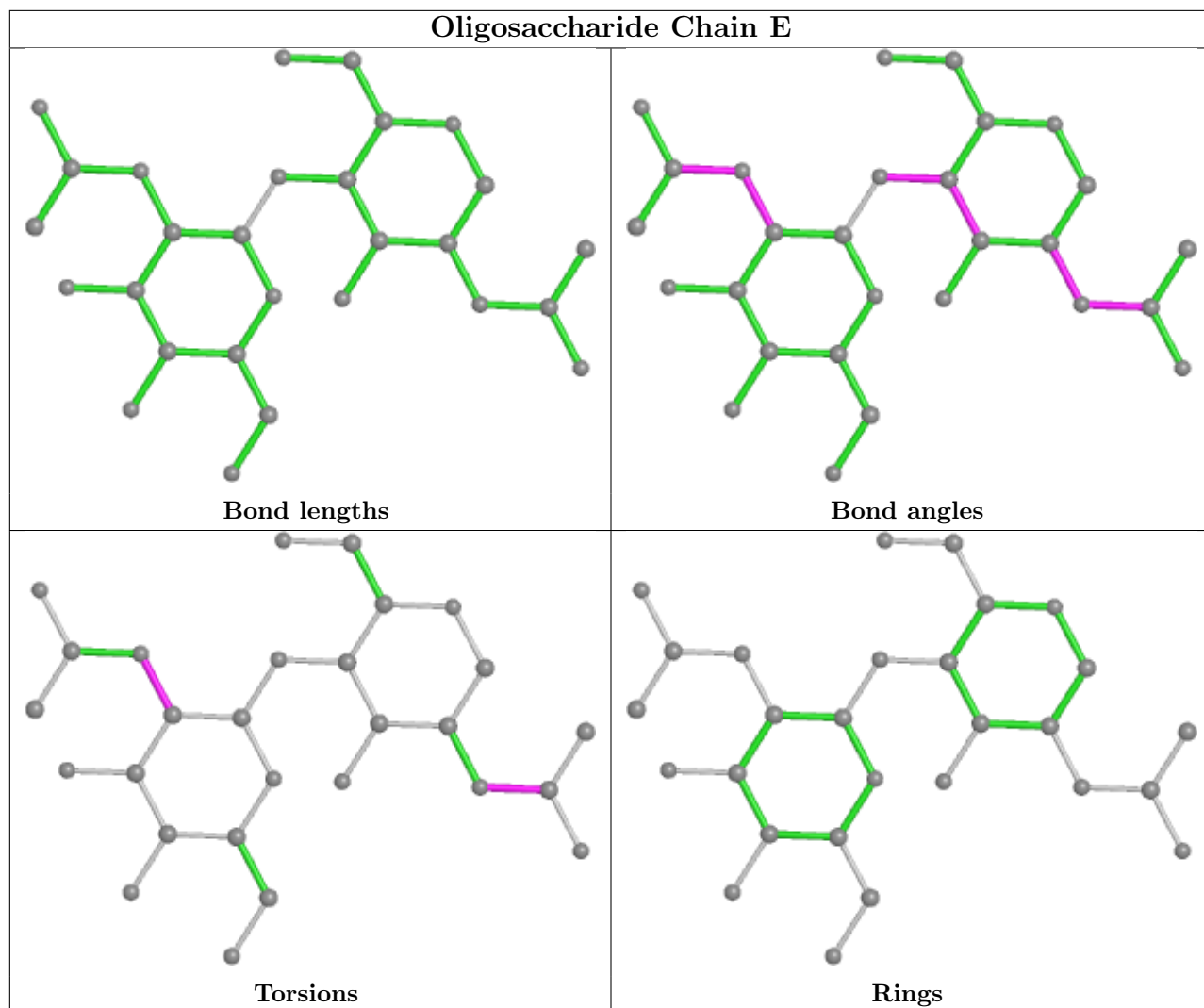


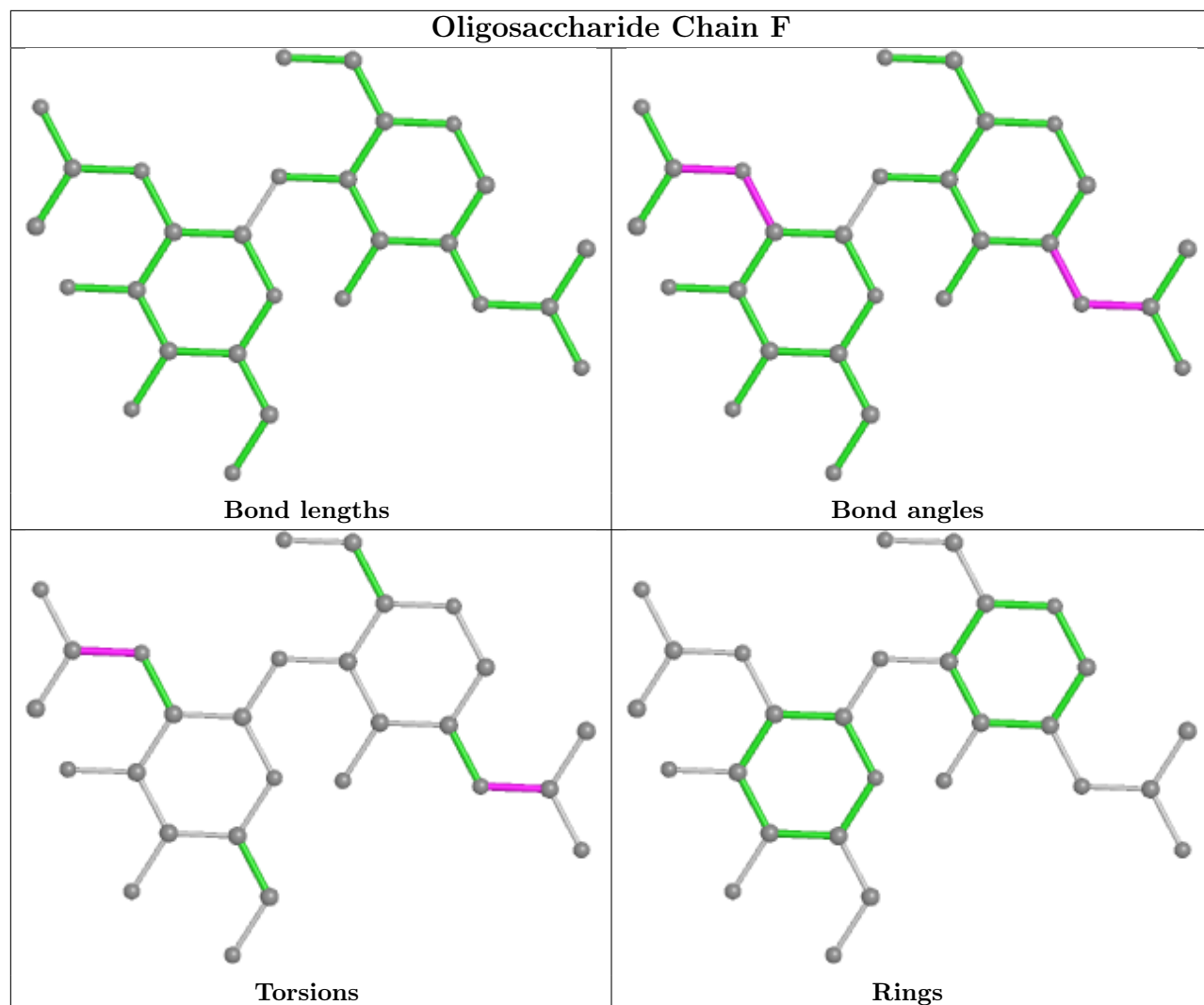


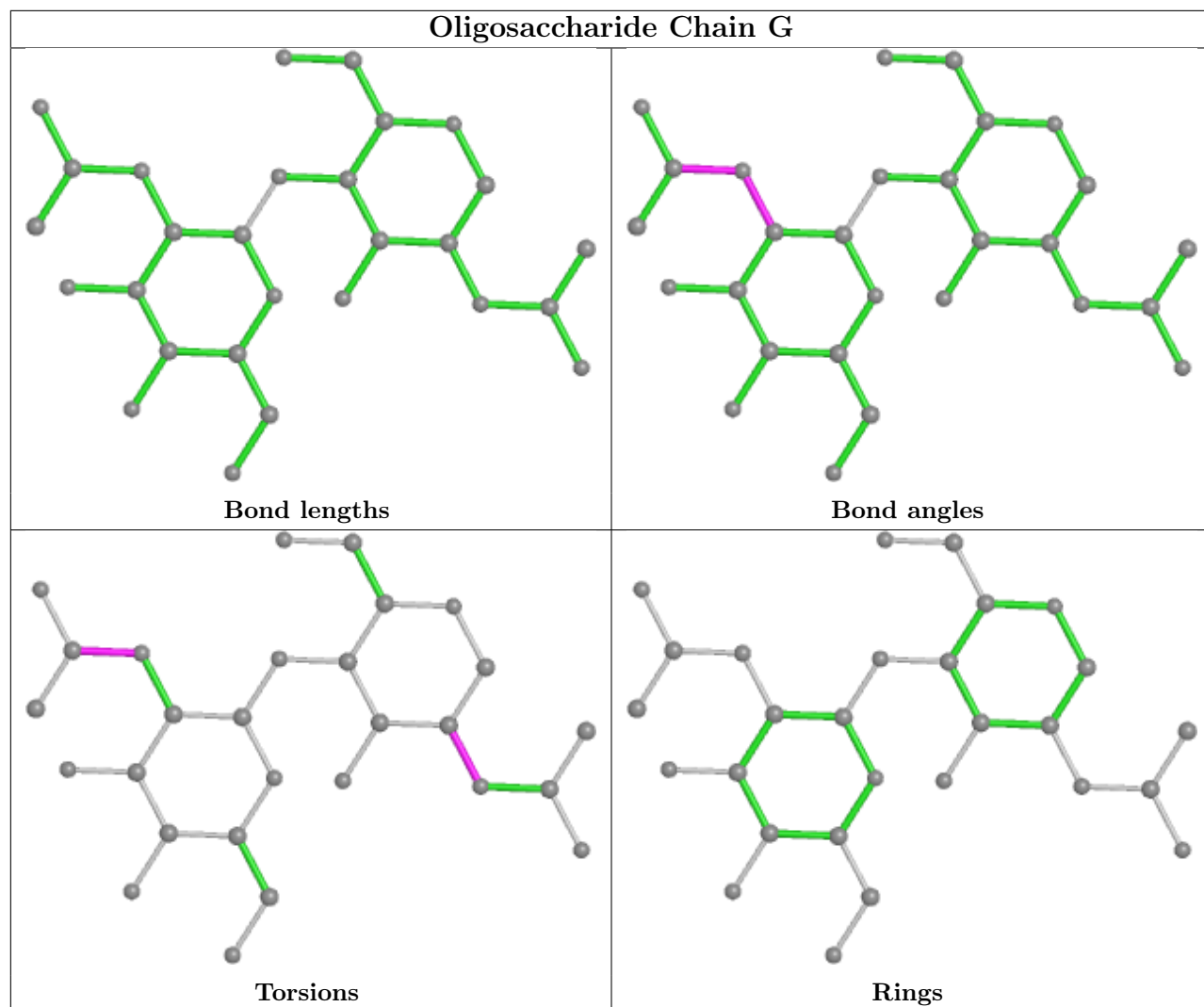


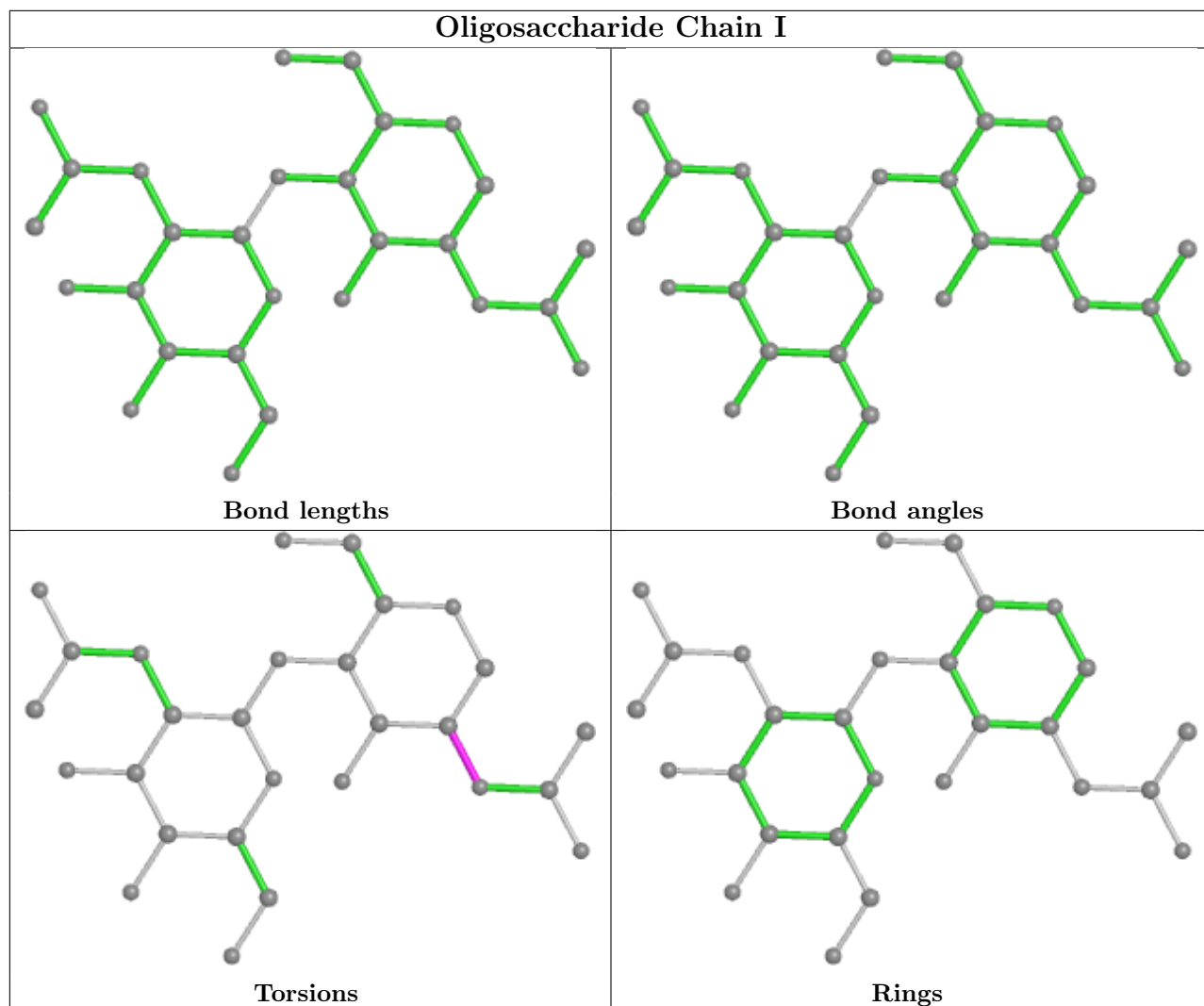


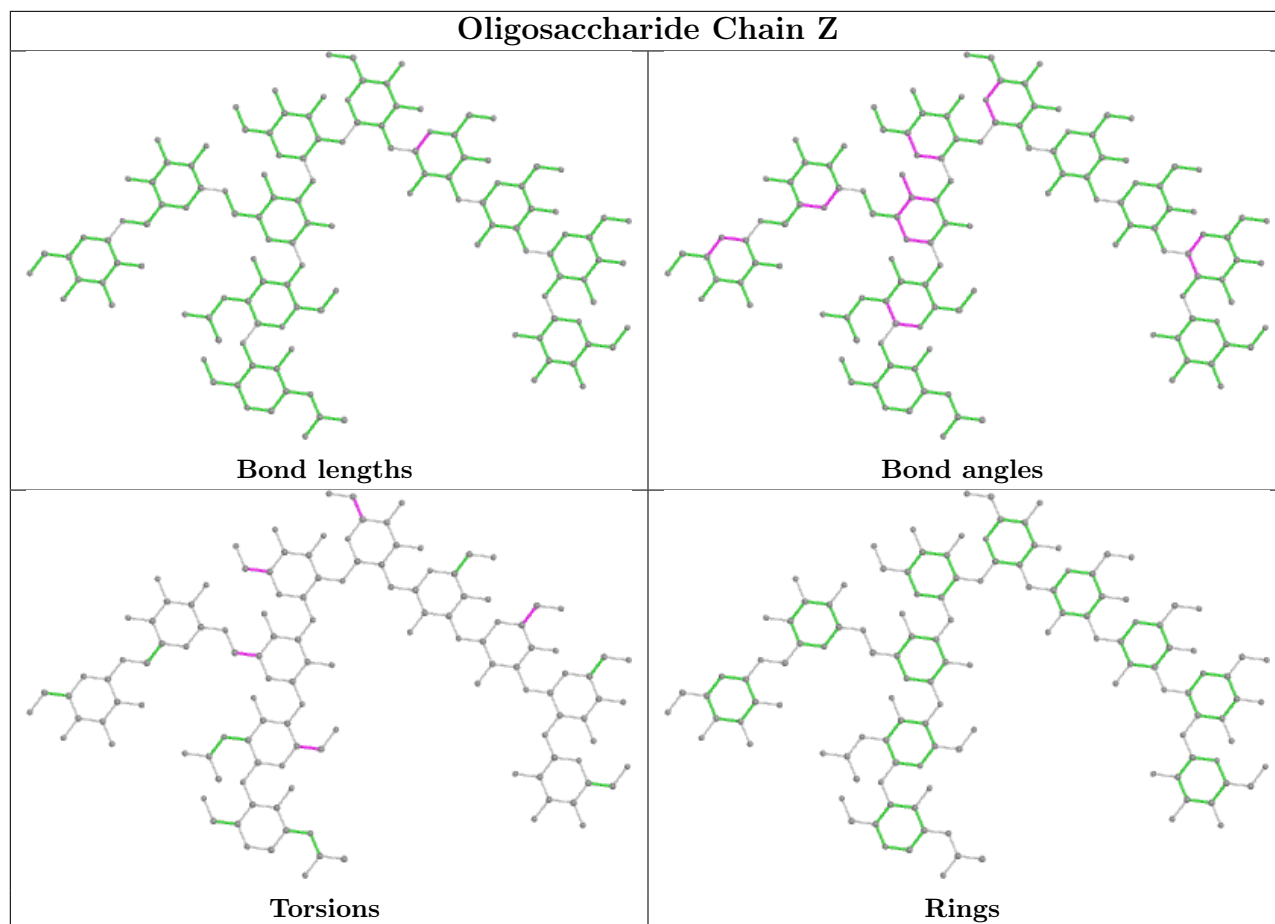












## 5.6 Ligand geometry [i](#)

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	n	201	-	31,31,31	0.35	0	48,48,48	0.81	1 (2%)
19	CLR	m	201	-	31,31,31	0.44	0	48,48,48	1.31	5 (10%)
19	CLR	o	202	-	31,31,31	0.46	0	48,48,48	1.08	4 (8%)
19	CLR	h	201	-	31,31,31	0.41	0	48,48,48	1.34	3 (6%)
14	PC1	P	501	-	53,53,53	0.49	0	59,61,61	0.48	1 (1%)
19	CLR	j	202	-	31,31,31	0.40	0	48,48,48	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	PTY	b	303	-	49,49,49	0.48	0	52,54,54	0.41	0
18	PTY	b	304	-	49,49,49	0.47	0	52,54,54	0.40	0
19	CLR	k	203	-	31,31,31	0.40	0	48,48,48	0.82	0
18	PTY	p	401	-	49,49,49	0.49	0	52,54,54	0.47	0
19	CLR	n	204	-	31,31,31	0.37	0	48,48,48	0.94	2 (4%)
19	CLR	i	202	-	31,31,31	0.40	0	48,48,48	0.75	2 (4%)
19	CLR	b	305	-	31,31,31	0.38	0	48,48,48	0.65	0
19	CLR	m	202	-	31,31,31	0.46	0	48,48,48	1.08	3 (6%)
18	PTY	e	101	-	49,49,49	0.46	0	52,54,54	0.42	0
19	CLR	j	203	-	31,31,31	0.42	0	48,48,48	0.92	4 (8%)
19	CLR	h	202	-	31,31,31	0.39	0	48,48,48	1.01	3 (6%)
19	CLR	l	202	-	31,31,31	0.42	0	48,48,48	1.10	5 (10%)
17	LP3	a	903	-	34,34,34	0.52	0	39,41,41	0.54	0
14	PC1	l	201	-	53,53,53	0.49	0	59,61,61	0.50	1 (1%)
14	PC1	b	302	-	53,53,53	0.50	0	59,61,61	0.54	1 (1%)
19	CLR	n	202	-	31,31,31	0.40	0	48,48,48	0.85	0
19	CLR	k	204	-	31,31,31	0.45	0	48,48,48	1.07	3 (6%)
19	CLR	i	201	-	31,31,31	0.42	0	48,48,48	1.18	2 (4%)
19	CLR	o	201	-	31,31,31	0.44	0	48,48,48	1.25	4 (8%)
15	WJP	a	901	-	31,33,34	1.61	7 (22%)	39,43,44	7.04	8 (20%)
19	CLR	i	203	-	31,31,31	0.57	0	48,48,48	1.24	4 (8%)
14	PC1	a	904	-	53,53,53	0.50	0	59,61,61	0.46	1 (1%)
19	CLR	k	201	-	31,31,31	0.45	0	48,48,48	1.10	3 (6%)
19	CLR	m	203	-	31,31,31	0.37	0	48,48,48	0.79	0
19	CLR	n	203	-	31,31,31	0.44	0	48,48,48	1.19	3 (6%)
18	PTY	a	906	-	49,49,49	0.46	0	52,54,54	0.37	0
19	CLR	o	203	-	31,31,31	0.39	0	48,48,48	1.21	2 (4%)
16	NAG	a	902	4	14,14,15	0.72	0	17,19,21	1.44	2 (11%)
14	PC1	b	301	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
18	PTY	p	403	-	49,49,49	0.46	0	52,54,54	0.37	0
19	CLR	i	204	-	31,31,31	0.38	0	48,48,48	0.73	1 (2%)
19	CLR	m	204	-	31,31,31	0.41	0	48,48,48	0.86	2 (4%)
19	CLR	j	205	-	31,31,31	0.38	0	48,48,48	0.78	0
18	PTY	a	905	-	49,49,49	0.46	0	52,54,54	0.38	0
19	CLR	m	205	-	31,31,31	0.39	0	48,48,48	1.10	4 (8%)
18	PTY	p	402	-	49,49,49	0.47	0	52,54,54	0.42	0
19	CLR	l	203	-	31,31,31	0.42	0	48,48,48	0.99	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLR	j	204	-	31,31,31	0.43	0	48,48,48	0.78	1 (2%)
18	PTY	j	201	-	49,49,49	0.47	0	52,54,54	0.41	0
19	CLR	l	204	-	31,31,31	0.40	0	48,48,48	0.66	0
19	CLR	k	202	-	31,31,31	0.40	0	48,48,48	0.96	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	n	201	-	-	3/10/68/68	0/4/4/4
19	CLR	m	201	-	-	4/10/68/68	0/4/4/4
19	CLR	o	202	-	-	8/10/68/68	0/4/4/4
19	CLR	h	201	-	-	6/10/68/68	0/4/4/4
14	PC1	P	501	-	-	19/57/57/57	-
19	CLR	j	202	-	-	4/10/68/68	0/4/4/4
18	PTY	b	303	-	-	26/53/53/53	-
18	PTY	b	304	-	-	24/53/53/53	-
19	CLR	k	203	-	-	2/10/68/68	0/4/4/4
18	PTY	p	401	-	-	23/53/53/53	-
19	CLR	n	204	-	-	9/10/68/68	0/4/4/4
19	CLR	i	202	-	-	5/10/68/68	0/4/4/4
19	CLR	b	305	-	-	10/10/68/68	0/4/4/4
19	CLR	m	202	-	-	5/10/68/68	0/4/4/4
18	PTY	e	101	-	-	21/53/53/53	-
19	CLR	j	203	-	-	7/10/68/68	0/4/4/4
19	CLR	h	202	-	-	7/10/68/68	0/4/4/4
19	CLR	l	202	-	-	9/10/68/68	0/4/4/4
17	LP3	a	903	-	-	15/36/36/36	-
14	PC1	l	201	-	-	22/57/57/57	-
14	PC1	b	302	-	-	20/57/57/57	-
19	CLR	n	202	-	-	3/10/68/68	0/4/4/4
19	CLR	k	204	-	-	7/10/68/68	0/4/4/4
19	CLR	i	201	-	-	10/10/68/68	0/4/4/4
19	CLR	o	201	-	-	8/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	WJP	a	901	-	-	11/37/37/40	-
19	CLR	i	203	-	-	6/10/68/68	0/4/4/4
14	PC1	a	904	-	-	24/57/57/57	-
19	CLR	k	201	-	-	5/10/68/68	0/4/4/4
19	CLR	m	203	-	-	5/10/68/68	0/4/4/4
19	CLR	n	203	-	-	8/10/68/68	0/4/4/4
18	PTY	a	906	-	-	20/53/53/53	-
19	CLR	o	203	-	-	6/10/68/68	0/4/4/4
16	NAG	a	902	4	-	2/6/23/26	0/1/1/1
14	PC1	b	301	-	-	24/57/57/57	-
18	PTY	p	403	-	-	27/53/53/53	-
19	CLR	i	204	-	-	9/10/68/68	0/4/4/4
19	CLR	m	204	-	-	5/10/68/68	0/4/4/4
19	CLR	j	205	-	-	4/10/68/68	0/4/4/4
18	PTY	a	905	-	-	19/53/53/53	-
19	CLR	m	205	-	-	5/10/68/68	0/4/4/4
18	PTY	p	402	-	-	26/53/53/53	-
19	CLR	l	203	-	-	3/10/68/68	0/4/4/4
19	CLR	j	204	-	-	8/10/68/68	0/4/4/4
18	PTY	j	201	-	-	23/53/53/53	-
19	CLR	l	204	-	-	9/10/68/68	0/4/4/4
19	CLR	k	202	-	-	7/10/68/68	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	901	WJP	C18-C16	3.48	1.58	1.51
15	a	901	WJP	C07-C06	3.03	1.58	1.50
15	a	901	WJP	P31-O32	2.99	1.66	1.54
15	a	901	WJP	C17-C16	2.82	1.57	1.50
15	a	901	WJP	C13-C11	2.69	1.56	1.51
15	a	901	WJP	C14-C15	2.30	1.57	1.50
15	a	901	WJP	C08-C06	2.10	1.55	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	901	WJP	C08-C06-C05	22.84	167.33	121.12
15	a	901	WJP	C17-C16-C18	-20.52	80.75	115.27
15	a	901	WJP	C18-C16-C15	-19.10	82.46	121.12
15	a	901	WJP	C07-C06-C08	-15.68	88.89	115.27
15	a	901	WJP	C17-C16-C15	15.39	163.16	123.68
15	a	901	WJP	C07-C06-C05	-7.95	103.29	123.68
15	a	901	WJP	C14-C15-C16	6.36	142.99	127.66
19	h	201	CLR	C1-C2-C3	6.24	118.47	110.47
19	o	203	CLR	C1-C2-C3	4.97	116.84	110.47
19	k	201	CLR	C1-C2-C3	4.82	116.65	110.47
19	n	203	CLR	C1-C2-C3	4.73	116.54	110.47
19	o	201	CLR	C1-C2-C3	4.61	116.38	110.47
19	o	202	CLR	C16-C17-C20	4.42	118.98	112.15
19	o	201	CLR	C2-C1-C10	4.31	122.09	112.74
19	h	201	CLR	C2-C1-C10	4.07	121.56	112.74
19	i	201	CLR	C1-C2-C3	4.02	115.63	110.47
19	m	201	CLR	C1-C2-C3	3.97	115.56	110.47
19	o	203	CLR	C2-C1-C10	3.97	121.33	112.74
19	m	201	CLR	C12-C11-C9	3.89	119.85	113.11
19	i	203	CLR	C1-C2-C3	3.87	115.43	110.47
19	k	204	CLR	C1-C2-C3	3.87	115.43	110.47
19	n	203	CLR	C2-C1-C10	3.81	121.00	112.74
19	l	202	CLR	C1-C2-C3	3.71	115.23	110.47
19	m	205	CLR	C1-C2-C3	3.43	114.87	110.47
16	a	902	NAG	C2-N2-C7	3.42	127.77	122.90
19	m	201	CLR	C2-C1-C10	3.39	120.09	112.74
19	m	202	CLR	C1-C2-C3	3.38	114.81	110.47
19	i	203	CLR	C2-C1-C10	3.37	120.03	112.74
19	k	204	CLR	C2-C1-C10	3.29	119.86	112.74
19	i	201	CLR	C2-C1-C10	3.25	119.77	112.74
16	a	902	NAG	C1-O5-C5	3.21	116.54	112.19
19	m	202	CLR	C2-C1-C10	3.17	119.62	112.74
19	l	202	CLR	C2-C1-C10	3.09	119.44	112.74
19	l	203	CLR	C1-C2-C3	3.07	114.41	110.47
19	l	203	CLR	C2-C1-C10	3.06	119.37	112.74
19	k	201	CLR	C2-C1-C10	3.01	119.25	112.74
19	m	201	CLR	C11-C12-C13	2.96	117.86	112.78
19	h	202	CLR	C16-C17-C20	2.91	116.65	112.15
19	h	202	CLR	C22-C20-C17	2.90	116.28	110.28
19	j	203	CLR	C21-C20-C17	2.82	117.23	112.92
15	a	901	WJP	P27-O30-P31	-2.75	123.41	132.83
19	k	201	CLR	C2-C3-C4	2.66	113.95	110.31
19	m	205	CLR	C2-C3-C4	2.63	113.91	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	o	201	CLR	C3-C4-C5	-2.57	107.67	112.03
19	j	203	CLR	C13-C17-C20	2.55	123.48	119.49
19	n	204	CLR	C16-C17-C13	-2.53	100.79	103.84
19	m	204	CLR	C16-C17-C20	2.53	116.06	112.15
19	o	202	CLR	C22-C20-C17	2.52	115.50	110.28
19	l	202	CLR	C16-C17-C13	-2.52	100.80	103.84
19	j	204	CLR	C21-C20-C17	2.50	116.75	112.92
19	i	202	CLR	C16-C17-C20	2.50	116.01	112.15
19	j	203	CLR	C12-C13-C14	-2.48	103.43	107.27
19	i	204	CLR	C16-C17-C20	2.45	115.94	112.15
19	l	202	CLR	C16-C17-C20	2.44	115.93	112.15
19	k	202	CLR	C3-C4-C5	2.44	116.16	112.03
19	n	203	CLR	C16-C17-C20	2.41	115.87	112.15
14	b	302	PC1	O12-P-O14	2.39	124.07	112.24
19	k	202	CLR	C4-C5-C10	2.35	119.55	116.42
14	l	201	PC1	O12-P-O14	2.35	123.87	112.24
19	n	204	CLR	C16-C17-C20	2.34	115.76	112.15
19	l	202	CLR	C22-C20-C17	2.33	115.11	110.28
14	P	501	PC1	O12-P-O14	2.33	123.75	112.24
14	a	904	PC1	O12-P-O14	2.33	123.74	112.24
19	i	203	CLR	C12-C13-C14	-2.31	103.69	107.27
19	k	204	CLR	C22-C20-C17	2.28	114.99	110.28
19	m	204	CLR	C2-C1-C10	2.26	117.63	112.74
14	b	301	PC1	O12-P-O14	2.24	123.31	112.24
19	m	201	CLR	C14-C8-C9	-2.20	106.14	109.09
19	m	205	CLR	C16-C17-C20	2.19	115.53	112.15
19	o	202	CLR	C21-C20-C22	2.18	113.78	110.36
19	i	203	CLR	C16-C17-C20	2.17	115.50	112.15
19	h	202	CLR	C16-C17-C13	-2.16	101.24	103.84
19	o	201	CLR	C16-C17-C20	2.08	115.37	112.15
19	h	201	CLR	C3-C4-C5	-2.05	108.54	112.03
19	m	205	CLR	C22-C20-C17	2.05	114.52	110.28
19	n	201	CLR	C13-C14-C8	2.04	117.40	114.38
19	m	202	CLR	C14-C8-C9	2.04	111.82	109.09
19	o	202	CLR	C21-C20-C17	-2.01	109.84	112.92
19	j	203	CLR	C15-C14-C13	2.01	106.27	103.84
19	i	202	CLR	C22-C20-C17	2.01	114.43	110.28

There are no chirality outliers.

All (533) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C1-O11-P-O14
14	a	904	PC1	C22-C21-O21-C2
14	b	301	PC1	C11-O13-P-O12
14	b	301	PC1	O22-C21-O21-C2
14	b	301	PC1	C22-C21-O21-C2
14	b	302	PC1	C11-O13-P-O14
14	b	302	PC1	O22-C21-O21-C2
14	b	302	PC1	C22-C21-O21-C2
14	l	201	PC1	C11-O13-P-O12
14	l	201	PC1	C11-O13-P-O14
14	l	201	PC1	C11-O13-P-O11
14	l	201	PC1	C1-O11-P-O13
14	l	201	PC1	C2-C1-O11-P
14	l	201	PC1	O22-C21-O21-C2
14	l	201	PC1	C22-C21-O21-C2
15	a	901	WJP	P27-O30-P31-O32
17	a	903	LP3	O4P-C4-C5-N
17	a	903	LP3	C1-O3P-P-O2P
18	a	905	PTY	C3-O11-P1-O13
18	a	905	PTY	C5-O14-P1-O12
18	a	906	PTY	C5-O14-P1-O11
18	b	303	PTY	N1-C2-C3-O11
18	b	303	PTY	C5-O14-P1-O12
18	b	303	PTY	C5-O14-P1-O13
18	b	304	PTY	N1-C2-C3-O11
18	b	304	PTY	C3-O11-P1-O12
18	b	304	PTY	C3-O11-P1-O13
18	b	304	PTY	C3-O11-P1-O14
18	b	304	PTY	C5-O14-P1-O12
18	e	101	PTY	N1-C2-C3-O11
18	e	101	PTY	O10-C8-O7-C6
18	j	201	PTY	N1-C2-C3-O11
18	j	201	PTY	O10-C8-O7-C6
18	j	201	PTY	C11-C8-O7-C6
18	p	401	PTY	N1-C2-C3-O11
18	p	401	PTY	C3-O11-P1-O12
18	p	401	PTY	C3-O11-P1-O13
18	p	402	PTY	N1-C2-C3-O11
18	p	402	PTY	C11-C8-O7-C6
18	p	402	PTY	C3-O11-P1-O13

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Mol	Chain	Res	Type	Atoms
18	p	403	PTY	C11-C8-O7-C6
18	p	403	PTY	C3-O11-P1-O12
18	p	403	PTY	C3-O11-P1-O13
18	p	403	PTY	C3-O11-P1-O14
19	h	202	CLR	C13-C17-C20-C21
19	h	202	CLR	C16-C17-C20-C22
19	j	204	CLR	C13-C17-C20-C22
14	b	302	PC1	O32-C31-O31-C3
14	b	301	PC1	O32-C31-O31-C3
18	p	402	PTY	O30-C30-O4-C1
19	h	202	CLR	C16-C17-C20-C21
19	h	202	CLR	C13-C17-C20-C22
19	h	201	CLR	C20-C22-C23-C24
14	a	904	PC1	O22-C21-O21-C2
18	p	402	PTY	O10-C8-O7-C6
18	p	403	PTY	O10-C8-O7-C6
14	b	302	PC1	C32-C31-O31-C3
18	j	201	PTY	C31-C30-O4-C1
18	p	402	PTY	C31-C30-O4-C1
14	P	501	PC1	C22-C21-O21-C2
18	e	101	PTY	C11-C8-O7-C6
19	o	202	CLR	C21-C20-C22-C23
19	i	203	CLR	C16-C17-C20-C21
19	m	204	CLR	C16-C17-C20-C21
19	i	203	CLR	C13-C17-C20-C21
19	m	204	CLR	C13-C17-C20-C21
19	i	203	CLR	C13-C17-C20-C22
19	m	204	CLR	C13-C17-C20-C22
14	a	904	PC1	O32-C31-O31-C3
14	a	904	PC1	C32-C31-O31-C3
14	b	301	PC1	C32-C31-O31-C3
18	j	201	PTY	O30-C30-O4-C1
19	m	204	CLR	C16-C17-C20-C22
19	i	201	CLR	C20-C22-C23-C24
19	o	201	CLR	C17-C20-C22-C23
18	p	401	PTY	C40-C41-C42-C43
19	n	203	CLR	C13-C17-C20-C22
19	i	204	CLR	C17-C20-C22-C23
19	k	203	CLR	C17-C20-C22-C23
19	i	201	CLR	C21-C20-C22-C23
19	i	204	CLR	C21-C20-C22-C23
19	m	201	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
19	o	201	CLR	C21-C20-C22-C23
19	i	203	CLR	C16-C17-C20-C22
19	j	202	CLR	C13-C17-C20-C22
19	i	201	CLR	C17-C20-C22-C23
19	l	202	CLR	C17-C20-C22-C23
19	l	204	CLR	C17-C20-C22-C23
19	m	201	CLR	C17-C20-C22-C23
19	m	202	CLR	C17-C20-C22-C23
15	a	901	WJP	C04-C05-C06-C08
19	m	202	CLR	C21-C20-C22-C23
18	p	401	PTY	C17-C18-C19-C20
19	j	203	CLR	C13-C17-C20-C22
19	o	202	CLR	C13-C17-C20-C22
19	h	202	CLR	C17-C20-C22-C23
19	j	203	CLR	C17-C20-C22-C23
16	a	902	NAG	C8-C7-N2-C2
16	a	902	NAG	O7-C7-N2-C2
18	a	906	PTY	O14-C5-C6-O7
18	p	401	PTY	C15-C16-C17-C18
19	n	202	CLR	C22-C23-C24-C25
19	o	201	CLR	C22-C23-C24-C25
19	o	202	CLR	C20-C22-C23-C24
19	j	203	CLR	C21-C20-C22-C23
19	k	203	CLR	C21-C20-C22-C23
19	l	202	CLR	C21-C20-C22-C23
19	l	204	CLR	C21-C20-C22-C23
18	b	304	PTY	C8-C11-C12-C13
19	o	202	CLR	C16-C17-C20-C21
19	o	202	CLR	C13-C17-C20-C21
19	i	202	CLR	C13-C17-C20-C22
17	a	903	LP3	C11-C12-C13-C14
19	k	204	CLR	C20-C22-C23-C24
19	h	201	CLR	C17-C20-C22-C23
19	h	202	CLR	C21-C20-C22-C23
19	l	203	CLR	C22-C23-C24-C25
19	n	201	CLR	C22-C23-C24-C25
18	p	401	PTY	C8-C11-C12-C13
15	a	901	WJP	C02-C03-C04-C05
19	l	202	CLR	C20-C22-C23-C24
19	m	203	CLR	C22-C23-C24-C25
19	n	203	CLR	C13-C17-C20-C21
19	l	202	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
18	j	201	PTY	C30-C31-C32-C33
18	p	402	PTY	C30-C31-C32-C33
19	j	203	CLR	C22-C23-C24-C25
19	b	305	CLR	C17-C20-C22-C23
19	j	205	CLR	C17-C20-C22-C23
19	k	202	CLR	C17-C20-C22-C23
19	h	201	CLR	C21-C20-C22-C23
14	a	904	PC1	C31-C32-C33-C34
18	b	303	PTY	C8-C11-C12-C13
19	b	305	CLR	C22-C23-C24-C25
19	i	202	CLR	C16-C17-C20-C21
19	n	203	CLR	C16-C17-C20-C21
19	j	202	CLR	C13-C17-C20-C21
19	j	203	CLR	C16-C17-C20-C22
19	j	204	CLR	C16-C17-C20-C22
19	m	204	CLR	C22-C23-C24-C25
19	n	204	CLR	C17-C20-C22-C23
19	b	305	CLR	C21-C20-C22-C23
19	j	205	CLR	C21-C20-C22-C23
19	b	305	CLR	C20-C22-C23-C24
15	a	901	WJP	C16-C18-C19-C20
19	k	201	CLR	C22-C23-C24-C25
19	m	201	CLR	C22-C23-C24-C25
19	j	202	CLR	C16-C17-C20-C21
19	j	204	CLR	C16-C17-C20-C21
19	i	202	CLR	C13-C17-C20-C21
19	i	201	CLR	C22-C23-C24-C25
19	k	201	CLR	C20-C22-C23-C24
19	m	201	CLR	C20-C22-C23-C24
19	k	202	CLR	C21-C20-C22-C23
19	j	203	CLR	C20-C22-C23-C24
19	n	203	CLR	C20-C22-C23-C24
14	a	904	PC1	C11-O13-P-O11
14	b	302	PC1	C11-O13-P-O11
14	b	302	PC1	C1-O11-P-O13
18	a	905	PTY	C3-O11-P1-O14
18	a	905	PTY	C5-O14-P1-O11
18	b	303	PTY	C5-O14-P1-O11
18	e	101	PTY	C5-O14-P1-O11
18	j	201	PTY	C3-O11-P1-O14
18	p	401	PTY	C3-O11-P1-O14
19	o	202	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	m	205	CLR	C13-C17-C20-C22
18	a	905	PTY	C31-C30-O4-C1
19	n	203	CLR	C16-C17-C20-C22
19	n	201	CLR	C21-C20-C22-C23
14	a	904	PC1	C3A-C3B-C3C-C3D
14	b	301	PC1	C2B-C2C-C2D-C2E
14	b	302	PC1	C23-C24-C25-C26
17	a	903	LP3	C12-C13-C14-C15
18	j	201	PTY	C38-C39-C40-C41
18	p	403	PTY	C20-C21-C22-C23
14	b	301	PC1	C21-C22-C23-C24
18	b	303	PTY	C20-C21-C22-C23
14	a	904	PC1	C35-C36-C37-C38
14	b	302	PC1	C26-C27-C28-C29
14	l	201	PC1	C3E-C3F-C3G-C3H
18	b	304	PTY	C16-C17-C18-C19
19	l	202	CLR	C13-C17-C20-C21
14	l	201	PC1	C36-C37-C38-C39
18	a	906	PTY	C18-C19-C20-C21
18	p	402	PTY	C34-C35-C36-C37
19	k	204	CLR	C22-C23-C24-C25
19	o	203	CLR	C22-C23-C24-C25
18	a	905	PTY	O30-C30-O4-C1
19	n	203	CLR	C23-C24-C25-C26
19	n	204	CLR	C23-C24-C25-C26
19	o	203	CLR	C23-C24-C25-C27
15	a	901	WJP	C07-C06-C08-C09
18	b	304	PTY	C24-C25-C26-C27
18	p	403	PTY	C15-C16-C17-C18
19	i	202	CLR	C20-C22-C23-C24
14	a	904	PC1	C2B-C2C-C2D-C2E
18	p	401	PTY	C31-C32-C33-C34
19	l	204	CLR	C16-C17-C20-C21
14	P	501	PC1	C28-C29-C2A-C2B
14	P	501	PC1	C21-C22-C23-C24
18	p	401	PTY	C25-C26-C27-C28
19	n	203	CLR	C23-C24-C25-C27
19	n	204	CLR	C23-C24-C25-C27
19	j	204	CLR	C20-C22-C23-C24
18	p	401	PTY	C24-C25-C26-C27
14	a	904	PC1	C24-C25-C26-C27
14	b	302	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
18	a	905	PTY	C22-C23-C24-C25
19	j	203	CLR	C16-C17-C20-C21
19	n	204	CLR	C21-C20-C22-C23
14	P	501	PC1	C25-C26-C27-C28
14	l	201	PC1	C26-C27-C28-C29
18	j	201	PTY	C33-C34-C35-C36
18	j	201	PTY	C34-C35-C36-C37
14	l	201	PC1	C39-C3A-C3B-C3C
18	b	303	PTY	C30-C31-C32-C33
19	n	204	CLR	C22-C23-C24-C25
14	P	501	PC1	C33-C34-C35-C36
17	a	903	LP3	O3P-C1-C2-O2
19	j	202	CLR	C22-C23-C24-C25
19	l	203	CLR	C17-C20-C22-C23
18	p	403	PTY	C23-C24-C25-C26
18	j	201	PTY	C15-C16-C17-C18
14	b	302	PC1	C2B-C2C-C2D-C2E
18	b	304	PTY	C20-C21-C22-C23
18	e	101	PTY	C12-C13-C14-C15
18	e	101	PTY	C34-C35-C36-C37
14	b	301	PC1	C32-C33-C34-C35
18	p	401	PTY	C35-C36-C37-C38
18	p	403	PTY	C19-C20-C21-C22
19	j	204	CLR	C22-C23-C24-C25
19	l	204	CLR	C13-C17-C20-C22
14	b	302	PC1	C2A-C2B-C2C-C2D
18	a	906	PTY	C12-C13-C14-C15
14	P	501	PC1	C32-C31-O31-C3
14	b	302	PC1	C37-C38-C39-C3A
19	l	202	CLR	C16-C17-C20-C21
19	l	204	CLR	C13-C17-C20-C21
18	p	402	PTY	C39-C40-C41-C42
19	l	204	CLR	C20-C22-C23-C24
19	j	204	CLR	C23-C24-C25-C26
18	b	304	PTY	O10-C8-O7-C6
14	l	201	PC1	C32-C31-O31-C3
18	b	304	PTY	C34-C35-C36-C37
18	p	402	PTY	C38-C39-C40-C41
18	p	403	PTY	C32-C33-C34-C35
14	a	904	PC1	C33-C34-C35-C36
19	m	202	CLR	C23-C24-C25-C27
18	b	304	PTY	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
18	j	201	PTY	C17-C18-C19-C20
18	a	905	PTY	C11-C8-O7-C6
18	b	303	PTY	C11-C8-O7-C6
18	b	304	PTY	C11-C8-O7-C6
18	b	303	PTY	O10-C8-O7-C6
19	m	205	CLR	C13-C17-C20-C21
14	b	301	PC1	C23-C24-C25-C26
14	P	501	PC1	C2E-C2F-C2G-C2H
19	k	201	CLR	C17-C20-C22-C23
14	b	302	PC1	C35-C36-C37-C38
18	p	402	PTY	C37-C38-C39-C40
14	P	501	PC1	O32-C31-O31-C3
19	b	305	CLR	C23-C24-C25-C27
19	l	204	CLR	C23-C24-C25-C27
19	n	202	CLR	C23-C24-C25-C26
19	o	203	CLR	C23-C24-C25-C26
18	a	905	PTY	O10-C8-O7-C6
14	b	301	PC1	C11-O13-P-O11
17	a	903	LP3	C1-O3P-P-O4P
18	p	403	PTY	C31-C32-C33-C34
18	a	906	PTY	O14-C5-C6-C1
18	p	403	PTY	O14-C5-C6-C1
19	i	201	CLR	C23-C24-C25-C26
19	l	204	CLR	C16-C17-C20-C22
14	b	301	PC1	C3E-C3F-C3G-C3H
14	P	501	PC1	C3C-C3D-C3E-C3F
15	a	901	WJP	C12-C11-C13-C14
18	b	303	PTY	C19-C20-C21-C22
18	p	403	PTY	C13-C14-C15-C16
19	m	205	CLR	C16-C17-C20-C21
14	b	301	PC1	C29-C2A-C2B-C2C
18	a	906	PTY	O4-C1-C6-C5
18	b	303	PTY	O4-C1-C6-C5
18	p	402	PTY	C16-C17-C18-C19
19	l	202	CLR	C16-C17-C20-C22
19	m	205	CLR	C16-C17-C20-C22
19	i	204	CLR	C13-C17-C20-C22
19	j	205	CLR	C20-C22-C23-C24
19	n	201	CLR	C20-C22-C23-C24
18	p	401	PTY	C22-C23-C24-C25
18	p	403	PTY	C37-C38-C39-C40
19	m	202	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	m	205	CLR	C22-C23-C24-C25
14	l	201	PC1	C3F-C3G-C3H-C3I
14	b	302	PC1	C29-C2A-C2B-C2C
14	b	301	PC1	C3A-C3B-C3C-C3D
14	b	301	PC1	C3-C2-O21-C21
19	l	203	CLR	C20-C22-C23-C24
14	l	201	PC1	O32-C31-O31-C3
18	j	201	PTY	O14-C5-C6-O7
19	m	202	CLR	C23-C24-C25-C26
14	l	201	PC1	C22-C23-C24-C25
18	e	101	PTY	C37-C38-C39-C40
19	i	204	CLR	C16-C17-C20-C21
19	i	204	CLR	C13-C17-C20-C21
18	p	402	PTY	C35-C36-C37-C38
18	b	303	PTY	C12-C13-C14-C15
18	b	303	PTY	O4-C1-C6-O7
14	b	301	PC1	C38-C39-C3A-C3B
19	m	203	CLR	C16-C17-C20-C21
18	a	905	PTY	C14-C15-C16-C17
19	h	201	CLR	C22-C23-C24-C25
15	a	901	WJP	C10-C11-C13-C14
19	i	202	CLR	C16-C17-C20-C22
19	l	204	CLR	C23-C24-C25-C26
19	m	203	CLR	C13-C17-C20-C21
18	a	906	PTY	C19-C20-C21-C22
19	i	204	CLR	C16-C17-C20-C22
18	e	101	PTY	C36-C37-C38-C39
18	p	402	PTY	C31-C32-C33-C34
15	a	901	WJP	C05-C06-C08-C09
18	j	201	PTY	C36-C37-C38-C39
18	p	401	PTY	C26-C27-C28-C29
14	b	301	PC1	C26-C27-C28-C29
18	b	304	PTY	C31-C30-O4-C1
19	k	201	CLR	C21-C20-C22-C23
18	p	402	PTY	C23-C24-C25-C26
14	l	201	PC1	C3A-C3B-C3C-C3D
19	j	204	CLR	C23-C24-C25-C27
19	l	202	CLR	C23-C24-C25-C26
17	a	903	LP3	C14-C15-C16-C17
14	a	904	PC1	C1-O11-P-O13
18	p	403	PTY	O14-C5-C6-O7
19	m	203	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
19	i	201	CLR	C23-C24-C25-C27
14	b	301	PC1	C22-C23-C24-C25
14	b	302	PC1	C2D-C2E-C2F-C2G
18	b	303	PTY	C40-C41-C42-C43
19	o	202	CLR	C17-C20-C22-C23
19	n	204	CLR	C13-C17-C20-C21
19	b	305	CLR	C13-C17-C20-C22
19	m	203	CLR	C13-C17-C20-C22
19	n	204	CLR	C13-C17-C20-C22
14	b	301	PC1	C2D-C2E-C2F-C2G
19	b	305	CLR	C23-C24-C25-C26
18	p	402	PTY	C15-C16-C17-C18
19	o	202	CLR	C16-C17-C20-C22
19	n	202	CLR	C23-C24-C25-C27
19	i	204	CLR	C22-C23-C24-C25
19	b	305	CLR	C13-C17-C20-C21
14	P	501	PC1	C23-C24-C25-C26
19	b	305	CLR	C16-C17-C20-C22
18	b	303	PTY	C37-C38-C39-C40
18	p	403	PTY	C41-C42-C43-C44
19	n	204	CLR	C16-C17-C20-C22
18	a	905	PTY	C23-C24-C25-C26
14	l	201	PC1	C3-C2-O21-C21
18	p	403	PTY	C33-C34-C35-C36
18	b	304	PTY	O30-C30-O4-C1
18	a	906	PTY	C31-C30-O4-C1
18	b	303	PTY	O14-C5-C6-O7
18	b	304	PTY	O14-C5-C6-O7
19	i	203	CLR	C22-C23-C24-C25
18	a	906	PTY	O4-C1-C6-O7
19	b	305	CLR	C16-C17-C20-C21
19	l	202	CLR	C23-C24-C25-C27
19	h	201	CLR	C23-C24-C25-C26
19	k	202	CLR	C22-C23-C24-C25
18	b	303	PTY	C41-C42-C43-C44
14	P	501	PC1	C1-O11-P-O13
18	b	304	PTY	C5-O14-P1-O11
14	a	904	PC1	C2-C1-O11-P
18	a	906	PTY	C6-C5-O14-P1
19	n	204	CLR	C16-C17-C20-C21
14	P	501	PC1	C11-O13-P-O12
14	a	904	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
14	b	301	PC1	C11-O13-P-O14
14	b	302	PC1	C1-O11-P-O14
14	l	201	PC1	C1-O11-P-O12
17	a	903	LP3	C1-O3P-P-O1P
18	a	905	PTY	C3-O11-P1-O12
18	a	906	PTY	C5-O14-P1-O12
18	e	101	PTY	C5-O14-P1-O13
18	j	201	PTY	C3-O11-P1-O13
19	o	201	CLR	C13-C17-C20-C21
19	i	204	CLR	C23-C24-C25-C26
18	b	304	PTY	O14-C5-C6-C1
18	j	201	PTY	O14-C5-C6-C1
18	p	401	PTY	O14-C5-C6-C1
18	p	402	PTY	C32-C33-C34-C35
19	o	201	CLR	C16-C17-C20-C22
19	o	201	CLR	C13-C17-C20-C22
14	l	201	PC1	C37-C38-C39-C3A
18	a	906	PTY	O30-C30-O4-C1
18	p	401	PTY	C2-C3-O11-P1
19	i	201	CLR	C13-C17-C20-C22
18	p	401	PTY	O14-C5-C6-O7
14	a	904	PC1	C2F-C2G-C2H-C2I
19	i	201	CLR	C16-C17-C20-C22
18	p	401	PTY	C19-C20-C21-C22
18	p	401	PTY	C21-C22-C23-C24
14	a	904	PC1	O13-C11-C12-N
14	b	301	PC1	O13-C11-C12-N
14	l	201	PC1	O13-C11-C12-N
18	j	201	PTY	O4-C1-C6-C5
18	j	201	PTY	O4-C1-C6-O7
19	k	202	CLR	C13-C17-C20-C22
14	l	201	PC1	C2A-C2B-C2C-C2D
19	i	201	CLR	C13-C17-C20-C21
19	j	204	CLR	C13-C17-C20-C21
19	k	202	CLR	C13-C17-C20-C21
19	h	201	CLR	C23-C24-C25-C27
18	j	201	PTY	C20-C21-C22-C23
18	j	201	PTY	C25-C26-C27-C28
18	e	101	PTY	C35-C36-C37-C38
18	e	101	PTY	C15-C16-C17-C18
14	b	302	PC1	C3-C2-O21-C21
19	o	201	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
18	e	101	PTY	C6-C5-O14-P1
14	a	904	PC1	C3E-C3F-C3G-C3H
19	k	202	CLR	C16-C17-C20-C22
18	a	906	PTY	C3-O11-P1-O14
18	b	303	PTY	C3-O11-P1-O14
18	p	401	PTY	C5-O14-P1-O11
18	p	402	PTY	C3-O11-P1-O14
18	p	402	PTY	C5-O14-P1-O11
18	p	402	PTY	C8-C11-C12-C13
18	e	101	PTY	C41-C42-C43-C44
18	p	403	PTY	C35-C36-C37-C38
18	j	201	PTY	C24-C25-C26-C27
19	i	204	CLR	C23-C24-C25-C27
17	a	903	LP3	C20-C21-C22-C23
18	p	403	PTY	C14-C15-C16-C17
18	a	905	PTY	C17-C18-C19-C20
18	p	401	PTY	O4-C30-C31-C32
19	i	201	CLR	C16-C17-C20-C21
19	k	204	CLR	C16-C17-C20-C22
18	e	101	PTY	C16-C17-C18-C19
14	b	301	PC1	C25-C26-C27-C28
18	b	303	PTY	C34-C35-C36-C37
19	k	204	CLR	C17-C20-C22-C23
18	j	201	PTY	C22-C23-C24-C25
18	p	401	PTY	C13-C14-C15-C16
18	b	303	PTY	C11-C12-C13-C14
18	p	402	PTY	C5-C6-O7-C8
19	o	201	CLR	C20-C22-C23-C24
14	b	301	PC1	C34-C35-C36-C37
18	p	402	PTY	C20-C21-C22-C23
18	e	101	PTY	C22-C23-C24-C25
18	p	403	PTY	C16-C17-C18-C19
19	k	204	CLR	C13-C17-C20-C21
18	a	906	PTY	C30-C31-C32-C33
18	a	906	PTY	O10-C8-O7-C6
14	a	904	PC1	C3D-C3E-C3F-C3G
19	h	202	CLR	C20-C22-C23-C24
18	b	304	PTY	C36-C37-C38-C39
18	a	905	PTY	C18-C19-C20-C21
14	a	904	PC1	C29-C2A-C2B-C2C
19	k	204	CLR	C13-C17-C20-C22
19	o	203	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
17	a	903	LP3	C25-C26-C27-C28
19	k	201	CLR	C23-C24-C25-C27
14	a	904	PC1	C32-C33-C34-C35
18	a	905	PTY	C19-C20-C21-C22
18	e	101	PTY	O14-C5-C6-O7
18	p	403	PTY	C24-C25-C26-C27
15	a	901	WJP	P31-O30-P27-O26
18	a	906	PTY	C34-C35-C36-C37
18	b	303	PTY	O14-C5-C6-C1
18	e	101	PTY	O14-C5-C6-C1
17	a	903	LP3	C15-C16-C17-C18
18	b	304	PTY	C14-C15-C16-C17
14	b	302	PC1	C2E-C2F-C2G-C2H
18	a	905	PTY	C12-C11-C8-O7
19	i	203	CLR	C20-C22-C23-C24
18	p	402	PTY	C13-C14-C15-C16
18	p	403	PTY	C36-C37-C38-C39
18	p	402	PTY	C1-C6-O7-C8
17	a	903	LP3	C17-C18-C19-C20
18	p	403	PTY	C12-C11-C8-O7
17	a	903	LP3	C19-C20-C21-C22
17	a	903	LP3	O3P-C1-C2-C3
18	e	101	PTY	C8-C11-C12-C13
15	a	901	WJP	P27-O30-P31-O34
14	P	501	PC1	C29-C2A-C2B-C2C
18	b	303	PTY	C24-C25-C26-C27
18	e	101	PTY	C12-C11-C8-O7
19	k	204	CLR	C21-C20-C22-C23
18	a	906	PTY	C25-C26-C27-C28
18	a	905	PTY	O4-C30-C31-C32
18	a	905	PTY	C12-C11-C8-O10
18	p	403	PTY	C12-C13-C14-C15
18	a	906	PTY	C11-C8-O7-C6
14	b	301	PC1	C36-C37-C38-C39
19	n	203	CLR	C22-C23-C24-C25
14	P	501	PC1	C3D-C3E-C3F-C3G
18	a	905	PTY	O30-C30-C31-C32
14	b	301	PC1	C39-C3A-C3B-C3C
18	p	401	PTY	C6-C5-O14-P1
18	a	906	PTY	C3-O11-P1-O13
18	b	303	PTY	C3-O11-P1-O13
18	b	304	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
18	p	402	PTY	C3-O11-P1-O12
18	p	402	PTY	C5-O14-P1-O13
18	p	403	PTY	C5-O14-P1-O13
18	j	201	PTY	C26-C27-C28-C29
19	o	203	CLR	C17-C20-C22-C23
19	k	202	CLR	C16-C17-C20-C21
15	a	901	WJP	P27-O30-P31-O33
18	b	304	PTY	C23-C24-C25-C26
18	p	403	PTY	C12-C11-C8-O10
14	a	904	PC1	C38-C39-C3A-C3B
17	a	903	LP3	C24-C25-C26-C27
18	e	101	PTY	C24-C25-C26-C27
14	a	904	PC1	C12-C11-O13-P
14	l	201	PC1	C12-C11-O13-P
18	b	304	PTY	C17-C18-C19-C20
18	b	303	PTY	C32-C33-C34-C35
18	p	403	PTY	C25-C26-C27-C28
18	e	101	PTY	C12-C11-C8-O10
19	j	205	CLR	C16-C17-C20-C22
19	o	203	CLR	C16-C17-C20-C22
18	b	303	PTY	O4-C30-C31-C32
14	P	501	PC1	C3B-C3C-C3D-C3E
14	P	501	PC1	C31-C32-C33-C34
14	a	904	PC1	C34-C35-C36-C37
18	b	304	PTY	C12-C11-C8-O7
18	b	303	PTY	O30-C30-C31-C32
18	a	906	PTY	O4-C30-C31-C32
14	b	302	PC1	C34-C35-C36-C37

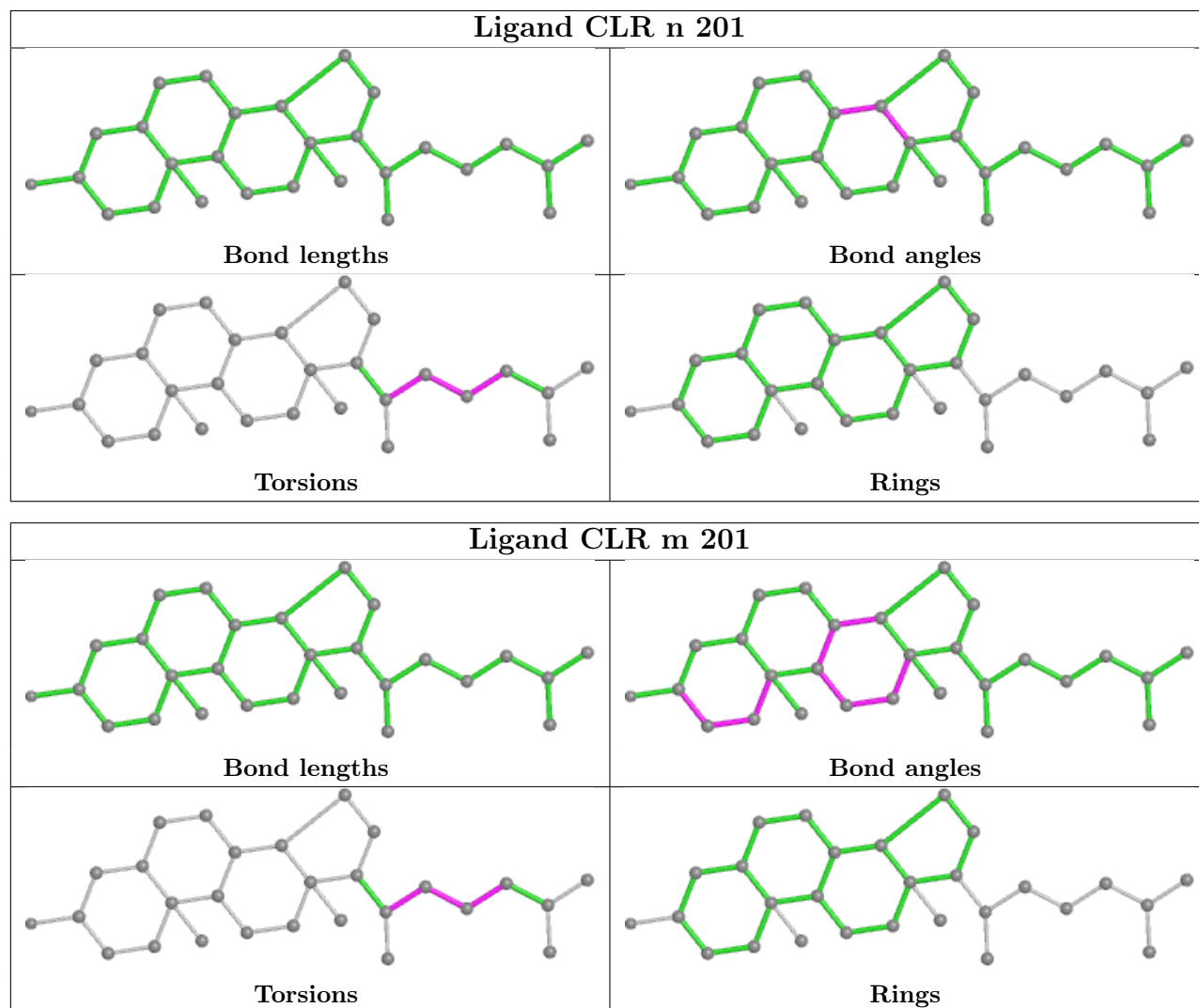
There are no ring outliers.

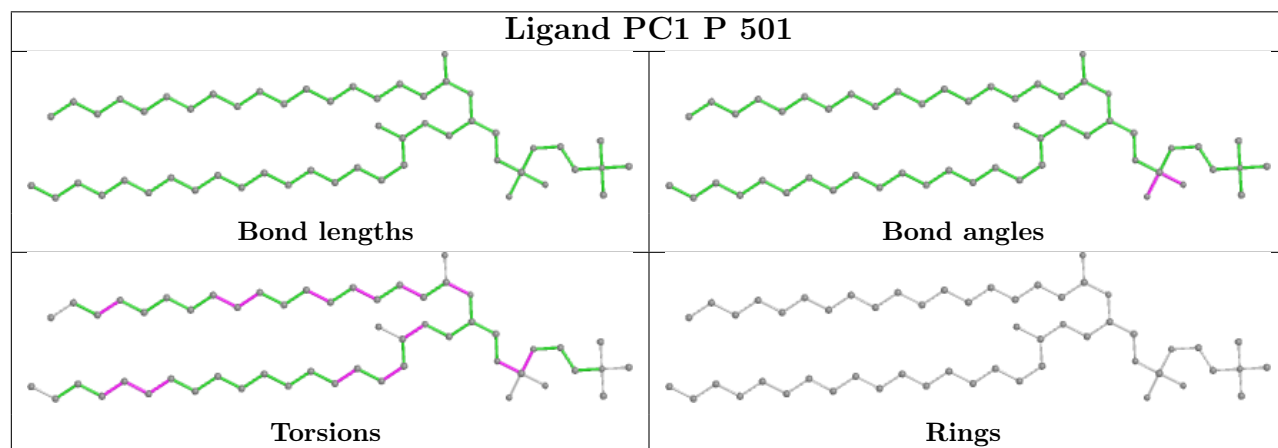
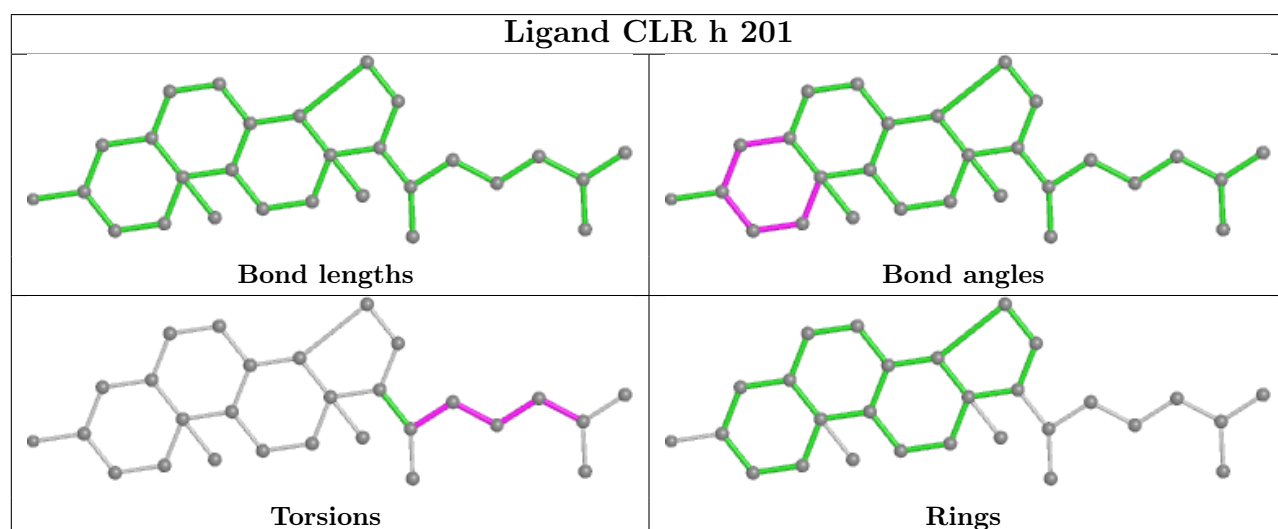
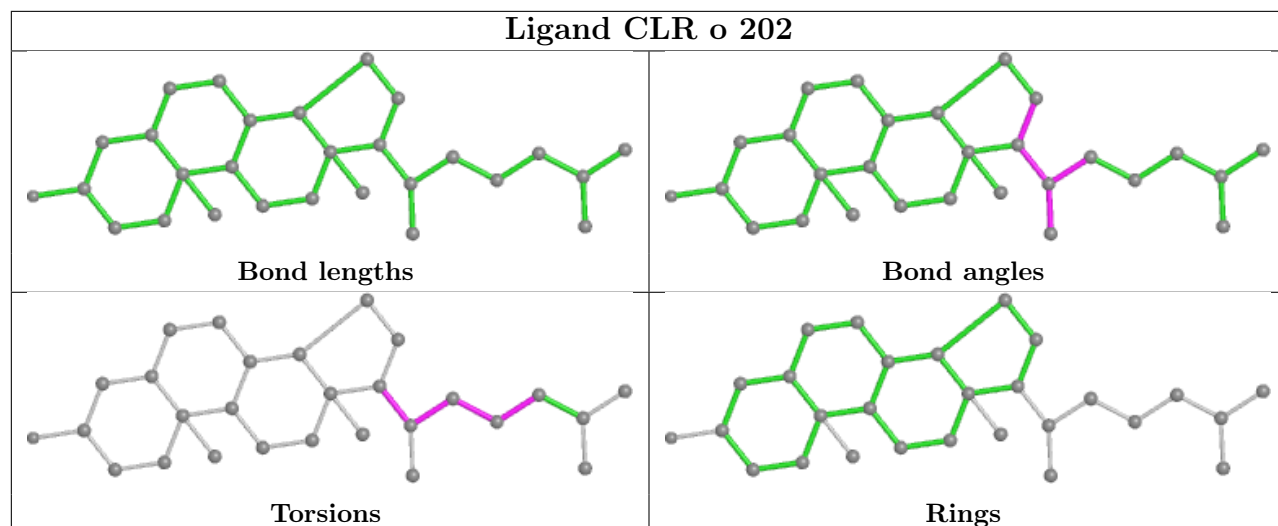
1 monomer is involved in 1 short contact:

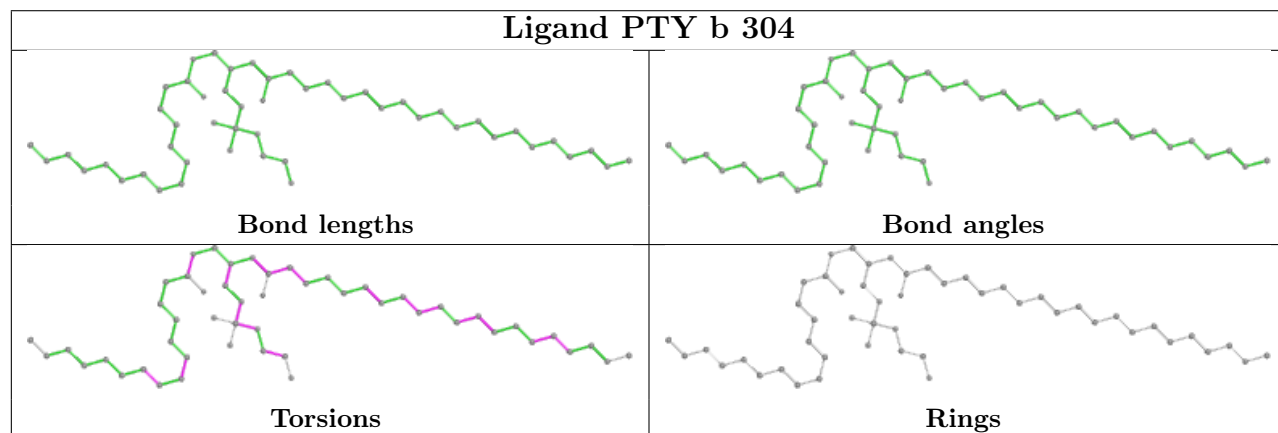
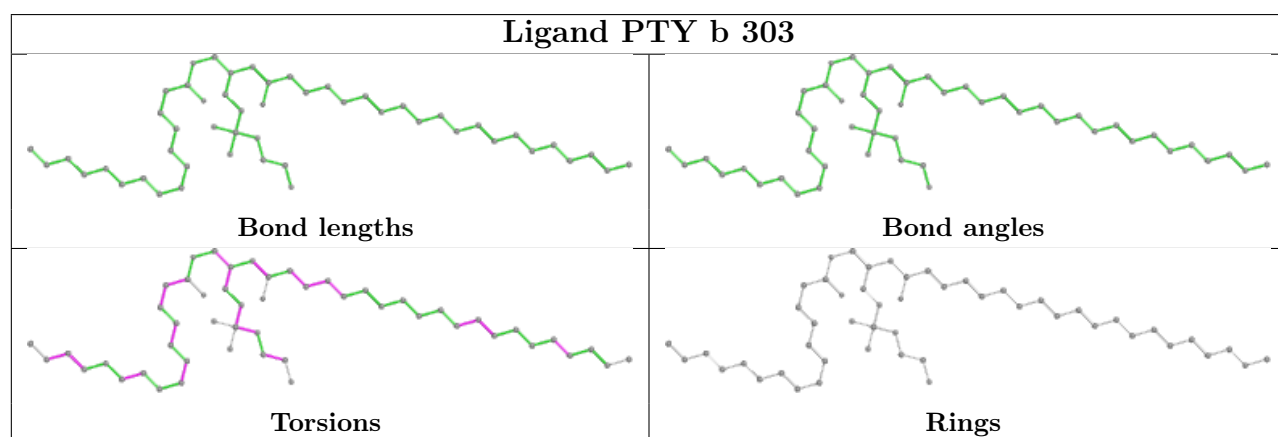
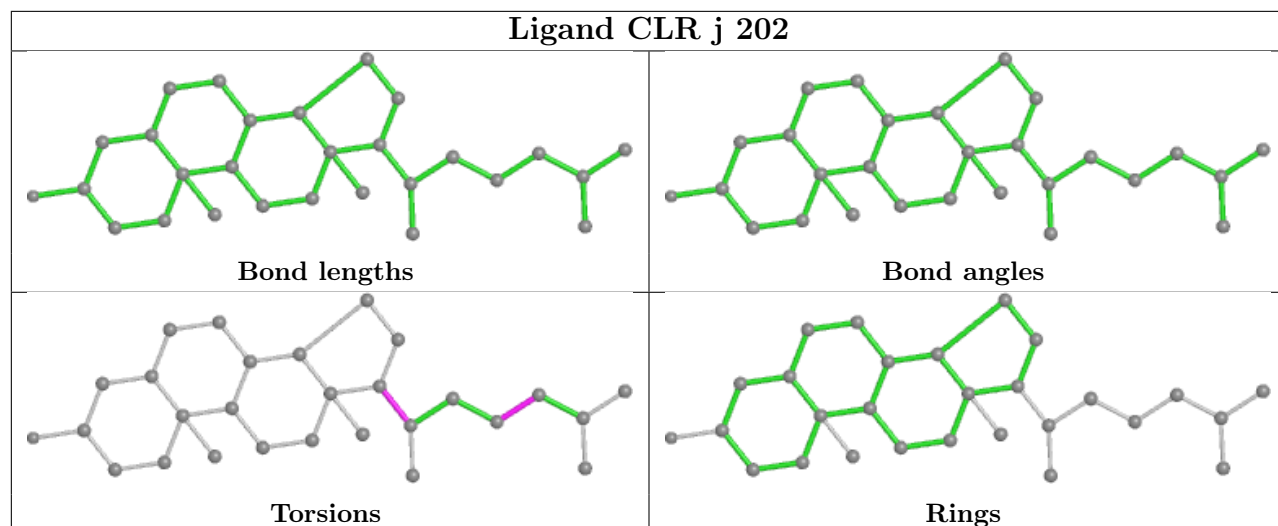
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	P	501	PC1	1	0

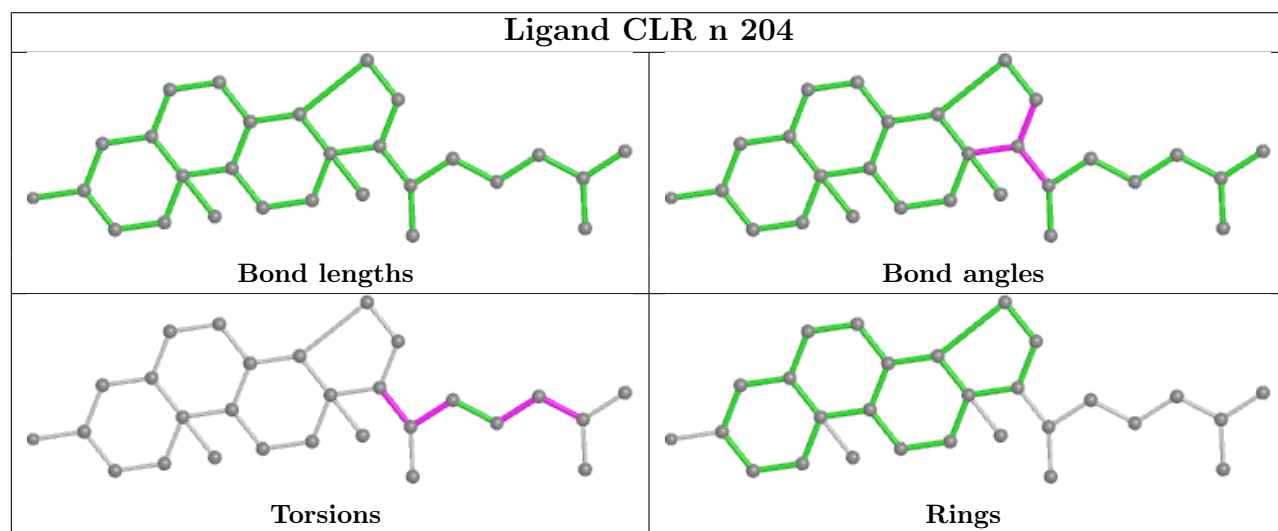
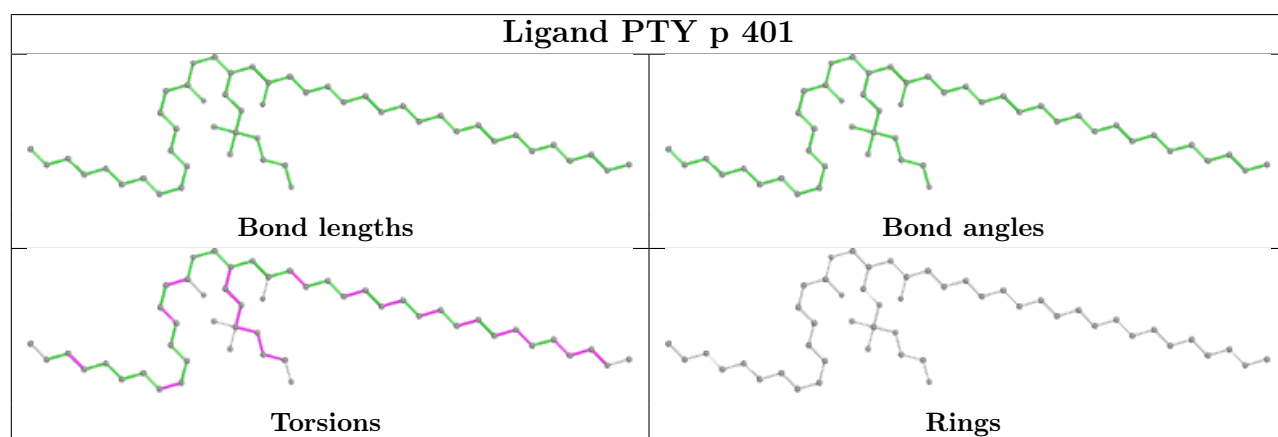
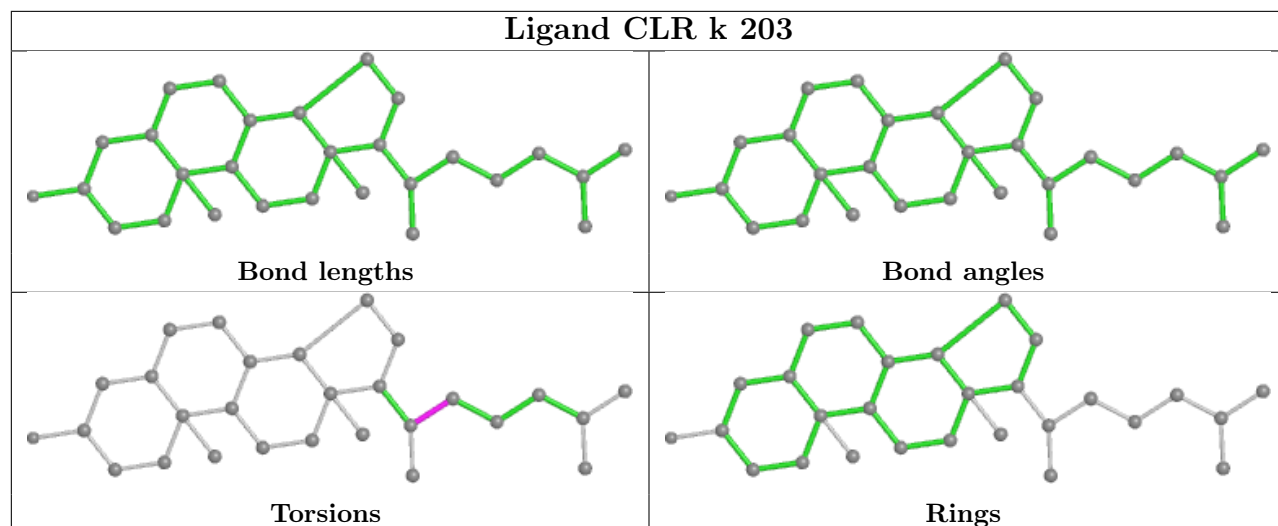
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

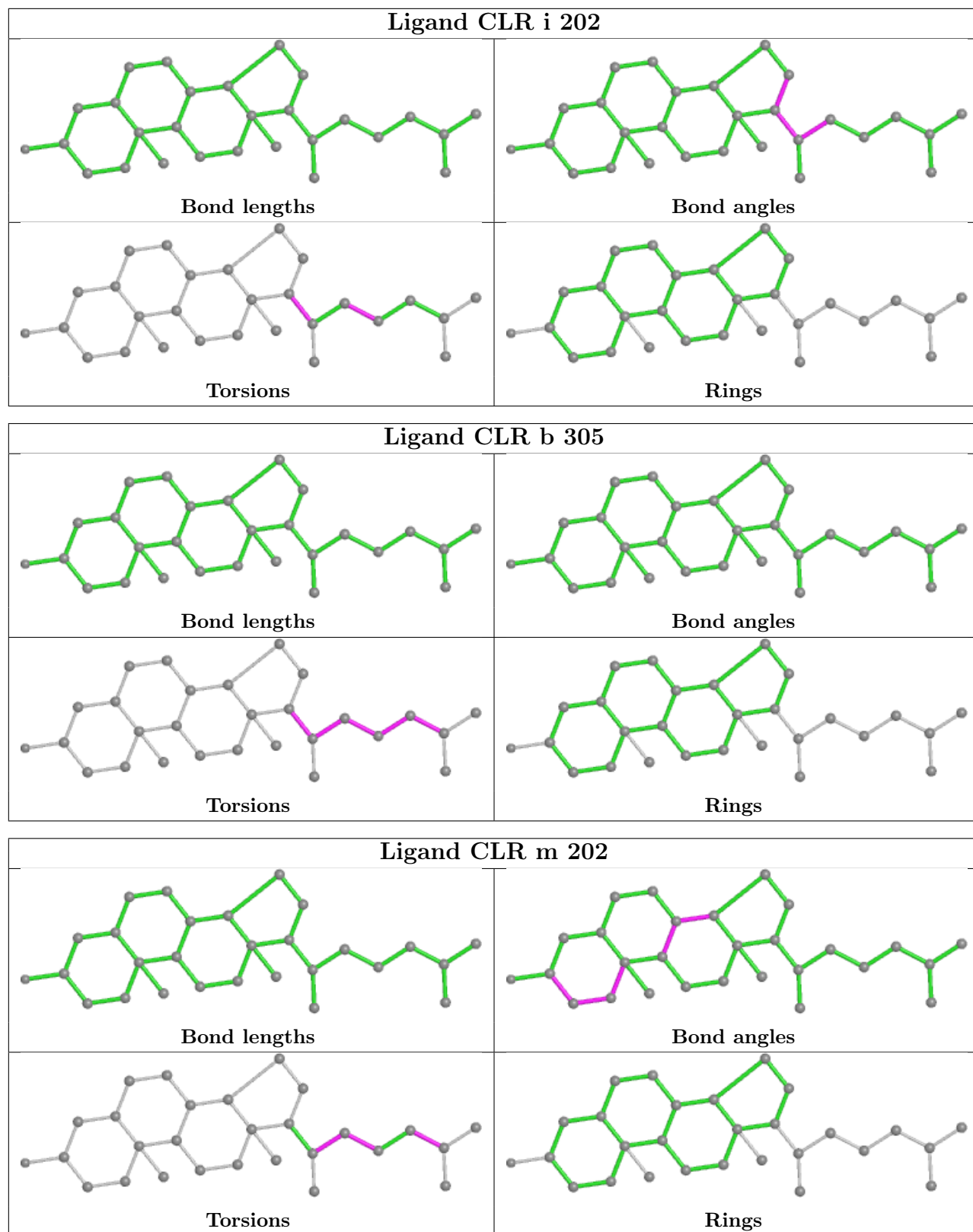
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

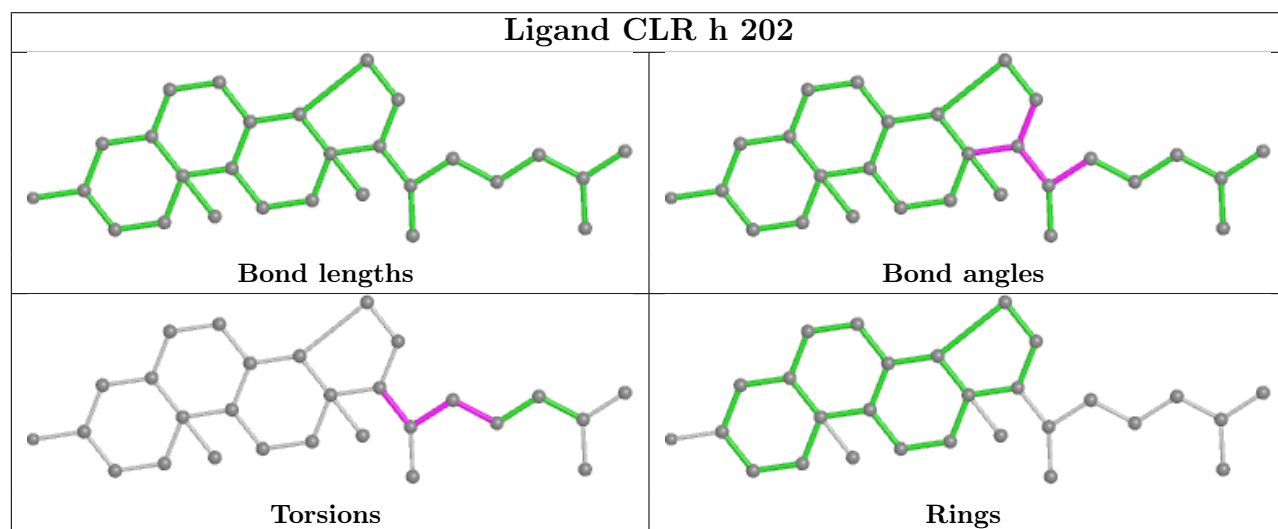
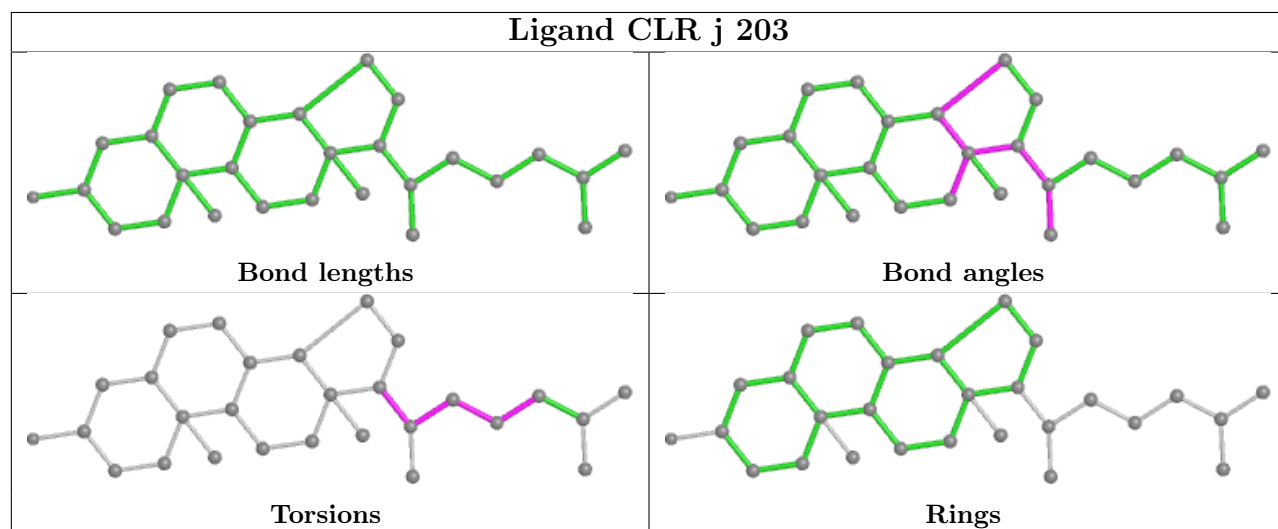
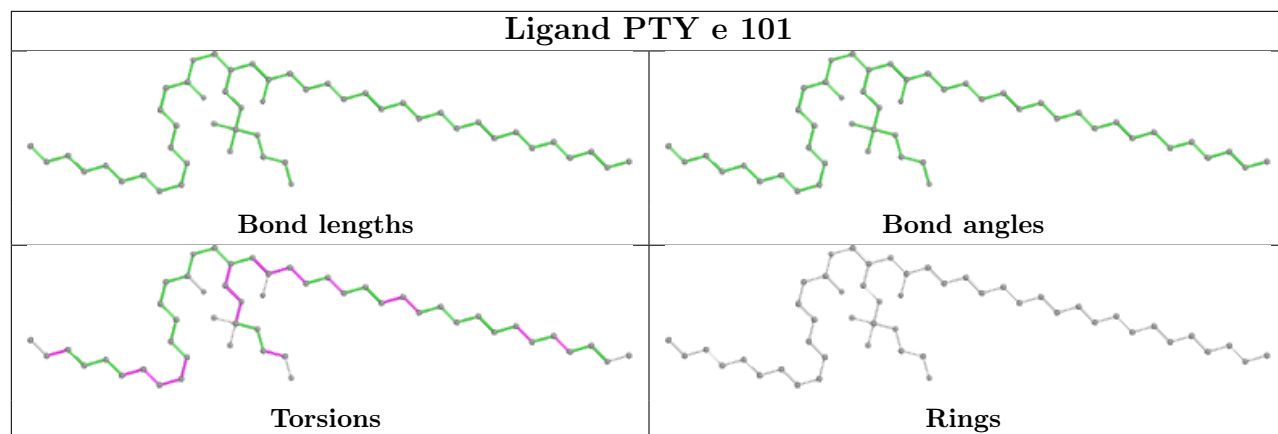


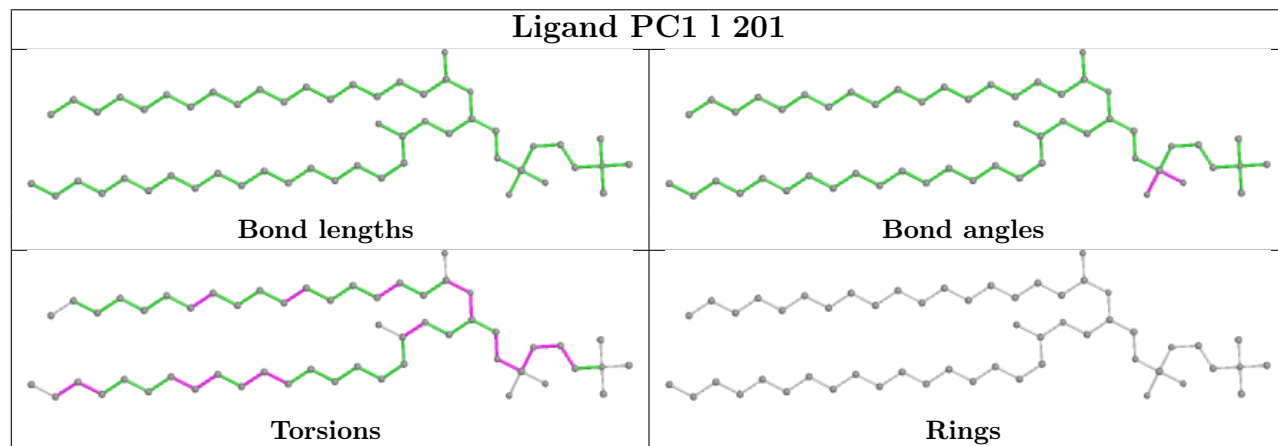
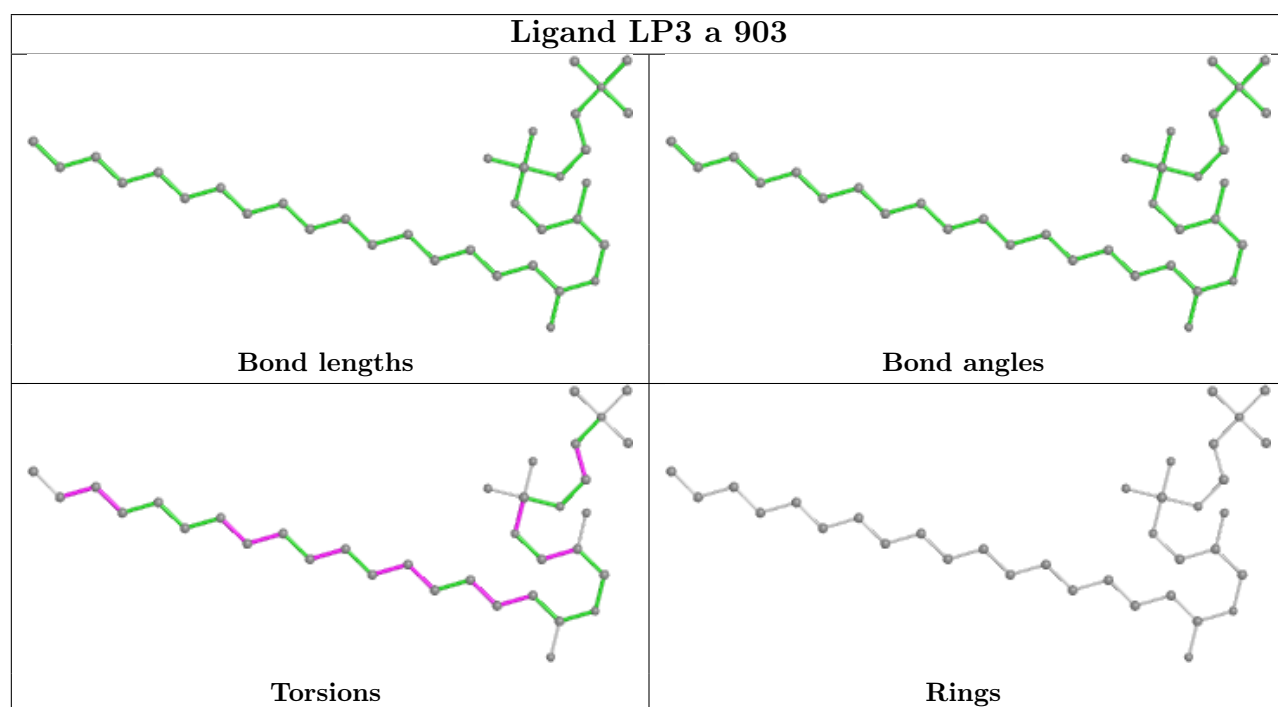
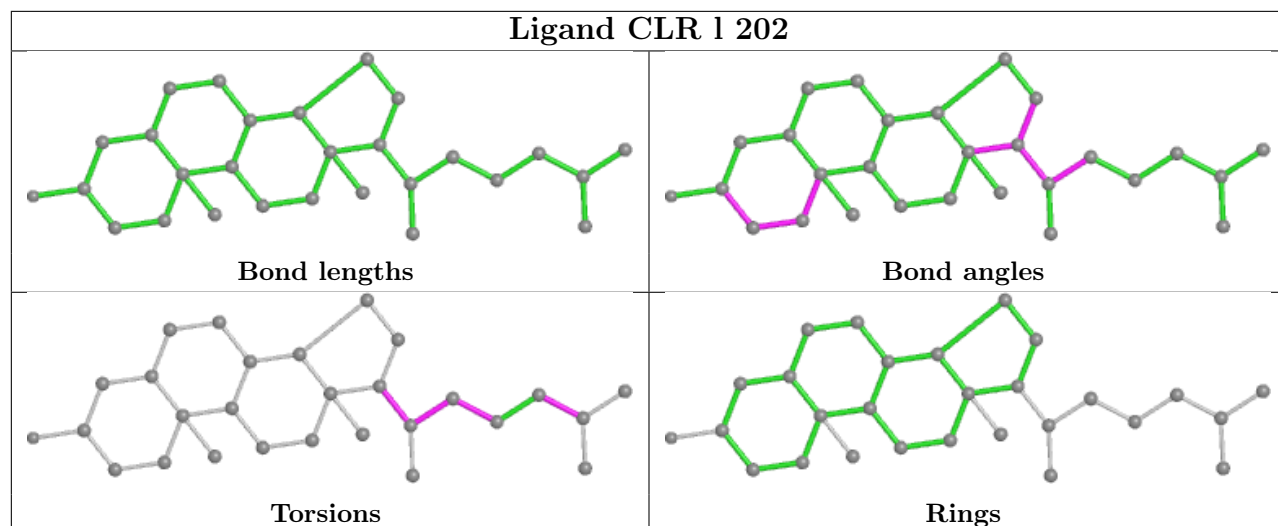




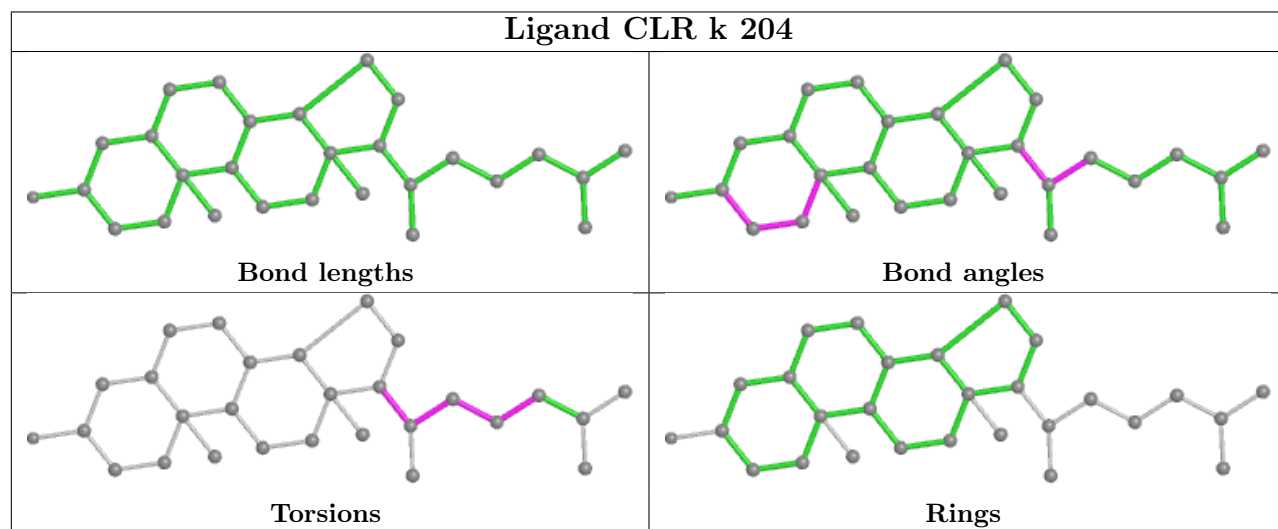
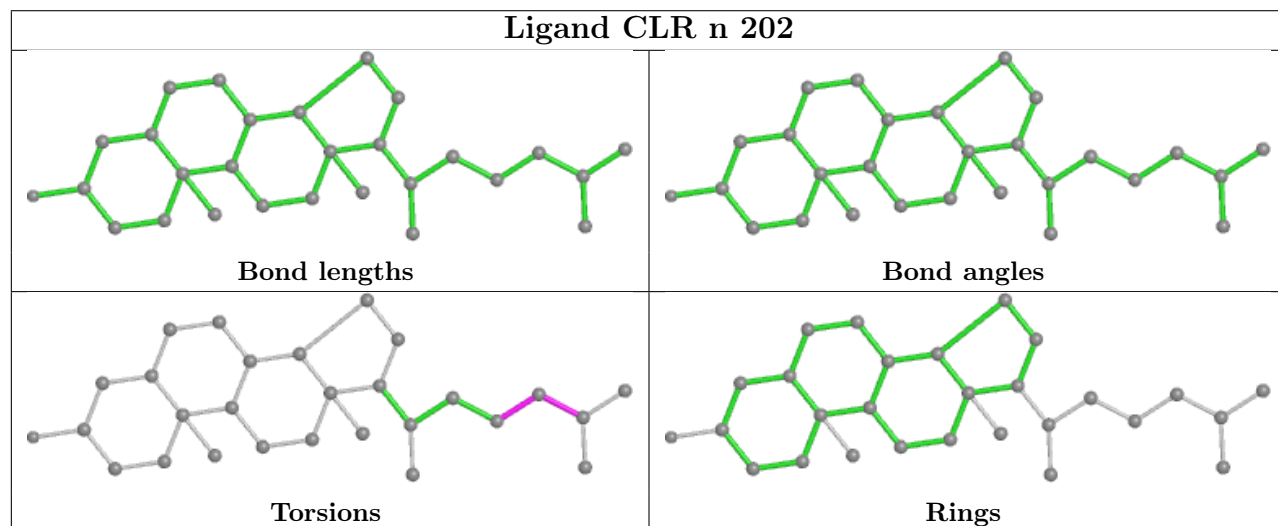
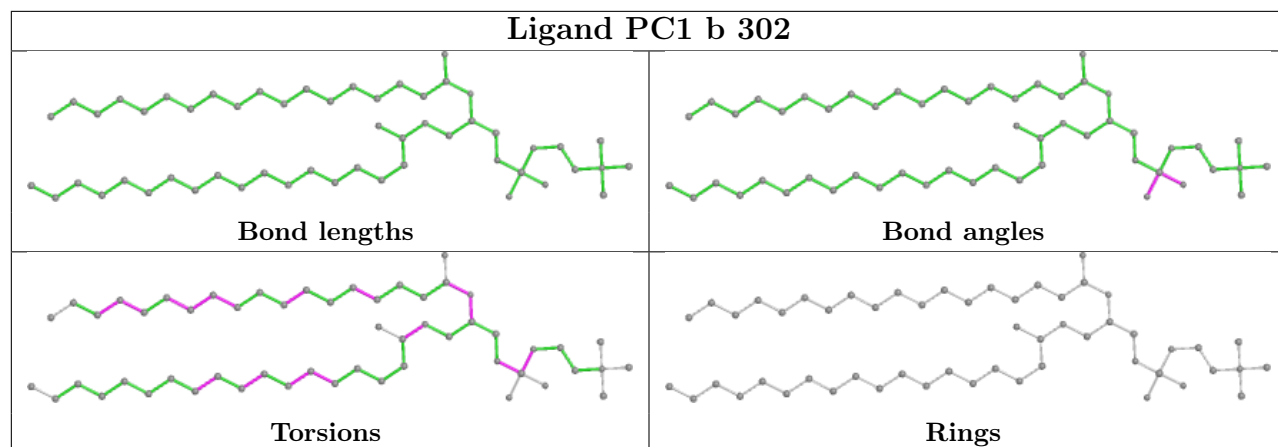


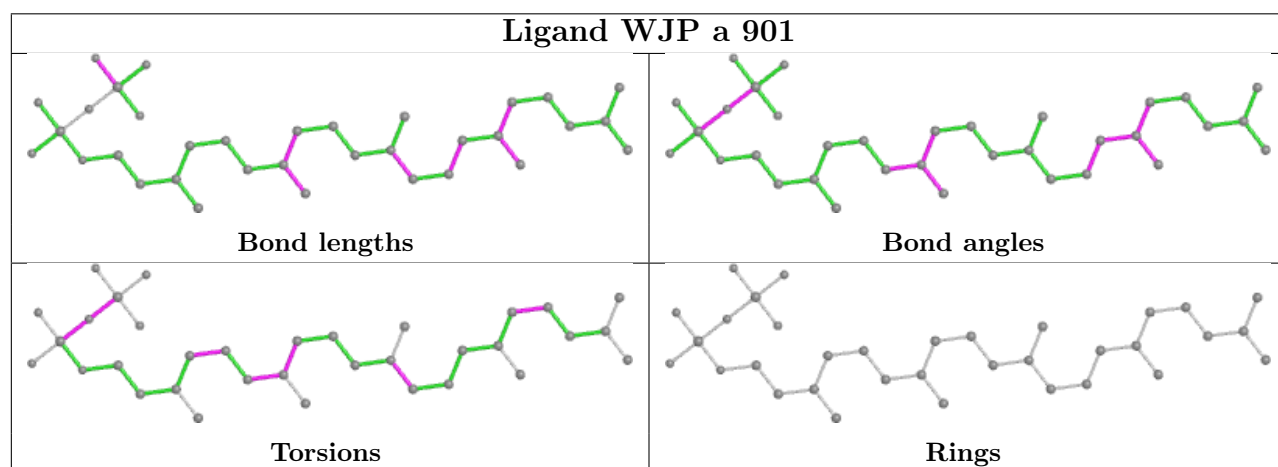
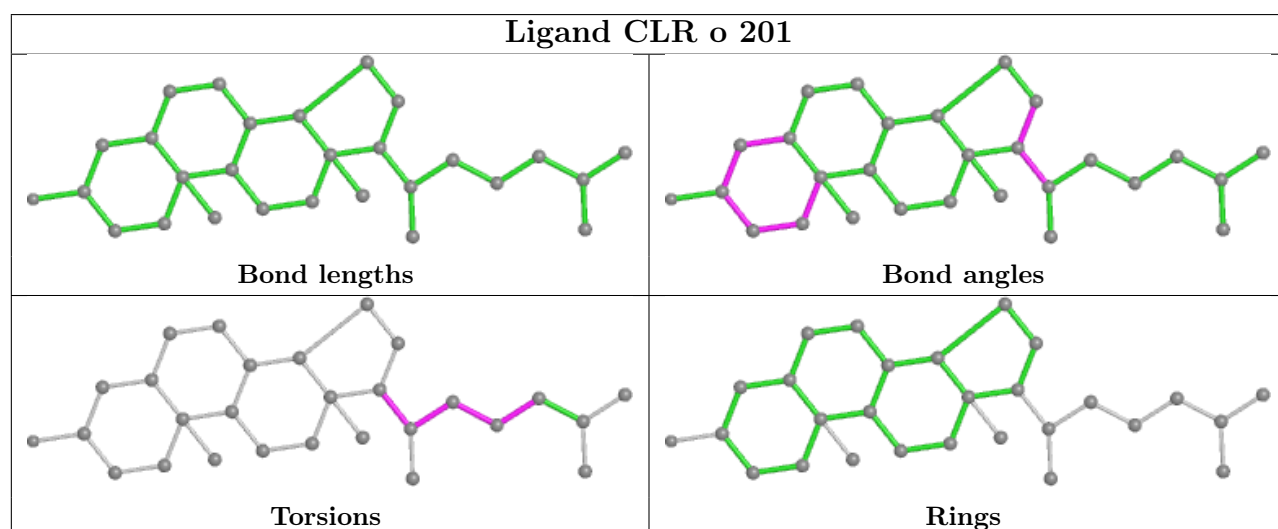
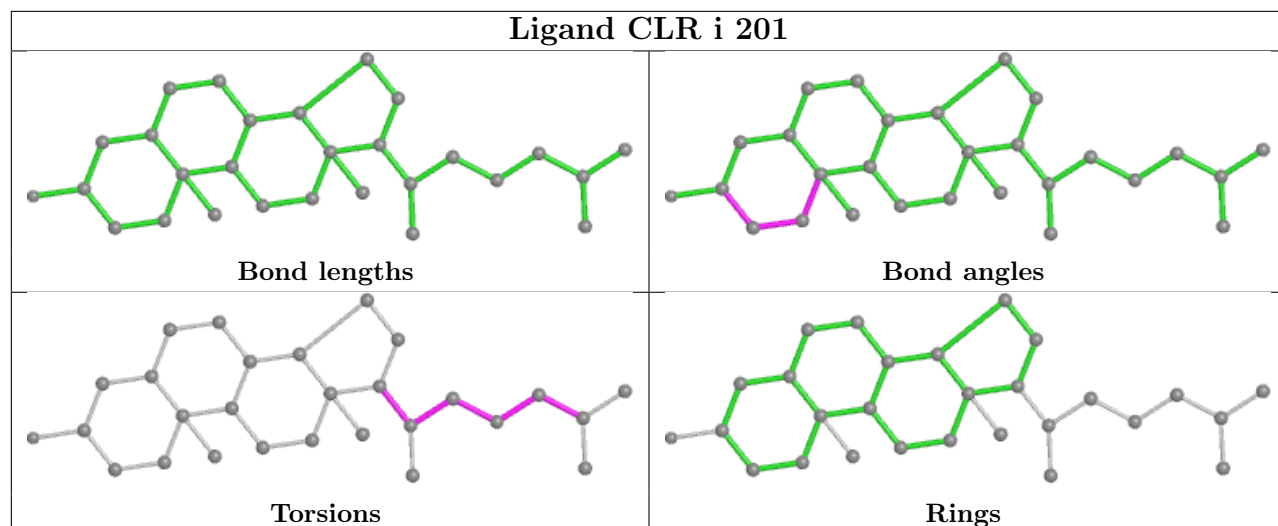


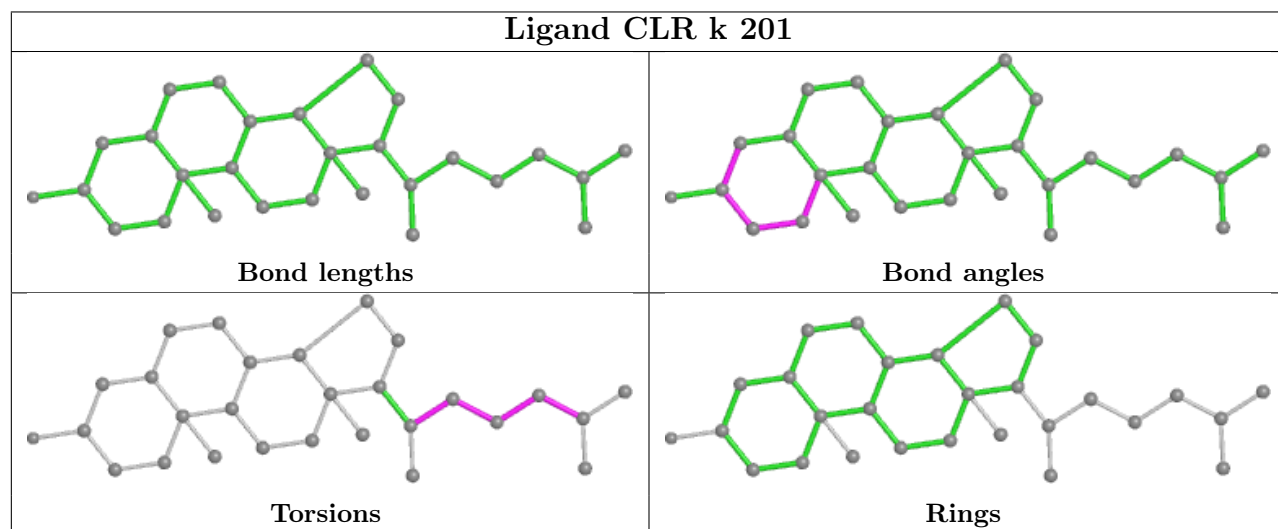
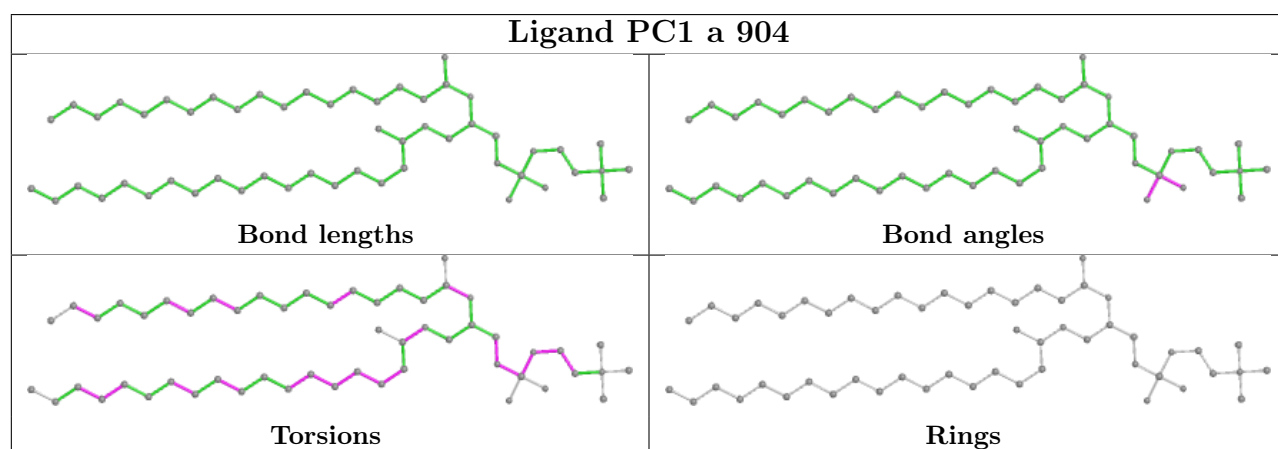
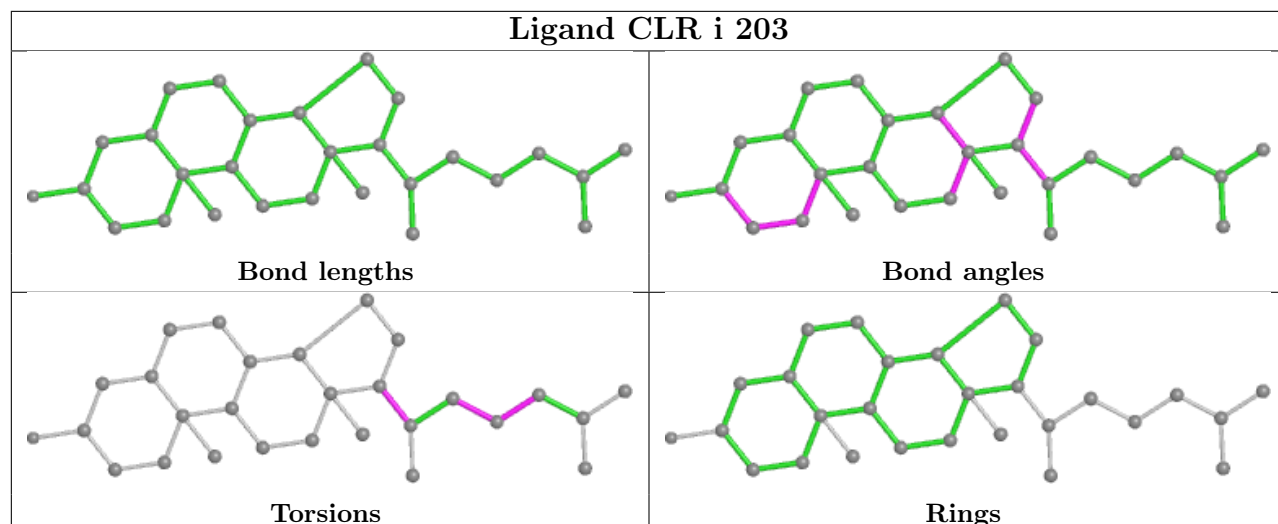


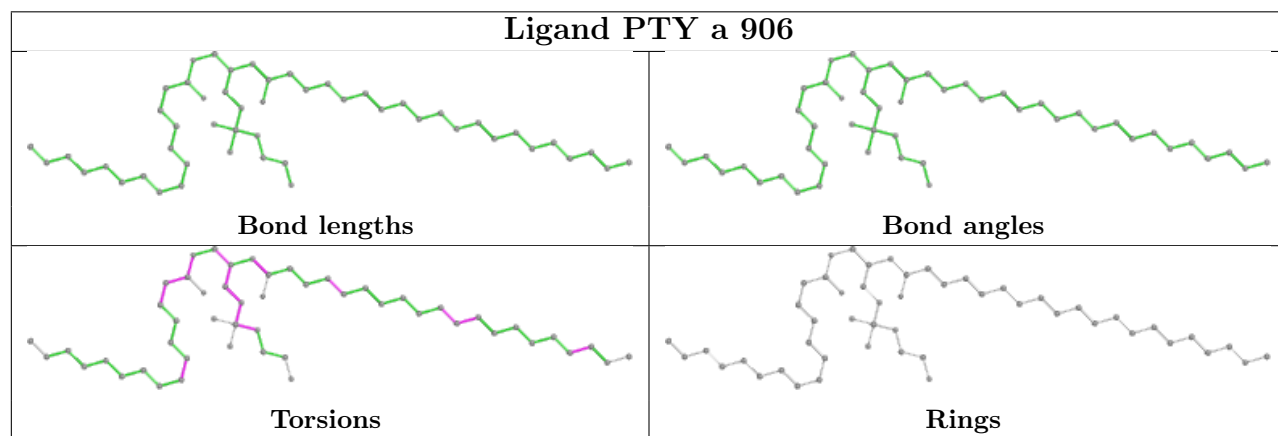
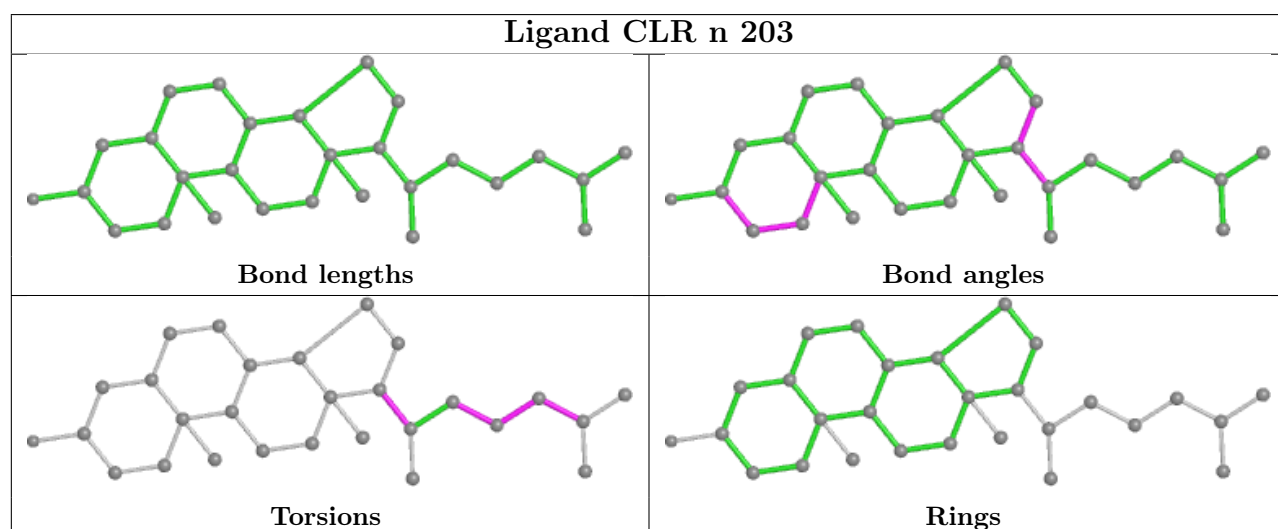
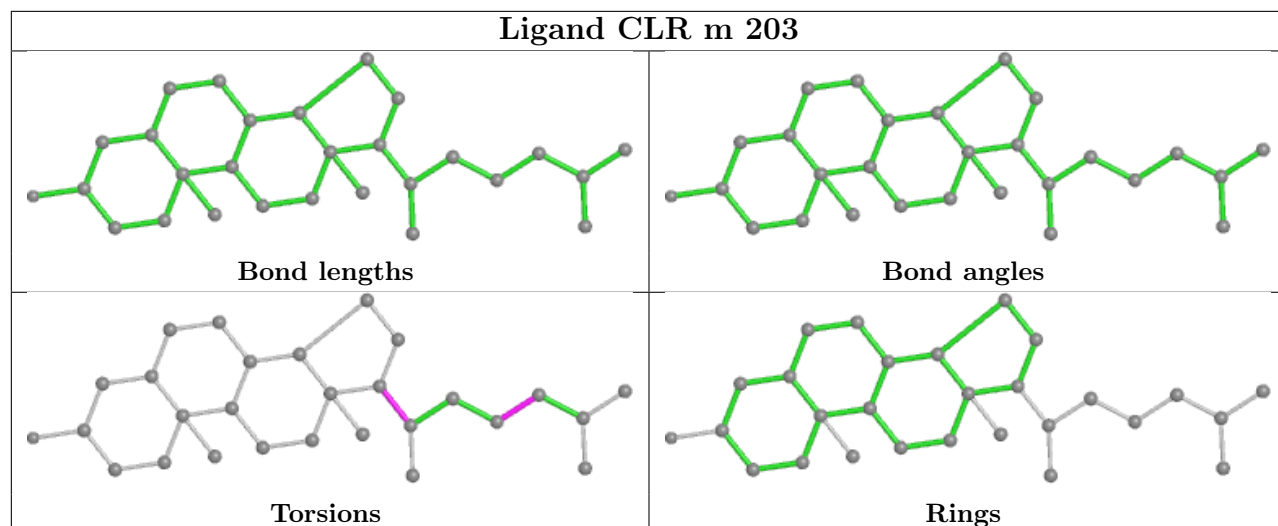


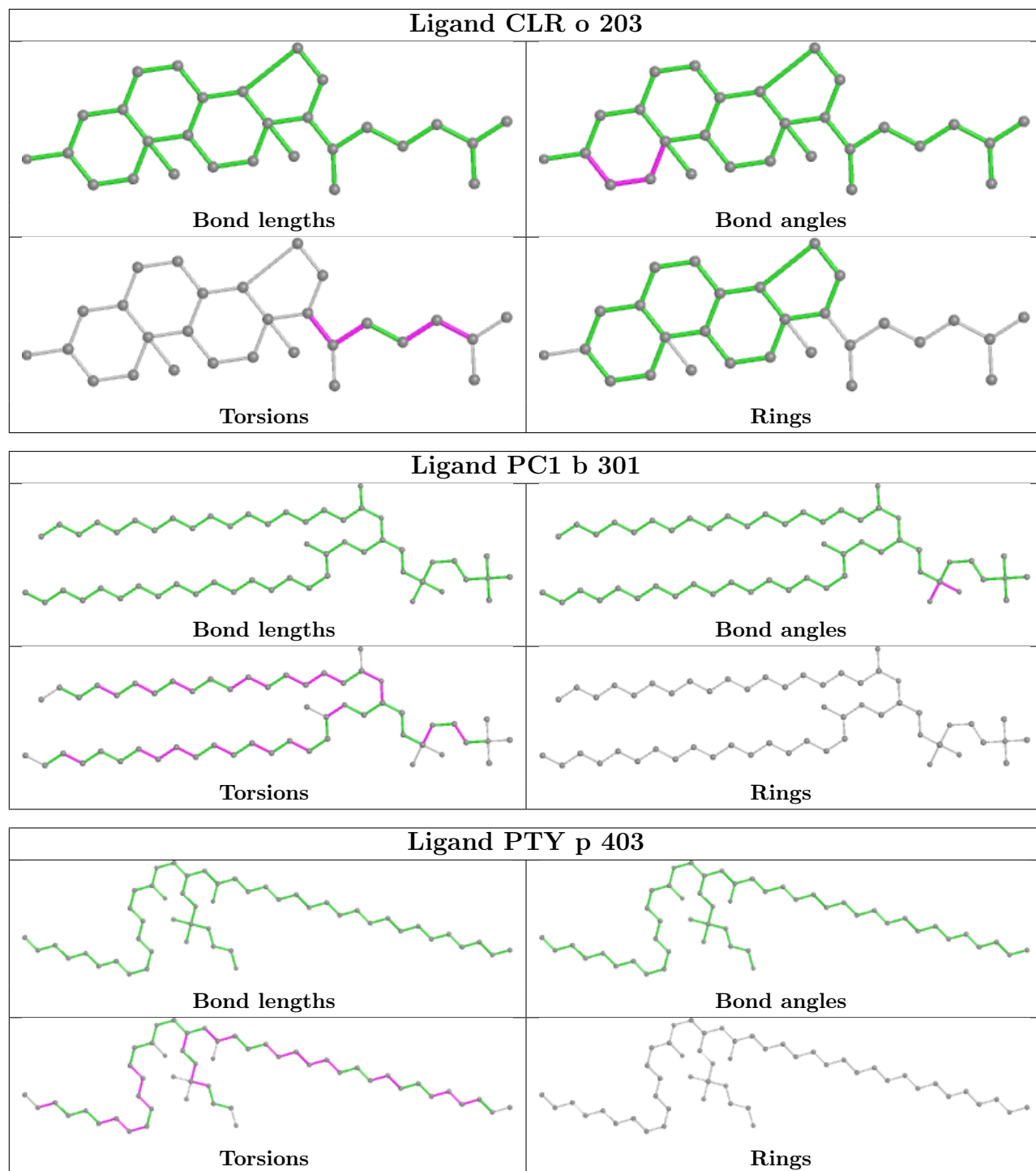


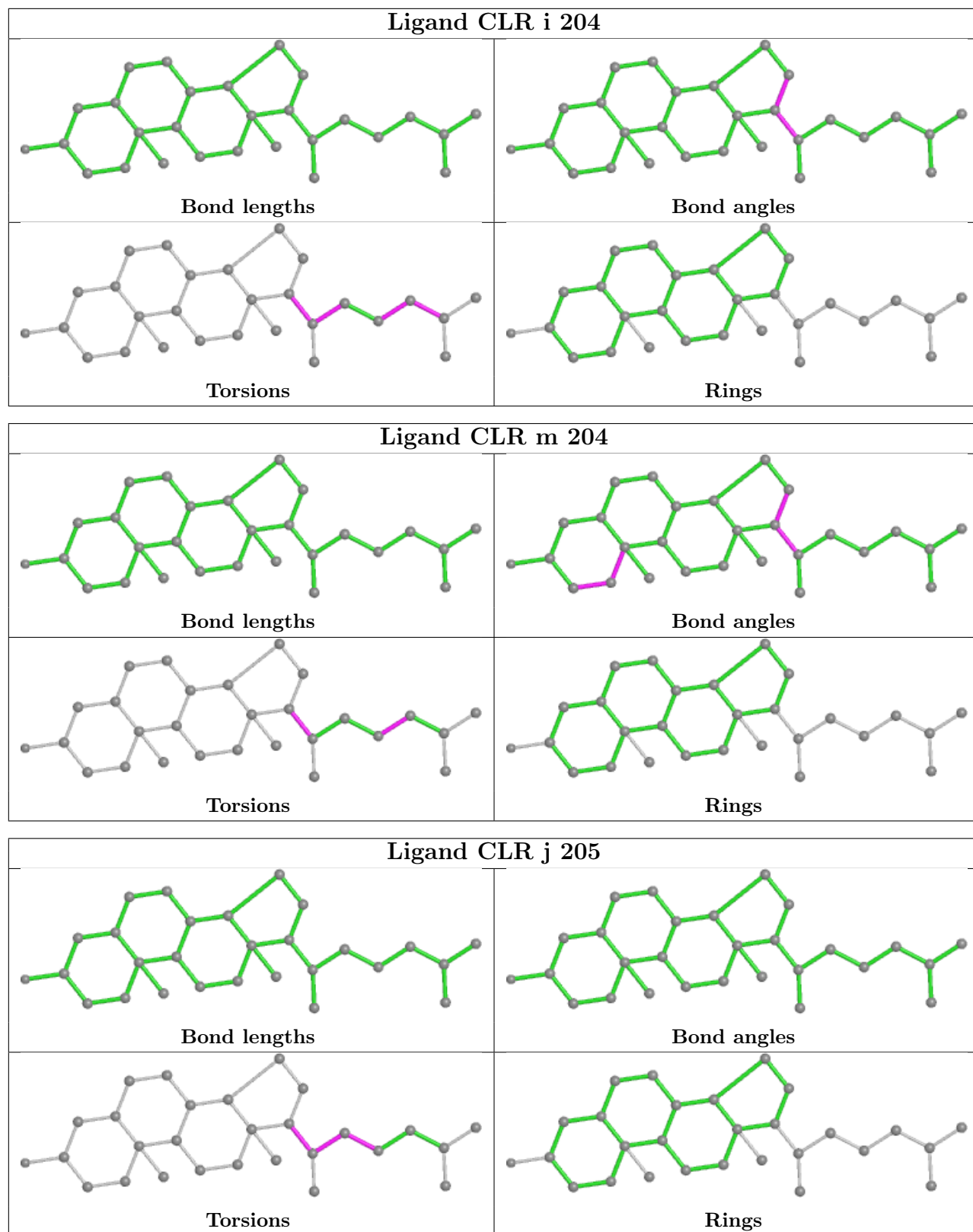


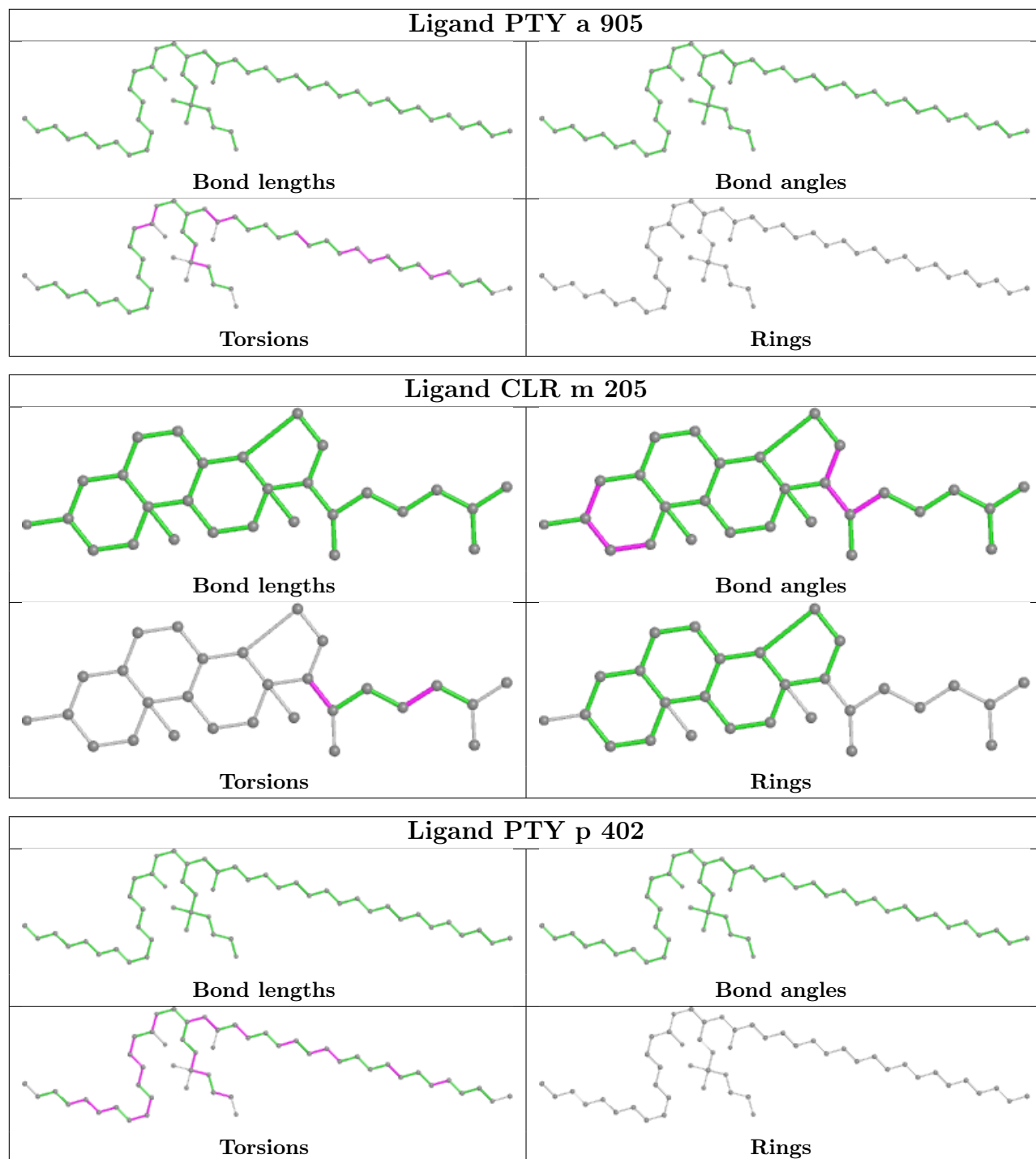


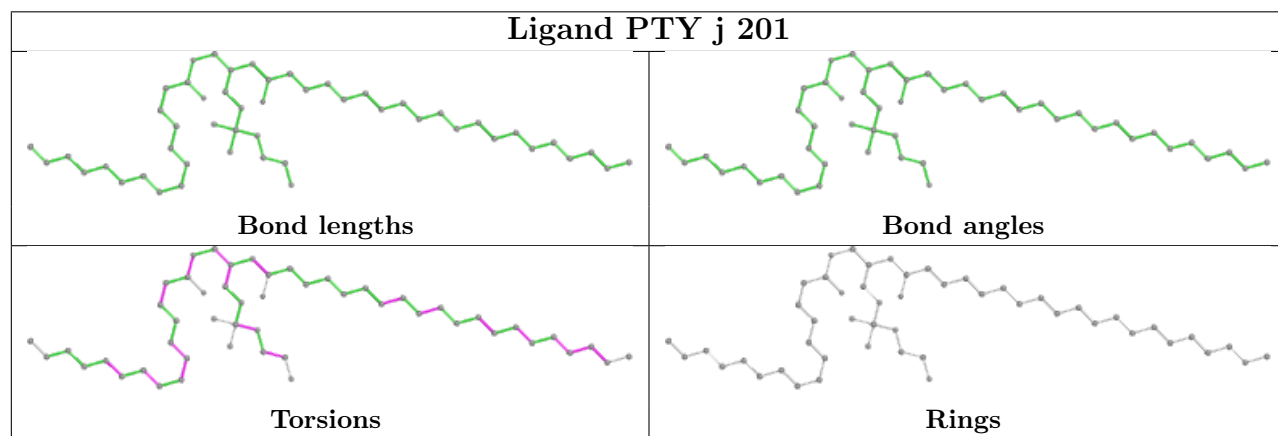
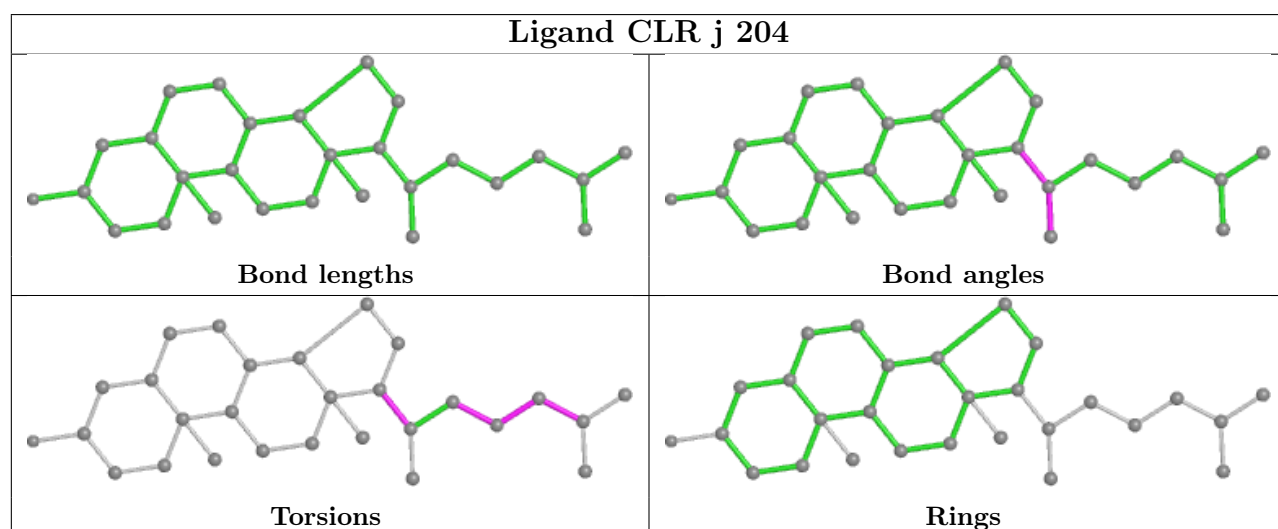
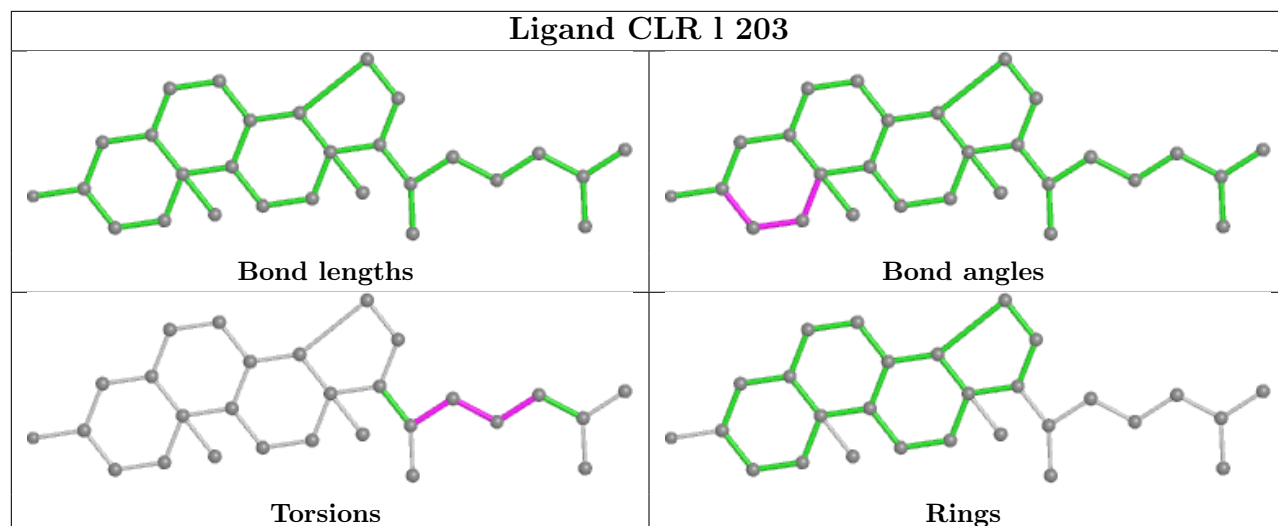




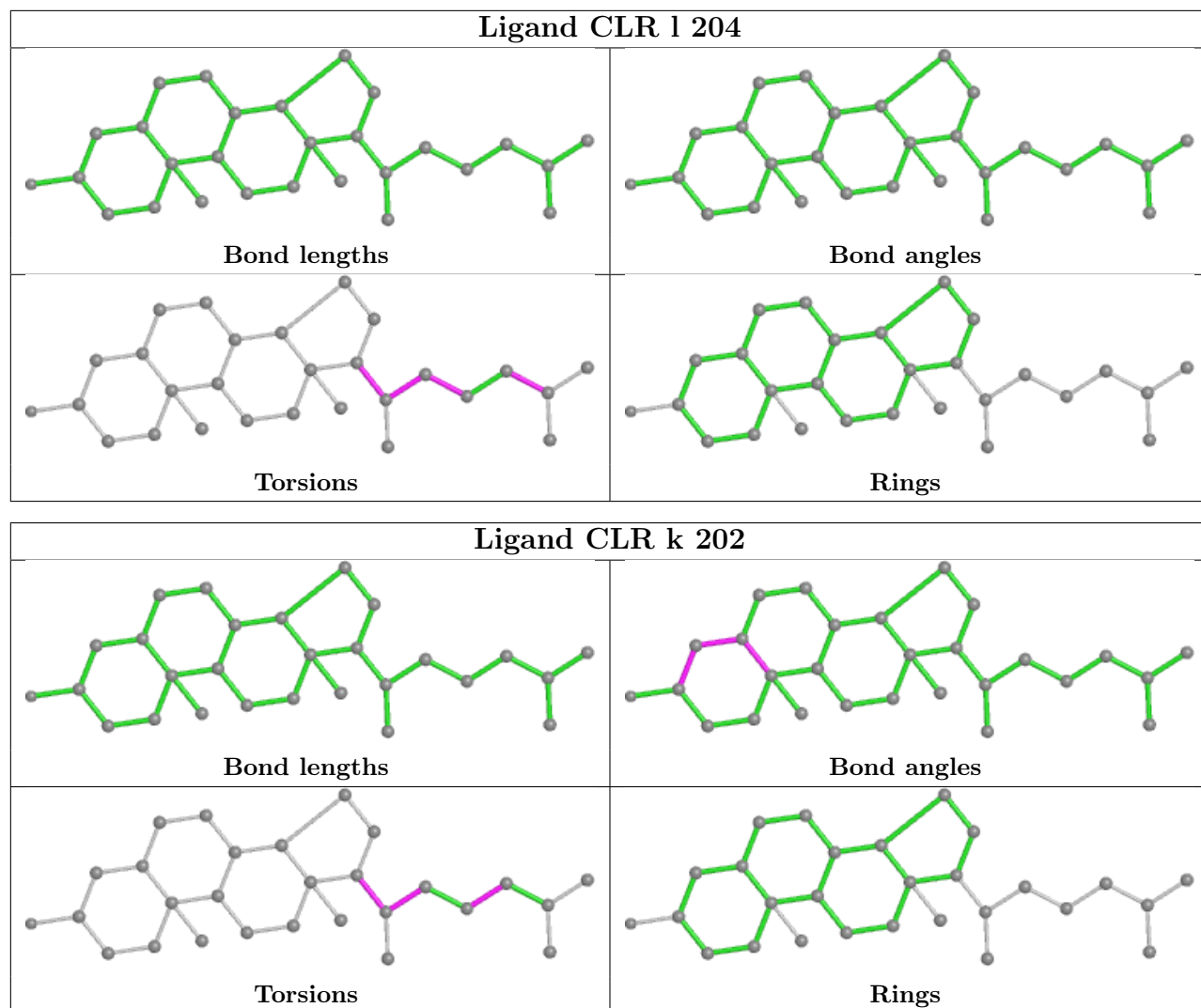












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

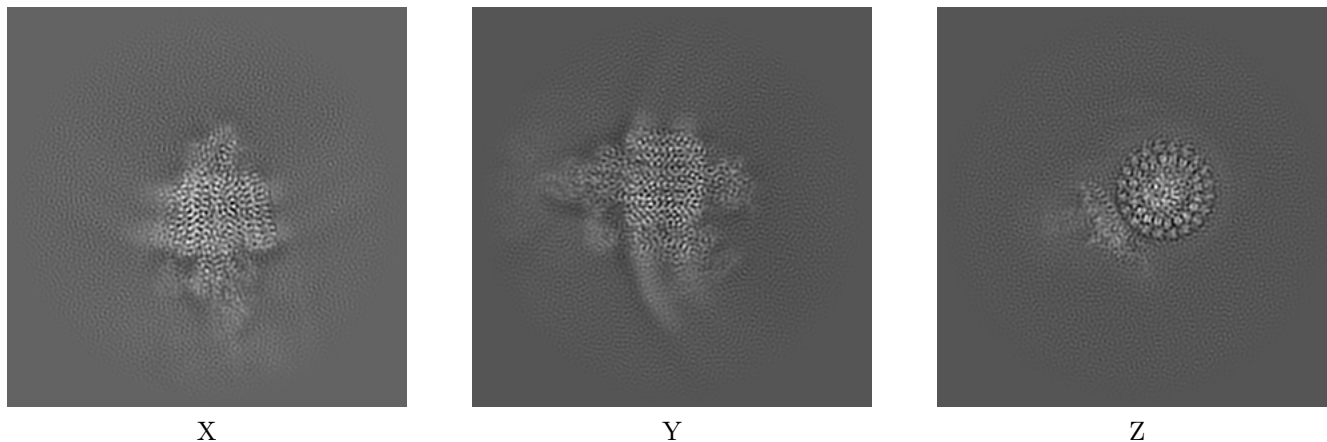
## 6 Map visualisation [i](#)

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

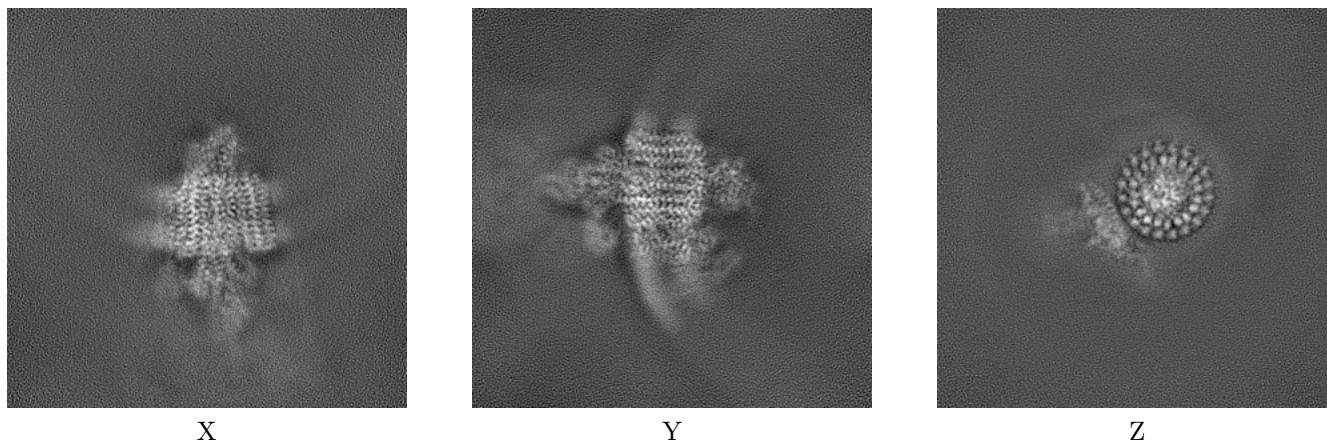
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



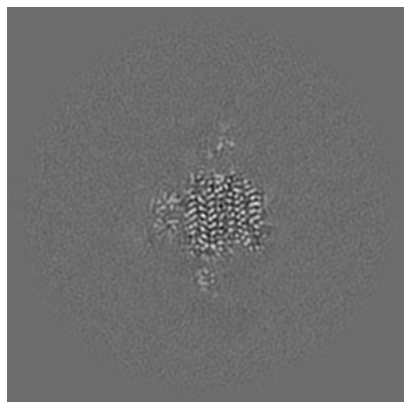
#### 6.1.2 Raw map



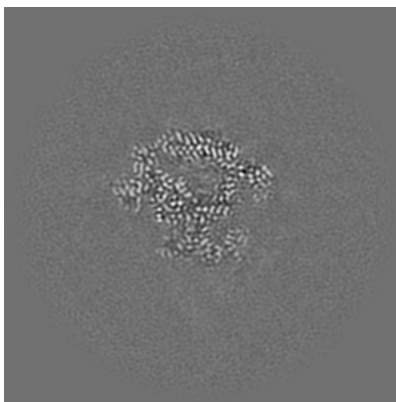
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

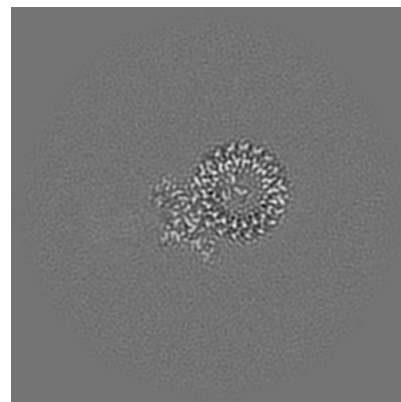
### 6.2.1 Primary map



X Index: 150

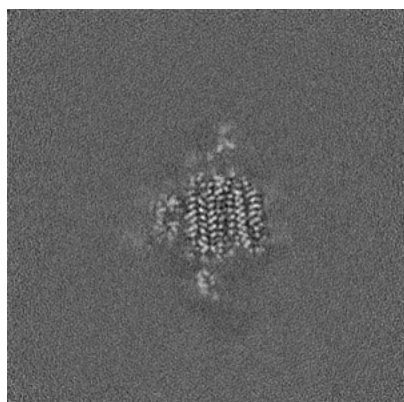


Y Index: 150

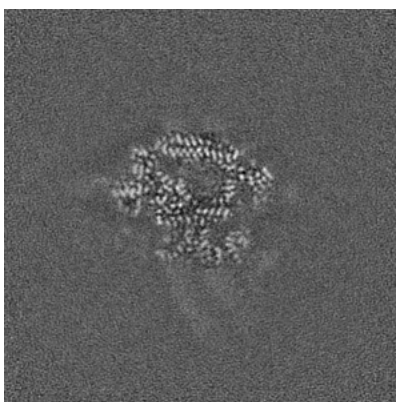


Z Index: 150

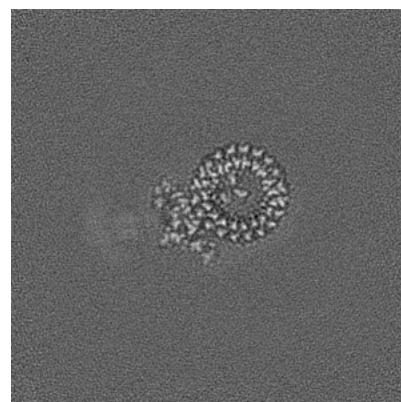
### 6.2.2 Raw map



X Index: 150



Y Index: 150

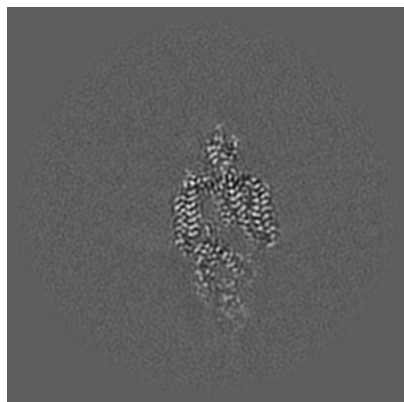


Z Index: 150

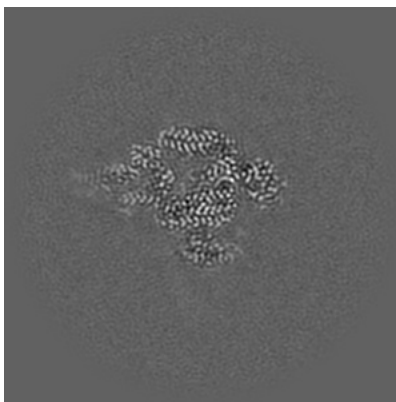
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

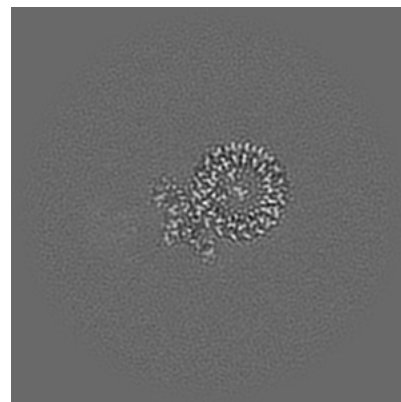
### 6.3.1 Primary map



X Index: 167

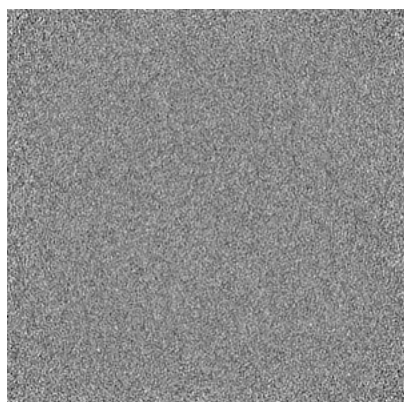


Y Index: 158

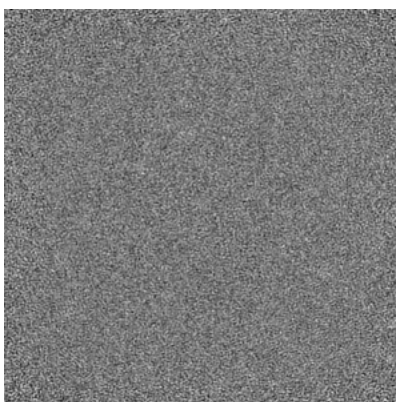


Z Index: 149

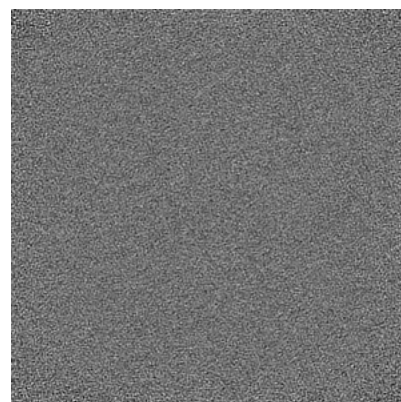
### 6.3.2 Raw map



X Index: 0



Y Index: 0



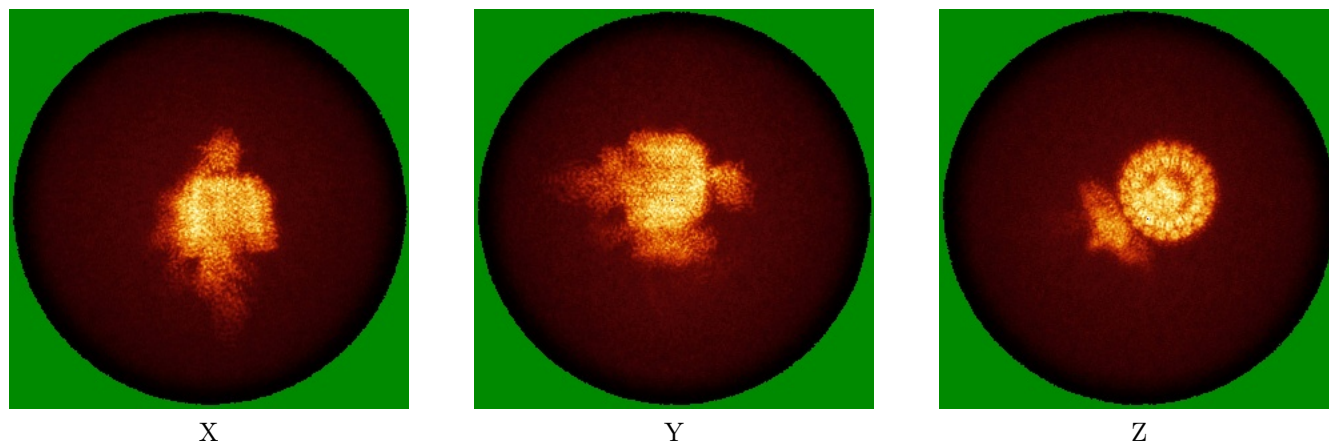
Z Index: 0

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

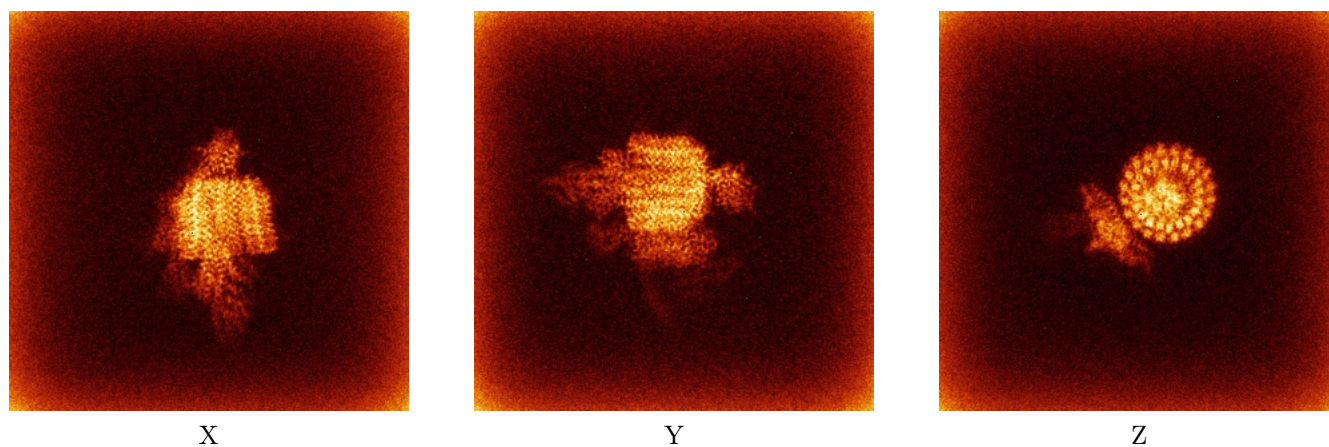


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



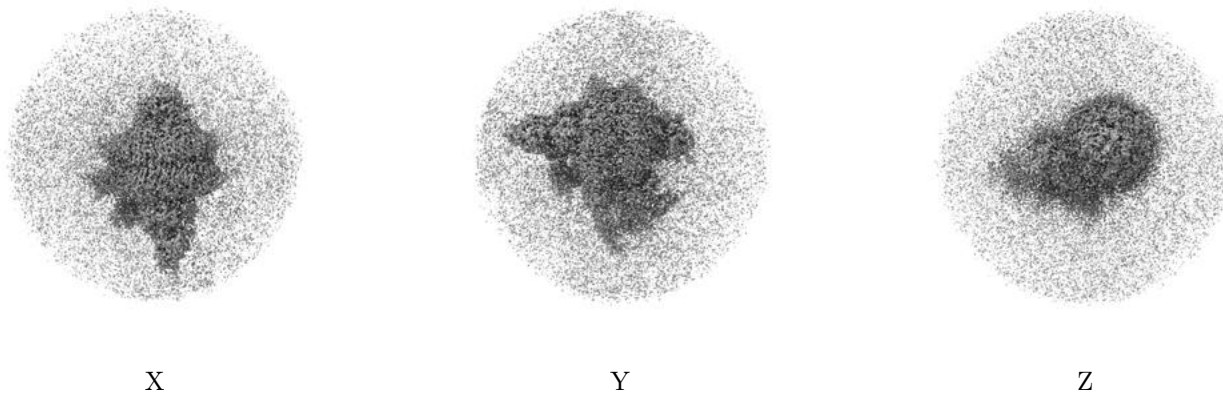
### 6.4.2 Raw map



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.

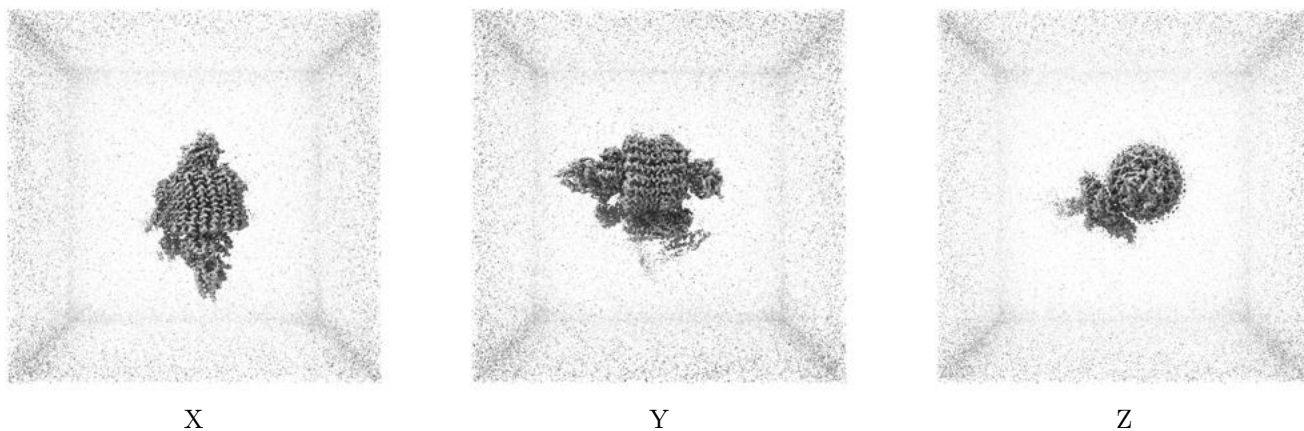
## 6.5 Orthogonal surface views [i](#)

### 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.

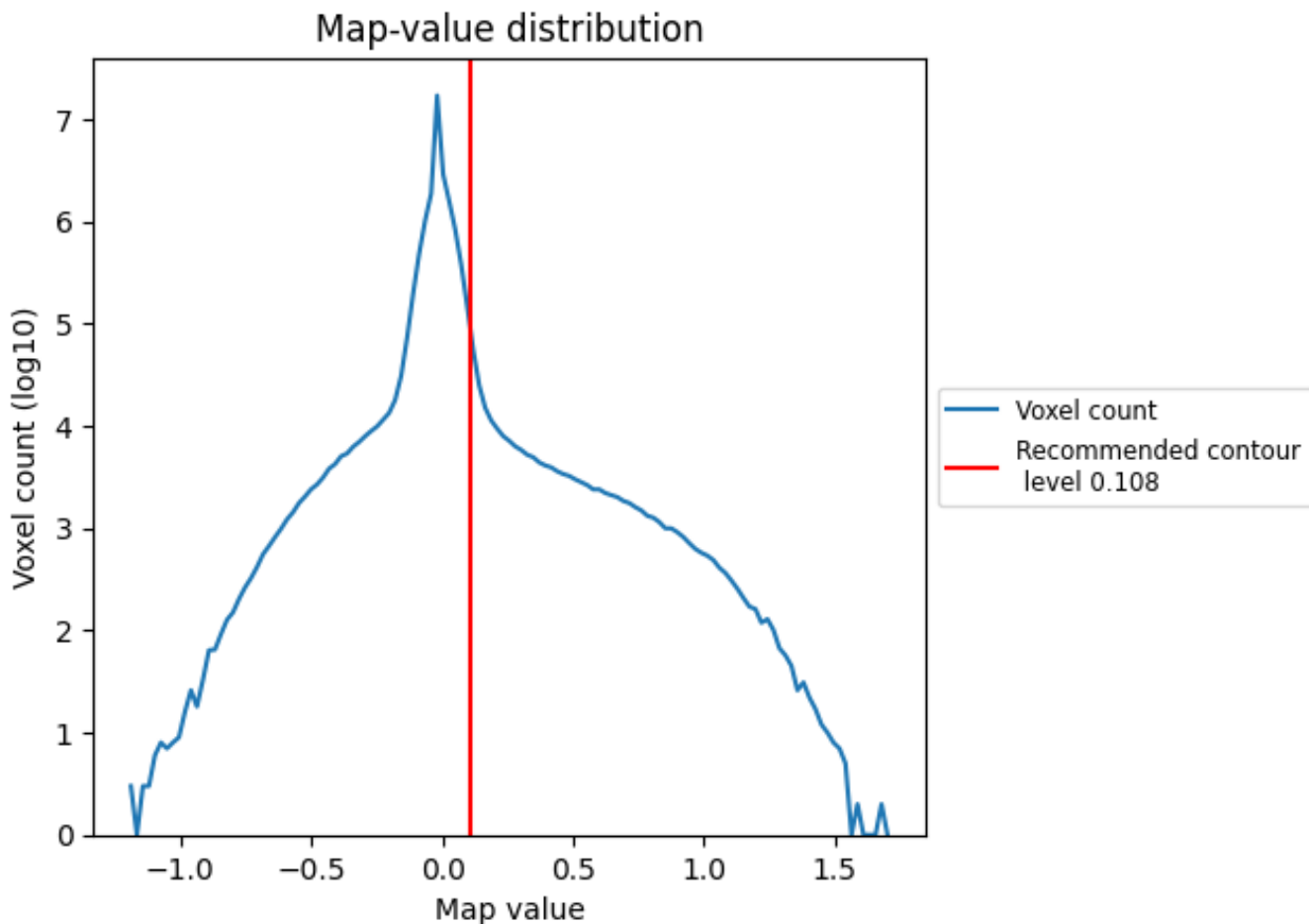
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

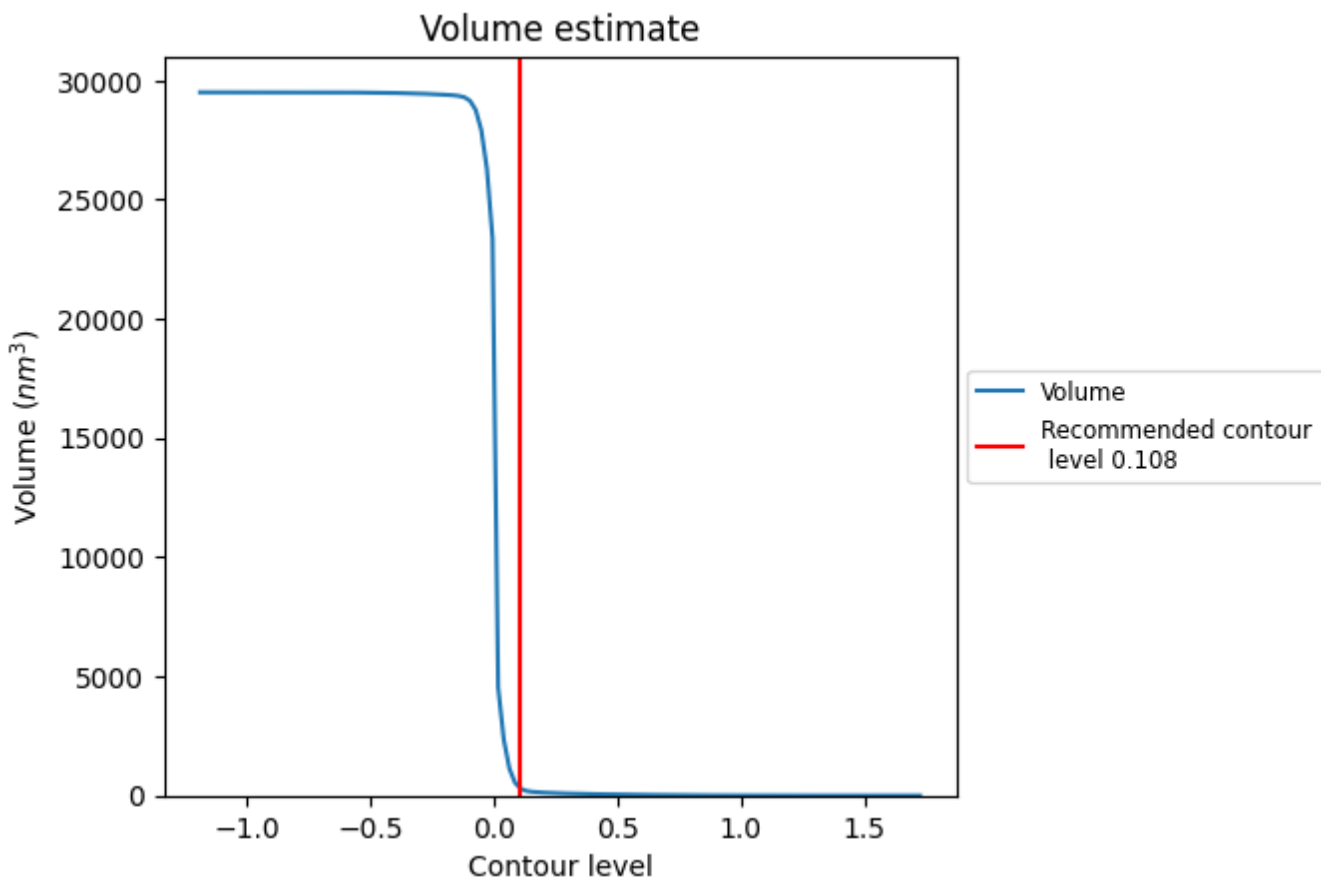
This section contains the results of statistical analysis of the map.

### 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](#)

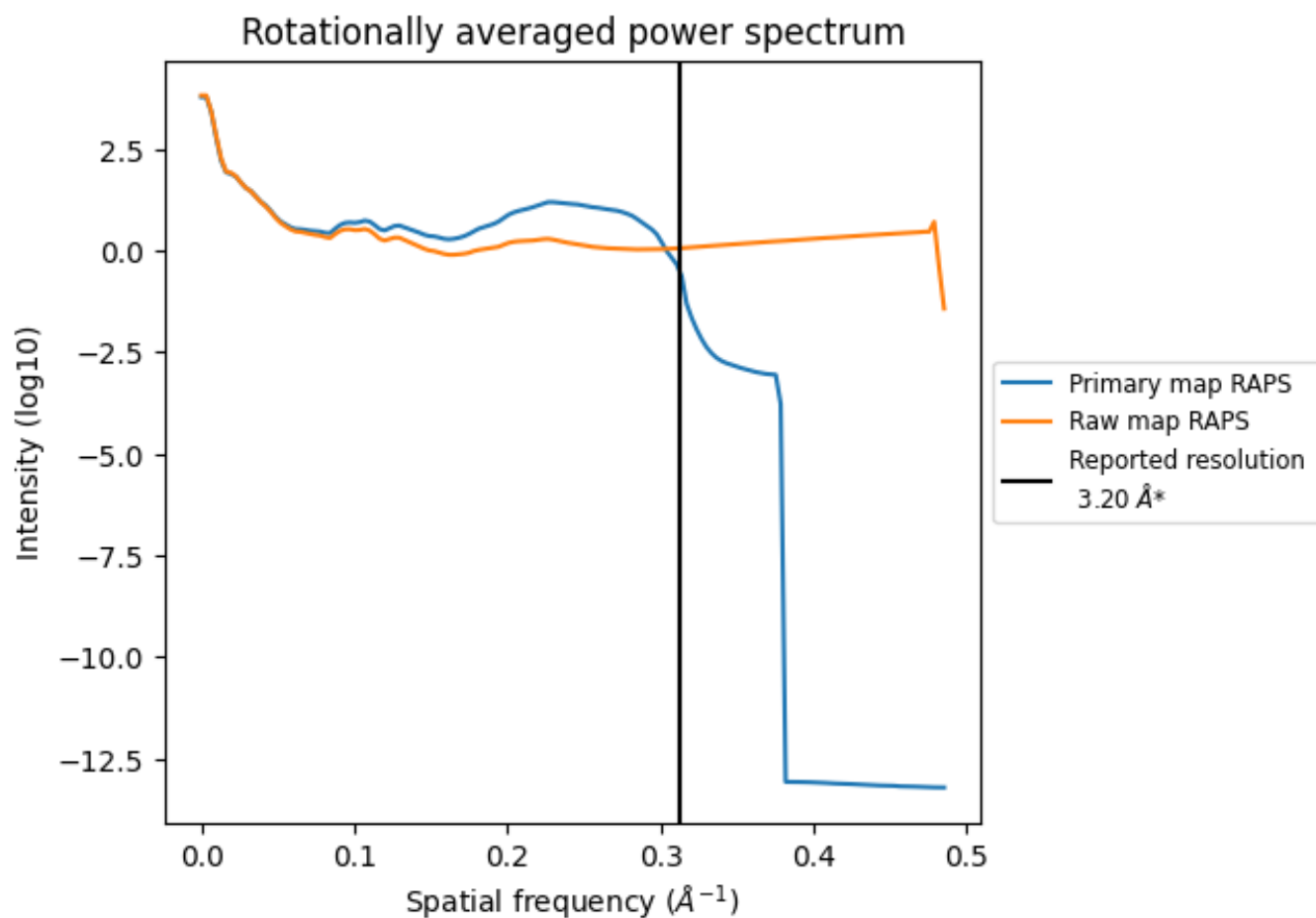


The volume at the recommended contour level is 291 nm<sup>3</sup>; this corresponds to an approximate mass of 263 kDa.

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 [i](#)

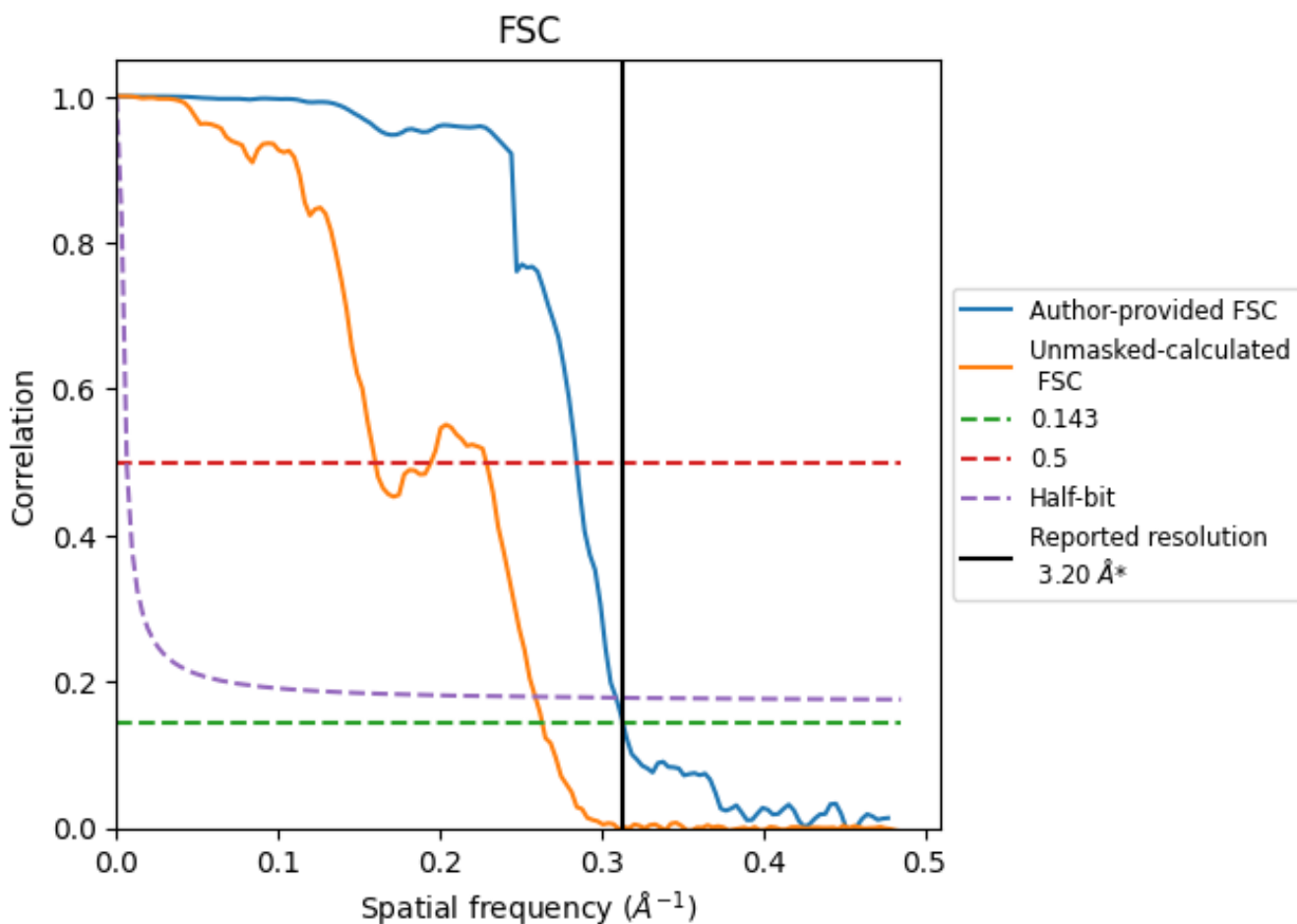


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

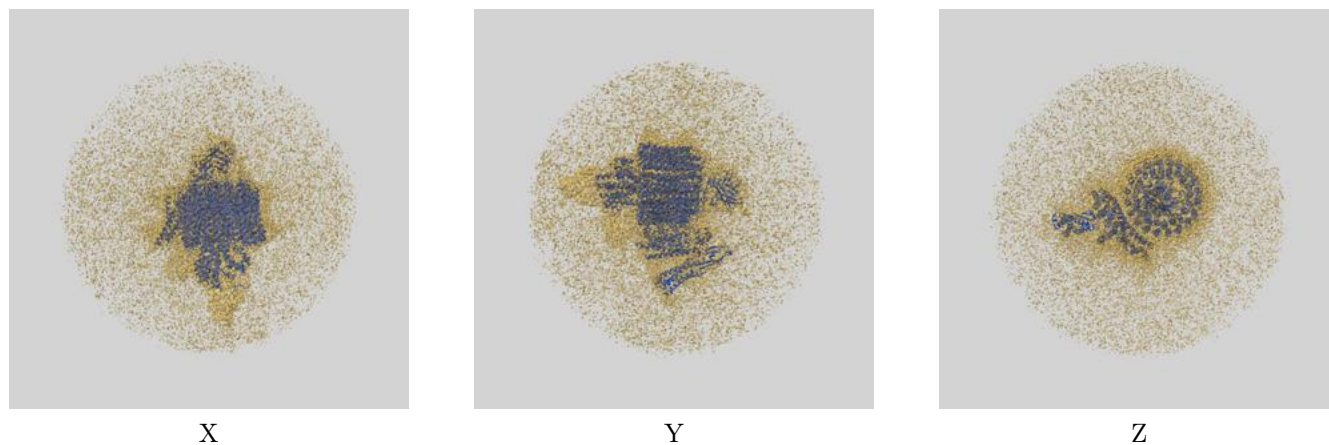
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.51	3.24
Unmasked-calculated*	3.80	6.25	3.86

\*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](#)

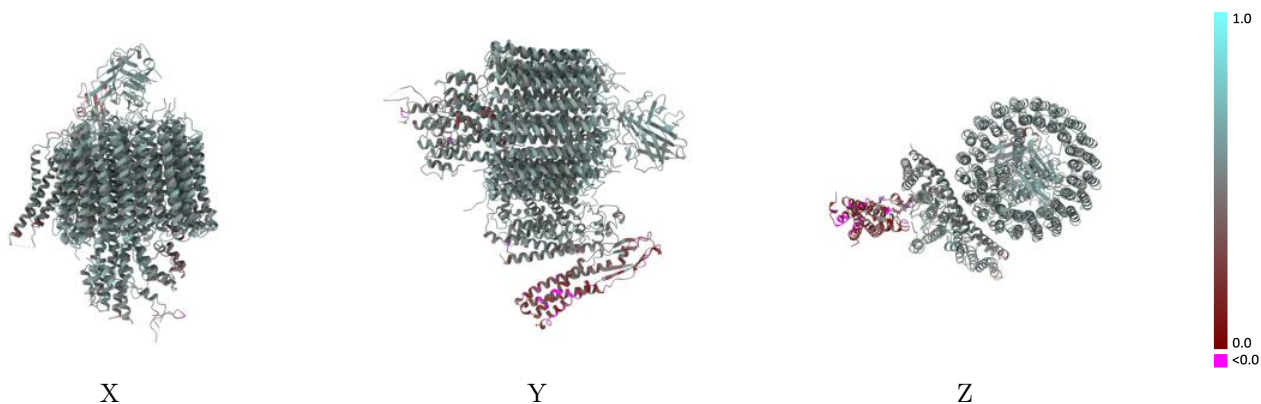
This section contains information regarding the fit between EMDB map EMD-44350 and PDB model 9B8O. Per-residue inclusion information can be found in section 3 on page 13.

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



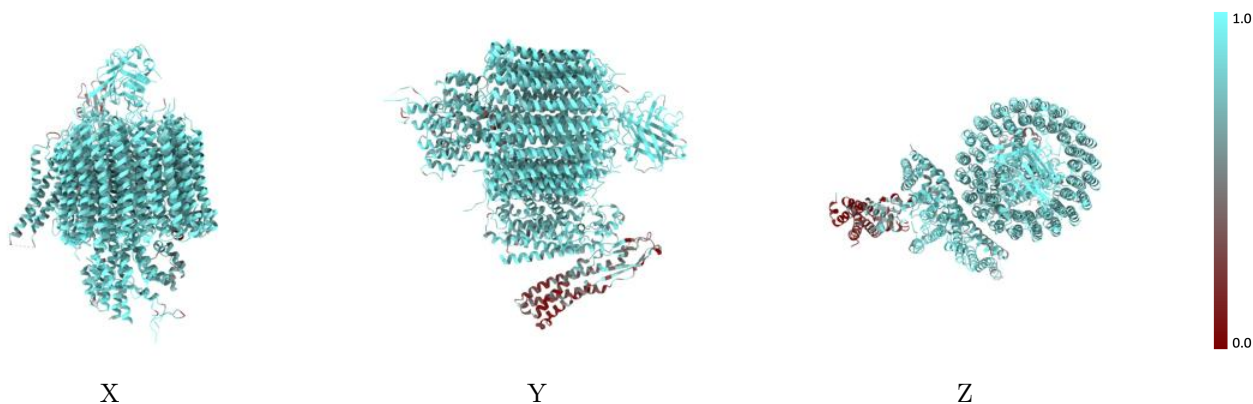
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



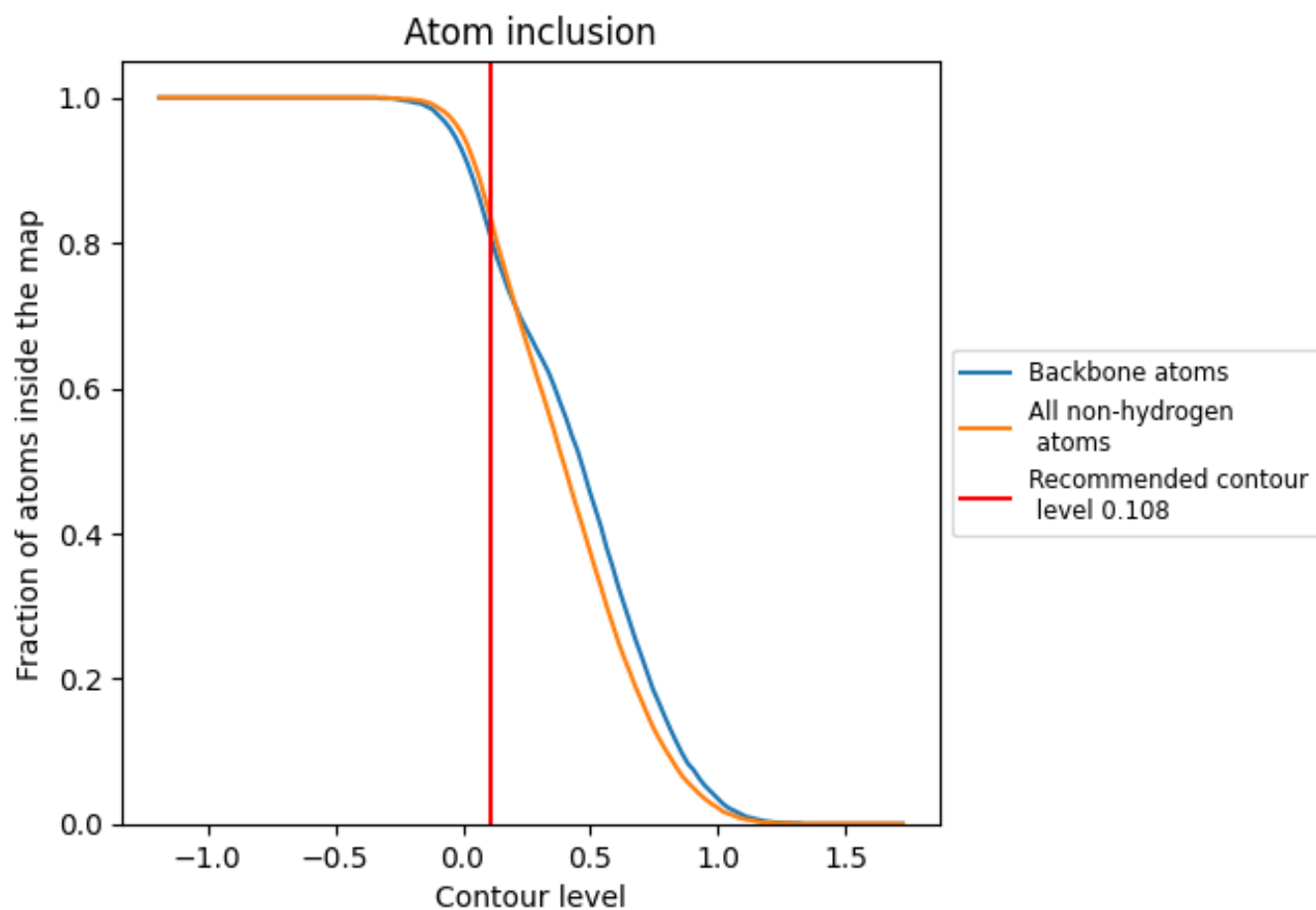
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

