



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:41 AM UTC

PDB ID : 6NZK / pdb_00006nzk
EMDB ID : EMD-0557
Title : Structural basis for human coronavirus attachment to sialic acid receptors
Authors : Tortorici, M.A.; Walls, A.C.; Lang, Y.; Wang, C.; Li, Z.; Koerhuis, D.; Boons, G.J.; Bosch, B.J.; Rey, F.A.; de Groot, R.; Veerler, D.
Deposited on : 2019-02-13
Resolution : 2.80 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:

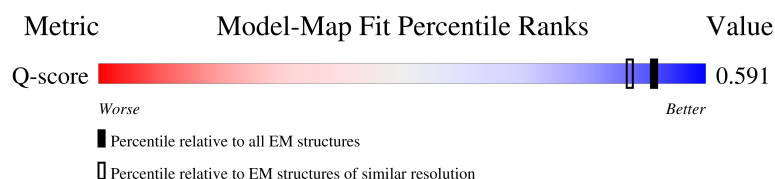
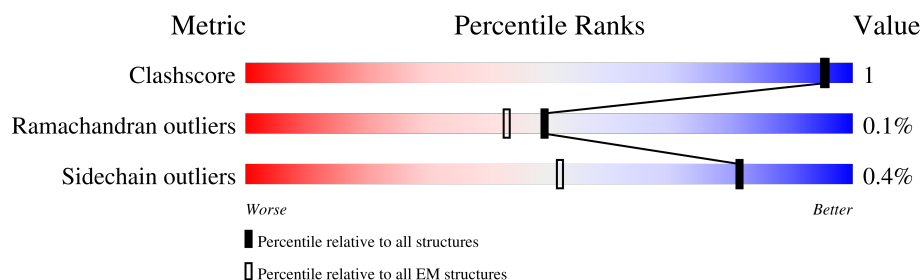
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.80 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	11806 (2.30 - 3.30)

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	1322	 6% 82% 7% 11%
1	B	1322	 6% 82% 7% 11%
1	C	1322	 6% 82% 7% 11%
2	D	3	 100% 33% 67%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	V	2	100%
			
4	c	2	100%
			
4	e	2	100%
			
4	f	2	100%
			

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29268 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 surface glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	B	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	C	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q696P8
A	-8	PRO	-	expression tag	UNP Q696P8
A	-7	MET	-	expression tag	UNP Q696P8
A	-6	GLY	-	expression tag	UNP Q696P8
A	-5	SER	-	expression tag	UNP Q696P8
A	-4	LEU	-	expression tag	UNP Q696P8
A	-3	GLN	-	expression tag	UNP Q696P8
A	-2	PRO	-	expression tag	UNP Q696P8
A	-1	LEU	-	expression tag	UNP Q696P8
A	0	ALA	-	expression tag	UNP Q696P8
A	1	THR	-	expression tag	UNP Q696P8
A	2	LEU	-	expression tag	UNP Q696P8
A	3	TYR	-	expression tag	UNP Q696P8
A	4	LEU	-	expression tag	UNP Q696P8
A	5	LEU	-	expression tag	UNP Q696P8
A	6	GLY	-	expression tag	UNP Q696P8
A	7	MET	-	expression tag	UNP Q696P8
A	8	LEU	-	expression tag	UNP Q696P8
A	9	VAL	-	expression tag	UNP Q696P8
A	10	ALA	-	expression tag	UNP Q696P8
A	11	SER	-	expression tag	UNP Q696P8
A	12	VAL	-	expression tag	UNP Q696P8
A	13	LEU	-	expression tag	UNP Q696P8
A	764	GLY	ARG	engineered mutation	UNP Q696P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	765	GLY	ARG	engineered mutation	UNP Q696P8
A	767	GLY	ARG	engineered mutation	UNP Q696P8
A	1274	LEU	-	expression tag	UNP Q696P8
A	1275	ILE	-	expression tag	UNP Q696P8
A	1276	LYS	-	expression tag	UNP Q696P8
A	1277	ARG	-	expression tag	UNP Q696P8
A	1278	MET	-	expression tag	UNP Q696P8
A	1279	LYS	-	expression tag	UNP Q696P8
A	1280	GLN	-	expression tag	UNP Q696P8
A	1281	ILE	-	expression tag	UNP Q696P8
A	1282	GLU	-	expression tag	UNP Q696P8
A	1283	ASP	-	expression tag	UNP Q696P8
A	1284	LYS	-	expression tag	UNP Q696P8
A	1285	ILE	-	expression tag	UNP Q696P8
A	1286	GLU	-	expression tag	UNP Q696P8
A	1287	GLU	-	expression tag	UNP Q696P8
A	1288	ILE	-	expression tag	UNP Q696P8
A	1289	GLU	-	expression tag	UNP Q696P8
A	1290	SER	-	expression tag	UNP Q696P8
A	1291	LYS	-	expression tag	UNP Q696P8
A	1292	GLN	-	expression tag	UNP Q696P8
A	1293	LYS	-	expression tag	UNP Q696P8
A	1294	LYS	-	expression tag	UNP Q696P8
A	1295	ILE	-	expression tag	UNP Q696P8
A	1296	GLU	-	expression tag	UNP Q696P8
A	1297	ASN	-	expression tag	UNP Q696P8
A	1298	GLU	-	expression tag	UNP Q696P8
A	1299	ILE	-	expression tag	UNP Q696P8
A	1300	ALA	-	expression tag	UNP Q696P8
A	1301	ARG	-	expression tag	UNP Q696P8
A	1302	ILE	-	expression tag	UNP Q696P8
A	1303	LYS	-	expression tag	UNP Q696P8
A	1304	LYS	-	expression tag	UNP Q696P8
A	1305	ILE	-	expression tag	UNP Q696P8
A	1306	LYS	-	expression tag	UNP Q696P8
A	1307	LEU	-	expression tag	UNP Q696P8
A	1308	VAL	-	expression tag	UNP Q696P8
A	1309	PRO	-	expression tag	UNP Q696P8
A	1310	ARG	-	expression tag	UNP Q696P8
A	1311	GLY	-	expression tag	UNP Q696P8
A	1312	SER	-	expression tag	UNP Q696P8
A	1313	LEU	-	expression tag	UNP Q696P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1314	GLU	-	expression tag	UNP Q696P8
A	1315	TRP	-	expression tag	UNP Q696P8
A	1316	SER	-	expression tag	UNP Q696P8
A	1317	HIS	-	expression tag	UNP Q696P8
A	1318	PRO	-	expression tag	UNP Q696P8
A	1319	GLN	-	expression tag	UNP Q696P8
A	1320	PHE	-	expression tag	UNP Q696P8
A	1321	GLU	-	expression tag	UNP Q696P8
A	1322	LYS	-	expression tag	UNP Q696P8
B	-9	MET	-	initiating methionine	UNP Q696P8
B	-8	PRO	-	expression tag	UNP Q696P8
B	-7	MET	-	expression tag	UNP Q696P8
B	-6	GLY	-	expression tag	UNP Q696P8
B	-5	SER	-	expression tag	UNP Q696P8
B	-4	LEU	-	expression tag	UNP Q696P8
B	-3	GLN	-	expression tag	UNP Q696P8
B	-2	PRO	-	expression tag	UNP Q696P8
B	-1	LEU	-	expression tag	UNP Q696P8
B	0	ALA	-	expression tag	UNP Q696P8
B	1	THR	-	expression tag	UNP Q696P8
B	2	LEU	-	expression tag	UNP Q696P8
B	3	TYR	-	expression tag	UNP Q696P8
B	4	LEU	-	expression tag	UNP Q696P8
B	5	LEU	-	expression tag	UNP Q696P8
B	6	GLY	-	expression tag	UNP Q696P8
B	7	MET	-	expression tag	UNP Q696P8
B	8	LEU	-	expression tag	UNP Q696P8
B	9	VAL	-	expression tag	UNP Q696P8
B	10	ALA	-	expression tag	UNP Q696P8
B	11	SER	-	expression tag	UNP Q696P8
B	12	VAL	-	expression tag	UNP Q696P8
B	13	LEU	-	expression tag	UNP Q696P8
B	764	GLY	ARG	engineered mutation	UNP Q696P8
B	765	GLY	ARG	engineered mutation	UNP Q696P8
B	767	GLY	ARG	engineered mutation	UNP Q696P8
B	1274	LEU	-	expression tag	UNP Q696P8
B	1275	ILE	-	expression tag	UNP Q696P8
B	1276	LYS	-	expression tag	UNP Q696P8
B	1277	ARG	-	expression tag	UNP Q696P8
B	1278	MET	-	expression tag	UNP Q696P8
B	1279	LYS	-	expression tag	UNP Q696P8
B	1280	GLN	-	expression tag	UNP Q696P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1281	ILE	-	expression tag	UNP Q696P8
B	1282	GLU	-	expression tag	UNP Q696P8
B	1283	ASP	-	expression tag	UNP Q696P8
B	1284	LYS	-	expression tag	UNP Q696P8
B	1285	ILE	-	expression tag	UNP Q696P8
B	1286	GLU	-	expression tag	UNP Q696P8
B	1287	GLU	-	expression tag	UNP Q696P8
B	1288	ILE	-	expression tag	UNP Q696P8
B	1289	GLU	-	expression tag	UNP Q696P8
B	1290	SER	-	expression tag	UNP Q696P8
B	1291	LYS	-	expression tag	UNP Q696P8
B	1292	GLN	-	expression tag	UNP Q696P8
B	1293	LYS	-	expression tag	UNP Q696P8
B	1294	LYS	-	expression tag	UNP Q696P8
B	1295	ILE	-	expression tag	UNP Q696P8
B	1296	GLU	-	expression tag	UNP Q696P8
B	1297	ASN	-	expression tag	UNP Q696P8
B	1298	GLU	-	expression tag	UNP Q696P8
B	1299	ILE	-	expression tag	UNP Q696P8
B	1300	ALA	-	expression tag	UNP Q696P8
B	1301	ARG	-	expression tag	UNP Q696P8
B	1302	ILE	-	expression tag	UNP Q696P8
B	1303	LYS	-	expression tag	UNP Q696P8
B	1304	LYS	-	expression tag	UNP Q696P8
B	1305	ILE	-	expression tag	UNP Q696P8
B	1306	LYS	-	expression tag	UNP Q696P8
B	1307	LEU	-	expression tag	UNP Q696P8
B	1308	VAL	-	expression tag	UNP Q696P8
B	1309	PRO	-	expression tag	UNP Q696P8
B	1310	ARG	-	expression tag	UNP Q696P8
B	1311	GLY	-	expression tag	UNP Q696P8
B	1312	SER	-	expression tag	UNP Q696P8
B	1313	LEU	-	expression tag	UNP Q696P8
B	1314	GLU	-	expression tag	UNP Q696P8
B	1315	TRP	-	expression tag	UNP Q696P8
B	1316	SER	-	expression tag	UNP Q696P8
B	1317	HIS	-	expression tag	UNP Q696P8
B	1318	PRO	-	expression tag	UNP Q696P8
B	1319	GLN	-	expression tag	UNP Q696P8
B	1320	PHE	-	expression tag	UNP Q696P8
B	1321	GLU	-	expression tag	UNP Q696P8
B	1322	LYS	-	expression tag	UNP Q696P8

Continued on next page...

Continued from previous page...

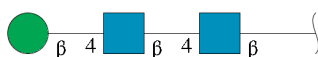
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	MET	-	initiating methionine	UNP Q696P8
C	-8	PRO	-	expression tag	UNP Q696P8
C	-7	MET	-	expression tag	UNP Q696P8
C	-6	GLY	-	expression tag	UNP Q696P8
C	-5	SER	-	expression tag	UNP Q696P8
C	-4	LEU	-	expression tag	UNP Q696P8
C	-3	GLN	-	expression tag	UNP Q696P8
C	-2	PRO	-	expression tag	UNP Q696P8
C	-1	LEU	-	expression tag	UNP Q696P8
C	0	ALA	-	expression tag	UNP Q696P8
C	1	THR	-	expression tag	UNP Q696P8
C	2	LEU	-	expression tag	UNP Q696P8
C	3	TYR	-	expression tag	UNP Q696P8
C	4	LEU	-	expression tag	UNP Q696P8
C	5	LEU	-	expression tag	UNP Q696P8
C	6	GLY	-	expression tag	UNP Q696P8
C	7	MET	-	expression tag	UNP Q696P8
C	8	LEU	-	expression tag	UNP Q696P8
C	9	VAL	-	expression tag	UNP Q696P8
C	10	ALA	-	expression tag	UNP Q696P8
C	11	SER	-	expression tag	UNP Q696P8
C	12	VAL	-	expression tag	UNP Q696P8
C	13	LEU	-	expression tag	UNP Q696P8
C	764	GLY	ARG	engineered mutation	UNP Q696P8
C	765	GLY	ARG	engineered mutation	UNP Q696P8
C	767	GLY	ARG	engineered mutation	UNP Q696P8
C	1274	LEU	-	expression tag	UNP Q696P8
C	1275	ILE	-	expression tag	UNP Q696P8
C	1276	LYS	-	expression tag	UNP Q696P8
C	1277	ARG	-	expression tag	UNP Q696P8
C	1278	MET	-	expression tag	UNP Q696P8
C	1279	LYS	-	expression tag	UNP Q696P8
C	1280	GLN	-	expression tag	UNP Q696P8
C	1281	ILE	-	expression tag	UNP Q696P8
C	1282	GLU	-	expression tag	UNP Q696P8
C	1283	ASP	-	expression tag	UNP Q696P8
C	1284	LYS	-	expression tag	UNP Q696P8
C	1285	ILE	-	expression tag	UNP Q696P8
C	1286	GLU	-	expression tag	UNP Q696P8
C	1287	GLU	-	expression tag	UNP Q696P8
C	1288	ILE	-	expression tag	UNP Q696P8
C	1289	GLU	-	expression tag	UNP Q696P8

Continued on next page...

Continued from previous page...

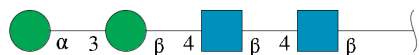
Chain	Residue	Modelled	Actual	Comment	Reference
C	1290	SER	-	expression tag	UNP Q696P8
C	1291	LYS	-	expression tag	UNP Q696P8
C	1292	GLN	-	expression tag	UNP Q696P8
C	1293	LYS	-	expression tag	UNP Q696P8
C	1294	LYS	-	expression tag	UNP Q696P8
C	1295	ILE	-	expression tag	UNP Q696P8
C	1296	GLU	-	expression tag	UNP Q696P8
C	1297	ASN	-	expression tag	UNP Q696P8
C	1298	GLU	-	expression tag	UNP Q696P8
C	1299	ILE	-	expression tag	UNP Q696P8
C	1300	ALA	-	expression tag	UNP Q696P8
C	1301	ARG	-	expression tag	UNP Q696P8
C	1302	ILE	-	expression tag	UNP Q696P8
C	1303	LYS	-	expression tag	UNP Q696P8
C	1304	LYS	-	expression tag	UNP Q696P8
C	1305	ILE	-	expression tag	UNP Q696P8
C	1306	LYS	-	expression tag	UNP Q696P8
C	1307	LEU	-	expression tag	UNP Q696P8
C	1308	VAL	-	expression tag	UNP Q696P8
C	1309	PRO	-	expression tag	UNP Q696P8
C	1310	ARG	-	expression tag	UNP Q696P8
C	1311	GLY	-	expression tag	UNP Q696P8
C	1312	SER	-	expression tag	UNP Q696P8
C	1313	LEU	-	expression tag	UNP Q696P8
C	1314	GLU	-	expression tag	UNP Q696P8
C	1315	TRP	-	expression tag	UNP Q696P8
C	1316	SER	-	expression tag	UNP Q696P8
C	1317	HIS	-	expression tag	UNP Q696P8
C	1318	PRO	-	expression tag	UNP Q696P8
C	1319	GLN	-	expression tag	UNP Q696P8
C	1320	PHE	-	expression tag	UNP Q696P8
C	1321	GLU	-	expression tag	UNP Q696P8
C	1322	LYS	-	expression tag	UNP Q696P8

- 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	E	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	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	O	3	Total	C	N	O	0	0
			39	22	2	15		
2	Q	3	Total	C	N	O	0	0
			39	22	2	15		
2	R	3	Total	C	N	O	0	0
			39	22	2	15		
2	W	3	Total	C	N	O	0	0
			39	22	2	15		
2	X	3	Total	C	N	O	0	0
			39	22	2	15		
2	Y	3	Total	C	N	O	0	0
			39	22	2	15		
2	a	3	Total	C	N	O	0	0
			39	22	2	15		
2	b	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	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	F	4	Total	C	N	O	0	0
			50	28	2	20		
3	J	4	Total	C	N	O	0	0
			50	28	2	20		

Continued on next page...

Continued from previous page...

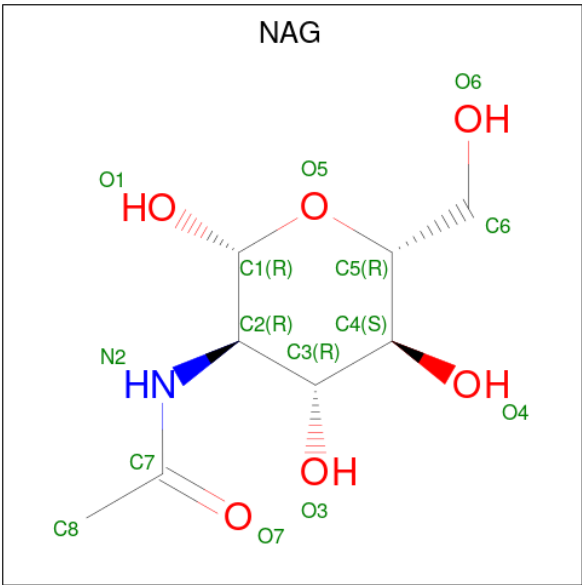
Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	4	Total	C	N	O	0	0
			50	28	2	20		
3	T	4	Total	C	N	O	0	0
			50	28	2	20		
3	Z	4	Total	C	N	O	0	0
			50	28	2	20		
3	d	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 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
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

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

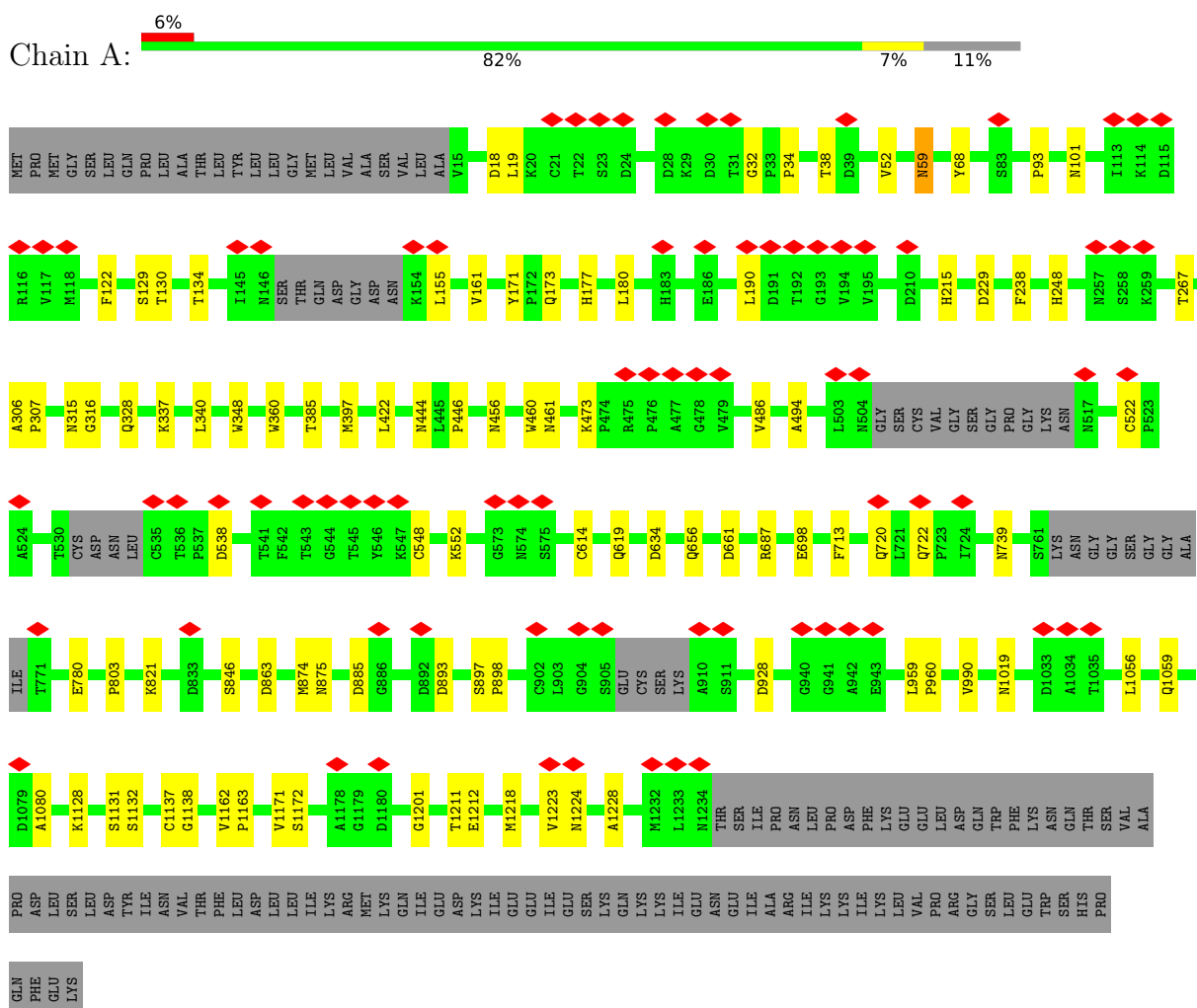
-
- The chemical structure shows a glucose molecule in its cyclic pyranose form, specifically the beta-D-glucopyranose isomer. The glucose ring is substituted with four acetyl groups (OAc) at the 2, 3, 4, and 6 positions. The anomeric carbon (C1) is linked to a methyl group (CH3) via an oxygen atom (O1A), forming a methyl glycoside. The stereochemistry is indicated by wedged and dashed bonds: C2(R), C3(R), C4(S), and C6(R) are shown with wedged bonds to their respective substituents, while C5(R) is shown with a dashed bond to its substituent. The acetyl groups are labeled with oxygen atoms O1B, O2, O3, and O4, and the methyl group is labeled with C11. The glucose ring carbons are labeled C1 through C6, and the acetyl carbonyl carbons are labeled C7 through C10. The methyl group is labeled C11.

Mol	Chain	Residues	Atoms	AltConf
7	A	132	Total O 132 132	0
7	B	132	Total O 132 132	0
7	C	132	Total O 132 132	0

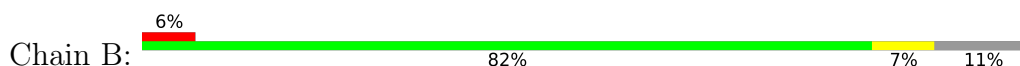
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike surface glycoprotein



- Molecule 1: Spike surface glycoprotein



LEU
LEU
ILE
LYS
ARG
MET
LYS
GLN
GLU
ASP
LYS
ILE
GLU
ILE
GLU
SER
LYS
GLN
LYS
ILE
GLU
ASN
GLU
ILE
ALA
ARG
ILE
LYS
LYS
LYS
LEU
VAL
PRO
ARG
GLY
SER
LEU
GLU
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- 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 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 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 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



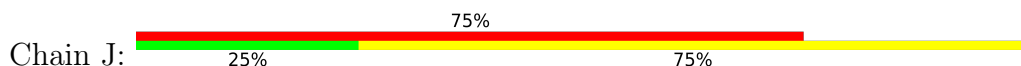
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



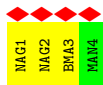
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



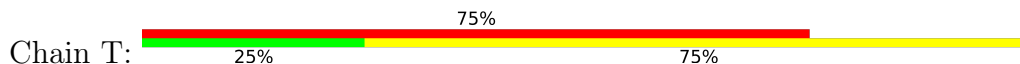
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



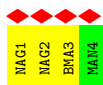
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



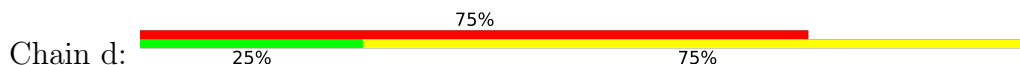
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





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



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



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



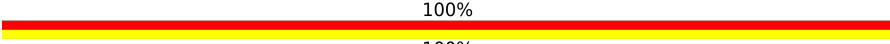
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

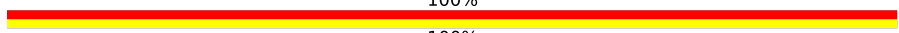


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%
100%



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

Chain f:  100%
100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	178356	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.030	Depositor
Minimum map value	-4.580	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	1	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.31	9/9359 (0.1%)	1.26	85/12744 (0.7%)
1	B	1.31	9/9359 (0.1%)	1.26	85/12744 (0.7%)
1	C	1.31	9/9359 (0.1%)	1.26	85/12744 (0.7%)
All	All	1.31	27/28077 (0.1%)	1.26	255/38232 (0.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	HIS	CB-CG	-7.81	1.39	1.50
1	A	215	HIS	CB-CG	-7.80	1.39	1.50
1	B	215	HIS	CB-CG	-7.80	1.39	1.50
1	B	444	ASN	CB-CG	-6.69	1.35	1.52
1	C	444	ASN	CB-CG	-6.69	1.35	1.52
1	A	444	ASN	CB-CG	-6.68	1.35	1.52
1	B	215	HIS	CG-CD2	-6.04	1.29	1.35
1	A	215	HIS	CG-CD2	-6.02	1.29	1.35
1	C	215	HIS	CG-CD2	-6.01	1.29	1.35
1	B	360	TRP	NE1-CE2	-5.91	1.30	1.37
1	A	360	TRP	NE1-CE2	-5.88	1.30	1.37
1	C	360	TRP	NE1-CE2	-5.86	1.31	1.37
1	A	348	TRP	NE1-CE2	-5.31	1.31	1.37
1	C	348	TRP	NE1-CE2	-5.31	1.31	1.37
1	B	348	TRP	NE1-CE2	-5.31	1.31	1.37
1	B	1128	LYS	CE-NZ	-5.12	1.33	1.49
1	C	173	GLN	CG-CD	-5.12	1.39	1.52
1	A	173	GLN	CG-CD	-5.11	1.39	1.52
1	A	1128	LYS	CE-NZ	-5.10	1.34	1.49
1	C	1128	LYS	CE-NZ	-5.10	1.34	1.49
1	B	173	GLN	CG-CD	-5.09	1.39	1.52
1	B	248	HIS	CB-CG	-5.05	1.43	1.50
1	A	460	TRP	NE1-CE2	-5.04	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	TRP	NE1-CE2	-5.03	1.31	1.37
1	C	248	HIS	CB-CG	-5.01	1.43	1.50
1	A	248	HIS	CB-CG	-5.00	1.43	1.50
1	C	460	TRP	NE1-CE2	-5.00	1.31	1.37

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	ASP	N-CA-C	10.11	127.61	113.56
1	C	893	ASP	N-CA-C	10.10	127.60	113.56
1	B	893	ASP	N-CA-C	10.09	127.58	113.56
1	B	134	THR	N-CA-C	-9.48	102.52	114.56
1	C	134	THR	N-CA-C	-9.47	102.53	114.56
1	A	134	THR	N-CA-C	-9.47	102.54	114.56
1	C	52	VAL	CA-CB-CG2	9.38	126.34	110.40
1	A	52	VAL	CA-CB-CG2	9.38	126.34	110.40
1	B	52	VAL	CA-CB-CG2	9.37	126.32	110.40
1	B	307	PRO	CA-C-N	8.50	128.37	120.21
1	B	307	PRO	C-N-CA	8.50	128.37	120.21
1	A	307	PRO	CA-C-N	8.48	128.35	120.21
1	A	307	PRO	C-N-CA	8.48	128.35	120.21
1	A	32	GLY	CA-C-N	8.47	129.10	120.38
1	A	32	GLY	C-N-CA	8.47	129.10	120.38
1	B	32	GLY	CA-C-N	8.45	129.09	120.38
1	B	32	GLY	C-N-CA	8.45	129.09	120.38
1	C	32	GLY	CA-C-N	8.45	129.08	120.38
1	C	32	GLY	C-N-CA	8.45	129.08	120.38
1	C	307	PRO	CA-C-N	8.45	128.32	120.21
1	C	307	PRO	C-N-CA	8.45	128.32	120.21
1	C	316	GLY	N-CA-C	8.26	128.19	114.48
1	A	316	GLY	N-CA-C	8.25	128.18	114.48
1	B	316	GLY	N-CA-C	8.21	128.11	114.48
1	A	1172	SER	CA-C-N	7.75	127.92	119.87
1	A	1172	SER	C-N-CA	7.75	127.92	119.87
1	B	1172	SER	CA-C-N	7.73	127.91	119.87
1	B	1172	SER	C-N-CA	7.73	127.91	119.87
1	C	1172	SER	CA-C-N	7.71	127.88	119.87
1	C	1172	SER	C-N-CA	7.71	127.88	119.87
1	A	960	PRO	CA-C-N	7.57	127.53	120.03
1	A	960	PRO	C-N-CA	7.57	127.53	120.03
1	B	960	PRO	CA-C-N	7.56	127.52	120.03
1	B	960	PRO	C-N-CA	7.56	127.52	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	960	PRO	CA-C-N	7.56	127.52	120.03
1	C	960	PRO	C-N-CA	7.56	127.52	120.03
1	B	1228	ALA	CA-C-N	7.31	127.47	119.87
1	B	1228	ALA	C-N-CA	7.31	127.47	119.87
1	C	1228	ALA	CA-C-N	7.30	127.46	119.87
1	C	1228	ALA	C-N-CA	7.30	127.46	119.87
1	A	18	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	1228	ALA	CA-C-N	7.26	127.42	119.87
1	A	1228	ALA	C-N-CA	7.26	127.42	119.87
1	B	18	ASP	CA-CB-CG	7.26	119.86	112.60
1	C	18	ASP	CA-CB-CG	7.25	119.86	112.60
1	B	122	PHE	CA-CB-CG	7.14	120.94	113.80
1	A	122	PHE	CA-CB-CG	7.12	120.92	113.80
1	C	122	PHE	CA-CB-CG	7.10	120.90	113.80
1	C	473	LYS	CA-C-N	7.07	127.64	120.14
1	C	473	LYS	C-N-CA	7.07	127.64	120.14
1	A	473	LYS	CA-C-N	7.05	127.62	120.14
1	A	473	LYS	C-N-CA	7.05	127.62	120.14
1	B	473	LYS	CA-C-N	7.05	127.62	120.14
1	B	473	LYS	C-N-CA	7.05	127.62	120.14
1	A	340	LEU	CA-C-N	7.04	127.00	120.03
1	A	340	LEU	C-N-CA	7.04	127.00	120.03
1	B	340	LEU	CA-C-N	7.03	126.99	120.03
1	B	340	LEU	C-N-CA	7.03	126.99	120.03
1	C	340	LEU	CA-C-N	7.01	126.97	120.03
1	C	340	LEU	C-N-CA	7.01	126.97	120.03
1	A	93	PRO	N-CA-C	-6.95	102.22	110.70
1	B	93	PRO	N-CA-C	-6.94	102.23	110.70
1	B	522	CYS	CA-C-N	6.94	126.90	120.03
1	B	522	CYS	C-N-CA	6.94	126.90	120.03
1	C	93	PRO	N-CA-C	-6.93	102.25	110.70
1	A	522	CYS	CA-C-N	6.92	126.88	120.03
1	A	522	CYS	C-N-CA	6.92	126.88	120.03
1	C	522	CYS	CA-C-N	6.89	126.85	120.03
1	C	522	CYS	C-N-CA	6.89	126.85	120.03
1	C	456	ASN	CA-C-N	6.84	126.99	119.87
1	C	456	ASN	C-N-CA	6.84	126.99	119.87
1	A	456	ASN	CA-C-N	6.83	126.97	119.87
1	A	456	ASN	C-N-CA	6.83	126.97	119.87
1	B	456	ASN	CA-C-N	6.79	126.93	119.87
1	B	456	ASN	C-N-CA	6.79	126.93	119.87
1	B	316	GLY	CA-C-N	-6.78	110.47	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	GLY	C-N-CA	-6.78	110.47	122.07
1	C	316	GLY	CA-C-N	-6.78	110.48	122.07
1	C	316	GLY	C-N-CA	-6.78	110.48	122.07
1	A	316	GLY	CA-C-N	-6.76	110.51	122.07
1	A	316	GLY	C-N-CA	-6.76	110.51	122.07
1	B	1138	GLY	N-CA-C	6.66	119.16	111.36
1	A	1138	GLY	N-CA-C	6.64	119.13	111.36
1	C	1138	GLY	N-CA-C	6.61	119.09	111.36
1	B	1171	VAL	N-CA-C	6.56	118.95	108.85
1	C	1171	VAL	N-CA-C	6.54	118.91	108.85
1	A	1171	VAL	N-CA-C	6.52	118.89	108.85
1	A	315	ASN	N-CA-C	6.50	120.64	110.17
1	C	315	ASN	N-CA-C	6.50	120.64	110.17
1	A	713	PHE	CA-CB-CG	-6.49	107.31	113.80
1	C	713	PHE	CA-CB-CG	-6.49	107.31	113.80
1	B	315	ASN	N-CA-C	6.48	120.61	110.17
1	B	713	PHE	CA-CB-CG	-6.48	107.32	113.80
1	B	990	VAL	CA-C-N	6.37	126.38	119.89
1	B	990	VAL	C-N-CA	6.37	126.38	119.89
1	A	990	VAL	CA-C-N	6.36	126.38	119.89
1	A	990	VAL	C-N-CA	6.36	126.38	119.89
1	C	990	VAL	CA-C-N	6.33	126.35	119.89
1	C	990	VAL	C-N-CA	6.33	126.35	119.89
1	B	461	ASN	CA-CB-CG	6.27	118.87	112.60
1	C	461	ASN	CA-CB-CG	6.25	118.85	112.60
1	A	461	ASN	CA-CB-CG	6.24	118.83	112.60
1	B	267	THR	CA-C-N	6.21	126.12	119.85
1	B	267	THR	C-N-CA	6.21	126.12	119.85
1	C	885	ASP	N-CA-C	-6.20	104.06	111.69
1	A	885	ASP	N-CA-C	-6.19	104.08	111.69
1	A	267	THR	CA-C-N	6.18	126.09	119.85
1	A	267	THR	C-N-CA	6.18	126.09	119.85
1	B	885	ASP	N-CA-C	-6.16	104.11	111.69
1	C	34	PRO	CA-C-N	6.14	126.11	119.78
1	C	34	PRO	C-N-CA	6.14	126.11	119.78
1	C	1162	VAL	N-CA-C	6.14	114.23	108.15
1	A	34	PRO	CA-C-N	6.13	126.10	119.78
1	A	34	PRO	C-N-CA	6.13	126.10	119.78
1	B	1162	VAL	N-CA-C	6.12	114.21	108.15
1	A	1162	VAL	N-CA-C	6.11	114.20	108.15
1	B	34	PRO	CA-C-N	6.11	126.08	119.78
1	B	34	PRO	C-N-CA	6.11	126.08	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	THR	CA-C-N	6.11	126.02	119.85
1	C	267	THR	C-N-CA	6.11	126.02	119.85
1	B	337	LYS	CA-C-N	6.03	126.22	120.31
1	B	337	LYS	C-N-CA	6.03	126.22	120.31
1	C	337	LYS	CA-C-N	5.99	126.18	120.31
1	C	337	LYS	C-N-CA	5.99	126.18	120.31
1	A	177	HIS	CA-C-N	5.98	126.41	119.47
1	A	177	HIS	C-N-CA	5.98	126.41	119.47
1	C	538	ASP	CA-C-N	5.98	125.60	119.56
1	C	538	ASP	C-N-CA	5.98	125.60	119.56
1	C	177	HIS	CA-C-N	5.97	126.40	119.47
1	C	177	HIS	C-N-CA	5.97	126.40	119.47
1	A	337	LYS	CA-C-N	5.97	126.16	120.31
1	A	337	LYS	C-N-CA	5.97	126.16	120.31
1	B	177	HIS	CA-C-N	5.97	126.39	119.47
1	B	177	HIS	C-N-CA	5.97	126.39	119.47
1	A	538	ASP	CA-C-N	5.95	125.57	119.56
1	A	538	ASP	C-N-CA	5.95	125.57	119.56
1	B	1056	LEU	N-CA-C	-5.95	105.68	113.12
1	A	1056	LEU	N-CA-C	-5.93	105.71	113.12
1	B	538	ASP	CA-C-N	5.93	125.55	119.56
1	B	538	ASP	C-N-CA	5.93	125.55	119.56
1	C	1056	LEU	N-CA-C	-5.91	105.73	113.12
1	C	722	GLN	CA-C-N	5.85	125.76	119.85
1	C	722	GLN	C-N-CA	5.85	125.76	119.85
1	B	1201	GLY	N-CA-C	-5.83	105.07	112.54
1	A	722	GLN	CA-C-N	5.83	125.74	119.85
1	A	722	GLN	C-N-CA	5.83	125.74	119.85
1	C	1201	GLY	N-CA-C	-5.83	105.08	112.54
1	A	1201	GLY	N-CA-C	-5.82	105.08	112.54
1	B	722	GLN	CA-C-N	5.81	125.72	119.85
1	B	722	GLN	C-N-CA	5.81	125.72	119.85
1	C	698	GLU	CA-C-N	5.75	125.95	120.31
1	C	698	GLU	C-N-CA	5.75	125.95	120.31
1	A	59	ASN	CA-CB-CG	5.75	118.35	112.60
1	B	959	LEU	CA-C-N	5.74	123.79	119.66
1	B	959	LEU	C-N-CA	5.74	123.79	119.66
1	C	959	LEU	CA-C-N	5.74	123.79	119.66
1	C	959	LEU	C-N-CA	5.74	123.79	119.66
1	C	59	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	698	GLU	CA-C-N	5.72	125.92	120.31
1	A	698	GLU	C-N-CA	5.72	125.92	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	GLU	CA-C-N	5.72	125.91	120.31
1	B	698	GLU	C-N-CA	5.72	125.91	120.31
1	C	494	ALA	CA-C-N	5.71	125.69	120.03
1	C	494	ALA	C-N-CA	5.71	125.69	120.03
1	B	59	ASN	CA-CB-CG	5.71	118.31	112.60
1	B	494	ALA	CA-C-N	5.71	125.69	120.03
1	B	494	ALA	C-N-CA	5.71	125.69	120.03
1	A	494	ALA	CA-C-N	5.70	125.67	120.03
1	A	494	ALA	C-N-CA	5.70	125.67	120.03
1	A	959	LEU	CA-C-N	5.69	123.75	119.66
1	A	959	LEU	C-N-CA	5.69	123.75	119.66
1	A	397	MET	N-CA-C	5.62	118.80	110.48
1	C	397	MET	N-CA-C	5.61	118.78	110.48
1	B	397	MET	N-CA-C	5.59	118.75	110.48
1	B	171	TYR	CA-C-N	5.59	125.35	119.76
1	B	171	TYR	C-N-CA	5.59	125.35	119.76
1	A	171	TYR	CA-C-N	5.58	125.34	119.76
1	A	171	TYR	C-N-CA	5.58	125.34	119.76
1	C	1137	CYS	N-CA-C	-5.55	101.44	110.20
1	A	1137	CYS	N-CA-C	-5.54	101.44	110.20
1	C	780	GLU	CA-C-N	5.53	125.15	119.56
1	C	780	GLU	C-N-CA	5.53	125.15	119.56
1	C	171	TYR	CA-C-N	5.52	125.28	119.76
1	C	171	TYR	C-N-CA	5.52	125.28	119.76
1	B	1137	CYS	N-CA-C	-5.52	101.48	110.20
1	A	780	GLU	CA-C-N	5.51	125.12	119.56
1	A	780	GLU	C-N-CA	5.51	125.12	119.56
1	B	874	MET	N-CA-C	5.47	120.05	112.45
1	C	874	MET	N-CA-C	5.46	120.05	112.45
1	A	874	MET	N-CA-C	5.46	120.04	112.45
1	B	780	GLU	CA-C-N	5.46	125.07	119.56
1	B	780	GLU	C-N-CA	5.46	125.07	119.56
1	C	68	TYR	CA-C-N	5.42	125.40	120.03
1	C	68	TYR	C-N-CA	5.42	125.40	120.03
1	A	68	TYR	CA-C-N	5.42	125.39	120.03
1	A	68	TYR	C-N-CA	5.42	125.39	120.03
1	B	68	TYR	CA-C-N	5.41	125.39	120.03
1	B	68	TYR	C-N-CA	5.41	125.39	120.03
1	C	306	ALA	CA-C-N	5.41	125.95	120.38
1	C	306	ALA	C-N-CA	5.41	125.95	120.38
1	B	1223	VAL	N-CA-C	5.41	117.85	111.09
1	A	306	ALA	CA-C-N	5.40	125.94	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ALA	C-N-CA	5.40	125.94	120.38
1	A	1223	VAL	N-CA-C	5.40	117.84	111.09
1	C	1223	VAL	N-CA-C	5.40	117.84	111.09
1	B	548	CYS	N-CA-C	-5.38	103.35	110.40
1	A	548	CYS	N-CA-C	-5.37	103.36	110.40
1	C	548	CYS	N-CA-C	-5.37	103.37	110.40
1	C	422	LEU	CA-C-N	-5.36	115.90	122.75
1	C	422	LEU	C-N-CA	-5.36	115.90	122.75
1	B	306	ALA	CA-C-N	5.34	125.88	120.38
1	B	306	ALA	C-N-CA	5.34	125.88	120.38
1	A	422	LEU	CA-C-N	-5.33	115.92	122.75
1	A	422	LEU	C-N-CA	-5.33	115.92	122.75
1	B	422	LEU	CA-C-N	-5.33	115.93	122.75
1	B	422	LEU	C-N-CA	-5.33	115.93	122.75
1	B	328	GLN	CA-C-N	5.30	125.22	119.76
1	B	328	GLN	C-N-CA	5.30	125.22	119.76
1	C	328	GLN	CA-C-N	5.28	125.20	119.76
1	C	328	GLN	C-N-CA	5.28	125.20	119.76
1	B	486	VAL	N-CA-C	5.27	115.89	108.36
1	A	328	GLN	CA-C-N	5.27	125.18	119.76
1	A	328	GLN	C-N-CA	5.27	125.18	119.76
1	A	486	VAL	N-CA-C	5.26	115.89	108.36
1	B	614	CYS	N-CA-C	5.26	117.82	109.50
1	A	444	ASN	N-CA-C	5.26	118.13	109.72
1	C	444	ASN	N-CA-C	5.26	118.13	109.72
1	A	614	CYS	N-CA-C	5.25	117.80	109.50
1	C	486	VAL	N-CA-C	5.25	115.87	108.36
1	C	614	CYS	N-CA-C	5.25	117.79	109.50
1	A	548	CYS	CB-CA-C	5.24	117.00	109.09
1	B	548	CYS	CB-CA-C	5.24	117.00	109.09
1	B	444	ASN	N-CA-C	5.24	118.10	109.72
1	C	548	CYS	CB-CA-C	5.21	116.96	109.09
1	C	101	ASN	N-CA-C	-5.21	107.05	113.41
1	B	101	ASN	N-CA-C	-5.18	107.09	113.41
1	A	101	ASN	N-CA-C	-5.17	107.10	113.41
1	A	656	GLN	N-CA-C	5.16	116.94	108.52
1	C	422	LEU	CB-CA-C	-5.16	104.47	111.95
1	A	422	LEU	CB-CA-C	-5.16	104.47	111.95
1	B	422	LEU	CB-CA-C	-5.15	104.48	111.95
1	B	656	GLN	N-CA-C	5.15	116.91	108.52
1	C	656	GLN	N-CA-C	5.14	116.90	108.52
1	B	1080	ALA	N-CA-C	5.14	116.88	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	ALA	N-CA-C	5.13	116.87	111.28
1	C	1080	ALA	N-CA-C	5.10	116.84	111.28
1	A	38	THR	N-CA-C	-5.05	106.96	113.23
1	C	1218	MET	CB-CA-C	5.05	119.35	109.35
1	A	1218	MET	CB-CA-C	5.05	119.34	109.35
1	B	38	THR	N-CA-C	-5.05	106.97	113.23
1	C	38	THR	N-CA-C	-5.04	106.98	113.23
1	B	1218	MET	CB-CA-C	5.03	119.32	109.35
1	B	180	LEU	N-CA-C	-5.03	105.89	112.23
1	A	180	LEU	N-CA-C	-5.01	105.92	112.23
1	C	180	LEU	N-CA-C	-5.00	105.92	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9150	0	8848	23	0
1	B	9150	0	8848	20	0
1	C	9150	0	8848	19	0
2	D	39	0	34	0	0
2	E	39	0	34	0	0
2	G	39	0	34	0	0
2	H	39	0	34	1	0
2	M	39	0	34	0	0
2	N	39	0	34	0	0
2	O	39	0	34	0	0
2	Q	39	0	34	0	0
2	R	39	0	34	0	0
2	W	39	0	34	0	0
2	X	39	0	34	0	0
2	Y	39	0	34	0	0
2	a	39	0	34	0	0
2	b	39	0	34	0	0
2	g	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	50	0	43	0	0
3	J	50	0	43	0	0
3	P	50	0	43	0	0
3	T	50	0	43	0	0
3	Z	50	0	43	0	0
3	d	50	0	43	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	c	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
5	A	70	0	65	1	0
5	B	70	0	65	1	0
5	C	70	0	65	1	0
6	A	25	0	0	0	0
6	B	25	0	0	0	0
6	C	25	0	0	0	0
7	A	132	0	0	5	0
7	B	132	0	0	5	0
7	C	132	0	0	5	0
All	All	29268	0	27732	56	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 1.

All (56) 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:C:190:LEU:HD12	7:C:5043:HOH:O	1.62	1.00
1:A:190:LEU:HD12	7:A:5043:HOH:O	1.62	0.98
1:B:190:LEU:HD12	7:B:5043:HOH:O	1.62	0.98
1:A:190:LEU:HA	7:A:5043:HOH:O	1.77	0.84
1:C:190:LEU:HA	7:C:5043:HOH:O	1.77	0.83
1:B:190:LEU:HA	7:B:5043:HOH:O	1.77	0.82
1:B:1059:GLN:NE2	1:C:846:SER:OG	2.28	0.67
1:A:846:SER:OG	1:C:1059:GLN:NE2	2.28	0.67
1:A:1059:GLN:NE2	1:B:846:SER:OG	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:O	7:A:5057:HOH:O	2.14	0.65
1:C:687:ARG:O	7:C:5057:HOH:O	2.14	0.64
1:B:687:ARG:O	7:B:5057:HOH:O	2.14	0.64
1:A:1019:ASN:HB3	7:A:5129:HOH:O	2.05	0.57
1:C:1019:ASN:HB3	7:C:5129:HOH:O	2.05	0.56
1:B:1019:ASN:HB3	7:B:5129:HOH:O	2.05	0.56
1:B:229:ASP:OD1	1:B:229:ASP:N	2.41	0.53
1:A:229:ASP:OD1	1:A:229:ASP:N	2.41	0.52
1:B:821:LYS:NZ	1:B:863:ASP:OD2	2.40	0.49
1:C:229:ASP:OD1	1:C:229:ASP:N	2.41	0.49
1:C:897:SER:N	1:C:898:PRO:CD	2.78	0.47
1:A:897:SER:N	1:A:898:PRO:CD	2.78	0.46
1:A:552:LYS:NZ	1:B:619:GLN:OE1	2.49	0.46
1:B:897:SER:N	1:B:898:PRO:CD	2.78	0.46
1:A:619:GLN:OE1	1:C:552:LYS:NZ	2.49	0.46
1:B:552:LYS:NZ	1:C:619:GLN:OE1	2.49	0.45
1:A:385:THR:HG22	7:A:5069:HOH:O	2.16	0.45
1:C:385:THR:HG22	7:C:5069:HOH:O	2.16	0.45
1:A:129:SER:OG	1:A:130:THR:N	2.49	0.45
1:A:821:LYS:NZ	1:A:863:ASP:OD2	2.40	0.45
1:B:155:LEU:HD21	5:B:3198:NAG:H82	2.00	0.44
1:B:385:THR:HG22	7:B:5069:HOH:O	2.16	0.43
1:A:155:LEU:HD21	5:A:3198:NAG:H82	2.00	0.43
1:A:739:ASN:OD1	1:A:739:ASN:C	2.60	0.43
1:C:155:LEU:HD21	5:C:3198:NAG:H82	2.00	0.43
1:B:928:ASP:N	1:B:928:ASP:OD1	2.52	0.43
1:C:129:SER:OG	1:C:130:THR:N	2.49	0.43
1:C:161:VAL:HG11	1:C:238:PHE:CE2	2.54	0.42
1:B:161:VAL:HG11	1:B:238:PHE:CE2	2.54	0.42
1:A:161:VAL:HG11	1:A:238:PHE:CE2	2.54	0.42
1:A:661:ASP:C	1:A:661:ASP:OD1	2.63	0.42
1:A:1211:THR:OG1	1:A:1212:GLU:N	2.53	0.42
1:B:1131:SER:OG	1:B:1132:SER:N	2.52	0.42
1:A:1131:SER:OG	1:A:1132:SER:N	2.52	0.42
1:B:661:ASP:OD1	1:B:661:ASP:C	2.63	0.42
1:A:928:ASP:OD1	1:A:928:ASP:N	2.52	0.41
1:C:803:PRO:HB3	1:C:1163:PRO:HB3	2.03	0.41
1:A:634:ASP:C	1:A:634:ASP:OD1	2.64	0.41
1:C:928:ASP:OD1	1:C:928:ASP:N	2.52	0.41
1:C:1211:THR:OG1	1:C:1212:GLU:N	2.53	0.41
1:C:634:ASP:C	1:C:634:ASP:OD1	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:PRO:HB3	1:A:1163:PRO:HB3	2.03	0.41
1:B:803:PRO:HB3	1:B:1163:PRO:HB3	2.03	0.41
1:B:1211:THR:OG1	1:B:1212:GLU:N	2.53	0.41
1:C:739:ASN:OD1	1:C:739:ASN:C	2.61	0.41
1:B:739:ASN:OD1	1:B:739:ASN:C	2.60	0.40
1:A:446:PRO:HG2	2:H:1:NAG:H82	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
1	B	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
1	C	1163/1322 (88%)	1143 (98%)	19 (2%)	1 (0%)	48	77
All	All	3489/3966 (88%)	3429 (98%)	57 (2%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	875	ASN
1	B	875	ASN
1	C	875	ASN

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1022/1151 (89%)	1018 (100%)	4 (0%)	84	94
1	B	1022/1151 (89%)	1018 (100%)	4 (0%)	84	94
1	C	1022/1151 (89%)	1018 (100%)	4 (0%)	84	94
All	All	3066/3453 (89%)	3054 (100%)	12 (0%)	81	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	59	ASN
1	A	720	GLN
1	A	1224	ASN
1	B	19	LEU
1	B	59	ASN
1	B	720	GLN
1	B	1224	ASN
1	C	19	LEU
1	C	59	ASN
1	C	720	GLN
1	C	1224	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	183	HIS
1	A	248	HIS
1	A	388	ASN
1	A	440	GLN
1	A	602	ASN
1	A	653	ASN
1	A	778	ASN
1	A	871	ASN
1	A	875	ASN
1	A	951	GLN
1	A	1049	ASN
1	A	1059	GLN
1	B	65	ASN
1	B	183	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	248	HIS
1	B	388	ASN
1	B	440	GLN
1	B	602	ASN
1	B	653	ASN
1	B	778	ASN
1	B	871	ASN
1	B	875	ASN
1	B	951	GLN
1	B	1049	ASN
1	B	1059	GLN
1	B	1092	ASN
1	C	182	ASN
1	C	183	HIS
1	C	248	HIS
1	C	388	ASN
1	C	440	GLN
1	C	602	ASN
1	C	653	ASN
1	C	778	ASN
1	C	850	ASN
1	C	871	ASN
1	C	875	ASN
1	C	951	GLN
1	C	1049	ASN
1	C	1059	GLN
1	C	1104	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

87 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	1,2	14,14,15	0.66	0	17,19,21	0.86	1 (5%)
2	NAG	D	2	2	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	NAG	E	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.72	0	17,19,21	1.20	2 (11%)
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	F	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	F	2	3	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
3	BMA	F	3	3	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	0.80	1 (6%)
2	NAG	G	1	1,2	14,14,15	0.65	0	17,19,21	1.23	3 (17%)
2	NAG	G	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	G	3	2	11,11,12	0.59	0	15,15,17	0.74	0
2	NAG	H	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	0.79	1 (5%)
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	1.43	3 (17%)
2	BMA	H	3	2	11,11,12	0.70	0	15,15,17	0.75	0
4	NAG	I	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	I	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	J	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	J	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.04	1 (6%)
3	MAN	J	4	3	11,11,12	0.70	0	15,15,17	0.77	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	0.79	0
4	NAG	K	2	4	14,14,15	0.81	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	L	1	1,4	14,14,15	0.79	1 (7%)	17,19,21	0.94	2 (11%)
4	NAG	L	2	4	14,14,15	0.99	1 (7%)	17,19,21	0.75	0
2	NAG	M	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	1.39	3 (17%)
2	NAG	M	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	M	3	2	11,11,12	0.72	0	15,15,17	0.68	0
2	NAG	N	1	1,2	14,14,15	0.66	0	17,19,21	0.85	1 (5%)
2	NAG	N	2	2	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	N	3	2	11,11,12	0.69	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	0.87	0
2	NAG	O	2	2	14,14,15	0.73	0	17,19,21	1.20	2 (11%)
2	BMA	O	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	P	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	P	2	3	14,14,15	0.81	0	17,19,21	1.53	2 (11%)
3	BMA	P	3	3	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
3	MAN	P	4	3	11,11,12	0.72	0	15,15,17	0.79	0
2	NAG	Q	1	1,2	14,14,15	0.65	0	17,19,21	1.23	3 (17%)
2	NAG	Q	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	Q	3	2	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	R	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	R	2	2	14,14,15	0.85	0	17,19,21	1.44	3 (17%)
2	BMA	R	3	2	11,11,12	0.71	0	15,15,17	0.75	0
4	NAG	S	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	S	2	4	14,14,15	0.78	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	T	1	1,3	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	T	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	T	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.04	1 (6%)
3	MAN	T	4	3	11,11,12	0.71	0	15,15,17	0.77	1 (6%)
4	NAG	U	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	0.79	0
4	NAG	U	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	V	1	1,4	14,14,15	0.79	1 (7%)	17,19,21	0.94	2 (11%)
4	NAG	V	2	4	14,14,15	1.00	1 (7%)	17,19,21	0.74	0
2	NAG	W	1	1,2	14,14,15	0.68	0	17,19,21	1.39	3 (17%)
2	NAG	W	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	W	3	2	11,11,12	0.72	0	15,15,17	0.68	0
2	NAG	X	1	1,2	14,14,15	0.66	0	17,19,21	0.86	1 (5%)
2	NAG	X	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	X	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	NAG	Y	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	0.86	0
2	NAG	Y	2	2	14,14,15	0.73	0	17,19,21	1.20	2 (11%)
2	BMA	Y	3	2	11,11,12	0.68	0	15,15,17	0.75	0
3	NAG	Z	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	Z	2	3	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
3	BMA	Z	3	3	11,11,12	0.67	0	15,15,17	0.94	1 (6%)
3	MAN	Z	4	3	11,11,12	0.73	0	15,15,17	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	a	1	1,2	14,14,15	0.65	0	17,19,21	1.24	3 (17%)
2	NAG	a	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	a	3	2	11,11,12	0.58	0	15,15,17	0.74	0
2	NAG	b	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	b	2	2	14,14,15	0.86	0	17,19,21	1.43	3 (17%)
2	BMA	b	3	2	11,11,12	0.71	0	15,15,17	0.75	0
4	NAG	c	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.31	2 (11%)
4	NAG	c	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	d	1	1,3	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	d	2	3	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
3	BMA	d	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.05	1 (6%)
3	MAN	d	4	3	11,11,12	0.72	0	15,15,17	0.76	1 (6%)
4	NAG	e	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	0.79	0
4	NAG	e	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	f	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	0.93	2 (11%)
4	NAG	f	2	4	14,14,15	0.99	1 (7%)	17,19,21	0.75	0
2	NAG	g	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	1.39	3 (17%)
2	NAG	g	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
2	BMA	g	3	2	11,11,12	0.71	0	15,15,17	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2	NAG	C1-C2	3.34	1.56	1.52
4	f	2	NAG	C1-C2	3.30	1.56	1.52
4	L	2	NAG	C1-C2	3.30	1.56	1.52
2	a	2	NAG	C1-C2	2.75	1.56	1.52
2	Q	2	NAG	C1-C2	2.74	1.56	1.52
2	G	2	NAG	C1-C2	2.74	1.56	1.52
2	b	1	NAG	C1-C2	2.68	1.56	1.52
2	R	1	NAG	C1-C2	2.66	1.56	1.52
4	K	2	NAG	C1-C2	2.66	1.56	1.52
2	H	1	NAG	C1-C2	2.65	1.56	1.52
4	U	2	NAG	C1-C2	2.63	1.55	1.52
4	e	2	NAG	C1-C2	2.63	1.55	1.52
4	c	1	NAG	C1-C2	2.58	1.55	1.52
3	Z	1	NAG	C1-C2	2.58	1.55	1.52
4	I	1	NAG	C1-C2	2.58	1.55	1.52
4	S	1	NAG	C1-C2	2.57	1.55	1.52
3	F	1	NAG	C1-C2	2.56	1.55	1.52
3	P	1	NAG	C1-C2	2.56	1.55	1.52
4	S	2	NAG	C1-C2	2.54	1.55	1.52
4	I	2	NAG	C1-C2	2.51	1.55	1.52
4	c	2	NAG	C1-C2	2.51	1.55	1.52
2	W	2	NAG	C1-C2	2.42	1.55	1.52
2	M	2	NAG	C1-C2	2.41	1.55	1.52
2	g	2	NAG	C1-C2	2.40	1.55	1.52
2	N	2	NAG	C1-C2	2.40	1.55	1.52
2	Y	1	NAG	C1-C2	2.39	1.55	1.52
2	O	1	NAG	C1-C2	2.39	1.55	1.52
4	V	1	NAG	C1-C2	2.39	1.55	1.52
2	D	2	NAG	C1-C2	2.38	1.55	1.52
4	L	1	NAG	C1-C2	2.38	1.55	1.52
2	E	1	NAG	C1-C2	2.37	1.55	1.52
2	X	2	NAG	C1-C2	2.35	1.55	1.52
4	f	1	NAG	C1-C2	2.30	1.55	1.52
4	U	1	NAG	C1-C2	2.15	1.55	1.52
3	T	3	BMA	C1-C2	2.14	1.57	1.52
3	d	3	BMA	C1-C2	2.12	1.57	1.52
4	K	1	NAG	C1-C2	2.12	1.55	1.52
4	e	1	NAG	C1-C2	2.12	1.55	1.52
3	J	3	BMA	C1-C2	2.10	1.57	1.52
2	g	1	NAG	C1-C2	2.02	1.55	1.52
2	M	1	NAG	C1-C2	2.01	1.55	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	2	NAG	C4-C3-C2	-4.36	104.63	111.02
3	P	2	NAG	C4-C3-C2	-4.36	104.63	111.02
3	F	2	NAG	C4-C3-C2	-4.35	104.64	111.02
2	W	1	NAG	C3-C4-C5	-3.57	103.76	110.23
2	M	1	NAG	C3-C4-C5	-3.57	103.77	110.23
4	c	1	NAG	C1-O5-C5	-3.57	107.41	112.19
2	g	1	NAG	C3-C4-C5	-3.56	103.77	110.23
4	I	1	NAG	C1-O5-C5	-3.55	107.42	112.19
4	S	1	NAG	C1-O5-C5	-3.55	107.43	112.19
2	a	1	NAG	C1-C2-N2	-3.18	105.43	110.43
2	G	1	NAG	C1-C2-N2	-3.14	105.48	110.43
2	Q	1	NAG	C1-C2-N2	-3.13	105.50	110.43
2	M	1	NAG	C4-C3-C2	3.05	115.49	111.02
3	Z	3	BMA	C2-C3-C4	-3.04	105.51	110.86
2	g	1	NAG	C4-C3-C2	3.04	115.48	111.02
2	W	1	NAG	C4-C3-C2	3.04	115.47	111.02
3	F	3	BMA	C2-C3-C4	-3.02	105.55	110.86
3	P	3	BMA	C2-C3-C4	-3.02	105.55	110.86
2	H	2	NAG	C3-C4-C5	-2.91	104.96	110.23
2	R	2	NAG	C3-C4-C5	-2.90	104.97	110.23
2	b	2	NAG	C3-C4-C5	-2.90	104.98	110.23
3	d	3	BMA	C2-C3-C4	-2.87	105.81	110.86
3	J	3	BMA	C2-C3-C4	-2.86	105.84	110.86
3	T	3	BMA	C2-C3-C4	-2.85	105.85	110.86
2	R	2	NAG	O4-C4-C3	2.70	116.75	110.38
2	H	2	NAG	O4-C4-C3	2.70	116.74	110.38
2	b	2	NAG	O4-C4-C3	2.70	116.74	110.38
2	M	2	NAG	C3-C4-C5	-2.62	105.48	110.23
2	g	2	NAG	C3-C4-C5	-2.62	105.48	110.23
4	e	2	NAG	C4-C3-C2	-2.61	107.20	111.02
2	W	2	NAG	C3-C4-C5	-2.60	105.51	110.23
2	W	2	NAG	O4-C4-C3	2.60	116.50	110.38
2	g	2	NAG	O4-C4-C3	2.59	116.48	110.38
4	U	2	NAG	C4-C3-C2	-2.59	107.22	111.02
3	P	2	NAG	O4-C4-C3	2.59	116.48	110.38
4	K	2	NAG	C4-C3-C2	-2.59	107.22	111.02
2	M	2	NAG	O4-C4-C3	2.58	116.47	110.38
3	F	2	NAG	O4-C4-C3	2.58	116.45	110.38
3	Z	2	NAG	O4-C4-C3	2.56	116.42	110.38
2	a	1	NAG	C3-C4-C5	-2.54	105.62	110.23
2	G	1	NAG	C3-C4-C5	-2.54	105.63	110.23
2	Q	1	NAG	C3-C4-C5	-2.53	105.65	110.23
4	f	1	NAG	C3-C4-C5	-2.45	105.78	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1	NAG	C3-C4-C5	-2.45	105.79	110.23
4	L	1	NAG	C3-C4-C5	-2.45	105.80	110.23
4	c	2	NAG	C4-C3-C2	-2.45	107.43	111.02
4	S	2	NAG	C4-C3-C2	-2.44	107.44	111.02
2	g	1	NAG	O4-C4-C3	-2.43	104.64	110.38
4	I	2	NAG	C4-C3-C2	-2.43	107.46	111.02
2	M	1	NAG	O4-C4-C3	-2.42	104.68	110.38
2	W	1	NAG	O4-C4-C3	-2.41	104.69	110.38
2	Q	2	NAG	C3-C4-C5	-2.38	105.91	110.23
2	G	2	NAG	C3-C4-C5	-2.38	105.91	110.23
4	c	1	NAG	C3-C4-C5	-2.37	105.93	110.23
4	S	1	NAG	C3-C4-C5	-2.37	105.93	110.23
2	R	2	NAG	O3-C3-C2	-2.37	104.48	109.40
4	I	1	NAG	C3-C4-C5	-2.37	105.94	110.23
2	a	2	NAG	C3-C4-C5	-2.37	105.94	110.23
2	H	2	NAG	O3-C3-C2	-2.37	104.48	109.40
3	T	2	NAG	C3-C4-C5	-2.36	105.94	110.23
3	P	1	NAG	C3-C4-C5	-2.36	105.96	110.23
2	b	2	NAG	O3-C3-C2	-2.35	104.51	109.40
3	J	2	NAG	C3-C4-C5	-2.35	105.97	110.23
3	d	2	NAG	C3-C4-C5	-2.35	105.97	110.23
3	F	1	NAG	C3-C4-C5	-2.34	105.98	110.23
2	N	2	NAG	C3-C4-C5	-2.34	105.99	110.23
3	Z	1	NAG	C3-C4-C5	-2.33	106.01	110.23
2	D	2	NAG	C3-C4-C5	-2.33	106.02	110.23
2	X	2	NAG	C3-C4-C5	-2.30	106.06	110.23
2	b	1	NAG	C3-C4-C5	-2.29	106.07	110.23
2	H	1	NAG	C3-C4-C5	-2.28	106.09	110.23
2	R	1	NAG	C3-C4-C5	-2.28	106.09	110.23
3	F	1	NAG	C1-O5-C5	-2.28	109.13	112.19
3	P	1	NAG	C1-O5-C5	-2.27	109.14	112.19
4	V	1	NAG	C1-O5-C5	2.26	115.21	112.19
3	Z	1	NAG	C1-O5-C5	-2.25	109.17	112.19
4	L	1	NAG	C1-O5-C5	2.25	115.20	112.19
2	Q	1	NAG	C1-O5-C5	-2.25	109.17	112.19
2	G	1	NAG	C1-O5-C5	-2.24	109.18	112.19
4	f	1	NAG	C1-O5-C5	2.23	115.18	112.19
2	a	1	NAG	C1-O5-C5	-2.23	109.20	112.19
2	Y	2	NAG	C4-C3-C2	-2.16	107.86	111.02
2	E	2	NAG	C4-C3-C2	-2.14	107.89	111.02
2	O	2	NAG	C4-C3-C2	-2.10	107.94	111.02
2	D	1	NAG	C3-C4-C5	-2.08	106.46	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1	NAG	C3-C4-C5	-2.08	106.46	110.23
2	N	1	NAG	C3-C4-C5	-2.07	106.48	110.23
3	J	4	MAN	C2-C3-C4	-2.05	107.26	110.86
3	T	4	MAN	C2-C3-C4	-2.04	107.28	110.86
2	D	2	NAG	C4-C3-C2	-2.04	108.03	111.02
3	d	4	MAN	C2-C3-C4	-2.04	107.28	110.86
2	O	2	NAG	C3-C4-C5	-2.03	106.55	110.23
2	X	2	NAG	C4-C3-C2	-2.03	108.05	111.02
2	Y	2	NAG	C3-C4-C5	-2.02	106.57	110.23
3	F	4	MAN	C2-C3-C4	-2.02	107.31	110.86
2	N	2	NAG	C4-C3-C2	-2.01	108.07	111.02
2	E	2	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	X	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
3	d	4	MAN	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	P	3	BMA	O5-C5-C6-O6
3	Z	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

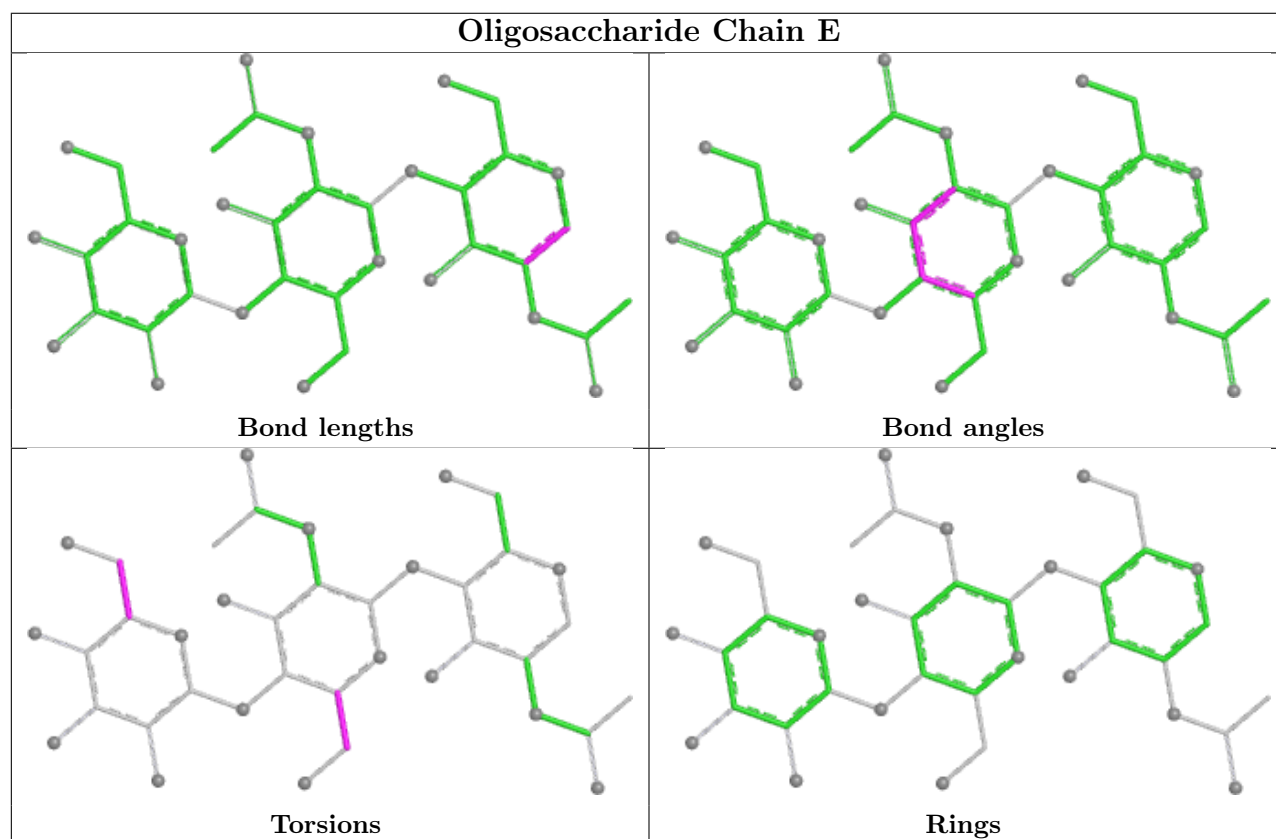
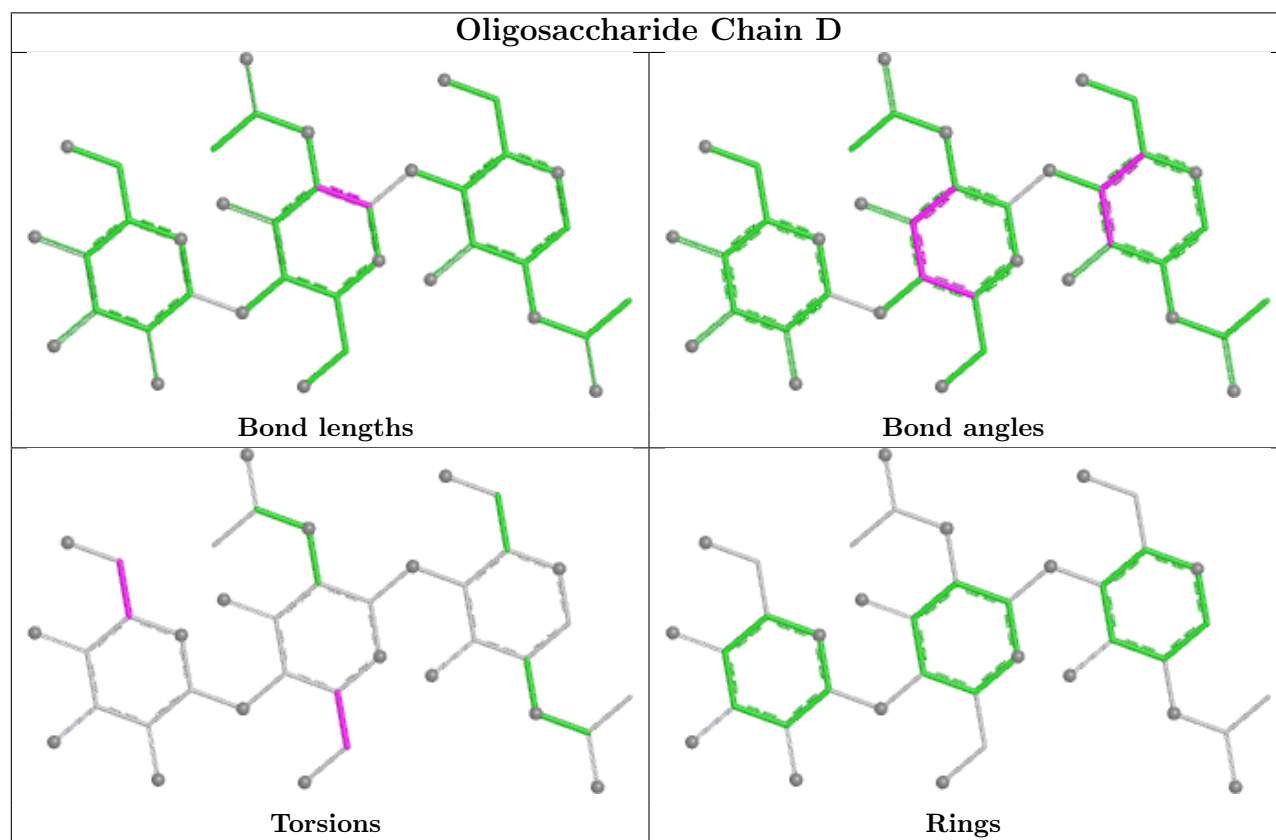
Mol	Chain	Res	Type	Atoms
2	G	3	BMA	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
2	W	3	BMA	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	g	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	P	4	MAN	O5-C5-C6-O6
3	Z	4	MAN	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	T	3	BMA	O5-C5-C6-O6
3	d	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	X	3	BMA	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	d	4	MAN	C4-C5-C6-O6
3	T	4	MAN	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6

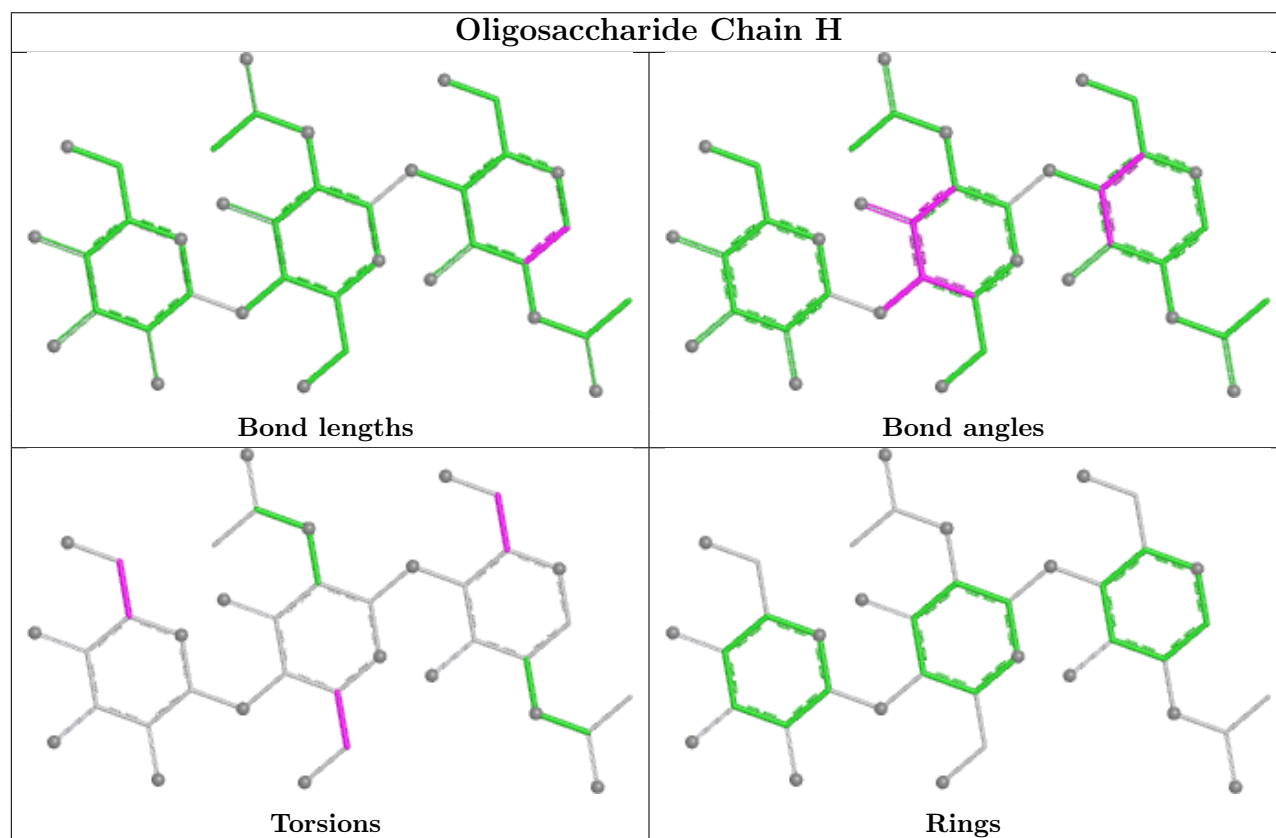
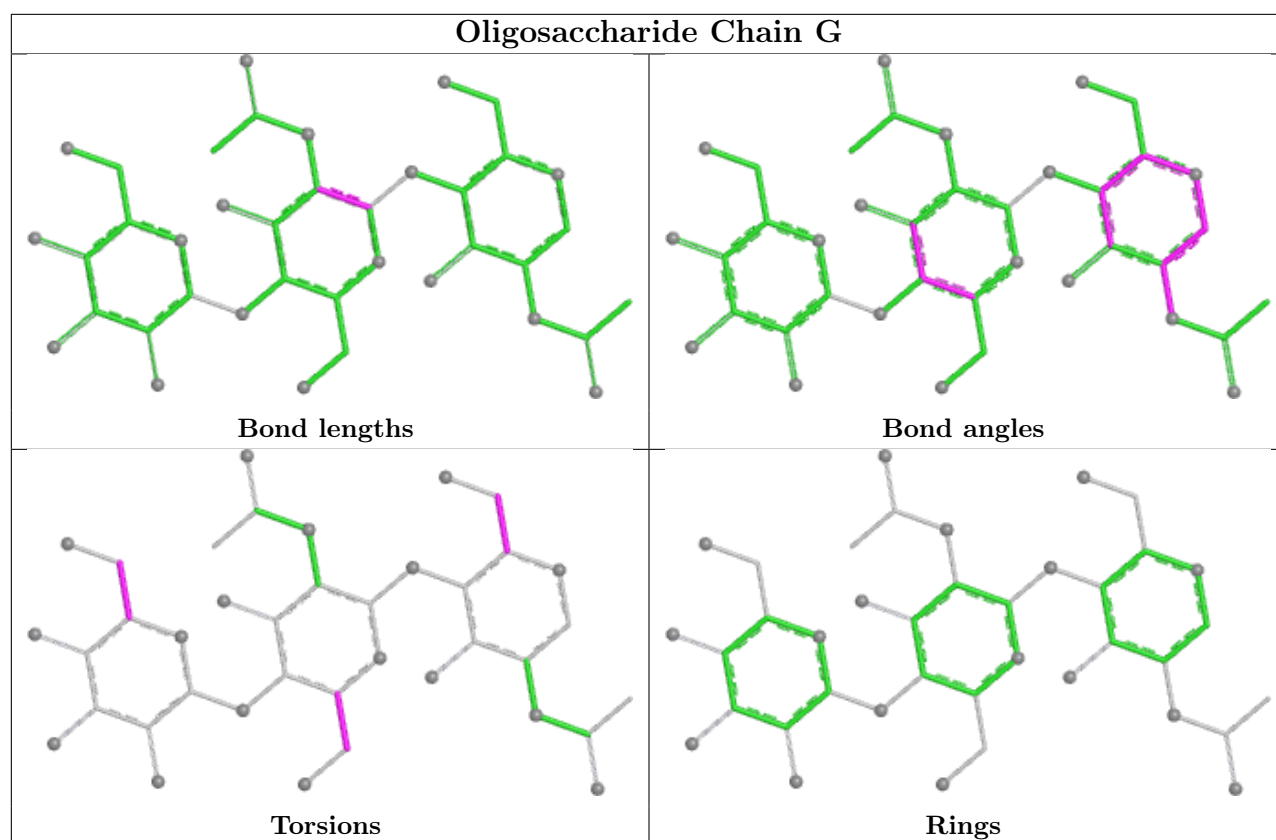
There are no ring outliers.

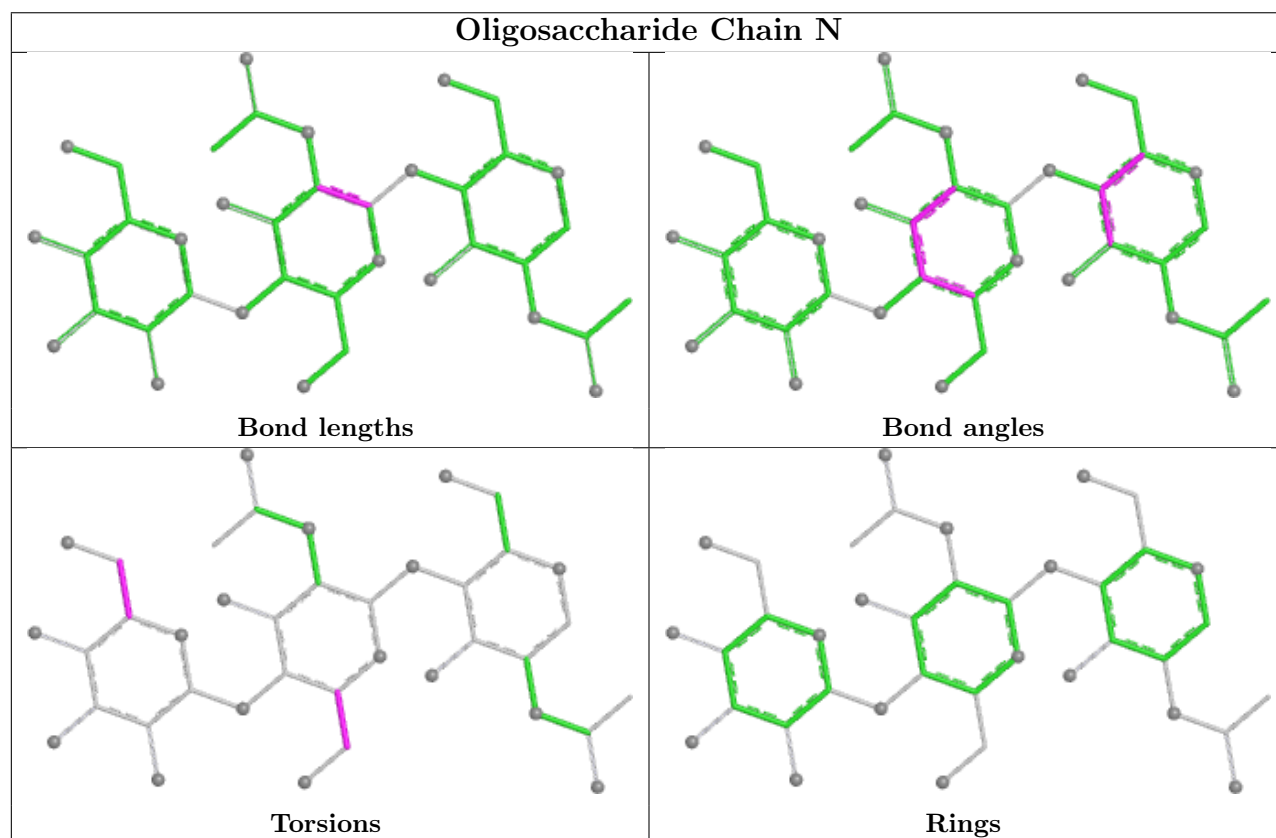
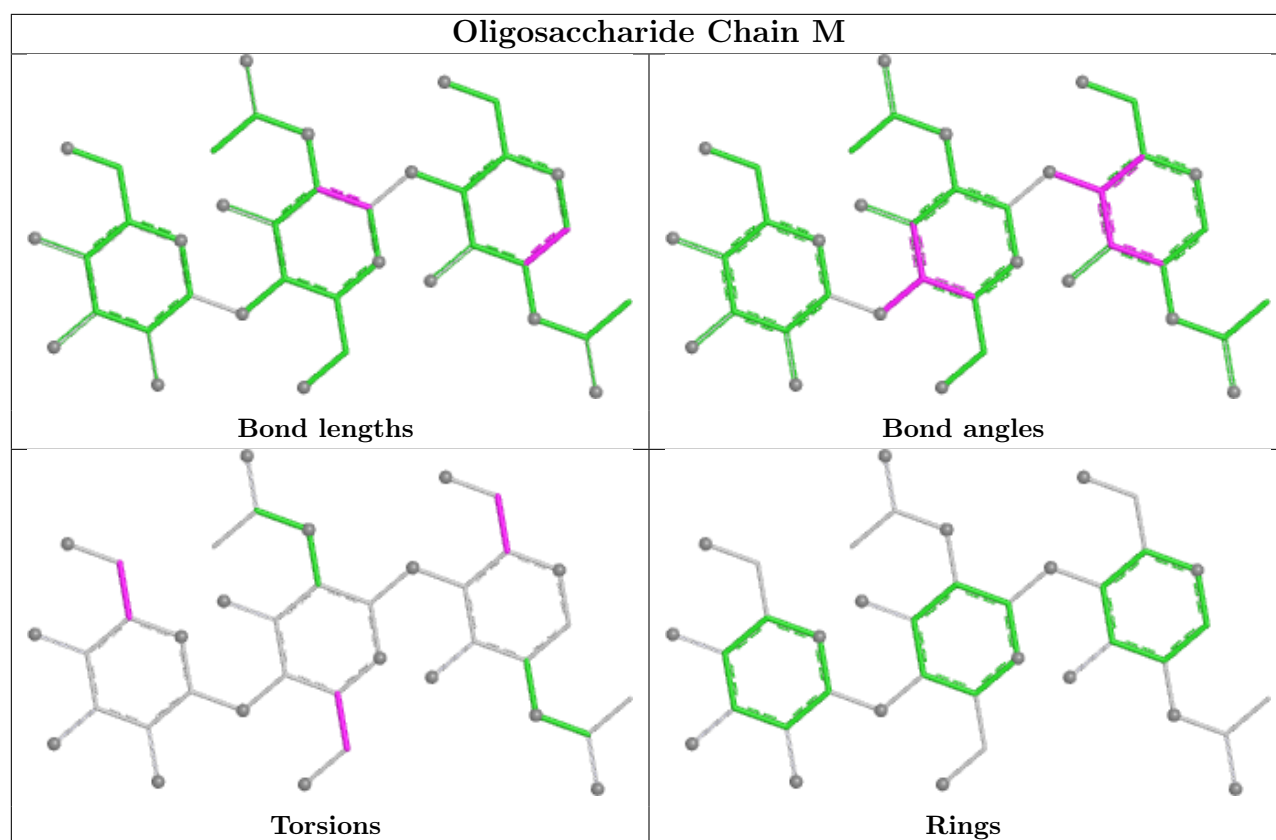
1 monomer is involved in 1 short contact:

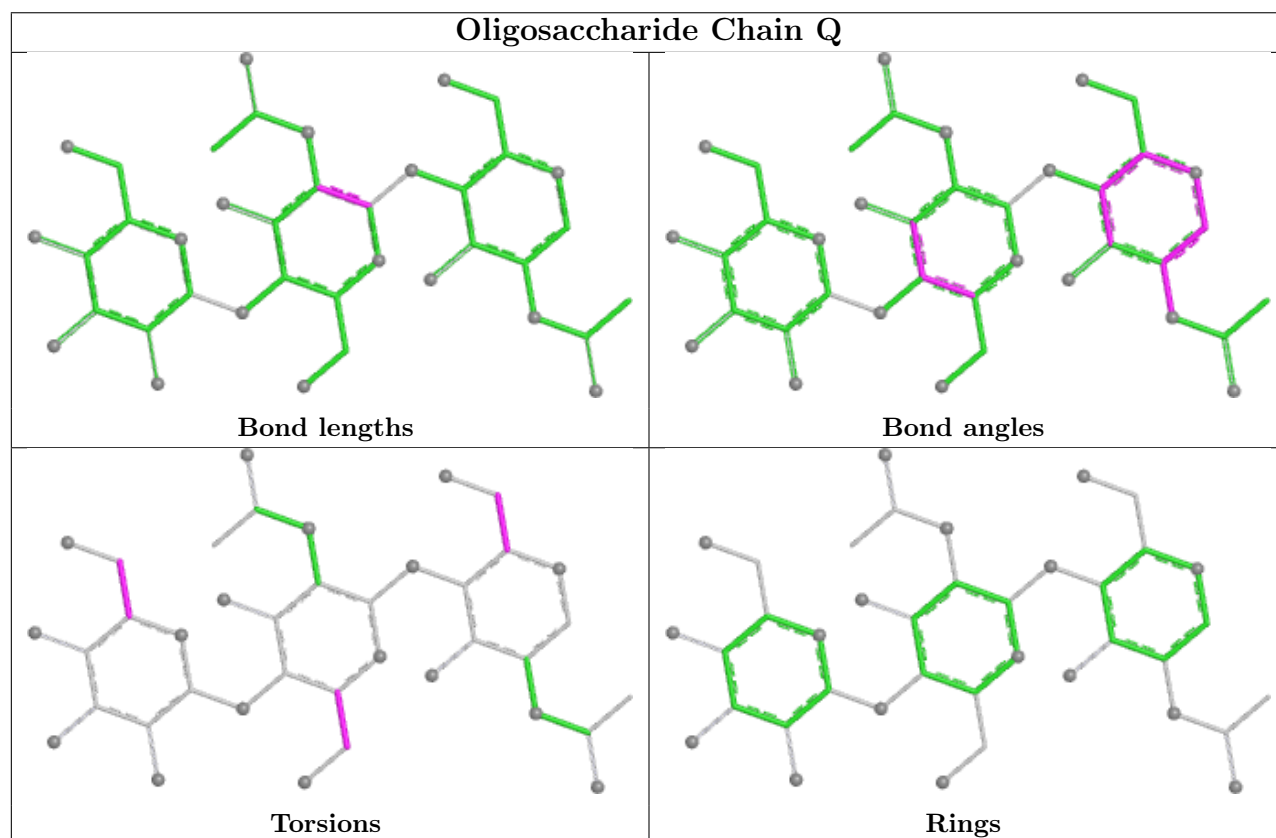
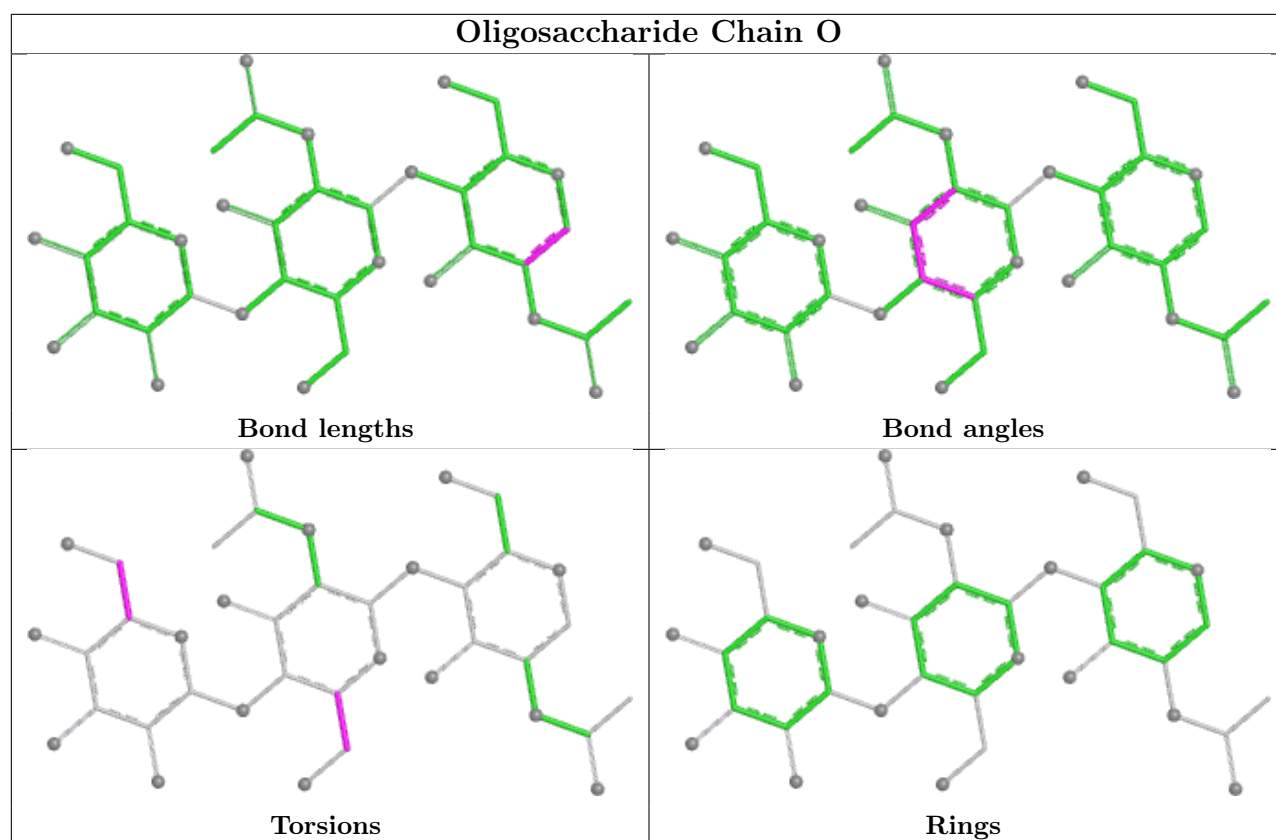
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

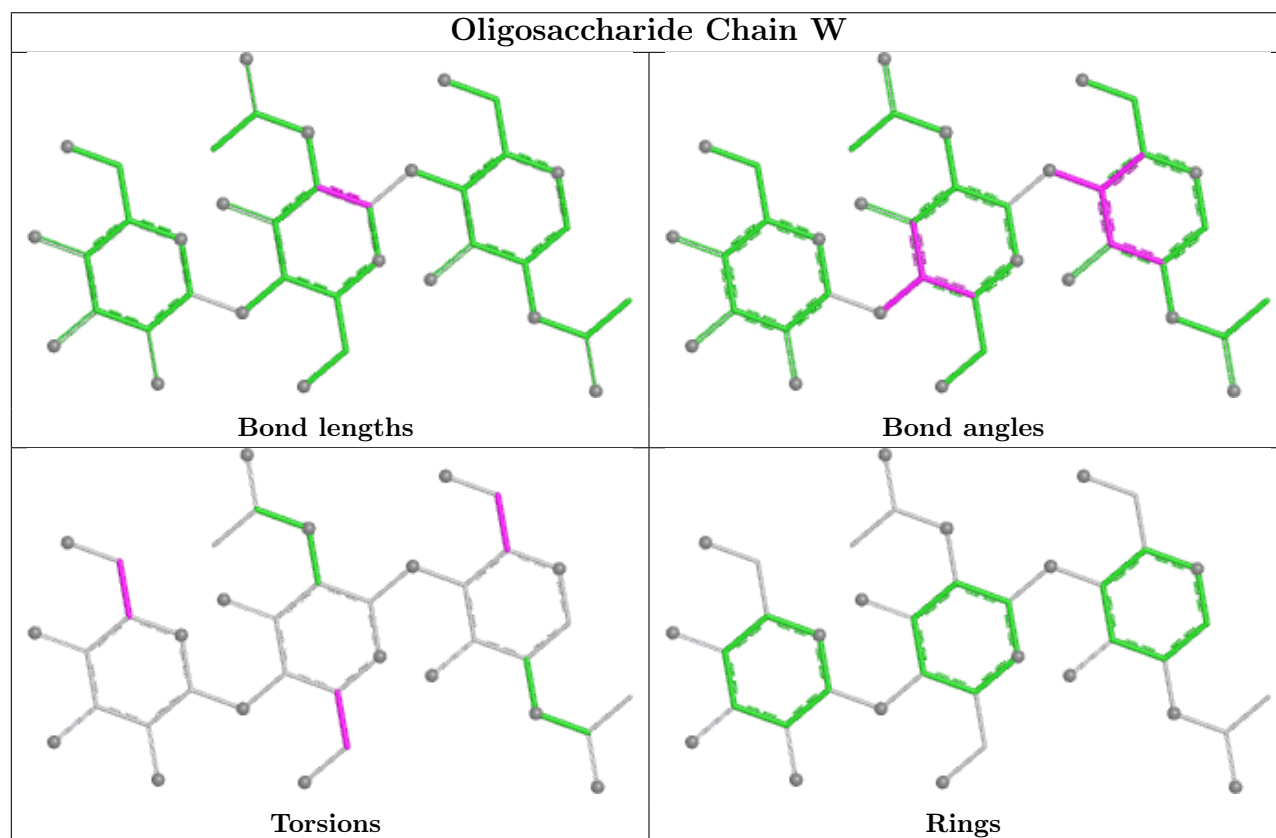
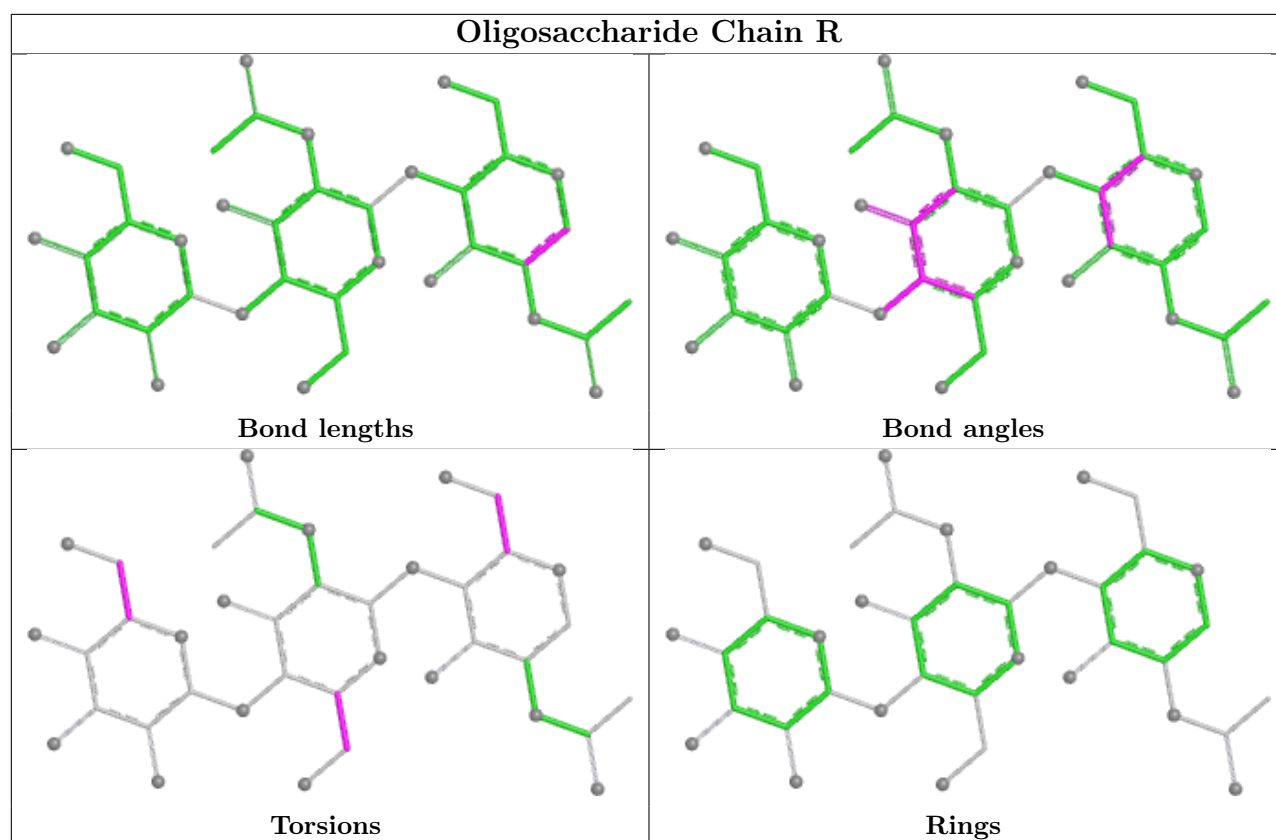
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

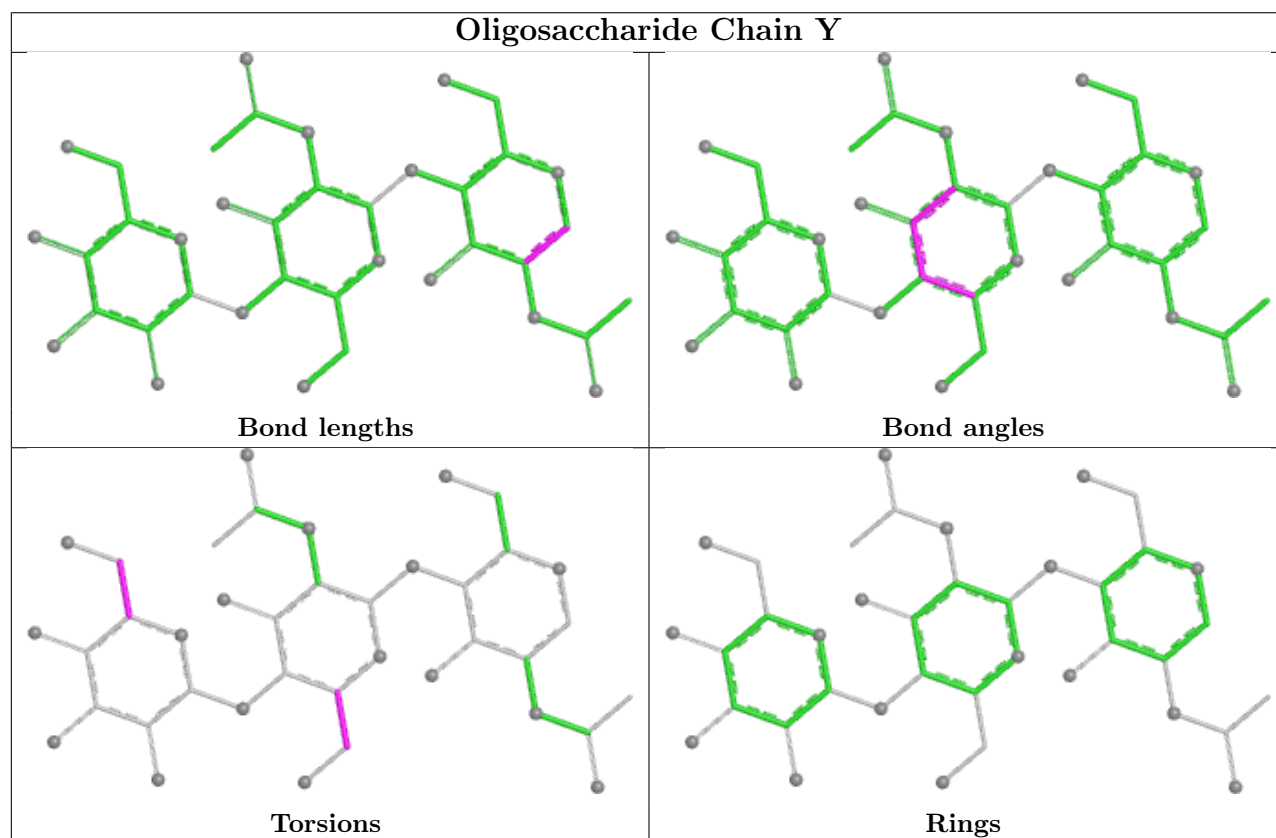
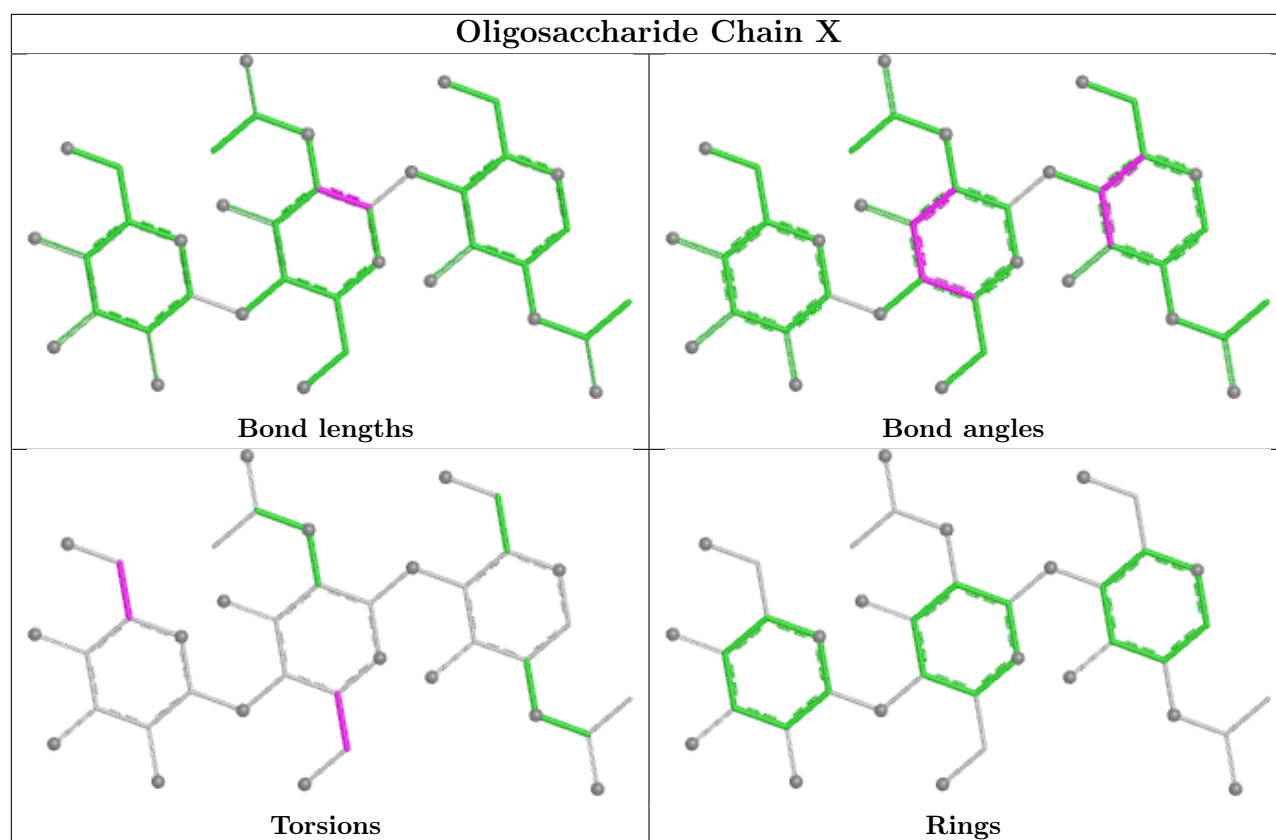


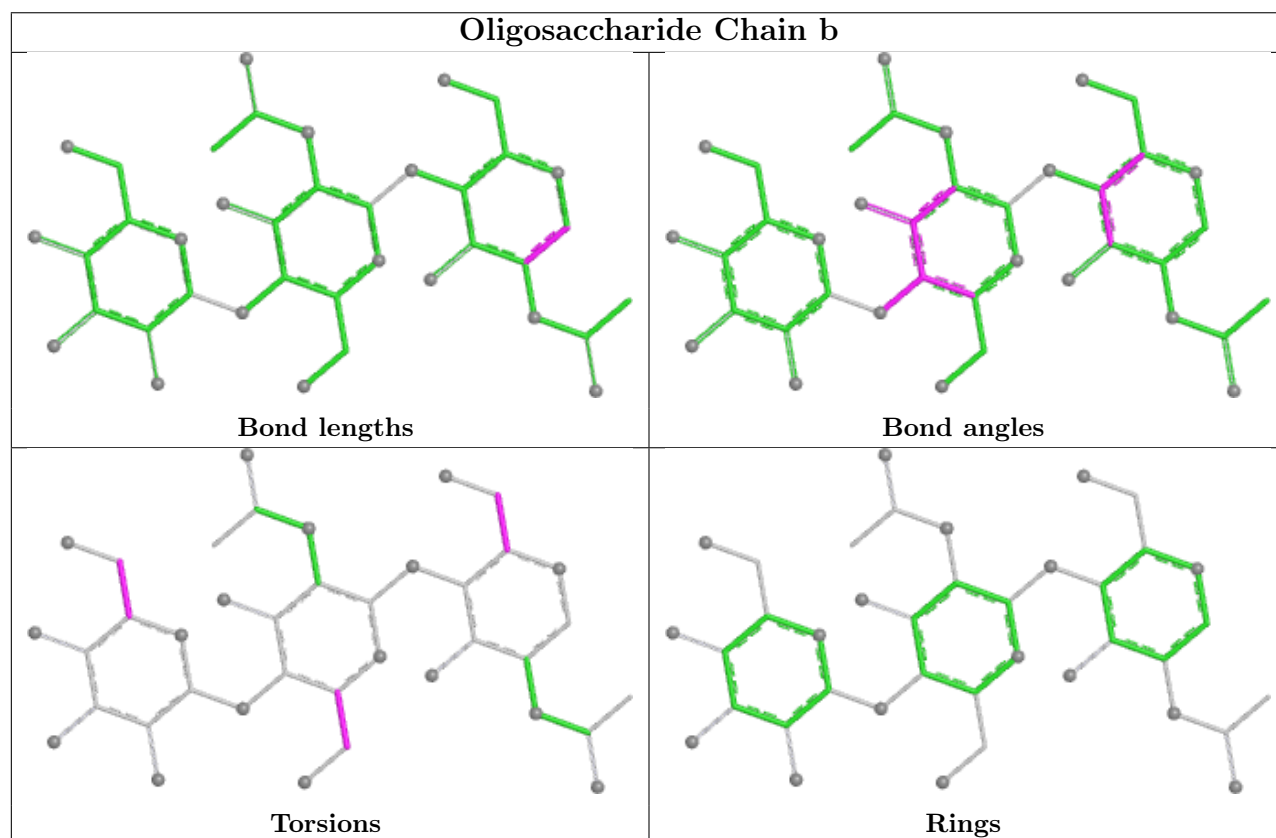
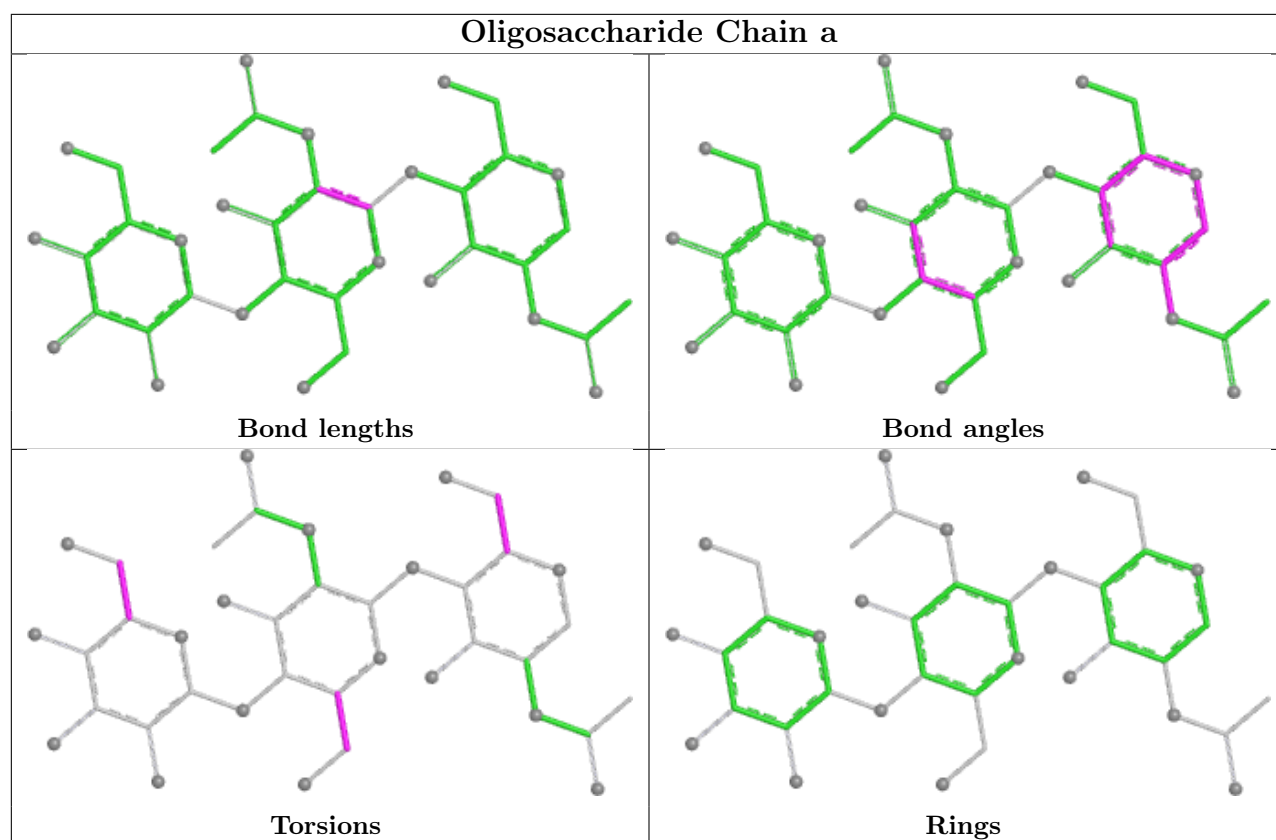


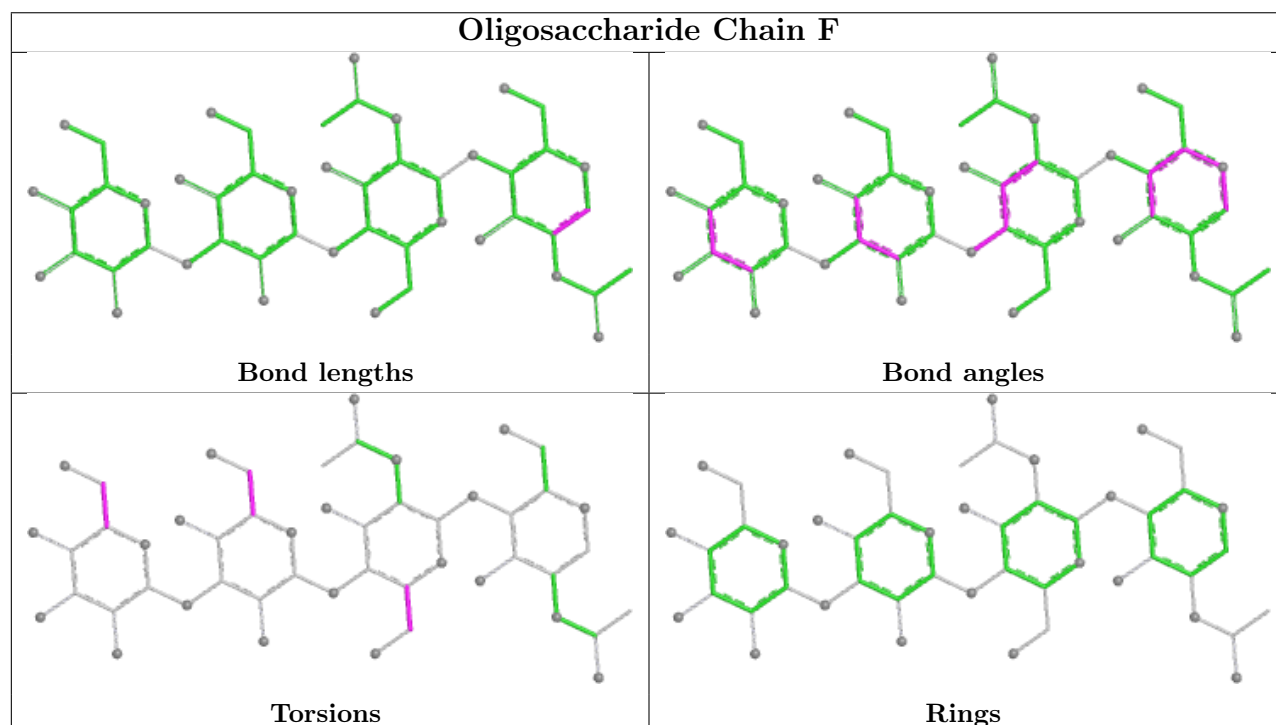
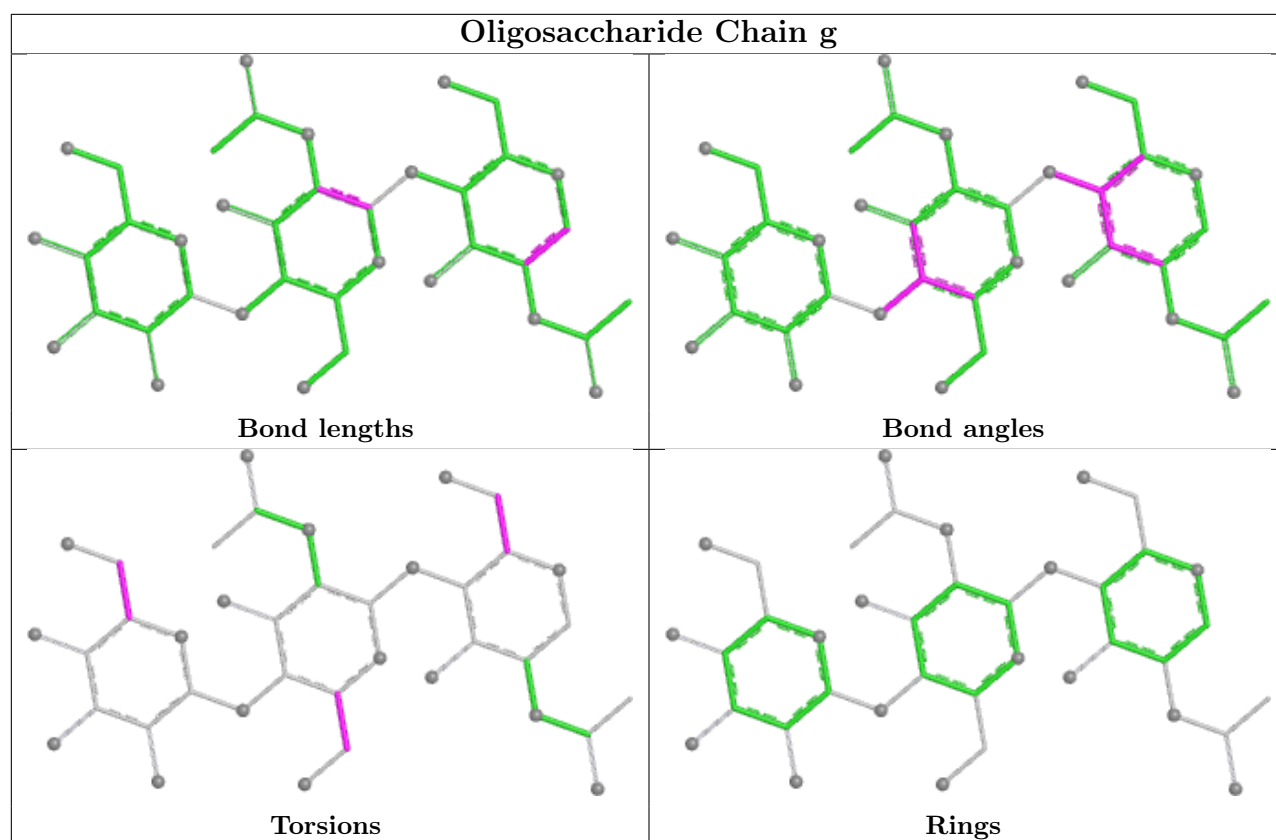


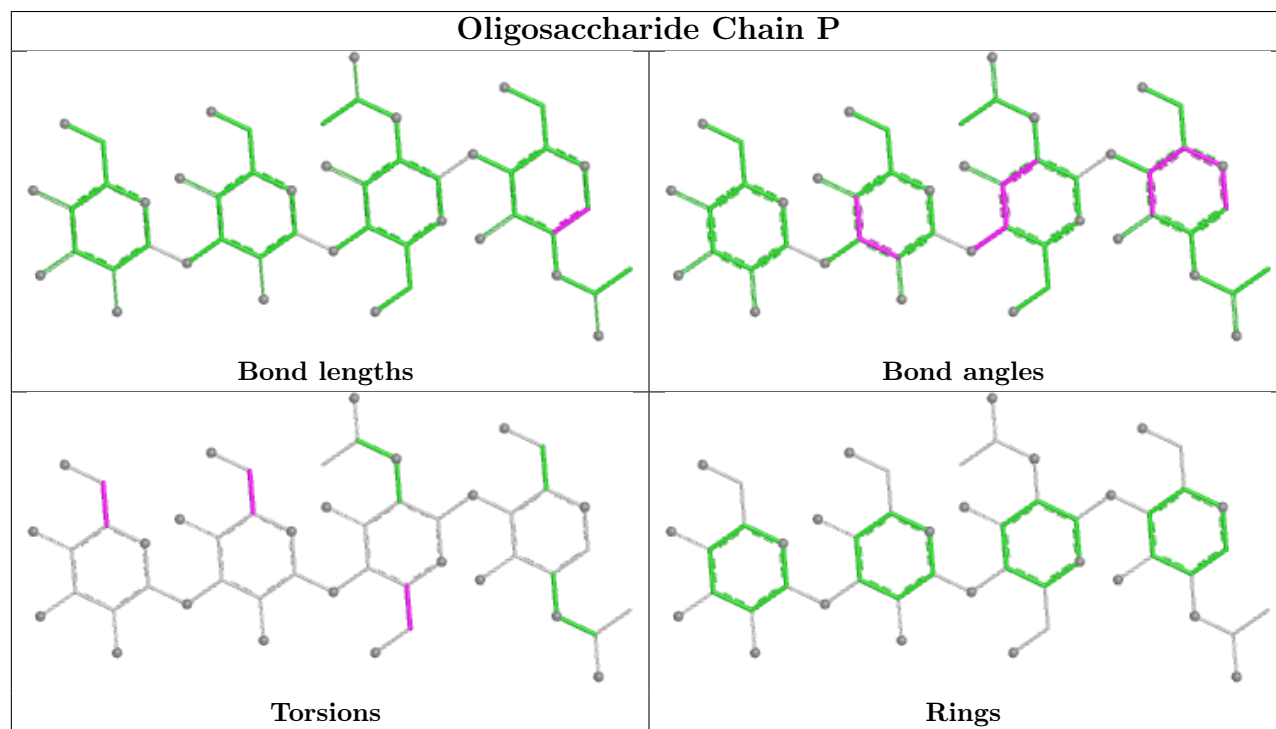
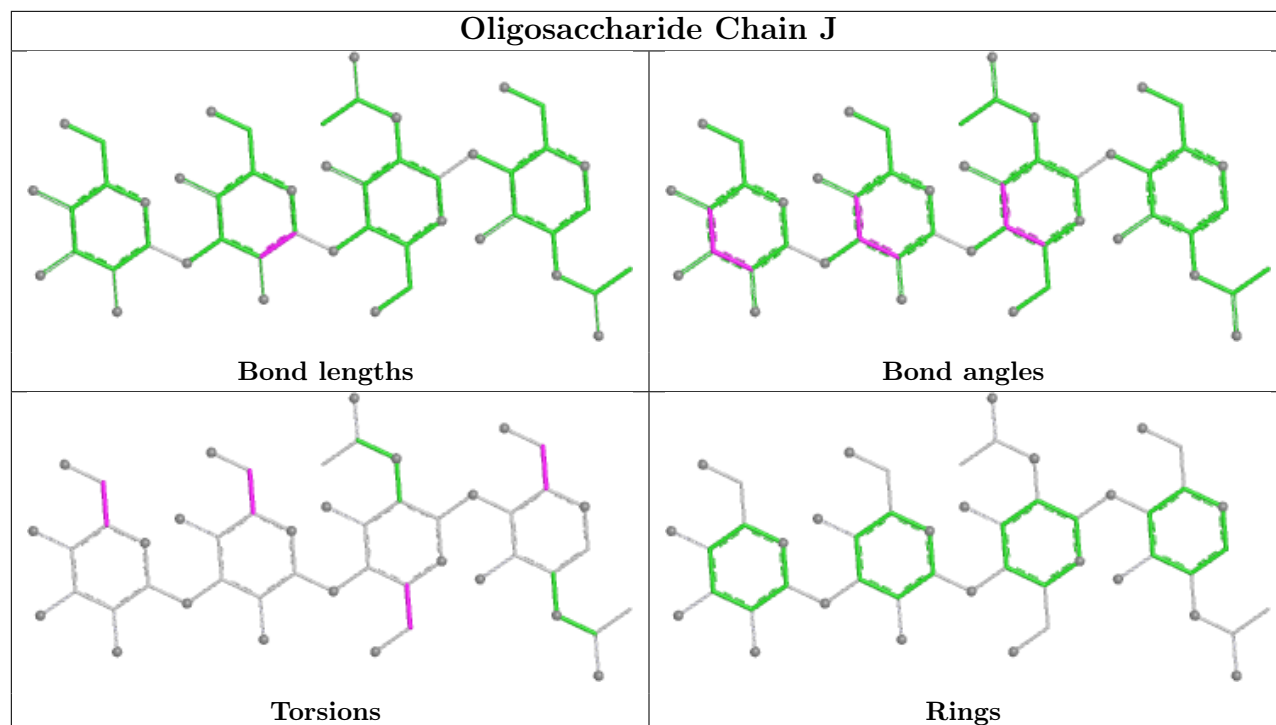


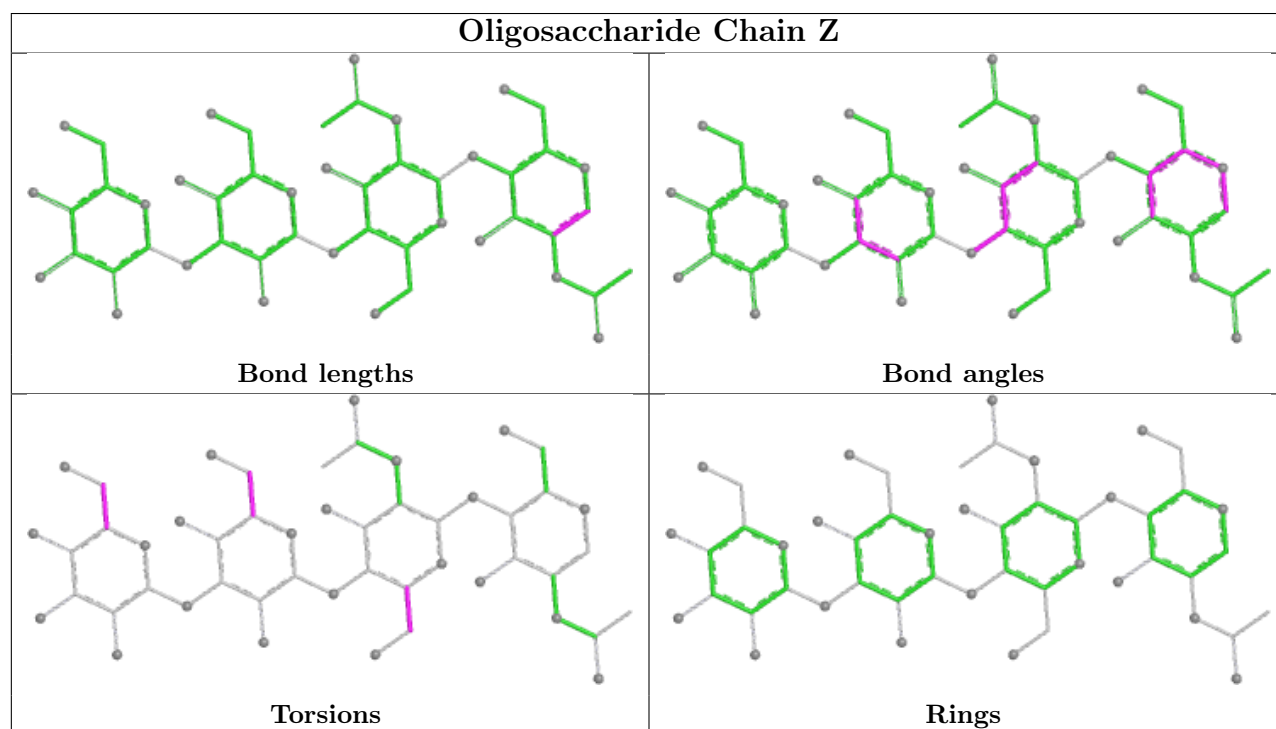
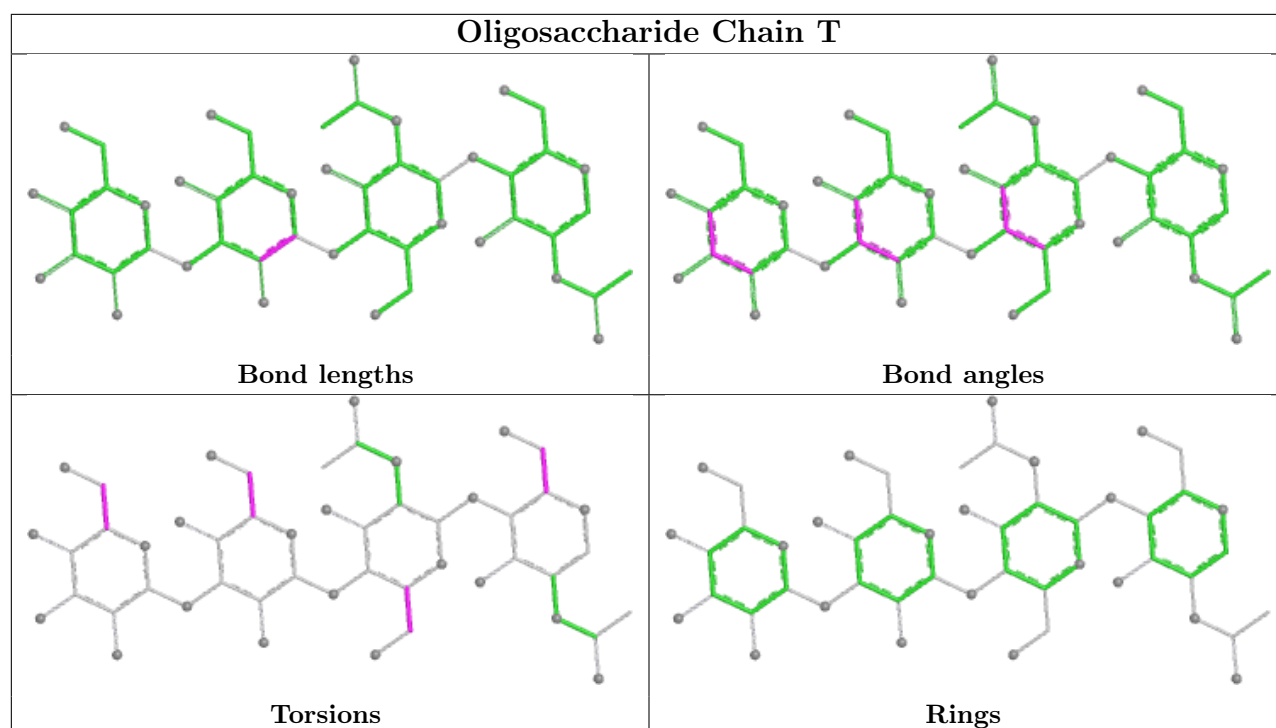


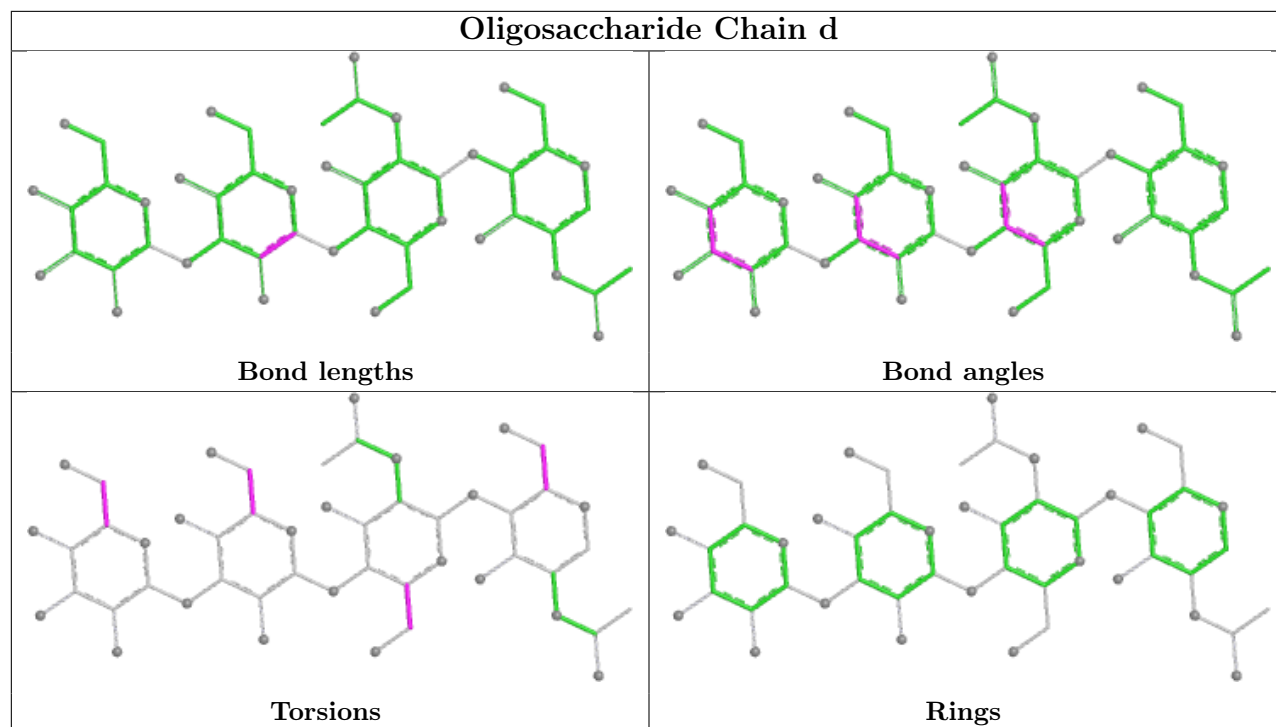


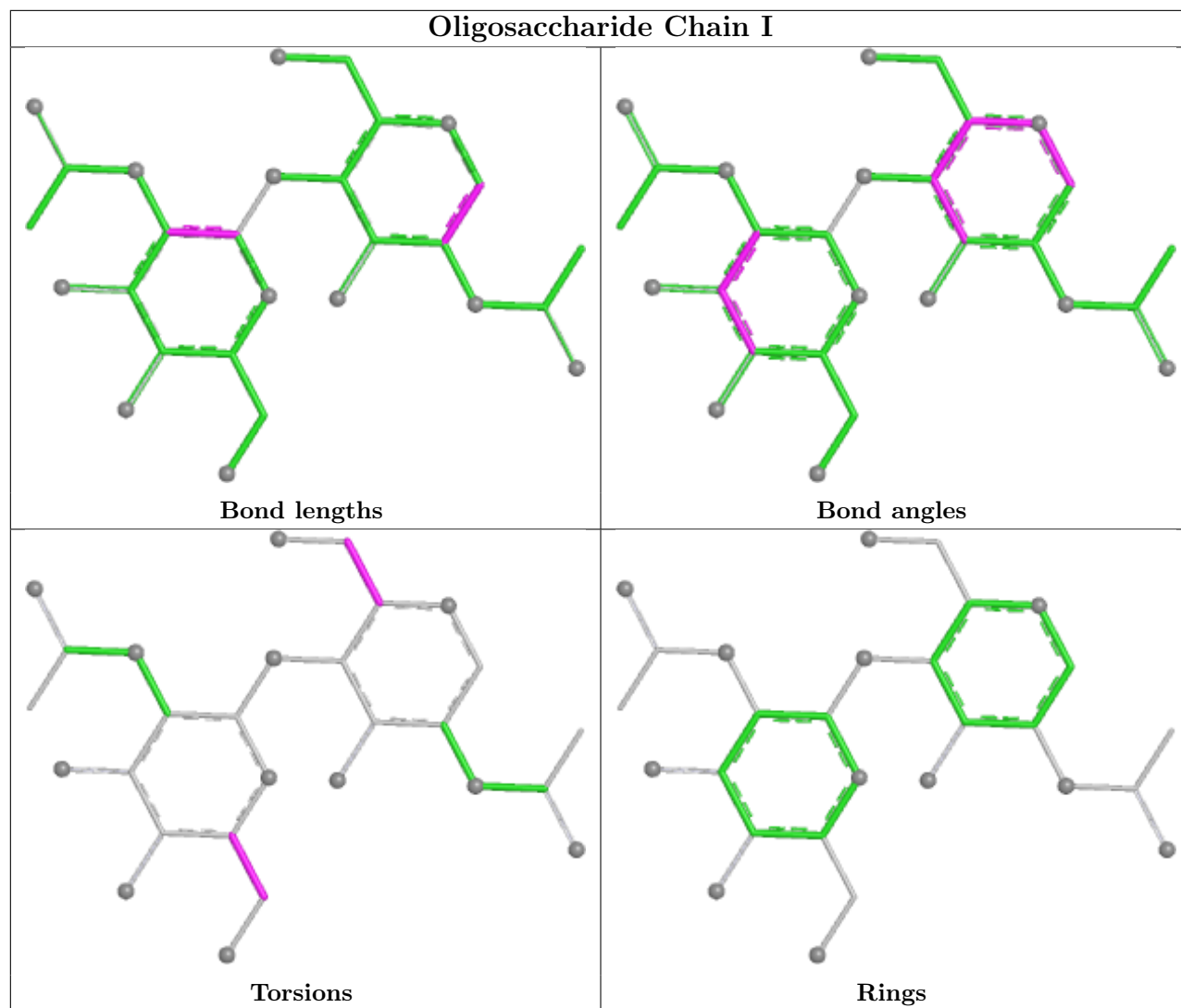


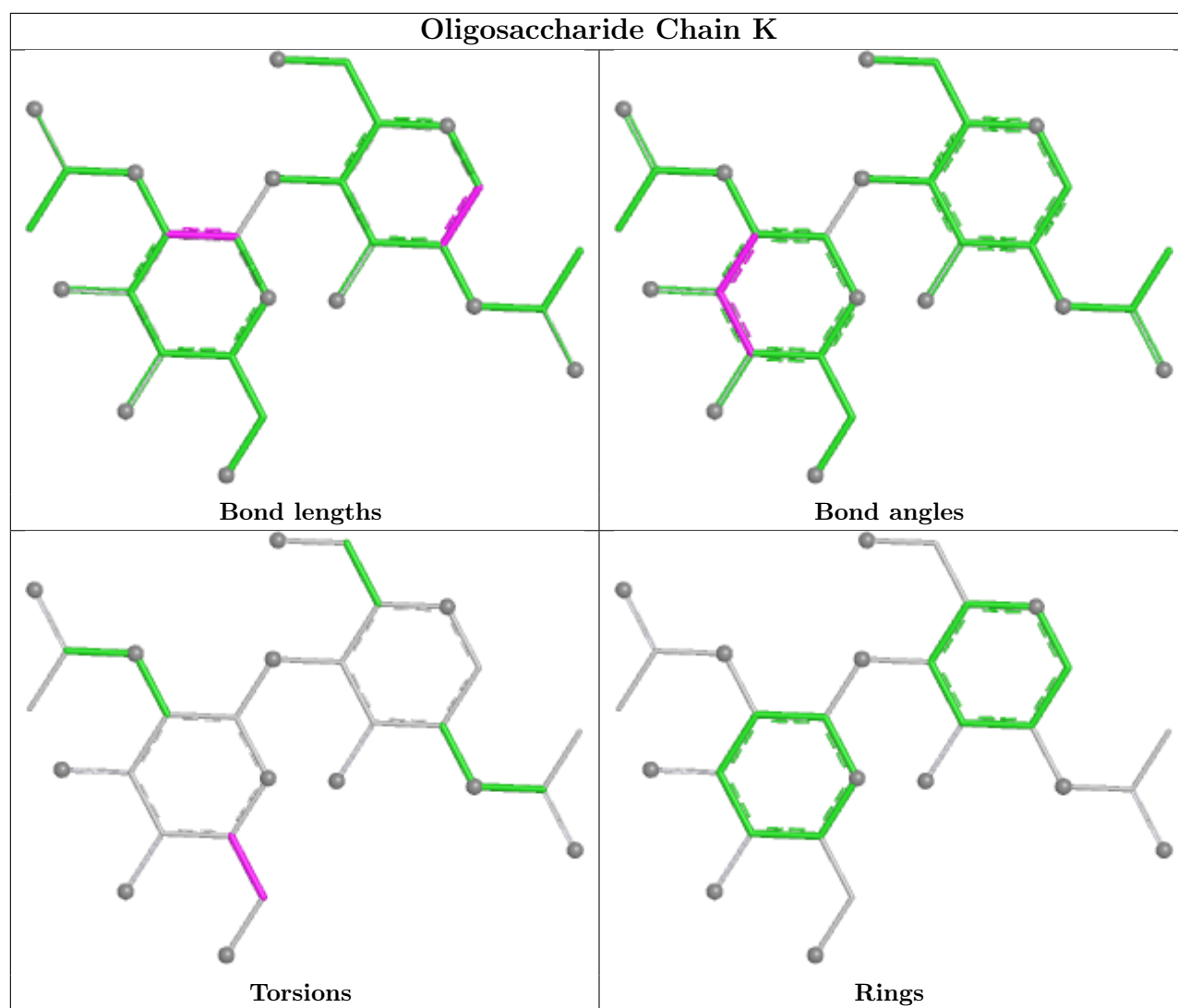


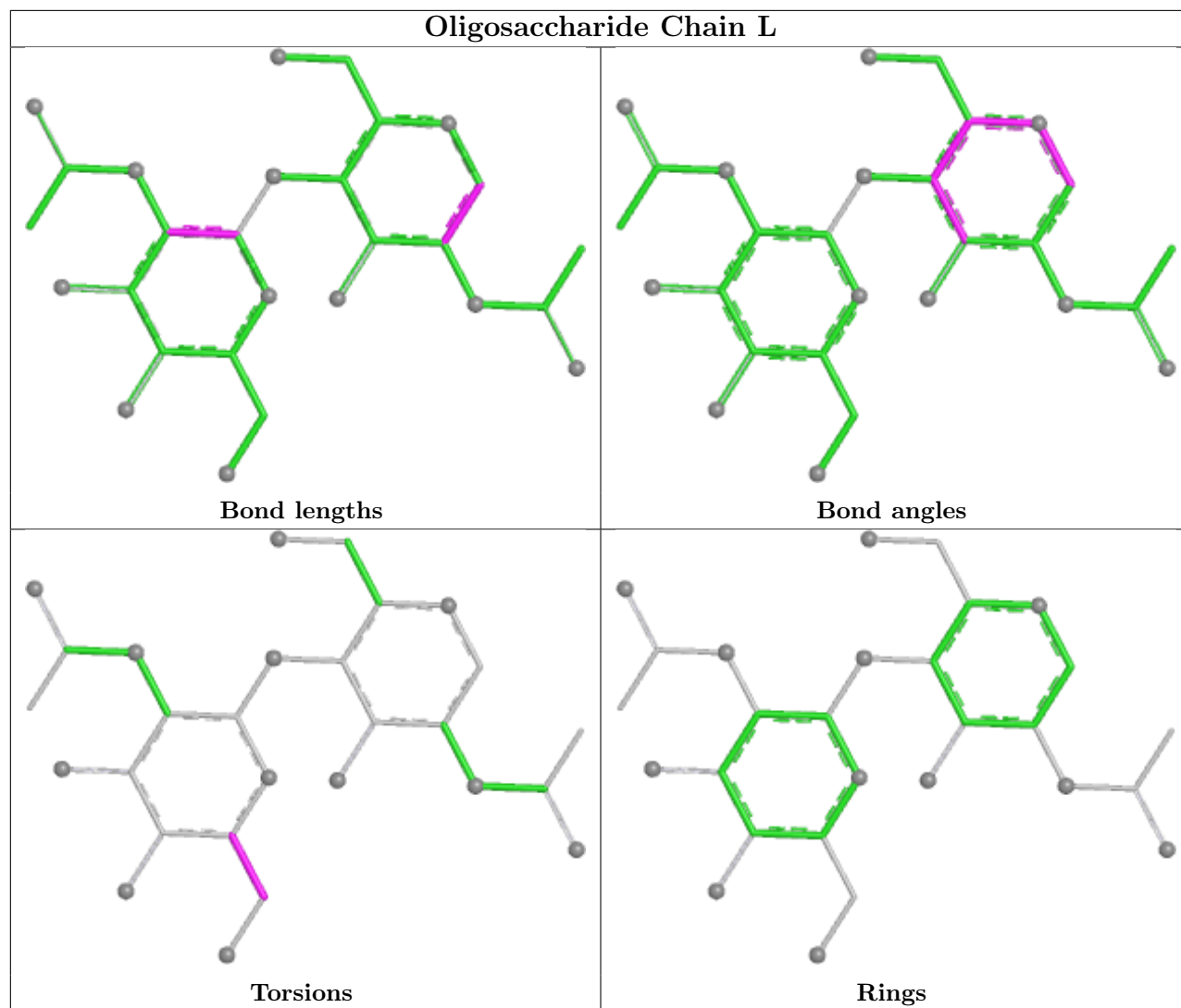


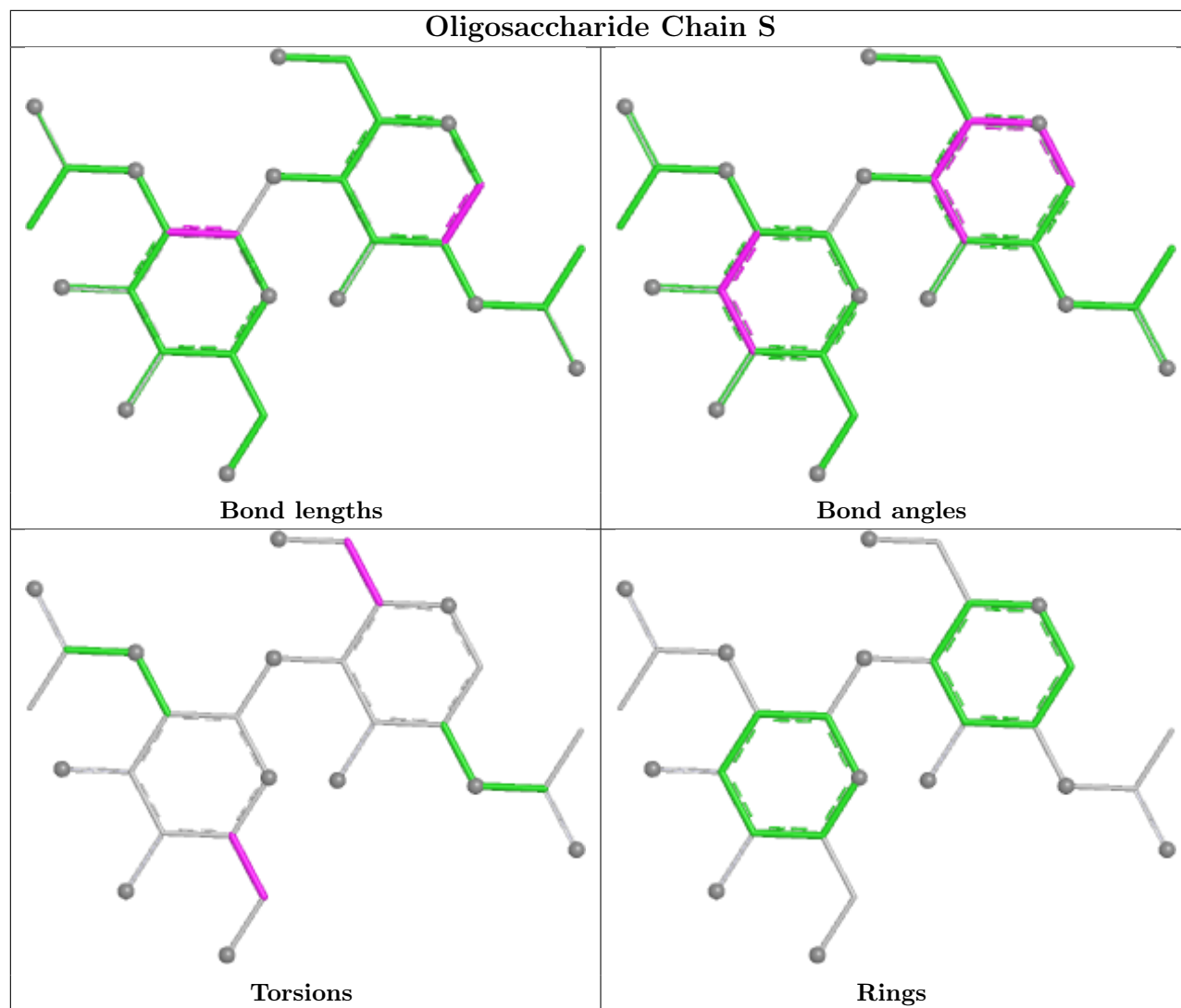


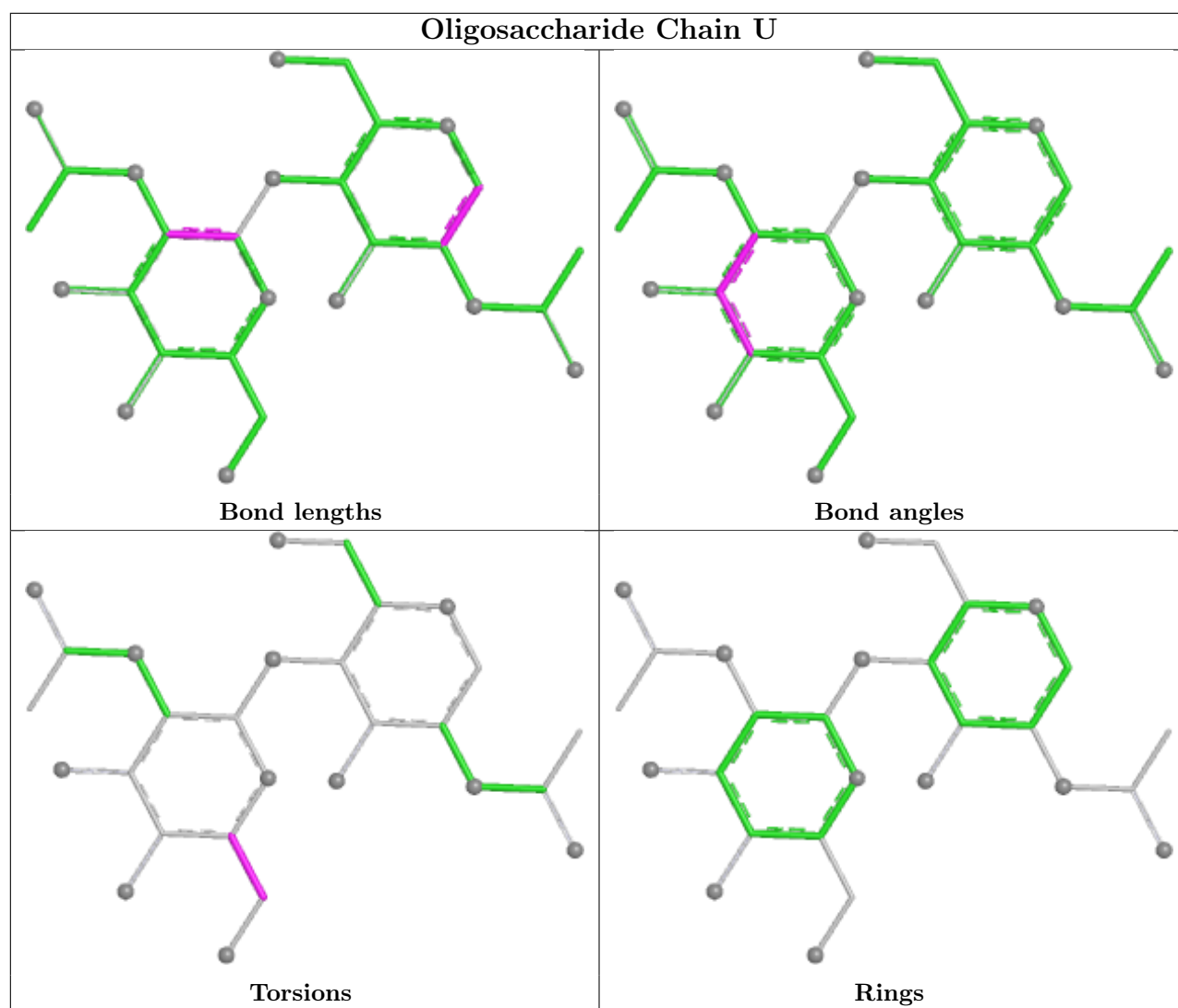


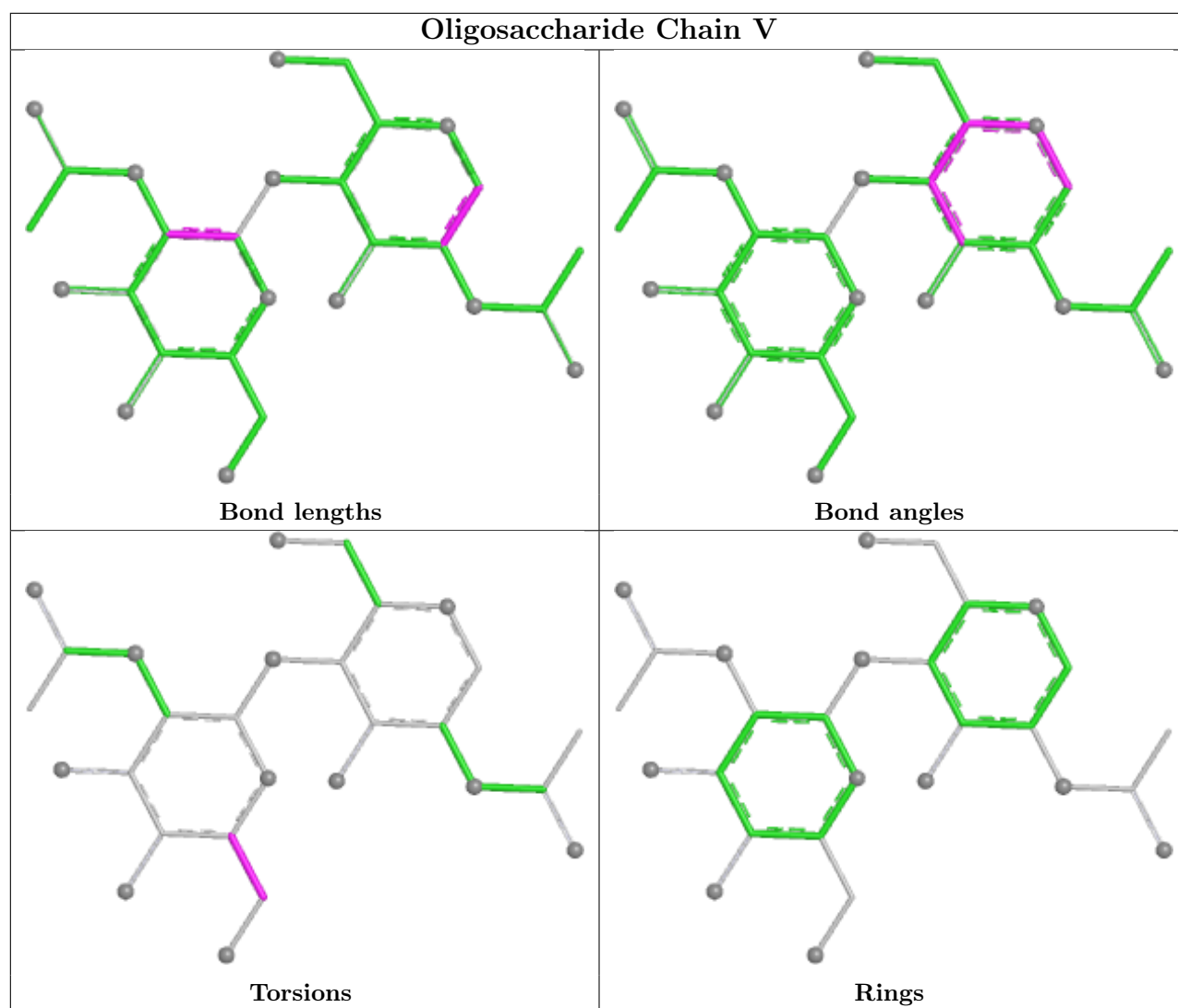


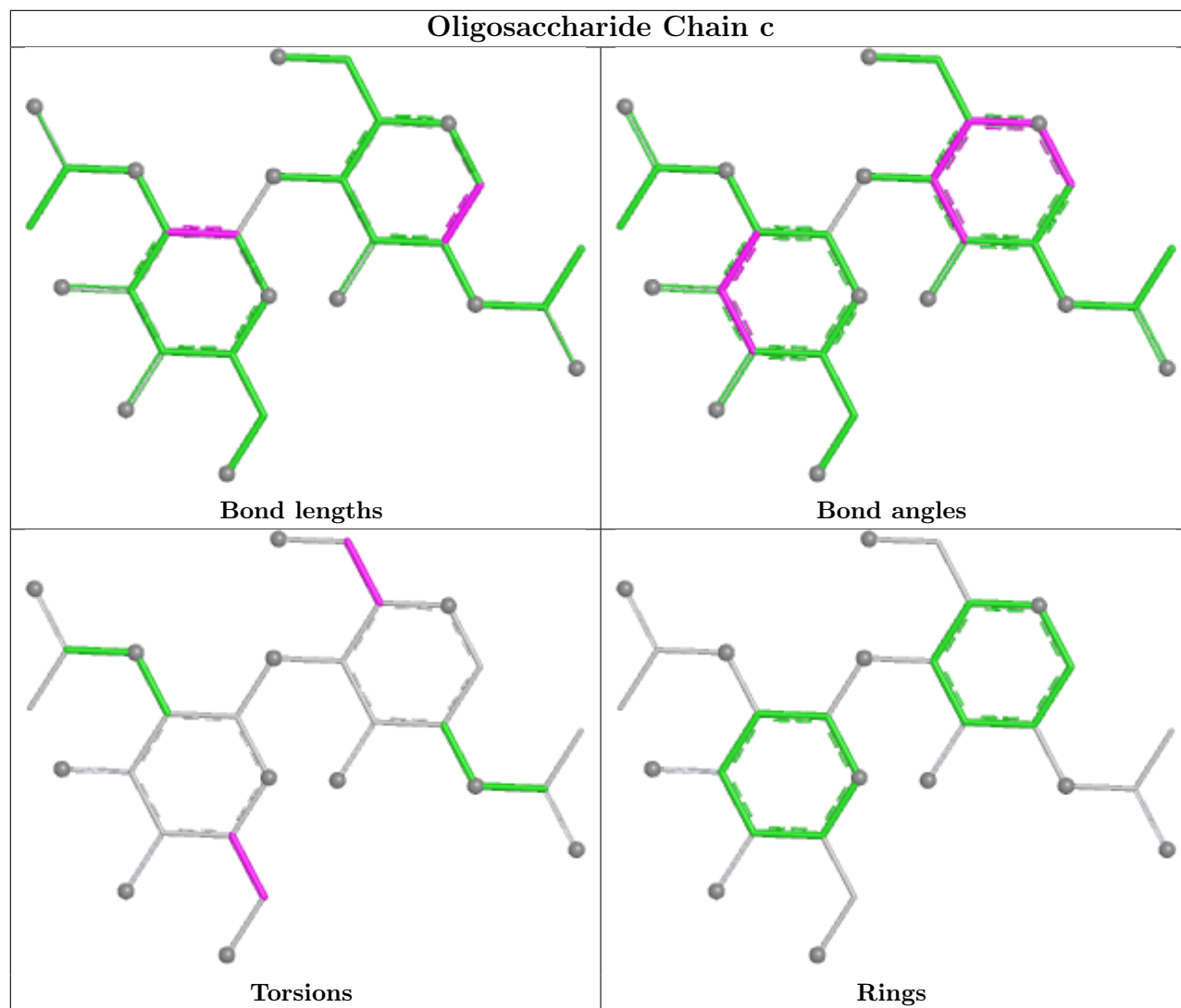


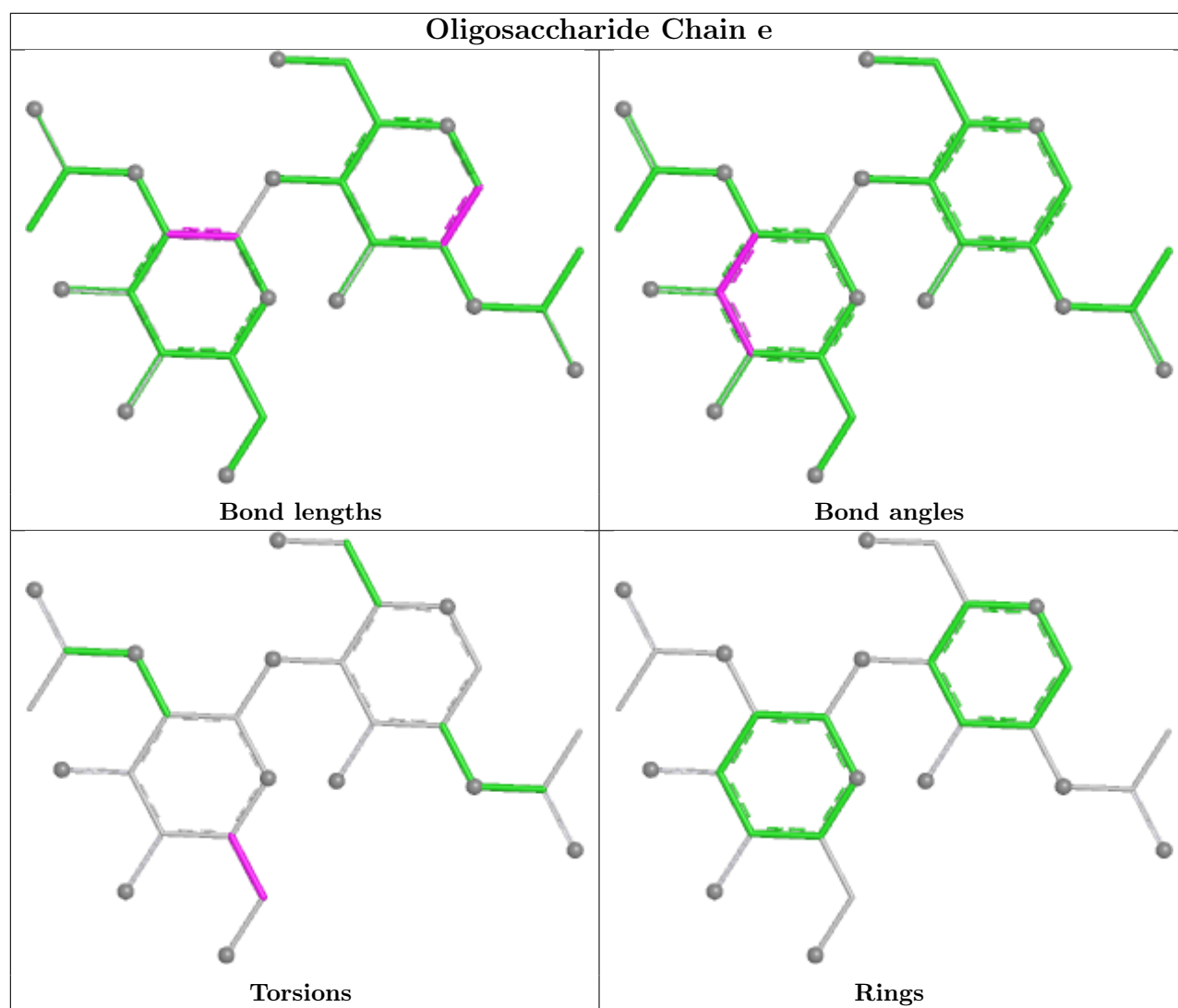


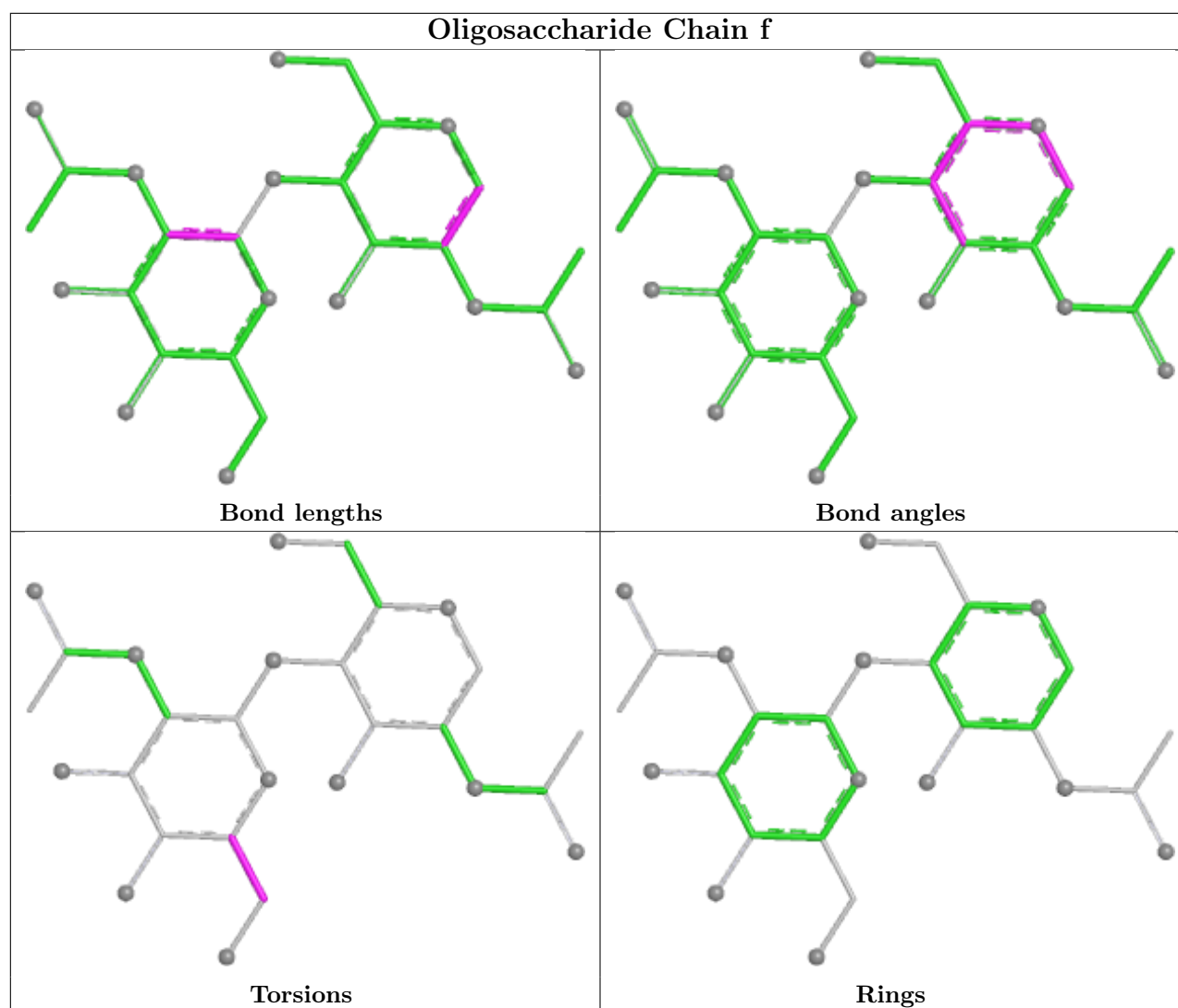












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
5	NAG	A	3200	1	14,14,15	0.76	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	B	3198	1	14,14,15	0.82	1 (7%)	17,19,21	0.61	0
5	NAG	A	3197	1	14,14,15	0.86	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	3200	1	14,14,15	0.76	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	A	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	C	3199	1	14,14,15	0.71	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	A	3199	1	14,14,15	0.70	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	C	3198	1	14,14,15	0.83	1 (7%)	17,19,21	0.61	0
5	NAG	B	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	B	3199	1	14,14,15	0.71	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	C	3201	1	14,14,15	1.03	1 (7%)	17,19,21	0.87	1 (5%)
6	MJJ	A	9999	-	25,25,25	2.34	8 (32%)	30,36,36	1.69	4 (13%)
5	NAG	C	3197	1	14,14,15	0.85	1 (7%)	17,19,21	1.01	1 (5%)
6	MJJ	C	9999	-	25,25,25	2.35	8 (32%)	30,36,36	1.69	4 (13%)
5	NAG	B	3200	1	14,14,15	0.77	1 (7%)	17,19,21	0.81	1 (5%)
5	NAG	A	3198	1	14,14,15	0.82	1 (7%)	17,19,21	0.61	0
6	MJJ	B	9999	-	25,25,25	2.34	8 (32%)	30,36,36	1.69	4 (13%)
5	NAG	B	3197	1	14,14,15	0.86	1 (7%)	17,19,21	1.01	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
5	NAG	A	3200	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3198	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3197	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3200	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3201	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3199	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3199	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3198	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3201	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3199	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3201	1	-	1/6/23/26	0/1/1/1
6	MJJ	A	9999	-	-	1/26/44/44	0/1/1/1
5	NAG	C	3197	1	-	2/6/23/26	0/1/1/1
6	MJJ	C	9999	-	-	1/26/44/44	0/1/1/1
5	NAG	B	3200	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3198	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MJJ	B	9999	-	-	1/26/44/44	0/1/1/1
5	NAG	B	3197	1	-	2/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	9999	MJJ	C4-C5	7.37	1.59	1.53
6	A	9999	MJJ	C4-C5	7.35	1.59	1.53
6	B	9999	MJJ	C4-C5	7.26	1.59	1.53
6	A	9999	MJJ	O1A-C1	3.77	1.33	1.22
6	C	9999	MJJ	O1A-C1	3.75	1.33	1.22
6	B	9999	MJJ	O1A-C1	3.75	1.33	1.22
5	C	3201	NAG	C1-C2	3.52	1.57	1.52
5	B	3201	NAG	C1-C2	3.52	1.57	1.52
5	A	3201	NAG	C1-C2	3.52	1.57	1.52
6	C	9999	MJJ	C6-C5	3.41	1.58	1.53
6	A	9999	MJJ	C6-C5	3.37	1.58	1.53
6	B	9999	MJJ	C6-C5	3.36	1.58	1.53
6	A	9999	MJJ	C8-C7	3.19	1.59	1.53
6	B	9999	MJJ	C8-C7	3.18	1.59	1.53
6	C	9999	MJJ	C8-C7	3.16	1.59	1.53
6	B	9999	MJJ	C7-C6	3.16	1.56	1.52
6	C	9999	MJJ	C7-C6	3.14	1.56	1.52
6	A	9999	MJJ	C7-C6	3.11	1.56	1.52
6	C	9999	MJJ	C3-C2	3.08	1.56	1.52
6	A	9999	MJJ	C3-C2	3.08	1.56	1.52
6	B	9999	MJJ	C3-C2	3.07	1.56	1.52
5	C	3198	NAG	C1-C2	2.77	1.56	1.52
5	A	3198	NAG	C1-C2	2.75	1.56	1.52
5	B	3198	NAG	C1-C2	2.75	1.56	1.52
5	A	3197	NAG	C1-C2	2.72	1.56	1.52
5	B	3197	NAG	C1-C2	2.71	1.56	1.52
5	C	3197	NAG	C1-C2	2.71	1.56	1.52
5	B	3200	NAG	C1-C2	2.53	1.55	1.52
5	A	3200	NAG	C1-C2	2.51	1.55	1.52
5	C	3200	NAG	C1-C2	2.51	1.55	1.52
6	C	9999	MJJ	O6-C6	2.39	1.47	1.44
6	A	9999	MJJ	O6-C6	2.36	1.47	1.44
6	B	9999	MJJ	O6-C6	2.34	1.47	1.44
6	C	9999	MJJ	O1B-C1	-2.18	1.22	1.30
6	A	9999	MJJ	O1B-C1	-2.18	1.22	1.30
6	B	9999	MJJ	O1B-C1	-2.18	1.22	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3199	NAG	C1-C2	2.15	1.55	1.52
5	B	3199	NAG	C1-C2	2.15	1.55	1.52
5	A	3199	NAG	C1-C2	2.10	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	9999	MJJ	O1B-C1-O1A	-4.98	107.93	123.86
6	C	9999	MJJ	O1B-C1-O1A	-4.97	107.95	123.86
6	B	9999	MJJ	O1B-C1-O1A	-4.97	107.95	123.86
6	A	9999	MJJ	CM2-O2-C2	4.86	121.78	115.46
6	C	9999	MJJ	CM2-O2-C2	4.84	121.75	115.46
6	B	9999	MJJ	CM2-O2-C2	4.84	121.75	115.46
5	B	3197	NAG	C4-C3-C2	-3.36	106.09	111.02
5	C	3197	NAG	C4-C3-C2	-3.35	106.11	111.02
5	A	3197	NAG	C4-C3-C2	-3.35	106.11	111.02
5	A	3201	NAG	C4-C3-C2	-2.89	106.78	111.02
5	C	3201	NAG	C4-C3-C2	-2.89	106.78	111.02
5	B	3201	NAG	C4-C3-C2	-2.89	106.79	111.02
5	A	3199	NAG	C4-C3-C2	-2.74	107.00	111.02
5	B	3199	NAG	C4-C3-C2	-2.73	107.02	111.02
5	C	3199	NAG	C4-C3-C2	-2.70	107.06	111.02
5	B	3200	NAG	C4-C3-C2	-2.63	107.17	111.02
5	A	3200	NAG	C4-C3-C2	-2.62	107.18	111.02
5	C	3200	NAG	C4-C3-C2	-2.61	107.19	111.02
6	C	9999	MJJ	O6-C2-C3	-2.32	108.23	111.35
6	A	9999	MJJ	O6-C2-C3	-2.31	108.24	111.35
6	B	9999	MJJ	O6-C2-C3	-2.30	108.26	111.35
6	C	9999	MJJ	C9-O9-CA9	2.18	122.47	117.08
6	B	9999	MJJ	C9-O9-CA9	2.17	122.43	117.08
6	A	9999	MJJ	C9-O9-CA9	2.16	122.42	117.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	9999	MJJ	O1B-C1-C2-O2
6	B	9999	MJJ	O1B-C1-C2-O2
6	C	9999	MJJ	O1B-C1-C2-O2
5	A	3197	NAG	C4-C5-C6-O6
5	B	3197	NAG	C4-C5-C6-O6
5	C	3197	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

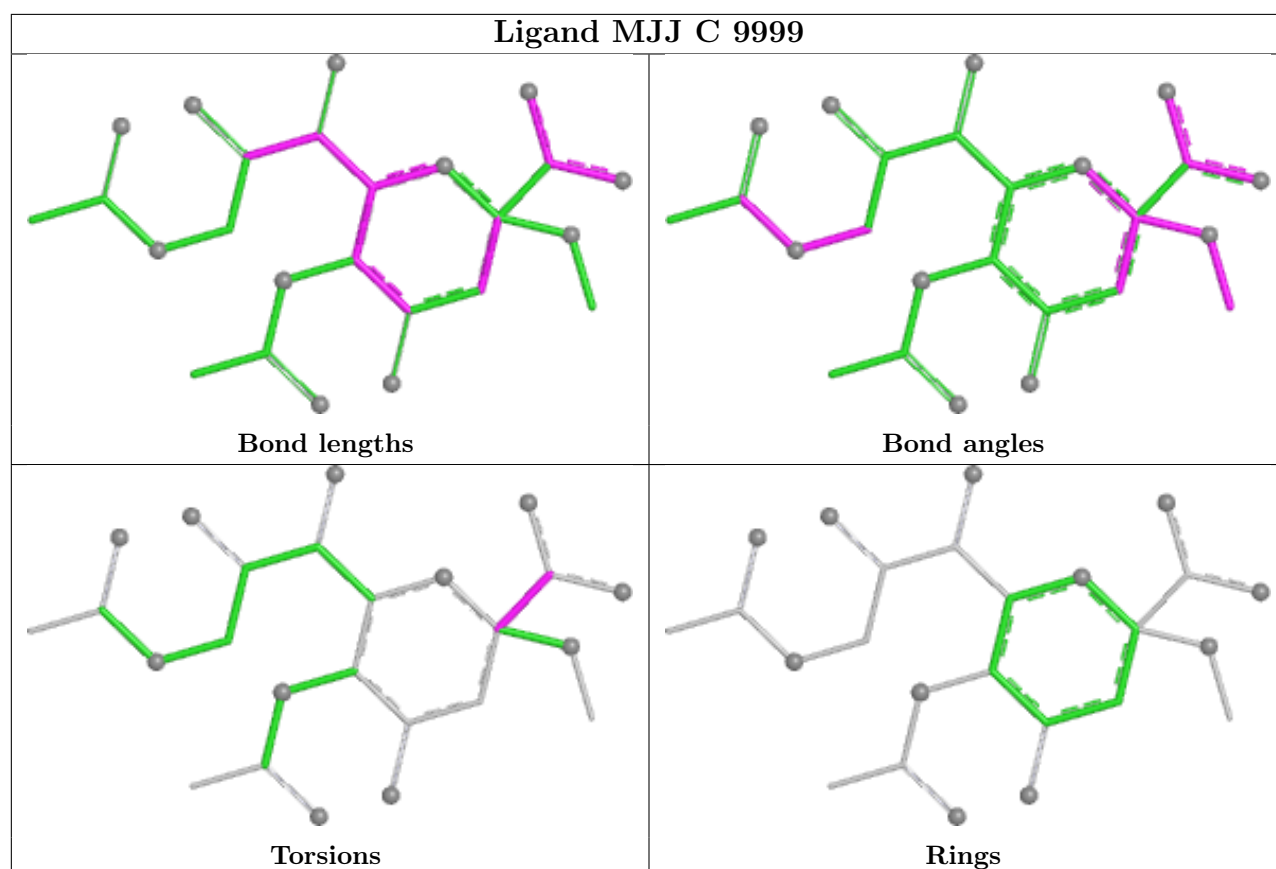
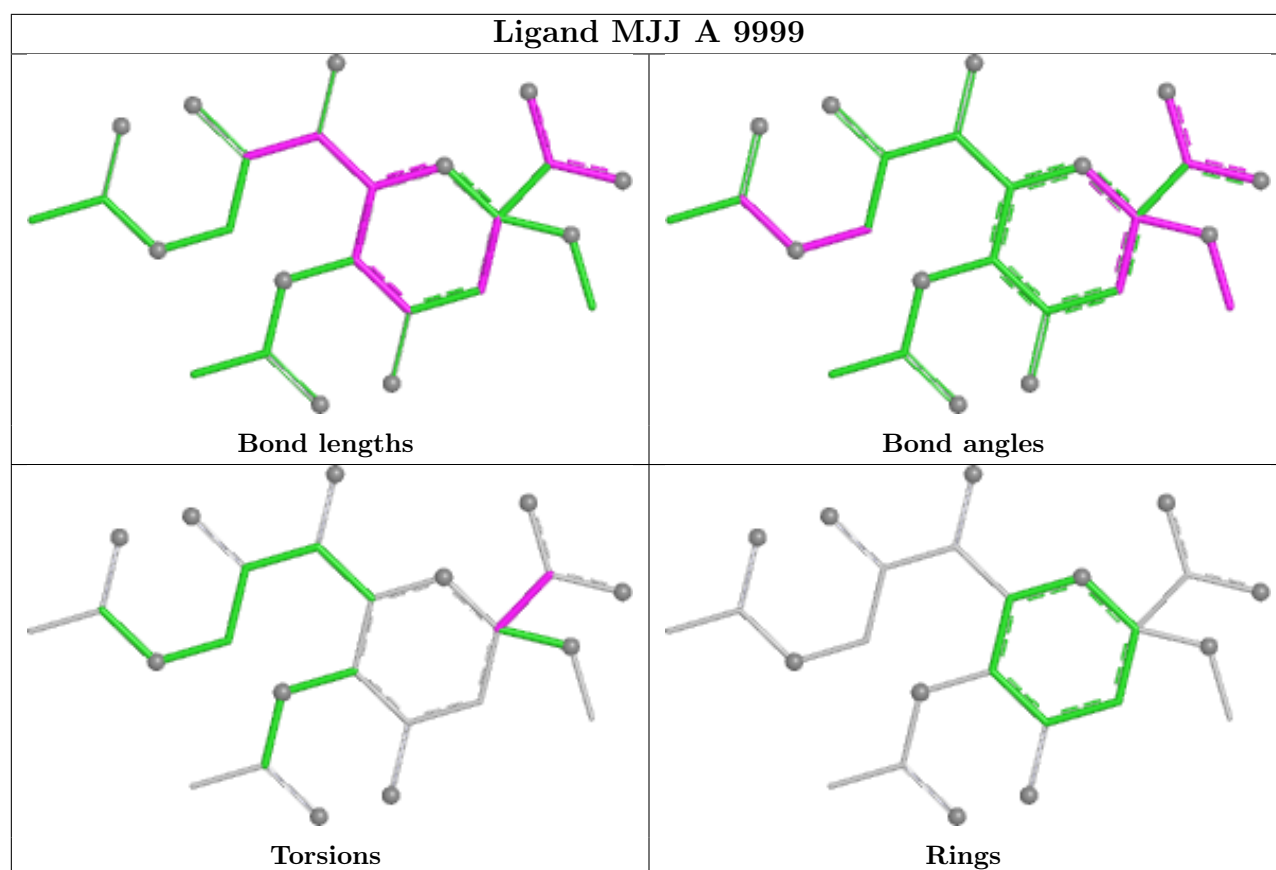
Mol	Chain	Res	Type	Atoms
5	A	3200	NAG	O5-C5-C6-O6
5	B	3200	NAG	O5-C5-C6-O6
5	C	3200	NAG	O5-C5-C6-O6
5	A	3197	NAG	O5-C5-C6-O6
5	B	3197	NAG	O5-C5-C6-O6
5	C	3197	NAG	O5-C5-C6-O6
5	A	3201	NAG	O5-C5-C6-O6
5	B	3201	NAG	O5-C5-C6-O6
5	C	3201	NAG	O5-C5-C6-O6
5	A	3200	NAG	C4-C5-C6-O6
5	B	3200	NAG	C4-C5-C6-O6
5	C	3200	NAG	C4-C5-C6-O6
5	A	3198	NAG	O5-C5-C6-O6
5	B	3198	NAG	O5-C5-C6-O6
5	C	3198	NAG	O5-C5-C6-O6
5	A	3199	NAG	O5-C5-C6-O6
5	B	3199	NAG	O5-C5-C6-O6
5	C	3199	NAG	O5-C5-C6-O6

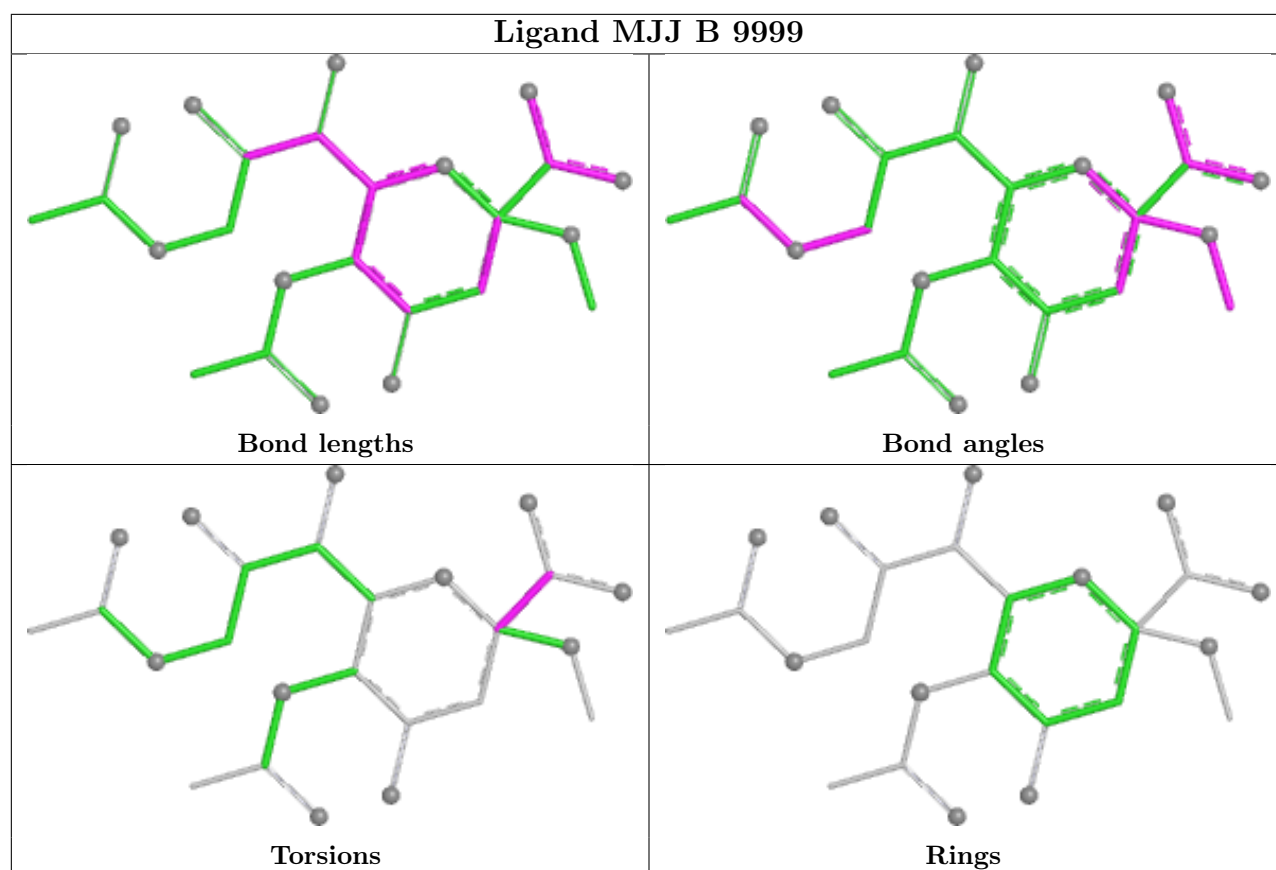
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3198	NAG	1	0
5	C	3198	NAG	1	0
5	A	3198	NAG	1	0

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





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.

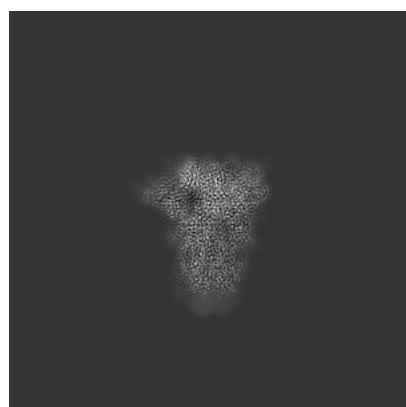
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0557. These allow visual inspection of the internal detail of the map and identification of artifacts.

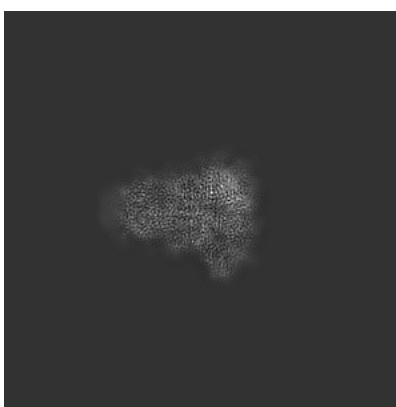
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

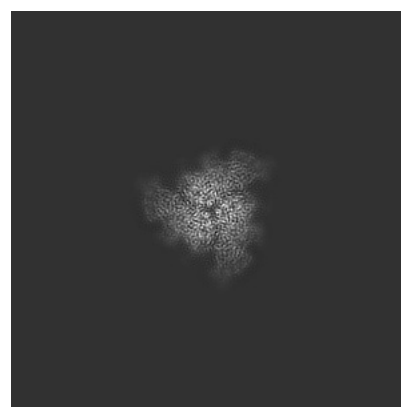
6.1.1 Primary map



X



Y

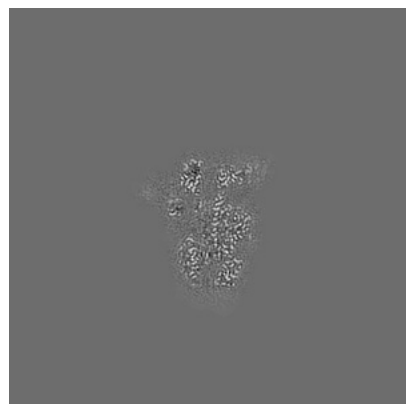


Z

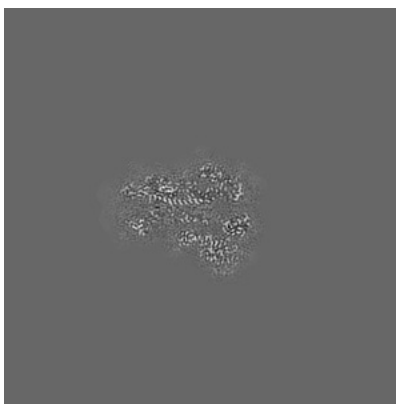
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

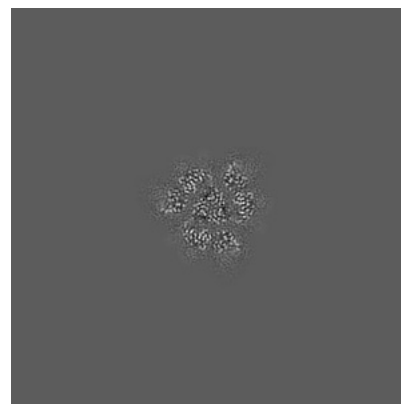
6.2.1 Primary map



X Index: 200



Y Index: 200

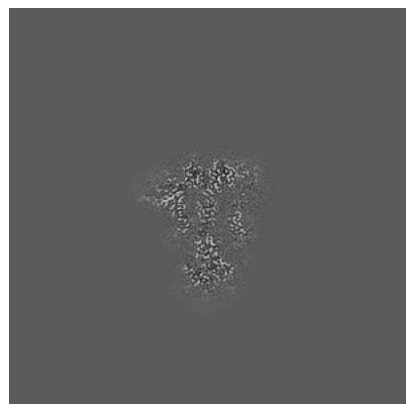


Z Index: 200

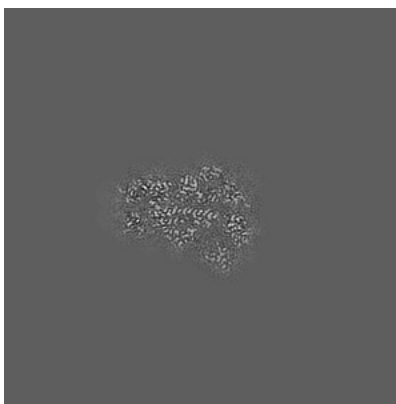
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

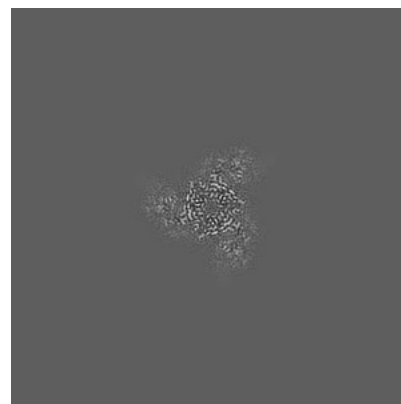
6.3.1 Primary map



X Index: 213



Y Index: 194

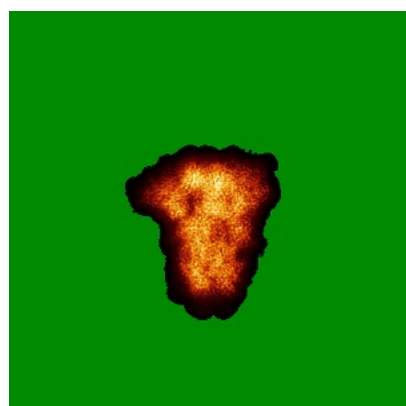


Z Index: 228

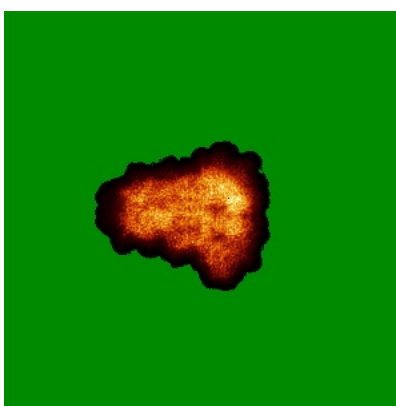
The images above show the largest variance slices of the map in three orthogonal directions.

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

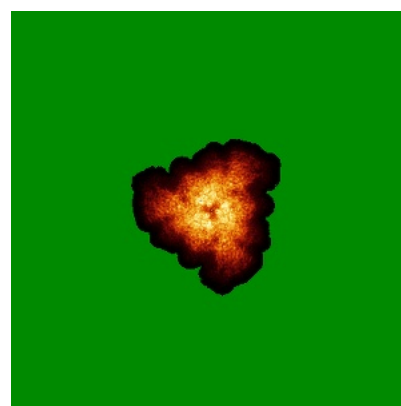
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

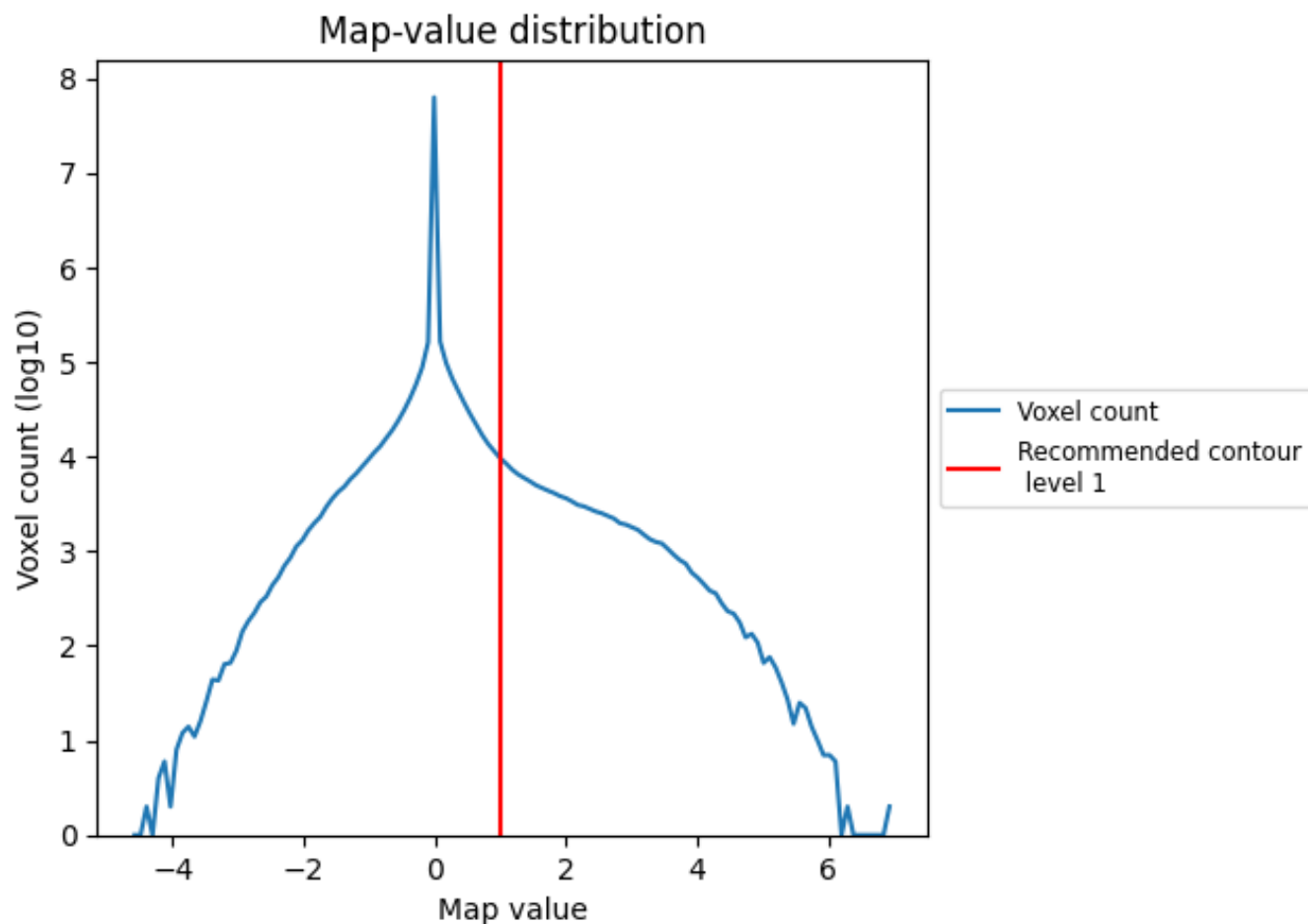
6.6 Mask visualisation

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

7 Map analysis [i](#)

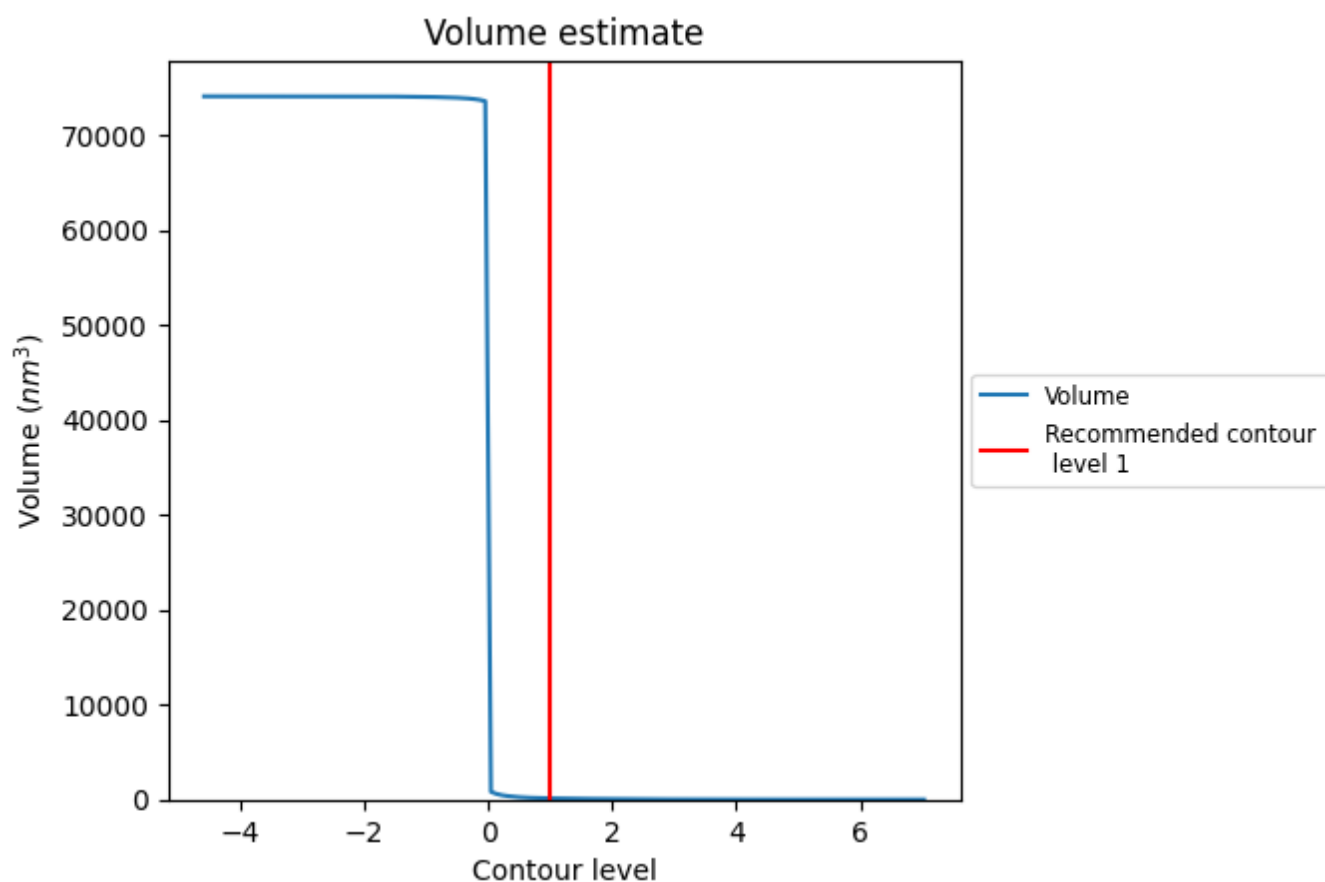
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

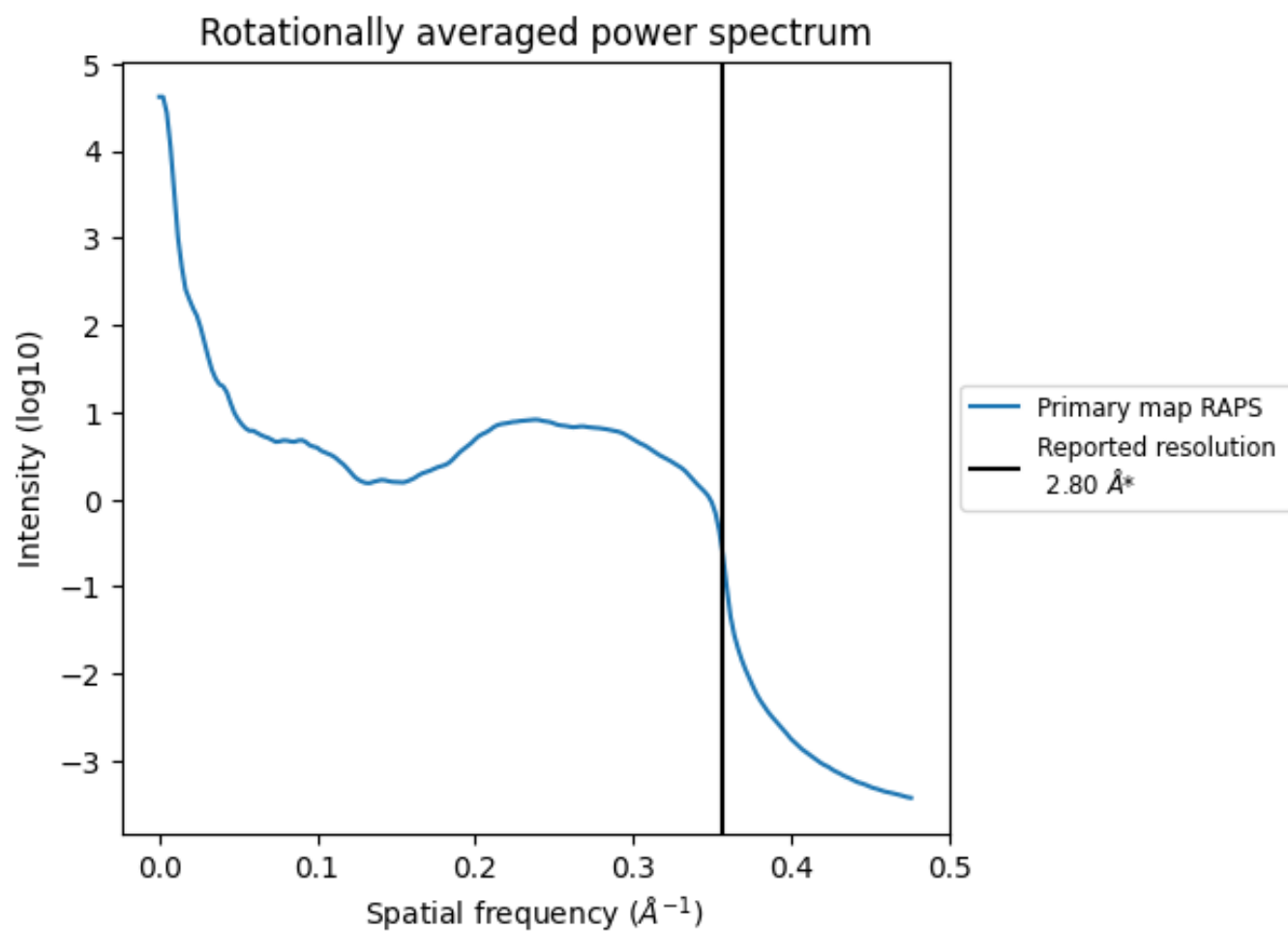
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 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 0.357 Å⁻¹

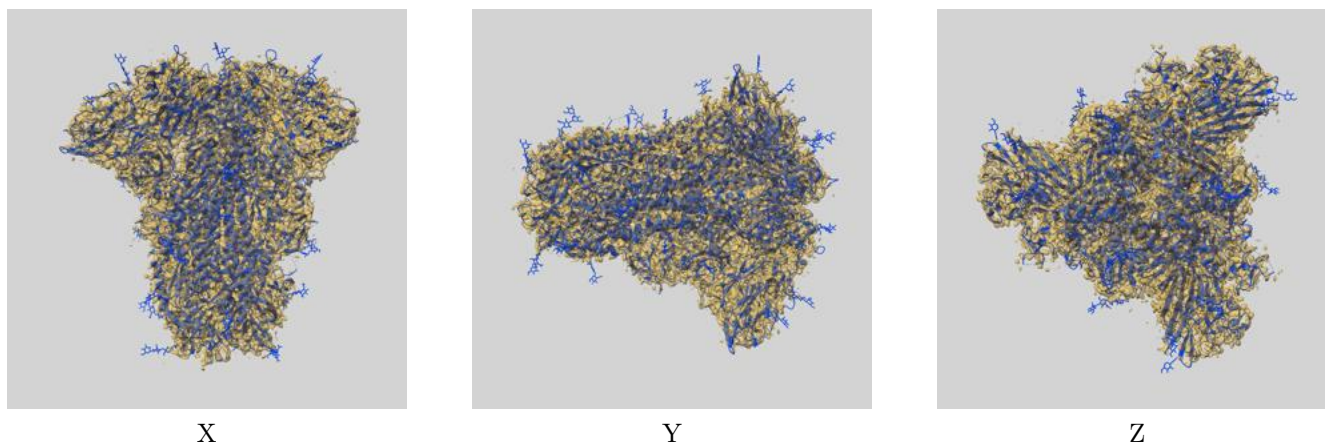
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

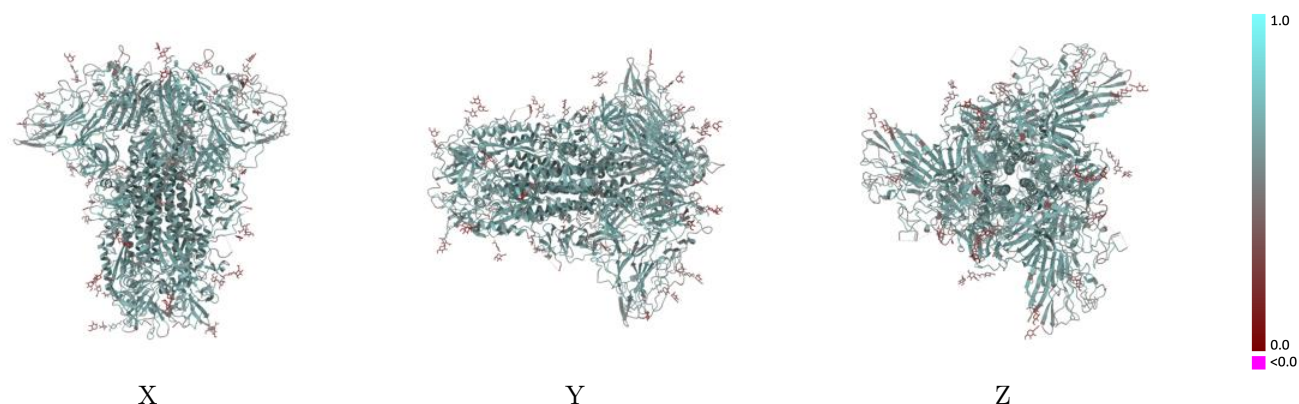
This section contains information regarding the fit between EMDB map EMD-0557 and PDB model 6NZK. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



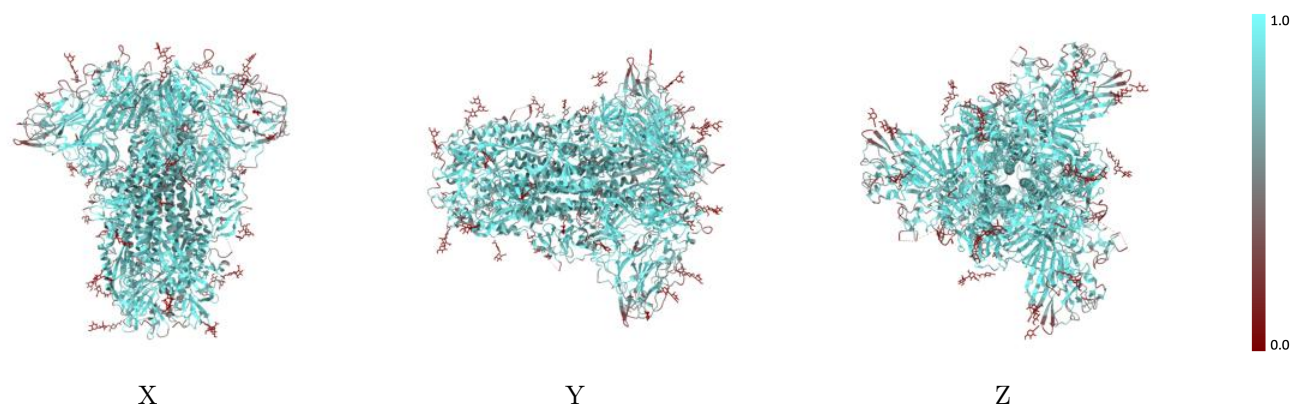
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



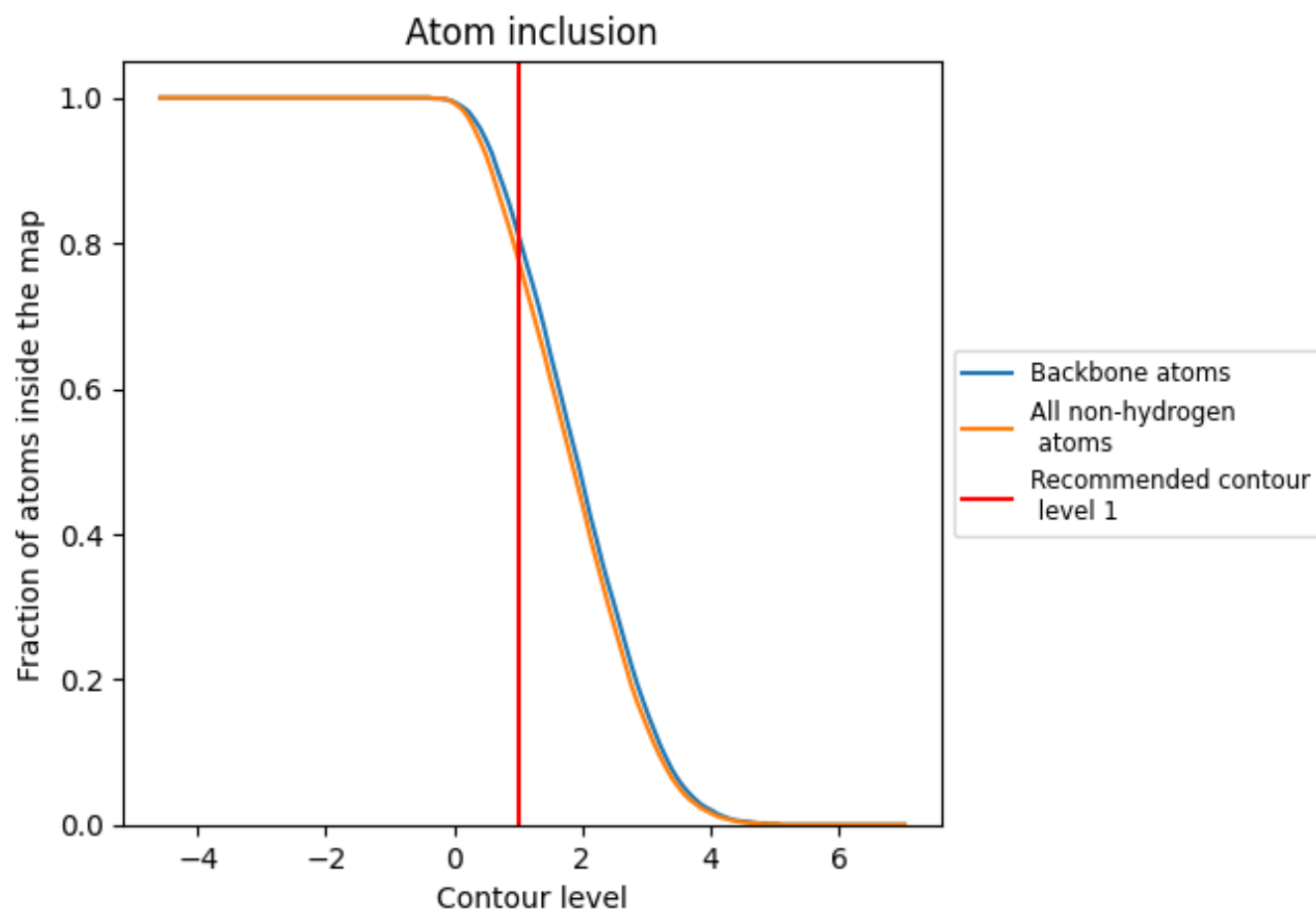
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.5910
A	 0.8090	 0.6030
B	 0.8070	 0.6030
C	 0.8100	 0.6030
D	 0.1030	 0.3390
E	 0.2310	 0.3880
F	 0.0400	 0.2490
G	 0.3330	 0.3100
H	 0.0260	 0.2520
I	 0.0000	 0.3210
J	 0.1600	 0.2880
K	 0.0000	 0.2340
L	 0.1790	 0.3520
M	 0.1030	 0.3800
N	 0.1030	 0.3190
O	 0.2310	 0.3980
P	 0.0400	 0.2670
Q	 0.3330	 0.3080
R	 0.0260	 0.2590
S	 0.0360	 0.3270
T	 0.1800	 0.2930
U	 0.0000	 0.2410
V	 0.1790	 0.3240
W	 0.0770	 0.3730
X	 0.1030	 0.3340
Y	 0.2050	 0.3910
Z	 0.0400	 0.2460
a	 0.3330	 0.2970
b	 0.0260	 0.2640
c	 0.0000	 0.3300
d	 0.1600	 0.2860
e	 0.0000	 0.2510
f	 0.1790	 0.3360
g	 0.0510	 0.3710

