



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:01 AM UTC

PDB ID : 6NB4 / pdb_00006nb4
EMDB ID : EMD-0402
Title : MERS-CoV S complex with human neutralizing LCA60 antibody Fab fragment (state 2)
Authors : Walls, A.C.; Xiong, X.; Park, Y.J.; Tortorici, M.A.; Snijder, S.; Quispe, J.; Cameroni, E.; Gopal, R.; Mian, D.; Lanzavecchia, A.; Zambon, M.; Rey, F.A.; Corti, D.; Veeler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-12-06
Resolution : 3.60 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:

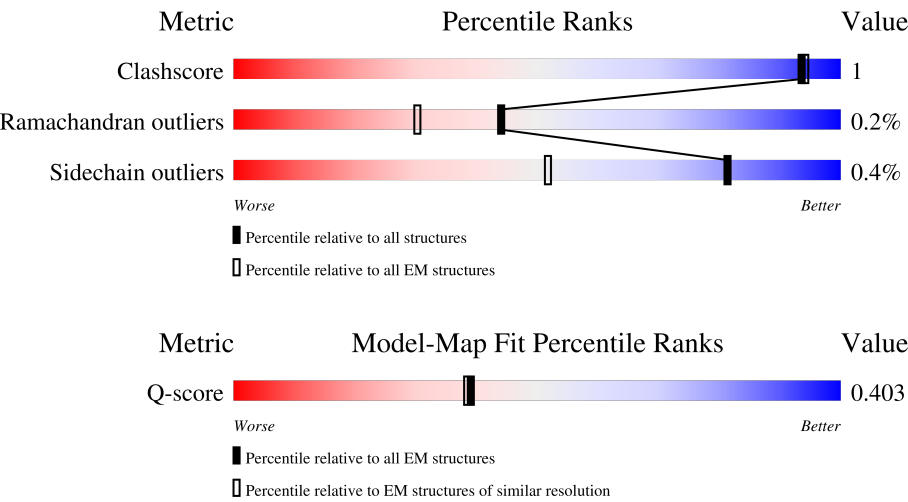
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1359	
1	B	1359	
1	C	1359	

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Mol	Chain	Length	Quality of chain
2	H	127	38% 94% ...
3	L	109	37% 94% ..
4	D	2	50% 50%
4	F	2	50% 100%
4	G	2	50% 100%
4	J	2	50% 100%
4	K	2	50% 100%
4	M	2	50% 100%
4	N	2	50% 100%
4	O	2	50% 100%
4	P	2	50% 100%
4	Q	2	100%
4	S	2	100%
4	T	2	50% 100%
4	V	2	50% 100%
4	Z	2	100%
4	a	2	100%
4	b	2	50% 100%
4	c	2	100%
4	d	2	50% 100%
4	e	2	100%
4	g	2	100%
4	h	2	50% 100%
4	j	2	50% 100%
4	l	2	100%

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Mol	Chain	Length	Quality of chain
4	m	2	50% 100%
4	n	2	100%
4	o	2	50% 100%
4	p	2	100%
5	E	5	20% 80% 20%
5	I	5	40% 100%
5	R	5	40% 100%
5	W	5	60% 100%
5	i	5	80% 20%
5	q	5	20% 100%
6	U	6	17% 83% 17%
7	X	4	25% 100%
7	f	4	25% 100%
8	Y	3	67% 100%
8	k	3	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26681 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	1169	Total	C	N	O	S	0	0
			9032	5739	1491	1752	50		
1	B	958	Total	C	N	O	S	0	0
			7402	4701	1232	1430	39		
1	C	959	Total	C	N	O	S	0	0
			7404	4699	1233	1433	39		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A140AYW5
A	-12	GLY	-	expression tag	UNP A0A140AYW5
A	-11	ILE	-	expression tag	UNP A0A140AYW5
A	-10	LEU	-	expression tag	UNP A0A140AYW5
A	-9	PRO	-	expression tag	UNP A0A140AYW5
A	-8	SER	-	expression tag	UNP A0A140AYW5
A	-7	PRO	-	expression tag	UNP A0A140AYW5
A	-6	GLY	-	expression tag	UNP A0A140AYW5
A	-5	MET	-	expression tag	UNP A0A140AYW5
A	-4	PRO	-	expression tag	UNP A0A140AYW5
A	-3	ALA	-	expression tag	UNP A0A140AYW5
A	-2	LEU	-	expression tag	UNP A0A140AYW5
A	-1	LEU	-	expression tag	UNP A0A140AYW5
A	0	SER	-	expression tag	UNP A0A140AYW5
A	1	LEU	-	expression tag	UNP A0A140AYW5
A	2	VAL	-	expression tag	UNP A0A140AYW5
A	3	SER	-	expression tag	UNP A0A140AYW5
A	4	LEU	-	expression tag	UNP A0A140AYW5
A	5	LEU	-	expression tag	UNP A0A140AYW5
A	6	SER	-	expression tag	UNP A0A140AYW5
A	7	VAL	-	expression tag	UNP A0A140AYW5
A	8	LEU	-	expression tag	UNP A0A140AYW5
A	9	LEU	-	expression tag	UNP A0A140AYW5
A	10	MET	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP A0A140AYW5
A	12	CYS	-	expression tag	UNP A0A140AYW5
A	13	VAL	-	expression tag	UNP A0A140AYW5
A	14	ALA	-	expression tag	UNP A0A140AYW5
A	15	GLU	-	expression tag	UNP A0A140AYW5
A	16	THR	-	expression tag	UNP A0A140AYW5
A	17	GLY	-	expression tag	UNP A0A140AYW5
A	18	THR	-	expression tag	UNP A0A140AYW5
A	529	ILE	THR	conflict	UNP A0A140AYW5
A	748	ALA	ARG	conflict	UNP A0A140AYW5
A	751	GLY	ARG	conflict	UNP A0A140AYW5
A	1020	GLN	ARG	conflict	UNP A0A140AYW5
A	1060	PRO	VAL	conflict	UNP A0A140AYW5
A	1061	PRO	LEU	conflict	UNP A0A140AYW5
A	1295	GLY	-	expression tag	UNP A0A140AYW5
A	1296	SER	-	expression tag	UNP A0A140AYW5
A	1297	GLY	-	expression tag	UNP A0A140AYW5
A	1298	ARG	-	expression tag	UNP A0A140AYW5
A	1299	GLU	-	expression tag	UNP A0A140AYW5
A	1300	ASN	-	expression tag	UNP A0A140AYW5
A	1301	LEU	-	expression tag	UNP A0A140AYW5
A	1302	TYR	-	expression tag	UNP A0A140AYW5
A	1303	PHE	-	expression tag	UNP A0A140AYW5
A	1304	GLN	-	expression tag	UNP A0A140AYW5
A	1305	GLY	-	expression tag	UNP A0A140AYW5
A	1306	GLY	-	expression tag	UNP A0A140AYW5
A	1307	GLY	-	expression tag	UNP A0A140AYW5
A	1308	GLY	-	expression tag	UNP A0A140AYW5
A	1309	SER	-	expression tag	UNP A0A140AYW5
A	1310	GLY	-	expression tag	UNP A0A140AYW5
A	1311	TYR	-	expression tag	UNP A0A140AYW5
A	1312	ILE	-	expression tag	UNP A0A140AYW5
A	1313	PRO	-	expression tag	UNP A0A140AYW5
A	1314	GLU	-	expression tag	UNP A0A140AYW5
A	1315	ALA	-	expression tag	UNP A0A140AYW5
A	1316	PRO	-	expression tag	UNP A0A140AYW5
A	1317	ARG	-	expression tag	UNP A0A140AYW5
A	1318	ASP	-	expression tag	UNP A0A140AYW5
A	1319	GLY	-	expression tag	UNP A0A140AYW5
A	1320	GLN	-	expression tag	UNP A0A140AYW5
A	1321	ALA	-	expression tag	UNP A0A140AYW5
A	1322	TYR	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1323	VAL	-	expression tag	UNP A0A140AYW5
A	1324	ARG	-	expression tag	UNP A0A140AYW5
A	1325	LYS	-	expression tag	UNP A0A140AYW5
A	1326	ASP	-	expression tag	UNP A0A140AYW5
A	1327	GLY	-	expression tag	UNP A0A140AYW5
A	1328	GLU	-	expression tag	UNP A0A140AYW5
A	1329	TRP	-	expression tag	UNP A0A140AYW5
A	1330	VAL	-	expression tag	UNP A0A140AYW5
A	1331	LEU	-	expression tag	UNP A0A140AYW5
A	1332	LEU	-	expression tag	UNP A0A140AYW5
A	1333	SER	-	expression tag	UNP A0A140AYW5
A	1334	THR	-	expression tag	UNP A0A140AYW5
A	1335	PHE	-	expression tag	UNP A0A140AYW5
A	1336	LEU	-	expression tag	UNP A0A140AYW5
A	1337	GLY	-	expression tag	UNP A0A140AYW5
A	1338	HIS	-	expression tag	UNP A0A140AYW5
A	1339	HIS	-	expression tag	UNP A0A140AYW5
A	1340	HIS	-	expression tag	UNP A0A140AYW5
A	1341	HIS	-	expression tag	UNP A0A140AYW5
A	1342	HIS	-	expression tag	UNP A0A140AYW5
A	1343	HIS	-	expression tag	UNP A0A140AYW5
A	1344	HIS	-	expression tag	UNP A0A140AYW5
A	1345	HIS	-	expression tag	UNP A0A140AYW5
B	-13	MET	-	initiating methionine	UNP A0A140AYW5
B	-12	GLY	-	expression tag	UNP A0A140AYW5
B	-11	ILE	-	expression tag	UNP A0A140AYW5
B	-10	LEU	-	expression tag	UNP A0A140AYW5
B	-9	PRO	-	expression tag	UNP A0A140AYW5
B	-8	SER	-	expression tag	UNP A0A140AYW5
B	-7	PRO	-	expression tag	UNP A0A140AYW5
B	-6	GLY	-	expression tag	UNP A0A140AYW5
B	-5	MET	-	expression tag	UNP A0A140AYW5
B	-4	PRO	-	expression tag	UNP A0A140AYW5
B	-3	ALA	-	expression tag	UNP A0A140AYW5
B	-2	LEU	-	expression tag	UNP A0A140AYW5
B	-1	LEU	-	expression tag	UNP A0A140AYW5
B	0	SER	-	expression tag	UNP A0A140AYW5
B	1	LEU	-	expression tag	UNP A0A140AYW5
B	2	VAL	-	expression tag	UNP A0A140AYW5
B	3	SER	-	expression tag	UNP A0A140AYW5
B	4	LEU	-	expression tag	UNP A0A140AYW5
B	5	LEU	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A0A140AYW5
B	7	VAL	-	expression tag	UNP A0A140AYW5
B	8	LEU	-	expression tag	UNP A0A140AYW5
B	9	LEU	-	expression tag	UNP A0A140AYW5
B	10	MET	-	expression tag	UNP A0A140AYW5
B	11	GLY	-	expression tag	UNP A0A140AYW5
B	12	CYS	-	expression tag	UNP A0A140AYW5
B	13	VAL	-	expression tag	UNP A0A140AYW5
B	14	ALA	-	expression tag	UNP A0A140AYW5
B	15	GLU	-	expression tag	UNP A0A140AYW5
B	16	THR	-	expression tag	UNP A0A140AYW5
B	17	GLY	-	expression tag	UNP A0A140AYW5
B	18	THR	-	expression tag	UNP A0A140AYW5
B	529	ILE	THR	conflict	UNP A0A140AYW5
B	748	ALA	ARG	conflict	UNP A0A140AYW5
B	751	GLY	ARG	conflict	UNP A0A140AYW5
B	1020	GLN	ARG	conflict	UNP A0A140AYW5
B	1060	PRO	VAL	conflict	UNP A0A140AYW5
B	1061	PRO	LEU	conflict	UNP A0A140AYW5
B	1295	GLY	-	expression tag	UNP A0A140AYW5
B	1296	SER	-	expression tag	UNP A0A140AYW5
B	1297	GLY	-	expression tag	UNP A0A140AYW5
B	1298	ARG	-	expression tag	UNP A0A140AYW5
B	1299	GLU	-	expression tag	UNP A0A140AYW5
B	1300	ASN	-	expression tag	UNP A0A140AYW5
B	1301	LEU	-	expression tag	UNP A0A140AYW5
B	1302	TYR	-	expression tag	UNP A0A140AYW5
B	1303	PHE	-	expression tag	UNP A0A140AYW5
B	1304	GLN	-	expression tag	UNP A0A140AYW5
B	1305	GLY	-	expression tag	UNP A0A140AYW5
B	1306	GLY	-	expression tag	UNP A0A140AYW5
B	1307	GLY	-	expression tag	UNP A0A140AYW5
B	1308	GLY	-	expression tag	UNP A0A140AYW5
B	1309	SER	-	expression tag	UNP A0A140AYW5
B	1310	GLY	-	expression tag	UNP A0A140AYW5
B	1311	TYR	-	expression tag	UNP A0A140AYW5
B	1312	ILE	-	expression tag	UNP A0A140AYW5
B	1313	PRO	-	expression tag	UNP A0A140AYW5
B	1314	GLU	-	expression tag	UNP A0A140AYW5
B	1315	ALA	-	expression tag	UNP A0A140AYW5
B	1316	PRO	-	expression tag	UNP A0A140AYW5
B	1317	ARG	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1318	ASP	-	expression tag	UNP A0A140AYW5
B	1319	GLY	-	expression tag	UNP A0A140AYW5
B	1320	GLN	-	expression tag	UNP A0A140AYW5
B	1321	ALA	-	expression tag	UNP A0A140AYW5
B	1322	TYR	-	expression tag	UNP A0A140AYW5
B	1323	VAL	-	expression tag	UNP A0A140AYW5
B	1324	ARG	-	expression tag	UNP A0A140AYW5
B	1325	LYS	-	expression tag	UNP A0A140AYW5
B	1326	ASP	-	expression tag	UNP A0A140AYW5
B	1327	GLY	-	expression tag	UNP A0A140AYW5
B	1328	GLU	-	expression tag	UNP A0A140AYW5
B	1329	TRP	-	expression tag	UNP A0A140AYW5
B	1330	VAL	-	expression tag	UNP A0A140AYW5
B	1331	LEU	-	expression tag	UNP A0A140AYW5
B	1332	LEU	-	expression tag	UNP A0A140AYW5
B	1333	SER	-	expression tag	UNP A0A140AYW5
B	1334	THR	-	expression tag	UNP A0A140AYW5
B	1335	PHE	-	expression tag	UNP A0A140AYW5
B	1336	LEU	-	expression tag	UNP A0A140AYW5
B	1337	GLY	-	expression tag	UNP A0A140AYW5
B	1338	HIS	-	expression tag	UNP A0A140AYW5
B	1339	HIS	-	expression tag	UNP A0A140AYW5
B	1340	HIS	-	expression tag	UNP A0A140AYW5
B	1341	HIS	-	expression tag	UNP A0A140AYW5
B	1342	HIS	-	expression tag	UNP A0A140AYW5
B	1343	HIS	-	expression tag	UNP A0A140AYW5
B	1344	HIS	-	expression tag	UNP A0A140AYW5
B	1345	HIS	-	expression tag	UNP A0A140AYW5
C	-13	MET	-	initiating methionine	UNP A0A140AYW5
C	-12	GLY	-	expression tag	UNP A0A140AYW5
C	-11	ILE	-	expression tag	UNP A0A140AYW5
C	-10	LEU	-	expression tag	UNP A0A140AYW5
C	-9	PRO	-	expression tag	UNP A0A140AYW5
C	-8	SER	-	expression tag	UNP A0A140AYW5
C	-7	PRO	-	expression tag	UNP A0A140AYW5
C	-6	GLY	-	expression tag	UNP A0A140AYW5
C	-5	MET	-	expression tag	UNP A0A140AYW5
C	-4	PRO	-	expression tag	UNP A0A140AYW5
C	-3	ALA	-	expression tag	UNP A0A140AYW5
C	-2	LEU	-	expression tag	UNP A0A140AYW5
C	-1	LEU	-	expression tag	UNP A0A140AYW5
C	0	SER	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LEU	-	expression tag	UNP A0A140AYW5
C	2	VAL	-	expression tag	UNP A0A140AYW5
C	3	SER	-	expression tag	UNP A0A140AYW5
C	4	LEU	-	expression tag	UNP A0A140AYW5
C	5	LEU	-	expression tag	UNP A0A140AYW5
C	6	SER	-	expression tag	UNP A0A140AYW5
C	7	VAL	-	expression tag	UNP A0A140AYW5
C	8	LEU	-	expression tag	UNP A0A140AYW5
C	9	LEU	-	expression tag	UNP A0A140AYW5
C	10	MET	-	expression tag	UNP A0A140AYW5
C	11	GLY	-	expression tag	UNP A0A140AYW5
C	12	CYS	-	expression tag	UNP A0A140AYW5
C	13	VAL	-	expression tag	UNP A0A140AYW5
C	14	ALA	-	expression tag	UNP A0A140AYW5
C	15	GLU	-	expression tag	UNP A0A140AYW5
C	16	THR	-	expression tag	UNP A0A140AYW5
C	17	GLY	-	expression tag	UNP A0A140AYW5
C	18	THR	-	expression tag	UNP A0A140AYW5
C	529	ILE	THR	conflict	UNP A0A140AYW5
C	748	ALA	ARG	conflict	UNP A0A140AYW5
C	751	GLY	ARG	conflict	UNP A0A140AYW5
C	1020	GLN	ARG	conflict	UNP A0A140AYW5
C	1060	PRO	VAL	conflict	UNP A0A140AYW5
C	1061	PRO	LEU	conflict	UNP A0A140AYW5
C	1295	GLY	-	expression tag	UNP A0A140AYW5
C	1296	SER	-	expression tag	UNP A0A140AYW5
C	1297	GLY	-	expression tag	UNP A0A140AYW5
C	1298	ARG	-	expression tag	UNP A0A140AYW5
C	1299	GLU	-	expression tag	UNP A0A140AYW5
C	1300	ASN	-	expression tag	UNP A0A140AYW5
C	1301	LEU	-	expression tag	UNP A0A140AYW5
C	1302	TYR	-	expression tag	UNP A0A140AYW5
C	1303	PHE	-	expression tag	UNP A0A140AYW5
C	1304	GLN	-	expression tag	UNP A0A140AYW5
C	1305	GLY	-	expression tag	UNP A0A140AYW5
C	1306	GLY	-	expression tag	UNP A0A140AYW5
C	1307	GLY	-	expression tag	UNP A0A140AYW5
C	1308	GLY	-	expression tag	UNP A0A140AYW5
C	1309	SER	-	expression tag	UNP A0A140AYW5
C	1310	GLY	-	expression tag	UNP A0A140AYW5
C	1311	TYR	-	expression tag	UNP A0A140AYW5
C	1312	ILE	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1313	PRO	-	expression tag	UNP A0A140AYW5
C	1314	GLU	-	expression tag	UNP A0A140AYW5
C	1315	ALA	-	expression tag	UNP A0A140AYW5
C	1316	PRO	-	expression tag	UNP A0A140AYW5
C	1317	ARG	-	expression tag	UNP A0A140AYW5
C	1318	ASP	-	expression tag	UNP A0A140AYW5
C	1319	GLY	-	expression tag	UNP A0A140AYW5
C	1320	GLN	-	expression tag	UNP A0A140AYW5
C	1321	ALA	-	expression tag	UNP A0A140AYW5
C	1322	TYR	-	expression tag	UNP A0A140AYW5
C	1323	VAL	-	expression tag	UNP A0A140AYW5
C	1324	ARG	-	expression tag	UNP A0A140AYW5
C	1325	LYS	-	expression tag	UNP A0A140AYW5
C	1326	ASP	-	expression tag	UNP A0A140AYW5
C	1327	GLY	-	expression tag	UNP A0A140AYW5
C	1328	GLU	-	expression tag	UNP A0A140AYW5
C	1329	TRP	-	expression tag	UNP A0A140AYW5
C	1330	VAL	-	expression tag	UNP A0A140AYW5
C	1331	LEU	-	expression tag	UNP A0A140AYW5
C	1332	LEU	-	expression tag	UNP A0A140AYW5
C	1333	SER	-	expression tag	UNP A0A140AYW5
C	1334	THR	-	expression tag	UNP A0A140AYW5
C	1335	PHE	-	expression tag	UNP A0A140AYW5
C	1336	LEU	-	expression tag	UNP A0A140AYW5
C	1337	GLY	-	expression tag	UNP A0A140AYW5
C	1338	HIS	-	expression tag	UNP A0A140AYW5
C	1339	HIS	-	expression tag	UNP A0A140AYW5
C	1340	HIS	-	expression tag	UNP A0A140AYW5
C	1341	HIS	-	expression tag	UNP A0A140AYW5
C	1342	HIS	-	expression tag	UNP A0A140AYW5
C	1343	HIS	-	expression tag	UNP A0A140AYW5
C	1344	HIS	-	expression tag	UNP A0A140AYW5
C	1345	HIS	-	expression tag	UNP A0A140AYW5

- Molecule 2 is a protein called LCA60 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	0	0
			738	467	134	135	2		

- Molecule 3 is a protein called LCA60 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			607	378	110	116	3		

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



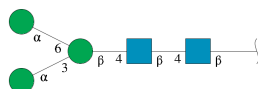
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	N	O		0	0
			28	16	2	10			
4	F	2	Total	C	N	O		0	0
			28	16	2	10			
4	G	2	Total	C	N	O		0	0
			28	16	2	10			
4	J	2	Total	C	N	O		0	0
			28	16	2	10			
4	K	2	Total	C	N	O		0	0
			28	16	2	10			
4	M	2	Total	C	N	O		0	0
			28	16	2	10			
4	N	2	Total	C	N	O		0	0
			28	16	2	10			
4	O	2	Total	C	N	O		0	0
			28	16	2	10			
4	P	2	Total	C	N	O		0	0
			28	16	2	10			
4	Q	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	T	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	Z	2	Total	C	N	O		0	0
			28	16	2	10			
4	a	2	Total	C	N	O		0	0
			28	16	2	10			
4	b	2	Total	C	N	O		0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	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	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	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	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



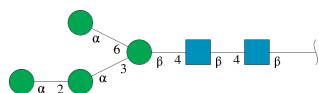
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	5	Total	C	N	O	0	0
			61	34	2	25		
5	I	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		
5	W	5	Total	C	N	O	0	0
			61	34	2	25		
5	i	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	q	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



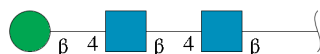
Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 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.



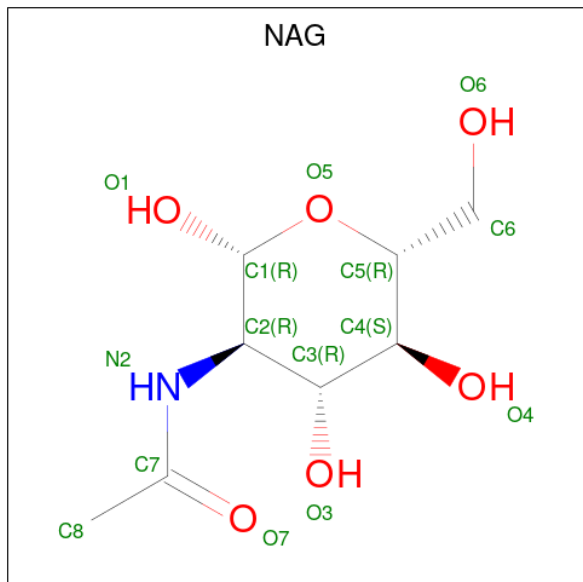
Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	4	Total	C	N	O	0	0
			50	28	2	20		
7	f	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 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.

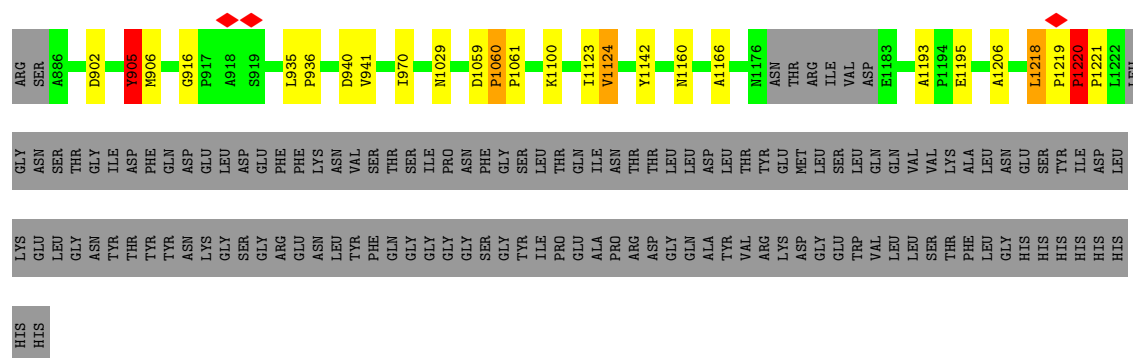


Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	3	Total	C	N	O	0	0
			39	22	2	15		
8	k	3	Total	C	N	O	0	0
			39	22	2	15		

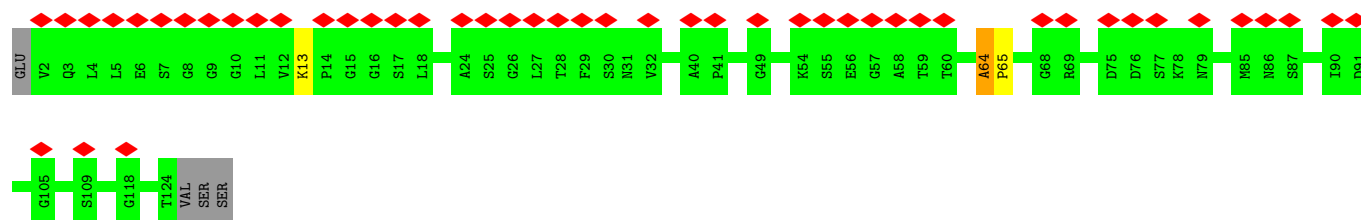
- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



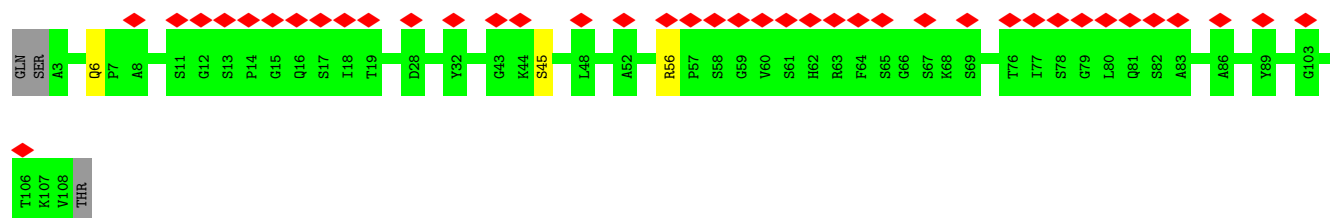
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	



- Molecule 2: LCA60 heavy chain



- Molecule 3: LCA60 light chain



- 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

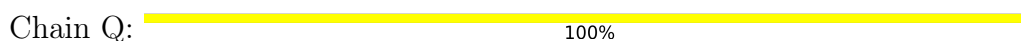




- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



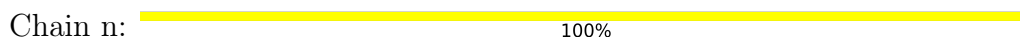
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- 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





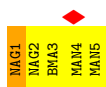
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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

Chain E: 20%
80%
20%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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

Chain I: 40%
100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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

Chain R: 40%
100%

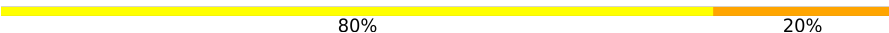


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 60%
100%

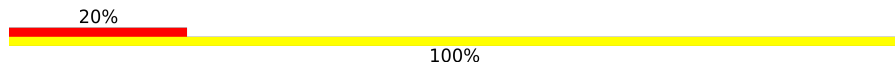


- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain i:  80% 20%



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain q:  20% 100%

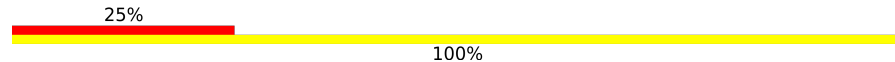


- Molecule 6: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain U:  17% 83% 17%

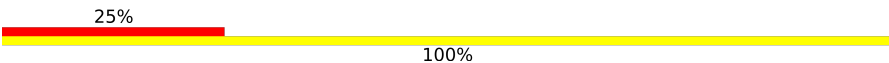


- Molecule 7: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  25% 100%

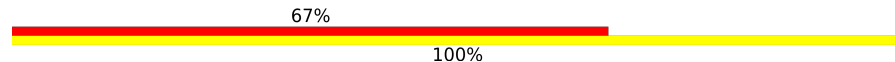


- Molecule 7: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain f:  25% 100%



- Molecule 8: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Y:  67% 100%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78719	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 ($e^-/\text{\AA}^2$)	45	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	4.392	Depositor
Minimum map value	-2.692	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	526.08, 526.08, 526.08	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, 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	0.68	1/9245 (0.0%)	0.96	108/12582 (0.9%)
1	B	0.67	1/7574 (0.0%)	0.93	78/10298 (0.8%)
1	C	0.68	1/7575 (0.0%)	0.95	74/10299 (0.7%)
2	H	0.58	0/759	0.90	4/1048 (0.4%)
3	L	0.52	0/622	1.05	6/859 (0.7%)
All	All	0.67	3/25775 (0.0%)	0.95	270/35086 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1220	PRO	CA-C	6.28	1.58	1.52
1	A	1220	PRO	CA-C	5.89	1.57	1.52
1	C	1220	PRO	CA-C	5.43	1.57	1.52

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	711	VAL	CB-CA-C	14.95	135.81	111.29
1	C	905	TYR	CB-CA-C	14.31	138.89	110.42
1	A	450	LEU	CB-CA-C	11.56	129.97	110.79
1	C	906	MET	N-CA-C	11.35	127.08	110.28
1	C	905	TYR	N-CA-C	-9.55	90.45	110.80
1	C	874	LEU	CD1-CG-CD2	9.33	131.33	110.80
1	A	874	LEU	CD1-CG-CD2	9.09	130.79	110.80
1	B	874	LEU	CD1-CG-CD2	9.06	130.73	110.80
1	A	451	SER	N-CA-C	8.86	123.50	112.87
1	C	906	MET	N-CA-CB	-8.29	97.79	109.97
1	A	22	GLY	CA-C-N	7.82	127.78	120.03
1	A	22	GLY	C-N-CA	7.82	127.78	120.03
1	C	22	GLY	CA-C-N	7.76	127.71	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	GLY	C-N-CA	7.76	127.71	120.03
1	A	1160	ASN	CA-C-N	7.71	127.43	119.56
1	A	1160	ASN	C-N-CA	7.71	127.43	119.56
1	B	22	GLY	CA-C-N	7.54	127.70	120.31
1	B	22	GLY	C-N-CA	7.54	127.70	120.31
1	B	1220	PRO	CB-CA-C	7.50	120.06	110.92
1	B	936	PRO	CA-C-N	7.48	127.39	120.21
1	B	936	PRO	C-N-CA	7.48	127.39	120.21
1	C	1219	PRO	N-CA-C	7.47	119.81	110.70
1	A	429	SER	CA-C-N	7.29	127.00	119.56
1	A	429	SER	C-N-CA	7.29	127.00	119.56
1	A	936	PRO	CA-C-N	7.23	127.18	120.03
1	A	936	PRO	C-N-CA	7.23	127.18	120.03
1	A	393	PRO	CA-C-N	7.20	127.63	119.92
1	A	393	PRO	C-N-CA	7.20	127.63	119.92
1	B	144	TYR	CA-C-N	7.16	127.08	119.85
1	B	144	TYR	C-N-CA	7.16	127.08	119.85
1	A	144	TYR	CA-C-N	7.12	127.29	120.31
1	A	144	TYR	C-N-CA	7.12	127.29	120.31
1	A	916	GLY	CA-C-N	7.10	127.02	119.85
1	A	916	GLY	C-N-CA	7.10	127.02	119.85
1	A	296	ILE	CA-C-N	7.06	127.05	119.78
1	A	296	ILE	C-N-CA	7.06	127.05	119.78
1	C	144	TYR	CA-C-N	7.05	126.98	119.85
1	C	144	TYR	C-N-CA	7.05	126.98	119.85
1	C	936	PRO	CA-C-N	7.02	126.98	120.03
1	C	936	PRO	C-N-CA	7.02	126.98	120.03
1	B	709	THR	CA-C-N	7.00	126.70	119.56
1	B	709	THR	C-N-CA	7.00	126.70	119.56
1	C	195	CYS	CA-C-N	6.99	127.58	119.47
1	C	195	CYS	C-N-CA	6.99	127.58	119.47
1	C	1160	ASN	CA-C-N	6.97	127.56	119.47
1	C	1160	ASN	C-N-CA	6.97	127.56	119.47
1	A	530	VAL	CA-C-N	6.93	126.86	120.21
1	A	530	VAL	C-N-CA	6.93	126.86	120.21
1	A	729	LEU	CA-C-N	6.93	127.48	120.14
1	A	729	LEU	C-N-CA	6.93	127.48	120.14
1	A	195	CYS	CA-C-N	6.89	127.46	119.47
1	A	195	CYS	C-N-CA	6.89	127.46	119.47
1	B	1193	ALA	CA-C-N	6.86	126.90	119.90
1	B	1193	ALA	C-N-CA	6.86	126.90	119.90
1	A	493	LYS	CA-C-N	6.84	127.24	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	LYS	C-N-CA	6.84	127.24	119.92
1	B	195	CYS	CA-C-N	6.83	127.40	119.47
1	B	195	CYS	C-N-CA	6.83	127.40	119.47
1	A	705	GLY	CA-C-N	6.81	126.73	119.85
1	A	705	GLY	C-N-CA	6.81	126.73	119.85
1	A	524	SER	CA-C-N	6.81	126.50	119.56
1	A	524	SER	C-N-CA	6.81	126.50	119.56
1	A	1142	TYR	CA-C-N	6.79	126.96	120.31
1	A	1142	TYR	C-N-CA	6.79	126.96	120.31
1	B	1142	TYR	CA-C-N	6.75	126.93	120.31
1	B	1142	TYR	C-N-CA	6.75	126.93	120.31
1	A	1219	PRO	N-CA-C	6.75	118.93	110.70
1	C	1142	TYR	CA-C-N	6.72	126.89	120.31
1	C	1142	TYR	C-N-CA	6.72	126.89	120.31
1	B	657	VAL	CA-C-N	6.71	126.67	119.76
1	B	657	VAL	C-N-CA	6.71	126.67	119.76
1	C	657	VAL	CA-C-N	6.70	126.66	119.76
1	C	657	VAL	C-N-CA	6.70	126.66	119.76
1	A	484	VAL	CA-C-N	6.66	126.63	120.03
1	A	484	VAL	C-N-CA	6.66	126.63	120.03
1	C	133	SER	CA-C-N	6.66	127.19	119.47
1	C	133	SER	C-N-CA	6.66	127.19	119.47
1	A	133	SER	CA-C-N	6.63	127.16	119.47
1	A	133	SER	C-N-CA	6.63	127.16	119.47
1	C	75	PHE	CA-C-N	6.62	126.58	120.03
1	C	75	PHE	C-N-CA	6.62	126.58	120.03
1	A	46	ARG	CA-C-N	6.60	126.56	120.03
1	A	46	ARG	C-N-CA	6.60	126.56	120.03
1	C	738	LEU	CA-C-N	6.58	126.76	120.31
1	C	738	LEU	C-N-CA	6.58	126.76	120.31
1	B	133	SER	CA-C-N	6.55	127.07	119.47
1	B	133	SER	C-N-CA	6.55	127.07	119.47
1	A	766	HIS	CA-C-N	6.55	126.51	120.03
1	A	766	HIS	C-N-CA	6.55	126.51	120.03
1	C	705	GLY	CA-C-N	6.53	127.06	120.14
1	C	705	GLY	C-N-CA	6.53	127.06	120.14
1	B	902	ASP	CA-C-N	6.52	126.43	119.85
1	B	902	ASP	C-N-CA	6.52	126.43	119.85
1	B	369	LYS	CA-C-N	6.50	126.46	119.76
1	B	369	LYS	C-N-CA	6.50	126.46	119.76
3	L	56	ARG	CA-C-N	6.50	126.47	119.78
3	L	56	ARG	C-N-CA	6.50	126.47	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1193	ALA	CA-C-N	6.47	126.50	119.90
1	A	1193	ALA	C-N-CA	6.47	126.50	119.90
1	C	1059	ASP	CA-C-N	6.41	126.98	120.38
1	C	1059	ASP	C-N-CA	6.41	126.98	120.38
1	C	766	HIS	CA-C-N	6.41	126.86	120.52
1	C	766	HIS	C-N-CA	6.41	126.86	120.52
1	A	782	ILE	CA-C-N	6.40	126.31	119.85
1	A	782	ILE	C-N-CA	6.40	126.31	119.85
1	C	296	ILE	CA-C-N	6.40	126.37	119.78
1	C	296	ILE	C-N-CA	6.40	126.37	119.78
1	C	902	ASP	CA-C-N	6.38	126.35	119.78
1	C	902	ASP	C-N-CA	6.38	126.35	119.78
1	A	738	LEU	CA-C-N	6.37	126.55	120.31
1	A	738	LEU	C-N-CA	6.37	126.55	120.31
1	A	970	ILE	CA-C-N	6.34	126.29	119.76
1	A	970	ILE	C-N-CA	6.34	126.29	119.76
1	B	766	HIS	CA-C-N	6.34	126.31	120.03
1	B	766	HIS	C-N-CA	6.34	126.31	120.03
1	A	709	THR	CA-C-N	6.34	127.76	119.84
1	A	709	THR	C-N-CA	6.34	127.76	119.84
1	A	902	ASP	CA-C-N	6.33	126.25	119.85
1	A	902	ASP	C-N-CA	6.33	126.25	119.85
1	A	451	SER	N-CA-CB	-6.33	98.80	110.32
1	A	1220	PRO	CB-CA-C	6.31	118.62	110.92
1	C	782	ILE	CA-C-N	6.30	126.22	119.85
1	C	782	ILE	C-N-CA	6.30	126.22	119.85
1	A	369	LYS	CA-C-N	6.30	126.25	119.76
1	A	369	LYS	C-N-CA	6.30	126.25	119.76
1	A	546	SER	CA-C-N	6.30	126.78	119.47
1	A	546	SER	C-N-CA	6.30	126.78	119.47
1	B	712	GLY	N-CA-C	-6.30	99.63	111.66
3	L	6	GLN	CA-C-N	6.29	126.26	119.78
3	L	6	GLN	C-N-CA	6.29	126.26	119.78
1	C	369	LYS	CA-C-N	6.29	126.20	119.85
1	C	369	LYS	C-N-CA	6.29	126.20	119.85
1	C	96	THR	CA-C-N	6.28	126.25	119.78
1	C	96	THR	C-N-CA	6.28	126.25	119.78
1	A	96	THR	CA-C-N	6.26	126.22	119.78
1	A	96	THR	C-N-CA	6.26	126.22	119.78
1	A	1206	ALA	CA-C-N	6.25	126.22	119.78
1	A	1206	ALA	C-N-CA	6.25	126.22	119.78
1	B	1219	PRO	N-CA-C	6.23	118.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	THR	CA-C-N	6.22	126.19	119.78
1	B	96	THR	C-N-CA	6.22	126.19	119.78
1	B	916	GLY	CA-C-N	6.21	126.72	120.14
1	B	916	GLY	C-N-CA	6.21	126.72	120.14
1	C	46	ARG	CA-C-N	6.20	126.17	120.03
1	C	46	ARG	C-N-CA	6.20	126.17	120.03
1	A	1059	ASP	CA-C-N	6.16	126.72	120.38
1	A	1059	ASP	C-N-CA	6.16	126.72	120.38
1	A	514	VAL	CA-C-N	6.13	126.15	119.89
1	A	514	VAL	C-N-CA	6.13	126.15	119.89
1	A	935	LEU	CA-C-N	6.12	126.68	120.38
1	A	935	LEU	C-N-CA	6.12	126.68	120.38
1	A	209	THR	CA-C-N	6.11	125.79	119.56
1	A	209	THR	C-N-CA	6.11	125.79	119.56
1	B	296	ILE	CA-C-N	6.10	126.06	119.78
1	B	296	ILE	C-N-CA	6.10	126.06	119.78
1	B	970	ILE	CA-C-N	6.09	126.03	119.76
1	B	970	ILE	C-N-CA	6.09	126.03	119.76
1	B	209	THR	CA-C-N	6.08	125.77	119.56
1	B	209	THR	C-N-CA	6.08	125.77	119.56
1	B	738	LEU	CA-C-N	6.08	126.00	119.85
1	B	738	LEU	C-N-CA	6.08	126.00	119.85
1	B	705	GLY	CA-C-N	6.07	126.58	120.14
1	B	705	GLY	C-N-CA	6.07	126.58	120.14
1	A	75	PHE	CA-C-N	6.07	125.98	119.85
1	A	75	PHE	C-N-CA	6.07	125.98	119.85
1	A	657	VAL	CA-C-N	6.06	125.82	119.76
1	A	657	VAL	C-N-CA	6.06	125.82	119.76
1	B	1206	ALA	CA-C-N	6.06	126.00	119.76
1	B	1206	ALA	C-N-CA	6.06	126.00	119.76
1	B	1160	ASN	CA-C-N	6.06	127.41	119.84
1	B	1160	ASN	C-N-CA	6.06	127.41	119.84
1	C	1206	ALA	CA-C-N	6.05	125.99	119.76
1	C	1206	ALA	C-N-CA	6.05	125.99	119.76
1	C	209	THR	CA-C-N	6.04	125.72	119.56
1	C	209	THR	C-N-CA	6.04	125.72	119.56
1	B	782	ILE	CA-C-N	6.02	125.93	119.85
1	B	782	ILE	C-N-CA	6.02	125.93	119.85
1	B	46	ARG	CA-C-N	6.01	125.98	120.03
1	B	46	ARG	C-N-CA	6.01	125.98	120.03
1	A	1166	ALA	CA-C-N	6.01	125.92	119.85
1	A	1166	ALA	C-N-CA	6.01	125.92	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	GLU	CA-C-N	6.00	125.94	119.76
1	A	875	GLU	C-N-CA	6.00	125.94	119.76
1	A	172	LEU	CA-C-N	5.99	125.93	119.76
1	A	172	LEU	C-N-CA	5.99	125.93	119.76
1	C	1193	ALA	CA-C-N	5.96	126.31	119.93
1	C	1193	ALA	C-N-CA	5.96	126.31	119.93
1	C	935	LEU	CA-C-N	5.95	126.51	120.38
1	C	935	LEU	C-N-CA	5.95	126.51	120.38
1	C	970	ILE	CA-C-N	5.90	125.83	119.76
1	C	970	ILE	C-N-CA	5.90	125.83	119.76
1	A	392	THR	CA-C-N	5.86	126.41	120.38
1	A	392	THR	C-N-CA	5.86	126.41	120.38
1	B	1060	PRO	CA-C-N	5.78	125.48	119.82
1	B	1060	PRO	C-N-CA	5.78	125.48	119.82
1	A	585	CYS	CA-C-N	5.77	125.75	120.21
1	A	585	CYS	C-N-CA	5.77	125.75	120.21
1	B	75	PHE	CA-C-N	5.77	125.67	119.85
1	B	75	PHE	C-N-CA	5.77	125.67	119.85
3	L	45	SER	CA-C-N	5.74	125.65	119.85
3	L	45	SER	C-N-CA	5.74	125.65	119.85
1	B	1059	ASP	CA-C-N	5.74	126.29	120.38
1	B	1059	ASP	C-N-CA	5.74	126.29	120.38
1	B	935	LEU	CA-C-N	5.72	126.28	120.38
1	B	935	LEU	C-N-CA	5.72	126.28	120.38
2	H	64	ALA	CA-C-N	5.72	125.39	119.56
2	H	64	ALA	C-N-CA	5.72	125.39	119.56
2	H	13	LYS	CA-C-N	5.72	125.73	119.90
2	H	13	LYS	C-N-CA	5.72	125.73	119.90
1	B	729	LEU	CA-C-N	5.71	126.20	120.14
1	B	729	LEU	C-N-CA	5.71	126.20	120.14
1	B	1195	GLU	CA-C-N	5.68	125.61	119.76
1	B	1195	GLU	C-N-CA	5.68	125.61	119.76
1	C	1218	LEU	CA-C-N	5.67	126.22	120.38
1	C	1218	LEU	C-N-CA	5.67	126.22	120.38
1	B	875	GLU	CA-C-N	5.67	125.59	119.76
1	B	875	GLU	C-N-CA	5.67	125.59	119.76
1	C	1220	PRO	N-CA-C	5.61	117.54	110.70
1	A	450	LEU	CB-CG-CD1	5.60	127.49	110.70
1	C	1166	ALA	CA-C-N	5.56	125.46	119.85
1	C	1166	ALA	C-N-CA	5.56	125.46	119.85
1	B	1166	ALA	CA-C-N	5.52	125.43	119.85
1	B	1166	ALA	C-N-CA	5.52	125.43	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	GLN	CA-C-N	5.51	126.72	119.84
1	A	319	GLN	C-N-CA	5.51	126.72	119.84
1	A	859	SER	CA-C-N	5.46	125.36	119.85
1	A	859	SER	C-N-CA	5.46	125.36	119.85
1	A	1060	PRO	CA-C-N	5.45	125.12	119.56
1	A	1060	PRO	C-N-CA	5.45	125.12	119.56
1	C	1060	PRO	CA-C-N	5.44	125.11	119.56
1	C	1060	PRO	C-N-CA	5.44	125.11	119.56
1	C	729	LEU	CA-C-N	5.43	126.63	119.84
1	C	729	LEU	C-N-CA	5.43	126.63	119.84
1	C	916	GLY	CA-C-N	5.43	125.35	119.76
1	C	916	GLY	C-N-CA	5.43	125.35	119.76
1	C	875	GLU	CA-C-N	5.42	125.34	119.76
1	C	875	GLU	C-N-CA	5.42	125.34	119.76
1	B	319	GLN	CA-C-N	5.42	126.61	119.84
1	B	319	GLN	C-N-CA	5.42	126.61	119.84
1	B	44	TRP	CA-C-N	5.41	125.72	119.93
1	B	44	TRP	C-N-CA	5.41	125.72	119.93
1	C	859	SER	CA-C-N	5.37	125.28	119.85
1	C	859	SER	C-N-CA	5.37	125.28	119.85
1	A	1195	GLU	CA-C-N	5.36	125.28	119.76
1	A	1195	GLU	C-N-CA	5.36	125.28	119.76
1	A	58	TYR	CA-C-N	5.35	125.66	119.93
1	A	58	TYR	C-N-CA	5.35	125.66	119.93
1	A	629	ARG	N-CA-C	5.32	119.39	113.01
1	A	44	TRP	CA-C-N	5.28	125.53	119.83
1	A	44	TRP	C-N-CA	5.28	125.53	119.83
1	B	1218	LEU	CA-C-N	5.27	125.81	120.38
1	B	1218	LEU	C-N-CA	5.27	125.81	120.38
1	C	1195	GLU	CA-C-N	5.22	125.14	119.76
1	C	1195	GLU	C-N-CA	5.22	125.14	119.76
1	B	188	GLU	CA-C-N	5.20	125.12	119.76
1	B	188	GLU	C-N-CA	5.20	125.12	119.76
1	A	188	GLU	CA-C-N	5.19	125.11	119.76
1	A	188	GLU	C-N-CA	5.19	125.11	119.76
1	C	188	GLU	CA-C-N	5.19	124.95	119.76
1	C	188	GLU	C-N-CA	5.19	124.95	119.76
1	A	1218	LEU	CA-C-N	5.16	125.69	120.38
1	A	1218	LEU	C-N-CA	5.16	125.69	120.38
1	B	859	SER	CA-C-N	5.13	125.03	119.85
1	B	859	SER	C-N-CA	5.13	125.03	119.85
1	C	1060	PRO	N-CA-C	5.10	116.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	SER	CA-C-N	5.05	124.50	119.24
1	A	386	SER	C-N-CA	5.05	124.50	119.24
1	B	113	ALA	CB-CA-C	-5.02	110.41	117.23
1	A	475	ASN	CA-C-N	5.01	125.24	119.83
1	A	475	ASN	C-N-CA	5.01	125.24	119.83

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	9032	0	8702	26	0
1	B	7402	0	7113	23	0
1	C	7404	0	7113	20	0
2	H	738	0	460	1	0
3	L	607	0	365	0	0
4	D	28	0	25	1	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	V	28	0	25	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	j	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	0	0
4	o	28	0	25	0	0
4	p	28	0	25	0	0
5	E	61	0	49	1	0
5	I	61	0	49	0	0
5	R	61	0	49	0	0
5	W	61	0	49	0	0
5	i	61	0	49	1	0
5	q	61	0	49	0	0
6	U	72	0	58	1	0
7	X	50	0	41	0	0
7	f	50	0	41	0	0
8	Y	39	0	33	0	0
8	k	39	0	33	0	0
9	A	56	0	52	0	0
9	B	14	0	13	0	0
9	C	56	0	52	0	0
All	All	26681	0	25045	65	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 (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:SER:HB2	1:C:905:TYR:O	1.23	1.31
1:B:676:SER:CB	1:C:905:TYR:O	1.99	1.10
1:C:592:ASN:N	1:C:592:ASN:OD1	2.28	0.66
1:B:1220:PRO:HB2	1:B:1221:PRO:HD3	1.81	0.61
1:A:419:SER:HG	1:A:483:THR:HG1	1.50	0.59
1:A:419:SER:OG	1:A:483:THR:OG1	2.25	0.55
1:A:462:GLY:N	1:A:463:PRO:CD	2.70	0.55
2:H:64:ALA:N	2:H:65:PRO:CD	2.71	0.54
1:B:306:ASP:OD1	1:B:308:LYS:NZ	2.41	0.54
1:B:1039:GLU:OE2	1:C:830:LYS:NZ	2.41	0.53
1:A:306:ASP:OD1	1:A:308:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:OE1	1:A:413:LYS:NZ	2.43	0.52
1:B:948:THR:OG1	1:B:1129:ASN:ND2	2.42	0.52
1:A:246:THR:O	1:A:269:ARG:NH2	2.44	0.51
1:C:1220:PRO:CG	1:C:1221:PRO:HD3	2.40	0.51
1:B:1220:PRO:CB	1:B:1221:PRO:HD3	2.40	0.51
1:C:306:ASP:OD1	1:C:308:LYS:NZ	2.44	0.50
1:A:386:SER:N	1:A:387:PRO:CD	2.75	0.50
1:A:709:THR:OG1	1:A:712:GLY:O	2.29	0.49
1:C:1220:PRO:HG2	1:C:1221:PRO:HD3	1.95	0.49
1:C:124:ALA:HB3	5:i:1:NAG:H82	1.95	0.49
1:B:124:ALA:HB3	6:U:1:NAG:H82	1.93	0.49
1:A:80:ASP:OD1	1:A:81:HIS:N	2.45	0.48
1:C:690:SER:O	1:C:691:ARG:C	2.55	0.48
1:B:119:ARG:NH1	1:B:316:TYR:OH	2.45	0.48
1:B:676:SER:HB3	1:C:905:TYR:O	2.05	0.47
1:B:83:ASP:OD2	1:B:110:LYS:NZ	2.48	0.47
1:A:124:ALA:HB3	5:E:1:NAG:H82	1.96	0.47
1:B:1219:PRO:HG2	1:B:1220:PRO:HD3	1.96	0.47
1:B:111:GLN:O	1:B:317:LYS:NZ	2.47	0.47
1:B:1218:LEU:H	1:B:1218:LEU:HD23	1.80	0.46
1:C:343:ASP:N	1:C:343:ASP:OD1	2.44	0.46
1:A:343:ASP:OD1	1:A:343:ASP:N	2.45	0.46
1:A:877:VAL:O	1:A:878:SER:C	2.58	0.46
1:C:1218:LEU:H	1:C:1218:LEU:HD23	1.80	0.46
1:A:940:ASP:OD1	1:A:941:VAL:N	2.50	0.45
1:B:677:VAL:HG12	1:B:679:CYS:H	1.82	0.44
1:C:83:ASP:OD2	1:C:110:LYS:NZ	2.50	0.44
1:A:83:ASP:OD2	1:A:110:LYS:NZ	2.48	0.44
1:A:1220:PRO:HB2	1:A:1221:PRO:HD3	1.99	0.44
1:C:1123:ILE:O	1:C:1124:VAL:C	2.61	0.44
1:A:505:ARG:NH2	1:A:549:GLU:O	2.49	0.43
1:B:1115:GLY:O	1:C:1100:LYS:NZ	2.49	0.43
1:B:877:VAL:O	1:B:878:SER:C	2.62	0.43
1:A:450:LEU:HD12	1:A:450:LEU:O	2.18	0.43
1:B:1220:PRO:HG2	1:B:1221:PRO:CD	2.49	0.43
1:C:800:GLN:HB2	1:C:1029:ASN:HD21	1.84	0.43
1:A:261:GLN:OE1	1:A:261:GLN:N	2.52	0.42
1:B:343:ASP:OD1	1:B:343:ASP:N	2.48	0.42
1:A:1060:PRO:N	1:A:1061:PRO:CD	2.82	0.41
1:A:1219:PRO:N	1:A:1220:PRO:CD	2.83	0.41
1:C:261:GLN:OE1	1:C:261:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1060:PRO:N	1:B:1061:PRO:CD	2.83	0.41
1:A:107:GLN:HB2	4:D:1:NAG:H82	2.02	0.41
1:A:328:SER:OG	1:A:330:ASP:OD1	2.37	0.41
1:C:877:VAL:O	1:C:878:SER:C	2.62	0.41
1:A:1220:PRO:HG2	1:A:1221:PRO:CD	2.51	0.41
1:C:1060:PRO:N	1:C:1061:PRO:CD	2.84	0.41
1:C:940:ASP:OD1	1:C:941:VAL:N	2.52	0.40
1:A:677:VAL:HG12	1:A:679:CYS:H	1.87	0.40
1:A:1220:PRO:CB	1:A:1221:PRO:HD3	2.51	0.40
1:B:202:THR:OG1	1:B:203:SER:N	2.54	0.40
1:B:1060:PRO:HB2	1:B:1061:PRO:HD3	2.04	0.40
1:B:1220:PRO:CB	1:B:1221:PRO:CD	2.99	0.40
1:A:1062:GLU:O	1:A:1063:GLN:C	2.64	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	1159/1359 (85%)	1123 (97%)	35 (3%)	1 (0%)	48	79
1	B	946/1359 (70%)	920 (97%)	24 (2%)	2 (0%)	43	72
1	C	947/1359 (70%)	921 (97%)	21 (2%)	5 (0%)	24	57
2	H	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
3	L	104/109 (95%)	100 (96%)	4 (4%)	0	100	100
All	All	3277/4313 (76%)	3183 (97%)	86 (3%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1220	PRO

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Mol	Chain	Res	Type
1	A	1220	PRO
1	C	905	TYR
1	C	1220	PRO
1	B	904	GLY
1	C	711	VAL
1	C	99	LYS
1	C	1124	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	1003/1167 (86%)	997 (99%)	6 (1%)	78	79
1	B	811/1167 (70%)	808 (100%)	3 (0%)	84	81
1	C	811/1167 (70%)	808 (100%)	3 (0%)	84	81
2	H	29/105 (28%)	29 (100%)	0	100	100
3	L	22/89 (25%)	22 (100%)	0	100	100
All	All	2676/3695 (72%)	2664 (100%)	12 (0%)	81	81

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

Mol	Chain	Res	Type
1	A	450	LEU
1	A	487	ASN
1	A	587	LYS
1	A	874	LEU
1	A	890	ILE
1	A	1033	LEU
1	B	592	ASN
1	B	728	LYS
1	B	874	LEU
1	C	62	ARG
1	C	592	ASN
1	C	874	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN
1	A	519	ASN
1	A	522	GLN
1	A	766	HIS
1	A	1212	GLN
1	B	81	HIS
1	B	91	HIS
1	B	766	HIS
1	B	836	HIS
1	B	1063	GLN
1	B	1129	ASN
1	C	81	HIS
1	C	91	HIS
1	C	628	GLN
1	C	766	HIS
1	C	836	HIS

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](#)

104 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	2.04	3 (21%)	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	2	4	14,14,15	2.10	2 (14%)	17,19,21	0.93	1 (5%)
5	NAG	E	1	1,5	14,14,15	2.05	4 (28%)	17,19,21	0.96	1 (5%)
5	NAG	E	2	5	14,14,15	2.14	5 (35%)	17,19,21	0.98	1 (5%)
5	BMA	E	3	5	11,11,12	1.91	3 (27%)	15,15,17	0.93	1 (6%)
5	MAN	E	4	5	11,11,12	1.76	1 (9%)	15,15,17	1.11	2 (13%)
5	MAN	E	5	5	11,11,12	1.81	2 (18%)	15,15,17	1.02	1 (6%)
4	NAG	F	1	1,4	14,14,15	2.05	3 (21%)	17,19,21	0.77	0
4	NAG	F	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	G	1	1,4	14,14,15	2.09	2 (14%)	17,19,21	0.79	0
4	NAG	G	2	4	14,14,15	2.10	1 (7%)	17,19,21	0.73	0
5	NAG	I	1	1,5	14,14,15	2.00	4 (28%)	17,19,21	1.06	1 (5%)
5	NAG	I	2	5	14,14,15	2.23	4 (28%)	17,19,21	0.98	1 (5%)
5	BMA	I	3	5	11,11,12	1.80	2 (18%)	15,15,17	1.09	1 (6%)
5	MAN	I	4	5	11,11,12	1.80	2 (18%)	15,15,17	0.99	1 (6%)
5	MAN	I	5	5	11,11,12	1.78	2 (18%)	15,15,17	1.16	2 (13%)
4	NAG	J	1	1,4	14,14,15	2.07	2 (14%)	17,19,21	0.84	0
4	NAG	J	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	K	1	1,4	14,14,15	2.01	3 (21%)	17,19,21	0.75	0
4	NAG	K	2	4	14,14,15	2.13	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	M	1	1,4	14,14,15	2.10	2 (14%)	17,19,21	0.73	0
4	NAG	M	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.91	1 (5%)
4	NAG	N	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	0.78	0
4	NAG	N	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	O	1	1,4	14,14,15	2.04	3 (21%)	17,19,21	0.95	1 (5%)
4	NAG	O	2	4	14,14,15	2.15	2 (14%)	17,19,21	0.99	1 (5%)
4	NAG	P	1	1,4	14,14,15	2.09	2 (14%)	17,19,21	0.81	0
4	NAG	P	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	Q	1	1,4	14,14,15	2.08	4 (28%)	17,19,21	0.85	1 (5%)
4	NAG	Q	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.90	1 (5%)
5	NAG	R	1	1,5	14,14,15	2.06	5 (35%)	17,19,21	1.12	2 (11%)
5	NAG	R	2	5	14,14,15	2.11	5 (35%)	17,19,21	1.06	1 (5%)
5	BMA	R	3	5	11,11,12	1.85	2 (18%)	15,15,17	1.05	1 (6%)
5	MAN	R	4	5	11,11,12	1.74	1 (9%)	15,15,17	1.13	2 (13%)
5	MAN	R	5	5	11,11,12	1.81	2 (18%)	15,15,17	1.12	2 (13%)
4	NAG	S	1	1,4	14,14,15	2.06	3 (21%)	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	S	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	T	1	1,4	14,14,15	2.09	4 (28%)	17,19,21	1.08	1 (5%)
4	NAG	T	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.90	1 (5%)
6	NAG	U	1	1,6	14,14,15	2.04	3 (21%)	17,19,21	0.94	1 (5%)
6	NAG	U	2	6	14,14,15	2.18	3 (21%)	17,19,21	0.95	0
6	BMA	U	3	6	11,11,12	1.82	2 (18%)	15,15,17	1.09	1 (6%)
6	MAN	U	4	6	11,11,12	1.53	1 (9%)	15,15,17	0.88	1 (6%)
6	MAN	U	5	6	11,11,12	1.78	2 (18%)	15,15,17	1.20	2 (13%)
6	MAN	U	6	6	11,11,12	1.82	2 (18%)	15,15,17	1.02	1 (6%)
4	NAG	V	1	1,4	14,14,15	2.04	3 (21%)	17,19,21	0.72	0
4	NAG	V	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.91	1 (5%)
5	NAG	W	1	1,5	14,14,15	2.10	3 (21%)	17,19,21	1.44	2 (11%)
5	NAG	W	2	5	14,14,15	2.21	5 (35%)	17,19,21	1.08	2 (11%)
5	BMA	W	3	5	11,11,12	1.89	2 (18%)	15,15,17	1.04	1 (6%)
5	MAN	W	4	5	11,11,12	1.83	3 (27%)	15,15,17	1.09	2 (13%)
5	MAN	W	5	5	11,11,12	1.76	1 (9%)	15,15,17	1.05	1 (6%)
7	NAG	X	1	1,7	14,14,15	2.05	4 (28%)	17,19,21	1.02	1 (5%)
7	NAG	X	2	7	14,14,15	2.19	5 (35%)	17,19,21	0.93	1 (5%)
7	BMA	X	3	7	11,11,12	1.83	2 (18%)	15,15,17	1.14	1 (6%)
7	MAN	X	4	7	11,11,12	1.77	2 (18%)	15,15,17	0.99	1 (6%)
8	NAG	Y	1	1,8	14,14,15	2.04	2 (14%)	17,19,21	0.76	0
8	NAG	Y	2	8	14,14,15	2.16	5 (35%)	17,19,21	1.14	2 (11%)
8	BMA	Y	3	8	11,11,12	1.77	1 (9%)	15,15,17	0.86	0
4	NAG	Z	1	1,4	14,14,15	2.02	4 (28%)	17,19,21	0.99	1 (5%)
4	NAG	Z	2	4	14,14,15	2.12	2 (14%)	17,19,21	1.02	1 (5%)
4	NAG	a	1	1,4	14,14,15	2.11	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	a	2	4	14,14,15	2.12	2 (14%)	17,19,21	1.00	1 (5%)
4	NAG	b	1	1,4	14,14,15	2.07	3 (21%)	17,19,21	0.86	0
4	NAG	b	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.81	1 (5%)
4	NAG	c	1	1,4	14,14,15	2.05	3 (21%)	17,19,21	0.71	0
4	NAG	c	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	d	1	1,4	14,14,15	2.08	3 (21%)	17,19,21	0.96	1 (5%)
4	NAG	d	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	e	1	1,4	14,14,15	2.11	4 (28%)	17,19,21	0.88	1 (5%)
4	NAG	e	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	f	1	1,7	14,14,15	2.04	4 (28%)	17,19,21	1.21	2 (11%)
7	NAG	f	2	7	14,14,15	2.08	4 (28%)	17,19,21	0.99	1 (5%)
7	BMA	f	3	7	11,11,12	1.81	2 (18%)	15,15,17	0.96	1 (6%)
7	MAN	f	4	7	11,11,12	1.82	2 (18%)	15,15,17	1.09	1 (6%)
4	NAG	g	1	1,4	14,14,15	2.09	2 (14%)	17,19,21	0.80	0
4	NAG	g	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	h	1	1,4	14,14,15	2.03	4 (28%)	17,19,21	0.95	1 (5%)
4	NAG	h	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.90	1 (5%)
5	NAG	i	1	1,5	14,14,15	2.06	4 (28%)	17,19,21	1.00	1 (5%)
5	NAG	i	2	5	14,14,15	2.20	5 (35%)	17,19,21	0.94	1 (5%)
5	BMA	i	3	5	11,11,12	1.79	2 (18%)	15,15,17	1.00	1 (6%)
5	MAN	i	4	5	11,11,12	1.79	2 (18%)	15,15,17	1.11	2 (13%)
5	MAN	i	5	5	11,11,12	1.79	2 (18%)	15,15,17	1.14	2 (13%)
4	NAG	j	1	1,4	14,14,15	2.09	4 (28%)	17,19,21	0.80	1 (5%)
4	NAG	j	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.87	1 (5%)
8	NAG	k	1	1,8	14,14,15	1.94	1 (7%)	17,19,21	0.95	1 (5%)
8	NAG	k	2	8	14,14,15	2.16	3 (21%)	17,19,21	0.85	1 (5%)
8	BMA	k	3	8	11,11,12	1.81	2 (18%)	15,15,17	1.06	1 (6%)
4	NAG	l	1	1,4	14,14,15	2.04	3 (21%)	17,19,21	0.78	1 (5%)
4	NAG	l	2	4	14,14,15	2.13	2 (14%)	17,19,21	0.91	1 (5%)
4	NAG	m	1	1,4	14,14,15	2.06	2 (14%)	17,19,21	0.68	0
4	NAG	m	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.94	1 (5%)
4	NAG	n	1	1,4	14,14,15	2.07	3 (21%)	17,19,21	0.77	0
4	NAG	n	2	4	14,14,15	2.12	2 (14%)	17,19,21	0.94	1 (5%)
4	NAG	o	1	1,4	14,14,15	2.08	3 (21%)	17,19,21	0.87	1 (5%)
4	NAG	o	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.80	1 (5%)
4	NAG	p	1	1,4	14,14,15	2.10	3 (21%)	17,19,21	0.87	1 (5%)
4	NAG	p	2	4	14,14,15	2.10	2 (14%)	17,19,21	0.88	1 (5%)
5	NAG	q	1	1,5	14,14,15	2.03	5 (35%)	17,19,21	1.06	1 (5%)
5	NAG	q	2	5	14,14,15	2.18	5 (35%)	17,19,21	1.17	2 (11%)
5	BMA	q	3	5	11,11,12	1.84	3 (27%)	15,15,17	0.98	1 (6%)
5	MAN	q	4	5	11,11,12	1.79	2 (18%)	15,15,17	1.05	1 (6%)
5	MAN	q	5	5	11,11,12	1.79	2 (18%)	15,15,17	1.07	1 (6%)

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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	1/2/19/22	0/1/1/1
5	MAN	E	5	5	-	1/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	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	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	1/2/19/22	0/1/1/1
5	MAN	R	5	5	-	1/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	1/2/19/22	0/1/1/1
6	MAN	U	5	6	-	1/2/19/22	0/1/1/1
6	MAN	U	6	6	-	1/2/19/22	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
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	BMA	W	3	5	-	1/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	0/1/1/1
5	MAN	W	5	5	-	1/2/19/22	0/1/1/1
7	NAG	X	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
7	BMA	X	3	7	-	1/2/19/22	0/1/1/1
7	MAN	X	4	7	-	1/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	2/2/19/22	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	1/6/23/26	0/1/1/1
7	NAG	f	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	BMA	f	3	7	-	1/2/19/22	0/1/1/1
7	MAN	f	4	7	-	2/2/19/22	0/1/1/1
4	NAG	g	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
5	NAG	i	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	i	2	5	-	0/6/23/26	0/1/1/1
5	BMA	i	3	5	-	2/2/19/22	0/1/1/1
5	MAN	i	4	5	-	2/2/19/22	0/1/1/1
5	MAN	i	5	5	-	1/2/19/22	0/1/1/1
4	NAG	j	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	j	2	4	-	1/6/23/26	0/1/1/1
8	NAG	k	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
8	BMA	k	3	8	-	1/2/19/22	0/1/1/1
4	NAG	l	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	m	2	4	-	1/6/23/26	0/1/1/1
4	NAG	n	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	2/6/23/26	0/1/1/1
4	NAG	o	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	2	4	-	1/6/23/26	0/1/1/1
5	NAG	q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	q	3	5	-	2/2/19/22	0/1/1/1
5	MAN	q	4	5	-	1/2/19/22	0/1/1/1
5	MAN	q	5	5	-	1/2/19/22	0/1/1/1

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	2	NAG	O5-C1	6.80	1.55	1.43
4	K	2	NAG	O5-C1	6.79	1.55	1.43
8	k	2	NAG	O5-C1	6.78	1.55	1.43
4	P	2	NAG	O5-C1	6.76	1.55	1.43
5	W	2	NAG	O5-C1	6.76	1.55	1.43
4	G	1	NAG	O5-C1	6.76	1.55	1.43
4	j	2	NAG	O5-C1	6.76	1.55	1.43
4	G	2	NAG	O5-C1	6.74	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	NAG	O5-C1	6.74	1.55	1.43
4	T	2	NAG	O5-C1	6.74	1.55	1.43
4	V	2	NAG	O5-C1	6.73	1.55	1.43
4	b	2	NAG	O5-C1	6.73	1.55	1.43
4	S	2	NAG	O5-C1	6.73	1.55	1.43
4	d	2	NAG	O5-C1	6.72	1.55	1.43
4	m	2	NAG	O5-C1	6.71	1.55	1.43
4	M	1	NAG	O5-C1	6.70	1.55	1.43
4	c	2	NAG	O5-C1	6.70	1.55	1.43
4	a	2	NAG	O5-C1	6.70	1.54	1.43
4	h	2	NAG	O5-C1	6.70	1.54	1.43
4	F	2	NAG	O5-C1	6.69	1.54	1.43
4	l	2	NAG	O5-C1	6.68	1.54	1.43
4	P	1	NAG	O5-C1	6.67	1.54	1.43
4	g	2	NAG	O5-C1	6.66	1.54	1.43
4	a	1	NAG	O5-C1	6.66	1.54	1.43
4	N	1	NAG	O5-C1	6.66	1.54	1.43
4	Z	2	NAG	O5-C1	6.65	1.54	1.43
4	n	1	NAG	O5-C1	6.65	1.54	1.43
4	p	2	NAG	O5-C1	6.64	1.54	1.43
4	Q	2	NAG	O5-C1	6.64	1.54	1.43
4	m	1	NAG	O5-C1	6.64	1.54	1.43
5	I	2	NAG	O5-C1	6.64	1.54	1.43
4	o	2	NAG	O5-C1	6.63	1.54	1.43
5	i	2	NAG	O5-C1	6.63	1.54	1.43
4	N	2	NAG	O5-C1	6.62	1.54	1.43
4	n	2	NAG	O5-C1	6.62	1.54	1.43
4	J	2	NAG	O5-C1	6.62	1.54	1.43
4	e	2	NAG	O5-C1	6.62	1.54	1.43
6	U	2	NAG	O5-C1	6.59	1.54	1.43
4	o	1	NAG	O5-C1	6.59	1.54	1.43
4	c	1	NAG	O5-C1	6.57	1.54	1.43
4	D	2	NAG	O5-C1	6.57	1.54	1.43
7	X	2	NAG	O5-C1	6.56	1.54	1.43
4	J	1	NAG	O5-C1	6.55	1.54	1.43
4	j	1	NAG	O5-C1	6.54	1.54	1.43
8	Y	1	NAG	O5-C1	6.54	1.54	1.43
4	g	1	NAG	O5-C1	6.53	1.54	1.43
4	b	1	NAG	O5-C1	6.51	1.54	1.43
4	l	1	NAG	O5-C1	6.51	1.54	1.43
4	D	1	NAG	O5-C1	6.51	1.54	1.43
5	E	2	NAG	O5-C1	6.49	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	1	NAG	O5-C1	6.45	1.54	1.43
4	p	1	NAG	O5-C1	6.45	1.54	1.43
4	S	1	NAG	O5-C1	6.43	1.54	1.43
4	e	1	NAG	O5-C1	6.42	1.54	1.43
6	U	1	NAG	O5-C1	6.40	1.54	1.43
5	q	2	NAG	O5-C1	6.39	1.54	1.43
5	W	1	NAG	O5-C1	6.37	1.54	1.43
4	F	1	NAG	O5-C1	6.36	1.54	1.43
4	Q	1	NAG	O5-C1	6.36	1.54	1.43
8	Y	2	NAG	O5-C1	6.36	1.54	1.43
7	f	2	NAG	O5-C1	6.35	1.54	1.43
4	O	1	NAG	O5-C1	6.34	1.54	1.43
4	T	1	NAG	O5-C1	6.33	1.54	1.43
4	V	1	NAG	O5-C1	6.33	1.54	1.43
5	E	1	NAG	O5-C1	6.33	1.54	1.43
4	K	1	NAG	O5-C1	6.31	1.54	1.43
5	R	2	NAG	O5-C1	6.31	1.54	1.43
5	i	1	NAG	O5-C1	6.29	1.54	1.43
7	X	1	NAG	O5-C1	6.29	1.54	1.43
4	Z	1	NAG	O5-C1	6.25	1.54	1.43
4	h	1	NAG	O5-C1	6.23	1.54	1.43
5	R	1	NAG	O5-C1	6.19	1.54	1.43
7	f	1	NAG	O5-C1	6.14	1.54	1.43
8	k	1	NAG	O5-C1	6.12	1.54	1.43
5	I	1	NAG	O5-C1	6.02	1.53	1.43
5	q	1	NAG	O5-C1	5.99	1.53	1.43
5	E	3	BMA	O2-C2	-4.36	1.34	1.43
5	W	3	BMA	O2-C2	-4.34	1.34	1.43
6	U	3	BMA	O2-C2	-4.28	1.34	1.43
5	R	3	BMA	O2-C2	-4.23	1.34	1.43
5	q	3	BMA	O2-C2	-4.20	1.34	1.43
6	U	6	MAN	O2-C2	-4.18	1.34	1.43
5	I	4	MAN	O2-C2	-4.16	1.34	1.43
7	f	4	MAN	O2-C2	-4.14	1.34	1.43
7	X	4	MAN	O2-C2	-4.14	1.34	1.43
5	R	5	MAN	O2-C2	-4.14	1.34	1.43
7	f	3	BMA	O2-C2	-4.13	1.34	1.43
5	i	3	BMA	O2-C2	-4.13	1.34	1.43
5	E	5	MAN	O2-C2	-4.12	1.34	1.43
5	q	5	MAN	O2-C2	-4.12	1.34	1.43
5	q	4	MAN	O2-C2	-4.12	1.34	1.43
7	X	3	BMA	O2-C2	-4.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	5	MAN	O2-C2	-4.12	1.34	1.43
6	U	5	MAN	O2-C2	-4.11	1.34	1.43
8	Y	3	BMA	O2-C2	-4.11	1.34	1.43
8	k	3	BMA	O2-C2	-4.11	1.34	1.43
5	i	4	MAN	O2-C2	-4.10	1.34	1.43
5	i	5	MAN	O2-C2	-4.09	1.34	1.43
5	E	4	MAN	O2-C2	-4.08	1.34	1.43
5	W	4	MAN	O2-C2	-4.08	1.34	1.43
5	R	4	MAN	O2-C2	-4.06	1.34	1.43
5	W	5	MAN	O2-C2	-4.05	1.34	1.43
5	I	3	BMA	O2-C2	-4.03	1.34	1.43
6	U	4	MAN	O2-C2	-2.99	1.37	1.43
8	Y	2	NAG	C4-C3	2.81	1.59	1.52
5	i	2	NAG	C3-C2	-2.72	1.46	1.52
6	U	2	NAG	C3-C2	-2.70	1.46	1.52
5	I	2	NAG	C3-C2	-2.63	1.47	1.52
5	q	2	NAG	C1-C2	-2.55	1.48	1.52
5	q	2	NAG	C4-C5	2.55	1.58	1.53
7	X	2	NAG	C3-C2	-2.52	1.47	1.52
5	W	2	NAG	C3-C2	-2.50	1.47	1.52
7	X	2	NAG	C1-C2	-2.47	1.49	1.52
5	I	2	NAG	C1-C2	-2.45	1.49	1.52
8	Y	2	NAG	C1-C2	-2.42	1.49	1.52
5	q	2	NAG	C4-C3	2.41	1.58	1.52
5	I	1	NAG	C4-C5	2.40	1.58	1.53
5	W	1	NAG	C4-C5	2.40	1.58	1.53
5	R	2	NAG	C3-C2	-2.38	1.47	1.52
7	f	2	NAG	C3-C2	-2.37	1.47	1.52
4	Q	1	NAG	C3-C2	-2.37	1.47	1.52
5	q	5	MAN	C2-C3	-2.37	1.48	1.52
4	M	1	NAG	C3-C2	-2.36	1.47	1.52
5	R	3	BMA	C2-C3	-2.36	1.48	1.52
5	R	2	NAG	C4-C5	2.35	1.58	1.53
8	k	3	BMA	C2-C3	-2.35	1.48	1.52
6	U	2	NAG	C1-C2	-2.35	1.49	1.52
4	e	1	NAG	C3-C2	-2.35	1.47	1.52
5	I	3	BMA	C2-C3	-2.34	1.48	1.52
5	E	2	NAG	C1-C2	-2.34	1.49	1.52
5	E	2	NAG	C3-C2	-2.34	1.47	1.52
4	p	1	NAG	C3-C2	-2.33	1.47	1.52
8	k	2	NAG	C3-C2	-2.33	1.47	1.52
5	q	4	MAN	C2-C3	-2.32	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	C3-C2	-2.31	1.47	1.52
5	E	3	BMA	C2-C3	-2.31	1.49	1.52
4	T	1	NAG	C3-C2	-2.30	1.47	1.52
5	q	2	NAG	C3-C2	-2.29	1.47	1.52
5	E	5	MAN	C2-C3	-2.29	1.49	1.52
4	d	1	NAG	C3-C2	-2.29	1.47	1.52
8	Y	1	NAG	C3-C2	-2.28	1.47	1.52
4	Z	1	NAG	C4-C5	2.27	1.57	1.53
4	a	1	NAG	C3-C2	-2.27	1.47	1.52
5	I	1	NAG	C4-C3	2.26	1.58	1.52
4	o	1	NAG	C3-C2	-2.26	1.47	1.52
5	I	2	NAG	C4-C5	2.26	1.57	1.53
5	R	5	MAN	C2-C3	-2.26	1.49	1.52
5	R	1	NAG	C4-C5	2.25	1.57	1.53
4	l	1	NAG	C3-C2	-2.25	1.47	1.52
7	f	1	NAG	C4-C5	2.25	1.57	1.53
5	q	1	NAG	C4-C5	2.24	1.57	1.53
5	q	1	NAG	C3-C2	-2.24	1.47	1.52
4	c	2	NAG	C3-C2	-2.24	1.47	1.52
5	W	1	NAG	C4-C3	2.23	1.58	1.52
5	R	1	NAG	C3-C2	-2.23	1.47	1.52
5	i	2	NAG	C1-C2	-2.23	1.49	1.52
7	f	1	NAG	C3-C2	-2.23	1.47	1.52
4	g	1	NAG	C3-C2	-2.22	1.47	1.52
5	I	4	MAN	C2-C3	-2.22	1.49	1.52
5	W	3	BMA	C2-C3	-2.22	1.49	1.52
4	P	1	NAG	C3-C2	-2.22	1.47	1.52
4	m	1	NAG	C3-C2	-2.22	1.47	1.52
7	X	1	NAG	C4-C5	2.22	1.57	1.53
5	i	3	BMA	C2-C3	-2.22	1.49	1.52
5	i	1	NAG	C4-C5	2.22	1.57	1.53
4	N	1	NAG	C3-C2	-2.22	1.47	1.52
5	W	2	NAG	C1-C2	-2.22	1.49	1.52
4	e	2	NAG	C3-C2	-2.22	1.47	1.52
6	U	3	BMA	C2-C3	-2.22	1.49	1.52
4	O	1	NAG	C3-C2	-2.22	1.47	1.52
5	q	3	BMA	C2-C3	-2.21	1.49	1.52
4	Z	1	NAG	C3-C2	-2.21	1.47	1.52
7	X	1	NAG	C3-C2	-2.20	1.47	1.52
4	V	1	NAG	C4-C3	2.20	1.58	1.52
5	i	1	NAG	C3-C2	-2.20	1.47	1.52
5	q	1	NAG	C4-C3	2.19	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	2	NAG	C3-C2	-2.19	1.47	1.52
4	g	2	NAG	C3-C2	-2.18	1.47	1.52
4	S	1	NAG	C3-C2	-2.18	1.47	1.52
4	Z	2	NAG	C3-C2	-2.18	1.47	1.52
4	l	2	NAG	C3-C2	-2.17	1.48	1.52
4	h	2	NAG	C3-C2	-2.17	1.48	1.52
4	n	2	NAG	C3-C2	-2.17	1.48	1.52
4	h	1	NAG	C4-C5	2.17	1.57	1.53
5	R	2	NAG	C1-C2	-2.16	1.49	1.52
7	f	4	MAN	C2-C3	-2.16	1.49	1.52
5	i	4	MAN	C2-C3	-2.16	1.49	1.52
5	E	1	NAG	C3-C2	-2.15	1.48	1.52
6	U	6	MAN	C2-C3	-2.15	1.49	1.52
7	X	4	MAN	C2-C3	-2.15	1.49	1.52
4	S	2	NAG	C3-C2	-2.15	1.48	1.52
4	J	2	NAG	C3-C2	-2.15	1.48	1.52
8	Y	2	NAG	C4-C5	2.15	1.57	1.53
4	j	1	NAG	C4-C3	2.14	1.57	1.52
4	O	2	NAG	C3-C2	-2.14	1.48	1.52
4	b	1	NAG	C3-C2	-2.13	1.48	1.52
4	j	2	NAG	C3-C2	-2.13	1.48	1.52
4	p	2	NAG	C3-C2	-2.13	1.48	1.52
5	W	2	NAG	C4-C3	2.13	1.57	1.52
4	D	2	NAG	C3-C2	-2.13	1.48	1.52
7	X	2	NAG	C4-C3	2.12	1.57	1.52
7	f	2	NAG	C4-C5	2.12	1.57	1.53
4	h	1	NAG	C4-C3	2.12	1.57	1.52
4	d	1	NAG	C4-C3	2.12	1.57	1.52
5	R	2	NAG	C4-C3	2.12	1.57	1.52
6	U	1	NAG	C3-C2	-2.12	1.48	1.52
4	Q	1	NAG	C1-C2	-2.11	1.49	1.52
4	V	2	NAG	C3-C2	-2.11	1.48	1.52
5	R	1	NAG	C1-C2	-2.11	1.49	1.52
5	I	5	MAN	C2-C3	-2.11	1.49	1.52
5	i	2	NAG	C4-C5	2.11	1.57	1.53
4	F	1	NAG	C3-C2	-2.10	1.48	1.52
5	W	2	NAG	C4-C5	2.10	1.57	1.53
4	e	1	NAG	C1-C2	-2.10	1.49	1.52
7	X	1	NAG	C4-C3	2.10	1.57	1.52
4	F	2	NAG	C3-C2	-2.09	1.48	1.52
4	Q	2	NAG	C3-C2	-2.09	1.48	1.52
4	j	1	NAG	C3-C2	-2.08	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	2	NAG	C4-C5	2.08	1.57	1.53
7	f	2	NAG	C1-C2	-2.08	1.49	1.52
4	b	2	NAG	C3-C2	-2.08	1.48	1.52
4	j	1	NAG	C4-C5	2.08	1.57	1.53
4	T	2	NAG	C3-C2	-2.08	1.48	1.52
5	i	5	MAN	C2-C3	-2.08	1.49	1.52
4	n	1	NAG	C3-C2	-2.07	1.48	1.52
4	G	1	NAG	C4-C3	2.07	1.57	1.52
4	Q	1	NAG	C4-C3	2.07	1.57	1.52
4	b	1	NAG	C4-C3	2.07	1.57	1.52
4	Z	1	NAG	C4-C3	2.07	1.57	1.52
7	X	2	NAG	C4-C5	2.07	1.57	1.53
6	U	5	MAN	C2-C3	-2.07	1.49	1.52
4	m	2	NAG	C3-C2	-2.06	1.48	1.52
4	N	2	NAG	C3-C2	-2.06	1.48	1.52
8	Y	2	NAG	C3-C2	-2.06	1.48	1.52
5	W	4	MAN	C2-C3	-2.06	1.49	1.52
4	p	1	NAG	C1-C2	-2.06	1.49	1.52
4	K	1	NAG	C3-C2	-2.06	1.48	1.52
4	o	1	NAG	C4-C3	2.06	1.57	1.52
7	f	3	BMA	C2-C3	-2.06	1.49	1.52
4	P	2	NAG	C3-C2	-2.06	1.48	1.52
4	D	1	NAG	C3-C2	-2.05	1.48	1.52
5	i	2	NAG	C4-C3	2.05	1.57	1.52
5	E	1	NAG	C4-C5	2.05	1.57	1.53
4	F	1	NAG	C4-C3	2.05	1.57	1.52
4	d	2	NAG	C3-C2	-2.05	1.48	1.52
5	i	1	NAG	C4-C3	2.05	1.57	1.52
7	X	3	BMA	C2-C3	-2.05	1.49	1.52
4	e	1	NAG	C4-C3	2.05	1.57	1.52
4	n	1	NAG	C4-C3	2.04	1.57	1.52
5	E	3	BMA	C6-C5	2.04	1.58	1.51
4	T	1	NAG	C4-C5	2.04	1.57	1.53
4	O	1	NAG	C4-C3	2.04	1.57	1.52
6	U	1	NAG	C4-C5	2.04	1.57	1.53
4	c	1	NAG	C3-C2	-2.04	1.48	1.52
4	V	1	NAG	C3-C2	-2.04	1.48	1.52
4	K	2	NAG	C3-C2	-2.04	1.48	1.52
5	I	1	NAG	C3-C2	-2.04	1.48	1.52
5	E	1	NAG	C4-C3	2.03	1.57	1.52
4	c	1	NAG	C4-C3	2.03	1.57	1.52
5	E	2	NAG	C4-C5	2.03	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	C4-C3	2.03	1.57	1.52
4	M	2	NAG	C3-C2	-2.03	1.48	1.52
4	K	1	NAG	C4-C3	2.02	1.57	1.52
5	q	1	NAG	C1-C2	-2.02	1.49	1.52
4	S	1	NAG	C4-C3	2.02	1.57	1.52
4	h	1	NAG	C3-C2	-2.02	1.48	1.52
4	N	1	NAG	C4-C3	2.02	1.57	1.52
4	T	1	NAG	C4-C3	2.01	1.57	1.52
5	q	3	BMA	C6-C5	2.01	1.58	1.51
5	R	1	NAG	C4-C3	2.01	1.57	1.52
4	l	1	NAG	C4-C3	2.00	1.57	1.52
4	o	2	NAG	C3-C2	-2.00	1.48	1.52
4	D	1	NAG	C4-C3	2.00	1.57	1.52
7	f	1	NAG	C4-C3	2.00	1.57	1.52
5	W	4	MAN	C6-C5	2.00	1.58	1.51

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	1	NAG	C3-C4-C5	-3.40	104.07	110.23
7	X	3	BMA	C2-C3-C4	-3.24	105.17	110.86
6	U	3	BMA	C2-C3-C4	-3.11	105.39	110.86
7	f	1	NAG	C3-C4-C5	-3.11	104.59	110.23
4	T	1	NAG	C1-O5-C5	-3.09	108.04	112.19
8	k	3	BMA	C2-C3-C4	-2.89	105.78	110.86
4	O	2	NAG	C4-C3-C2	-2.88	106.79	111.02
4	a	2	NAG	C4-C3-C2	-2.86	106.83	111.02
5	I	3	BMA	C2-C3-C4	-2.80	105.93	110.86
5	I	1	NAG	C3-C4-C5	-2.80	105.15	110.23
4	O	1	NAG	C1-O5-C5	-2.79	108.45	112.19
5	q	2	NAG	C4-C3-C2	-2.79	106.94	111.02
7	X	1	NAG	C3-C4-C5	-2.74	105.26	110.23
4	Z	2	NAG	C4-C3-C2	-2.71	107.04	111.02
5	W	3	BMA	C2-C3-C4	-2.69	106.13	110.86
5	i	3	BMA	C2-C3-C4	-2.69	106.13	110.86
4	D	2	NAG	C4-C3-C2	-2.66	107.12	111.02
5	i	5	MAN	C2-C3-C4	-2.65	106.19	110.86
5	q	1	NAG	C3-C4-C5	-2.65	105.42	110.23
4	m	2	NAG	C4-C3-C2	-2.64	107.14	111.02
6	U	5	MAN	C1-C2-C3	2.64	113.49	109.64
5	W	2	NAG	C3-C4-C5	-2.62	105.49	110.23
7	f	3	BMA	C2-C3-C4	-2.61	106.27	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	3	BMA	C2-C3-C4	-2.61	106.28	110.86
5	R	5	MAN	C2-C3-C4	-2.60	106.29	110.86
5	R	1	NAG	C3-C4-C5	-2.59	105.54	110.23
4	n	2	NAG	C4-C3-C2	-2.58	107.23	111.02
4	l	2	NAG	C4-C3-C2	-2.57	107.25	111.02
4	e	2	NAG	C4-C3-C2	-2.56	107.26	111.02
4	J	2	NAG	C4-C3-C2	-2.56	107.27	111.02
4	h	2	NAG	C4-C3-C2	-2.55	107.28	111.02
4	M	2	NAG	C4-C3-C2	-2.53	107.31	111.02
4	T	2	NAG	C4-C3-C2	-2.52	107.32	111.02
5	q	3	BMA	C2-C3-C4	-2.52	106.43	110.86
5	W	1	NAG	C1-O5-C5	2.51	115.56	112.19
4	d	1	NAG	C4-C3-C2	-2.51	107.34	111.02
5	q	4	MAN	C2-C3-C4	-2.50	106.46	110.86
6	U	5	MAN	C2-C3-C4	-2.48	106.50	110.86
8	k	1	NAG	C1-O5-C5	-2.48	108.87	112.19
5	R	4	MAN	C2-C3-C4	-2.48	106.50	110.86
5	E	1	NAG	C3-C4-C5	-2.48	105.74	110.23
4	F	2	NAG	C4-C3-C2	-2.47	107.40	111.02
4	h	1	NAG	C1-O5-C5	-2.47	108.88	112.19
5	I	5	MAN	C2-C3-C4	-2.46	106.53	110.86
5	q	5	MAN	C2-C3-C4	-2.45	106.56	110.86
4	c	2	NAG	C4-C3-C2	-2.44	107.44	111.02
5	i	4	MAN	C2-C3-C4	-2.40	106.64	110.86
5	R	4	MAN	C1-C2-C3	2.39	113.12	109.64
4	V	2	NAG	C4-C3-C2	-2.38	107.53	111.02
5	W	5	MAN	C2-C3-C4	-2.38	106.68	110.86
5	E	3	BMA	C2-C3-C4	-2.35	106.72	110.86
4	d	2	NAG	C4-C3-C2	-2.35	107.58	111.02
4	p	2	NAG	C4-C3-C2	-2.34	107.58	111.02
4	Q	2	NAG	C4-C3-C2	-2.33	107.60	111.02
5	i	1	NAG	C3-C4-C5	-2.33	106.00	110.23
5	I	2	NAG	C1-O5-C5	-2.33	109.07	112.19
4	g	2	NAG	C4-C3-C2	-2.32	107.61	111.02
4	K	2	NAG	C4-C3-C2	-2.32	107.61	111.02
4	Q	1	NAG	C3-C4-C5	-2.32	106.03	110.23
4	S	2	NAG	C4-C3-C2	-2.32	107.62	111.02
5	R	2	NAG	C4-C3-C2	-2.31	107.64	111.02
4	N	2	NAG	C4-C3-C2	-2.30	107.65	111.02
8	Y	2	NAG	C1-O5-C5	-2.29	109.12	112.19
7	f	2	NAG	C1-O5-C5	-2.28	109.13	112.19
4	e	1	NAG	C3-C4-C5	-2.28	106.11	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	2	NAG	C3-C4-C5	-2.27	106.12	110.23
5	i	4	MAN	C1-C2-C3	2.25	112.92	109.64
4	p	1	NAG	C3-C4-C5	-2.25	106.15	110.23
5	E	4	MAN	C2-C3-C4	-2.25	106.91	110.86
7	f	1	NAG	C4-C3-C2	2.24	114.30	111.02
4	P	2	NAG	C4-C3-C2	-2.24	107.74	111.02
6	U	1	NAG	C3-C4-C5	-2.24	106.18	110.23
4	Z	1	NAG	C3-C4-C5	-2.23	106.18	110.23
5	I	4	MAN	C2-C3-C4	-2.23	106.94	110.86
5	W	4	MAN	C2-C3-C4	-2.21	106.98	110.86
6	U	6	MAN	C2-C3-C4	-2.20	106.98	110.86
4	o	1	NAG	C4-C3-C2	-2.20	107.79	111.02
4	j	2	NAG	C4-C3-C2	-2.20	107.80	111.02
7	X	2	NAG	C3-C4-C5	-2.19	106.25	110.23
5	E	5	MAN	C2-C3-C4	-2.18	107.02	110.86
5	E	4	MAN	C1-C2-C3	2.18	112.82	109.64
5	i	5	MAN	C1-C2-C3	2.18	112.82	109.64
4	l	1	NAG	C1-O5-C5	-2.16	109.29	112.19
5	R	5	MAN	C1-C2-C3	2.15	112.77	109.64
5	i	2	NAG	C3-C4-C5	-2.14	106.35	110.23
7	X	4	MAN	C2-C3-C4	-2.14	107.10	110.86
4	j	1	NAG	C3-C4-C5	-2.14	106.36	110.23
7	f	4	MAN	C2-C3-C4	-2.14	107.11	110.86
5	W	2	NAG	C1-O5-C5	-2.11	109.36	112.19
4	b	2	NAG	C4-C3-C2	-2.11	107.93	111.02
5	I	5	MAN	C1-C2-C3	2.10	112.71	109.64
5	W	4	MAN	C1-C2-C3	2.10	112.71	109.64
4	D	1	NAG	C1-O5-C5	-2.08	109.40	112.19
5	q	2	NAG	C1-O5-C5	-2.08	109.40	112.19
4	o	2	NAG	C4-C3-C2	-2.05	108.01	111.02
5	E	2	NAG	C3-C4-C5	-2.04	106.54	110.23
8	k	2	NAG	C3-C4-C5	-2.04	106.54	110.23
6	U	4	MAN	C2-C3-C4	-2.03	107.29	110.86
4	a	1	NAG	C1-O5-C5	-2.03	109.47	112.19
5	R	1	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	q	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	l	2	NAG	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	o	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	n	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
5	i	4	MAN	O5-C5-C6-O6
7	f	4	MAN	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
7	f	4	MAN	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
5	q	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
5	q	3	BMA	C4-C5-C6-O6
5	q	2	NAG	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
5	i	5	MAN	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
5	R	5	MAN	O5-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	P	2	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
8	k	3	BMA	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6
5	i	3	BMA	O5-C5-C6-O6
6	U	6	MAN	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
8	Y	3	BMA	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
7	f	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
4	l	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	n	2	NAG	C4-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
4	o	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
7	X	3	BMA	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
5	q	5	MAN	O5-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
5	q	4	MAN	O5-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6

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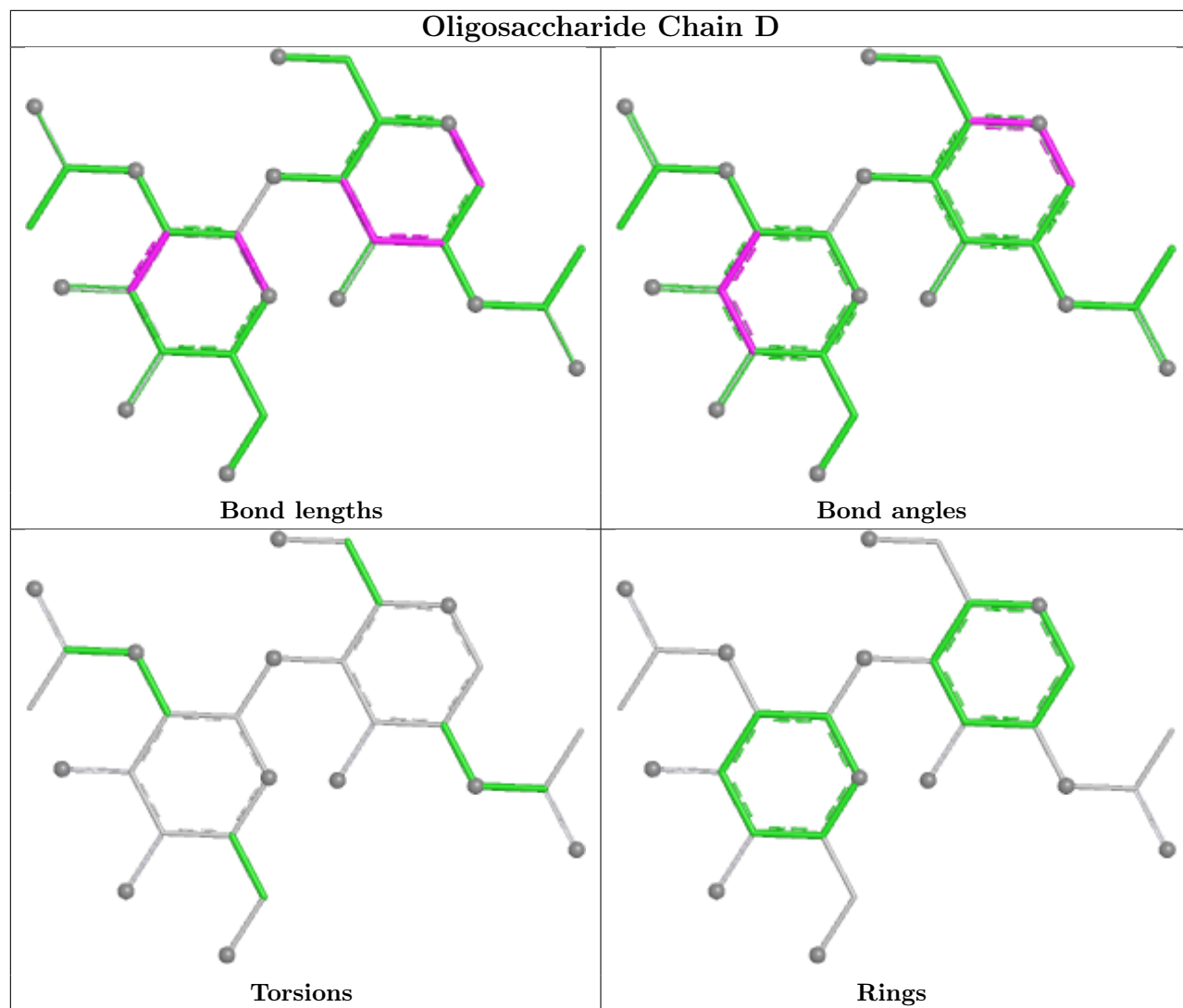
Mol	Chain	Res	Type	Atoms
4	d	2	NAG	C4-C5-C6-O6
5	q	1	NAG	O5-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	i	3	BMA	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
5	i	4	MAN	C4-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6

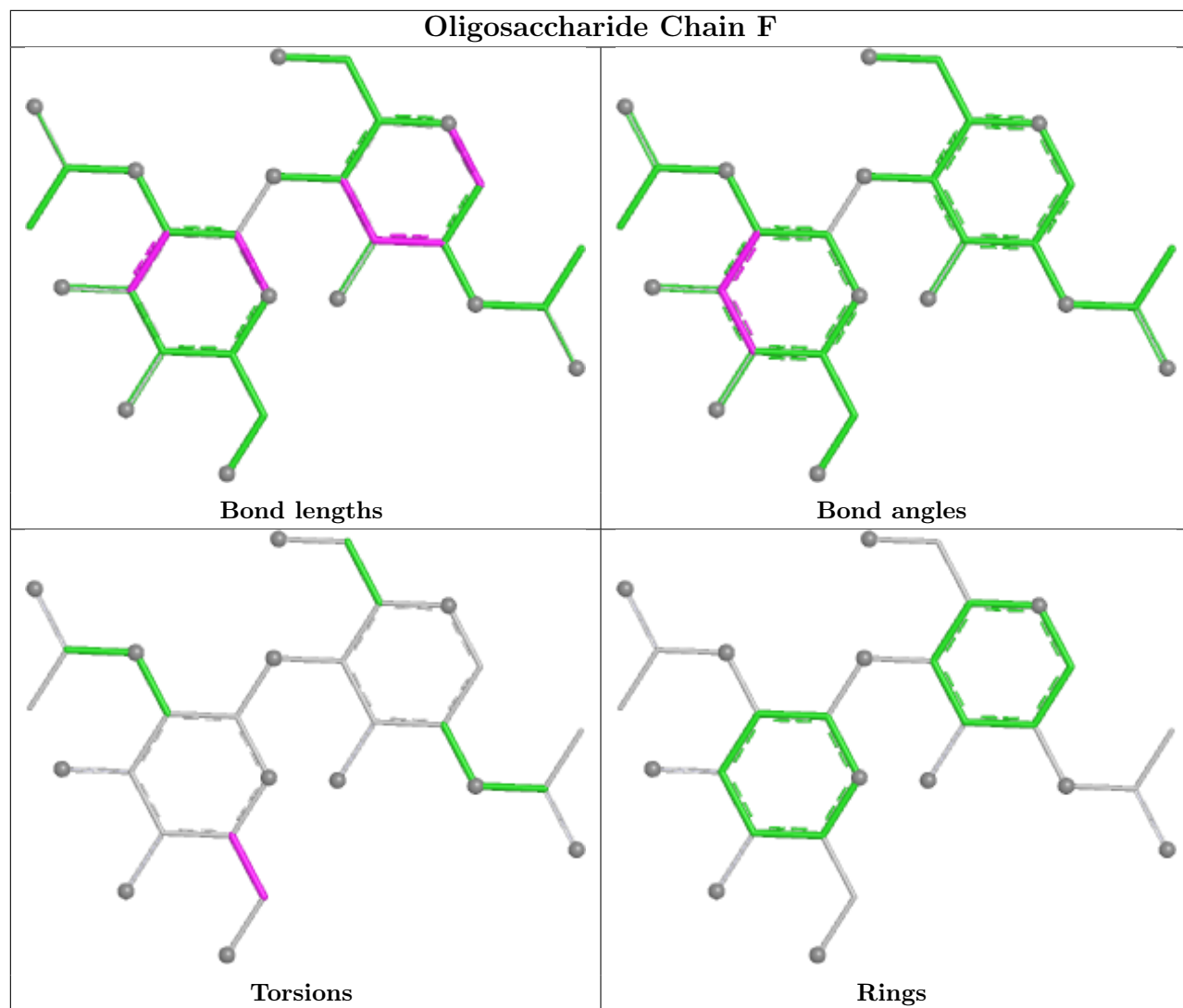
There are no ring outliers.

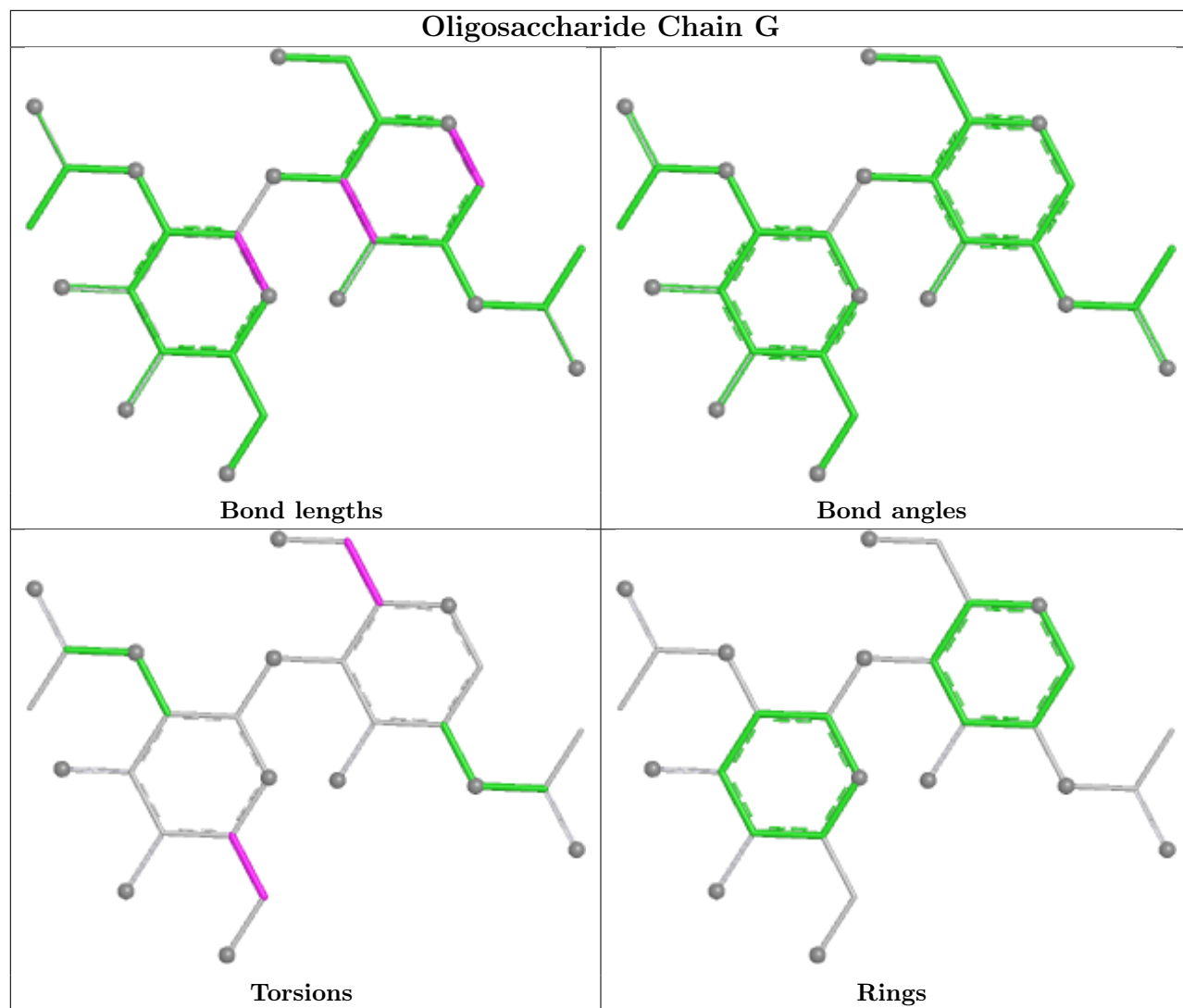
4 monomers are involved in 4 short contacts:

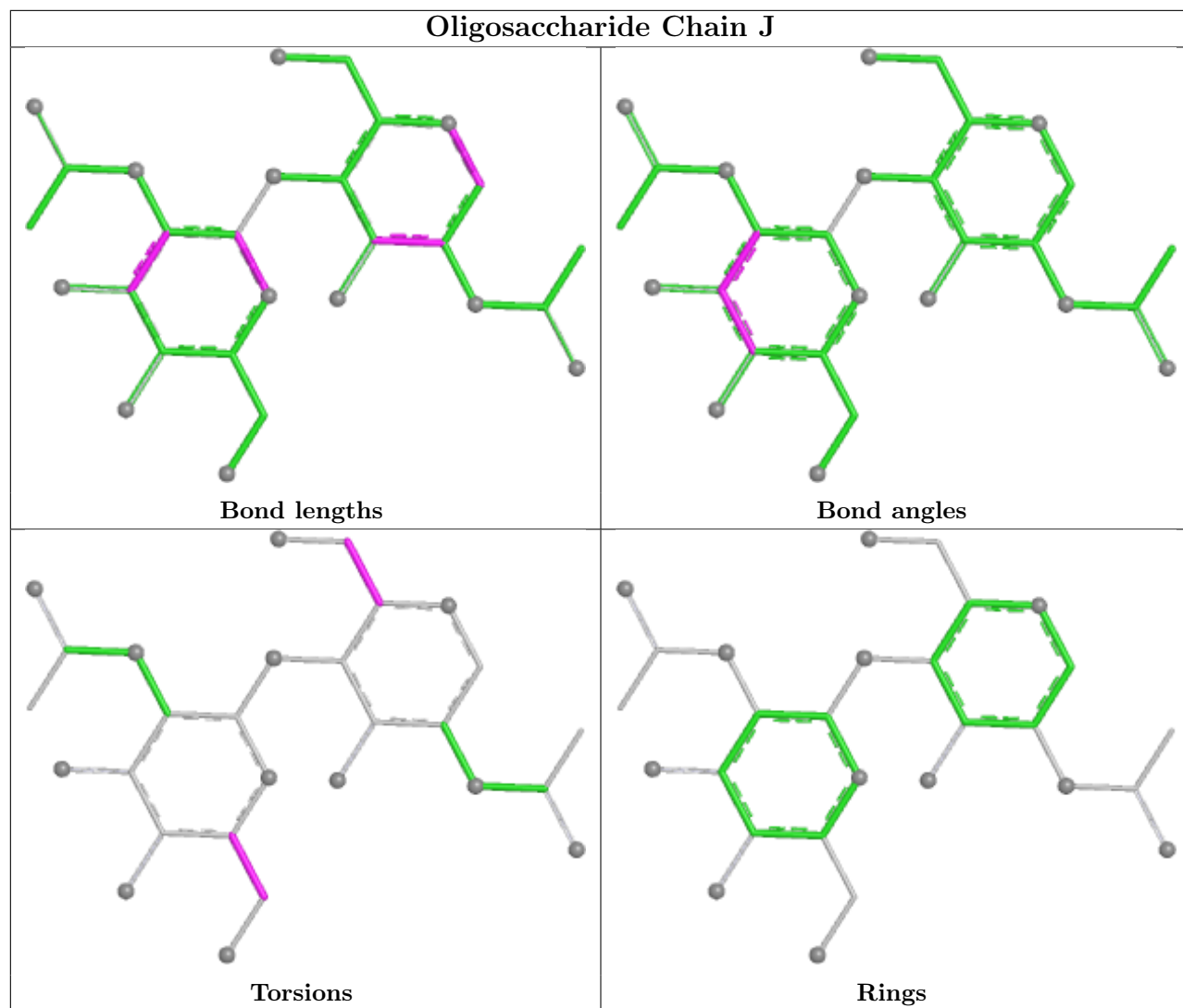
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	i	1	NAG	1	0
5	E	1	NAG	1	0
6	U	1	NAG	1	0

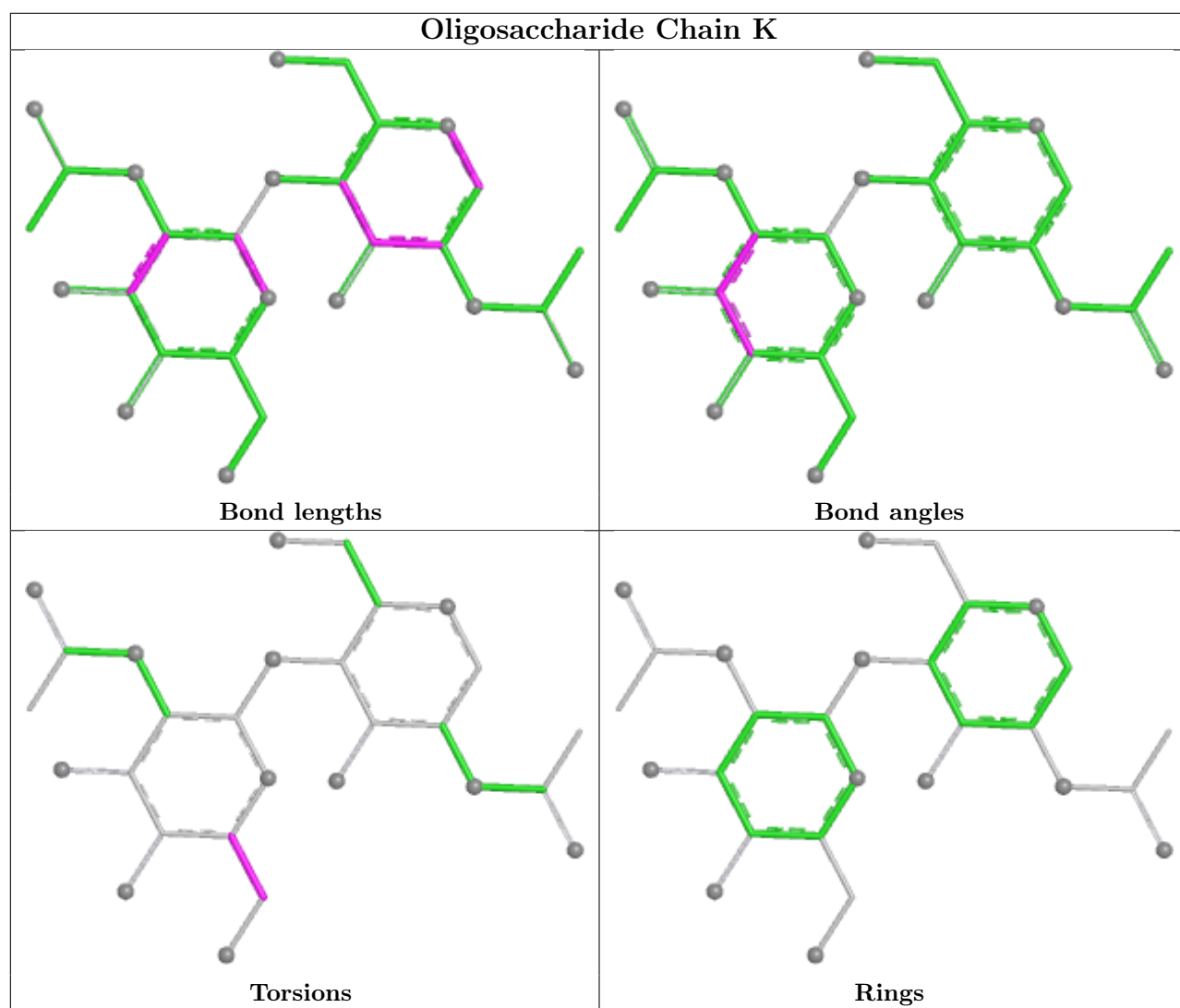
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

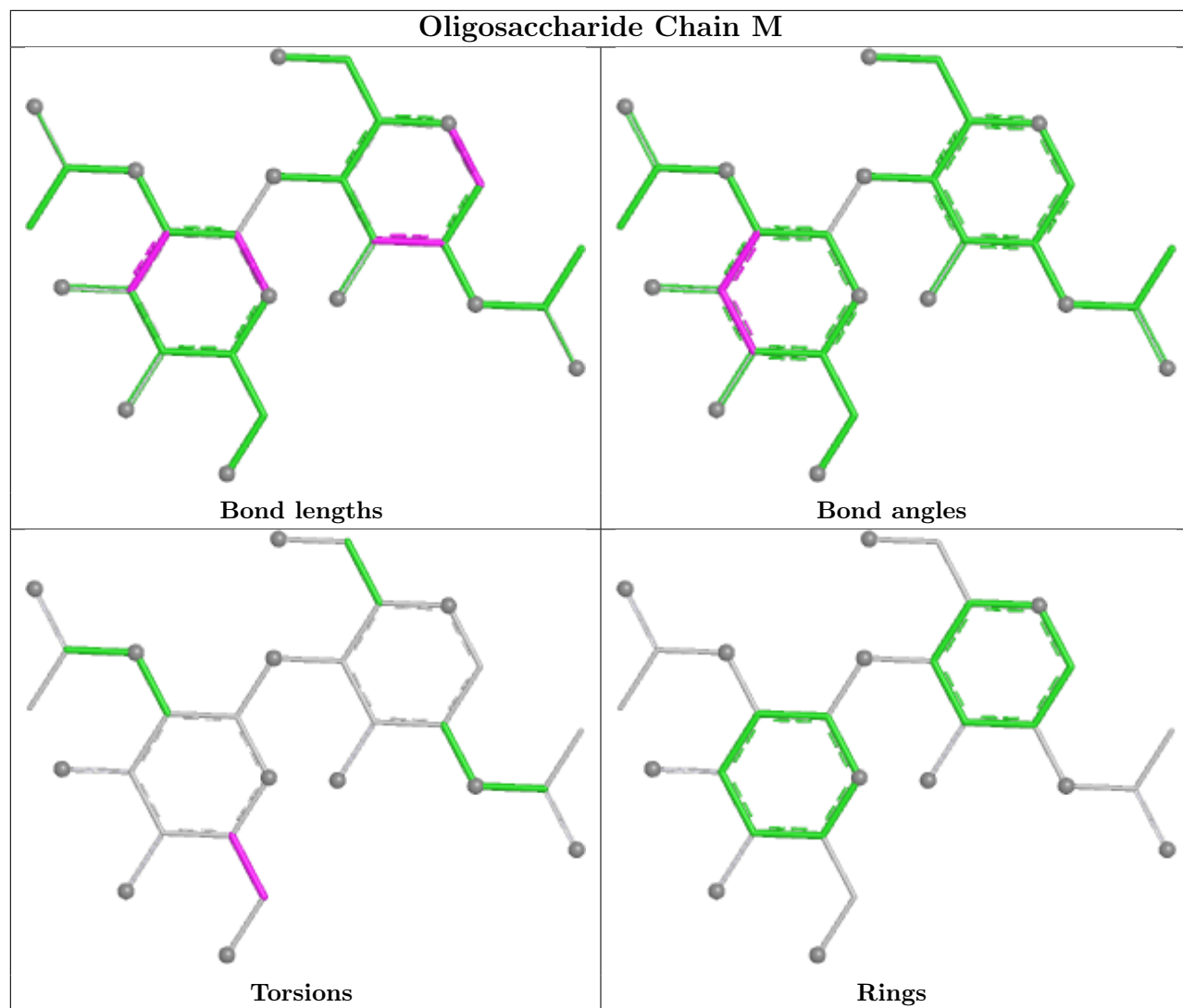


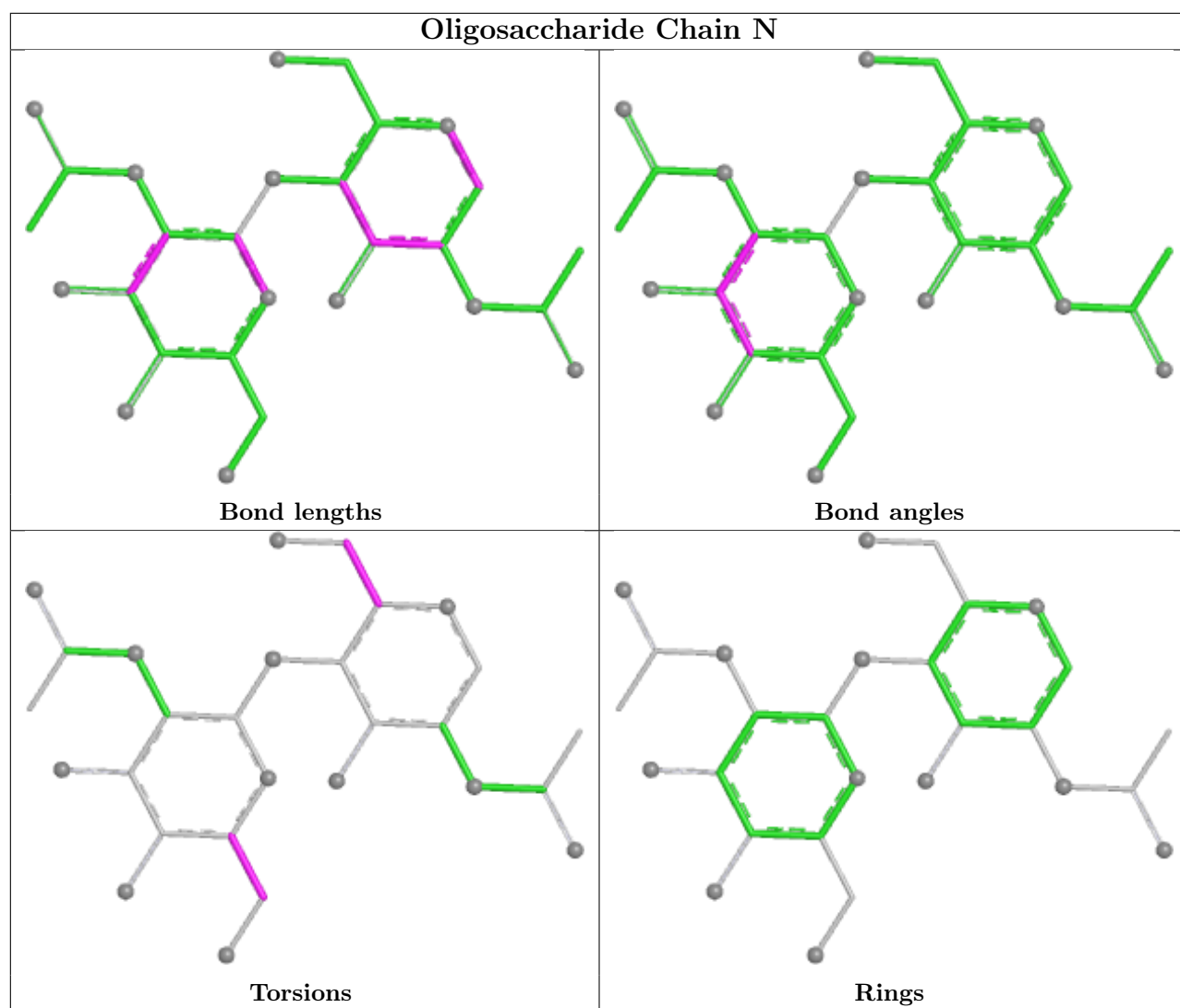


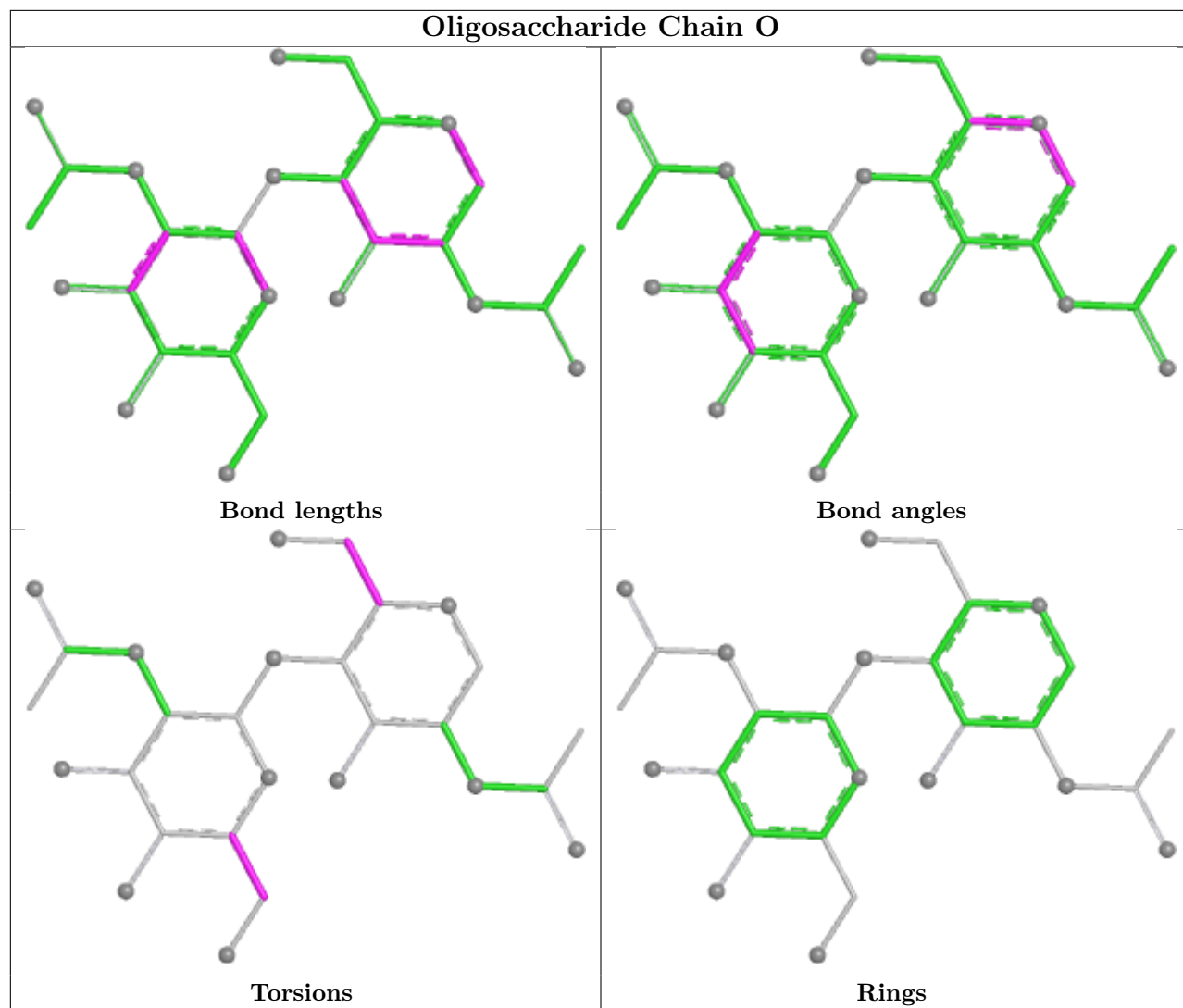


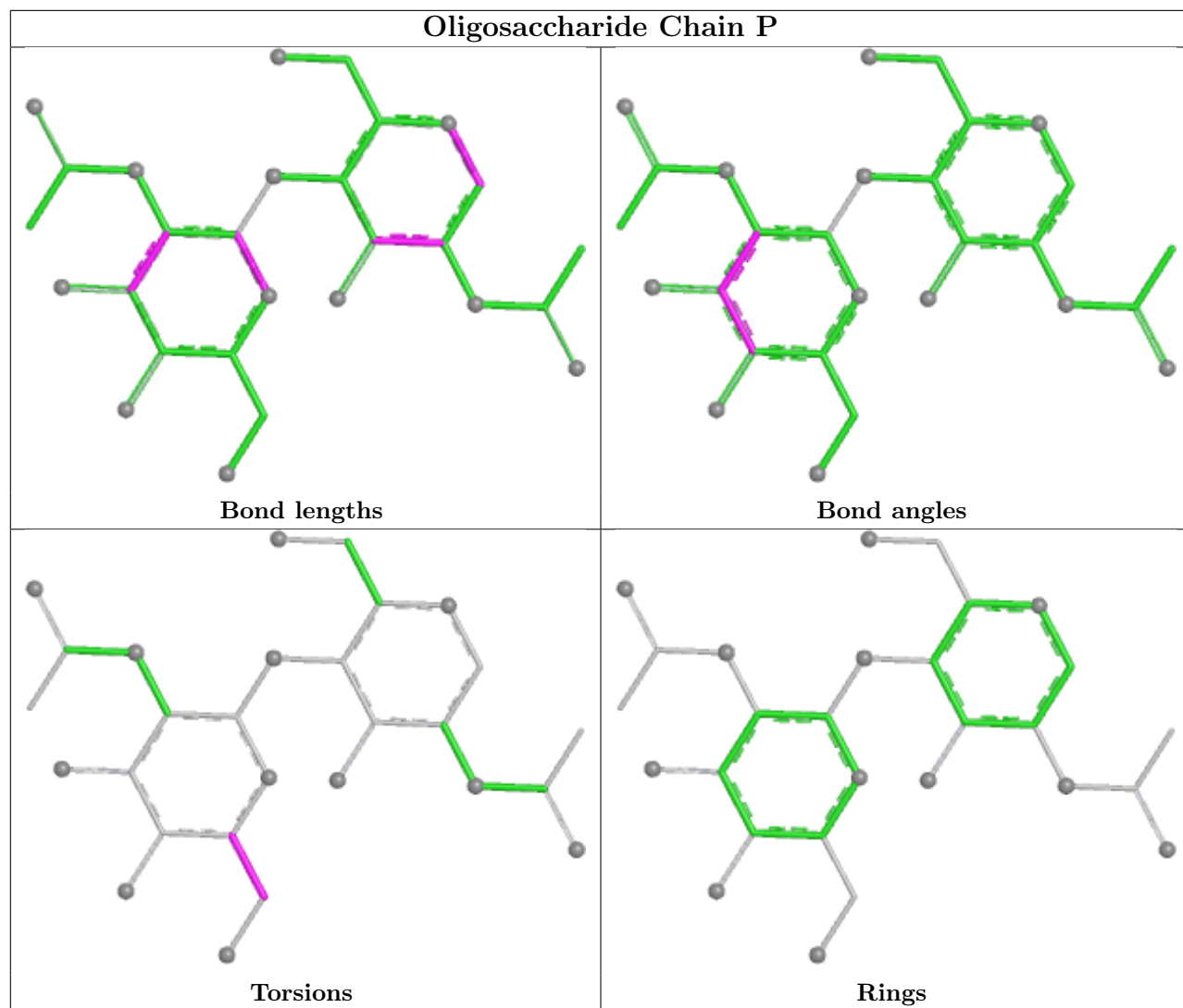


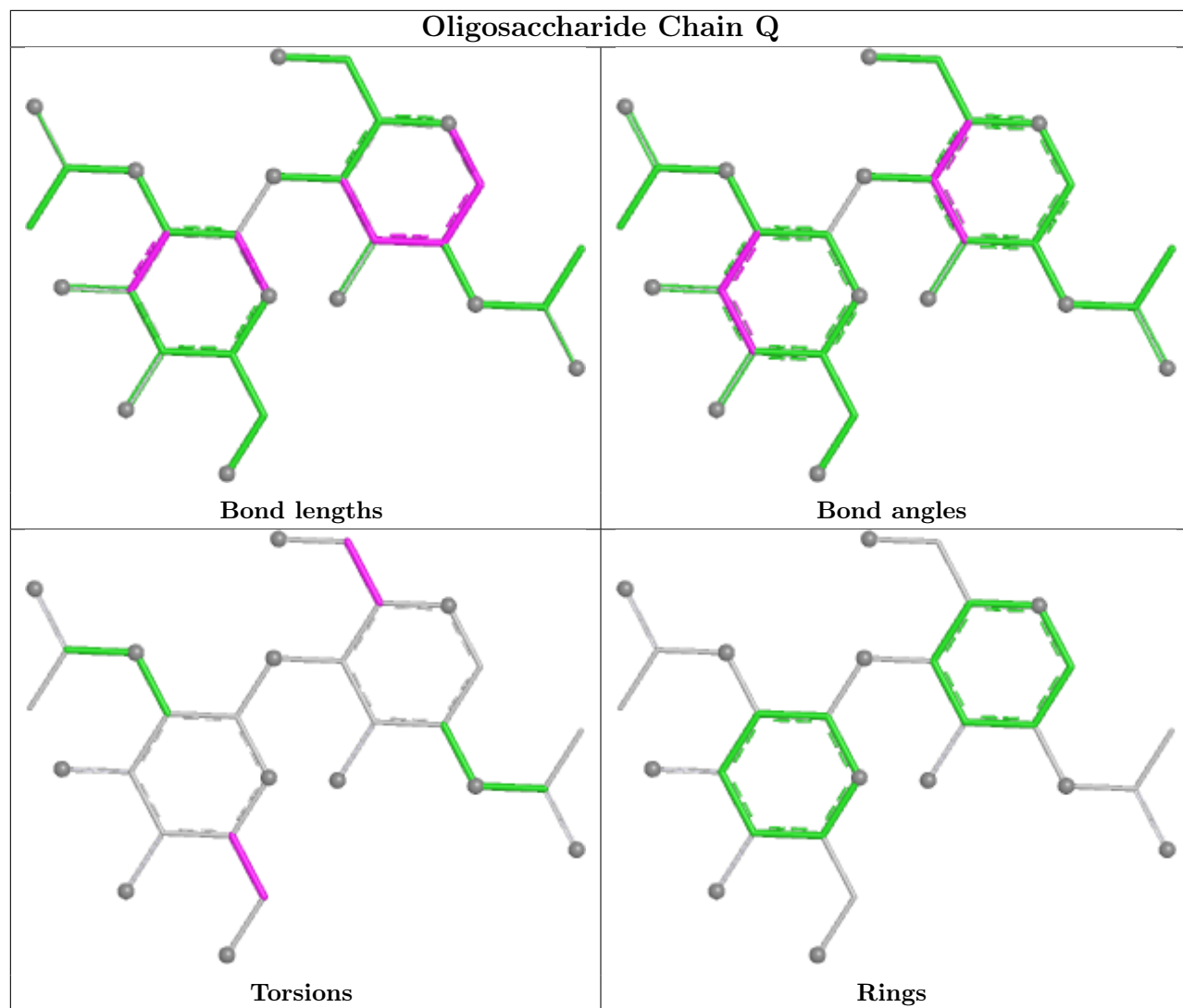


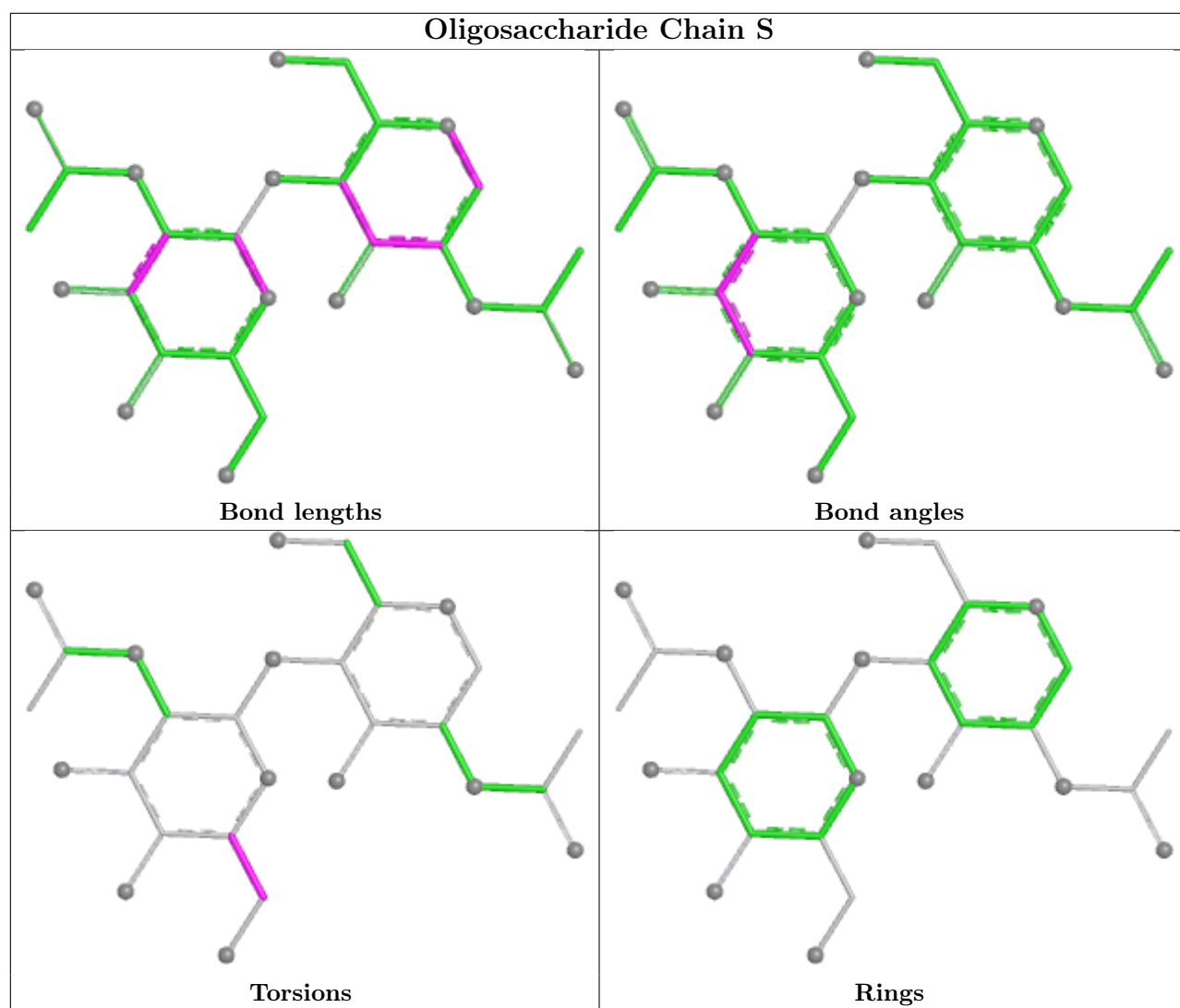


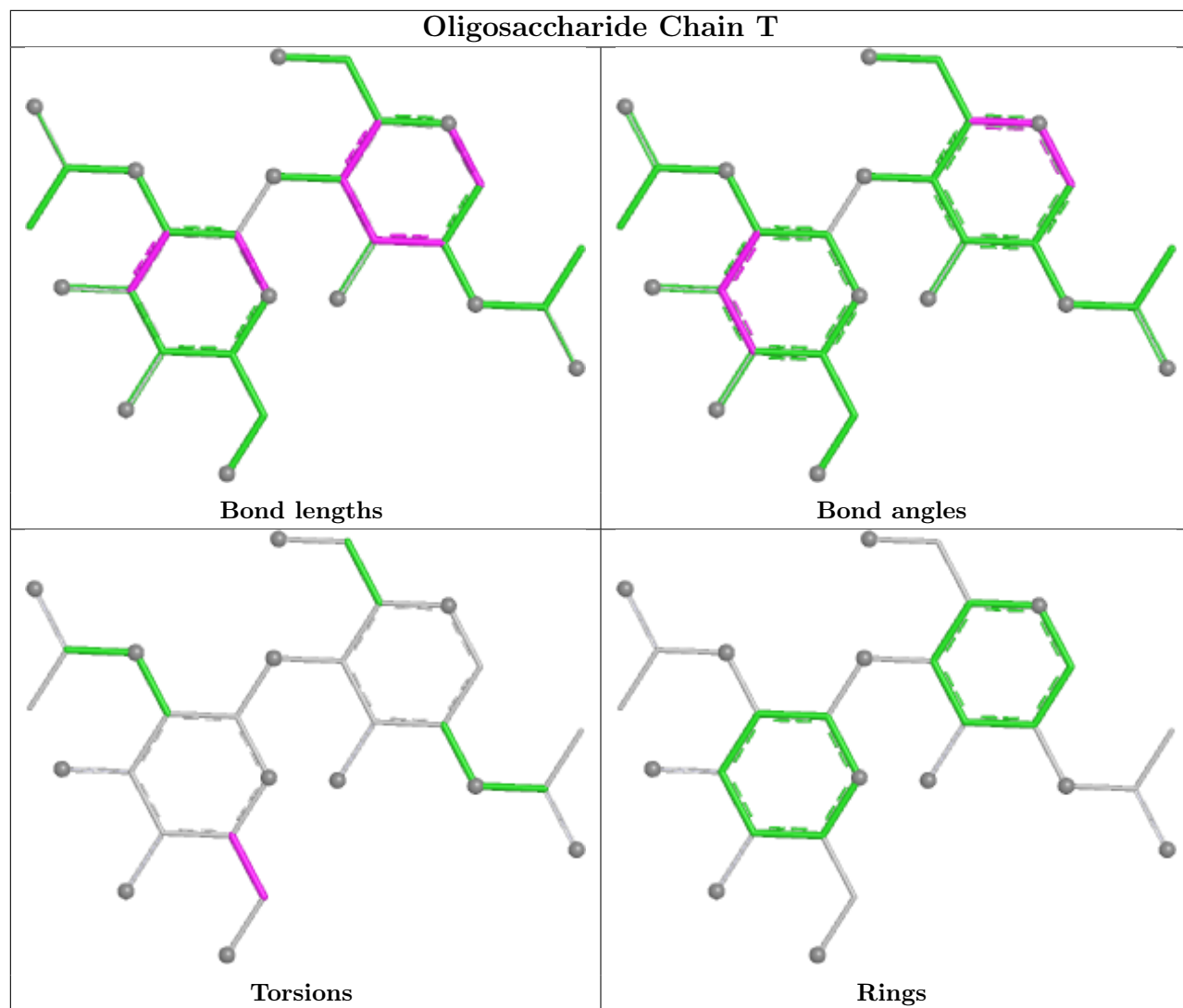


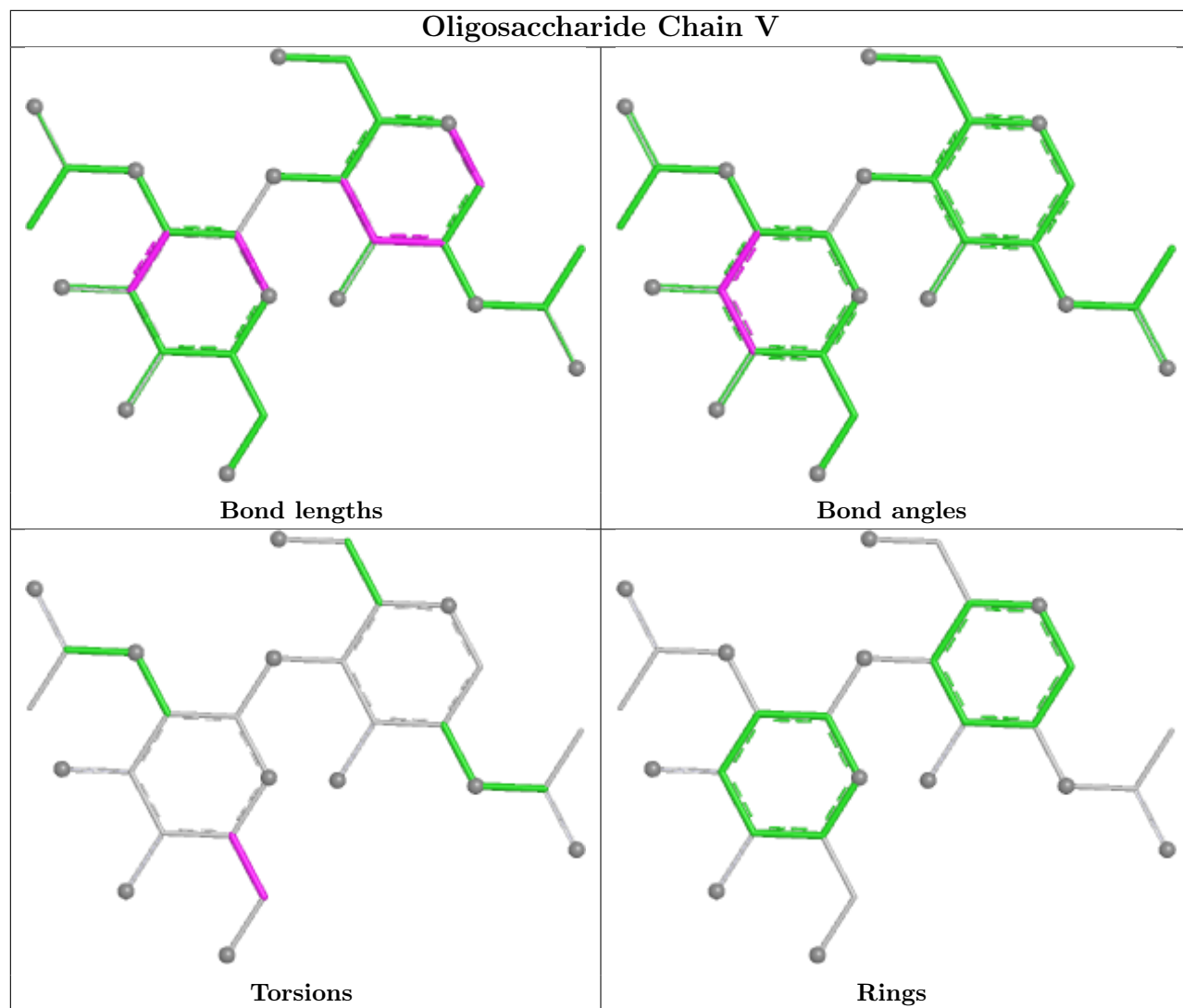


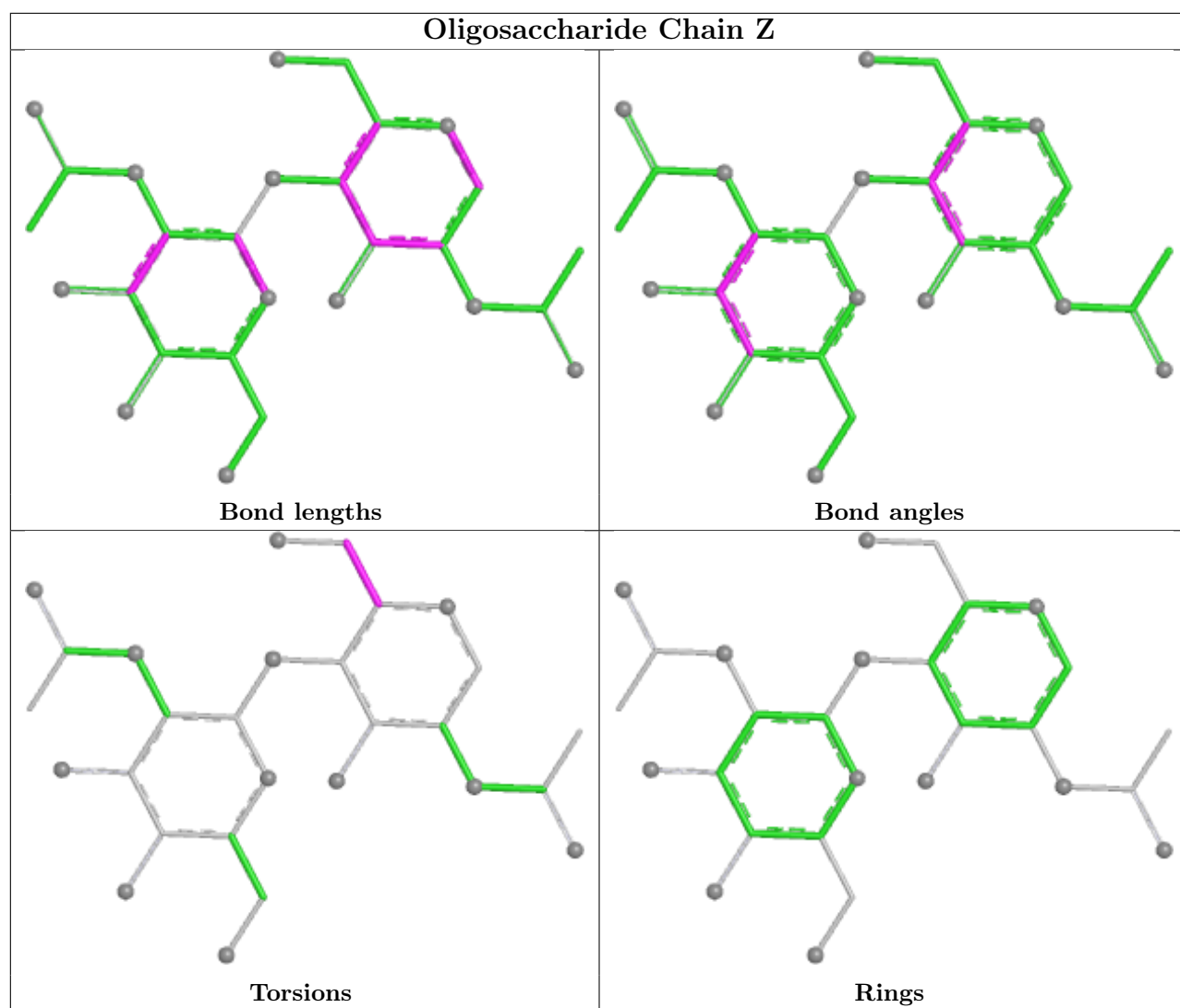


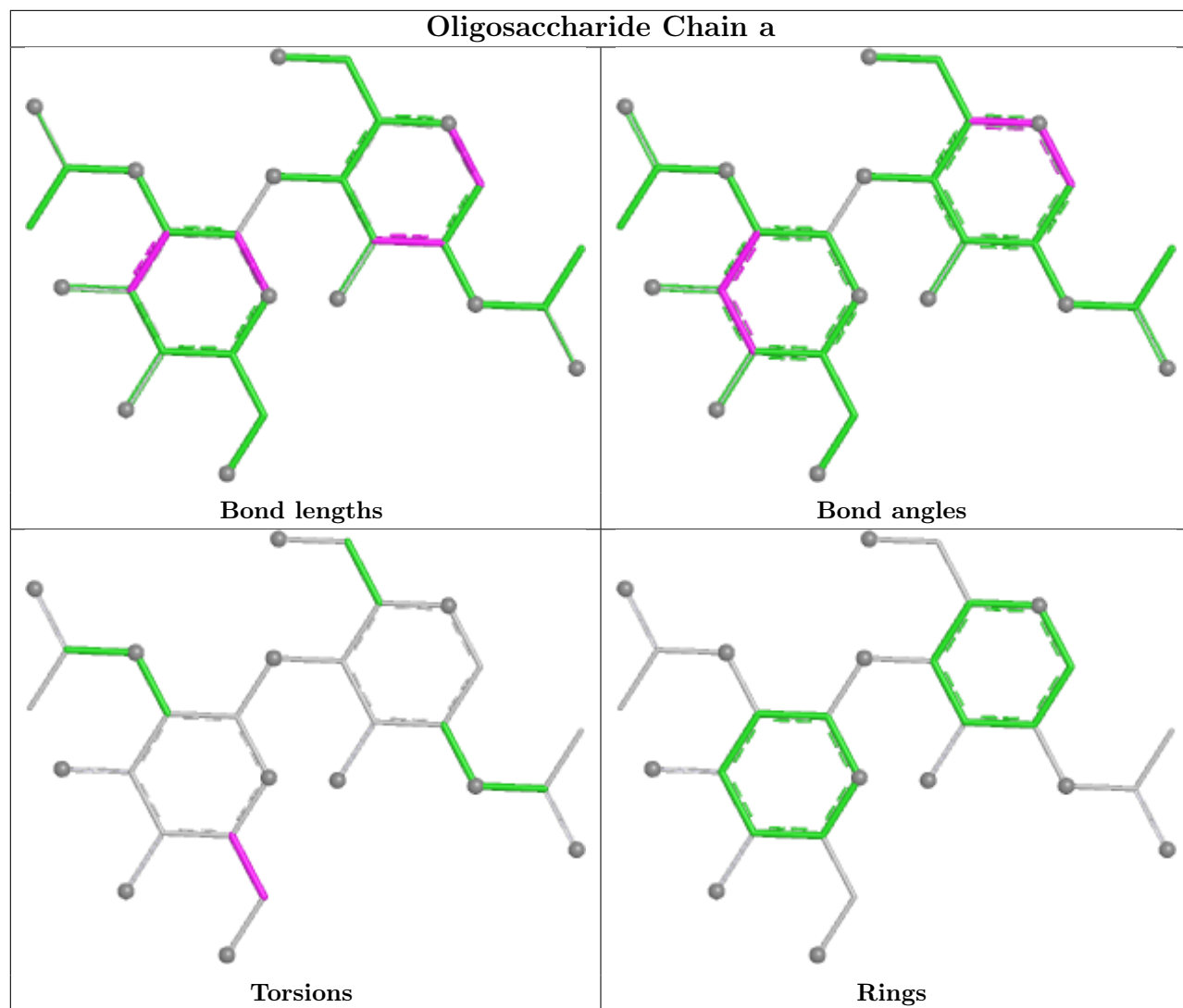


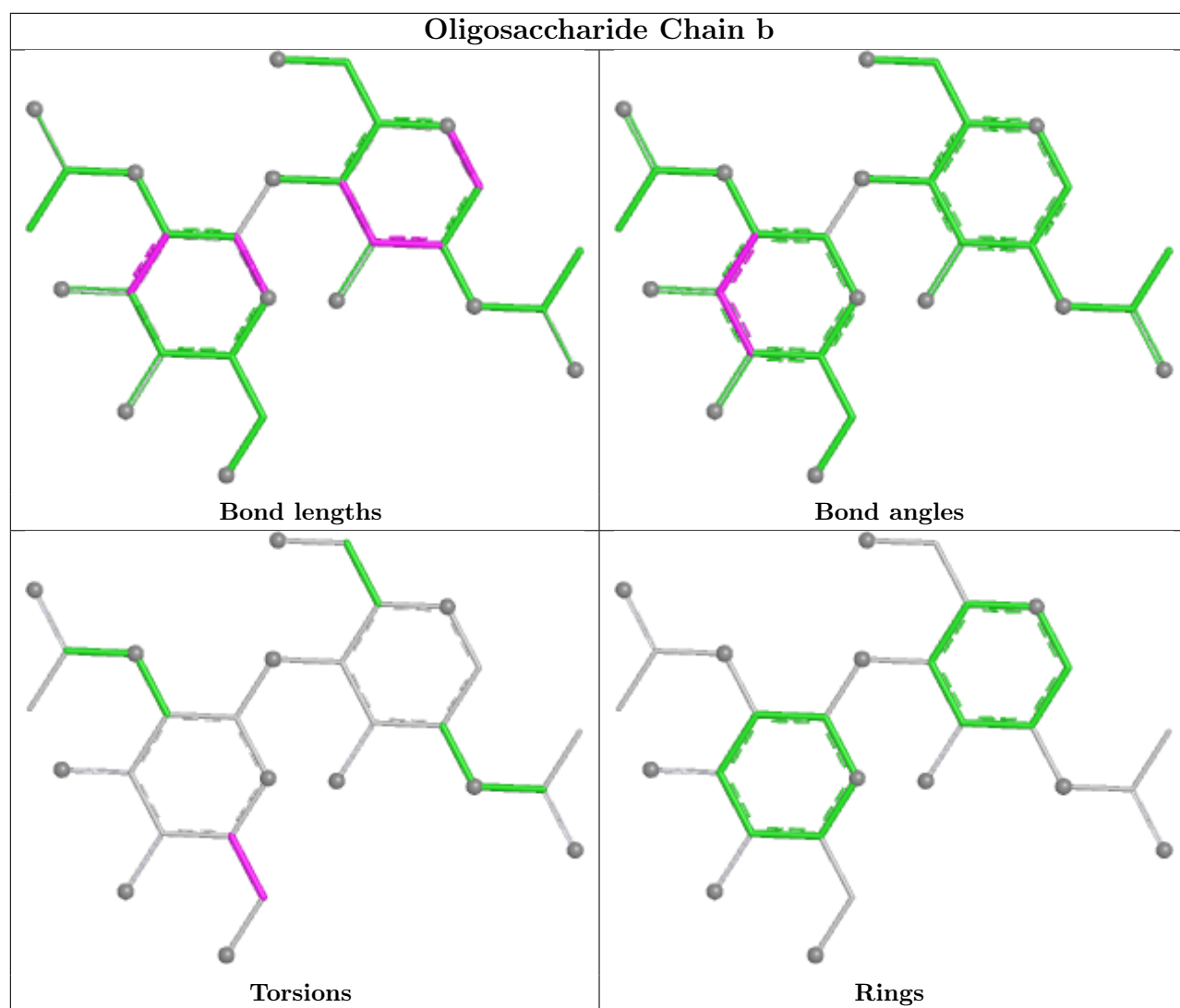


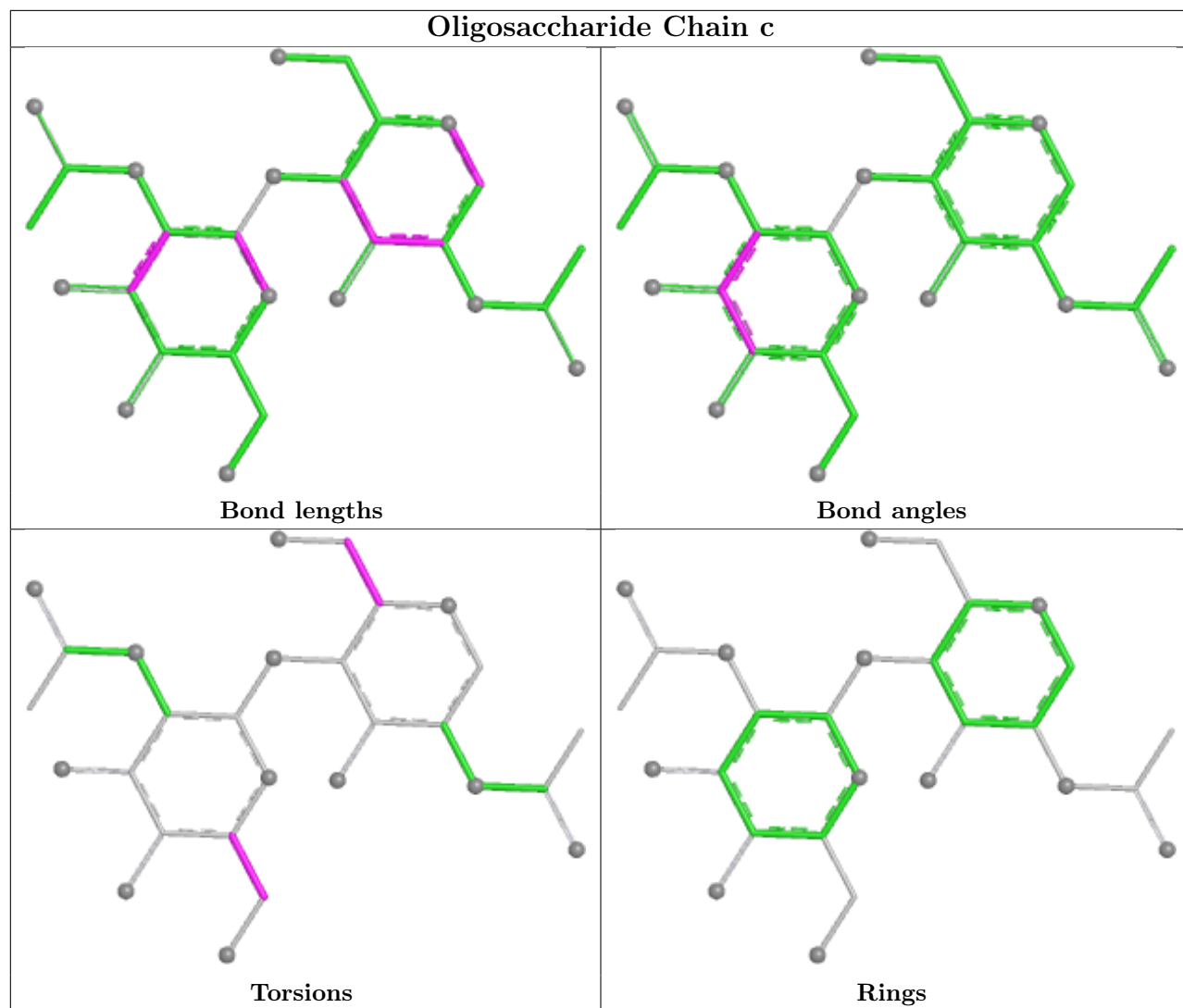


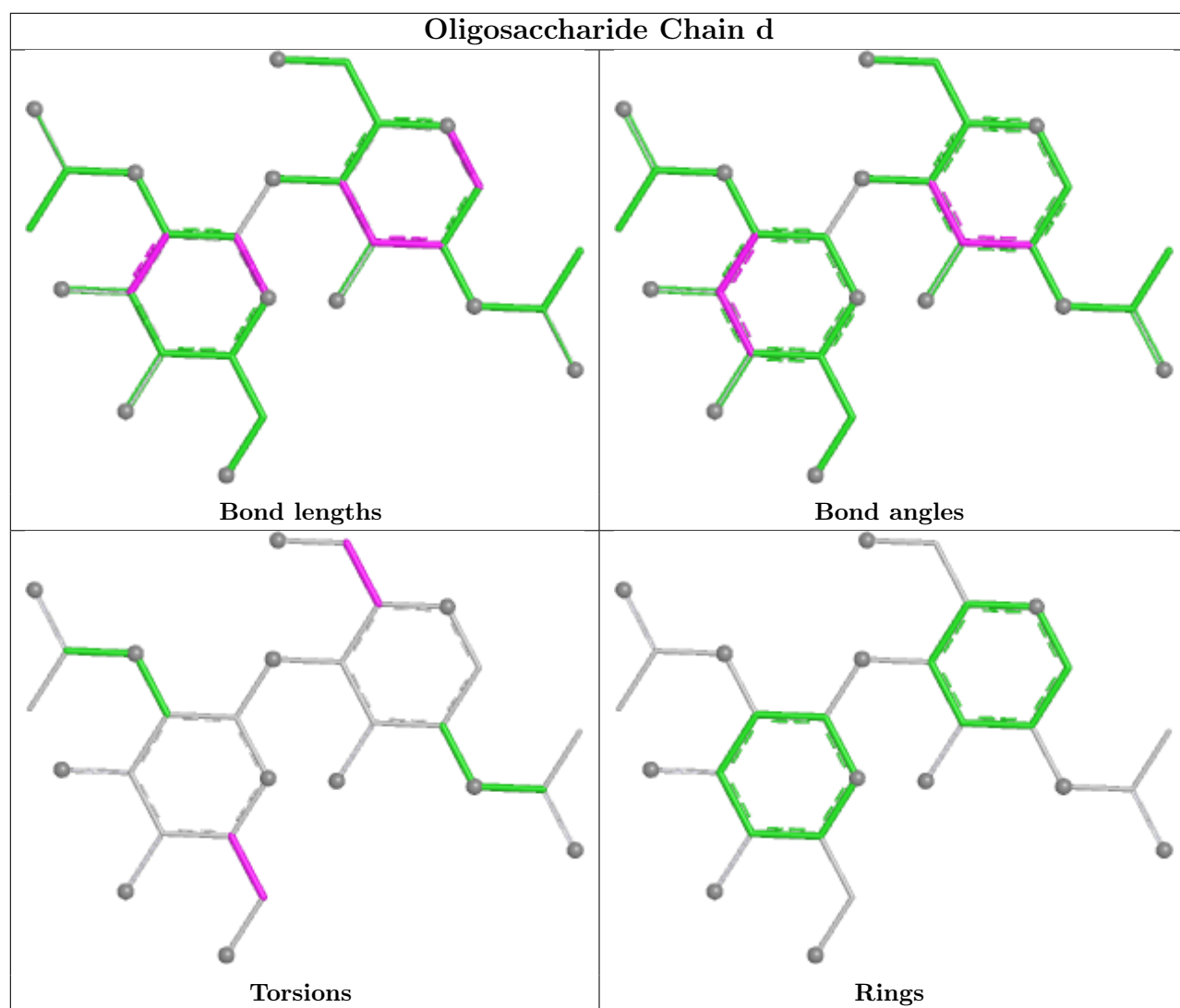


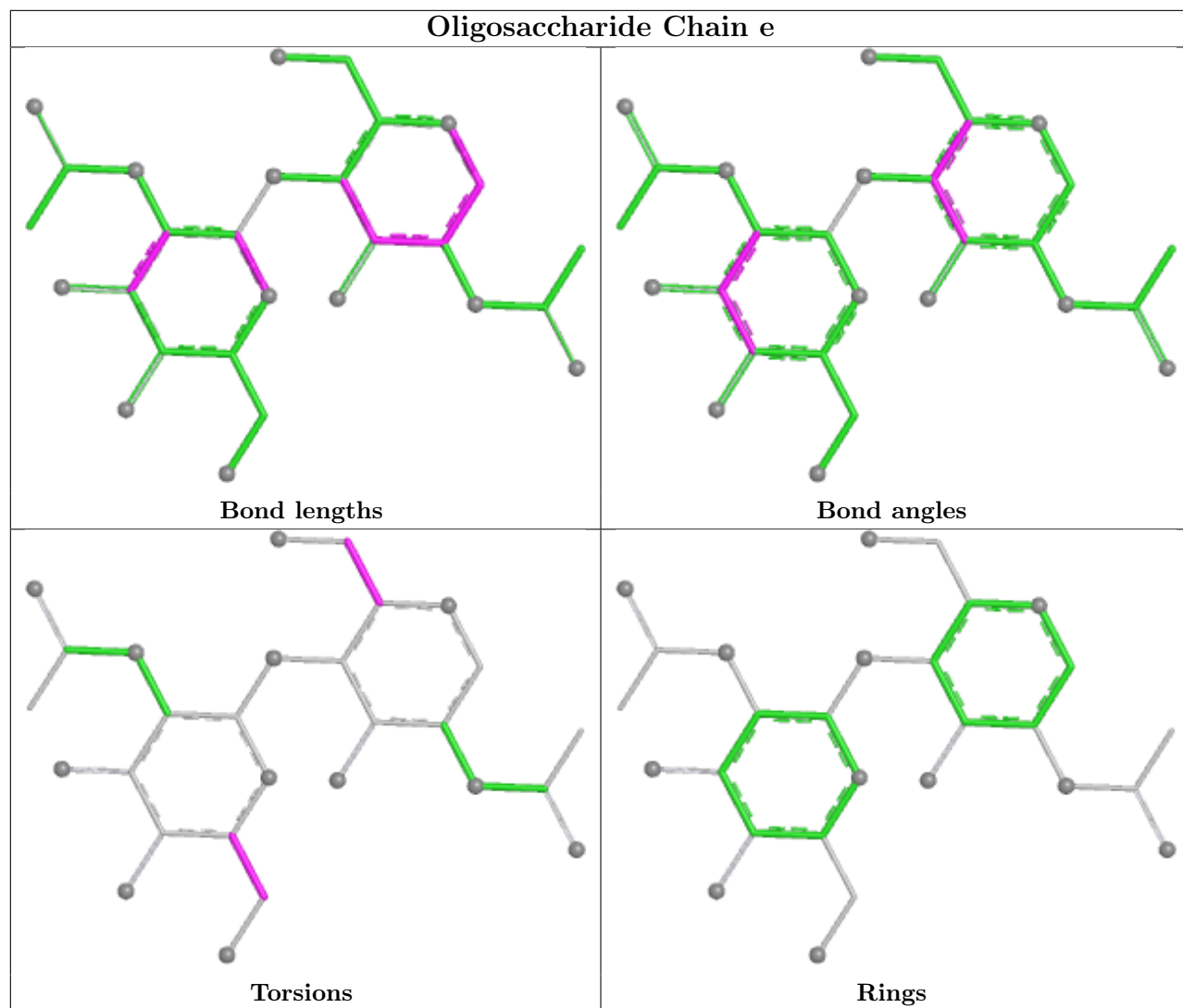


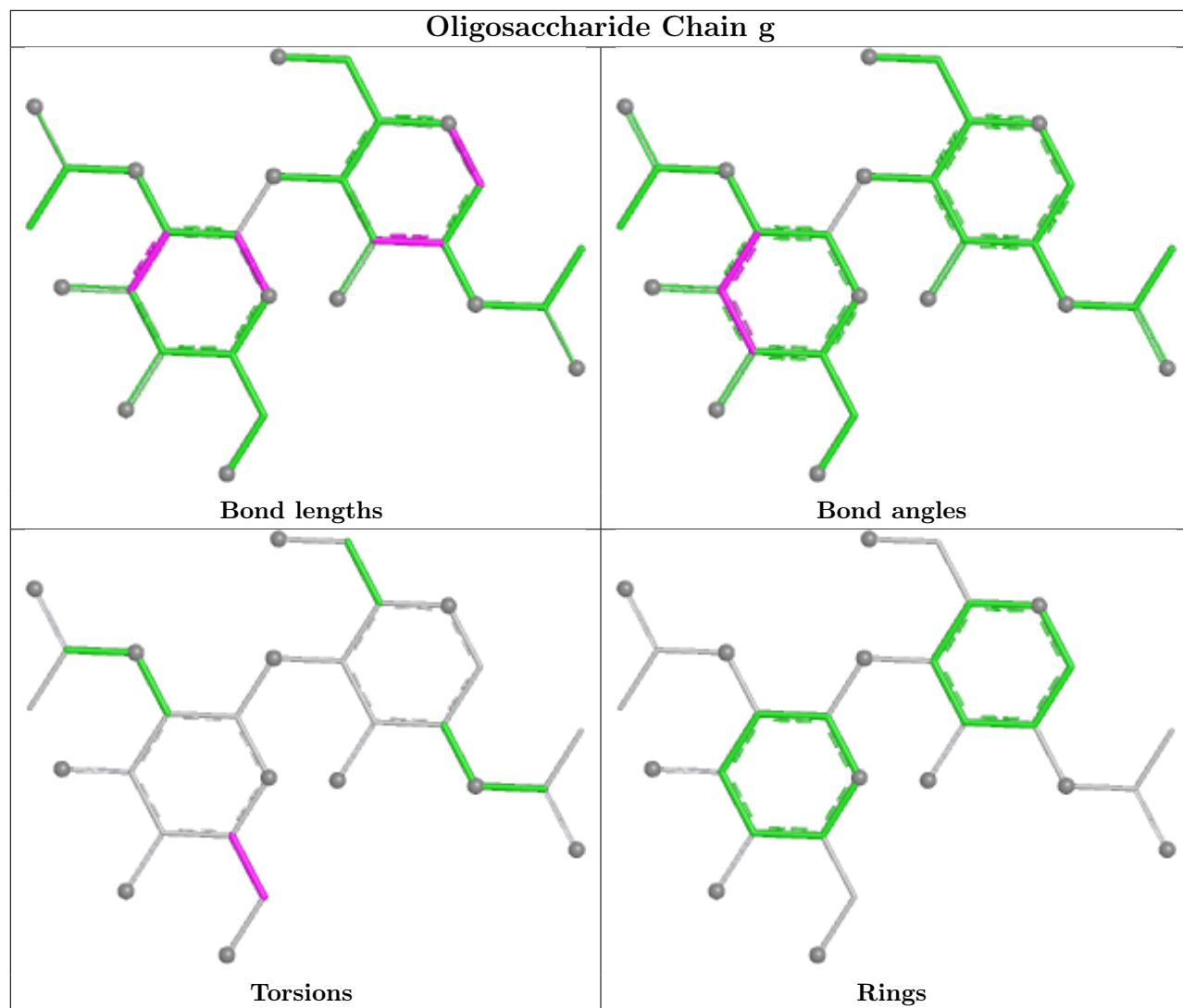


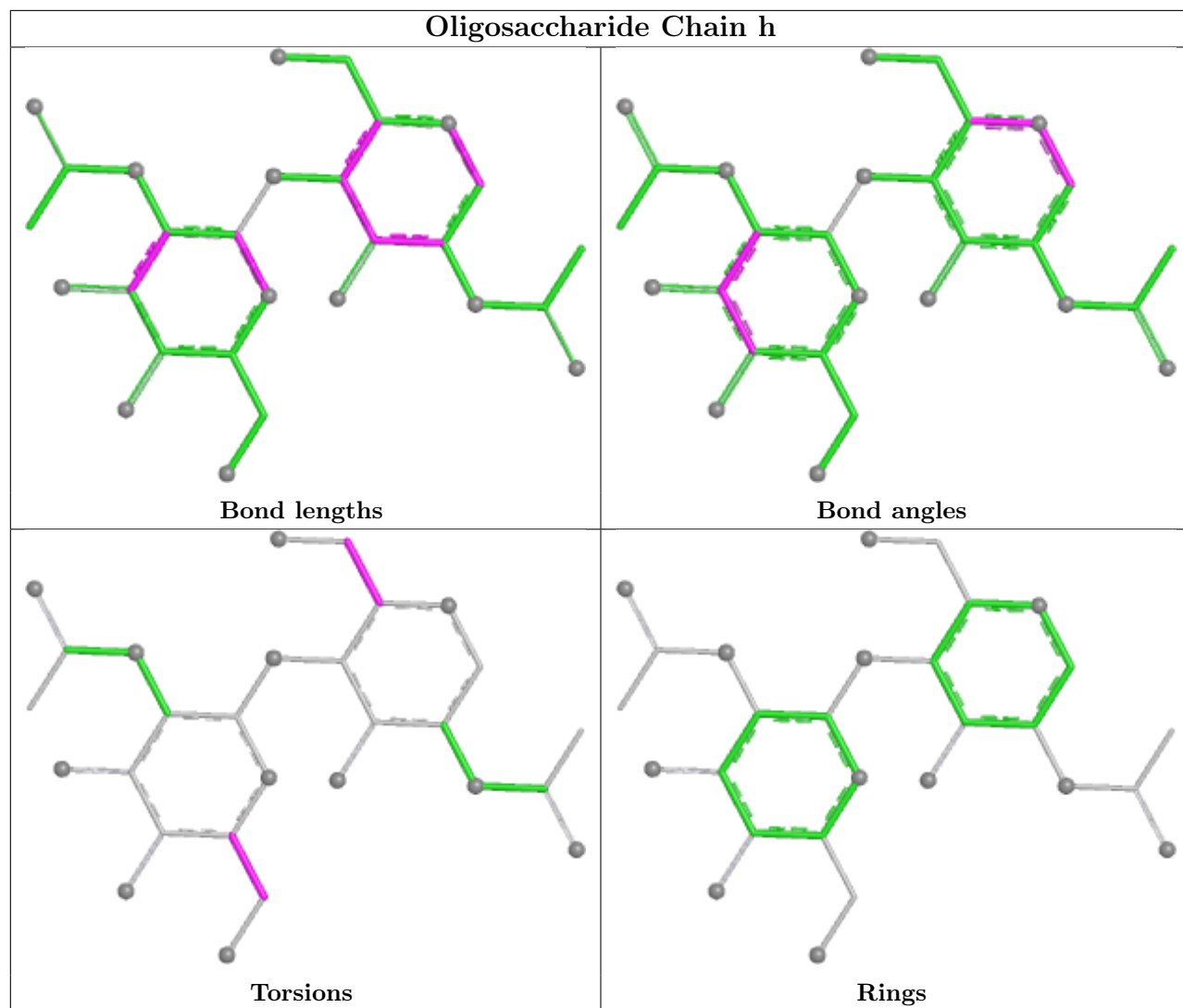


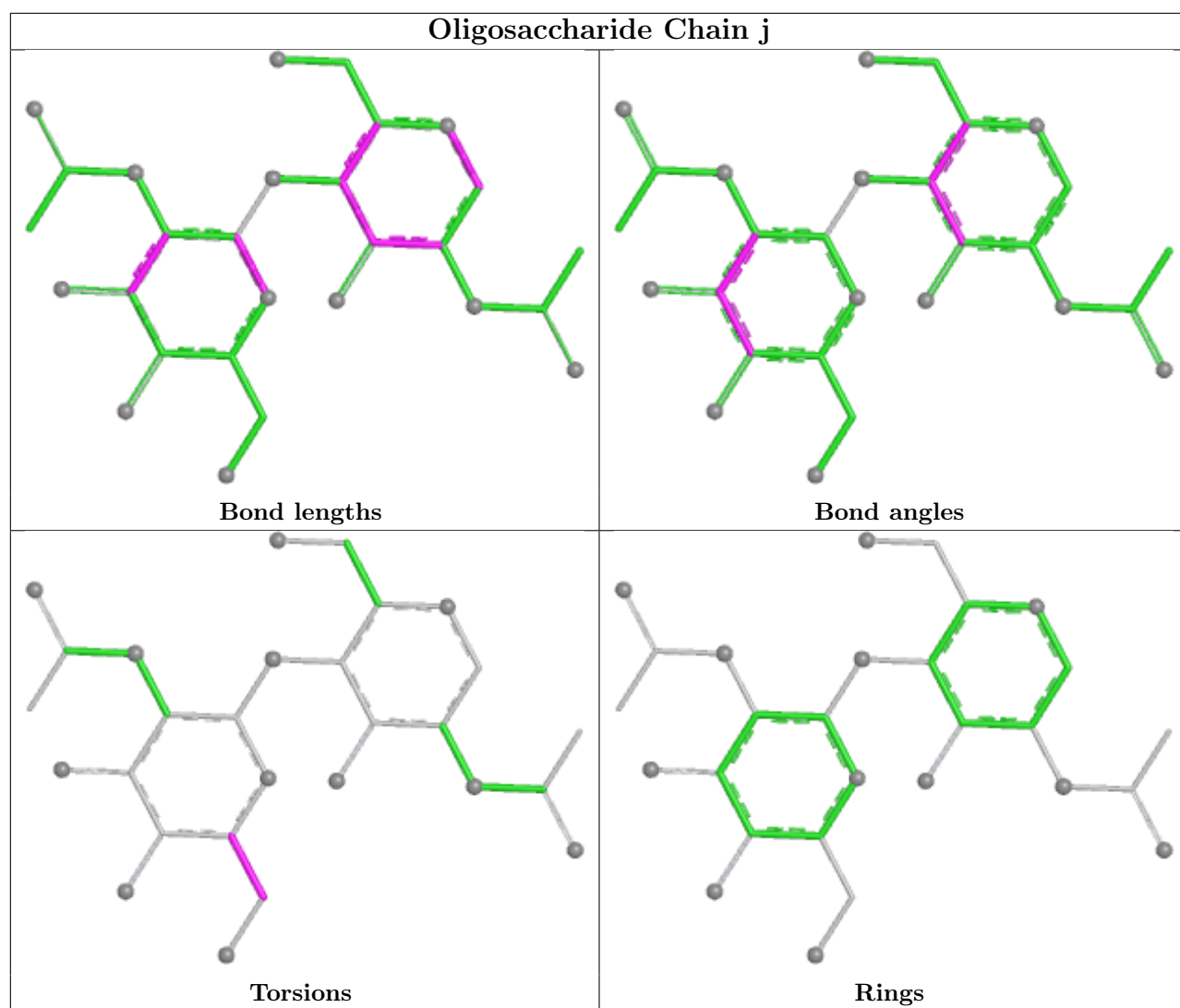


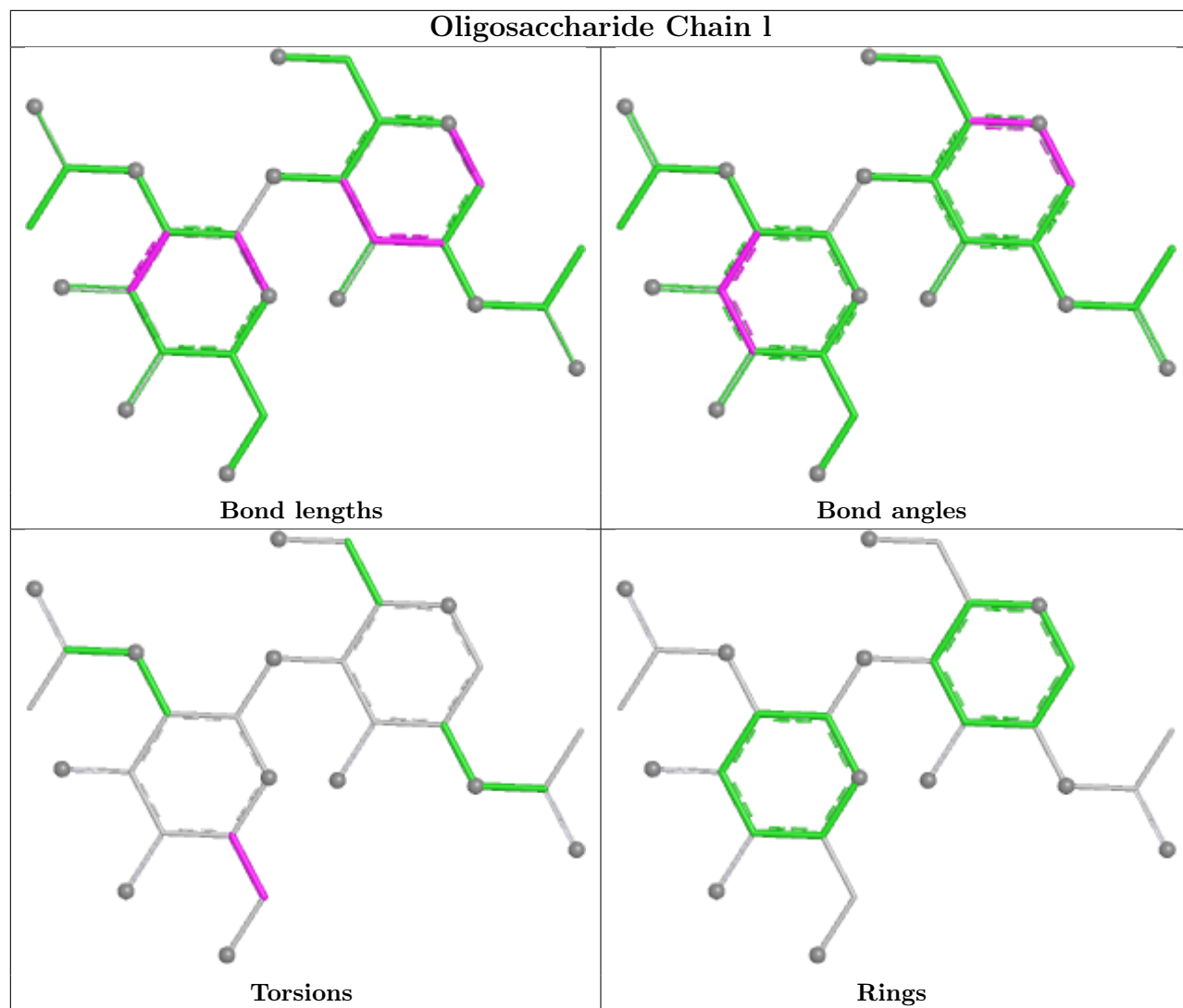


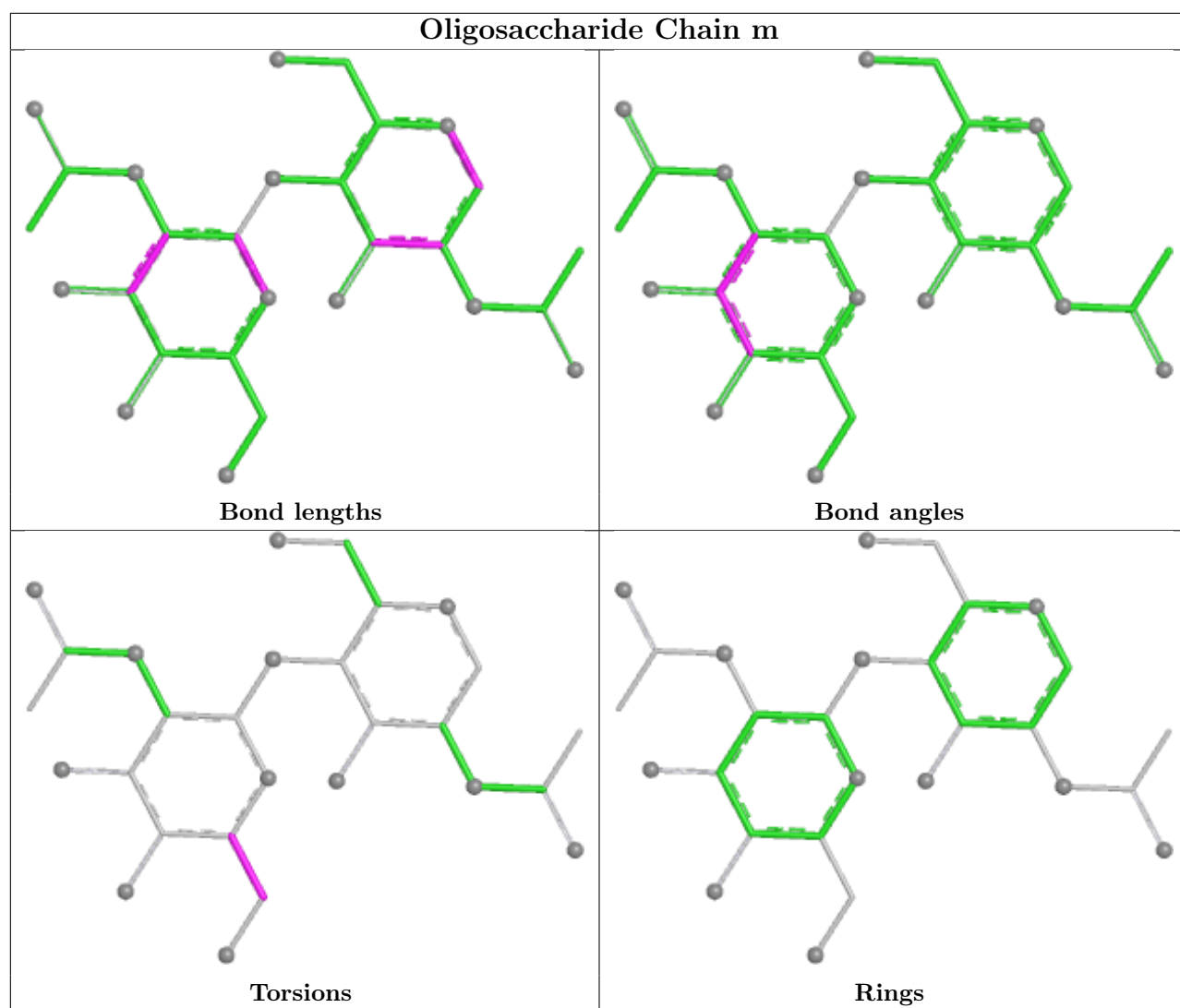


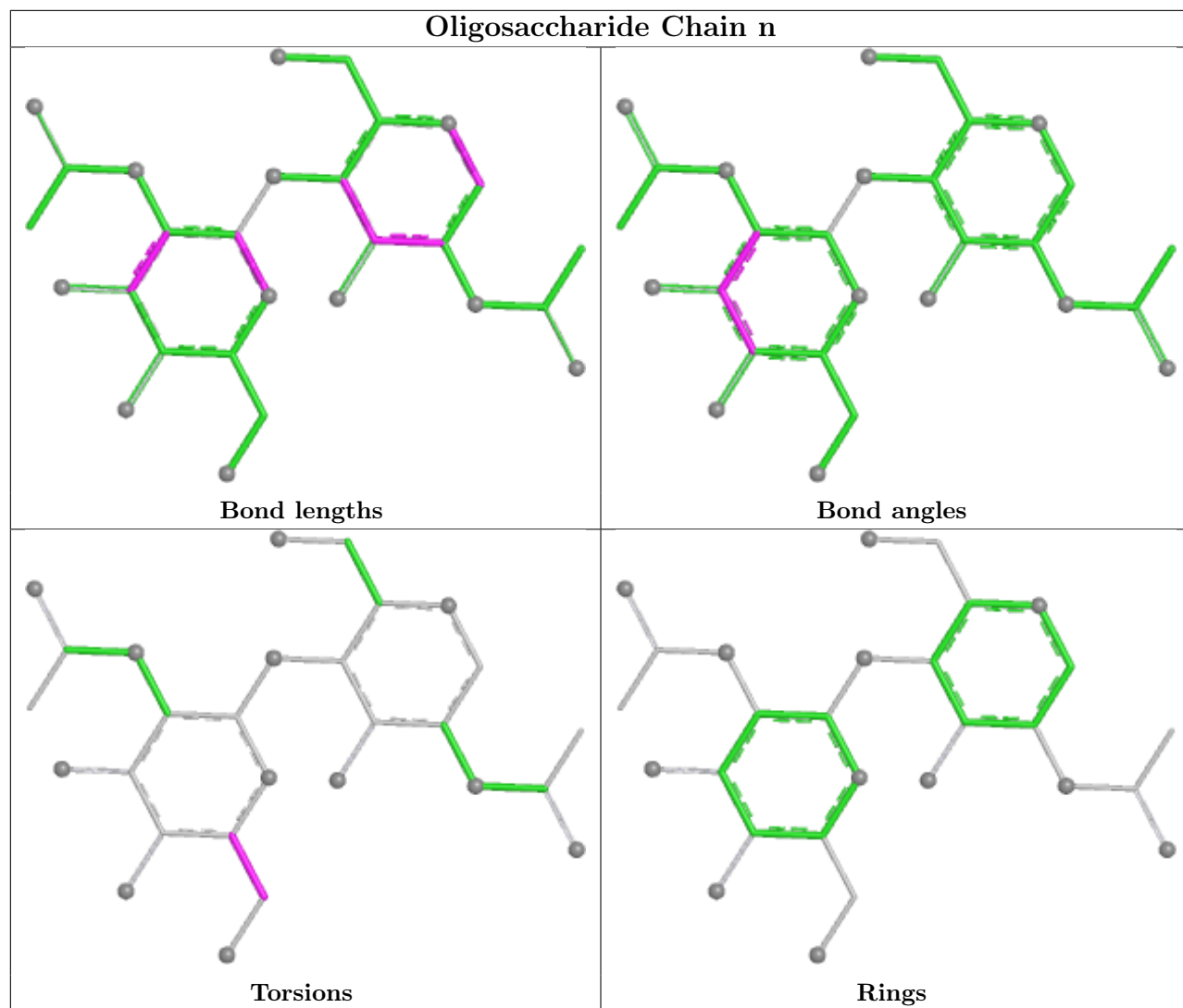


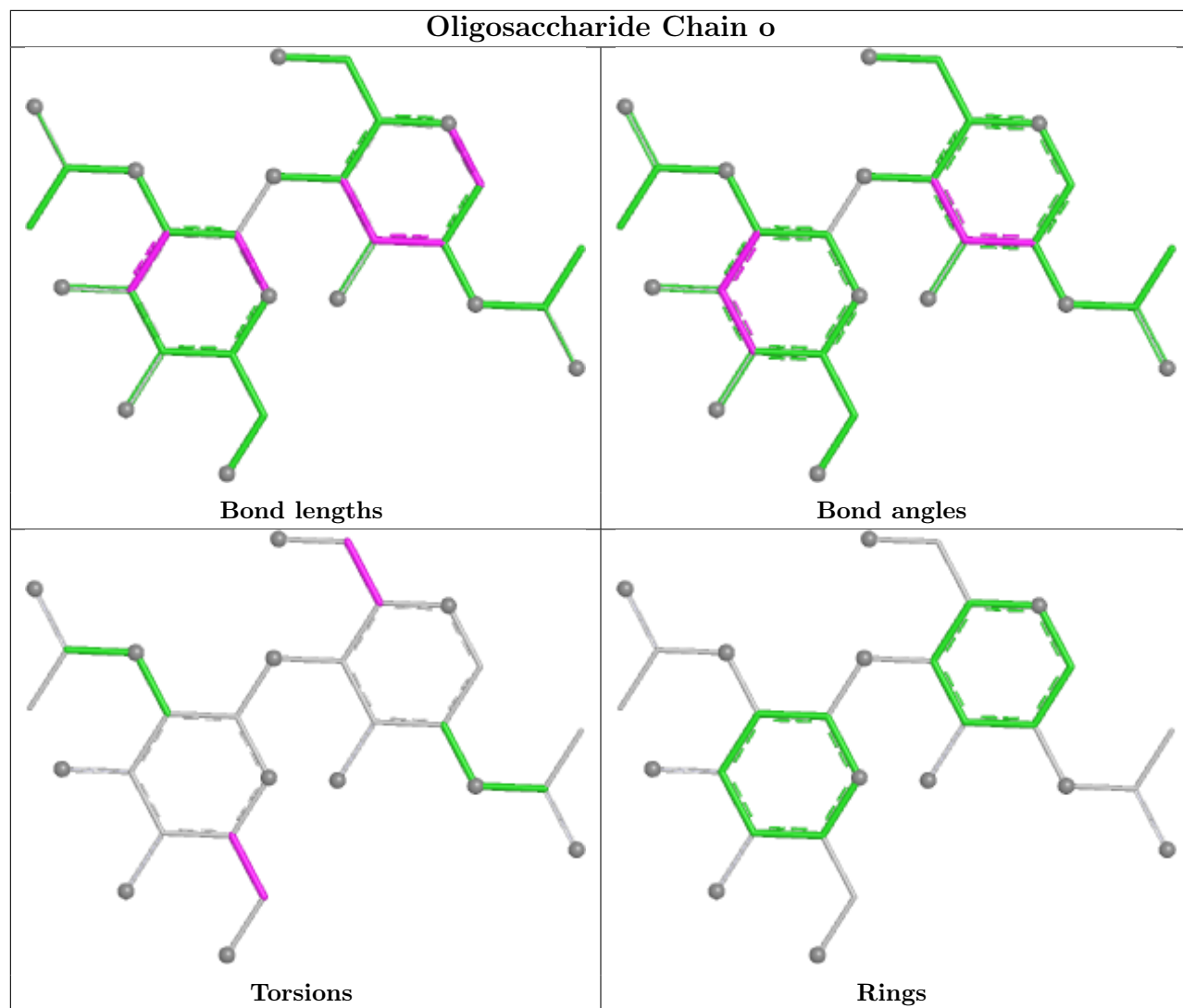


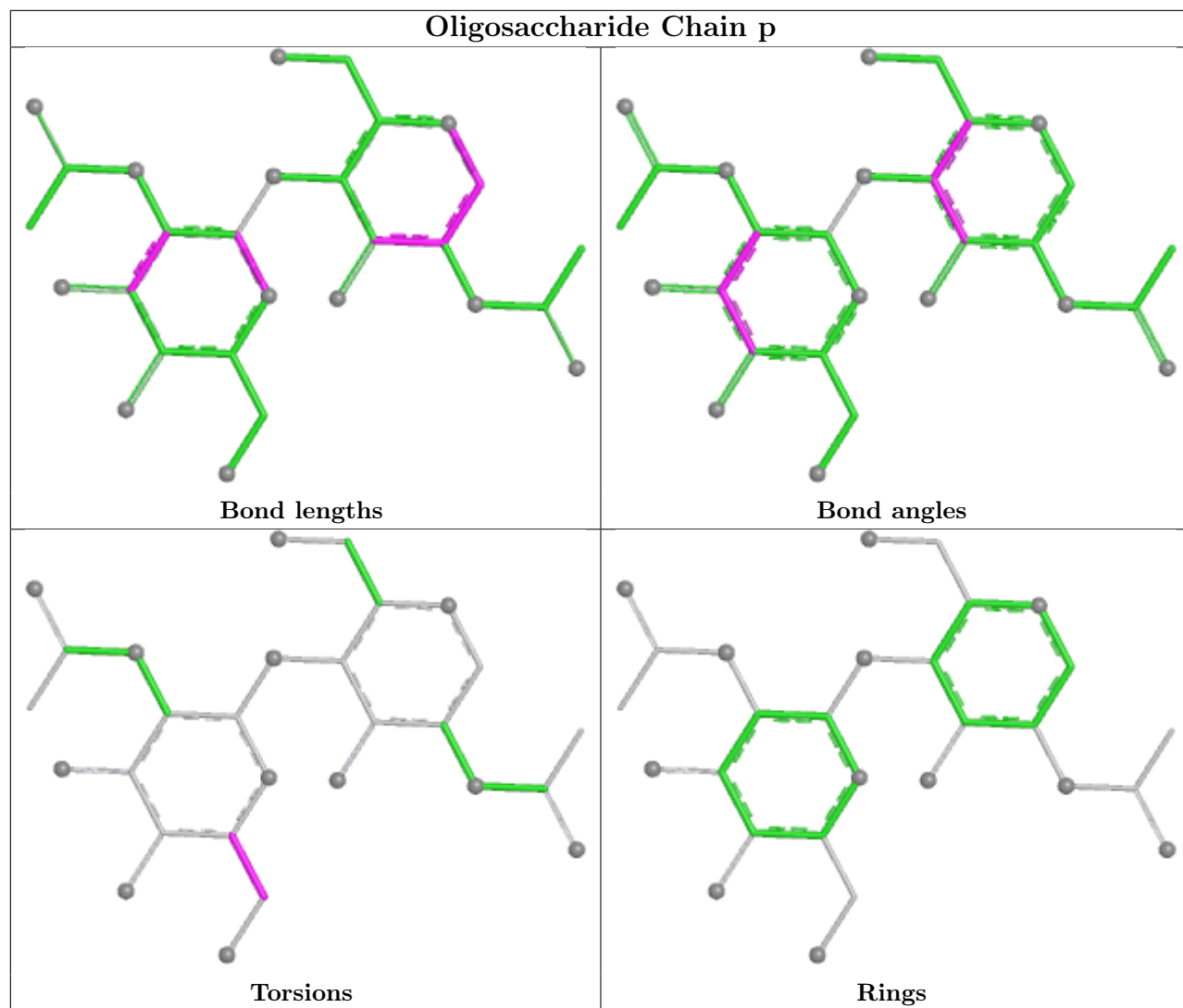


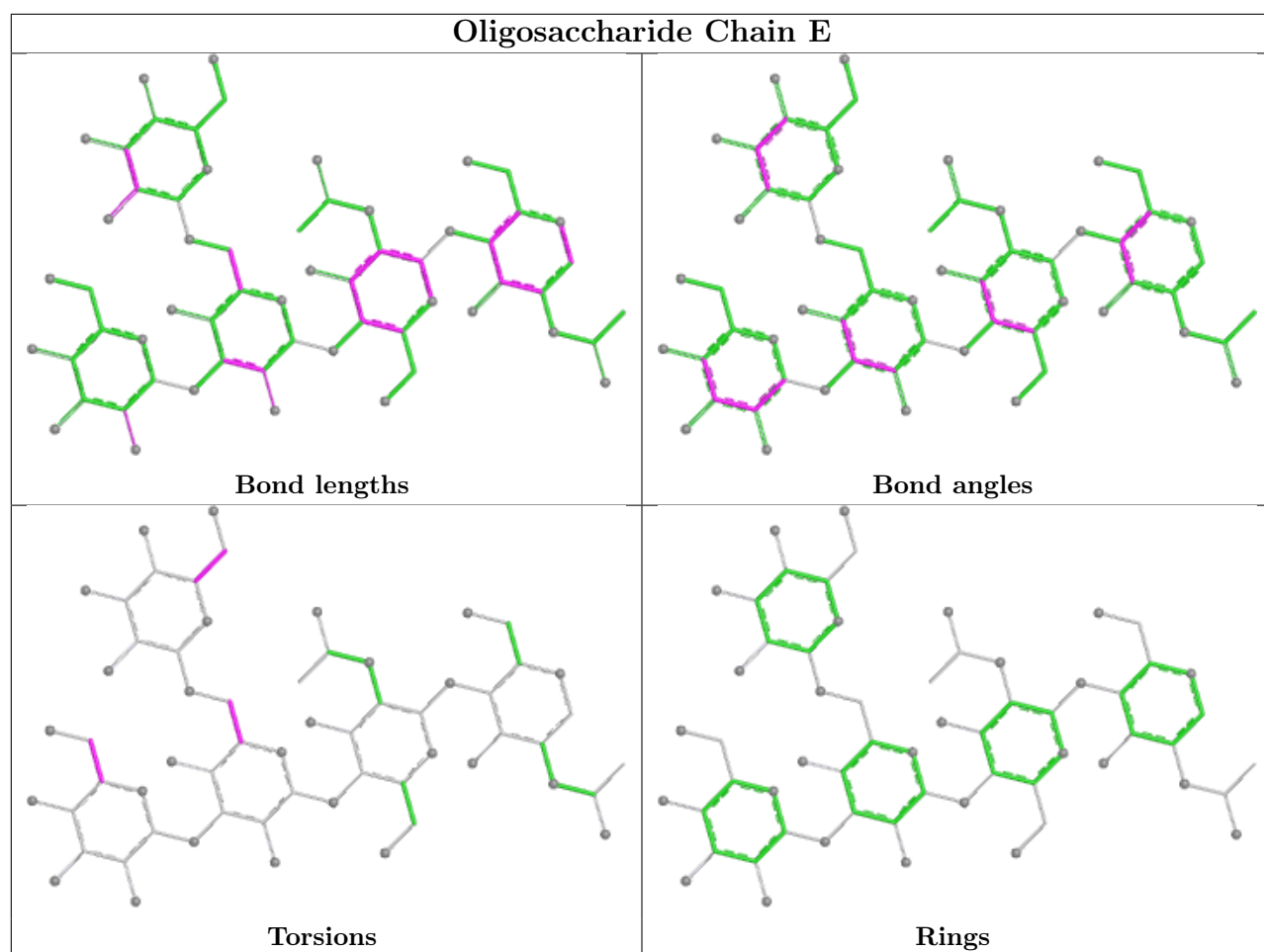


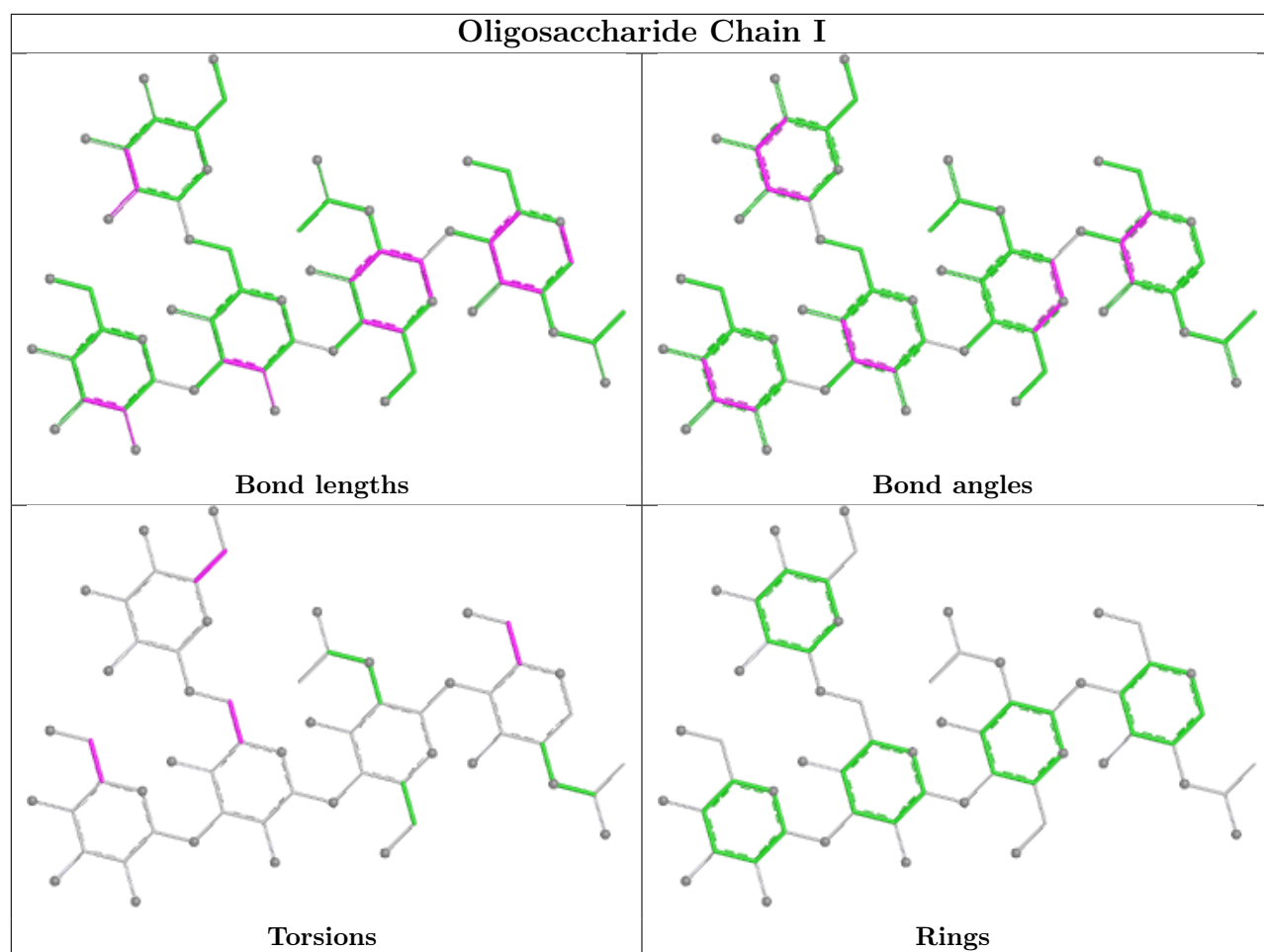


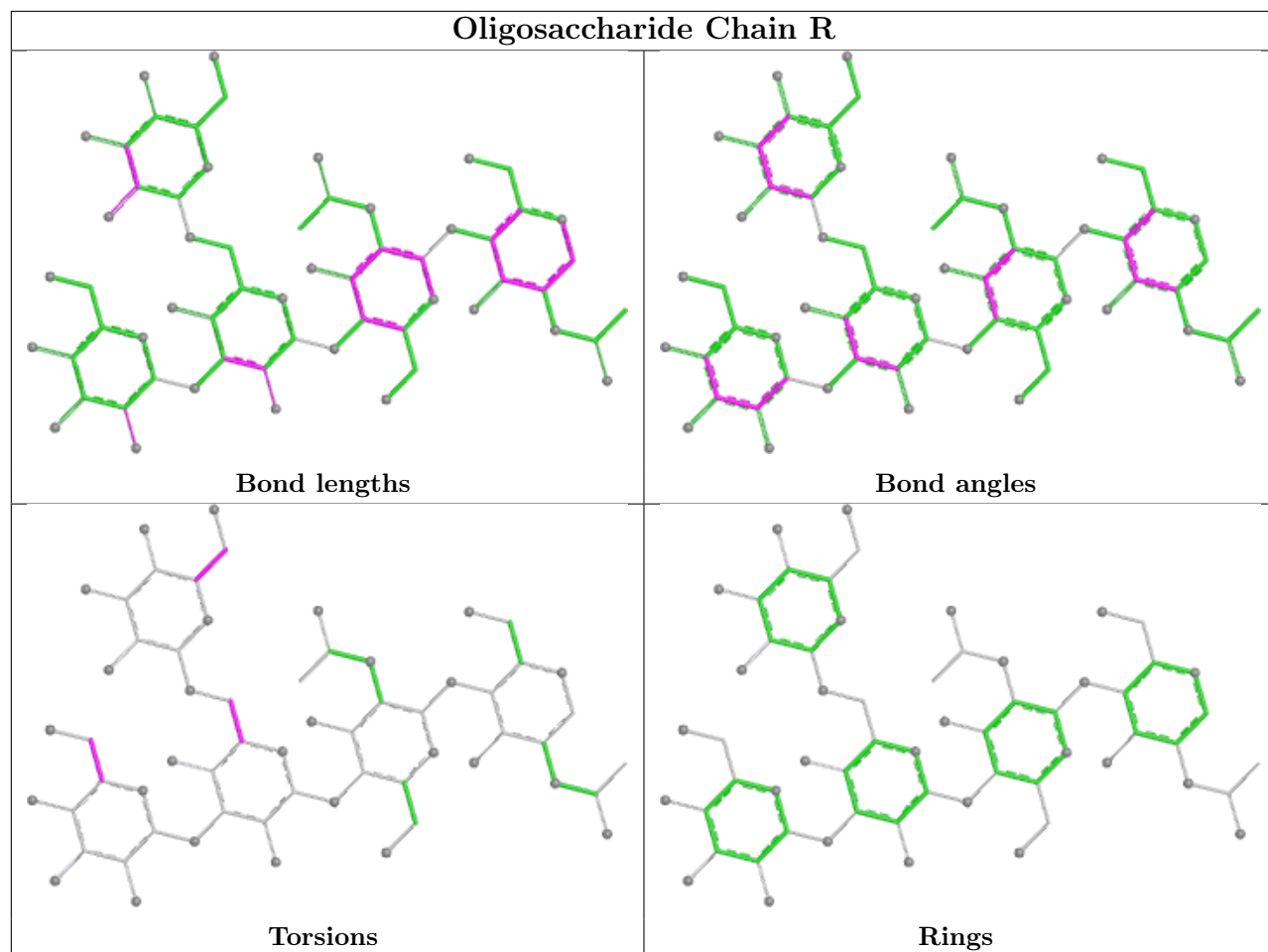


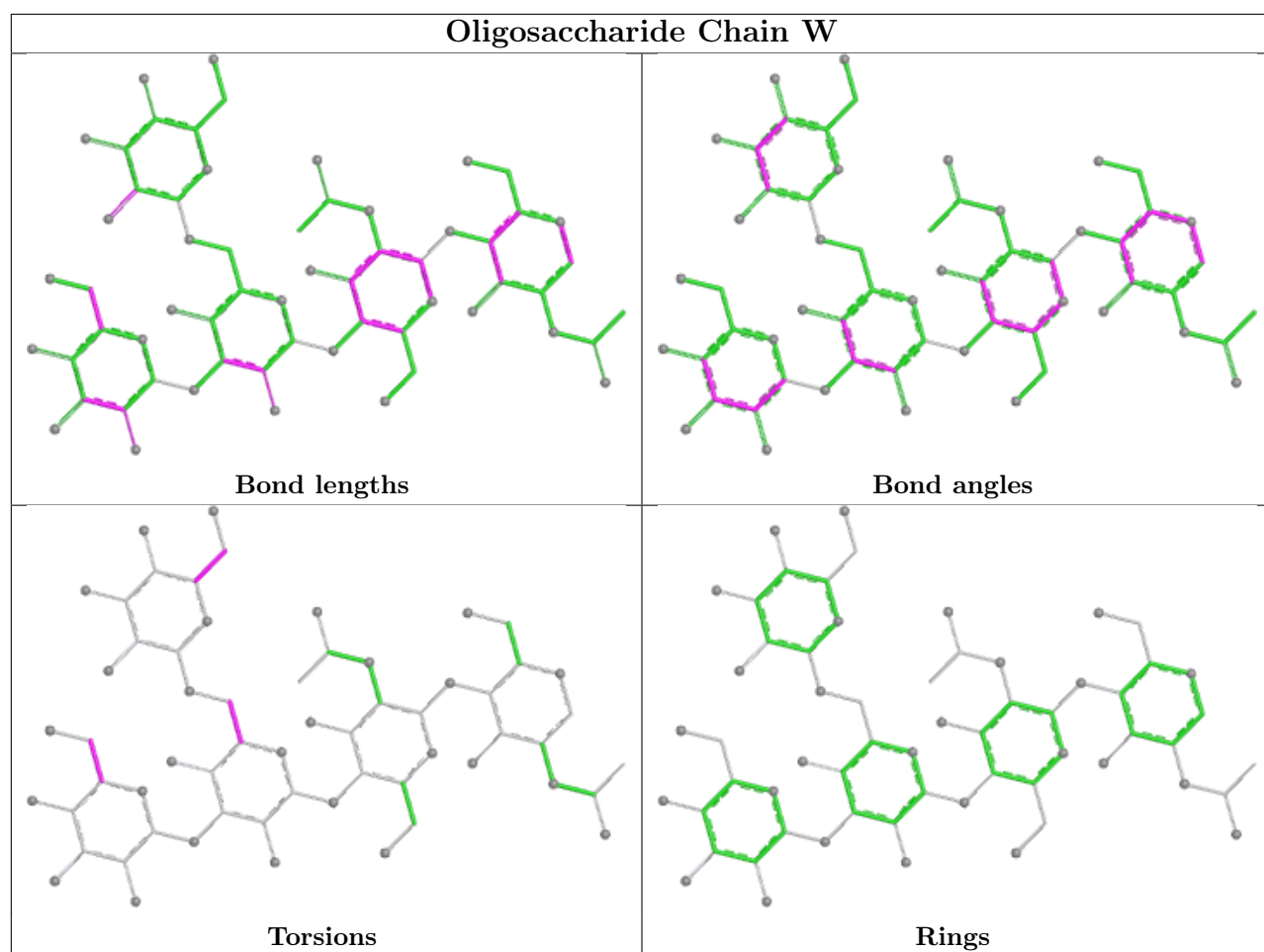


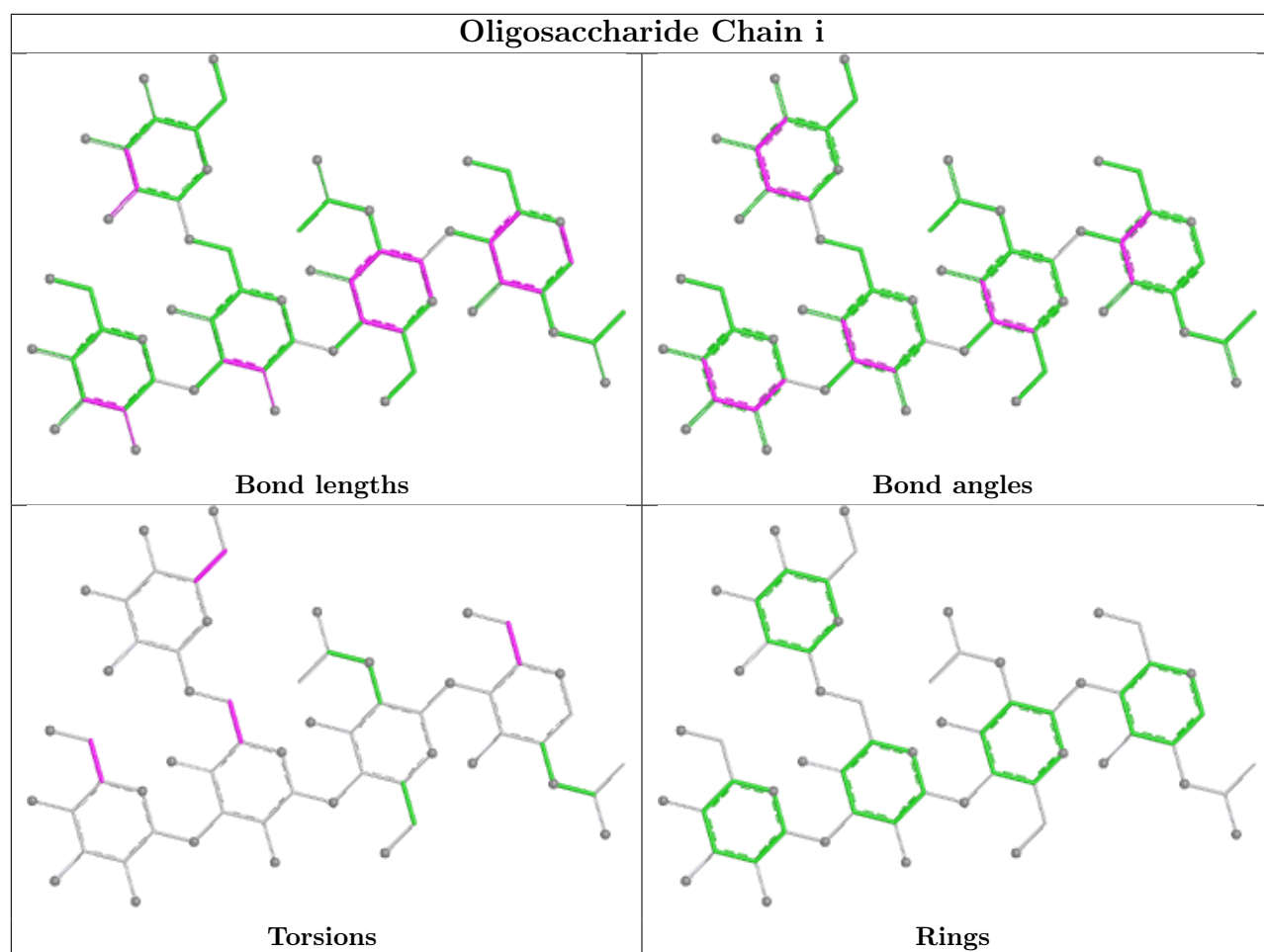


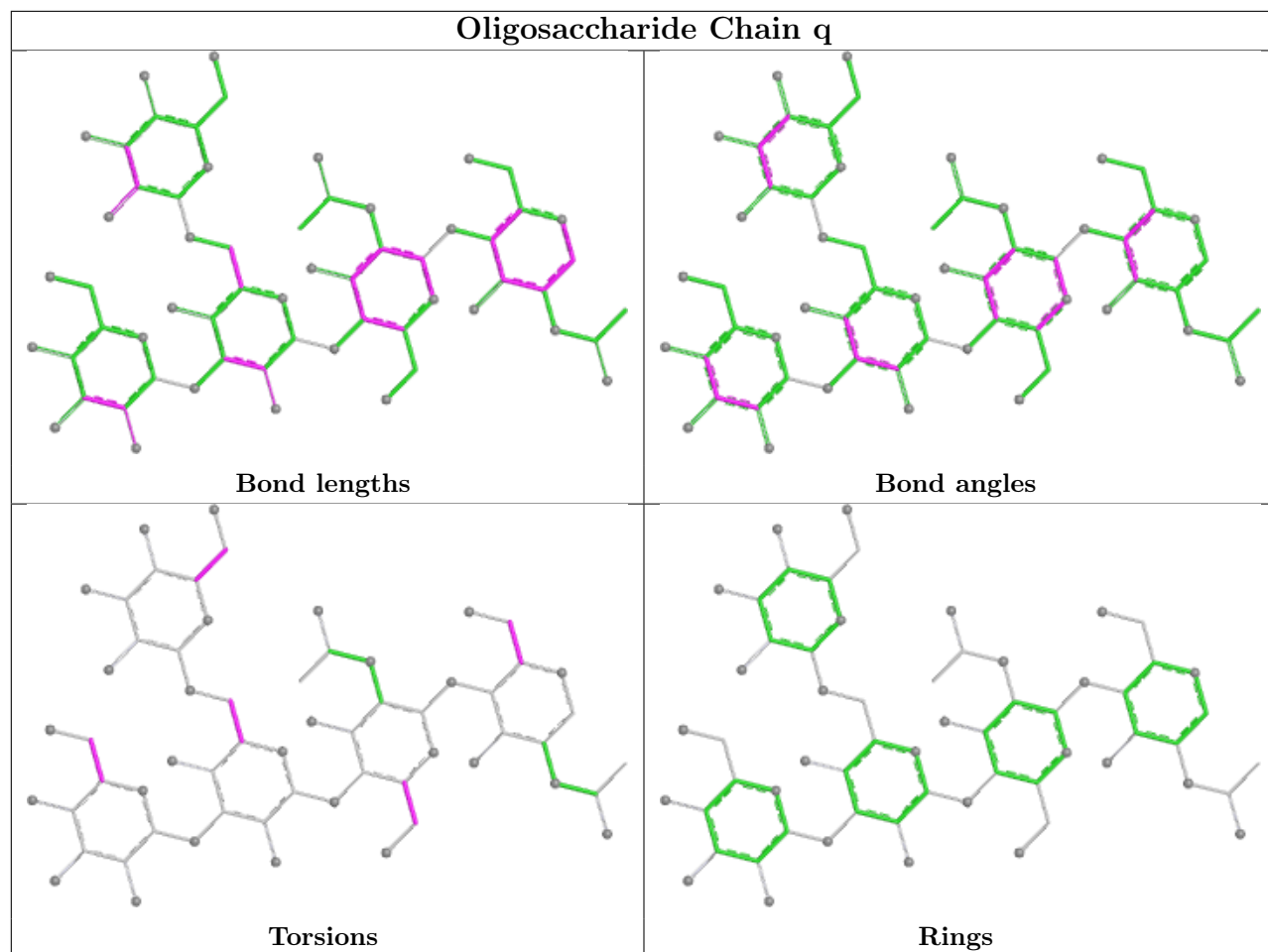


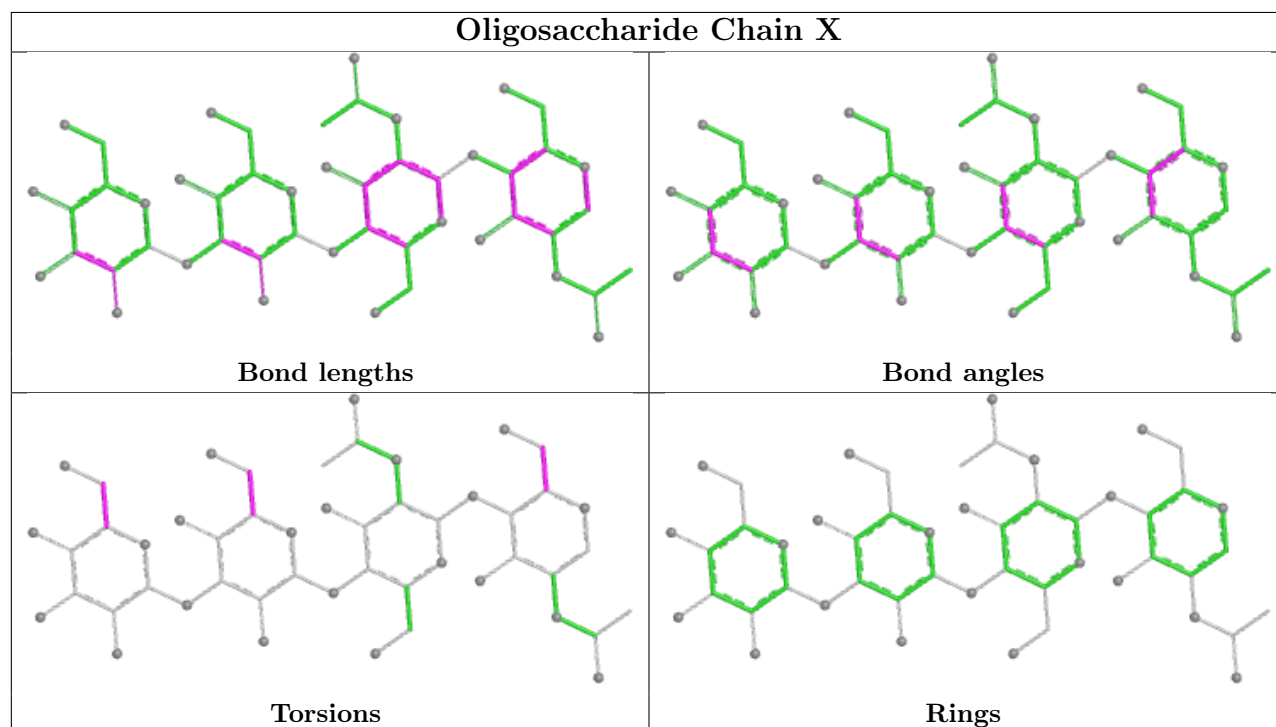
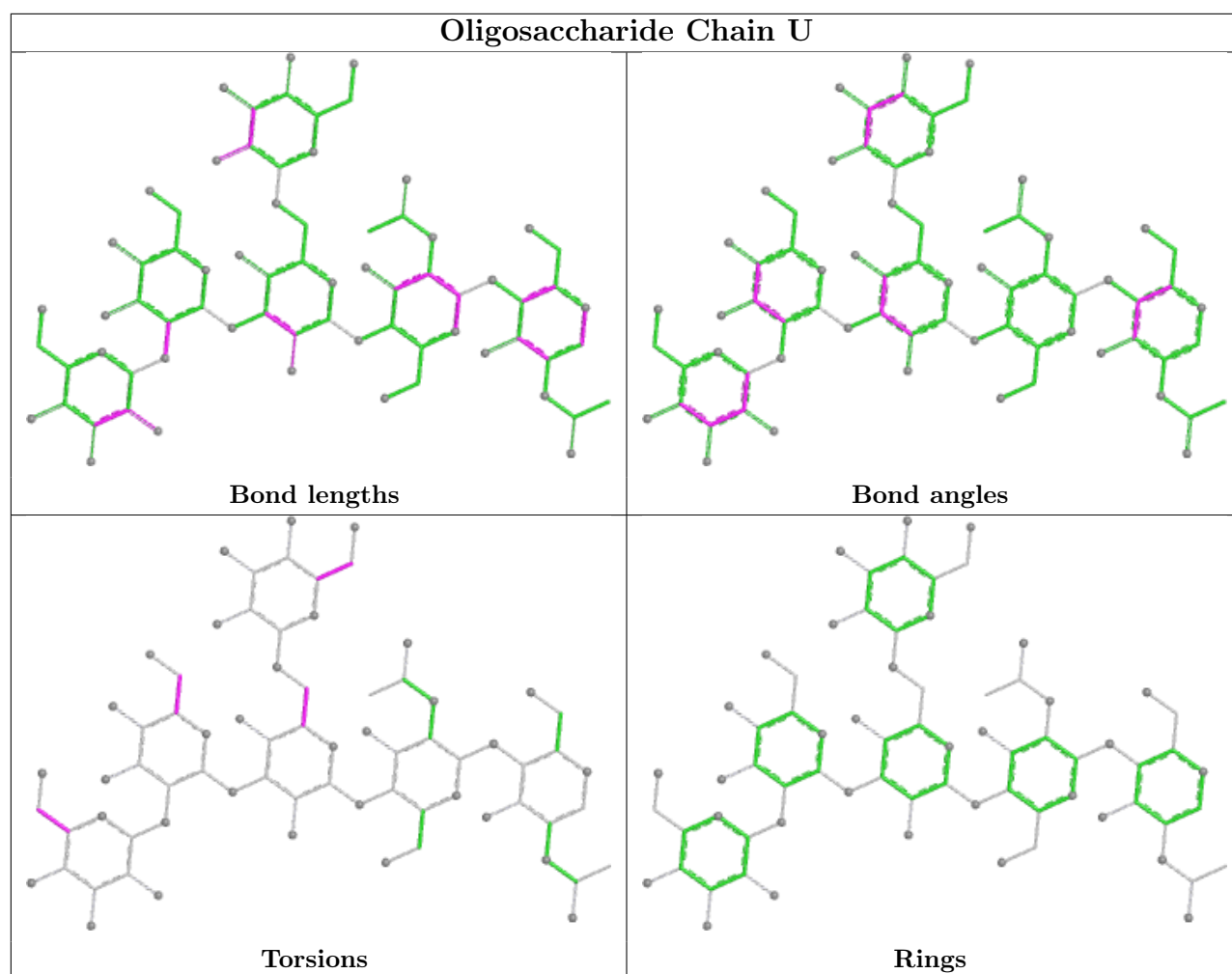


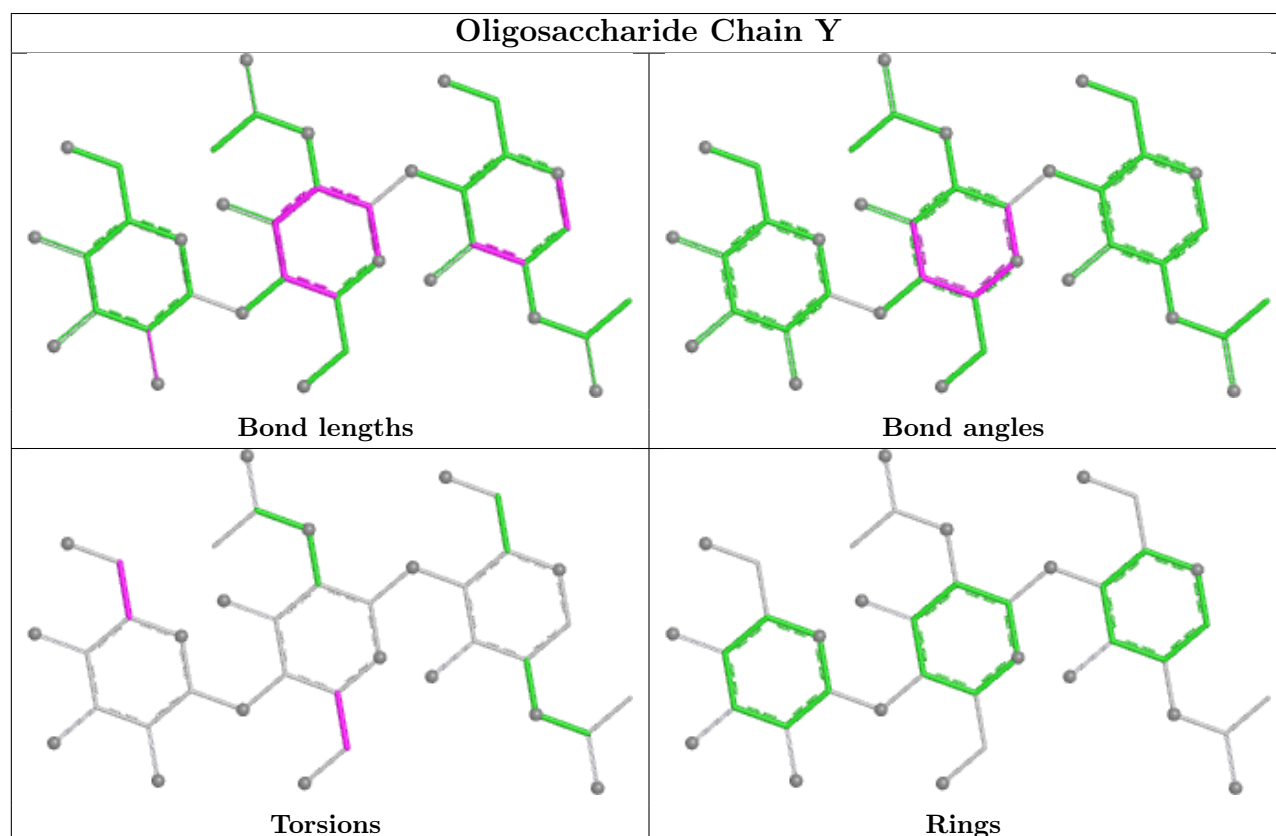
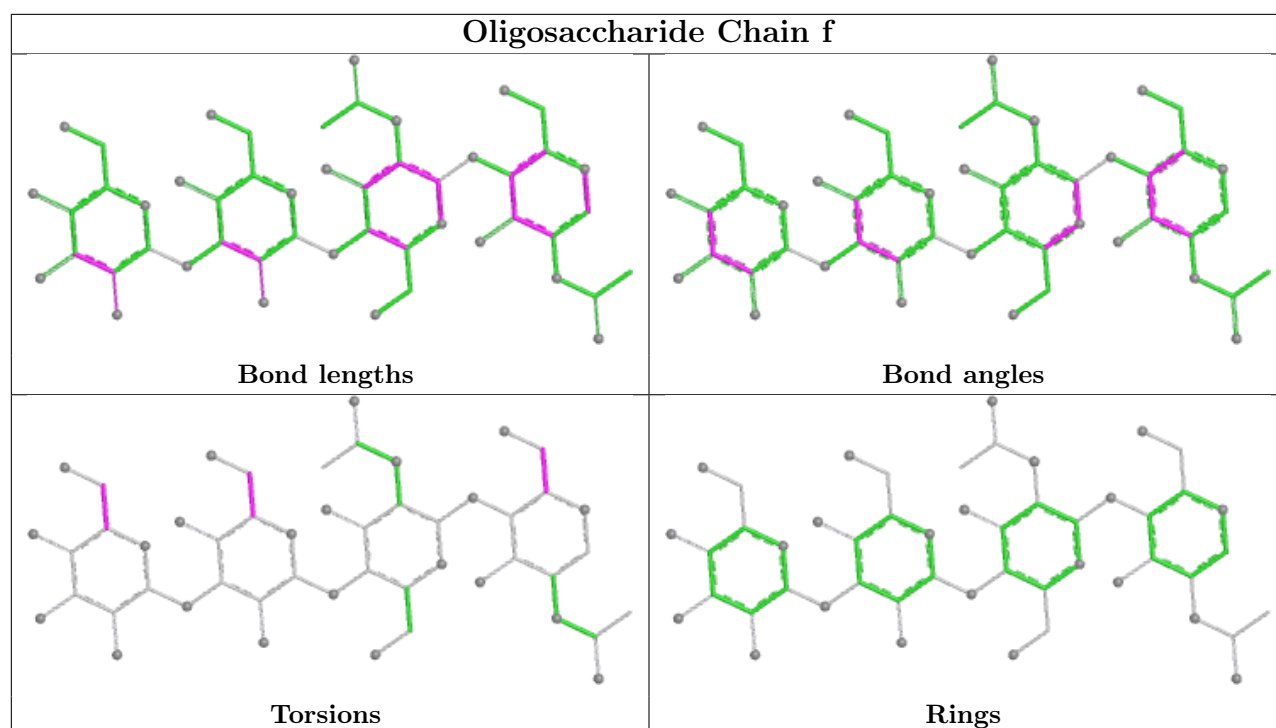


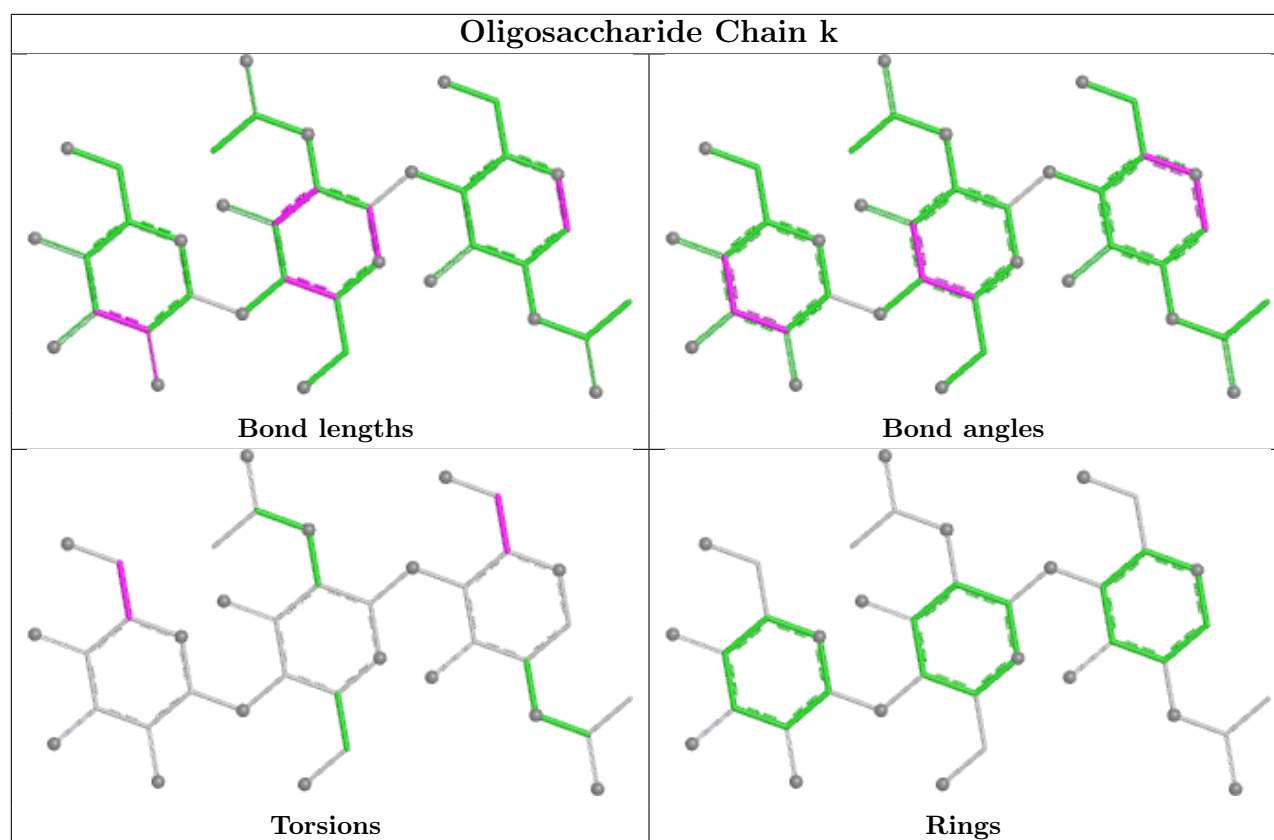












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
9	NAG	B	1433	1	14,14,15	2.06	2 (14%)	17,19,21	0.87	1 (5%)
9	NAG	C	1412	1	14,14,15	2.08	2 (14%)	17,19,21	0.76	0
9	NAG	C	1419	1	14,14,15	2.07	2 (14%)	17,19,21	0.92	1 (5%)
9	NAG	A	1423	1	14,14,15	2.10	2 (14%)	17,19,21	0.76	0
9	NAG	A	1401	1	14,14,15	2.07	2 (14%)	17,19,21	0.89	1 (5%)
9	NAG	C	1416	1	14,14,15	2.07	2 (14%)	17,19,21	0.99	1 (5%)
9	NAG	C	1424	1	14,14,15	2.03	2 (14%)	17,19,21	1.03	2 (11%)
9	NAG	A	1424	1	14,14,15	2.06	2 (14%)	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	1418	1	14,14,15	2.12	2 (14%)	17,19,21	0.81	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
9	NAG	B	1433	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1412	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1419	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1423	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1416	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1424	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1424	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1418	1	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1423	NAG	O5-C1	6.79	1.55	1.43
9	A	1418	NAG	O5-C1	6.75	1.55	1.43
9	C	1412	NAG	O5-C1	6.68	1.54	1.43
9	C	1419	NAG	O5-C1	6.66	1.54	1.43
9	A	1424	NAG	O5-C1	6.65	1.54	1.43
9	C	1416	NAG	O5-C1	6.63	1.54	1.43
9	B	1433	NAG	O5-C1	6.59	1.54	1.43
9	A	1401	NAG	O5-C1	6.55	1.54	1.43
9	C	1424	NAG	O5-C1	6.46	1.54	1.43
9	A	1401	NAG	C3-C2	-2.27	1.47	1.52
9	C	1424	NAG	C3-C2	-2.19	1.47	1.52
9	C	1416	NAG	C3-C2	-2.19	1.47	1.52
9	C	1419	NAG	C3-C2	-2.13	1.48	1.52
9	B	1433	NAG	C3-C2	-2.12	1.48	1.52
9	A	1424	NAG	C3-C2	-2.11	1.48	1.52
9	A	1418	NAG	C3-C2	-2.09	1.48	1.52
9	C	1412	NAG	C3-C2	-2.05	1.48	1.52
9	A	1423	NAG	C3-C2	-2.03	1.48	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1416	NAG	C4-C3-C2	-2.88	106.79	111.02
9	C	1424	NAG	C4-C3-C2	-2.69	107.08	111.02
9	C	1419	NAG	C4-C3-C2	-2.41	107.48	111.02
9	C	1424	NAG	C1-O5-C5	-2.41	108.95	112.19
9	A	1401	NAG	C4-C3-C2	-2.27	107.70	111.02
9	B	1433	NAG	C4-C3-C2	-2.23	107.75	111.02
9	A	1418	NAG	C4-C3-C2	-2.05	108.02	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1412	NAG	O5-C5-C6-O6
9	A	1401	NAG	O5-C5-C6-O6
9	A	1424	NAG	O5-C5-C6-O6
9	C	1412	NAG	C4-C5-C6-O6
9	C	1419	NAG	O5-C5-C6-O6
9	C	1416	NAG	O5-C5-C6-O6
9	B	1433	NAG	O5-C5-C6-O6
9	C	1424	NAG	O5-C5-C6-O6
9	A	1401	NAG	C4-C5-C6-O6
9	A	1424	NAG	C4-C5-C6-O6
9	A	1423	NAG	C4-C5-C6-O6
9	A	1423	NAG	O5-C5-C6-O6
9	A	1418	NAG	O5-C5-C6-O6
9	C	1419	NAG	C4-C5-C6-O6
9	A	1418	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-0402. These allow visual inspection of the internal detail of the map and identification of artifacts.

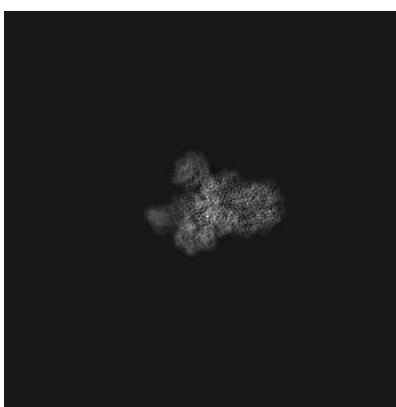
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

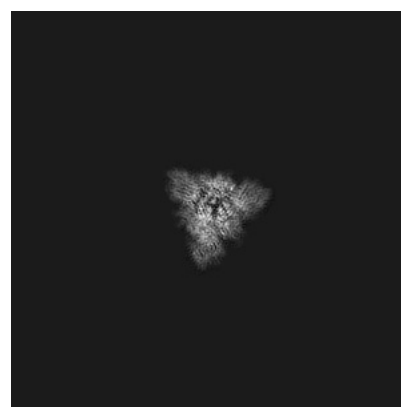
6.1.1 Primary map



X



Y



Z

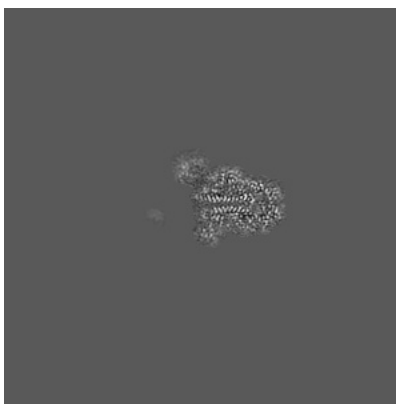
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

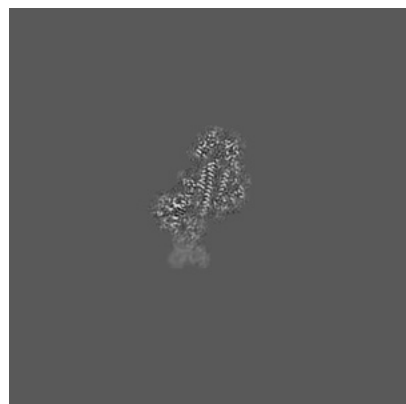


Z Index: 192

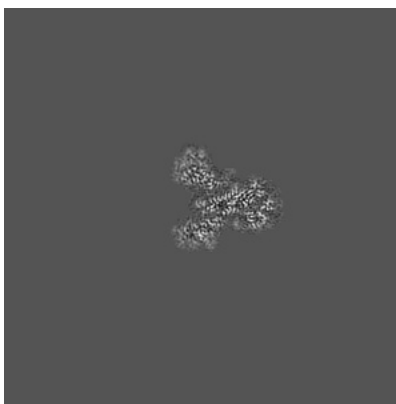
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

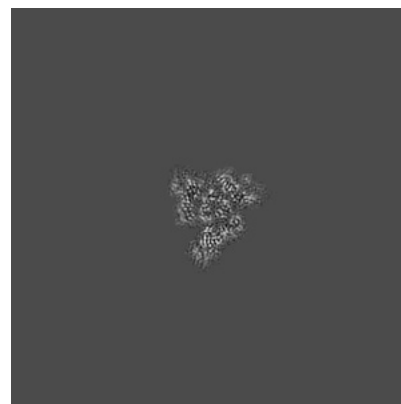
6.3.1 Primary map



X Index: 189



Y Index: 206

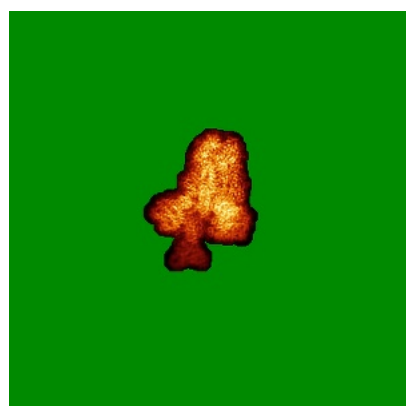


Z Index: 195

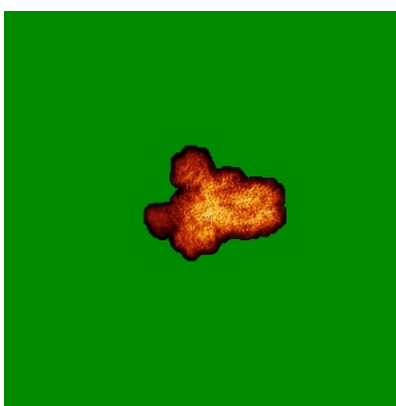
The images above show the largest variance slices of the map in three orthogonal directions.

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

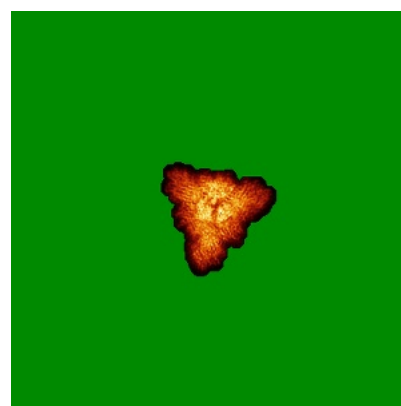
6.4.1 Primary map



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.

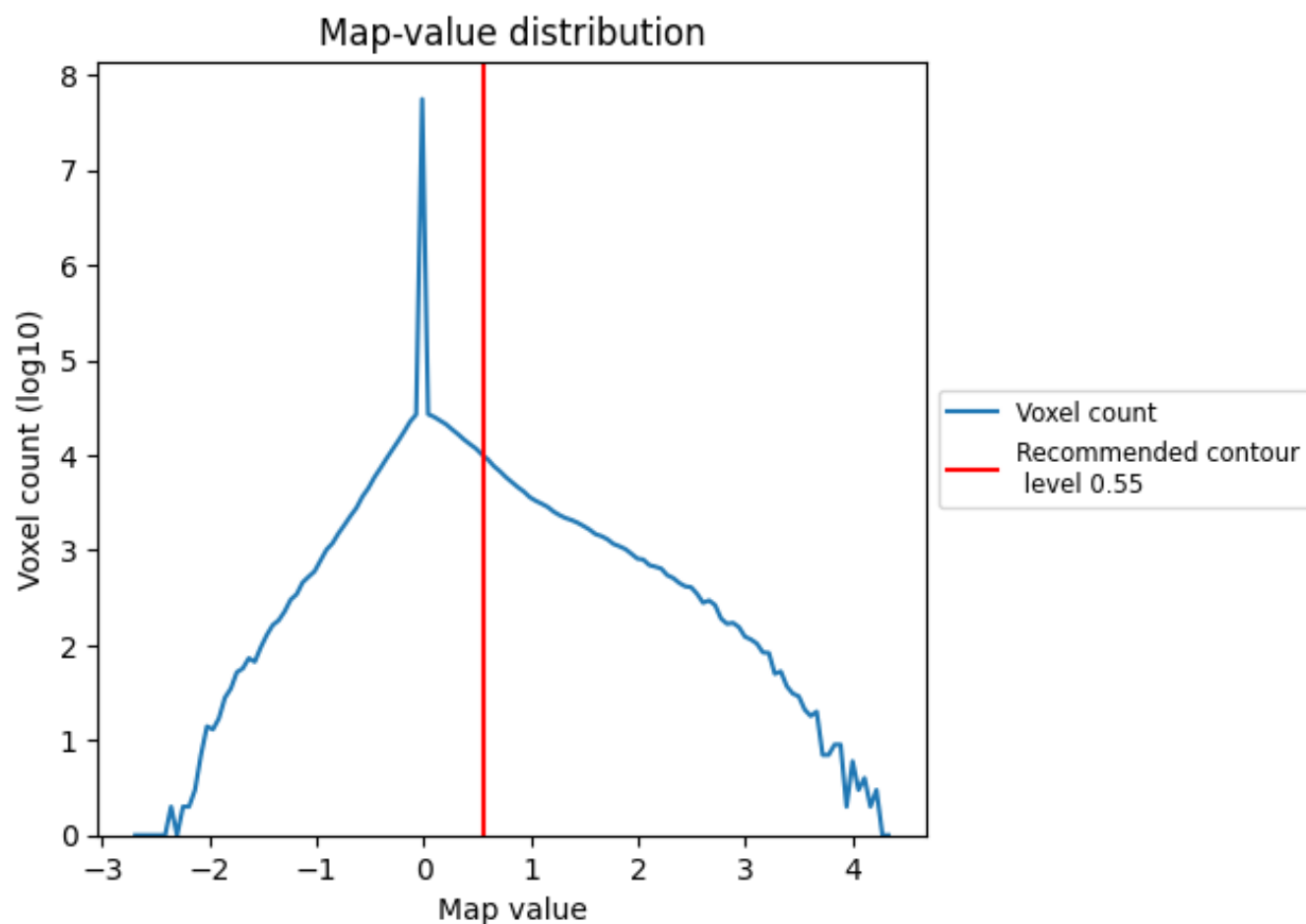
6.6 Mask visualisation

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

7 Map analysis [i](#)

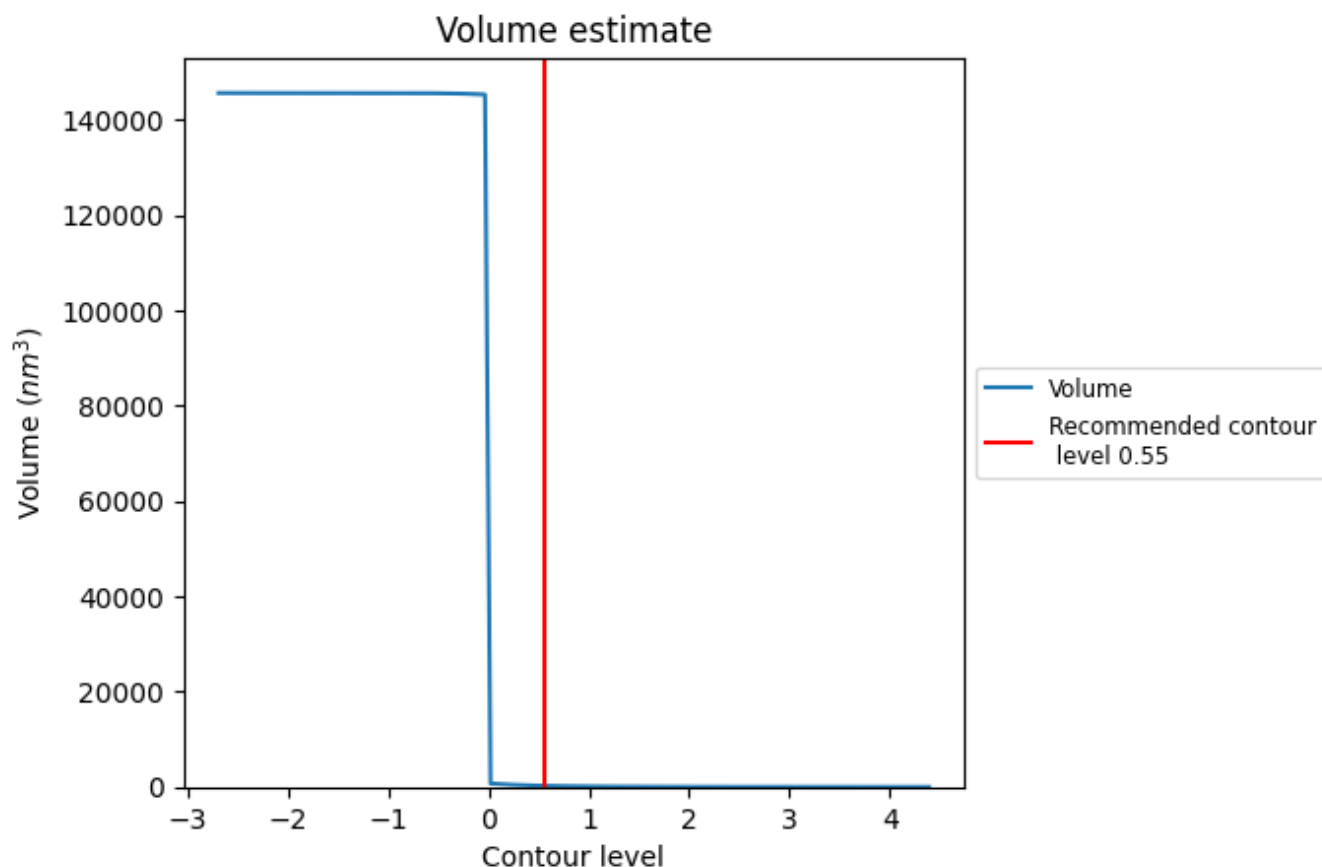
This section contains the results of statistical analysis of the map.

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.

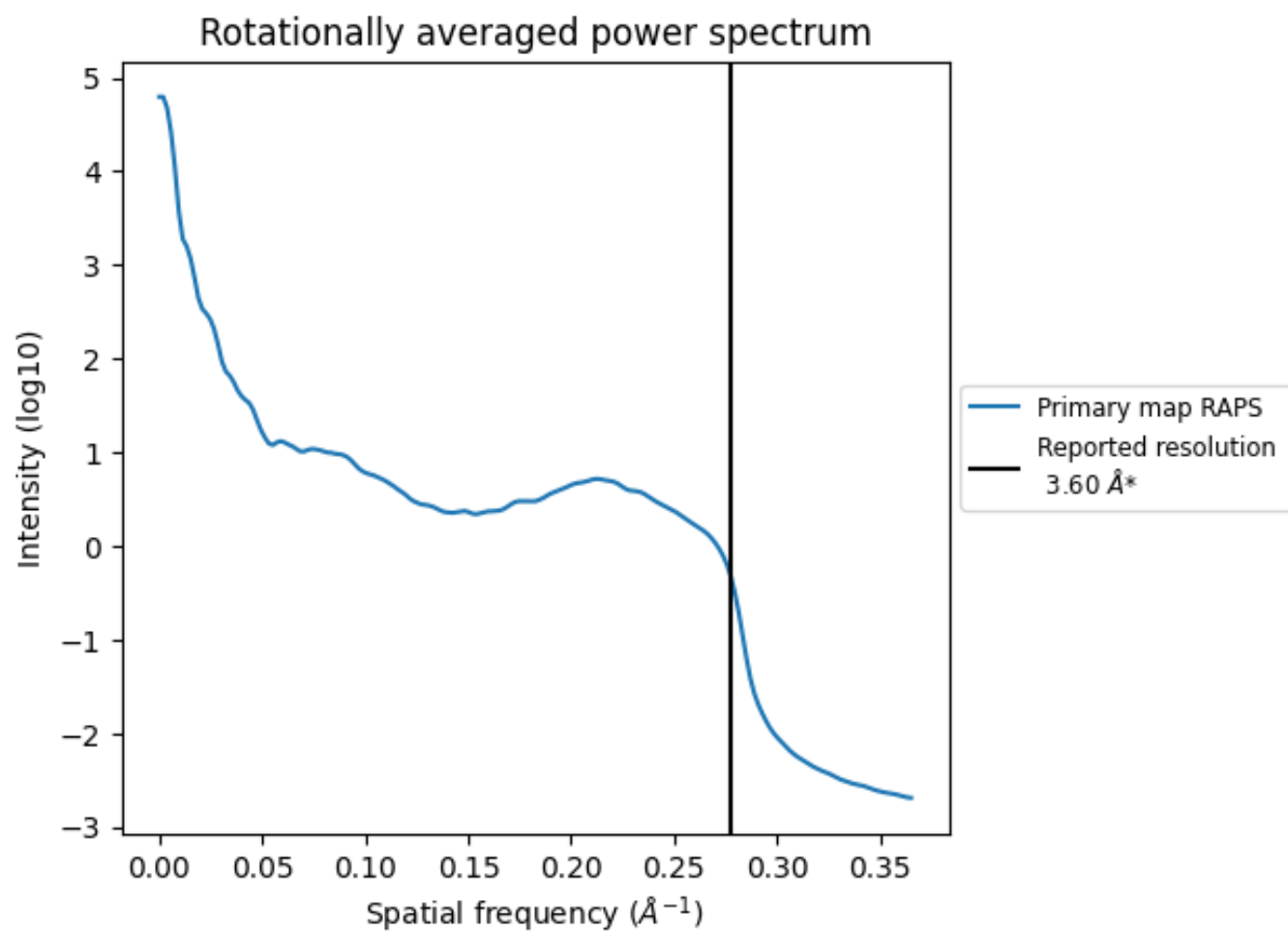
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm^3 ; this corresponds to an approximate mass of 225 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 0.278 Å⁻¹

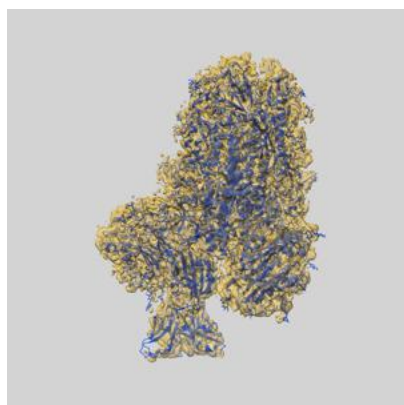
8 Fourier-Shell correlation

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

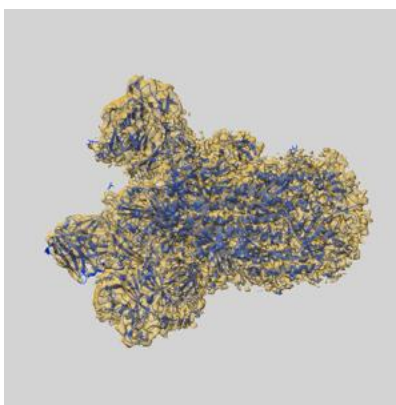
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0402 and PDB model 6NB4. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

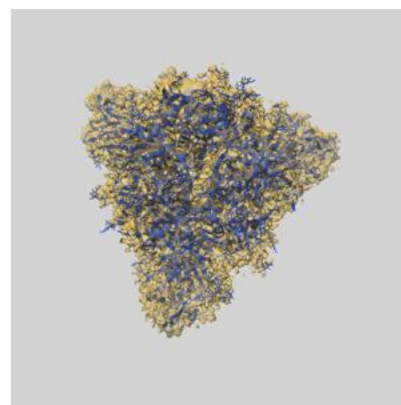
9.1 Map-model overlay [i](#)



X



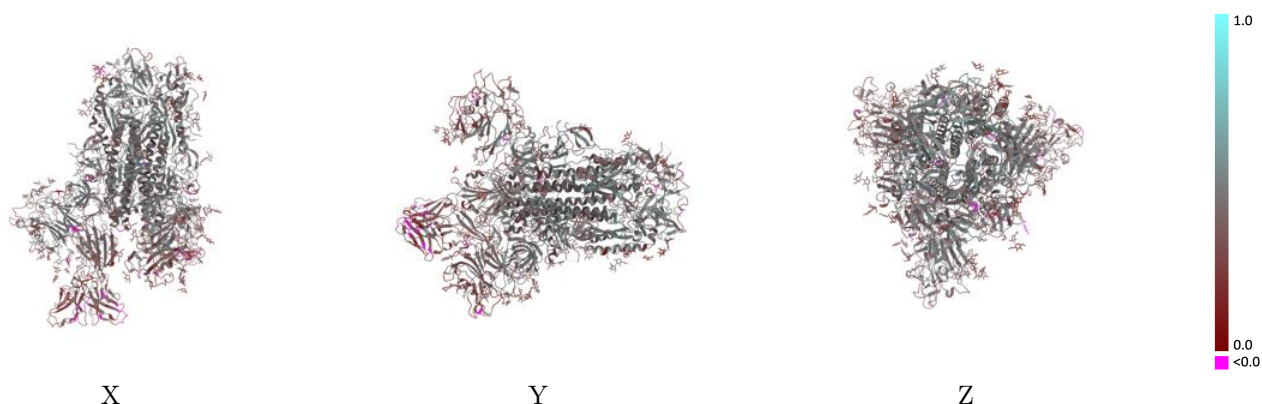
Y



Z

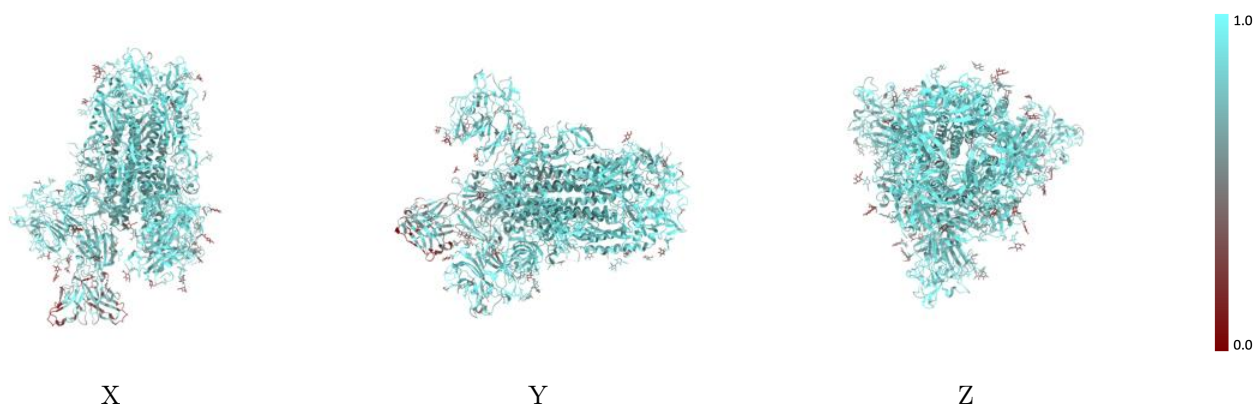
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



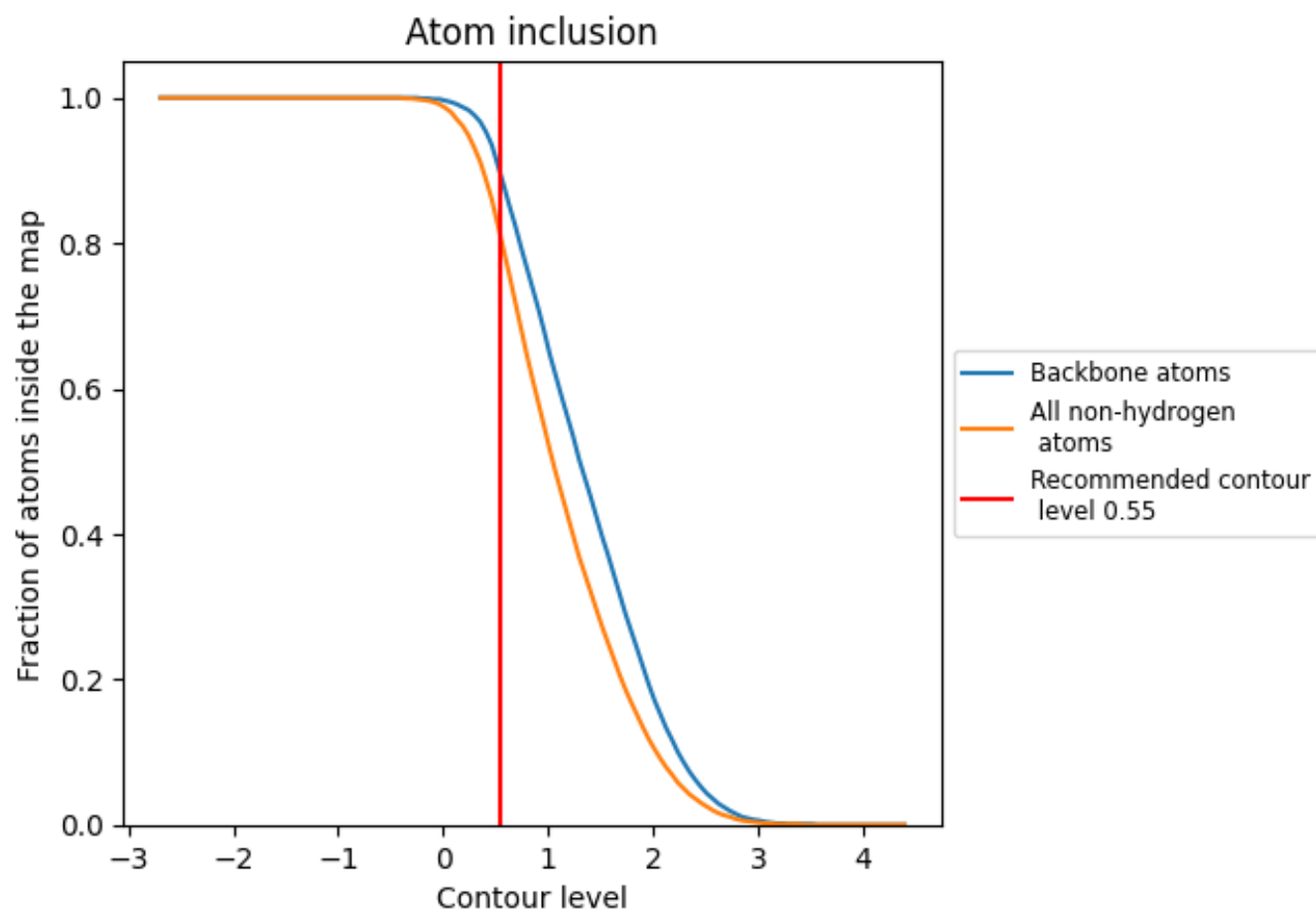
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.4030
A	 0.8150	 0.4040
B	 0.8550	 0.4390
C	 0.8420	 0.4190
D	 0.3930	 0.2620
E	 0.7540	 0.3250
F	 0.5710	 0.2810
G	 0.5000	 0.2960
H	 0.5630	 0.2410
I	 0.5570	 0.2200
J	 0.4640	 0.2740
K	 0.4290	 0.3230
L	 0.5400	 0.2410
M	 0.5000	 0.1700
N	 0.5710	 0.2850
O	 0.3570	 0.1710
P	 0.5000	 0.2440
Q	 0.6790	 0.3340
R	 0.5740	 0.2500
S	 0.6070	 0.3640
T	 0.4290	 0.2590
U	 0.7360	 0.3320
V	 0.5000	 0.2820
W	 0.4590	 0.2050
X	 0.6600	 0.2530
Y	 0.2820	 0.2280
Z	 0.5360	 0.1630
a	 0.1790	 0.2570
b	 0.4640	 0.3150
c	 0.5710	 0.2800
d	 0.4290	 0.2960
e	 0.7860	 0.3710
f	 0.6600	 0.2900
g	 0.6070	 0.3790
h	 0.3570	 0.3050



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Chain	Atom inclusion	Q-score
i	 0.7210	 0.2640
j	 0.3930	 0.3000
k	 0.6670	 0.2790
l	 0.5710	 0.2790
m	 0.5000	 0.3270
n	 0.7140	 0.3380
o	 0.5710	 0.2500
p	 0.7140	 0.3600
q	 0.5740	 0.2900