



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:04 AM UTC

PDB ID : 9J5U / pdb_00009j5u
EMDB ID : EMD-61152
Title : Cryo-EM structure of Bat SARS-like coronavirus Khosta-2 spike protein
Authors : Pan, X.Q.; Li, L.J.; Liu, K.F.; Qi, J.X.; Gao, G.F.
Deposited on : 2024-08-13
Resolution : 2.25 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

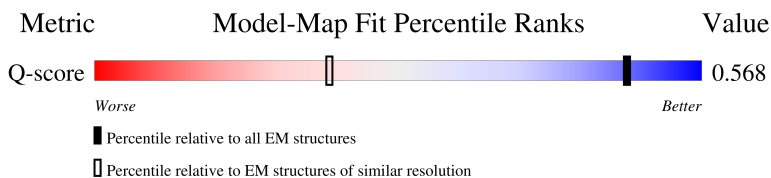
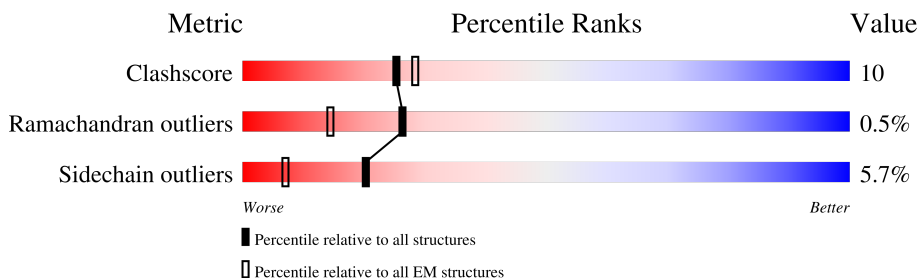
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 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	3458 (1.75 - 2.75)

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	A	1229	 7% 70% 18% • 10%
1	B	1229	 11% 69% 18% • 10%
1	C	1229	 7% 69% 18% • 10%
2	D	3	 100% 67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	
2	G	3	
2	J	3	
3	E	4	
3	H	4	
3	N	4	
3	S	4	
3	Y	4	
3	a	4	
4	I	4	
5	K	2	
5	M	2	
5	O	2	
5	P	2	
5	Q	2	
5	R	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	
5	Z	2	
5	b	2	
6	L	2	
6	T	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27152 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1103	Total	C	N	O	S	0	0
			8597	5472	1435	1642	48		
1	B	1103	Total	C	N	O	S	0	0
			8597	5472	1435	1642	48		
1	C	1103	Total	C	N	O	S	0	0
			8597	5472	1435	1642	48		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	797	PRO	PHE	conflict	UNP A0A8E6HRK4
A	872	PRO	ALA	conflict	UNP A0A8E6HRK4
A	879	PRO	ALA	conflict	UNP A0A8E6HRK4
A	922	PRO	ALA	conflict	UNP A0A8E6HRK4
A	966	PRO	LYS	conflict	UNP A0A8E6HRK4
A	967	PRO	VAL	conflict	UNP A0A8E6HRK4
A	1195	GLY	-	expression tag	UNP A0A8E6HRK4
A	1196	GLY	-	expression tag	UNP A0A8E6HRK4
A	1197	GLY	-	expression tag	UNP A0A8E6HRK4
A	1198	SER	-	expression tag	UNP A0A8E6HRK4
A	1199	GLY	-	expression tag	UNP A0A8E6HRK4
A	1200	GLY	-	expression tag	UNP A0A8E6HRK4
A	1201	GLY	-	expression tag	UNP A0A8E6HRK4
A	1202	SER	-	expression tag	UNP A0A8E6HRK4
A	1203	GLY	-	expression tag	UNP A0A8E6HRK4
A	1204	TYR	-	expression tag	UNP A0A8E6HRK4
A	1205	ILE	-	expression tag	UNP A0A8E6HRK4
A	1206	PRO	-	expression tag	UNP A0A8E6HRK4
A	1207	GLU	-	expression tag	UNP A0A8E6HRK4
A	1208	ALA	-	expression tag	UNP A0A8E6HRK4
A	1209	PRO	-	expression tag	UNP A0A8E6HRK4
A	1210	ARG	-	expression tag	UNP A0A8E6HRK4
A	1211	ASP	-	expression tag	UNP A0A8E6HRK4
A	1212	GLY	-	expression tag	UNP A0A8E6HRK4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1213	GLN	-	expression tag	UNP A0A8E6HRK4
A	1214	ALA	-	expression tag	UNP A0A8E6HRK4
A	1215	TYR	-	expression tag	UNP A0A8E6HRK4
A	1216	VAL	-	expression tag	UNP A0A8E6HRK4
A	1217	ARG	-	expression tag	UNP A0A8E6HRK4
A	1218	LYS	-	expression tag	UNP A0A8E6HRK4
A	1219	ASP	-	expression tag	UNP A0A8E6HRK4
A	1220	GLY	-	expression tag	UNP A0A8E6HRK4
A	1221	GLU	-	expression tag	UNP A0A8E6HRK4
A	1222	TRP	-	expression tag	UNP A0A8E6HRK4
A	1223	VAL	-	expression tag	UNP A0A8E6HRK4
A	1224	LEU	-	expression tag	UNP A0A8E6HRK4
A	1225	LEU	-	expression tag	UNP A0A8E6HRK4
A	1226	SER	-	expression tag	UNP A0A8E6HRK4
A	1227	THR	-	expression tag	UNP A0A8E6HRK4
A	1228	PHE	-	expression tag	UNP A0A8E6HRK4
A	1229	LEU	-	expression tag	UNP A0A8E6HRK4
A	1230	GLY	-	expression tag	UNP A0A8E6HRK4
A	1231	GLY	-	expression tag	UNP A0A8E6HRK4
A	1232	GLY	-	expression tag	UNP A0A8E6HRK4
A	1233	SER	-	expression tag	UNP A0A8E6HRK4
A	1234	ALA	-	expression tag	UNP A0A8E6HRK4
A	1235	TRP	-	expression tag	UNP A0A8E6HRK4
A	1236	SER	-	expression tag	UNP A0A8E6HRK4
A	1237	HIS	-	expression tag	UNP A0A8E6HRK4
A	1238	PRO	-	expression tag	UNP A0A8E6HRK4
A	1239	GLN	-	expression tag	UNP A0A8E6HRK4
A	1240	PHE	-	expression tag	UNP A0A8E6HRK4
A	1241	GLU	-	expression tag	UNP A0A8E6HRK4
A	1242	LYS	-	expression tag	UNP A0A8E6HRK4
B	797	PRO	PHE	conflict	UNP A0A8E6HRK4
B	872	PRO	ALA	conflict	UNP A0A8E6HRK4
B	879	PRO	ALA	conflict	UNP A0A8E6HRK4
B	922	PRO	ALA	conflict	UNP A0A8E6HRK4
B	966	PRO	LYS	conflict	UNP A0A8E6HRK4
B	967	PRO	VAL	conflict	UNP A0A8E6HRK4
B	1195	GLY	-	expression tag	UNP A0A8E6HRK4
B	1196	GLY	-	expression tag	UNP A0A8E6HRK4
B	1197	GLY	-	expression tag	UNP A0A8E6HRK4
B	1198	SER	-	expression tag	UNP A0A8E6HRK4
B	1199	GLY	-	expression tag	UNP A0A8E6HRK4
B	1200	GLY	-	expression tag	UNP A0A8E6HRK4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	GLY	-	expression tag	UNP A0A8E6HRK4
B	1202	SER	-	expression tag	UNP A0A8E6HRK4
B	1203	GLY	-	expression tag	UNP A0A8E6HRK4
B	1204	TYR	-	expression tag	UNP A0A8E6HRK4
B	1205	ILE	-	expression tag	UNP A0A8E6HRK4
B	1206	PRO	-	expression tag	UNP A0A8E6HRK4
B	1207	GLU	-	expression tag	UNP A0A8E6HRK4
B	1208	ALA	-	expression tag	UNP A0A8E6HRK4
B	1209	PRO	-	expression tag	UNP A0A8E6HRK4
B	1210	ARG	-	expression tag	UNP A0A8E6HRK4
B	1211	ASP	-	expression tag	UNP A0A8E6HRK4
B	1212	GLY	-	expression tag	UNP A0A8E6HRK4
B	1213	GLN	-	expression tag	UNP A0A8E6HRK4
B	1214	ALA	-	expression tag	UNP A0A8E6HRK4
B	1215	TYR	-	expression tag	UNP A0A8E6HRK4
B	1216	VAL	-	expression tag	UNP A0A8E6HRK4
B	1217	ARG	-	expression tag	UNP A0A8E6HRK4
B	1218	LYS	-	expression tag	UNP A0A8E6HRK4
B	1219	ASP	-	expression tag	UNP A0A8E6HRK4
B	1220	GLY	-	expression tag	UNP A0A8E6HRK4
B	1221	GLU	-	expression tag	UNP A0A8E6HRK4
B	1222	TRP	-	expression tag	UNP A0A8E6HRK4
B	1223	VAL	-	expression tag	UNP A0A8E6HRK4
B	1224	LEU	-	expression tag	UNP A0A8E6HRK4
B	1225	LEU	-	expression tag	UNP A0A8E6HRK4
B	1226	SER	-	expression tag	UNP A0A8E6HRK4
B	1227	THR	-	expression tag	UNP A0A8E6HRK4
B	1228	PHE	-	expression tag	UNP A0A8E6HRK4
B	1229	LEU	-	expression tag	UNP A0A8E6HRK4
B	1230	GLY	-	expression tag	UNP A0A8E6HRK4
B	1231	GLY	-	expression tag	UNP A0A8E6HRK4
B	1232	GLY	-	expression tag	UNP A0A8E6HRK4
B	1233	SER	-	expression tag	UNP A0A8E6HRK4
B	1234	ALA	-	expression tag	UNP A0A8E6HRK4
B	1235	TRP	-	expression tag	UNP A0A8E6HRK4
B	1236	SER	-	expression tag	UNP A0A8E6HRK4
B	1237	HIS	-	expression tag	UNP A0A8E6HRK4
B	1238	PRO	-	expression tag	UNP A0A8E6HRK4
B	1239	GLN	-	expression tag	UNP A0A8E6HRK4
B	1240	PHE	-	expression tag	UNP A0A8E6HRK4
B	1241	GLU	-	expression tag	UNP A0A8E6HRK4
B	1242	LYS	-	expression tag	UNP A0A8E6HRK4

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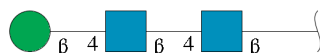
Chain	Residue	Modelled	Actual	Comment	Reference
C	797	PRO	PHE	conflict	UNP A0A8E6HRK4
C	872	PRO	ALA	conflict	UNP A0A8E6HRK4
C	879	PRO	ALA	conflict	UNP A0A8E6HRK4
C	922	PRO	ALA	conflict	UNP A0A8E6HRK4
C	966	PRO	LYS	conflict	UNP A0A8E6HRK4
C	967	PRO	VAL	conflict	UNP A0A8E6HRK4
C	1195	GLY	-	expression tag	UNP A0A8E6HRK4
C	1196	GLY	-	expression tag	UNP A0A8E6HRK4
C	1197	GLY	-	expression tag	UNP A0A8E6HRK4
C	1198	SER	-	expression tag	UNP A0A8E6HRK4
C	1199	GLY	-	expression tag	UNP A0A8E6HRK4
C	1200	GLY	-	expression tag	UNP A0A8E6HRK4
C	1201	GLY	-	expression tag	UNP A0A8E6HRK4
C	1202	SER	-	expression tag	UNP A0A8E6HRK4
C	1203	GLY	-	expression tag	UNP A0A8E6HRK4
C	1204	TYR	-	expression tag	UNP A0A8E6HRK4
C	1205	ILE	-	expression tag	UNP A0A8E6HRK4
C	1206	PRO	-	expression tag	UNP A0A8E6HRK4
C	1207	GLU	-	expression tag	UNP A0A8E6HRK4
C	1208	ALA	-	expression tag	UNP A0A8E6HRK4
C	1209	PRO	-	expression tag	UNP A0A8E6HRK4
C	1210	ARG	-	expression tag	UNP A0A8E6HRK4
C	1211	ASP	-	expression tag	UNP A0A8E6HRK4
C	1212	GLY	-	expression tag	UNP A0A8E6HRK4
C	1213	GLN	-	expression tag	UNP A0A8E6HRK4
C	1214	ALA	-	expression tag	UNP A0A8E6HRK4
C	1215	TYR	-	expression tag	UNP A0A8E6HRK4
C	1216	VAL	-	expression tag	UNP A0A8E6HRK4
C	1217	ARG	-	expression tag	UNP A0A8E6HRK4
C	1218	LYS	-	expression tag	UNP A0A8E6HRK4
C	1219	ASP	-	expression tag	UNP A0A8E6HRK4
C	1220	GLY	-	expression tag	UNP A0A8E6HRK4
C	1221	GLU	-	expression tag	UNP A0A8E6HRK4
C	1222	TRP	-	expression tag	UNP A0A8E6HRK4
C	1223	VAL	-	expression tag	UNP A0A8E6HRK4
C	1224	LEU	-	expression tag	UNP A0A8E6HRK4
C	1225	LEU	-	expression tag	UNP A0A8E6HRK4
C	1226	SER	-	expression tag	UNP A0A8E6HRK4
C	1227	THR	-	expression tag	UNP A0A8E6HRK4
C	1228	PHE	-	expression tag	UNP A0A8E6HRK4
C	1229	LEU	-	expression tag	UNP A0A8E6HRK4
C	1230	GLY	-	expression tag	UNP A0A8E6HRK4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1231	GLY	-	expression tag	UNP A0A8E6HRK4
C	1232	GLY	-	expression tag	UNP A0A8E6HRK4
C	1233	SER	-	expression tag	UNP A0A8E6HRK4
C	1234	ALA	-	expression tag	UNP A0A8E6HRK4
C	1235	TRP	-	expression tag	UNP A0A8E6HRK4
C	1236	SER	-	expression tag	UNP A0A8E6HRK4
C	1237	HIS	-	expression tag	UNP A0A8E6HRK4
C	1238	PRO	-	expression tag	UNP A0A8E6HRK4
C	1239	GLN	-	expression tag	UNP A0A8E6HRK4
C	1240	PHE	-	expression tag	UNP A0A8E6HRK4
C	1241	GLU	-	expression tag	UNP A0A8E6HRK4
C	1242	LYS	-	expression tag	UNP A0A8E6HRK4

- Molecule 2 is an oligosaccharide called 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	G	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
3	E	4	Total	C	N	O	0	0
			50	28	2	20		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	4	Total	C	N	O	0	0
			50	28	2	20		
3	N	4	Total	C	N	O	0	0
			50	28	2	20		
3	S	4	Total	C	N	O	0	0
			50	28	2	20		
3	Y	4	Total	C	N	O	0	0
			50	28	2	20		
3	a	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is an oligosaccharide called 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
4	I	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 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
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	2	Total	C	N	O	0	0
			25	14	1	10		
6	T	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



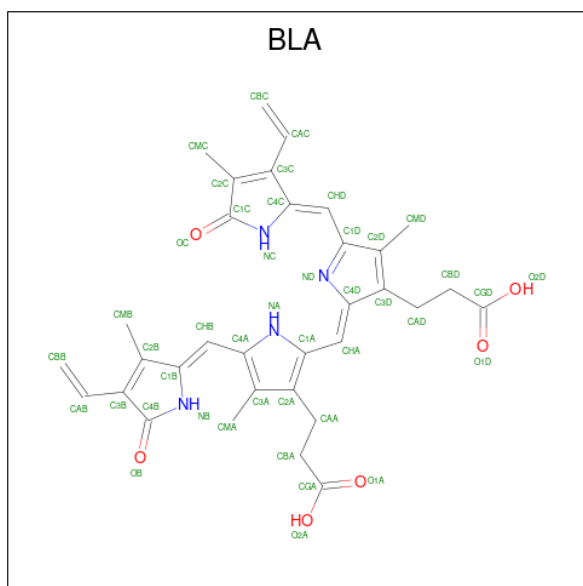
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7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

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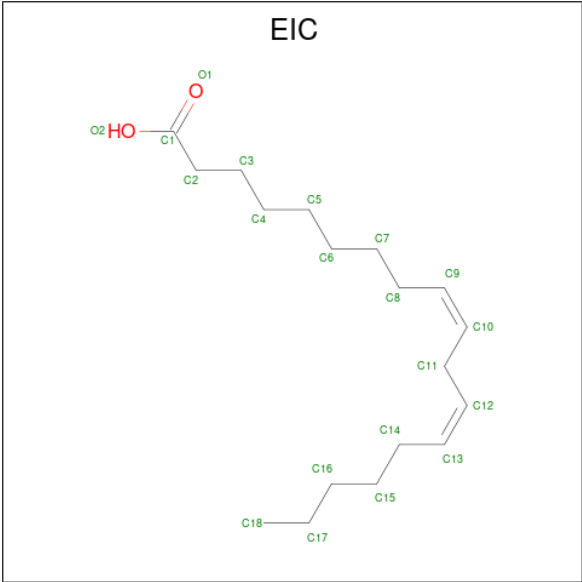
Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



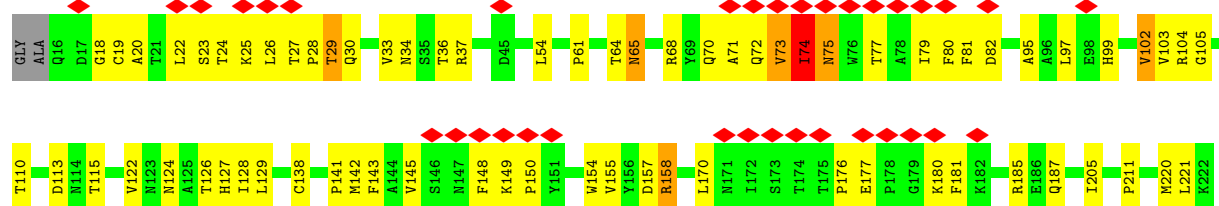
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			43	33	4	6	
8	B	1	Total	C	N	O	0
			43	33	4	6	
8	C	1	Total	C	N	O	0
			43	33	4	6	

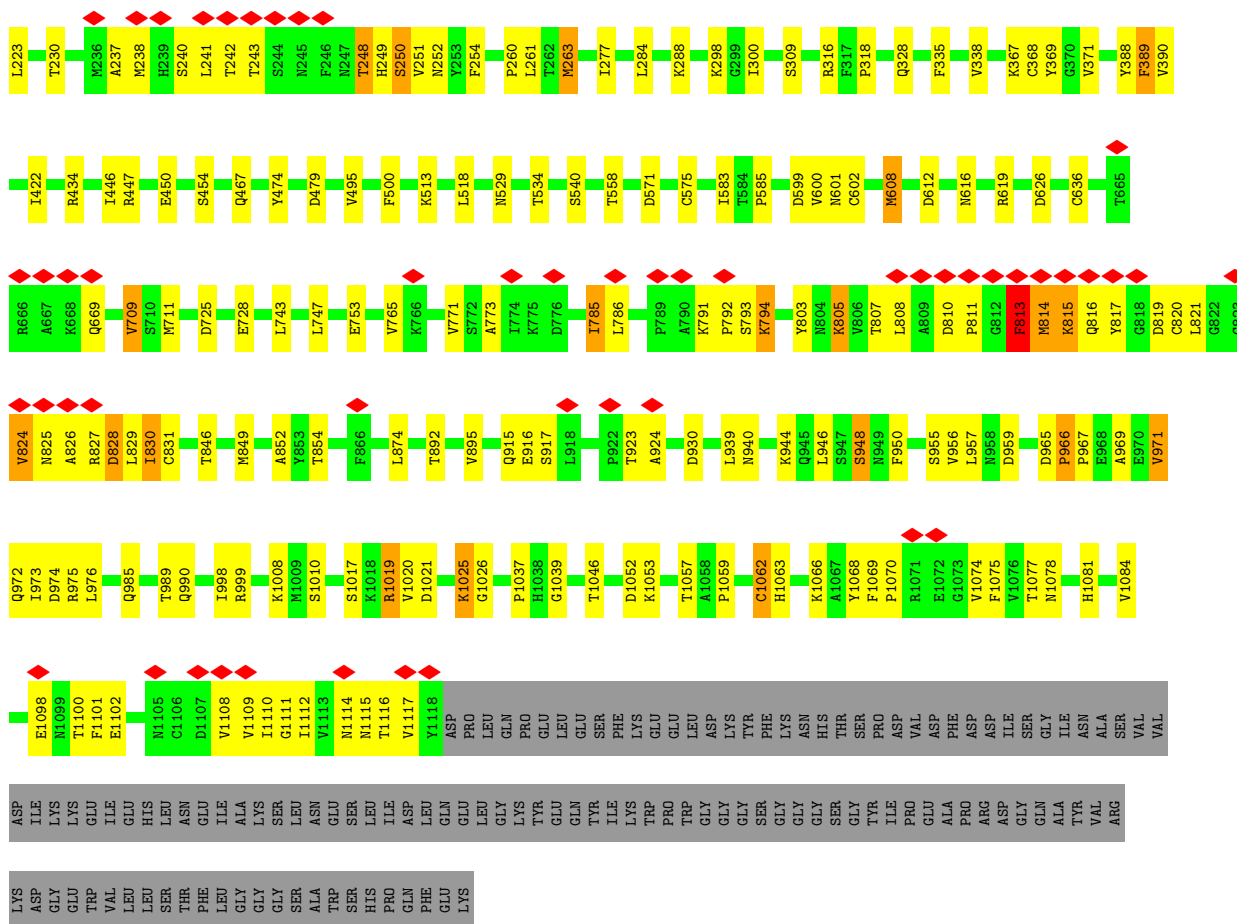
- Molecule 9 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	

Chain B: 11% 69% 18% 10%





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



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



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

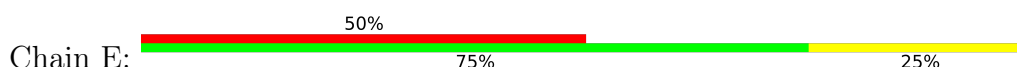




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



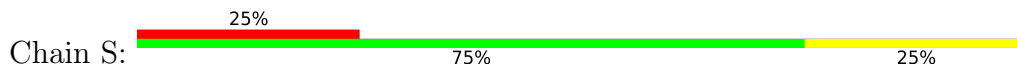
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



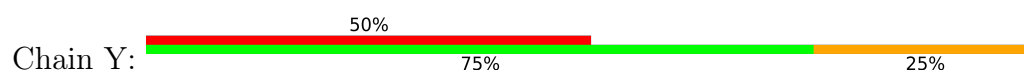
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



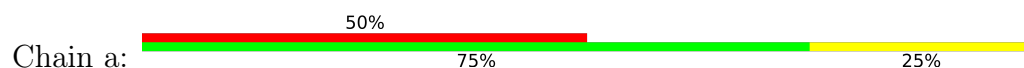
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



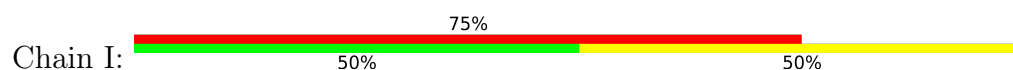
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: 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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

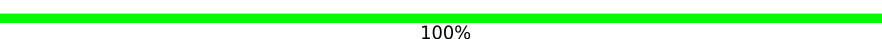


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

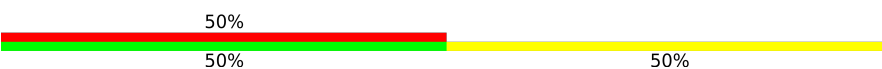


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

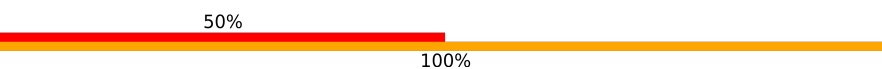


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	468039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.599	Depositor
Minimum map value	-0.556	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	457.6, 457.6, 457.6	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA, NAG, MAN, EIC, 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	A	0.45	0/8804	0.75	6/11997 (0.1%)
1	B	0.45	1/8804 (0.0%)	0.75	7/11997 (0.1%)
1	C	0.42	0/8804	0.72	17/11997 (0.1%)
All	All	0.44	1/26412 (0.0%)	0.74	30/35991 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1013	VAL	N-CA	5.01	1.51	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	971	VAL	N-CA-C	-7.83	105.13	112.96
1	C	73	VAL	CB-CA-C	7.26	119.27	111.35
1	C	75	ASN	N-CA-C	6.90	118.88	111.36
1	C	794	LYS	N-CA-C	-6.66	105.05	112.57
1	C	73	VAL	N-CA-C	-6.62	99.25	108.12
1	A	1078	ASN	CA-CB-CG	6.61	119.21	112.60
1	B	917	SER	N-CA-C	-6.58	106.46	114.75
1	B	959	ASP	N-CA-C	-6.31	105.51	113.72
1	C	966	PRO	N-CA-C	6.24	118.31	110.70
1	A	867	THR	N-CA-C	-6.21	106.01	113.97
1	C	917	SER	N-CA-C	-6.07	107.10	114.75
1	A	946	LEU	N-CA-C	-6.03	105.69	113.16
1	C	826	ALA	N-CA-C	-5.91	104.91	111.71
1	B	577	TYR	CB-CA-C	5.89	118.47	109.34
1	B	470	THR	CB-CA-C	-5.63	99.75	113.15
1	B	22	LEU	CA-C-O	-5.52	114.11	120.24
1	C	74	ILE	CB-CA-C	-5.52	103.88	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	826	ALA	N-CA-C	-5.50	105.19	111.14
1	A	88	PHE	CA-CB-CG	5.47	119.28	113.80
1	C	601	ASN	N-CA-CB	5.36	117.89	110.17
1	C	1069	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	389	PHE	N-CA-C	5.32	114.86	107.73
1	C	64	THR	CA-C-N	-5.23	114.45	122.87
1	C	64	THR	C-N-CA	-5.23	114.45	122.87
1	A	335	PHE	CB-CA-C	5.12	116.08	108.87
1	A	974	ASP	N-CA-C	-5.11	107.18	113.41
1	B	795	ARG	N-CA-C	-5.10	100.73	109.24
1	C	967	PRO	N-CA-C	5.08	121.25	114.18
1	C	1019	ARG	CB-CA-C	5.03	118.53	109.64
1	C	1017	SER	N-CA-C	5.02	116.76	110.24

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	8597	0	8356	190	0
1	B	8597	0	8358	181	0
1	C	8597	0	8355	188	0
2	D	39	0	34	1	0
2	F	39	0	34	0	0
2	G	39	0	34	1	0
2	J	39	0	34	2	0
3	E	50	0	43	0	0
3	H	50	0	43	2	0
3	N	50	0	43	0	0
3	S	50	0	43	1	0
3	Y	50	0	43	2	0
3	a	50	0	43	1	0
4	I	50	0	43	0	0
5	K	28	0	25	1	0
5	M	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	1	0
5	R	28	0	25	1	0
5	U	28	0	25	0	0
5	V	28	0	25	1	0
5	W	28	0	25	2	0
5	X	28	0	25	2	0
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
6	L	25	0	22	1	0
6	T	25	0	22	0	0
7	A	98	0	91	2	0
7	B	84	0	78	2	0
7	C	98	0	91	1	0
8	A	43	0	32	6	0
8	B	43	0	32	6	0
8	C	43	0	32	4	0
9	A	20	0	31	0	0
9	B	40	0	62	1	0
All	All	27152	0	26299	554	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 10.

All (554) 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:A:241:LEU:HD22	1:A:249:HIS:CE1	1.62	1.33
1:B:104:ARG:HH12	1:B:125:ALA:CB	1.61	1.13
1:B:104:ARG:NH1	1:B:125:ALA:HB2	1.64	1.10
1:A:145:VAL:HB	1:A:240:SER:HB2	1.34	1.09
1:C:126:THR:HG22	1:C:127:HIS:CE1	1.91	1.05
1:A:1061:ILE:HD12	1:A:1068:TYR:HD1	1.23	1.01
1:B:22:LEU:HG	1:B:140:GLU:HG3	1.44	0.96
1:B:104:ARG:HH12	1:B:125:ALA:HB2	0.80	0.95
1:A:241:LEU:HD22	1:A:249:HIS:HE1	1.14	0.95
1:A:1061:ILE:HD12	1:A:1068:TYR:CD1	2.02	0.93
1:A:241:LEU:CD2	1:A:249:HIS:HE1	1.83	0.91
1:A:334:GLN:NE2	1:A:335:PHE:O	2.02	0.91
1:C:791:LYS:HG3	1:C:792:PRO:HD2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:O	1:B:250:SER:HA	1.70	0.90
1:C:786:LEU:HD11	1:C:794:LYS:HG2	1.54	0.90
1:A:176:PRO:HG2	1:A:241:LEU:HD13	1.54	0.88
1:C:126:THR:HG22	1:C:127:HIS:ND1	1.87	0.88
1:A:241:LEU:CD2	1:A:249:HIS:CE1	2.52	0.88
1:C:956:VAL:HG23	1:C:959:ASP:HB2	1.52	0.87
1:A:1063:HIS:HB3	1:A:1068:TYR:CE1	2.10	0.86
1:B:1063:HIS:HB2	1:B:1117:VAL:CG2	2.07	0.85
1:C:1063:HIS:CB	1:C:1117:VAL:HG22	2.05	0.84
1:B:142:MET:HB2	1:B:237:ALA:HA	1.58	0.83
1:C:24:THR:HB	1:C:79:ILE:H	1.41	0.83
1:B:32:GLN:HE22	1:B:65:ASN:HD22	1.26	0.83
1:C:26:LEU:HB2	1:C:80:PHE:HB3	1.60	0.81
1:C:102:VAL:HG11	1:C:251:VAL:HG11	1.63	0.80
1:A:1061:ILE:CD1	1:A:1068:TYR:CD1	2.64	0.80
1:C:956:VAL:CG2	1:C:959:ASP:HB2	2.11	0.80
1:C:126:THR:CG2	1:C:127:HIS:CE1	2.65	0.79
1:A:1063:HIS:HB3	1:A:1068:TYR:HE1	1.44	0.78
1:C:28:PRO:HB3	1:C:30:GLN:HE22	1.47	0.78
1:A:145:VAL:HB	1:A:240:SER:CB	2.11	0.78
1:A:26:LEU:HB2	1:A:80:PHE:HB2	1.66	0.78
1:A:104:ARG:HD2	1:A:237:ALA:HB3	1.66	0.78
1:A:145:VAL:CB	1:A:240:SER:HB2	2.12	0.76
1:C:22:LEU:HD23	1:C:25:LYS:HB2	1.66	0.76
1:C:1068:TYR:CD2	1:C:1117:VAL:HB	2.21	0.76
1:B:79:ILE:HD13	1:B:248:THR:HG21	1.69	0.75
1:B:143:PHE:HB2	1:B:237:ALA:HB1	1.68	0.75
1:B:201:SER:HB3	1:B:217:LEU:HD13	1.69	0.74
1:A:71:ALA:O	1:A:250:SER:HA	1.88	0.74
1:A:606:PRO:HB3	1:A:611:MET:HE2	1.68	0.74
1:B:442:ARG:NH1	1:B:452:ASP:OD2	2.20	0.74
1:A:241:LEU:HD22	1:A:249:HIS:NE2	2.01	0.74
1:B:1063:HIS:HB2	1:B:1117:VAL:HG23	1.69	0.74
1:B:298:LYS:HG3	1:B:585:PRO:HA	1.71	0.73
1:B:786:LEU:H	1:B:786:LEU:HD22	1.53	0.73
1:C:72:GLN:NE2	1:C:73:VAL:O	2.24	0.71
1:C:794:LYS:HE3	1:C:852:ALA:HB2	1.73	0.70
1:C:28:PRO:HA	1:C:82:ASP:OD1	1.92	0.70
1:B:30:GLN:NE2	1:B:82:ASP:OD1	2.24	0.70
1:C:102:VAL:HG13	1:C:238:MET:HE2	1.73	0.70
1:A:333:THR:HG23	1:A:335:PHE:HE1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:CYS:HA	1:C:824:VAL:HG13	1.75	0.68
1:C:73:VAL:HA	1:C:79:ILE:HD13	1.76	0.68
1:C:79:ILE:HG12	1:C:248:THR:HG21	1.76	0.68
1:C:1063:HIS:CG	1:C:1117:VAL:HG22	2.29	0.68
1:C:102:VAL:HG12	1:C:103:VAL:N	2.07	0.67
1:A:176:PRO:HG2	1:A:241:LEU:CD1	2.24	0.67
1:A:145:VAL:HG22	1:A:150:PRO:HA	1.76	0.67
1:C:1020:VAL:HG23	1:C:1021:ASP:H	1.60	0.67
1:A:923:THR:OG1	1:A:924:ALA:N	2.28	0.66
1:B:1063:HIS:HB2	1:B:1117:VAL:HG21	1.77	0.66
1:C:20:ALA:HB2	1:C:154:TRP:CE3	2.31	0.66
1:C:1063:HIS:ND1	1:C:1117:VAL:HG22	2.11	0.66
1:A:248:THR:HG23	1:A:249:HIS:O	1.96	0.65
1:C:1063:HIS:HB2	1:C:1117:VAL:HG22	1.78	0.65
1:A:605:VAL:HA	1:A:608:MET:HE2	1.78	0.65
1:A:28:PRO:HB3	1:A:82:ASP:CG	2.22	0.65
1:B:102:VAL:HG11	1:B:251:VAL:HG11	1.78	0.65
1:A:124:ASN:C	1:A:126:THR:H	2.04	0.64
1:B:709:VAL:HG13	1:B:1039:GLY:HA2	1.80	0.64
1:B:104:ARG:NH1	1:B:125:ALA:CA	2.61	0.64
1:A:145:VAL:HG13	1:A:149:LYS:N	2.12	0.64
1:B:806:VAL:HG21	1:B:1037:PRO:HG2	1.80	0.64
1:B:1117:VAL:O	1:B:1118:TYR:C	2.40	0.64
1:B:22:LEU:HB3	1:B:25:LYS:HD3	1.80	0.63
1:B:104:ARG:NH1	1:B:125:ALA:CB	2.40	0.63
1:A:121:VAL:HG13	1:A:130:ILE:HG12	1.80	0.63
1:C:141:PRO:HB3	1:C:155:VAL:HG13	1.80	0.63
1:A:916:GLU:HA	1:A:919:THR:HG22	1.81	0.62
1:B:787:PRO:HG3	1:B:797:PRO:HG3	1.80	0.62
1:B:38:ARG:HH21	1:B:211:PRO:HB2	1.65	0.62
1:C:26:LEU:H	1:C:80:PHE:CB	2.12	0.62
1:A:102:VAL:HG13	1:A:238:MET:HB2	1.82	0.62
1:C:26:LEU:HB2	1:C:80:PHE:CB	2.28	0.62
1:C:102:VAL:HG11	1:C:251:VAL:CG1	2.28	0.62
1:A:38:ARG:NH2	1:A:186:GLU:OE2	2.30	0.62
1:A:949:ASN:HD22	1:A:951:GLY:H	1.47	0.62
1:B:25:LYS:HZ1	1:B:81:PHE:HB2	1.65	0.61
1:B:75:ASN:C	1:B:77:THR:H	2.09	0.61
1:A:602:CYS:HB3	1:A:629:MET:HE3	1.82	0.61
1:B:145:VAL:H	1:B:240:SER:HB2	1.66	0.61
1:B:74:ILE:HD11	1:B:80:PHE:HD1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:GLN:HE21	1:A:915:GLN:HE22	1.48	0.60
1:A:101:ASN:ND2	1:A:173:SER:O	2.34	0.60
1:A:141:PRO:HB2	1:A:235:VAL:HG22	1.83	0.60
1:A:1061:ILE:CD1	1:A:1068:TYR:HD1	2.00	0.60
1:A:143:PHE:HB2	1:A:237:ALA:HB1	1.83	0.60
1:A:298:LYS:HG3	1:A:585:PRO:HA	1.84	0.60
1:A:185:ARG:CZ	8:A:1307:BLA:HHD	2.32	0.60
1:C:1063:HIS:CB	1:C:1117:VAL:CG2	2.80	0.59
1:A:73:VAL:HG22	1:A:79:ILE:HB	1.83	0.59
1:C:368:CYS:HB3	1:C:371:VAL:O	2.01	0.59
1:A:239:HIS:ND1	1:A:247:ASN:HA	2.17	0.59
1:A:605:VAL:HG22	1:A:608:MET:CE	2.33	0.59
1:A:102:VAL:HG13	1:A:238:MET:HE2	1.84	0.59
1:B:152:LYS:HZ3	1:B:154:TRP:HZ2	1.51	0.59
1:C:811:PRO:HG2	1:C:816:GLN:HG2	1.84	0.59
1:C:923:THR:OG1	1:C:924:ALA:N	2.33	0.59
1:C:1059:PRO:HD2	1:C:1111:GLY:O	2.02	0.59
1:A:545:GLN:HB2	1:A:548:GLN:HG3	1.84	0.59
1:B:923:THR:OG1	1:B:924:ALA:N	2.36	0.59
1:C:1062:CYS:SG	1:C:1112:ILE:HD11	2.42	0.59
1:C:612:ASP:OD1	1:C:612:ASP:N	2.34	0.59
1:B:805:LYS:NZ	1:B:918:LEU:O	2.30	0.59
1:C:124:ASN:CG	1:C:129:LEU:HD11	2.27	0.59
1:A:1068:TYR:HB3	1:A:1100:THR:CG2	2.33	0.58
1:C:709:VAL:HG13	1:C:1039:GLY:HA2	1.84	0.58
1:C:1098:GLU:OE1	1:C:1098:GLU:N	2.36	0.58
1:A:949:ASN:ND2	1:A:951:GLY:H	2.02	0.58
1:B:787:PRO:HD3	1:B:797:PRO:HD3	1.86	0.58
1:C:1068:TYR:CE1	1:C:1102:GLU:HB2	2.38	0.58
1:C:1068:TYR:CE2	1:C:1117:VAL:HB	2.38	0.58
1:B:97:LEU:HD21	1:B:205:ILE:HD11	1.84	0.58
1:A:605:VAL:HG22	1:A:608:MET:HE2	1.86	0.58
1:C:61:PRO:HG3	1:C:261:LEU:HD11	1.85	0.58
1:A:20:ALA:HB2	1:A:154:TRP:CE3	2.39	0.57
1:A:617:ASP:O	1:A:620:VAL:HG12	2.04	0.57
1:A:985:GLN:O	1:A:989:THR:HG22	2.04	0.57
1:B:120:ILE:HG13	1:B:135:PHE:CE2	2.39	0.57
1:A:333:THR:HG23	1:A:335:PHE:CE1	2.38	0.57
1:C:251:VAL:C	1:C:252:ASN:HD22	2.12	0.57
1:A:956:VAL:HG23	1:A:959:ASP:HB2	1.87	0.56
1:B:143:PHE:HB2	1:B:237:ALA:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:GLN:HE22	7:B:1307:NAG:H3	1.71	0.56
1:C:626:ASP:OD1	1:C:626:ASP:N	2.36	0.56
1:A:146:SER:HB3	1:A:149:LYS:HB2	1.86	0.56
1:A:970:GLU:HA	1:A:973:ILE:HG12	1.88	0.56
1:A:26:LEU:CB	1:A:80:PHE:HB2	2.35	0.56
1:B:185:ARG:HH21	8:B:1309:BLA:HMD3	1.71	0.56
1:C:300:ILE:HG13	1:C:583:ILE:HG12	1.88	0.56
1:C:102:VAL:HG13	1:C:238:MET:CE	2.35	0.56
1:C:157:ASP:OD1	1:C:157:ASP:N	2.38	0.56
1:B:1020:VAL:HG23	1:B:1021:ASP:H	1.69	0.56
1:B:34:ASN:O	1:B:66:ILE:HG12	2.06	0.56
1:A:806:VAL:HG21	1:A:1037:PRO:HG2	1.86	0.55
1:A:784:GLN:NE2	1:A:915:GLN:HE22	2.03	0.55
1:C:128:ILE:HD11	1:C:170:LEU:HD13	1.87	0.55
1:A:238:MET:CE	1:A:249:HIS:HB2	2.37	0.55
1:B:220:MET:SD	8:B:1309:BLA:HBB	2.47	0.55
1:A:834:LYS:HB2	1:B:577:TYR:HE1	1.69	0.55
1:A:1020:VAL:HG23	1:A:1021:ASP:H	1.71	0.55
1:B:708:PRO:O	1:B:1001:SER:OG	2.24	0.55
1:B:930:ASP:O	1:B:934:GLN:HG2	2.07	0.55
1:A:28:PRO:HB3	1:A:82:ASP:OD2	2.07	0.55
1:C:1026:GLY:HA3	1:C:1046:THR:CG2	2.35	0.55
1:A:1117:VAL:O	1:A:1118:TYR:C	2.50	0.55
5:X:1:NAG:H61	5:X:2:NAG:C7	2.36	0.55
5:W:1:NAG:H4	5:W:2:NAG:N2	2.22	0.55
1:A:465:CYS:SG	1:A:466:ASN:N	2.79	0.54
1:A:984:LEU:O	1:A:988:VAL:HG13	2.06	0.54
1:C:1026:GLY:HA3	1:C:1046:THR:HG21	1.88	0.54
1:B:176:PRO:HG3	1:B:241:LEU:HD22	1.89	0.54
1:A:124:ASN:C	1:A:126:THR:N	2.66	0.54
1:B:985:GLN:O	1:B:989:THR:HG23	2.08	0.54
1:C:68:ARG:NH2	1:C:252:ASN:OD1	2.34	0.54
1:A:22:LEU:HD21	1:A:142:MET:HE1	1.90	0.54
1:A:26:LEU:HB2	1:A:80:PHE:CB	2.38	0.54
1:A:145:VAL:HG13	1:A:149:LYS:H	1.73	0.54
1:B:242:THR:HG22	1:B:243:THR:H	1.73	0.54
1:A:820:CYS:SG	1:A:831:CYS:HB2	2.49	0.53
1:B:17:ASP:HB2	1:B:154:TRP:HD1	1.73	0.53
1:B:101:ASN:ND2	1:B:173:SER:O	2.41	0.53
1:A:141:PRO:HB3	1:A:155:VAL:HG23	1.89	0.53
1:A:238:MET:HE1	1:A:249:HIS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LYS:HB2	1:C:599:ASP:OD1	2.08	0.53
1:C:241:LEU:HB2	1:C:249:HIS:HE1	1.73	0.53
1:C:1078:ASN:OD1	1:C:1081:HIS:HB2	2.09	0.53
1:C:143:PHE:HB2	1:C:237:ALA:HB1	1.90	0.53
1:C:1052:ASP:N	1:C:1052:ASP:OD1	2.40	0.53
1:A:98:GLU:HB3	1:A:251:VAL:HG23	1.90	0.53
1:A:143:PHE:H	1:A:237:ALA:HB1	1.74	0.53
1:C:725:ASP:OD1	1:C:725:ASP:N	2.41	0.52
1:A:474:TYR:CE2	2:J:1:NAG:H83	2.44	0.52
1:A:1066:LYS:HB3	1:A:1102:GLU:OE1	2.09	0.52
1:B:22:LEU:HG	1:B:140:GLU:CG	2.31	0.52
1:C:1025:LYS:O	1:C:1046:THR:HG21	2.10	0.52
1:B:427:THR:HG21	1:B:494:ARG:HD2	1.91	0.52
1:A:788:ASP:OD2	1:A:789:PRO:HD2	2.09	0.52
1:C:73:VAL:HB	1:C:248:THR:HG23	1.91	0.52
1:A:125:ALA:HA	1:A:172:ILE:HG22	1.91	0.52
1:A:600:VAL:HG11	1:A:608:MET:SD	2.50	0.52
1:B:172:ILE:HB	8:B:1309:BLA:HBC2	1.92	0.52
1:C:104:ARG:HD3	1:C:237:ALA:HB3	1.92	0.52
1:C:1081:HIS:CD2	5:Q:1:NAG:H5	2.44	0.52
1:A:145:VAL:HG22	1:A:150:PRO:CA	2.40	0.52
1:B:44:ASP:OD2	1:B:48:ARG:NH2	2.40	0.52
1:A:280:SER:O	1:A:280:SER:OG	2.28	0.52
8:A:1307:BLA:HBC1	8:A:1307:BLA:HA	1.76	0.51
1:B:902:GLN:O	1:B:906:GLN:HG3	2.10	0.51
1:A:728:GLU:CD	1:A:728:GLU:H	2.19	0.51
1:A:802:LEU:HA	1:A:805:LYS:HZ3	1.76	0.51
1:B:855:SER:O	1:B:859:SER:OG	2.24	0.51
1:C:19:CYS:HA	1:C:138:CYS:SG	2.50	0.51
1:C:102:VAL:CG2	1:C:238:MET:HE1	2.41	0.51
1:C:242:THR:HG22	1:C:243:THR:H	1.76	0.51
1:B:22:LEU:HD12	1:B:25:LYS:NZ	2.26	0.51
1:B:894:ASN:H	1:B:894:ASN:ND2	2.08	0.51
1:C:113:ASP:OD1	1:C:115:THR:OG1	2.25	0.51
1:A:145:VAL:H	1:A:240:SER:HA	1.75	0.51
1:A:933:ASN:O	1:A:937:ILE:HG23	2.10	0.51
1:B:894:ASN:HD21	1:C:1101:PHE:HE2	1.59	0.51
1:B:102:VAL:HG21	1:B:251:VAL:HB	1.93	0.50
1:B:806:VAL:CG2	1:B:1037:PRO:HG2	2.41	0.50
1:A:930:ASP:O	1:A:934:GLN:HG2	2.11	0.50
1:A:398:GLN:NE2	1:A:405:GLY:HA3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:MET:SD	1:C:249:HIS:N	2.74	0.50
1:C:241:LEU:HD13	1:C:249:HIS:CE1	2.47	0.50
1:A:600:VAL:HG11	1:A:608:MET:CE	2.41	0.50
1:B:809:ALA:O	1:B:810:ASP:C	2.55	0.50
1:B:892:THR:O	1:B:895:VAL:HG13	2.10	0.50
1:A:709:VAL:HG23	1:A:1039:GLY:HA2	1.91	0.50
1:B:71:ALA:HB3	1:B:251:VAL:HG12	1.94	0.50
1:B:616:ASN:HA	1:B:619:ARG:HH11	1.76	0.50
1:B:715:ALA:HB3	1:B:839:THR:HG23	1.92	0.50
1:B:753:GLU:OE1	1:B:999:ARG:HD3	2.10	0.50
1:A:555:ALA:HB1	1:C:946:LEU:HD11	1.93	0.50
1:B:1020:VAL:HG23	1:B:1021:ASP:N	2.26	0.50
1:B:1083:PHE:HZ	5:M:1:NAG:H62	1.77	0.50
1:C:129:LEU:HD21	7:C:1308:NAG:O5	2.12	0.50
1:C:298:LYS:HG3	1:C:585:PRO:HA	1.92	0.50
1:B:820:CYS:HA	1:B:824:VAL:HG13	1.92	0.50
1:A:956:VAL:HG21	1:A:959:ASP:CG	2.36	0.50
1:B:145:VAL:HB	1:B:150:PRO:HA	1.93	0.50
1:B:666:ARG:NH1	1:B:669:GLN:HG3	2.27	0.50
1:A:120:ILE:HD12	1:A:135:PHE:CE2	2.47	0.49
1:B:185:ARG:NH2	8:B:1309:BLA:HMD3	2.27	0.49
1:B:345:ARG:HG3	1:B:345:ARG:HH11	1.76	0.49
1:C:1063:HIS:HB2	1:C:1117:VAL:CG2	2.42	0.49
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.76	0.49
1:B:17:ASP:HB2	1:B:154:TRP:CD1	2.48	0.49
1:B:893:GLN:HE22	1:C:1070:PRO:HG2	1.77	0.49
1:A:172:ILE:HD13	8:A:1307:BLA:HAD1	1.93	0.49
1:A:70:GLN:N	1:A:70:GLN:OE1	2.46	0.49
1:A:230:THR:O	1:A:231:ARG:HG3	2.13	0.49
1:B:74:ILE:HD12	1:B:78:ALA:O	2.13	0.49
1:B:141:PRO:HA	1:B:154:TRP:O	2.13	0.49
1:C:37:ARG:HG3	5:K:2:NAG:H81	1.93	0.49
1:C:368:CYS:HB3	1:C:371:VAL:HG23	1.95	0.49
1:A:172:ILE:HD13	8:A:1307:BLA:HMD1	1.94	0.49
1:B:236:MET:C	1:B:238:MET:H	2.21	0.49
1:C:26:LEU:HD13	1:C:74:ILE:HD11	1.95	0.49
1:C:75:ASN:O	1:C:77:THR:N	2.46	0.49
1:C:260:PRO:O	1:C:261:LEU:HG	2.13	0.49
1:A:145:VAL:N	1:A:240:SER:HB2	2.28	0.49
1:B:75:ASN:C	1:B:77:THR:N	2.69	0.49
1:B:815:LYS:HE3	1:C:599:ASP:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:HB3	1:A:251:VAL:HG12	1.94	0.48
1:A:143:PHE:H	1:A:237:ALA:CB	2.26	0.48
1:A:149:LYS:O	1:A:150:PRO:C	2.56	0.48
1:B:103:VAL:O	8:B:1309:BLA:HMC3	2.12	0.48
1:B:447:ARG:NH1	3:S:1:NAG:H82	2.28	0.48
1:B:1066:LYS:HB3	1:B:1102:GLU:OE1	2.12	0.48
1:B:813:PHE:HE2	1:B:831:CYS:HB3	1.77	0.48
1:C:1063:HIS:HB2	1:C:1117:VAL:HG13	1.95	0.48
5:V:1:NAG:H61	5:V:2:NAG:O5	2.13	0.48
1:A:51:LEU:HD12	1:A:52:ARG:H	1.78	0.48
1:B:1010:SER:O	1:C:1020:VAL:HG21	2.13	0.48
1:B:54:LEU:HD12	1:B:292:LYS:HE2	1.94	0.48
1:B:894:ASN:O	1:B:898:GLU:HG3	2.13	0.48
1:A:1061:ILE:HD11	1:A:1068:TYR:CD1	2.47	0.48
1:C:105:GLY:HA3	1:C:122:VAL:HG12	1.94	0.48
1:C:241:LEU:HD13	1:C:249:HIS:ND1	2.28	0.48
1:A:430:ILE:HG22	1:A:431:ASP:OD1	2.14	0.48
1:B:36:THR:HG23	1:B:38:ARG:HG3	1.95	0.48
1:B:40:PHE:HD2	1:B:216:VAL:HG22	1.77	0.48
2:D:1:NAG:H61	2:D:2:NAG:C7	2.43	0.48
1:A:304:SER:OG	1:A:305:ASN:N	2.47	0.48
1:C:180:LYS:HB3	1:C:180:LYS:HE3	1.59	0.48
1:C:540:SER:HB2	1:C:571:ASP:CG	2.38	0.48
1:C:753:GLU:OE2	1:C:999:ARG:HD3	2.13	0.48
1:C:1020:VAL:HG23	1:C:1021:ASP:N	2.27	0.48
1:C:65:ASN:OD1	1:C:65:ASN:N	2.46	0.47
1:B:902:GLN:NE2	7:B:1307:NAG:H3	2.29	0.47
1:C:148:PHE:O	1:C:149:LYS:NZ	2.41	0.47
1:C:474:TYR:CE2	2:G:1:NAG:H83	2.48	0.47
1:A:600:VAL:HG21	1:A:608:MET:SD	2.54	0.47
1:A:868:PHE:HD1	1:A:868:PHE:H	1.62	0.47
1:B:107:ILE:HD13	1:B:120:ILE:HG12	1.94	0.47
1:B:341:TRP:O	1:B:451:ARG:NH1	2.48	0.47
1:B:786:LEU:HD22	1:B:786:LEU:N	2.24	0.47
1:C:102:VAL:HG11	1:C:251:VAL:CB	2.44	0.47
1:A:849:MET:HG3	1:B:679:LEU:HD11	1.96	0.47
1:B:100:SER:O	1:B:100:SER:OG	2.31	0.47
1:B:238:MET:SD	1:B:249:HIS:HB2	2.55	0.47
1:B:726:SER:OG	1:B:728:GLU:OE1	2.26	0.47
1:C:1053:LYS:HE2	1:C:1053:LYS:HB2	1.64	0.47
1:B:89:ASN:HB3	1:B:90:ASP:H	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ASP:OD1	1:A:612:ASP:N	2.47	0.47
1:A:220:MET:O	1:A:221:LEU:HD23	2.15	0.47
1:B:35:SER:HB3	1:B:66:ILE:HG23	1.97	0.47
1:B:1068:TYR:CZ	1:B:1102:GLU:HG3	2.50	0.47
1:C:23:SER:O	1:C:24:THR:C	2.57	0.47
1:A:894:ASN:O	1:A:898:GLU:HG3	2.15	0.47
1:A:1053:LYS:HB3	1:A:1053:LYS:HE3	1.64	0.47
1:C:102:VAL:CG1	1:C:238:MET:CE	2.92	0.47
1:B:984:LEU:O	1:B:988:VAL:HG23	2.15	0.47
1:B:1013:VAL:HG12	1:B:1014:LEU:HD22	1.97	0.47
6:L:1:NAG:H4	6:L:2:BMA:H4	1.96	0.47
1:A:702:VAL:HA	1:A:1044:HIS:O	2.15	0.47
1:A:899:ASN:O	1:A:903:ILE:HG13	2.15	0.47
1:B:325:PRO:O	9:B:1308:EIC:H181	2.15	0.47
1:C:1066:LYS:HB3	1:C:1102:GLU:OE1	2.15	0.47
1:A:86:ILE:HG22	1:A:87:PRO:HD2	1.97	0.46
1:A:298:LYS:NZ	1:A:650:ASP:OD1	2.44	0.46
1:C:828:ASP:HB3	1:C:830:ILE:HD12	1.97	0.46
1:A:1020:VAL:HG21	1:C:1010:SER:O	2.15	0.46
1:B:22:LEU:HA	1:B:22:LEU:HD22	1.57	0.46
1:B:142:MET:SD	1:B:239:HIS:HB2	2.55	0.46
1:B:467:GLN:N	1:B:467:GLN:OE1	2.49	0.46
1:A:155:VAL:HG13	1:A:156:TYR:CD2	2.51	0.46
1:B:788:ASP:CG	1:B:791:LYS:HD3	2.40	0.46
1:B:812:GLY:O	1:B:813:PHE:C	2.58	0.46
1:C:71:ALA:O	1:C:250:SER:HA	2.14	0.46
1:C:1063:HIS:HB3	1:C:1117:VAL:CG2	2.45	0.46
1:C:1063:HIS:HB3	1:C:1117:VAL:HG22	1.93	0.46
1:A:21:THR:C	1:A:22:LEU:HD22	2.41	0.46
1:B:1077:THR:OG1	1:B:1081:HIS:O	2.32	0.46
1:C:185:ARG:HG2	8:C:1307:BLA:HMB1	1.97	0.46
1:B:16:GLN:HA	1:B:156:TYR:O	2.16	0.46
1:B:248:THR:OG1	1:B:249:HIS:N	2.48	0.46
1:C:803:TYR:CE1	1:C:1037:PRO:HG3	2.51	0.46
1:A:242:THR:OG1	1:A:243:THR:N	2.47	0.46
1:A:312:LEU:HD23	1:A:313:ASP:N	2.30	0.46
1:A:956:VAL:CG2	1:A:959:ASP:CG	2.89	0.46
1:C:29:THR:HG21	1:C:70:GLN:HG2	1.97	0.46
1:C:81:PHE:HZ	1:C:238:MET:HB3	1.80	0.46
1:A:930:ASP:OD1	1:A:930:ASP:N	2.48	0.46
1:B:318:PRO:HD3	1:B:529:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:HA	1:C:230:THR:HG22	1.97	0.46
1:C:773:ALA:HA	1:C:785:ILE:HD11	1.98	0.46
1:A:150:PRO:HD3	1:A:174:THR:HG21	1.98	0.46
1:C:145:VAL:HG22	1:C:240:SER:O	2.15	0.46
1:A:129:LEU:CD1	7:A:1308:NAG:O7	2.64	0.46
1:B:174:THR:O	1:B:174:THR:OG1	2.34	0.45
1:B:367:LYS:HD2	1:B:368:CYS:N	2.31	0.45
1:C:128:ILE:HD11	8:C:1307:BLA:HAC	1.98	0.45
1:C:805:LYS:HB3	1:C:805:LYS:HE2	1.57	0.45
1:A:61:PRO:HG3	1:A:261:LEU:HD11	1.97	0.45
1:A:695:PRO:HD3	1:C:874:LEU:HD21	1.99	0.45
1:B:559:ASP:OD1	1:B:559:ASP:N	2.49	0.45
1:A:786:LEU:HD23	1:A:787:PRO:HD2	1.97	0.45
1:A:788:ASP:CG	1:A:789:PRO:HD2	2.41	0.45
1:B:36:THR:OG1	1:B:37:ARG:N	2.49	0.45
1:B:748:ALA:O	1:B:752:VAL:HG12	2.16	0.45
1:C:187:GLN:HE22	8:C:1307:BLA:HBB2	1.81	0.45
1:C:447:ARG:HB2	1:C:450:GLU:OE1	2.16	0.45
1:A:145:VAL:HG21	1:A:174:THR:CG2	2.47	0.45
1:B:200:HIS:CD2	1:B:201:SER:H	2.35	0.45
1:C:81:PHE:CZ	1:C:238:MET:HB3	2.51	0.45
1:C:142:MET:HE3	1:C:142:MET:HB2	1.82	0.45
1:A:682:ASP:OD1	1:A:683:SER:N	2.50	0.45
1:C:26:LEU:H	1:C:80:PHE:HB2	1.82	0.45
1:A:559:ASP:OD1	1:A:559:ASP:N	2.49	0.45
1:B:70:GLN:OE1	1:B:252:ASN:HB3	2.16	0.45
1:B:268:SER:HB3	1:B:272:THR:H	1.82	0.45
1:A:417:GLU:CD	1:A:417:GLU:H	2.24	0.45
1:A:1054:ASN:OD1	1:A:1055:PHE:N	2.49	0.45
1:A:1061:ILE:HD11	1:A:1068:TYR:HB2	1.98	0.45
1:C:1068:TYR:HB3	1:C:1100:THR:CG2	2.47	0.45
1:A:660:LYS:HG2	1:A:675:TYR:HE1	1.82	0.45
1:B:957:LEU:HD22	1:B:973:ILE:HG12	1.98	0.45
1:C:158:ARG:HD3	1:C:158:ARG:HA	1.88	0.45
1:C:939:LEU:HD23	1:C:939:LEU:HA	1.86	0.45
1:A:962:SER:O	1:B:379:LEU:HD21	2.17	0.45
1:A:1025:LYS:O	1:A:1046:THR:HG21	2.17	0.45
1:C:26:LEU:HD22	1:C:74:ILE:HD13	1.98	0.45
1:C:176:PRO:HD3	1:C:241:LEU:HD23	1.99	0.45
1:C:1025:LYS:HA	1:C:1025:LYS:HD3	1.60	0.45
1:A:95:ALA:HB3	1:A:254:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HB2	1:A:237:ALA:HA	2.00	0.44
1:A:148:PHE:CE1	1:A:176:PRO:HD2	2.52	0.44
1:A:263:MET:HE3	1:A:263:MET:HB3	1.83	0.44
1:B:331:ASN:HD21	3:a:1:NAG:C1	2.30	0.44
1:B:629:MET:HG3	1:B:638:VAL:HG22	2.00	0.44
1:B:817:TYR:CD1	1:B:817:TYR:N	2.85	0.44
1:B:501:GLU:OE1	1:B:501:GLU:HA	2.17	0.44
1:C:447:ARG:NH1	3:Y:1:NAG:H82	2.33	0.44
1:A:1082:TRP:NE1	1:A:1113:VAL:HG11	2.33	0.44
1:B:22:LEU:HD12	1:B:25:LYS:HZ2	1.83	0.44
1:C:26:LEU:HB3	1:C:27:THR:H	1.64	0.44
1:C:328:GLN:OE1	1:C:328:GLN:N	2.51	0.44
1:B:123:ASN:HD22	8:B:1309:BLA:HBB2	1.82	0.44
1:B:786:LEU:H	1:B:786:LEU:CD2	2.26	0.44
1:C:102:VAL:CG1	1:C:251:VAL:HG11	2.43	0.44
1:C:284:LEU:O	1:C:288:LYS:HG3	2.18	0.44
1:C:318:PRO:HD3	1:C:529:ASN:OD1	2.17	0.44
1:C:829:LEU:HD13	1:C:940:ASN:HD21	1.83	0.44
3:H:3:BMA:H3	3:H:4:MAN:H2	1.71	0.44
1:B:24:THR:O	1:B:25:LYS:HB2	2.18	0.44
1:C:338:VAL:HG23	1:C:389:PHE:CD1	2.53	0.44
1:A:813:PHE:C	1:A:815:LYS:N	2.76	0.44
1:B:957:LEU:CD2	1:B:973:ILE:HG12	2.48	0.44
1:B:1078:ASN:OD1	1:B:1081:HIS:HB2	2.17	0.43
1:C:1068:TYR:CD2	1:C:1100:THR:HG21	2.53	0.43
2:J:1:NAG:H61	2:J:2:NAG:C7	2.47	0.43
1:C:447:ARG:HH11	3:Y:1:NAG:H82	1.81	0.43
1:C:846:THR:OG1	1:C:849:MET:HG3	2.18	0.43
5:W:1:NAG:H4	5:W:2:NAG:HN2	1.82	0.43
1:B:201:SER:HB3	1:B:217:LEU:CD1	2.42	0.43
1:B:702:VAL:HA	1:B:1044:HIS:O	2.18	0.43
1:C:948:SER:C	1:C:955:SER:HG	2.26	0.43
1:C:985:GLN:O	1:C:989:THR:HG22	2.18	0.43
1:A:241:LEU:O	1:A:242:THR:HG22	2.18	0.43
1:A:815:LYS:HA	1:A:815:LYS:HD3	1.38	0.43
1:A:834:LYS:HB2	1:B:577:TYR:CE1	2.52	0.43
1:B:816:GLN:HE21	1:B:816:GLN:HB3	1.58	0.43
1:B:1052:ASP:OD1	1:B:1052:ASP:N	2.50	0.43
1:A:172:ILE:CD1	8:A:1307:BLA:HAD1	2.49	0.43
1:C:18:GLY:H	1:C:154:TRP:HD1	1.65	0.43
1:C:248:THR:OG1	1:C:249:HIS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:ASP:O	1:C:829:LEU:C	2.60	0.43
1:C:972:GLN:HE21	1:C:972:GLN:HB3	1.54	0.43
1:A:1068:TYR:CE1	1:A:1117:VAL:HG21	2.54	0.43
1:C:930:ASP:OD1	1:C:930:ASP:N	2.52	0.43
1:B:322:ASN:O	1:B:350:VAL:HG12	2.18	0.43
1:B:891:VAL:CG1	1:B:895:VAL:HG11	2.49	0.43
1:C:915:GLN:HG3	1:C:916:GLU:OE2	2.17	0.43
1:A:203:GLU:HG3	1:A:205:ILE:HG23	2.01	0.43
1:A:124:ASN:O	1:A:126:THR:N	2.52	0.43
1:C:97:LEU:HG	1:C:181:PHE:CD2	2.53	0.43
1:C:205:ILE:HD13	1:C:211:PRO:HG2	2.00	0.43
1:C:367:LYS:HG2	1:C:369:TYR:CE1	2.53	0.43
1:C:728:GLU:H	1:C:728:GLU:CD	2.25	0.43
1:A:365:THR:CG2	1:A:424:ALA:HB3	2.49	0.43
1:B:100:SER:HB2	1:B:176:PRO:HA	2.01	0.43
1:B:113:ASP:OD1	1:B:115:THR:HG22	2.19	0.43
1:B:141:PRO:O	1:B:142:MET:HB3	2.19	0.43
1:C:99:HIS:CD2	1:C:99:HIS:C	2.96	0.43
1:C:1068:TYR:HD2	1:C:1100:THR:HG21	1.83	0.43
1:A:813:PHE:C	1:A:815:LYS:H	2.27	0.42
1:A:969:ALA:O	1:A:973:ILE:HG23	2.19	0.42
1:B:91:GLY:HA3	1:B:258:LEU:HD12	2.01	0.42
1:B:236:MET:HE2	1:B:236:MET:HB3	1.92	0.42
1:B:263:MET:HE3	1:B:263:MET:HB3	1.82	0.42
1:A:157:ASP:OD1	1:A:157:ASP:N	2.49	0.42
1:B:817:TYR:N	1:B:817:TYR:HD1	2.17	0.42
1:B:1098:GLU:N	1:B:1098:GLU:OE1	2.53	0.42
1:C:105:GLY:HA3	1:C:122:VAL:HA	2.00	0.42
1:C:126:THR:CG2	1:C:127:HIS:ND1	2.70	0.42
1:A:166:ARG:HG3	1:A:166:ARG:NH1	2.34	0.42
1:B:44:ASP:OD1	1:B:44:ASP:C	2.62	0.42
1:C:54:LEU:HD12	1:C:54:LEU:HA	1.78	0.42
1:C:815:LYS:HD3	1:C:815:LYS:HA	1.38	0.42
1:A:145:VAL:HA	1:A:151:TYR:H	1.84	0.42
1:A:200:HIS:NE2	8:A:1307:BLA:HBC2	2.33	0.42
1:B:302:GLN:HE22	1:B:598:GLN:NE2	2.17	0.42
1:B:1068:TYR:HB3	1:B:1100:THR:CG2	2.48	0.42
1:C:54:LEU:HD12	1:C:263:MET:O	2.20	0.42
1:C:1114:ASN:O	1:C:1115:ASN:HB2	2.19	0.42
1:A:145:VAL:HG21	1:A:174:THR:HG21	2.02	0.42
1:B:1008:LYS:HB2	1:B:1008:LYS:HE2	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:HB3	1:C:254:PHE:HB2	2.00	0.42
1:C:220:MET:HG2	1:C:221:LEU:HG	2.00	0.42
1:C:600:VAL:HG21	1:C:608:MET:HE3	2.01	0.42
1:C:616:ASN:HA	1:C:619:ARG:HD2	2.01	0.42
1:C:892:THR:O	1:C:895:VAL:HG22	2.19	0.42
1:C:965:ASP:HB2	1:C:966:PRO:HD2	2.02	0.42
1:C:33:VAL:HG12	1:C:34:ASN:N	2.35	0.42
1:C:971:VAL:HA	1:C:974:ASP:OD2	2.19	0.42
1:C:1075:PHE:CE1	1:C:1084:VAL:HG22	2.55	0.42
1:A:23:SER:C	1:A:25:LYS:H	2.28	0.42
1:B:270:ASN:OD1	1:B:272:THR:HG23	2.20	0.42
1:B:787:PRO:HD3	1:B:796:SER:HA	2.02	0.42
1:C:944:LYS:NZ	1:C:944:LYS:HB2	2.34	0.42
1:C:969:ALA:O	1:C:973:ILE:HG13	2.20	0.42
1:A:21:THR:O	1:A:22:LEU:HD13	2.20	0.42
1:A:1007:THR:O	1:A:1011:GLU:HG3	2.20	0.42
1:B:794:LYS:HD2	1:B:848:ASP:OD1	2.19	0.42
1:B:1071:ARG:O	1:B:1072:GLU:HG3	2.19	0.42
1:B:1081:HIS:CD2	5:M:1:NAG:H5	2.54	0.42
3:H:1:NAG:H62	3:H:2:NAG:C7	2.50	0.42
1:A:815:LYS:HZ2	1:B:599:ASP:HA	1.85	0.42
1:B:660:LYS:HG2	1:B:675:TYR:HE1	1.84	0.42
1:C:669:GLN:N	1:C:669:GLN:OE1	2.53	0.42
1:C:711:MET:SD	1:C:998:ILE:HG13	2.60	0.42
5:R:1:NAG:H61	5:R:2:NAG:C7	2.50	0.42
1:A:345:ARG:HG3	1:A:345:ARG:NH1	2.34	0.42
1:A:643:ASP:HB2	1:A:673:LEU:HD11	2.02	0.42
1:B:36:THR:OG1	5:X:1:NAG:H62	2.20	0.42
1:A:79:ILE:CD1	1:A:248:THR:HG21	2.50	0.41
1:A:365:THR:HG23	1:A:424:ALA:HB3	2.02	0.41
1:B:112:LEU:HD13	1:B:112:LEU:HA	1.86	0.41
1:C:70:GLN:HE22	1:C:72:GLN:HB3	1.85	0.41
1:C:145:VAL:HB	1:C:150:PRO:HA	2.01	0.41
1:C:971:VAL:HG12	1:C:975:ARG:NH2	2.34	0.41
1:A:238:MET:HE3	1:A:249:HIS:C	2.45	0.41
1:A:247:ASN:CG	1:A:248:THR:H	2.28	0.41
1:A:1085:THR:OG1	1:A:1086:GLN:N	2.53	0.41
1:B:30:GLN:HE22	1:B:84:PRO:HG3	1.84	0.41
1:B:1063:HIS:ND1	1:B:1064:LYS:HD2	2.35	0.41
1:C:434:ARG:HH21	1:C:479:ASP:CG	2.28	0.41
1:A:895:VAL:O	1:A:899:ASN:ND2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:OG1	1:C:37:ARG:N	2.54	0.41
1:B:33:VAL:HG21	1:B:254:PHE:CE2	2.55	0.41
1:B:143:PHE:H	1:B:237:ALA:CB	2.33	0.41
1:B:1011:GLU:OE1	1:C:1019:ARG:HB3	2.19	0.41
1:B:22:LEU:O	1:B:23:SER:CB	2.67	0.41
1:B:417:GLU:CD	1:B:417:GLU:H	2.29	0.41
1:C:369:TYR:CE1	1:C:422:ILE:HD12	2.55	0.41
1:A:210:LEU:H	1:A:210:LEU:HD23	1.86	0.41
1:A:284:LEU:O	1:A:288:LYS:HG3	2.21	0.41
1:A:542:LYS:C	1:A:543:LYS:HD2	2.46	0.41
1:A:334:GLN:C	1:A:334:GLN:CD	2.88	0.41
1:B:814:MET:HB2	1:C:599:ASP:O	2.21	0.41
1:C:371:VAL:HG21	1:C:500:PHE:HE2	1.86	0.41
1:A:146:SER:N	1:A:149:LYS:O	2.48	0.41
1:A:238:MET:HG3	1:A:248:THR:OG1	2.21	0.41
1:A:774:ILE:HD12	1:A:774:ILE:C	2.45	0.41
1:A:1071:ARG:NH1	1:A:1100:THR:O	2.54	0.41
1:A:1091:GLN:NE2	1:B:1101:PHE:HZ	2.19	0.41
1:B:40:PHE:CE1	1:B:263:MET:HE2	2.55	0.41
1:C:950:PHE:HD2	1:C:976:LEU:HD23	1.85	0.41
1:A:803:TYR:CE1	1:A:1037:PRO:HG3	2.56	0.41
1:B:86:ILE:CD1	1:B:255:VAL:HG11	2.51	0.41
1:B:236:MET:C	1:B:238:MET:N	2.78	0.41
1:B:1107:ASP:O	1:B:1109:VAL:N	2.50	0.41
1:C:220:MET:O	1:C:221:LEU:HD23	2.21	0.41
1:C:221:LEU:HD13	1:C:223:LEU:HD21	2.02	0.41
1:C:316:ARG:HD2	1:C:518:LEU:HD13	2.02	0.41
1:C:335:PHE:CE2	1:C:388:TYR:HB2	2.56	0.41
1:C:602:CYS:HB2	1:C:636:CYS:HB2	1.51	0.41
1:C:813:PHE:HD1	1:C:813:PHE:HA	1.77	0.41
1:A:105:GLY:CA	1:A:121:VAL:O	2.69	0.41
1:B:719:ASN:OD1	1:B:730:SER:OG	2.31	0.41
1:B:73:VAL:HG22	1:B:248:THR:HG23	2.02	0.40
1:B:120:ILE:HG22	1:B:122:VAL:HG22	2.03	0.40
1:C:25:LYS:N	1:C:79:ILE:O	2.49	0.40
1:A:907:PHE:O	1:A:911:ILE:HG13	2.21	0.40
1:C:335:PHE:HB3	1:C:390:VAL:HG23	2.03	0.40
1:A:145:VAL:H	1:A:240:SER:HB2	1.86	0.40
7:A:1304:NAG:H82	1:C:814:MET:O	2.22	0.40
1:A:51:LEU:HD12	1:A:52:ARG:N	2.36	0.40
1:A:316:ARG:HD2	1:A:518:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PHE:O	1:A:330:PHE:HB2	2.22	0.40
1:A:973:ILE:O	1:A:977:ILE:HG13	2.21	0.40
1:B:81:PHE:HZ	1:B:238:MET:HB3	1.86	0.40
1:B:788:ASP:O	1:B:790:ALA:N	2.54	0.40
1:C:170:LEU:HD13	8:C:1307:BLA:HAC	2.04	0.40
1:A:171:ASN:OD1	1:A:171:ASN:N	2.45	0.40
1:B:806:VAL:HG21	1:B:1037:PRO:CG	2.49	0.40
1:C:747:LEU:HD23	1:C:747:LEU:HA	1.86	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	1101/1229 (90%)	1011 (92%)	81 (7%)	9 (1%)	16	14
1	B	1101/1229 (90%)	1007 (92%)	89 (8%)	5 (0%)	24	24
1	C	1101/1229 (90%)	1006 (91%)	93 (8%)	2 (0%)	43	50
All	All	3303/3687 (90%)	3024 (92%)	263 (8%)	16 (0%)	26	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	SER
1	B	813	PHE
1	A	75	ASN
1	A	827	ARG
1	A	150	PRO
1	A	125	ALA
1	A	789	PRO
1	A	810	ASP
1	B	25	LYS

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Mol	Chain	Res	Type
1	B	237	ALA
1	A	246	PHE
1	A	813	PHE
1	C	813	PHE
1	A	19	CYS
1	B	812	GLY
1	C	1108	VAL

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	965/1070 (90%)	910 (94%)	55 (6%)	18	19
1	B	965/1070 (90%)	911 (94%)	54 (6%)	19	20
1	C	965/1070 (90%)	910 (94%)	55 (6%)	18	19
All	All	2895/3210 (90%)	2731 (94%)	164 (6%)	20	19

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	64	THR
1	A	75	ASN
1	A	79	ILE
1	A	80	PHE
1	A	86	ILE
1	A	89	ASN
1	A	92	VAL
1	A	116	THR
1	A	133	CYS
1	A	142	MET
1	A	150	PRO
1	A	241	LEU
1	A	242	THR
1	A	248	THR

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Mol	Chain	Res	Type
1	A	308	VAL
1	A	315	VAL
1	A	334	GLN
1	A	365	THR
1	A	371	VAL
1	A	513	LYS
1	A	518	LEU
1	A	531	LEU
1	A	560	SER
1	A	561	VAL
1	A	604	ASP
1	A	608	MET
1	A	615	SER
1	A	632	THR
1	A	663	THR
1	A	668	LYS
1	A	741	GLN
1	A	771	VAL
1	A	794	LYS
1	A	796	SER
1	A	813	PHE
1	A	815	LYS
1	A	821	LEU
1	A	824	VAL
1	A	827	ARG
1	A	830	ILE
1	A	831	CYS
1	A	868	PHE
1	A	899	ASN
1	A	909	LYS
1	A	966	PRO
1	A	971	VAL
1	A	988	VAL
1	A	998	ILE
1	A	1017	SER
1	A	1046	THR
1	A	1064	LYS
1	A	1066	LYS
1	A	1112	ILE
1	A	1116	THR
1	B	22	LEU
1	B	73	VAL

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Mol	Chain	Res	Type
1	B	74	ILE
1	B	100	SER
1	B	110	THR
1	B	133	CYS
1	B	149	LYS
1	B	152	LYS
1	B	155	VAL
1	B	234	VAL
1	B	236	MET
1	B	259	LYS
1	B	261	LEU
1	B	263	MET
1	B	315	VAL
1	B	329	VAL
1	B	371	VAL
1	B	433	LYS
1	B	467	GLN
1	B	508	THR
1	B	560	SER
1	B	573	THR
1	B	577	TYR
1	B	607	THR
1	B	709	VAL
1	B	770	LYS
1	B	774	ILE
1	B	795	ARG
1	B	798	ILE
1	B	806	VAL
1	B	807	THR
1	B	813	PHE
1	B	815	LYS
1	B	816	GLN
1	B	817	TYR
1	B	821	LEU
1	B	824	VAL
1	B	825	ASN
1	B	830	ILE
1	B	875	GLN
1	B	887	ASN
1	B	894	ASN
1	B	895	VAL
1	B	896	LEU

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Mol	Chain	Res	Type
1	B	901	LYS
1	B	954	SER
1	B	955	SER
1	B	964	LEU
1	B	970	GLU
1	B	971	VAL
1	B	1021	ASP
1	B	1064	LYS
1	B	1066	LYS
1	B	1116	THR
1	C	29	THR
1	C	65	ASN
1	C	74	ILE
1	C	102	VAL
1	C	158	ARG
1	C	177	GLU
1	C	248	THR
1	C	250	SER
1	C	263	MET
1	C	277	ILE
1	C	309	SER
1	C	446	ILE
1	C	454	SER
1	C	467	GLN
1	C	495	VAL
1	C	513	LYS
1	C	534	THR
1	C	558	THR
1	C	575	CYS
1	C	608	MET
1	C	709	VAL
1	C	743	LEU
1	C	765	VAL
1	C	771	VAL
1	C	785	ILE
1	C	793	SER
1	C	805	LYS
1	C	807	THR
1	C	808	LEU
1	C	810	ASP
1	C	813	PHE
1	C	814	MET

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Mol	Chain	Res	Type
1	C	815	LYS
1	C	817	TYR
1	C	819	ASP
1	C	821	LEU
1	C	824	VAL
1	C	825	ASN
1	C	827	ARG
1	C	828	ASP
1	C	830	ILE
1	C	831	CYS
1	C	854	THR
1	C	948	SER
1	C	957	LEU
1	C	990	GLN
1	C	1008	LYS
1	C	1025	LYS
1	C	1057	THR
1	C	1062	CYS
1	C	1074	VAL
1	C	1077	THR
1	C	1109	VAL
1	C	1110	ILE
1	C	1116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	ASN
1	A	395	HIS
1	A	471	HIS
1	A	549	GLN
1	A	690	ASN
1	A	784	GLN
1	A	908	ASN
1	A	949	ASN
1	A	1034	GLN
1	A	1063	HIS
1	B	32	GLN
1	B	252	ASN
1	B	305	ASN
1	B	545	GLN
1	B	598	GLN

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Mol	Chain	Res	Type
1	B	754	GLN
1	B	893	GLN
1	B	902	GLN
1	B	929	GLN
1	B	1016	GLN
1	C	30	GLN
1	C	70	GLN
1	C	89	ASN
1	C	101	ASN
1	C	187	GLN
1	C	200	HIS
1	C	245	ASN
1	C	249	HIS
1	C	305	ASN
1	C	662	GLN
1	C	902	GLN
1	C	940	ASN
1	C	945	GLN
1	C	972	GLN
1	C	1028	HIS
1	C	1034	GLN
1	C	1081	HIS

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 ⓘ

68 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	0.46	0	17,19,21	0.85	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.73	0
2	BMA	D	3	2	11,11,12	0.25	0	15,15,17	0.56	0
3	NAG	E	1	3,1	14,14,15	0.50	0	17,19,21	0.79	1 (5%)
3	NAG	E	2	3	14,14,15	0.50	0	17,19,21	0.76	0
3	BMA	E	3	3	11,11,12	0.25	0	15,15,17	0.62	0
3	MAN	E	4	3	11,11,12	0.22	0	15,15,17	0.58	0
2	NAG	F	1	2,1	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	0.81	0
2	BMA	F	3	2	11,11,12	0.24	0	15,15,17	0.57	0
2	NAG	G	1	2,1	14,14,15	0.48	0	17,19,21	0.95	2 (11%)
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	0.88	1 (5%)
2	BMA	G	3	2	11,11,12	0.30	0	15,15,17	0.60	0
3	NAG	H	1	3,1	14,14,15	0.45	0	17,19,21	0.59	0
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	0.69	0
3	BMA	H	3	3	11,11,12	0.21	0	15,15,17	0.77	0
3	MAN	H	4	3	11,11,12	0.21	0	15,15,17	0.54	0
4	NAG	I	1	4,1	14,14,15	0.72	0	17,19,21	1.02	1 (5%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	0.97	1 (5%)
4	BMA	I	3	4	11,11,12	0.20	0	15,15,17	0.74	0
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.63	0
2	NAG	J	1	2,1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
2	NAG	J	2	2	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
2	BMA	J	3	2	11,11,12	0.26	0	15,15,17	0.64	0
5	NAG	K	1	5,1	14,14,15	0.49	0	17,19,21	0.89	1 (5%)
5	NAG	K	2	5	14,14,15	0.35	0	17,19,21	0.68	0
6	NAG	L	1	6,1	14,14,15	0.37	0	17,19,21	1.11	2 (11%)
6	BMA	L	2	6	11,11,12	0.52	0	15,15,17	1.13	1 (6%)
5	NAG	M	1	5,1	14,14,15	0.39	0	17,19,21	0.53	0
5	NAG	M	2	5	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
3	NAG	N	1	3,1	14,14,15	0.39	0	17,19,21	0.66	1 (5%)
3	NAG	N	2	3	14,14,15	0.38	0	17,19,21	0.59	0
3	BMA	N	3	3	11,11,12	0.27	0	15,15,17	0.63	0
3	MAN	N	4	3	11,11,12	0.34	0	15,15,17	1.04	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.41	0	17,19,21	0.67	0
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	0.45	0
5	NAG	P	1	5,1	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
5	NAG	P	2	5	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	Q	1	5,1	14,14,15	0.40	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Q	2	5	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
5	NAG	R	1	5,1	14,14,15	0.43	0	17,19,21	0.97	0
5	NAG	R	2	5	14,14,15	0.33	0	17,19,21	0.66	0
3	NAG	S	1	3,1	14,14,15	0.40	0	17,19,21	0.83	0
3	NAG	S	2	3	14,14,15	0.40	0	17,19,21	0.64	0
3	BMA	S	3	3	11,11,12	0.41	0	15,15,17	0.67	0
3	MAN	S	4	3	11,11,12	0.33	0	15,15,17	0.52	0
6	NAG	T	1	6,1	14,14,15	0.72	0	17,19,21	0.90	0
6	BMA	T	2	6	11,11,12	0.42	0	15,15,17	0.60	0
5	NAG	U	1	5,1	14,14,15	0.39	0	17,19,21	0.82	0
5	NAG	U	2	5	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	V	1	5,1	14,14,15	0.37	0	17,19,21	1.81	4 (23%)
5	NAG	V	2	5	14,14,15	0.39	0	17,19,21	0.68	0
5	NAG	W	1	5,1	14,14,15	0.39	0	17,19,21	0.76	0
5	NAG	W	2	5	14,14,15	0.41	0	17,19,21	0.84	0
5	NAG	X	1	5,1	14,14,15	0.49	0	17,19,21	1.17	1 (5%)
5	NAG	X	2	5	14,14,15	0.29	0	17,19,21	0.66	0
3	NAG	Y	1	3,1	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
3	NAG	Y	2	3	14,14,15	0.40	0	17,19,21	0.63	0
3	BMA	Y	3	3	11,11,12	0.33	0	15,15,17	0.56	0
3	MAN	Y	4	3	11,11,12	0.34	0	15,15,17	0.57	0
5	NAG	Z	1	5,1	14,14,15	0.39	0	17,19,21	0.60	0
5	NAG	Z	2	5	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	a	1	3	14,14,15	0.61	0	17,19,21	0.96	0
3	NAG	a	2	3	14,14,15	0.40	0	17,19,21	0.88	0
3	BMA	a	3	3	11,11,12	0.25	0	15,15,17	0.68	0
3	MAN	a	4	3	11,11,12	0.25	0	15,15,17	0.61	0
5	NAG	b	1	5,1	14,14,15	0.41	0	17,19,21	0.64	0
5	NAG	b	2	5	14,14,15	0.38	0	17,19,21	0.79	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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	BMA	L	2	6	-	2/2/19/22	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	4/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	S	4	3	-	2/2/19/22	0/1/1/1
6	NAG	T	1	6,1	-	0/6/23/26	0/1/1/1
6	BMA	T	2	6	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	3/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Y	4	3	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
3	MAN	a	4	3	-	1/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	1	NAG	C1-C2-N2	4.80	117.99	110.43
5	V	1	NAG	C2-N2-C7	3.39	127.45	122.90
6	L	1	NAG	C1-O5-C5	3.29	116.60	112.19
2	J	1	NAG	C1-C2-N2	-3.18	105.43	110.43
5	X	1	NAG	C2-N2-C7	-3.12	118.72	122.90
3	N	4	MAN	C1-O5-C5	3.05	116.27	112.19
5	M	2	NAG	C1-C2-N2	3.04	115.22	110.43
5	V	1	NAG	O4-C4-C3	-2.77	103.84	110.38
6	L	2	BMA	C1-C2-C3	2.75	113.64	109.64
5	Q	2	NAG	C1-C2-N2	2.63	114.57	110.43
3	Y	1	NAG	C1-C2-N2	2.58	114.49	110.43
5	P	1	NAG	C2-N2-C7	2.53	126.30	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	1	NAG	C1-O5-C5	2.40	115.41	112.19
4	I	1	NAG	C2-N2-C7	-2.36	119.74	122.90
2	G	1	NAG	C1-C2-N2	-2.35	106.73	110.43
2	G	1	NAG	C4-C3-C2	-2.31	107.63	111.02
5	b	2	NAG	C2-N2-C7	2.26	125.92	122.90
3	Y	1	NAG	C1-O5-C5	2.24	115.19	112.19
6	L	1	NAG	O5-C1-C2	-2.13	107.99	111.29
3	E	1	NAG	C1-O5-C5	2.12	115.02	112.19
2	J	2	NAG	C4-C3-C2	-2.10	107.94	111.02
3	N	4	MAN	C1-C2-C3	2.09	112.69	109.64
2	F	1	NAG	C1-O5-C5	2.09	114.99	112.19
5	K	1	NAG	C2-N2-C7	-2.05	120.15	122.90
2	G	2	NAG	C4-C3-C2	-2.01	108.07	111.02
3	N	1	NAG	C1-O5-C5	2.01	114.88	112.19
4	I	2	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
5	V	1	NAG	C1-C2-N2-C7
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
6	L	2	BMA	C4-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2

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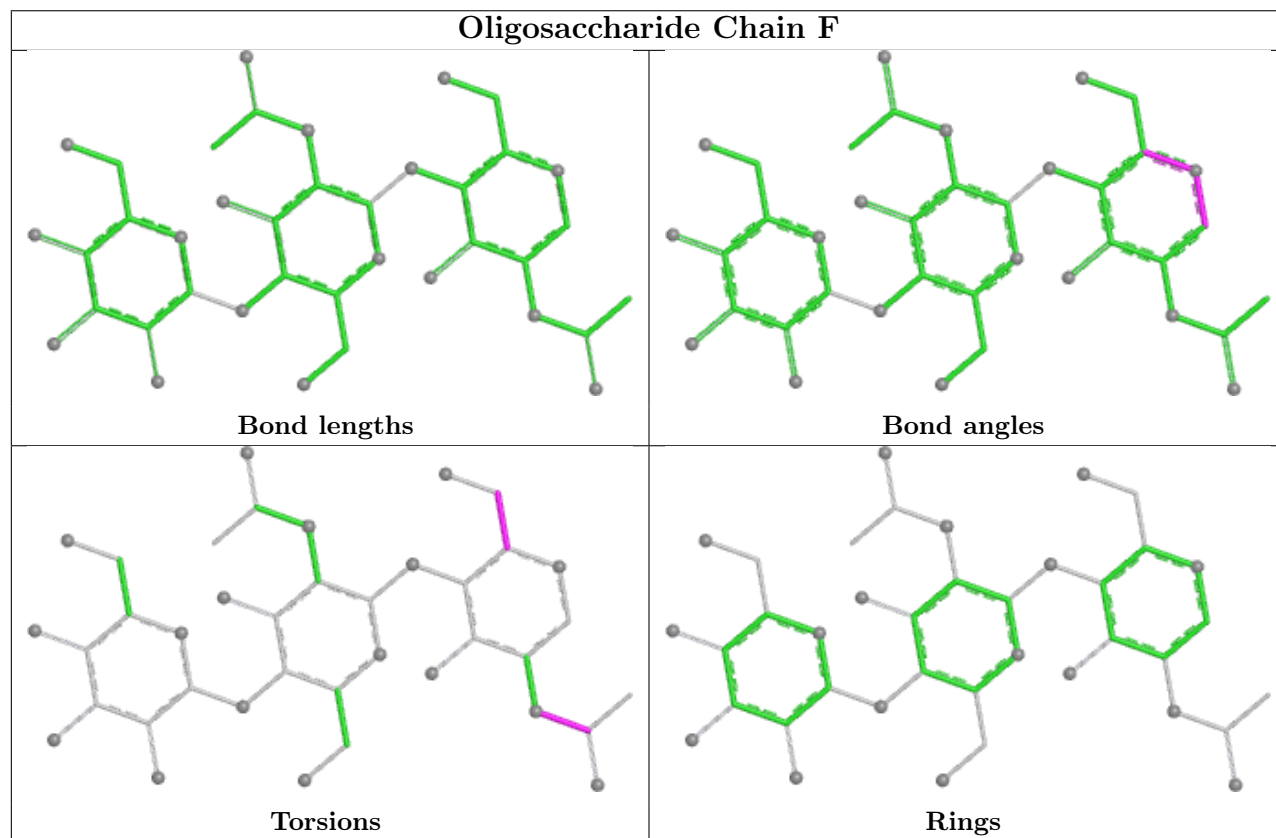
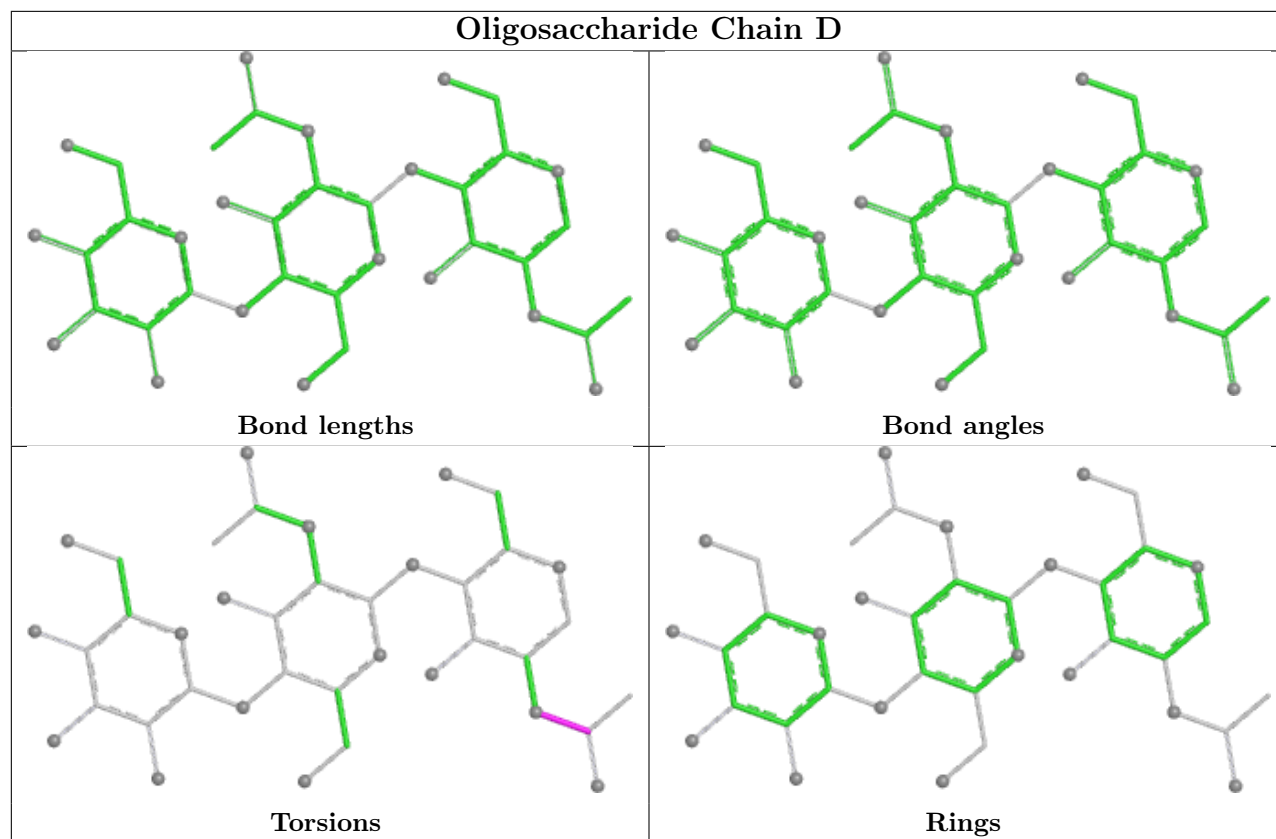
Mol	Chain	Res	Type	Atoms
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
6	L	2	BMA	O5-C5-C6-O6
5	Q	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	U	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
3	Y	4	MAN	O5-C5-C6-O6
3	a	4	MAN	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	O7-C7-N2-C2
3	S	4	MAN	C4-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
3	Y	1	NAG	C8-C7-N2-C2
2	G	1	NAG	C3-C2-N2-C7
2	J	2	NAG	C8-C7-N2-C2
3	S	4	MAN	O5-C5-C6-O6
5	K	1	NAG	C1-C2-N2-C7
2	J	2	NAG	O7-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2

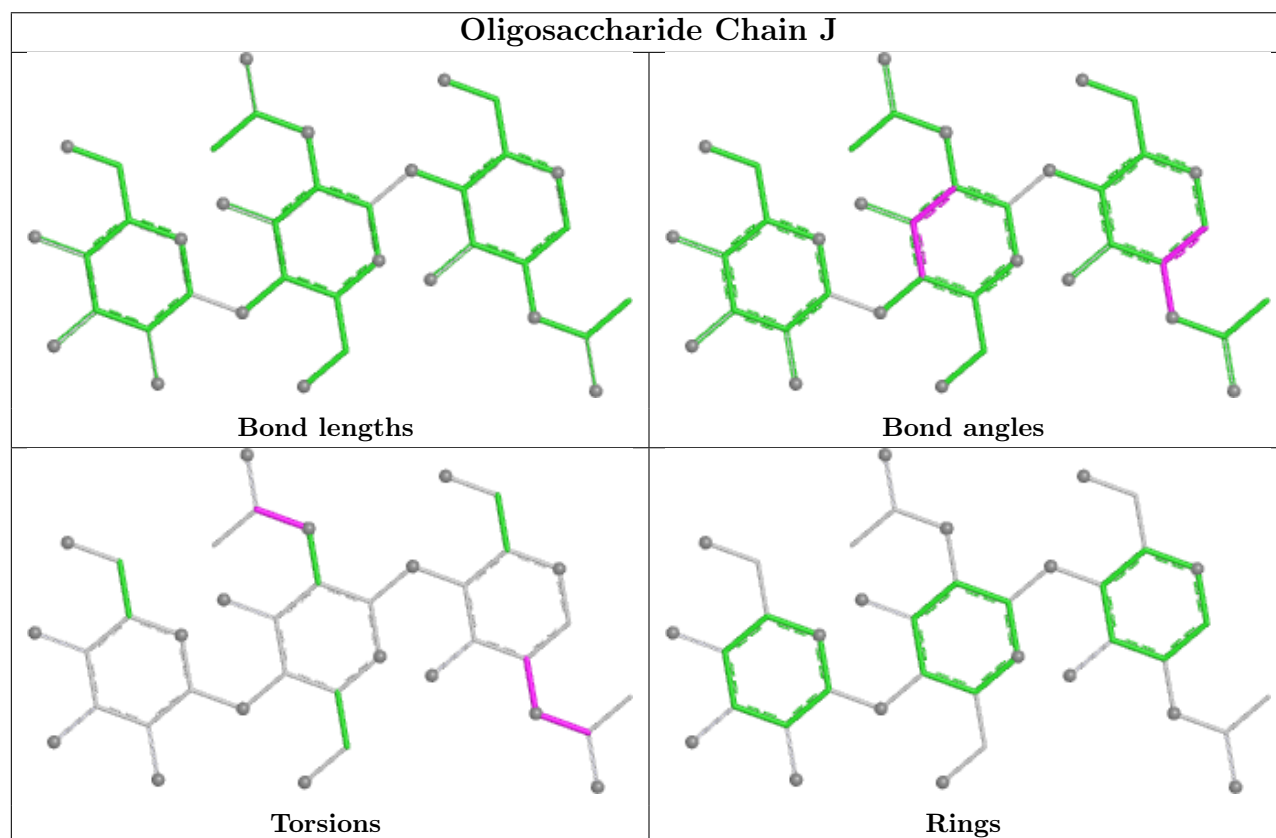
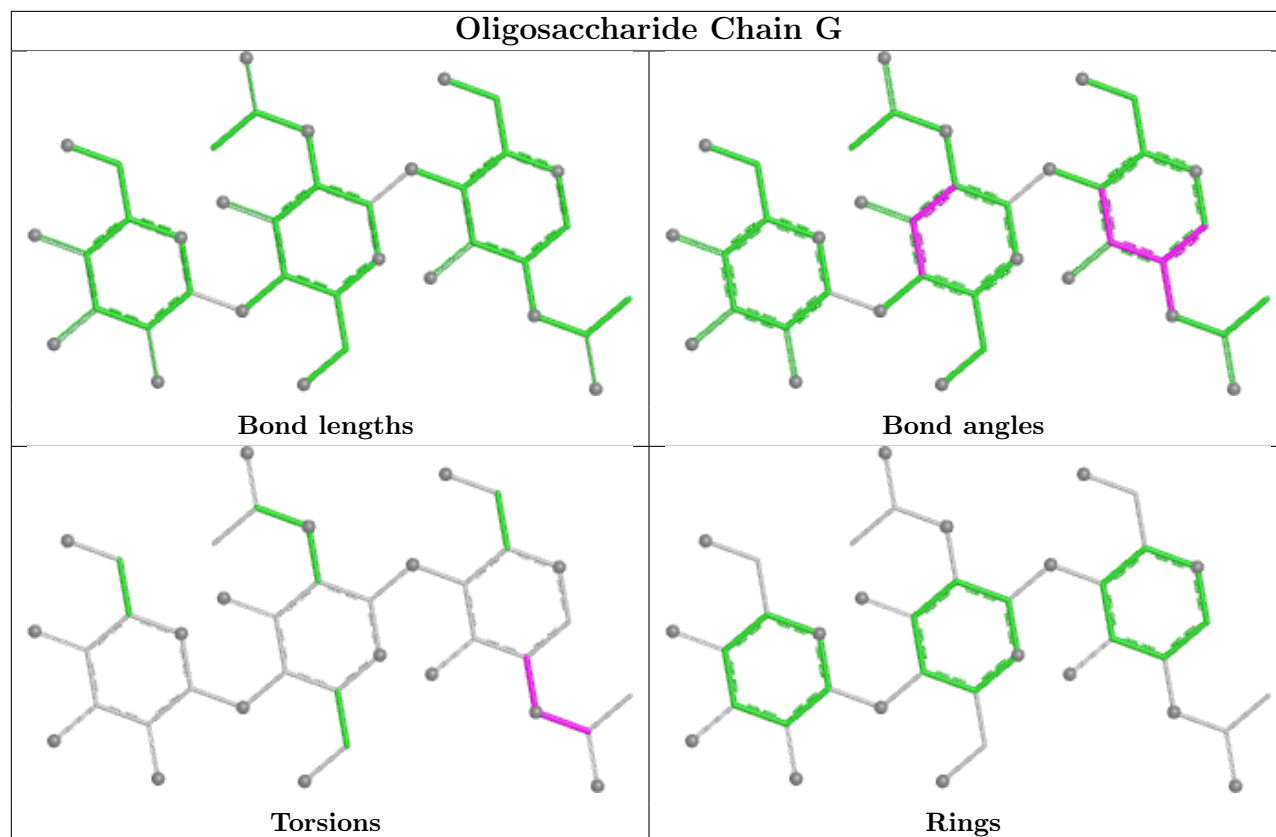
There are no ring outliers.

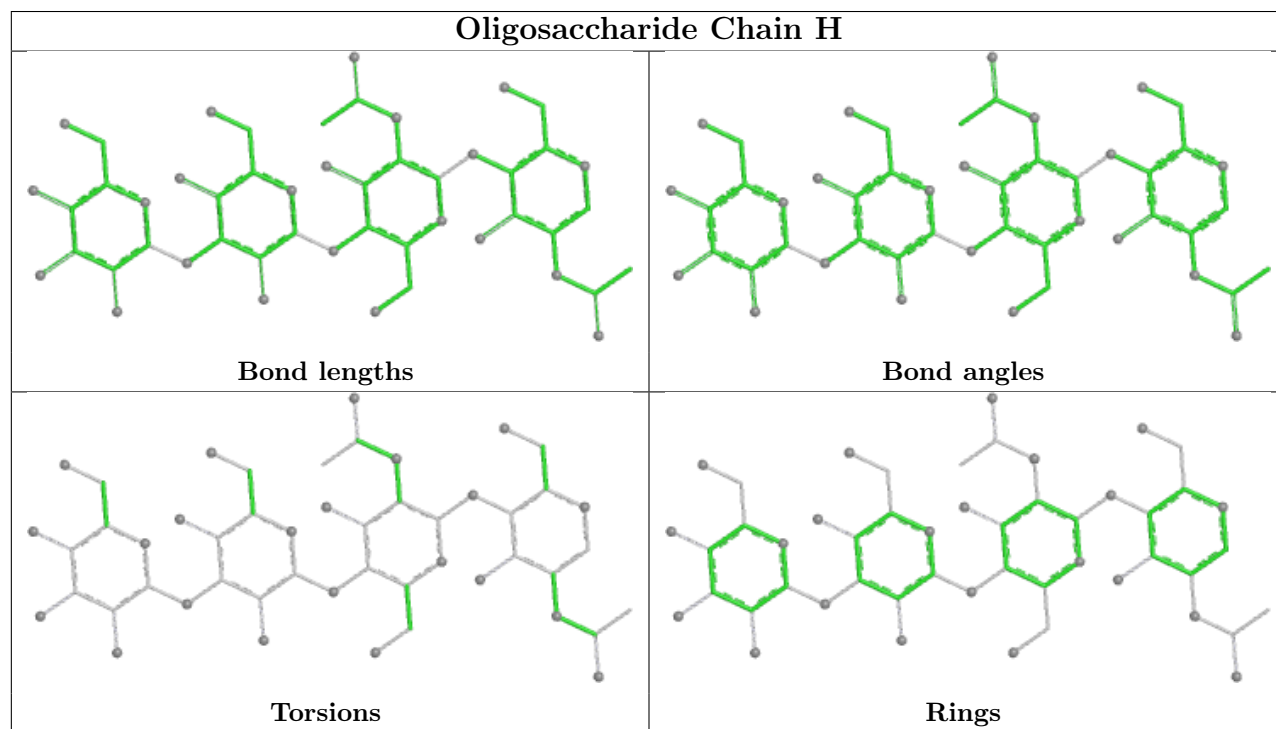
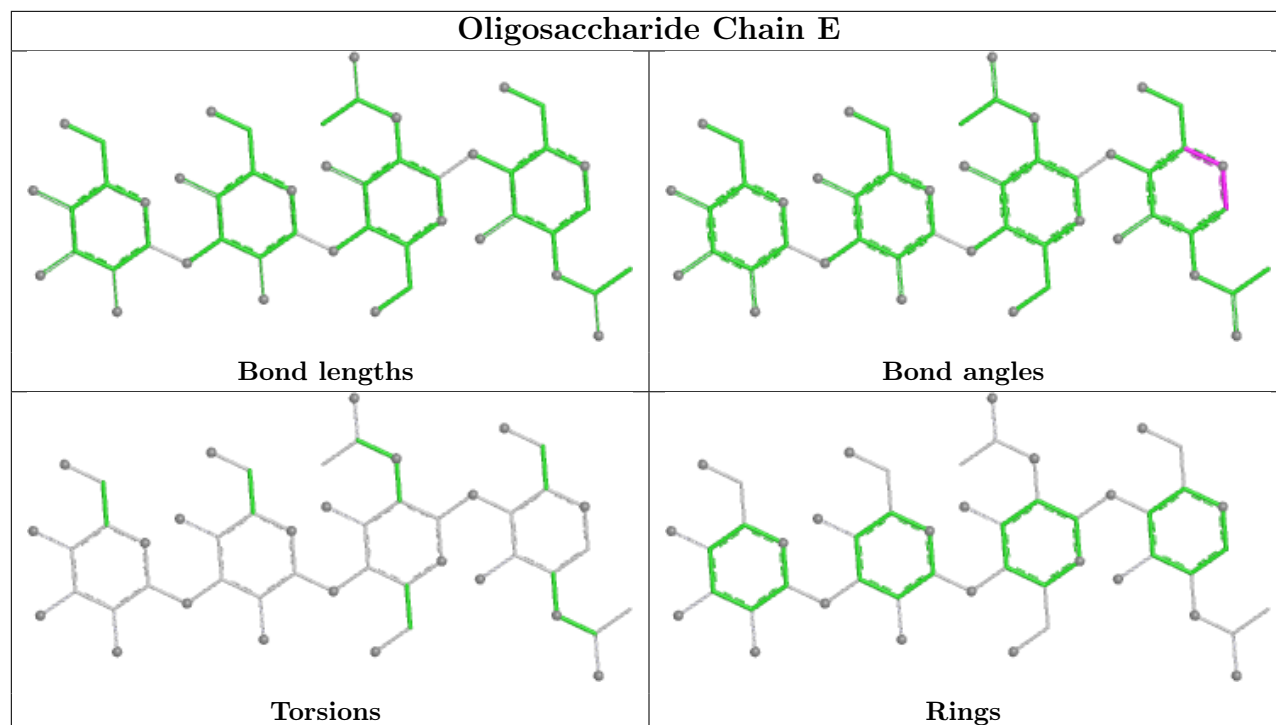
25 monomers are involved in 21 short contacts:

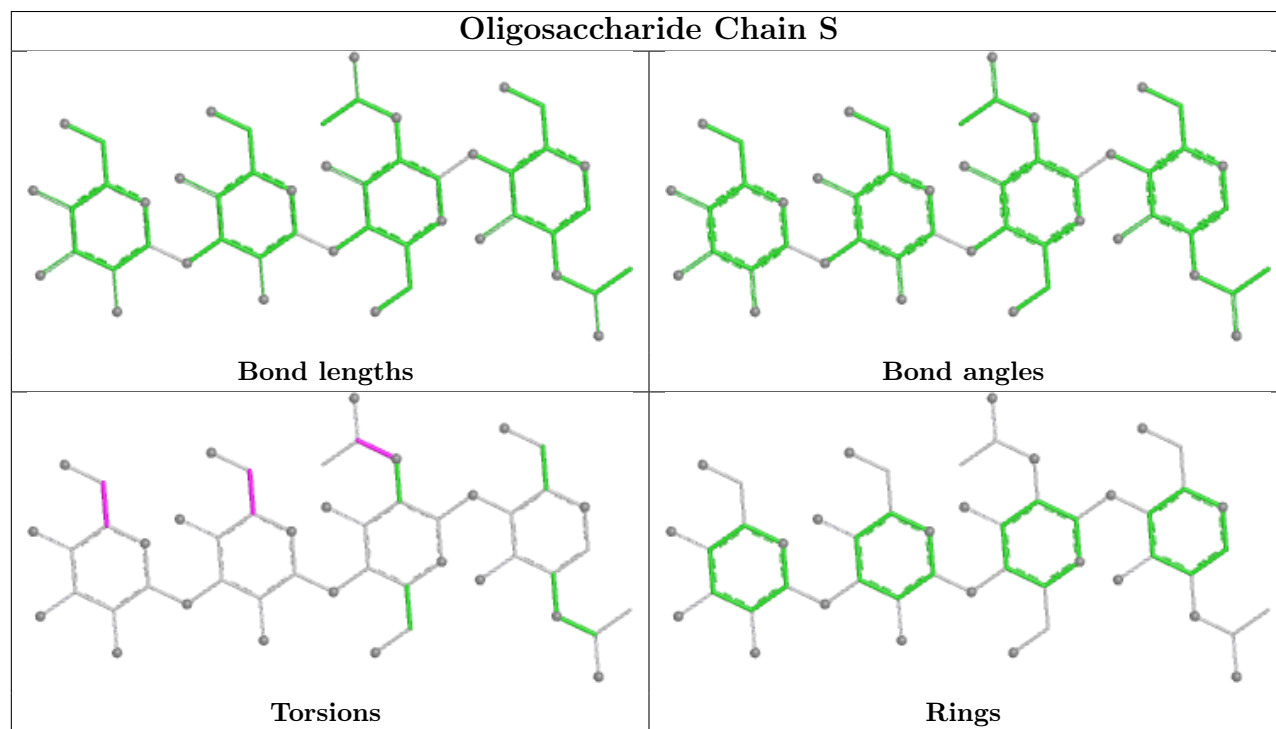
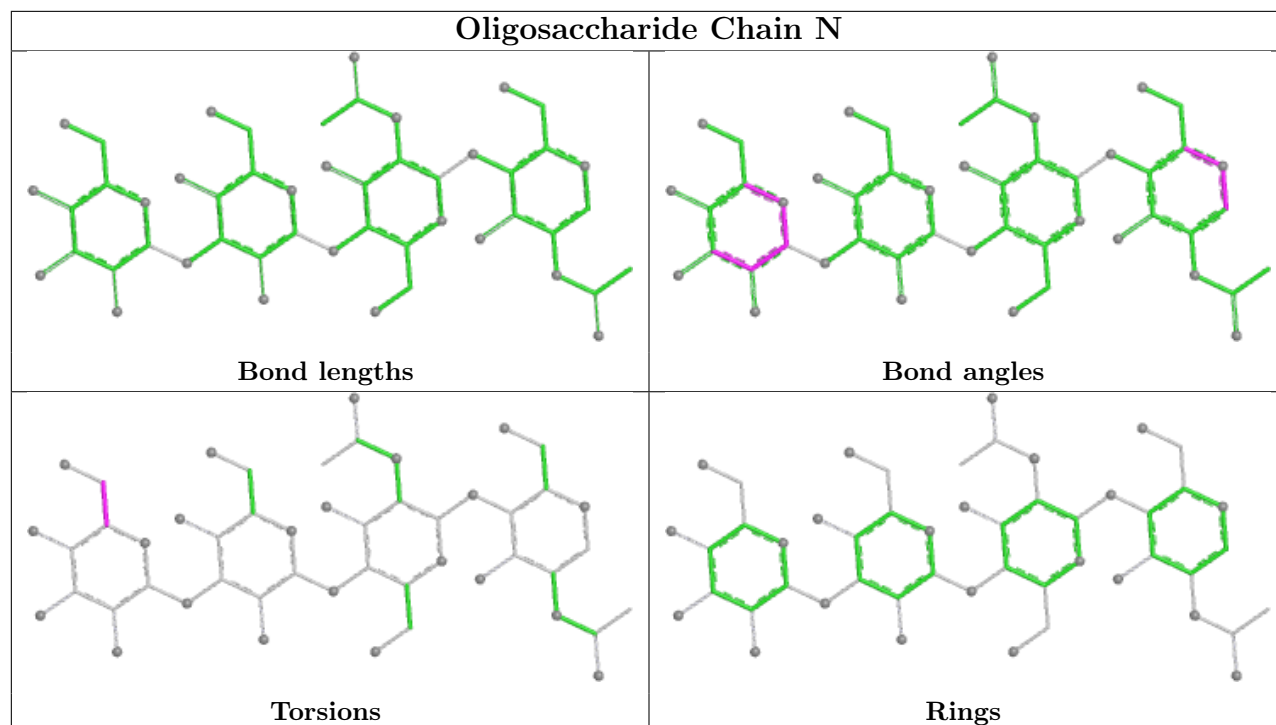
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	H	2	NAG	1	0
3	H	3	BMA	1	0
6	L	1	NAG	1	0
5	V	1	NAG	1	0
6	L	2	BMA	1	0
3	S	1	NAG	1	0
3	H	4	MAN	1	0
5	Q	1	NAG	1	0
5	R	1	NAG	1	0
5	X	2	NAG	1	0
5	V	2	NAG	1	0
5	R	2	NAG	1	0
2	J	1	NAG	2	0
2	G	1	NAG	1	0
2	D	1	NAG	1	0
5	W	1	NAG	2	0
5	K	2	NAG	1	0
5	M	1	NAG	2	0
5	W	2	NAG	2	0
3	Y	1	NAG	2	0
2	J	2	NAG	1	0
3	a	1	NAG	1	0
5	X	1	NAG	2	0
2	D	2	NAG	1	0

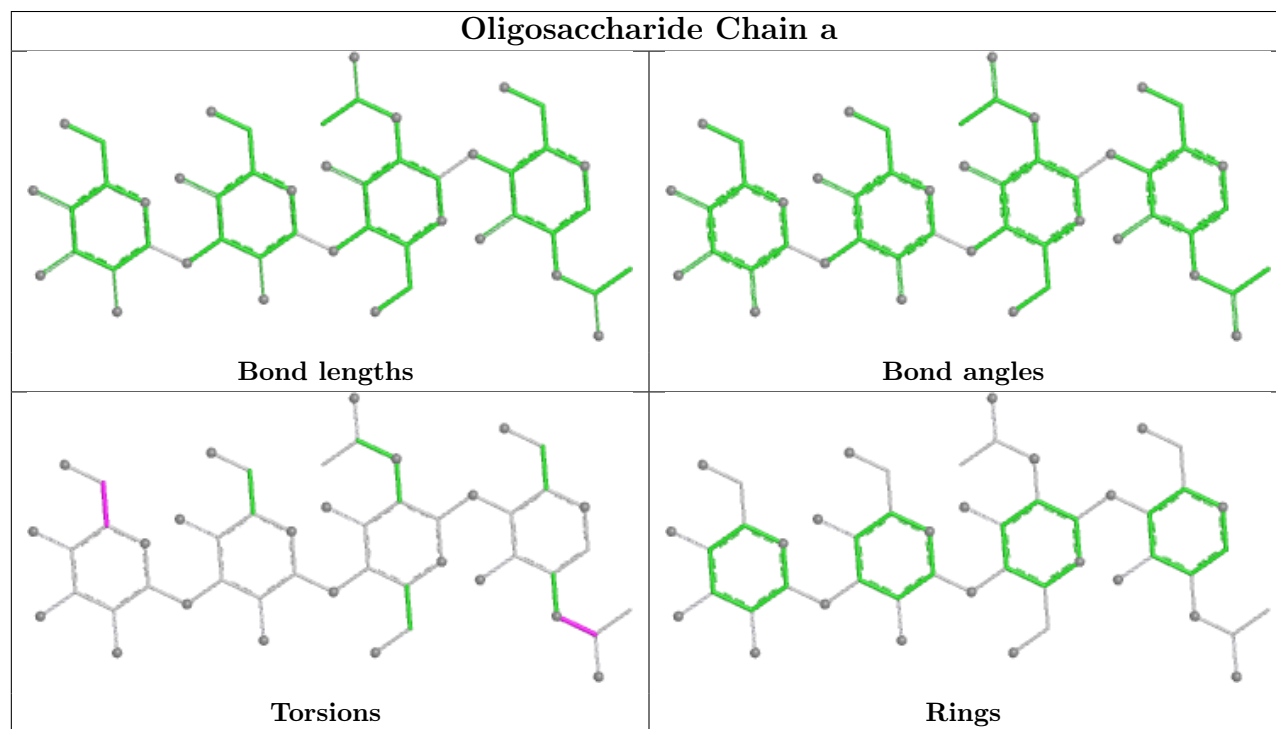
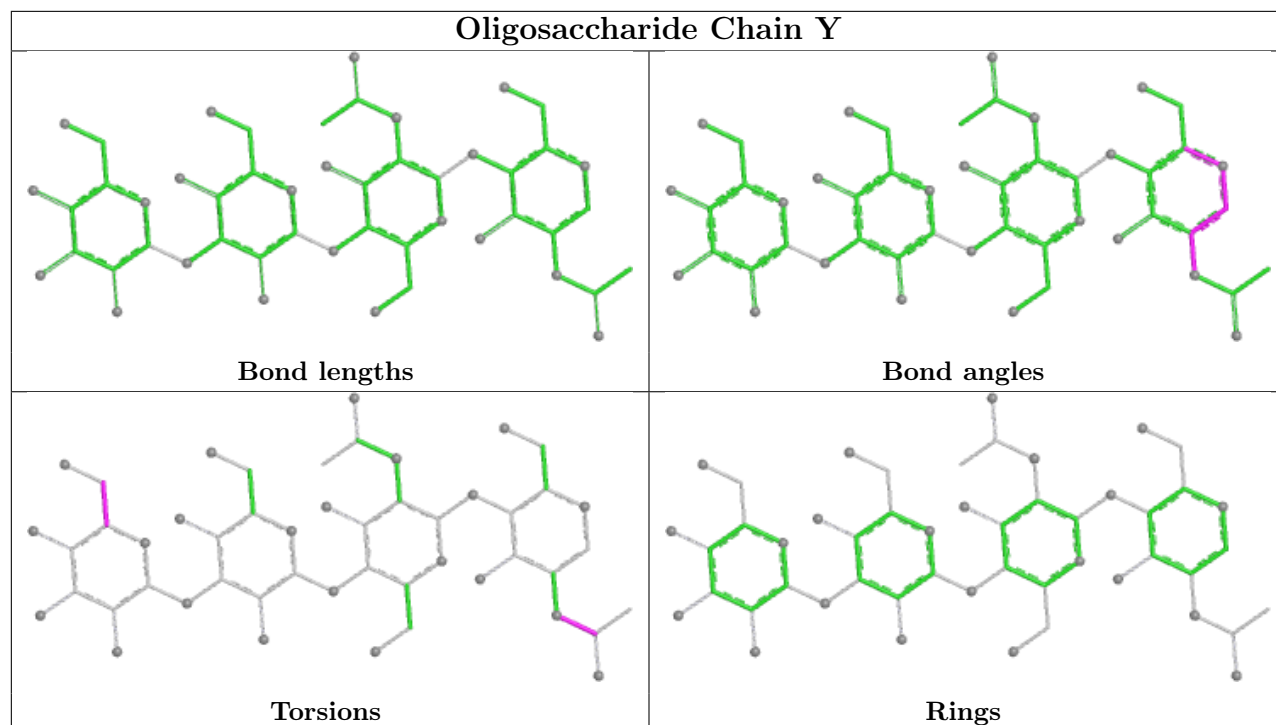
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

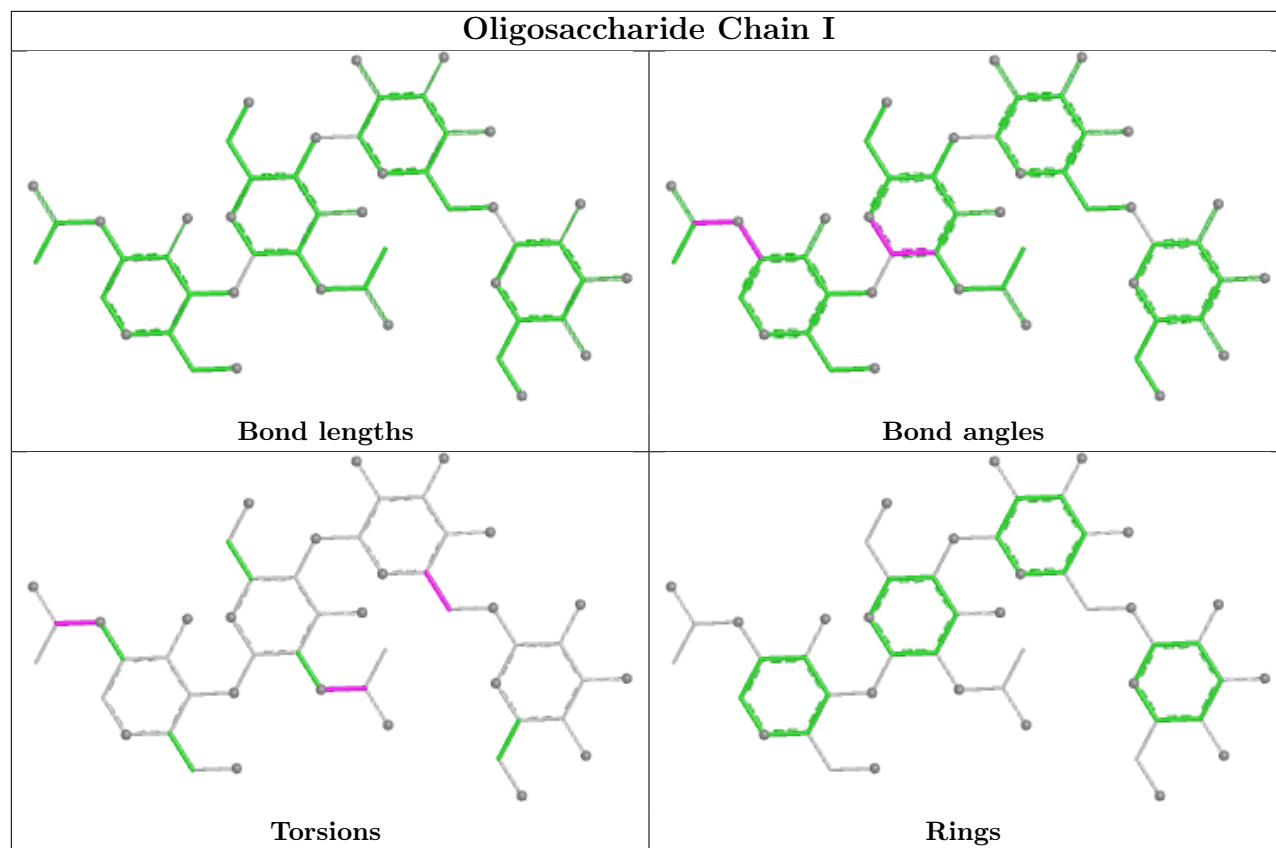


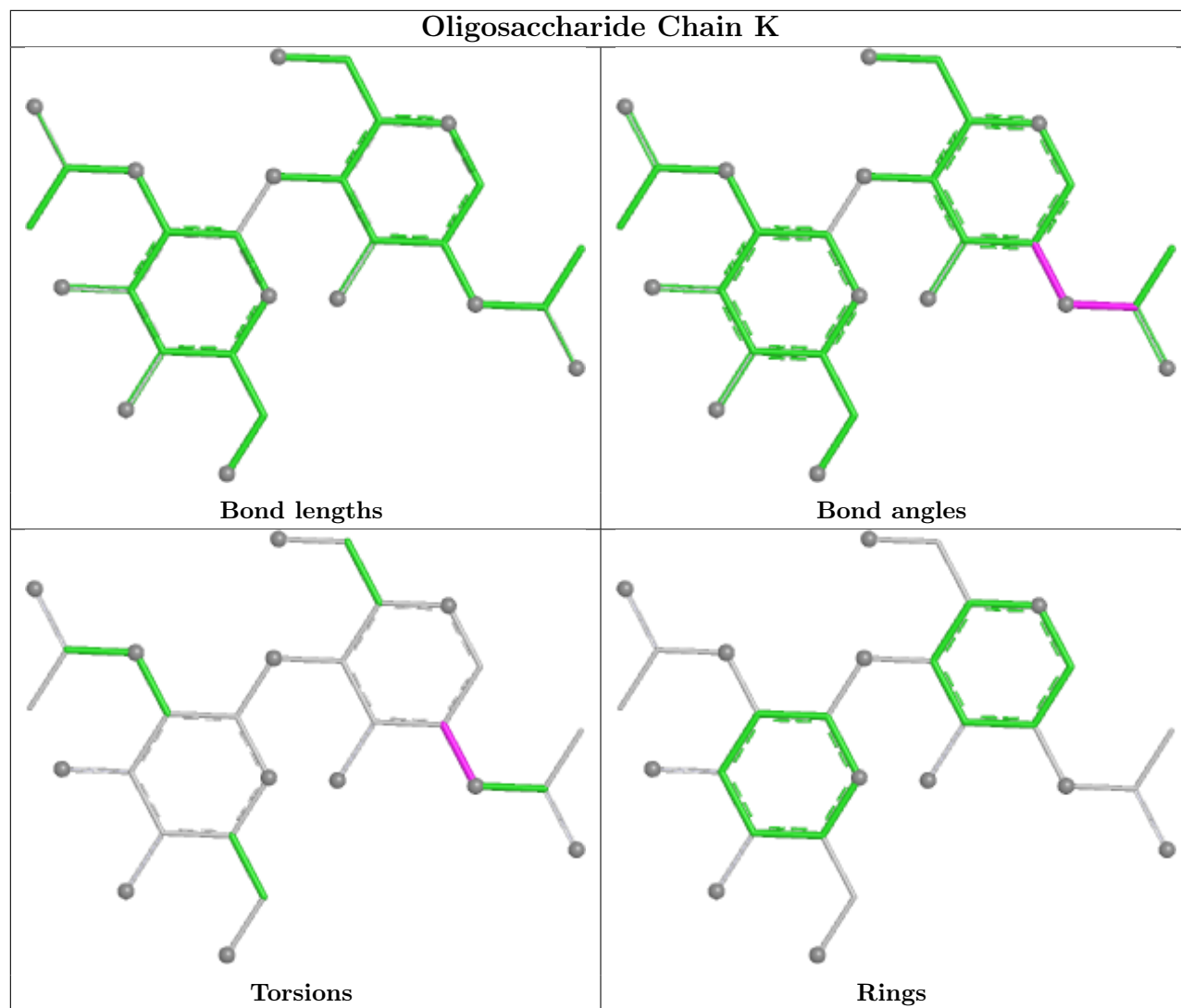


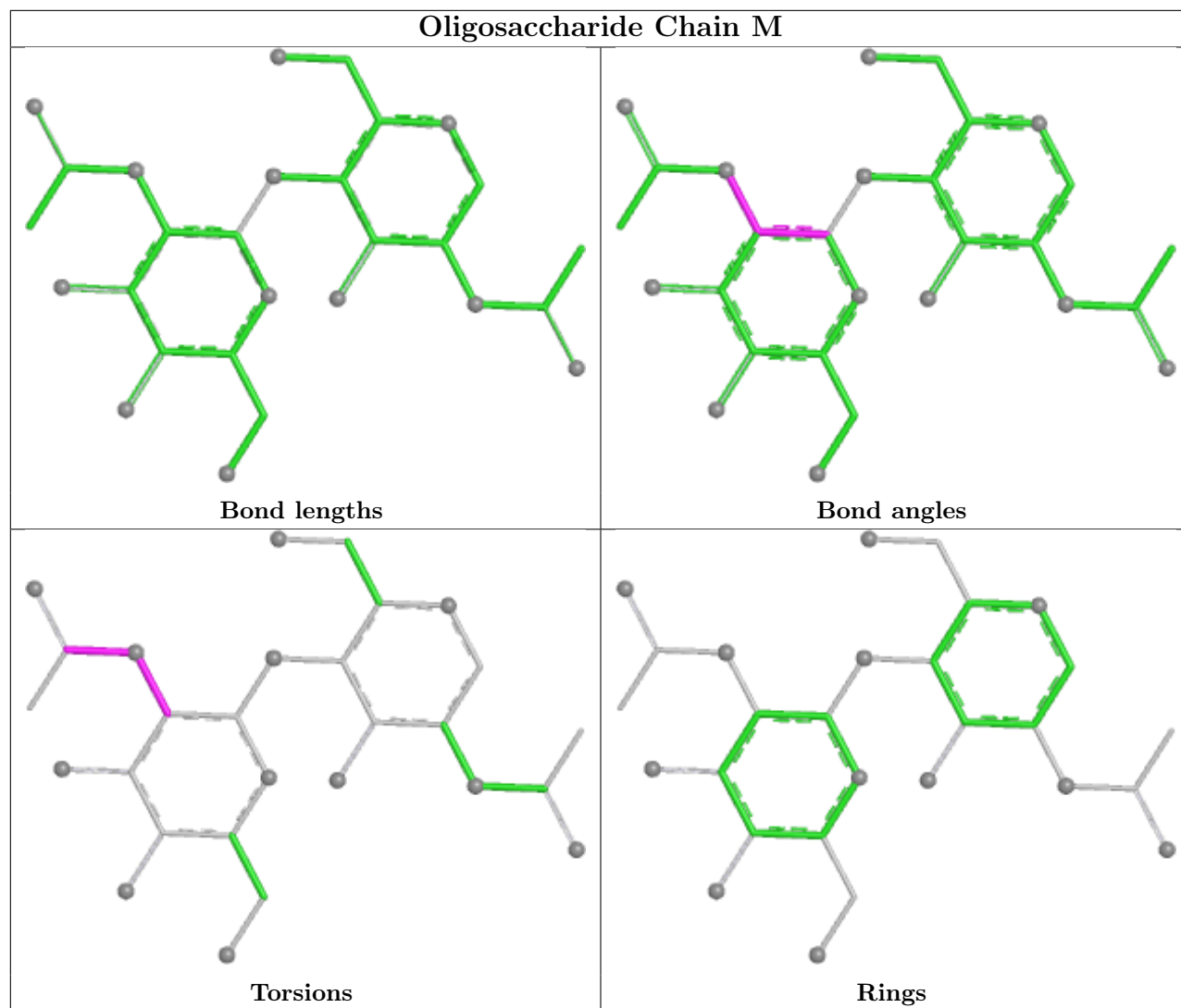


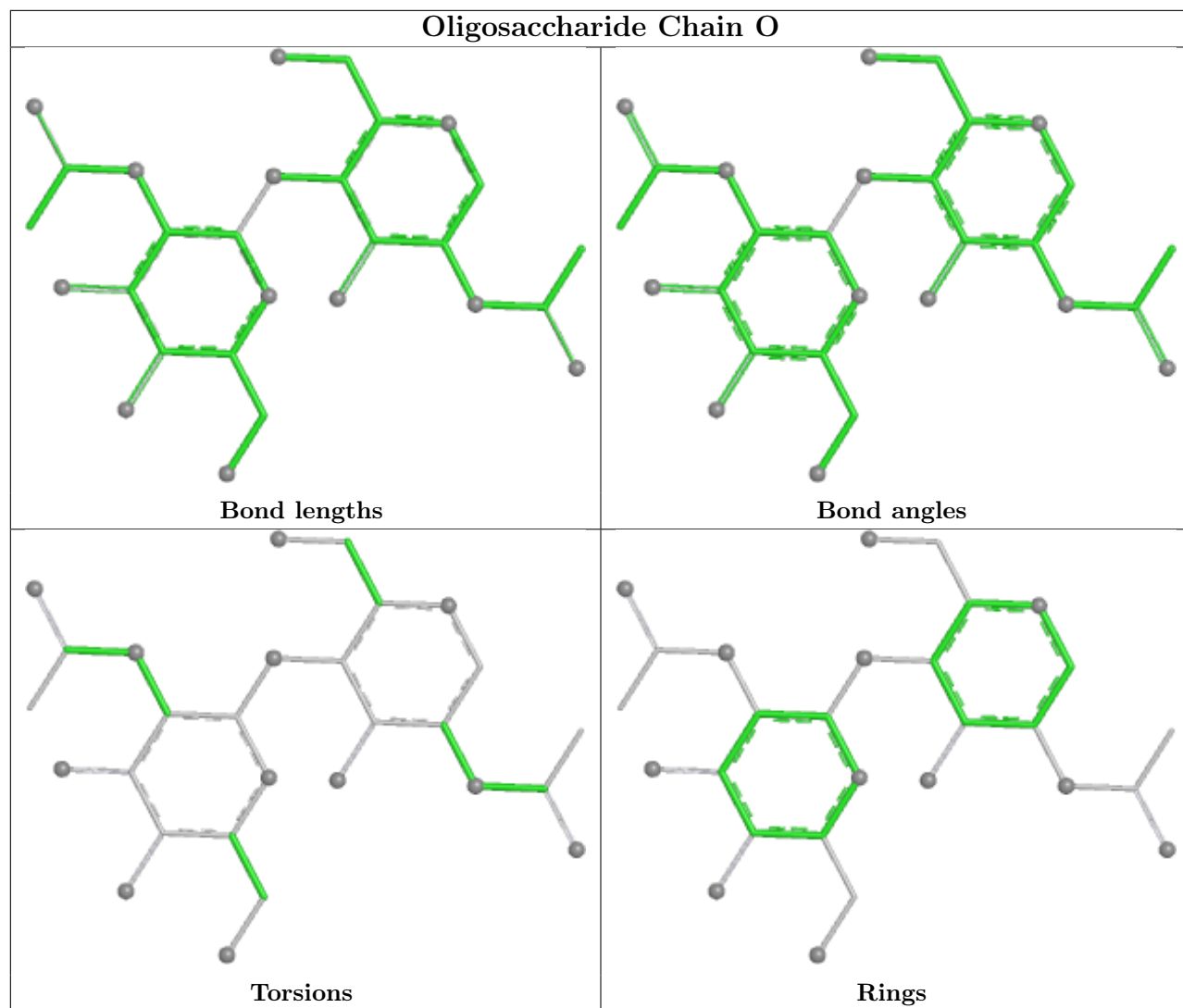


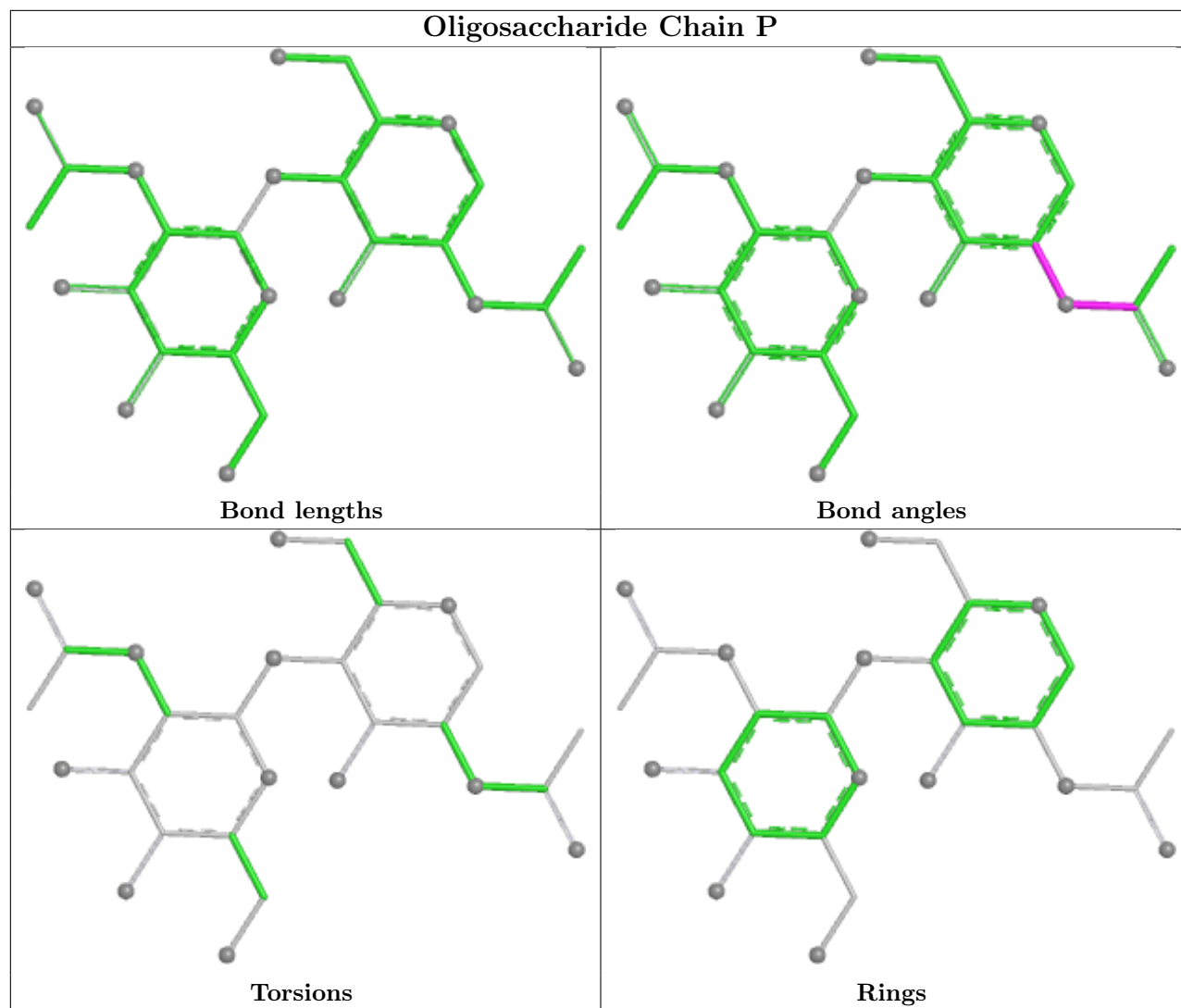


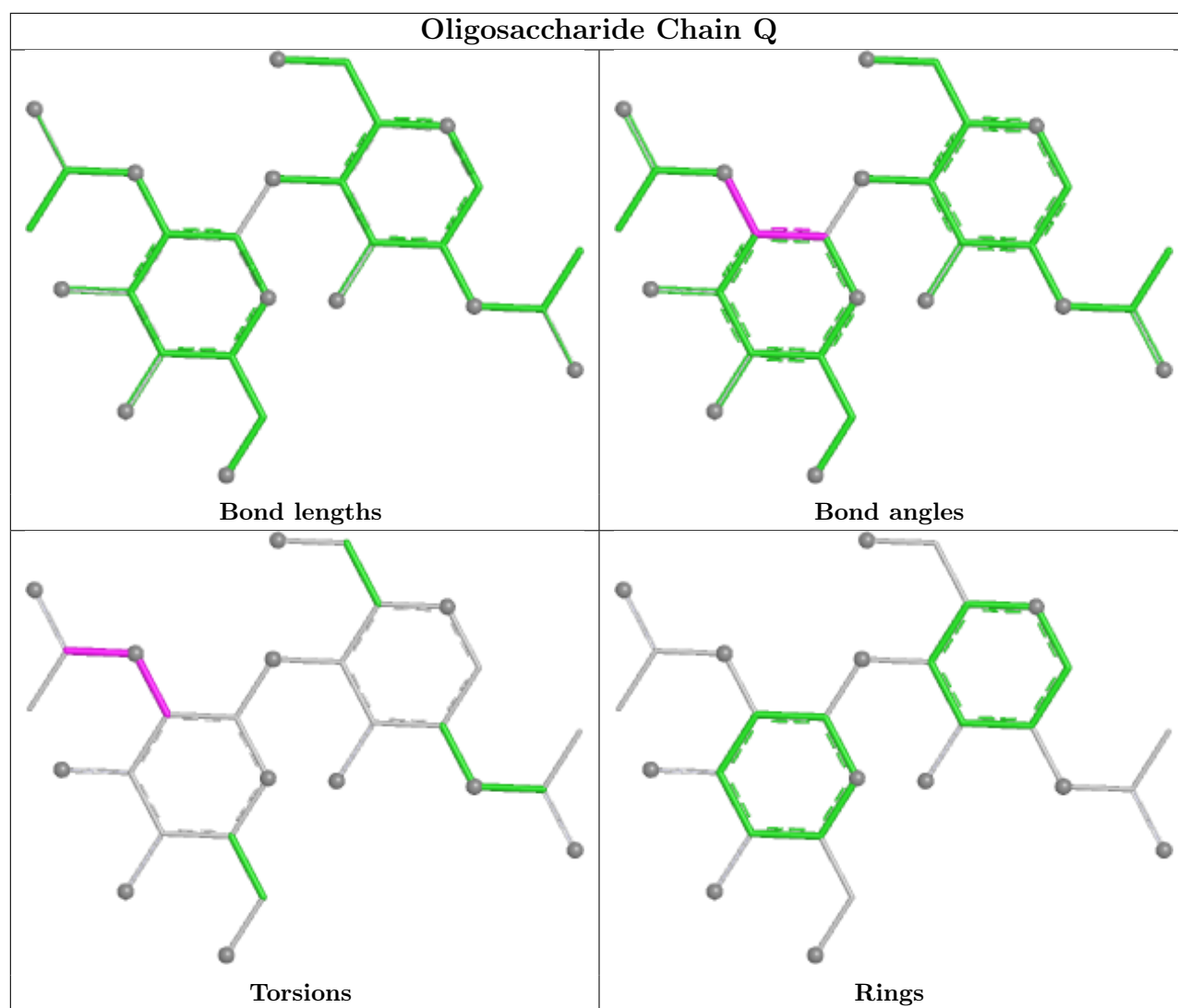


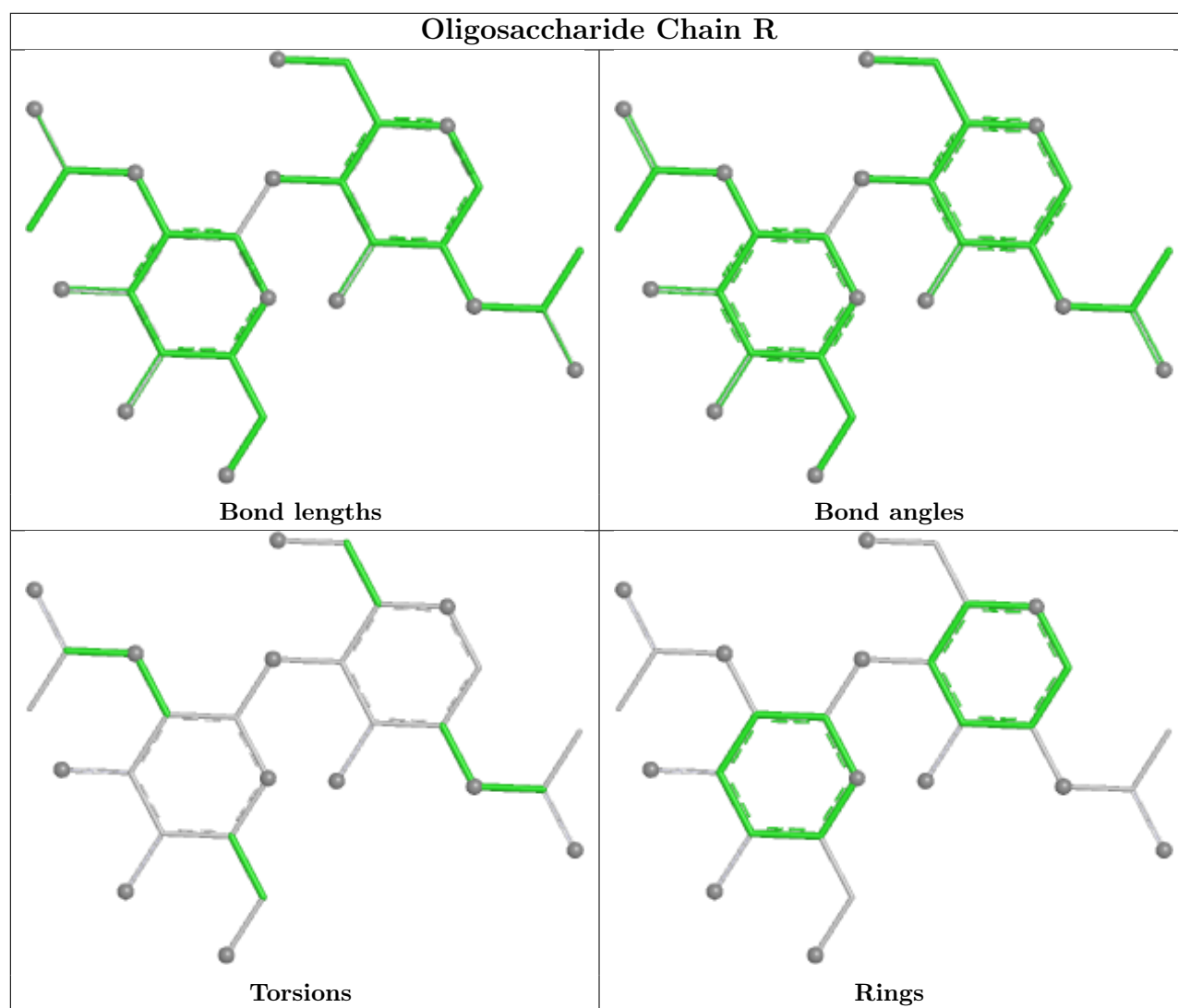


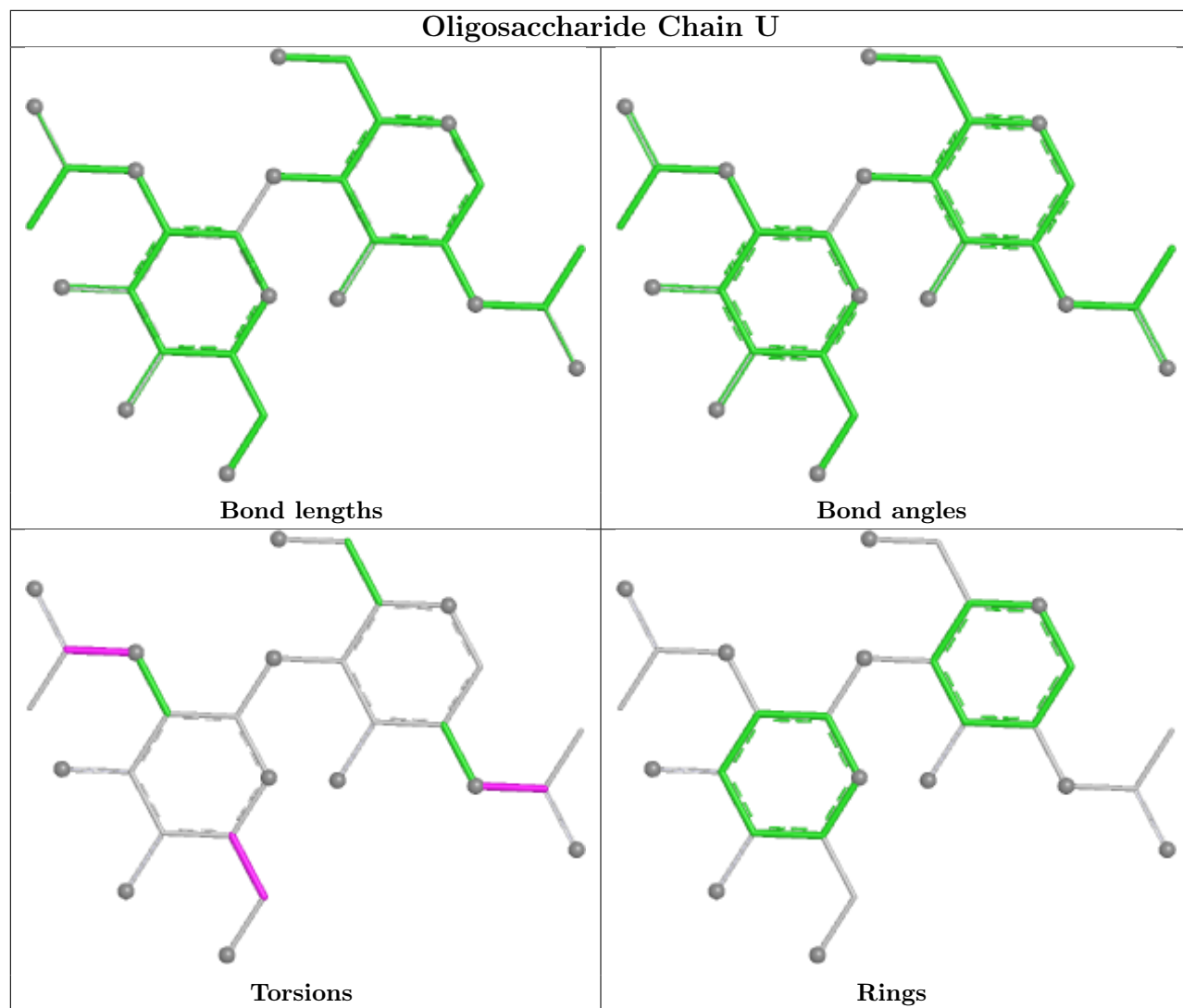


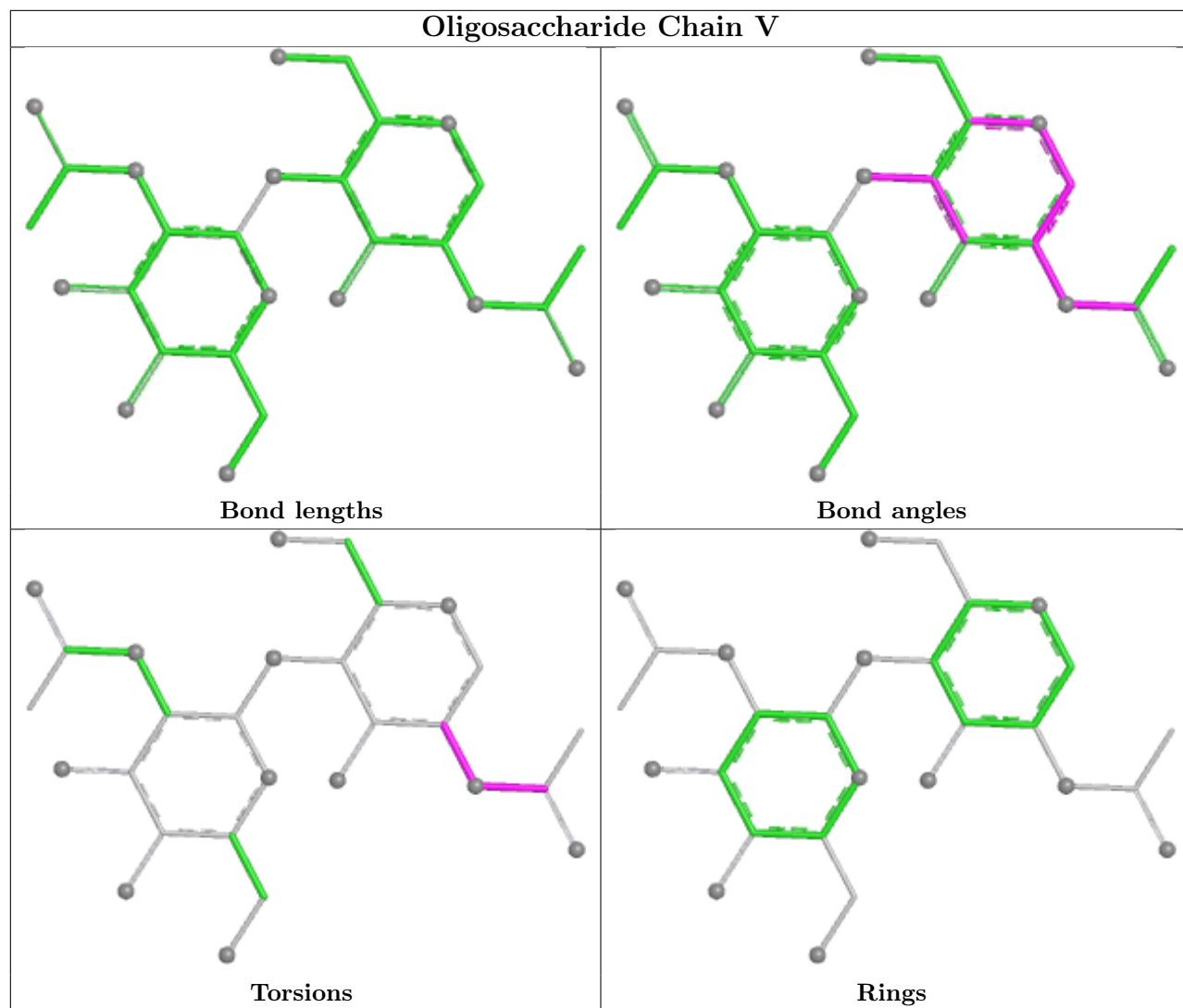


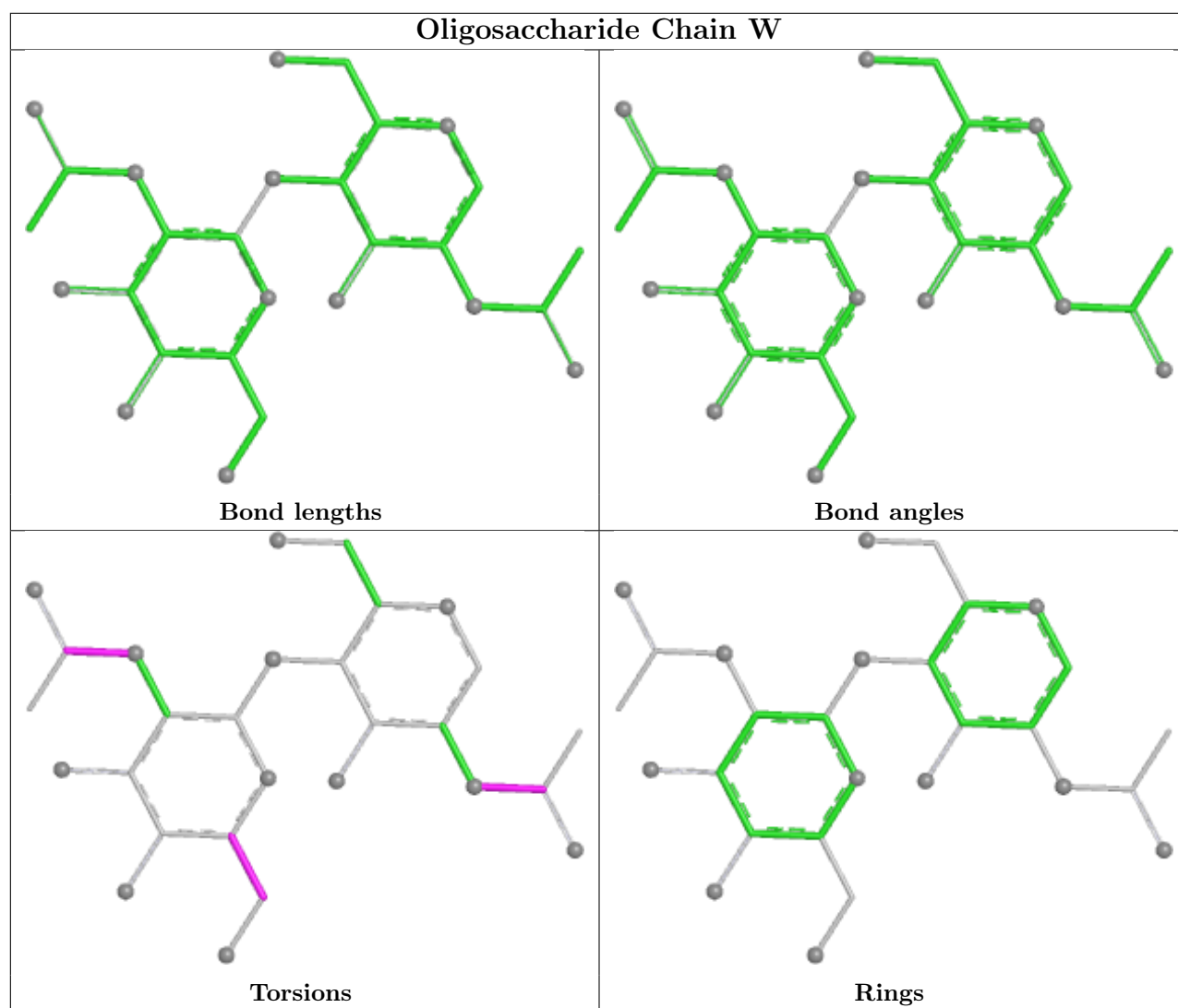


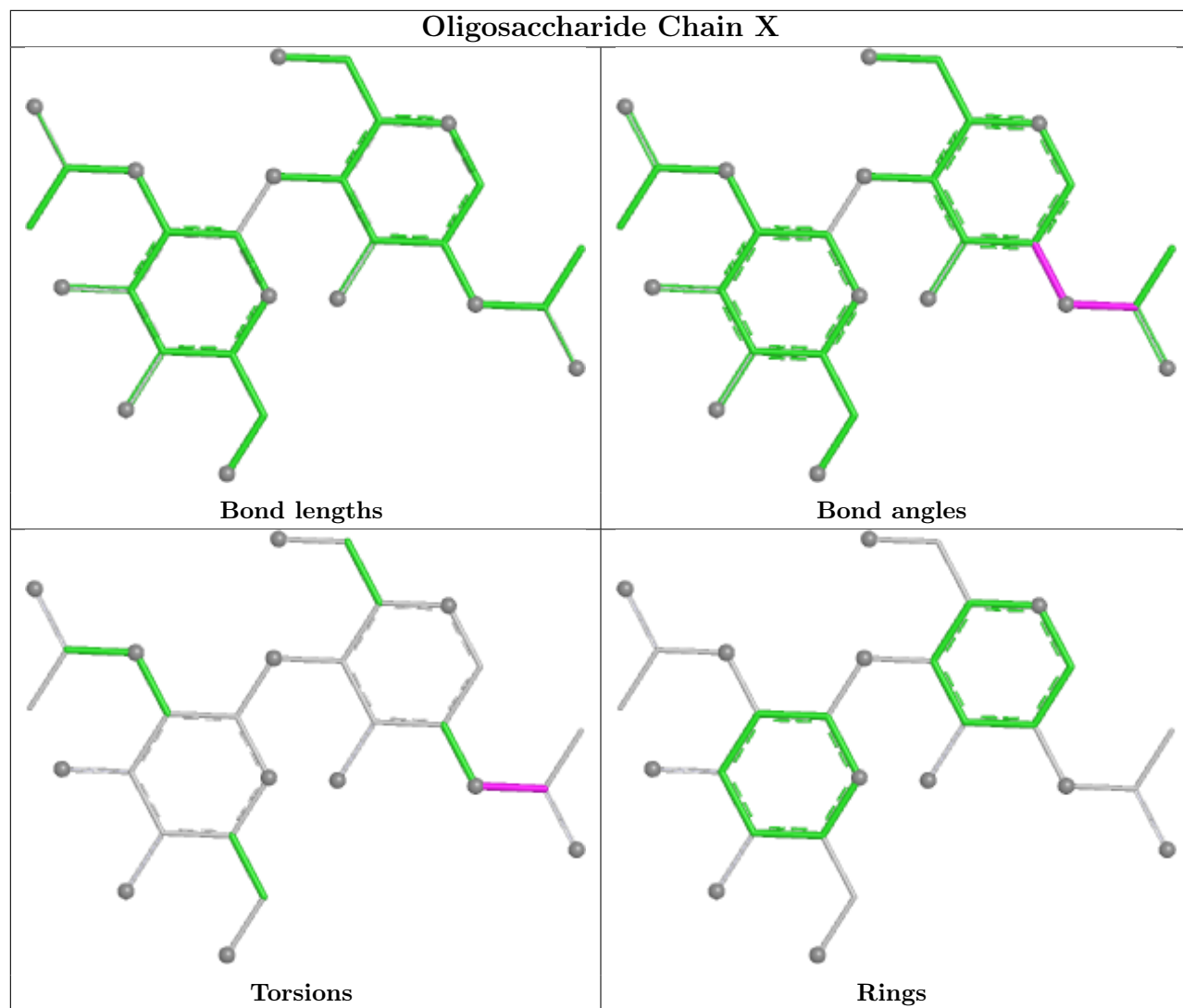


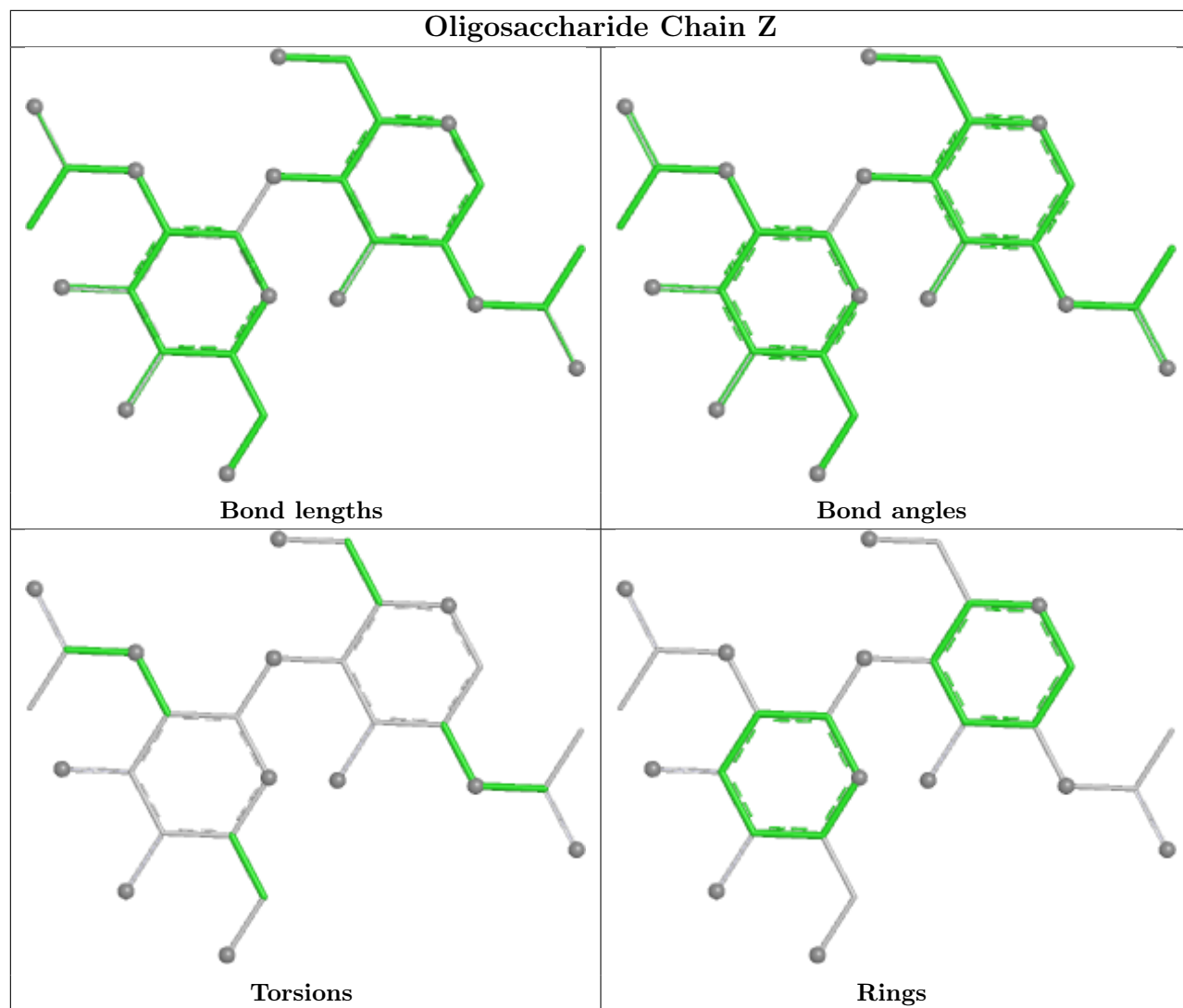


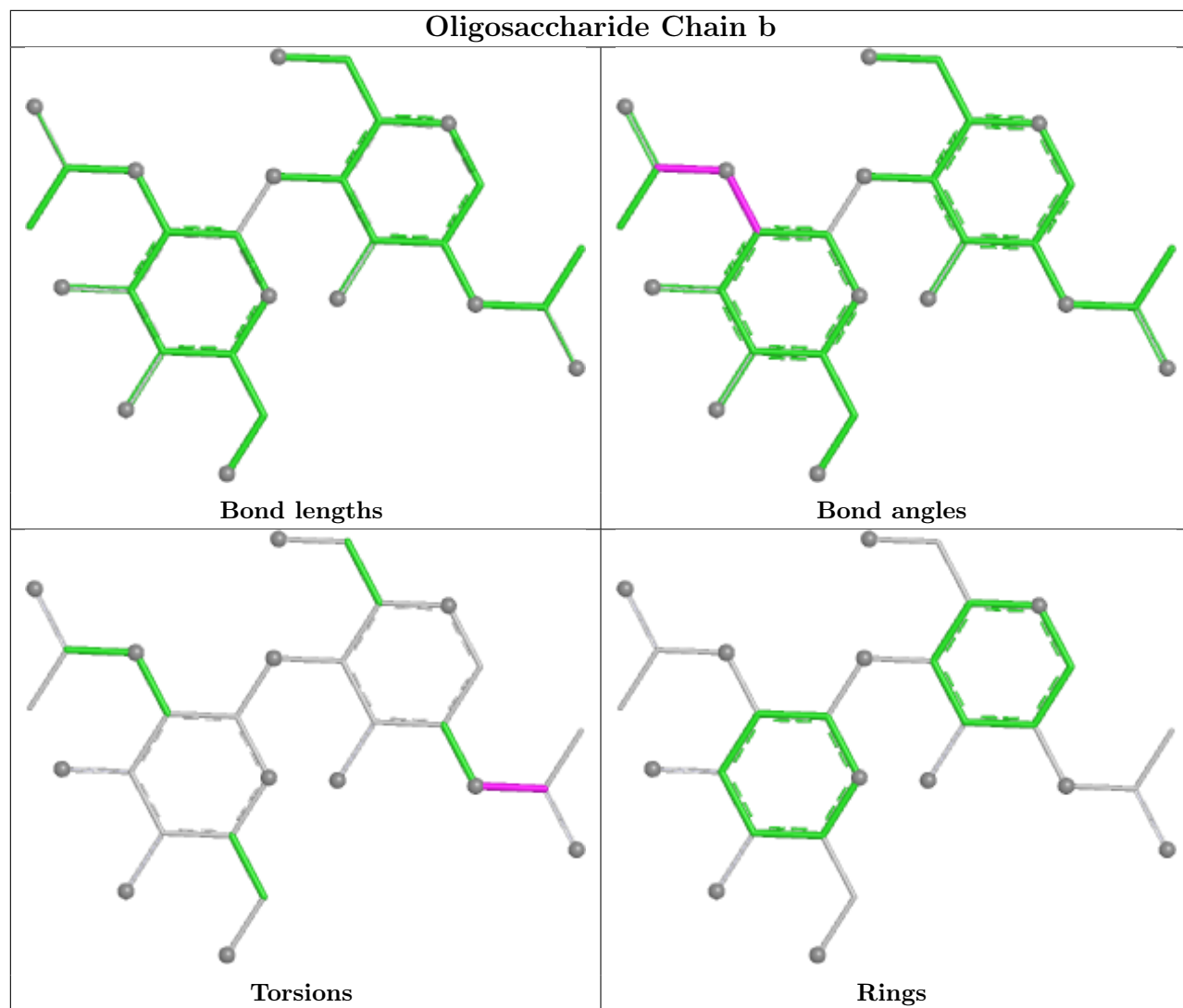


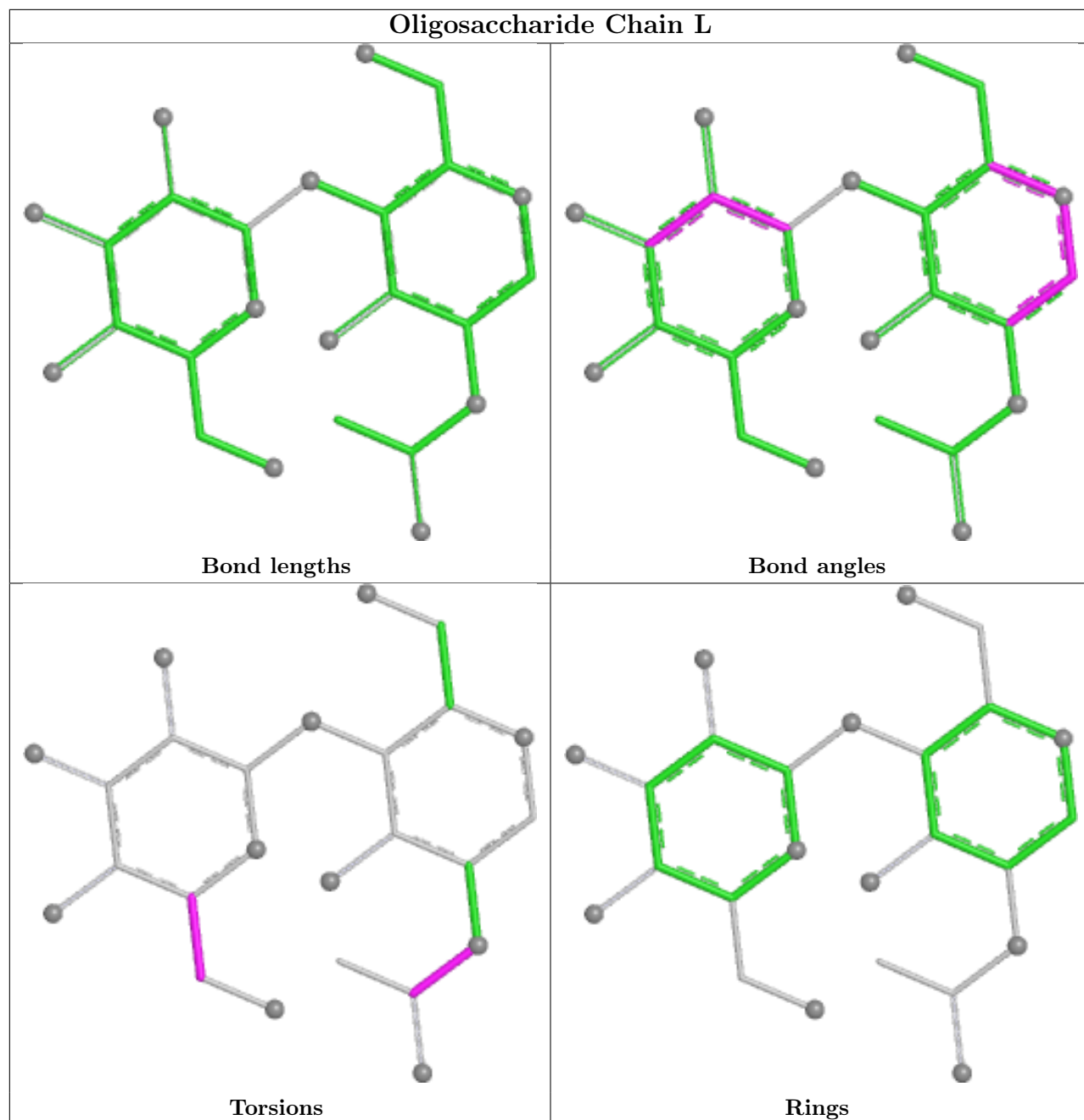


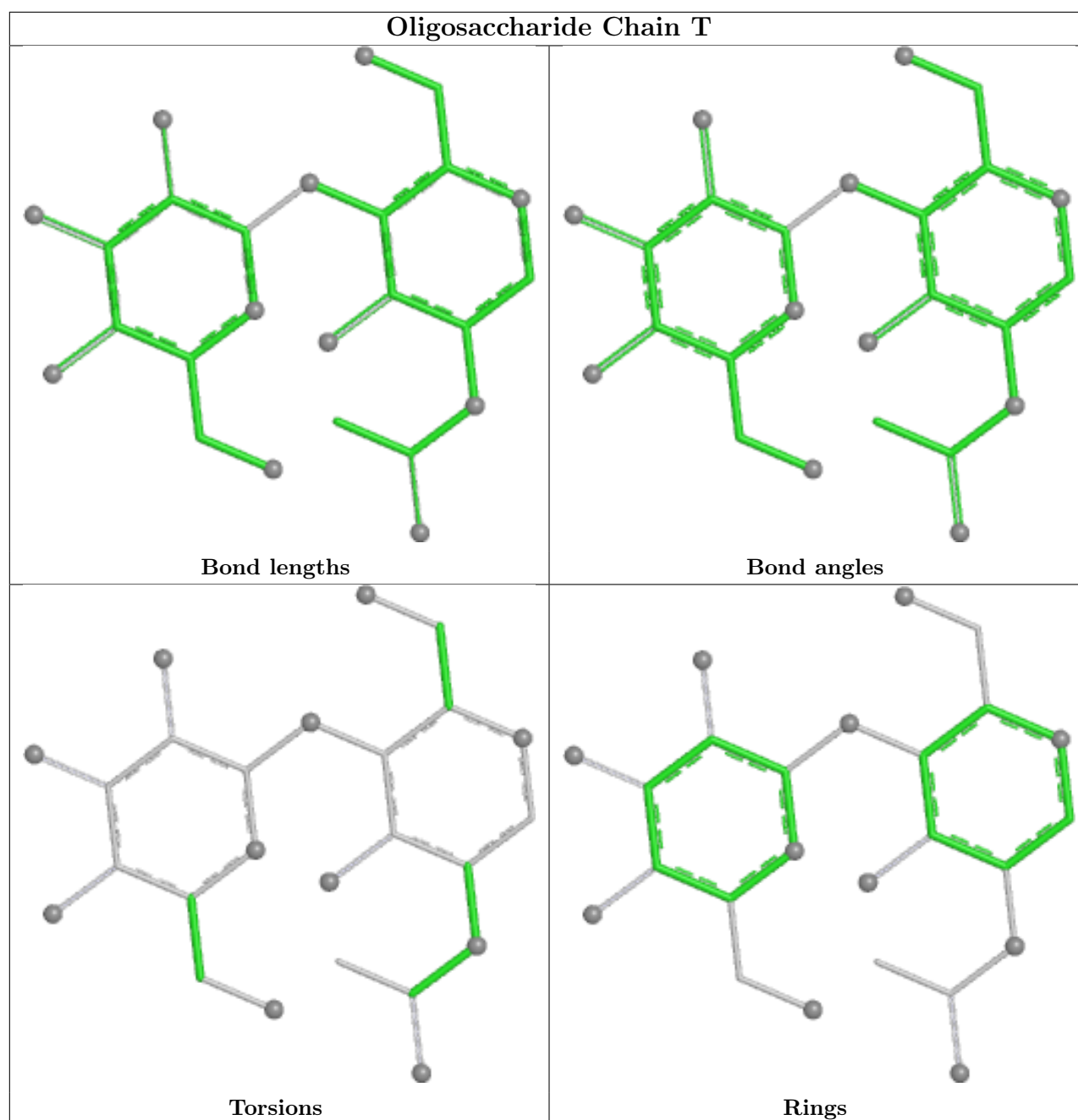












5.6 Ligand geometry [i](#)

26 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
7	NAG	B	1303	1	14,14,15	0.33	0	17,19,21	1.20	2 (11%)
8	BLA	A	1307	-	46,46,46	1.10	4 (8%)	66,67,67	1.19	5 (7%)
7	NAG	C	1306	1	14,14,15	0.39	0	17,19,21	0.41	0
9	EIC	A	1309	-	19,19,19	0.56	0	19,19,19	0.52	0
7	NAG	A	1303	1	14,14,15	0.49	0	17,19,21	0.73	0
7	NAG	B	1305	1	14,14,15	0.36	0	17,19,21	0.71	0
7	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.56	0
9	EIC	B	1308	-	19,19,19	0.55	0	19,19,19	0.55	0
7	NAG	B	1306	1	14,14,15	0.37	0	17,19,21	0.63	0
7	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.76	0
8	BLA	B	1309	-	46,46,46	1.09	3 (6%)	66,67,67	1.07	5 (7%)
7	NAG	A	1306	1	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
7	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.72	0
7	NAG	B	1304	1	14,14,15	0.44	0	17,19,21	0.83	2 (11%)
7	NAG	C	1302	1	14,14,15	0.38	0	17,19,21	0.41	0
7	NAG	C	1304	1	14,14,15	0.38	0	17,19,21	0.44	0
7	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	0.84	0
7	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
7	NAG	C	1301	1	14,14,15	0.45	0	17,19,21	1.33	3 (17%)
7	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.80	0
9	EIC	B	1301	-	19,19,19	0.55	0	19,19,19	0.47	0
7	NAG	C	1303	1	14,14,15	0.38	0	17,19,21	0.40	0
7	NAG	C	1308	1	14,14,15	0.40	0	17,19,21	0.76	0
8	BLA	C	1307	-	46,46,46	1.04	4 (8%)	66,67,67	1.13	5 (7%)
7	NAG	C	1305	1	14,14,15	0.42	0	17,19,21	0.58	0
7	NAG	B	1307	1	14,14,15	0.51	0	17,19,21	0.75	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
7	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
8	BLA	A	1307	-	-	13/26/74/74	0/4/4/4
7	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
9	EIC	A	1309	-	-	8/17/17/17	-
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EIC	B	1308	-	-	5/17/17/17	-
7	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
8	BLA	B	1309	-	-	10/26/74/74	0/4/4/4
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
9	EIC	B	1301	-	-	7/17/17/17	-
7	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
8	BLA	C	1307	-	-	14/26/74/74	0/4/4/4
7	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1309	BLA	CAC-C3C	-2.96	1.39	1.47
8	A	1307	BLA	CAB-C3B	-2.93	1.39	1.47
8	C	1307	BLA	CAB-C3B	-2.90	1.39	1.47
8	A	1307	BLA	CAC-C3C	-2.89	1.39	1.47
8	C	1307	BLA	CAC-C3C	-2.79	1.39	1.47
8	B	1309	BLA	CAB-C3B	-2.78	1.40	1.47
8	B	1309	BLA	C3B-C2B	2.45	1.42	1.37
8	A	1307	BLA	C3C-C4C	-2.29	1.41	1.45
8	A	1307	BLA	C3B-C2B	2.21	1.41	1.37
8	C	1307	BLA	C3B-C2B	2.09	1.41	1.37
8	C	1307	BLA	C3C-C2C	2.03	1.41	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1307	BLA	CMB-C2B-C1B	4.19	129.25	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1309	BLA	CMC-C2C-C1C	4.04	129.65	121.21
8	C	1307	BLA	CMB-C2B-C1B	3.95	128.97	124.16
7	C	1301	NAG	C1-O5-C5	3.73	117.19	112.19
8	A	1307	BLA	CMC-C2C-C1C	3.73	129.01	121.21
7	B	1303	NAG	O5-C1-C2	-3.57	105.77	111.29
8	C	1307	BLA	CMC-C2C-C1C	3.51	128.54	121.21
8	B	1309	BLA	C4C-NC-C1C	-3.20	106.74	110.66
8	B	1309	BLA	CMB-C2B-C1B	2.98	127.78	124.16
8	A	1307	BLA	C4D-C3D-C2D	-2.71	103.80	106.73
8	C	1307	BLA	C4C-NC-C1C	-2.57	107.51	110.66
7	B	1303	NAG	C2-N2-C7	-2.55	119.48	122.90
8	C	1307	BLA	C1A-CHA-C4D	-2.53	122.70	128.22
8	C	1307	BLA	C4C-CHD-C1D	2.51	134.21	128.06
8	A	1307	BLA	C1A-CHA-C4D	-2.50	122.77	128.22
7	C	1301	NAG	O5-C1-C2	-2.47	107.48	111.29
7	A	1306	NAG	C2-N2-C7	-2.46	119.61	122.90
8	B	1309	BLA	C4A-CHB-C1B	-2.29	124.24	130.82
8	A	1307	BLA	C4C-NC-C1C	-2.21	107.95	110.66
8	B	1309	BLA	C4B-C3B-C2B	-2.16	105.15	107.92
7	B	1304	NAG	C2-N2-C7	-2.06	120.14	122.90
7	C	1301	NAG	C2-N2-C7	-2.05	120.15	122.90
7	B	1304	NAG	C4-C3-C2	-2.04	108.03	111.02
7	A	1302	NAG	C2-N2-C7	-2.02	120.20	122.90

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1301	NAG	C1-C2-N2-C7
7	A	1301	NAG	C8-C7-N2-C2
7	A	1301	NAG	O7-C7-N2-C2
7	A	1303	NAG	C8-C7-N2-C2
7	A	1303	NAG	O7-C7-N2-C2
7	B	1305	NAG	O7-C7-N2-C2
7	C	1301	NAG	C8-C7-N2-C2
7	C	1301	NAG	O7-C7-N2-C2
8	A	1307	BLA	ND-C4D-CHA-C1A
8	A	1307	BLA	C3D-C4D-CHA-C1A
8	A	1307	BLA	NC-C4C-CHD-C1D
8	A	1307	BLA	C3C-C4C-CHD-C1D
8	A	1307	BLA	ND-C1D-CHD-C4C
8	A	1307	BLA	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
8	B	1309	BLA	NB-C1B-CHB-C4A
8	B	1309	BLA	C2B-C1B-CHB-C4A
8	B	1309	BLA	C3C-C4C-CHD-C1D
8	C	1307	BLA	NB-C1B-CHB-C4A
8	C	1307	BLA	C2B-C1B-CHB-C4A
8	C	1307	BLA	NC-C4C-CHD-C1D
8	C	1307	BLA	C3C-C4C-CHD-C1D
7	A	1302	NAG	C8-C7-N2-C2
7	A	1302	NAG	O7-C7-N2-C2
7	B	1302	NAG	C8-C7-N2-C2
7	B	1302	NAG	O7-C7-N2-C2
7	B	1305	NAG	C8-C7-N2-C2
8	A	1307	BLA	NB-C1B-CHB-C4A
8	B	1309	BLA	NC-C4C-CHD-C1D
8	A	1307	BLA	C2B-C1B-CHB-C4A
7	B	1303	NAG	C8-C7-N2-C2
7	B	1303	NAG	C4-C5-C6-O6
9	B	1308	EIC	C11-C10-C9-C8
9	B	1308	EIC	C11-C12-C13-C14
7	B	1303	NAG	O5-C5-C6-O6
7	A	1306	NAG	C8-C7-N2-C2
7	B	1303	NAG	O7-C7-N2-C2
7	C	1305	NAG	C8-C7-N2-C2
7	C	1305	NAG	O7-C7-N2-C2
7	A	1306	NAG	O7-C7-N2-C2
8	C	1307	BLA	C2A-CAA-CBA-CGA
8	C	1307	BLA	C2C-C3C-CAC-CBC
9	B	1301	EIC	C5-C6-C7-C8
9	A	1309	EIC	C5-C6-C7-C8
9	A	1309	EIC	C11-C12-C13-C14
7	B	1307	NAG	C8-C7-N2-C2
9	A	1309	EIC	C9-C10-C11-C12
8	C	1307	BLA	C3D-C4D-CHA-C1A
9	A	1309	EIC	C12-C13-C14-C15
8	C	1307	BLA	ND-C4D-CHA-C1A
9	A	1309	EIC	C11-C10-C9-C8
7	B	1307	NAG	O7-C7-N2-C2
9	B	1301	EIC	C12-C13-C14-C15
8	C	1307	BLA	C4C-C3C-CAC-CBC
8	B	1309	BLA	C3D-C4D-CHA-C1A
9	A	1309	EIC	C7-C8-C9-C10
8	A	1307	BLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	1307	BLA	CAA-CBA-CGA-O2A
8	C	1307	BLA	CAA-CBA-CGA-O1A
8	C	1307	BLA	CAA-CBA-CGA-O2A
9	B	1301	EIC	O1-C1-C2-C3
8	A	1307	BLA	CAD-CBD-CGD-O1D
8	B	1309	BLA	ND-C4D-CHA-C1A
7	A	1308	NAG	C1-C2-N2-C7
7	C	1308	NAG	C1-C2-N2-C7
8	A	1307	BLA	CAD-CBD-CGD-O2D
9	B	1301	EIC	O2-C1-C2-C3
9	B	1301	EIC	C11-C10-C9-C8
9	B	1308	EIC	O2-C1-C2-C3
8	B	1309	BLA	CAD-CBD-CGD-O2D
8	C	1307	BLA	CAD-CBD-CGD-O2D
8	B	1309	BLA	CAA-CBA-CGA-O2A
8	C	1307	BLA	CAD-CBD-CGD-O1D
9	B	1301	EIC	C15-C16-C17-C18
8	B	1309	BLA	CAA-CBA-CGA-O1A
8	B	1309	BLA	CAD-CBD-CGD-O1D
9	B	1308	EIC	O1-C1-C2-C3
9	B	1308	EIC	C1-C2-C3-C4
8	C	1307	BLA	C2A-C1A-CHA-C4D
9	A	1309	EIC	O2-C1-C2-C3
9	A	1309	EIC	O1-C1-C2-C3
8	A	1307	BLA	C2A-C1A-CHA-C4D
9	B	1301	EIC	C4-C5-C6-C7

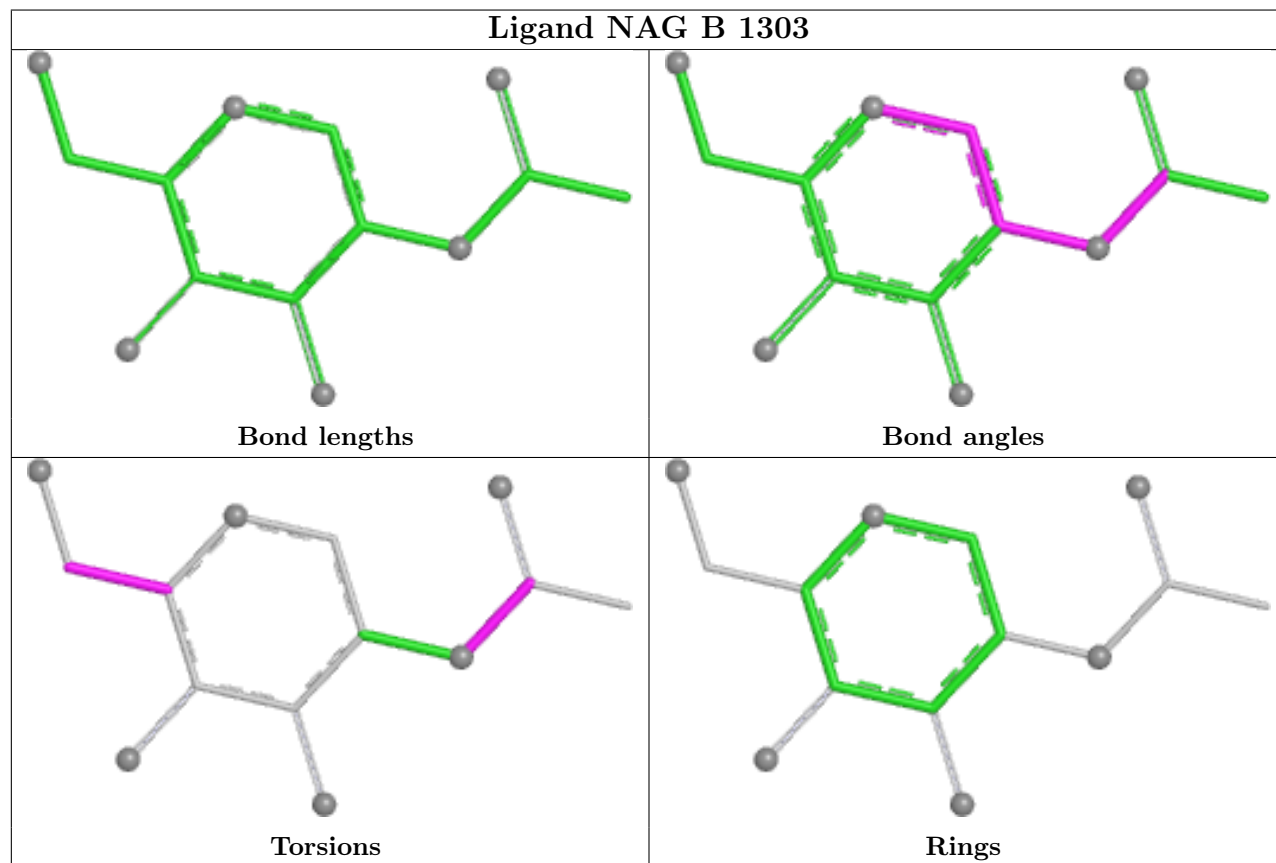
There are no ring outliers.

8 monomers are involved in 22 short contacts:

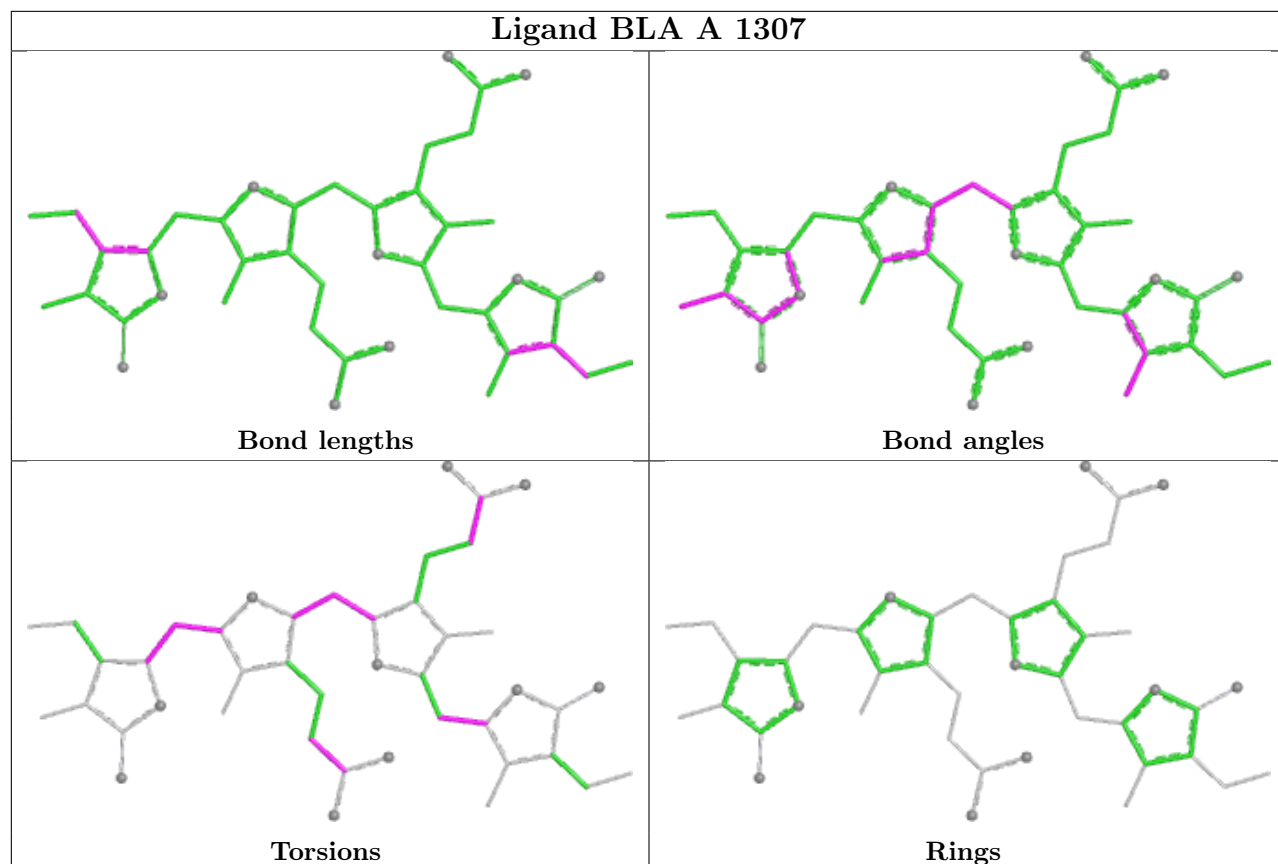
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1307	BLA	6	0
9	B	1308	EIC	1	0
7	A	1308	NAG	1	0
8	B	1309	BLA	6	0
7	A	1304	NAG	1	0
7	C	1308	NAG	1	0
8	C	1307	BLA	4	0
7	B	1307	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

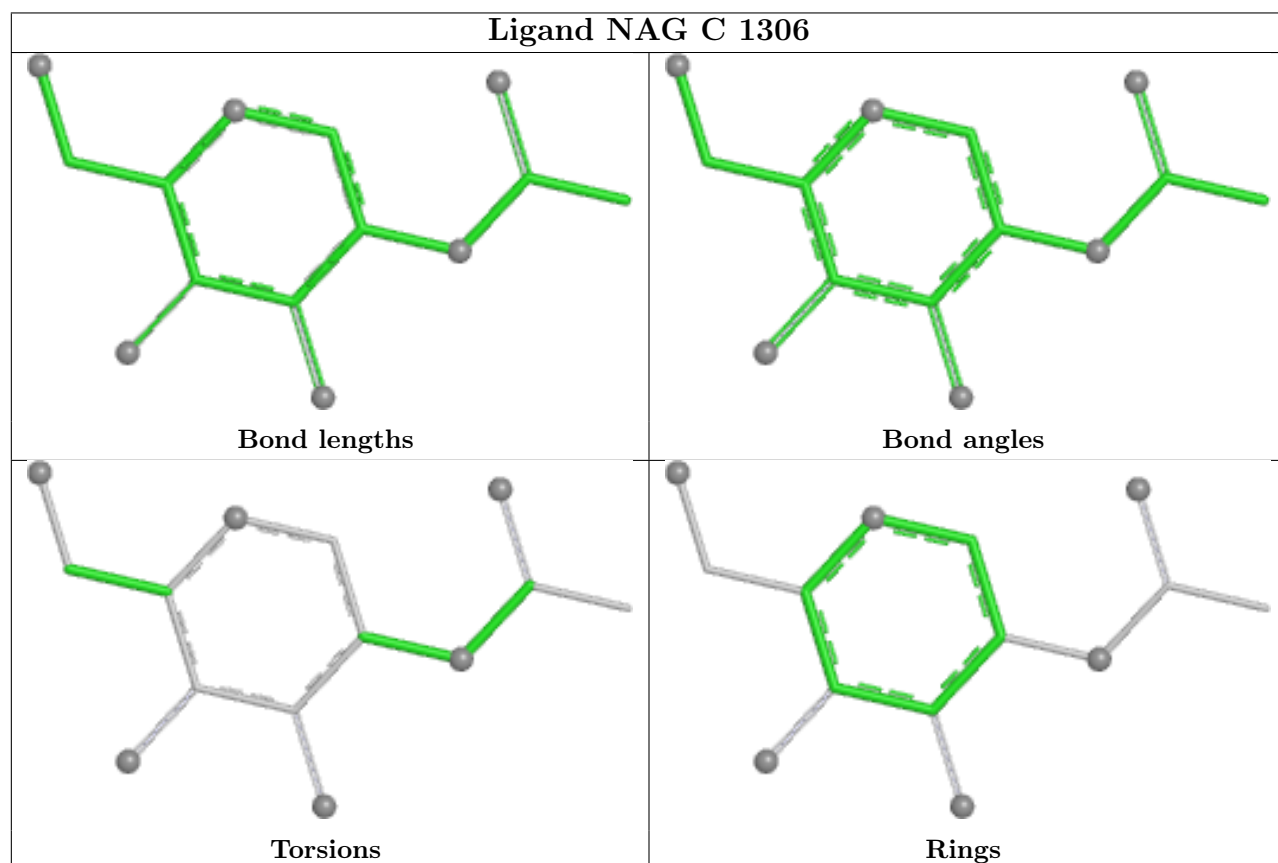
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

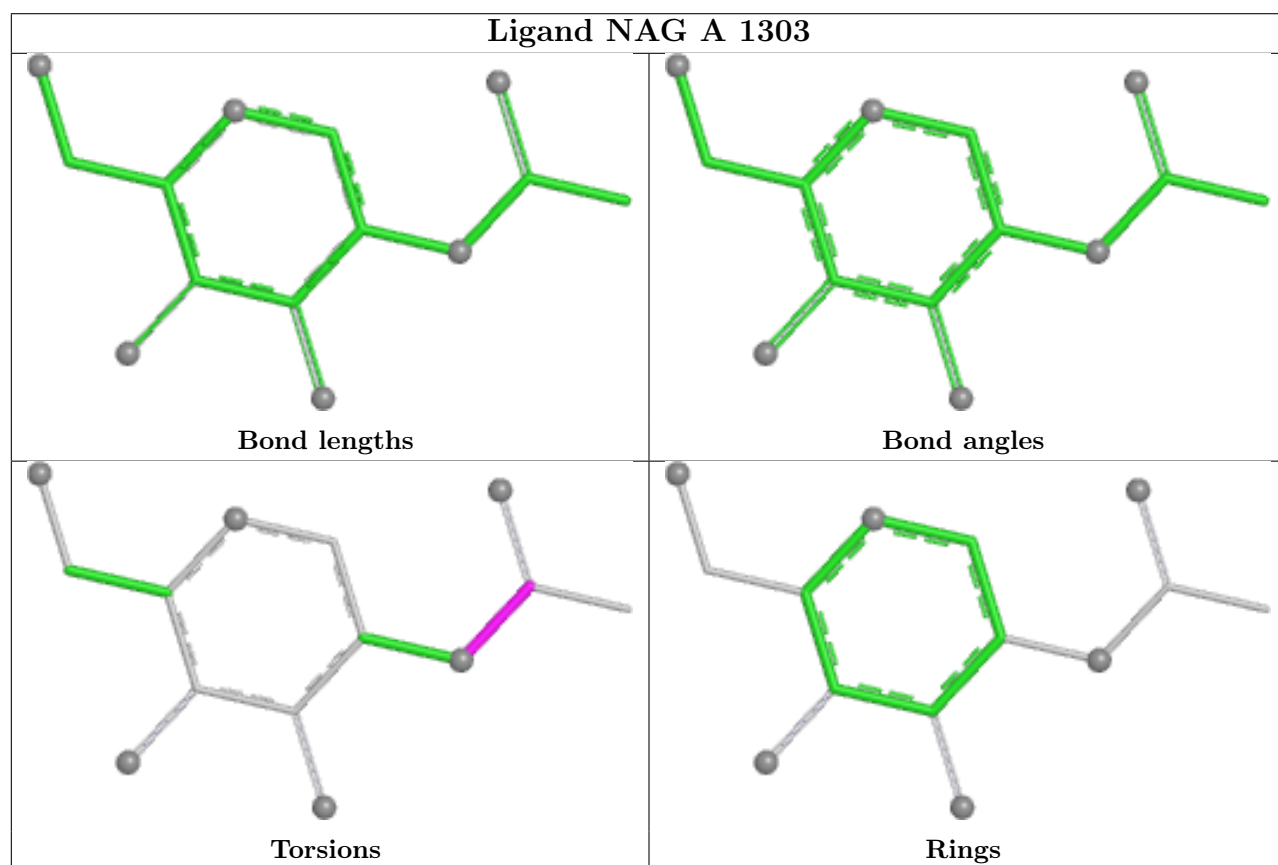
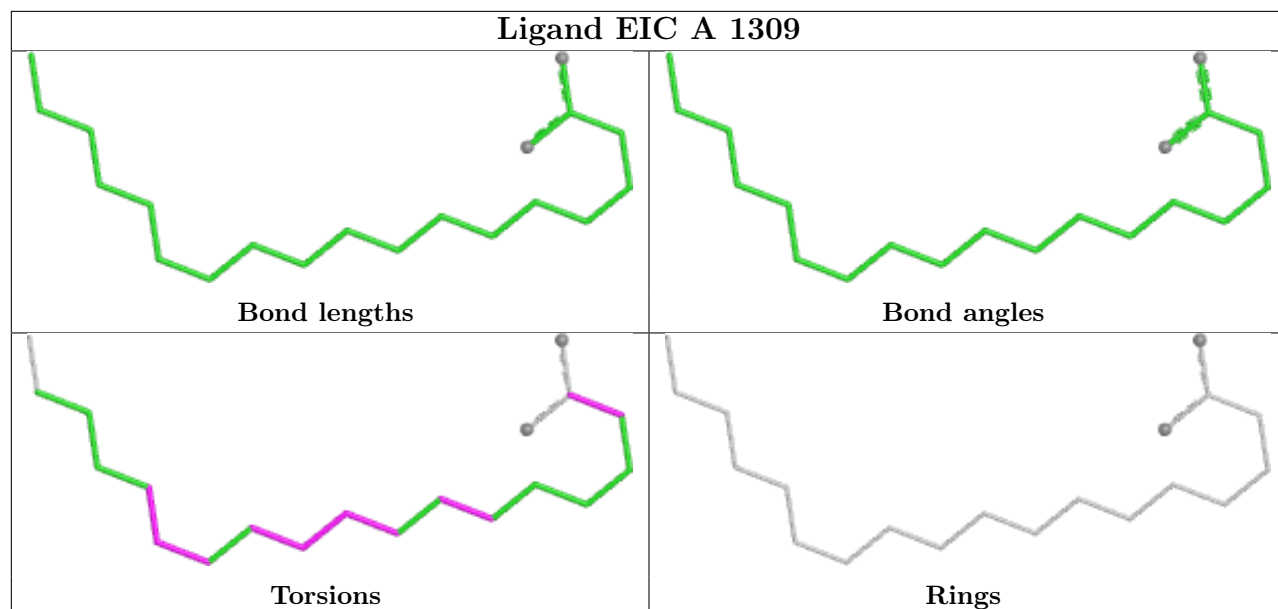


Ligand BLA A 1307

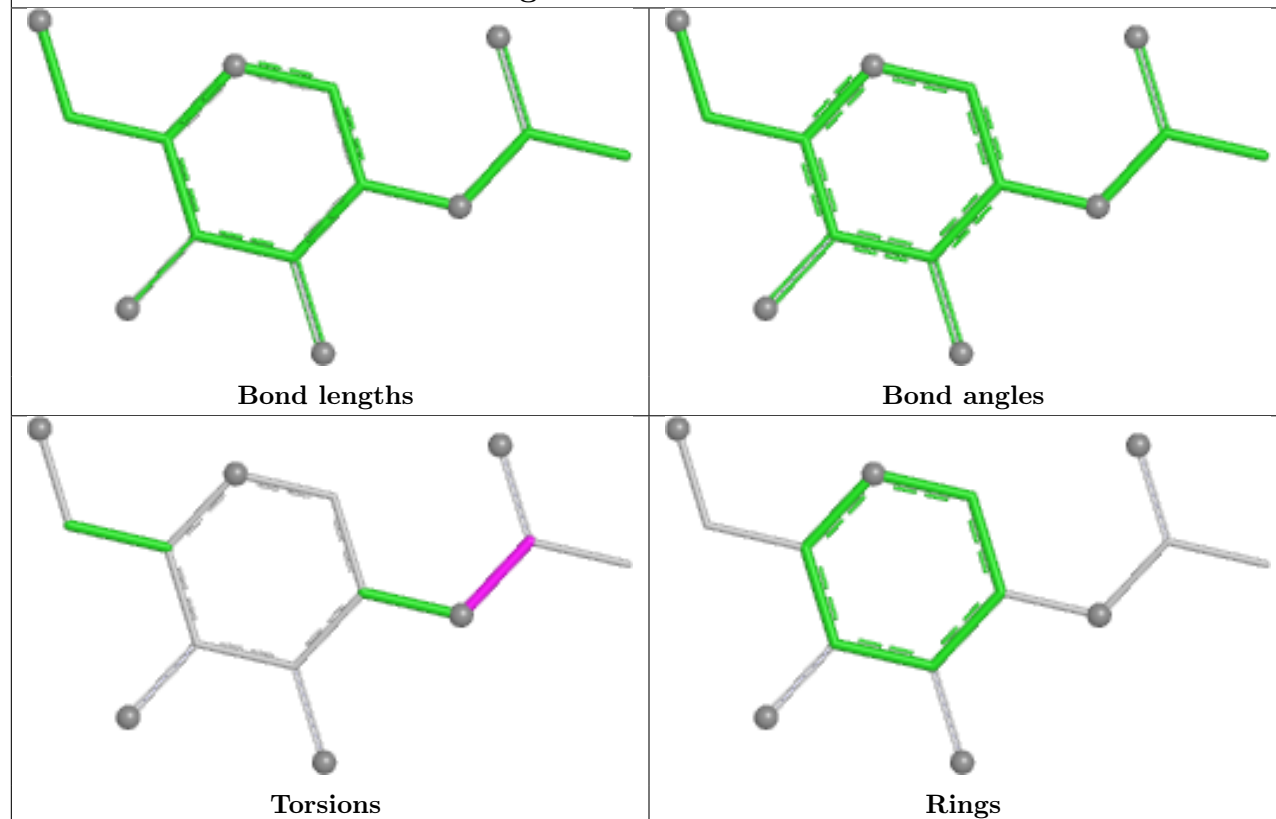


Ligand NAG C 1306

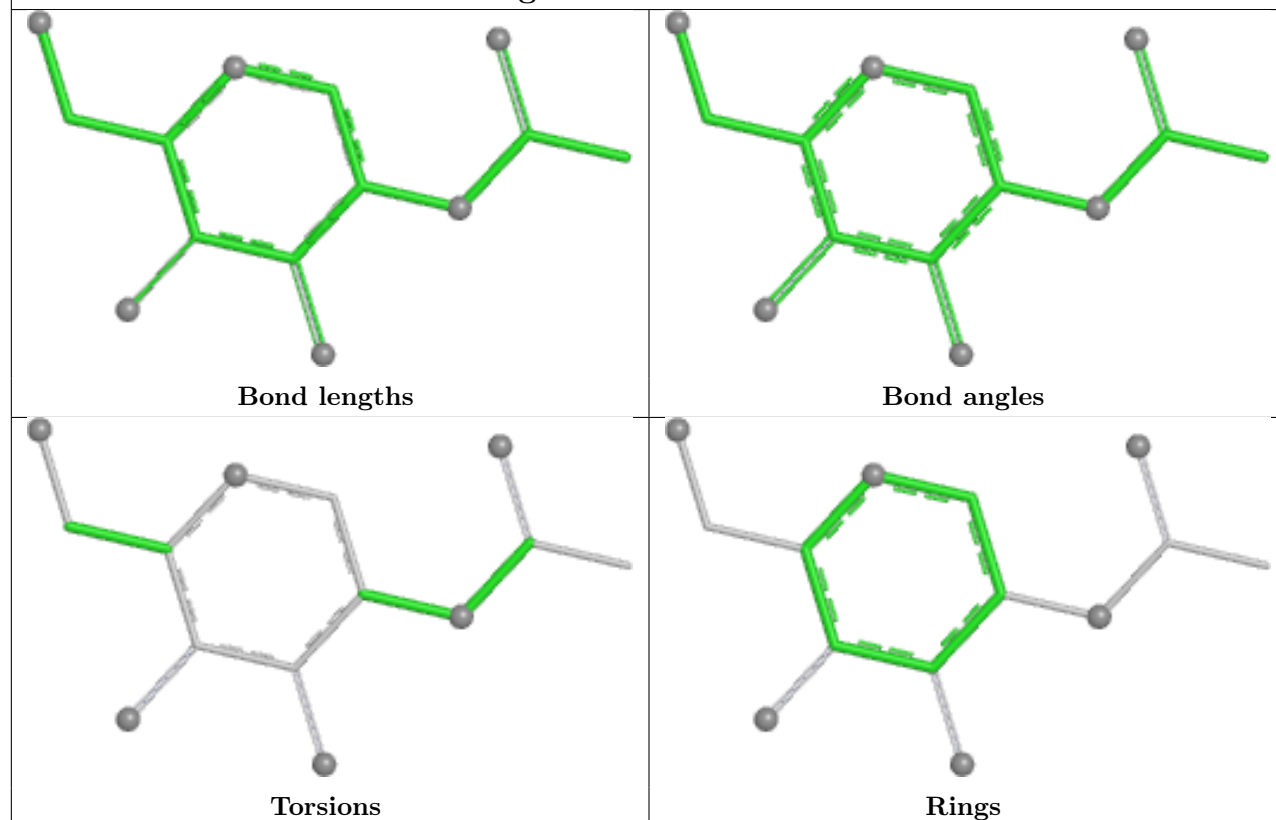


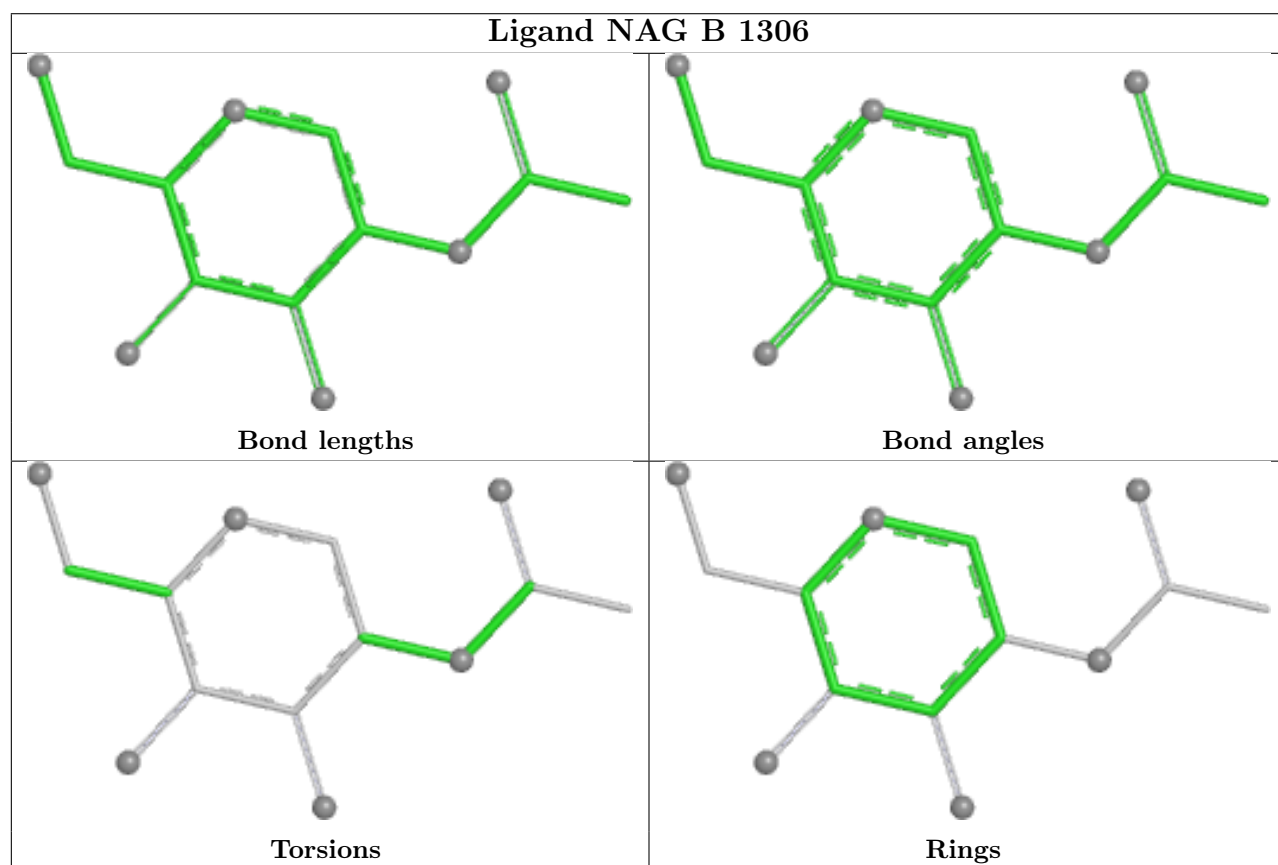
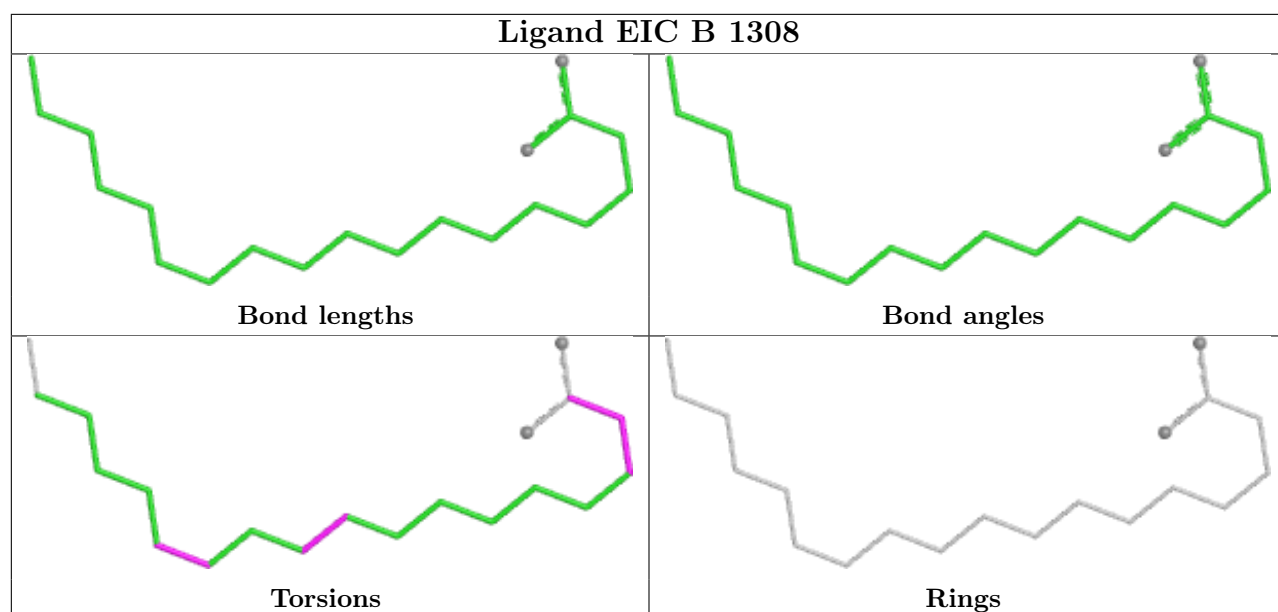


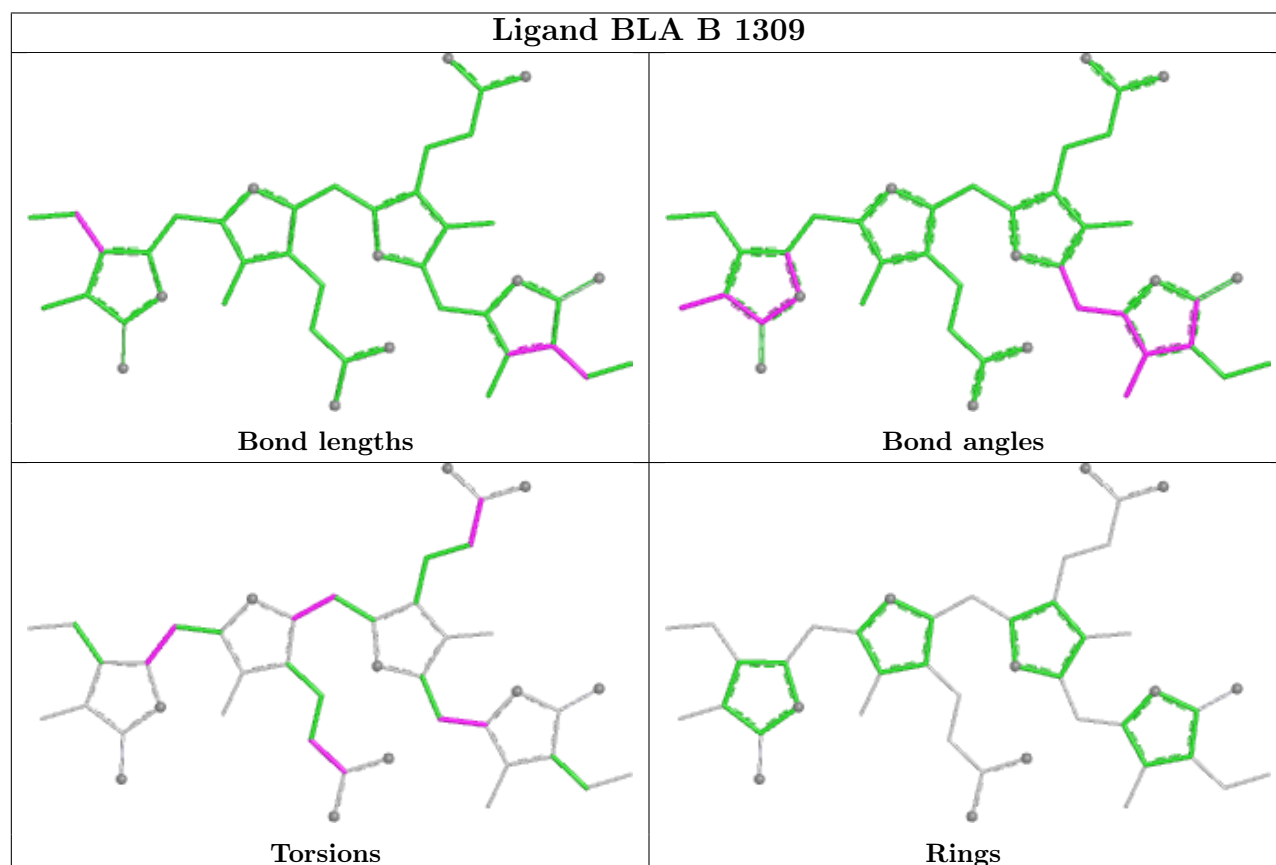
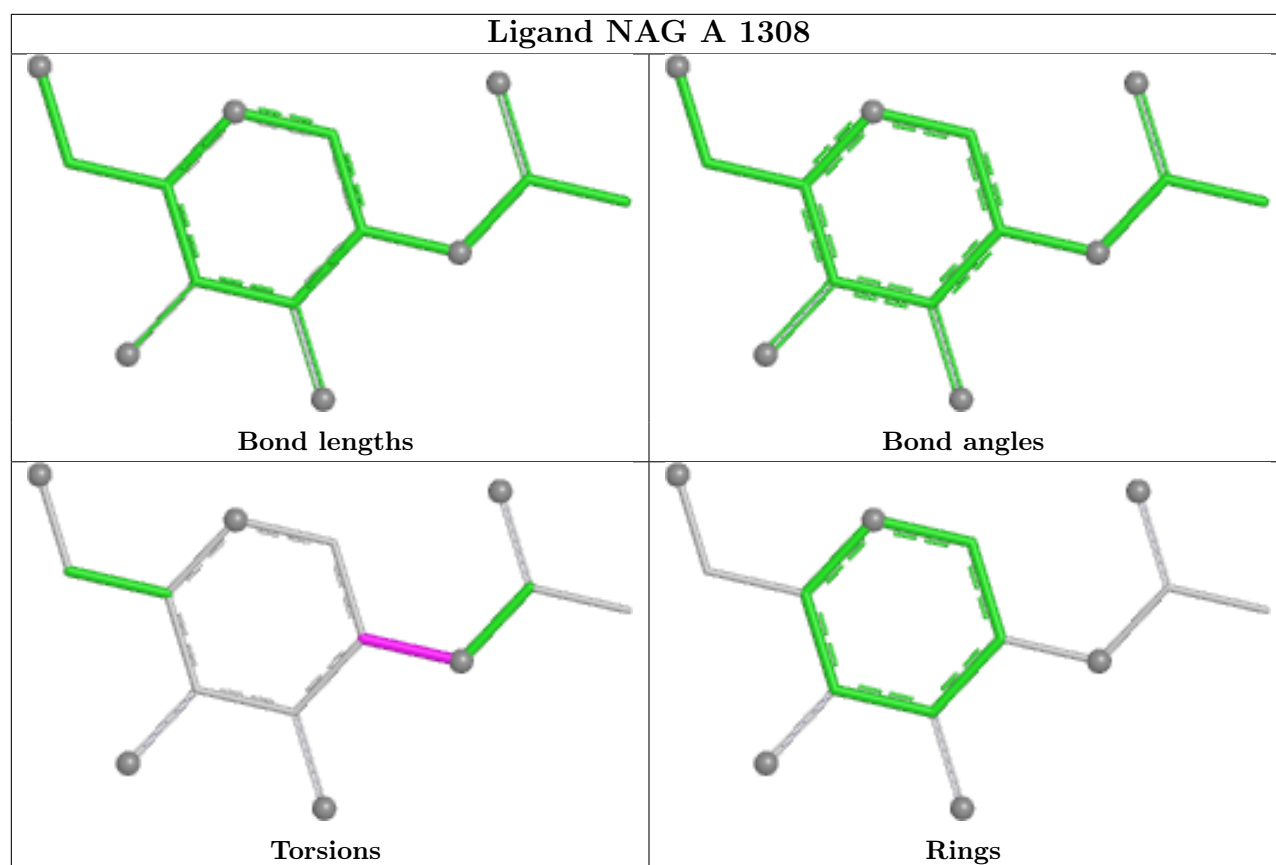
Ligand NAG B 1305



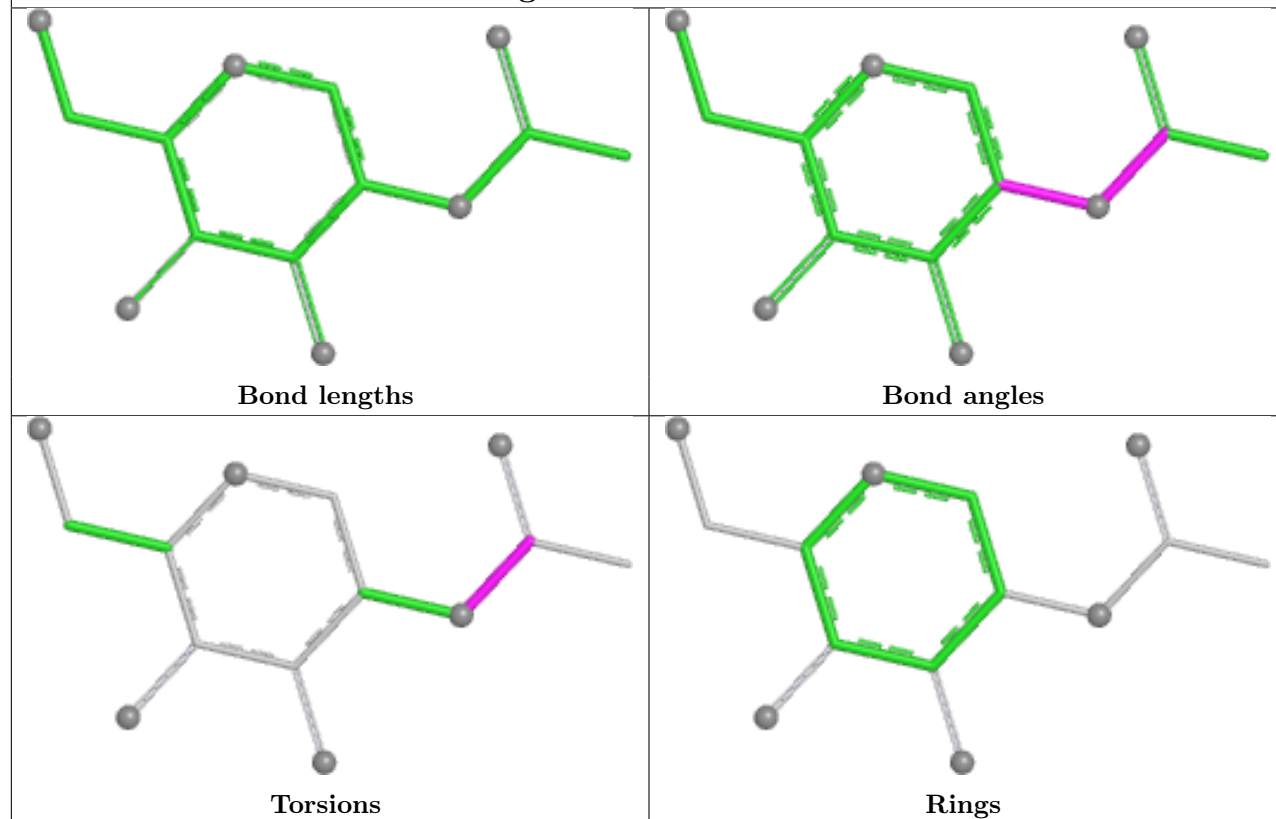
Ligand NAG A 1305



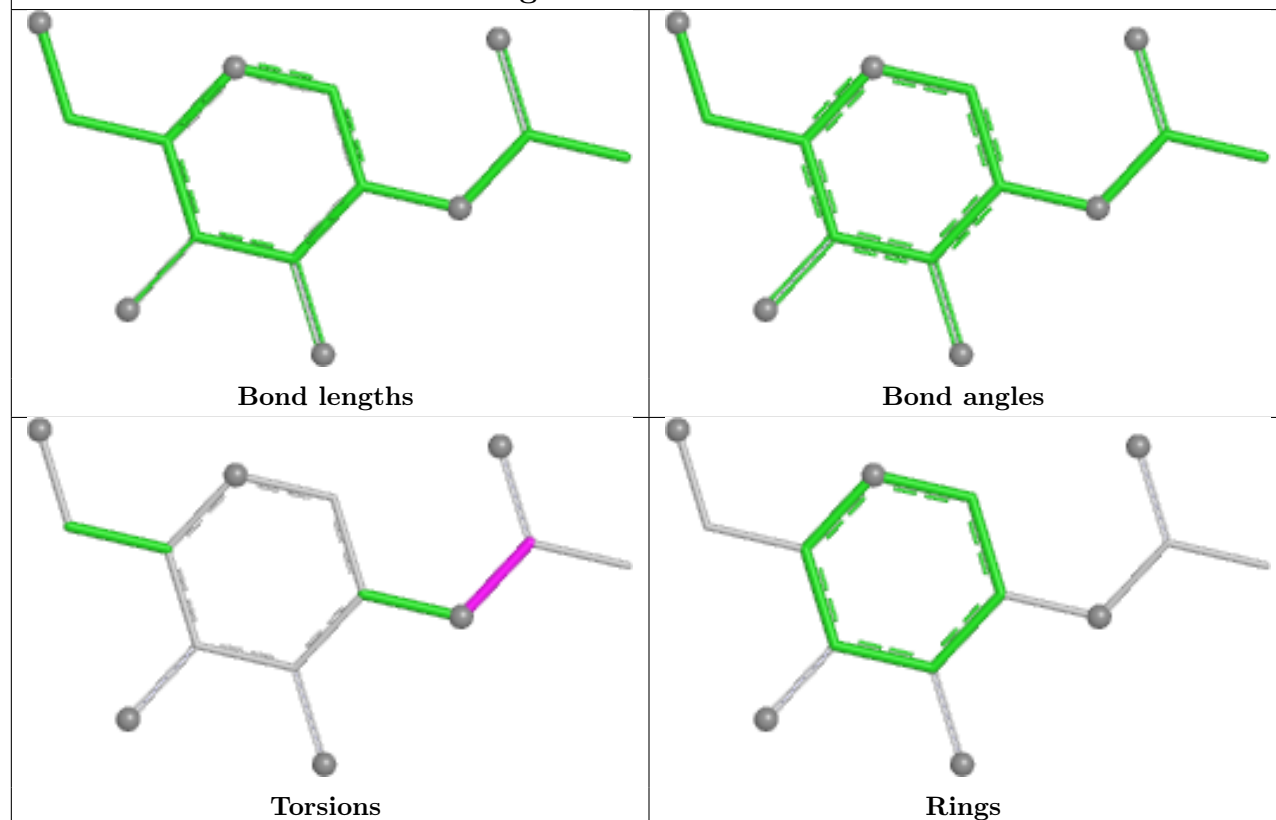


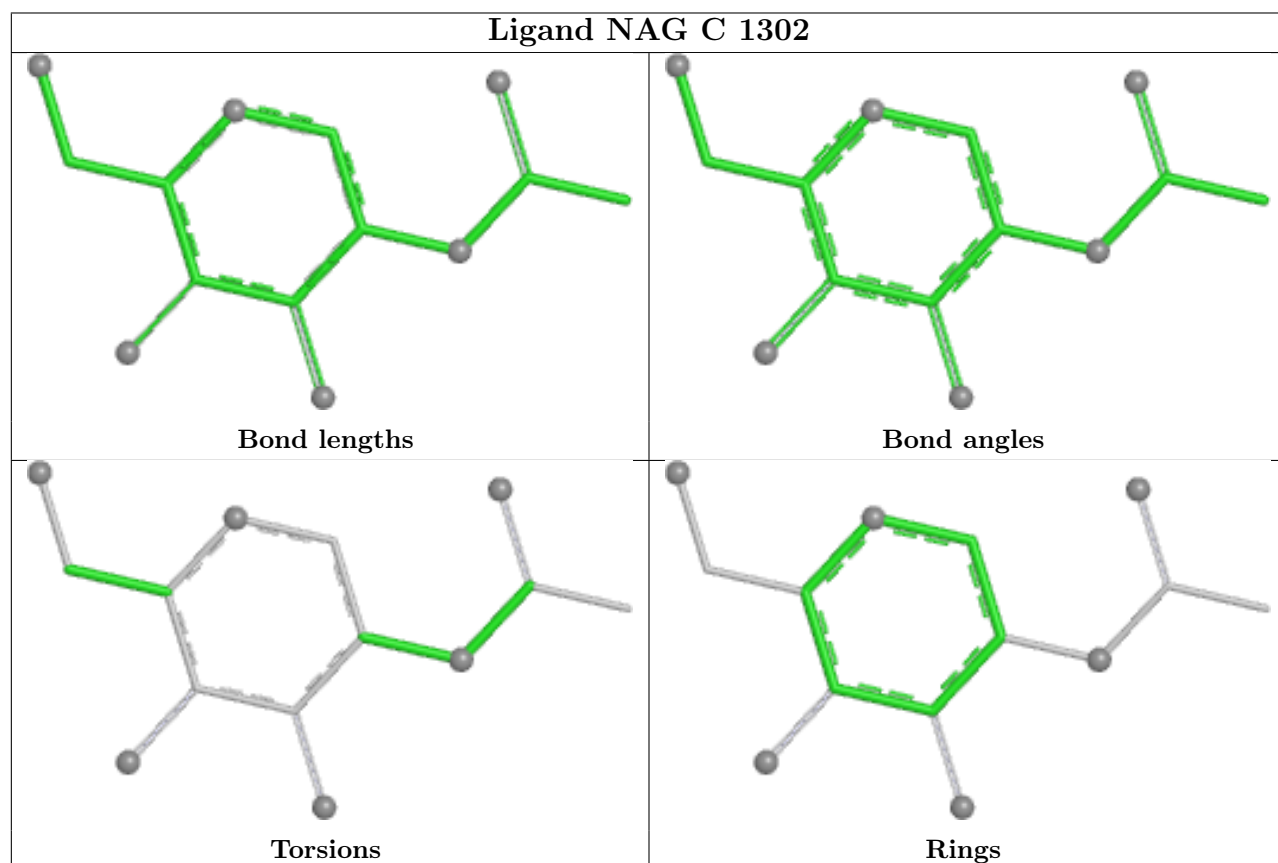
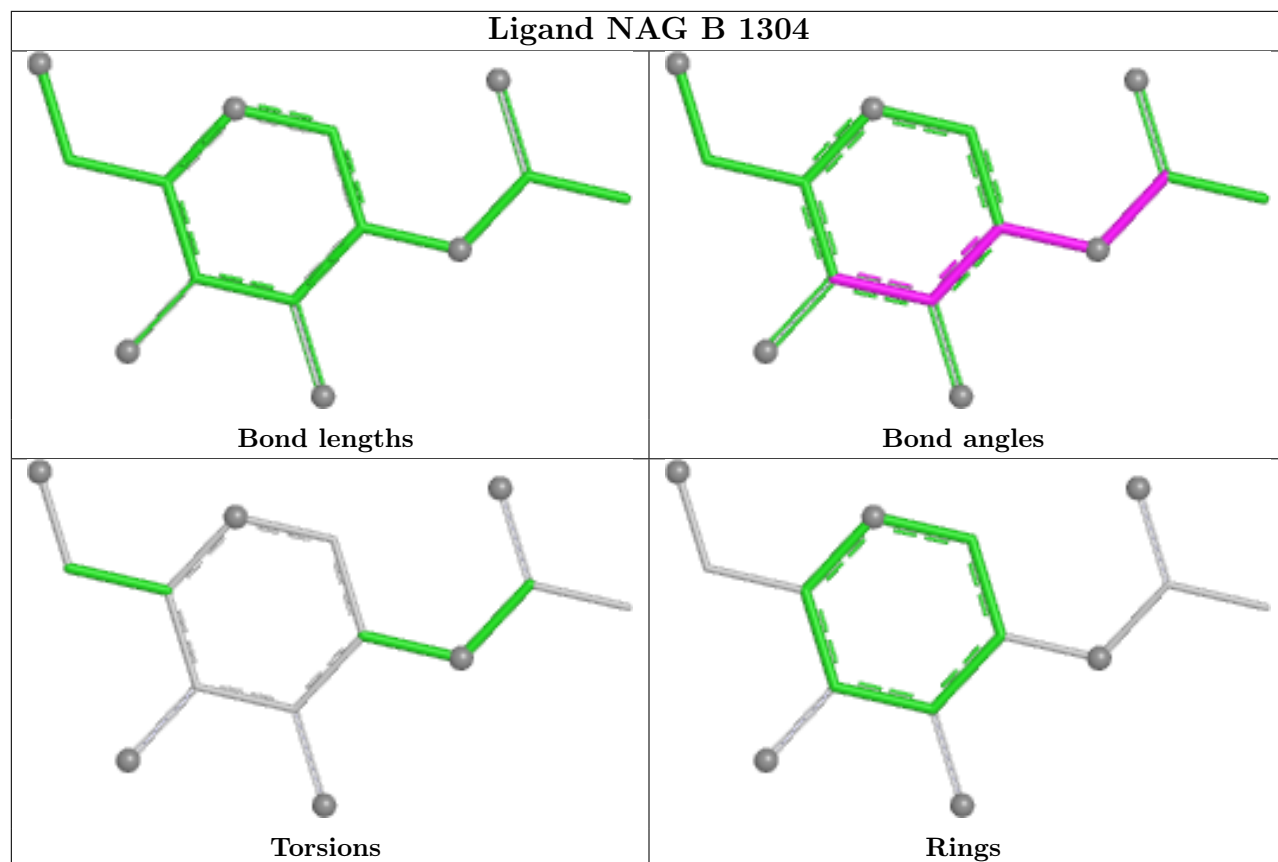


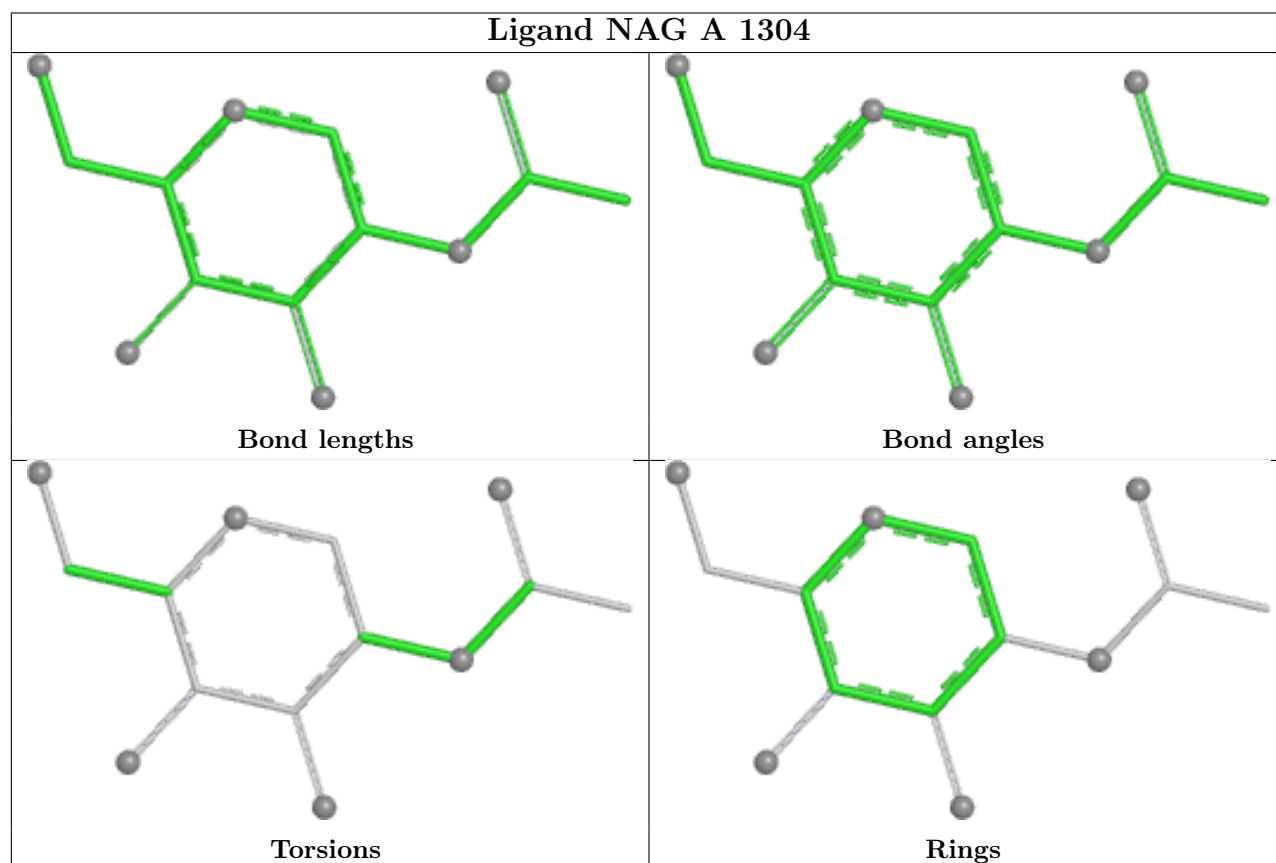
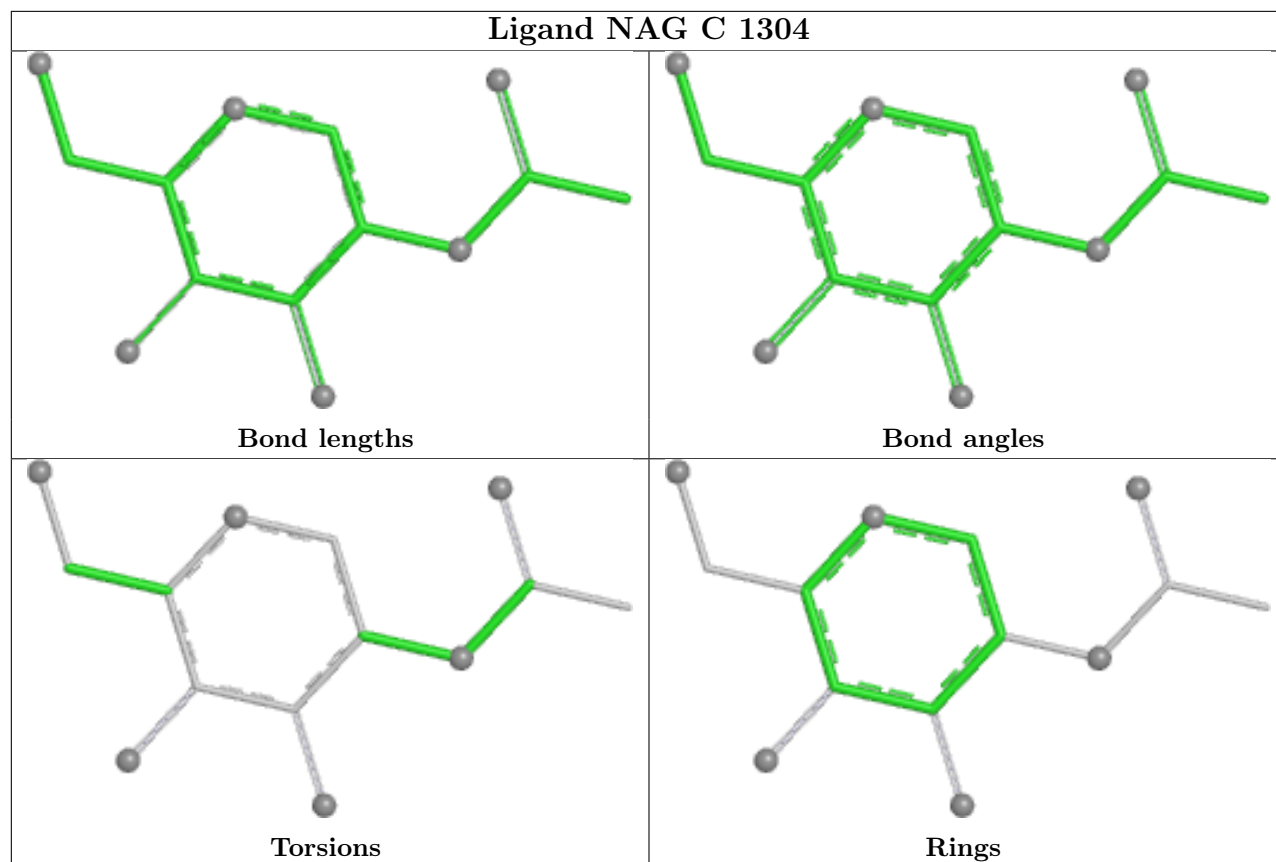
Ligand NAG A 1306



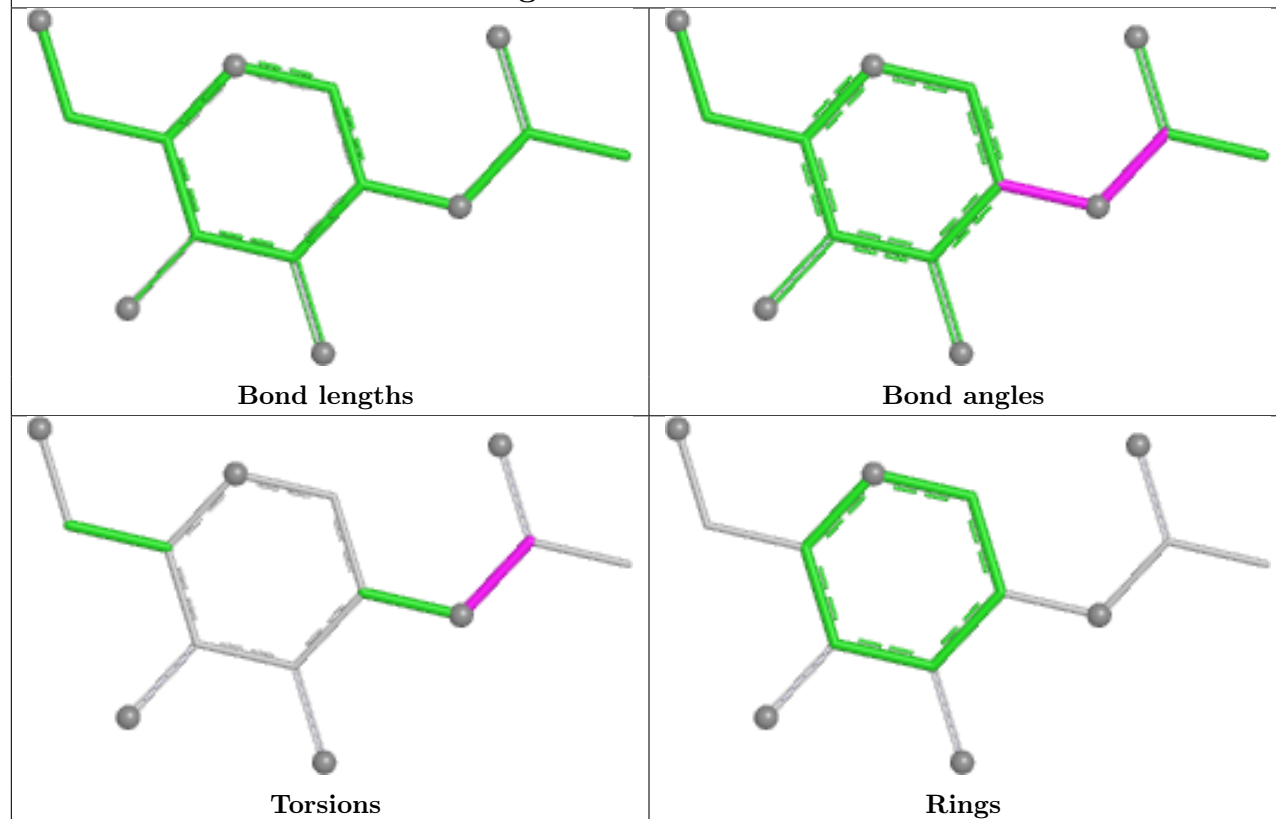
Ligand NAG B 1302



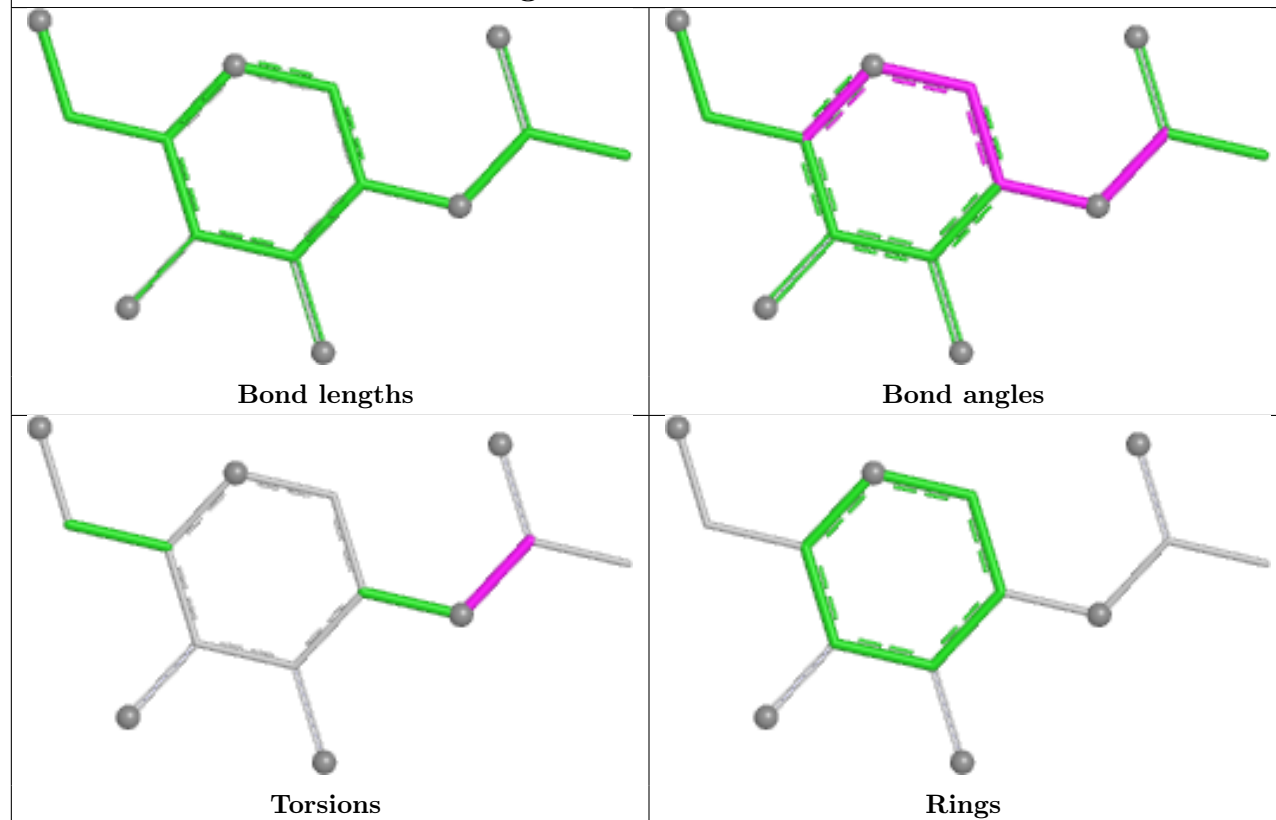


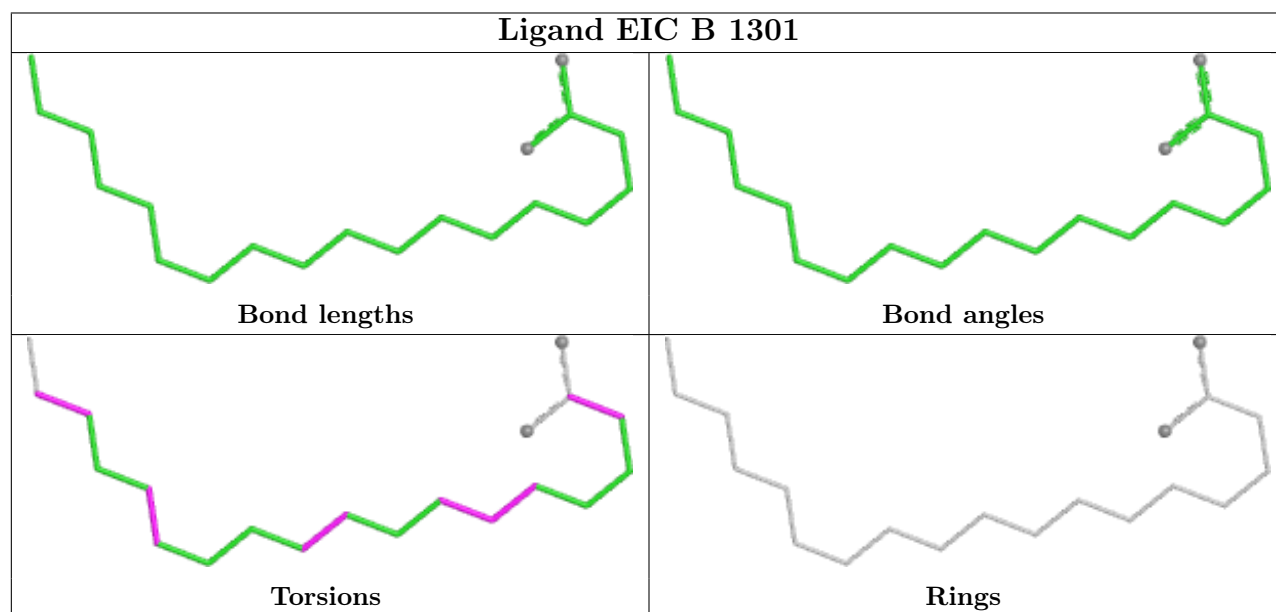
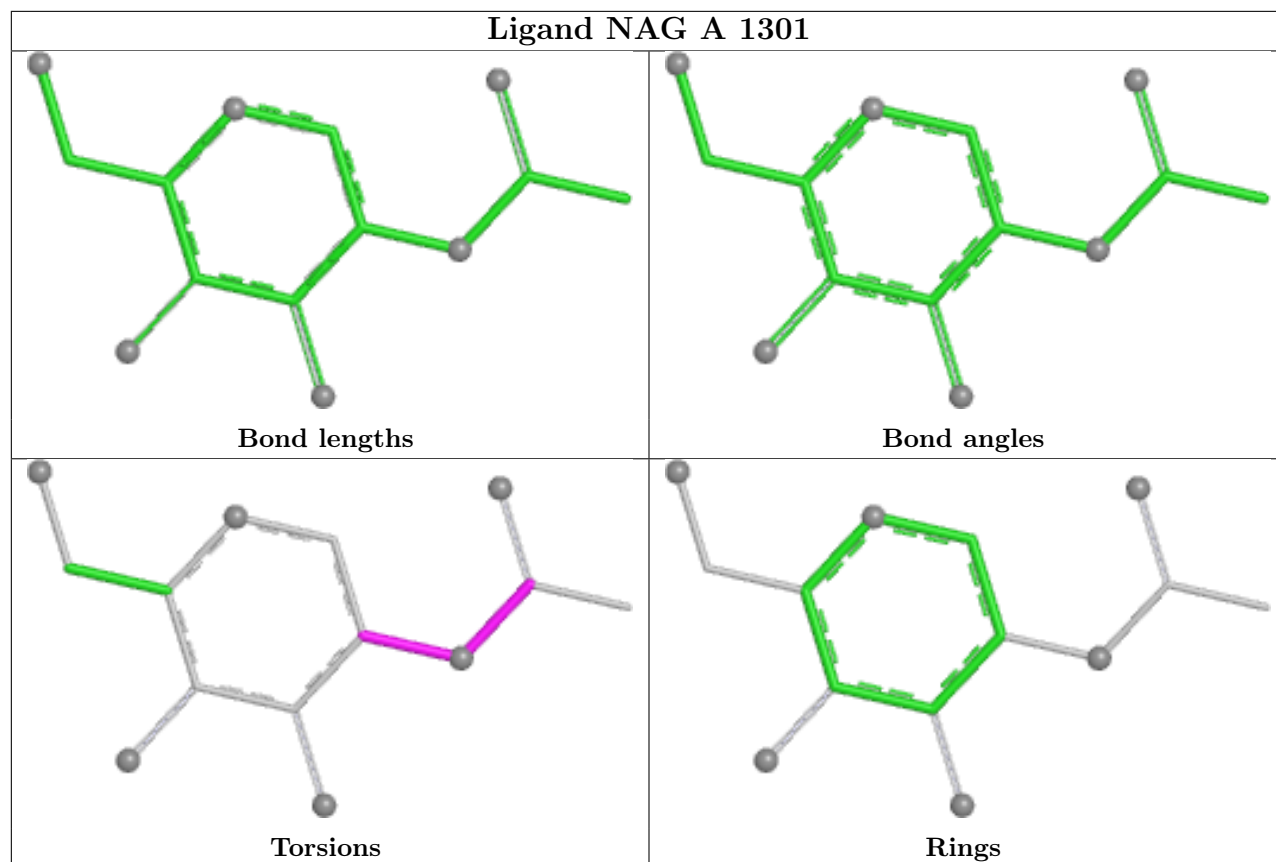


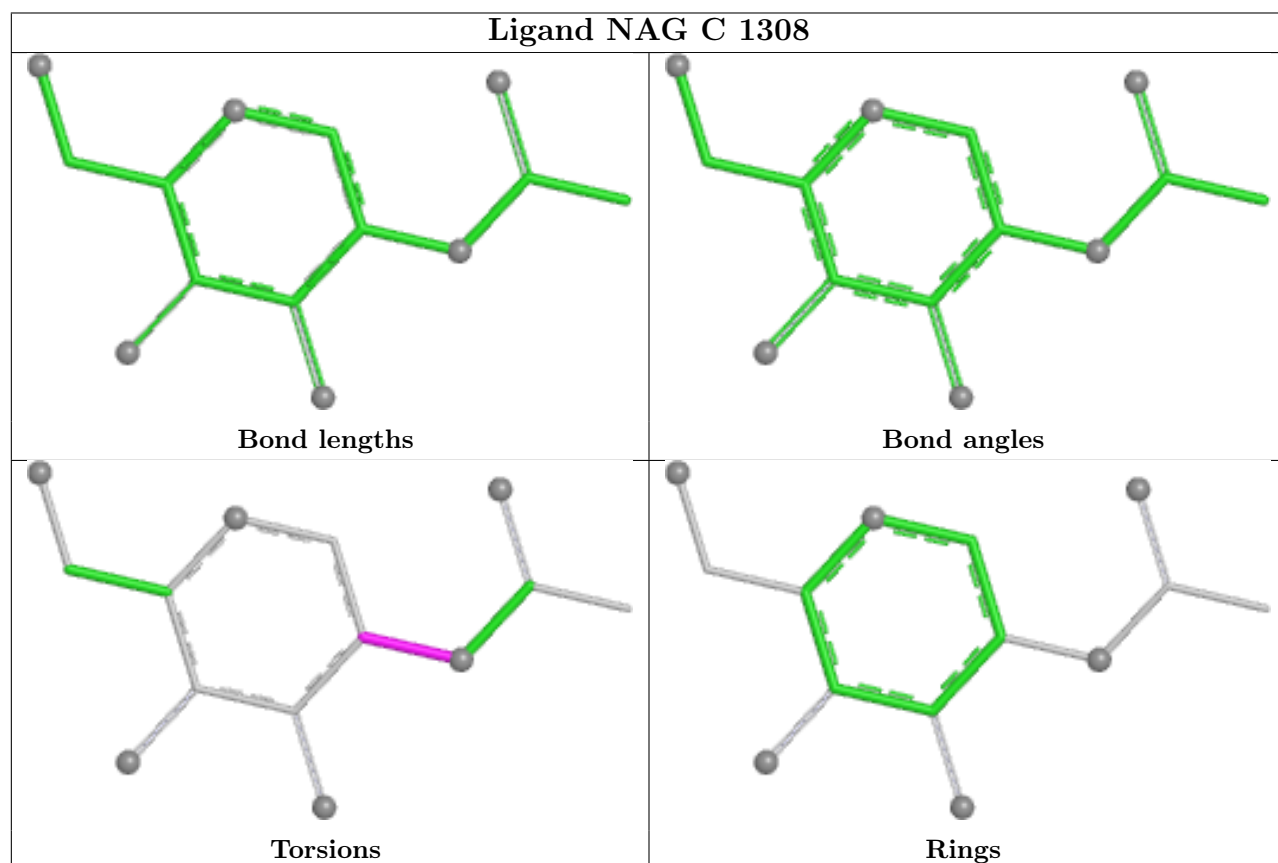
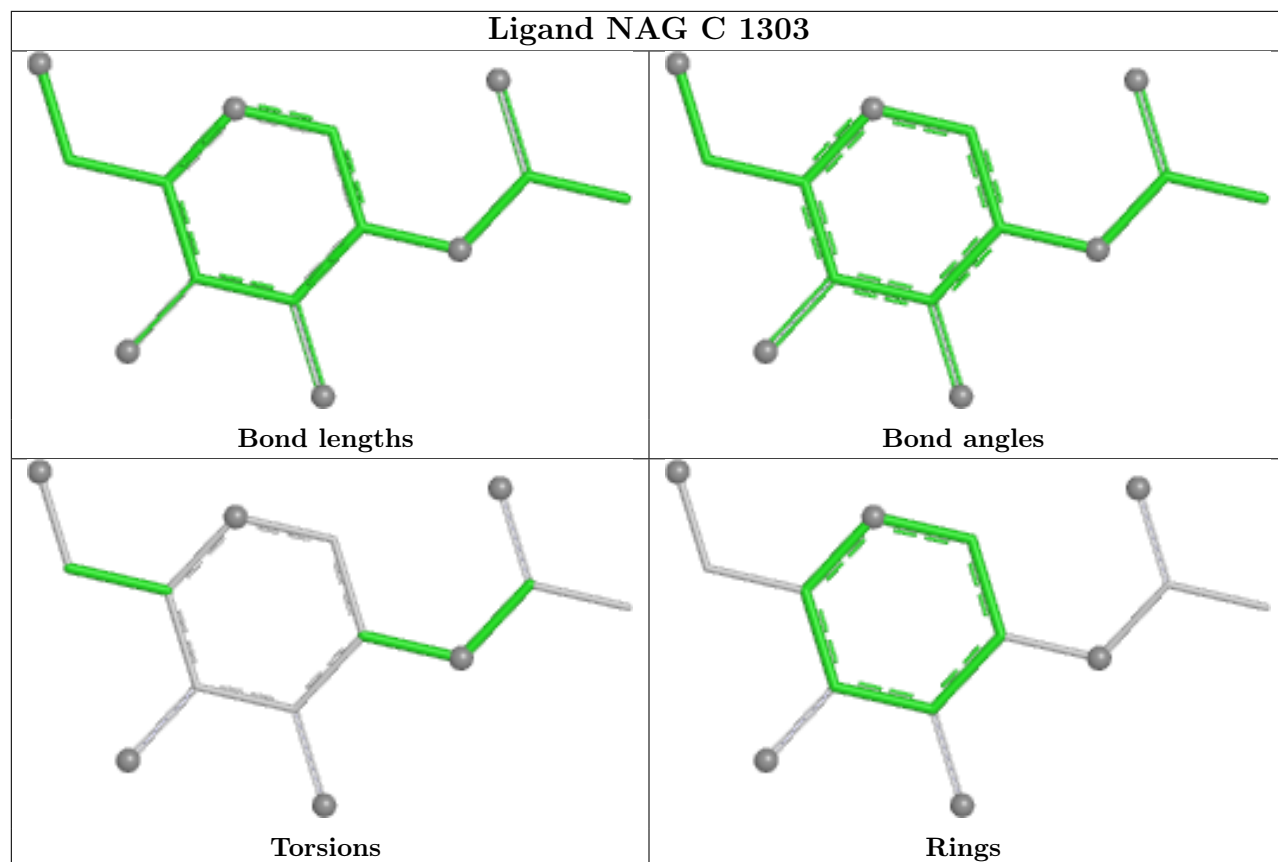
Ligand NAG A 1302



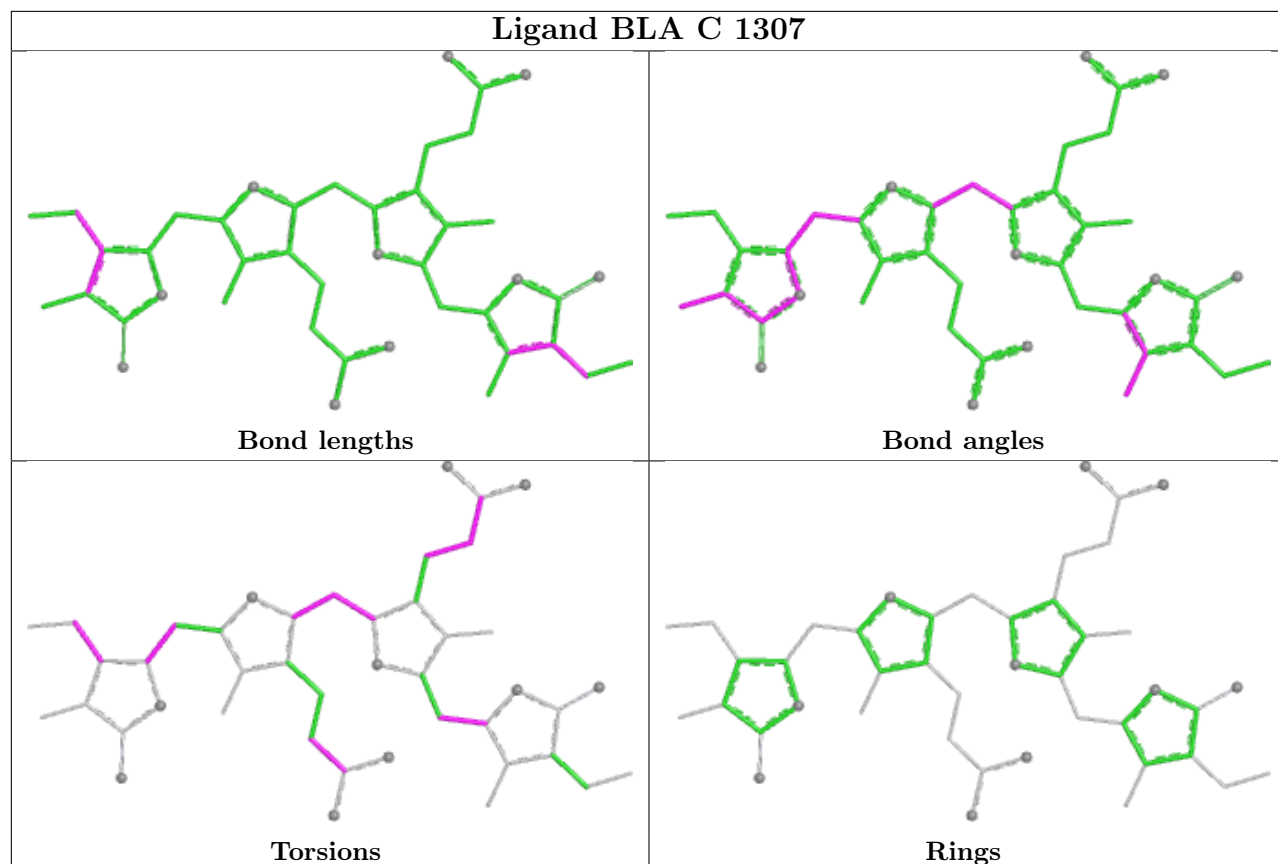
Ligand NAG C 1301



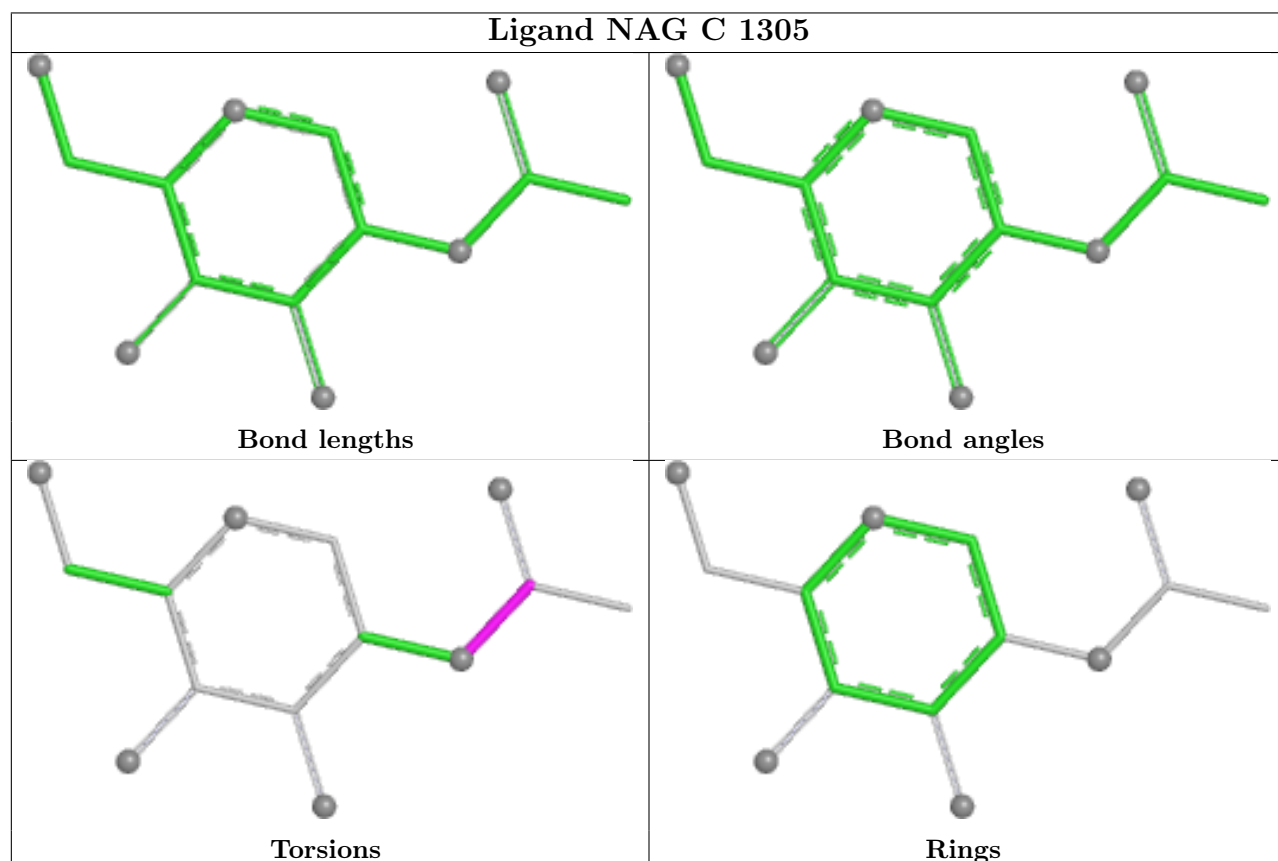


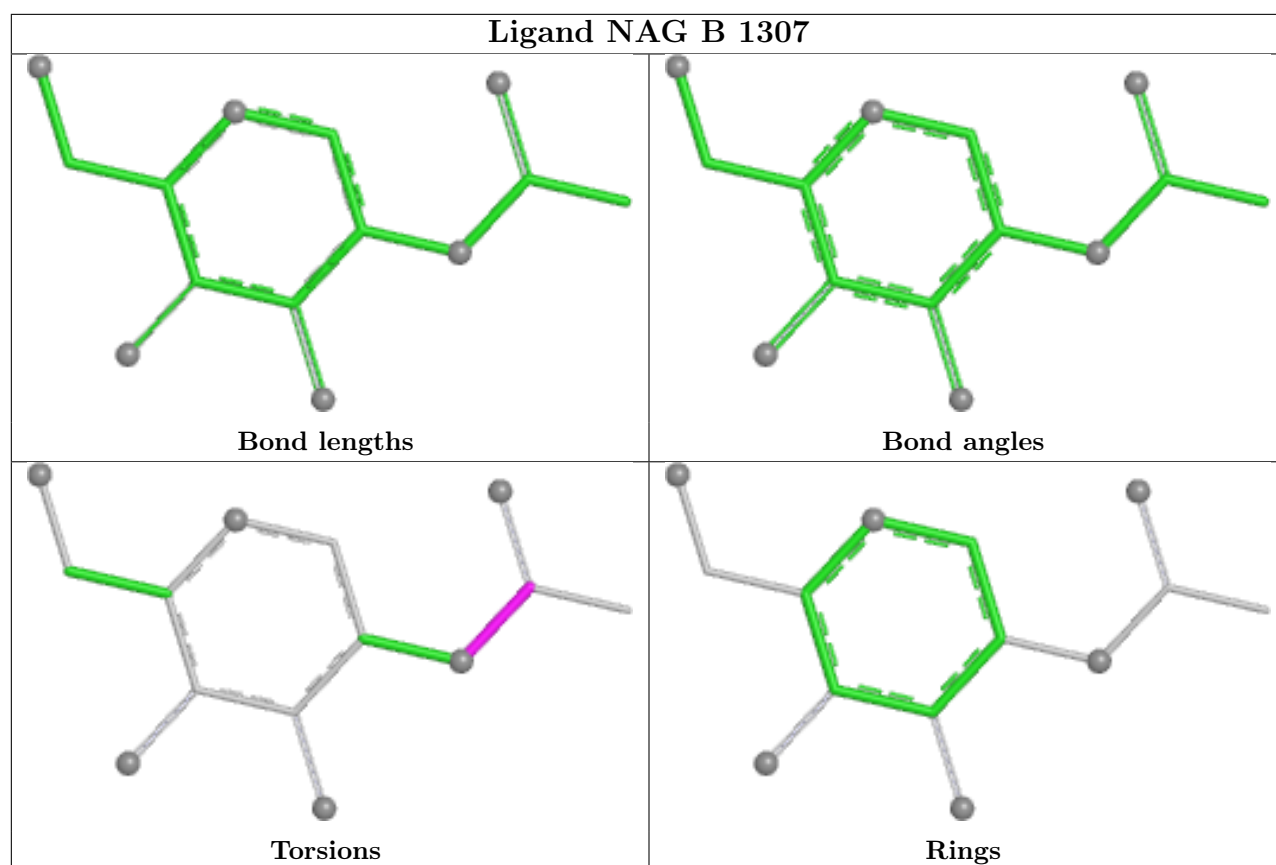


Ligand BLA C 1307



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.

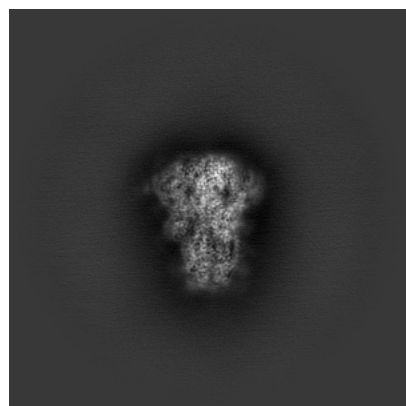
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61152. These allow visual inspection of the internal detail of the map and identification of artifacts.

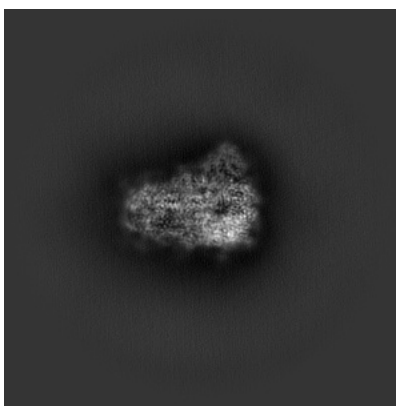
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

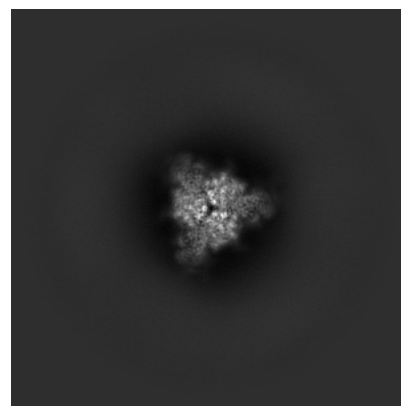
6.1.1 Primary map



X

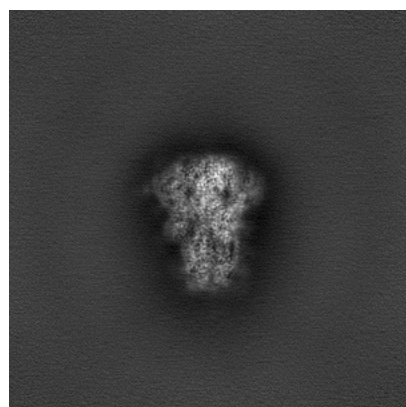


Y

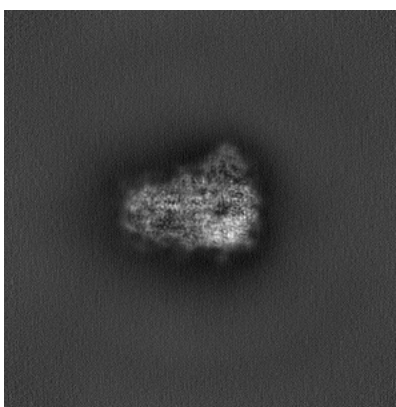


Z

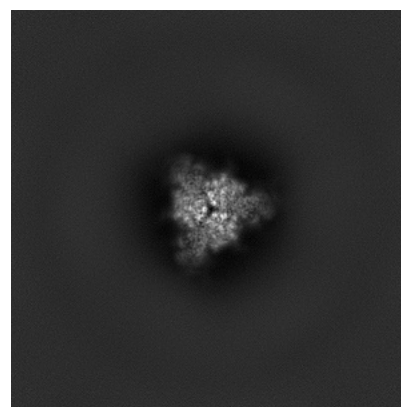
6.1.2 Raw map



X



Y

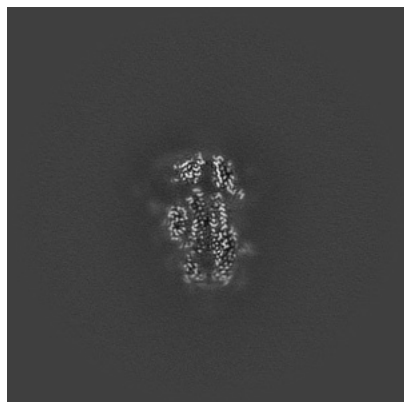


Z

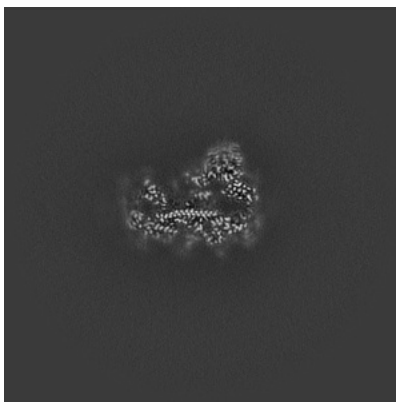
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

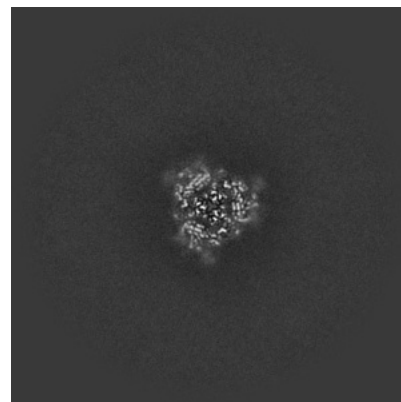
6.2.1 Primary map



X Index: 260

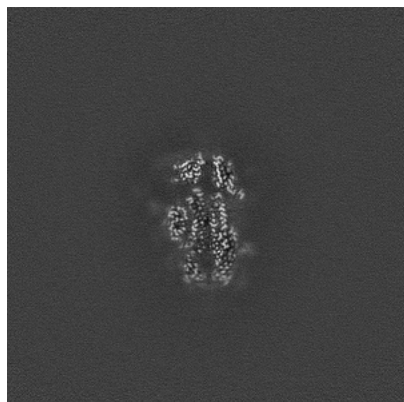


Y Index: 260

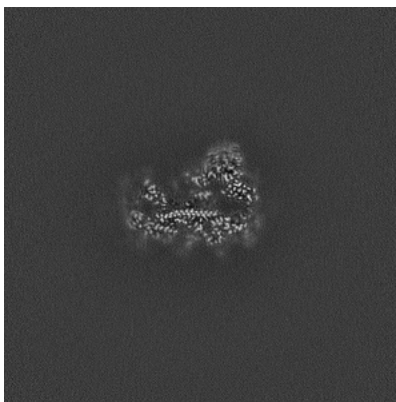


Z Index: 260

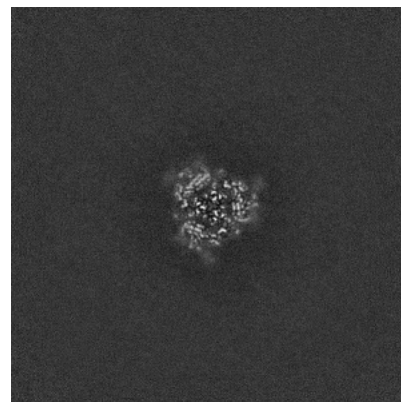
6.2.2 Raw map



X Index: 260



Y Index: 260

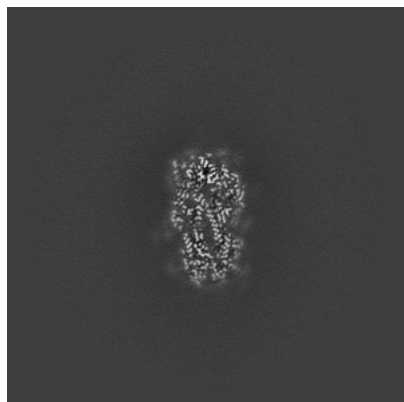


Z Index: 260

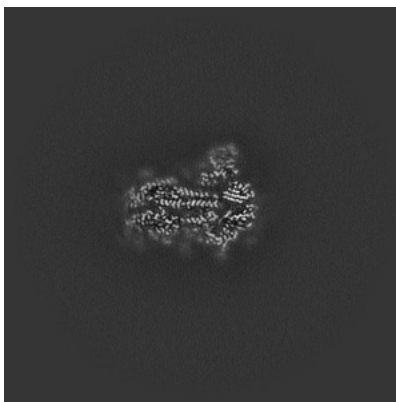
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

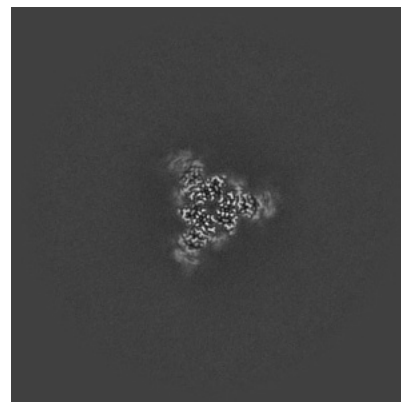
6.3.1 Primary map



X Index: 274

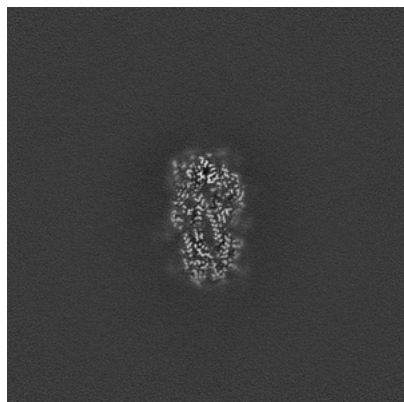


Y Index: 252

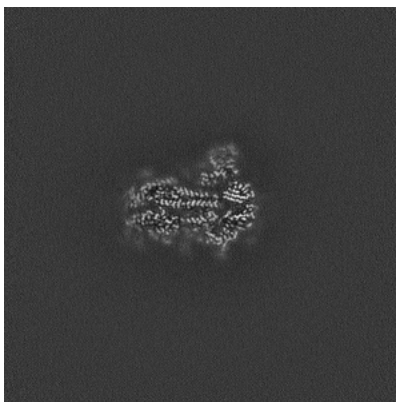


Z Index: 296

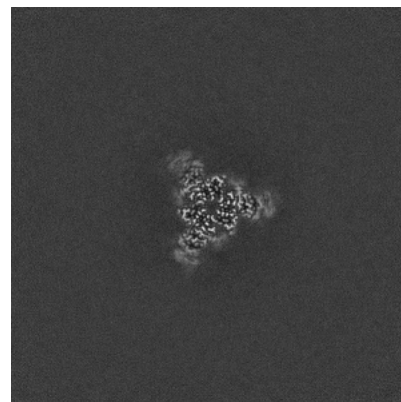
6.3.2 Raw map



X Index: 274



Y Index: 252

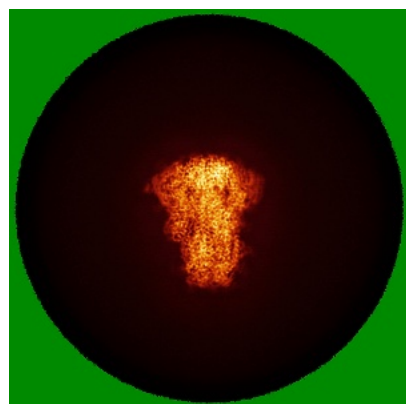


Z Index: 296

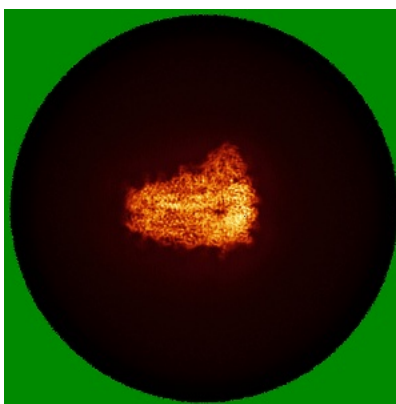
The images above show the largest variance slices of the map in three orthogonal directions.

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

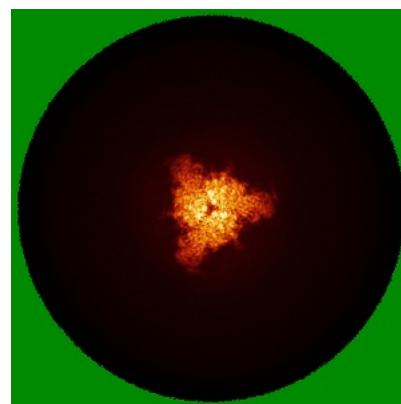
6.4.1 Primary map



X

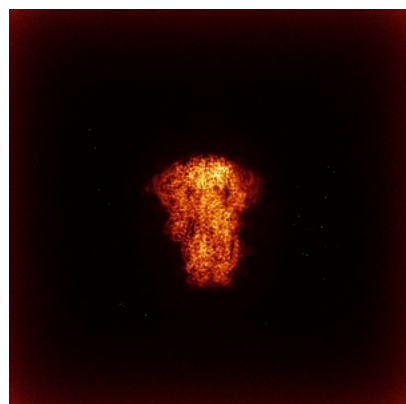


Y

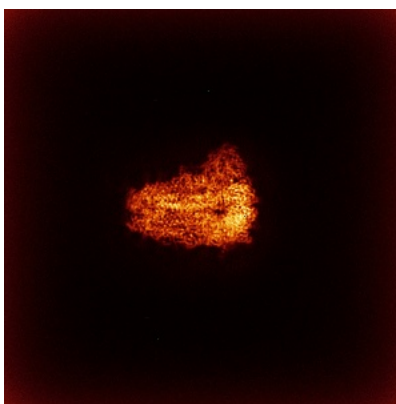


Z

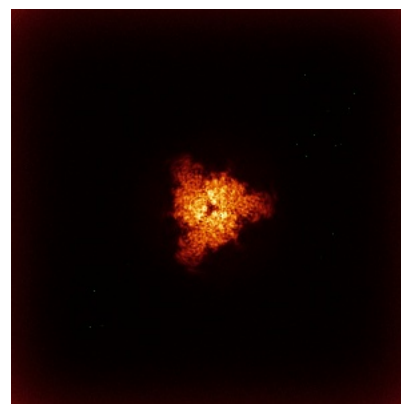
6.4.2 Raw map



X



Y

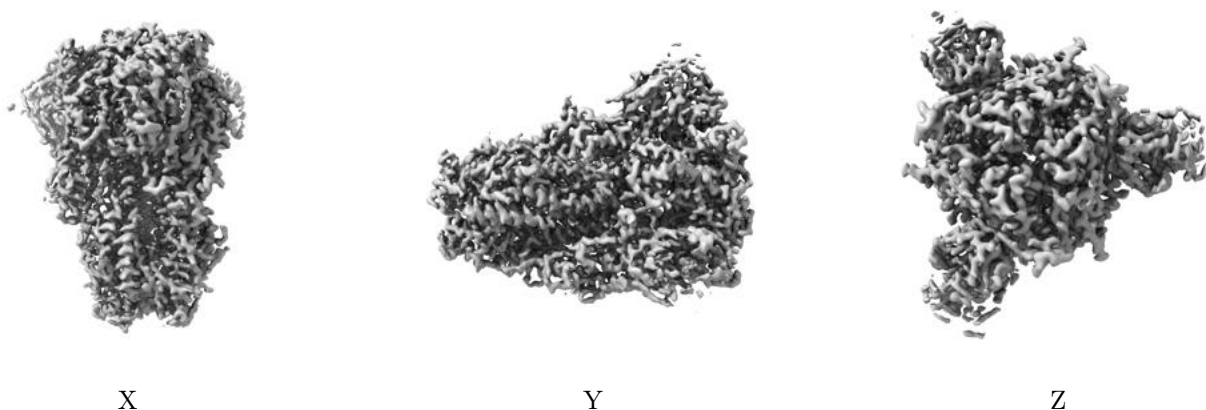


Z

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.

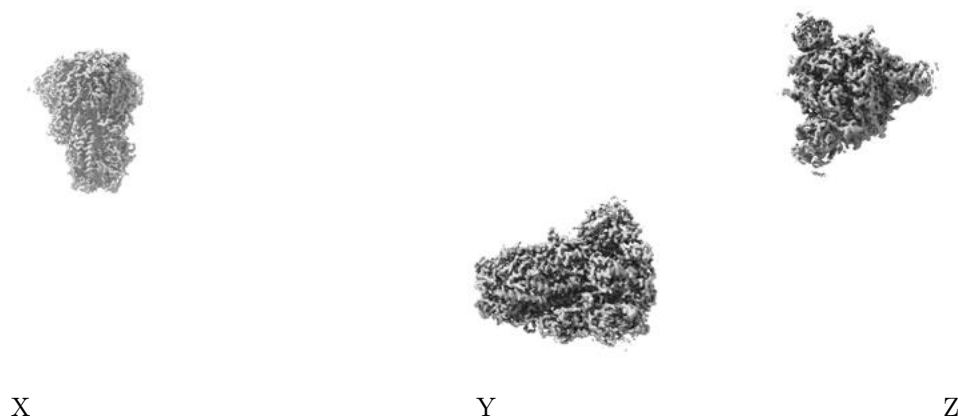
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. 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.

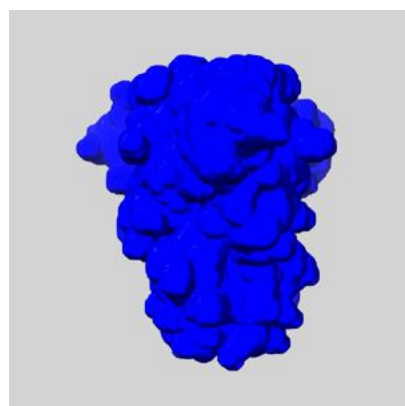
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

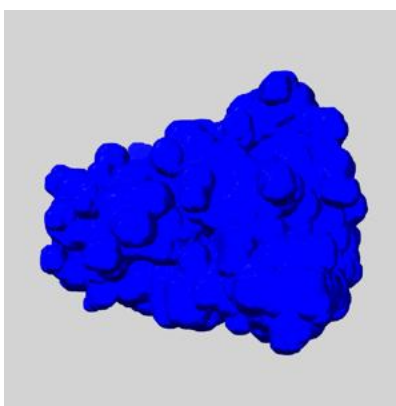
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

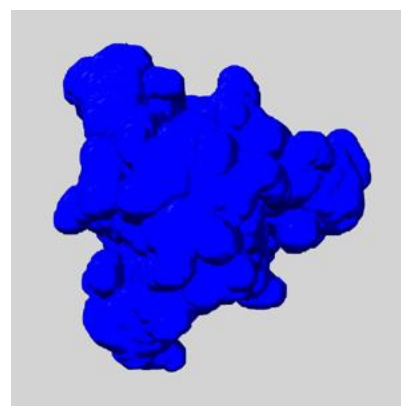
6.6.1 emd_61152_msk_1.map [i](#)



X



Y

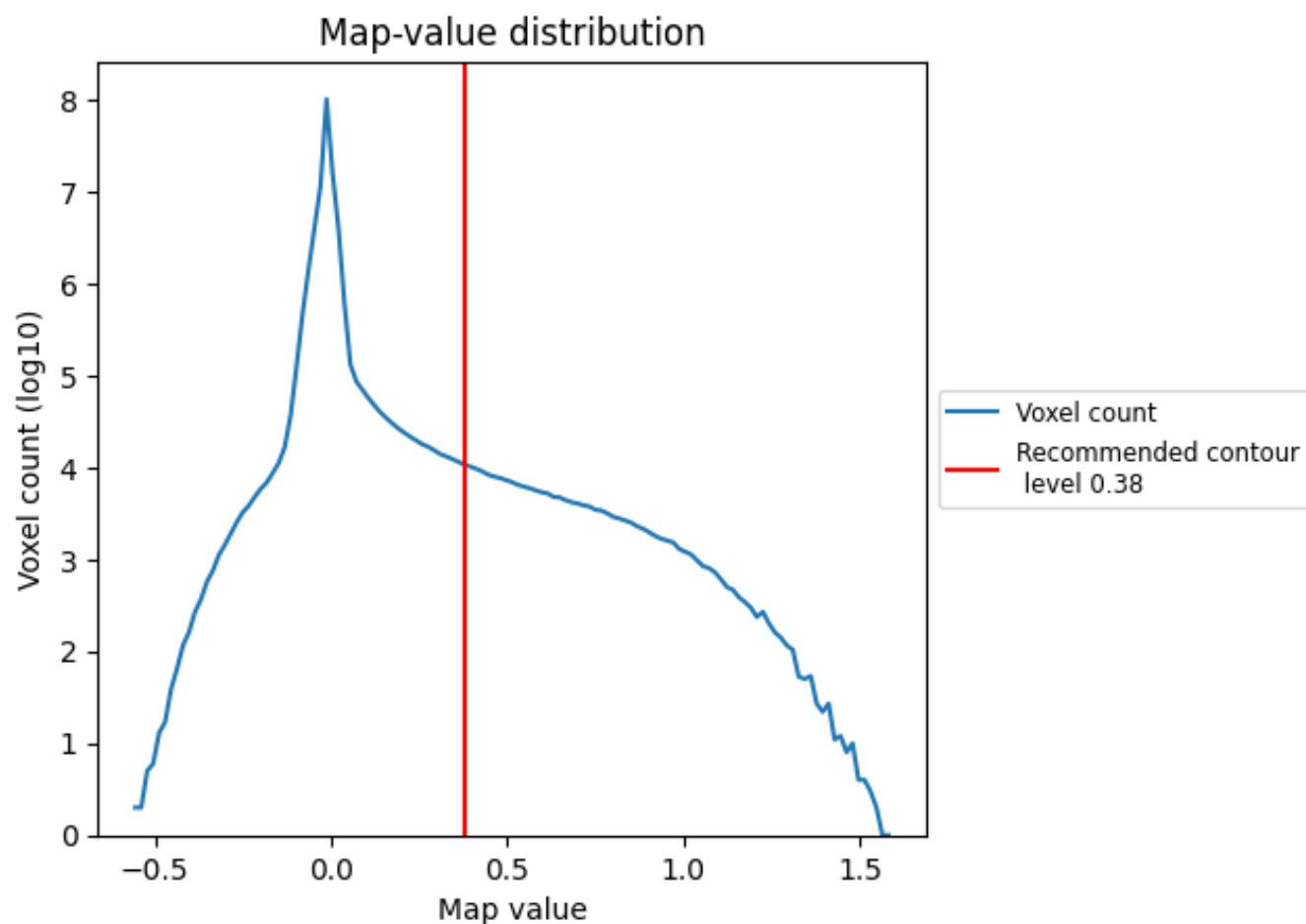


Z

7 Map analysis [i](#)

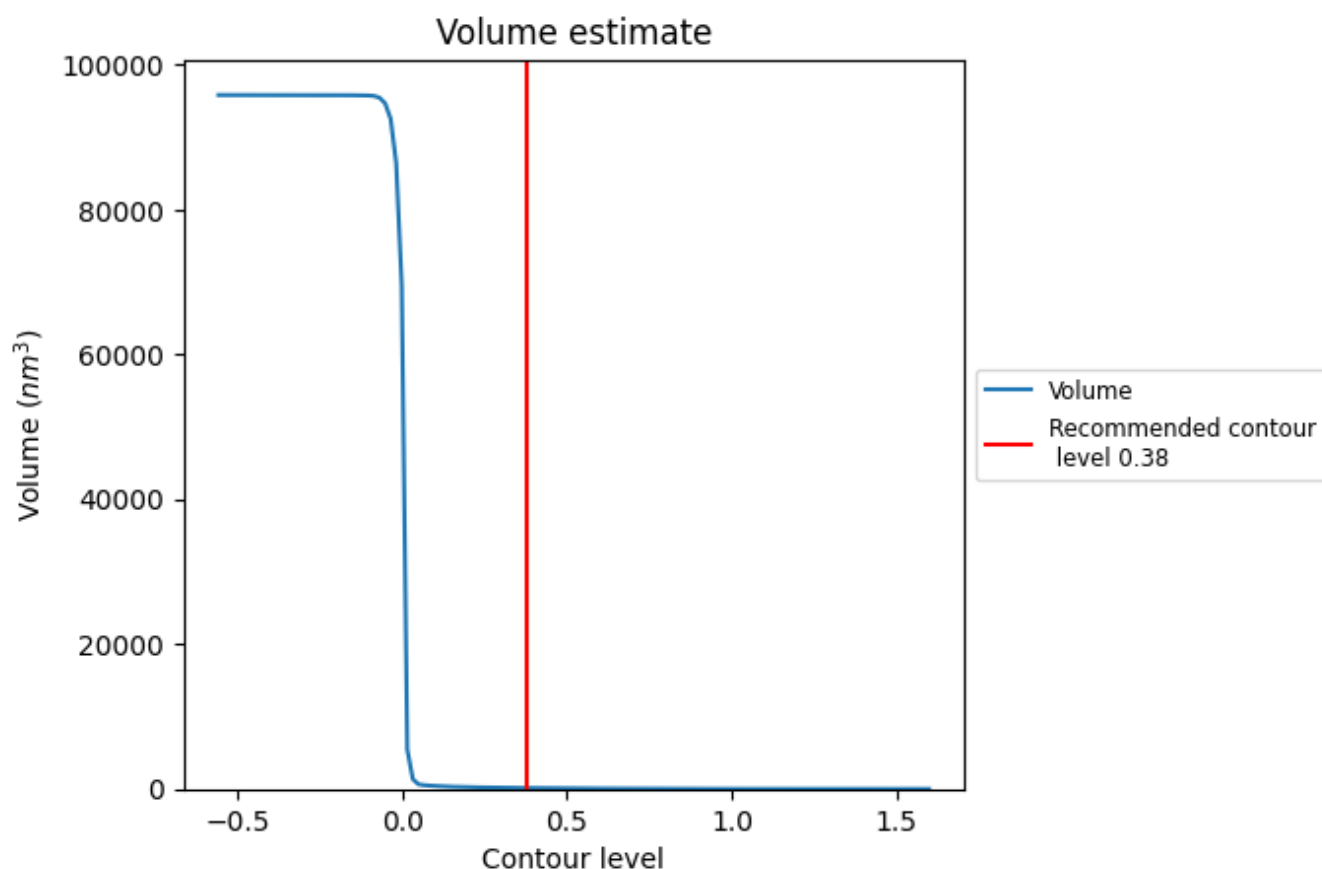
This section contains the results of statistical analysis of the map.

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.

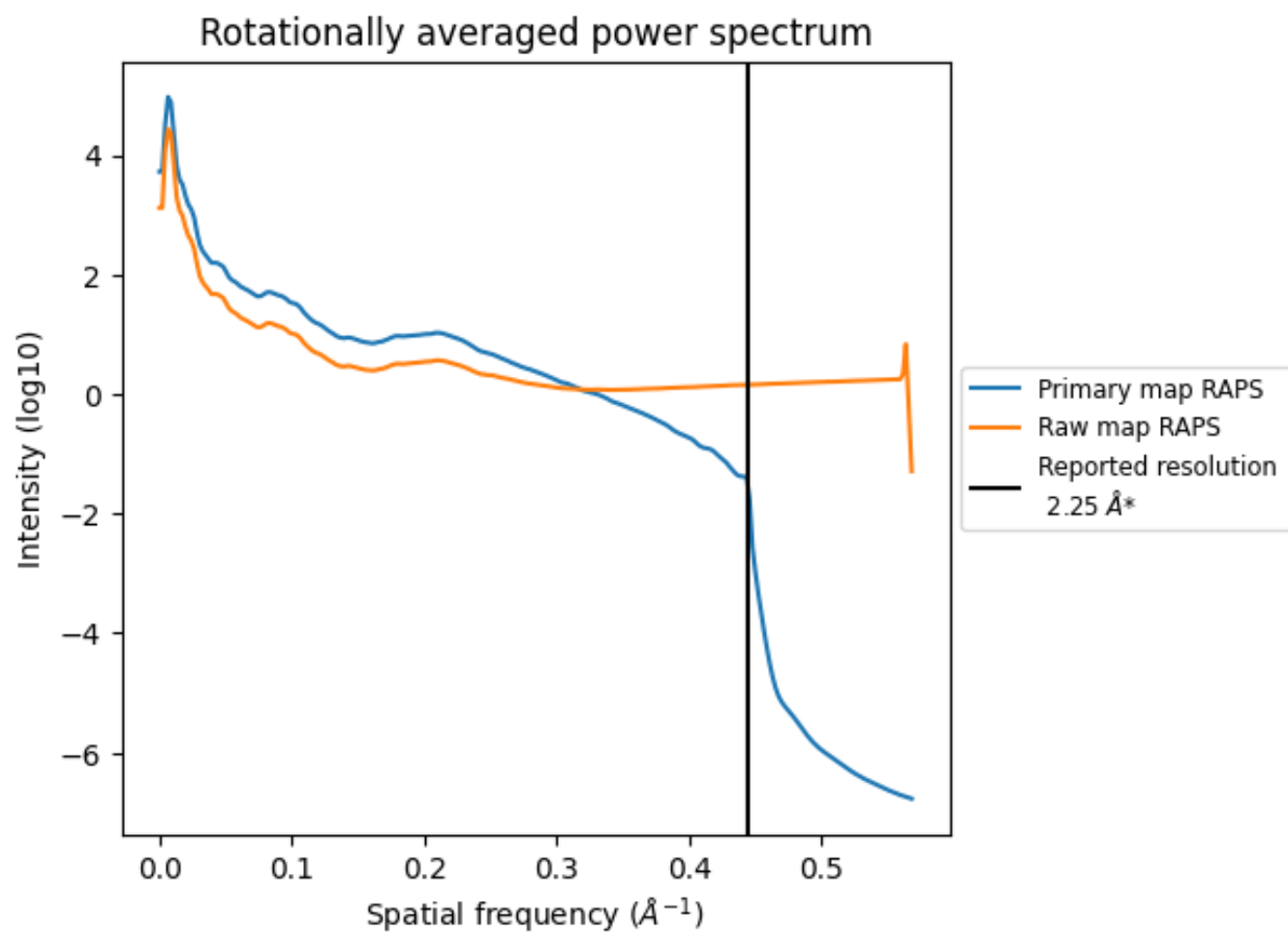
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 114 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 ⓘ

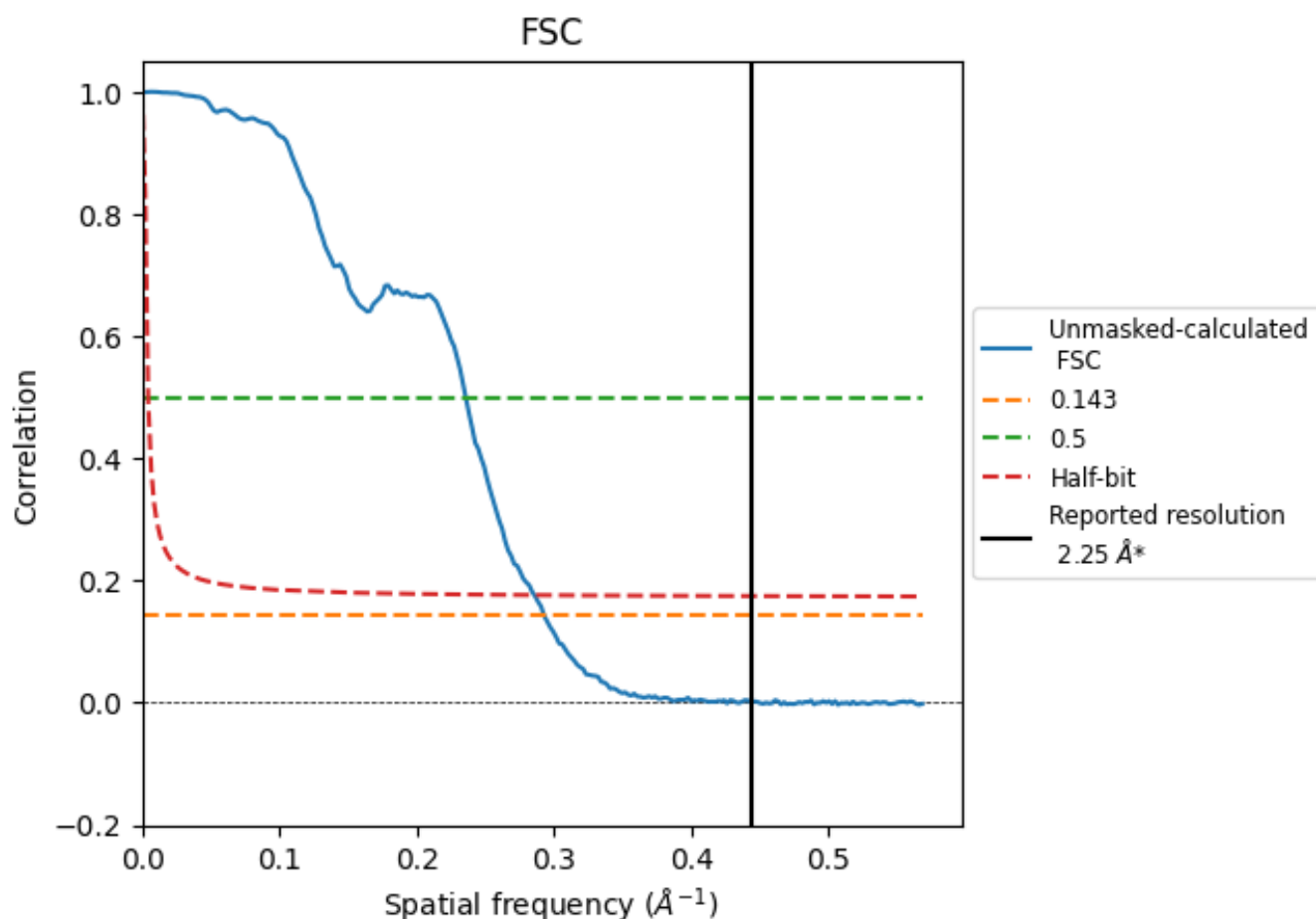


*Reported resolution corresponds to spatial frequency of $0.444 \text{ \AA}^{-1}$

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 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

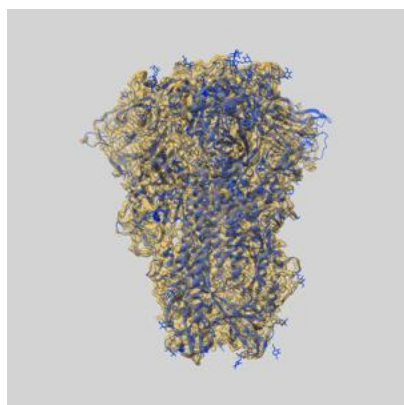
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	4.24	3.50

*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 3.42 differs from the reported value 2.25 by more than 10 %

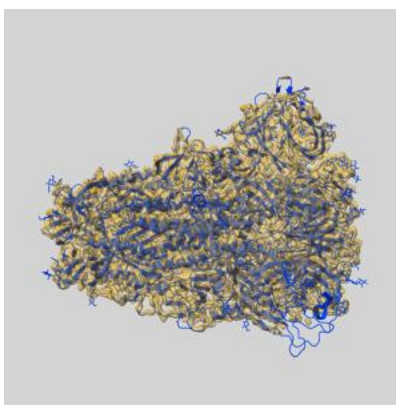
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61152 and PDB model 9J5U. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

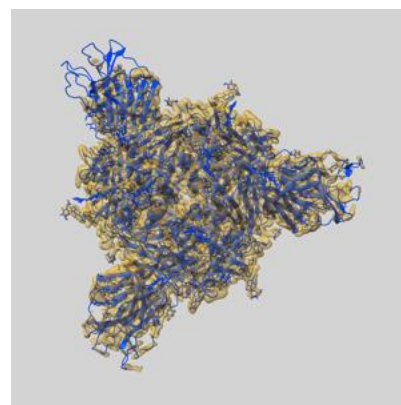
9.1 Map-model overlay [i](#)



X



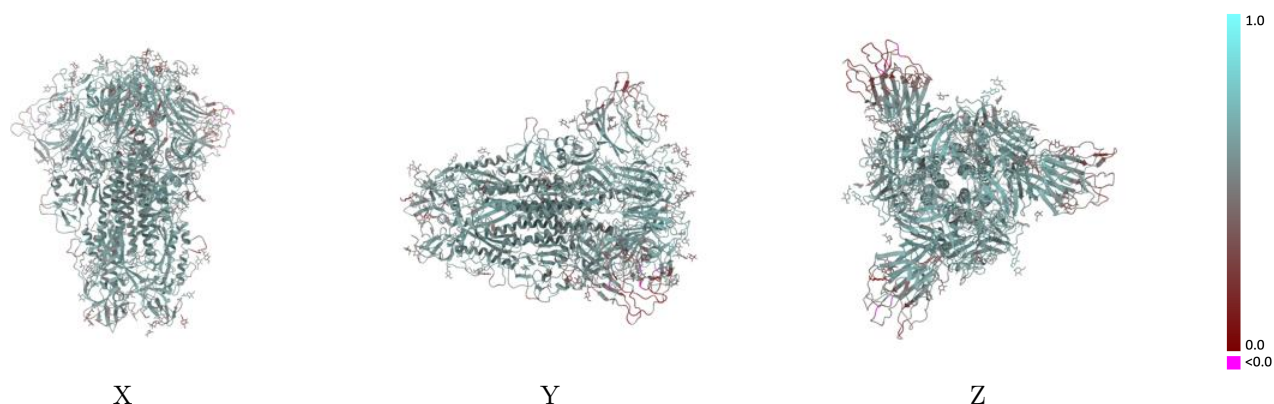
Y



Z

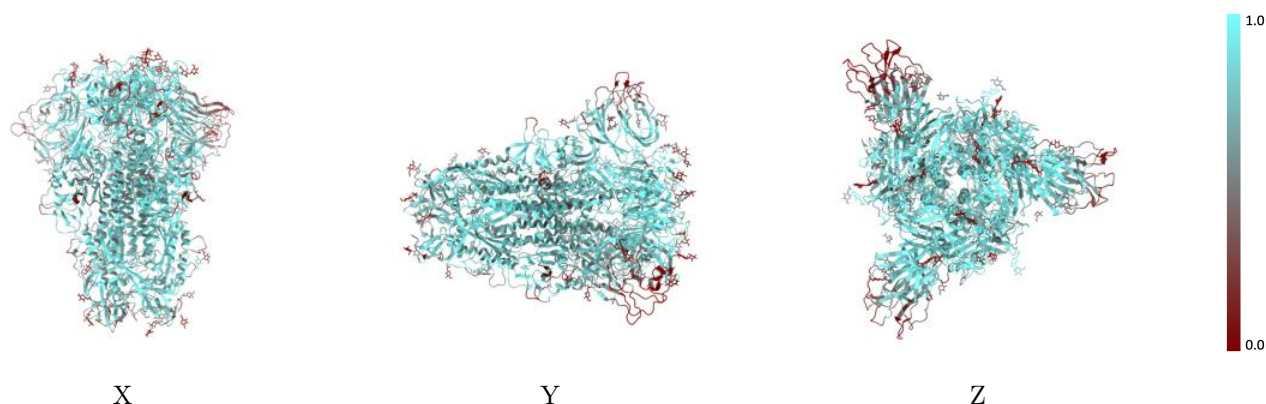
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



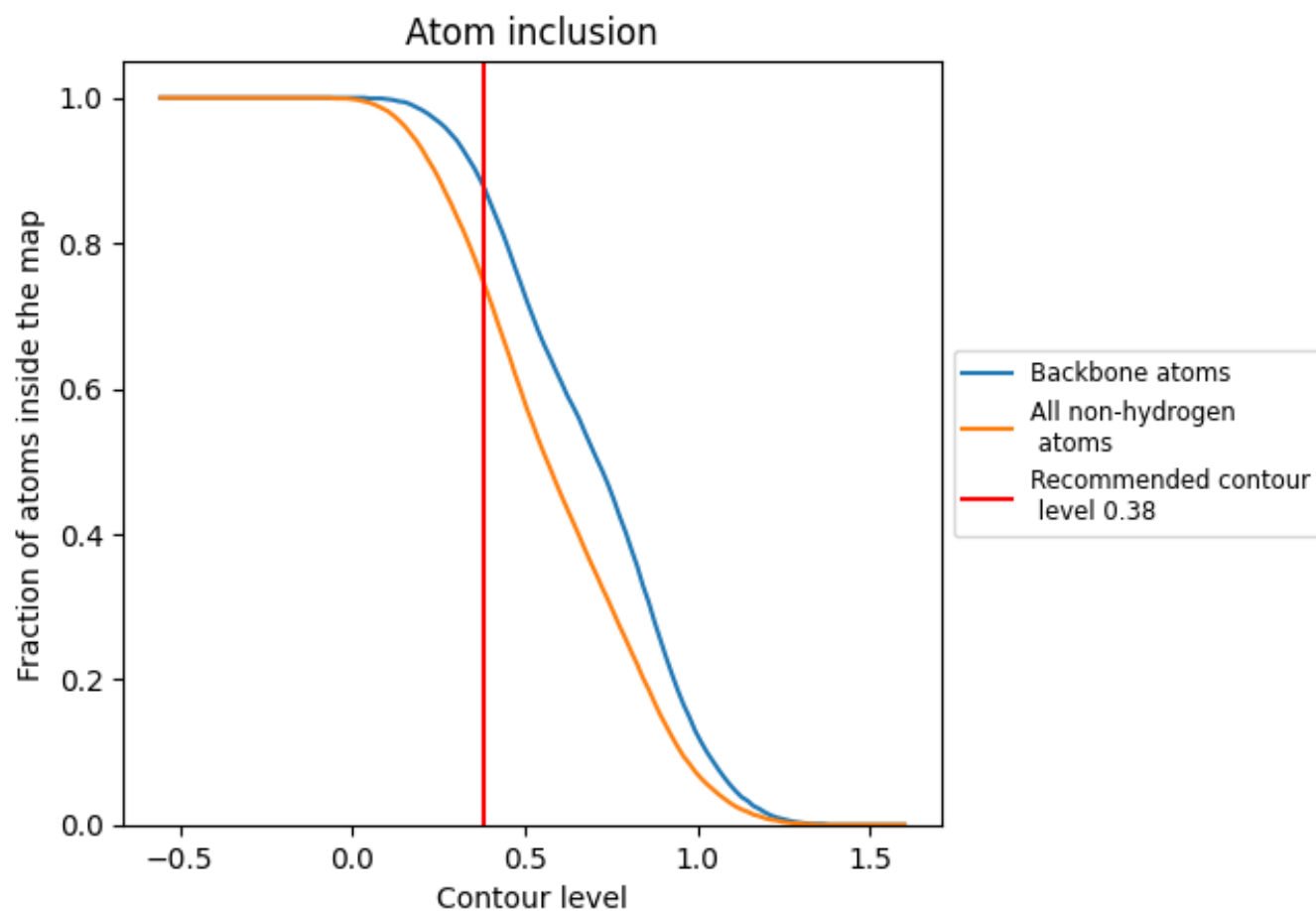
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 75% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.5680
A	 0.7770	 0.5790
B	 0.7220	 0.5580
C	 0.7790	 0.5800
D	 0.0510	 0.3370
E	 0.3800	 0.5190
F	 0.0510	 0.4290
G	 0.2050	 0.4540
H	 0.0800	 0.3630
I	 0.3000	 0.4430
J	 0.2310	 0.4430
K	 0.3570	 0.4670
L	 0.4000	 0.2970
M	 0.2140	 0.4590
N	 0.6800	 0.5350
O	 0.7500	 0.5770
P	 0.3570	 0.4430
Q	 0.1790	 0.4520
R	 0.2500	 0.4630
S	 0.6200	 0.4750
T	 0.8800	 0.5690
U	 0.3570	 0.5230
V	 0.3570	 0.3600
W	 0.0360	 0.2310
X	 0.2500	 0.2560
Y	 0.4800	 0.4970
Z	 0.7860	 0.5680
a	 0.3800	 0.5180
b	 0.4290	 0.4750

