



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:32 PM UTC

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

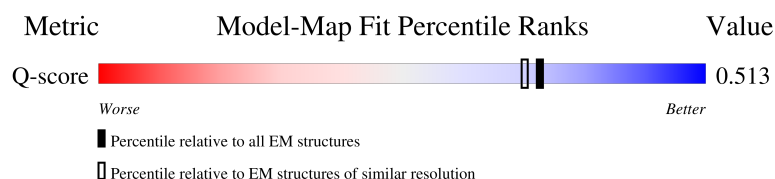
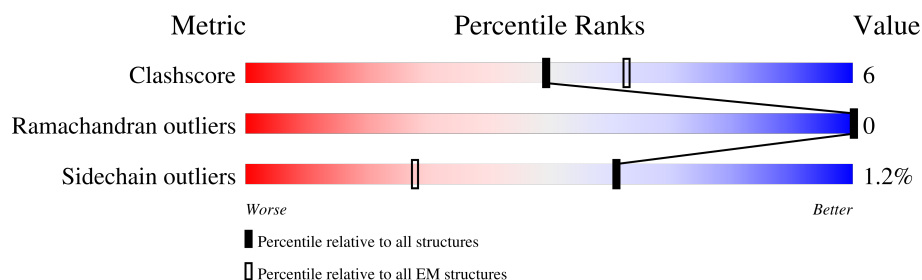
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

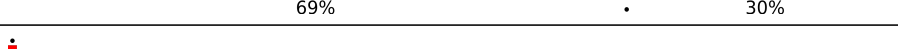
The reported resolution of this entry is 3.20 Å.

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



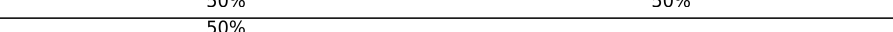
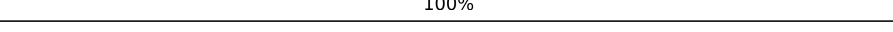
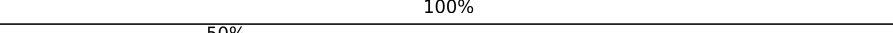
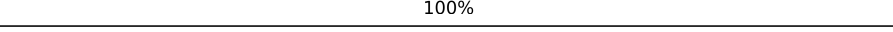
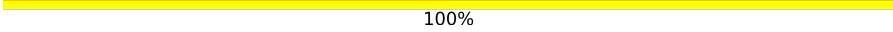
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	H	247	
2	P	463	
3	U	307	
4	a	826	

Continued on next page...

Continued from previous page...

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

2 Entry composition [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⁺-transporting V1 subunit D.

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

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

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

- Molecule 3 is a protein called Synaptophysin.

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Rnasek protein.

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

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

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

- Molecule 10 is a protein called Renin receptor.

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

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

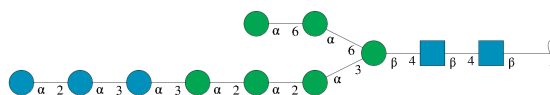
Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	10	Total	C	N	O	0	0
			82	48	19	15		

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



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

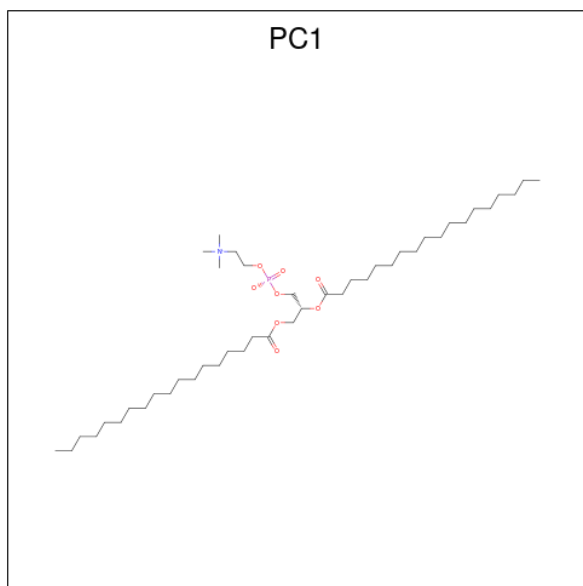
- Molecule 13 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-be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



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

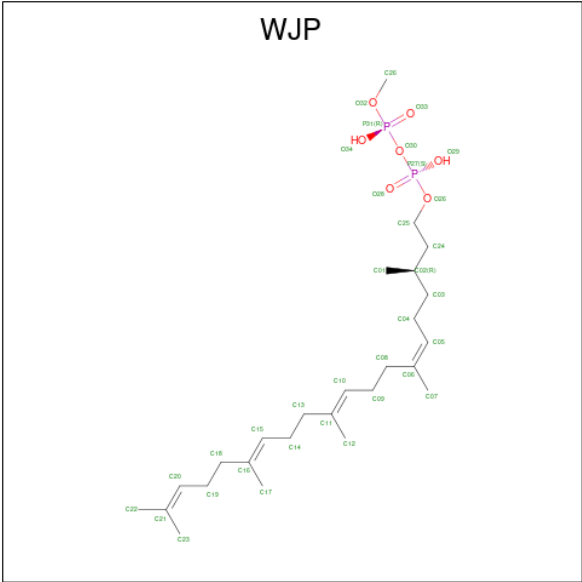
- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

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



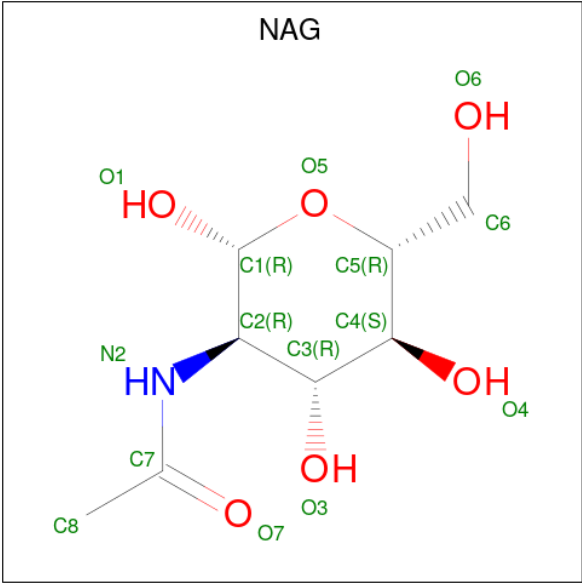
Mol	Chain	Residues	Atoms					AltConf
14	P	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
14	l	1	Total	C	N	O	P	0
			54	44	1	8	1	

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



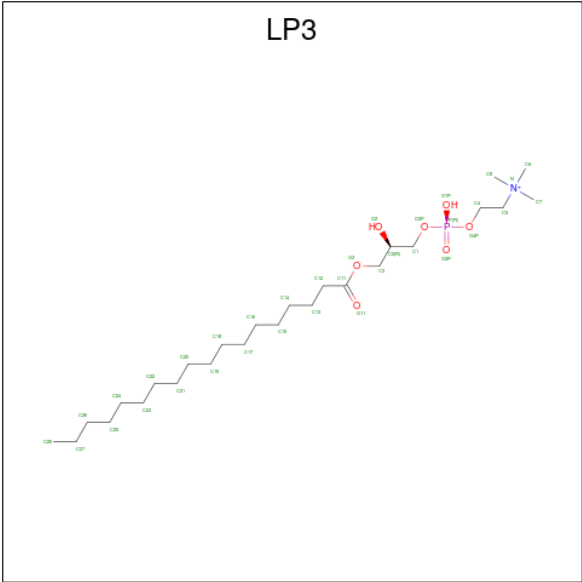
Mol	Chain	Residues	Atoms				AltConf
15	a	1	Total	C	O	P	0
			34	25	7	2	

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



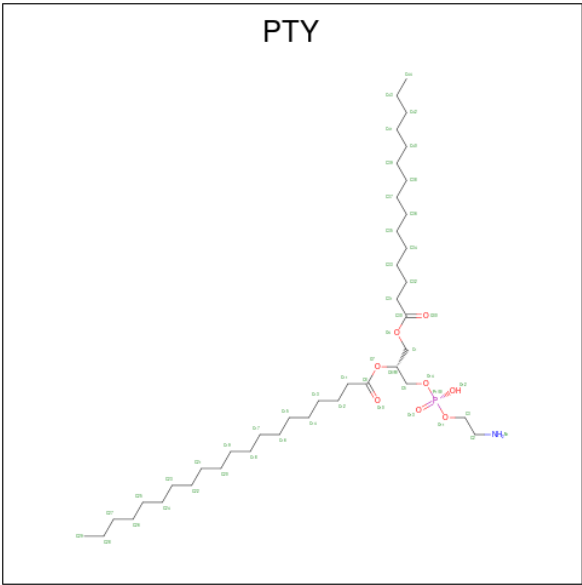
Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 17 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (CCD ID: LP3) (formula: $C_{26}H_{55}NO_7P$).



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

- Molecule 18 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



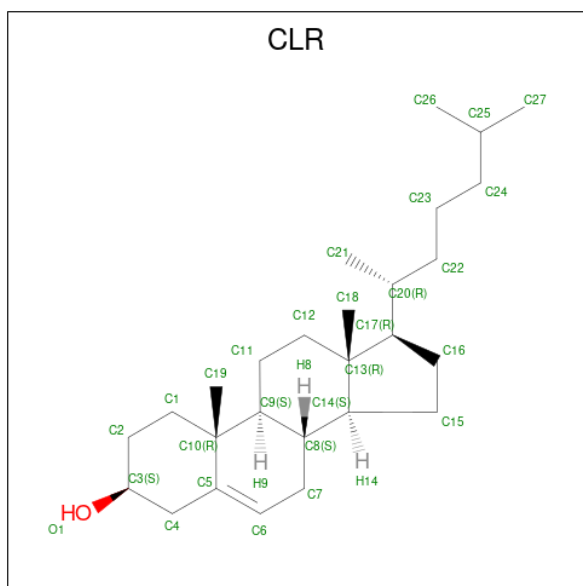
Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
18	b	1	Total	C	N	O	P	0
			50	40	1	8	1	

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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



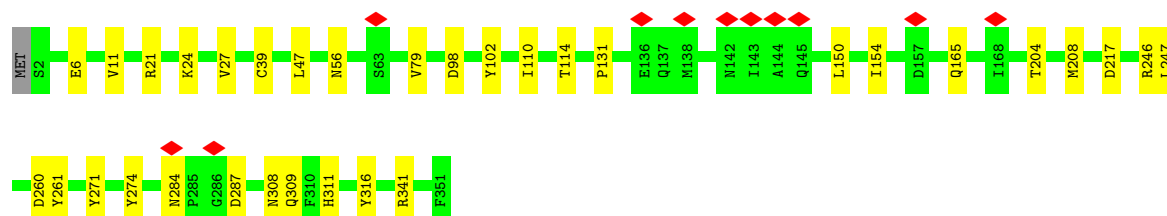
- Molecule 5: ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a

Chain b:  84% 14% ..



- Molecule 6: V-type proton ATPase subunit

Chain d:  90% 9%



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

Chain e:  84% 15% .



- Molecule 8: Rnasek protein

Chain f:  88% 12%



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

Chain g:  78% 19% .



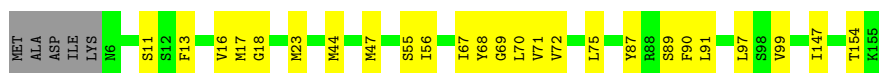
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h:  85% 12% .

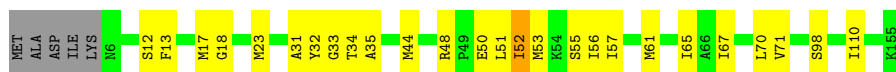
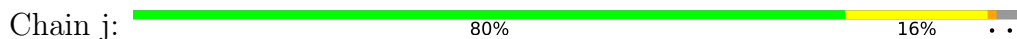


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

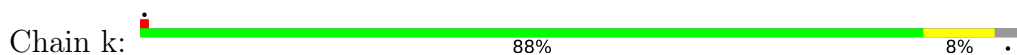
Chain i:  81% 16% .



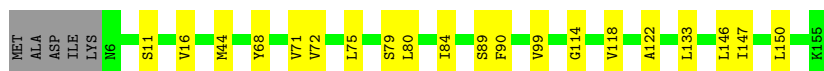
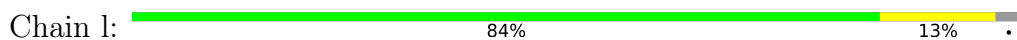
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



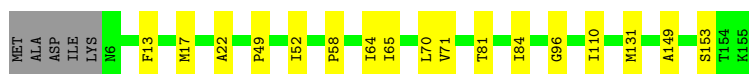
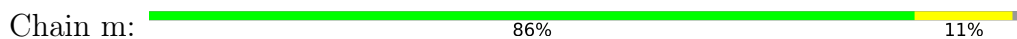
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



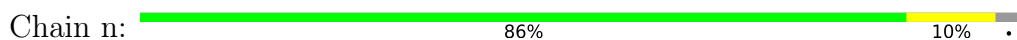
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



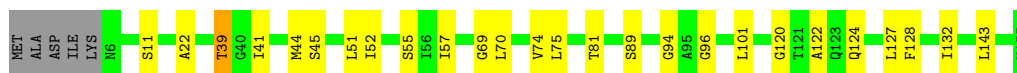
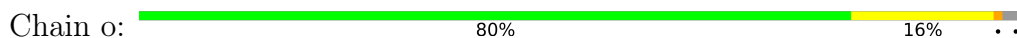
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c



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

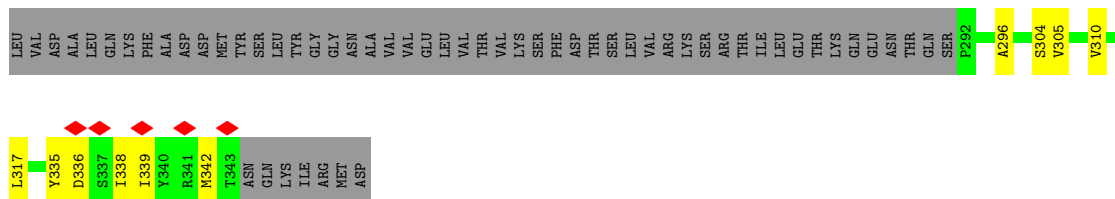


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit c

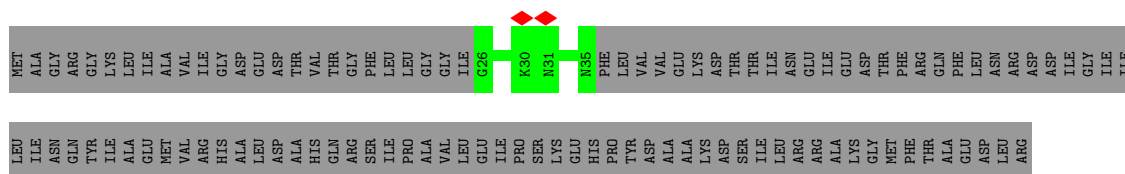


- Molecule 10: Renin receptor





Chain L: 8% 92%



Chain A: 50% 50%



Chain B:



Chain C: 100%



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



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



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



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



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



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



MAG1	MAG2	BM43	MAN4	MAN5	MAN6	GLC7	GLC8	GLC9	MAN10	MAN11
------	------	------	------	------	------	------	------	------	-------	-------



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198533	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-1.189	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	309.0, 309.0, 309.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Continued on next page...

Continued from previous page...

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

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

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:n:51:LEU:O	9:n:55:SER:OG	1.97	0.81
9:h:17:MET:O	9:h:21:SER:OG	2.00	0.79
6:d:217:ASP:OD2	6:d:274:TYR:OH	2.00	0.79
9:j:71:VAL:HG11	19:j:204:CLR:H182	1.68	0.76
9:i:23:MET:HE3	9:i:23:MET:O	1.86	0.74
5:b:77:ILE:HG21	9:g:117:GLY:HA2	1.69	0.74
7:e:2:THR:N	7:e:81:GLU:OE2	2.20	0.73
4:a:363:THR:OG1	4:a:384:GLY:O	2.06	0.72
9:j:71:VAL:HG13	19:j:203:CLR:H161	1.71	0.72
9:h:48:ARG:NH1	9:h:122:ALA:O	2.23	0.72
9:j:67:ILE:HG23	19:j:202:CLR:H271	1.71	0.71
9:o:120:GLY:O	9:o:124:GLN:N	2.25	0.70
6:d:260:ASP:OD1	6:d:261:TYR:N	2.24	0.70
5:b:55:GLY:O	5:b:59:SER:OG	2.10	0.69
4:a:748:ALA:HB2	9:g:143:LEU:HD11	1.75	0.67
4:a:757:TRP:CE3	4:a:761:ILE:HD11	2.30	0.66
9:j:51:LEU:O	9:j:55:SER:OG	2.09	0.66
4:a:477:SER:OG	4:a:520:ASP:OD1	2.12	0.66
10:p:310:VAL:HG11	18:p:401:PTY:H151	1.78	0.66
6:d:21:ARG:NH2	6:d:308:ASN:O	2.29	0.65
19:m:201:CLR:H191	19:n:204:CLR:H182	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:424:LEU:HD12	5:b:48:MET:HE1	1.80	0.64
5:b:41:LEU:O	5:b:135:TYR:OH	2.15	0.63
6:d:208:MET:HE1	6:d:316:TYR:CD1	2.34	0.63
19:h:201:CLR:H213	9:i:147:ILE:HD13	1.81	0.63
12:D:1:NAG:O3	12:D:2:NAG:O5	2.15	0.63
9:g:44:MET:HG3	9:g:122:ALA:HB2	1.82	0.62
9:i:71:VAL:HG21	19:i:203:CLR:H231	1.82	0.62
9:l:11:SER:O	9:l:89:SER:OG	2.09	0.61
9:i:47:MET:HE2	9:i:47:MET:HA	1.82	0.61
9:o:75:LEU:HD11	19:o:203:CLR:H193	1.82	0.61
4:a:757:TRP:CD2	4:a:761:ILE:HD11	2.36	0.61
19:j:204:CLR:H151	19:j:205:CLR:H181	1.83	0.61
9:n:11:SER:O	9:n:89:SER:OG	2.18	0.61
2:P:344:ASN:O	2:P:346:SER:N	2.36	0.59
10:p:338:ILE:HG22	10:p:342:MET:HG2	1.85	0.59
19:k:202:CLR:H9	19:k:203:CLR:H6	1.85	0.58
4:a:594:LYS:NZ	15:a:901:WJP:O29	2.36	0.58
5:b:24:ILE:HG23	5:b:28:ILE:HD12	1.86	0.58
4:a:641:ILE:O	4:a:645:MET:HG2	2.03	0.58
9:n:143:LEU:HD11	19:n:204:CLR:H231	1.84	0.58
9:i:154:THR:HG21	19:i:203:CLR:H192	1.86	0.57
4:a:592:PHE:O	4:a:596:THR:HG23	2.04	0.57
2:P:429:MET:HE1	9:g:17:MET:HE3	1.86	0.57
9:j:23:MET:HE3	9:j:23:MET:O	2.05	0.57
2:P:381:ASN:OD1	12:F:1:NAG:H82	2.04	0.56
12:G:1:NAG:O3	12:G:2:NAG:O5	2.21	0.56
6:d:79:VAL:HG21	6:d:131:PRO:HB2	1.87	0.56
9:l:150:LEU:HD12	19:l:204:CLR:H231	1.86	0.56
7:e:74:TRP:HZ3	8:f:58:ILE:HD12	1.70	0.56
4:a:802:HIS:CE1	9:g:140:VAL:HG11	2.41	0.56
9:k:47:MET:SD	9:k:47:MET:N	2.77	0.56
4:a:576:GLU:HG3	4:a:651:MET:HE3	1.87	0.55
9:i:147:ILE:HG12	19:i:204:CLR:H183	1.88	0.55
7:e:28:VAL:O	7:e:34:ARG:NH2	2.40	0.55
19:n:201:CLR:H183	19:o:202:CLR:H182	1.89	0.55
9:o:44:MET:HG3	9:o:122:ALA:HB2	1.88	0.54
4:a:498:SER:O	7:e:70:ASN:ND2	2.41	0.54
4:a:751:GLN:HG3	9:g:150:LEU:HD13	1.90	0.54
4:a:755:VAL:HG11	9:g:71:VAL:HG22	1.89	0.54
2:P:410:ASP:OD1	2:P:410:ASP:N	2.41	0.53
9:k:16:VAL:HG11	9:l:90:PHE:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:m:58:PRO:HG3	9:m:131:MET:HE3	1.89	0.53
18:p:401:PTY:O12	18:p:401:PTY:N1	2.42	0.53
5:b:62:VAL:HG13	9:g:141:LEU:HB3	1.91	0.52
9:l:75:LEU:HD21	19:l:203:CLR:H9	1.91	0.52
19:i:201:CLR:H181	19:i:202:CLR:H161	1.91	0.52
2:P:270:VAL:CG1	2:P:279:LEU:HD11	2.39	0.52
9:k:71:VAL:HG22	19:k:202:CLR:H161	1.92	0.52
6:d:247:LEU:HD23	6:d:271:TYR:CE1	2.44	0.52
9:k:11:SER:O	9:k:89:SER:OG	2.24	0.52
9:g:11:SER:O	9:g:89:SER:OG	2.26	0.52
4:a:620:SER:O	4:a:620:SER:OG	2.18	0.51
9:k:44:MET:HG3	9:k:122:ALA:HB2	1.92	0.51
2:P:314:THR:HG23	2:P:314:THR:O	2.09	0.51
9:h:16:VAL:HG11	9:i:90:PHE:O	2.11	0.51
9:k:150:LEU:HB3	19:k:204:CLR:H191	1.92	0.51
2:P:310:LEU:HD23	2:P:311:PHE:CG	2.45	0.51
5:b:81:VAL:HG13	9:g:123:GLN:HB3	1.93	0.51
6:d:284:ASN:ND2	6:d:287:ASP:OD2	2.44	0.51
4:a:535:SER:OG	13:Z:1:NAG:H82	2.10	0.51
4:a:557:LEU:HD22	4:a:573:PHE:CE2	2.46	0.51
6:d:246:ARG:NH1	6:d:274:TYR:OH	2.44	0.51
3:U:30:PHE:O	3:U:31:ALA:HB3	2.10	0.51
6:d:98:ASP:O	6:d:102:TYR:CD1	2.64	0.51
9:i:13:PHE:O	9:i:16:VAL:HG22	2.11	0.50
9:i:75:LEU:HD23	19:i:202:CLR:H11	1.93	0.50
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
4:a:377:ILE:HG23	4:a:804:LEU:CD2	2.42	0.50
7:e:2:THR:HG23	7:e:2:THR:O	2.11	0.50
4:a:547:ILE:HD13	7:e:50:LEU:HD11	1.93	0.50
4:a:392:ALA:O	4:a:396:VAL:HG23	2.12	0.50
4:a:723:ILE:HG21	5:b:178:ILE:HD12	1.94	0.50
9:h:79:SER:O	9:h:79:SER:OG	2.22	0.50
2:P:328:VAL:HG12	2:P:328:VAL:O	2.12	0.49
9:m:49:PRO:O	9:m:52:ILE:HD12	2.11	0.49
2:P:352:VAL:HG22	2:P:378:LEU:HD23	1.94	0.49
9:g:16:VAL:HG22	9:g:80:LEU:HD13	1.94	0.49
9:i:70:LEU:HD21	19:i:201:CLR:H261	1.93	0.49
4:a:594:LYS:NZ	13:Z:1:NAG:O5	2.40	0.49
9:l:79:SER:O	9:l:79:SER:OG	2.29	0.49
9:o:45:SER:HB2	9:o:52:ILE:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:72:HIS:O	4:a:482:ARG:NH2	2.44	0.49
6:d:110:ILE:O	6:d:114:THR:OG1	2.28	0.48
9:g:137:PHE:O	9:g:140:VAL:HG22	2.13	0.48
9:m:13:PHE:CE1	9:m:17:MET:HE3	2.48	0.48
8:f:35:VAL:HG12	8:f:35:VAL:O	2.13	0.48
9:j:52:ILE:HD11	9:k:130:GLY:HA3	1.95	0.48
9:l:16:VAL:CG1	9:l:80:LEU:HD21	2.43	0.48
9:o:11:SER:O	9:o:89:SER:OG	2.30	0.48
4:a:609:LEU:N	15:a:901:WJP:O28	2.46	0.48
5:b:59:SER:HB2	9:g:101:LEU:HD23	1.95	0.48
19:o:202:CLR:H272	19:o:202:CLR:H213	1.96	0.48
8:f:15:GLY:O	8:f:19:SER:OG	2.28	0.48
19:l:204:CLR:H221	19:l:204:CLR:H262	1.95	0.48
4:a:805:ARG:NH2	4:a:810:GLU:OE2	2.46	0.47
9:j:23:MET:HG2	9:k:148:VAL:HG21	1.96	0.47
6:d:165:GLN:HA	6:d:165:GLN:OE1	2.15	0.47
5:b:69:ILE:HD12	9:g:141:LEU:HD11	1.96	0.47
9:m:65:ILE:HD11	9:m:110:ILE:HD12	1.94	0.47
4:a:802:HIS:NE2	9:g:140:VAL:HG11	2.28	0.47
18:e:101:PTY:HN11	18:e:101:PTY:P1	2.38	0.47
9:m:81:THR:CG2	9:m:84:ILE:HG23	2.45	0.47
4:a:368:ASN:OD1	4:a:369:LYS:N	2.44	0.47
2:P:330:ALA:HB3	14:b:301:PC1:H131	1.97	0.47
9:m:149:ALA:O	9:m:153:SER:N	2.45	0.46
9:h:114:GLY:O	9:h:118:VAL:HG22	2.15	0.46
5:b:173:PHE:CZ	5:b:177:LEU:HD13	2.50	0.46
7:e:14:THR:OG1	7:e:49:TYR:OH	2.05	0.46
9:j:57:ILE:O	9:j:61:MET:HG2	2.16	0.46
9:n:74:VAL:HG11	19:n:201:CLR:H72	1.97	0.46
9:h:23:MET:HE3	9:h:23:MET:O	2.16	0.46
9:m:81:THR:HG23	9:m:84:ILE:HG23	1.96	0.46
2:P:282:LEU:O	2:P:286:VAL:HG21	2.16	0.46
5:b:63:VAL:HG22	9:g:105:ALA:HB2	1.98	0.46
5:b:36:ASP:HB3	5:b:39:TRP:HB3	1.98	0.46
19:n:204:CLR:H162	19:n:204:CLR:H262	1.98	0.46
4:a:399:PHE:HB3	4:a:400:PRO:HD3	1.97	0.45
4:a:417:THR:HG23	4:a:454:GLY:C	2.41	0.45
5:b:107:MET:HG3	5:b:144:VAL:HG21	1.98	0.45
6:d:204:THR:HA	6:d:311:HIS:HB2	1.97	0.45
1:H:64:GLU:OE2	1:H:64:GLU:HA	2.17	0.45
18:a:906:PTY:H391	7:e:44:THR:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:47:LEU:C	6:d:47:LEU:HD23	2.41	0.45
6:d:309:GLN:OE1	9:o:39:THR:OG1	2.32	0.45
9:i:11:SER:O	9:i:89:SER:OG	2.23	0.45
9:n:150:LEU:HD12	19:n:204:CLR:H122	1.98	0.45
4:a:377:ILE:HG23	4:a:804:LEU:HD21	1.97	0.45
4:a:489:ASN:OD1	4:a:489:ASN:N	2.49	0.45
9:i:56:ILE:HG22	9:i:56:ILE:O	2.15	0.45
9:k:85:THR:HG23	9:k:88:ARG:H	1.81	0.45
9:n:57:ILE:O	9:n:61:MET:HG2	2.16	0.45
5:b:64:GLY:HA3	5:b:149:LEU:HA	1.98	0.45
9:g:75:LEU:HD23	9:g:75:LEU:O	2.17	0.45
2:P:403:GLU:HG2	12:C:2:NAG:H82	1.97	0.45
4:a:606:ALA:O	13:Z:2:NAG:H82	2.16	0.45
9:h:56:ILE:O	9:h:56:ILE:CG2	2.64	0.45
9:j:70:LEU:HD23	19:j:202:CLR:H273	1.98	0.45
9:o:57:ILE:HG21	9:o:132:ILE:HD12	1.99	0.45
9:l:114:GLY:O	9:l:118:VAL:HG22	2.16	0.45
9:m:65:ILE:CD1	9:m:110:ILE:HD12	2.47	0.45
19:i:201:CLR:H263	19:i:201:CLR:H20	1.98	0.45
19:n:201:CLR:H151	19:n:202:CLR:H152	1.99	0.44
6:d:11:VAL:O	9:g:36:LYS:NZ	2.47	0.44
9:j:13:PHE:CE1	9:j:17:MET:HE3	2.52	0.44
8:f:44:VAL:HG21	8:f:62:TYR:CE2	2.52	0.44
9:l:44:MET:HG3	9:l:122:ALA:HB2	1.99	0.44
12:I:1:NAG:O3	12:I:2:NAG:O5	2.24	0.44
9:l:68:TYR:HE1	19:l:203:CLR:H273	1.82	0.44
2:P:343:SER:O	2:P:344:ASN:C	2.58	0.44
4:a:527:THR:N	7:e:67:GLN:O	2.48	0.44
19:h:201:CLR:H183	19:h:202:CLR:H212	1.99	0.44
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
4:a:417:THR:HG21	4:a:458:ILE:HD12	2.00	0.44
4:a:713:ASP:OD1	4:a:713:ASP:N	2.51	0.44
9:g:17:MET:HE1	9:h:97:LEU:CD1	2.48	0.44
4:a:406:MET:SD	4:a:745:LEU:HD22	2.58	0.43
2:P:376:SER:O	2:P:376:SER:OG	2.29	0.43
4:a:619:PHE:CE2	4:a:641:ILE:HG21	2.52	0.43
2:P:279:LEU:HD21	2:P:310:LEU:HD11	2.00	0.43
19:h:201:CLR:H272	19:i:204:CLR:H263	1.99	0.43
9:l:71:VAL:HG21	19:l:203:CLR:H232	1.99	0.43
4:a:743:TRP:CH2	5:b:109:ILE:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:34:THR:O	9:j:35:ALA:C	2.61	0.43
5:b:59:SER:O	5:b:63:VAL:HG23	2.18	0.43
5:b:70:TYR:C	5:b:70:TYR:CD1	2.96	0.43
9:j:48:ARG:NH2	9:j:50:GLU:OE2	2.52	0.43
12:A:1:NAG:O3	12:A:2:NAG:O5	2.30	0.43
4:a:648:VAL:HB	4:a:649:PRO:HD3	2.00	0.43
19:i:203:CLR:H221	19:i:203:CLR:H262	2.01	0.43
9:j:17:MET:O	9:j:18:GLY:C	2.60	0.43
9:j:31:ALA:O	9:j:32:TYR:C	2.62	0.43
4:a:401:PHE:O	4:a:405:VAL:HG23	2.18	0.43
9:i:44:MET:HE1	9:i:55:SER:OG	2.19	0.43
9:i:71:VAL:HG21	19:i:203:CLR:C23	2.47	0.43
19:i:204:CLR:H162	19:i:204:CLR:H262	2.00	0.43
9:m:64:ILE:HG23	19:m:203:CLR:H261	2.00	0.43
2:P:343:SER:HB2	12:A:1:NAG:H81	2.01	0.43
14:P:501:PC1:H2B2	18:b:303:PTY:H293	2.00	0.43
4:a:606:ALA:O	13:Z:1:NAG:O6	2.33	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
4:a:719:VAL:O	4:a:723:ILE:HG12	2.18	0.42
2:P:352:VAL:HG22	2:P:378:LEU:CD2	2.48	0.42
6:d:150:LEU:CD2	6:d:154:ILE:HD11	2.49	0.42
8:f:31:ILE:O	8:f:35:VAL:HG23	2.19	0.42
9:h:75:LEU:HD12	19:h:202:CLR:H42	2.01	0.42
10:p:335:TYR:HB2	10:p:338:ILE:HD12	2.00	0.42
9:j:12:SER:O	9:j:13:PHE:C	2.63	0.42
9:j:32:TYR:O	9:j:33:GLY:C	2.61	0.42
9:m:70:LEU:O	9:m:71:VAL:C	2.63	0.42
9:n:16:VAL:CG1	9:o:94:GLY:HA3	2.49	0.42
7:e:75:TYR:CD2	8:f:41:ILE:HD12	2.54	0.42
2:P:257:THR:O	2:P:257:THR:HG22	2.19	0.42
9:i:17:MET:O	9:i:18:GLY:C	2.63	0.42
2:P:278:ASP:OD1	2:P:279:LEU:N	2.53	0.42
5:b:42:THR:HG23	5:b:123:PRO:HB3	2.01	0.42
2:P:267:ASN:ND2	12:E:1:NAG:H83	2.34	0.42
9:j:33:GLY:O	9:j:34:THR:C	2.62	0.42
9:i:71:VAL:HG11	19:i:203:CLR:H183	2.02	0.42
9:l:68:TYR:CE1	19:l:203:CLR:H273	2.54	0.42
9:l:84:ILE:HG23	9:l:84:ILE:O	2.19	0.42
9:o:22:ALA:HB2	9:o:96:GLY:HA2	2.02	0.42
4:a:543:ILE:HG12	4:a:588:VAL:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:782:ALA:O	4:a:785:THR:HG22	2.20	0.42
9:i:97:LEU:HD21	10:p:317:LEU:HD21	2.00	0.42
9:o:143:LEU:HD11	19:o:202:CLR:H232	2.02	0.42
5:b:24:ILE:CG2	5:b:28:ILE:HD12	2.50	0.41
9:i:87:TYR:CZ	9:i:91:LEU:HD11	2.55	0.41
9:j:70:LEU:O	9:j:71:VAL:C	2.63	0.41
19:o:201:CLR:H6	19:o:202:CLR:H9	2.01	0.41
2:P:412:ALA:O	14:b:302:PC1:H152	2.19	0.41
9:l:16:VAL:HG13	9:l:80:LEU:HD21	2.01	0.41
9:n:71:VAL:HG22	19:n:202:CLR:H17	2.01	0.41
2:P:267:ASN:HD22	12:E:1:NAG:H83	1.86	0.41
9:g:140:VAL:HA	9:g:143:LEU:HB3	2.03	0.41
19:m:201:CLR:H192	19:n:204:CLR:H191	2.01	0.41
9:g:49:PRO:HB2	9:h:126:ARG:HE	1.86	0.41
9:o:69:GLY:O	9:o:70:LEU:C	2.64	0.41
9:h:72:VAL:HG21	9:h:99:VAL:HG21	2.03	0.41
9:n:44:MET:HE1	9:n:51:LEU:HB3	2.01	0.41
2:P:408:ALA:CB	10:p:296:ALA:HB2	2.50	0.41
9:l:146:LEU:O	9:l:147:ILE:C	2.63	0.41
9:n:24:VAL:HG13	9:o:101:LEU:HB3	2.02	0.41
10:p:336:ASP:HA	10:p:339:ILE:HD12	2.03	0.41
6:d:56:ASN:OD1	6:d:56:ASN:C	2.64	0.41
9:j:65:ILE:CD1	9:j:110:ILE:HD12	2.51	0.41
19:j:203:CLR:H121	19:j:203:CLR:H222	2.02	0.41
12:D:1:NAG:HO3	12:D:2:NAG:C1	2.30	0.41
9:g:60:VAL:HG22	9:h:137:PHE:CZ	2.56	0.41
9:n:67:ILE:O	9:n:68:TYR:C	2.63	0.41
3:U:72:HIS:O	4:a:482:ARG:NH1	2.52	0.41
4:a:505:PRO:HG2	4:a:600:ALA:HB2	2.02	0.41
9:g:51:LEU:O	9:g:55:SER:OG	2.33	0.41
9:i:56:ILE:O	9:i:56:ILE:CG2	2.69	0.41
9:j:52:ILE:HG23	9:j:53:MET:N	2.36	0.41
9:m:22:ALA:HB2	9:m:96:GLY:HA2	2.03	0.41
9:o:41:ILE:HG12	9:o:55:SER:OG	2.21	0.41
5:b:77:ILE:HG22	5:b:77:ILE:O	2.21	0.41
9:i:67:ILE:O	9:i:68:TYR:C	2.64	0.41
9:o:51:LEU:O	9:o:52:ILE:C	2.64	0.41
6:d:24:LYS:O	6:d:27:VAL:HG22	2.22	0.40
6:d:39:CYS:O	6:d:341:ARG:NH2	2.51	0.40
9:h:52:ILE:HG23	9:h:53:MET:N	2.37	0.40
19:m:201:CLR:H183	19:n:204:CLR:H263	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:501:PC1:H141	10:p:305:VAL:HG23	2.02	0.40
4:a:713:ASP:OD2	4:a:716:ASP:HB2	2.22	0.40
9:g:20:SER:O	9:g:24:VAL:HG23	2.22	0.40
9:i:68:TYR:O	9:i:69:GLY:C	2.64	0.40
9:j:52:ILE:HD12	9:k:127:LEU:HA	2.03	0.40
2:P:339:LEU:HD21	2:P:388:MET:HE1	2.02	0.40
9:g:88:ARG:NH1	9:g:155:LYS:O	2.49	0.40
9:i:72:VAL:HG21	9:i:99:VAL:HG21	2.03	0.40
9:j:56:ILE:O	9:j:56:ILE:CG2	2.70	0.40
5:b:196:LEU:CD1	9:o:74:VAL:HG22	2.51	0.40
9:l:72:VAL:HG21	9:l:99:VAL:HG21	2.04	0.40
9:n:70:LEU:O	9:n:71:VAL:C	2.64	0.40
4:a:427:GLU:O	4:a:431:LEU:HG	2.22	0.40
5:b:154:CYS:O	5:b:158:VAL:HG23	2.21	0.40
19:b:305:CLR:H262	19:b:305:CLR:H231	1.99	0.40
9:j:44:MET:HE1	9:j:52:ILE:HA	2.04	0.40
9:o:127:LEU:O	9:o:128:PHE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	f	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
9	g	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
9	h	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
9	i	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
9	j	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
9	k	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
9	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
9	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	n	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
9	o	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
10	p	50/350 (14%)	50 (100%)	0	0	100	100
11	L	8/119 (7%)	7 (88%)	1 (12%)	0	100	100
All	All	2986/4430 (67%)	2879 (96%)	107 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	43/212 (20%)	43 (100%)	0	100	100
2	P	182/395 (46%)	179 (98%)	3 (2%)	55	75
3	U	24/241 (10%)	24 (100%)	0	100	100
4	a	367/732 (50%)	358 (98%)	9 (2%)	42	69
5	b	156/158 (99%)	152 (97%)	4 (3%)	40	69
6	d	305/306 (100%)	304 (100%)	1 (0%)	86	88
7	e	67/68 (98%)	67 (100%)	0	100	100
8	f	72/72 (100%)	70 (97%)	2 (3%)	38	68
9	g	109/113 (96%)	107 (98%)	2 (2%)	51	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	h	109/113 (96%)	108 (99%)	1 (1%)	70	81
9	i	109/113 (96%)	109 (100%)	0	100	100
9	j	109/113 (96%)	107 (98%)	2 (2%)	51	74
9	k	109/113 (96%)	109 (100%)	0	100	100
9	l	109/113 (96%)	108 (99%)	1 (1%)	70	81
9	m	109/113 (96%)	109 (100%)	0	100	100
9	n	109/113 (96%)	109 (100%)	0	100	100
9	o	109/113 (96%)	107 (98%)	2 (2%)	51	74
10	p	47/313 (15%)	46 (98%)	1 (2%)	47	71
11	L	9/100 (9%)	9 (100%)	0	100	100
All	All	2253/3614 (62%)	2225 (99%)	28 (1%)	61	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	297	ASN
2	P	321	LEU
2	P	410	ASP
4	a	367	THR
4	a	388	GLU
4	a	489	ASN
4	a	491	THR
4	a	502	GLN
4	a	524	ASN
4	a	636	ILE
4	a	725	THR
4	a	741	ARG
5	b	70	TYR
5	b	142	LEU
5	b	154	CYS
5	b	188	LEU
6	d	6	GLU
8	f	17	VAL
8	f	89	LEU
9	g	6	ASN
9	g	154	THR
9	h	61	MET
9	j	52	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	j	98	SER
9	l	133	LEU
9	o	39	THR
9	o	81	THR
10	p	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	85	GLN
2	P	364	HIS
2	P	391	HIS
4	a	365	ASN
4	a	601	HIS
4	a	662	GLN
5	b	197	GLN
6	d	84	HIS
6	d	324	GLN
8	f	56	GLN
9	j	78	ASN
9	k	92	GLN
9	m	124	GLN
9	o	123	GLN
10	p	330	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

27 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	NAG	A	1	12	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
12	NAG	A	2	12	14,14,15	0.69	0	17,19,21	0.86	0
12	NAG	B	1	12,2	14,14,15	0.76	0	17,19,21	1.26	3 (17%)
12	NAG	B	2	12	14,14,15	0.79	0	17,19,21	1.04	1 (5%)
12	NAG	C	1	12,2	14,14,15	0.79	0	17,19,21	1.17	2 (11%)
12	NAG	C	2	12	14,14,15	0.75	0	17,19,21	0.79	0
12	NAG	D	1	12,2	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
12	NAG	D	2	12	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
12	NAG	E	1	12,2	14,14,15	0.76	0	17,19,21	1.42	2 (11%)
12	NAG	E	2	12	14,14,15	0.69	0	17,19,21	1.28	1 (5%)
12	NAG	F	1	12	14,14,15	0.72	0	17,19,21	1.35	1 (5%)
12	NAG	F	2	12	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
12	NAG	G	1	12,2	14,14,15	0.75	0	17,19,21	0.88	0
12	NAG	G	2	12	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
12	NAG	I	1	12	14,14,15	0.75	0	17,19,21	0.72	0
12	NAG	I	2	12	14,14,15	0.69	0	17,19,21	0.81	0
13	NAG	Z	1	13	14,14,15	0.77	0	17,19,21	0.79	0
13	MAN	Z	10	13	11,11,12	0.71	0	15,15,17	1.06	1 (6%)
13	MAN	Z	11	13	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
13	NAG	Z	2	13	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
13	BMA	Z	3	13	11,11,12	0.80	0	15,15,17	2.30	3 (20%)
13	MAN	Z	4	13	11,11,12	0.65	0	15,15,17	1.34	1 (6%)
13	MAN	Z	5	13	11,11,12	0.72	0	15,15,17	1.26	1 (6%)
13	MAN	Z	6	13	11,11,12	0.82	1 (9%)	15,15,17	0.97	1 (6%)
13	GLC	Z	7	13	11,11,12	0.65	0	15,15,17	0.52	0
13	GLC	Z	8	13	11,11,12	0.59	0	15,15,17	0.70	0
13	GLC	Z	9	13	11,11,12	0.59	0	15,15,17	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	1	12	-	2/6/23/26	0/1/1/1
12	NAG	A	2	12	-	0/6/23/26	0/1/1/1
12	NAG	B	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	2	12	-	0/6/23/26	0/1/1/1
12	NAG	C	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	C	2	12	-	0/6/23/26	0/1/1/1
12	NAG	D	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	2	12	-	1/6/23/26	0/1/1/1
12	NAG	E	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	E	2	12	-	1/6/23/26	0/1/1/1
12	NAG	F	1	12	-	2/6/23/26	0/1/1/1
12	NAG	F	2	12	-	2/6/23/26	0/1/1/1
12	NAG	G	1	12,2	-	1/6/23/26	0/1/1/1
12	NAG	G	2	12	-	2/6/23/26	0/1/1/1
12	NAG	I	1	12	-	2/6/23/26	0/1/1/1
12	NAG	I	2	12	-	0/6/23/26	0/1/1/1
13	NAG	Z	1	13	-	0/6/23/26	0/1/1/1
13	MAN	Z	10	13	-	0/2/19/22	0/1/1/1
13	MAN	Z	11	13	-	0/2/19/22	0/1/1/1
13	NAG	Z	2	13	-	2/6/23/26	0/1/1/1
13	BMA	Z	3	13	-	1/2/19/22	0/1/1/1
13	MAN	Z	4	13	-	2/2/19/22	0/1/1/1
13	MAN	Z	5	13	-	2/2/19/22	0/1/1/1
13	MAN	Z	6	13	-	0/2/19/22	0/1/1/1
13	GLC	Z	7	13	-	1/2/19/22	0/1/1/1
13	GLC	Z	8	13	-	0/2/19/22	0/1/1/1
13	GLC	Z	9	13	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

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

All (26) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	5	MAN	C1-O5-C5	3.51	116.89	112.19
12	D	2	NAG	O5-C1-C2	-3.46	105.94	111.29
12	G	2	NAG	C2-N2-C7	3.32	127.34	122.90
13	Z	3	BMA	C3-C4-C5	3.25	116.13	110.23
12	F	2	NAG	C2-N2-C7	3.22	127.21	122.90
12	B	2	NAG	O5-C1-C2	-2.87	106.84	111.29
12	D	2	NAG	C2-N2-C7	2.87	126.75	122.90
13	Z	10	MAN	C1-O5-C5	2.87	116.03	112.19
12	A	1	NAG	C2-N2-C7	2.86	126.73	122.90
12	C	1	NAG	O4-C4-C3	-2.82	103.72	110.38
13	Z	11	MAN	C1-O5-C5	2.44	115.45	112.19
12	B	1	NAG	O4-C4-C3	-2.43	104.66	110.38
13	Z	3	BMA	O4-C4-C3	-2.39	104.75	110.38
12	E	1	NAG	O4-C4-C3	-2.29	104.97	110.38
12	D	1	NAG	C4-C3-C2	-2.25	107.72	111.02
12	D	1	NAG	C1-O5-C5	2.22	115.17	112.19
12	B	1	NAG	O5-C1-C2	-2.20	107.89	111.29
13	Z	2	NAG	O5-C1-C2	-2.12	108.01	111.29
12	C	1	NAG	O5-C1-C2	-2.09	108.06	111.29
12	B	1	NAG	C1-O5-C5	2.02	114.89	112.19
13	Z	6	MAN	C1-O5-C5	2.02	114.89	112.19

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	G	1	NAG	C1-C2-N2-C7
12	I	1	NAG	C1-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
13	Z	4	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

Continued on next page...

Continued from previous page...

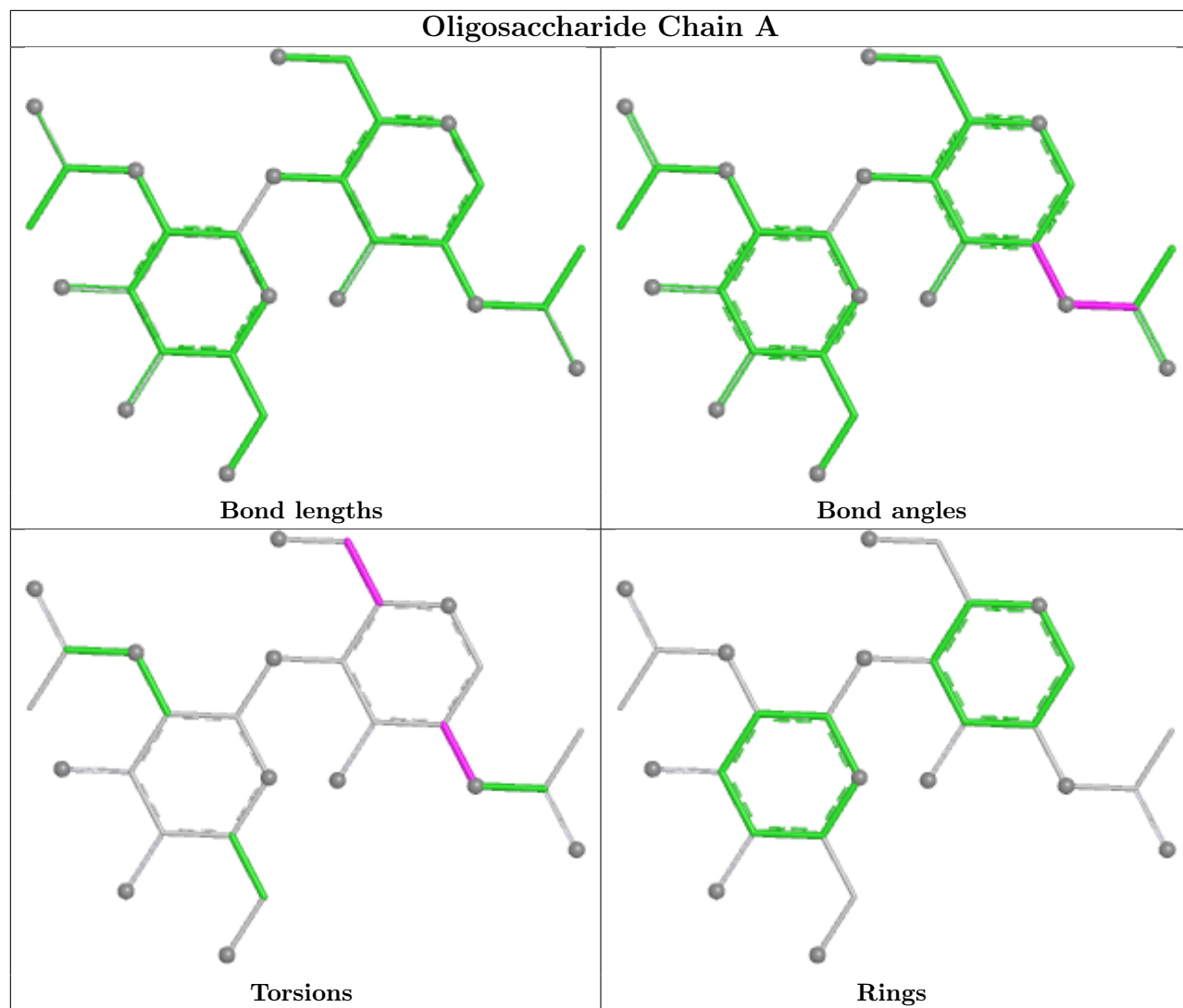
Mol	Chain	Res	Type	Atoms
12	F	2	NAG	O7-C7-N2-C2
12	G	2	NAG	C8-C7-N2-C2
12	G	2	NAG	O7-C7-N2-C2
13	Z	7	GLC	O5-C5-C6-O6
12	A	1	NAG	O5-C5-C6-O6
12	I	1	NAG	C3-C2-N2-C7
13	Z	3	BMA	O5-C5-C6-O6

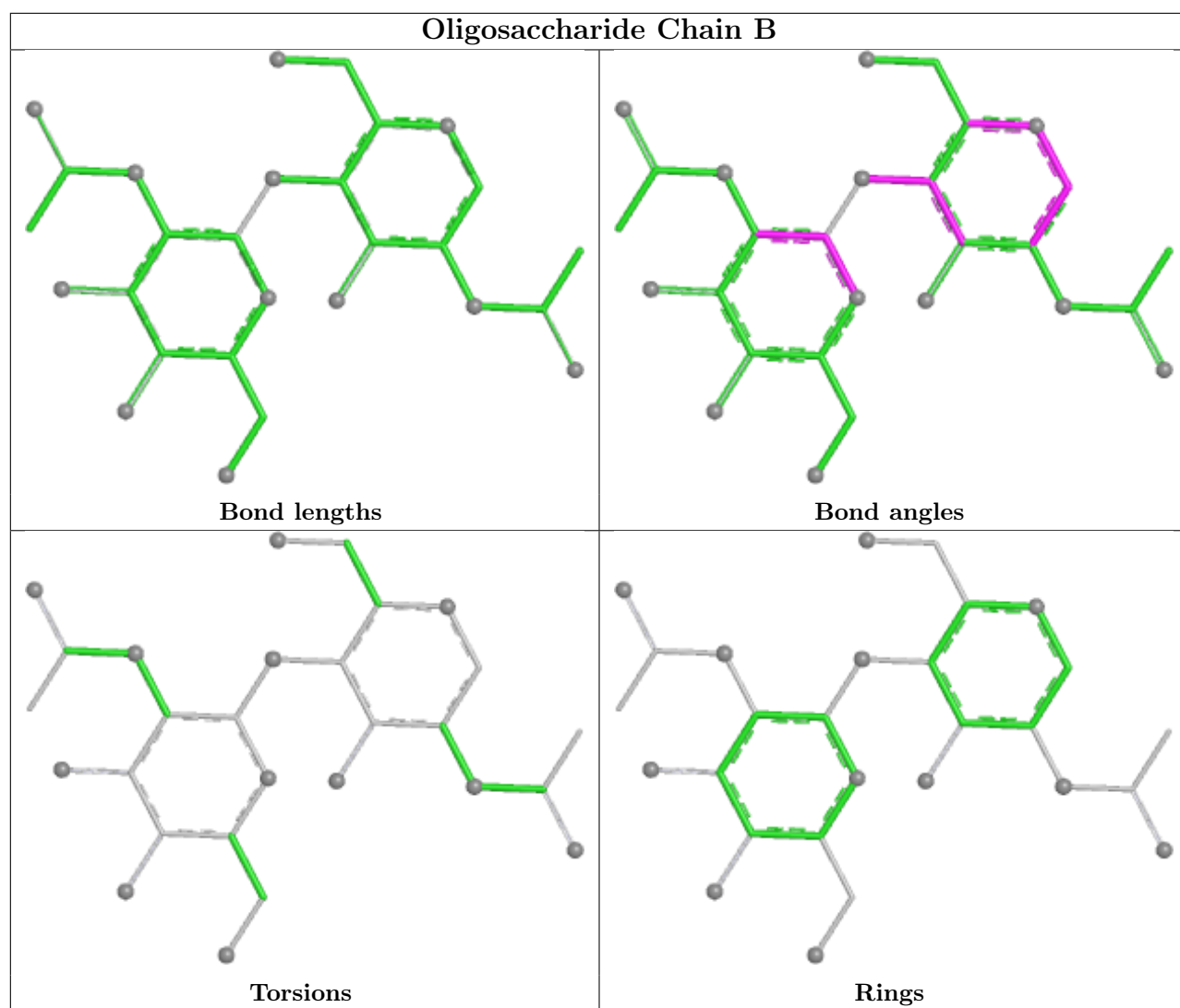
There are no ring outliers.

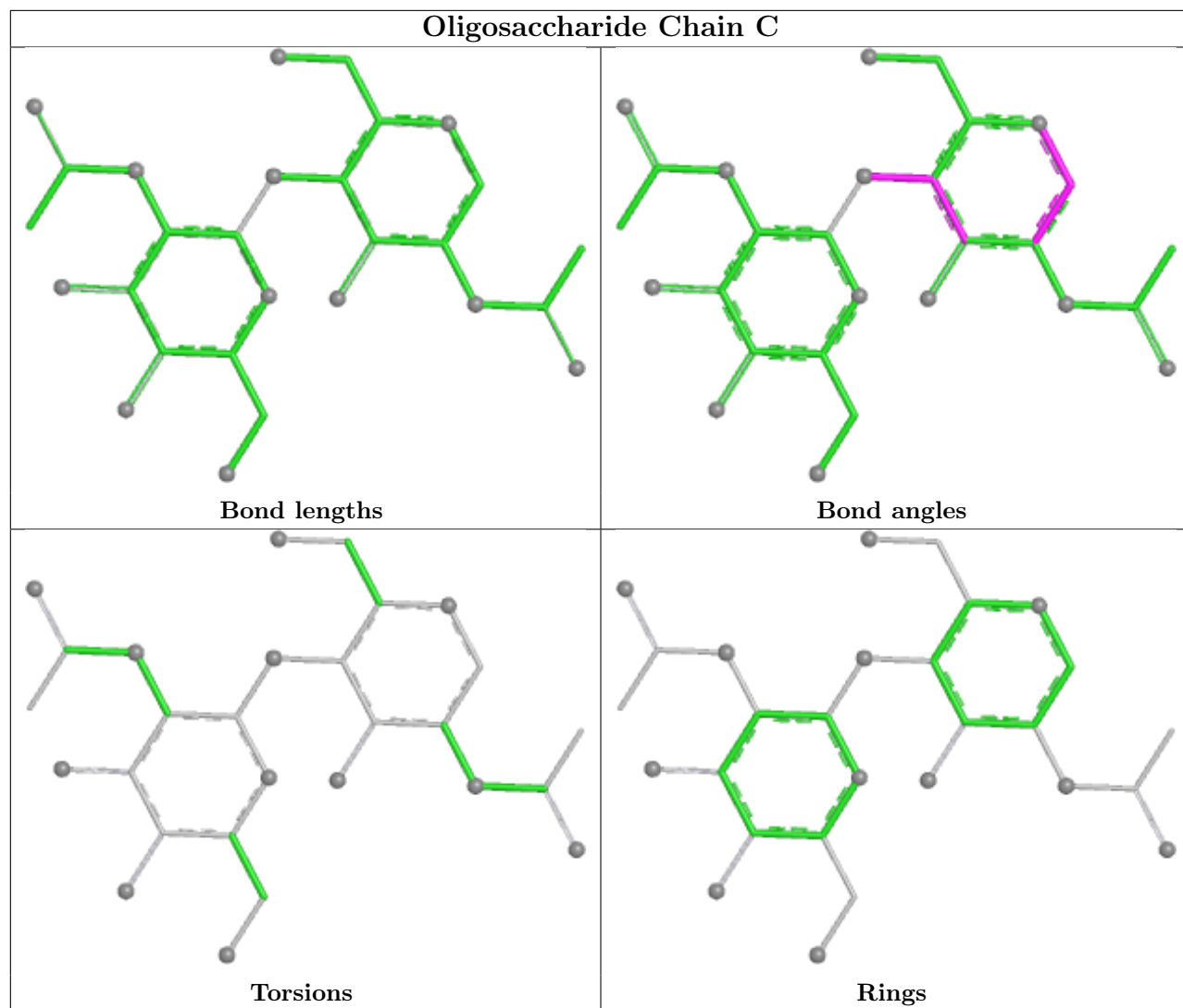
13 monomers are involved in 14 short contacts:

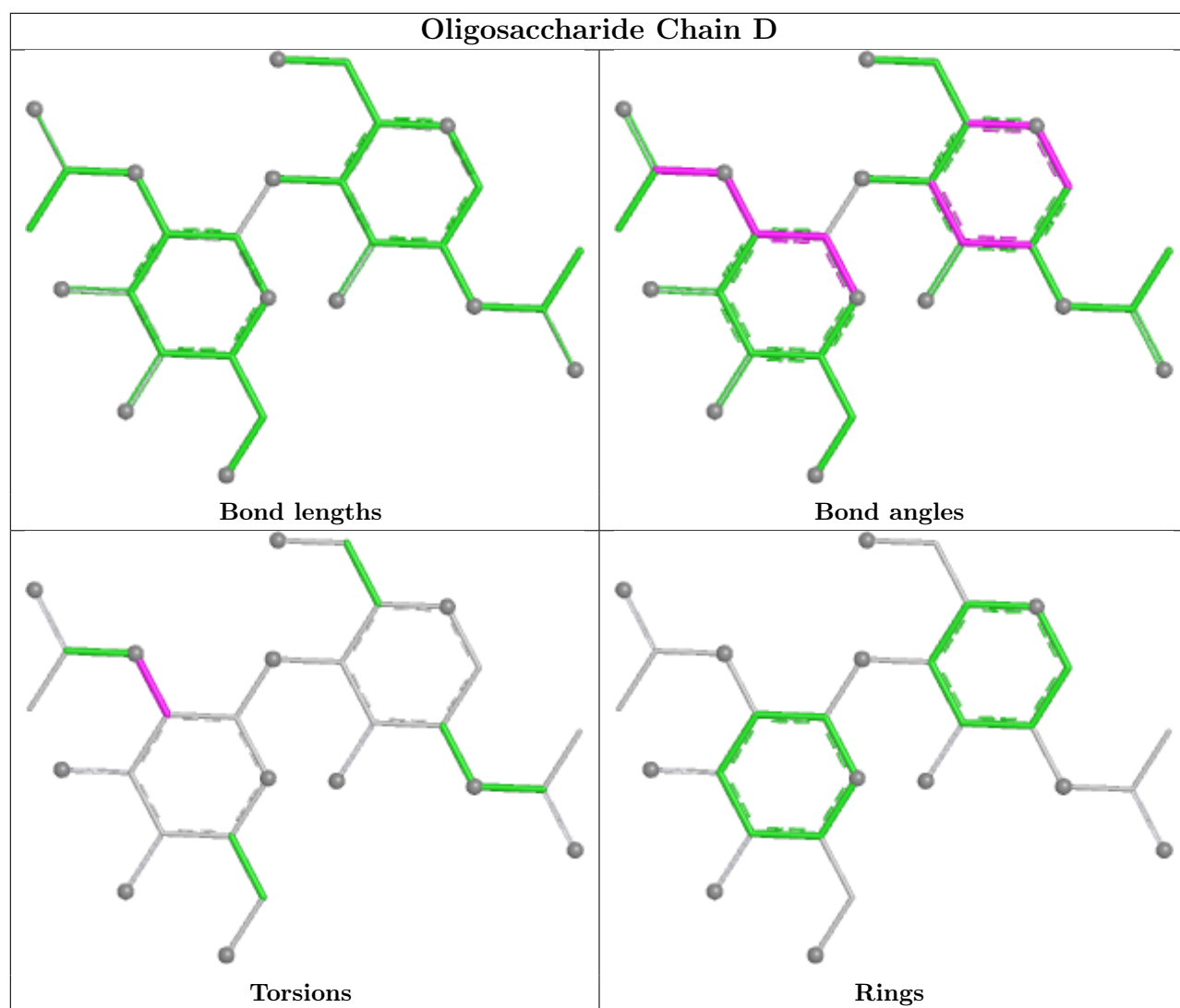
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	2	NAG	1	0
12	C	2	NAG	1	0
12	E	1	NAG	2	0
12	F	1	NAG	1	0
13	Z	1	NAG	3	0
12	D	1	NAG	2	0
12	I	2	NAG	1	0
12	G	1	NAG	1	0
13	Z	2	NAG	1	0
12	G	2	NAG	1	0
12	D	2	NAG	2	0
12	I	1	NAG	1	0
12	A	1	NAG	2	0

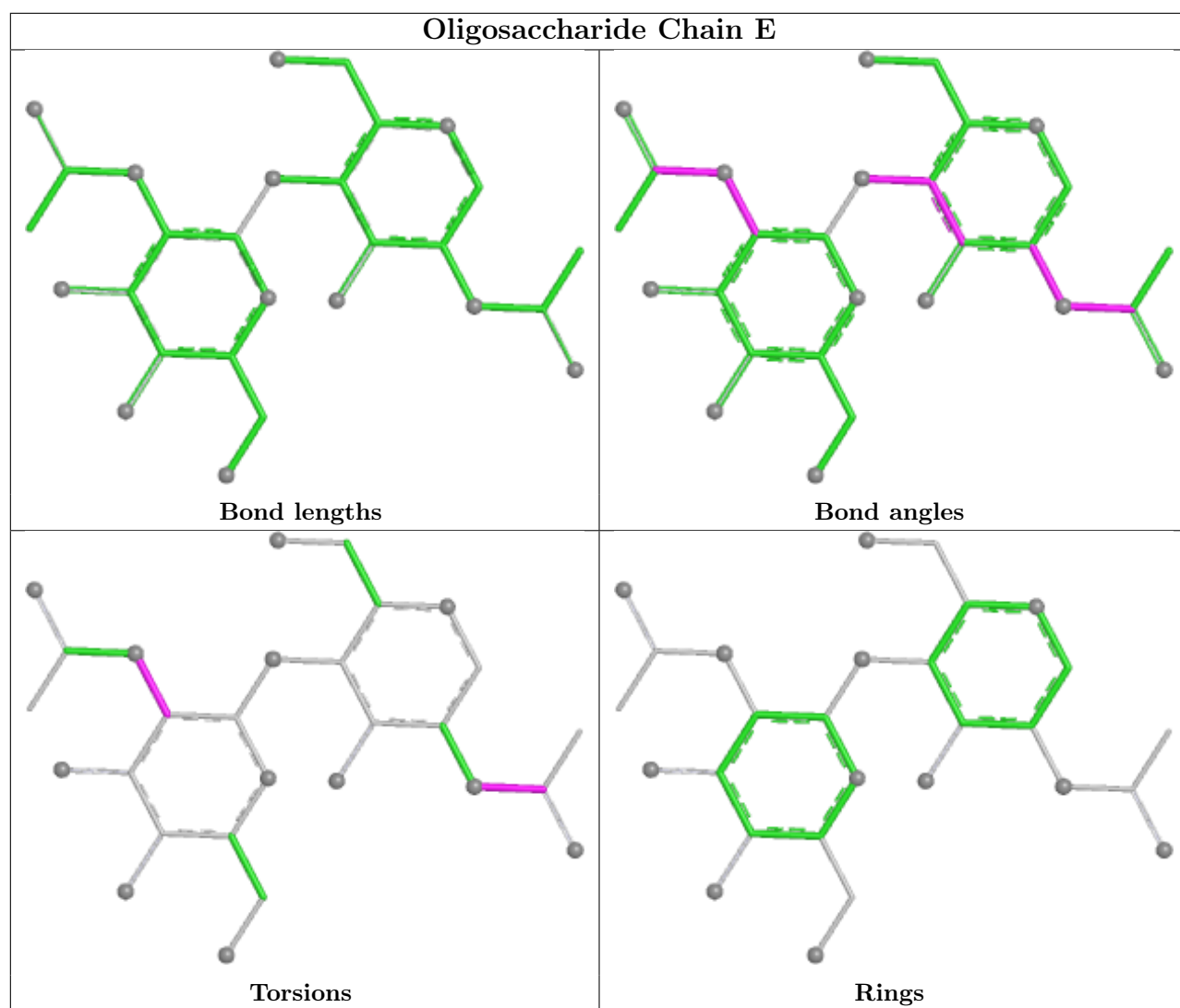
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

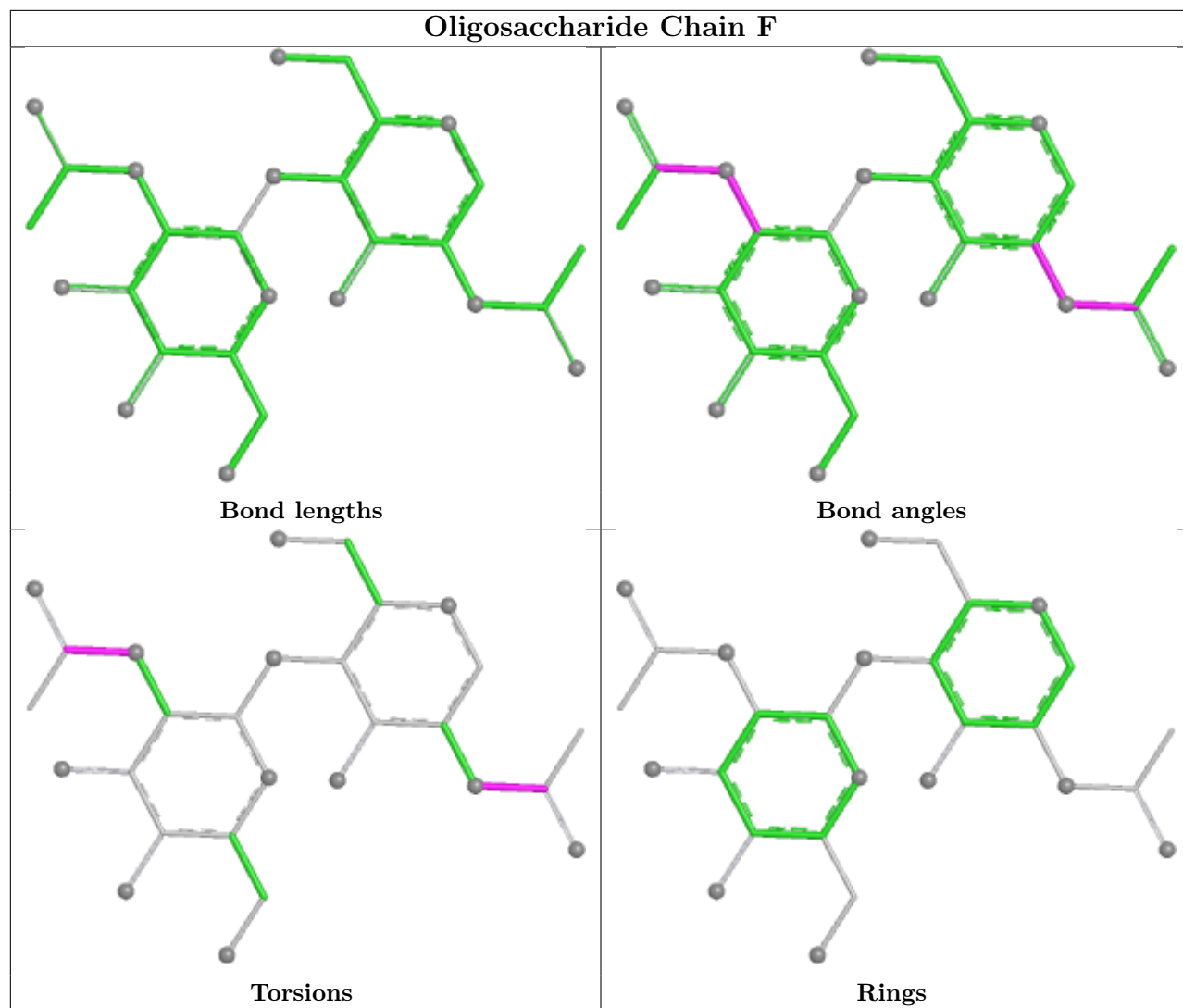


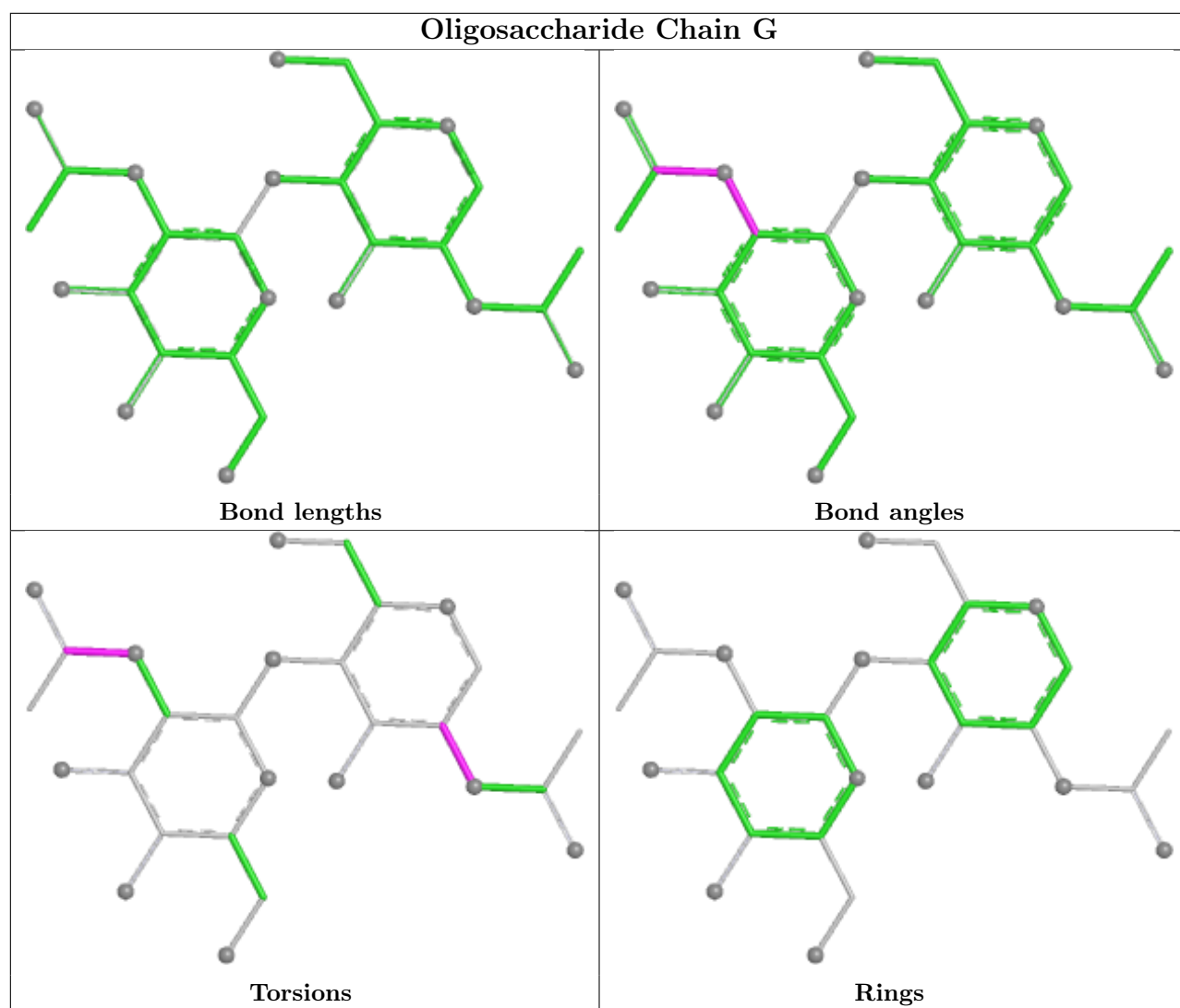


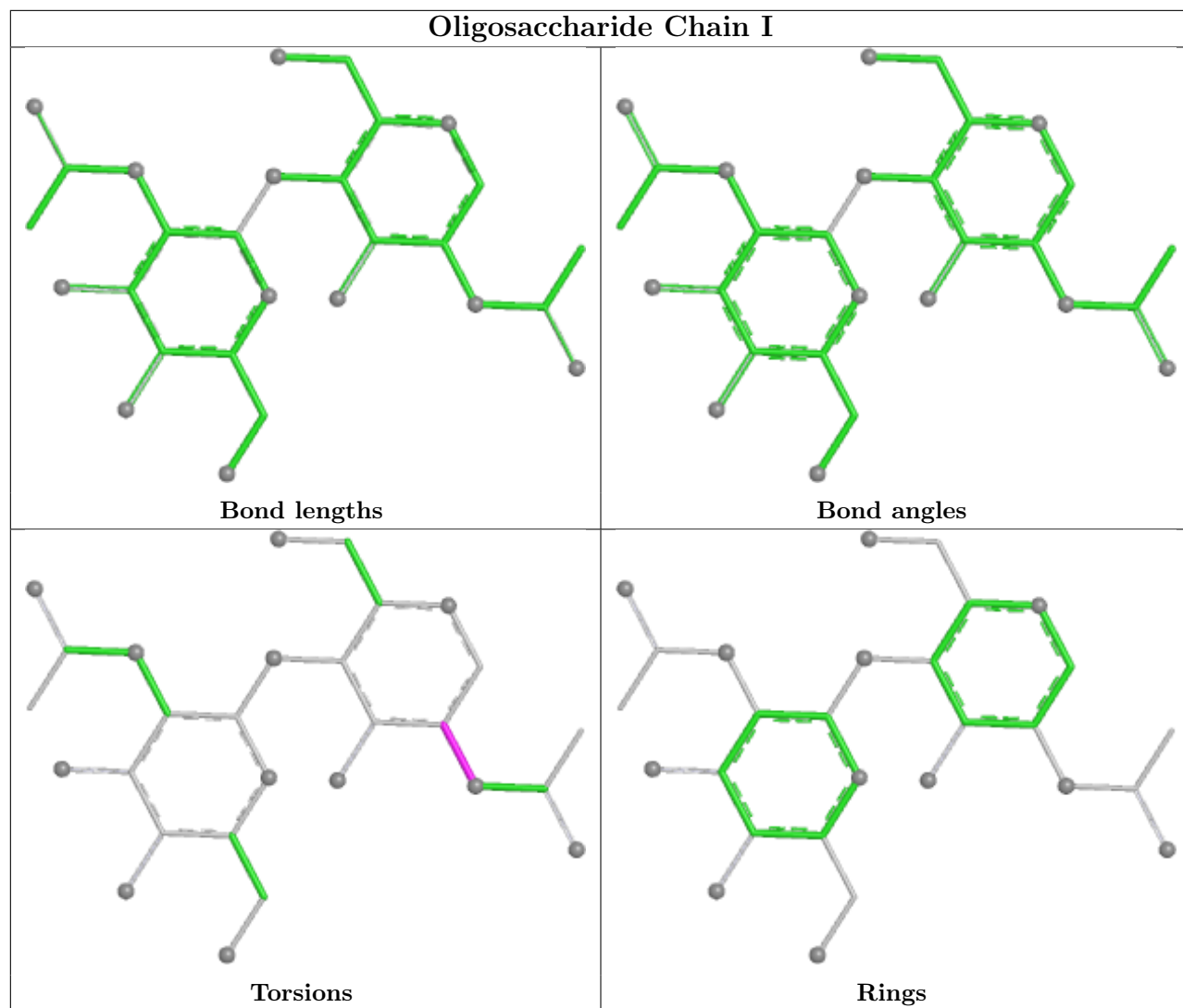


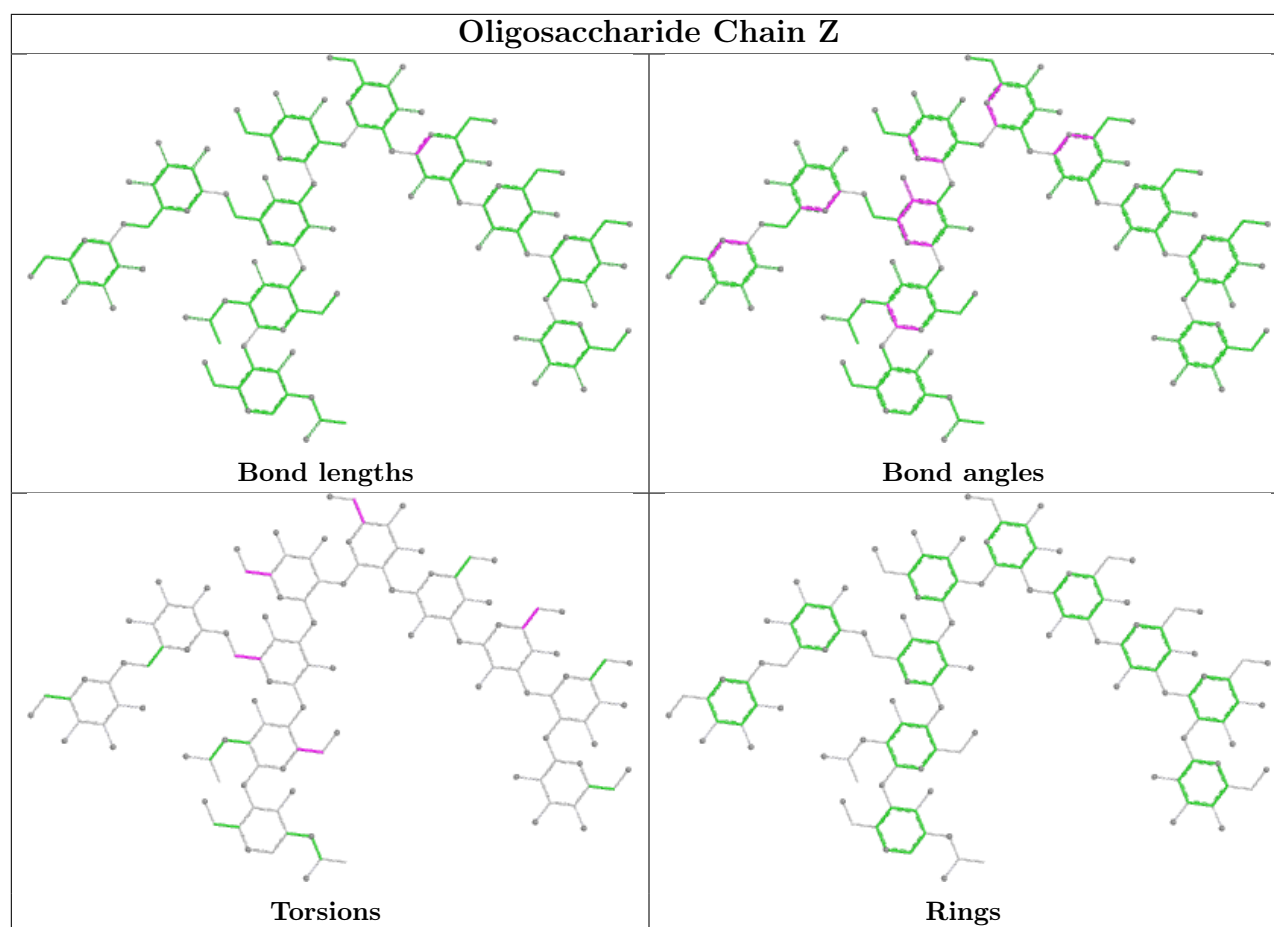












5.6 Ligand geometry [i](#)

47 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	901	WJP	P27-O30	5.01	1.64	1.59
15	a	901	WJP	C18-C16	3.50	1.58	1.51
15	a	901	WJP	C07-C06	3.18	1.58	1.50
15	a	901	WJP	P31-O32	3.11	1.66	1.54
15	a	901	WJP	C17-C16	2.96	1.57	1.50
15	a	901	WJP	C13-C11	2.71	1.56	1.51
15	a	901	WJP	C14-C15	2.47	1.57	1.50
15	a	901	WJP	C08-C06	2.12	1.55	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	901	WJP	C08-C06-C05	20.56	167.33	121.17
15	a	901	WJP	C17-C16-C18	-19.86	80.75	115.23
15	a	901	WJP	C18-C16-C15	-17.24	82.46	121.17
15	a	901	WJP	C17-C16-C15	15.39	163.16	123.63
15	a	901	WJP	C07-C06-C08	-15.17	88.89	115.23
15	a	901	WJP	C07-C06-C05	-7.92	103.29	123.63
15	a	901	WJP	C14-C15-C16	6.71	142.99	127.62
19	h	201	CLR	C1-C2-C3	6.03	118.47	110.48
19	o	203	CLR	C1-C2-C3	4.80	116.84	110.48
19	k	201	CLR	C1-C2-C3	4.66	116.65	110.48
19	n	203	CLR	C1-C2-C3	4.57	116.54	110.48
19	o	202	CLR	C16-C17-C20	4.50	118.98	112.18
19	o	201	CLR	C1-C2-C3	4.45	116.38	110.48
19	o	201	CLR	C2-C1-C10	4.37	122.09	112.78
19	h	201	CLR	C2-C1-C10	4.12	121.56	112.78
19	o	203	CLR	C2-C1-C10	4.02	121.33	112.78
19	m	201	CLR	C12-C11-C9	3.95	119.85	113.14
19	i	201	CLR	C1-C2-C3	3.88	115.63	110.48
19	n	203	CLR	C2-C1-C10	3.86	121.00	112.78
19	m	201	CLR	C1-C2-C3	3.84	115.56	110.48
19	i	203	CLR	C1-C2-C3	3.74	115.43	110.48
19	k	204	CLR	C1-C2-C3	3.74	115.43	110.48
16	a	902	NAG	C2-N2-C7	3.63	127.77	122.90
19	l	202	CLR	C1-C2-C3	3.58	115.23	110.48
19	m	201	CLR	C2-C1-C10	3.43	120.09	112.78
19	i	203	CLR	C2-C1-C10	3.40	120.03	112.78
19	k	204	CLR	C2-C1-C10	3.32	119.86	112.78
19	m	205	CLR	C1-C2-C3	3.31	114.87	110.48
19	i	201	CLR	C2-C1-C10	3.28	119.77	112.78
19	m	202	CLR	C1-C2-C3	3.27	114.81	110.48
16	a	902	NAG	C1-O5-C5	3.25	116.54	112.19
19	m	202	CLR	C2-C1-C10	3.21	119.62	112.78
19	l	202	CLR	C2-C1-C10	3.13	119.44	112.78
19	l	203	CLR	C2-C1-C10	3.09	119.37	112.78
19	k	201	CLR	C2-C1-C10	3.04	119.25	112.78
19	m	201	CLR	C11-C12-C13	3.03	117.86	112.74
19	l	203	CLR	C1-C2-C3	2.96	114.41	110.48
19	h	202	CLR	C16-C17-C20	2.96	116.65	112.18
19	j	203	CLR	C21-C20-C17	2.90	117.23	112.88
19	h	202	CLR	C22-C20-C17	2.87	116.28	110.33
19	o	201	CLR	C3-C4-C5	-2.75	107.67	112.05
19	k	201	CLR	C2-C3-C4	2.60	113.95	110.29
19	n	204	CLR	C16-C17-C13	-2.59	100.79	103.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	203	CLR	C13-C17-C20	2.58	123.48	119.50
19	l	202	CLR	C16-C17-C13	-2.58	100.80	103.84
19	k	202	CLR	C3-C4-C5	2.58	116.16	112.05
19	j	204	CLR	C21-C20-C17	2.57	116.75	112.88
19	m	205	CLR	C2-C3-C4	2.57	113.91	110.29
19	m	204	CLR	C16-C17-C20	2.57	116.06	112.18
19	j	203	CLR	C12-C13-C14	-2.55	103.43	107.25
19	i	202	CLR	C16-C17-C20	2.53	116.01	112.18
14	b	302	PC1	O12-P-O14	2.50	124.07	112.44
19	o	202	CLR	C22-C20-C17	2.49	115.50	110.33
19	i	204	CLR	C16-C17-C20	2.49	115.94	112.18
19	l	202	CLR	C16-C17-C20	2.48	115.93	112.18
14	l	201	PC1	O12-P-O14	2.46	123.87	112.44
19	n	203	CLR	C16-C17-C20	2.44	115.87	112.18
19	k	202	CLR	C4-C5-C10	2.44	119.55	116.42
14	P	501	PC1	O12-P-O14	2.43	123.75	112.44
14	a	904	PC1	O12-P-O14	2.43	123.74	112.44
19	i	203	CLR	C12-C13-C14	-2.37	103.69	107.25
19	n	204	CLR	C16-C17-C20	2.37	115.76	112.18
14	b	301	PC1	O12-P-O14	2.34	123.31	112.44
19	l	202	CLR	C22-C20-C17	2.30	115.11	110.33
19	m	204	CLR	C2-C1-C10	2.28	117.63	112.78
19	m	201	CLR	C14-C8-C9	-2.25	106.14	109.09
19	k	204	CLR	C22-C20-C17	2.25	114.99	110.33
19	o	202	CLR	C21-C20-C22	2.22	113.78	110.34
19	m	205	CLR	C16-C17-C20	2.22	115.53	112.18
19	h	202	CLR	C16-C17-C13	-2.21	101.24	103.84
19	h	201	CLR	C3-C4-C5	-2.21	108.54	112.05
19	i	203	CLR	C16-C17-C20	2.20	115.50	112.18
19	o	201	CLR	C16-C17-C20	2.11	115.37	112.18
19	k	203	CLR	C3-C4-C5	2.10	115.40	112.05
19	n	201	CLR	C13-C14-C8	2.10	117.40	114.41
19	o	203	CLR	C3-C4-C5	-2.10	108.71	112.05
19	m	202	CLR	C14-C8-C9	2.09	111.82	109.09
19	j	203	CLR	C15-C14-C13	2.06	106.27	103.84
19	j	204	CLR	C13-C14-C8	2.04	117.31	114.41
19	o	202	CLR	C21-C20-C17	-2.03	109.84	112.88
19	m	205	CLR	C22-C20-C17	2.02	114.52	110.33
15	a	901	WJP	C09-C10-C11	-2.01	123.03	127.62
19	n	201	CLR	C17-C13-C14	-2.00	97.80	100.10

There are no chirality outliers.

All (522) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	P	501	PC1	C11-O13-P-O12
14	P	501	PC1	C11-O13-P-O11
14	P	501	PC1	C1-O11-P-O14
14	P	501	PC1	O22-C21-O21-C2
14	a	904	PC1	C11-O13-P-O11
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	C11-O13-P-O11
14	b	302	PC1	C1-O11-P-O13
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-O12
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	C3-O11-P1-O14
18	a	905	PTY	C5-O14-P1-O11
18	a	905	PTY	C5-O14-P1-O12
18	a	906	PTY	C5-O14-P1-O11
18	a	906	PTY	C5-O14-P1-O12
18	b	303	PTY	N1-C2-C3-O11
18	b	303	PTY	C5-O14-P1-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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	101	PTY	C5-O14-P1-O11
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	j	201	PTY	C3-O11-P1-O14
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	401	PTY	C3-O11-P1-O14
18	p	402	PTY	N1-C2-C3-O11
18	p	402	PTY	C11-C8-O7-C6
18	p	402	PTY	C3-O11-P1-O13
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
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	o	201	CLR	C17-C20-C22-C23
19	i	203	CLR	C13-C17-C20-C21
19	m	204	CLR	C13-C17-C20-C21
19	i	203	CLR	C13-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	m	204	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	C20-C22-C23-C24
19	i	201	CLR	C21-C20-C22-C23
19	i	204	CLR	C21-C20-C22-C23
19	m	201	CLR	C21-C20-C22-C23
19	o	201	CLR	C21-C20-C22-C23
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
19	m	202	CLR	C21-C20-C22-C23
19	i	203	CLR	C16-C17-C20-C21
19	m	204	CLR	C16-C17-C20-C21
19	n	203	CLR	C13-C17-C20-C22
19	h	202	CLR	C17-C20-C22-C23
19	j	203	CLR	C17-C20-C22-C23
18	p	401	PTY	C40-C41-C42-C43
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	m	204	CLR	C16-C17-C20-C22
19	h	201	CLR	C17-C20-C22-C23
18	a	906	PTY	O14-C5-C6-O7
19	n	202	CLR	C22-C23-C24-C25
19	o	201	CLR	C22-C23-C24-C25
19	o	202	CLR	C20-C22-C23-C24
16	a	902	NAG	C8-C7-N2-C2
16	a	902	NAG	O7-C7-N2-C2
15	a	901	WJP	C02-C03-C04-C05
17	a	903	LP3	C11-C12-C13-C14
15	a	901	WJP	C04-C05-C06-C08
19	j	202	CLR	C13-C17-C20-C22
19	b	305	CLR	C17-C20-C22-C23
19	j	205	CLR	C17-C20-C22-C23
19	k	202	CLR	C17-C20-C22-C23
18	p	401	PTY	C17-C18-C19-C20
19	h	202	CLR	C21-C20-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	p	401	PTY	C8-C11-C12-C13
15	a	901	WJP	C16-C18-C19-C20
19	l	203	CLR	C22-C23-C24-C25
19	o	202	CLR	C13-C17-C20-C21
18	p	401	PTY	C15-C16-C17-C18
18	p	402	PTY	C30-C31-C32-C33
19	i	203	CLR	C16-C17-C20-C22
19	k	204	CLR	C20-C22-C23-C24
19	o	202	CLR	C13-C17-C20-C22
19	h	201	CLR	C21-C20-C22-C23
19	j	203	CLR	C22-C23-C24-C25
19	l	202	CLR	C20-C22-C23-C24
19	n	201	CLR	C22-C23-C24-C25
14	a	904	PC1	C31-C32-C33-C34
18	j	201	PTY	C30-C31-C32-C33
19	m	203	CLR	C22-C23-C24-C25
19	j	202	CLR	C13-C17-C20-C21
19	n	203	CLR	C13-C17-C20-C21
18	b	303	PTY	C8-C11-C12-C13
19	i	202	CLR	C13-C17-C20-C22
19	l	202	CLR	C13-C17-C20-C22
19	b	305	CLR	C21-C20-C22-C23
19	j	205	CLR	C21-C20-C22-C23
19	m	204	CLR	C22-C23-C24-C25
19	b	305	CLR	C22-C23-C24-C25
19	n	203	CLR	C16-C17-C20-C21
19	o	202	CLR	C16-C17-C20-C21
19	j	203	CLR	C13-C17-C20-C22
19	n	204	CLR	C17-C20-C22-C23
19	k	202	CLR	C21-C20-C22-C23
19	b	305	CLR	C20-C22-C23-C24
18	a	905	PTY	C31-C30-O4-C1
19	k	201	CLR	C22-C23-C24-C25
19	m	201	CLR	C20-C22-C23-C24
19	m	201	CLR	C22-C23-C24-C25
19	j	202	CLR	C16-C17-C20-C21
19	i	201	CLR	C22-C23-C24-C25
19	k	201	CLR	C20-C22-C23-C24
19	j	203	CLR	C20-C22-C23-C24
19	n	203	CLR	C20-C22-C23-C24
19	o	202	CLR	C22-C23-C24-C25
19	j	204	CLR	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	i	202	CLR	C13-C17-C20-C21
19	m	205	CLR	C13-C17-C20-C22
19	n	201	CLR	C21-C20-C22-C23
18	a	905	PTY	O30-C30-O4-C1
19	i	202	CLR	C16-C17-C20-C21
19	n	204	CLR	C23-C24-C25-C26
19	o	203	CLR	C22-C23-C24-C25
19	l	202	CLR	C13-C17-C20-C21
19	n	203	CLR	C23-C24-C25-C26
19	o	203	CLR	C23-C24-C25-C27
19	i	202	CLR	C20-C22-C23-C24
14	a	904	PC1	C3A-C3B-C3C-C3D
14	b	302	PC1	C23-C24-C25-C26
14	l	201	PC1	C3E-C3F-C3G-C3H
17	a	903	LP3	C12-C13-C14-C15
18	j	201	PTY	C38-C39-C40-C41
14	b	301	PC1	C21-C22-C23-C24
14	a	904	PC1	C35-C36-C37-C38
14	b	301	PC1	C2B-C2C-C2D-C2E
18	a	906	PTY	C18-C19-C20-C21
18	p	403	PTY	C20-C21-C22-C23
19	l	204	CLR	C16-C17-C20-C21
19	j	204	CLR	C20-C22-C23-C24
19	k	204	CLR	C22-C23-C24-C25
18	b	303	PTY	C20-C21-C22-C23
19	n	203	CLR	C23-C24-C25-C27
19	n	204	CLR	C23-C24-C25-C27
19	j	203	CLR	C16-C17-C20-C22
18	p	402	PTY	C34-C35-C36-C37
17	a	903	LP3	O3P-C1-C2-O2
18	b	304	PTY	C16-C17-C18-C19
18	b	304	PTY	C24-C25-C26-C27
14	b	302	PC1	C26-C27-C28-C29
19	n	204	CLR	C21-C20-C22-C23
19	j	204	CLR	C16-C17-C20-C22
14	a	904	PC1	C2B-C2C-C2D-C2E
14	P	501	PC1	C32-C31-O31-C3
19	l	203	CLR	C17-C20-C22-C23
18	p	401	PTY	C24-C25-C26-C27
14	P	501	PC1	C21-C22-C23-C24
19	n	204	CLR	C22-C23-C24-C25
14	l	201	PC1	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	j	201	PTY	C33-C34-C35-C36
18	j	201	PTY	C34-C35-C36-C37
18	a	905	PTY	C22-C23-C24-C25
19	j	204	CLR	C23-C24-C25-C26
14	P	501	PC1	C25-C26-C27-C28
19	n	203	CLR	C16-C17-C20-C22
19	j	202	CLR	C22-C23-C24-C25
18	p	403	PTY	C15-C16-C17-C18
18	b	303	PTY	C30-C31-C32-C33
14	l	201	PC1	C39-C3A-C3B-C3C
18	p	401	PTY	C31-C32-C33-C34
14	P	501	PC1	C28-C29-C2A-C2B
14	l	201	PC1	C32-C31-O31-C3
18	p	403	PTY	C23-C24-C25-C26
19	j	204	CLR	C22-C23-C24-C25
19	l	204	CLR	C13-C17-C20-C22
14	P	501	PC1	C33-C34-C35-C36
18	p	401	PTY	C25-C26-C27-C28
19	l	202	CLR	C16-C17-C20-C21
19	l	204	CLR	C13-C17-C20-C21
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	e	101	PTY	C12-C13-C14-C15
18	b	304	PTY	O10-C8-O7-C6
14	b	301	PC1	C32-C33-C34-C35
18	p	403	PTY	C19-C20-C21-C22
14	a	904	PC1	C24-C25-C26-C27
14	b	302	PC1	C2A-C2B-C2C-C2D
19	b	305	CLR	C23-C24-C25-C27
19	m	202	CLR	C23-C24-C25-C27
19	n	202	CLR	C23-C24-C25-C26
19	o	203	CLR	C23-C24-C25-C26
15	a	901	WJP	C07-C06-C08-C09
14	b	302	PC1	C39-C3A-C3B-C3C
19	l	204	CLR	C20-C22-C23-C24
18	p	402	PTY	C39-C40-C41-C42
19	i	201	CLR	C23-C24-C25-C26
14	P	501	PC1	O32-C31-O31-C3
19	m	205	CLR	C13-C17-C20-C21
18	p	402	PTY	C38-C39-C40-C41
14	l	201	PC1	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	p	403	PTY	C32-C33-C34-C35
19	l	204	CLR	C23-C24-C25-C27
14	a	904	PC1	C33-C34-C35-C36
14	b	302	PC1	C2B-C2C-C2D-C2E
18	b	304	PTY	C19-C20-C21-C22
18	e	101	PTY	C34-C35-C36-C37
18	j	201	PTY	C15-C16-C17-C18
18	j	201	PTY	C17-C18-C19-C20
18	b	304	PTY	C20-C21-C22-C23
18	p	401	PTY	C35-C36-C37-C38
19	j	203	CLR	C16-C17-C20-C21
14	b	301	PC1	C23-C24-C25-C26
14	b	302	PC1	C37-C38-C39-C3A
18	a	906	PTY	C12-C13-C14-C15
18	a	906	PTY	O14-C5-C6-C1
18	p	403	PTY	O14-C5-C6-C1
18	b	303	PTY	O10-C8-O7-C6
14	b	302	PC1	C35-C36-C37-C38
18	p	402	PTY	C37-C38-C39-C40
19	m	205	CLR	C16-C17-C20-C21
18	b	304	PTY	C34-C35-C36-C37
18	p	403	PTY	C31-C32-C33-C34
19	k	201	CLR	C17-C20-C22-C23
18	a	905	PTY	O10-C8-O7-C6
19	n	201	CLR	C20-C22-C23-C24
18	a	906	PTY	O4-C1-C6-C5
18	b	303	PTY	O4-C1-C6-C5
14	b	301	PC1	C3E-C3F-C3G-C3H
19	i	204	CLR	C13-C17-C20-C22
14	b	301	PC1	C29-C2A-C2B-C2C
19	m	202	CLR	C23-C24-C25-C26
18	p	402	PTY	C16-C17-C18-C19
14	l	201	PC1	O32-C31-O31-C3
19	j	205	CLR	C20-C22-C23-C24
19	m	202	CLR	C20-C22-C23-C24
19	m	205	CLR	C22-C23-C24-C25
19	i	204	CLR	C16-C17-C20-C21
19	i	204	CLR	C13-C17-C20-C21
14	b	301	PC1	C3-C2-O21-C21
14	P	501	PC1	C2E-C2F-C2G-C2H
19	l	204	CLR	C16-C17-C20-C22
19	l	204	CLR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	m	203	CLR	C16-C17-C20-C21
18	j	201	PTY	O14-C5-C6-O7
19	l	202	CLR	C16-C17-C20-C22
19	m	205	CLR	C16-C17-C20-C22
14	P	501	PC1	C3C-C3D-C3E-C3F
18	b	303	PTY	C19-C20-C21-C22
18	p	403	PTY	C13-C14-C15-C16
18	b	303	PTY	O4-C1-C6-O7
18	e	101	PTY	C37-C38-C39-C40
18	p	401	PTY	C22-C23-C24-C25
14	l	201	PC1	C3F-C3G-C3H-C3I
18	p	402	PTY	C35-C36-C37-C38
19	m	203	CLR	C13-C17-C20-C21
14	b	302	PC1	C29-C2A-C2B-C2C
18	p	403	PTY	C37-C38-C39-C40
14	b	301	PC1	C3A-C3B-C3C-C3D
14	b	301	PC1	C38-C39-C3A-C3B
19	l	203	CLR	C20-C22-C23-C24
15	a	901	WJP	C12-C11-C13-C14
18	a	905	PTY	C14-C15-C16-C17
18	b	304	PTY	C31-C30-O4-C1
14	l	201	PC1	C22-C23-C24-C25
18	b	303	PTY	C12-C13-C14-C15
18	a	906	PTY	C19-C20-C21-C22
19	h	201	CLR	C22-C23-C24-C25
19	k	201	CLR	C21-C20-C22-C23
19	i	202	CLR	C16-C17-C20-C22
18	p	402	PTY	C31-C32-C33-C34
18	p	401	PTY	C26-C27-C28-C29
18	e	101	PTY	C36-C37-C38-C39
19	j	204	CLR	C23-C24-C25-C27
18	j	201	PTY	C36-C37-C38-C39
15	a	901	WJP	C05-C06-C08-C09
19	n	204	CLR	C13-C17-C20-C21
18	p	403	PTY	O14-C5-C6-O7
19	i	204	CLR	C16-C17-C20-C22
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	C26-C27-C28-C29
18	p	402	PTY	C23-C24-C25-C26
19	l	202	CLR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a	901	WJP	C10-C11-C13-C14
17	a	903	LP3	C14-C15-C16-C17
14	l	201	PC1	C3A-C3B-C3C-C3D
14	b	301	PC1	C22-C23-C24-C25
18	b	303	PTY	C40-C41-C42-C43
19	i	201	CLR	C23-C24-C25-C27
14	b	302	PC1	C2D-C2E-C2F-C2G
19	b	305	CLR	C13-C17-C20-C21
19	o	202	CLR	C17-C20-C22-C23
19	i	204	CLR	C22-C23-C24-C25
18	b	304	PTY	O30-C30-O4-C1
19	m	203	CLR	C16-C17-C20-C22
14	b	301	PC1	C2D-C2E-C2F-C2G
19	b	305	CLR	C23-C24-C25-C26
18	p	403	PTY	C41-C42-C43-C44
18	a	906	PTY	C31-C30-O4-C1
19	l	202	CLR	C23-C24-C25-C27
18	p	402	PTY	C15-C16-C17-C18
19	i	203	CLR	C22-C23-C24-C25
14	l	201	PC1	C3-C2-O21-C21
14	P	501	PC1	C23-C24-C25-C26
19	n	202	CLR	C23-C24-C25-C27
19	b	305	CLR	C16-C17-C20-C21
18	b	303	PTY	C37-C38-C39-C40
18	b	303	PTY	O14-C5-C6-O7
18	b	304	PTY	O14-C5-C6-O7
19	o	202	CLR	C16-C17-C20-C22
18	a	905	PTY	C23-C24-C25-C26
18	p	401	PTY	C2-C3-O11-P1
19	b	305	CLR	C16-C17-C20-C22
18	a	906	PTY	O4-C1-C6-O7
18	p	403	PTY	C33-C34-C35-C36
19	n	204	CLR	C16-C17-C20-C22
19	k	202	CLR	C22-C23-C24-C25
19	n	204	CLR	C16-C17-C20-C21
14	a	904	PC1	O13-C11-C12-N
14	b	301	PC1	O13-C11-C12-N
14	l	201	PC1	O13-C11-C12-N
19	o	201	CLR	C13-C17-C20-C21
19	i	204	CLR	C23-C24-C25-C26
19	o	201	CLR	C13-C17-C20-C22
19	i	201	CLR	C13-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	906	PTY	O30-C30-O4-C1
18	b	303	PTY	C41-C42-C43-C44
18	b	304	PTY	O14-C5-C6-C1
18	j	201	PTY	O14-C5-C6-C1
18	p	401	PTY	O14-C5-C6-C1
19	h	201	CLR	C23-C24-C25-C26
19	k	202	CLR	C13-C17-C20-C22
18	p	402	PTY	C32-C33-C34-C35
19	h	201	CLR	C23-C24-C25-C27
19	o	201	CLR	C16-C17-C20-C22
18	p	401	PTY	O14-C5-C6-O7
14	l	201	PC1	C37-C38-C39-C3A
19	i	201	CLR	C13-C17-C20-C21
19	j	204	CLR	C13-C17-C20-C21
19	k	202	CLR	C13-C17-C20-C21
18	j	201	PTY	O4-C1-C6-O7
14	a	904	PC1	C2F-C2G-C2H-C2I
18	j	201	PTY	O4-C1-C6-C5
19	i	201	CLR	C16-C17-C20-C22
18	p	401	PTY	C19-C20-C21-C22
19	o	201	CLR	C16-C17-C20-C21
18	p	401	PTY	C21-C22-C23-C24
14	a	904	PC1	C11-O13-P-O14
14	b	301	PC1	C11-O13-P-O14
14	b	301	PC1	C11-O13-P-O11
14	b	302	PC1	C1-O11-P-O14
14	l	201	PC1	C1-O11-P-O13
17	a	903	LP3	C1-O3P-P-O1P
17	a	903	LP3	C1-O3P-P-O4P
18	a	905	PTY	C3-O11-P1-O12
18	a	906	PTY	C3-O11-P1-O13
18	b	303	PTY	C3-O11-P1-O13
18	b	304	PTY	C5-O14-P1-O11
18	e	101	PTY	C5-O14-P1-O13
18	j	201	PTY	C3-O11-P1-O13
18	p	402	PTY	C3-O11-P1-O14
18	p	402	PTY	C5-O14-P1-O13
18	p	403	PTY	C5-O14-P1-O13
14	a	904	PC1	C2-C1-O11-P
14	l	201	PC1	C2A-C2B-C2C-C2D
14	b	302	PC1	C3-C2-O21-C21
18	j	201	PTY	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	j	201	PTY	C25-C26-C27-C28
18	e	101	PTY	C35-C36-C37-C38
19	i	204	CLR	C23-C24-C25-C27
19	k	202	CLR	C16-C17-C20-C22
18	e	101	PTY	C15-C16-C17-C18
14	a	904	PC1	C3E-C3F-C3G-C3H
18	p	402	PTY	C8-C11-C12-C13
18	e	101	PTY	C41-C42-C43-C44
19	i	201	CLR	C16-C17-C20-C21
18	a	906	PTY	C6-C5-O14-P1
18	j	201	PTY	C24-C25-C26-C27
18	p	403	PTY	C35-C36-C37-C38
19	k	204	CLR	C16-C17-C20-C22
17	a	903	LP3	C20-C21-C22-C23
18	a	905	PTY	C17-C18-C19-C20
18	p	403	PTY	C14-C15-C16-C17
18	e	101	PTY	C16-C17-C18-C19
18	p	402	PTY	C5-C6-O7-C8
19	o	201	CLR	C20-C22-C23-C24
18	p	401	PTY	O4-C30-C31-C32
19	k	204	CLR	C13-C17-C20-C21
18	p	401	PTY	C13-C14-C15-C16
19	h	202	CLR	C20-C22-C23-C24
14	b	301	PC1	C25-C26-C27-C28
18	e	101	PTY	C6-C5-O14-P1
18	b	303	PTY	C34-C35-C36-C37
18	j	201	PTY	C22-C23-C24-C25
14	b	301	PC1	C34-C35-C36-C37
18	b	303	PTY	C11-C12-C13-C14
18	e	101	PTY	C22-C23-C24-C25
19	k	204	CLR	C17-C20-C22-C23
18	p	403	PTY	C16-C17-C18-C19
19	k	204	CLR	C13-C17-C20-C22
18	p	402	PTY	C20-C21-C22-C23
18	a	905	PTY	C18-C19-C20-C21
15	a	901	WJP	P31-O30-P27-O26
18	b	304	PTY	C36-C37-C38-C39
14	a	904	PC1	C3D-C3E-C3F-C3G
18	a	906	PTY	O10-C8-O7-C6
18	e	101	PTY	O14-C5-C6-O7
17	a	903	LP3	C25-C26-C27-C28
19	k	201	CLR	C23-C24-C25-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	o	203	CLR	C13-C17-C20-C21
14	a	904	PC1	C29-C2A-C2B-C2C
18	a	905	PTY	C19-C20-C21-C22
14	a	904	PC1	C32-C33-C34-C35
18	b	303	PTY	O14-C5-C6-C1
18	e	101	PTY	O14-C5-C6-C1
18	p	403	PTY	C24-C25-C26-C27
18	a	906	PTY	C34-C35-C36-C37
14	b	302	PC1	C2E-C2F-C2G-C2H
18	a	906	PTY	C30-C31-C32-C33
18	b	304	PTY	C14-C15-C16-C17
18	p	402	PTY	C13-C14-C15-C16
15	a	901	WJP	P27-O30-P31-O34
18	p	402	PTY	C1-C6-O7-C8
17	a	903	LP3	C15-C16-C17-C18
19	i	203	CLR	C20-C22-C23-C24
18	p	403	PTY	C36-C37-C38-C39
17	a	903	LP3	C17-C18-C19-C20
18	a	905	PTY	C12-C11-C8-O7
17	a	903	LP3	C19-C20-C21-C22
19	n	203	CLR	C22-C23-C24-C25
14	P	501	PC1	C29-C2A-C2B-C2C
18	b	303	PTY	C24-C25-C26-C27
18	a	906	PTY	C11-C8-O7-C6
18	p	403	PTY	C12-C11-C8-O7
14	b	301	PC1	C36-C37-C38-C39
18	a	906	PTY	C25-C26-C27-C28
19	k	204	CLR	C21-C20-C22-C23
18	p	403	PTY	C12-C13-C14-C15
19	k	202	CLR	C16-C17-C20-C21
18	e	101	PTY	C8-C11-C12-C13
18	e	101	PTY	C12-C11-C8-O7
14	P	501	PC1	C3D-C3E-C3F-C3G
15	a	901	WJP	P27-O30-P31-O33
18	a	905	PTY	O4-C30-C31-C32
14	b	301	PC1	C39-C3A-C3B-C3C
18	b	304	PTY	C23-C24-C25-C26
18	j	201	PTY	C26-C27-C28-C29
18	p	401	PTY	C6-C5-O14-P1
18	a	905	PTY	C12-C11-C8-O10
18	b	304	PTY	C17-C18-C19-C20
14	a	904	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	903	LP3	C24-C25-C26-C27
19	j	205	CLR	C16-C17-C20-C22
19	o	203	CLR	C16-C17-C20-C22
14	a	904	PC1	C34-C35-C36-C37
18	e	101	PTY	C24-C25-C26-C27
18	a	905	PTY	O30-C30-C31-C32
18	b	303	PTY	C32-C33-C34-C35
18	p	403	PTY	C25-C26-C27-C28
19	o	203	CLR	C17-C20-C22-C23
14	P	501	PC1	C3B-C3C-C3D-C3E
14	P	501	PC1	C3E-C3F-C3G-C3H
18	b	303	PTY	O4-C30-C31-C32
14	b	301	PC1	C3C-C3D-C3E-C3F
18	b	304	PTY	C12-C11-C8-O7
18	e	101	PTY	C12-C11-C8-O10
18	p	403	PTY	C12-C11-C8-O10
14	P	501	PC1	C31-C32-C33-C34
14	b	302	PC1	C27-C28-C29-C2A

There are no ring outliers.

32 monomers are involved in 57 short contacts:

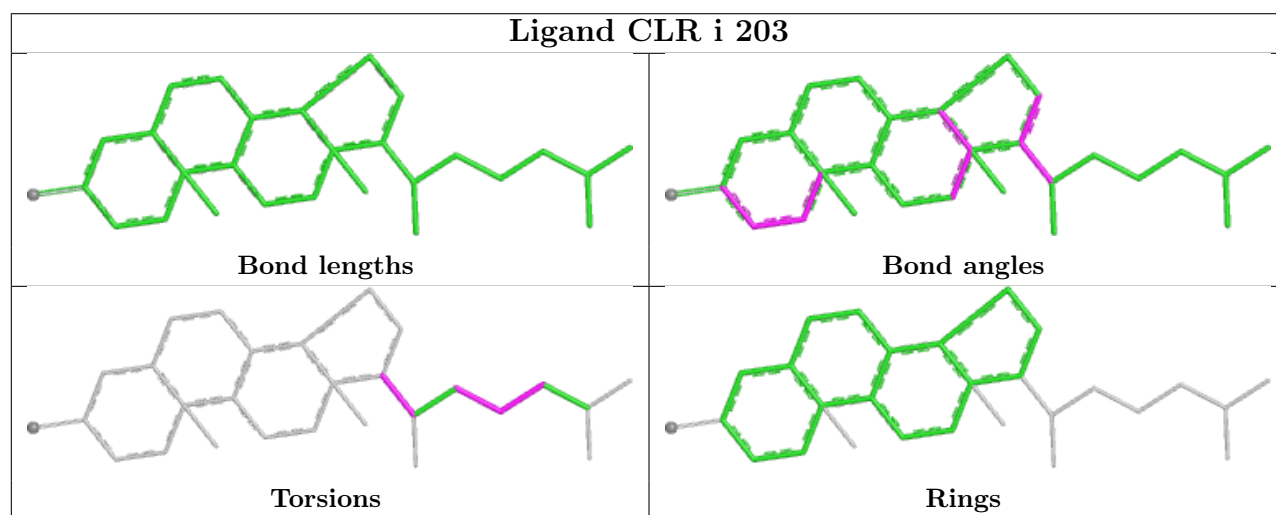
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	i	203	CLR	5	0
19	k	203	CLR	1	0
19	o	203	CLR	1	0
18	e	101	PTY	1	0
19	o	202	CLR	4	0
14	b	302	PC1	1	0
19	b	305	CLR	1	0
14	P	501	PC1	3	0
19	m	203	CLR	1	0
19	j	202	CLR	2	0
19	i	202	CLR	2	0
19	h	202	CLR	2	0
19	o	201	CLR	1	0
15	a	901	WJP	2	0
19	n	201	CLR	3	0
19	m	201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

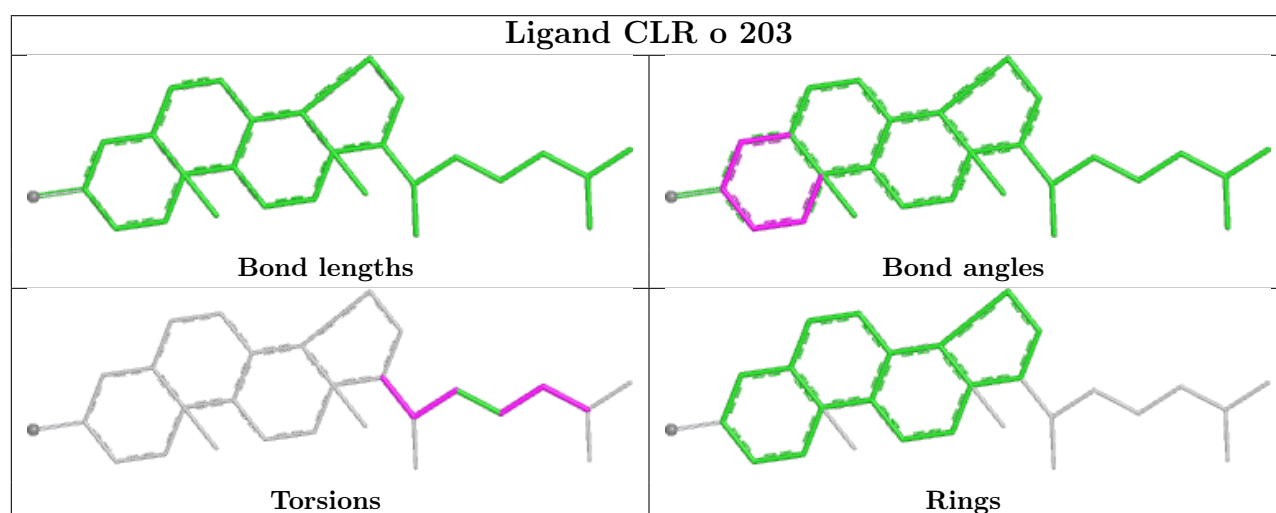
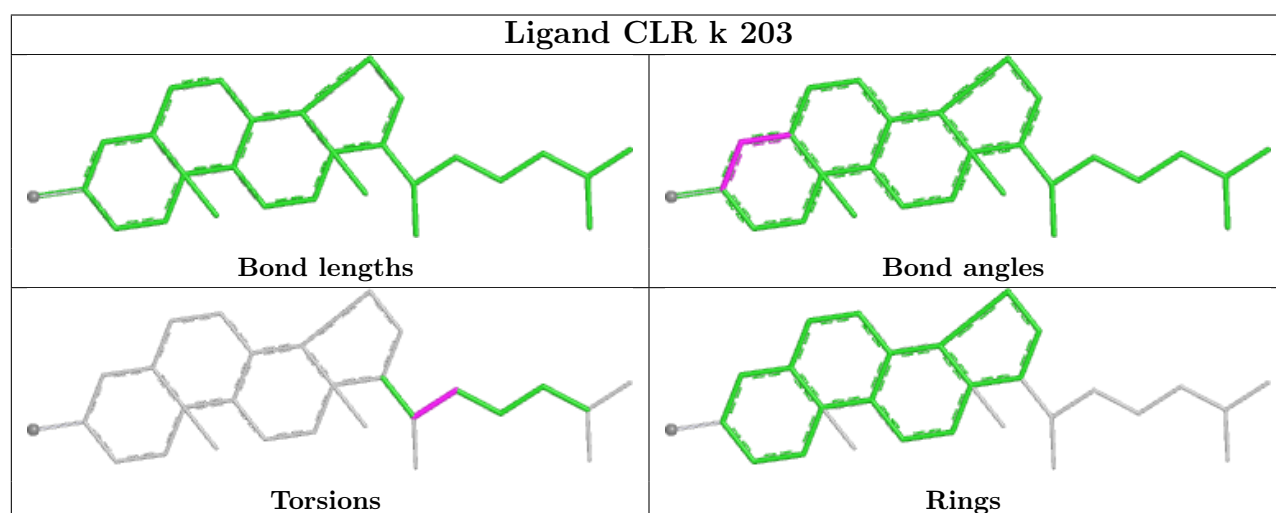
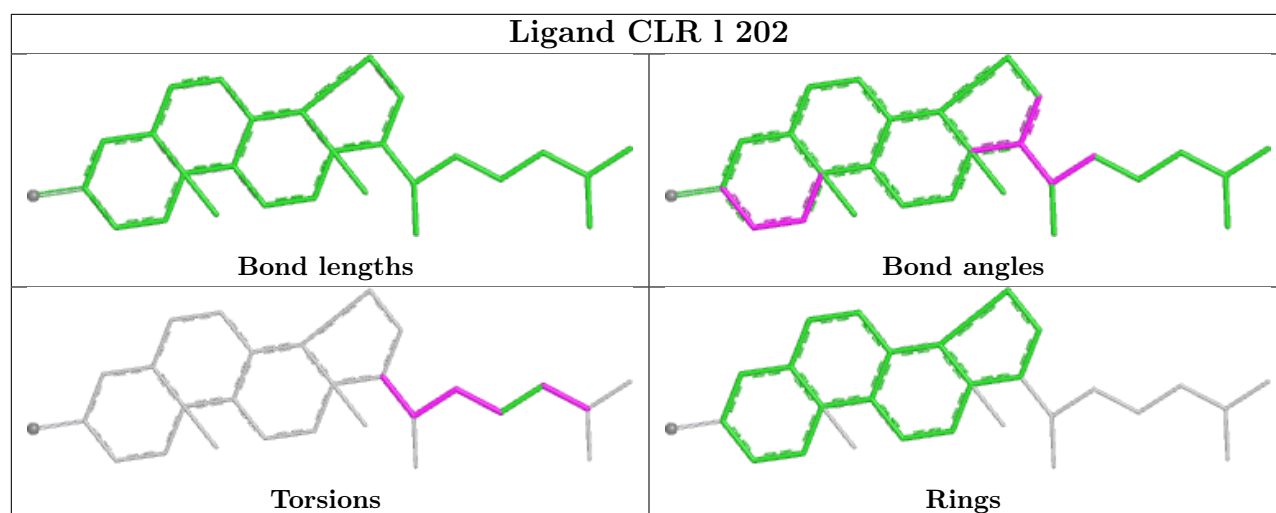
Continued on next page...

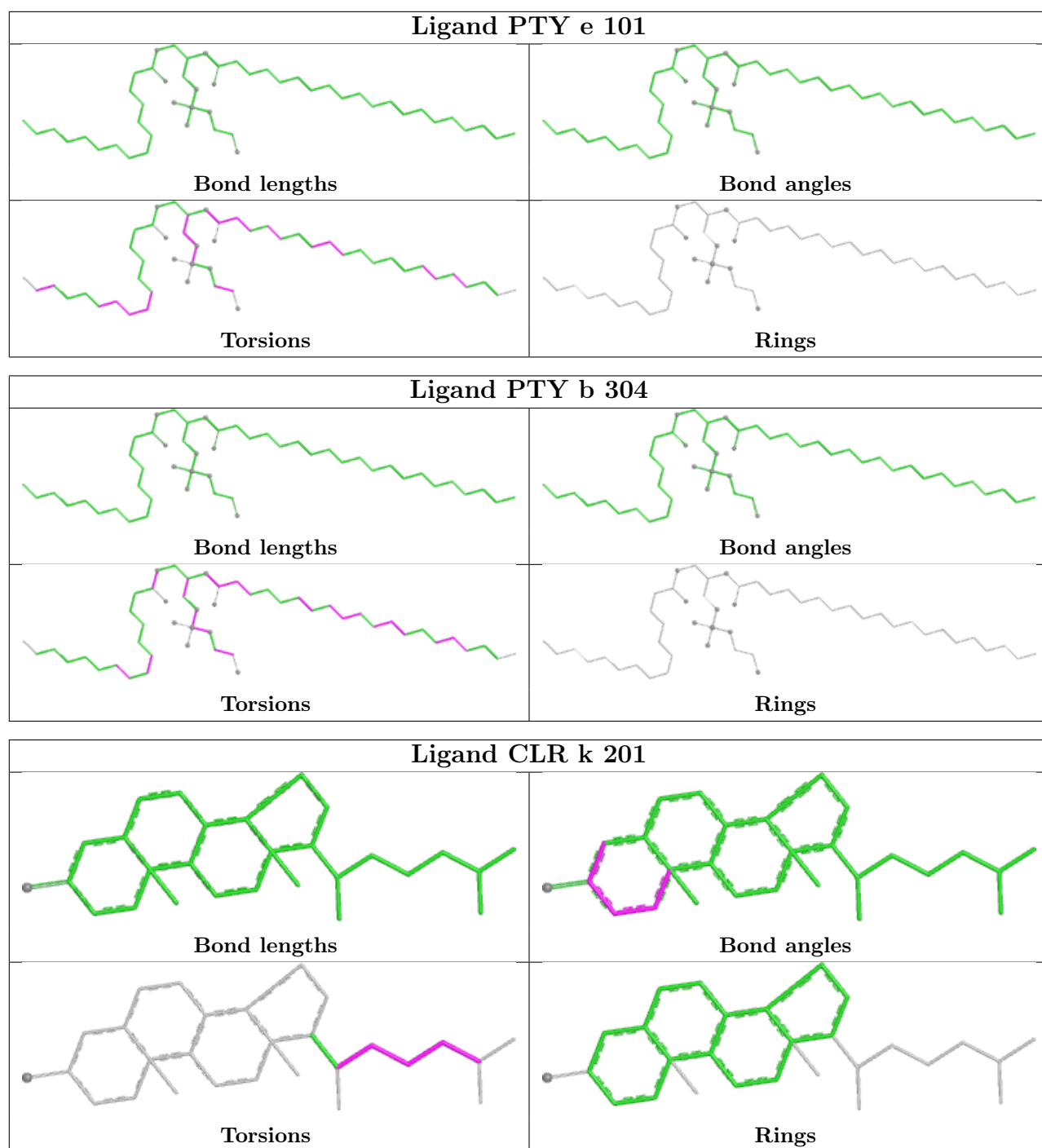
Continued from previous page...

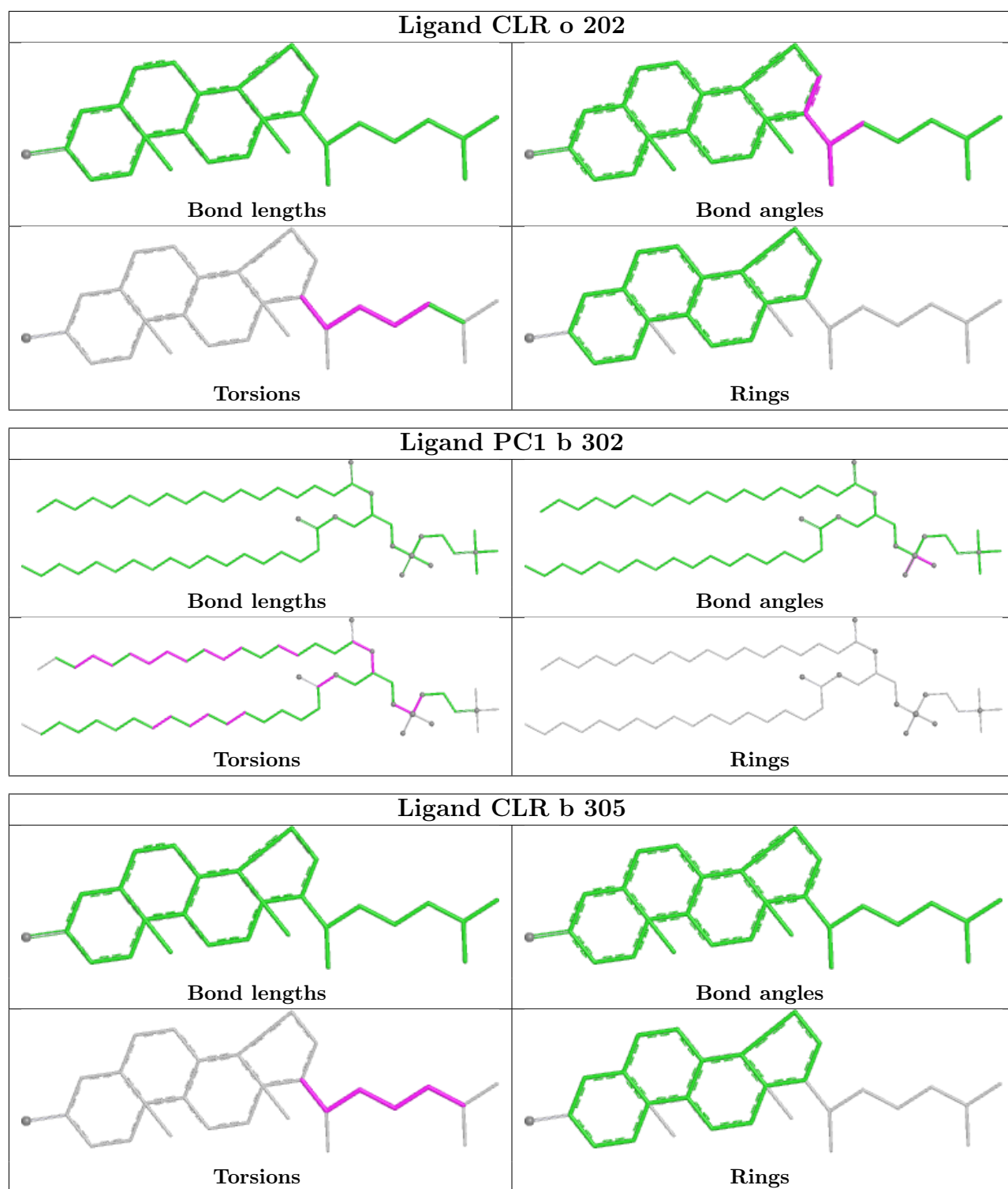
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	h	201	CLR	3	0
19	l	204	CLR	2	0
19	i	201	CLR	3	0
19	j	204	CLR	2	0
18	a	906	PTY	1	0
19	n	204	CLR	6	0
19	j	203	CLR	2	0
19	n	202	CLR	2	0
18	b	303	PTY	1	0
19	l	203	CLR	4	0
19	j	205	CLR	1	0
14	b	301	PC1	1	0
19	k	202	CLR	2	0

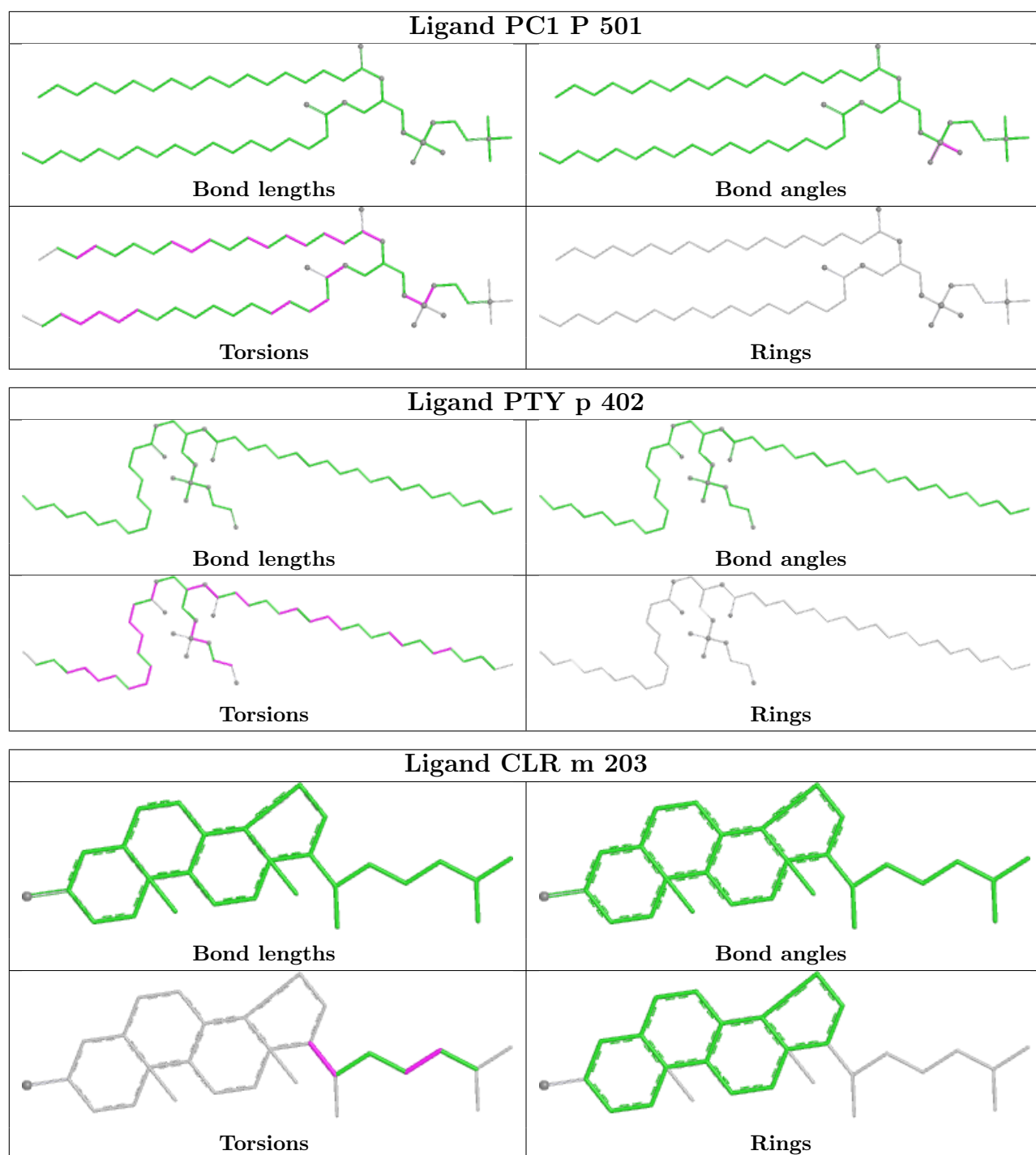
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

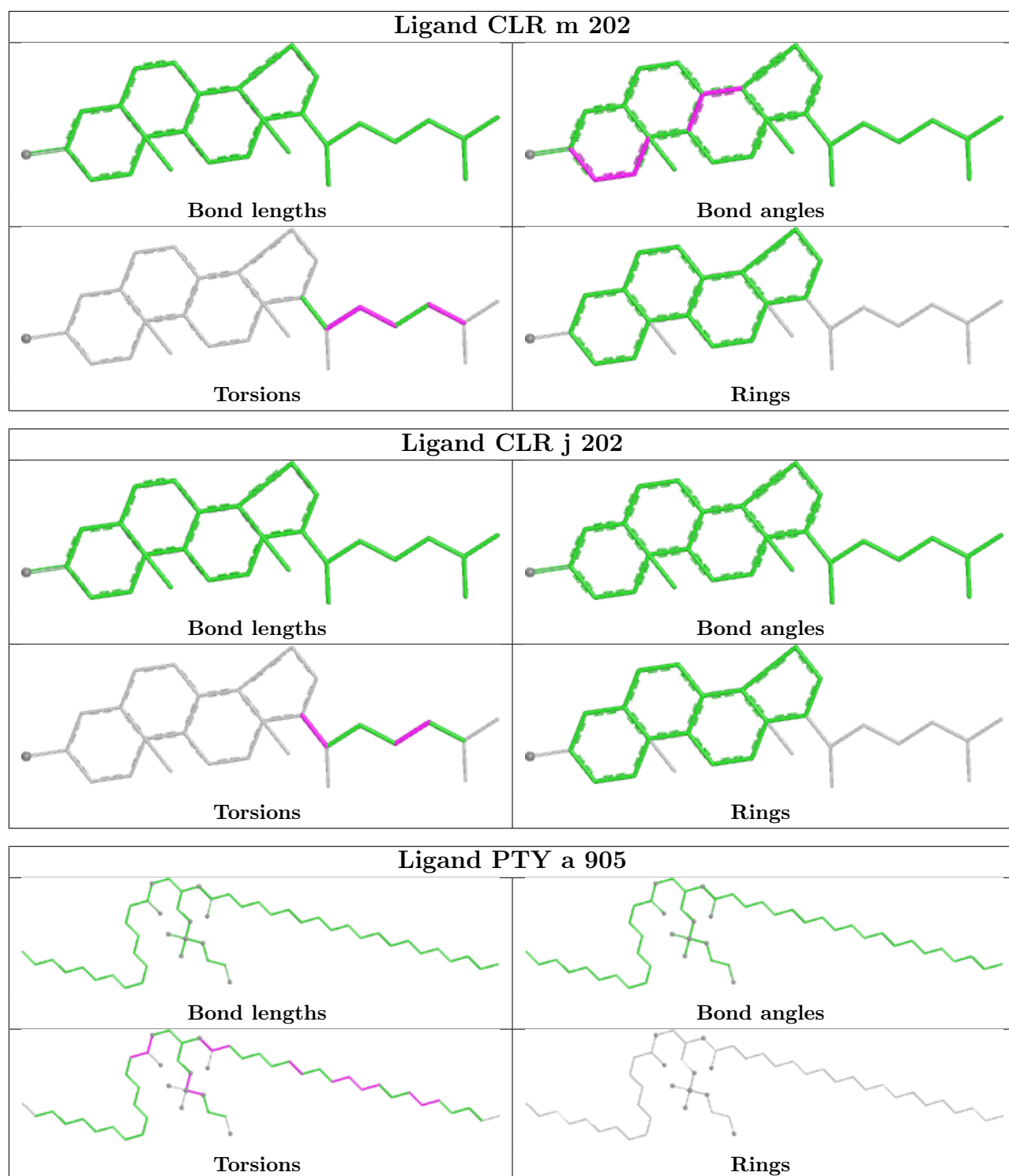


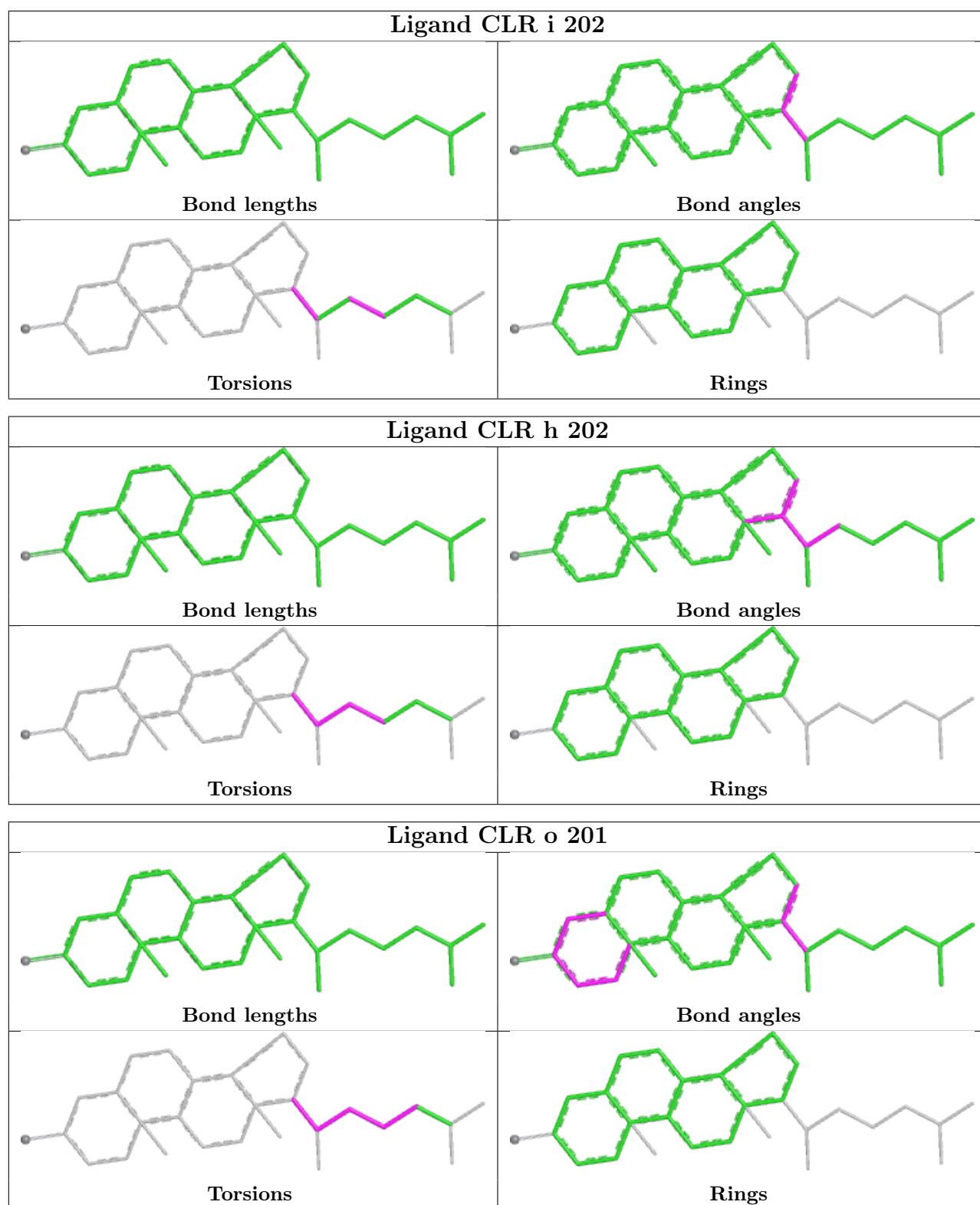


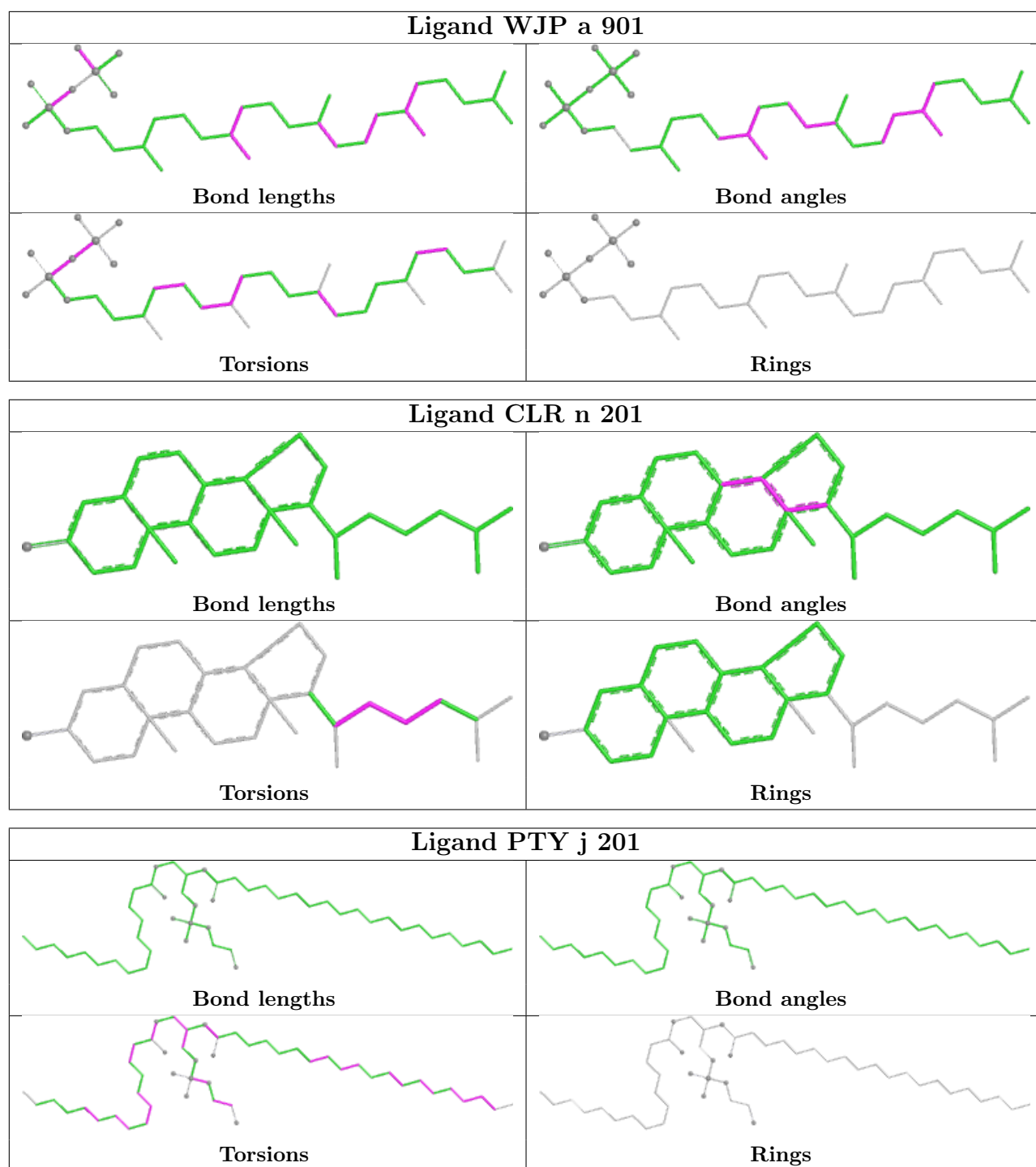


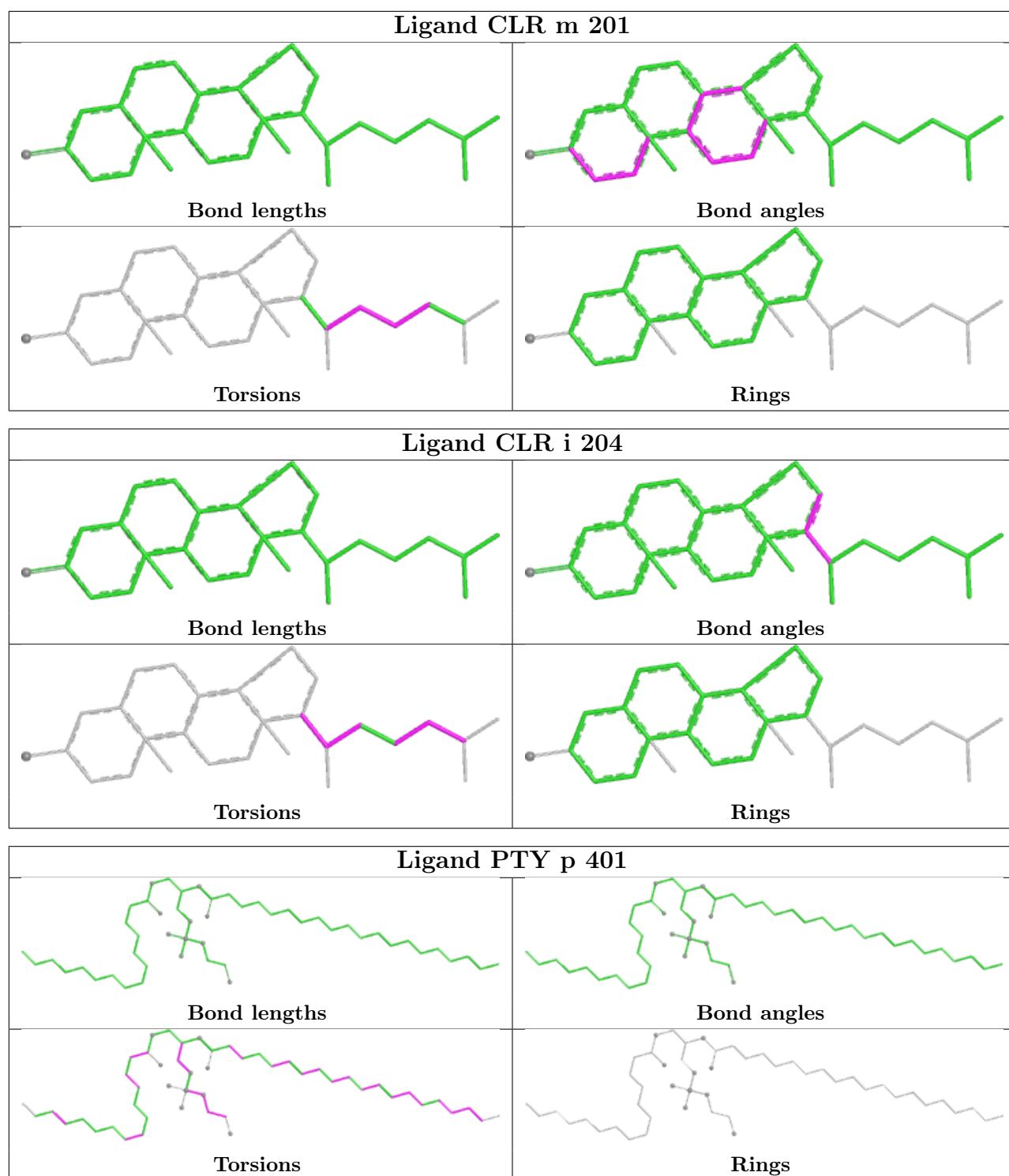


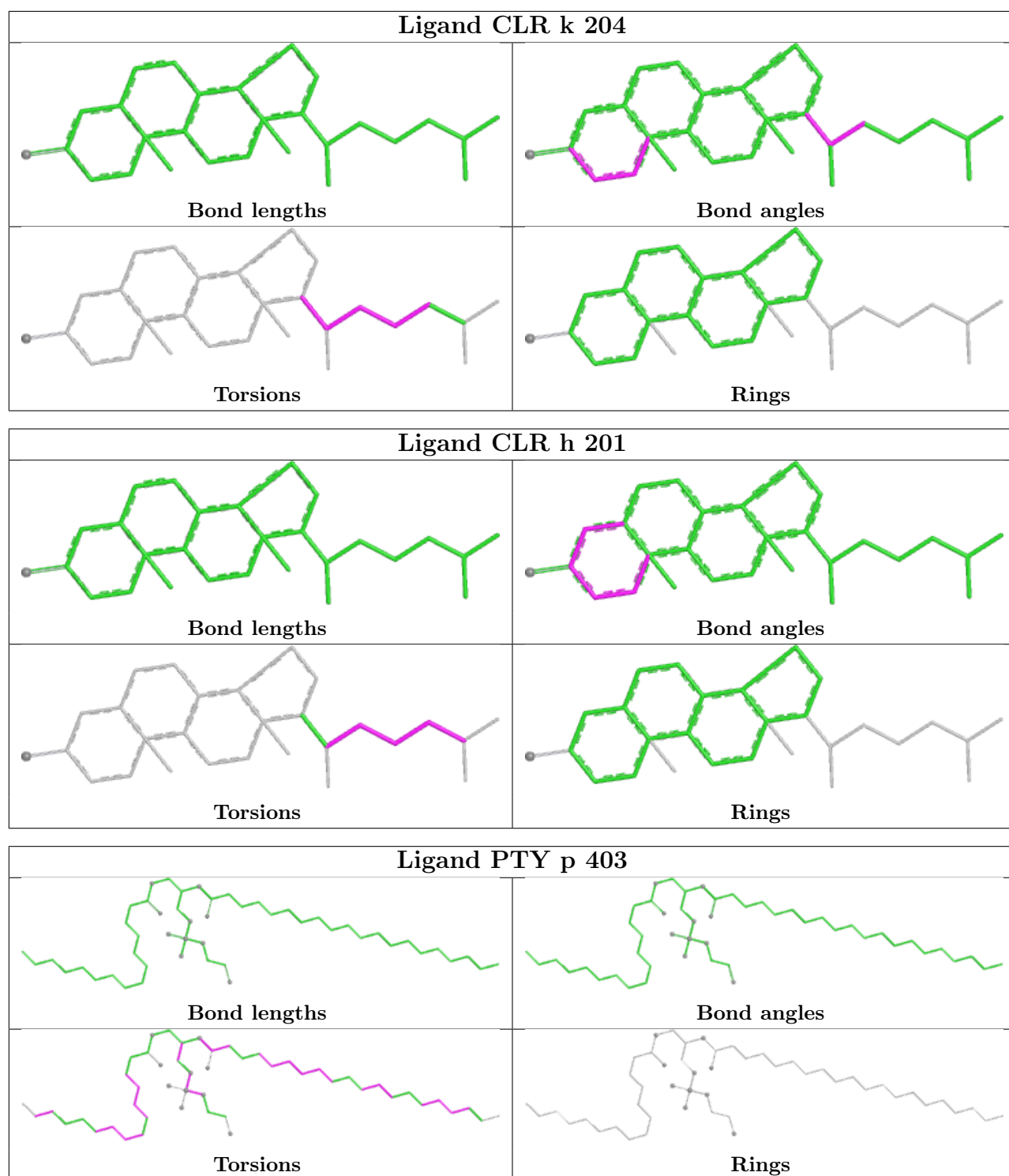


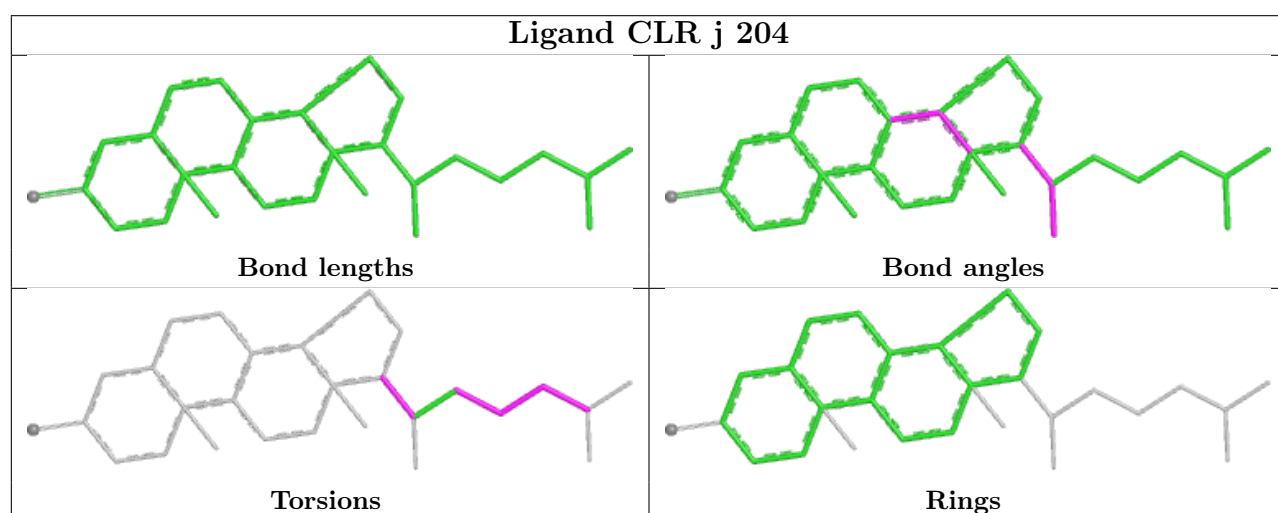
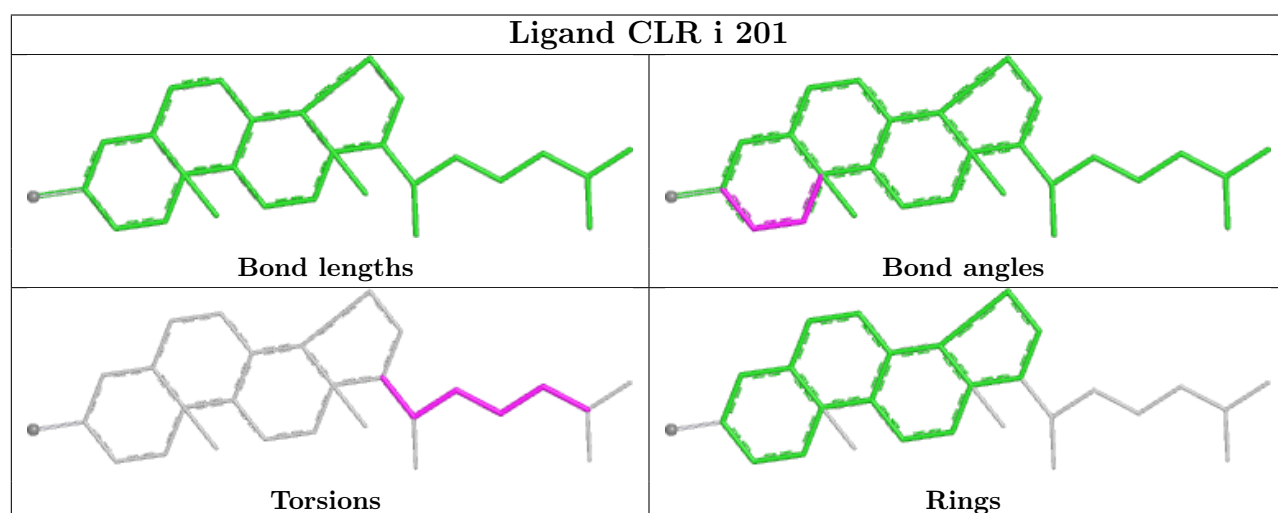
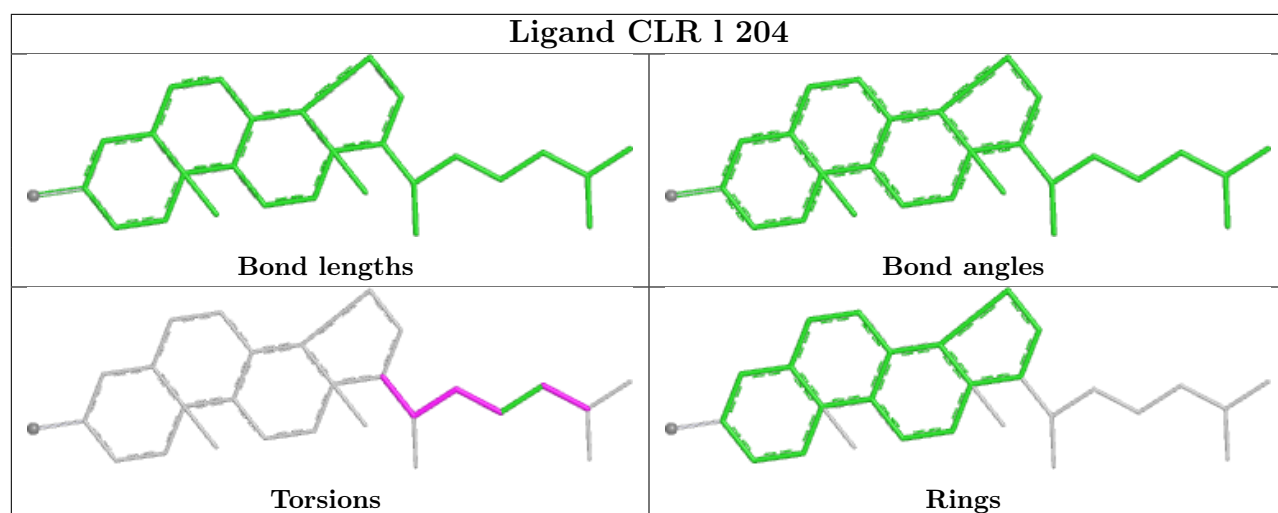


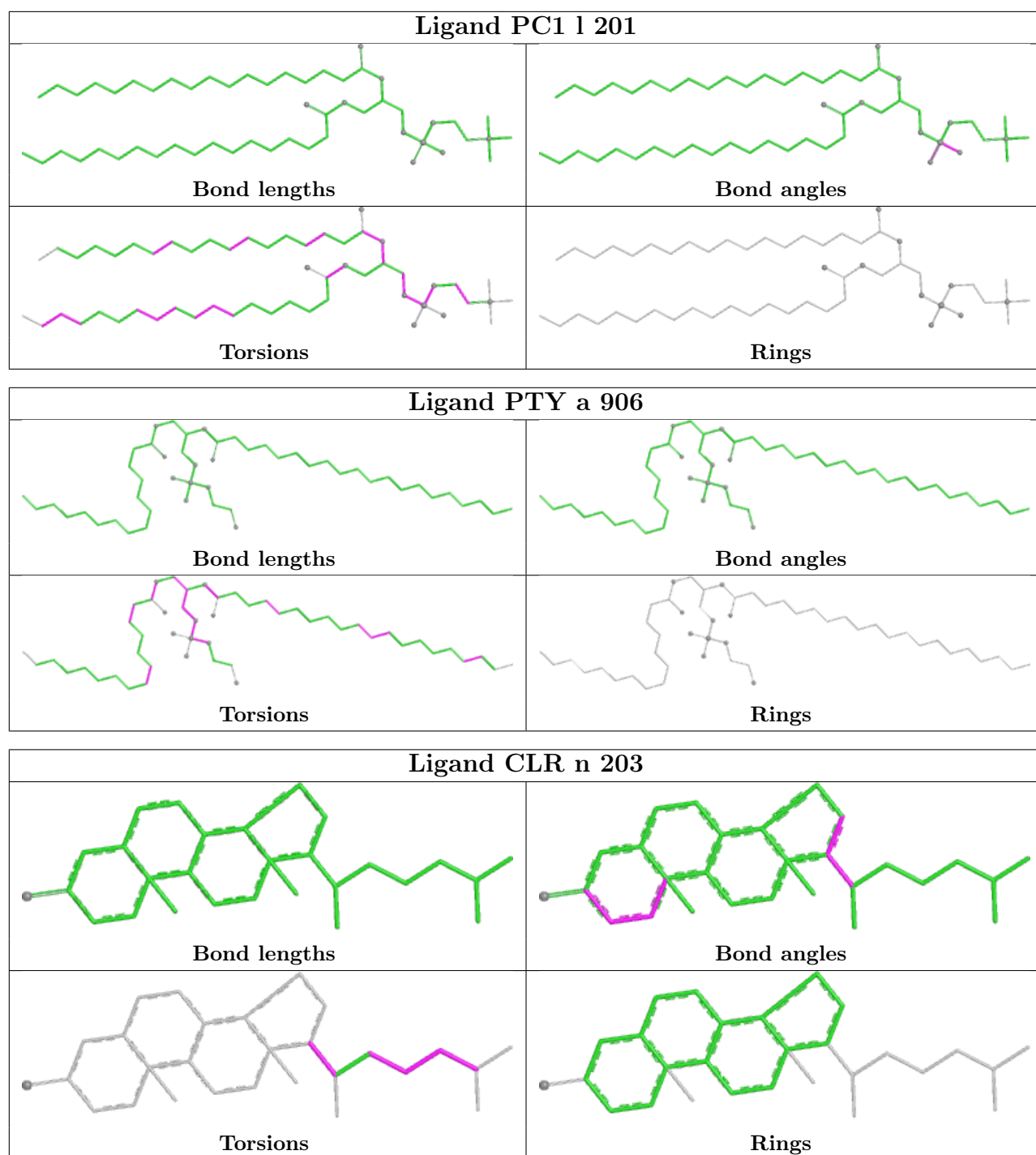


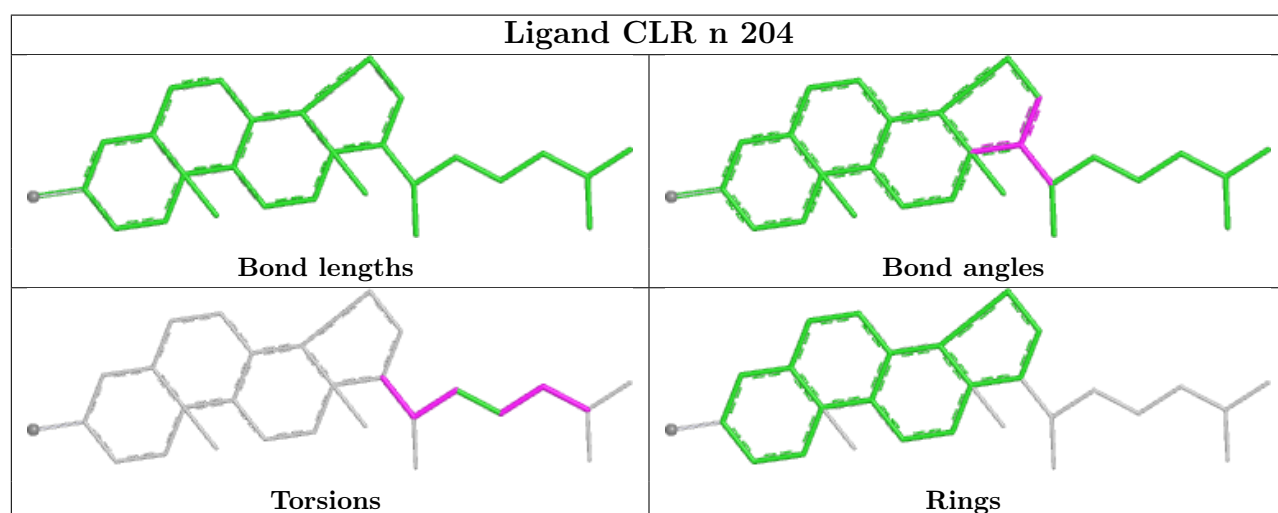
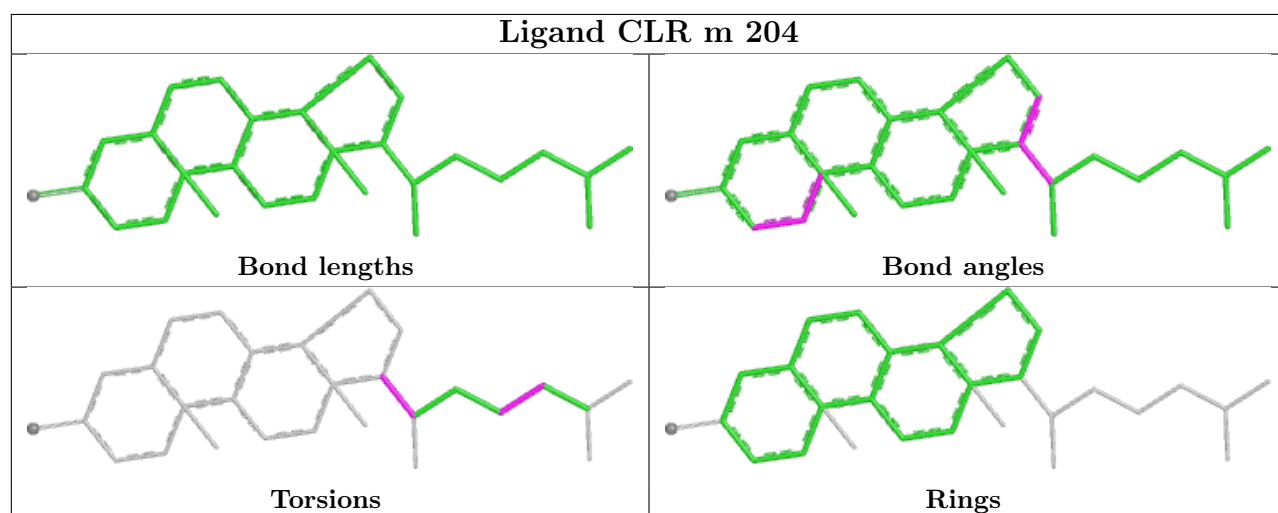
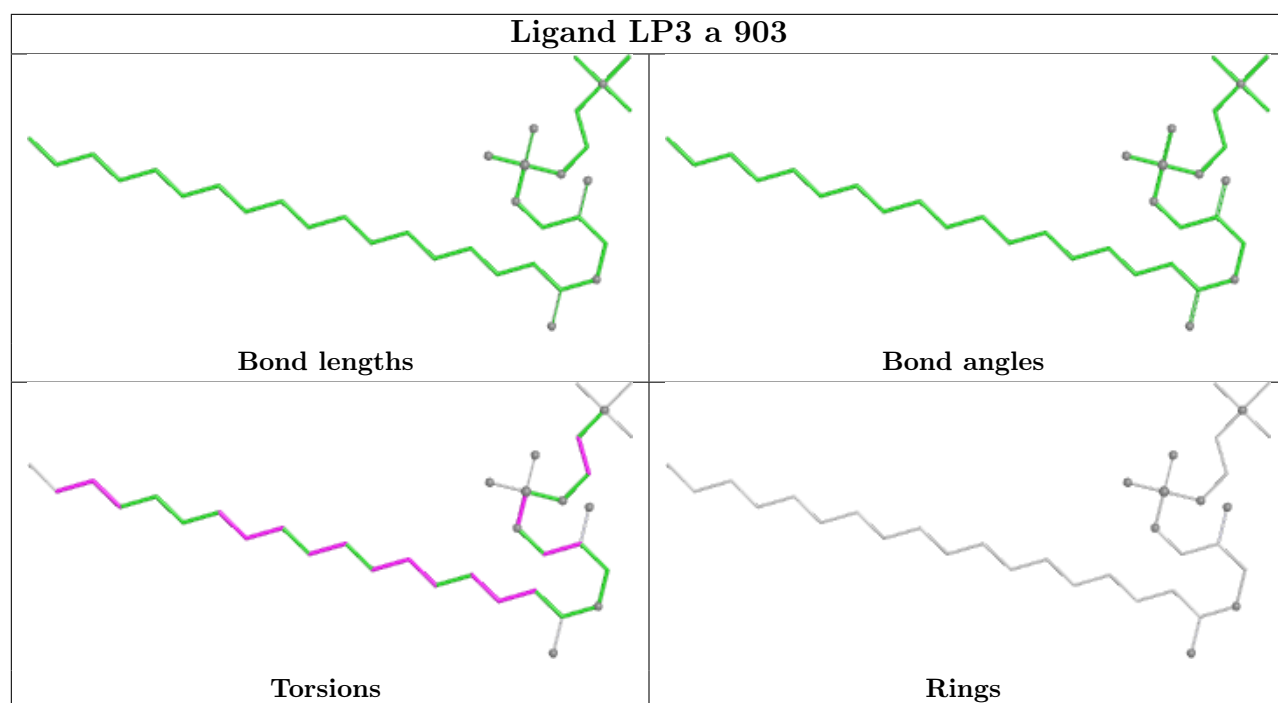


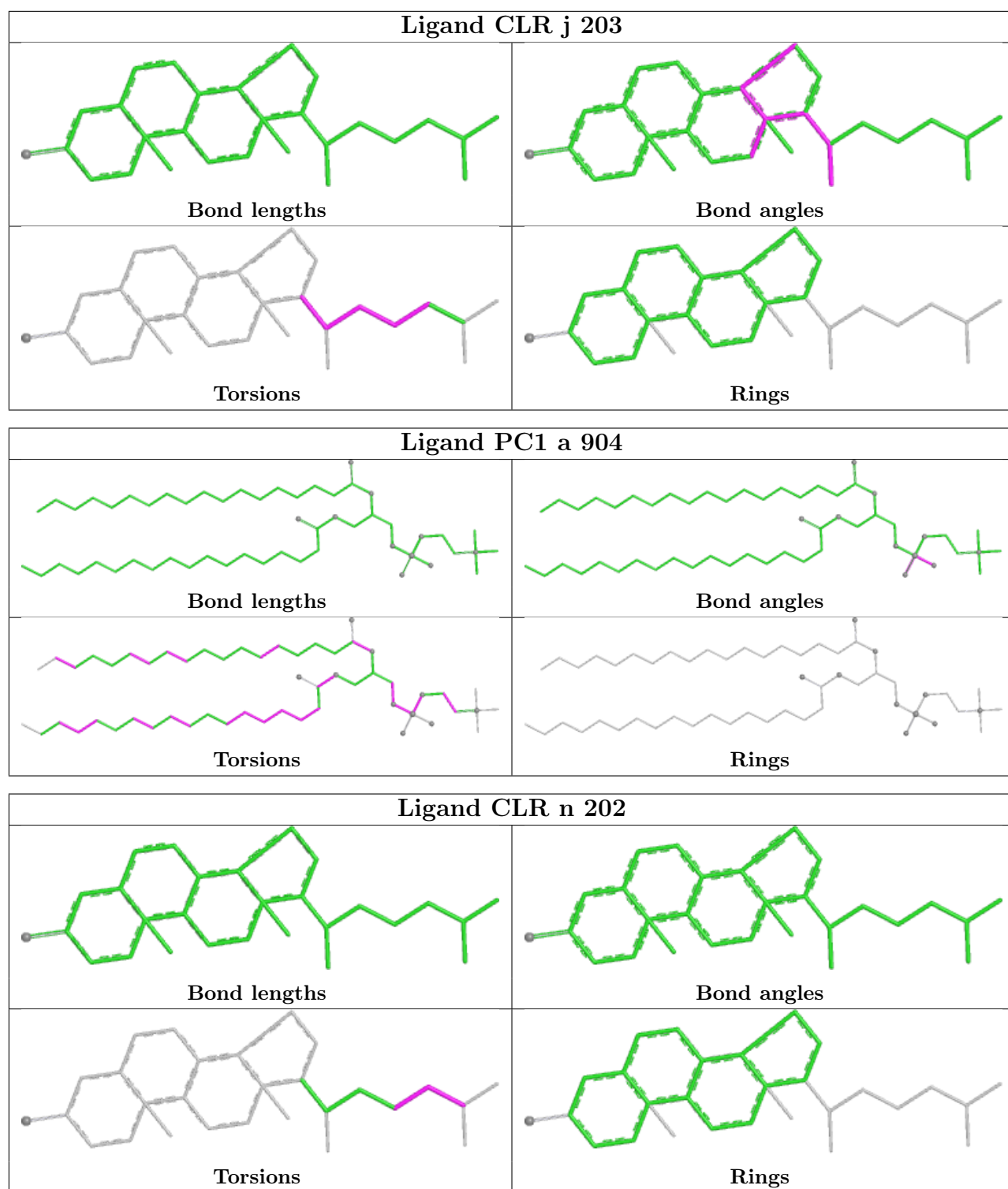


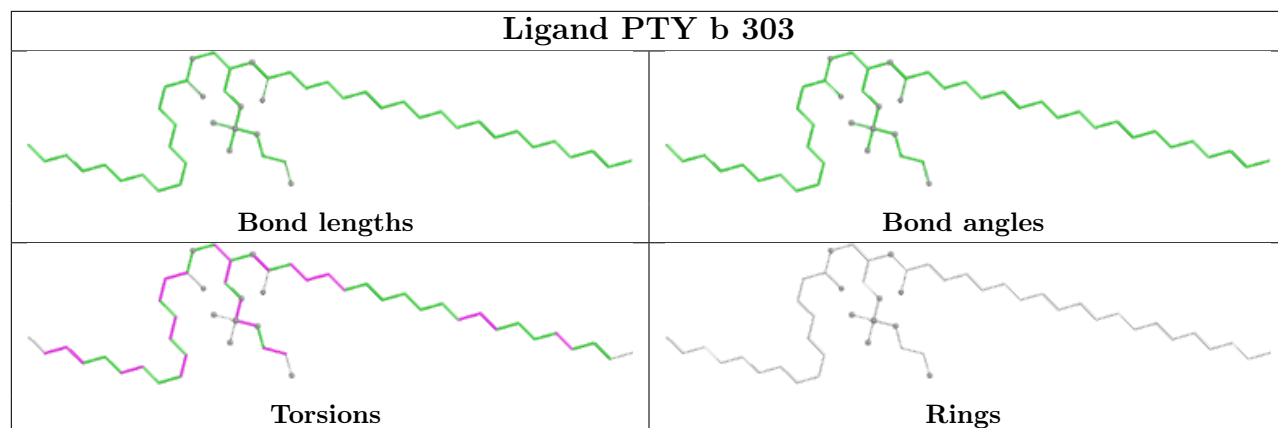
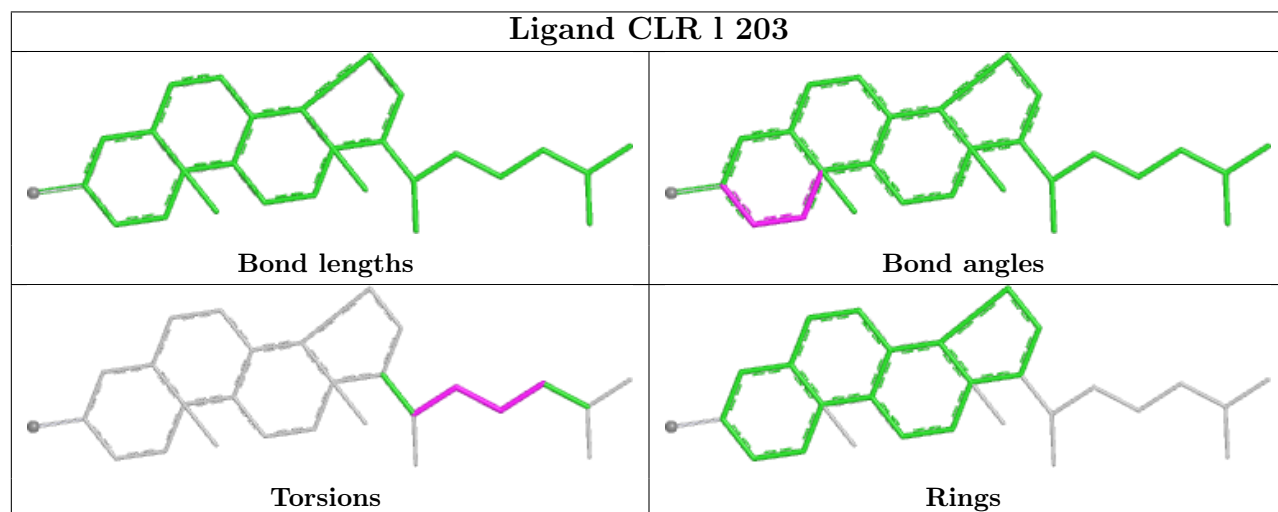
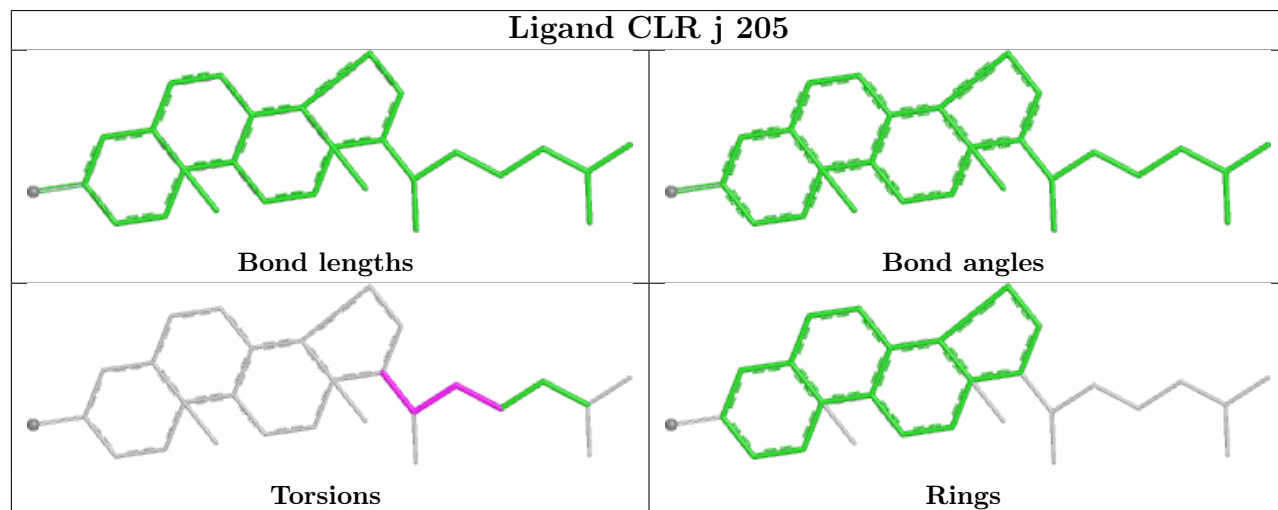


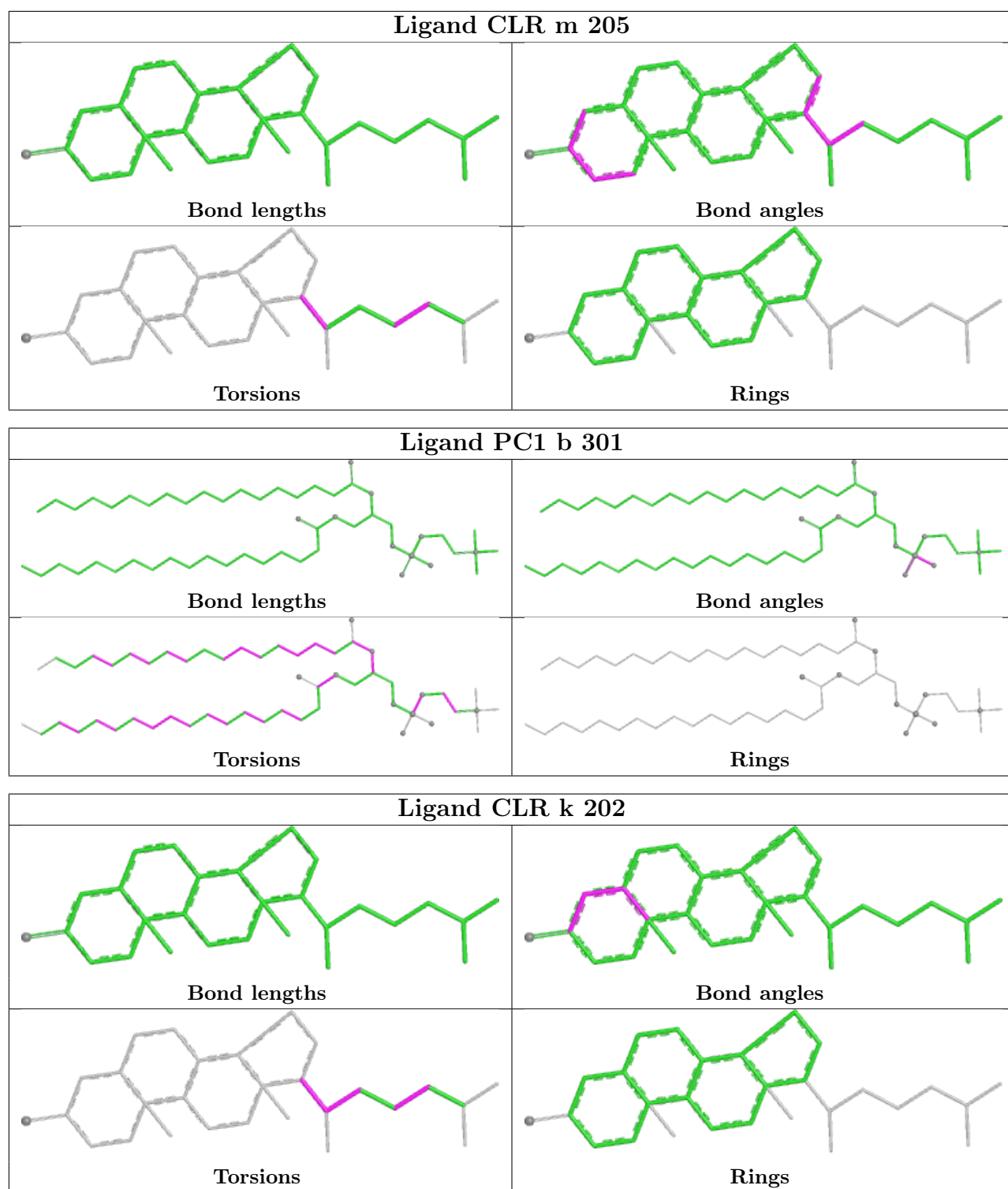








Ligand PTY b 303**Ligand CLR l 203****Ligand CLR j 205**



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

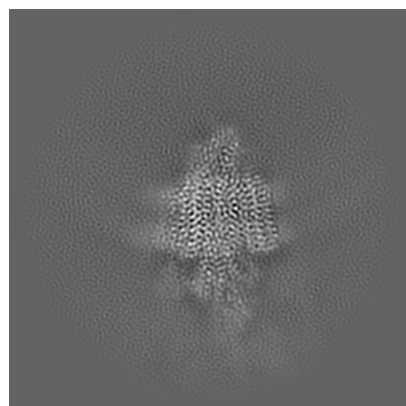
6 Map visualisation [i](#)

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

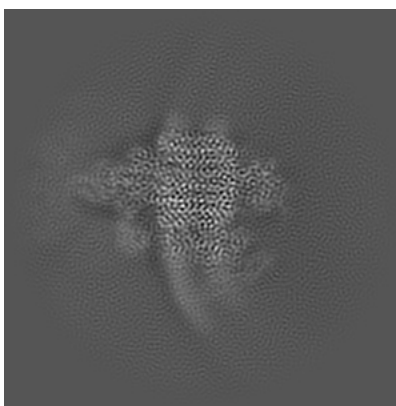
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

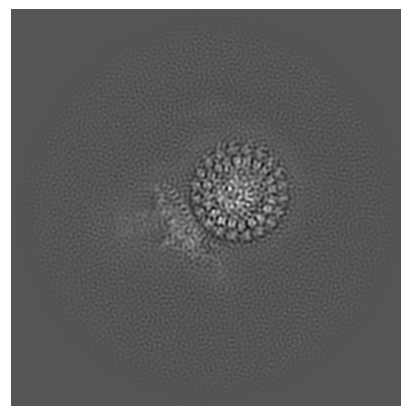
6.1.1 Primary map



X

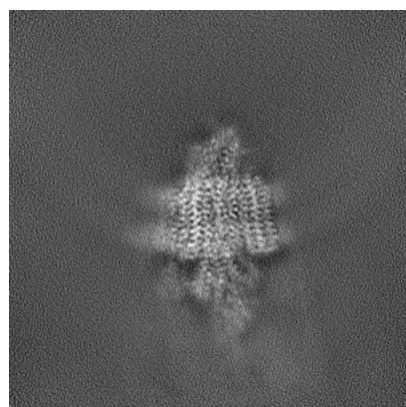


Y

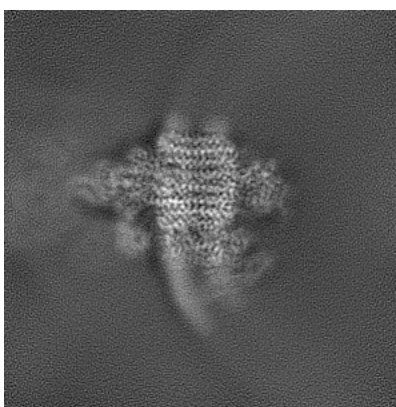


Z

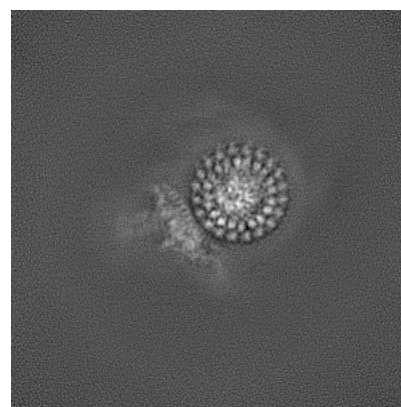
6.1.2 Raw map



X



Y

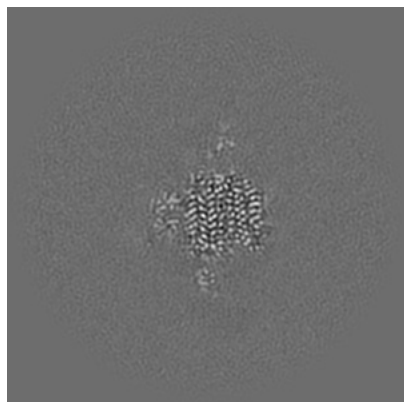


Z

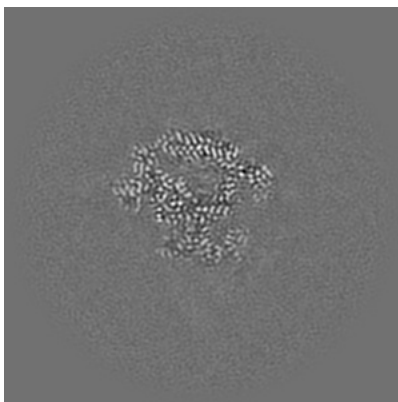
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

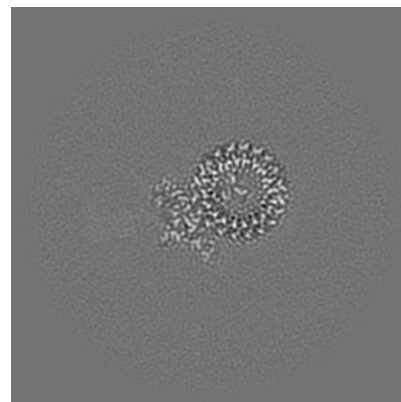
6.2.1 Primary map



X Index: 150

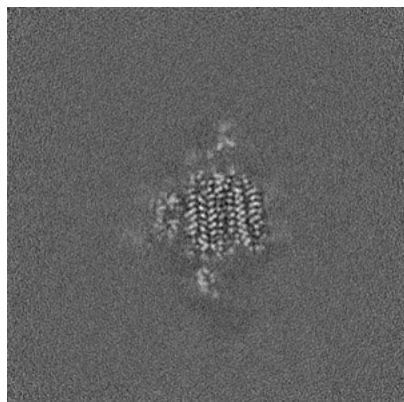


Y Index: 150

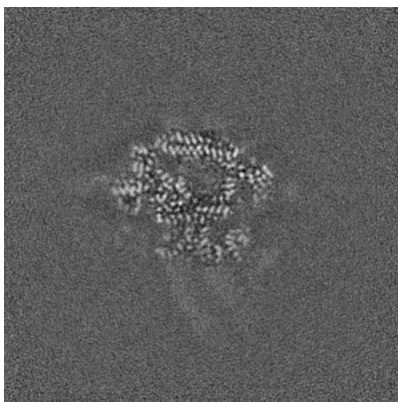


Z Index: 150

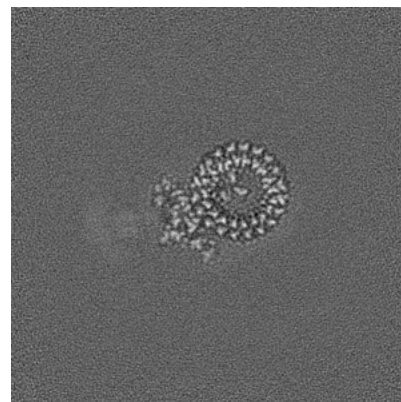
6.2.2 Raw map



X Index: 150



Y Index: 150

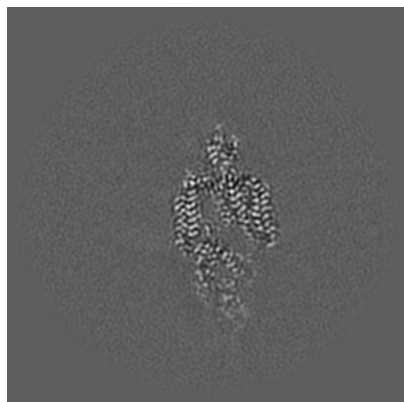


Z Index: 150

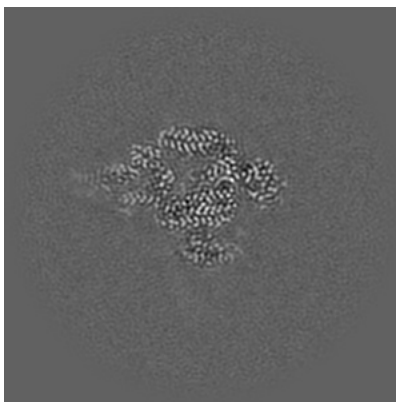
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

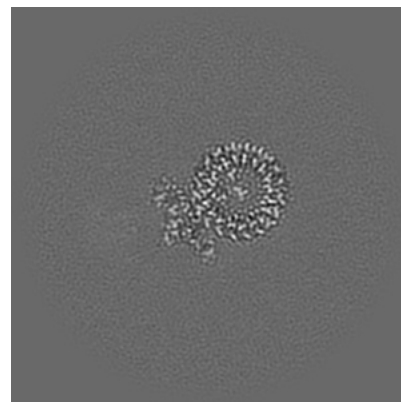
6.3.1 Primary map



X Index: 167

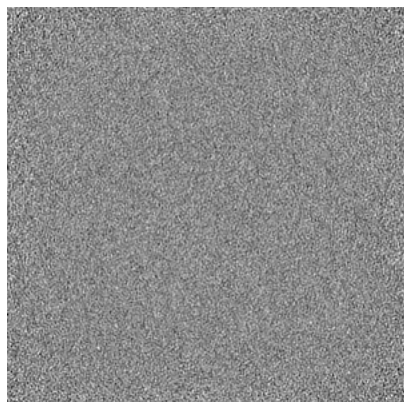


Y Index: 158

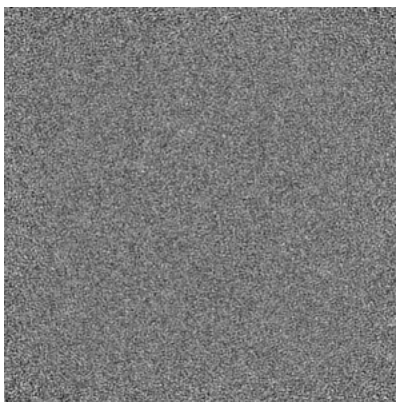


Z Index: 149

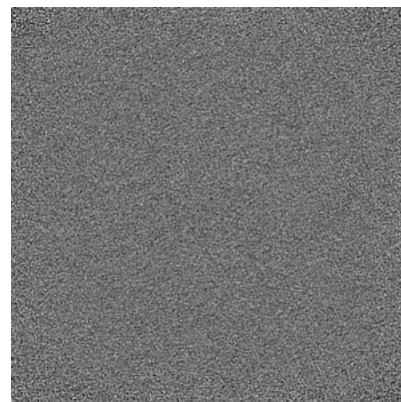
6.3.2 Raw map



X Index: 0



Y Index: 0

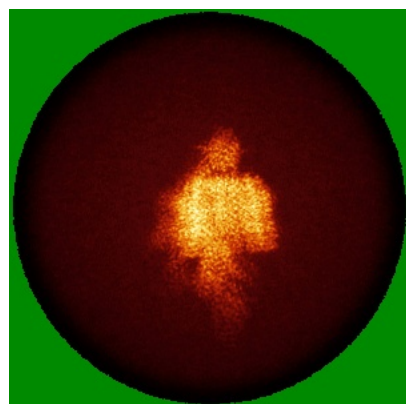


Z Index: 0

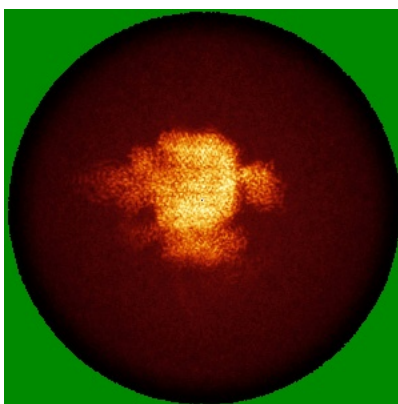
The images above show the largest variance slices of the map in three orthogonal directions.

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

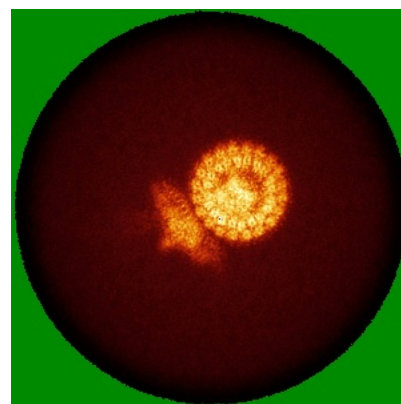
6.4.1 Primary map



X

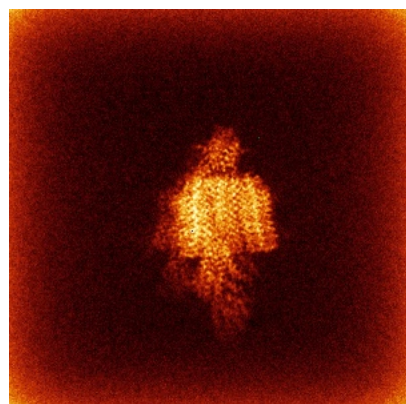


Y

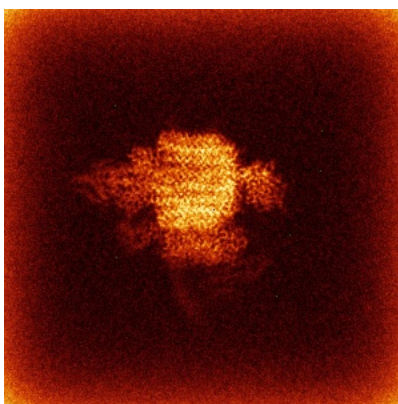


Z

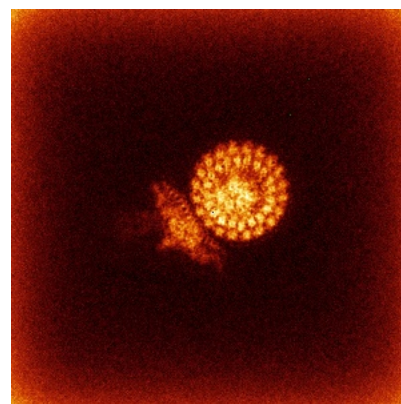
6.4.2 Raw map



X



Y

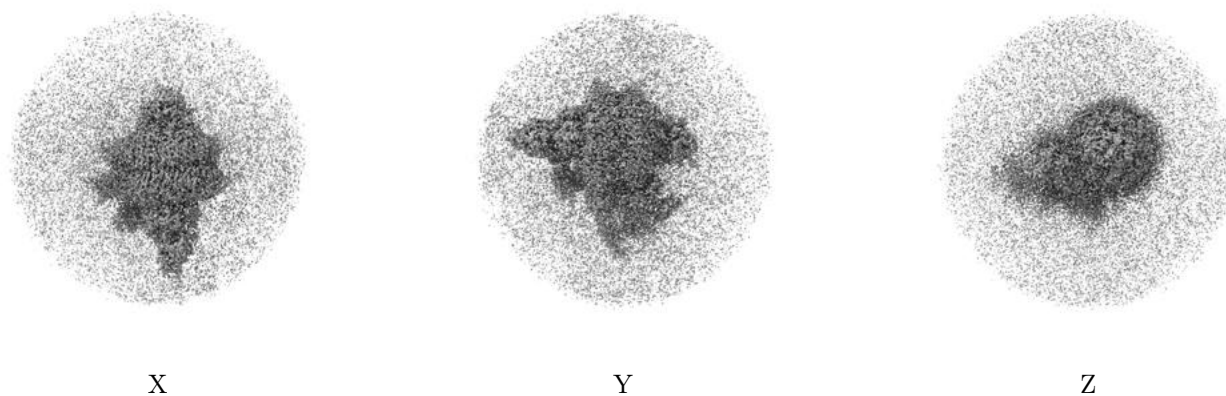


Z

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

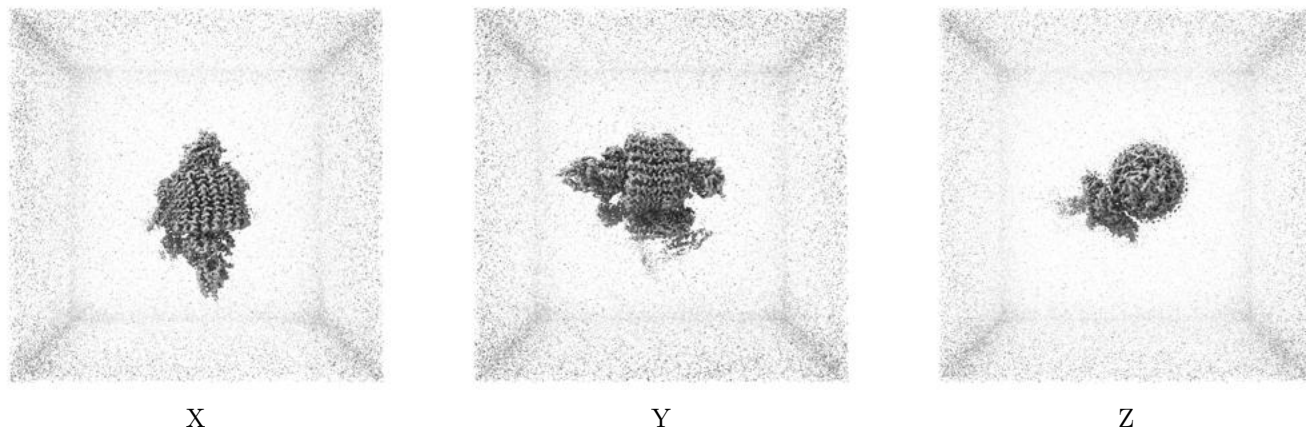
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

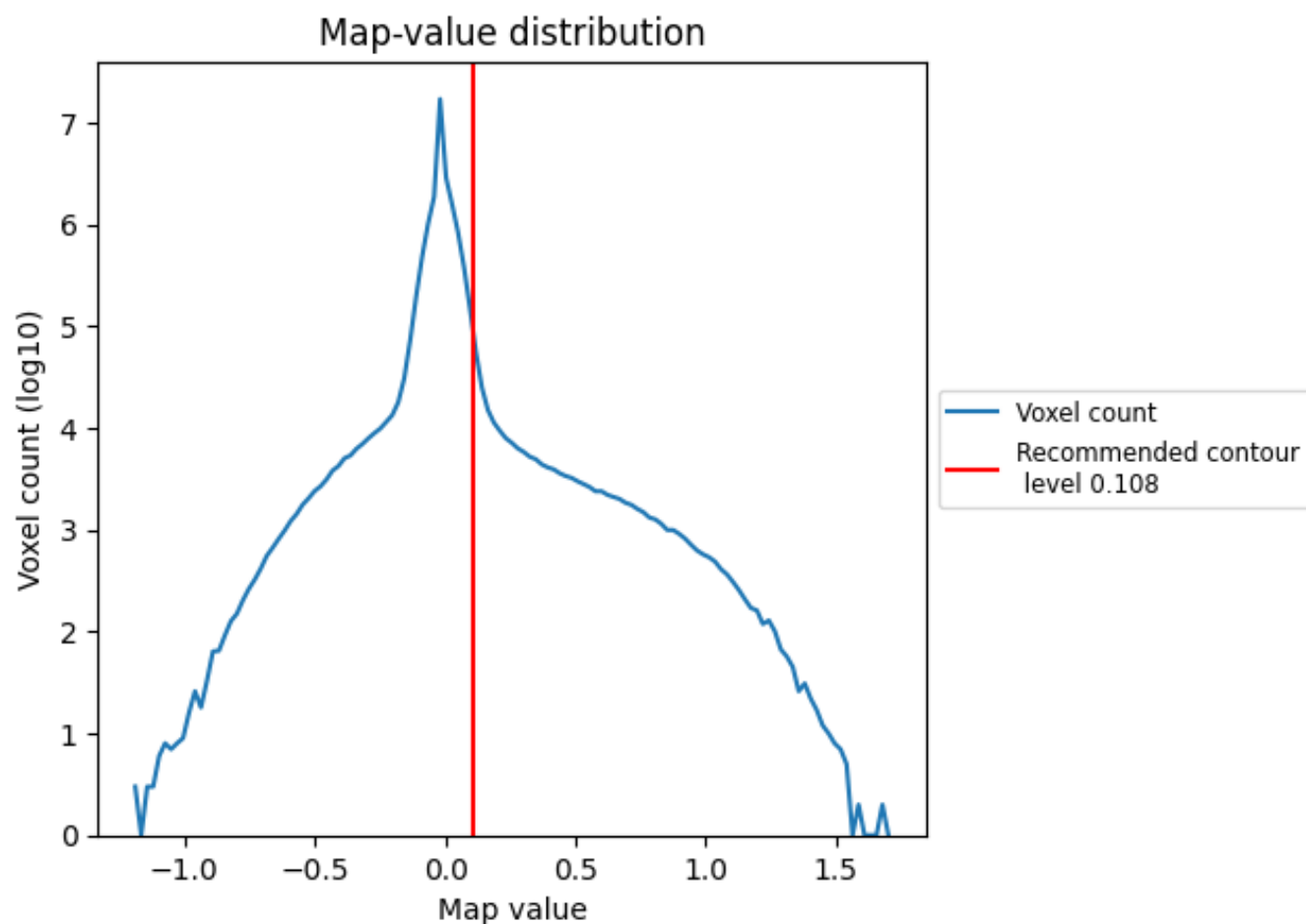
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

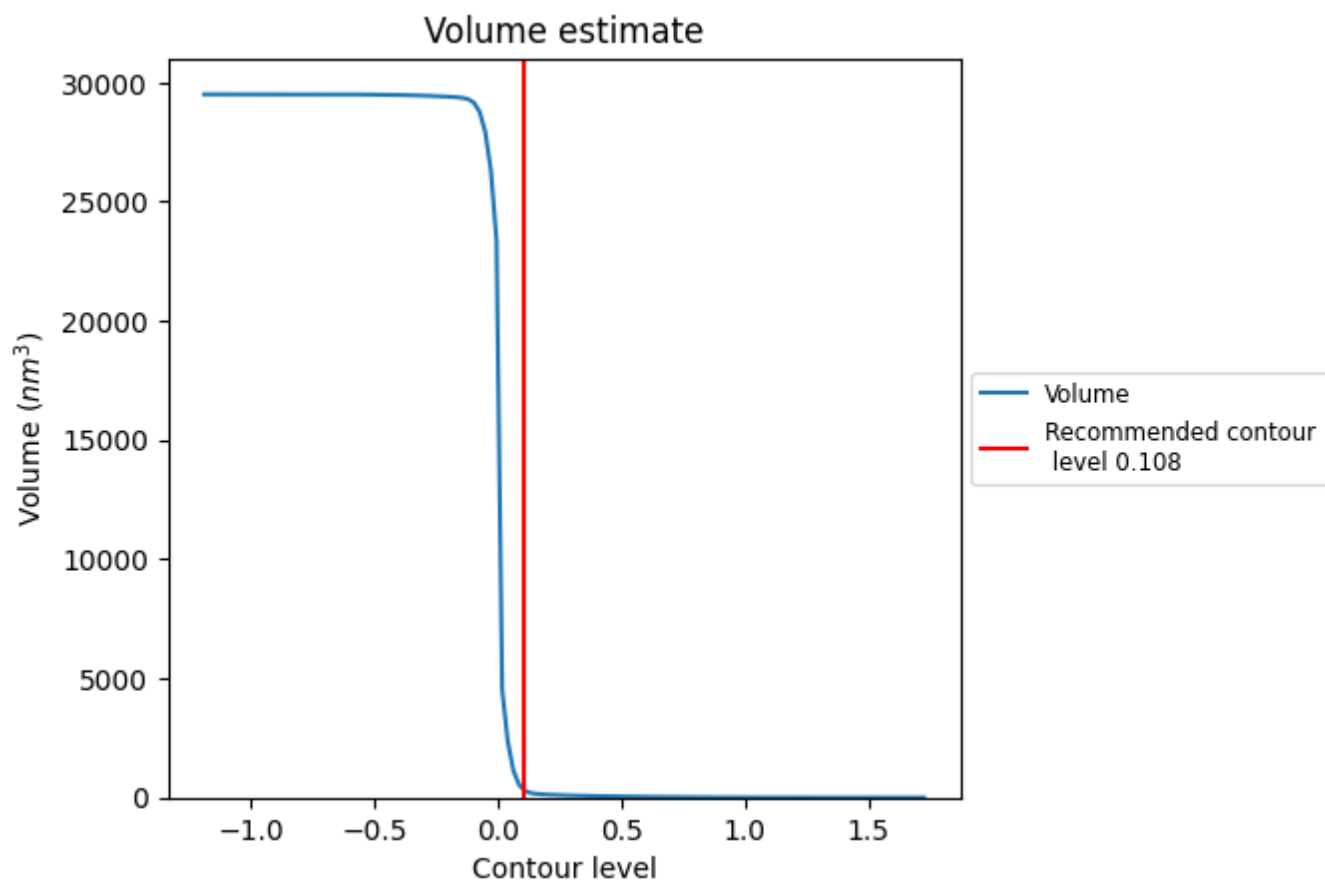
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

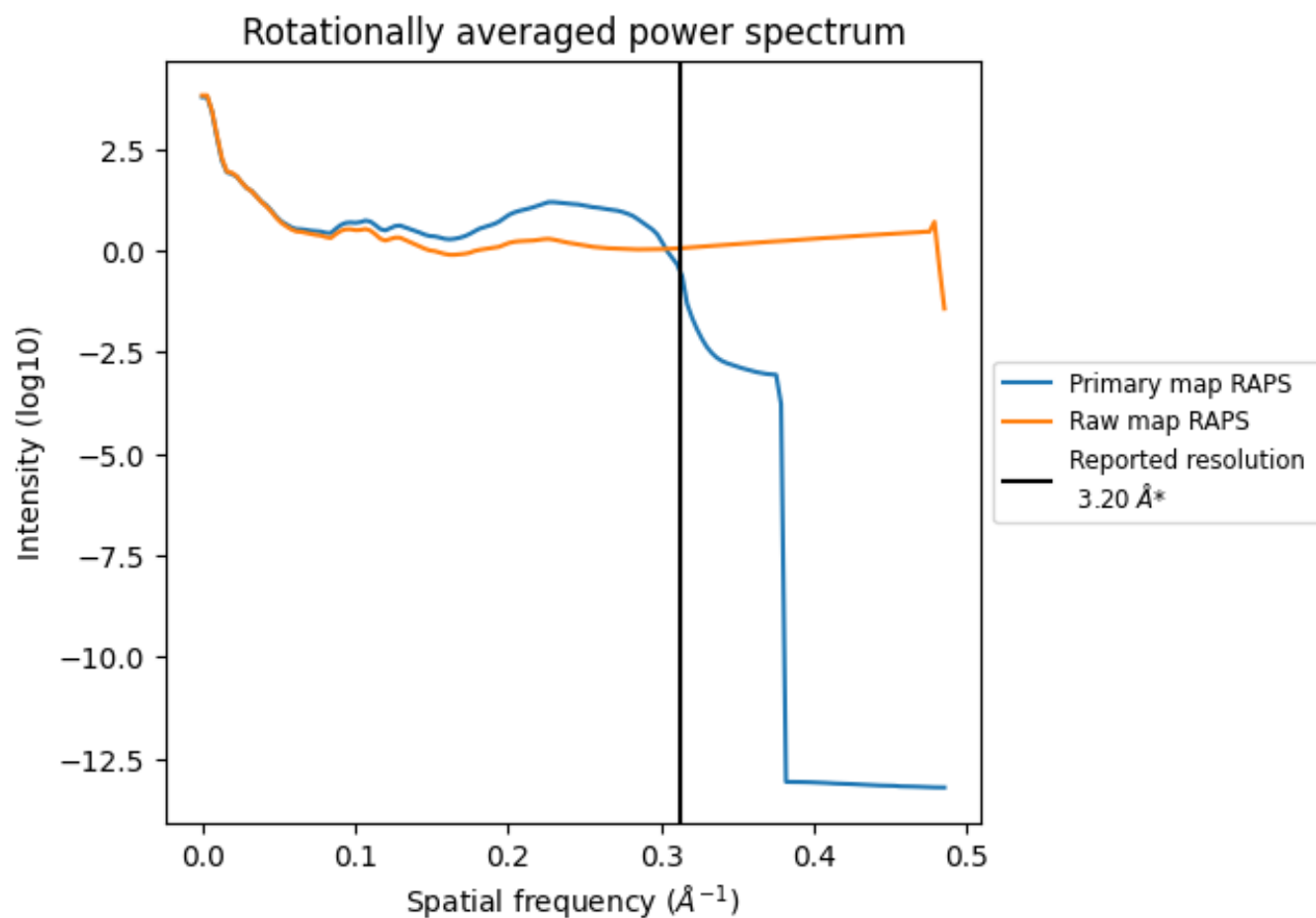
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

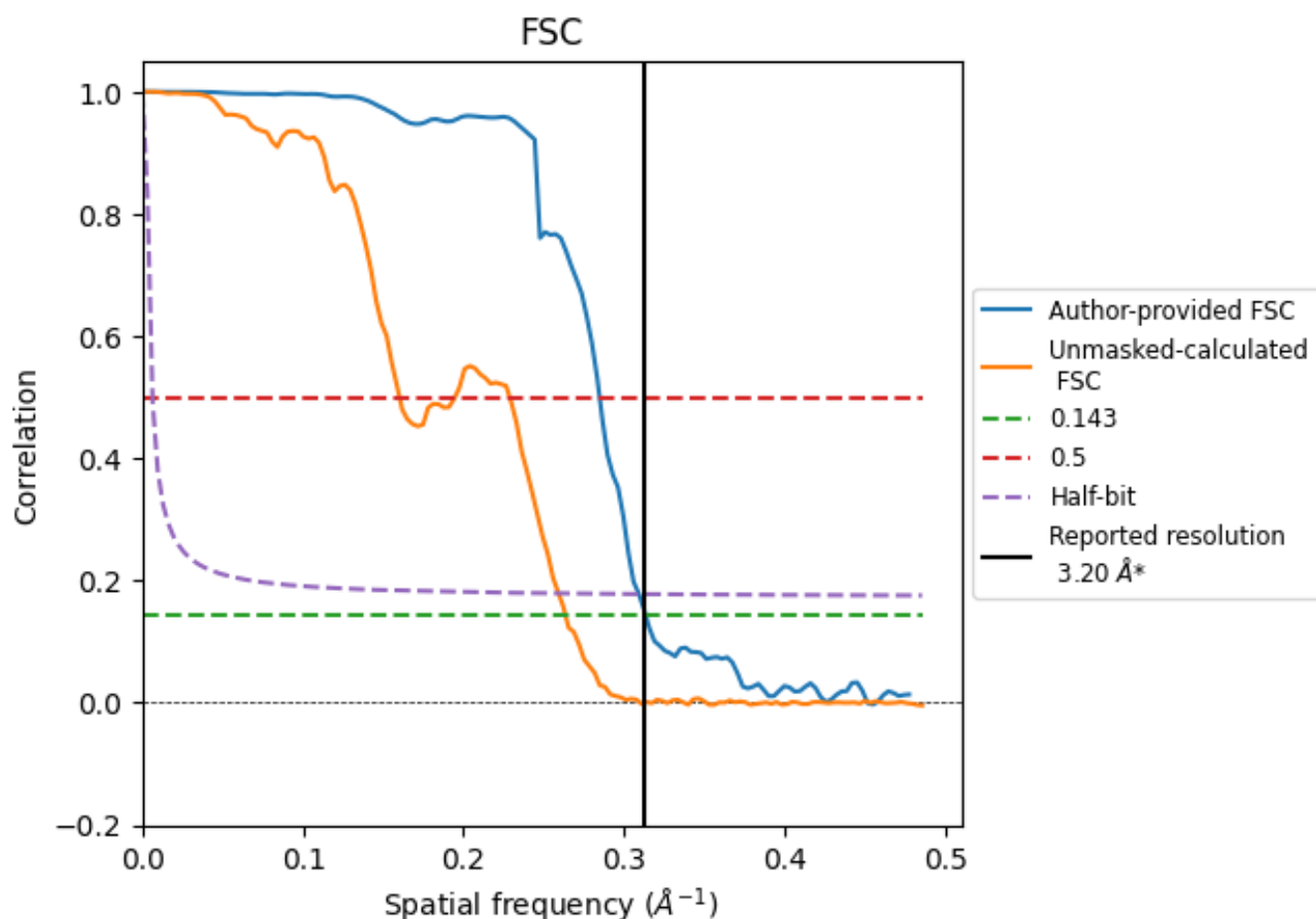


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

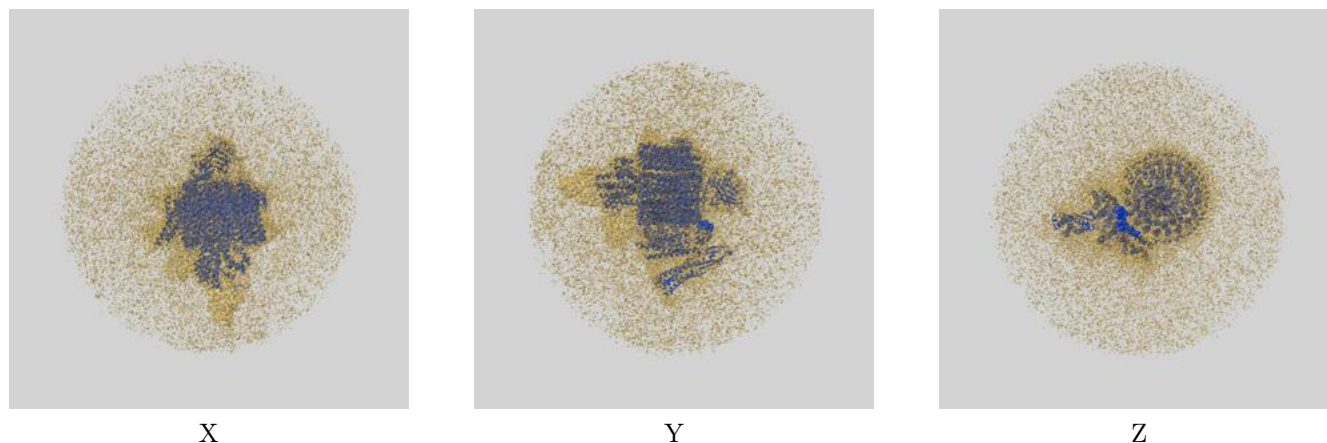
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.51	3.24
Unmasked-calculated*	3.80	6.25	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

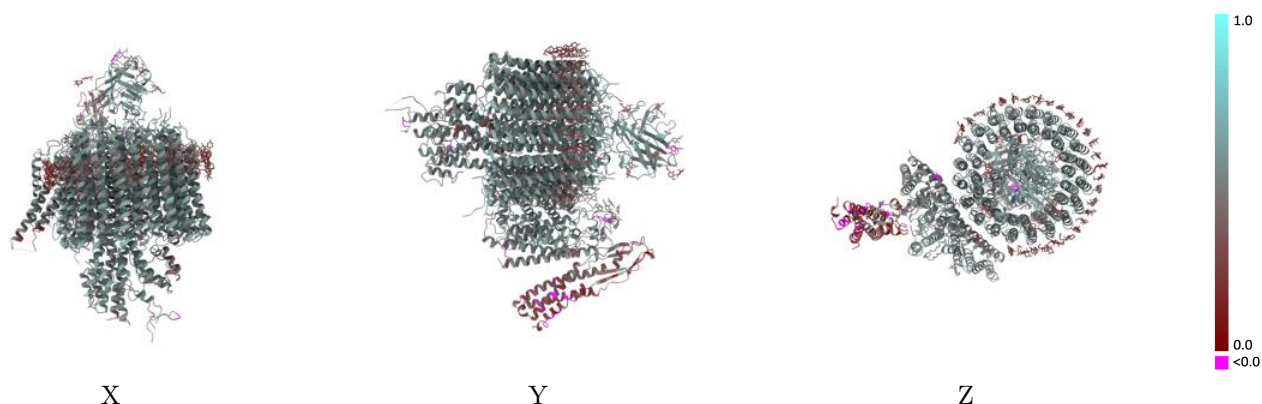
This section contains information regarding the fit between EMDB map EMD-44350 and PDB model 9B8O. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



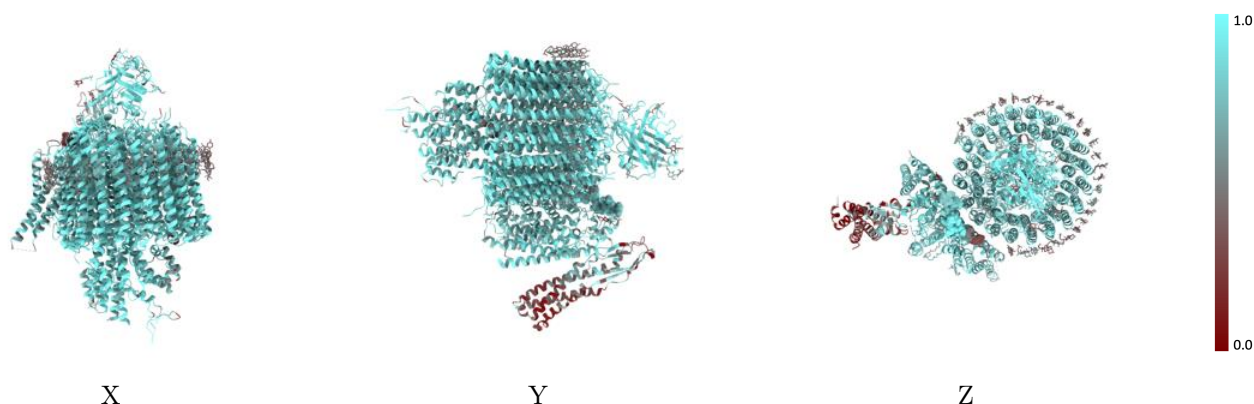
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



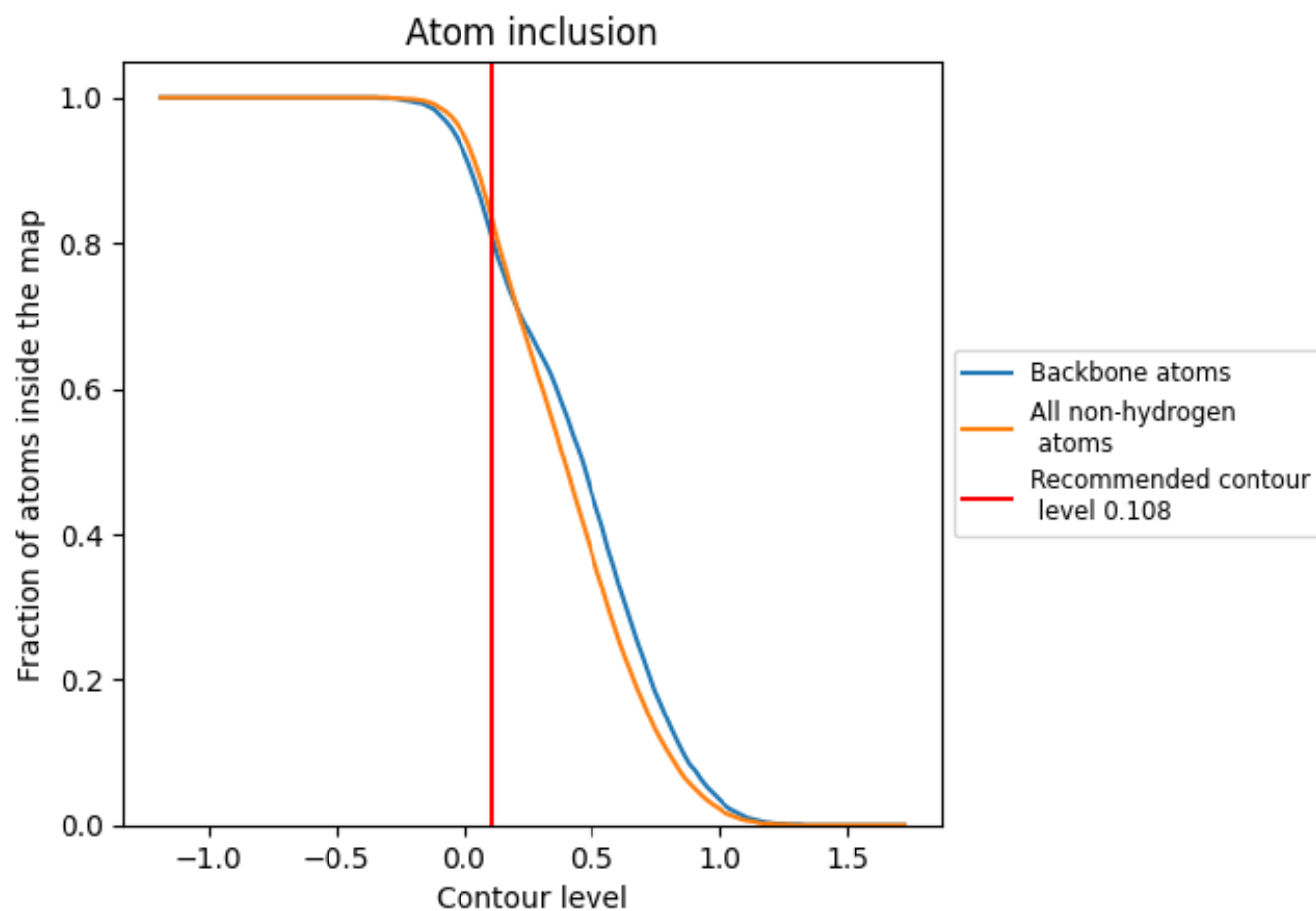
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.108).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.108) and Q-score for the entire model and for each chain.

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

