



Full wwPDB EM Validation Report ⓘ

Jun 11, 2026 – 10:08 AM EDT

PDB ID : 9YX6 / pdb_00009yx6
EMDB ID : EMD-73395
Title : SARS-CoV-2 BA.3.2.1 spike, flexible conformation
Authors : Wang, Y.; Hu, Y.; Chen, Z.; Liang, B.; Xie, X.
Deposited on : 2025-10-26
Resolution : 3.03 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

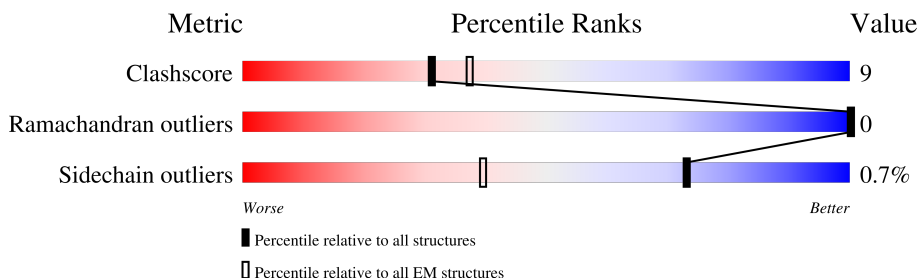
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1271	58% 17% 25%
1	B	1271	48% 13% 39%
1	C	1271	61% 15% 23%
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	100%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50%50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21789 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 SARS-Cov-2 BA.3.2.1 spike.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7463	4800	1233	1398	32		
1	B	779	Total	C	N	O	S	0	0
			6070	3889	1003	1153	25		
1	C	978	Total	C	N	O	S	0	0
			7682	4937	1271	1440	34		

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



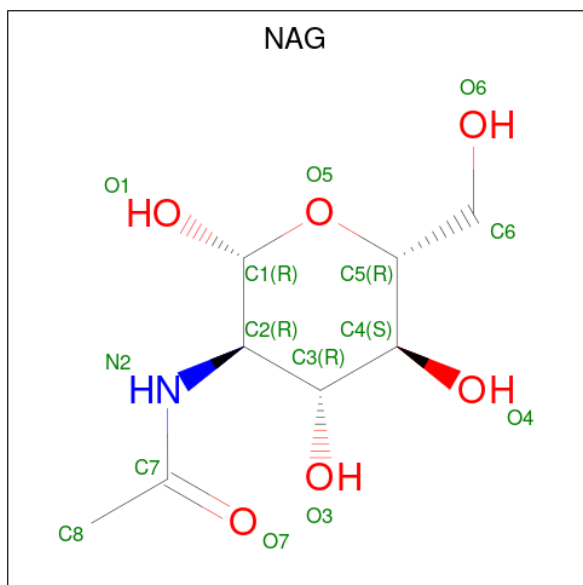
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



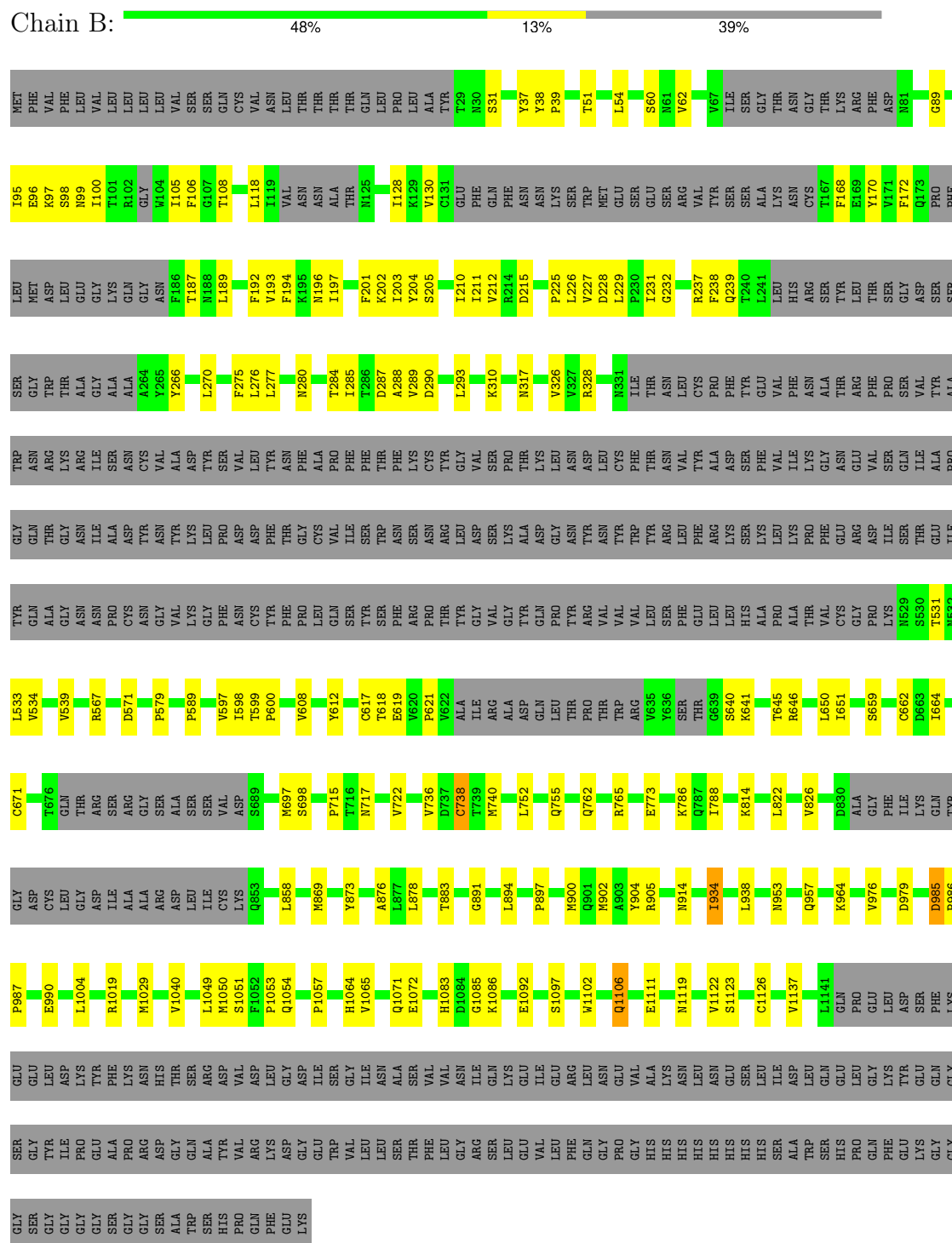
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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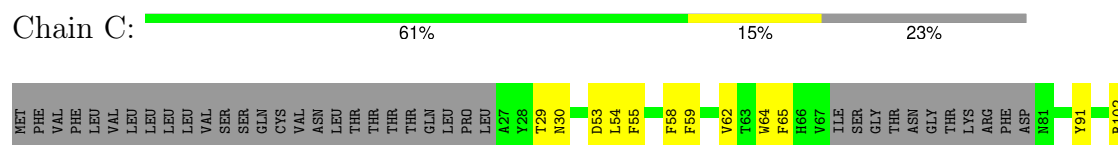
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

• Molecule 1: SARS-Cov-2 BA.3.2.1 spike



• Molecule 1: SARS-Cov-2 BA.3.2.1 spike







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

Chain G:  50% 50%



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

Chain H:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M: 


MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143152	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 ($e^-/\text{\AA}^2$)	39.84	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	10500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/7641	0.33	0/10394
1	B	0.13	0/6198	0.32	0/8429
1	C	0.17	0/7862	0.33	0/10692
All	All	0.17	0/21701	0.33	0/29515

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	A	7463	0	7295	147	0
1	B	6070	0	5991	116	0
1	C	7682	0	7521	146	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	A	70	0	65	1	0
3	B	112	0	104	0	0
3	C	112	0	104	0	0
All	All	21789	0	21330	381	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 9.

All (381) 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)
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.17	1.14
1:B:599:THR:CG2	1:B:608:VAL:HG12	1.89	1.02
1:B:599:THR:HG22	1:B:608:VAL:CG1	1.94	0.95
1:B:203:ILE:HG12	1:B:227:VAL:HG22	1.55	0.89
1:B:869:MET:HE2	1:C:699:LEU:HD21	1.59	0.83
1:A:118:LEU:HD23	1:A:118:LEU:O	1.77	0.83
1:C:418:ILE:HG23	1:C:422:ASN:HD22	1.49	0.77
1:C:659:SER:HB3	1:C:698:SER:HB3	1.66	0.76
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.68	0.75
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.67	0.75
1:A:319:ARG:NH2	1:C:740:MET:SD	2.59	0.74
1:C:420:ASP:HB2	1:C:460:LYS:HD2	1.69	0.74
1:B:599:THR:CG2	1:B:608:VAL:CG1	2.62	0.73
1:A:737:ASP:OD2	1:B:317:ASN:ND2	2.23	0.71
1:C:328:ARG:HH12	1:C:581:THR:HG23	1.57	0.69
1:B:196:ASN:HB3	1:B:201:PHE:HD1	1.57	0.69
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.59	0.68
1:B:869:MET:HE1	1:C:697:MET:HG3	1.76	0.68
1:A:1101:HIS:CE1	2:G:1:NAG:H3	2.29	0.67
1:B:192:PHE:HA	1:B:204:TYR:O	1.95	0.67
1:B:752:LEU:HD21	1:B:990:GLU:HG2	1.77	0.67
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.78	0.66
1:A:736:VAL:HG22	1:A:767:LEU:HD12	1.77	0.66
1:A:902:MET:HB3	1:A:916:LEU:HD11	1.76	0.66
1:B:170:TYR:HB3	1:B:172:PHE:CE1	2.31	0.66
1:B:618:THR:HG23	1:B:619:GLU:HG3	1.77	0.66
1:B:130:VAL:HB	1:B:168:PHE:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.78	0.65
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.30	0.65
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.77	0.65
1:B:659:SER:HB3	1:B:698:SER:HB3	1.79	0.64
1:B:869:MET:CE	1:C:699:LEU:HD21	2.27	0.64
1:A:118:LEU:HD13	1:A:129:LYS:HE3	1.79	0.64
1:B:128:ILE:HD13	1:B:229:LEU:HD11	1.80	0.63
1:A:521:PRO:HB3	1:A:564:GLN:HG3	1.80	0.63
1:C:59:PHE:HD2	1:C:293:LEU:HD21	1.64	0.63
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.32	0.63
1:A:126:VAL:HG12	1:A:174:PRO:HD3	1.81	0.62
1:A:346:ARG:HH12	1:A:348:PRO:HA	1.64	0.62
1:B:95:ILE:HG12	1:B:189:LEU:HD13	1.80	0.62
1:A:236:THR:HG22	1:A:237:ARG:HG3	1.81	0.62
1:B:736:VAL:HG22	1:B:858:LEU:HD22	1.82	0.62
1:C:454:ARG:NH2	1:C:469:SER:OG	2.33	0.62
1:B:1106:GLN:NE2	1:B:1111:GLU:OE1	2.32	0.62
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.82	0.61
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.80	0.61
1:A:364:ASP:OD1	1:A:366:SER:OG	2.18	0.61
1:B:869:MET:HE1	1:C:697:MET:CG	2.31	0.61
1:C:412:PRO:HG3	1:C:429:PHE:HD2	1.66	0.61
1:C:58:PHE:HB2	1:C:293:LEU:HD22	1.83	0.60
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.82	0.60
1:C:578:ASP:OD1	1:C:583:ASP:N	2.34	0.60
1:C:1093:GLY:O	1:C:1107:ARG:NH1	2.35	0.60
1:A:736:VAL:HG12	1:A:858:LEU:HD23	1.84	0.60
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.83	0.60
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.84	0.60
1:B:914:ASN:ND2	1:C:1123:SER:OG	2.35	0.60
1:C:422:ASN:HD21	1:C:453:TYR:HB2	1.66	0.59
1:B:212:VAL:HG13	1:B:215:ASP:H	1.68	0.59
1:C:280:ASN:OD1	1:C:284:THR:N	2.31	0.59
1:B:736:VAL:HG11	1:B:1004:LEU:HD11	1.85	0.59
1:C:428:ASP:OD1	1:C:428:ASP:N	2.35	0.58
1:A:998:THR:O	1:A:1002:GLN:HG2	2.03	0.58
1:C:206:LYS:HB3	1:C:223:LEU:HG	1.85	0.58
1:A:444:LYS:HG2	1:A:444:LYS:O	2.03	0.58
1:B:883:THR:HG23	1:C:707:TYR:HB2	1.85	0.58
1:A:747:THR:O	1:A:751:ASN:ND2	2.37	0.58
1:A:984:LEU:HD13	1:A:988:GLU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ILE:HG23	1:A:931:ILE:HD11	1.86	0.57
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.85	0.57
1:A:402:ILE:CG2	1:A:418:ILE:HD13	2.34	0.57
1:B:280:ASN:OD1	1:B:284:THR:N	2.38	0.57
1:B:762:GLN:OE1	1:B:765:ARG:NH1	2.38	0.57
1:C:119:ILE:HG13	1:C:128:ILE:HG23	1.86	0.57
1:C:349:SER:OG	1:C:452:TRP:O	2.22	0.56
1:A:106:PHE:HB3	1:A:235:ILE:HD11	1.88	0.56
1:B:211:ILE:HG22	1:B:211:ILE:O	2.05	0.56
1:A:118:LEU:HD13	1:A:129:LYS:CE	2.35	0.56
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.24	0.56
1:B:762:GLN:HE22	1:C:957:GLN:HE22	1.52	0.56
1:A:348:PRO:HG3	1:A:354:ASN:HB2	1.86	0.56
1:A:980:ILE:HG23	1:A:992:GLN:HB2	1.88	0.56
1:C:454:ARG:NH1	1:C:467:ASP:O	2.38	0.56
1:A:866:THR:OG1	1:A:869:MET:HG3	2.07	0.55
1:A:118:LEU:HD23	1:A:120:VAL:HG13	1.88	0.55
1:A:34:ARG:NH2	1:A:191:GLU:OE2	2.40	0.55
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.88	0.55
1:B:231:ILE:O	1:C:357:ARG:NH1	2.35	0.54
1:A:125:ASN:ND2	1:A:172:PHE:O	2.35	0.54
1:B:617:CYS:HA	1:B:621:PRO:HD3	1.90	0.54
1:A:298:GLU:OE2	1:A:316:SER:OG	2.13	0.54
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.89	0.54
1:C:462:LYS:NZ	1:C:463:PRO:O	2.39	0.54
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.90	0.54
1:C:1051:SER:OG	1:C:1064:HIS:ND1	2.34	0.54
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.34	0.54
1:C:197:ILE:O	1:C:199:GLY:N	2.41	0.54
1:B:1092:GLU:N	1:B:1092:GLU:OE2	2.40	0.54
1:C:312:ILE:HD12	1:C:598:ILE:HD11	1.89	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.36	0.53
1:B:193:VAL:O	1:B:203:ILE:HA	2.07	0.53
1:C:125:ASN:HA	1:C:172:PHE:HD2	1.73	0.53
1:C:446:ASP:HB3	1:C:499:PRO:HA	1.90	0.53
1:A:320:VAL:HG22	1:A:621:PRO:HG3	1.91	0.53
1:C:452:TRP:HB3	1:C:492:LEU:HD22	1.91	0.53
1:B:786:LYS:NZ	1:B:891:GLY:O	2.41	0.53
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.34	0.53
1:A:918:GLU:OE2	1:B:1123:SER:OG	2.26	0.52
1:A:1094:VAL:HG23	1:C:900:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:SER:HA	1:C:132:GLU:HB3	1.92	0.52
1:C:724:THR:HG23	1:C:934:ILE:HD12	1.91	0.52
1:B:976:VAL:HG12	1:B:979:ASP:H	1.74	0.52
1:C:126:VAL:H	1:C:172:PHE:HB3	1.74	0.52
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.75	0.52
1:C:295:PRO:O	1:C:299:THR:HG23	2.10	0.52
1:A:402:ILE:HD13	1:A:410:ILE:HD11	1.91	0.52
1:B:287:ASP:OD1	1:B:288:ALA:N	2.43	0.52
1:A:1101:HIS:HE1	2:G:1:NAG:H3	1.70	0.52
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.92	0.52
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.91	0.52
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.29	0.51
1:A:855:PHE:CD1	1:B:589:PRO:HG2	2.45	0.51
1:C:102:ARG:NH1	1:C:243:HIS:O	2.43	0.51
1:C:456:PHE:HB2	1:C:491:PRO:HB3	1.93	0.51
1:A:980:ILE:CG2	1:A:992:GLN:HB2	2.41	0.51
1:C:204:TYR:HA	1:C:225:PRO:HA	1.92	0.51
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.93	0.51
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.46	0.51
1:B:599:THR:HG22	1:B:608:VAL:CB	2.41	0.51
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.46	0.51
1:C:411:ALA:HB3	1:C:414:GLN:HB2	1.93	0.51
1:C:496:SER:HB2	1:C:498:ARG:HH12	1.74	0.51
1:A:280:ASN:OD1	1:A:284:THR:N	2.43	0.51
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.91	0.51
1:B:187:THR:HB	1:B:210:ILE:HG13	1.93	0.51
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.92	0.51
1:A:240:THR:OG1	1:A:241:LEU:N	2.44	0.50
1:A:360:ASN:H	1:A:523:THR:HG23	1.75	0.50
1:A:751:ASN:HA	1:A:754:LEU:HD23	1.93	0.50
1:A:353:TRP:CH2	1:A:466:ARG:HB2	2.46	0.50
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.47	0.50
1:C:303:LEU:HD22	1:C:308:VAL:HG12	1.94	0.50
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.29	0.50
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.39	0.50
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.93	0.50
1:A:90:VAL:HG12	1:A:92:PHE:H	1.77	0.50
1:A:128:ILE:HG21	1:A:229:LEU:HD11	1.94	0.50
1:A:402:ILE:HG21	1:A:418:ILE:HD13	1.94	0.50
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.44	0.50
1:A:618:THR:OG1	1:A:619:GLU:OE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.40	0.49
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.94	0.49
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.38	0.49
1:B:1085:GLY:O	1:B:1126:CYS:N	2.41	0.49
1:A:897:PRO:HB2	1:A:900:MET:HG3	1.94	0.49
1:C:903:ALA:HB2	1:C:916:LEU:HD22	1.94	0.49
1:A:987:PRO:HG3	1:C:413:GLY:O	2.12	0.49
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.93	0.49
1:C:1050:MET:HG2	1:C:1065:VAL:HB	1.95	0.49
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.95	0.49
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	1.95	0.49
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.94	0.49
1:A:737:ASP:OD1	1:A:739:THR:OG1	2.30	0.49
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.95	0.49
1:B:740:MET:HE1	1:C:319:ARG:HH12	1.78	0.49
1:C:336:CYS:HB2	1:C:338:PHE:CE2	2.47	0.49
1:A:118:LEU:N	1:A:129:LYS:O	2.46	0.49
1:A:347:PHE:HB2	1:A:401:VAL:HG23	1.95	0.49
1:A:973:ILE:HG21	1:A:983:ARG:HD3	1.95	0.49
1:B:640:SER:O	1:B:641:LYS:HG3	2.13	0.49
1:C:338:PHE:HE2	1:C:363:ALA:HA	1.78	0.49
1:C:375:PHE:N	1:C:435:SER:O	2.44	0.49
1:B:897:PRO:HB2	1:B:900:MET:HG3	1.95	0.48
1:B:277:LEU:HD13	1:B:285:ILE:HD13	1.95	0.48
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.95	0.48
1:C:276:LEU:HB3	1:C:289:VAL:HG23	1.95	0.48
1:A:126:VAL:H	1:A:174:PRO:HD3	1.78	0.48
1:B:986:PRO:N	1:B:987:PRO:HD2	2.29	0.48
1:C:342:PHE:CZ	1:C:368:LEU:HD13	2.48	0.48
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.96	0.48
1:C:1115:ILE:HG22	1:C:1137:VAL:HG12	1.96	0.48
1:C:335:LEU:HD13	1:C:362:VAL:HB	1.95	0.48
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.95	0.48
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.95	0.48
1:C:599:THR:HG23	1:C:608:VAL:HG12	1.95	0.48
1:A:739:THR:O	1:A:744:GLY:N	2.47	0.47
1:B:1086:LYS:HB3	1:B:1122:VAL:HG13	1.96	0.47
1:C:497:PHE:HB3	1:C:507:PRO:HD3	1.95	0.47
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.80	0.47
1:A:324:GLU:H	1:A:539:VAL:HG12	1.79	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ASN:HD21	1:A:579:PRO:HG3	1.80	0.47
1:A:619:GLU:OE2	1:A:619:GLU:N	2.48	0.47
1:C:113:LYS:O	1:C:113:LYS:NZ	2.36	0.47
1:A:354:ASN:O	1:A:398:ASP:HA	2.15	0.47
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.80	0.47
1:C:425:LEU:HD21	1:C:512:VAL:HG11	1.96	0.47
1:A:95:ILE:HD12	1:A:189:LEU:HB2	1.97	0.47
1:A:724:THR:HG23	1:A:934:ILE:HD12	1.97	0.47
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.96	0.47
1:A:989:ALA:O	1:A:990:GLU:C	2.57	0.47
1:B:205:SER:HB3	1:B:226:LEU:HD13	1.95	0.47
1:C:29:THR:HG22	1:C:30:ASN:N	2.30	0.47
1:C:295:PRO:HG3	1:C:633:TRP:HE3	1.79	0.47
1:A:456:PHE:HE2	1:A:489:TYR:HD2	1.62	0.47
1:C:205:SER:HB3	1:C:226:LEU:HD22	1.96	0.47
1:A:605:SER:OG	1:A:606:ASN:N	2.47	0.47
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.48	0.47
1:B:645:THR:OG1	1:B:646:ARG:N	2.48	0.47
1:A:203:ILE:HB	1:A:227:VAL:HB	1.96	0.47
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.96	0.47
1:A:28:TYR:CD2	1:A:63:THR:HA	2.50	0.46
1:A:435:SER:HB2	1:A:510:VAL:HG22	1.96	0.46
1:C:190:ARG:HB3	1:C:192:PHE:CZ	2.50	0.46
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.96	0.46
1:A:745:ASP:OD1	1:A:745:ASP:O	2.32	0.46
1:C:731:MET:HG2	1:C:1018:ILE:HG13	1.98	0.46
1:A:403:LYS:HG2	1:A:497:PHE:HE1	1.80	0.46
1:B:215:ASP:OD1	1:B:266:TYR:OH	2.30	0.46
1:A:29:THR:HB	1:A:62:VAL:HG23	1.98	0.46
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.96	0.46
1:C:716:THR:HG21	1:C:1073:LYS:HD3	1.97	0.46
1:A:443:SER:O	1:A:443:SER:OG	2.31	0.46
1:B:275:PHE:HB3	1:B:277:LEU:HD21	1.98	0.46
1:B:904:TYR:CZ	1:C:1107:ARG:HD3	2.51	0.46
1:B:37:TYR:OH	1:B:54:LEU:O	2.26	0.46
1:C:353:TRP:O	1:C:466:ARG:NH2	2.43	0.46
1:A:1043:CYS:HB2	1:A:1048:HIS:CD2	2.51	0.46
1:C:964:LYS:HB2	1:C:964:LYS:HE3	1.77	0.46
1:C:58:PHE:CB	1:C:293:LEU:HD22	2.45	0.45
1:C:340:GLU:OE1	1:C:340:GLU:N	2.34	0.45
1:A:919:ASN:O	1:A:923:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:HG22	1:C:315:THR:HG21	1.98	0.45
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.85	0.45
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.51	0.45
1:B:31:SER:N	1:B:60:SER:O	2.42	0.45
1:C:29:THR:HB	1:C:62:VAL:HG13	1.98	0.45
1:B:964:LYS:NZ	1:C:571:ASP:OD2	2.38	0.45
1:C:105:ILE:HD13	1:C:241:LEU:HD21	1.99	0.45
1:A:870:ILE:HG22	1:A:1055:SER:HB2	1.99	0.45
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	1.99	0.45
1:B:814:LYS:HA	1:B:814:LYS:HD3	1.81	0.44
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.52	0.44
1:C:492:LEU:HD23	1:C:492:LEU:HA	1.83	0.44
1:C:786:LYS:NZ	1:C:891:GLY:O	2.49	0.44
1:B:204:TYR:HA	1:B:225:PRO:HA	1.99	0.44
1:B:211:ILE:O	1:B:211:ILE:CG2	2.65	0.44
1:A:659:SER:HB3	1:A:698:SER:HB2	1.99	0.44
1:A:697:MET:HB2	1:C:869:MET:HE1	2.00	0.44
1:B:755:GLN:HE22	1:C:969:LYS:HD2	1.82	0.44
1:C:902:MET:HE3	1:C:1049:LEU:HD13	1.99	0.44
1:B:869:MET:HE2	1:C:699:LEU:CD2	2.39	0.44
1:A:40:ASP:OD1	1:A:40:ASP:C	2.60	0.44
1:B:98:SER:OG	1:B:99:ASN:N	2.50	0.44
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.98	0.44
1:C:900:MET:HE2	1:C:900:MET:HB3	1.80	0.44
1:A:445:ALA:H	1:A:499:PRO:HD3	1.83	0.44
1:A:1035:GLY:HA3	1:B:1040:VAL:HG21	1.99	0.44
1:B:95:ILE:HG12	1:B:189:LEU:CD1	2.48	0.44
1:B:105:ILE:HG22	1:B:118:LEU:HD23	1.99	0.44
1:A:53:ASP:OD1	1:A:54:LEU:N	2.46	0.44
1:B:612:TYR:HE2	1:B:651:ILE:HD12	1.83	0.44
1:C:357:ARG:NE	1:C:396:TYR:HE1	2.15	0.44
1:C:414:GLN:NE2	1:C:415:THR:O	2.51	0.44
1:C:578:ASP:OD2	1:C:581:THR:OG1	2.27	0.44
1:C:1076:THR:O	1:C:1097:SER:N	2.48	0.44
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.84	0.44
1:C:353:TRP:CD1	1:C:353:TRP:H	2.35	0.44
1:C:880:GLY:O	1:C:884:SER:OG	2.30	0.43
1:A:118:LEU:O	1:A:118:LEU:CD2	2.57	0.43
1:B:717:ASN:HD22	1:B:1071:GLN:NE2	2.17	0.43
1:B:953:ASN:O	1:B:957:GLN:HG2	2.18	0.43
1:C:556:ASN:OD1	1:C:556:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:O	1:A:328:ARG:HD2	2.19	0.43
1:A:439:ASN:O	1:A:443:SER:OG	2.31	0.43
1:B:822:LEU:HD21	1:B:938:LEU:HD13	2.00	0.43
1:A:329:PHE:CD2	1:A:528:LYS:HB2	2.53	0.43
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.54	0.43
1:A:928:ASN:HA	1:A:931:ILE:HG22	2.00	0.43
1:C:977:LEU:HD23	1:C:977:LEU:HA	1.81	0.43
1:B:38:TYR:CE1	1:B:285:ILE:HG13	2.53	0.43
1:C:119:ILE:HA	1:C:127:VAL:O	2.19	0.43
1:C:902:MET:HB3	1:C:916:LEU:HD11	2.01	0.43
1:A:358:ILE:HB	1:A:395:VAL:HB	2.00	0.43
1:B:788:ILE:HG23	1:B:876:ALA:HB2	2.01	0.43
1:C:55:PHE:C	1:C:270:LEU:HD12	2.43	0.43
1:C:65:PHE:HB3	1:C:265:TYR:CZ	2.54	0.43
1:C:317:ASN:OD1	1:C:317:ASN:N	2.52	0.43
1:A:516:GLU:OE2	1:A:519:HIS:HB3	2.19	0.43
1:B:697:MET:HE3	1:B:697:MET:HB2	1.83	0.43
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.44	0.43
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.53	0.43
1:B:567:ARG:HD2	1:B:571:ASP:HA	2.00	0.43
1:B:738:CYS:C	1:B:740:MET:H	2.25	0.43
1:C:113:LYS:HG3	1:C:114:THR:HG23	2.00	0.43
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.00	0.43
1:C:528:LYS:HD3	1:C:528:LYS:HA	1.65	0.43
1:A:403:LYS:HG3	1:A:495:TYR:CE1	2.53	0.43
1:A:448:ASN:OD1	1:A:494:SER:OG	2.34	0.43
1:B:231:ILE:HG22	1:B:232:GLY:H	1.84	0.42
1:C:338:PHE:CZ	1:C:365:TYR:HE1	2.37	0.42
1:C:353:TRP:CZ2	1:C:466:ARG:HB3	2.54	0.42
1:C:451:TYR:O	1:C:495:TYR:N	2.47	0.42
1:C:759:PHE:O	1:C:763:LEU:HG	2.18	0.42
1:A:87:ASN:OD1	1:A:87:ASN:N	2.51	0.42
1:A:402:ILE:HB	1:A:418:ILE:CD1	2.49	0.42
1:A:921:LYS:HE3	1:A:921:LYS:HB3	1.81	0.42
1:C:103:GLY:O	1:C:104:TRP:HD1	2.02	0.42
1:C:383:SER:HB3	1:C:386:LYS:HD2	1.99	0.42
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.83	0.42
1:A:125:ASN:HD21	1:A:171:VAL:HG13	1.83	0.42
1:A:328:ARG:NH1	1:A:533:LEU:HB2	2.34	0.42
1:B:822:LEU:O	1:B:826:VAL:HG23	2.18	0.42
1:B:276:LEU:HB3	1:B:289:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HB3	1:B:579:PRO:HD2	2.01	0.42
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.31	0.42
1:C:402:ILE:HD11	1:C:418:ILE:HG21	2.01	0.42
1:C:979:ASP:OD1	1:C:979:ASP:C	2.62	0.42
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.29	0.42
1:A:984:LEU:HD13	1:A:988:GLU:CB	2.48	0.42
1:B:985:ASP:N	1:C:383:SER:HB2	2.34	0.42
1:C:460:LYS:HD3	1:C:460:LYS:HA	1.78	0.42
1:A:290:ASP:O	1:A:297:SER:HB3	2.19	0.42
1:B:62:VAL:HG21	1:B:266:TYR:HB3	2.02	0.42
1:C:988:GLU:OE1	1:C:988:GLU:N	2.53	0.42
1:A:189:LEU:HB3	1:A:208:THR:HB	2.02	0.42
1:A:900:MET:HE2	1:A:900:MET:HB3	1.93	0.42
1:B:1050:MET:HG2	1:B:1065:VAL:HB	2.01	0.42
1:A:117:LEU:HG	1:A:130:VAL:HB	2.01	0.42
1:A:468:ILE:HD12	1:A:468:ILE:HA	1.88	0.42
1:A:742:ILE:HA	1:A:1000:ARG:HD3	2.02	0.42
1:A:91:TYR:N	1:A:268:GLY:O	2.51	0.41
1:B:96:GLU:HB2	1:B:100:ILE:HD13	2.02	0.41
1:B:934:ILE:HD12	1:B:934:ILE:HA	1.90	0.41
1:B:1029:MET:HE2	1:B:1029:MET:HB2	1.92	0.41
1:A:547:THR:HG23	1:C:978:ASN:HB3	2.02	0.41
1:A:878:LEU:HD11	1:A:1054:GLN:HE22	1.86	0.41
1:B:197:ILE:HD12	1:B:197:ILE:O	2.20	0.41
1:B:873:TYR:CE2	1:C:699:LEU:HD22	2.55	0.41
1:B:964:LYS:HD3	1:B:964:LYS:HA	1.75	0.41
1:B:326:VAL:HA	1:B:531:THR:HG21	2.02	0.41
1:B:894:LEU:HB3	1:C:713:ALA:HB3	2.03	0.41
1:C:312:ILE:HG23	1:C:312:ILE:O	2.19	0.41
1:A:418:ILE:HA	1:A:422:ASN:HB2	2.02	0.41
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.31	0.41
1:B:108:THR:O	1:B:237:ARG:NH2	2.45	0.41
1:B:597:VAL:HG12	1:B:599:THR:HG23	2.02	0.41
1:C:371:PHE:HB3	1:C:374:PHE:HZ	1.85	0.41
1:A:91:TYR:O	1:A:91:TYR:CG	2.72	0.41
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.02	0.41
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.31	0.41
1:C:328:ARG:NH1	1:C:580:GLN:HB2	2.36	0.41
1:A:350:VAL:HA	1:A:400:PHE:HB2	2.02	0.41
1:A:1129:VAL:HG13	1:C:917:TYR:HB3	2.02	0.41
1:B:290:ASP:OD2	1:B:293:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HG12	1:C:406:GLU:HB2	2.03	0.41
1:A:40:ASP:OD1	1:A:42:VAL:N	2.54	0.41
1:A:128:ILE:HB	1:A:170:TYR:HB2	2.03	0.41
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.48	0.41
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.87	0.41
1:C:943:SER:O	1:C:943:SER:OG	2.29	0.41
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.86	0.41
1:B:534:VAL:HG23	1:B:539:VAL:HG11	2.03	0.41
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.56	0.41
1:A:277:LEU:HD22	1:A:285:ILE:HD13	2.03	0.40
1:A:298:GLU:OE2	1:A:316:SER:CB	2.69	0.40
1:A:943:SER:O	1:A:943:SER:OG	2.36	0.40
1:B:902:MET:HE3	1:B:1049:LEU:HD13	2.03	0.40
1:B:650:LEU:HD12	1:B:650:LEU:HA	1.92	0.40
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.90	0.40
1:A:52:GLN:OE1	1:A:52:GLN:HA	2.21	0.40
1:B:97:LYS:HE3	1:B:97:LYS:HB3	1.89	0.40
1:B:105:ILE:HG12	1:B:239:GLN:HB3	2.03	0.40
1:B:671:CYS:SG	1:B:697:MET:HB3	2.62	0.40
1:B:878:LEU:HD11	1:B:1054:GLN:NE2	2.35	0.40
1:B:1083:HIS:CG	1:B:1137:VAL:HG22	2.56	0.40
1:A:281:GLU:OE2	3:A:1304:NAG:N2	2.45	0.40
1:A:738:CYS:O	1:A:742:ILE:N	2.50	0.40
1:C:202:LYS:HE2	1:C:202:LYS:HB2	1.87	0.40
1:C:369:TYR:OH	1:C:384:PRO:O	2.31	0.40
1:C:752:LEU:HD23	1:C:752:LEU:HA	1.77	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	A	921/1271 (72%)	882 (96%)	39 (4%)	0	100	100
1	B	755/1271 (59%)	728 (96%)	27 (4%)	0	100	100
1	C	950/1271 (75%)	918 (97%)	32 (3%)	0	100	100
All	All	2626/3813 (69%)	2528 (96%)	98 (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	A	833/1106 (75%)	832 (100%)	1 (0%)	88	91
1	B	686/1106 (62%)	681 (99%)	5 (1%)	76	84
1	C	859/1106 (78%)	848 (99%)	11 (1%)	61	79
All	All	2378/3318 (72%)	2361 (99%)	17 (1%)	73	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1106	GLN
1	B	738	CYS
1	B	934	ILE
1	B	985	ASP
1	B	1106	GLN
1	B	1119	ASN
1	C	131	CYS
1	C	207	HIS
1	C	277	LEU
1	C	317	ASN
1	C	368	LEU
1	C	428	ASP
1	C	524	VAL
1	C	529	ASN
1	C	563	GLN

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Mol	Chain	Res	Type
1	C	617	CYS
1	C	955	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	388	ASN
1	A	422	ASN
1	A	448	ASN
1	A	856	ASN
1	A	960	ASN
1	A	1088	HIS
1	A	1135	ASN
1	B	30	ASN
1	B	271	GLN
1	B	607	GLN
1	B	613	GLN
1	B	755	GLN
1	B	907	ASN
1	B	949	GLN
1	C	196	ASN
1	C	422	ASN
1	C	755	GLN
1	C	913	GLN
1	C	957	GLN
1	C	1106	GLN
1	C	1135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.74	0	17,19,21	0.80	0
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.76	0
2	NAG	E	1	2,1	14,14,15	0.75	0	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.72	0	17,19,21	0.80	0
2	NAG	F	1	2,1	14,14,15	0.74	0	17,19,21	0.82	0
2	NAG	F	2	2	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
2	NAG	G	2	2	14,14,15	0.38	0	17,19,21	0.50	0
2	NAG	H	1	2,1	14,14,15	0.75	0	17,19,21	0.87	0
2	NAG	H	2	2	14,14,15	0.71	0	17,19,21	0.80	0
2	NAG	I	1	2,1	14,14,15	0.73	0	17,19,21	0.77	0
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	0.79	0
2	NAG	J	1	2,1	14,14,15	0.73	0	17,19,21	0.86	0
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.81	0
2	NAG	K	1	2,1	14,14,15	0.73	0	17,19,21	0.83	0
2	NAG	K	2	2	14,14,15	0.72	0	17,19,21	0.86	0
2	NAG	L	1	2,1	14,14,15	0.75	0	17,19,21	0.81	0
2	NAG	L	2	2	14,14,15	0.72	0	17,19,21	0.80	0
2	NAG	M	1	2,1	14,14,15	0.70	0	17,19,21	0.97	0
2	NAG	M	2	2	14,14,15	0.72	0	17,19,21	1.19	1 (5%)

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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	3.11	127.07	122.90
2	M	2	NAG	C2-N2-C7	3.05	126.99	122.90
2	G	1	NAG	C1-C2-N2	2.58	114.50	110.43
2	G	1	NAG	C2-N2-C7	2.57	126.34	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6

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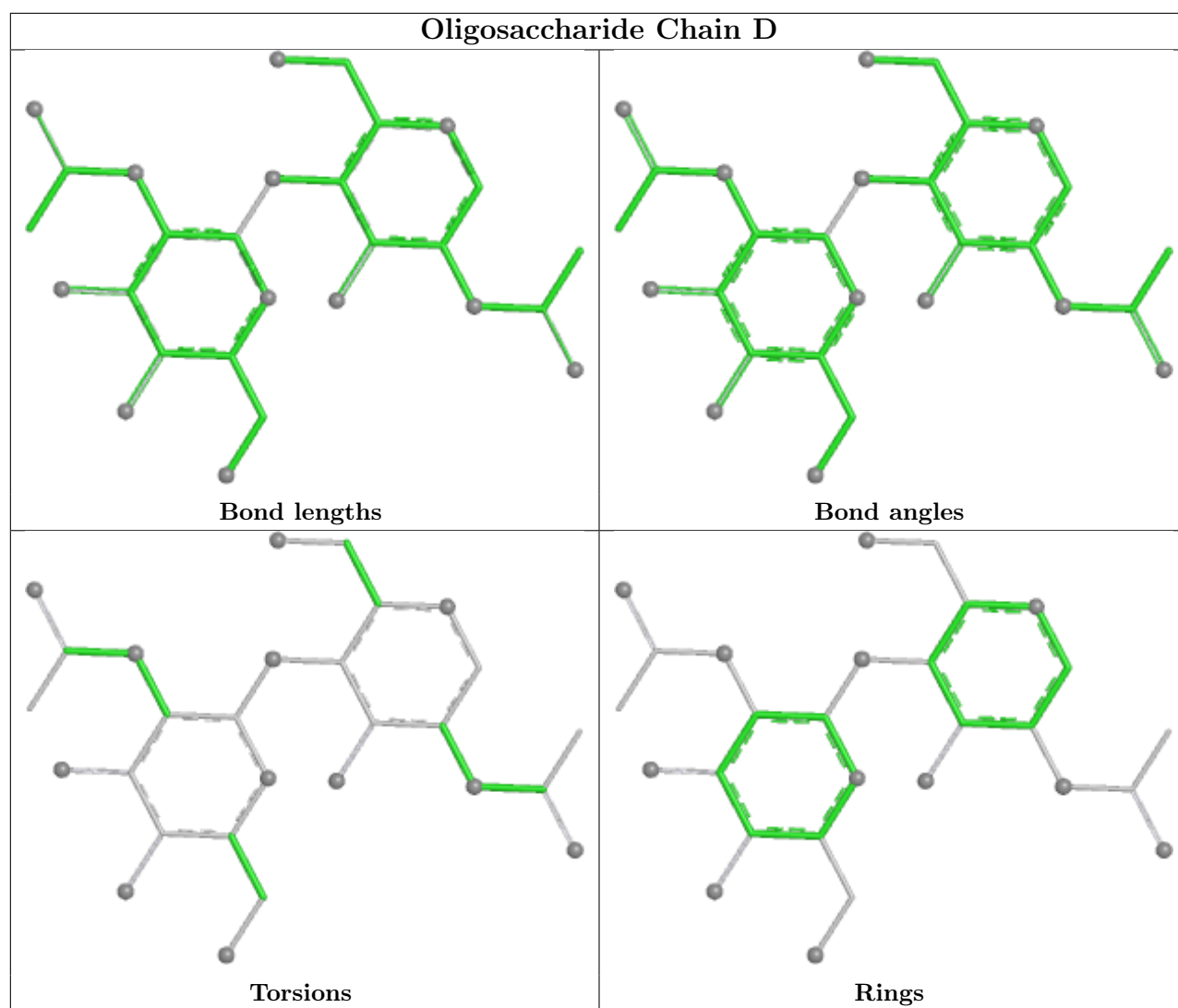
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	M	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	M	2	NAG	C3-C2-N2-C7

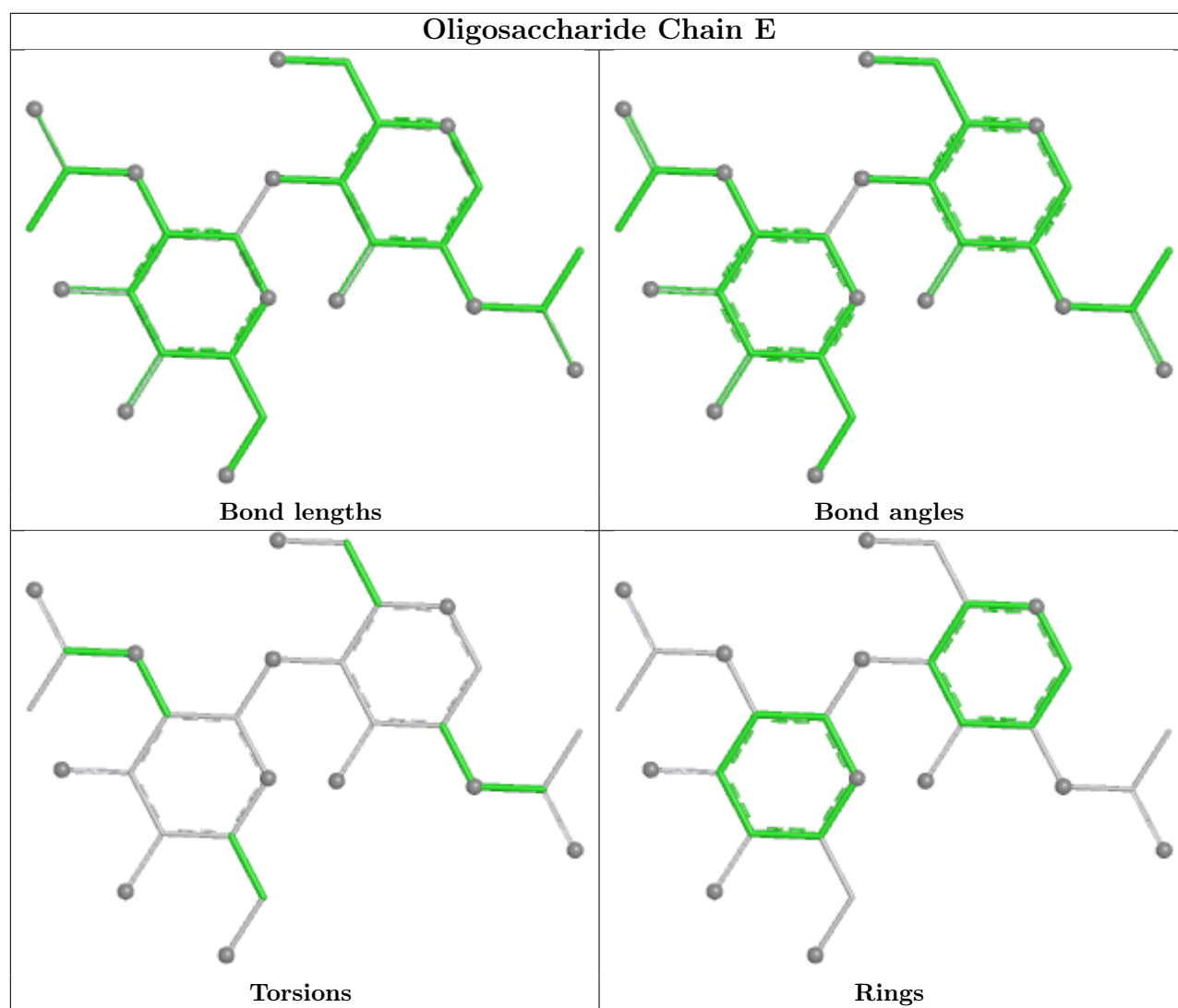
There are no ring outliers.

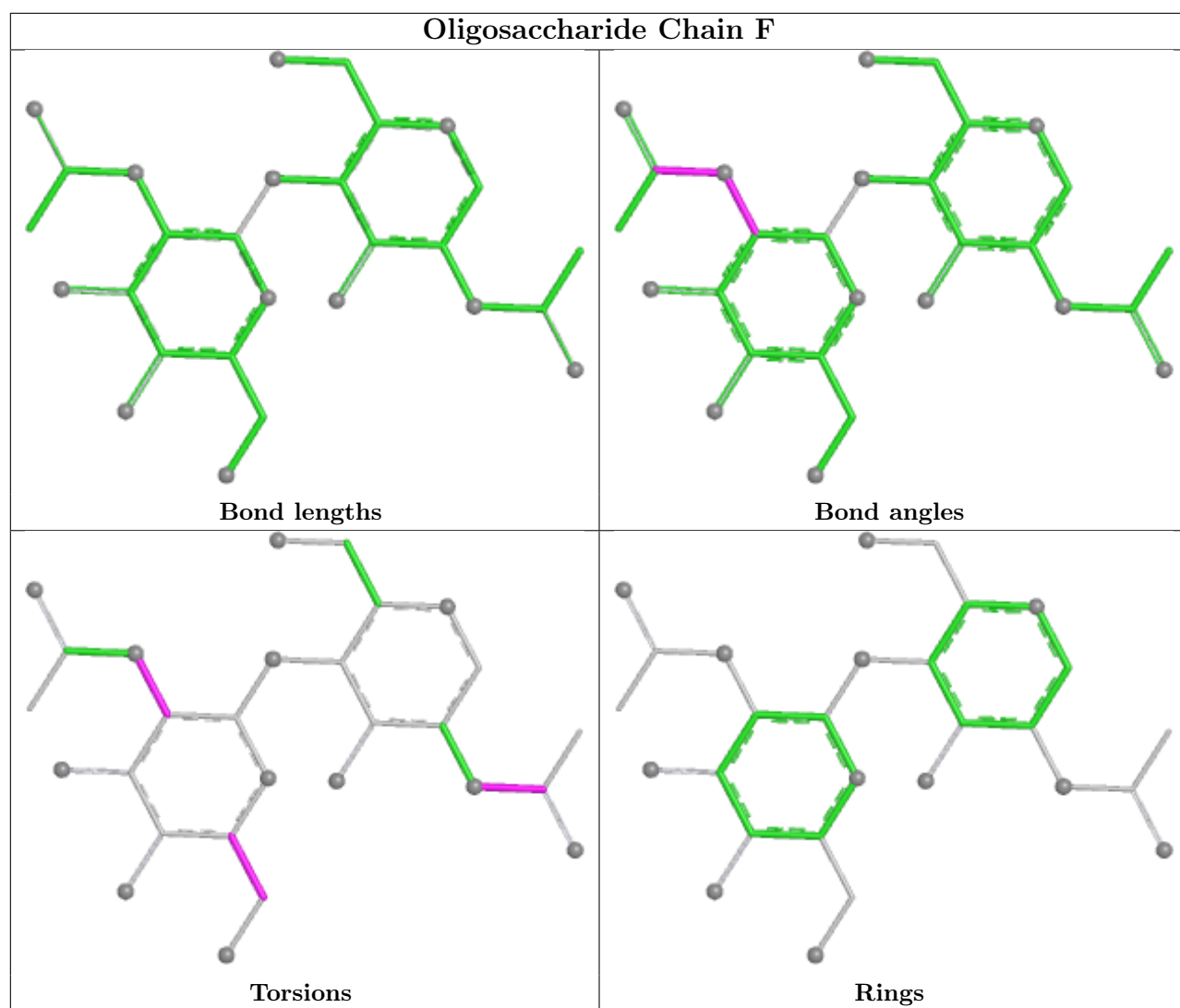
1 monomer is involved in 2 short contacts:

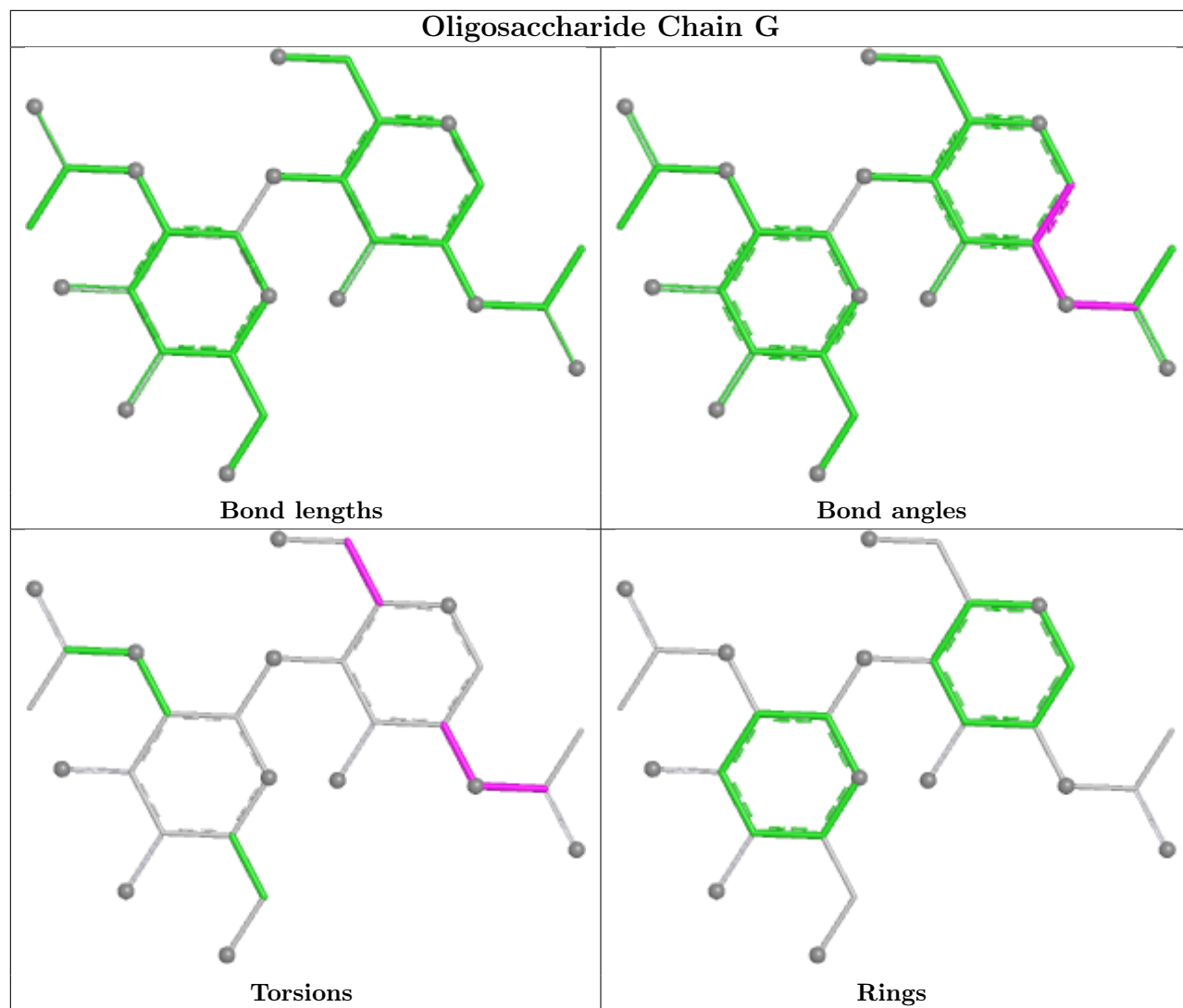
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0

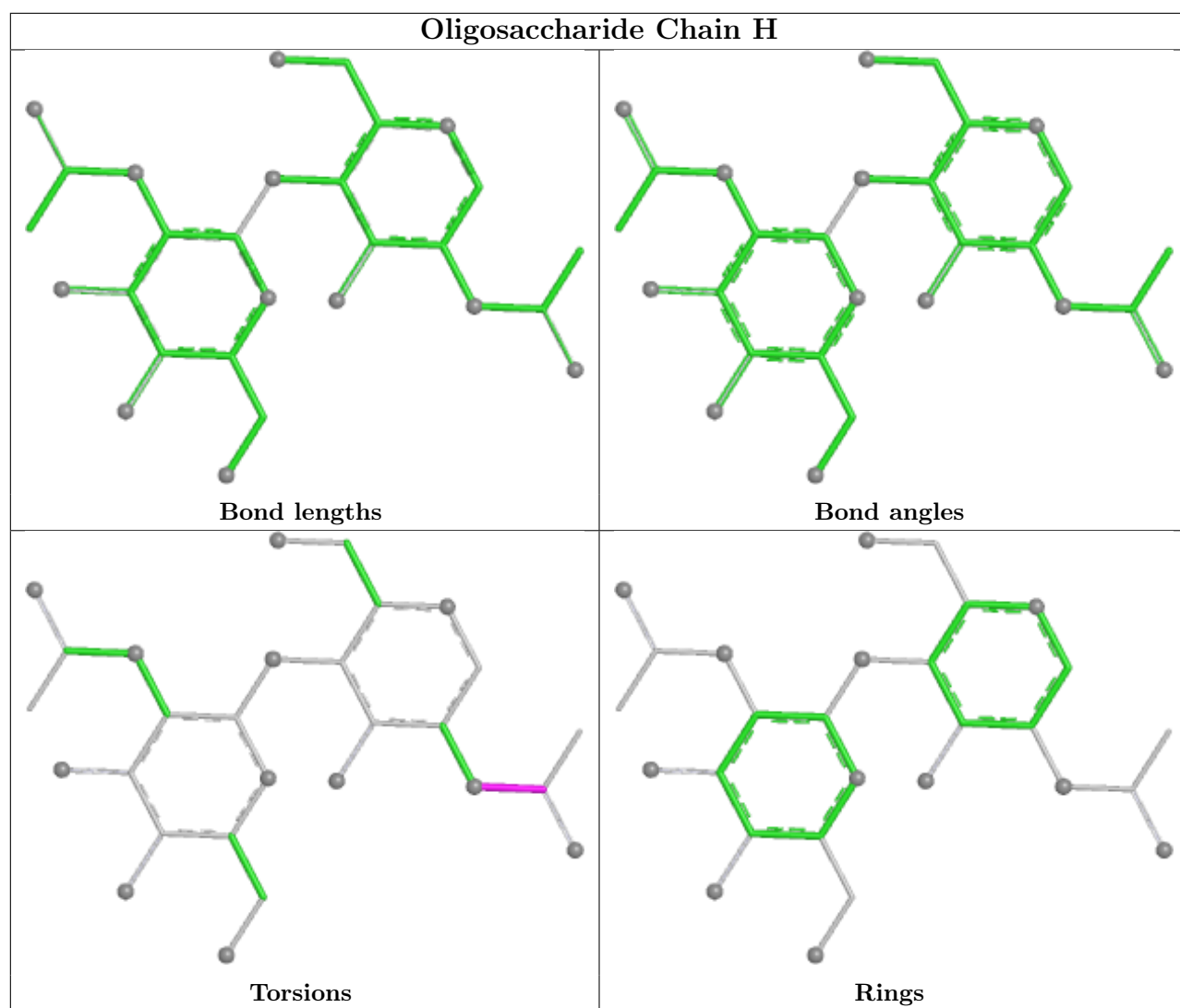
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

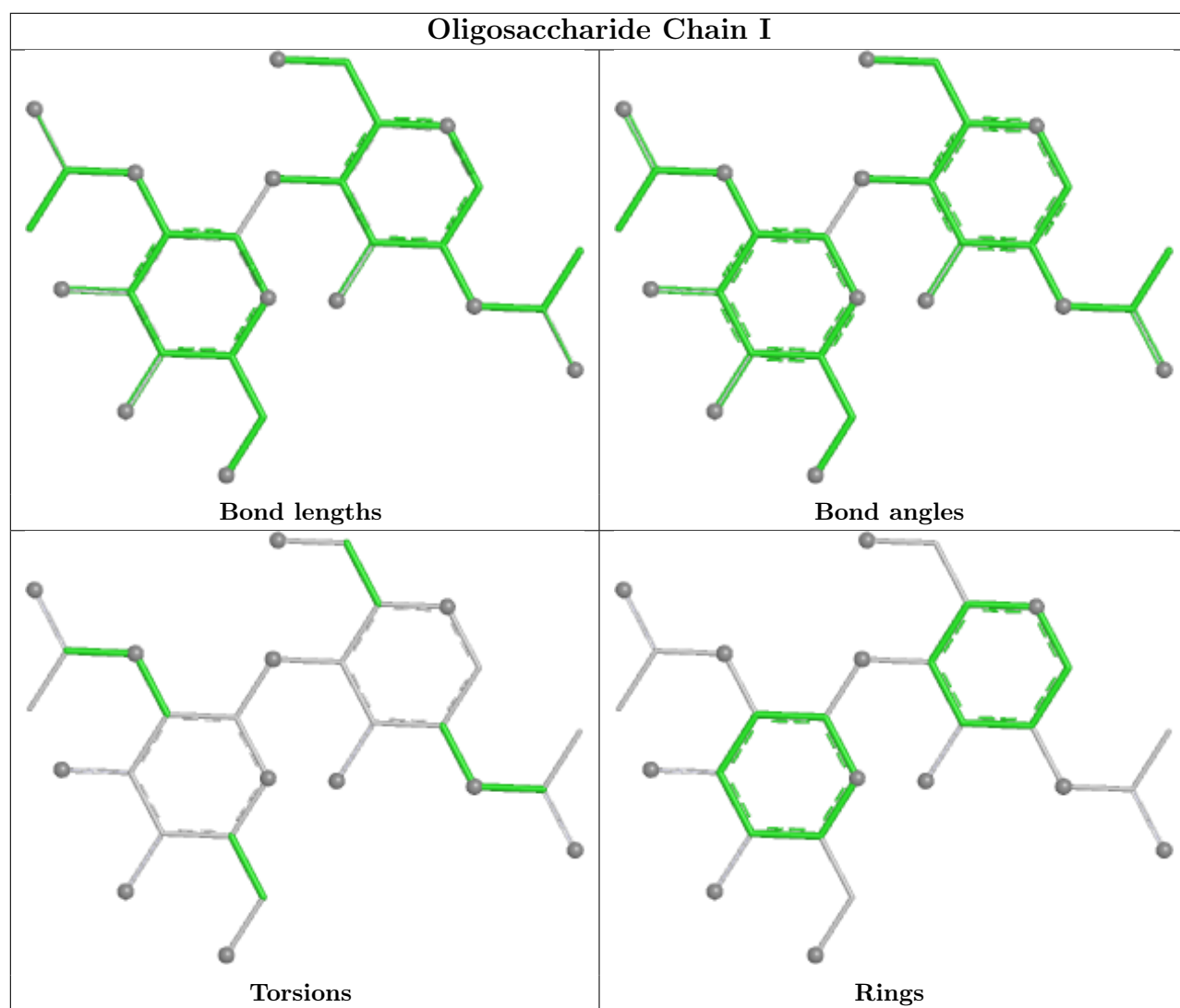


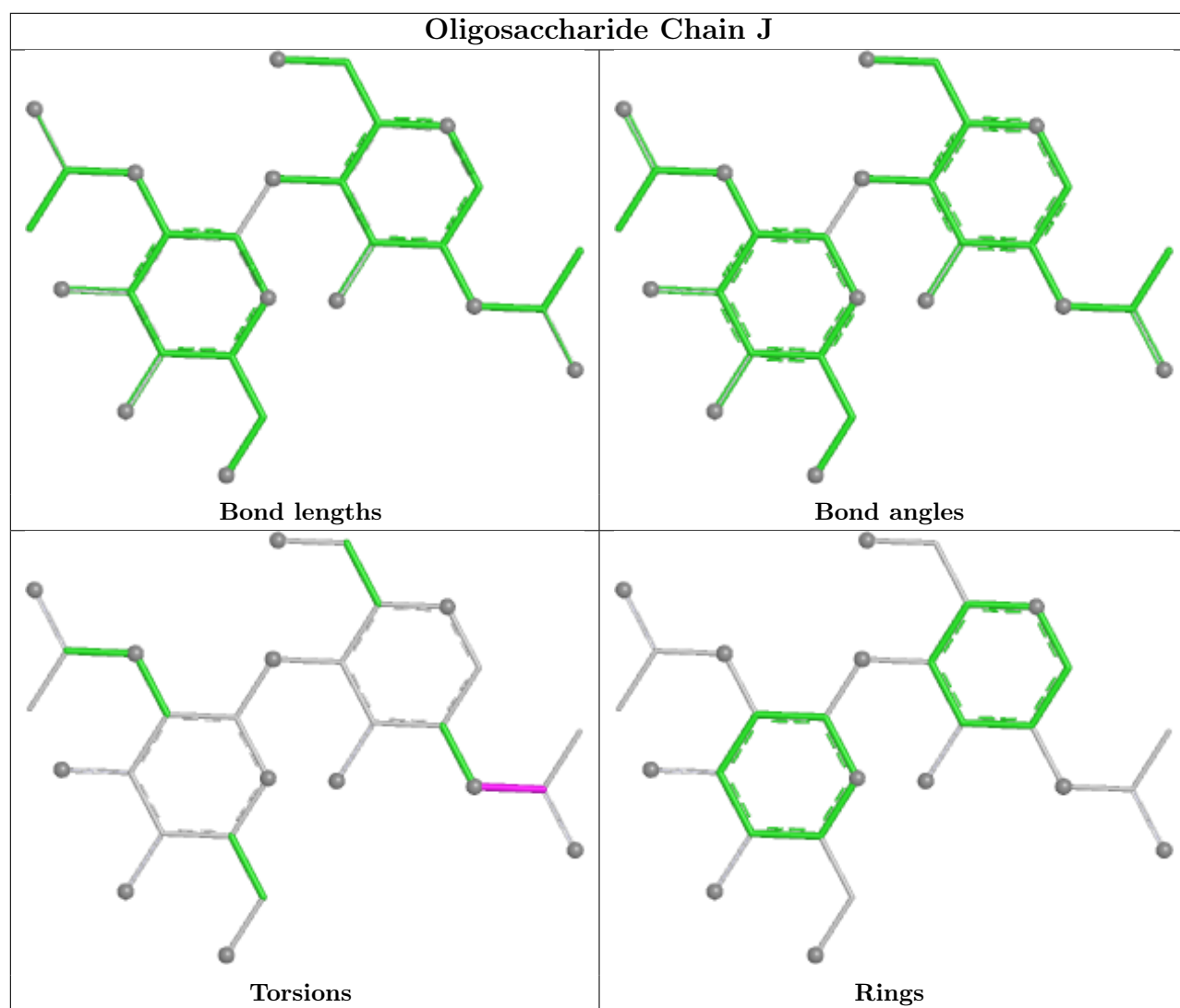


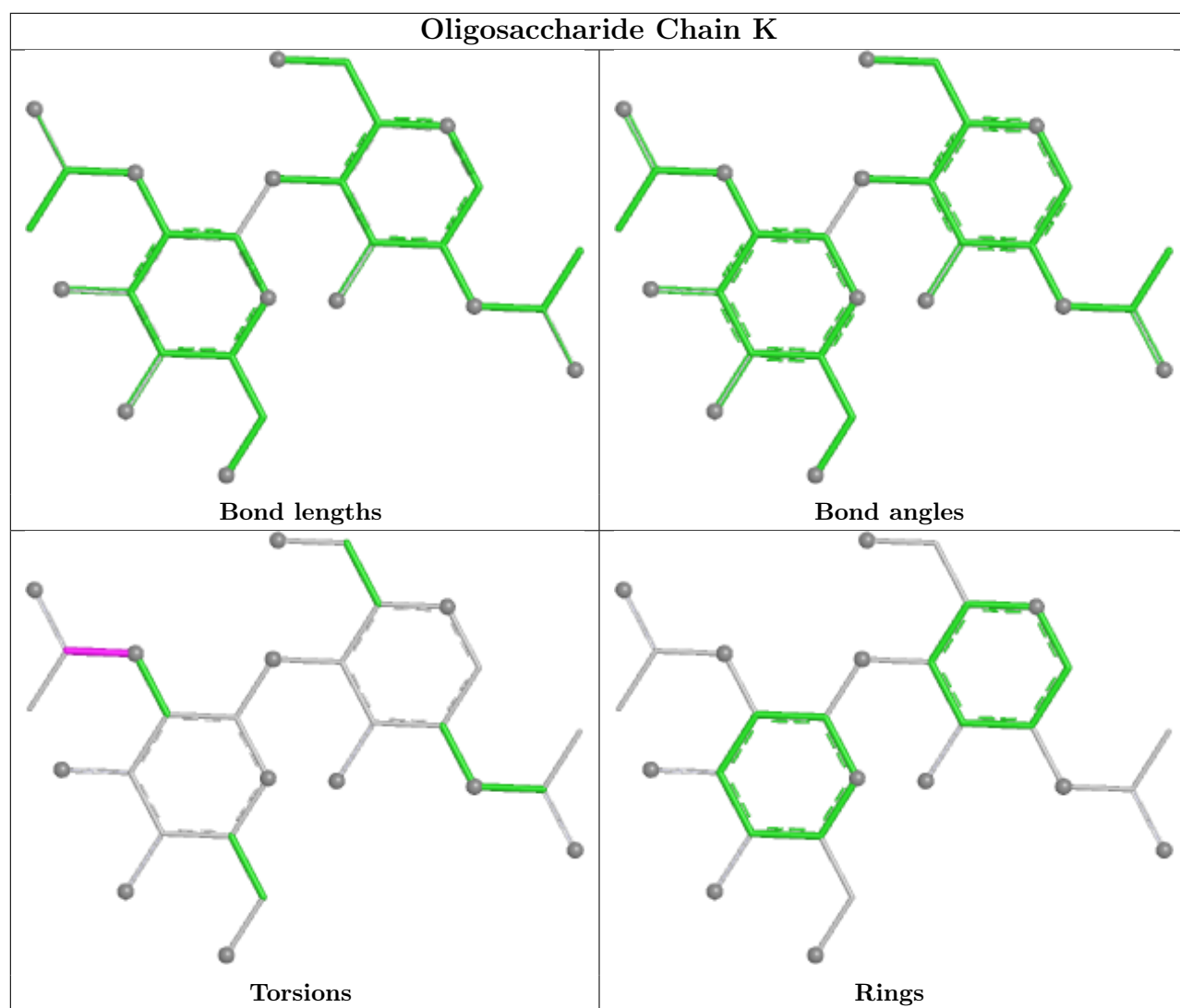


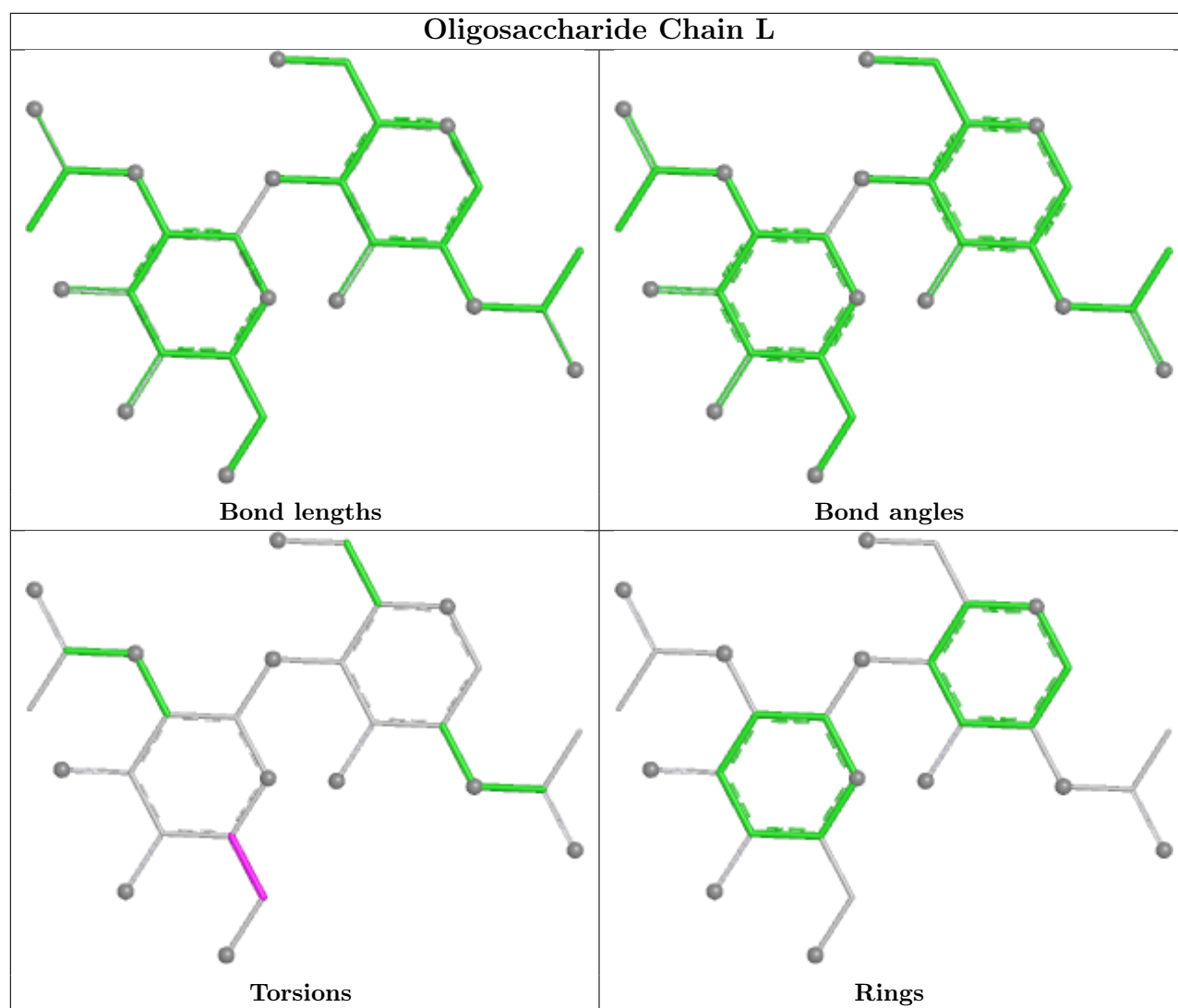


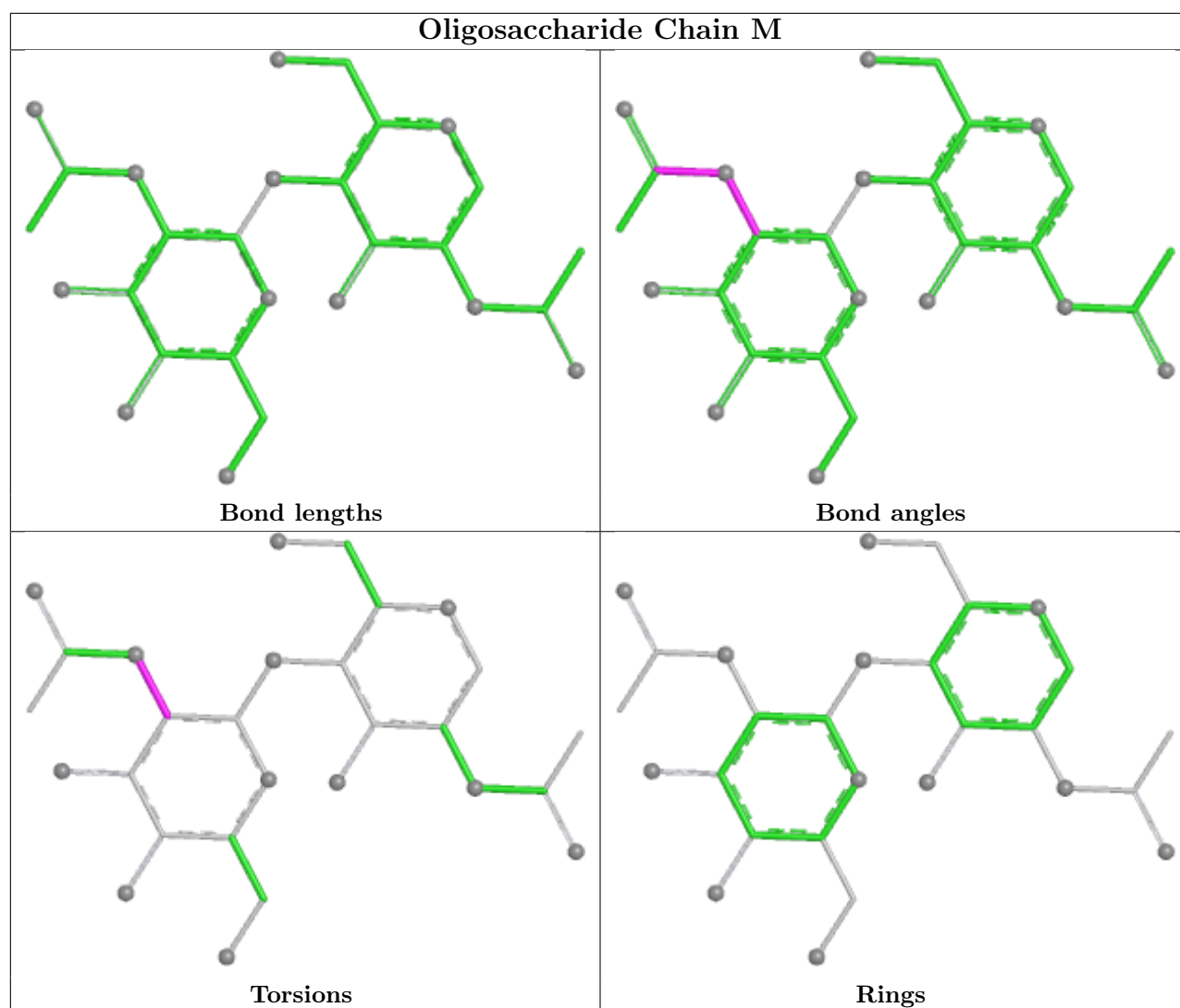












5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
3	NAG	C	1307	1	14,14,15	0.72	0	17,19,21	0.85	0
3	NAG	C	1304	1	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
3	NAG	B	1305	1	14,14,15	0.75	0	17,19,21	2.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1302	1	14,14,15	0.72	0	17,19,21	0.89	0
3	NAG	C	1303	1	14,14,15	0.72	0	17,19,21	2.37	3 (17%)
3	NAG	B	1304	1	14,14,15	0.70	0	17,19,21	0.82	0
3	NAG	A	1305	1	14,14,15	0.71	0	17,19,21	0.85	0
3	NAG	A	1303	1	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	C	1301	1	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	B	1307	1	14,14,15	0.71	0	17,19,21	0.84	0
3	NAG	A	1302	1	14,14,15	0.70	0	17,19,21	0.85	0
3	NAG	B	1303	1	14,14,15	0.71	0	17,19,21	0.73	0
3	NAG	A	1304	1	14,14,15	0.70	0	17,19,21	0.76	0
3	NAG	B	1302	1	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
3	NAG	A	1301	1	14,14,15	0.72	0	17,19,21	1.13	1 (5%)
3	NAG	B	1306	1	14,14,15	0.75	0	17,19,21	0.90	0
3	NAG	C	1308	1	14,14,15	0.71	0	17,19,21	0.75	0
3	NAG	B	1301	1	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	C	1306	1	14,14,15	0.71	0	17,19,21	1.23	1 (5%)
3	NAG	B	1308	1	14,14,15	0.69	0	17,19,21	0.83	0
3	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	0.44	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
3	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	5/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1305	NAG	C2-N2-C7	8.40	134.16	122.90
3	C	1303	NAG	C2-N2-C7	8.35	134.09	122.90
3	C	1304	NAG	C2-N2-C7	3.22	127.22	122.90
3	C	1306	NAG	C2-N2-C7	3.13	127.10	122.90
3	A	1301	NAG	C2-N2-C7	3.08	127.03	122.90
3	B	1305	NAG	C8-C7-N2	2.61	120.44	116.12
3	C	1303	NAG	C8-C7-N2	2.53	120.32	116.12
3	C	1303	NAG	C1-C2-N2	2.38	114.19	110.43
3	B	1305	NAG	C1-C2-N2	2.29	114.05	110.43
3	B	1302	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1305	NAG	C8-C7-N2-C2
3	A	1305	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1305	NAG	C8-C7-N2-C2
3	B	1305	NAG	O7-C7-N2-C2
3	B	1307	NAG	C8-C7-N2-C2
3	B	1307	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	1303	NAG	C8-C7-N2-C2
3	C	1303	NAG	O7-C7-N2-C2
3	C	1307	NAG	C8-C7-N2-C2
3	C	1307	NAG	O7-C7-N2-C2
3	B	1304	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	C1-C2-N2-C7
3	C	1304	NAG	C1-C2-N2-C7
3	A	1301	NAG	C3-C2-N2-C7
3	C	1306	NAG	C3-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	C	1303	NAG	C1-C2-N2-C7
3	C	1306	NAG	C1-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7
3	C	1304	NAG	C3-C2-N2-C7

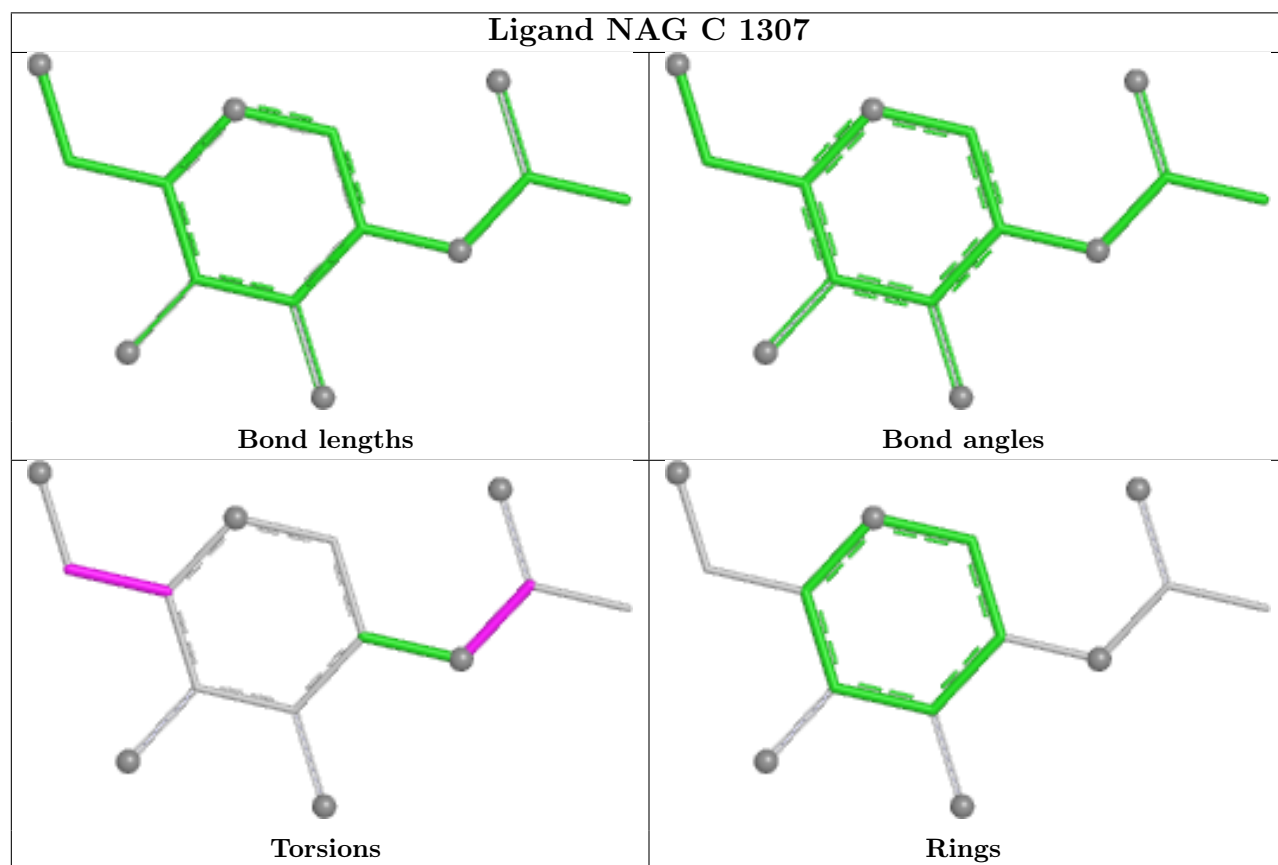
There are no ring outliers.

1 monomer is involved in 1 short contact:

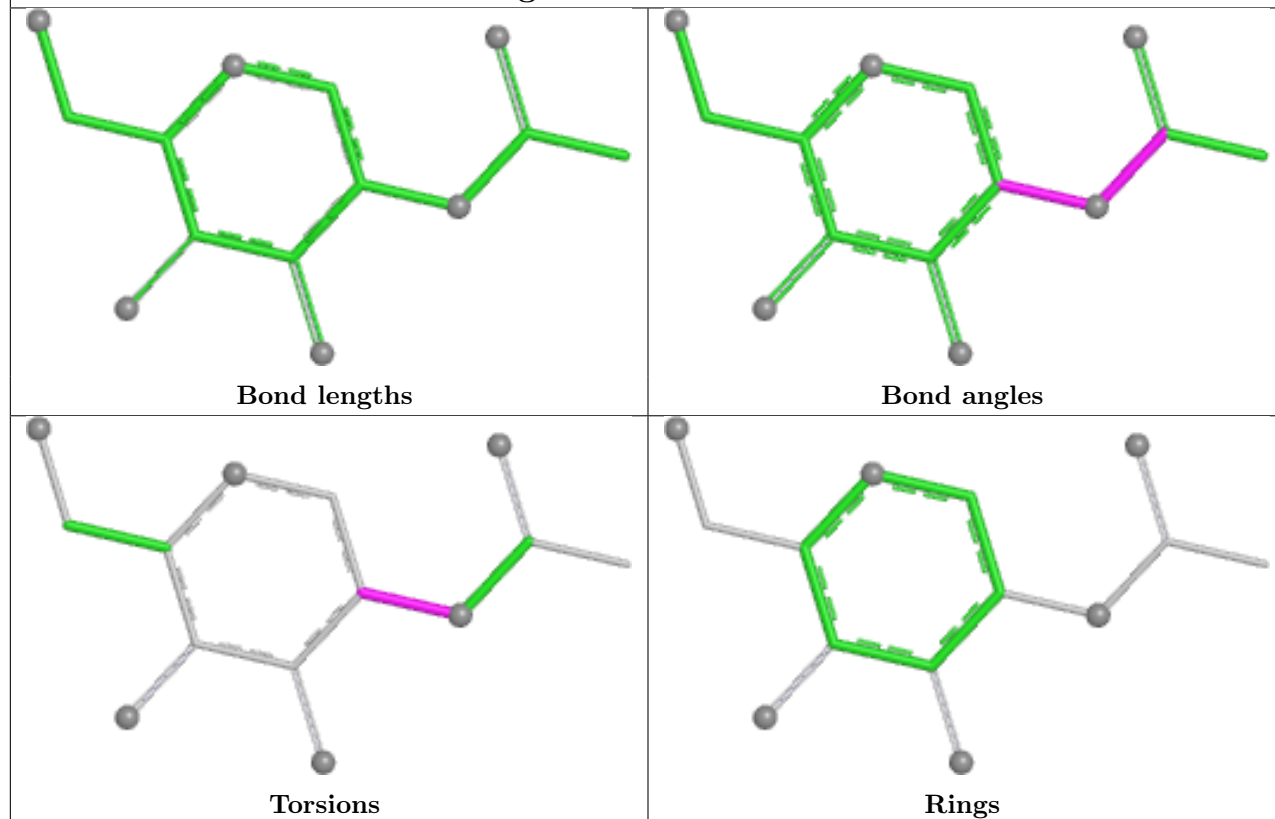
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1304	NAG	1	0

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

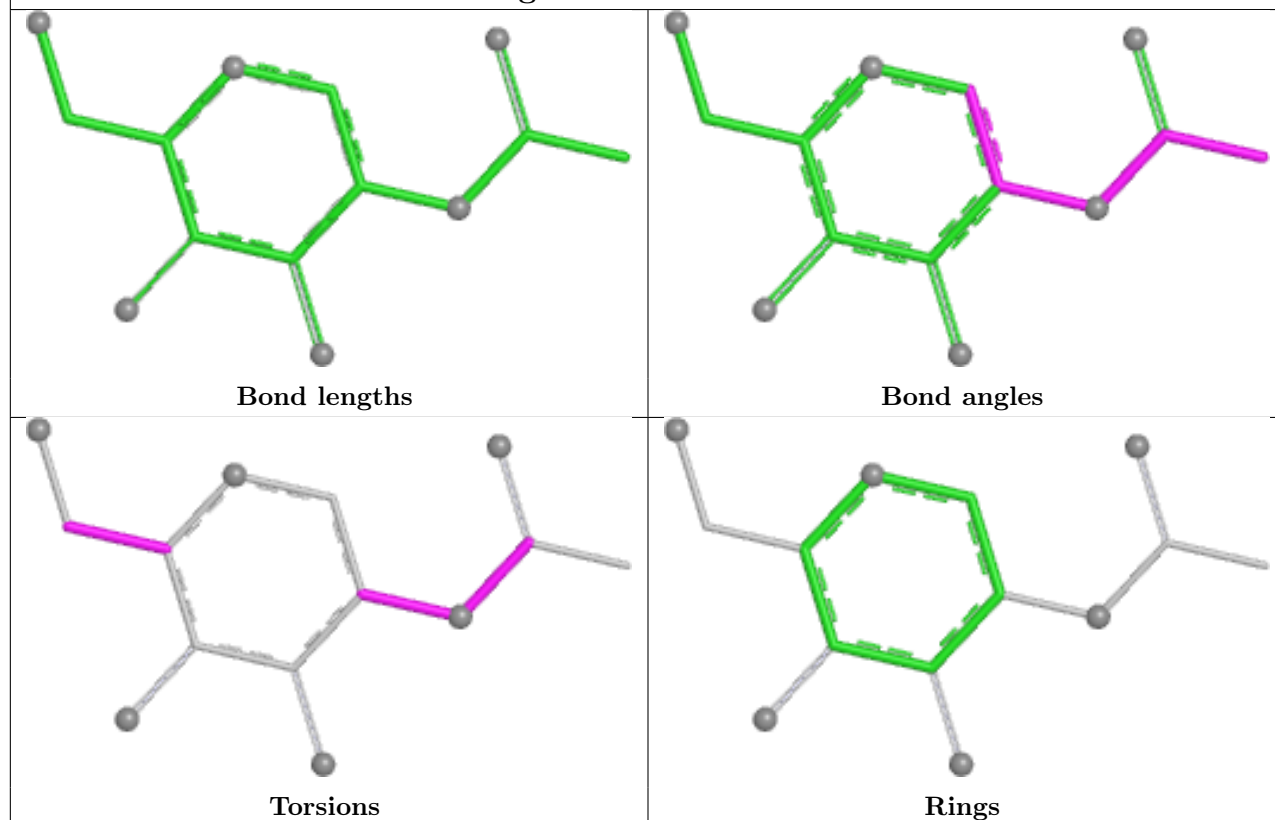
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

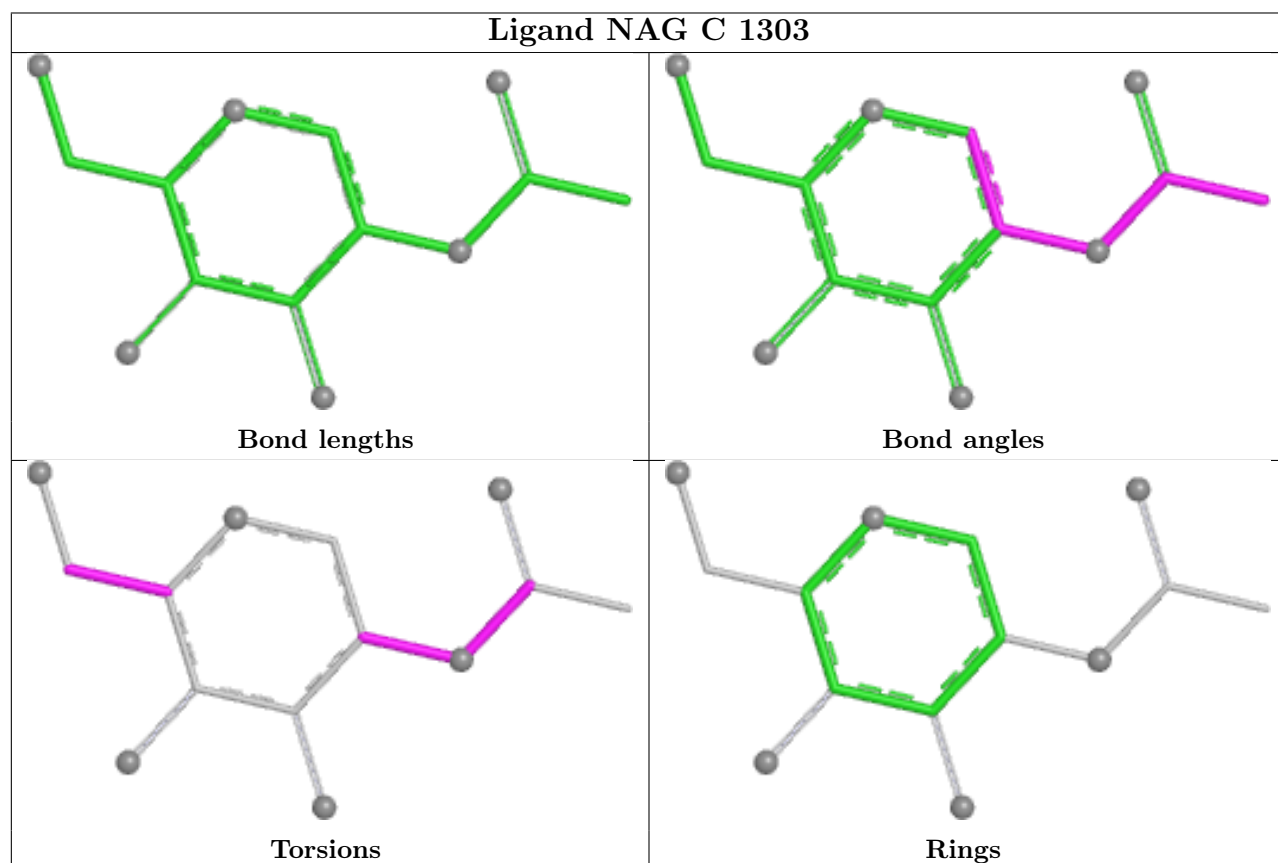
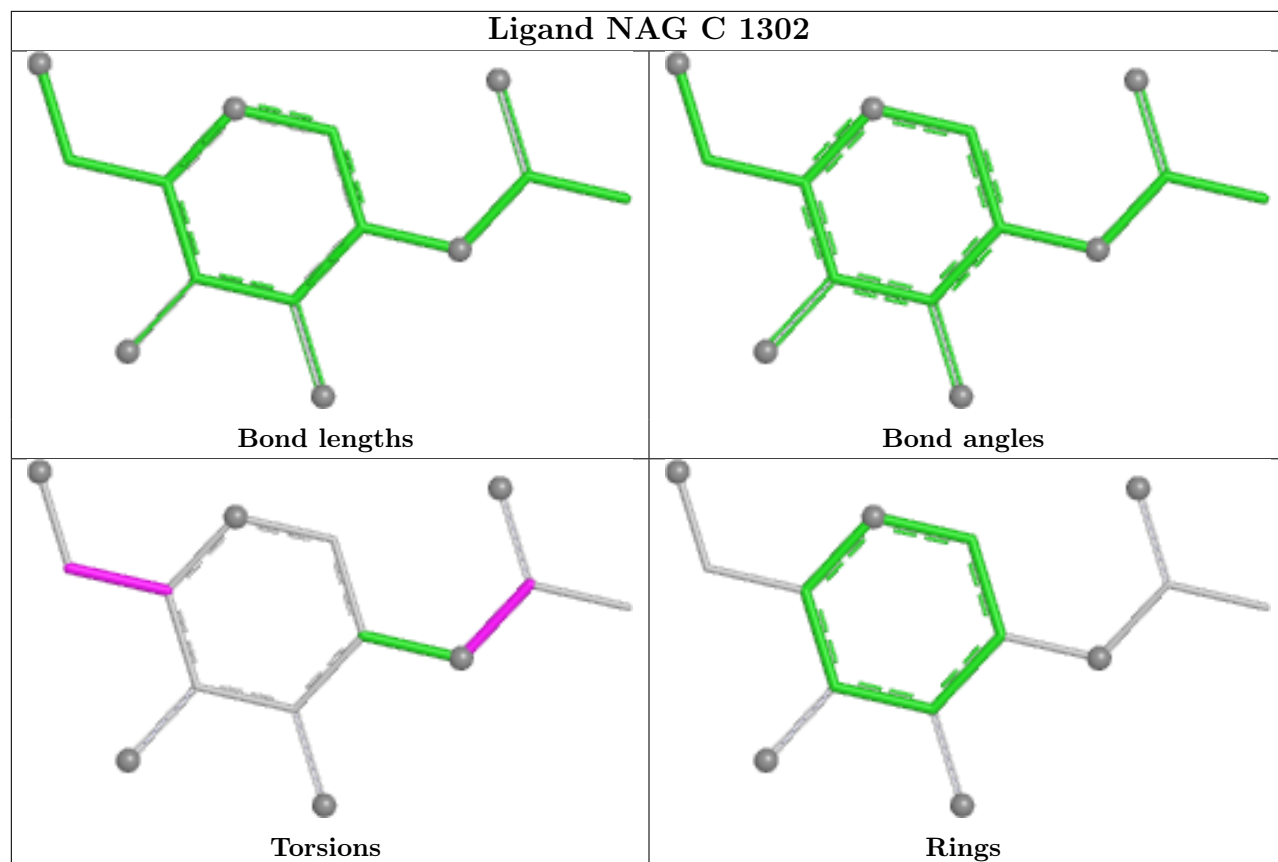


Ligand NAG C 1304

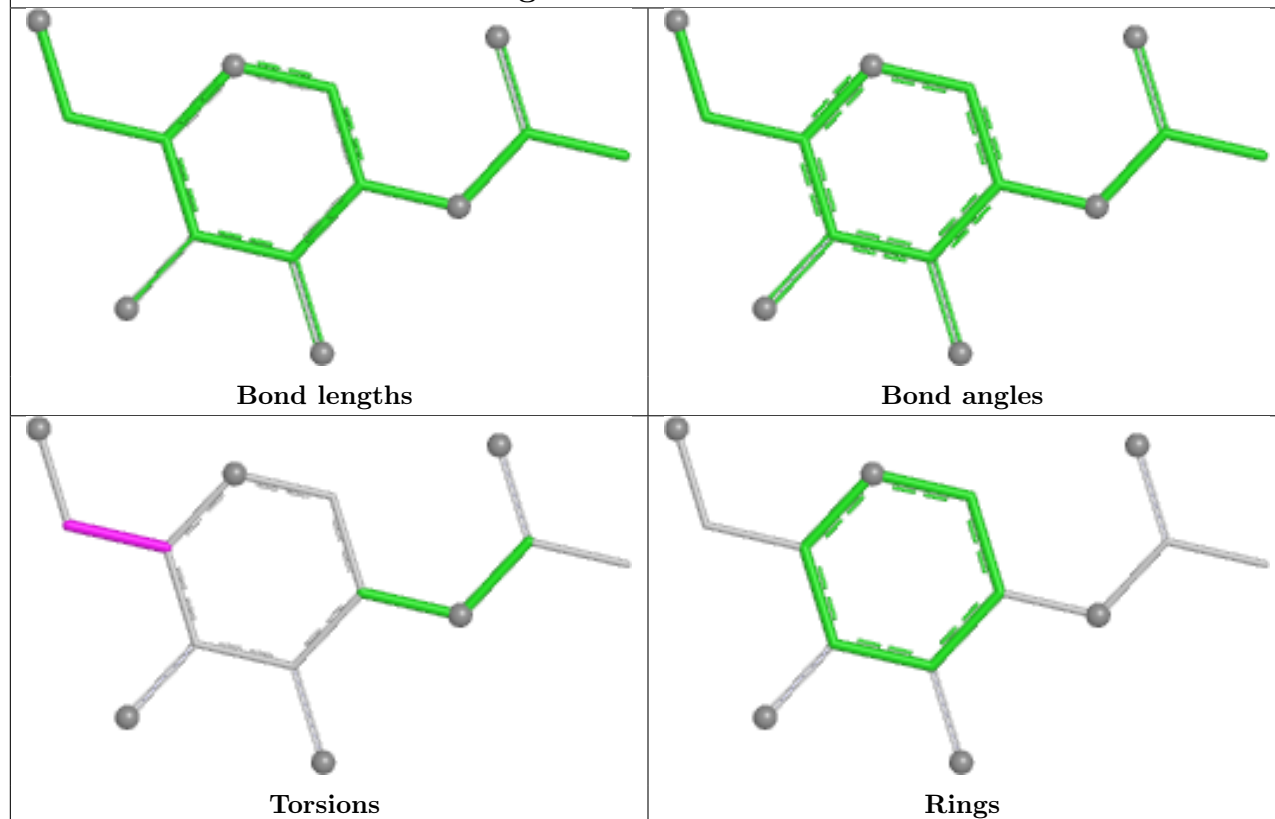


Ligand NAG B 1305

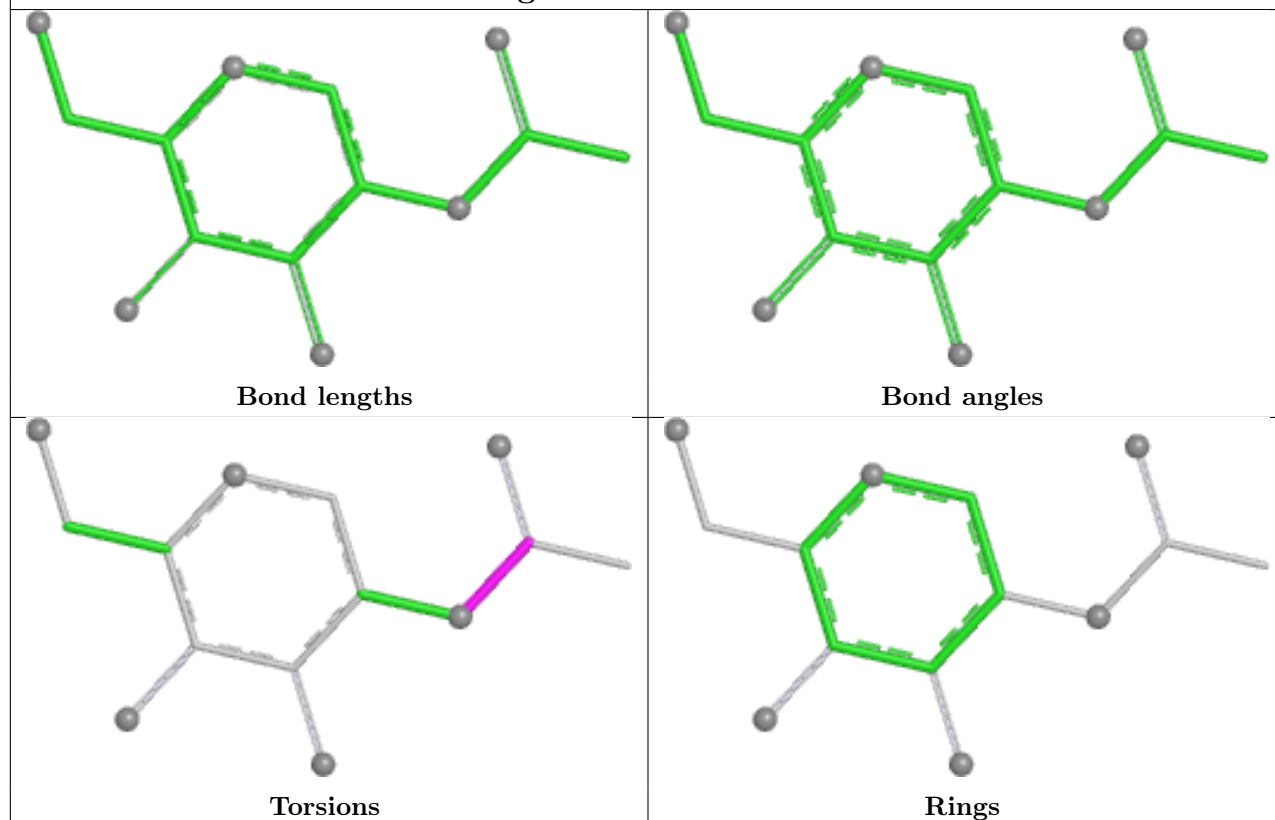




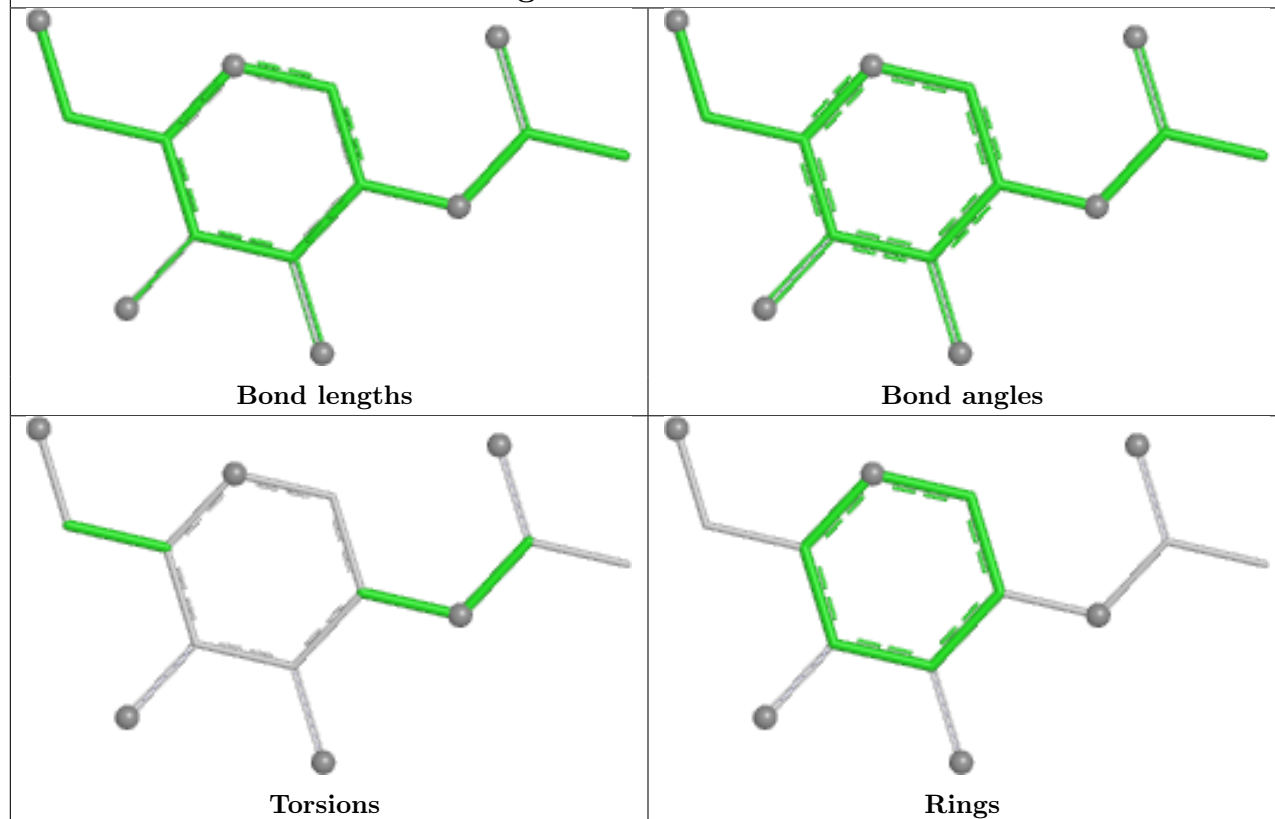
Ligand NAG B 1304



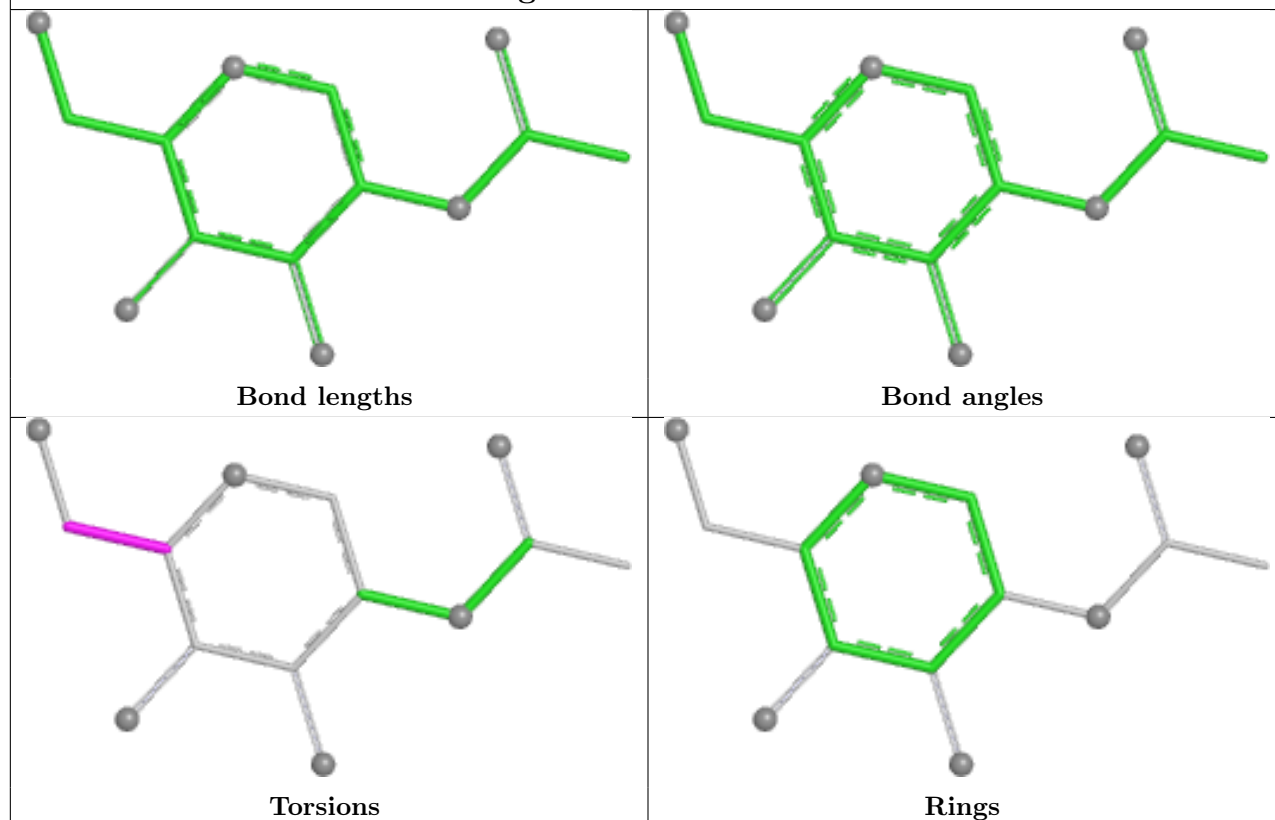
Ligand NAG A 1305



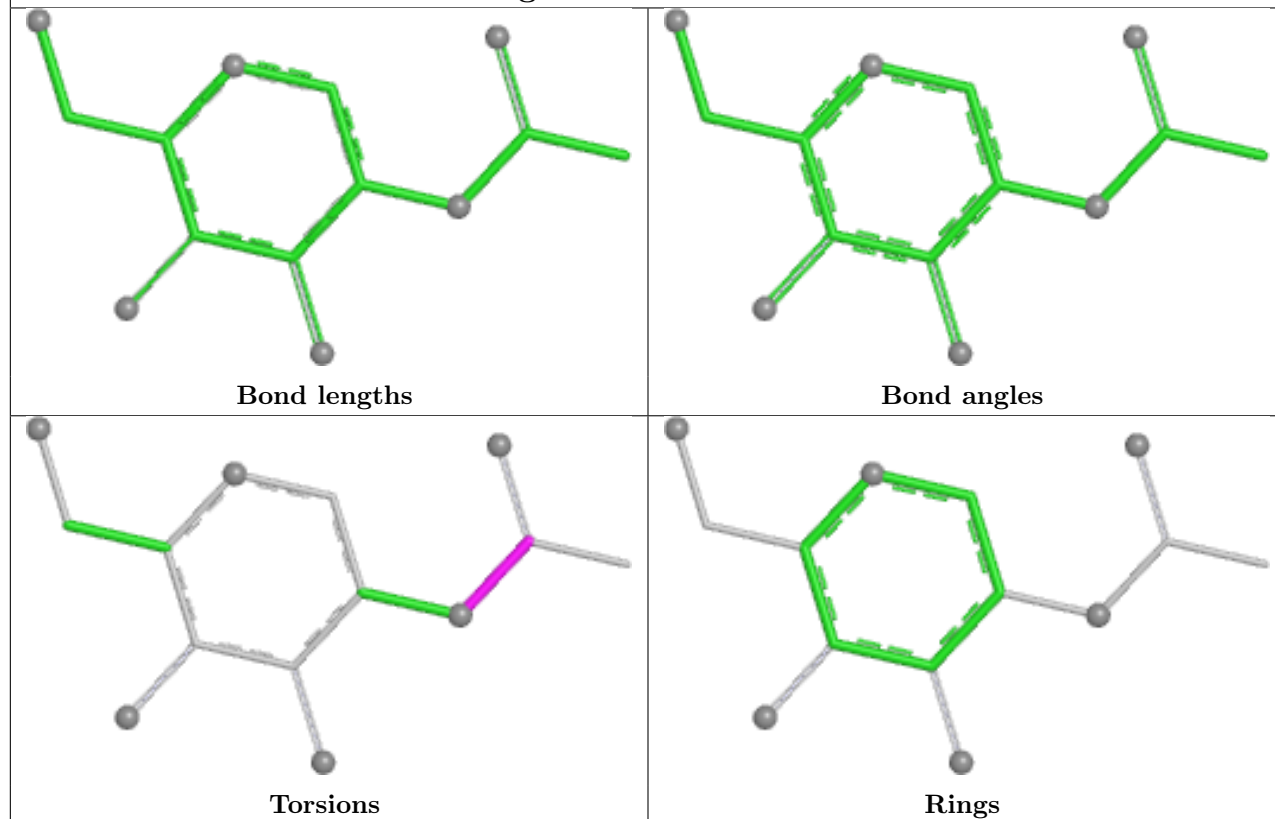
Ligand NAG A 1303



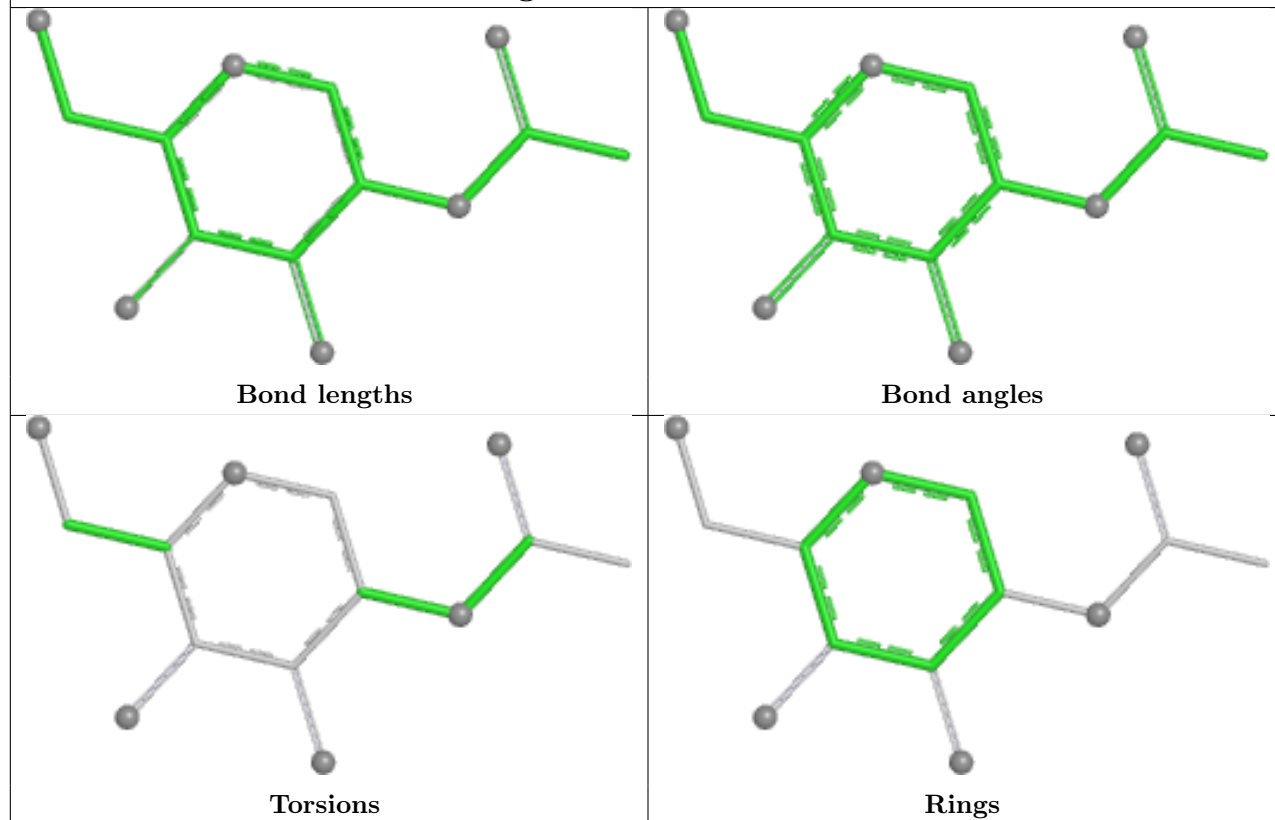
Ligand NAG C 1301



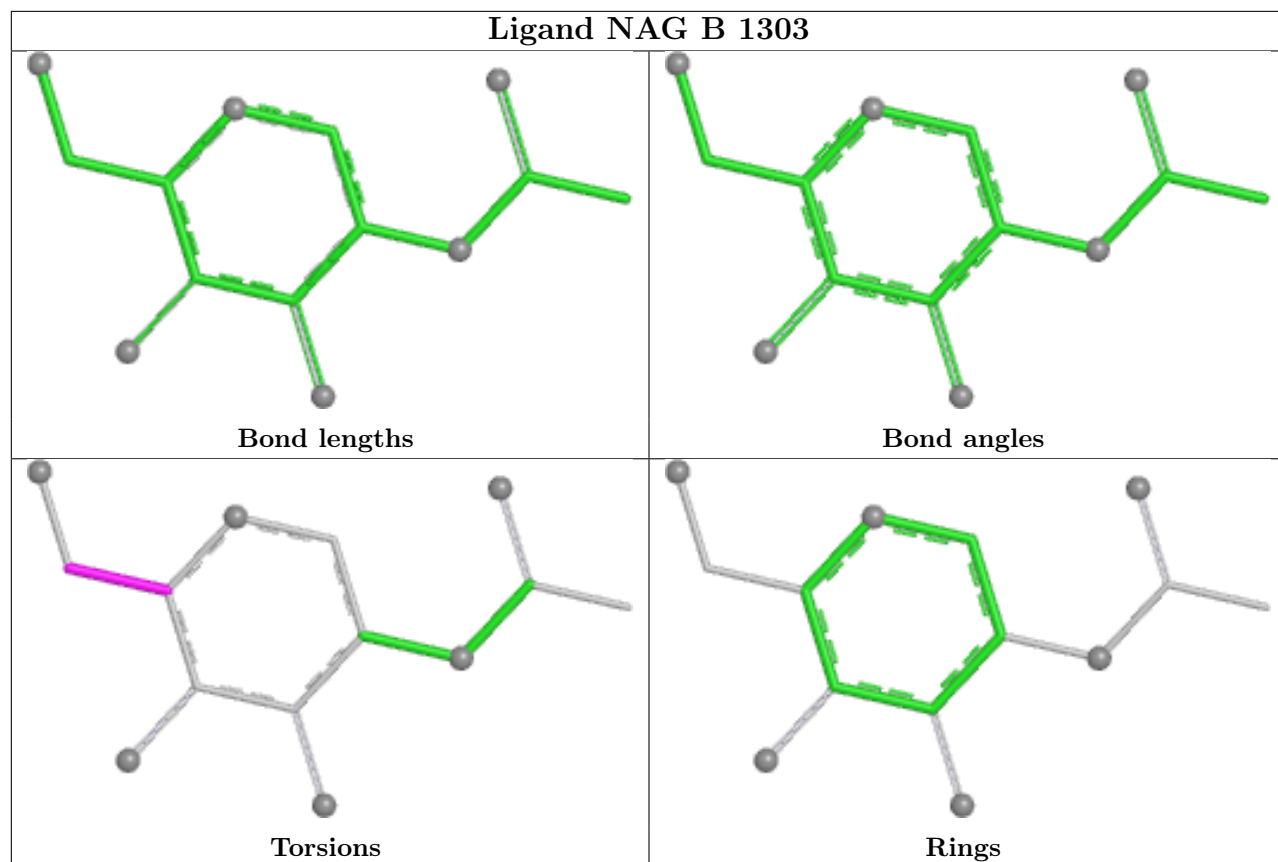
Ligand NAG B 1307



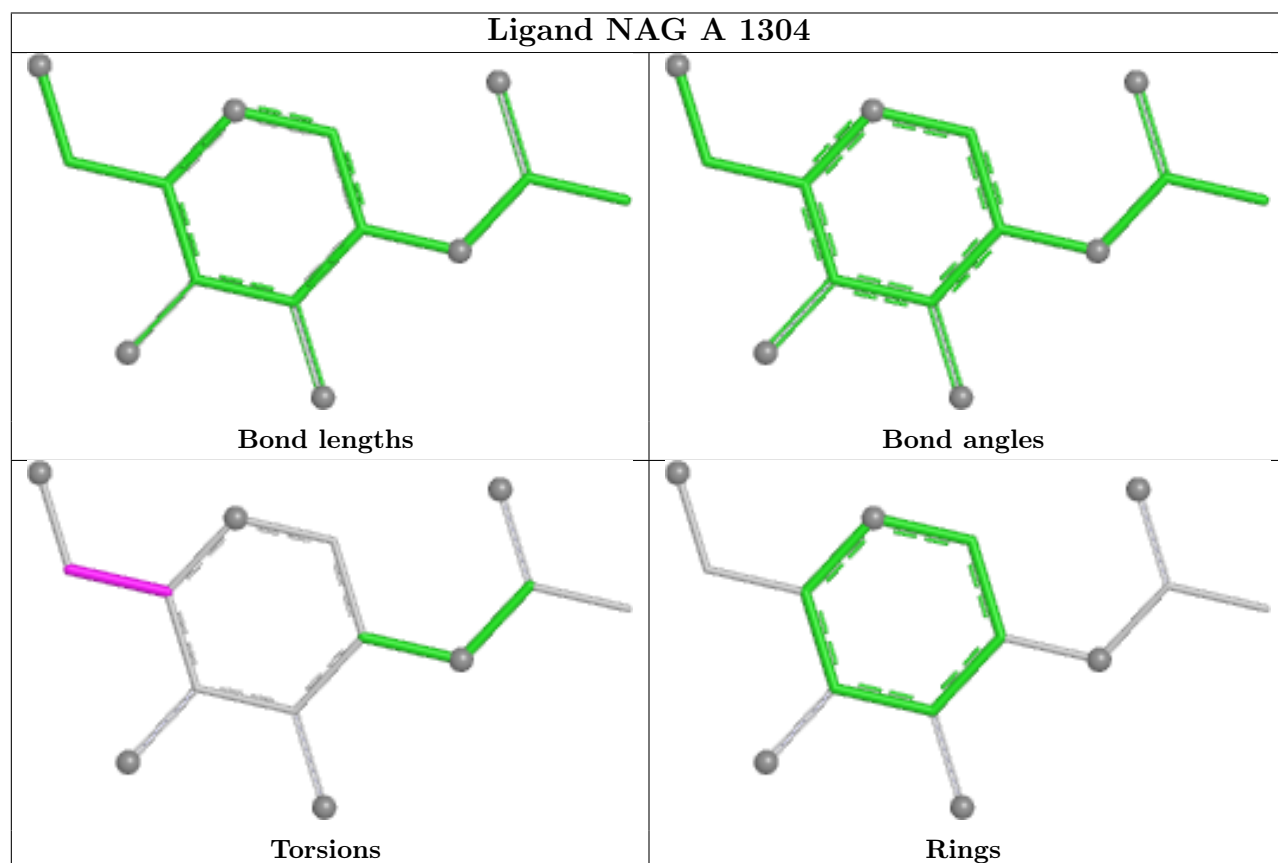
Ligand NAG A 1302



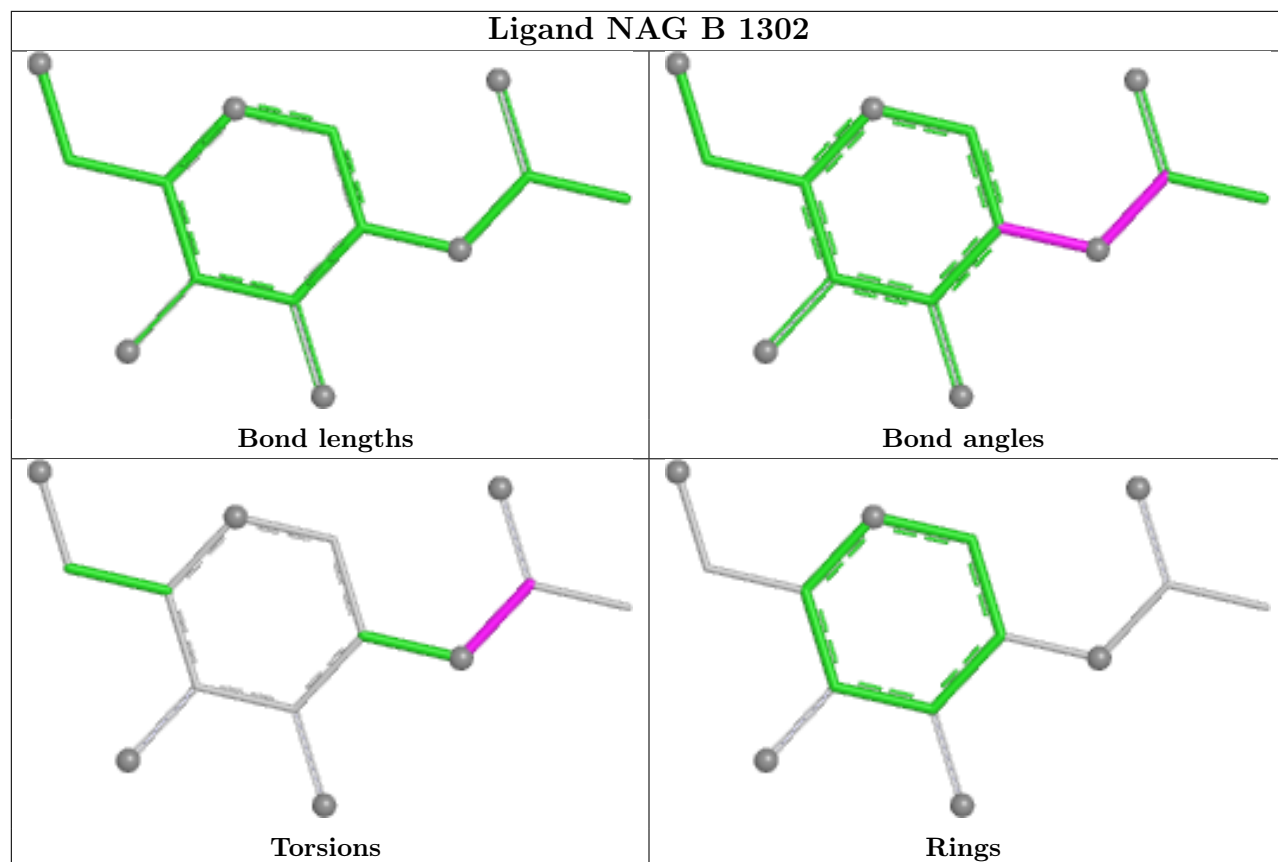
Ligand NAG B 1303



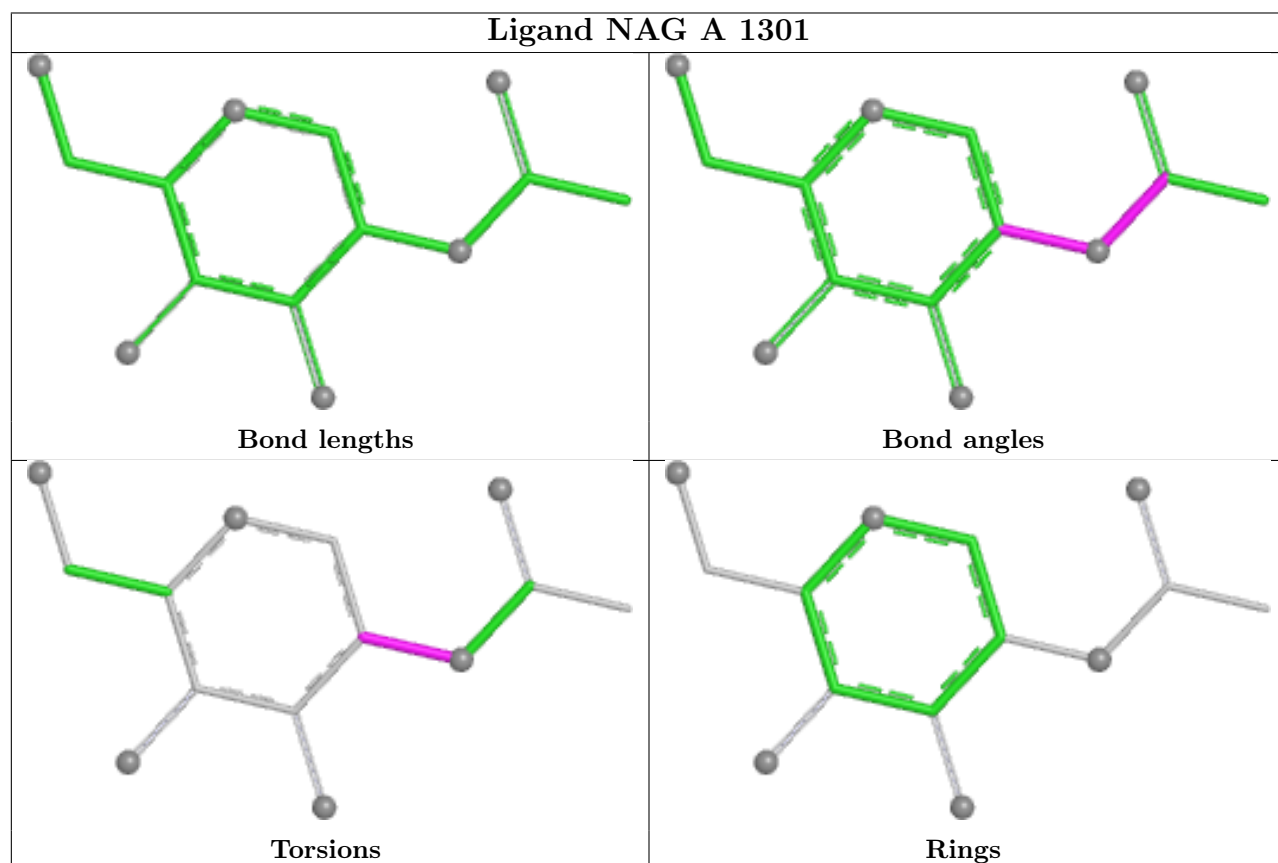
Ligand NAG A 1304



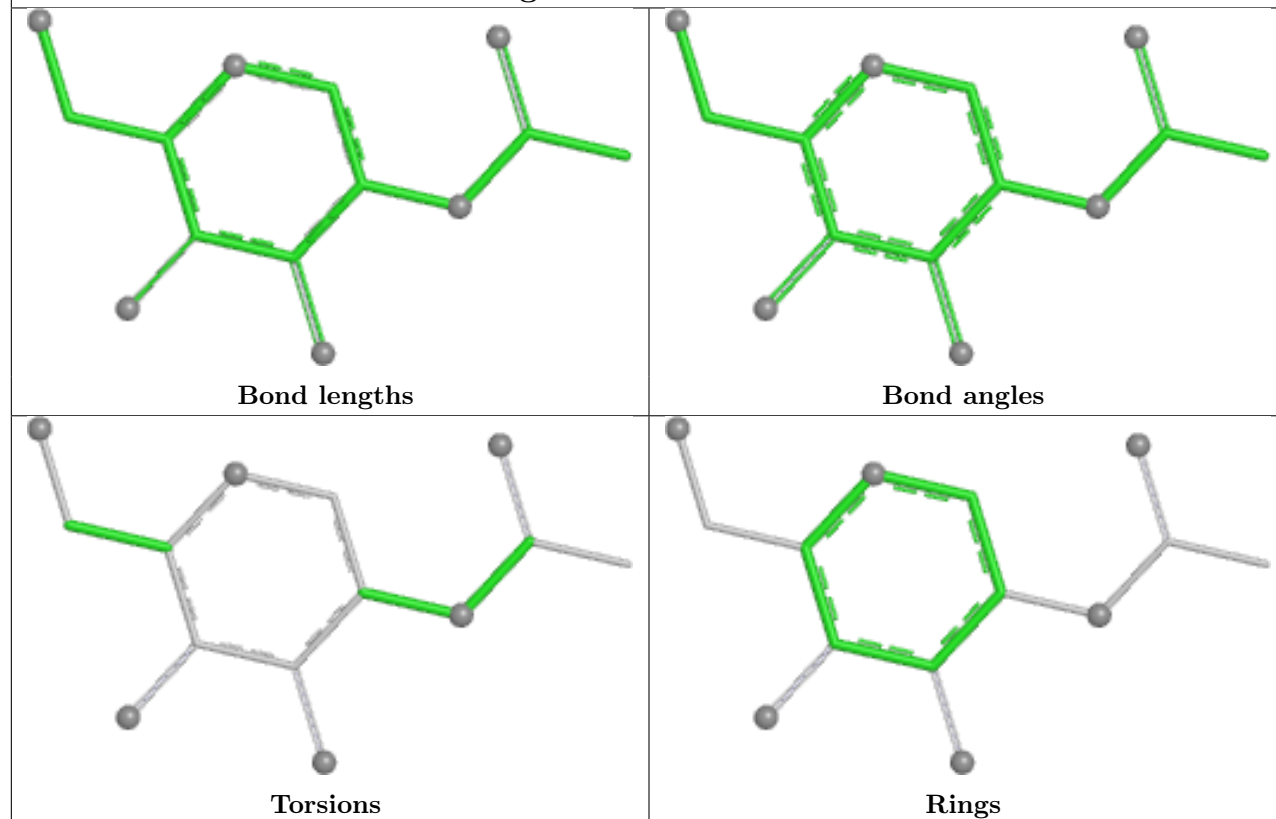
Ligand NAG B 1302



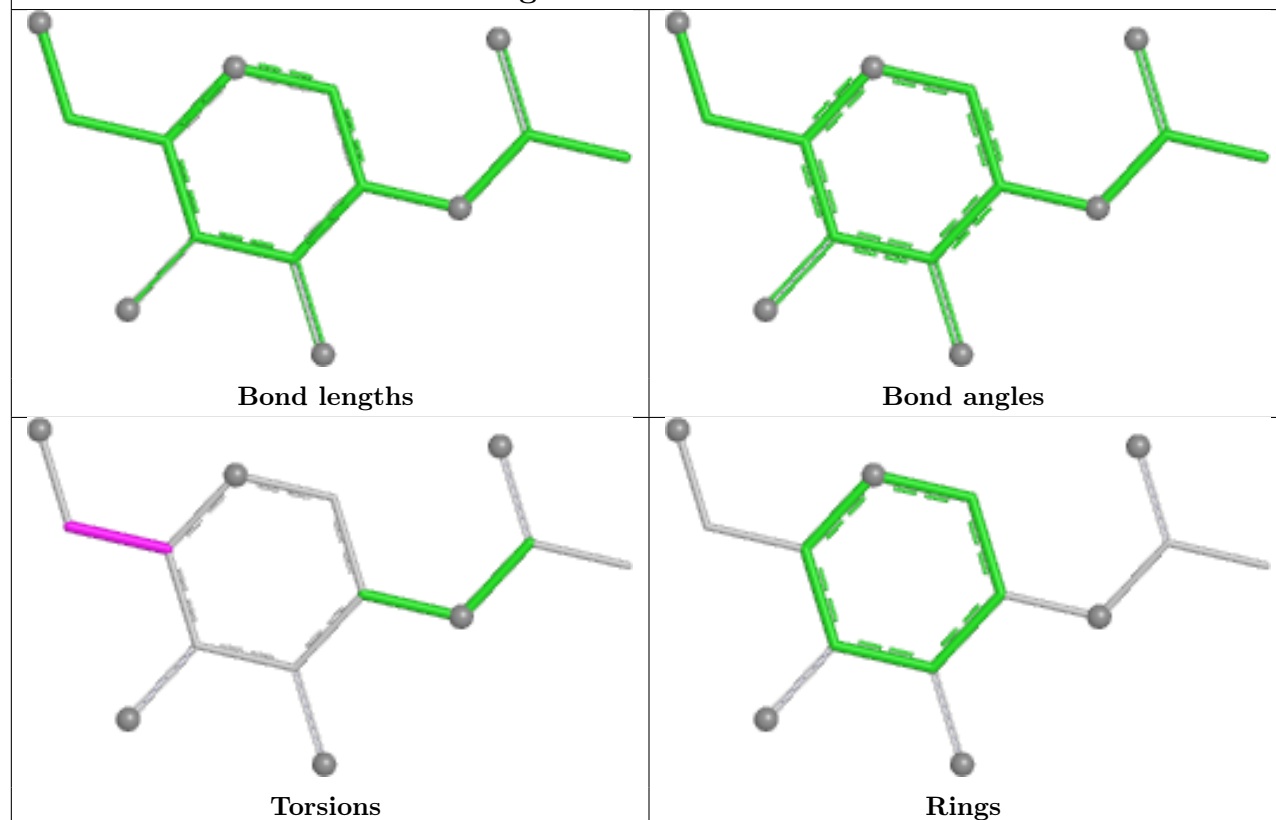
Ligand NAG A 1301



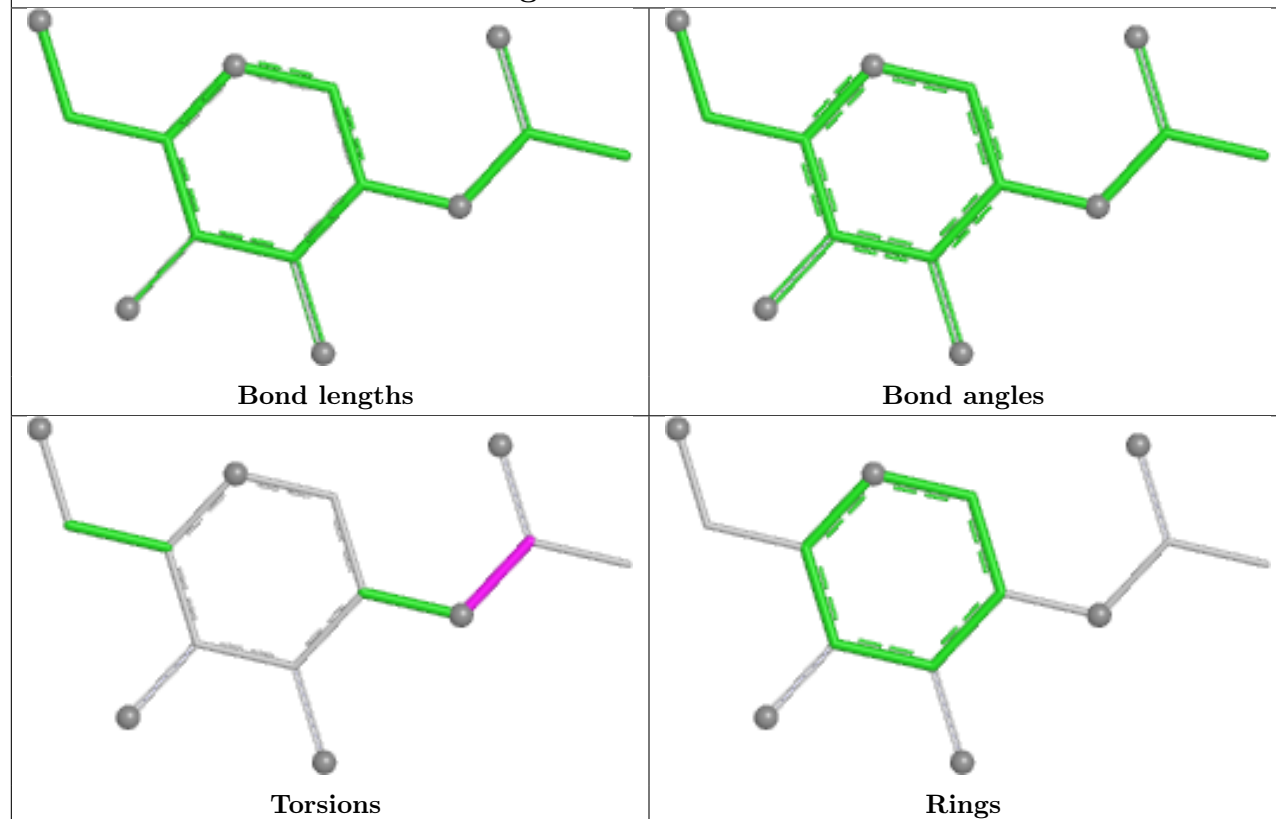
Ligand NAG B 1306



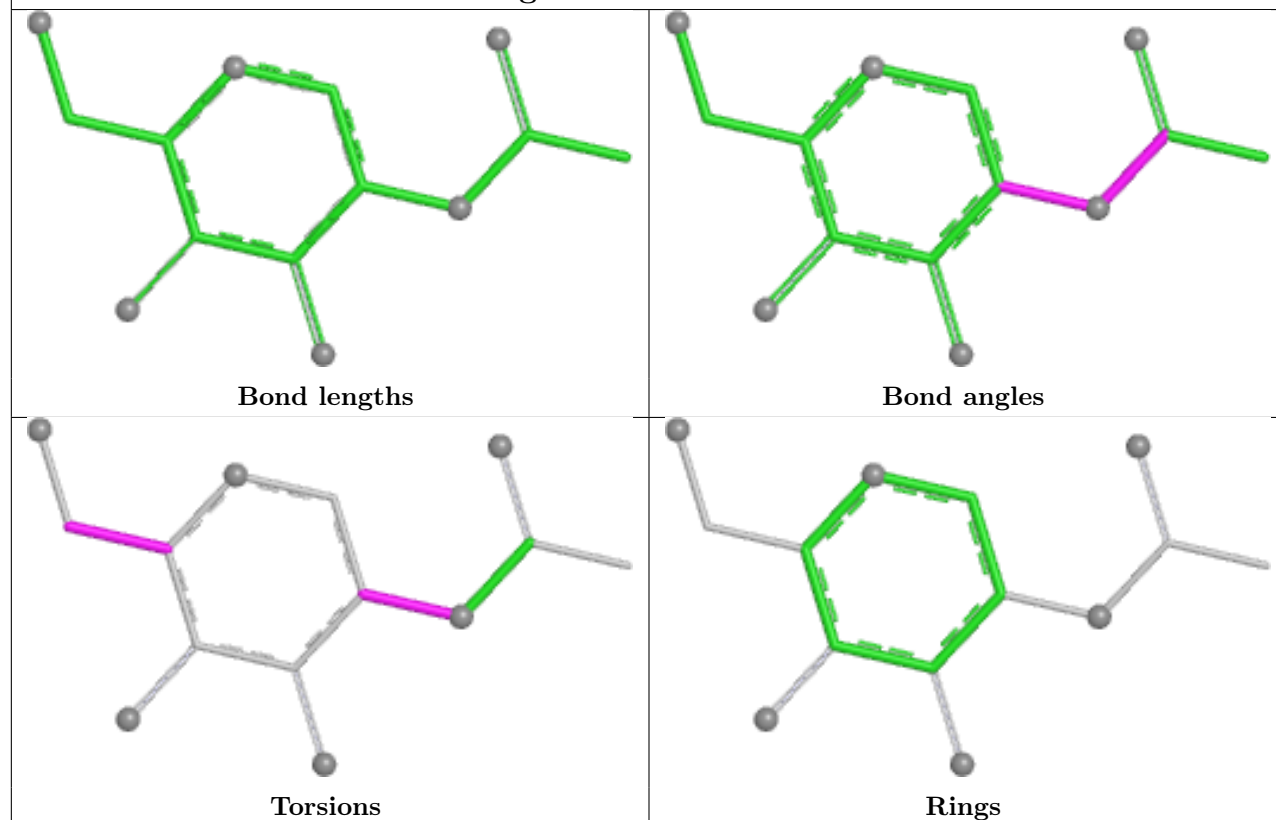
Ligand NAG C 1308



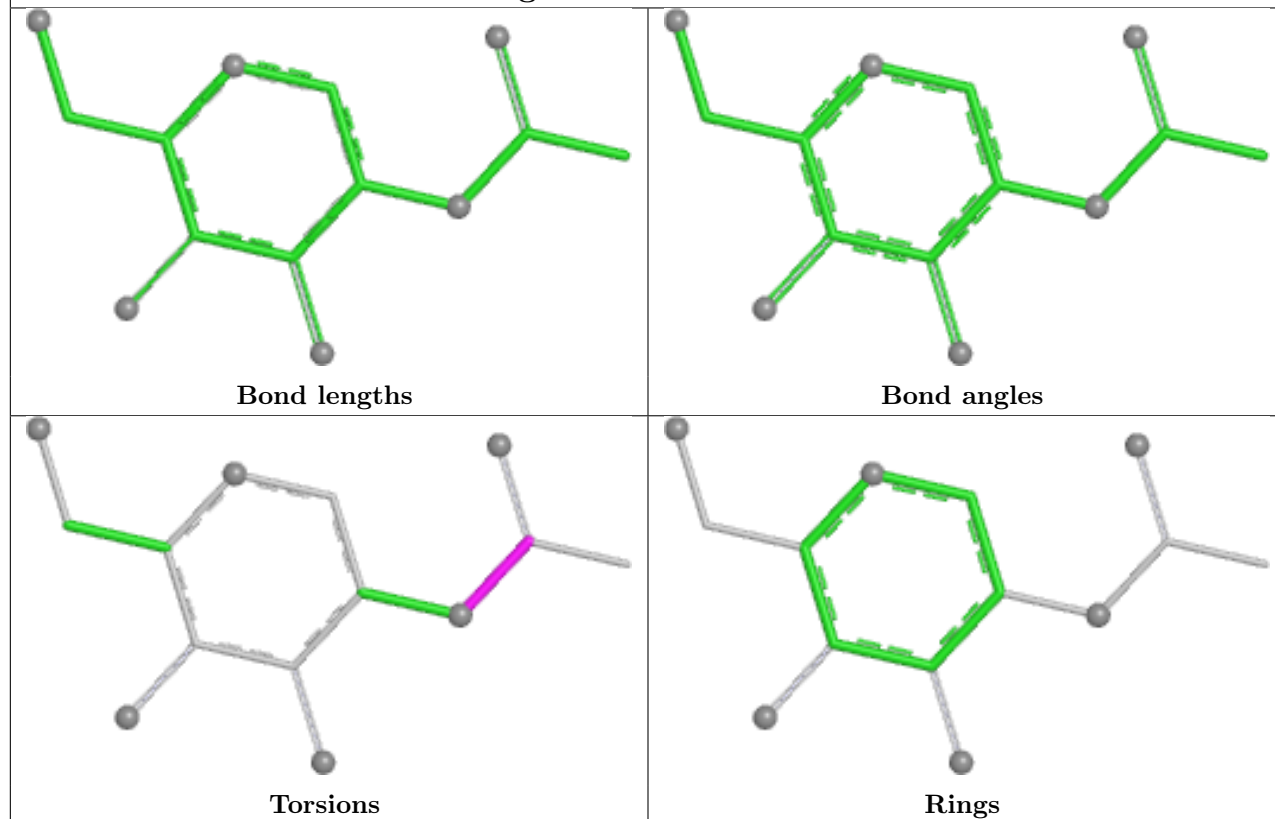
Ligand NAG B 1301



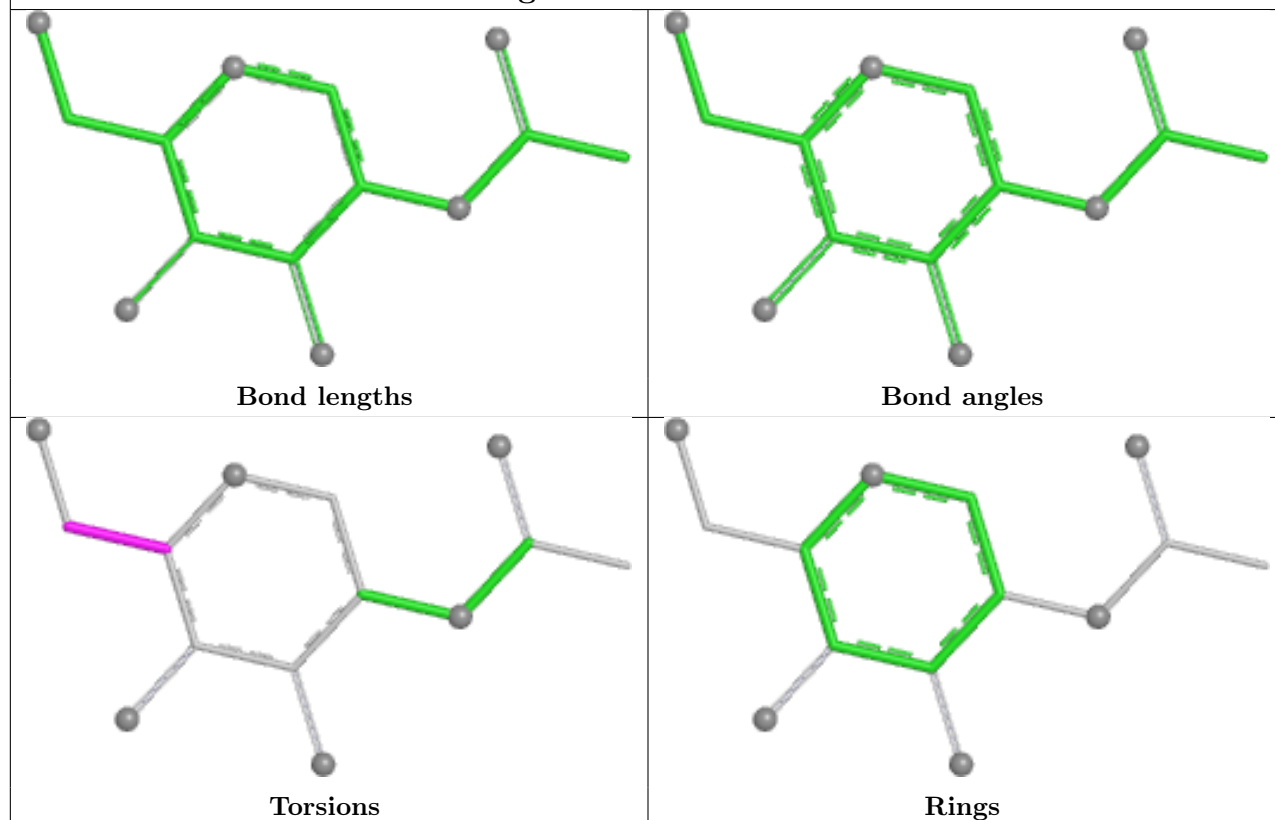
Ligand NAG C 1306



Ligand NAG B 1308



Ligand NAG C 1305



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.