



Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 03:25 PM EDT

PDB ID : 9YPD / pdb_00009ypd
EMDB ID : EMD-73294
Title : The ligand free HCoV-HKU1 spike structure obtained from data collected on 100 kV Tundra at 180kX magnification with Falcon C detector
Authors : Pathirage, R.; Acharya, P.
Deposited on : 2025-10-14
Resolution : 3.72 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:

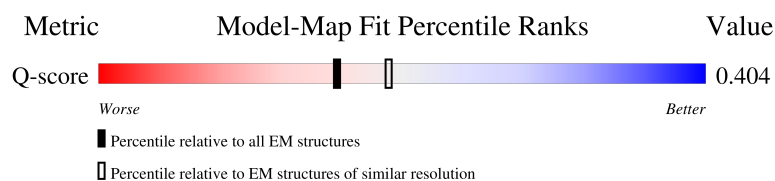
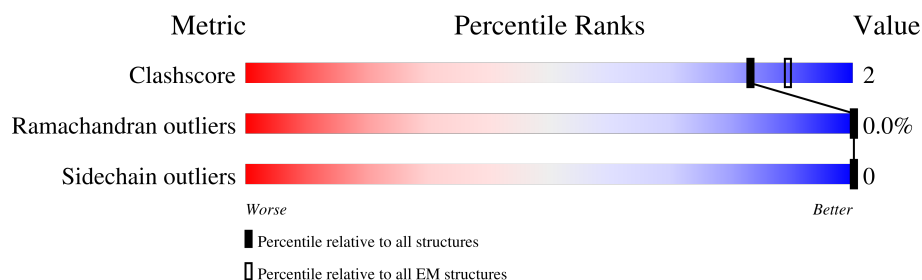
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.72 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.



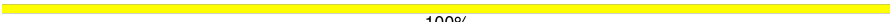
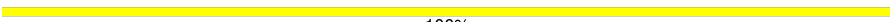
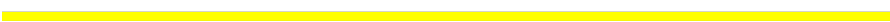
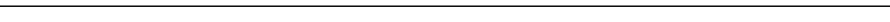
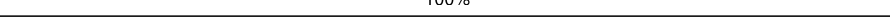
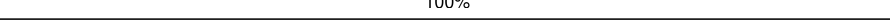
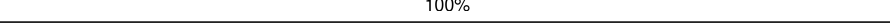
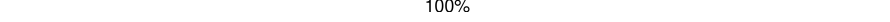
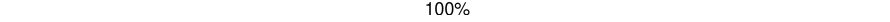
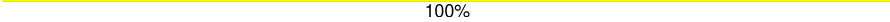
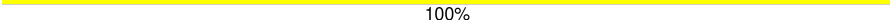
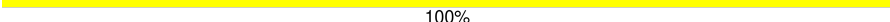
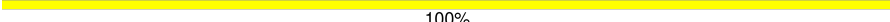
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10474 (3.22 - 4.22)

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	1357	 82% 6% 12%
1	B	1357	 82% 6% 12%
1	C	1357	 82% 6% 12%
2	D	2	 100%

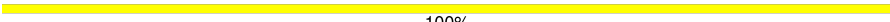
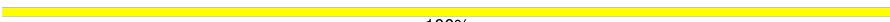
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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
2	G	2	 50% 50%
2	I	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	P	2	 50% 50%
2	R	2	 100%
2	U	2	 100%
2	V	2	 100%
2	W	2	 100%
2	X	2	 100%
2	Y	2	 50% 50%
2	a	2	 100%
2	d	2	 100%
2	e	2	 100%
3	H	5	 100%
3	Q	5	 100%
3	Z	5	 100%
4	J	3	 100%
4	K	3	 100%
4	S	3	 100%
4	T	3	 100%

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Mol	Chain	Length	Quality of chain
4	b	3	 100%
4	c	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29516 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	1195	Total	C	N	O	S	0	0
			9373	5981	1535	1799	58		
1	B	1195	Total	C	N	O	S	0	0
			9373	5981	1535	1799	58		
1	C	1195	Total	C	N	O	S	0	0
			9373	5981	1535	1799	58		

There are 321 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP E0YJ44
A	-9	PRO	-	expression tag	UNP E0YJ44
A	-8	MET	-	expression tag	UNP E0YJ44
A	-7	GLY	-	expression tag	UNP E0YJ44
A	-6	SER	-	expression tag	UNP E0YJ44
A	-5	LEU	-	expression tag	UNP E0YJ44
A	-4	GLN	-	expression tag	UNP E0YJ44
A	-3	PRO	-	expression tag	UNP E0YJ44
A	-2	LEU	-	expression tag	UNP E0YJ44
A	-1	ALA	-	expression tag	UNP E0YJ44
A	0	THR	-	expression tag	UNP E0YJ44
A	1	LEU	-	expression tag	UNP E0YJ44
A	2	TYR	-	expression tag	UNP E0YJ44
A	3	LEU	-	expression tag	UNP E0YJ44
A	4	LEU	-	expression tag	UNP E0YJ44
A	5	GLY	-	expression tag	UNP E0YJ44
A	6	MET	-	expression tag	UNP E0YJ44
A	7	LEU	-	expression tag	UNP E0YJ44
A	8	VAL	-	expression tag	UNP E0YJ44
A	9	ALA	-	expression tag	UNP E0YJ44
A	10	SER	-	expression tag	UNP E0YJ44
A	11	VAL	-	expression tag	UNP E0YJ44
A	756	GLY	ARG	conflict	UNP E0YJ44
A	757	GLY	ARG	conflict	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
A	758	SER	LYS	conflict	UNP E0YJ44
A	759	GLY	ARG	conflict	UNP E0YJ44
A	760	SER	ARG	conflict	UNP E0YJ44
A	1267	GLY	-	expression tag	UNP E0YJ44
A	1268	SER	-	expression tag	UNP E0YJ44
A	1269	GLY	-	expression tag	UNP E0YJ44
A	1270	TYR	-	expression tag	UNP E0YJ44
A	1271	ILE	-	expression tag	UNP E0YJ44
A	1272	PRO	-	expression tag	UNP E0YJ44
A	1273	GLU	-	expression tag	UNP E0YJ44
A	1274	ALA	-	expression tag	UNP E0YJ44
A	1275	PRO	-	expression tag	UNP E0YJ44
A	1276	ARG	-	expression tag	UNP E0YJ44
A	1277	ASP	-	expression tag	UNP E0YJ44
A	1278	GLY	-	expression tag	UNP E0YJ44
A	1279	GLN	-	expression tag	UNP E0YJ44
A	1280	ALA	-	expression tag	UNP E0YJ44
A	1281	TYR	-	expression tag	UNP E0YJ44
A	1282	VAL	-	expression tag	UNP E0YJ44
A	1283	ARG	-	expression tag	UNP E0YJ44
A	1284	LYS	-	expression tag	UNP E0YJ44
A	1285	ASP	-	expression tag	UNP E0YJ44
A	1286	GLY	-	expression tag	UNP E0YJ44
A	1287	GLU	-	expression tag	UNP E0YJ44
A	1288	TRP	-	expression tag	UNP E0YJ44
A	1289	VAL	-	expression tag	UNP E0YJ44
A	1290	LEU	-	expression tag	UNP E0YJ44
A	1291	LEU	-	expression tag	UNP E0YJ44
A	1292	SER	-	expression tag	UNP E0YJ44
A	1293	THR	-	expression tag	UNP E0YJ44
A	1294	PHE	-	expression tag	UNP E0YJ44
A	1295	LEU	-	expression tag	UNP E0YJ44
A	1296	GLY	-	expression tag	UNP E0YJ44
A	1297	ARG	-	expression tag	UNP E0YJ44
A	1298	SER	-	expression tag	UNP E0YJ44
A	1299	LEU	-	expression tag	UNP E0YJ44
A	1300	GLU	-	expression tag	UNP E0YJ44
A	1301	VAL	-	expression tag	UNP E0YJ44
A	1302	LEU	-	expression tag	UNP E0YJ44
A	1303	PHE	-	expression tag	UNP E0YJ44
A	1304	GLN	-	expression tag	UNP E0YJ44
A	1305	GLY	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1306	PRO	-	expression tag	UNP E0YJ44
A	1307	GLY	-	expression tag	UNP E0YJ44
A	1308	HIS	-	expression tag	UNP E0YJ44
A	1309	HIS	-	expression tag	UNP E0YJ44
A	1310	HIS	-	expression tag	UNP E0YJ44
A	1311	HIS	-	expression tag	UNP E0YJ44
A	1312	HIS	-	expression tag	UNP E0YJ44
A	1313	HIS	-	expression tag	UNP E0YJ44
A	1314	HIS	-	expression tag	UNP E0YJ44
A	1315	HIS	-	expression tag	UNP E0YJ44
A	1316	SER	-	expression tag	UNP E0YJ44
A	1317	ALA	-	expression tag	UNP E0YJ44
A	1318	TRP	-	expression tag	UNP E0YJ44
A	1319	SER	-	expression tag	UNP E0YJ44
A	1320	HIS	-	expression tag	UNP E0YJ44
A	1321	PRO	-	expression tag	UNP E0YJ44
A	1322	GLN	-	expression tag	UNP E0YJ44
A	1323	PHE	-	expression tag	UNP E0YJ44
A	1324	GLU	-	expression tag	UNP E0YJ44
A	1325	LYS	-	expression tag	UNP E0YJ44
A	1326	GLY	-	expression tag	UNP E0YJ44
A	1327	GLY	-	expression tag	UNP E0YJ44
A	1328	GLY	-	expression tag	UNP E0YJ44
A	1329	SER	-	expression tag	UNP E0YJ44
A	1330	GLY	-	expression tag	UNP E0YJ44
A	1331	GLY	-	expression tag	UNP E0YJ44
A	1332	GLY	-	expression tag	UNP E0YJ44
A	1333	GLY	-	expression tag	UNP E0YJ44
A	1334	SER	-	expression tag	UNP E0YJ44
A	1335	GLY	-	expression tag	UNP E0YJ44
A	1336	GLY	-	expression tag	UNP E0YJ44
A	1337	SER	-	expression tag	UNP E0YJ44
A	1338	ALA	-	expression tag	UNP E0YJ44
A	1339	TRP	-	expression tag	UNP E0YJ44
A	1340	SER	-	expression tag	UNP E0YJ44
A	1341	HIS	-	expression tag	UNP E0YJ44
A	1342	PRO	-	expression tag	UNP E0YJ44
A	1343	GLN	-	expression tag	UNP E0YJ44
A	1344	PHE	-	expression tag	UNP E0YJ44
A	1345	GLU	-	expression tag	UNP E0YJ44
A	1346	LYS	-	expression tag	UNP E0YJ44
B	-10	MET	-	initiating methionine	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	PRO	-	expression tag	UNP E0YJ44
B	-8	MET	-	expression tag	UNP E0YJ44
B	-7	GLY	-	expression tag	UNP E0YJ44
B	-6	SER	-	expression tag	UNP E0YJ44
B	-5	LEU	-	expression tag	UNP E0YJ44
B	-4	GLN	-	expression tag	UNP E0YJ44
B	-3	PRO	-	expression tag	UNP E0YJ44
B	-2	LEU	-	expression tag	UNP E0YJ44
B	-1	ALA	-	expression tag	UNP E0YJ44
B	0	THR	-	expression tag	UNP E0YJ44
B	1	LEU	-	expression tag	UNP E0YJ44
B	2	TYR	-	expression tag	UNP E0YJ44
B	3	LEU	-	expression tag	UNP E0YJ44
B	4	LEU	-	expression tag	UNP E0YJ44
B	5	GLY	-	expression tag	UNP E0YJ44
B	6	MET	-	expression tag	UNP E0YJ44
B	7	LEU	-	expression tag	UNP E0YJ44
B	8	VAL	-	expression tag	UNP E0YJ44
B	9	ALA	-	expression tag	UNP E0YJ44
B	10	SER	-	expression tag	UNP E0YJ44
B	11	VAL	-	expression tag	UNP E0YJ44
B	756	GLY	ARG	conflict	UNP E0YJ44
B	757	GLY	ARG	conflict	UNP E0YJ44
B	758	SER	LYS	conflict	UNP E0YJ44
B	759	GLY	ARG	conflict	UNP E0YJ44
B	760	SER	ARG	conflict	UNP E0YJ44
B	1267	GLY	-	expression tag	UNP E0YJ44
B	1268	SER	-	expression tag	UNP E0YJ44
B	1269	GLY	-	expression tag	UNP E0YJ44
B	1270	TYR	-	expression tag	UNP E0YJ44
B	1271	ILE	-	expression tag	UNP E0YJ44
B	1272	PRO	-	expression tag	UNP E0YJ44
B	1273	GLU	-	expression tag	UNP E0YJ44
B	1274	ALA	-	expression tag	UNP E0YJ44
B	1275	PRO	-	expression tag	UNP E0YJ44
B	1276	ARG	-	expression tag	UNP E0YJ44
B	1277	ASP	-	expression tag	UNP E0YJ44
B	1278	GLY	-	expression tag	UNP E0YJ44
B	1279	GLN	-	expression tag	UNP E0YJ44
B	1280	ALA	-	expression tag	UNP E0YJ44
B	1281	TYR	-	expression tag	UNP E0YJ44
B	1282	VAL	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1283	ARG	-	expression tag	UNP E0YJ44
B	1284	LYS	-	expression tag	UNP E0YJ44
B	1285	ASP	-	expression tag	UNP E0YJ44
B	1286	GLY	-	expression tag	UNP E0YJ44
B	1287	GLU	-	expression tag	UNP E0YJ44
B	1288	TRP	-	expression tag	UNP E0YJ44
B	1289	VAL	-	expression tag	UNP E0YJ44
B	1290	LEU	-	expression tag	UNP E0YJ44
B	1291	LEU	-	expression tag	UNP E0YJ44
B	1292	SER	-	expression tag	UNP E0YJ44
B	1293	THR	-	expression tag	UNP E0YJ44
B	1294	PHE	-	expression tag	UNP E0YJ44
B	1295	LEU	-	expression tag	UNP E0YJ44
B	1296	GLY	-	expression tag	UNP E0YJ44
B	1297	ARG	-	expression tag	UNP E0YJ44
B	1298	SER	-	expression tag	UNP E0YJ44
B	1299	LEU	-	expression tag	UNP E0YJ44
B	1300	GLU	-	expression tag	UNP E0YJ44
B	1301	VAL	-	expression tag	UNP E0YJ44
B	1302	LEU	-	expression tag	UNP E0YJ44
B	1303	PHE	-	expression tag	UNP E0YJ44
B	1304	GLN	-	expression tag	UNP E0YJ44
B	1305	GLY	-	expression tag	UNP E0YJ44
B	1306	PRO	-	expression tag	UNP E0YJ44
B	1307	GLY	-	expression tag	UNP E0YJ44
B	1308	HIS	-	expression tag	UNP E0YJ44
B	1309	HIS	-	expression tag	UNP E0YJ44
B	1310	HIS	-	expression tag	UNP E0YJ44
B	1311	HIS	-	expression tag	UNP E0YJ44
B	1312	HIS	-	expression tag	UNP E0YJ44
B	1313	HIS	-	expression tag	UNP E0YJ44
B	1314	HIS	-	expression tag	UNP E0YJ44
B	1315	HIS	-	expression tag	UNP E0YJ44
B	1316	SER	-	expression tag	UNP E0YJ44
B	1317	ALA	-	expression tag	UNP E0YJ44
B	1318	TRP	-	expression tag	UNP E0YJ44
B	1319	SER	-	expression tag	UNP E0YJ44
B	1320	HIS	-	expression tag	UNP E0YJ44
B	1321	PRO	-	expression tag	UNP E0YJ44
B	1322	GLN	-	expression tag	UNP E0YJ44
B	1323	PHE	-	expression tag	UNP E0YJ44
B	1324	GLU	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1325	LYS	-	expression tag	UNP E0YJ44
B	1326	GLY	-	expression tag	UNP E0YJ44
B	1327	GLY	-	expression tag	UNP E0YJ44
B	1328	GLY	-	expression tag	UNP E0YJ44
B	1329	SER	-	expression tag	UNP E0YJ44
B	1330	GLY	-	expression tag	UNP E0YJ44
B	1331	GLY	-	expression tag	UNP E0YJ44
B	1332	GLY	-	expression tag	UNP E0YJ44
B	1333	GLY	-	expression tag	UNP E0YJ44
B	1334	SER	-	expression tag	UNP E0YJ44
B	1335	GLY	-	expression tag	UNP E0YJ44
B	1336	GLY	-	expression tag	UNP E0YJ44
B	1337	SER	-	expression tag	UNP E0YJ44
B	1338	ALA	-	expression tag	UNP E0YJ44
B	1339	TRP	-	expression tag	UNP E0YJ44
B	1340	SER	-	expression tag	UNP E0YJ44
B	1341	HIS	-	expression tag	UNP E0YJ44
B	1342	PRO	-	expression tag	UNP E0YJ44
B	1343	GLN	-	expression tag	UNP E0YJ44
B	1344	PHE	-	expression tag	UNP E0YJ44
B	1345	GLU	-	expression tag	UNP E0YJ44
B	1346	LYS	-	expression tag	UNP E0YJ44
C	-10	MET	-	initiating methionine	UNP E0YJ44
C	-9	PRO	-	expression tag	UNP E0YJ44
C	-8	MET	-	expression tag	UNP E0YJ44
C	-7	GLY	-	expression tag	UNP E0YJ44
C	-6	SER	-	expression tag	UNP E0YJ44
C	-5	LEU	-	expression tag	UNP E0YJ44
C	-4	GLN	-	expression tag	UNP E0YJ44
C	-3	PRO	-	expression tag	UNP E0YJ44
C	-2	LEU	-	expression tag	UNP E0YJ44
C	-1	ALA	-	expression tag	UNP E0YJ44
C	0	THR	-	expression tag	UNP E0YJ44
C	1	LEU	-	expression tag	UNP E0YJ44
C	2	TYR	-	expression tag	UNP E0YJ44
C	3	LEU	-	expression tag	UNP E0YJ44
C	4	LEU	-	expression tag	UNP E0YJ44
C	5	GLY	-	expression tag	UNP E0YJ44
C	6	MET	-	expression tag	UNP E0YJ44
C	7	LEU	-	expression tag	UNP E0YJ44
C	8	VAL	-	expression tag	UNP E0YJ44
C	9	ALA	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
C	10	SER	-	expression tag	UNP E0YJ44
C	11	VAL	-	expression tag	UNP E0YJ44
C	756	GLY	ARG	conflict	UNP E0YJ44
C	757	GLY	ARG	conflict	UNP E0YJ44
C	758	SER	LYS	conflict	UNP E0YJ44
C	759	GLY	ARG	conflict	UNP E0YJ44
C	760	SER	ARG	conflict	UNP E0YJ44
C	1267	GLY	-	expression tag	UNP E0YJ44
C	1268	SER	-	expression tag	UNP E0YJ44
C	1269	GLY	-	expression tag	UNP E0YJ44
C	1270	TYR	-	expression tag	UNP E0YJ44
C	1271	ILE	-	expression tag	UNP E0YJ44
C	1272	PRO	-	expression tag	UNP E0YJ44
C	1273	GLU	-	expression tag	UNP E0YJ44
C	1274	ALA	-	expression tag	UNP E0YJ44
C	1275	PRO	-	expression tag	UNP E0YJ44
C	1276	ARG	-	expression tag	UNP E0YJ44
C	1277	ASP	-	expression tag	UNP E0YJ44
C	1278	GLY	-	expression tag	UNP E0YJ44
C	1279	GLN	-	expression tag	UNP E0YJ44
C	1280	ALA	-	expression tag	UNP E0YJ44
C	1281	TYR	-	expression tag	UNP E0YJ44
C	1282	VAL	-	expression tag	UNP E0YJ44
C	1283	ARG	-	expression tag	UNP E0YJ44
C	1284	LYS	-	expression tag	UNP E0YJ44
C	1285	ASP	-	expression tag	UNP E0YJ44
C	1286	GLY	-	expression tag	UNP E0YJ44
C	1287	GLU	-	expression tag	UNP E0YJ44
C	1288	TRP	-	expression tag	UNP E0YJ44
C	1289	VAL	-	expression tag	UNP E0YJ44
C	1290	LEU	-	expression tag	UNP E0YJ44
C	1291	LEU	-	expression tag	UNP E0YJ44
C	1292	SER	-	expression tag	UNP E0YJ44
C	1293	THR	-	expression tag	UNP E0YJ44
C	1294	PHE	-	expression tag	UNP E0YJ44
C	1295	LEU	-	expression tag	UNP E0YJ44
C	1296	GLY	-	expression tag	UNP E0YJ44
C	1297	ARG	-	expression tag	UNP E0YJ44
C	1298	SER	-	expression tag	UNP E0YJ44
C	1299	LEU	-	expression tag	UNP E0YJ44
C	1300	GLU	-	expression tag	UNP E0YJ44
C	1301	VAL	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	LEU	-	expression tag	UNP E0YJ44
C	1303	PHE	-	expression tag	UNP E0YJ44
C	1304	GLN	-	expression tag	UNP E0YJ44
C	1305	GLY	-	expression tag	UNP E0YJ44
C	1306	PRO	-	expression tag	UNP E0YJ44
C	1307	GLY	-	expression tag	UNP E0YJ44
C	1308	HIS	-	expression tag	UNP E0YJ44
C	1309	HIS	-	expression tag	UNP E0YJ44
C	1310	HIS	-	expression tag	UNP E0YJ44
C	1311	HIS	-	expression tag	UNP E0YJ44
C	1312	HIS	-	expression tag	UNP E0YJ44
C	1313	HIS	-	expression tag	UNP E0YJ44
C	1314	HIS	-	expression tag	UNP E0YJ44
C	1315	HIS	-	expression tag	UNP E0YJ44
C	1316	SER	-	expression tag	UNP E0YJ44
C	1317	ALA	-	expression tag	UNP E0YJ44
C	1318	TRP	-	expression tag	UNP E0YJ44
C	1319	SER	-	expression tag	UNP E0YJ44
C	1320	HIS	-	expression tag	UNP E0YJ44
C	1321	PRO	-	expression tag	UNP E0YJ44
C	1322	GLN	-	expression tag	UNP E0YJ44
C	1323	PHE	-	expression tag	UNP E0YJ44
C	1324	GLU	-	expression tag	UNP E0YJ44
C	1325	LYS	-	expression tag	UNP E0YJ44
C	1326	GLY	-	expression tag	UNP E0YJ44
C	1327	GLY	-	expression tag	UNP E0YJ44
C	1328	GLY	-	expression tag	UNP E0YJ44
C	1329	SER	-	expression tag	UNP E0YJ44
C	1330	GLY	-	expression tag	UNP E0YJ44
C	1331	GLY	-	expression tag	UNP E0YJ44
C	1332	GLY	-	expression tag	UNP E0YJ44
C	1333	GLY	-	expression tag	UNP E0YJ44
C	1334	SER	-	expression tag	UNP E0YJ44
C	1335	GLY	-	expression tag	UNP E0YJ44
C	1336	GLY	-	expression tag	UNP E0YJ44
C	1337	SER	-	expression tag	UNP E0YJ44
C	1338	ALA	-	expression tag	UNP E0YJ44
C	1339	TRP	-	expression tag	UNP E0YJ44
C	1340	SER	-	expression tag	UNP E0YJ44
C	1341	HIS	-	expression tag	UNP E0YJ44
C	1342	PRO	-	expression tag	UNP E0YJ44
C	1343	GLN	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1344	PHE	-	expression tag	UNP E0YJ44
C	1345	GLU	-	expression tag	UNP E0YJ44
C	1346	LYS	-	expression tag	UNP E0YJ44

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



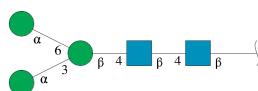
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		

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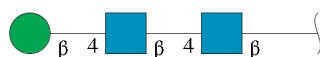
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	H	5	Total	C	N	O	0	0
			61	34	2	25		
3	Q	5	Total	C	N	O	0	0
			61	34	2	25		
3	Z	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 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.



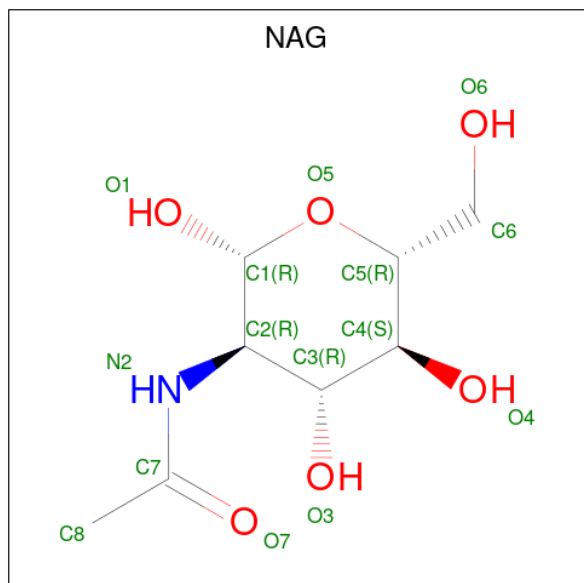
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	b	3	Total	C	N	O	0	0
			39	22	2	15		
4	c	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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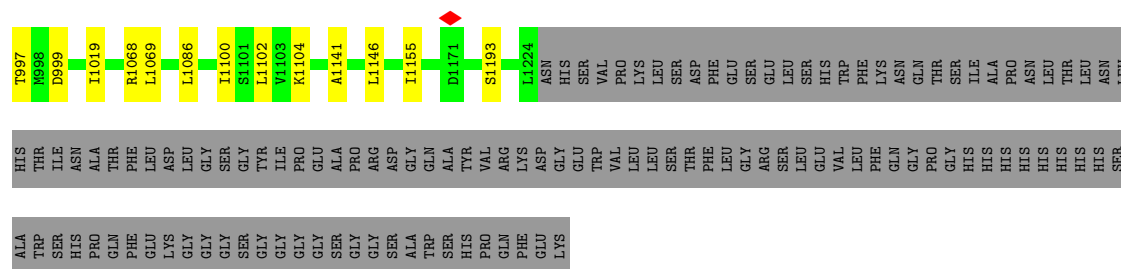
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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

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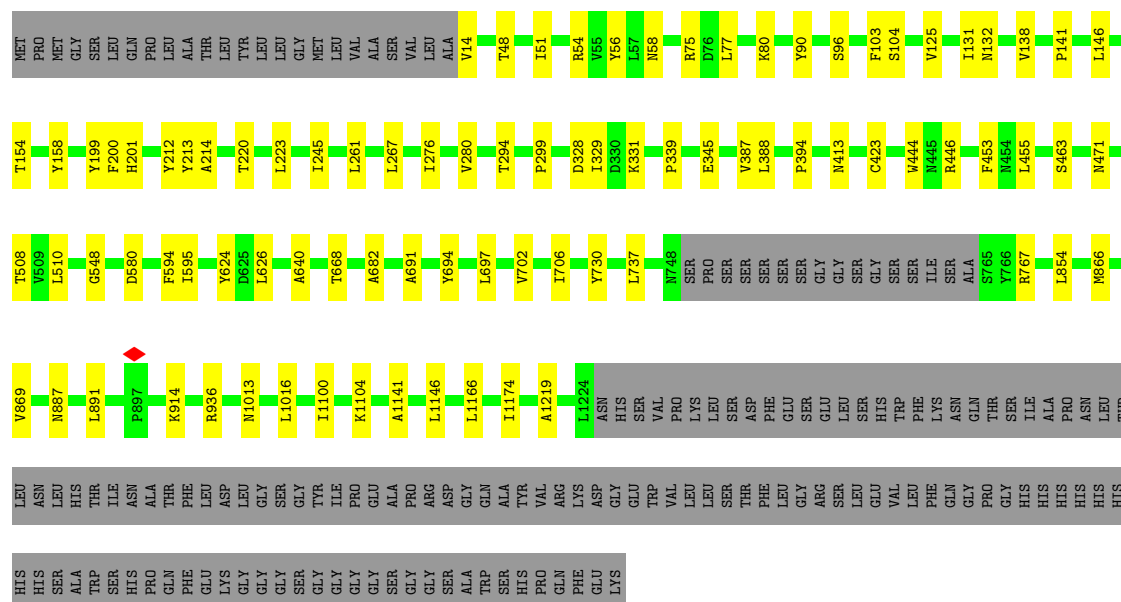
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	



- Molecule 1: Spike glycoprotein

Chain C: 82% 6% 12%



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

Chain D: 100%



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

Chain E: 100%



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

Chain F: 100%

MAG1
MAG2

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

Chain G:  50% 50%MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain L:  100%MAG1
MAG2

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

Chain M:  100%MAG1
MAG2

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

Chain N:  100%MAG1
MAG2

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

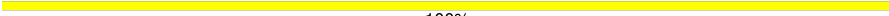
Chain O:  100%MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain X:  100%

MAG1
MAG2

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

Chain Y:  50% 50%



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

Chain a:  100%



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

Chain d:  100%



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

Chain e:  100%



- Molecule 3: 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 H:  100%



- Molecule 3: 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 Q:  100%



- Molecule 3: 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 Z:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain J:  100%

MAG1
MAG2
BMA3

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

Chain K:  100%

MAG1
MAG2
BMA3

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

Chain S:  100%

MAG1
MAG2
BMA3

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

Chain T:  100%

MAG1
MAG2
BMA3

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

Chain b:  100%

MAG1
MAG2
BMA3

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

Chain c:  100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	149190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TUNDRA	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.16	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	2.500	Depositor
Minimum map value	-1.341	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.181	Depositor
Map size ($\text{\AA}$)	376.32, 376.32, 376.32	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.47, 1.47, 1.47	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/9603	0.45	0/13070
1	B	0.18	0/9603	0.48	0/13070
1	C	0.17	0/9603	0.45	0/13070
All	All	0.18	0/28809	0.46	0/39210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9373	0	9000	46	0
1	B	9373	0	9000	49	0
1	C	9373	0	8999	52	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	R	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	a	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
3	H	61	0	52	0	0
3	Q	61	0	52	0	0
3	Z	61	0	52	0	0
4	J	39	0	34	0	0
4	K	39	0	34	0	0
4	S	39	0	34	0	0
4	T	39	0	34	0	0
4	b	39	0	34	0	0
4	c	39	0	34	0	0
5	A	154	0	143	0	0
5	B	140	0	130	0	0
5	C	154	0	143	0	0
All	All	29516	0	28250	141	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 2.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.81	0.62
1:B:853:LEU:HB3	1:B:1104:LYS:HZ1	1.64	0.62
1:B:447:ARG:HD2	1:C:131:ILE:HG13	1.79	0.62
1:A:127:GLY:HA2	1:A:232:LEU:HD22	1.84	0.60
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.84	0.60
1:B:338:VAL:HG21	1:B:590:ILE:HD12	1.84	0.59
1:C:854:LEU:HD21	1:C:1100:ILE:HD11	1.84	0.59
1:B:387:VAL:HB	1:B:595:ILE:HB	1.83	0.59
1:B:854:LEU:HD21	1:B:1100:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:CYS:HB2	1:C:594:PHE:HB2	1.86	0.58
1:A:682:ALA:HB1	1:A:737:LEU:HD13	1.86	0.57
1:B:125:VAL:HG12	1:B:138:VAL:HG22	1.87	0.56
1:A:694:TYR:HB3	1:A:697:LEU:HD12	1.88	0.56
1:A:15:ILE:HD11	1:A:159:PRO:HG3	1.89	0.55
1:B:682:ALA:HB3	1:B:691:ALA:HB3	1.88	0.55
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.89	0.54
1:C:14:VAL:HG12	1:C:90:TYR:HB3	1.89	0.54
1:A:682:ALA:HB3	1:A:691:ALA:HB3	1.91	0.53
1:C:508:THR:HG22	1:C:510:LEU:H	1.73	0.53
1:A:447:ARG:HH11	1:B:131:ILE:HD13	1.73	0.52
1:B:682:ALA:HB1	1:B:737:LEU:HD13	1.90	0.52
1:C:339:PRO:HG3	1:C:345:GLU:HG2	1.91	0.52
1:C:682:ALA:HB3	1:C:691:ALA:HB3	1.91	0.52
1:A:328:ASP:HB3	1:A:331:LYS:HB2	1.91	0.52
1:A:453:PHE:HB3	1:A:455:LEU:HD13	1.93	0.51
1:C:1141:ALA:HB2	1:C:1146:LEU:HB2	1.93	0.51
1:A:126:ILE:HG22	1:A:235:TYR:HB2	1.93	0.51
1:B:640:ALA:HB3	1:B:668:THR:HG21	1.93	0.50
1:B:51:ILE:HB	1:B:54:ARG:HB2	1.93	0.50
1:B:997:THR:HG22	1:B:999:ASP:H	1.75	0.50
1:C:75:ARG:HH21	1:C:77:LEU:HD11	1.76	0.50
1:B:75:ARG:HH21	1:B:77:LEU:HD11	1.77	0.50
1:C:267:LEU:HB3	1:C:280:VAL:HB	1.93	0.49
1:B:213:TYR:HB2	1:B:223:LEU:HD22	1.95	0.49
1:C:90:TYR:HE2	1:C:158:TYR:HA	1.76	0.49
1:C:328:ASP:HB3	1:C:331:LYS:HB2	1.94	0.49
1:A:58:ASN:HD22	1:A:936:ARG:HH12	1.61	0.49
1:A:199:TYR:HB2	1:A:214:ALA:HB3	1.93	0.49
1:A:129:VAL:HG13	1:C:471:ASN:HB2	1.94	0.49
1:B:850:VAL:HG13	1:B:1100:ILE:HG21	1.94	0.49
1:A:394:PRO:HB3	1:A:580:ASP:HB3	1.94	0.48
1:B:214:ALA:HB2	1:B:220:THR:HA	1.95	0.48
1:A:809:THR:HB	1:A:1144:GLY:HA2	1.94	0.48
1:B:556:CYS:HB2	1:B:570:SER:H	1.78	0.48
1:A:651:TYR:HD2	1:B:54:ARG:HG3	1.76	0.48
1:A:90:TYR:HE2	1:A:158:TYR:HA	1.79	0.48
1:A:387:VAL:HB	1:A:595:ILE:HB	1.96	0.48
1:B:702:VAL:HG13	1:B:703:LEU:HD12	1.95	0.48
1:C:104:SER:HB3	1:C:200:PHE:HB2	1.95	0.48
1:C:1166:LEU:HD12	1:C:1219:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:PRO:HB3	1:B:580:ASP:HB3	1.96	0.48
1:B:199:TYR:HB2	1:B:214:ALA:HB3	1.96	0.47
1:C:213:TYR:HB2	1:C:223:LEU:HD22	1.96	0.47
1:C:866:MET:HB2	1:C:869:VAL:HB	1.96	0.47
1:C:444:TRP:HE1	1:C:548:GLY:HA3	1.79	0.47
1:A:556:CYS:HB2	1:A:569:CYS:HB3	1.67	0.47
1:B:453:PHE:HB3	1:B:455:LEU:HD13	1.97	0.47
1:C:132:ASN:HB3	1:C:154:THR:HA	1.97	0.47
1:C:887:ASN:H	1:C:1013:ASN:HD21	1.62	0.47
1:A:1167:CYS:HA	1:A:1173:GLY:HA2	1.97	0.46
1:A:75:ARG:HH21	1:A:77:LEU:HD11	1.80	0.46
1:A:624:TYR:HB2	1:A:626:LEU:HG	1.97	0.46
1:A:839:PHE:HD2	1:A:1086:LEU:HD13	1.80	0.46
1:B:694:TYR:HB3	1:B:697:LEU:HD12	1.98	0.46
1:B:132:ASN:HB3	1:B:154:THR:HG22	1.97	0.46
1:C:387:VAL:HB	1:C:595:ILE:HB	1.97	0.46
1:A:866:MET:HB2	1:A:869:VAL:HB	1.97	0.46
1:B:48:THR:HG21	1:B:276:ILE:HG21	1.98	0.45
1:B:938:LEU:HA	1:B:941:VAL:HG12	1.97	0.45
1:C:214:ALA:HB2	1:C:220:THR:HA	1.97	0.45
1:B:1068:ARG:HG3	1:B:1069:LEU:HD12	1.99	0.45
1:C:48:THR:HG21	1:C:276:ILE:HG21	1.99	0.45
1:B:87:THR:HG22	1:B:91:GLN:HE22	1.81	0.45
1:B:610:LEU:HD11	2:P:2:NAG:H83	1.98	0.45
1:C:141:PRO:HB3	1:C:146:LEU:HD23	1.98	0.45
1:C:453:PHE:HB3	1:C:455:LEU:HD13	1.98	0.45
1:B:995:GLY:HA3	1:B:1193:SER:HB3	1.97	0.45
1:C:682:ALA:HB1	1:C:737:LEU:HD13	1.98	0.45
1:A:214:ALA:HB2	1:A:220:THR:HA	1.99	0.45
1:B:267:LEU:HB3	1:B:280:VAL:HB	1.98	0.45
1:B:1141:ALA:HB2	1:B:1146:LEU:HB2	1.99	0.45
1:A:446:ARG:HA	1:A:446:ARG:HD3	1.73	0.44
1:A:48:THR:HG21	1:A:276:ILE:HG21	1.98	0.44
1:C:80:LYS:HE3	1:C:245:ILE:HB	2.00	0.43
1:C:199:TYR:HB2	1:C:214:ALA:HB3	2.00	0.43
1:C:624:TYR:HB2	1:C:626:LEU:HG	2.00	0.43
1:C:702:VAL:O	1:C:706:ILE:HB	2.17	0.43
1:A:16:GLY:HA3	1:A:157:GLU:HA	1.99	0.43
1:A:1166:LEU:HD12	1:A:1219:ALA:HB3	2.00	0.43
1:C:694:TYR:HB3	1:C:697:LEU:HD12	2.00	0.43
1:B:644:ASN:H	1:B:647:GLN:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ASN:HD22	1:C:936:ARG:HH12	1.66	0.43
1:C:329:ILE:HG23	1:C:388:LEU:HD11	2.01	0.43
1:A:1089:LEU:HD23	1:A:1089:LEU:HA	1.90	0.43
1:A:1166:LEU:HA	1:A:1216:PHE:HB3	2.00	0.43
1:B:75:ARG:HH22	1:B:96:SER:HB3	1.84	0.43
1:B:294:THR:HG21	1:B:299:PRO:HB3	1.99	0.43
1:B:524:PRO:HA	1:B:527:ALA:HB2	1.99	0.43
1:A:875:LEU:HD21	1:A:968:VAL:HG11	2.00	0.43
1:B:1102:LEU:HD11	1:C:1104:LYS:HD2	2.00	0.43
1:B:343:ASN:HB3	1:B:441:PRO:HD3	2.01	0.42
1:C:294:THR:HG21	1:C:299:PRO:HB3	2.01	0.42
1:C:702:VAL:HG23	1:C:706:ILE:HD12	2.00	0.42
1:B:839:PHE:HD2	1:B:1086:LEU:HD13	1.83	0.42
1:A:1183:LYS:HD2	1:A:1186:ASP:HA	2.00	0.42
1:C:51:ILE:HB	1:C:54:ARG:HB2	2.00	0.42
1:C:891:LEU:HD11	1:C:1016:LEU:HD11	2.01	0.42
1:A:521:LEU:HA	1:A:522:PRO:HA	1.90	0.42
1:A:702:VAL:HG22	1:A:706:ILE:HD12	2.01	0.42
1:A:917:LEU:HD12	1:A:917:LEU:HA	1.91	0.42
1:C:103:PHE:HB2	1:C:261:LEU:HD21	2.02	0.42
1:A:506:SER:HA	1:A:516:CYS:HA	2.01	0.42
1:A:727:LEU:HD11	1:A:767:ARG:HD2	2.01	0.42
1:C:394:PRO:HB3	1:C:580:ASP:HB3	2.01	0.42
1:C:730:TYR:HE2	1:C:767:ARG:HH22	1.68	0.42
1:B:698:LYS:HA	1:B:698:LYS:HD2	1.95	0.41
1:C:125:VAL:HG12	1:C:138:VAL:HG22	2.01	0.41
1:B:342:LEU:HD12	1:B:461:VAL:HG13	2.01	0.41
1:C:640:ALA:HB3	1:C:668:THR:HG21	2.02	0.41
1:A:213:TYR:HB2	1:A:223:LEU:HD22	2.00	0.41
1:A:421:SER:HB2	1:A:596:LEU:HB2	2.03	0.41
1:A:878:ASN:HA	1:A:895:LEU:HB3	2.02	0.41
1:C:413:ASN:HD21	1:C:463:SER:H	1.67	0.41
1:A:341:PRO:HB2	1:A:413:ASN:HB3	2.03	0.41
1:A:833:LEU:HD13	1:A:1082:ILE:HD12	2.03	0.41
1:B:861:VAL:HA	1:B:864:THR:HG22	2.03	0.41
1:B:917:LEU:HD12	1:B:917:LEU:HA	1.95	0.41
1:C:914:LYS:HD3	1:C:914:LYS:HA	1.97	0.41
1:C:75:ARG:HH22	1:C:96:SER:HB3	1.86	0.41
1:C:730:TYR:HD2	1:C:767:ARG:HH12	1.69	0.41
1:C:1174:ILE:HD12	1:C:1174:ILE:HA	1.96	0.41
1:B:727:LEU:HD13	1:B:767:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:LEU:HD23	1:B:854:LEU:HA	1.76	0.40
1:B:1019:ILE:HD12	1:B:1019:ILE:HA	1.97	0.40
1:C:446:ARG:HA	1:C:446:ARG:HD3	1.76	0.40
1:A:342:LEU:HD12	1:A:461:VAL:HG13	2.04	0.40
1:A:854:LEU:HD11	1:A:1100:ILE:HD12	2.03	0.40
1:B:651:TYR:HB2	1:C:56:TYR:HE1	1.87	0.40
1:A:294:THR:HG21	1:A:299:PRO:HB3	2.04	0.40
1:B:799:THR:HG22	1:B:1155:ILE:HD11	2.03	0.40
1:C:80:LYS:HA	1:C:80:LYS:HD2	1.87	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	1191/1357 (88%)	1135 (95%)	56 (5%)	0	100	100
1	B	1191/1357 (88%)	1134 (95%)	56 (5%)	1 (0%)	48	78
1	C	1191/1357 (88%)	1130 (95%)	61 (5%)	0	100	100
All	All	3573/4071 (88%)	3399 (95%)	173 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	583	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1072/1203 (89%)	1072 (100%)	0	100	100
1	B	1072/1203 (89%)	1072 (100%)	0	100	100
1	C	1072/1203 (89%)	1072 (100%)	0	100	100
All	All	3216/3609 (89%)	3216 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	364	HIS
1	A	395	ASN
1	A	611	GLN
1	A	803	GLN
1	A	887	ASN
1	A	945	ASN
1	A	1187	HIS
1	B	243	ASN
1	B	255	GLN
1	B	372	ASN
1	B	607	ASN
1	B	611	GLN
1	B	887	ASN
1	B	1004	ASN
1	B	1038	ASN
1	B	1077	GLN
1	C	251	ASN
1	C	371	ASN
1	C	395	ASN
1	C	593	ASN
1	C	696	ASN
1	C	867	GLN
1	C	887	ASN
1	C	927	ASN
1	C	1013	ASN
1	C	1130	ASN
1	C	1187	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

71 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2,1	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
2	NAG	D	2	2	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.80	0	17,19,21	1.50	3 (17%)
2	NAG	F	2	2	14,14,15	0.69	0	17,19,21	0.95	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.75	0	17,19,21	0.95	0
2	NAG	G	2	2	14,14,15	0.74	0	17,19,21	1.76	3 (17%)
3	NAG	H	1	3,1	14,14,15	0.77	0	17,19,21	1.28	2 (11%)
3	NAG	H	2	3	14,14,15	0.74	0	17,19,21	1.75	2 (11%)
3	BMA	H	3	3	11,11,12	0.93	1 (9%)	15,15,17	2.38	3 (20%)
3	MAN	H	4	3	11,11,12	0.73	0	15,15,17	1.36	1 (6%)
3	MAN	H	5	3	11,11,12	0.66	0	15,15,17	1.46	1 (6%)
2	NAG	I	1	2,1	14,14,15	0.70	0	17,19,21	1.80	4 (23%)
2	NAG	I	2	2	14,14,15	0.69	0	17,19,21	0.99	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.72	0	17,19,21	1.27	1 (5%)
4	NAG	J	2	4	14,14,15	0.72	0	17,19,21	1.29	2 (11%)
4	BMA	J	3	4	11,11,12	0.92	1 (9%)	15,15,17	2.62	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	1	4,1	14,14,15	0.74	0	17,19,21	1.11	3 (17%)
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	1.51	2 (11%)
4	BMA	K	3	4	11,11,12	0.94	1 (9%)	15,15,17	2.36	4 (26%)
2	NAG	L	1	2,1	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
2	NAG	L	2	2	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.69	0	17,19,21	1.21	2 (11%)
2	NAG	M	2	2	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	N	2	2	14,14,15	0.73	0	17,19,21	0.98	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.78	0	17,19,21	1.25	2 (11%)
2	NAG	O	2	2	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
2	NAG	P	1	2,1	14,14,15	0.75	0	17,19,21	0.90	0
2	NAG	P	2	2	14,14,15	0.75	0	17,19,21	1.72	3 (17%)
3	NAG	Q	1	3,1	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
3	NAG	Q	2	3	14,14,15	0.71	0	17,19,21	1.77	4 (23%)
3	BMA	Q	3	3	11,11,12	0.91	1 (9%)	15,15,17	2.56	4 (26%)
3	MAN	Q	4	3	11,11,12	0.69	0	15,15,17	1.46	1 (6%)
3	MAN	Q	5	3	11,11,12	0.69	0	15,15,17	1.31	1 (6%)
2	NAG	R	1	2,1	14,14,15	0.69	0	17,19,21	1.77	3 (17%)
2	NAG	R	2	2	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
4	NAG	S	1	4,1	14,14,15	0.74	0	17,19,21	1.77	4 (23%)
4	NAG	S	2	4	14,14,15	0.70	0	17,19,21	1.40	2 (11%)
4	BMA	S	3	4	11,11,12	0.92	1 (9%)	15,15,17	2.67	5 (33%)
4	NAG	T	1	4,1	14,14,15	0.72	0	17,19,21	1.13	1 (5%)
4	NAG	T	2	4	14,14,15	0.72	0	17,19,21	1.74	3 (17%)
4	BMA	T	3	4	11,11,12	0.92	1 (9%)	15,15,17	2.63	4 (26%)
2	NAG	U	1	2,1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	U	2	2	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
2	NAG	V	1	2,1	14,14,15	0.69	0	17,19,21	1.24	2 (11%)
2	NAG	V	2	2	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
2	NAG	W	1	2,1	14,14,15	0.72	0	17,19,21	1.02	1 (5%)
2	NAG	W	2	2	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
2	NAG	X	1	2,1	14,14,15	0.80	0	17,19,21	1.42	3 (17%)
2	NAG	X	2	2	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
2	NAG	Y	1	2,1	14,14,15	0.74	0	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Y	2	2	14,14,15	0.75	0	17,19,21	1.76	4 (23%)
3	NAG	Z	1	3,1	14,14,15	0.76	0	17,19,21	1.24	2 (11%)
3	NAG	Z	2	3	14,14,15	0.69	0	17,19,21	1.74	3 (17%)
3	BMA	Z	3	3	11,11,12	0.91	1 (9%)	15,15,17	2.56	5 (33%)
3	MAN	Z	4	3	11,11,12	0.68	0	15,15,17	1.41	1 (6%)
3	MAN	Z	5	3	11,11,12	0.73	0	15,15,17	1.20	1 (6%)
2	NAG	a	1	2,1	14,14,15	0.68	0	17,19,21	1.77	3 (17%)
2	NAG	a	2	2	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
4	NAG	b	1	4,1	14,14,15	0.71	0	17,19,21	1.25	1 (5%)
4	NAG	b	2	4	14,14,15	0.71	0	17,19,21	1.23	1 (5%)
4	BMA	b	3	4	11,11,12	0.92	1 (9%)	15,15,17	2.57	4 (26%)
4	NAG	c	1	4,1	14,14,15	0.72	0	17,19,21	1.07	3 (17%)
4	NAG	c	2	4	14,14,15	0.71	0	17,19,21	1.28	1 (5%)
4	BMA	c	3	4	11,11,12	0.93	1 (9%)	15,15,17	2.40	4 (26%)
2	NAG	d	1	2,1	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
2	NAG	d	2	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
2	NAG	e	1	2,1	14,14,15	0.69	0	17,19,21	1.23	2 (11%)
2	NAG	e	2	2	14,14,15	0.71	0	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	0/1/1/1

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	C2-C3	2.26	1.55	1.52
4	S	3	BMA	C2-C3	2.19	1.55	1.52
4	T	3	BMA	C2-C3	2.19	1.55	1.52
4	K	3	BMA	C2-C3	2.18	1.55	1.52
4	c	3	BMA	C2-C3	2.17	1.55	1.52
4	b	3	BMA	C2-C3	2.17	1.55	1.52
4	J	3	BMA	C2-C3	2.17	1.55	1.52
3	Q	3	BMA	C2-C3	2.15	1.55	1.52
3	Z	3	BMA	C2-C3	2.14	1.55	1.52

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	3	BMA	C1-O5-C5	8.42	123.46	112.19
4	T	3	BMA	C1-O5-C5	8.37	123.40	112.19
4	J	3	BMA	C1-O5-C5	8.35	123.38	112.19
4	b	3	BMA	C1-O5-C5	8.09	123.02	112.19
3	Q	3	BMA	C1-O5-C5	8.01	122.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	3	BMA	C1-O5-C5	7.91	122.78	112.19
4	c	3	BMA	C1-O5-C5	7.24	121.89	112.19
3	H	3	BMA	C1-O5-C5	7.19	121.82	112.19
4	K	3	BMA	C1-O5-C5	7.04	121.62	112.19
4	S	1	NAG	O5-C1-C2	-5.42	102.90	111.29
2	R	1	NAG	C2-N2-C7	5.16	129.82	122.90
3	Q	2	NAG	C2-N2-C7	5.15	129.80	122.90
3	Z	2	NAG	C2-N2-C7	5.11	129.74	122.90
3	H	2	NAG	C2-N2-C7	5.10	129.74	122.90
2	a	1	NAG	C2-N2-C7	5.10	129.74	122.90
2	I	1	NAG	C2-N2-C7	5.07	129.69	122.90
4	T	2	NAG	C2-N2-C7	4.99	129.59	122.90
2	P	2	NAG	C2-N2-C7	4.96	129.54	122.90
3	H	5	MAN	C1-O5-C5	4.93	118.79	112.19
2	Y	2	NAG	C2-N2-C7	4.92	129.50	122.90
2	G	2	NAG	C2-N2-C7	4.90	129.47	122.90
3	Q	4	MAN	C1-O5-C5	4.80	118.61	112.19
3	Z	4	MAN	C1-O5-C5	4.60	118.35	112.19
3	Q	5	MAN	C1-O5-C5	4.16	117.77	112.19
3	H	4	MAN	C1-O5-C5	4.05	117.62	112.19
4	J	1	NAG	C1-O5-C5	3.97	117.51	112.19
2	F	1	NAG	C1-O5-C5	3.79	117.27	112.19
4	b	1	NAG	C1-O5-C5	3.73	117.19	112.19
3	Z	5	MAN	C1-O5-C5	3.54	116.94	112.19
4	T	3	BMA	C2-C3-C4	3.46	116.95	110.86
4	S	3	BMA	C2-C3-C4	3.44	116.92	110.86
4	b	3	BMA	C2-C3-C4	3.43	116.90	110.86
4	J	3	BMA	C2-C3-C4	3.43	116.89	110.86
4	c	3	BMA	C2-C3-C4	3.40	116.84	110.86
3	Q	3	BMA	C2-C3-C4	3.40	116.84	110.86
3	H	3	BMA	C2-C3-C4	3.39	116.82	110.86
4	K	3	BMA	C2-C3-C4	3.38	116.80	110.86
4	S	2	NAG	O5-C1-C2	-3.37	106.08	111.29
3	Z	3	BMA	C2-C3-C4	3.36	116.77	110.86
4	K	2	NAG	C2-N2-C7	3.30	127.32	122.90
4	b	2	NAG	C2-N2-C7	3.29	127.31	122.90
2	V	1	NAG	C2-N2-C7	3.28	127.29	122.90
2	e	1	NAG	C2-N2-C7	3.24	127.25	122.90
2	M	1	NAG	C2-N2-C7	3.23	127.22	122.90
2	D	1	NAG	C1-O5-C5	3.08	116.31	112.19
4	J	2	NAG	C2-N2-C7	3.00	126.91	122.90
2	X	1	NAG	C1-O5-C5	2.97	116.17	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2	NAG	C2-N2-C7	2.82	126.67	122.90
2	O	1	NAG	C1-O5-C5	2.78	115.91	112.19
2	a	2	NAG	C1-O5-C5	2.73	115.84	112.19
2	R	2	NAG	C1-O5-C5	2.72	115.83	112.19
4	T	2	NAG	C1-O5-C5	2.70	115.81	112.19
2	I	2	NAG	C1-O5-C5	2.68	115.78	112.19
4	J	2	NAG	O5-C1-C2	-2.67	107.16	111.29
2	X	2	NAG	C1-O5-C5	2.67	115.77	112.19
3	H	1	NAG	C4-C3-C2	2.63	114.87	111.02
4	S	3	BMA	C3-C4-C5	2.56	114.87	110.23
2	X	1	NAG	C2-N2-C7	2.54	126.30	122.90
2	O	2	NAG	C1-O5-C5	2.53	115.58	112.19
2	U	2	NAG	C1-O5-C5	2.49	115.53	112.19
2	M	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	d	2	NAG	C1-O5-C5	2.47	115.49	112.19
2	F	1	NAG	O5-C1-C2	-2.46	107.48	111.29
2	I	1	NAG	O5-C1-C2	-2.46	107.49	111.29
4	S	1	NAG	C4-C3-C2	2.45	114.61	111.02
2	L	1	NAG	C1-O5-C5	2.42	115.44	112.19
4	S	1	NAG	O4-C4-C3	-2.42	104.66	110.38
2	L	2	NAG	C1-O5-C5	2.39	115.39	112.19
2	V	1	NAG	C1-O5-C5	2.37	115.36	112.19
2	d	1	NAG	C1-O5-C5	2.37	115.36	112.19
3	Z	3	BMA	C3-C4-C5	2.34	114.48	110.23
2	N	1	NAG	C1-O5-C5	2.34	115.32	112.19
3	Z	2	NAG	O5-C1-C2	-2.33	107.69	111.29
2	G	2	NAG	O7-C7-N2	2.33	126.09	121.98
2	Y	2	NAG	C1-O5-C5	2.32	115.30	112.19
2	a	1	NAG	O5-C1-C2	-2.31	107.72	111.29
2	F	2	NAG	C1-O5-C5	2.30	115.27	112.19
2	G	2	NAG	C1-O5-C5	2.30	115.27	112.19
4	T	1	NAG	O5-C1-C2	-2.30	107.74	111.29
2	E	1	NAG	C1-O5-C5	2.30	115.27	112.19
3	Z	1	NAG	C4-C3-C2	2.29	114.37	111.02
4	K	1	NAG	C4-C3-C2	2.28	114.36	111.02
2	R	1	NAG	O5-C1-C2	-2.28	107.76	111.29
3	H	2	NAG	O7-C7-N2	2.27	125.99	121.98
3	Z	2	NAG	O7-C7-N2	2.27	125.99	121.98
2	V	2	NAG	C1-O5-C5	2.26	115.21	112.19
2	P	2	NAG	C1-O5-C5	2.26	115.21	112.19
2	e	1	NAG	C1-O5-C5	2.26	115.21	112.19
2	e	2	NAG	C1-O5-C5	2.25	115.20	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	3	BMA	C3-C4-C5	2.25	114.31	110.23
4	T	3	BMA	C3-C4-C5	2.25	114.31	110.23
4	S	1	NAG	C1-C2-N2	2.25	113.97	110.43
3	Q	2	NAG	O5-C1-C2	-2.25	107.81	111.29
4	J	3	BMA	C3-C4-C5	2.25	114.30	110.23
2	a	1	NAG	O7-C7-N2	2.24	125.95	121.98
2	I	1	NAG	O7-C7-N2	2.24	125.93	121.98
4	c	3	BMA	C3-C4-C5	2.23	114.28	110.23
2	Y	2	NAG	O7-C7-N2	2.23	125.92	121.98
2	R	1	NAG	O7-C7-N2	2.22	125.91	121.98
2	D	2	NAG	C1-O5-C5	2.22	115.17	112.19
3	Q	2	NAG	O7-C7-N2	2.22	125.91	121.98
4	K	3	BMA	C3-C4-C5	2.22	114.25	110.23
2	X	1	NAG	C4-C3-C2	2.22	114.27	111.02
4	T	2	NAG	O7-C7-N2	2.21	125.89	121.98
2	E	2	NAG	C1-O5-C5	2.21	115.15	112.19
3	Z	3	BMA	O3-C3-C2	-2.20	105.56	110.05
3	H	1	NAG	O4-C4-C3	-2.20	105.19	110.38
2	P	2	NAG	O7-C7-N2	2.19	125.85	121.98
2	O	1	NAG	C2-N2-C7	2.18	125.83	122.90
4	K	2	NAG	O4-C4-C3	-2.18	105.23	110.38
2	N	2	NAG	C1-O5-C5	2.18	115.11	112.19
2	U	1	NAG	C1-O5-C5	2.17	115.10	112.19
2	M	1	NAG	C1-O5-C5	2.17	115.10	112.19
2	I	1	NAG	C1-O5-C5	2.17	115.09	112.19
2	W	2	NAG	C1-O5-C5	2.17	115.09	112.19
3	Q	3	BMA	O3-C3-C2	-2.17	105.63	110.05
4	K	3	BMA	O3-C3-C2	-2.16	105.65	110.05
3	Q	3	BMA	C3-C4-C5	2.13	114.10	110.23
3	H	3	BMA	O3-C3-C2	-2.13	105.70	110.05
4	K	1	NAG	O4-C4-C3	-2.13	105.35	110.38
4	S	3	BMA	O4-C4-C3	-2.11	105.41	110.38
4	c	3	BMA	O3-C3-C2	-2.10	105.76	110.05
4	c	2	NAG	O4-C4-C3	-2.10	105.42	110.38
4	c	1	NAG	O4-C4-C3	-2.10	105.43	110.38
4	c	1	NAG	O5-C1-C2	-2.10	108.05	111.29
2	Y	2	NAG	C1-C2-N2	2.07	113.70	110.43
3	Z	1	NAG	O4-C4-C3	-2.07	105.50	110.38
3	Q	1	NAG	C1-O5-C5	2.07	114.96	112.19
4	J	3	BMA	O3-C3-C2	-2.06	105.85	110.05
3	Q	2	NAG	C1-O5-C5	2.06	114.94	112.19
4	c	1	NAG	C4-C3-C2	2.05	114.02	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	3	BMA	O3-C3-C2	-2.04	105.90	110.05
3	Z	3	BMA	O4-C4-C3	-2.04	105.58	110.38
4	T	3	BMA	O3-C3-C2	-2.03	105.90	110.05
4	K	1	NAG	O5-C1-C2	-2.03	108.15	111.29
2	W	1	NAG	C1-O5-C5	2.03	114.90	112.19
4	b	3	BMA	O3-C3-C2	-2.02	105.93	110.05
2	F	1	NAG	C1-C2-N2	2.01	113.61	110.43

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Z	4	MAN	C4-C5-C6-O6
3	Q	4	MAN	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	Z	4	MAN	O5-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	e	1	NAG	C8-C7-N2-C2
2	e	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	b	2	NAG	C8-C7-N2-C2
4	b	2	NAG	O7-C7-N2-C2
4	b	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	c	3	BMA	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Q	5	MAN	C4-C5-C6-O6
3	Q	5	MAN	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7
2	R	1	NAG	C3-C2-N2-C7
2	a	1	NAG	C3-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	H	5	MAN	C4-C5-C6-O6
4	T	3	BMA	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	R	1	NAG	C1-C2-N2-C7
2	Y	2	NAG	C1-C2-N2-C7
2	a	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
3	Z	2	NAG	C1-C2-N2-C7
4	T	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	Y	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
3	H	5	MAN	O5-C5-C6-O6

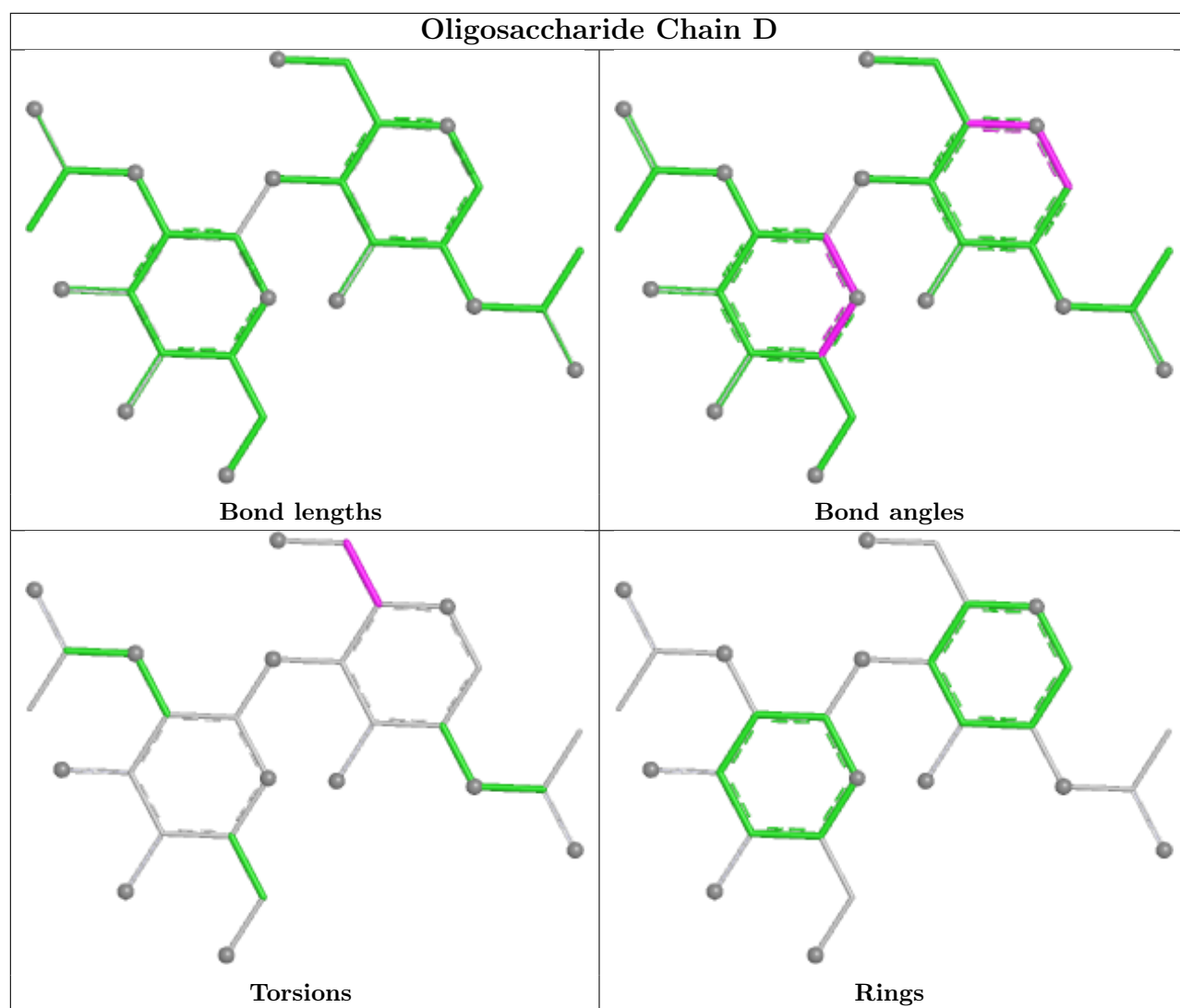
All (2) ring outliers are listed below:

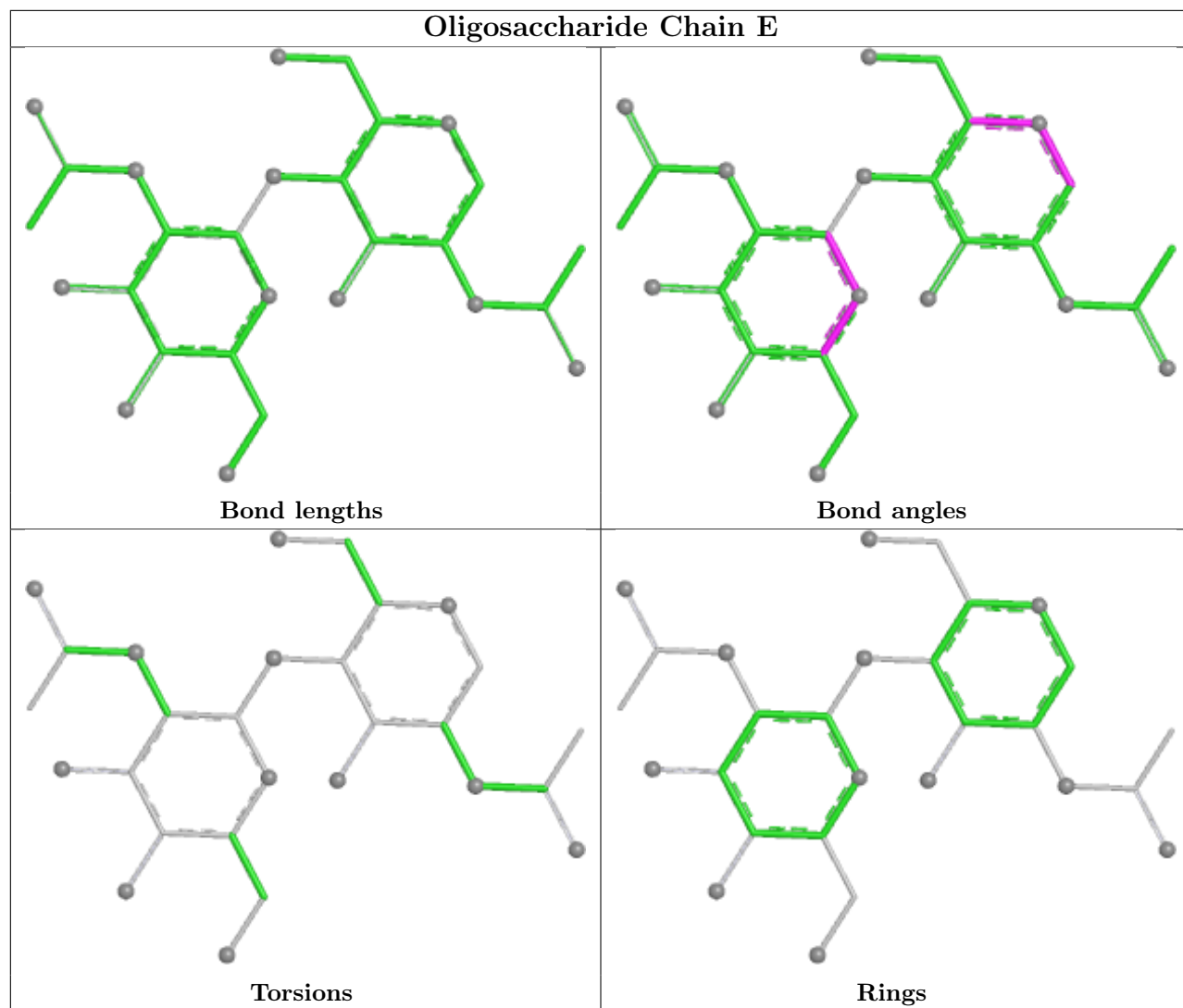
Mol	Chain	Res	Type	Atoms
3	Z	4	MAN	C1-C2-C3-C4-C5-O5
3	Q	4	MAN	C1-C2-C3-C4-C5-O5

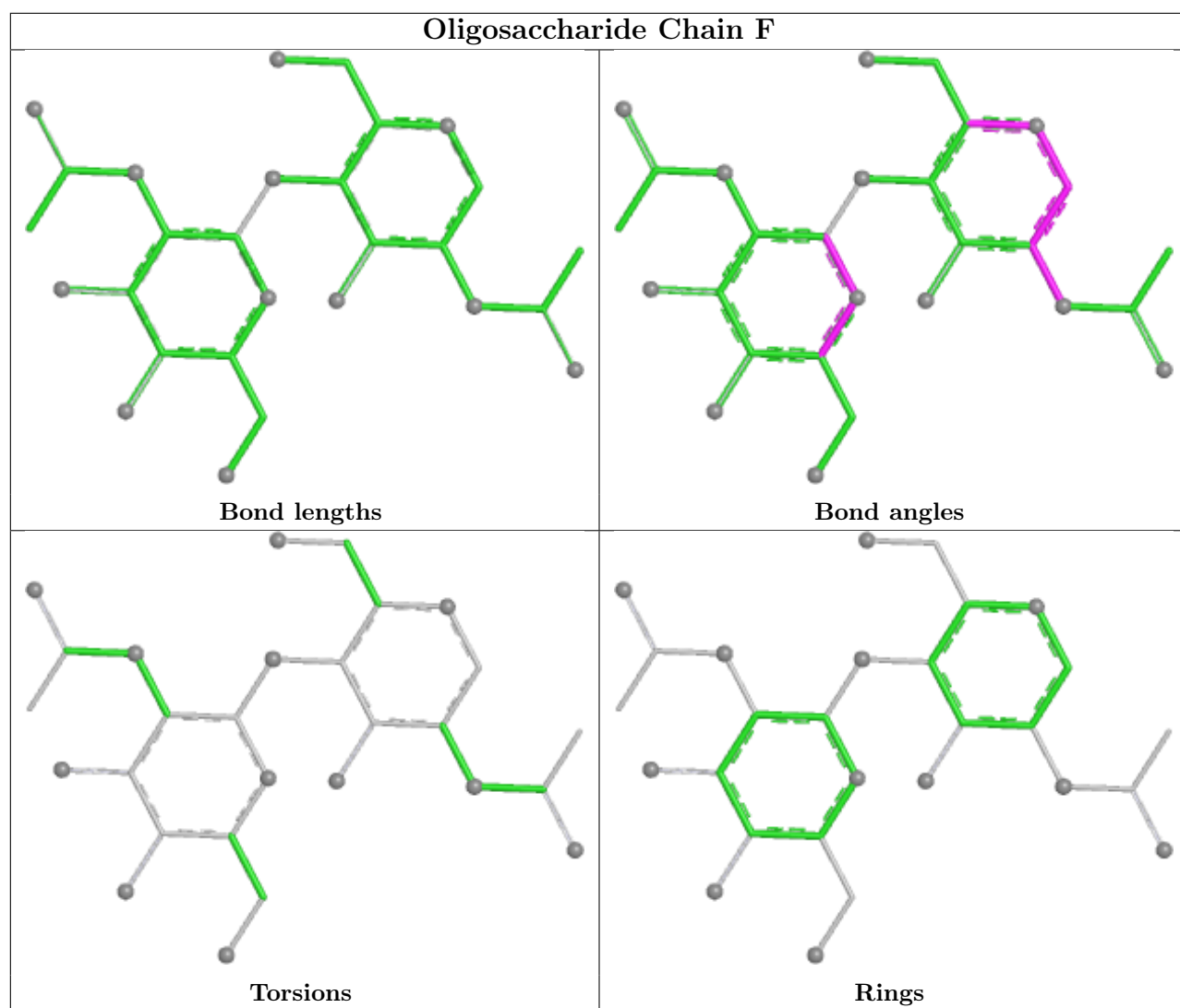
1 monomer is involved in 1 short contact:

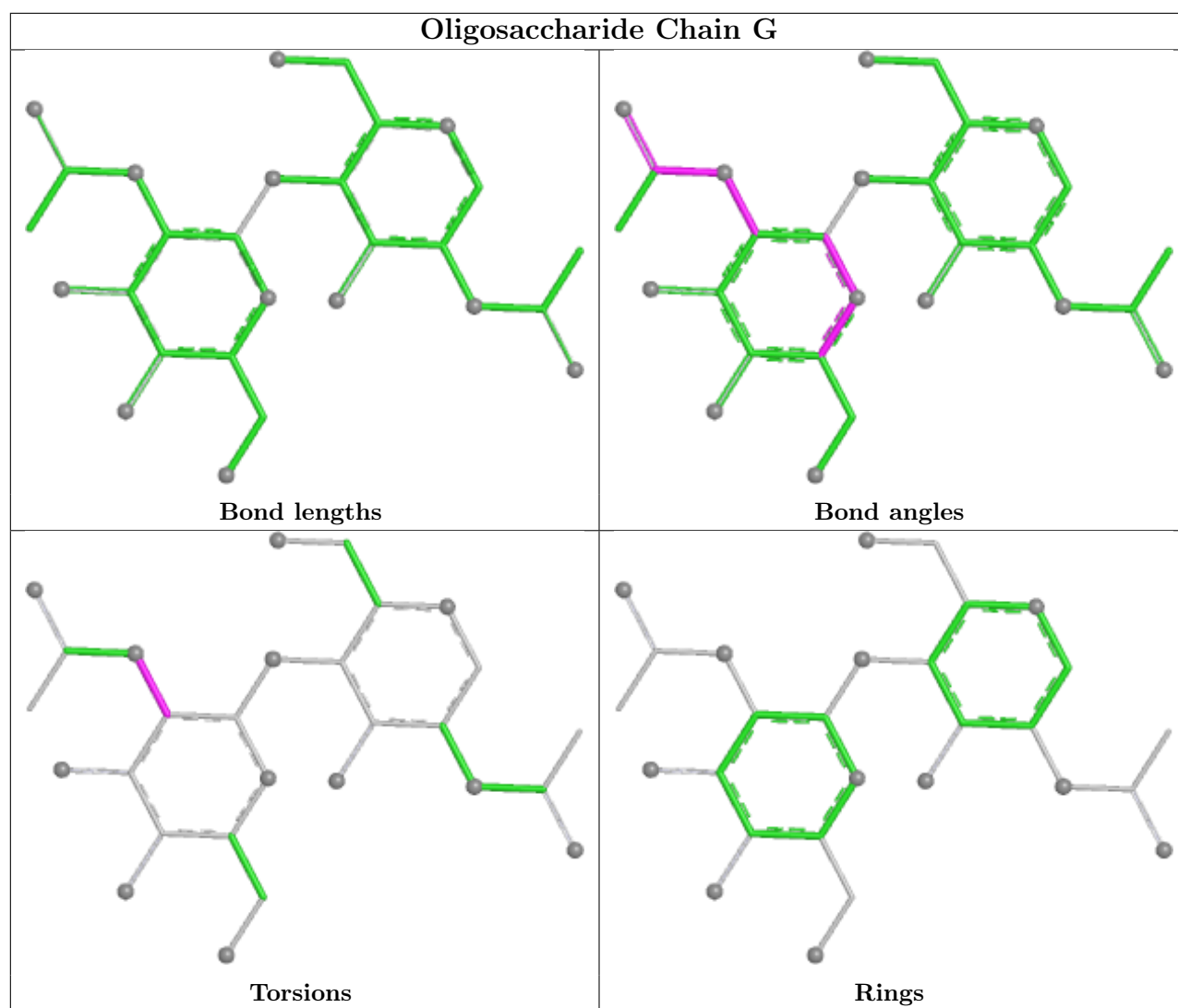
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	2	NAG	1	0

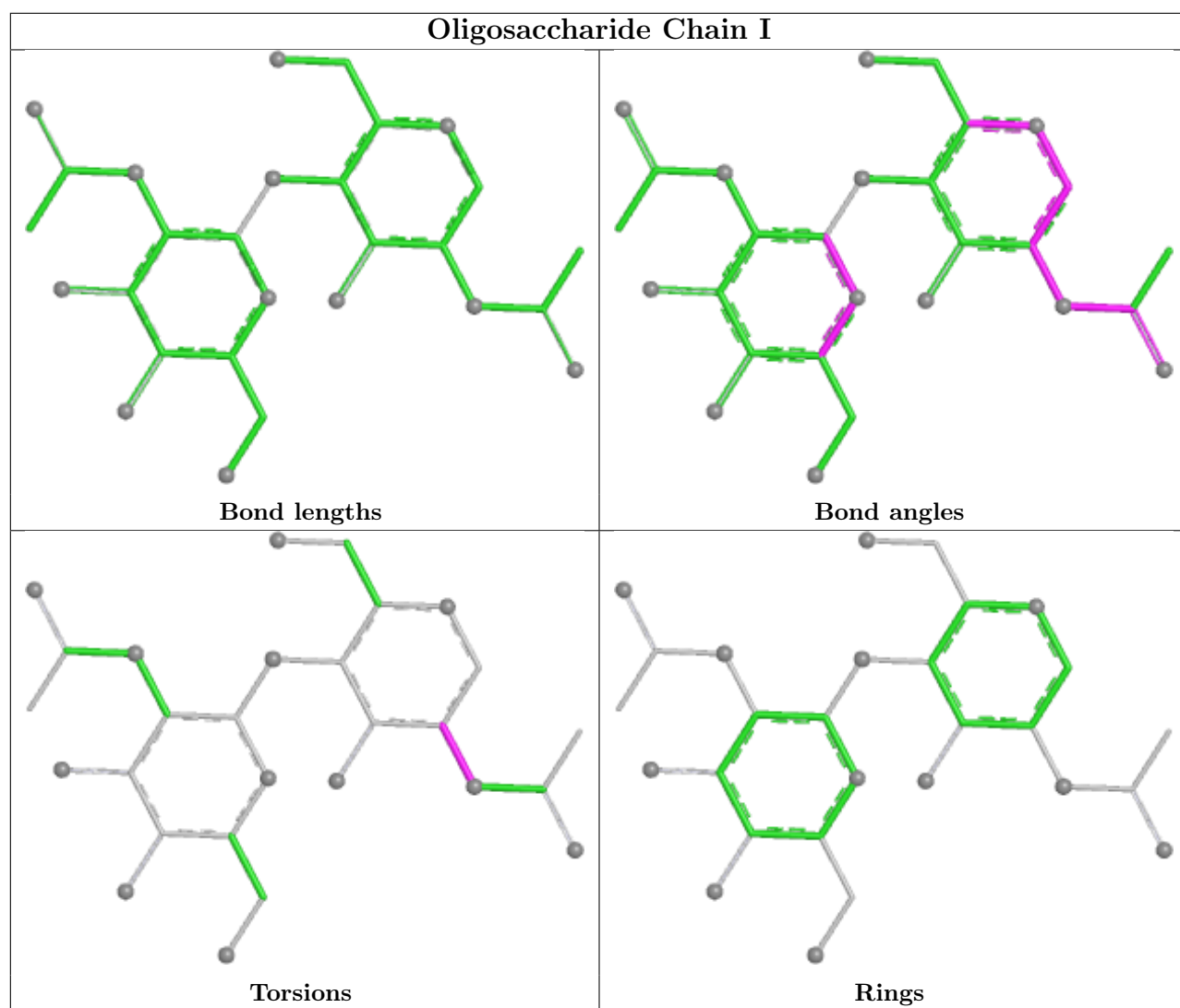
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

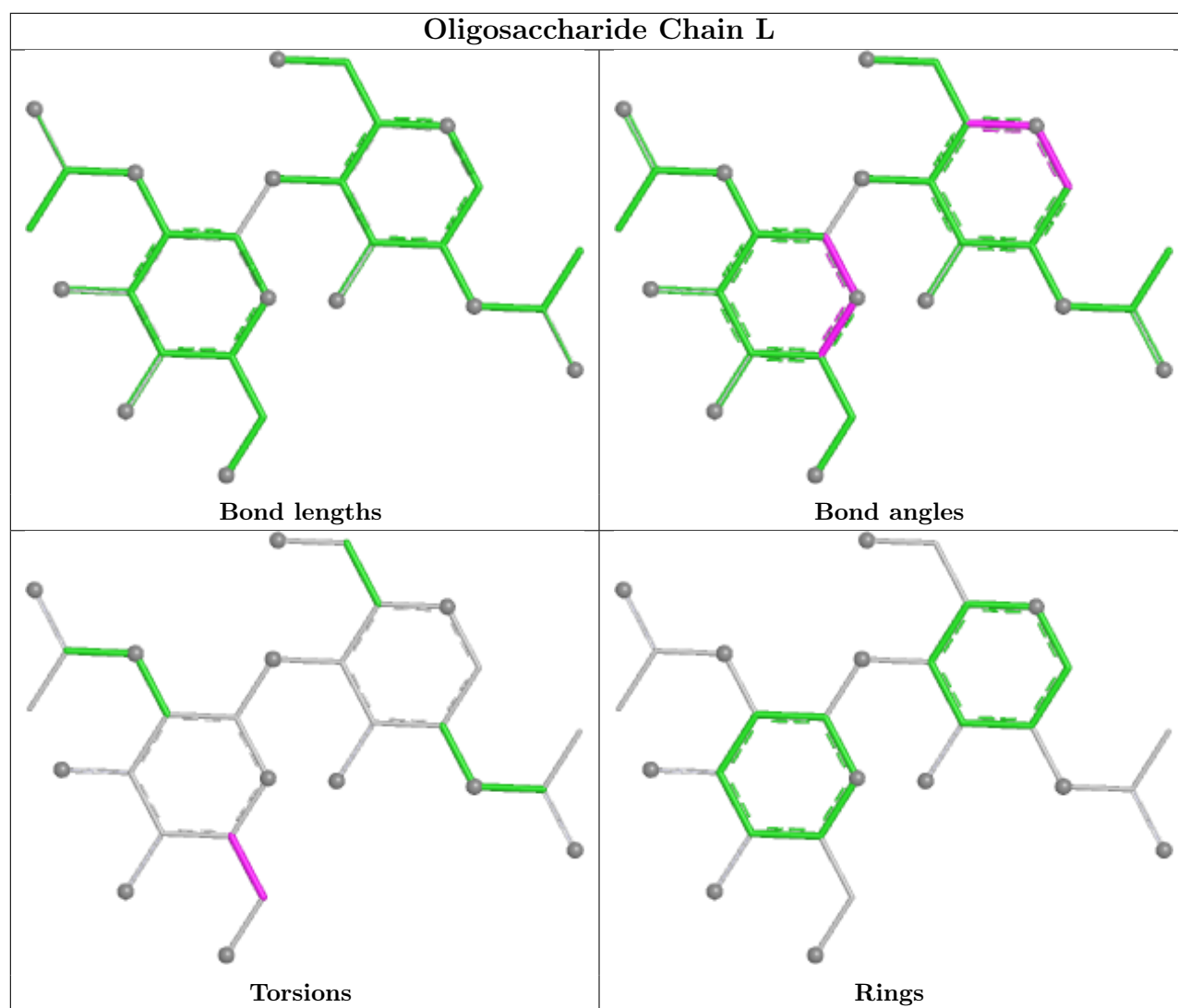


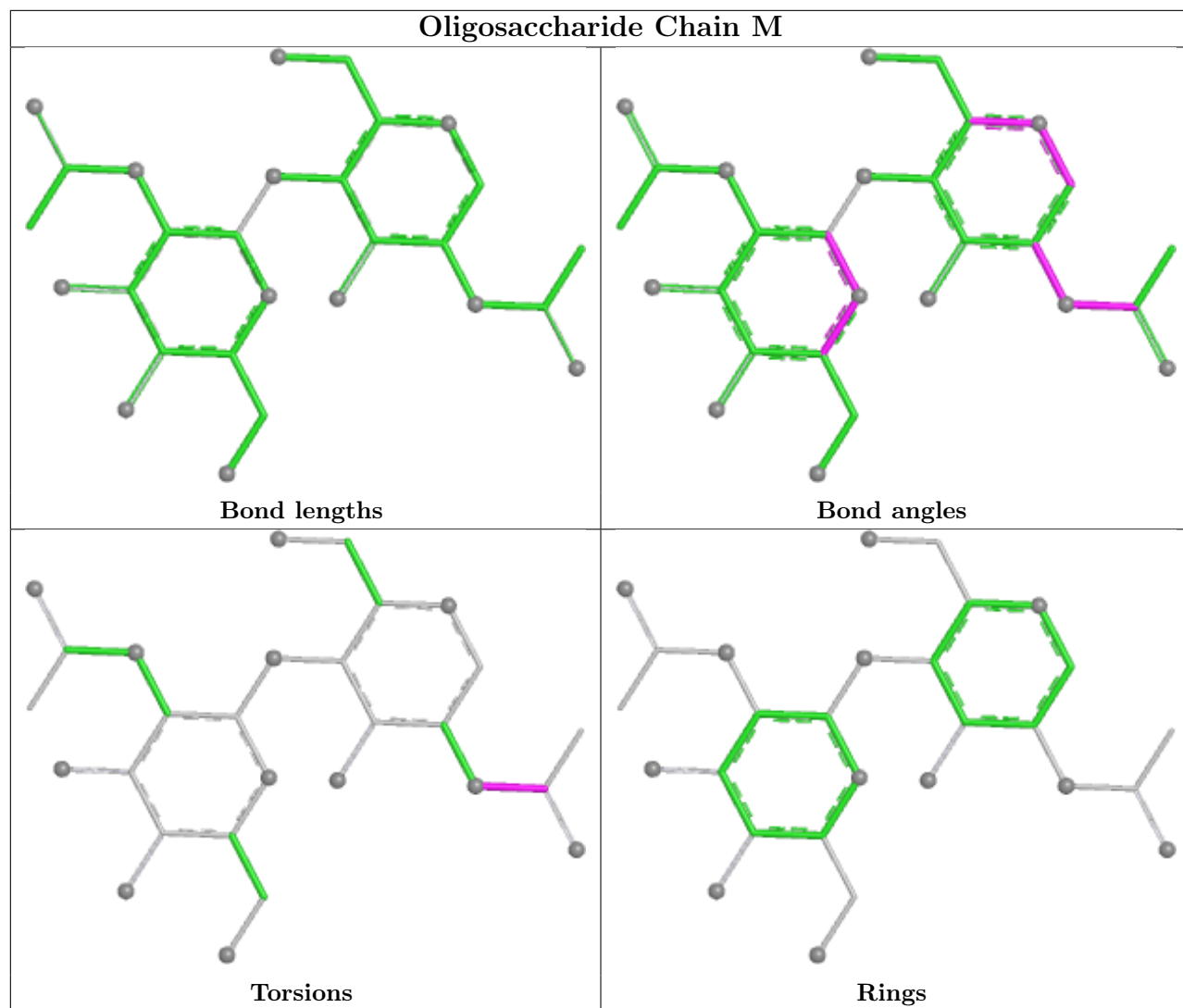


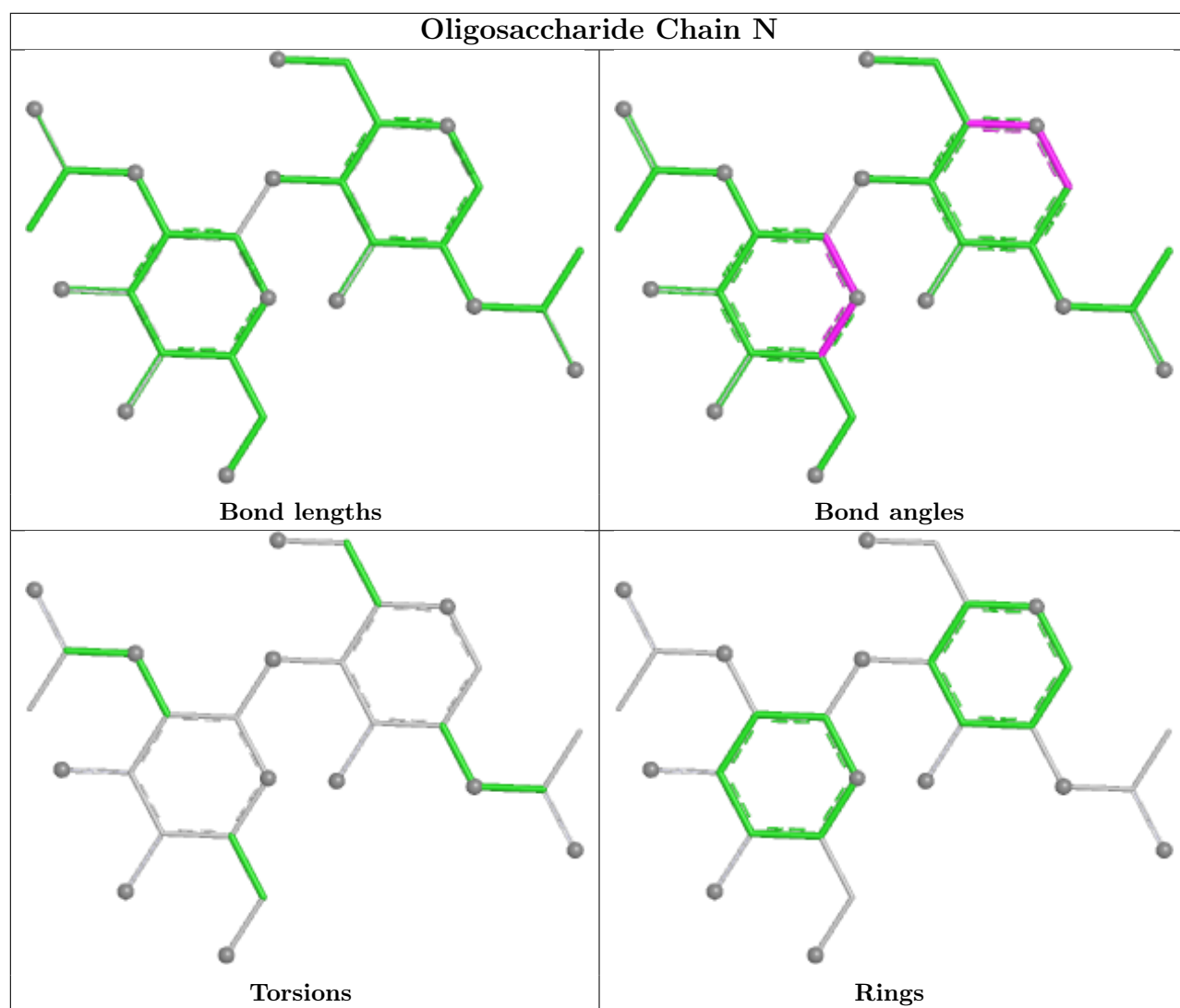


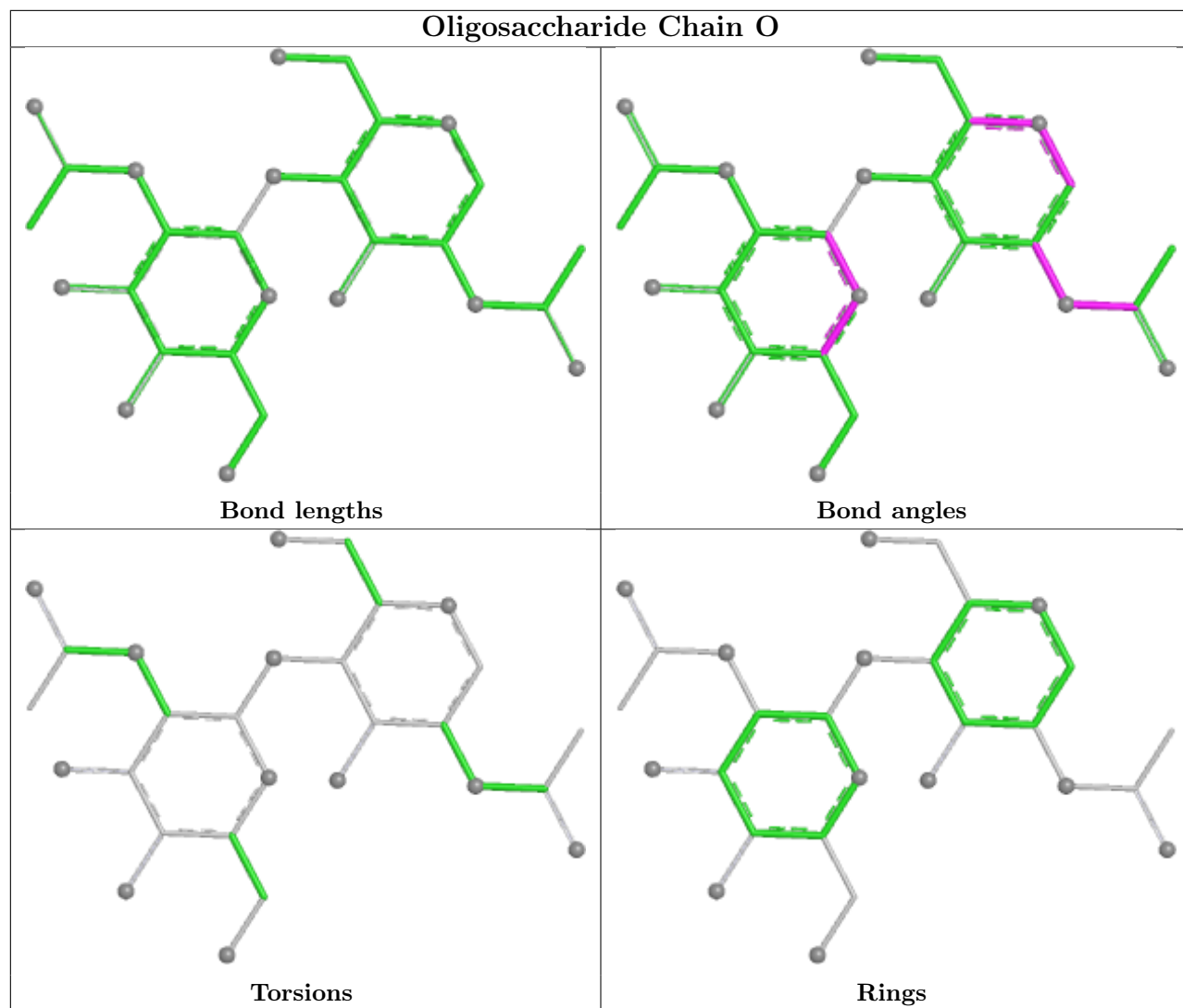


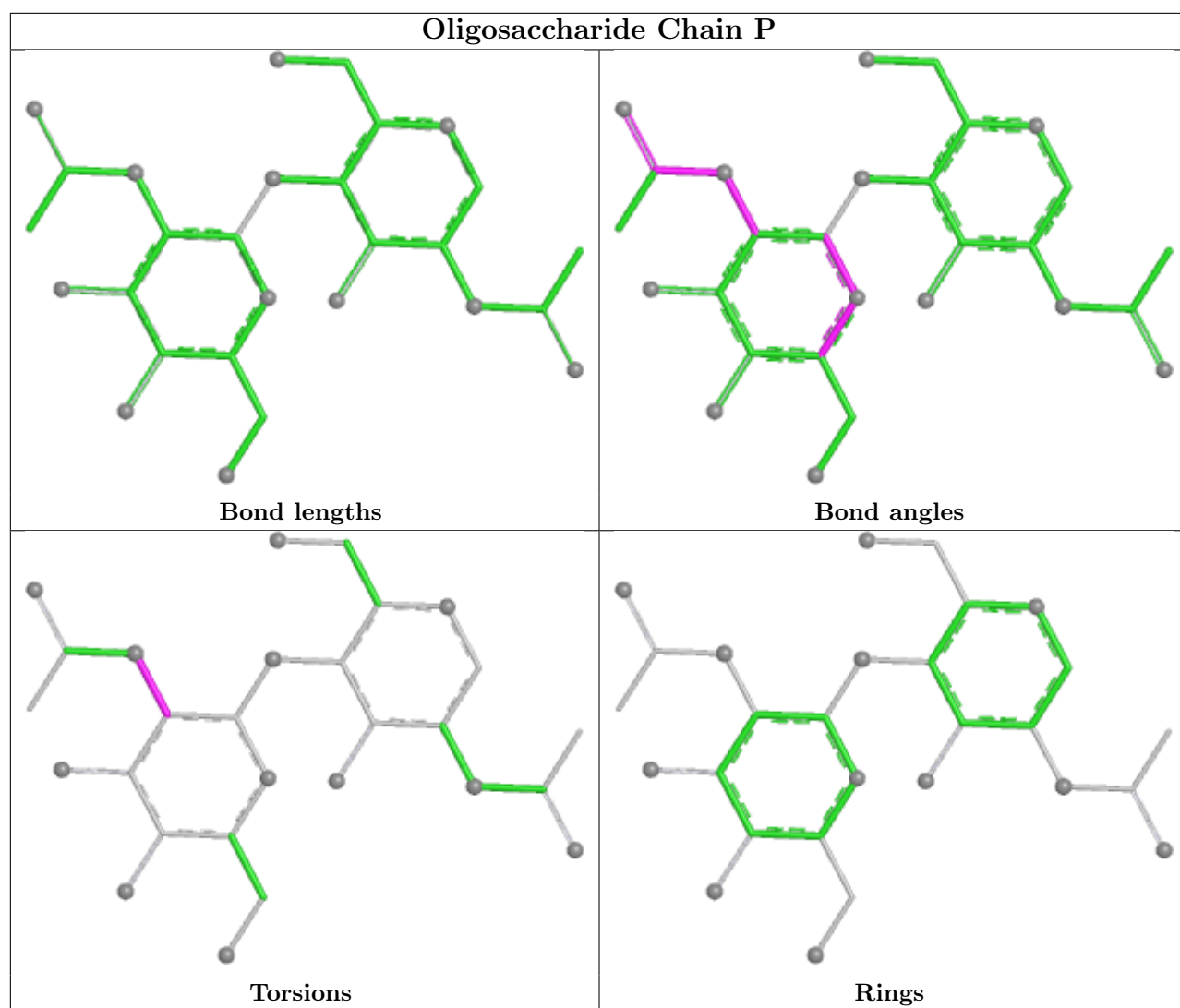


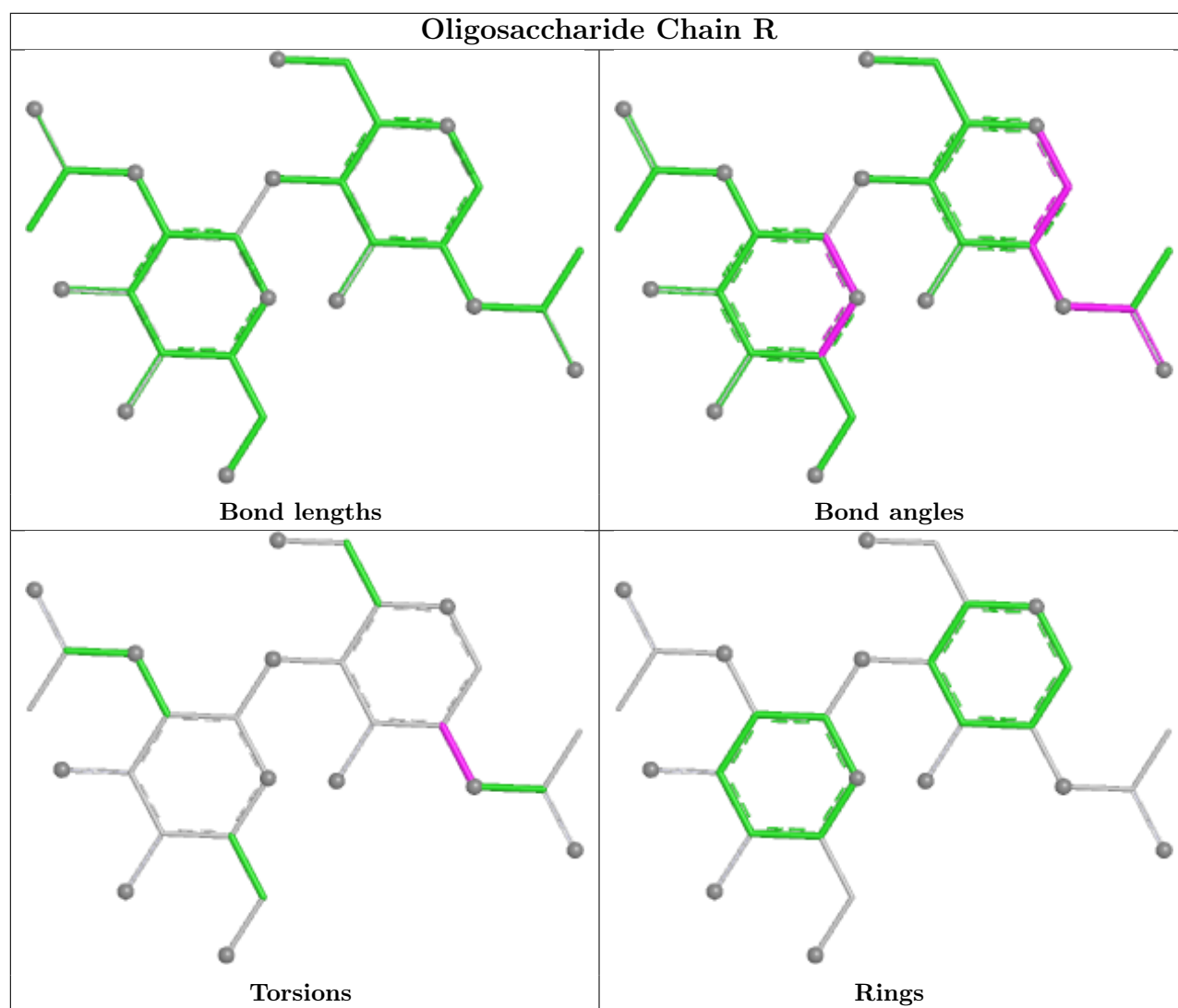


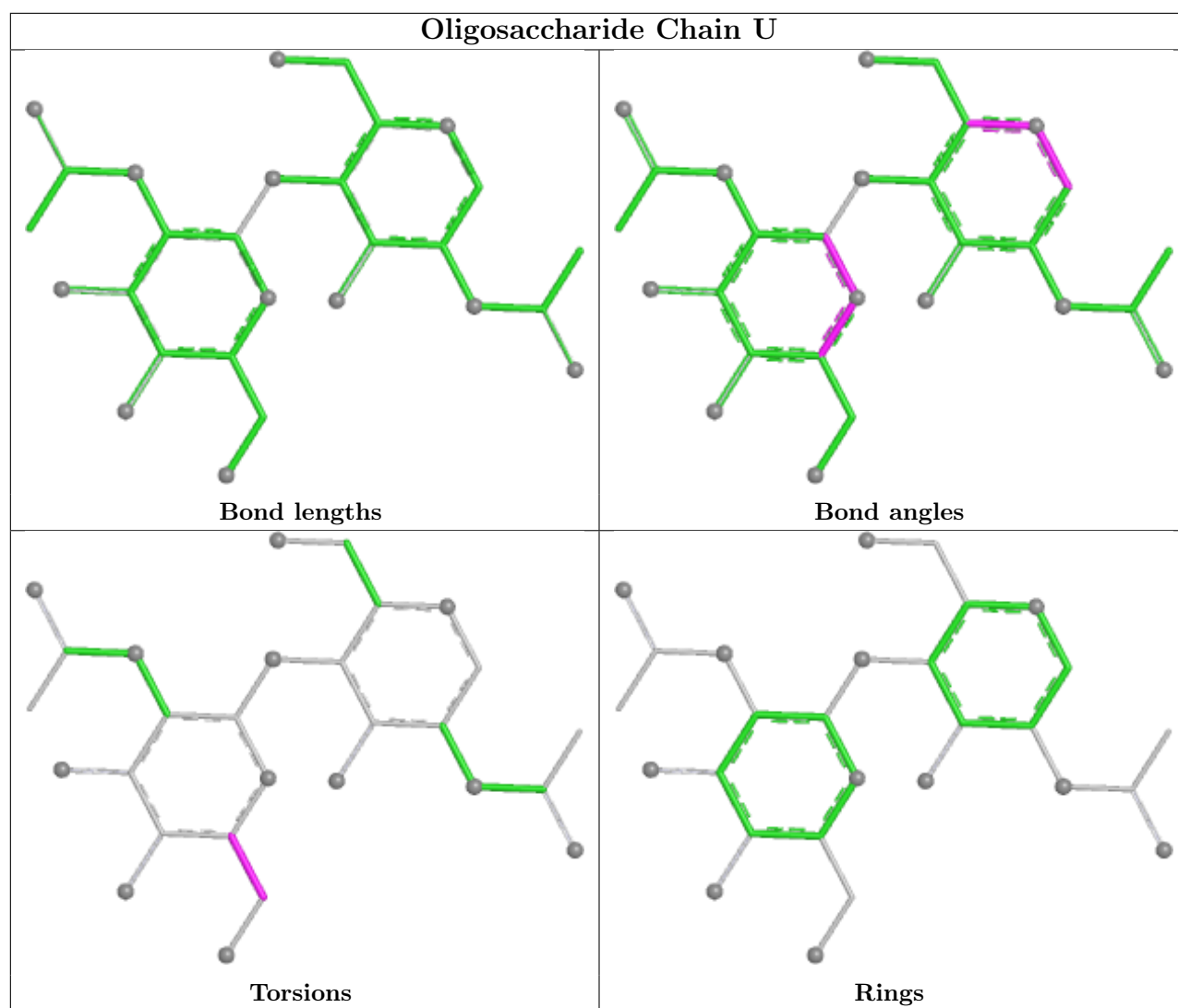


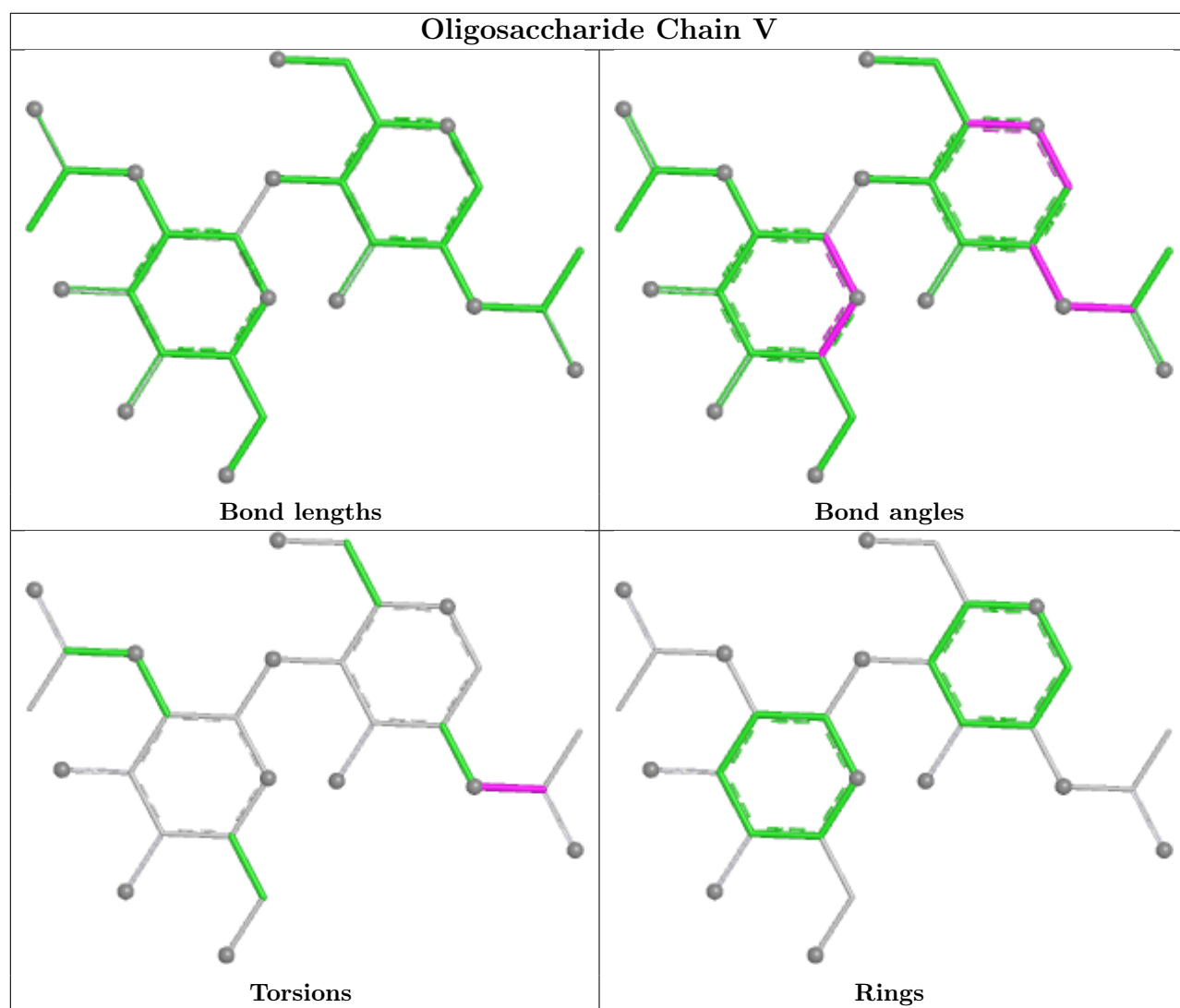


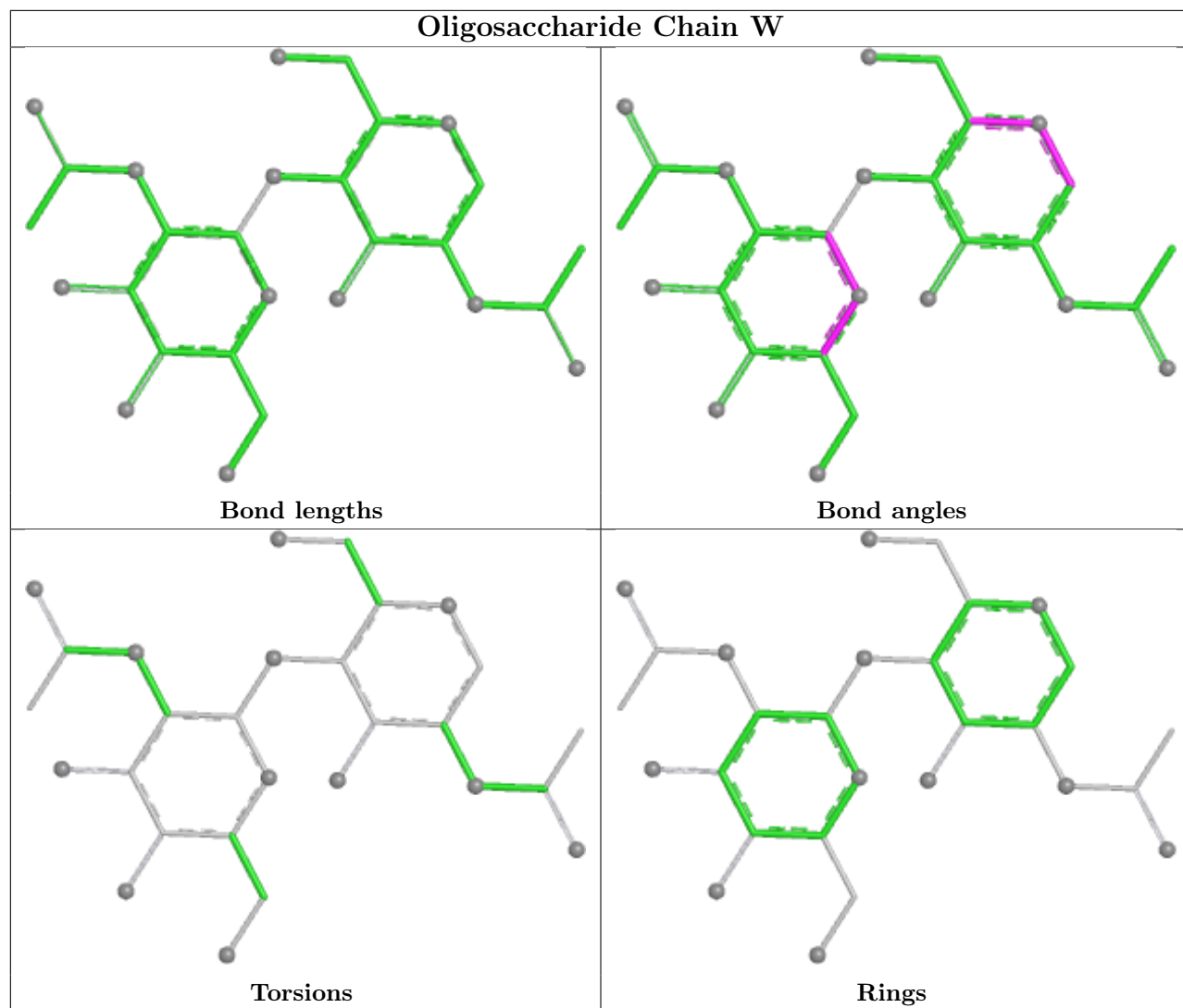


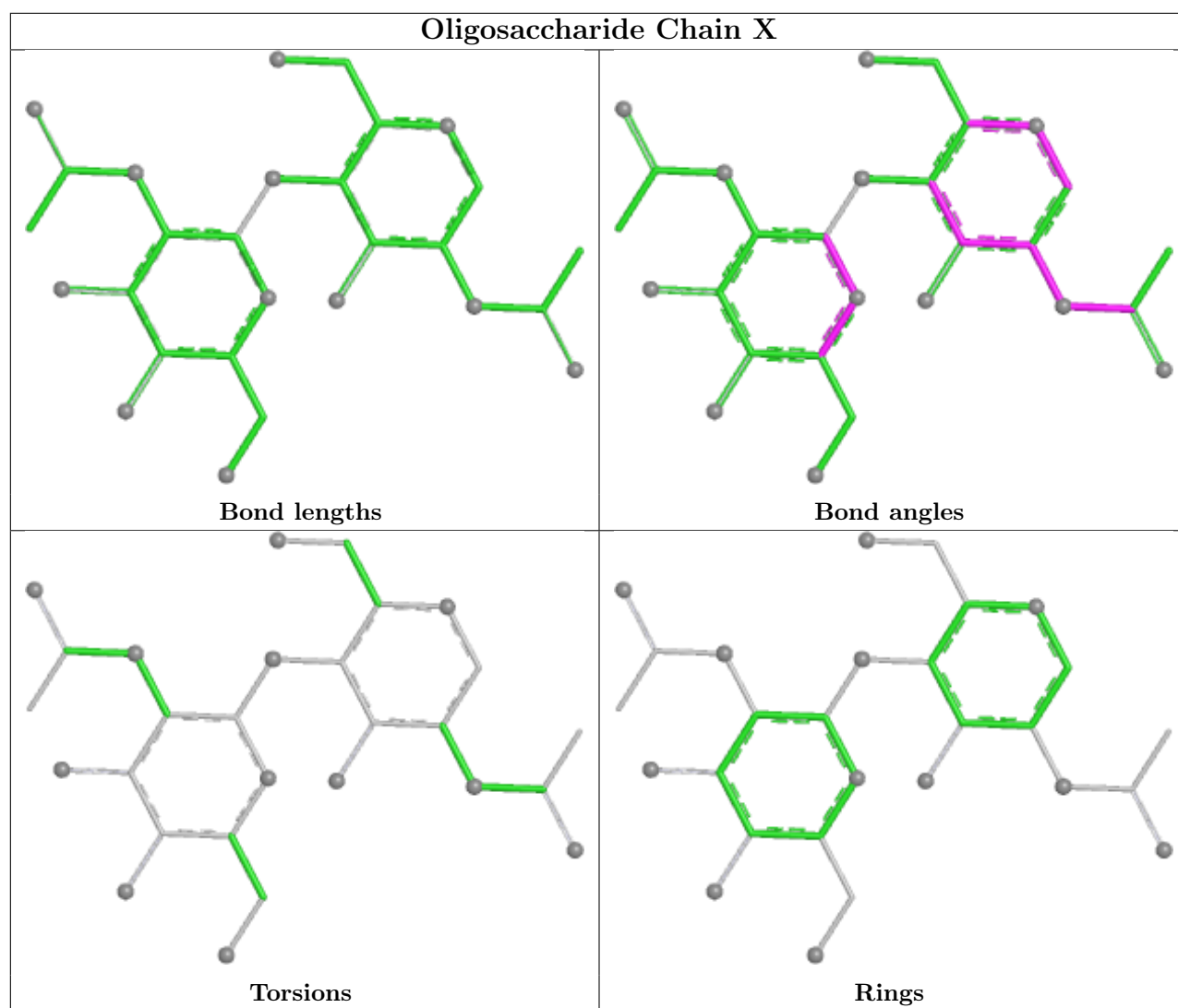


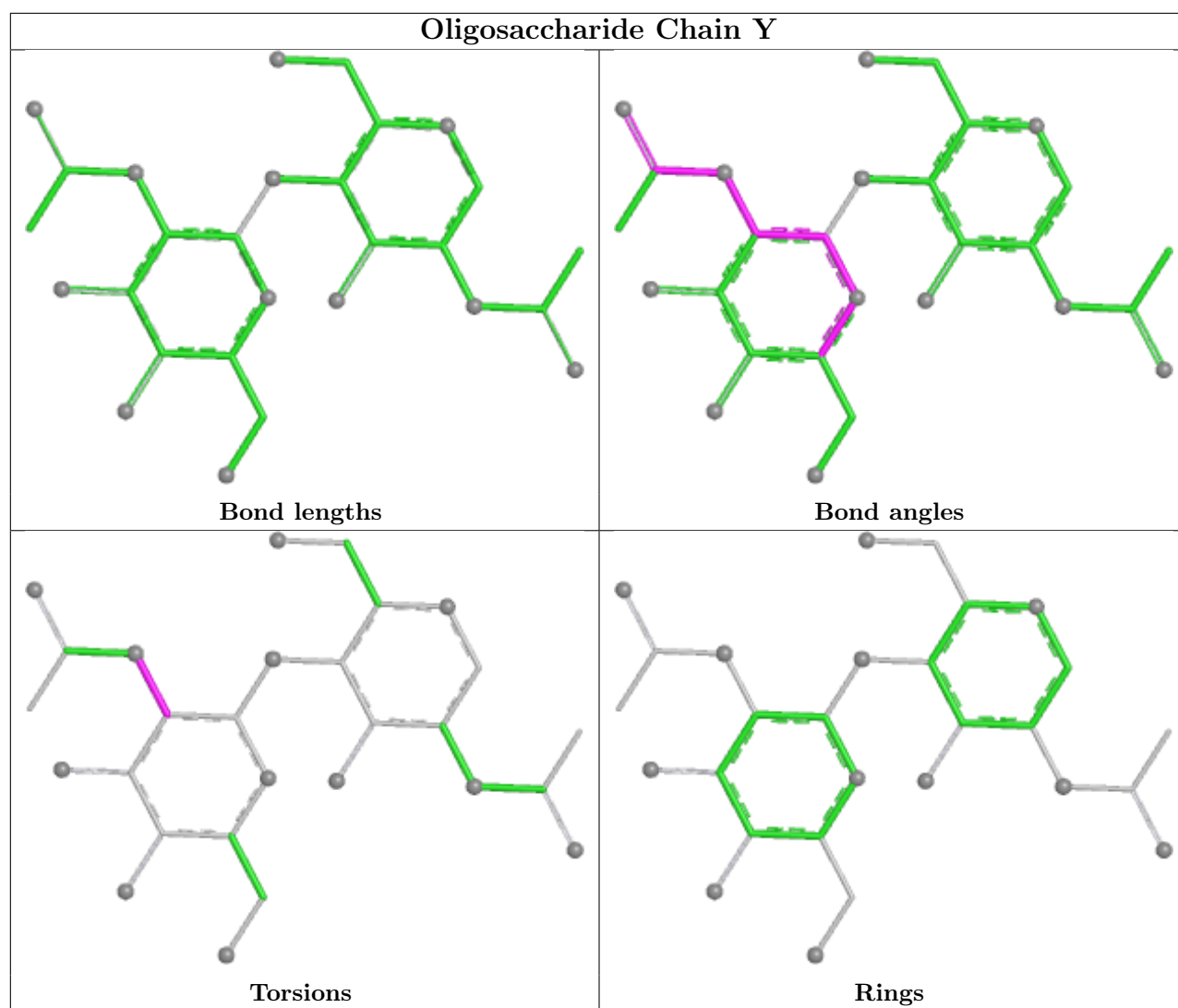


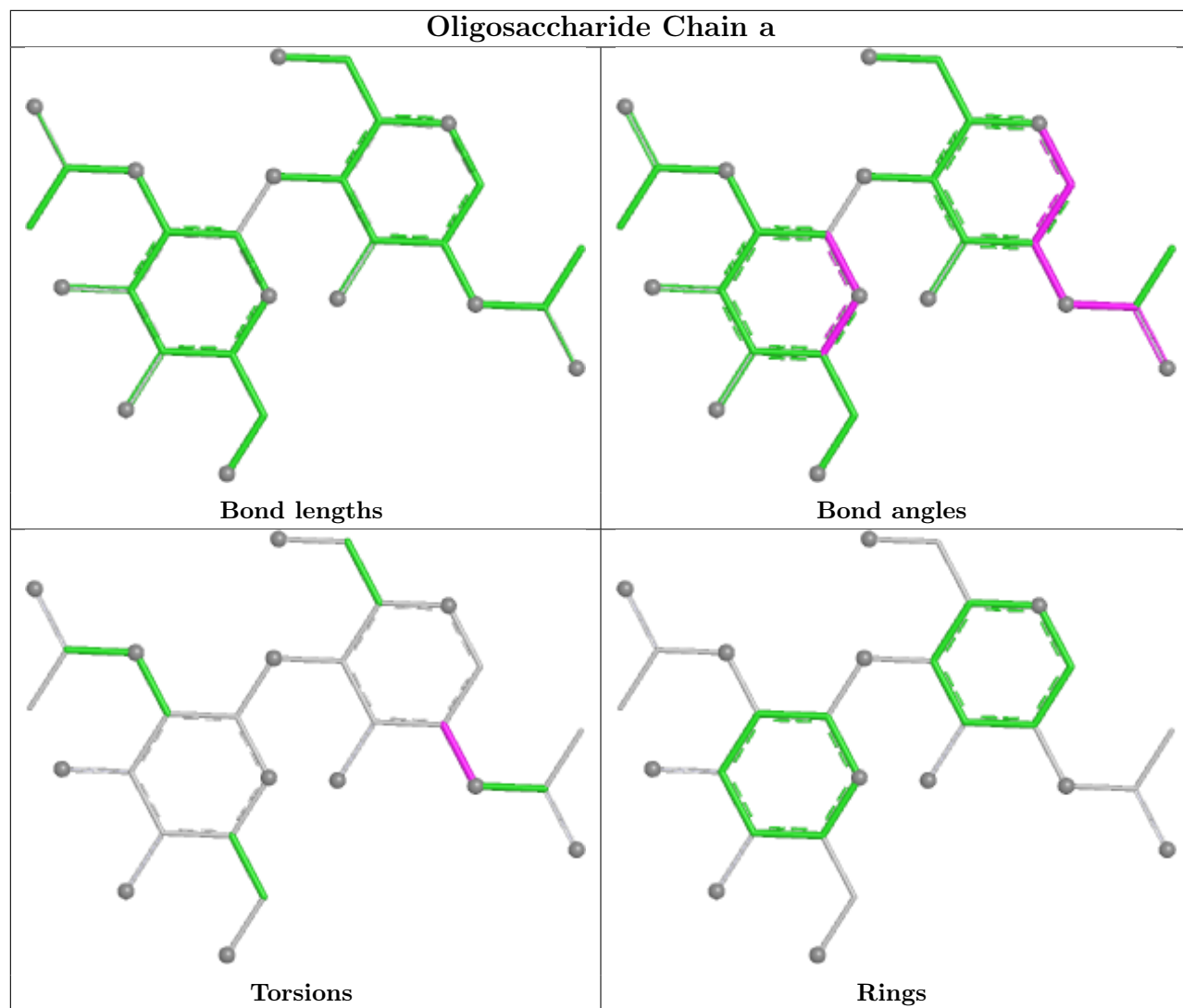


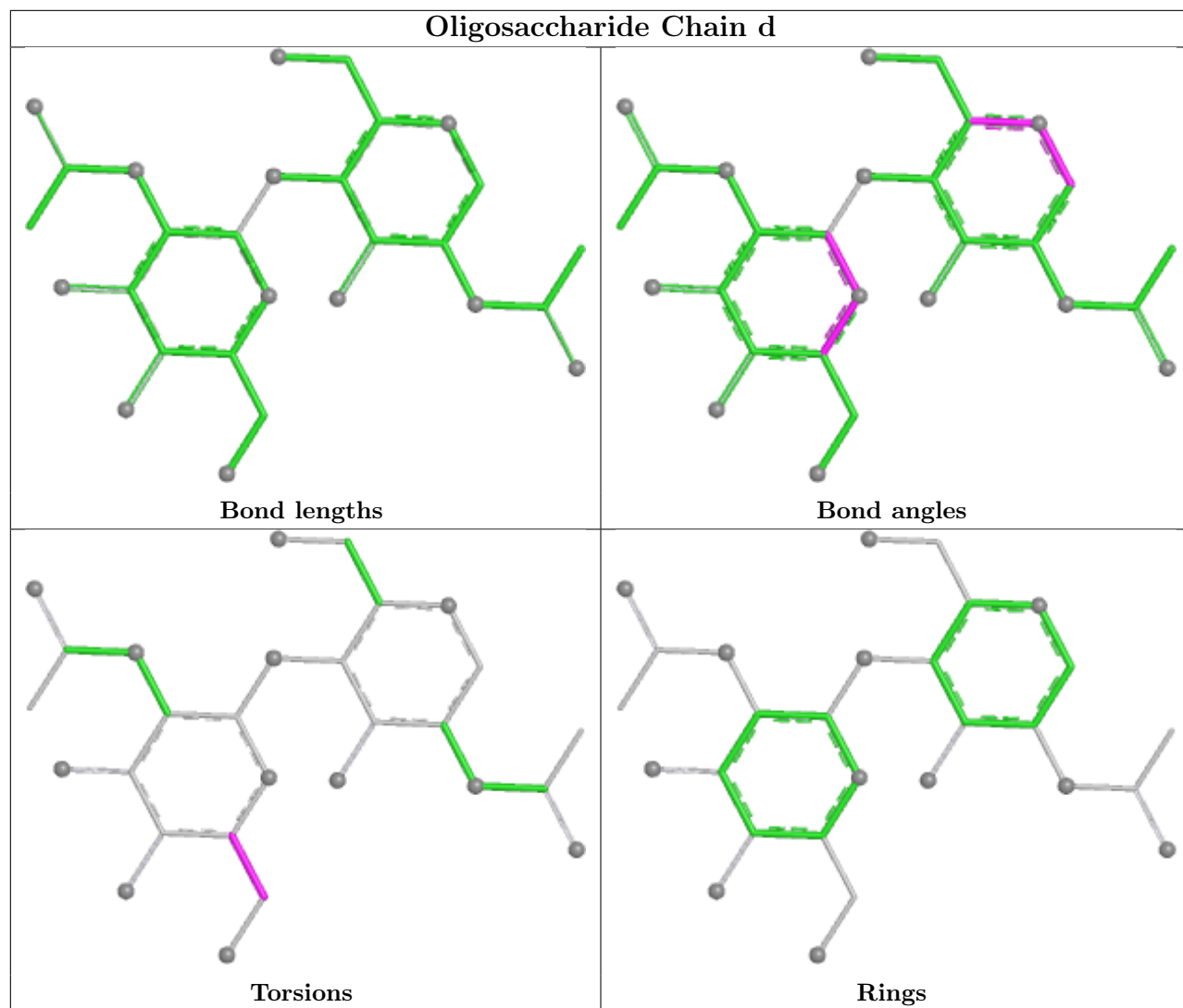


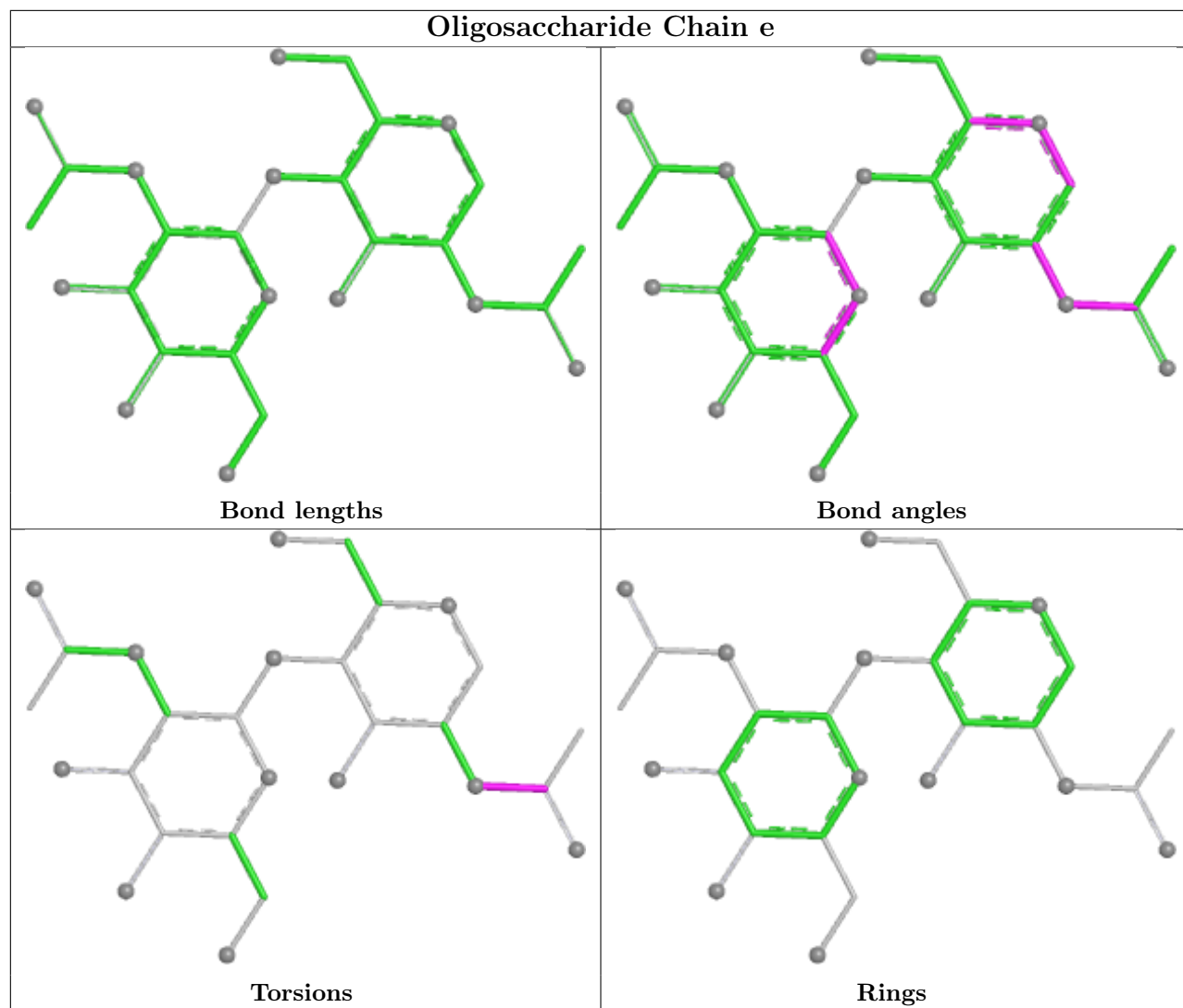


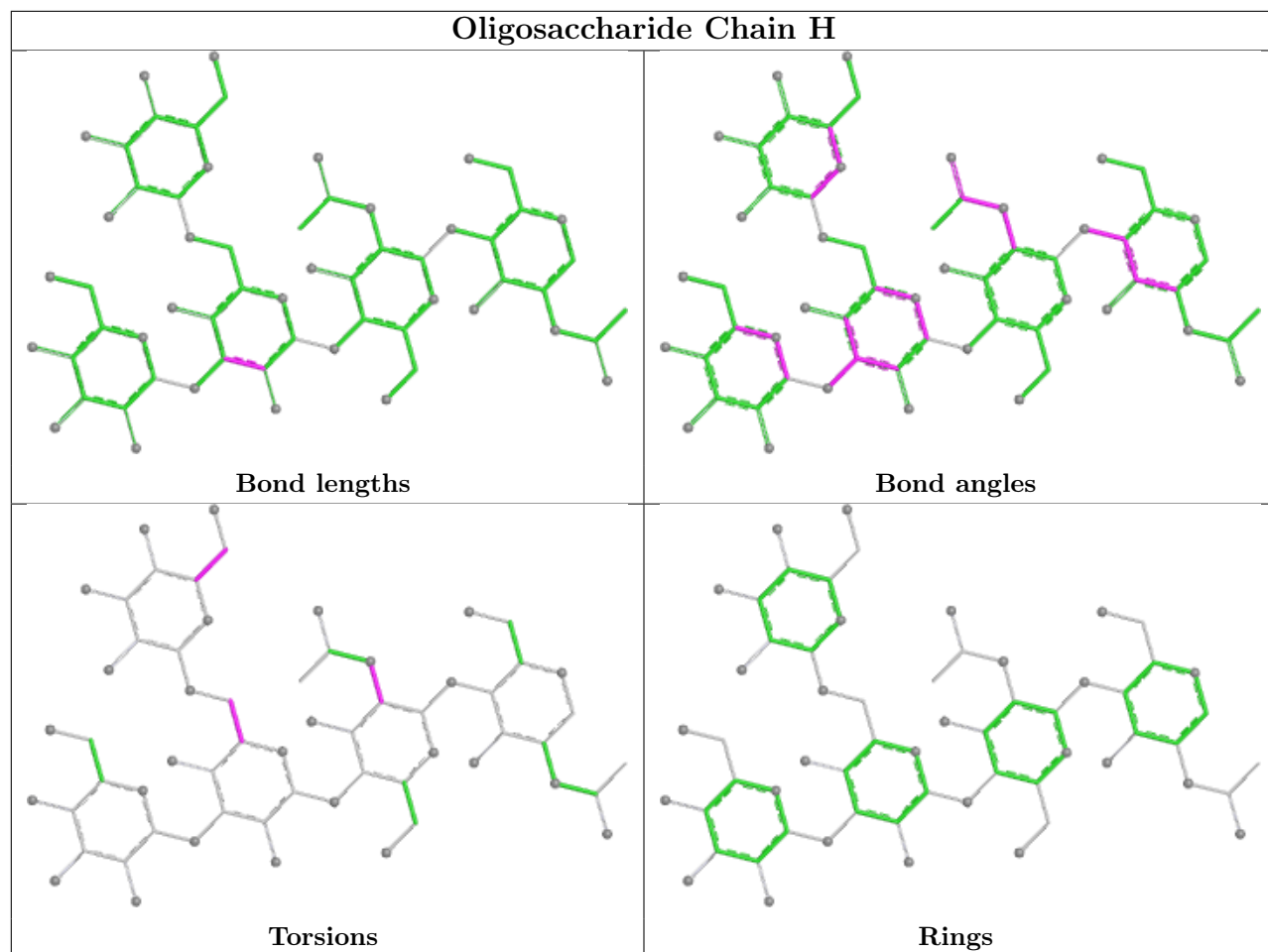


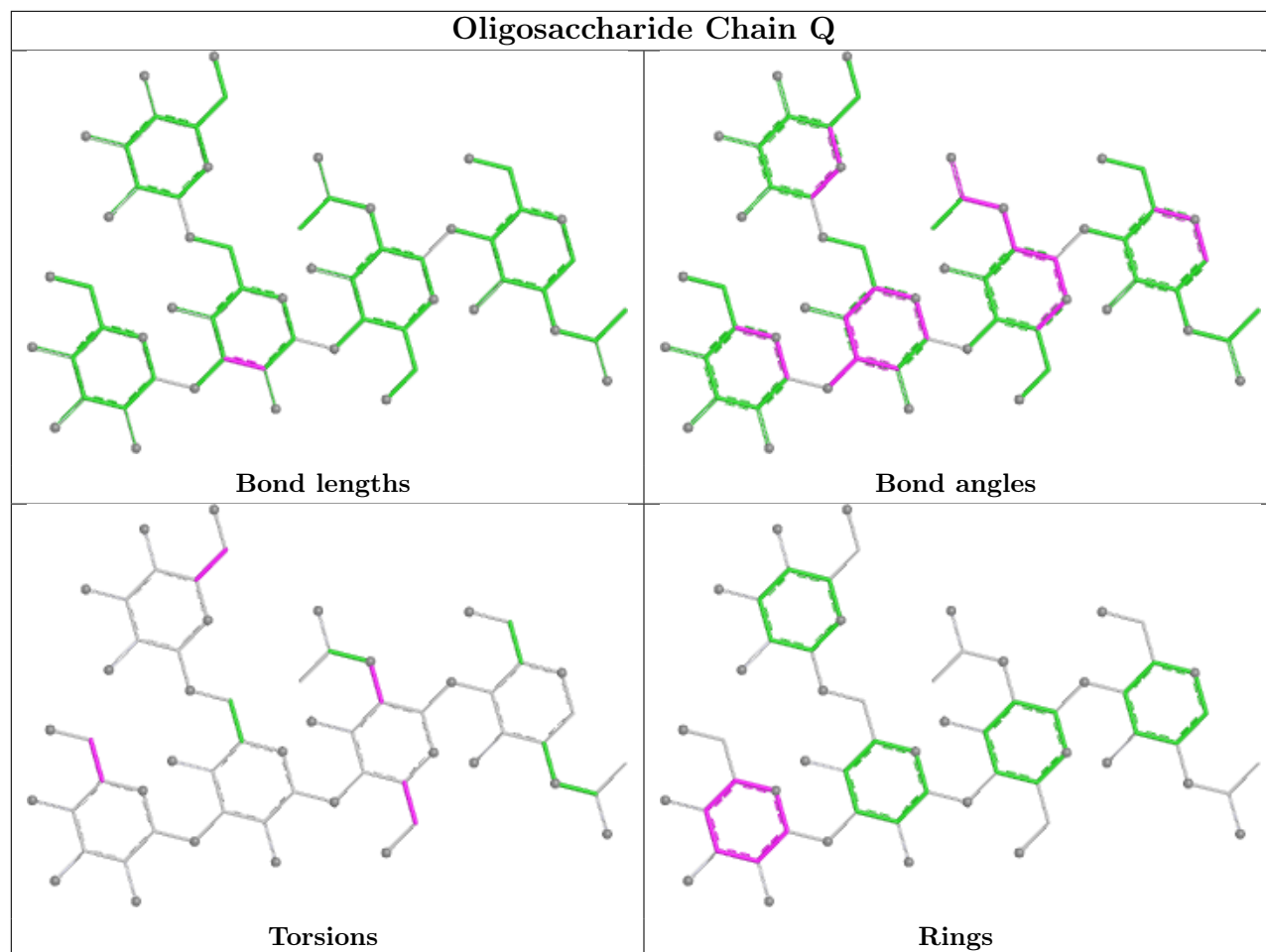


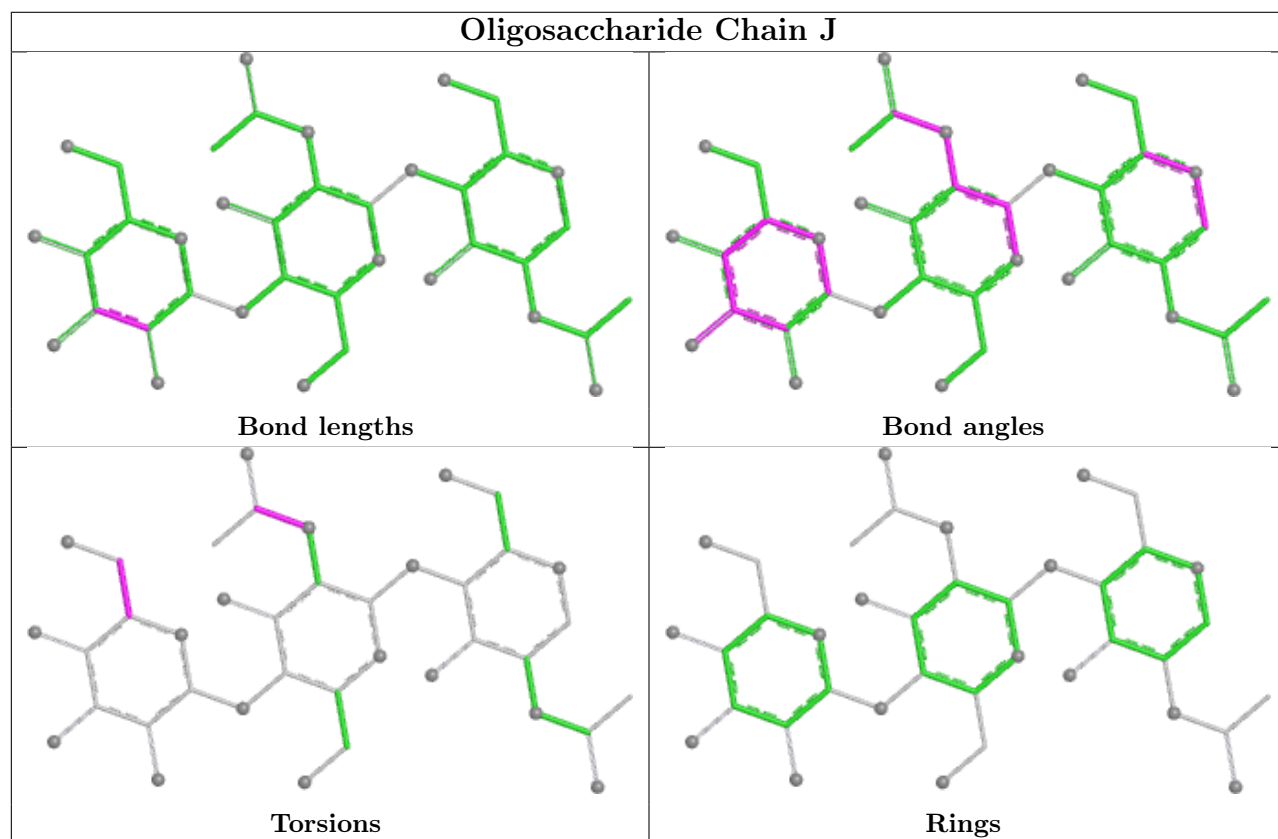
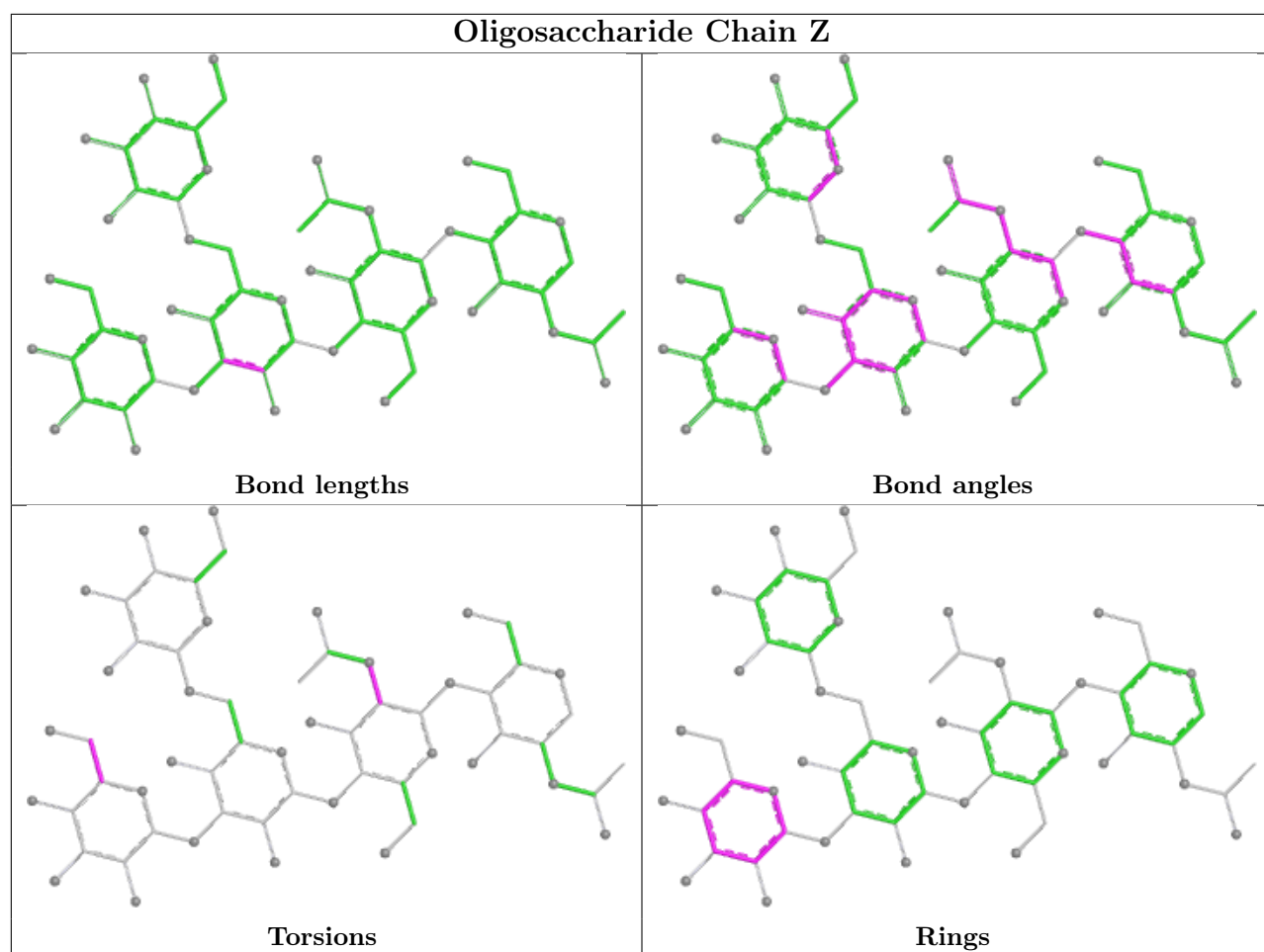


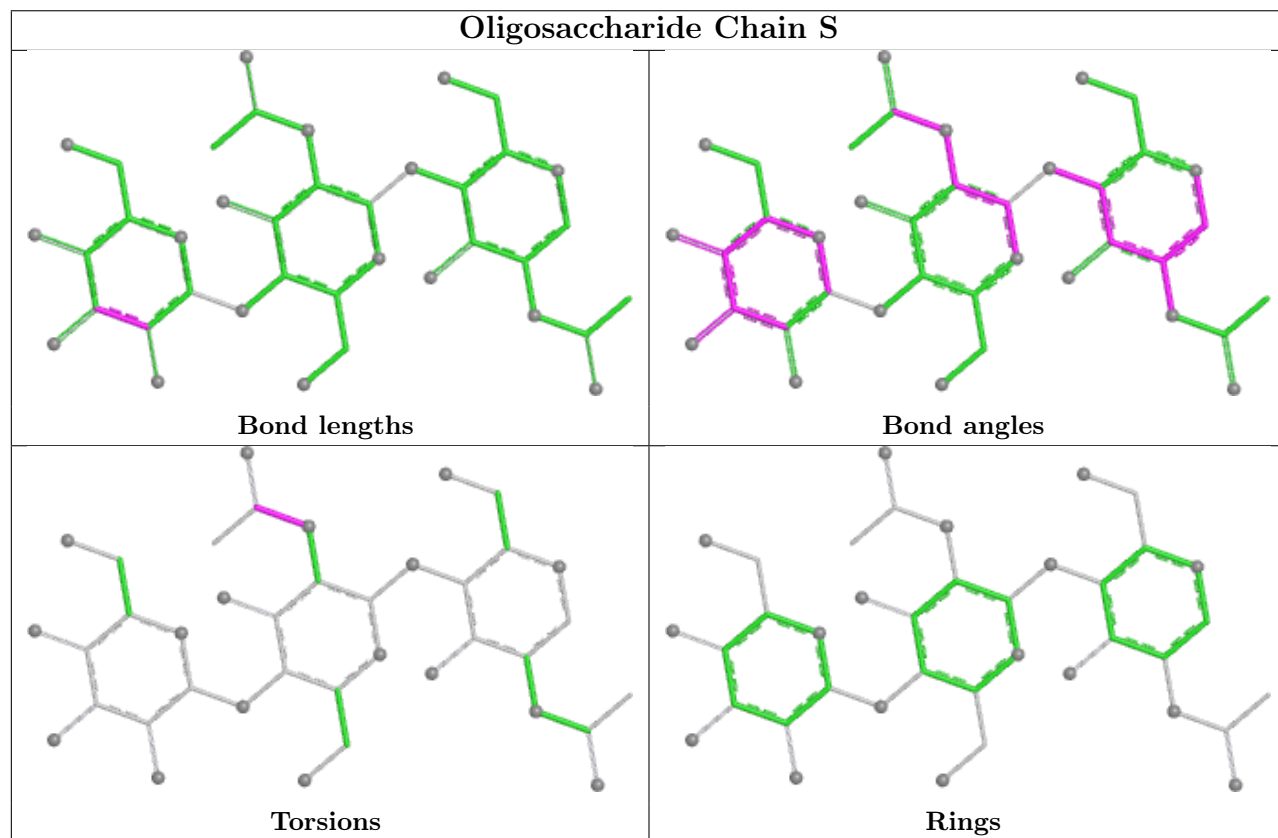
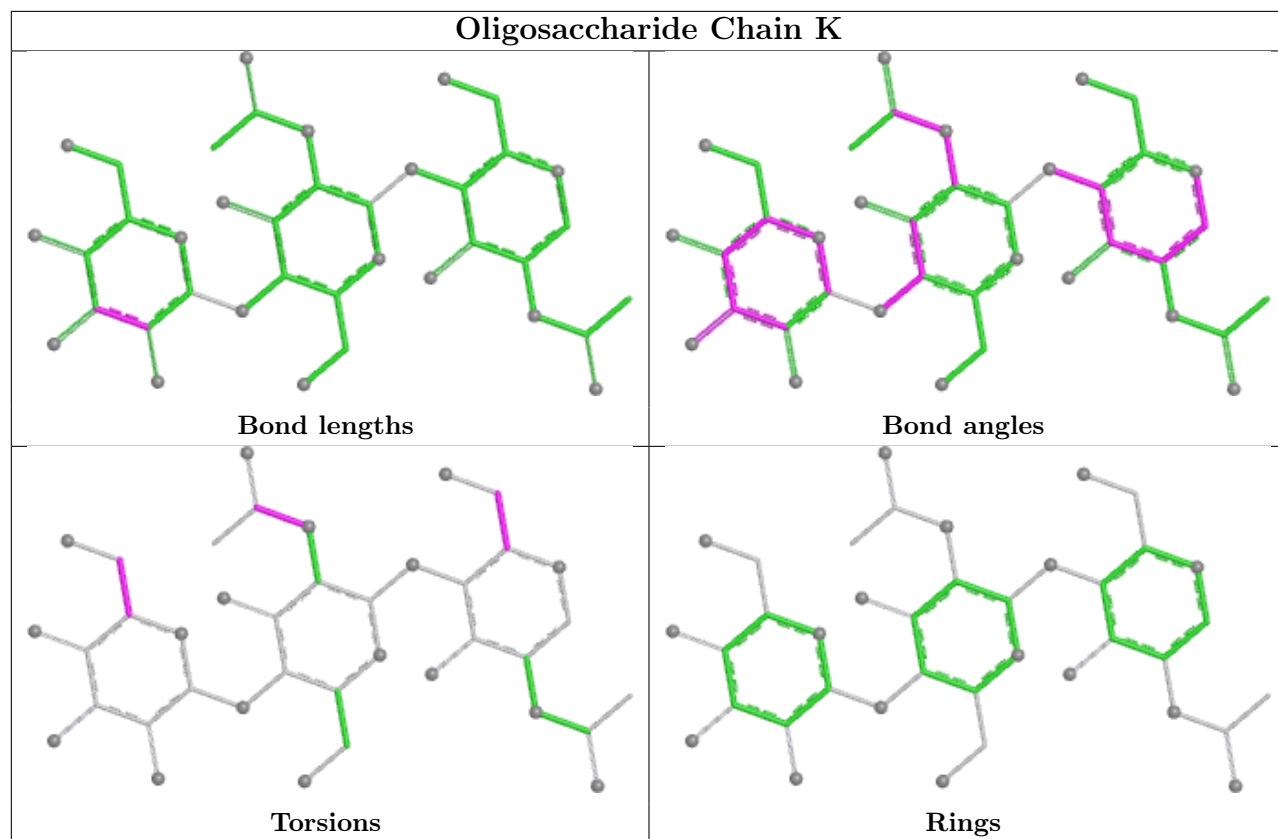


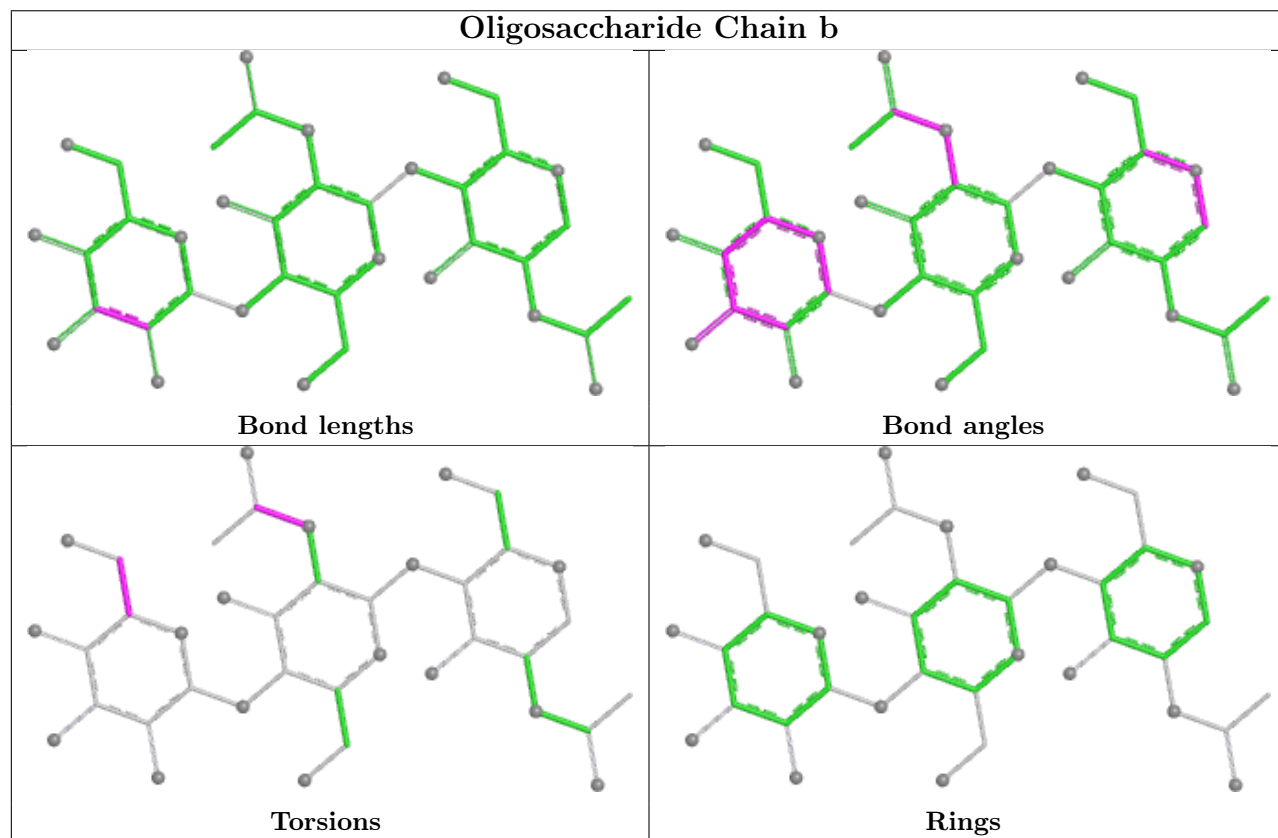
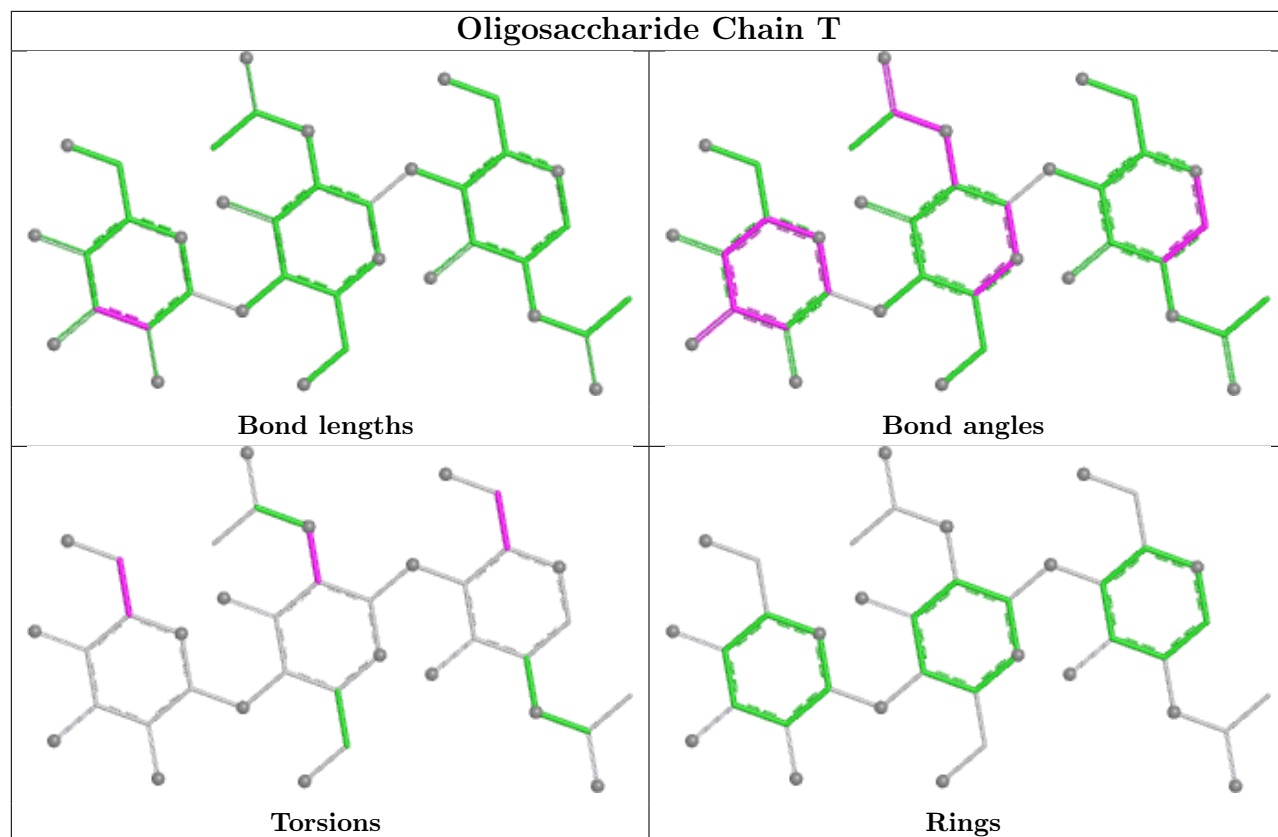


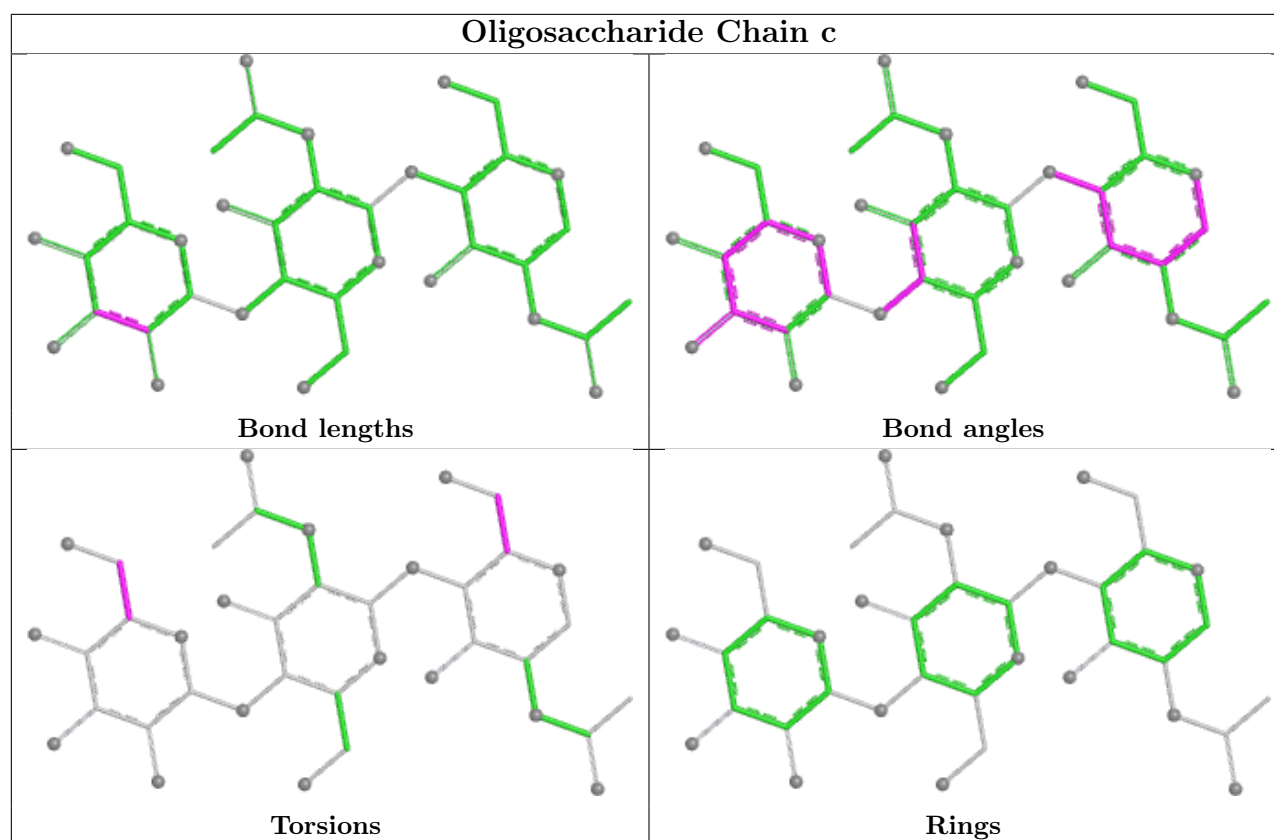












5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	1402	1	14,14,15	0.71	0	17,19,21	1.32	2 (11%)
5	NAG	B	1407	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
5	NAG	B	1405	1	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
5	NAG	B	1410	1	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
5	NAG	C	1410	1	14,14,15	0.77	0	17,19,21	1.13	1 (5%)
5	NAG	A	1406	1	14,14,15	0.71	0	17,19,21	1.19	1 (5%)
5	NAG	B	1404	1	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
5	NAG	A	1409	1	14,14,15	0.72	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1408	1	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
5	NAG	A	1401	1	14,14,15	0.74	0	17,19,21	1.32	2 (11%)
5	NAG	A	1410	1	14,14,15	0.79	0	17,19,21	1.17	2 (11%)
5	NAG	B	1401	1	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
5	NAG	C	1404	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
5	NAG	C	1411	1	14,14,15	0.91	1 (7%)	17,19,21	2.10	3 (17%)
5	NAG	C	1409	1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
5	NAG	C	1406	1	14,14,15	0.71	0	17,19,21	1.25	2 (11%)
5	NAG	A	1408	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
5	NAG	B	1402	1	14,14,15	0.69	0	17,19,21	1.35	2 (11%)
5	NAG	B	1403	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
5	NAG	A	1402	1	14,14,15	0.71	0	17,19,21	1.26	2 (11%)
5	NAG	A	1407	1	14,14,15	0.73	0	17,19,21	1.32	2 (11%)
5	NAG	C	1405	1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
5	NAG	A	1404	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
5	NAG	A	1403	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
5	NAG	A	1411	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
5	NAG	C	1403	1	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
5	NAG	B	1406	1	14,14,15	0.74	0	17,19,21	1.30	2 (11%)
5	NAG	C	1408	1	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
5	NAG	C	1407	1	14,14,15	0.67	0	17,19,21	1.26	2 (11%)
5	NAG	B	1409	1	14,14,15	0.78	0	17,19,21	1.08	1 (5%)
5	NAG	A	1405	1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
5	NAG	C	1401	1	14,14,15	0.71	0	17,19,21	1.25	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1411	NAG	C1-C2	2.73	1.56	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1411	NAG	C1-O5-C5	6.45	120.83	112.19
5	C	1411	NAG	C2-N2-C7	4.49	128.91	122.90
5	A	1401	NAG	C2-N2-C7	3.48	127.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1406	NAG	C2-N2-C7	3.45	127.53	122.90
5	C	1401	NAG	C2-N2-C7	3.41	127.46	122.90
5	A	1407	NAG	C2-N2-C7	3.39	127.44	122.90
5	A	1406	NAG	C2-N2-C7	3.36	127.41	122.90
5	B	1401	NAG	C2-N2-C7	3.34	127.38	122.90
5	C	1407	NAG	O5-C1-C2	-3.32	106.15	111.29
5	B	1405	NAG	C2-N2-C7	3.29	127.31	122.90
5	B	1402	NAG	C1-O5-C5	3.27	116.56	112.19
5	C	1402	NAG	C2-N2-C7	3.26	127.27	122.90
5	B	1402	NAG	C2-N2-C7	3.24	127.25	122.90
5	A	1402	NAG	C2-N2-C7	3.22	127.21	122.90
5	C	1406	NAG	C2-N2-C7	3.17	127.14	122.90
5	C	1402	NAG	C1-O5-C5	3.14	116.39	112.19
5	B	1401	NAG	C1-O5-C5	3.03	116.25	112.19
5	C	1403	NAG	C1-O5-C5	2.95	116.14	112.19
5	A	1401	NAG	C1-O5-C5	2.94	116.12	112.19
5	A	1402	NAG	C1-O5-C5	2.91	116.08	112.19
5	A	1407	NAG	C1-O5-C5	2.88	116.05	112.19
5	C	1408	NAG	C1-O5-C5	2.86	116.02	112.19
5	A	1408	NAG	C1-O5-C5	2.83	115.98	112.19
5	C	1407	NAG	C2-N2-C7	2.80	126.65	122.90
5	A	1410	NAG	C1-O5-C5	2.75	115.88	112.19
5	A	1404	NAG	C1-O5-C5	2.73	115.84	112.19
5	C	1404	NAG	C1-O5-C5	2.72	115.83	112.19
5	C	1410	NAG	C1-O5-C5	2.70	115.81	112.19
5	B	1403	NAG	C1-O5-C5	2.68	115.78	112.19
5	B	1407	NAG	C1-O5-C5	2.68	115.78	112.19
5	B	1406	NAG	C1-O5-C5	2.65	115.74	112.19
5	A	1403	NAG	C1-O5-C5	2.65	115.73	112.19
5	C	1406	NAG	C1-O5-C5	2.64	115.72	112.19
5	C	1401	NAG	C1-O5-C5	2.61	115.69	112.19
5	A	1411	NAG	O5-C1-C2	-2.49	107.44	111.29
5	A	1405	NAG	C1-O5-C5	2.40	115.41	112.19
5	C	1405	NAG	C1-O5-C5	2.33	115.31	112.19
5	A	1409	NAG	C1-O5-C5	2.32	115.30	112.19
5	B	1408	NAG	C1-O5-C5	2.30	115.27	112.19
5	C	1409	NAG	C1-O5-C5	2.21	115.14	112.19
5	B	1404	NAG	C1-O5-C5	2.18	115.11	112.19
5	B	1410	NAG	O5-C1-C2	-2.11	108.03	111.29
5	A	1410	NAG	C2-N2-C7	2.06	125.66	122.90
5	C	1411	NAG	C3-C4-C5	-2.05	106.51	110.23
5	B	1409	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1401	NAG	C8-C7-N2-C2
5	A	1401	NAG	O7-C7-N2-C2
5	A	1402	NAG	C8-C7-N2-C2
5	A	1402	NAG	O7-C7-N2-C2
5	A	1406	NAG	C8-C7-N2-C2
5	A	1406	NAG	O7-C7-N2-C2
5	A	1407	NAG	C8-C7-N2-C2
5	A	1407	NAG	O7-C7-N2-C2
5	B	1401	NAG	C8-C7-N2-C2
5	B	1401	NAG	O7-C7-N2-C2
5	B	1402	NAG	C8-C7-N2-C2
5	B	1402	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	B	1406	NAG	C8-C7-N2-C2
5	B	1406	NAG	O7-C7-N2-C2
5	C	1401	NAG	C8-C7-N2-C2
5	C	1401	NAG	O7-C7-N2-C2
5	C	1402	NAG	C8-C7-N2-C2
5	C	1402	NAG	O7-C7-N2-C2
5	C	1406	NAG	C8-C7-N2-C2
5	C	1406	NAG	O7-C7-N2-C2
5	C	1407	NAG	C8-C7-N2-C2
5	C	1407	NAG	O7-C7-N2-C2
5	C	1411	NAG	C8-C7-N2-C2
5	C	1411	NAG	O7-C7-N2-C2
5	C	1403	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

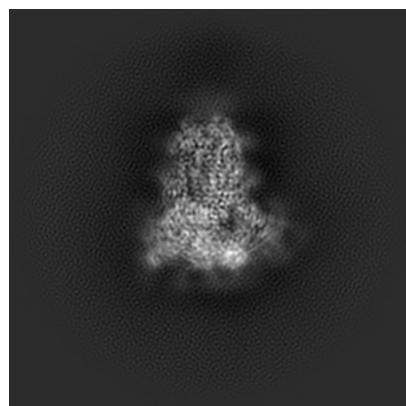
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73294. These allow visual inspection of the internal detail of the map and identification of artifacts.

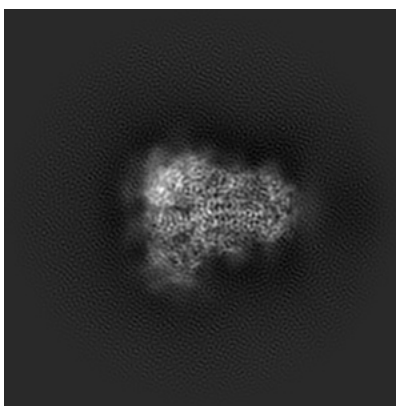
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

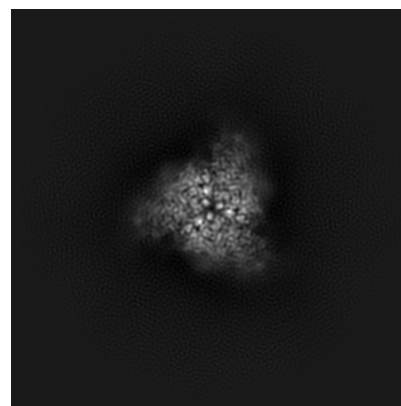
6.1.1 Primary map



X

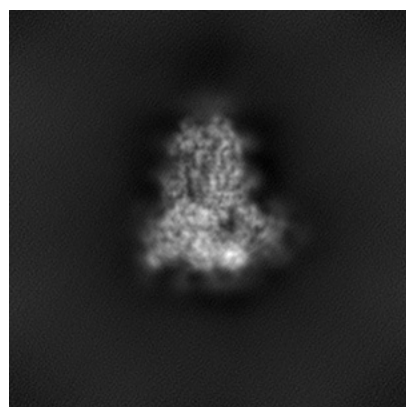


Y

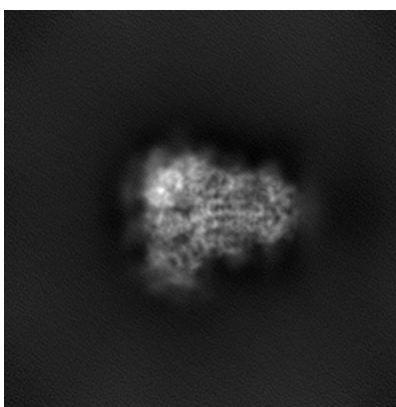


Z

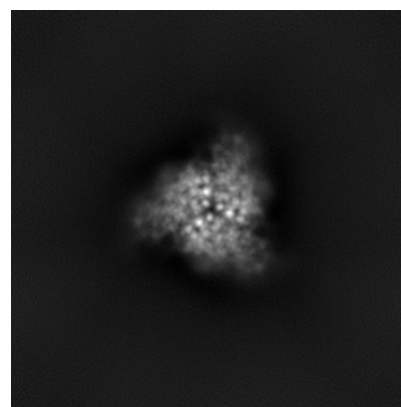
6.1.2 Raw map



X



Y

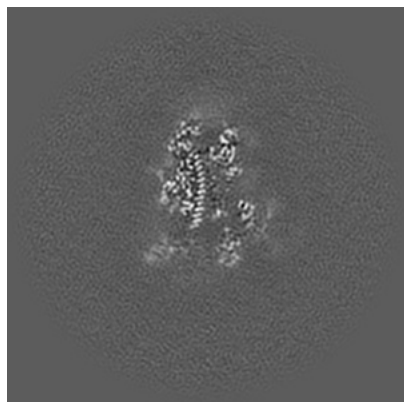


Z

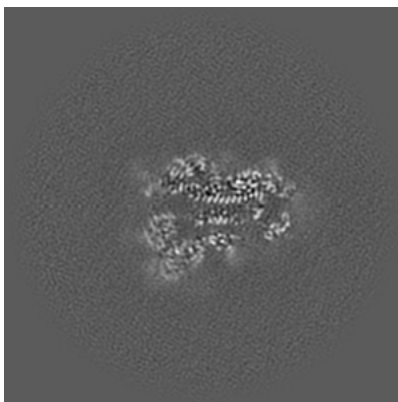
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

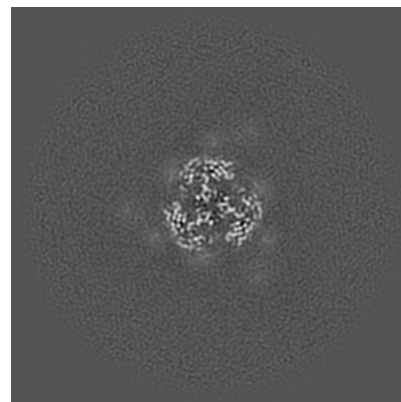
6.2.1 Primary map



X Index: 128

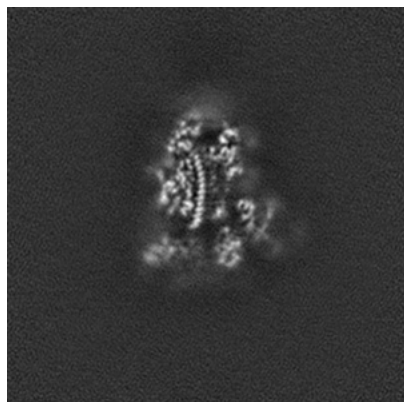


Y Index: 128

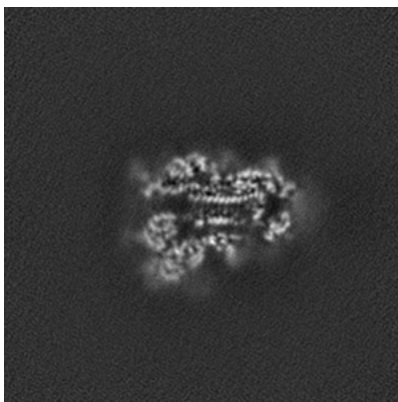


Z Index: 128

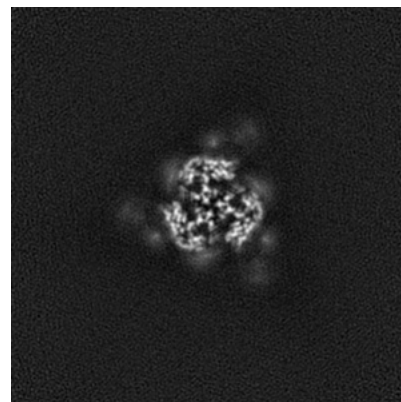
6.2.2 Raw map



X Index: 128



Y Index: 128

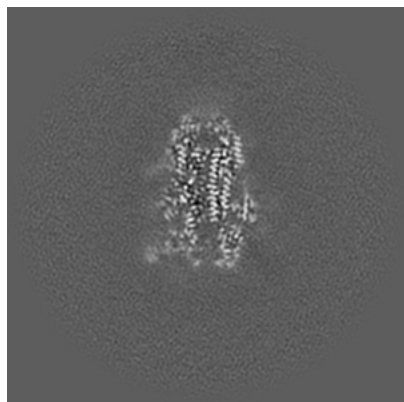


Z Index: 128

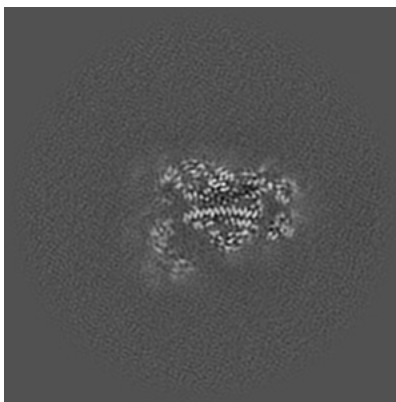
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

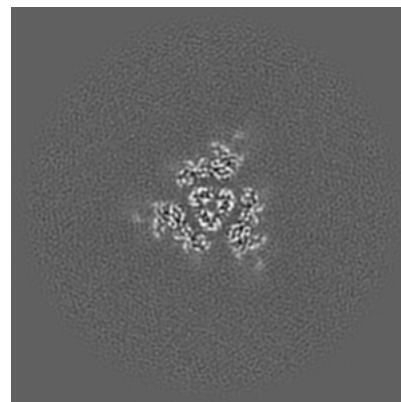
6.3.1 Primary map



X Index: 124

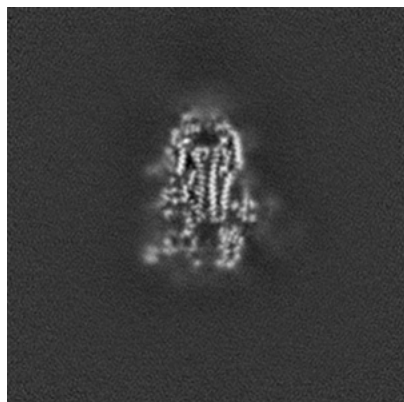


Y Index: 132

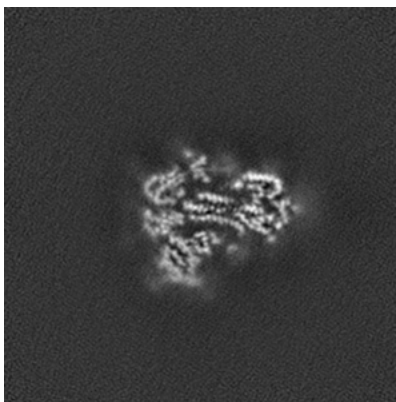


Z Index: 123

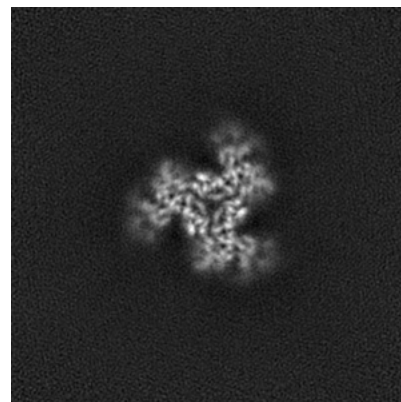
6.3.2 Raw map



X Index: 125



Y Index: 121

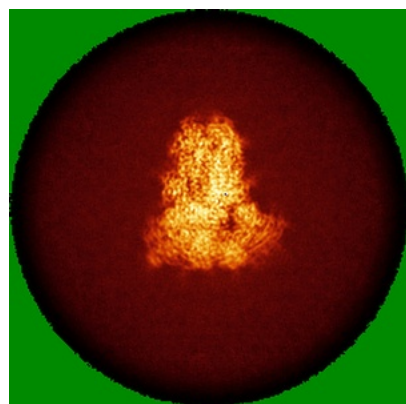


Z Index: 100

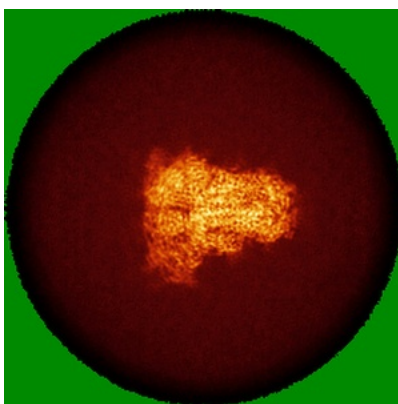
The images above show the largest variance slices of the map in three orthogonal directions.

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

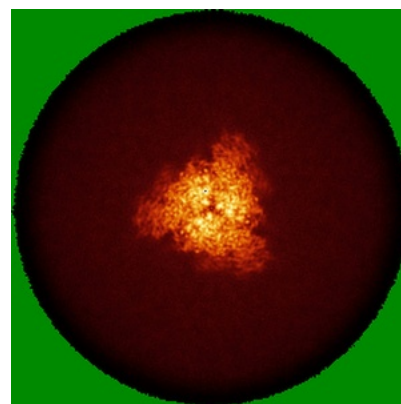
6.4.1 Primary map



X

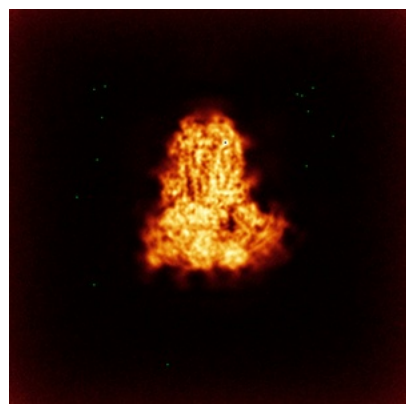


Y

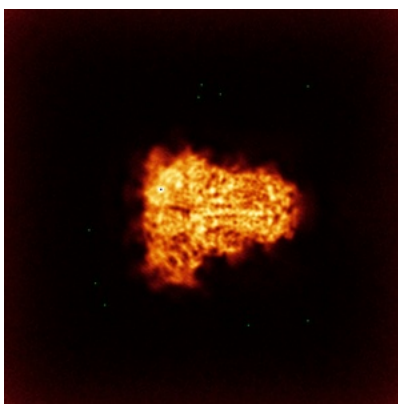


Z

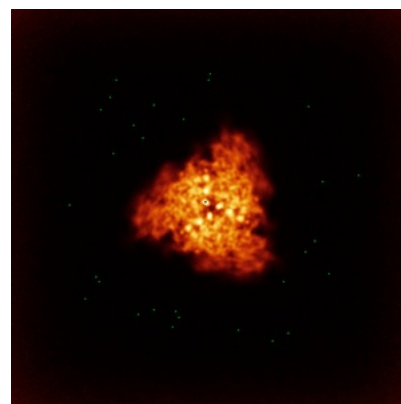
6.4.2 Raw map



X



Y

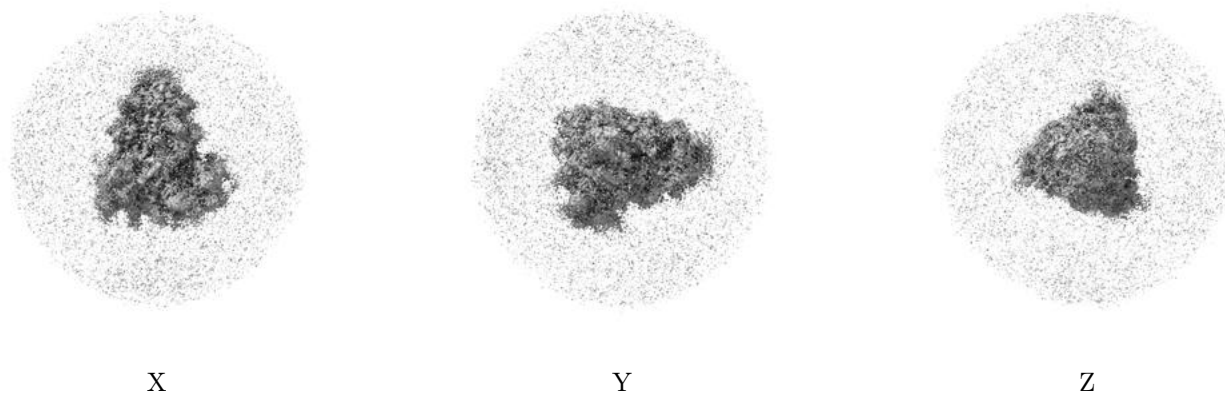


Z

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

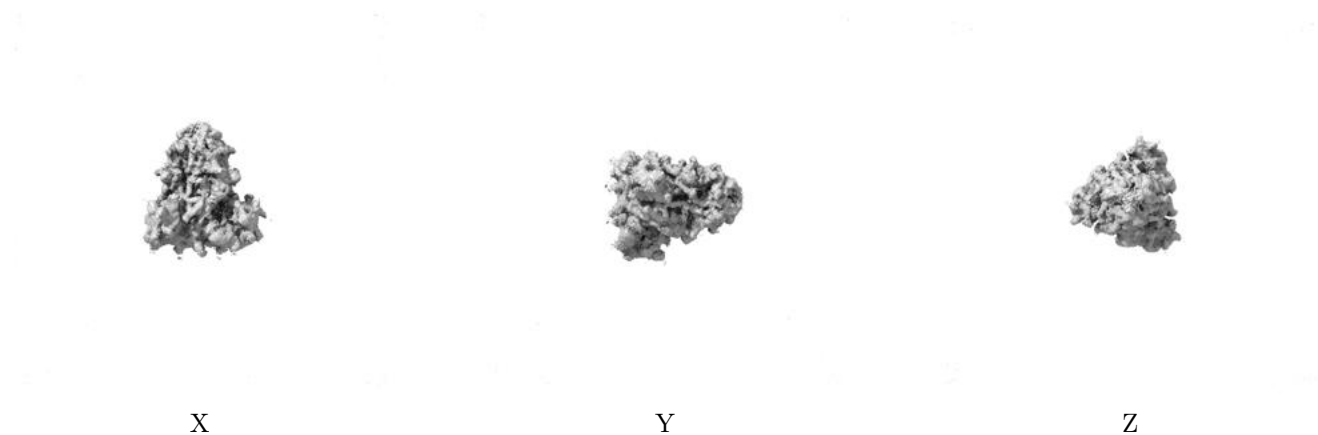
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.181. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

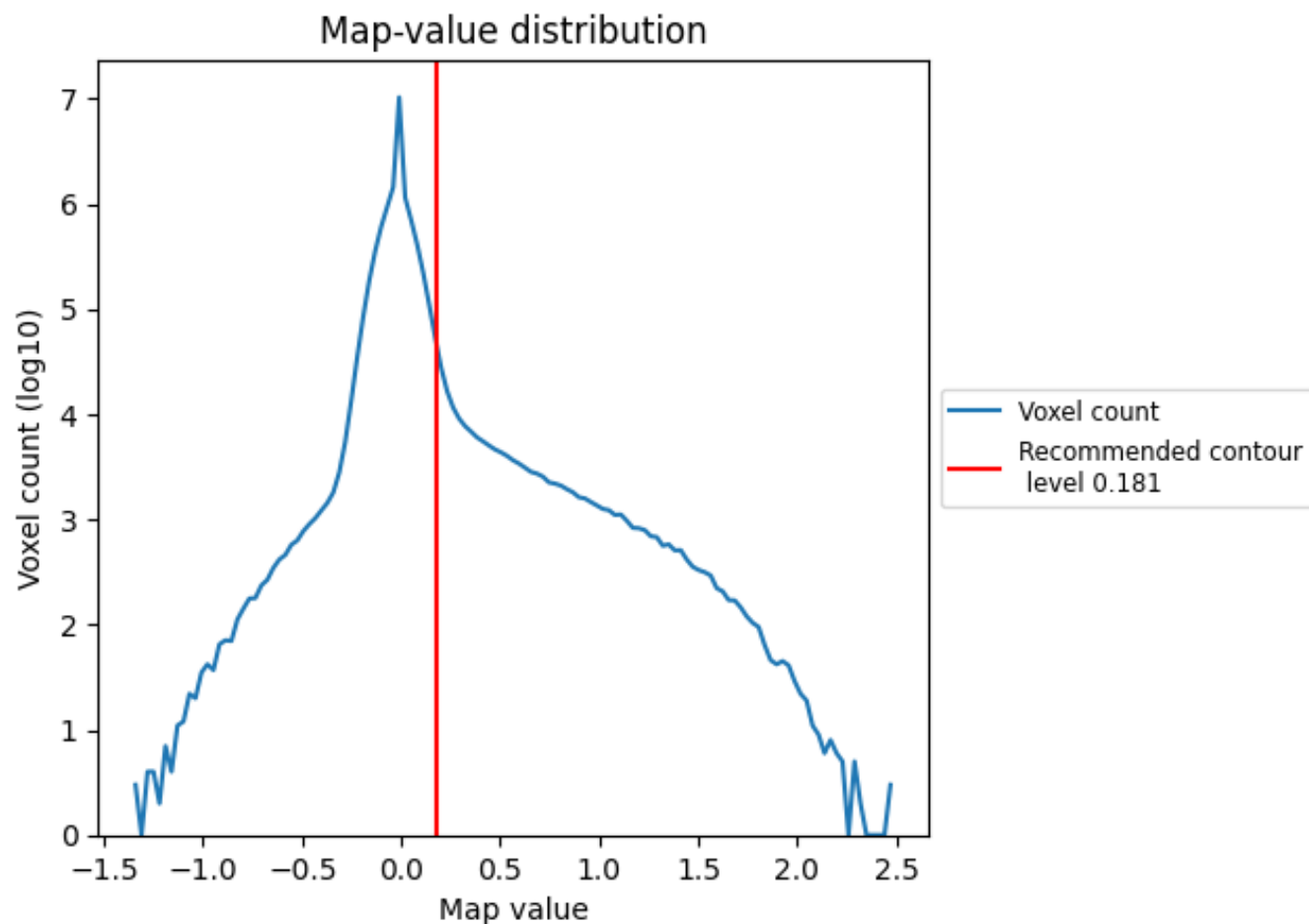
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

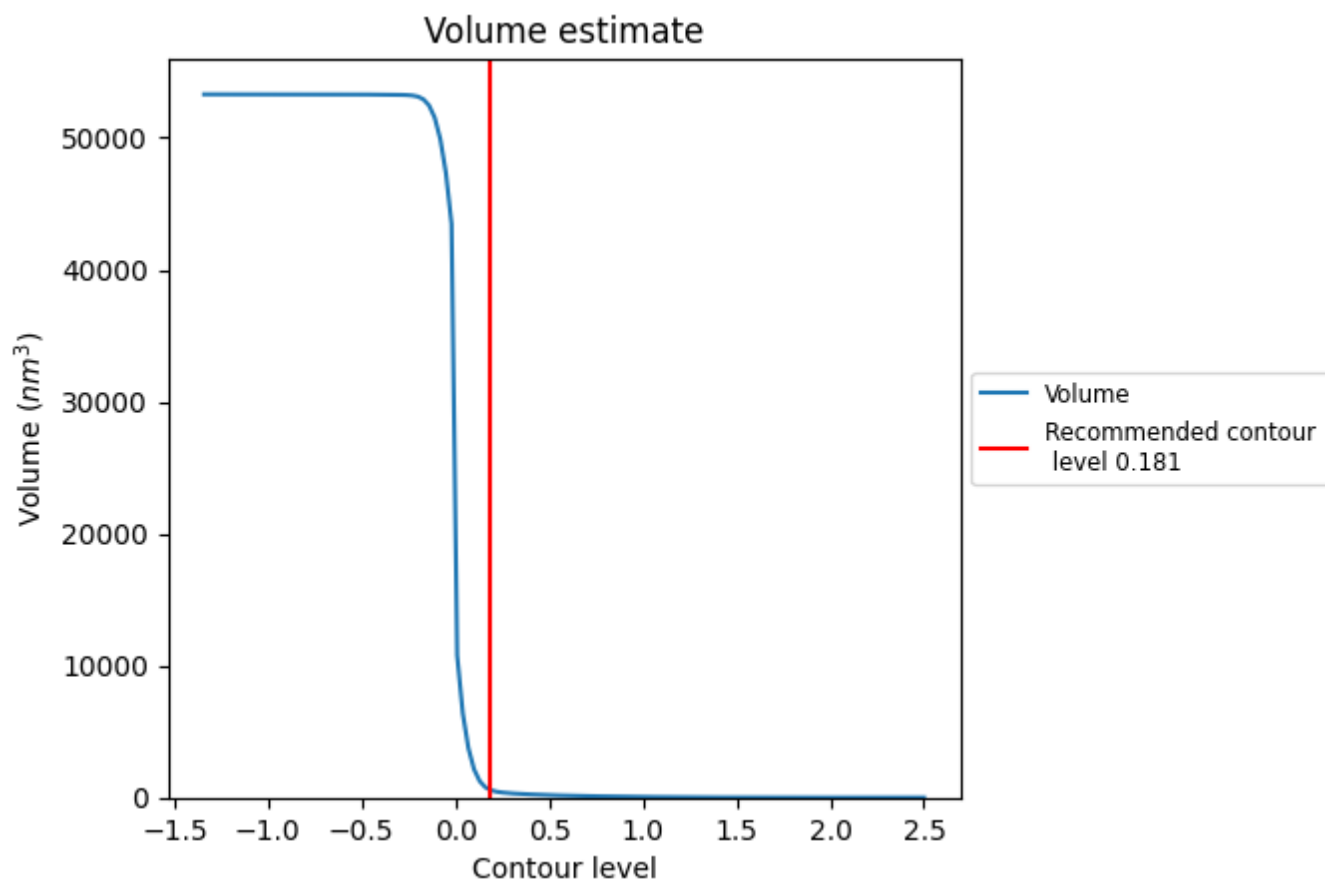
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

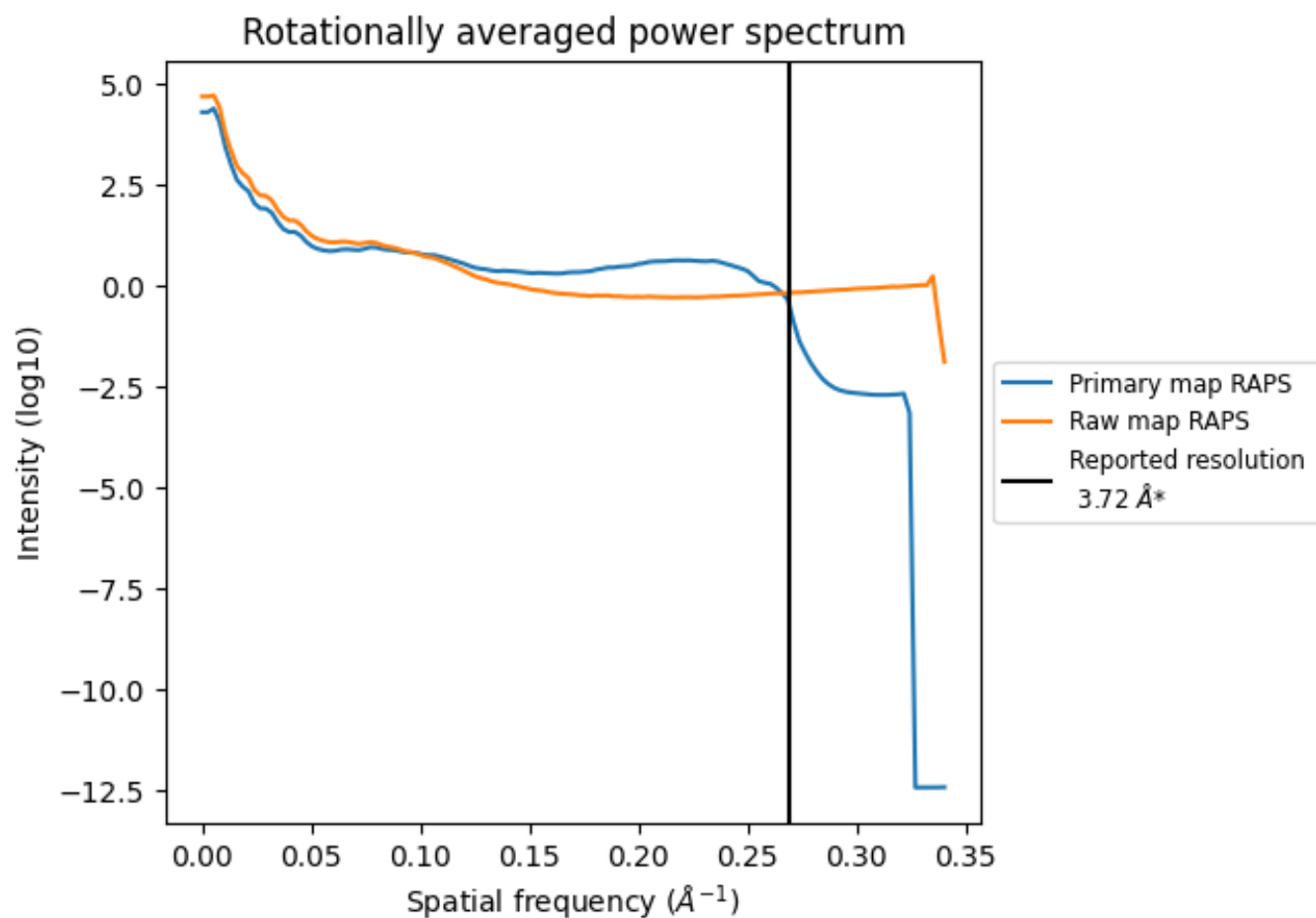
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 623 nm^3 ; this corresponds to an approximate mass of 563 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 ⓘ

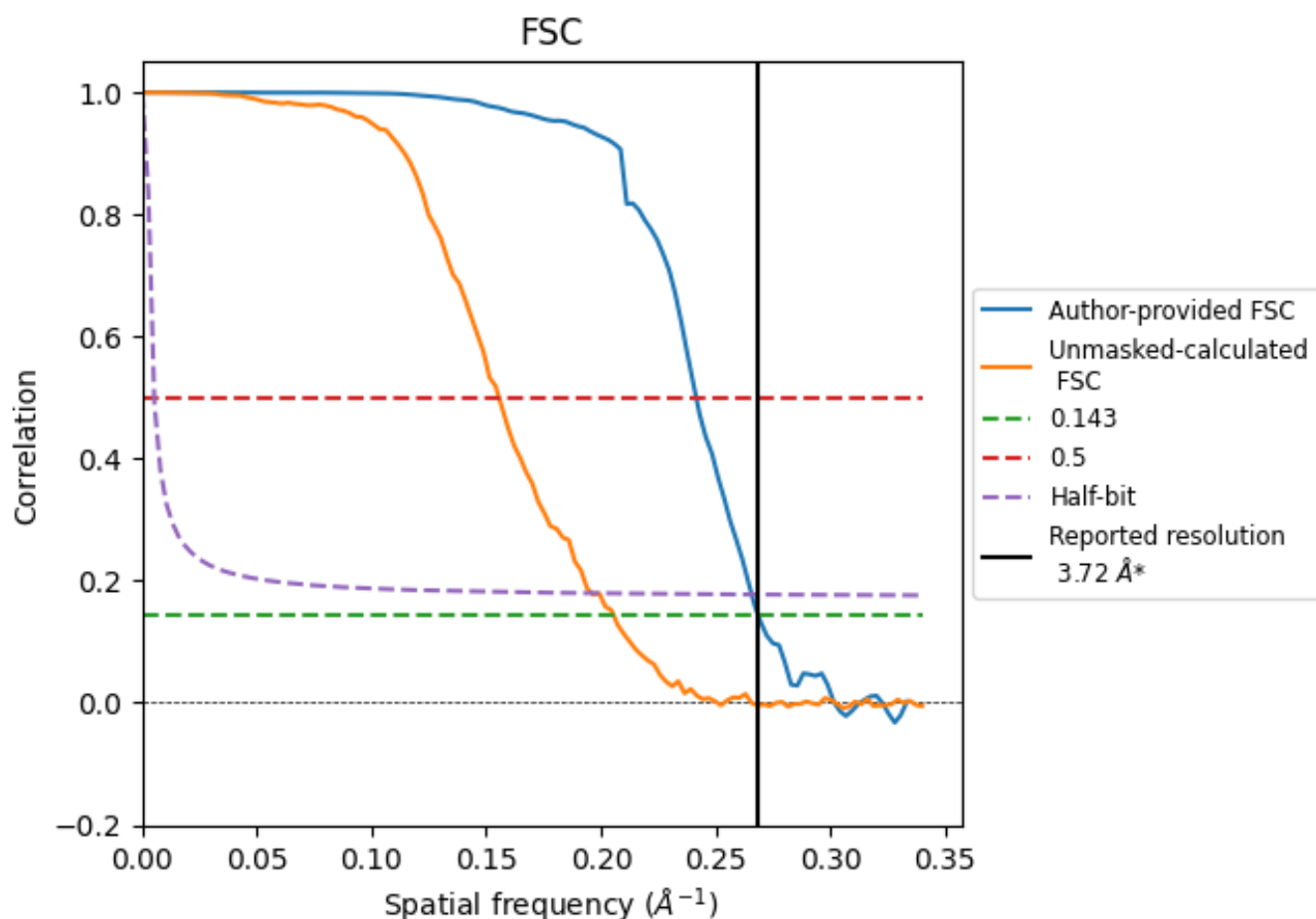


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.269 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

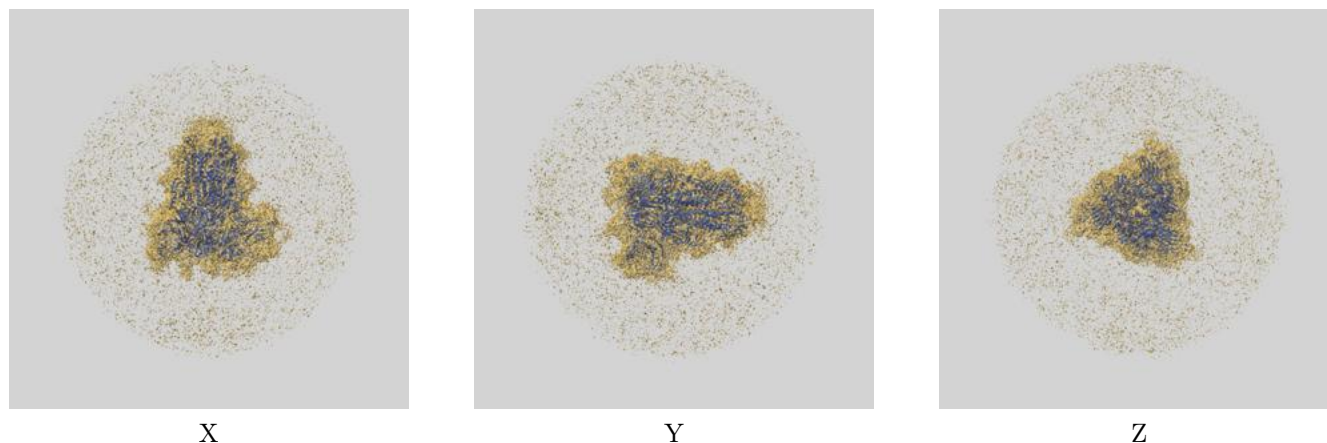
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.72	4.14	3.76
Unmasked-calculated*	4.86	6.43	5.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.86 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

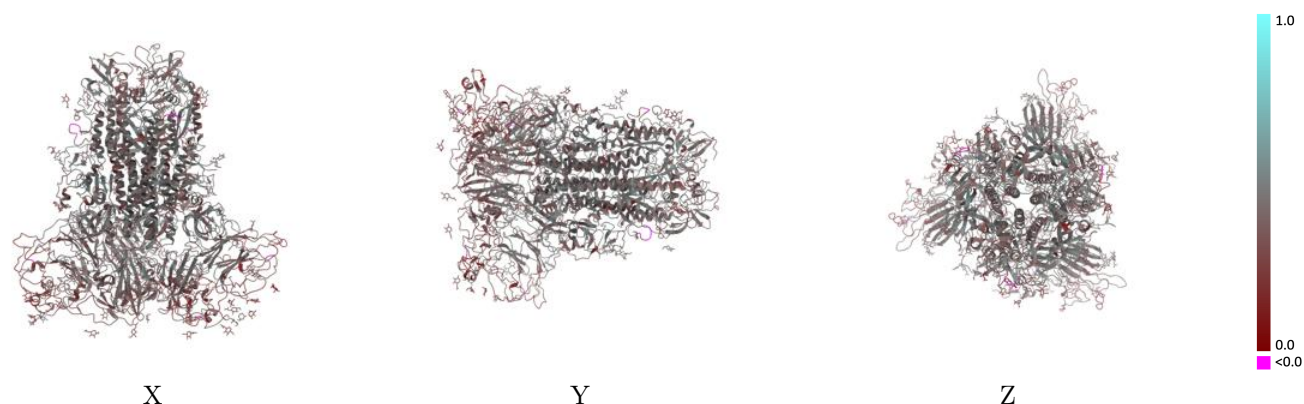
This section contains information regarding the fit between EMDB map EMD-73294 and PDB model 9YPD. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



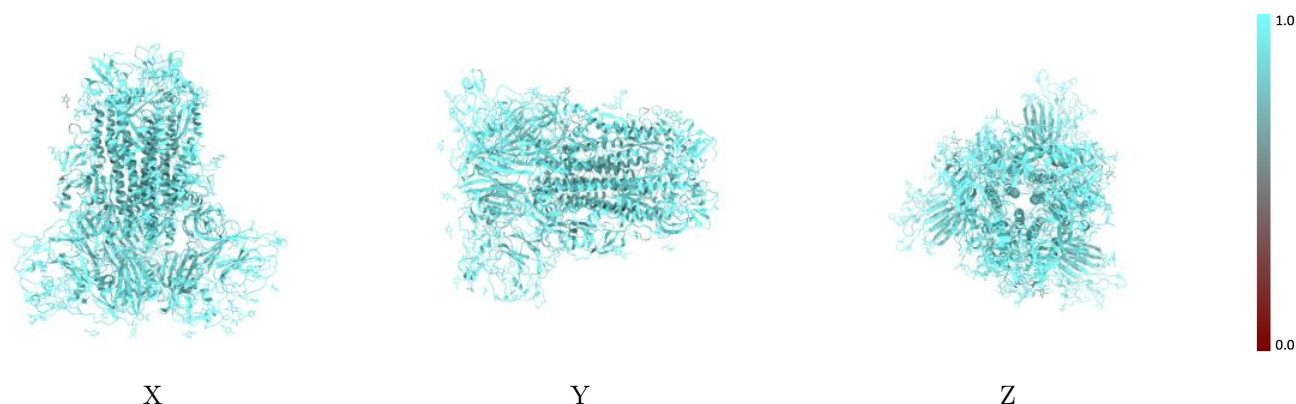
The images above show the 3D surface view of the map at the recommended contour level 0.181 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



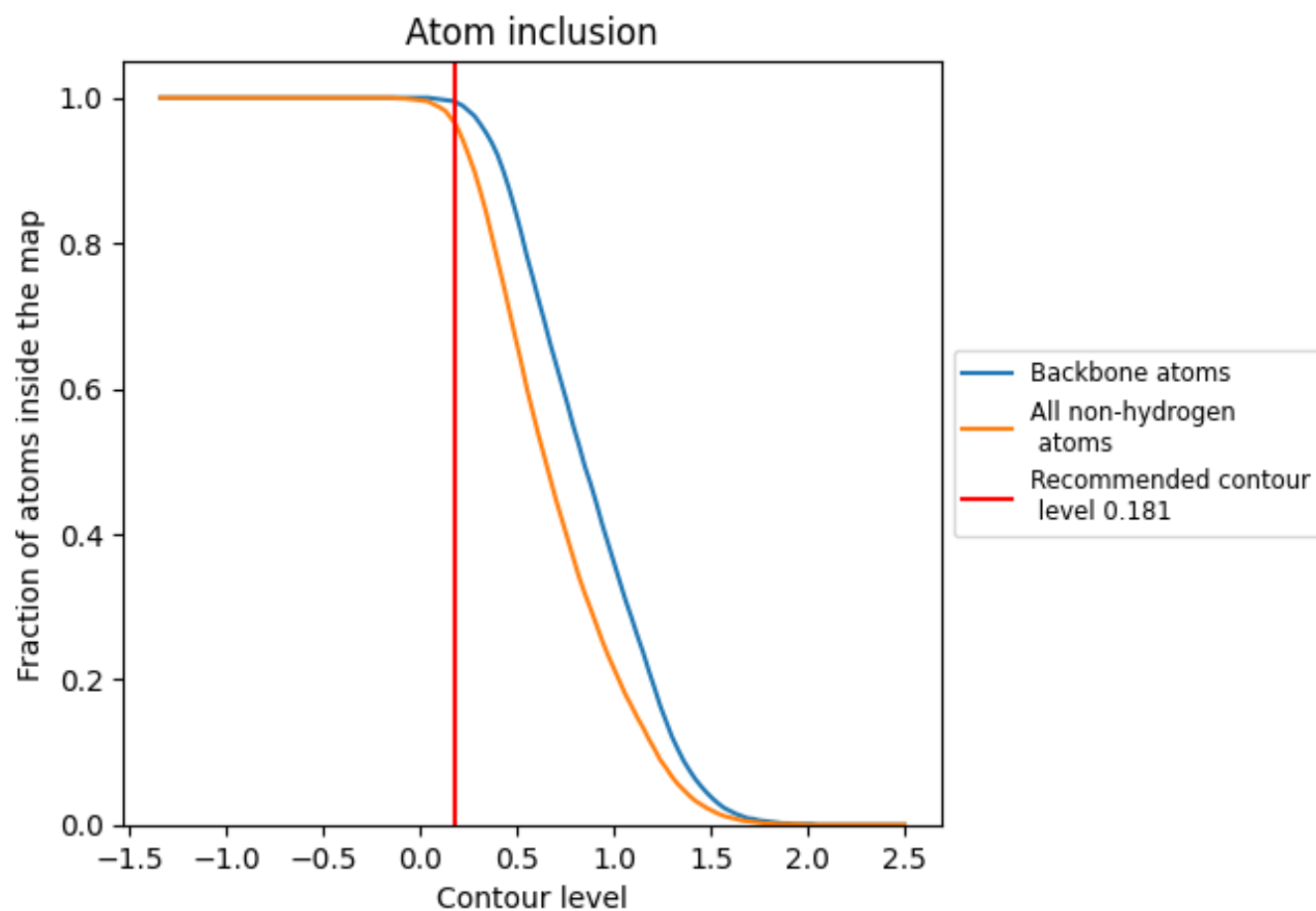
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.181).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.181) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4040
A	 0.9650	 0.4060
B	 0.9630	 0.4040
C	 0.9660	 0.4060
D	 1.0000	 0.4210
E	 1.0000	 0.4070
F	 0.8210	 0.2890
G	 0.9290	 0.3670
H	 0.9340	 0.3500
I	 0.9290	 0.3970
J	 0.9740	 0.4060
K	 0.8720	 0.2950
L	 0.9640	 0.4100
M	 1.0000	 0.3960
N	 1.0000	 0.4150
O	 0.8930	 0.2760
P	 0.8570	 0.3490
Q	 0.9840	 0.3640
R	 0.9290	 0.3990
S	 0.9740	 0.3950
T	 0.9490	 0.3570
U	 0.9640	 0.4370
V	 1.0000	 0.4050
W	 1.0000	 0.3740
X	 0.8210	 0.2760
Y	 0.8210	 0.3570
Z	 0.9510	 0.3600
a	 0.9290	 0.3830
b	 1.0000	 0.4240
c	 0.8720	 0.2850
d	 0.9640	 0.4300
e	 1.0000	 0.4050

