



## Full wwPDB EM Validation Report ⓘ

May 10, 2025 – 01:45 PM EDT

PDB ID : 9BSY / pdb\_00009bsy  
EMDB ID : EMD-44876  
Title : Cryo-EM structure of HCoV-HKU1 glycoprotein in complex with 9O-acetyl GD3 sialoglycan (DAU state)  
Authors : Jin, M.; Rini, J.M.  
Deposited on : 2024-05-14  
Resolution : 2.58 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

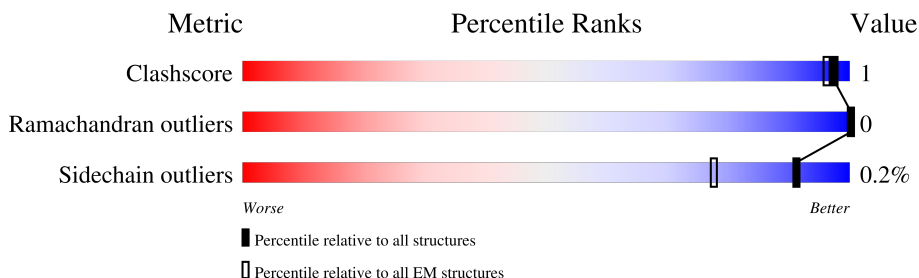
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



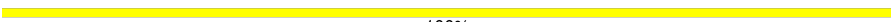

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1348	<div> <div>5%</div> <div>87%</div> <div>11%</div> </div>
1	B	1348	<div> <div>86%</div> <div>11%</div> </div>
1	C	1348	<div> <div>86%</div> <div>11%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	G	2	<div> <div>100%</div> </div>
2	H	2	<div> <div>100%</div> </div>
2	I	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
3	F	5	 100%
3	Q	5	 100%
4	P	3	 100%
4	R	3	 100%
4	V	3	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29304 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	1194	Total	C	N	O	S	0	0
			9369	5977	1535	1799	58		
1	B	1194	Total	C	N	O	S	0	0
			9369	5977	1535	1799	58		
1	C	1194	Total	C	N	O	S	0	0
			9369	5977	1535	1799	58		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	PRO	THR	conflict	UNP Q5MQD0
A	1071	PRO	ALA	conflict	UNP Q5MQD0
A	1072	PRO	LEU	conflict	UNP Q5MQD0
A	1299	SER	-	expression tag	UNP Q5MQD0
A	1300	GLY	-	expression tag	UNP Q5MQD0
A	1301	GLY	-	expression tag	UNP Q5MQD0
A	1302	TYR	-	expression tag	UNP Q5MQD0
A	1303	ILE	-	expression tag	UNP Q5MQD0
A	1304	PRO	-	expression tag	UNP Q5MQD0
A	1305	GLU	-	expression tag	UNP Q5MQD0
A	1306	ALA	-	expression tag	UNP Q5MQD0
A	1307	PRO	-	expression tag	UNP Q5MQD0
A	1308	ARG	-	expression tag	UNP Q5MQD0
A	1309	ASP	-	expression tag	UNP Q5MQD0
A	1310	GLY	-	expression tag	UNP Q5MQD0
A	1311	GLN	-	expression tag	UNP Q5MQD0
A	1312	ALA	-	expression tag	UNP Q5MQD0
A	1313	TYR	-	expression tag	UNP Q5MQD0
A	1314	VAL	-	expression tag	UNP Q5MQD0
A	1315	ARG	-	expression tag	UNP Q5MQD0
A	1316	LYS	-	expression tag	UNP Q5MQD0
A	1317	ASP	-	expression tag	UNP Q5MQD0
A	1318	GLY	-	expression tag	UNP Q5MQD0
A	1319	GLU	-	expression tag	UNP Q5MQD0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1320	TRP	-	expression tag	UNP Q5MQD0
A	1321	VAL	-	expression tag	UNP Q5MQD0
A	1322	LEU	-	expression tag	UNP Q5MQD0
A	1323	LEU	-	expression tag	UNP Q5MQD0
A	1324	SER	-	expression tag	UNP Q5MQD0
A	1325	THR	-	expression tag	UNP Q5MQD0
A	1326	PHE	-	expression tag	UNP Q5MQD0
A	1327	LEU	-	expression tag	UNP Q5MQD0
A	1328	ASN	-	expression tag	UNP Q5MQD0
A	1329	SER	-	expression tag	UNP Q5MQD0
A	1330	GLY	-	expression tag	UNP Q5MQD0
A	1331	ARG	-	expression tag	UNP Q5MQD0
A	1332	ALA	-	expression tag	UNP Q5MQD0
A	1333	HIS	-	expression tag	UNP Q5MQD0
A	1334	HIS	-	expression tag	UNP Q5MQD0
A	1335	HIS	-	expression tag	UNP Q5MQD0
A	1336	HIS	-	expression tag	UNP Q5MQD0
A	1337	HIS	-	expression tag	UNP Q5MQD0
A	1338	HIS	-	expression tag	UNP Q5MQD0
A	1339	GLY	-	expression tag	UNP Q5MQD0
A	1340	ALA	-	expression tag	UNP Q5MQD0
A	1341	GLY	-	expression tag	UNP Q5MQD0
A	1342	GLY	-	expression tag	UNP Q5MQD0
A	1343	LEU	-	expression tag	UNP Q5MQD0
A	1344	ASN	-	expression tag	UNP Q5MQD0
A	1345	ASP	-	expression tag	UNP Q5MQD0
A	1346	ILE	-	expression tag	UNP Q5MQD0
A	1347	PHE	-	expression tag	UNP Q5MQD0
A	1348	GLU	-	expression tag	UNP Q5MQD0
A	1349	ALA	-	expression tag	UNP Q5MQD0
A	1350	GLN	-	expression tag	UNP Q5MQD0
A	1351	LYS	-	expression tag	UNP Q5MQD0
A	1352	ILE	-	expression tag	UNP Q5MQD0
A	1353	GLU	-	expression tag	UNP Q5MQD0
A	1354	TRP	-	expression tag	UNP Q5MQD0
A	1355	HIS	-	expression tag	UNP Q5MQD0
A	1356	GLU	-	expression tag	UNP Q5MQD0
A	1357	ASP	-	expression tag	UNP Q5MQD0
A	1358	THR	-	expression tag	UNP Q5MQD0
A	1359	ALA	-	expression tag	UNP Q5MQD0
A	1360	ALA	-	expression tag	UNP Q5MQD0
A	1361	ALA	-	expression tag	UNP Q5MQD0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1026	PRO	THR	conflict	UNP Q5MQD0
B	1071	PRO	ALA	conflict	UNP Q5MQD0
B	1072	PRO	LEU	conflict	UNP Q5MQD0
B	1299	SER	-	expression tag	UNP Q5MQD0
B	1300	GLY	-	expression tag	UNP Q5MQD0
B	1301	GLY	-	expression tag	UNP Q5MQD0
B	1302	TYR	-	expression tag	UNP Q5MQD0
B	1303	ILE	-	expression tag	UNP Q5MQD0
B	1304	PRO	-	expression tag	UNP Q5MQD0
B	1305	GLU	-	expression tag	UNP Q5MQD0
B	1306	ALA	-	expression tag	UNP Q5MQD0
B	1307	PRO	-	expression tag	UNP Q5MQD0
B	1308	ARG	-	expression tag	UNP Q5MQD0
B	1309	ASP	-	expression tag	UNP Q5MQD0
B	1310	GLY	-	expression tag	UNP Q5MQD0
B	1311	GLN	-	expression tag	UNP Q5MQD0
B	1312	ALA	-	expression tag	UNP Q5MQD0
B	1313	TYR	-	expression tag	UNP Q5MQD0
B	1314	VAL	-	expression tag	UNP Q5MQD0
B	1315	ARG	-	expression tag	UNP Q5MQD0
B	1316	LYS	-	expression tag	UNP Q5MQD0
B	1317	ASP	-	expression tag	UNP Q5MQD0
B	1318	GLY	-	expression tag	UNP Q5MQD0
B	1319	GLU	-	expression tag	UNP Q5MQD0
B	1320	TRP	-	expression tag	UNP Q5MQD0
B	1321	VAL	-	expression tag	UNP Q5MQD0
B	1322	LEU	-	expression tag	UNP Q5MQD0
B	1323	LEU	-	expression tag	UNP Q5MQD0
B	1324	SER	-	expression tag	UNP Q5MQD0
B	1325	THR	-	expression tag	UNP Q5MQD0
B	1326	PHE	-	expression tag	UNP Q5MQD0
B	1327	LEU	-	expression tag	UNP Q5MQD0
B	1328	ASN	-	expression tag	UNP Q5MQD0
B	1329	SER	-	expression tag	UNP Q5MQD0
B	1330	GLY	-	expression tag	UNP Q5MQD0
B	1331	ARG	-	expression tag	UNP Q5MQD0
B	1332	ALA	-	expression tag	UNP Q5MQD0
B	1333	HIS	-	expression tag	UNP Q5MQD0
B	1334	HIS	-	expression tag	UNP Q5MQD0
B	1335	HIS	-	expression tag	UNP Q5MQD0
B	1336	HIS	-	expression tag	UNP Q5MQD0
B	1337	HIS	-	expression tag	UNP Q5MQD0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1338	HIS	-	expression tag	UNP Q5MQD0
B	1339	GLY	-	expression tag	UNP Q5MQD0
B	1340	ALA	-	expression tag	UNP Q5MQD0
B	1341	GLY	-	expression tag	UNP Q5MQD0
B	1342	GLY	-	expression tag	UNP Q5MQD0
B	1343	LEU	-	expression tag	UNP Q5MQD0
B	1344	ASN	-	expression tag	UNP Q5MQD0
B	1345	ASP	-	expression tag	UNP Q5MQD0
B	1346	ILE	-	expression tag	UNP Q5MQD0
B	1347	PHE	-	expression tag	UNP Q5MQD0
B	1348	GLU	-	expression tag	UNP Q5MQD0
B	1349	ALA	-	expression tag	UNP Q5MQD0
B	1350	GLN	-	expression tag	UNP Q5MQD0
B	1351	LYS	-	expression tag	UNP Q5MQD0
B	1352	ILE	-	expression tag	UNP Q5MQD0
B	1353	GLU	-	expression tag	UNP Q5MQD0
B	1354	TRP	-	expression tag	UNP Q5MQD0
B	1355	HIS	-	expression tag	UNP Q5MQD0
B	1356	GLU	-	expression tag	UNP Q5MQD0
B	1357	ASP	-	expression tag	UNP Q5MQD0
B	1358	THR	-	expression tag	UNP Q5MQD0
B	1359	ALA	-	expression tag	UNP Q5MQD0
B	1360	ALA	-	expression tag	UNP Q5MQD0
B	1361	ALA	-	expression tag	UNP Q5MQD0
C	1026	PRO	THR	conflict	UNP Q5MQD0
C	1071	PRO	ALA	conflict	UNP Q5MQD0
C	1072	PRO	LEU	conflict	UNP Q5MQD0
C	1299	SER	-	expression tag	UNP Q5MQD0
C	1300	GLY	-	expression tag	UNP Q5MQD0
C	1301	GLY	-	expression tag	UNP Q5MQD0
C	1302	TYR	-	expression tag	UNP Q5MQD0
C	1303	ILE	-	expression tag	UNP Q5MQD0
C	1304	PRO	-	expression tag	UNP Q5MQD0
C	1305	GLU	-	expression tag	UNP Q5MQD0
C	1306	ALA	-	expression tag	UNP Q5MQD0
C	1307	PRO	-	expression tag	UNP Q5MQD0
C	1308	ARG	-	expression tag	UNP Q5MQD0
C	1309	ASP	-	expression tag	UNP Q5MQD0
C	1310	GLY	-	expression tag	UNP Q5MQD0
C	1311	GLN	-	expression tag	UNP Q5MQD0
C	1312	ALA	-	expression tag	UNP Q5MQD0
C	1313	TYR	-	expression tag	UNP Q5MQD0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1314	VAL	-	expression tag	UNP Q5MQD0
C	1315	ARG	-	expression tag	UNP Q5MQD0
C	1316	LYS	-	expression tag	UNP Q5MQD0
C	1317	ASP	-	expression tag	UNP Q5MQD0
C	1318	GLY	-	expression tag	UNP Q5MQD0
C	1319	GLU	-	expression tag	UNP Q5MQD0
C	1320	TRP	-	expression tag	UNP Q5MQD0
C	1321	VAL	-	expression tag	UNP Q5MQD0
C	1322	LEU	-	expression tag	UNP Q5MQD0
C	1323	LEU	-	expression tag	UNP Q5MQD0
C	1324	SER	-	expression tag	UNP Q5MQD0
C	1325	THR	-	expression tag	UNP Q5MQD0
C	1326	PHE	-	expression tag	UNP Q5MQD0
C	1327	LEU	-	expression tag	UNP Q5MQD0
C	1328	ASN	-	expression tag	UNP Q5MQD0
C	1329	SER	-	expression tag	UNP Q5MQD0
C	1330	GLY	-	expression tag	UNP Q5MQD0
C	1331	ARG	-	expression tag	UNP Q5MQD0
C	1332	ALA	-	expression tag	UNP Q5MQD0
C	1333	HIS	-	expression tag	UNP Q5MQD0
C	1334	HIS	-	expression tag	UNP Q5MQD0
C	1335	HIS	-	expression tag	UNP Q5MQD0
C	1336	HIS	-	expression tag	UNP Q5MQD0
C	1337	HIS	-	expression tag	UNP Q5MQD0
C	1338	HIS	-	expression tag	UNP Q5MQD0
C	1339	GLY	-	expression tag	UNP Q5MQD0
C	1340	ALA	-	expression tag	UNP Q5MQD0
C	1341	GLY	-	expression tag	UNP Q5MQD0
C	1342	GLY	-	expression tag	UNP Q5MQD0
C	1343	LEU	-	expression tag	UNP Q5MQD0
C	1344	ASN	-	expression tag	UNP Q5MQD0
C	1345	ASP	-	expression tag	UNP Q5MQD0
C	1346	ILE	-	expression tag	UNP Q5MQD0
C	1347	PHE	-	expression tag	UNP Q5MQD0
C	1348	GLU	-	expression tag	UNP Q5MQD0
C	1349	ALA	-	expression tag	UNP Q5MQD0
C	1350	GLN	-	expression tag	UNP Q5MQD0
C	1351	LYS	-	expression tag	UNP Q5MQD0
C	1352	ILE	-	expression tag	UNP Q5MQD0
C	1353	GLU	-	expression tag	UNP Q5MQD0
C	1354	TRP	-	expression tag	UNP Q5MQD0
C	1355	HIS	-	expression tag	UNP Q5MQD0

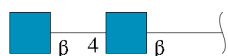
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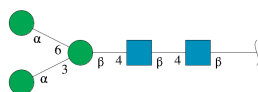
Chain	Residue	Modelled	Actual	Comment	Reference
C	1356	GLU	-	expression tag	UNP Q5MQD0
C	1357	ASP	-	expression tag	UNP Q5MQD0
C	1358	THR	-	expression tag	UNP Q5MQD0
C	1359	ALA	-	expression tag	UNP Q5MQD0
C	1360	ALA	-	expression tag	UNP Q5MQD0
C	1361	ALA	-	expression tag	UNP Q5MQD0

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



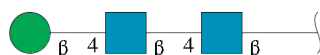
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16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



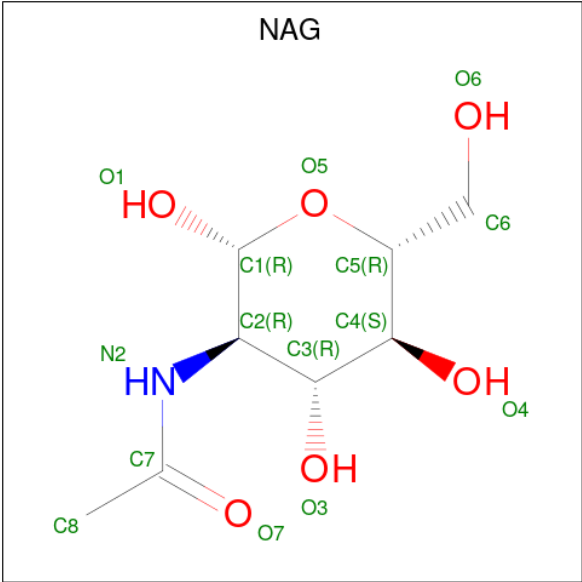
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	5	Total	C	N	O	0	0
			61	34	2	25		
3	Q	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	P	3	Total	C	N	O	0	0
			39	22	2	15		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	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<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



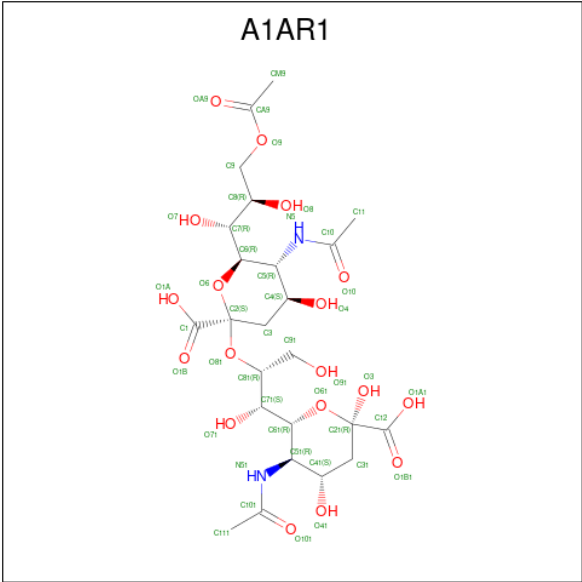
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

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

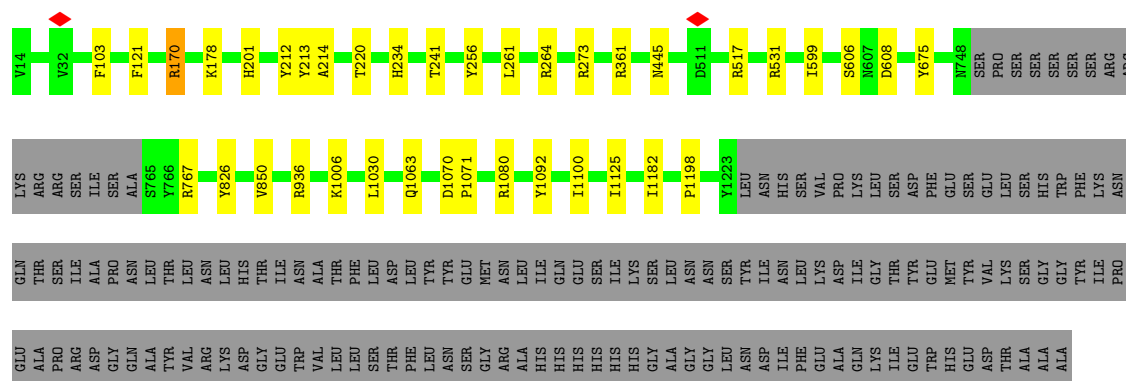
- Molecule 6 is 5-acetamido-8-O-(5-acetamido-9-O-acetyl-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranonosyl)-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid (CCD ID: A1AR1) (formula: C<sub>24</sub>H<sub>38</sub>N<sub>2</sub>O<sub>18</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			44	24	2	18	
6	B	1	Total	C	N	O	0
			44	24	2	18	
6	C	1	Total	C	N	O	0
			44	24	2	18	



Chain C:  86% 11%

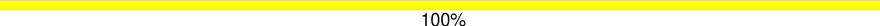


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

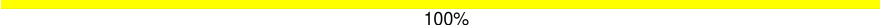
NAG1  
NAG2

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

Chain E:  100%

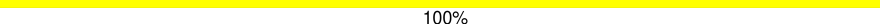
NAG1  
NAG2

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

Chain G:  100%

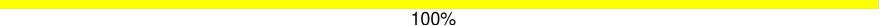
NAG1  
NAG2

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

Chain H:  100%

NAG1  
NAG2

- 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 J:  100%MAG1  
MAG2

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

Chain K:  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 S:  100%

MAG1  
MAG2

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

Chain T:  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 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 F:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- 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%


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 P:  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 R:  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 V:  100%

MAG1  
MAG2  
BMA3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	158150	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 ( $e^-/\text{\AA}^2$ )	36	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.993	Depositor
Minimum map value	-0.631	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	362.56, 362.56, 362.56	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.03, 1.03, 1.03	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, A1AR1

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	0.70	2/9603 (0.0%)	1.19	7/13073 (0.1%)
1	B	0.68	0/9603	1.19	11/13073 (0.1%)
1	C	0.66	0/9603	1.16	13/13073 (0.1%)
All	All	0.68	2/28809 (0.0%)	1.18	31/39219 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	7
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	HIS	CE1-NE2	-5.68	1.26	1.32
1	A	398	ARG	CZ-NH2	-5.36	1.26	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1125	ILE	N-CA-C	7.58	117.54	110.42
1	A	1125	ILE	N-CA-C	7.44	117.42	110.42
1	C	1125	ILE	N-CA-C	7.31	117.29	110.42
1	C	1080	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	C	517	ARG	NE-CZ-NH2	6.45	125.01	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	936	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	A	1186	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	243	ASN	N-CA-C	-5.89	103.33	111.81
1	C	1070	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	1071	PRO	N-CA-C	5.80	117.78	110.70
1	C	767	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	B	23	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	882	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	121	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	170	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	C	1071	PRO	N-CA-C	5.41	117.29	110.70
1	B	163	CYS	N-CA-CB	-5.36	101.85	110.69
1	C	234	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	C	273	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	234	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	264	ARG	N-CA-CB	-5.22	101.68	111.13
1	C	170	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	218	MET	N-CA-CB	-5.17	105.96	111.29
1	C	1063	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	366	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	445	ASN	CA-CB-CG	5.08	117.69	112.60
1	B	936	ARG	CD-NE-CZ	5.07	131.49	124.40
1	B	521	LEU	CB-CA-C	5.06	116.15	108.86
1	A	1050	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	142	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	C	445	ASN	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	TYR	Sidechain
1	A	675	TYR	Sidechain
1	B	1092	TYR	Sidechain
1	B	256	TYR	Sidechain
1	B	273	ARG	Sidechain
1	C	1092	TYR	Sidechain
1	C	256	TYR	Sidechain
1	C	264	ARG	Sidechain
1	C	361	ARG	Sidechain
1	C	531	ARG	Sidechain
1	C	675	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	826	TYR	Sidechain

## 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	9369	0	8988	12	0
1	B	9369	0	8983	13	0
1	C	9369	0	8982	9	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
3	F	61	0	52	0	0
3	Q	61	0	52	0	0
4	P	39	0	34	0	0
4	R	39	0	34	0	0
4	V	39	0	34	0	0
5	A	98	0	91	0	0
5	B	182	0	169	0	0
5	C	154	0	143	0	0
6	A	44	0	0	0	0
6	B	44	0	0	0	0
6	C	44	0	0	0	0
All	All	29304	0	27912	31	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 (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:CD1	1:A:359:LEU:HD23	2.27	0.64
1:B:866:MET:HE3	1:B:962:TYR:HA	1.82	0.62
1:A:356:LEU:HD13	1:A:359:LEU:HD23	1.83	0.60
1:C:214:ALA:HB2	1:C:220:THR:HA	1.85	0.59
1:B:80:LYS:HE3	1:B:245:ILE:HB	1.85	0.57
1:C:606:SER:OG	1:C:608:ASP:OD2	2.24	0.56
1:B:214:ALA:HB2	1:B:220:THR:HA	1.88	0.56
1:B:244:ALA:HB1	1:B:250:ASP:OD2	2.07	0.55
1:A:356:LEU:HD12	1:A:359:LEU:HB3	1.93	0.51
1:A:214:ALA:HB2	1:A:220:THR:HA	1.92	0.50
1:C:178:LYS:HA	1:C:178:LYS:HE2	1.93	0.50
1:C:1182:ILE:HD11	1:C:1198:PRO:HB3	1.94	0.49
1:A:971:MET:HG3	1:A:972:PHE:CD2	2.51	0.46
1:A:651:TYR:CE1	1:B:54:ARG:HD2	2.51	0.45
1:B:850:VAL:HG13	1:B:1100:ILE:HG13	1.99	0.45
1:A:657:ILE:H	1:A:657:ILE:HD12	1.82	0.45
1:A:1068:ARG:HD3	1:C:599:ILE:HD13	1.99	0.45
1:C:170:ARG:HD2	1:C:241:THR:HG21	2.00	0.44
1:C:201:HIS:HB2	1:C:212:TYR:HB2	2.00	0.44
1:B:866:MET:HE1	1:B:965:ALA:HB3	1.99	0.44
1:B:79:LEU:HD13	1:B:89:TRP:HB3	1.99	0.43
1:A:103:PHE:HB2	1:A:261:LEU:HD21	2.01	0.43
1:B:18:PHE:CE1	1:B:176:PHE:CD2	3.07	0.42
1:B:130:PHE:HA	1:B:136:THR:HG21	2.01	0.42
1:C:103:PHE:HB2	1:C:261:LEU:HD21	2.02	0.42
1:A:651:TYR:CD1	1:B:54:ARG:HD2	2.55	0.41
1:A:356:LEU:HD12	1:A:359:LEU:HD23	2.00	0.41
1:B:201:HIS:HB2	1:B:212:TYR:HB2	2.02	0.41
1:B:739:MET:HA	1:B:739:MET:HE2	2.02	0.41
1:C:850:VAL:HG13	1:C:1100:ILE:HG12	2.03	0.40
1:A:850:VAL:HG13	1:A:1100:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1190/1348 (88%)	1146 (96%)	44 (4%)	0	100	100
1	B	1190/1348 (88%)	1162 (98%)	28 (2%)	0	100	100
1	C	1190/1348 (88%)	1158 (97%)	32 (3%)	0	100	100
All	All	3570/4044 (88%)	3466 (97%)	104 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1073/1207 (89%)	1072 (100%)	1 (0%)	92	98
1	B	1073/1207 (89%)	1070 (100%)	3 (0%)	91	97
1	C	1073/1207 (89%)	1070 (100%)	3 (0%)	91	97
All	All	3219/3621 (89%)	3212 (100%)	7 (0%)	91	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	B	355	ASN
1	B	849	GLU
1	B	1076	VAL
1	C	213	TYR

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Mol	Chain	Res	Type
1	C	1006	LYS
1	C	1030	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	243	ASN
1	A	424	GLN
1	A	593	ASN
1	A	644	ASN
1	A	648	ASN
1	A	656	ASN
1	A	696	ASN
1	A	711	GLN
1	A	860	HIS
1	A	945	ASN
1	A	1040	ASN
1	A	1126	ASN
1	B	175	HIS
1	B	248	ASN
1	B	364	HIS
1	B	424	GLN
1	B	644	ASN
1	B	711	GLN
1	B	842	ASN
1	B	860	HIS
1	B	876	ASN
1	B	878	ASN
1	B	958	GLN
1	B	992	ASN
1	B	1004	ASN
1	B	1083	ASN
1	C	73	ASN
1	C	424	GLN
1	C	593	ASN
1	C	644	ASN
1	C	711	GLN
1	C	945	ASN
1	C	1004	ASN
1	C	1014	ASN
1	C	1045	ASN

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Mol	Chain	Res	Type
1	C	1083	ASN
1	C	1095	GLN
1	C	1126	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

47 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	1.22	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	D	2	2	14,14,15	1.27	2 (14%)	17,19,21	0.86	0
2	NAG	E	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	1.24	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	F	1	3,1	14,14,15	1.12	1 (7%)	17,19,21	0.95	0
3	NAG	F	2	3	14,14,15	1.16	1 (7%)	17,19,21	0.80	0
3	BMA	F	3	3	11,11,12	1.36	2 (18%)	15,15,17	1.25	3 (20%)
3	MAN	F	4	3	11,11,12	1.44	2 (18%)	15,15,17	0.91	1 (6%)
3	MAN	F	5	3	11,11,12	1.38	2 (18%)	15,15,17	0.99	1 (6%)
2	NAG	G	1	2,1	14,14,15	1.17	2 (14%)	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	1.26	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	H	1	2,1	14,14,15	1.23	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	H	2	2	14,14,15	1.36	3 (21%)	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	0.70	0
2	NAG	I	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.68	0
2	NAG	J	1	2,1	14,14,15	1.34	3 (21%)	17,19,21	0.71	0
2	NAG	J	2	2	14,14,15	1.29	2 (14%)	17,19,21	0.69	0
2	NAG	K	1	2,1	14,14,15	1.30	3 (21%)	17,19,21	0.81	0
2	NAG	K	2	2	14,14,15	1.40	2 (14%)	17,19,21	0.76	0
2	NAG	L	1	2,1	14,14,15	1.17	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	L	2	2	14,14,15	1.25	1 (7%)	17,19,21	1.13	1 (5%)
2	NAG	M	1	2,1	14,14,15	1.21	2 (14%)	17,19,21	0.87	1 (5%)
2	NAG	M	2	2	14,14,15	1.49	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	N	1	2,1	14,14,15	1.12	1 (7%)	17,19,21	0.83	0
2	NAG	N	2	2	14,14,15	1.14	1 (7%)	17,19,21	0.68	0
2	NAG	O	1	2,1	14,14,15	1.18	1 (7%)	17,19,21	0.62	0
2	NAG	O	2	2	14,14,15	1.24	1 (7%)	17,19,21	0.83	0
4	NAG	P	1	1,4	14,14,15	1.17	1 (7%)	17,19,21	0.62	0
4	NAG	P	2	4	14,14,15	1.24	2 (14%)	17,19,21	1.22	1 (5%)
4	BMA	P	3	4	11,11,12	1.21	1 (9%)	15,15,17	0.86	1 (6%)
3	NAG	Q	1	3,1	14,14,15	1.08	1 (7%)	17,19,21	1.01	0
3	NAG	Q	2	3	14,14,15	1.22	1 (7%)	17,19,21	0.77	1 (5%)
3	BMA	Q	3	3	11,11,12	1.42	3 (27%)	15,15,17	0.81	1 (6%)
3	MAN	Q	4	3	11,11,12	1.37	2 (18%)	15,15,17	1.17	1 (6%)
3	MAN	Q	5	3	11,11,12	1.38	2 (18%)	15,15,17	0.99	1 (6%)
4	NAG	R	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	0.56	0
4	NAG	R	2	4	14,14,15	1.27	2 (14%)	17,19,21	0.90	1 (5%)
4	BMA	R	3	4	11,11,12	1.23	1 (9%)	15,15,17	0.94	1 (6%)
2	NAG	S	1	2,1	14,14,15	1.21	2 (14%)	17,19,21	0.85	1 (5%)
2	NAG	S	2	2	14,14,15	1.28	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	T	1	2,1	14,14,15	1.20	1 (7%)	17,19,21	0.78	0
2	NAG	T	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.84	1 (5%)
2	NAG	U	1	2,1	14,14,15	1.18	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	U	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.63	0
4	NAG	V	1	1,4	14,14,15	1.11	2 (14%)	17,19,21	0.75	1 (5%)
4	NAG	V	2	4	14,14,15	1.33	4 (28%)	17,19,21	0.66	0
4	BMA	V	3	4	11,11,12	1.22	1 (9%)	15,15,17	0.72	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	MAN	O5-C5	3.32	1.49	1.43
2	K	2	NAG	O5-C5	3.12	1.49	1.43
3	F	5	MAN	O5-C5	3.11	1.49	1.43
2	M	2	NAG	C1-C2	3.07	1.56	1.52
3	Q	4	MAN	O5-C5	3.05	1.49	1.43
2	D	2	NAG	O5-C5	3.05	1.49	1.43
2	G	2	NAG	O5-C5	3.03	1.49	1.43
3	Q	5	MAN	O5-C5	3.02	1.49	1.43
2	H	2	NAG	O5-C5	2.97	1.49	1.43
2	O	2	NAG	O5-C5	2.93	1.49	1.43
2	U	2	NAG	O5-C5	2.90	1.49	1.43
2	I	2	NAG	O5-C5	2.86	1.49	1.43
2	S	2	NAG	O5-C5	2.85	1.49	1.43
2	L	2	NAG	O5-C5	2.83	1.48	1.43
2	E	2	NAG	O5-C5	2.82	1.48	1.43
2	T	2	NAG	O5-C5	2.81	1.48	1.43
4	R	3	BMA	O5-C5	2.75	1.48	1.43
3	Q	3	BMA	O5-C5	2.74	1.48	1.43
2	M	2	NAG	O5-C1	2.66	1.48	1.43
4	P	3	BMA	O5-C5	2.62	1.48	1.43
2	N	1	NAG	O5-C5	2.60	1.48	1.43
2	M	2	NAG	O5-C5	2.59	1.48	1.43
4	V	3	BMA	O5-C5	2.58	1.48	1.43
2	H	1	NAG	O5-C5	2.58	1.48	1.43
2	J	2	NAG	O5-C5	2.54	1.48	1.43
3	F	3	BMA	O3-C3	2.53	1.49	1.43
2	D	1	NAG	O5-C5	2.53	1.48	1.43
4	R	2	NAG	O5-C5	2.52	1.48	1.43
2	J	1	NAG	O5-C5	2.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O5-C1	2.50	1.47	1.43
2	H	2	NAG	O5-C1	2.46	1.47	1.43
2	K	1	NAG	O5-C5	2.44	1.48	1.43
3	Q	2	NAG	O5-C5	2.40	1.48	1.43
2	K	2	NAG	O5-C1	2.37	1.47	1.43
4	V	1	NAG	O5-C5	2.37	1.48	1.43
4	P	2	NAG	O4-C4	2.36	1.48	1.43
2	S	1	NAG	O5-C5	2.30	1.47	1.43
4	P	1	NAG	O5-C5	2.29	1.47	1.43
4	V	2	NAG	C1-C2	2.28	1.55	1.52
2	K	1	NAG	C1-C2	2.27	1.55	1.52
2	U	1	NAG	O5-C5	2.27	1.47	1.43
2	G	1	NAG	O5-C5	2.26	1.47	1.43
3	F	5	MAN	O5-C1	2.25	1.47	1.43
4	P	2	NAG	O5-C5	2.23	1.47	1.43
3	Q	4	MAN	O5-C1	2.22	1.47	1.43
2	T	1	NAG	O5-C5	2.22	1.47	1.43
3	Q	3	BMA	O3-C3	2.22	1.48	1.43
4	V	2	NAG	O5-C1	2.21	1.47	1.43
3	F	3	BMA	O5-C5	2.21	1.47	1.43
2	O	1	NAG	O5-C5	2.20	1.47	1.43
3	F	4	MAN	O5-C1	2.18	1.47	1.43
3	Q	5	MAN	O5-C1	2.17	1.47	1.43
2	I	1	NAG	O5-C5	2.17	1.47	1.43
3	Q	1	NAG	O5-C5	2.17	1.47	1.43
2	J	1	NAG	C1-C2	2.16	1.55	1.52
2	L	1	NAG	O5-C5	2.15	1.47	1.43
2	N	2	NAG	O5-C5	2.15	1.47	1.43
4	R	2	NAG	O4-C4	2.15	1.48	1.43
2	E	1	NAG	O5-C5	2.13	1.47	1.43
4	V	2	NAG	O5-C5	2.12	1.47	1.43
2	M	1	NAG	O4-C4	2.11	1.48	1.43
2	S	1	NAG	O4-C4	2.11	1.48	1.43
4	V	2	NAG	O4-C4	2.11	1.48	1.43
2	H	1	NAG	O4-C4	2.10	1.48	1.43
4	V	1	NAG	O4-C4	2.09	1.48	1.43
3	F	2	NAG	O5-C5	2.09	1.47	1.43
2	U	2	NAG	O5-C1	2.08	1.47	1.43
2	M	1	NAG	C1-C2	2.07	1.55	1.52
2	H	2	NAG	C1-C2	2.06	1.55	1.52
2	J	2	NAG	O5-C1	2.05	1.47	1.43
3	F	1	NAG	C1-C2	2.04	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	O4-C4	2.04	1.48	1.43
3	Q	3	BMA	O5-C1	2.03	1.47	1.43
2	D	2	NAG	O5-C1	2.03	1.47	1.43
2	G	1	NAG	O4-C4	2.03	1.48	1.43
2	J	1	NAG	O4-C4	2.01	1.47	1.43
4	R	1	NAG	O4-C4	2.00	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	2	NAG	C1-O5-C5	4.71	118.49	112.19
3	Q	4	MAN	C1-O5-C5	3.60	117.02	112.19
2	S	2	NAG	C1-O5-C5	3.51	116.89	112.19
3	F	3	BMA	O3-C3-C4	3.25	118.03	110.38
4	R	2	NAG	C1-O5-C5	3.18	116.45	112.19
2	E	2	NAG	C1-O5-C5	3.13	116.39	112.19
4	R	3	BMA	C1-O5-C5	3.04	116.26	112.19
3	F	5	MAN	C1-O5-C5	2.95	116.14	112.19
2	L	2	NAG	C1-O5-C5	2.92	116.11	112.19
2	H	1	NAG	C1-O5-C5	2.89	116.05	112.19
3	F	4	MAN	C1-O5-C5	2.88	116.04	112.19
2	U	1	NAG	C1-O5-C5	2.83	115.98	112.19
3	Q	5	MAN	C1-O5-C5	2.81	115.96	112.19
2	H	2	NAG	O5-C1-C2	-2.72	107.08	111.29
2	D	1	NAG	C2-N2-C7	2.56	126.33	122.90
2	S	1	NAG	C1-O5-C5	2.54	115.59	112.19
2	M	2	NAG	C1-O5-C5	2.53	115.58	112.19
4	P	3	BMA	C1-O5-C5	2.42	115.43	112.19
2	G	2	NAG	C1-O5-C5	2.37	115.36	112.19
2	H	2	NAG	C1-C2-N2	2.33	114.10	110.43
3	F	3	BMA	C6-C5-C4	2.22	118.48	113.02
2	T	2	NAG	C1-O5-C5	2.20	115.14	112.19
3	Q	3	BMA	C1-O5-C5	2.19	115.12	112.19
3	Q	2	NAG	C1-O5-C5	2.17	115.09	112.19
2	L	1	NAG	C2-N2-C7	2.14	125.77	122.90
4	V	1	NAG	C1-O5-C5	2.02	114.90	112.19
3	F	3	BMA	O3-C3-C2	-2.02	105.94	110.05
2	M	1	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

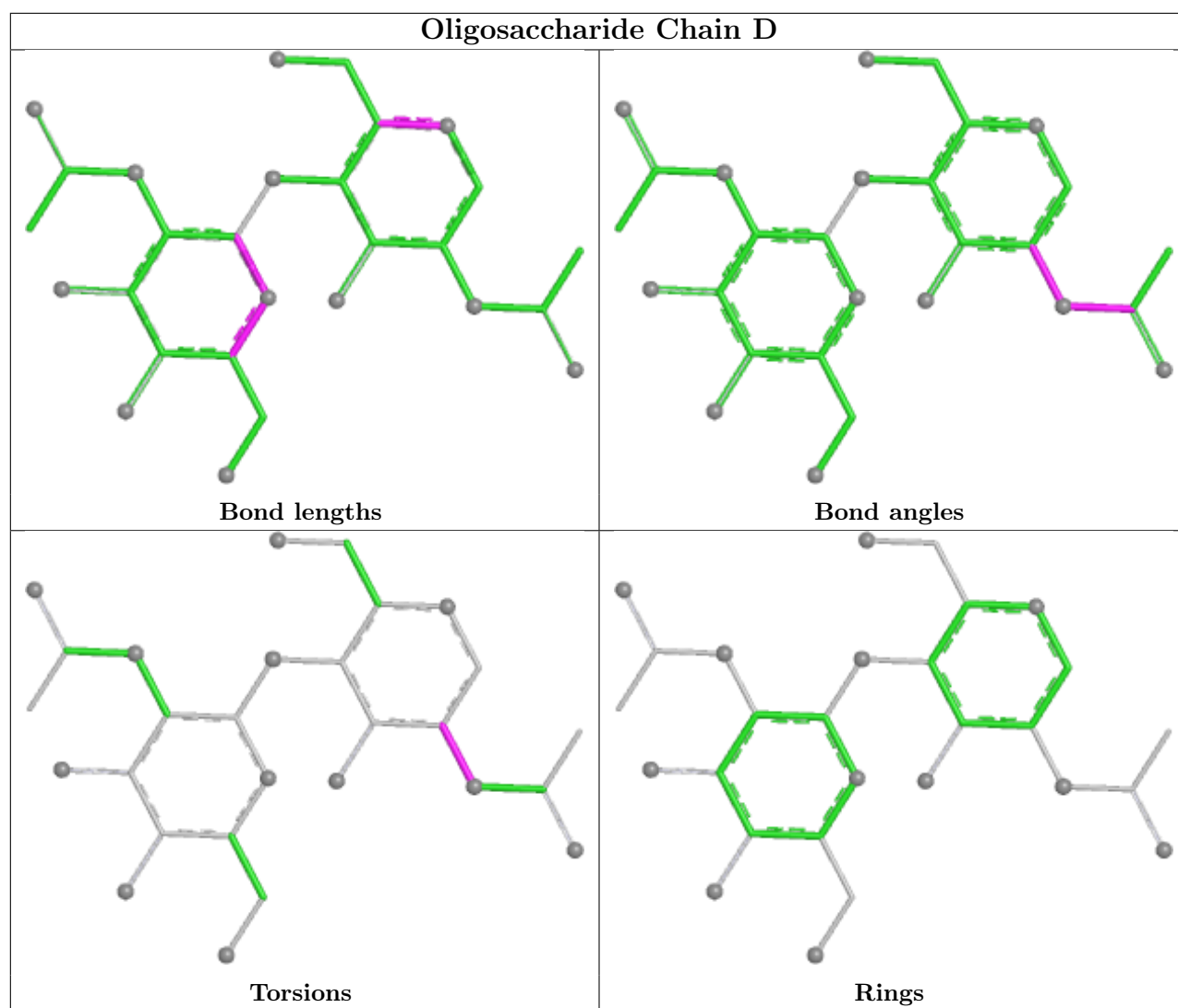
All (16) torsion outliers are listed below:

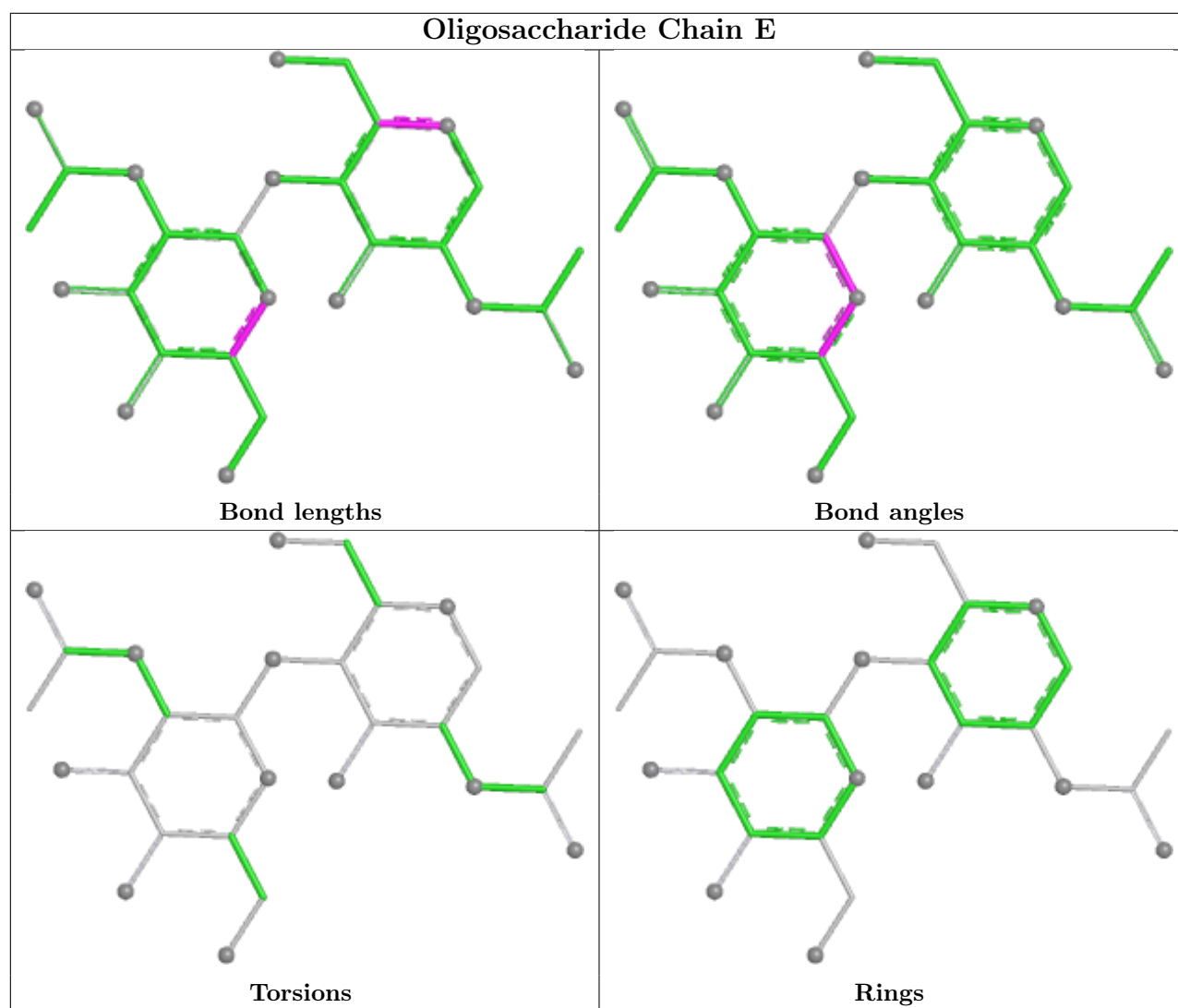
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C1-C2-N2-C7
4	R	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
3	F	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7
2	H	1	NAG	C1-C2-N2-C7
2	J	1	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7

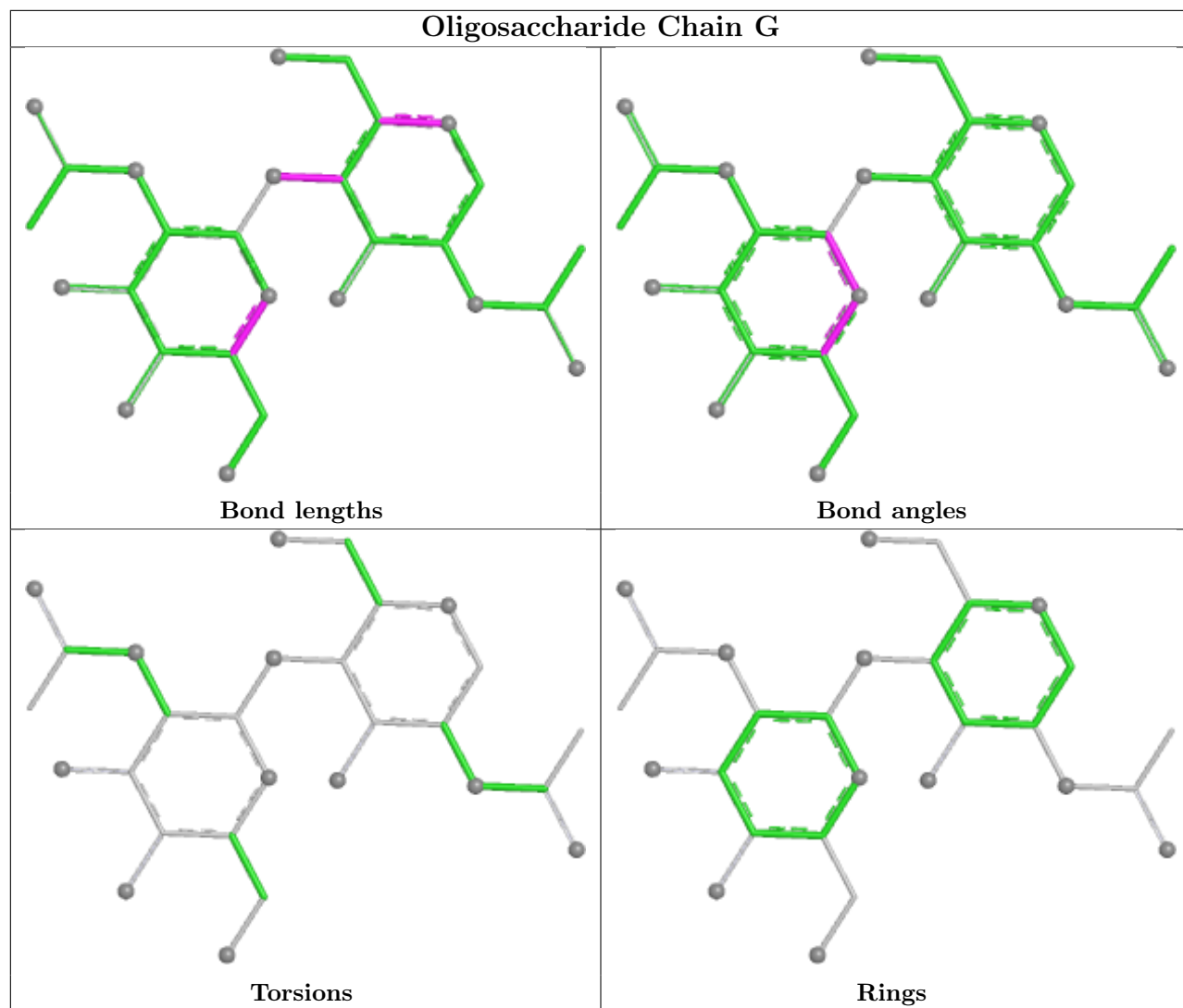
There are no ring outliers.

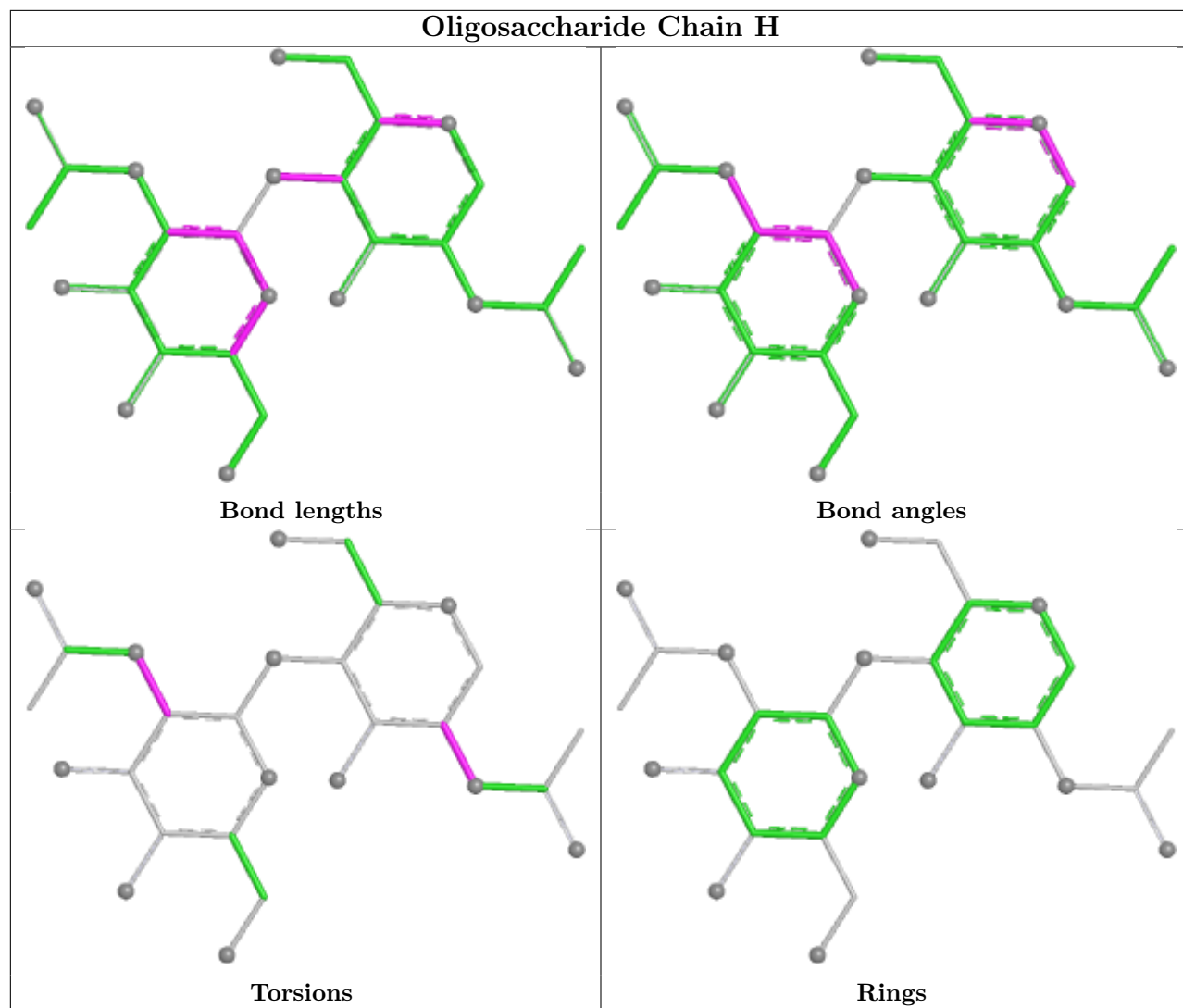
No monomer is involved in short contacts.

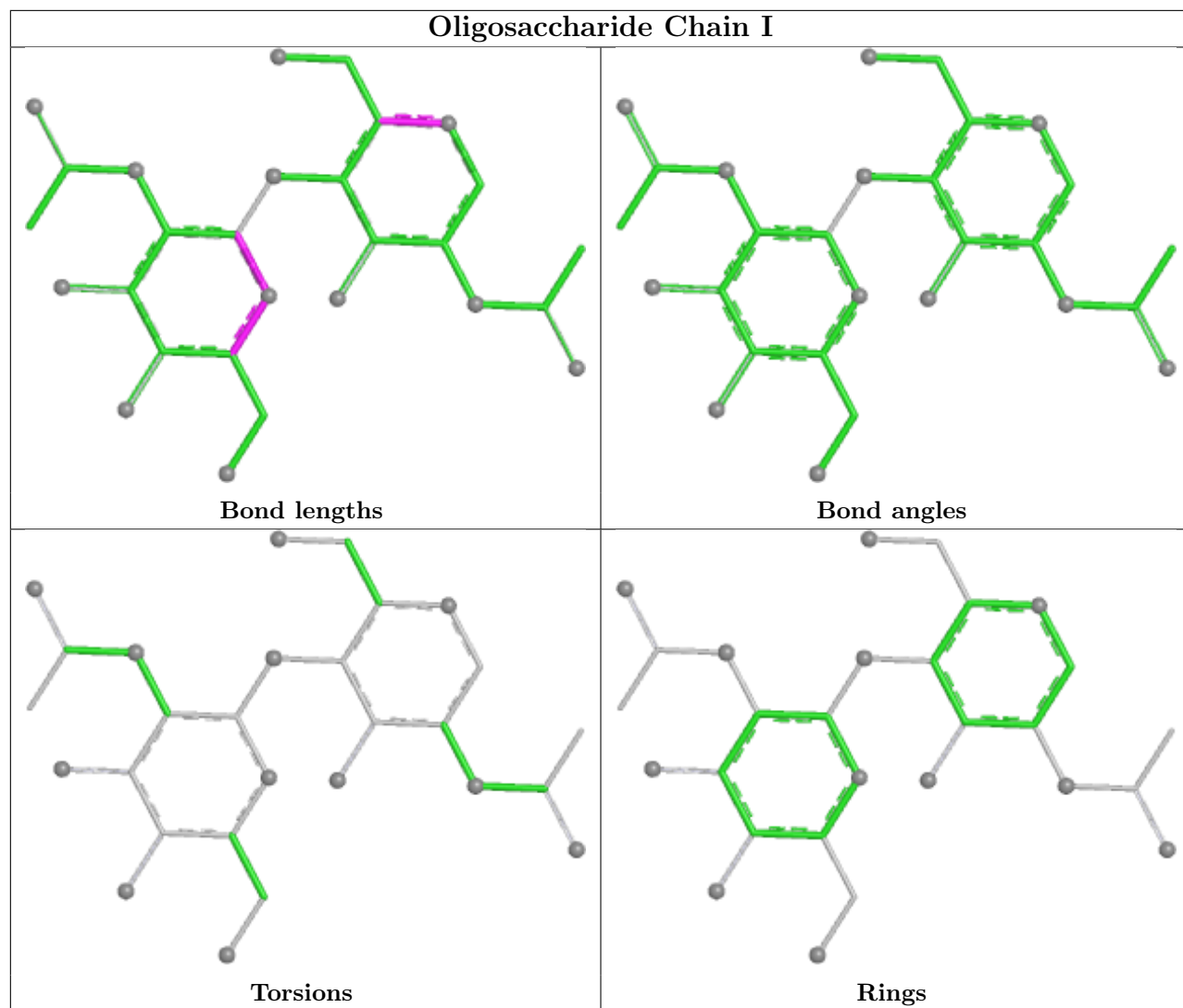
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



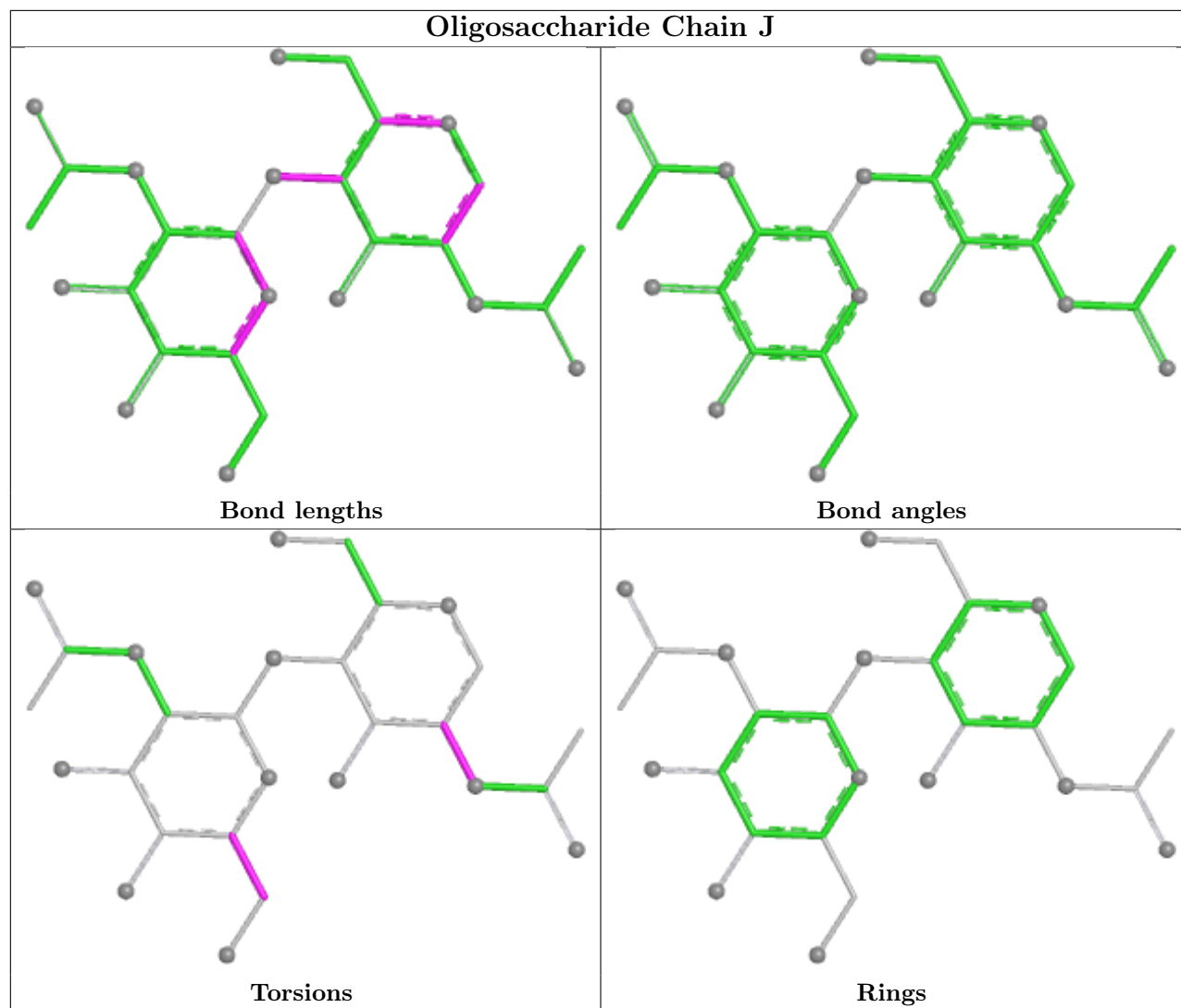


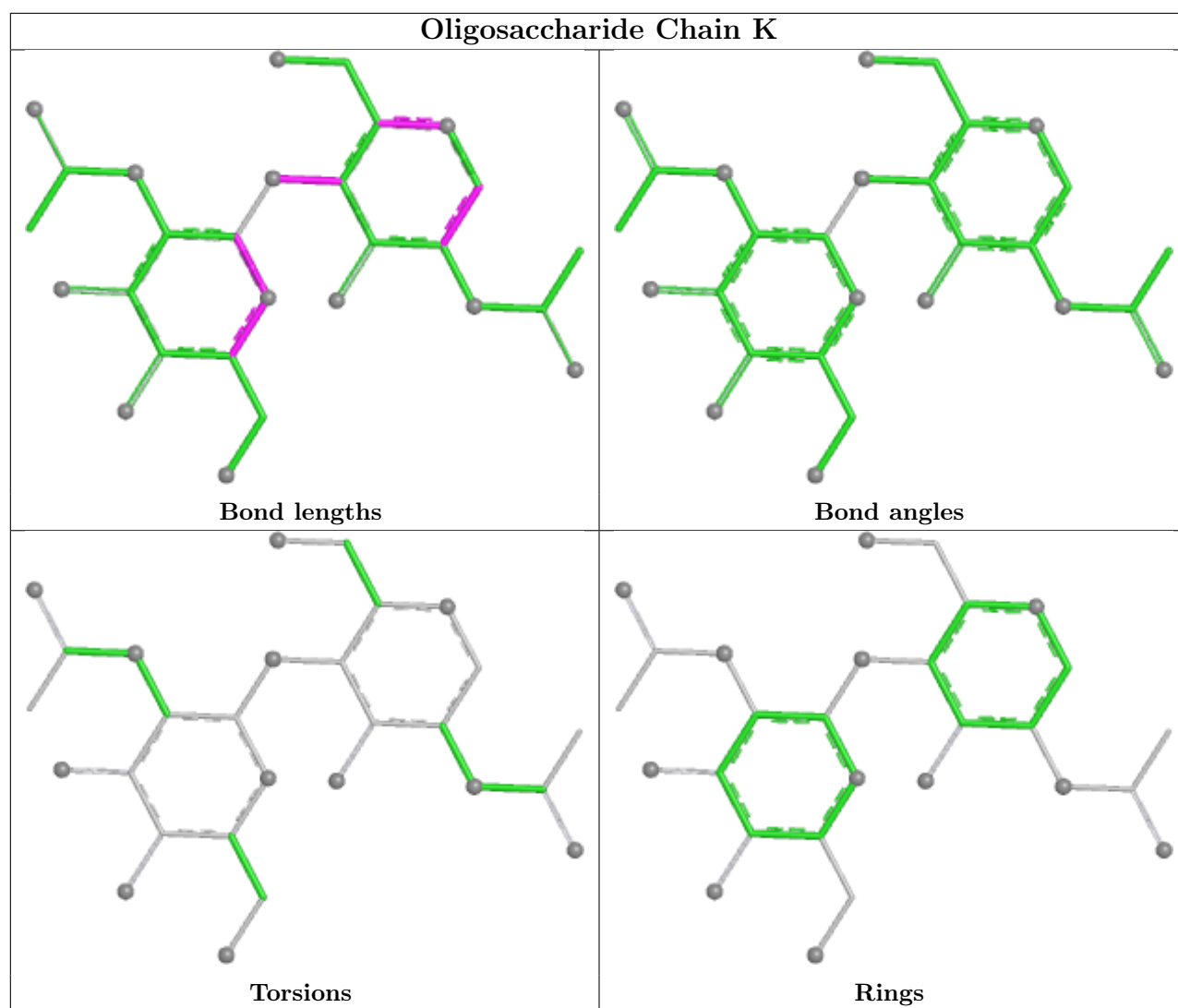


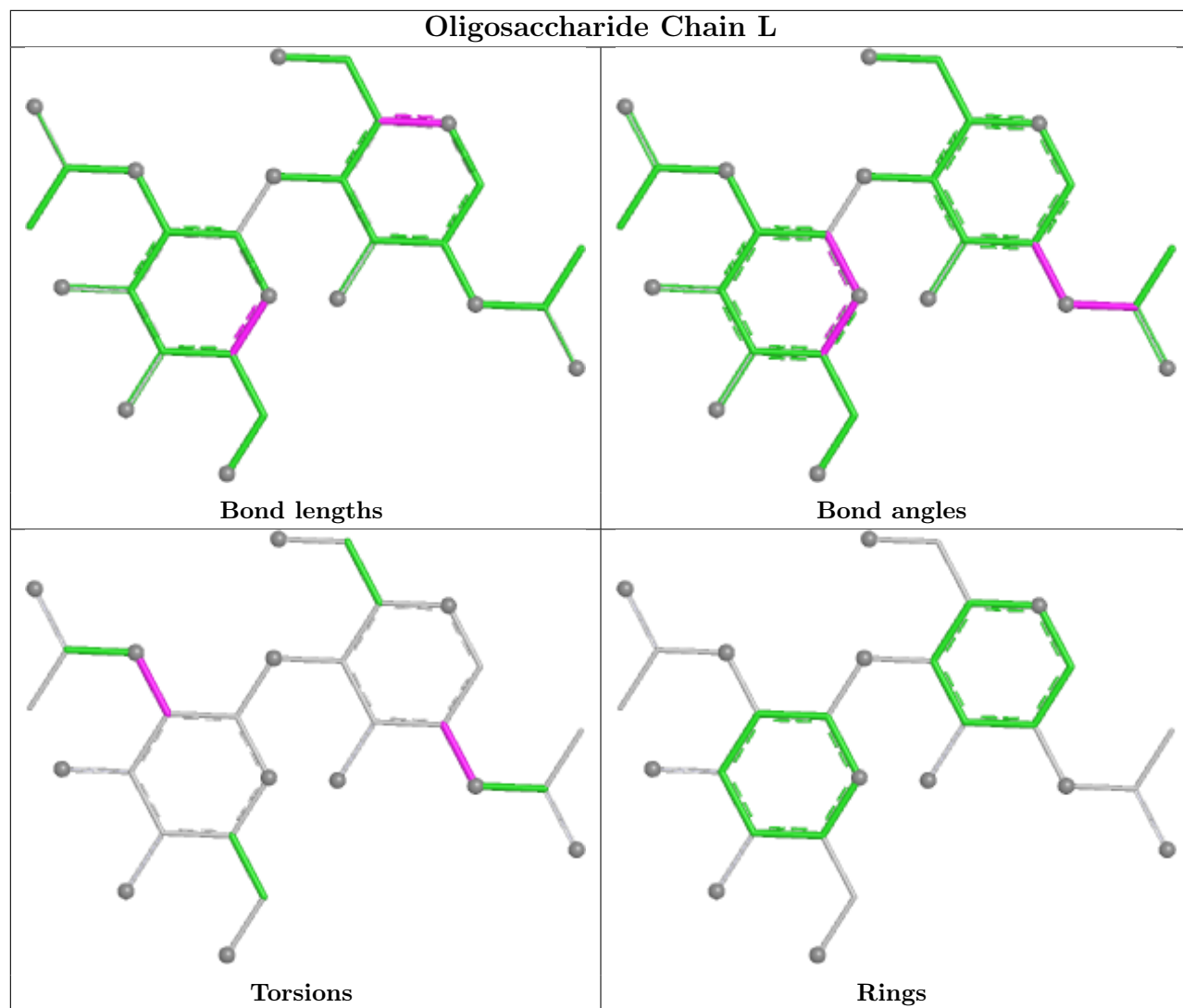


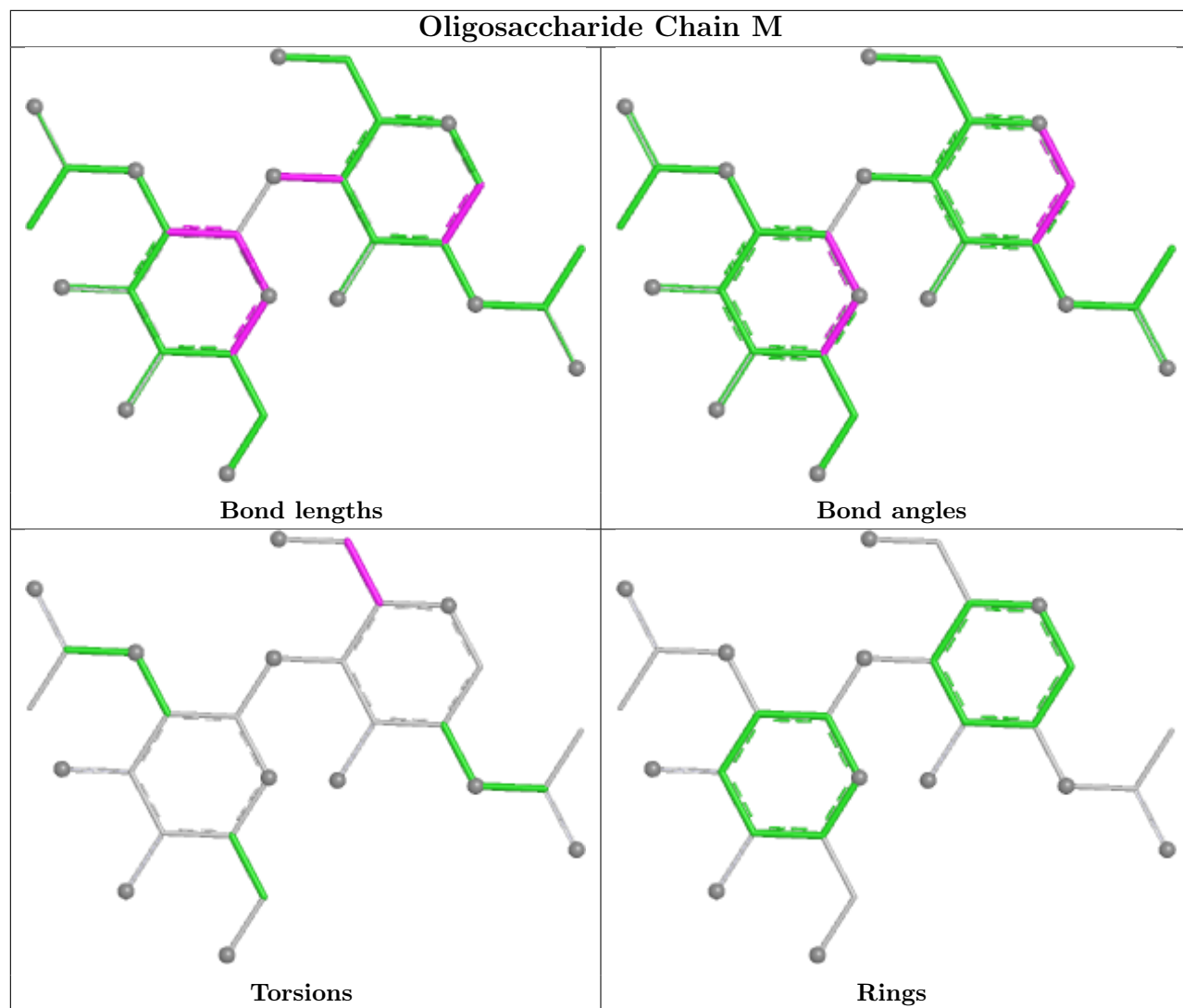


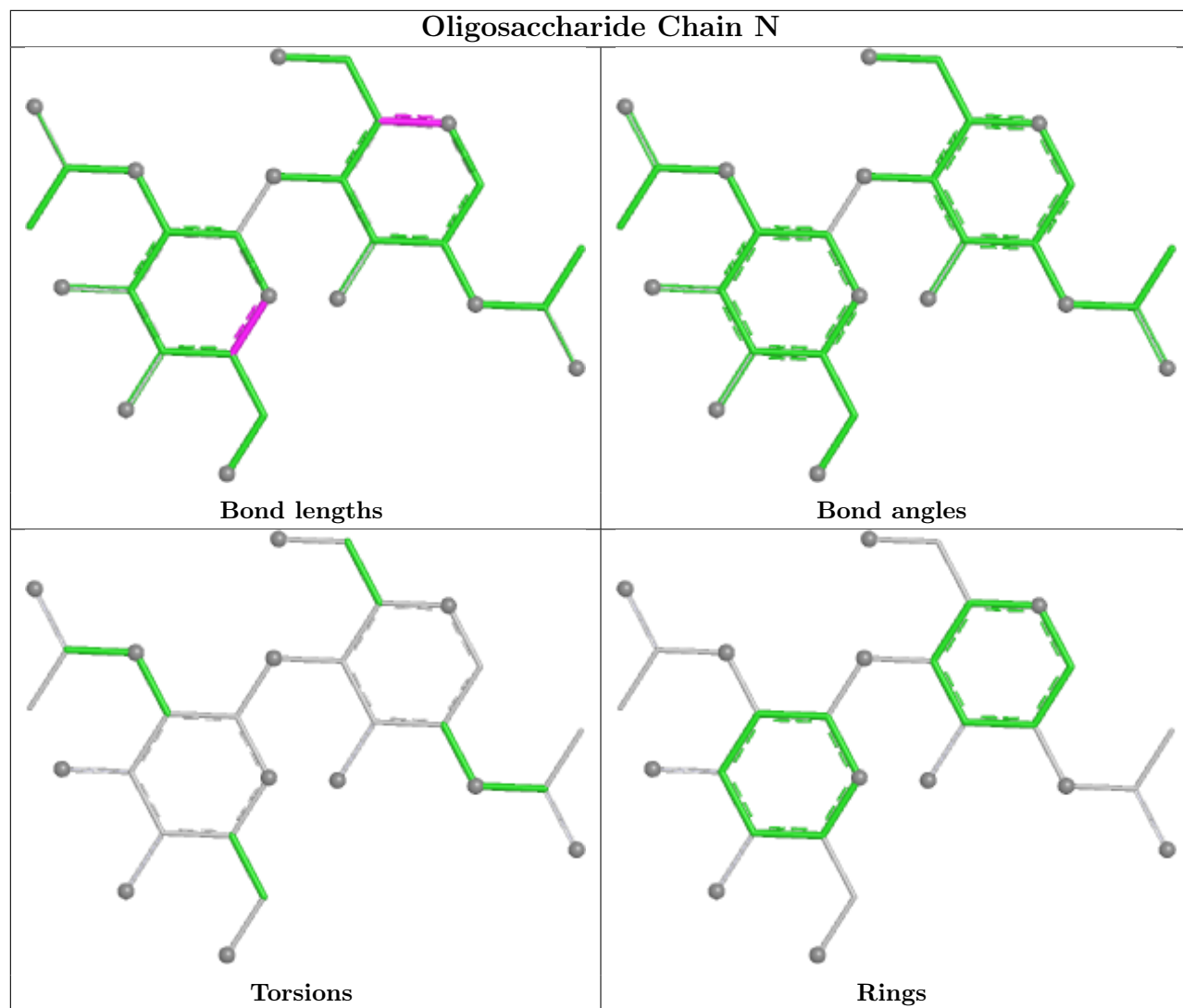


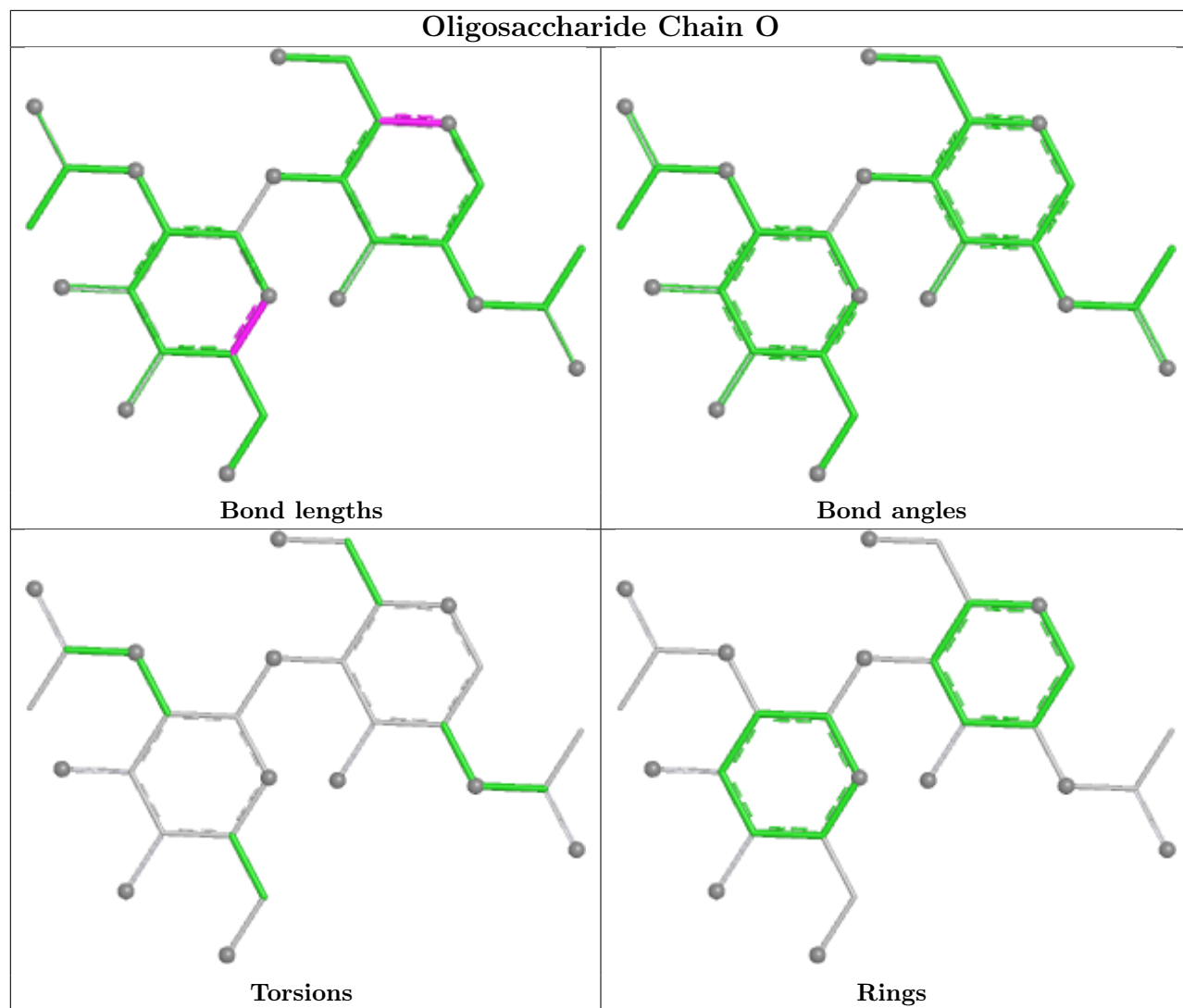


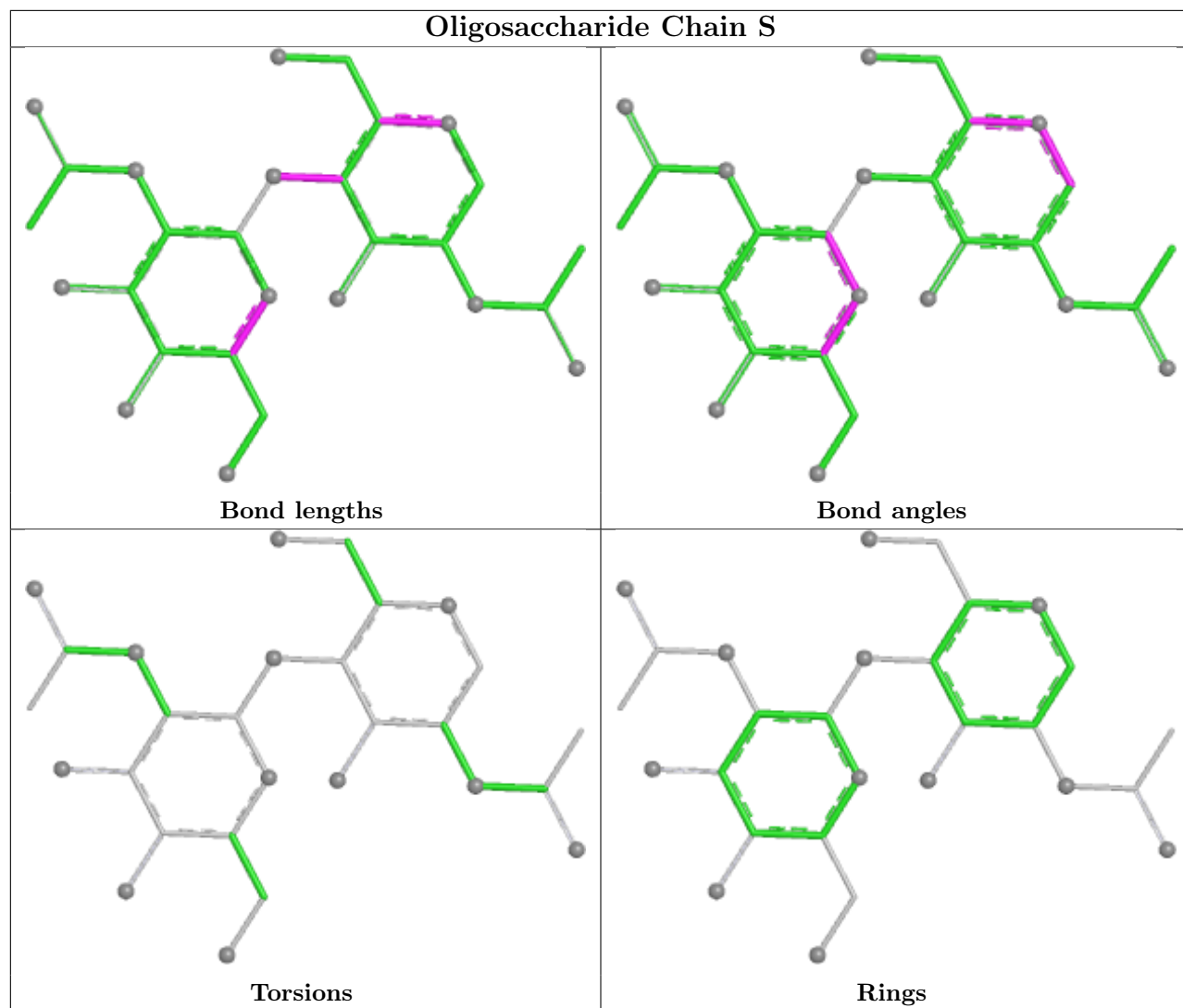


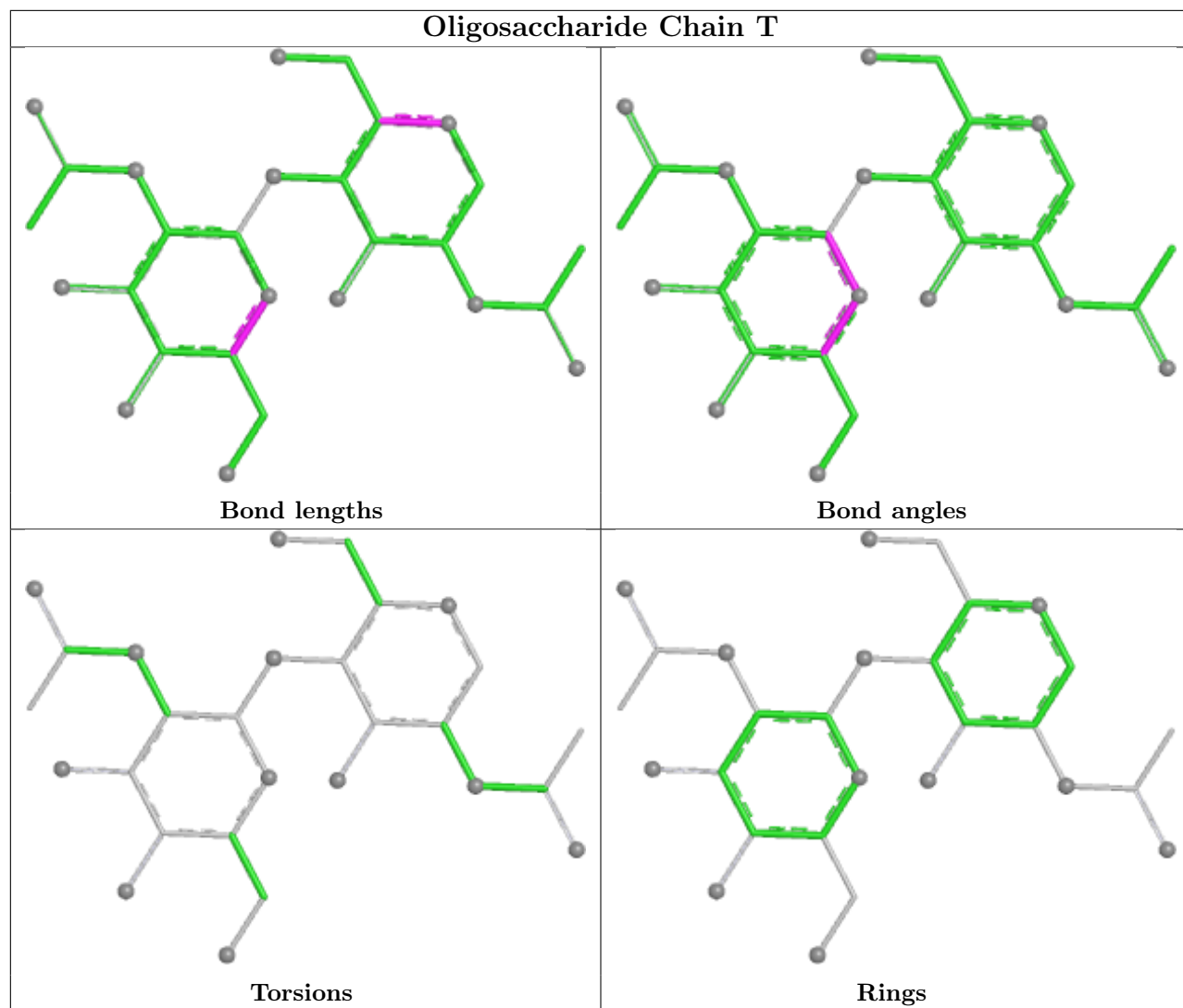




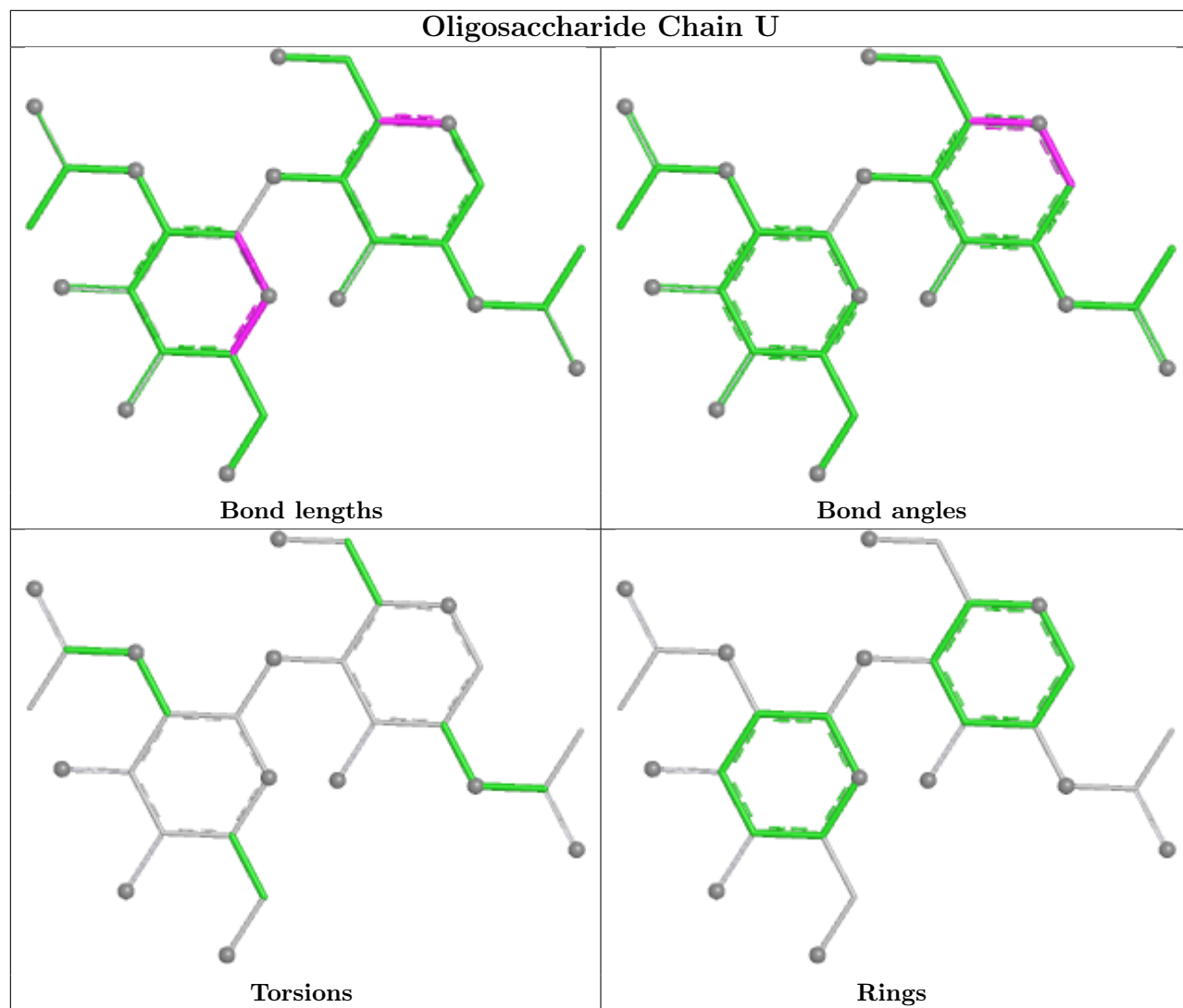


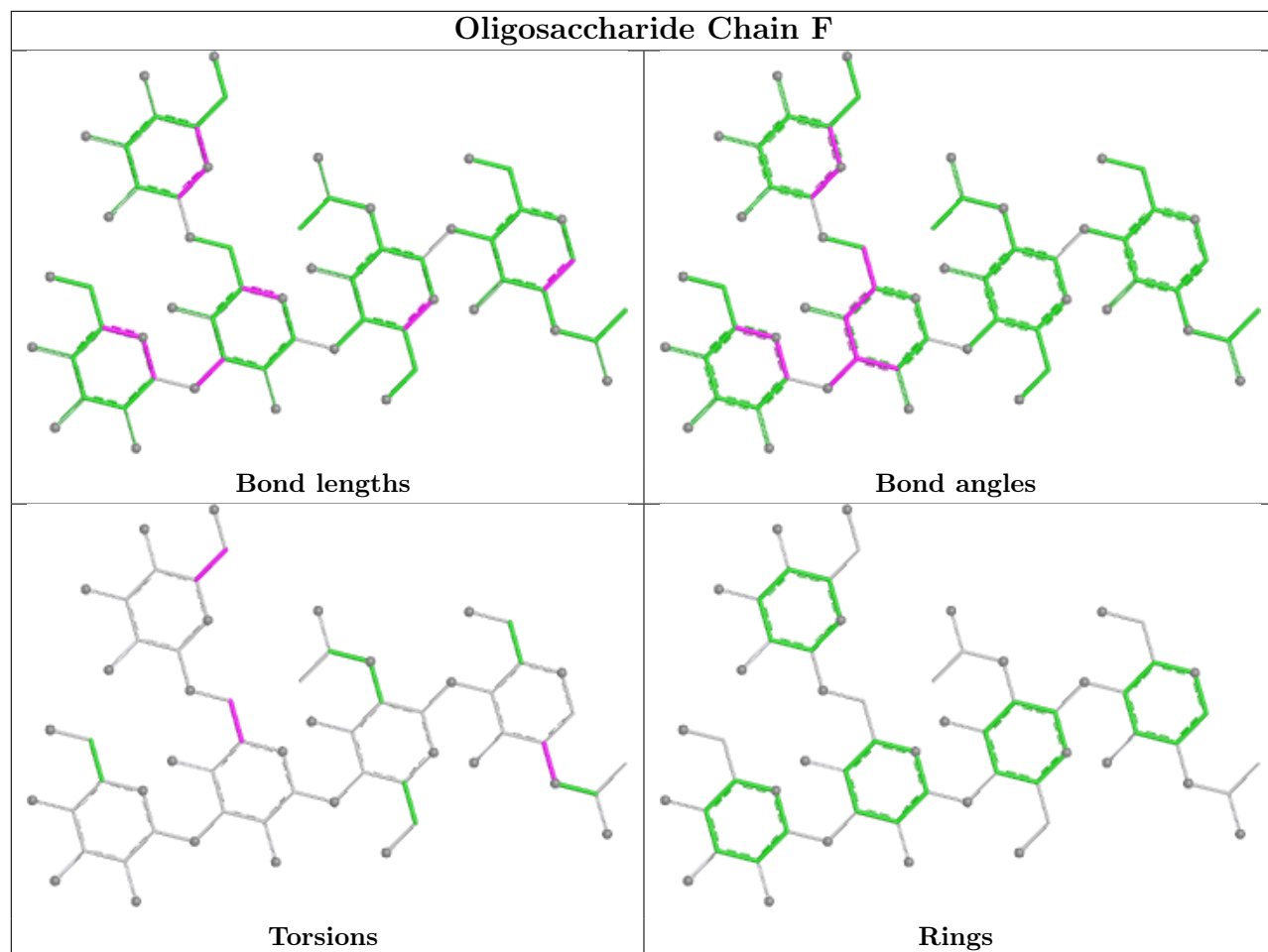




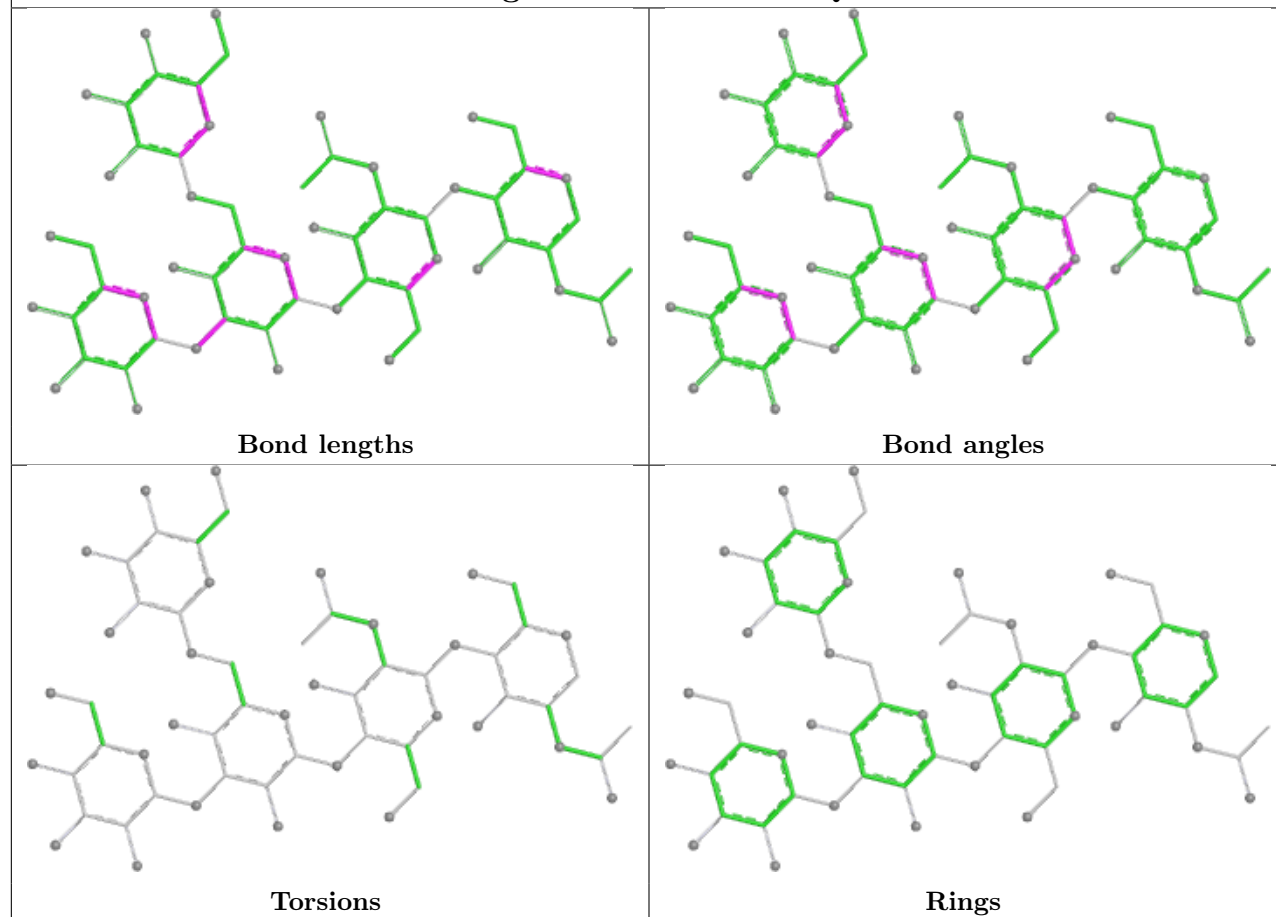




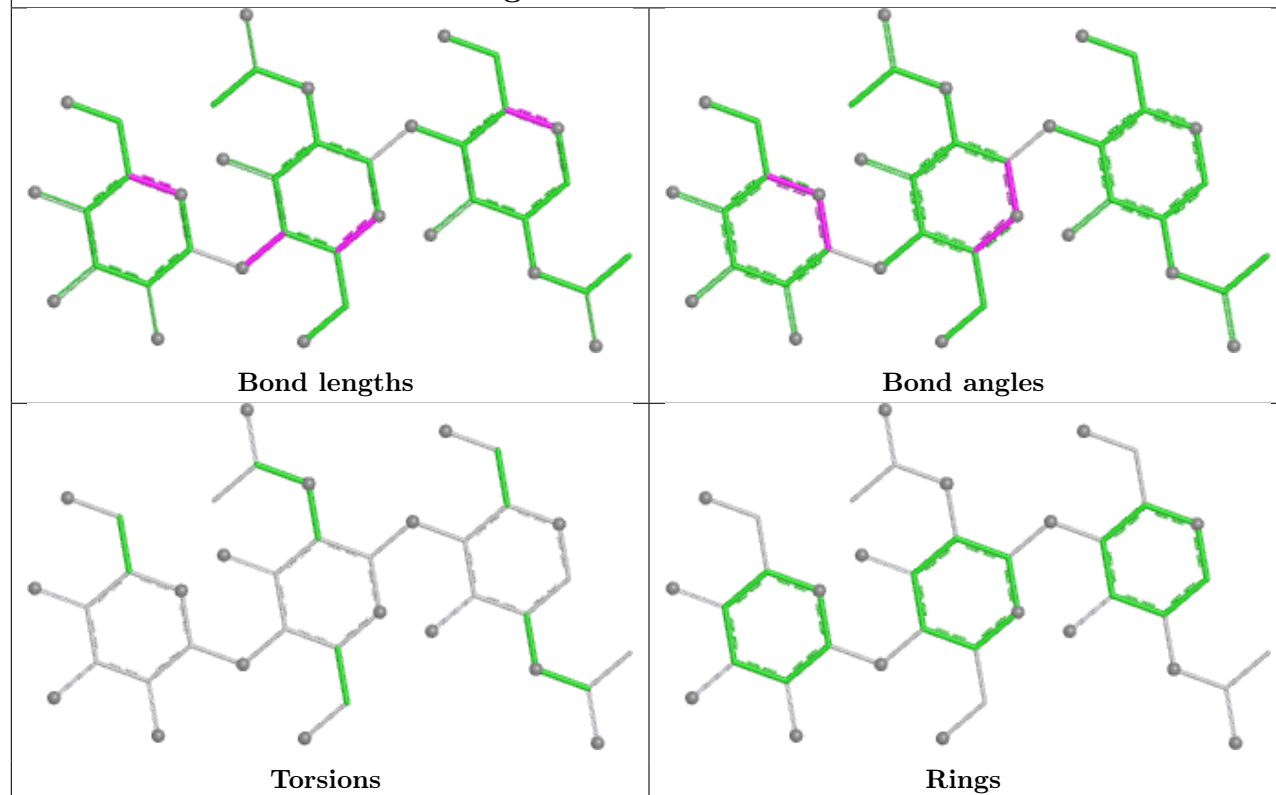


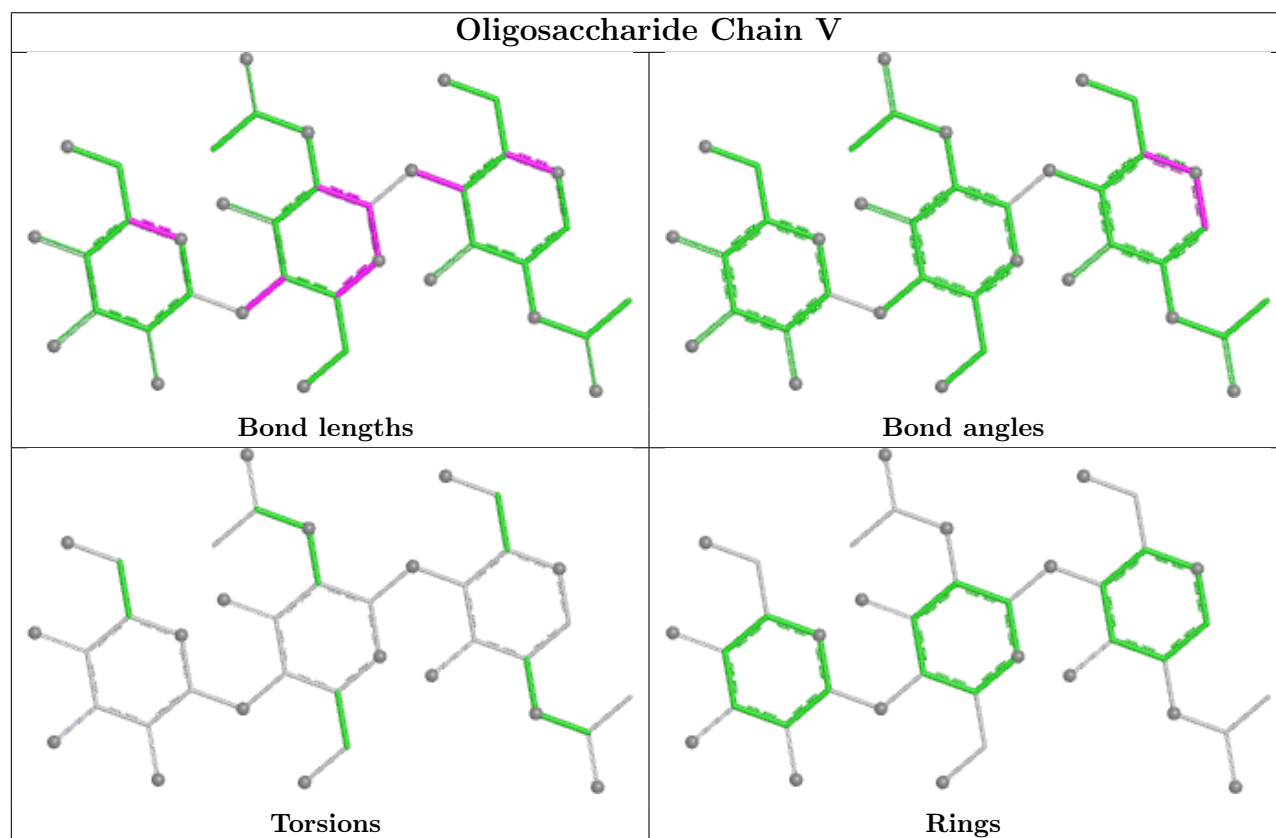
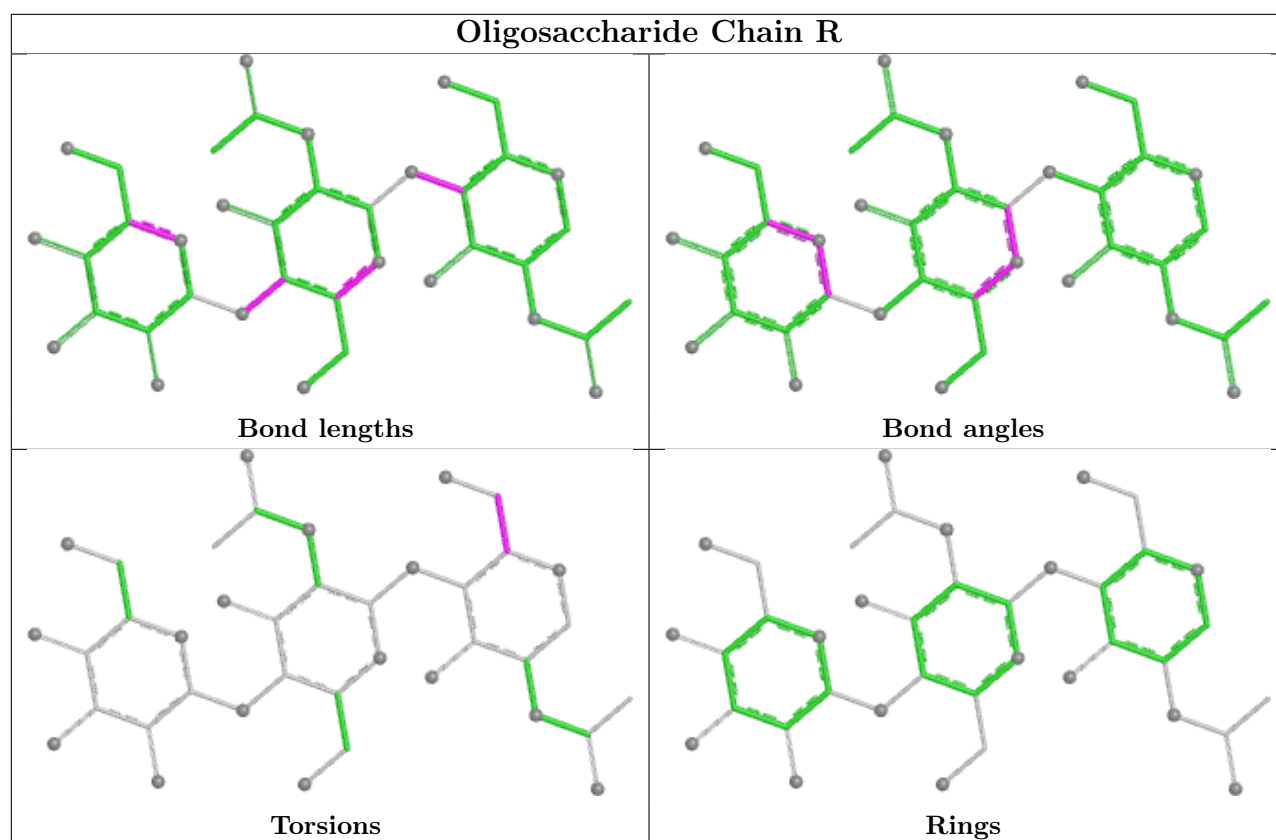


## Oligosaccharide Chain Q



## Oligosaccharide Chain P





## 5.6 Ligand geometry

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	A	1404	1	14,14,15	1.27	1 (7%)	17,19,21	0.83	0
5	NAG	B	1410	1	14,14,15	1.23	2 (14%)	17,19,21	0.91	1 (5%)
5	NAG	C	1408	1	14,14,15	1.17	1 (7%)	17,19,21	0.66	0
5	NAG	B	1407	1	14,14,15	1.19	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	B	1409	1	14,14,15	1.35	3 (21%)	17,19,21	0.75	1 (5%)
5	NAG	A	1405	1	14,14,15	1.27	1 (7%)	17,19,21	0.74	0
5	NAG	B	1403	1	14,14,15	1.18	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	B	1412	1	14,14,15	1.19	1 (7%)	17,19,21	0.75	0
5	NAG	B	1404	1	14,14,15	1.22	2 (14%)	17,19,21	0.98	1 (5%)
5	NAG	C	1401	1	14,14,15	1.25	2 (14%)	17,19,21	0.84	1 (5%)
5	NAG	C	1404	1	14,14,15	1.16	1 (7%)	17,19,21	0.82	0
6	A1AR1	B	1414	-	44,45,45	1.91	14 (31%)	55,67,67	1.46	6 (10%)
6	A1AR1	C	1412	-	44,45,45	1.73	11 (25%)	55,67,67	1.32	5 (9%)
6	A1AR1	A	1408	-	44,45,45	1.75	11 (25%)	55,67,67	1.27	4 (7%)
5	NAG	B	1401	1	14,14,15	1.19	1 (7%)	17,19,21	0.70	1 (5%)
5	NAG	A	1406	1	14,14,15	1.20	1 (7%)	17,19,21	0.67	0
5	NAG	B	1408	1	14,14,15	1.25	1 (7%)	17,19,21	0.62	0
5	NAG	B	1413	1	14,14,15	1.24	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	C	1405	1	14,14,15	1.28	2 (14%)	17,19,21	0.67	0
5	NAG	C	1410	1	14,14,15	1.16	1 (7%)	17,19,21	0.69	0
5	NAG	C	1402	1	14,14,15	1.29	1 (7%)	17,19,21	0.75	0
5	NAG	A	1407	1	14,14,15	1.22	2 (14%)	17,19,21	1.13	1 (5%)
5	NAG	C	1406	1	14,14,15	1.23	1 (7%)	17,19,21	0.84	0
5	NAG	A	1403	1	14,14,15	1.26	1 (7%)	17,19,21	0.73	1 (5%)
5	NAG	C	1409	1	14,14,15	1.33	2 (14%)	17,19,21	0.76	0
5	NAG	B	1411	1	14,14,15	1.18	1 (7%)	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	1411	1	14,14,15	1.19	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	A	1401	1	14,14,15	1.21	1 (7%)	17,19,21	0.73	0
5	NAG	B	1402	1	14,14,15	1.28	1 (7%)	17,19,21	0.72	0
5	NAG	B	1406	1	14,14,15	1.06	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	C	1407	1	14,14,15	1.09	1 (7%)	17,19,21	0.77	0
5	NAG	C	1403	1	14,14,15	1.23	1 (7%)	17,19,21	0.65	0
5	NAG	B	1405	1	14,14,15	1.28	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	A	1402	1	14,14,15	1.16	1 (7%)	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1412	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
6	A1AR1	B	1414	-	-	13/47/84/84	0/2/2/2
6	A1AR1	C	1412	-	-	11/47/84/84	0/2/2/2
6	A1AR1	A	1408	-	-	8/47/84/84	0/2/2/2
5	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1413	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	0/6/23/26	0/1/1/1

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

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1414	A1AR1	C21-C12	5.25	1.61	1.53
6	B	1414	A1AR1	O3-C21	4.52	1.46	1.39
6	A	1408	A1AR1	C21-C12	4.43	1.60	1.53
6	C	1412	A1AR1	C21-C12	4.24	1.60	1.53
6	C	1412	A1AR1	O3-C21	4.08	1.45	1.39
6	A	1408	A1AR1	O3-C21	4.03	1.45	1.39
6	A	1408	A1AR1	C41-C51	3.80	1.56	1.53
6	B	1414	A1AR1	C41-C51	3.55	1.56	1.53
6	B	1414	A1AR1	C31-C21	3.50	1.56	1.51
6	B	1414	A1AR1	C4-C5	3.42	1.56	1.53
6	C	1412	A1AR1	C9-C8	3.37	1.56	1.51
6	C	1412	A1AR1	C31-C21	3.28	1.56	1.51
6	C	1412	A1AR1	C4-C5	3.24	1.56	1.53
6	A	1408	A1AR1	C31-C21	3.23	1.56	1.51
6	C	1412	A1AR1	C41-C51	3.15	1.56	1.53
6	A	1408	A1AR1	C4-C5	3.15	1.56	1.53
5	C	1409	NAG	O5-C5	3.04	1.49	1.43
5	C	1405	NAG	O5-C5	3.02	1.49	1.43
5	B	1404	NAG	O5-C5	2.97	1.49	1.43
5	B	1409	NAG	O5-C5	2.96	1.49	1.43
5	B	1402	NAG	O5-C5	2.90	1.49	1.43
5	A	1405	NAG	O5-C5	2.88	1.49	1.43
6	B	1414	A1AR1	C3-C2	2.85	1.56	1.52
5	C	1406	NAG	O5-C5	2.85	1.49	1.43
5	B	1405	NAG	O5-C5	2.84	1.49	1.43
5	C	1404	NAG	O5-C5	2.81	1.48	1.43
5	B	1408	NAG	O5-C5	2.80	1.48	1.43
5	C	1403	NAG	O5-C5	2.79	1.48	1.43
5	A	1403	NAG	O5-C5	2.78	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1404	NAG	O5-C5	2.78	1.48	1.43
5	B	1411	NAG	O5-C5	2.78	1.48	1.43
5	C	1402	NAG	O5-C5	2.77	1.48	1.43
5	B	1407	NAG	O5-C5	2.75	1.48	1.43
6	B	1414	A1AR1	O61-C21	2.71	1.45	1.43
5	A	1402	NAG	O5-C5	2.69	1.48	1.43
5	A	1406	NAG	O5-C5	2.66	1.48	1.43
6	A	1408	A1AR1	C9-C8	2.66	1.55	1.51
6	B	1414	A1AR1	C9-C8	2.65	1.55	1.51
5	C	1408	NAG	O5-C5	2.65	1.48	1.43
6	C	1412	A1AR1	C3-C2	2.65	1.55	1.52
5	B	1412	NAG	O5-C5	2.63	1.48	1.43
6	B	1414	A1AR1	C71-C61	2.63	1.56	1.52
6	A	1408	A1AR1	O61-C21	2.59	1.45	1.43
5	C	1401	NAG	O5-C5	2.58	1.48	1.43
5	A	1401	NAG	O5-C5	2.57	1.48	1.43
5	C	1407	NAG	O5-C5	2.57	1.48	1.43
5	B	1401	NAG	O5-C5	2.55	1.48	1.43
5	B	1403	NAG	O5-C5	2.55	1.48	1.43
5	B	1413	NAG	O5-C5	2.55	1.48	1.43
6	C	1412	A1AR1	O61-C21	2.54	1.45	1.43
5	B	1410	NAG	O5-C5	2.52	1.48	1.43
6	C	1412	A1AR1	C2-C1	2.51	1.60	1.54
6	A	1408	A1AR1	C3-C2	2.50	1.55	1.52
6	A	1408	A1AR1	C2-C1	2.48	1.60	1.54
5	C	1411	NAG	O5-C5	2.48	1.48	1.43
5	C	1410	NAG	O5-C5	2.46	1.48	1.43
6	C	1412	A1AR1	O1A-C1	-2.41	1.21	1.30
5	B	1406	NAG	O5-C5	2.39	1.48	1.43
6	B	1414	A1AR1	C2-C1	2.35	1.60	1.54
6	A	1408	A1AR1	O1A-C1	-2.35	1.22	1.30
6	B	1414	A1AR1	O1A-C1	-2.33	1.22	1.30
5	A	1407	NAG	O5-C5	2.31	1.47	1.43
5	C	1401	NAG	C1-C2	2.28	1.55	1.52
5	A	1407	NAG	C1-C2	2.25	1.55	1.52
5	B	1409	NAG	C1-C2	2.21	1.55	1.52
6	C	1412	A1AR1	O1A1-C12	-2.21	1.22	1.30
6	A	1408	A1AR1	O1A1-C12	-2.19	1.22	1.30
6	B	1414	A1AR1	O1A1-C12	-2.18	1.22	1.30
5	B	1410	NAG	C1-C2	2.13	1.55	1.52
6	B	1414	A1AR1	C8-C7	2.05	1.57	1.53
5	B	1404	NAG	O5-C1	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1409	NAG	O5-C1	2.04	1.47	1.43
6	B	1414	A1AR1	C7-C6	2.04	1.55	1.52
5	C	1405	NAG	O5-C1	2.03	1.47	1.43
5	C	1409	NAG	O5-C1	2.01	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1414	A1AR1	O6-C2-C3	-4.38	105.47	111.35
6	B	1414	A1AR1	O6-C6-C5	-4.23	105.97	109.84
6	B	1414	A1AR1	O3-C21-C31	-3.98	103.42	109.44
6	C	1412	A1AR1	O6-C2-C3	-3.60	106.51	111.35
6	A	1408	A1AR1	O6-C6-C5	-3.54	106.60	109.84
5	A	1407	NAG	C1-O5-C5	3.53	116.92	112.19
6	A	1408	A1AR1	O1B1-C12-C21	-3.39	118.20	123.85
6	A	1408	A1AR1	O6-C2-C3	-3.28	106.94	111.35
6	C	1412	A1AR1	O1B1-C12-C21	-3.27	118.39	123.85
6	B	1414	A1AR1	O1B1-C12-C21	-3.14	118.61	123.85
5	C	1411	NAG	C1-O5-C5	3.05	116.28	112.19
5	B	1404	NAG	C1-O5-C5	3.01	116.22	112.19
6	C	1412	A1AR1	O6-C6-C5	-2.99	107.11	109.84
5	A	1402	NAG	C1-O5-C5	2.89	116.06	112.19
5	B	1406	NAG	C1-O5-C5	2.89	116.06	112.19
6	C	1412	A1AR1	O9-C9-C8	2.85	114.10	108.20
5	B	1403	NAG	C1-O5-C5	2.76	115.89	112.19
5	B	1407	NAG	C1-O5-C5	2.61	115.69	112.19
6	B	1414	A1AR1	C9-O9-CA9	2.52	123.30	117.08
5	B	1410	NAG	C1-O5-C5	2.47	115.50	112.19
6	A	1408	A1AR1	O3-C21-C31	-2.46	105.72	109.44
6	C	1412	A1AR1	O3-C21-C31	-2.37	105.85	109.44
5	C	1401	NAG	C1-O5-C5	2.27	115.23	112.19
5	B	1409	NAG	C1-O5-C5	2.25	115.21	112.19
5	B	1405	NAG	C1-O5-C5	2.20	115.13	112.19
5	B	1413	NAG	O5-C1-C2	-2.14	107.98	111.29
6	B	1414	A1AR1	C31-C41-C51	2.08	112.93	109.72
5	B	1401	NAG	C1-O5-C5	2.01	114.88	112.19
5	A	1403	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

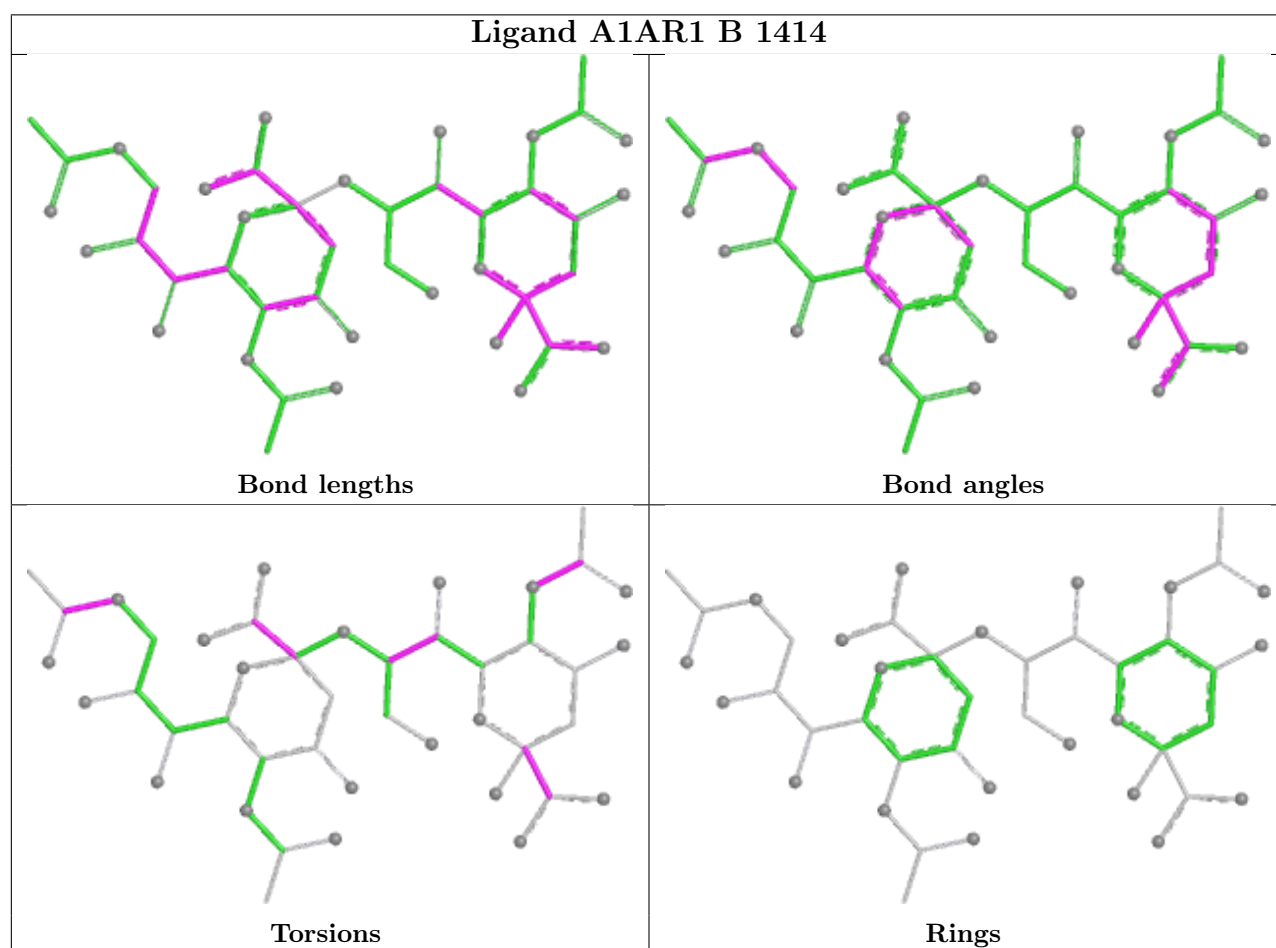
All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1408	A1AR1	O1A-C1-C2-O81
6	B	1414	A1AR1	O1A1-C12-C21-O61
6	B	1414	A1AR1	O1A-C1-C2-O81
6	B	1414	A1AR1	C61-C71-C81-C91
6	B	1414	A1AR1	O71-C71-C81-C91
6	B	1414	A1AR1	O71-C71-C81-O81
6	B	1414	A1AR1	C111-C101-N51-C51
6	B	1414	A1AR1	O101-C101-N51-C51
6	C	1412	A1AR1	C7-C8-C9-O9
6	C	1412	A1AR1	O8-C8-C9-O9
6	C	1412	A1AR1	O1A-C1-C2-O81
6	C	1412	A1AR1	C111-C101-N51-C51
6	C	1412	A1AR1	O101-C101-N51-C51
6	C	1412	A1AR1	OA9-CA9-O9-C9
6	C	1412	A1AR1	CM9-CA9-O9-C9
6	A	1408	A1AR1	C111-C101-N51-C51
6	A	1408	A1AR1	O101-C101-N51-C51
6	B	1414	A1AR1	CM9-CA9-O9-C9
6	A	1408	A1AR1	C61-C71-C81-C91
6	C	1412	A1AR1	C61-C71-C81-C91
6	B	1414	A1AR1	OA9-CA9-O9-C9
6	B	1414	A1AR1	O1B-C1-C2-O81
6	A	1408	A1AR1	O71-C71-C81-O81
6	C	1412	A1AR1	C61-C71-C81-O81
6	C	1412	A1AR1	O71-C71-C81-O81
5	B	1411	NAG	C4-C5-C6-O6
5	A	1402	NAG	C1-C2-N2-C7
5	A	1403	NAG	C1-C2-N2-C7
5	A	1405	NAG	C1-C2-N2-C7
5	A	1406	NAG	C1-C2-N2-C7
5	B	1403	NAG	C1-C2-N2-C7
6	B	1414	A1AR1	O1A-C1-C2-O6
6	A	1408	A1AR1	C61-C71-C81-O81
6	B	1414	A1AR1	C61-C71-C81-O81
5	C	1401	NAG	C4-C5-C6-O6
6	B	1414	A1AR1	O1A1-C12-C21-O3
5	A	1407	NAG	C4-C5-C6-O6
5	A	1407	NAG	O5-C5-C6-O6
5	B	1411	NAG	O5-C5-C6-O6
6	A	1408	A1AR1	O1A1-C12-C21-C31
6	C	1412	A1AR1	O1A1-C12-C21-C31
6	A	1408	A1AR1	O71-C71-C81-C91

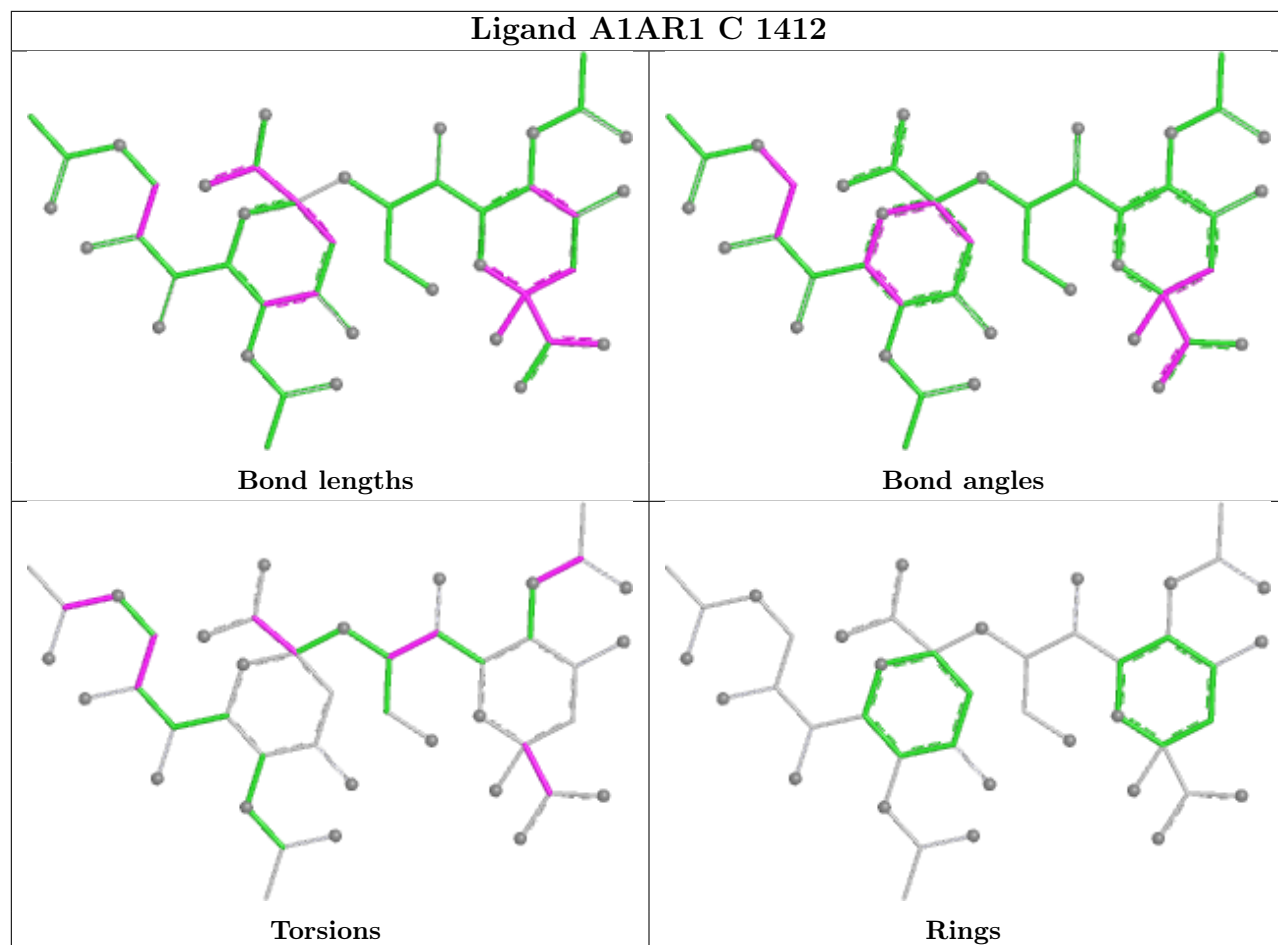
There are no ring outliers.

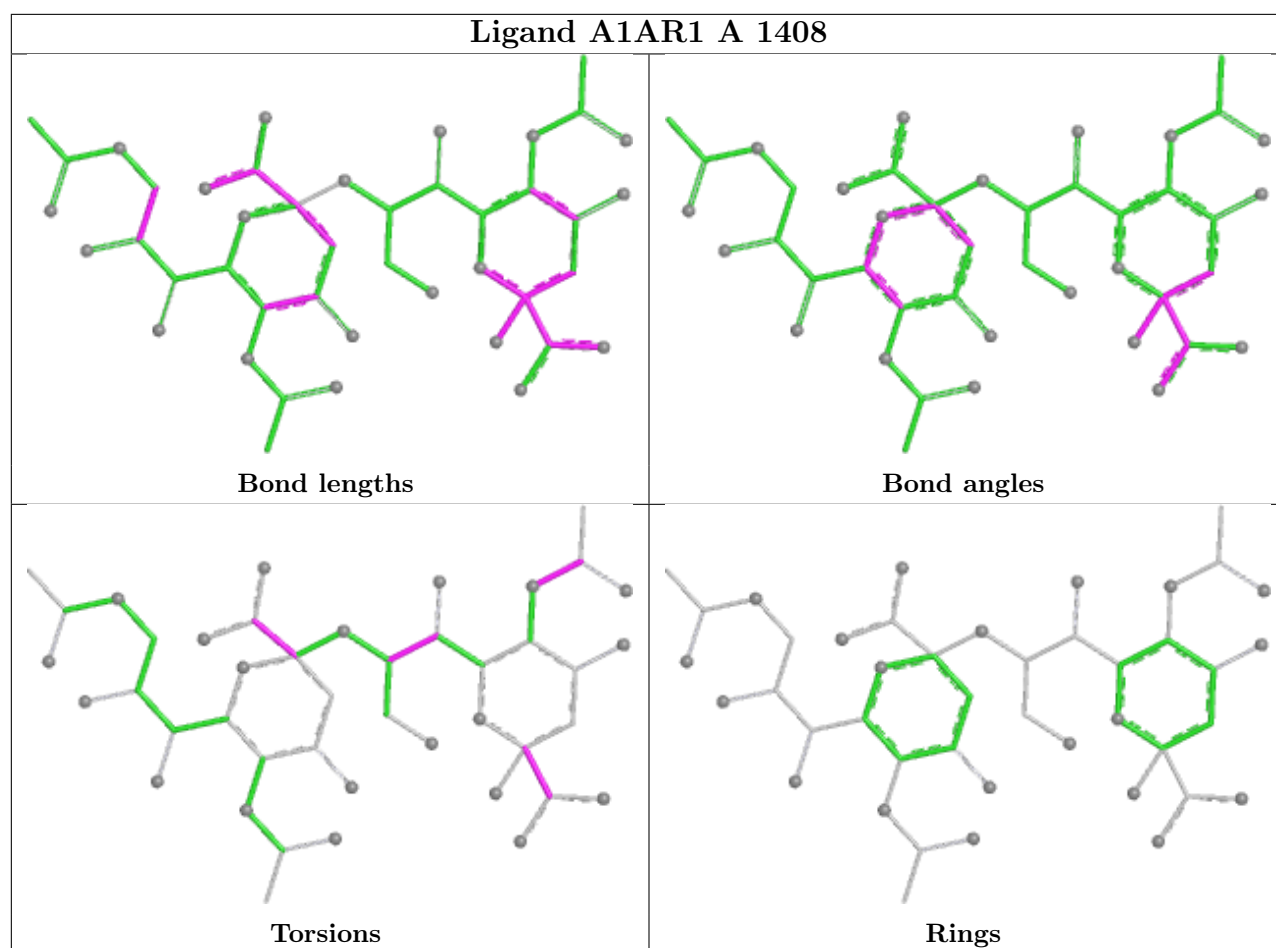
No monomer is involved in short contacts.

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



## Ligand A1AR1 C 1412





## 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.

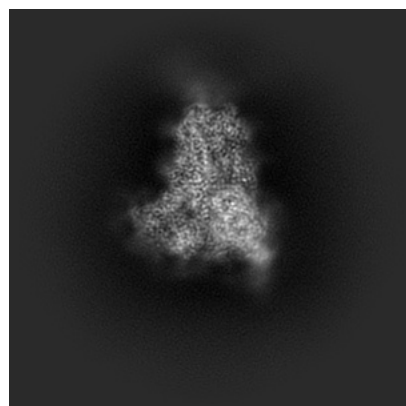
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44876. These allow visual inspection of the internal detail of the map and identification of artifacts.

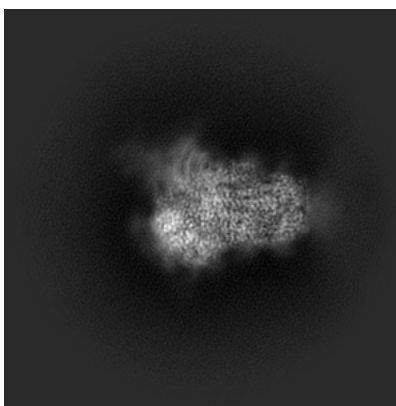
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

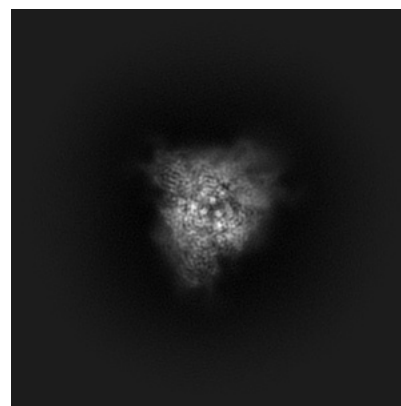
#### 6.1.1 Primary map



X

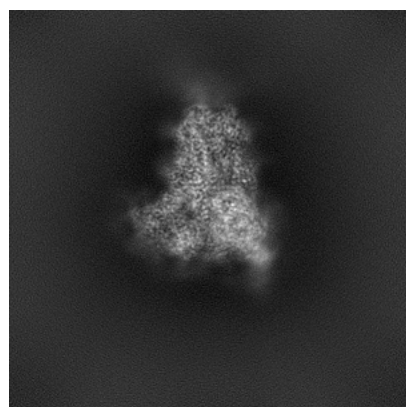


Y

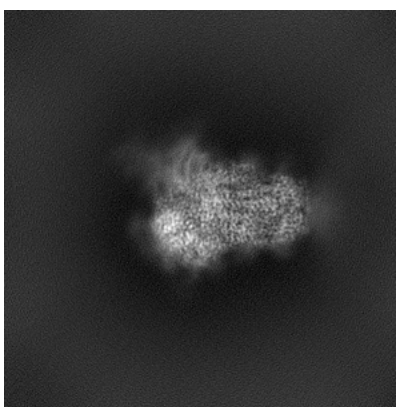


Z

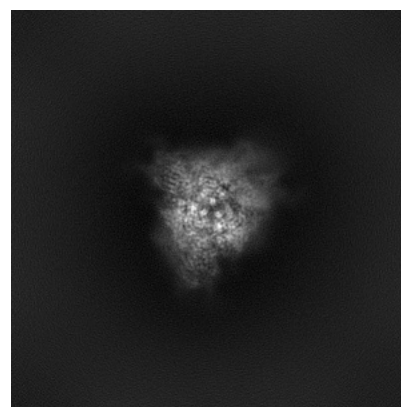
#### 6.1.2 Raw map



X



Y

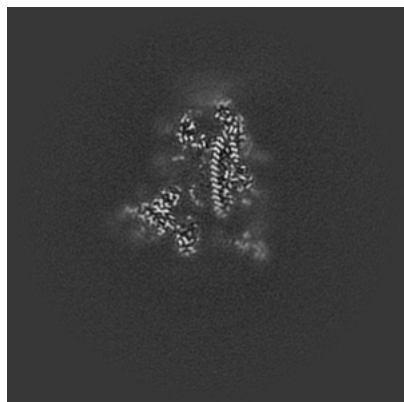


Z

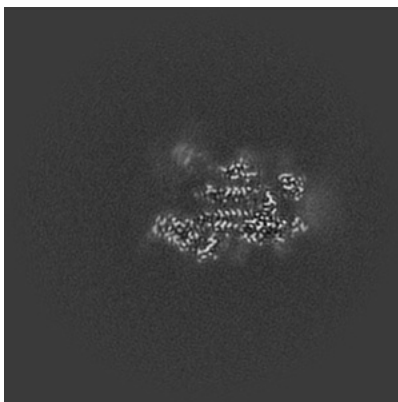
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

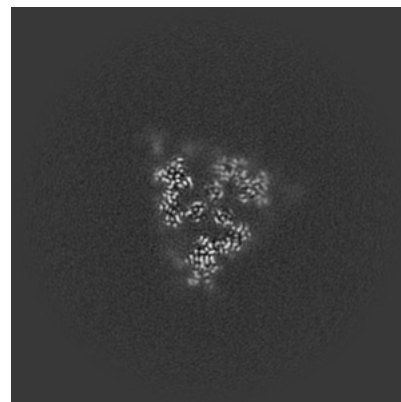
### 6.2.1 Primary map



X Index: 176

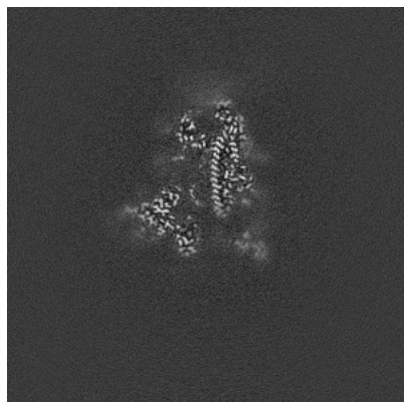


Y Index: 176

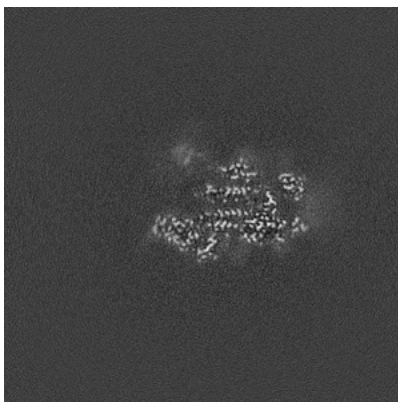


Z Index: 176

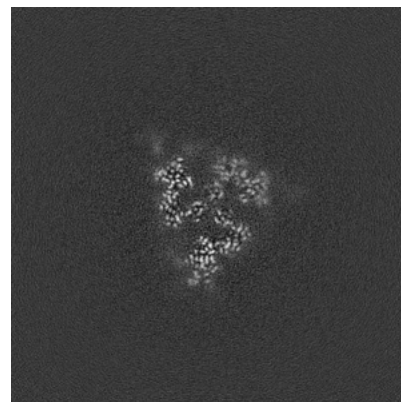
### 6.2.2 Raw map



X Index: 176



Y Index: 176



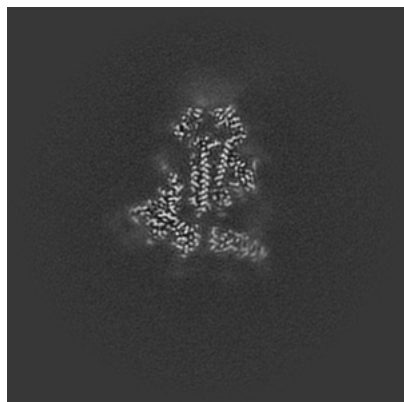
Z Index: 176

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

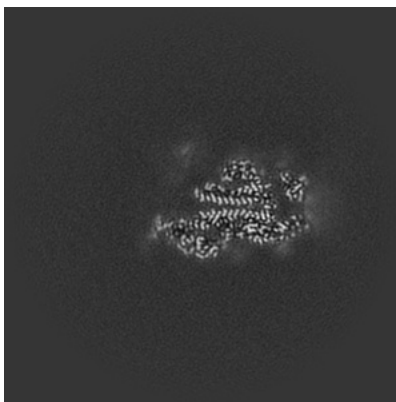


## 6.3 Largest variance slices [i](#)

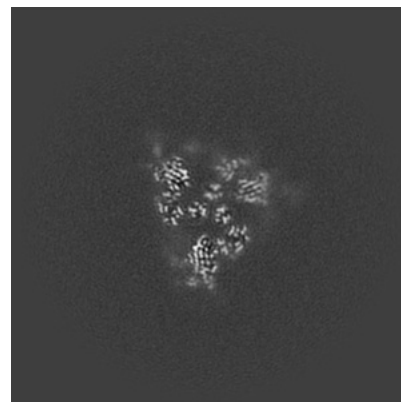
### 6.3.1 Primary map



X Index: 170

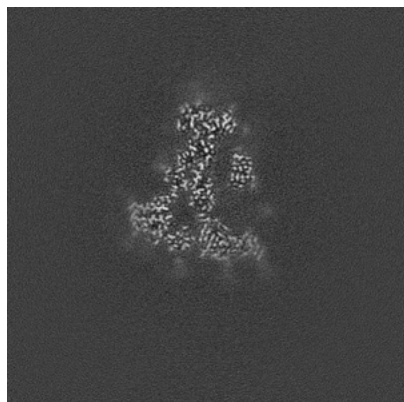


Y Index: 173

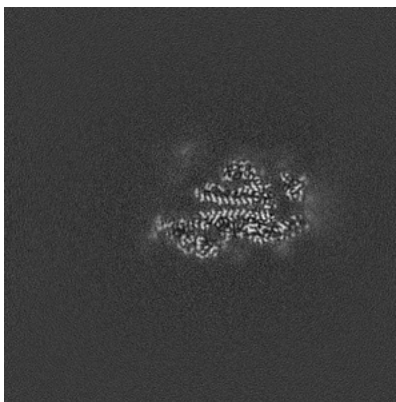


Z Index: 174

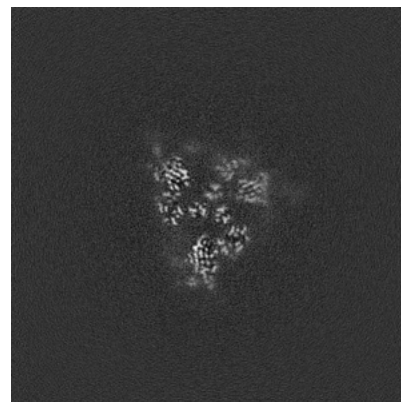
### 6.3.2 Raw map



X Index: 162



Y Index: 173



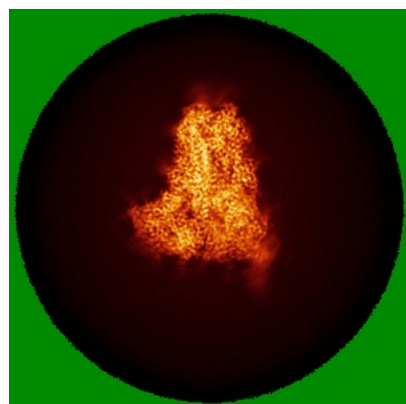
Z Index: 174

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

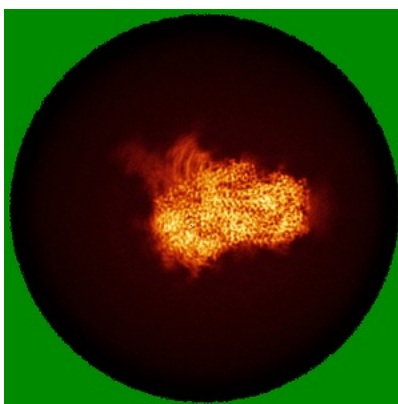


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

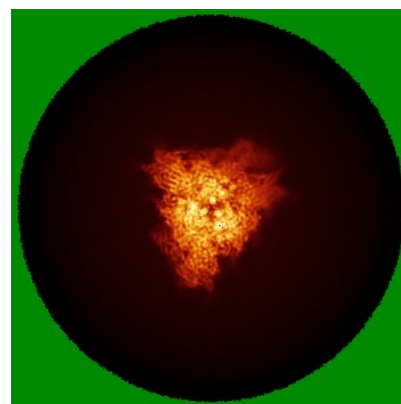
### 6.4.1 Primary map



X

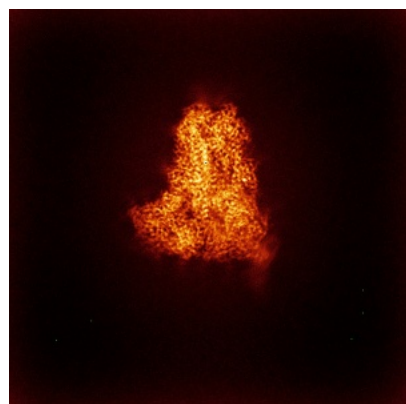


Y

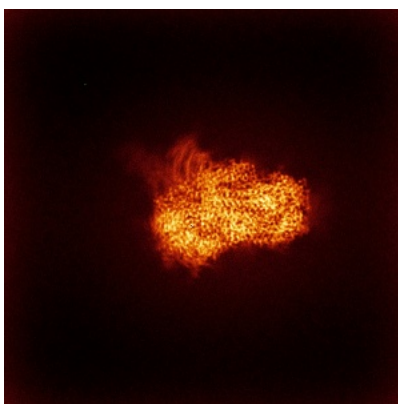


Z

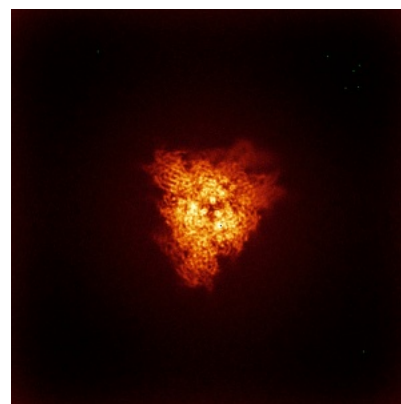
### 6.4.2 Raw map



X



Y

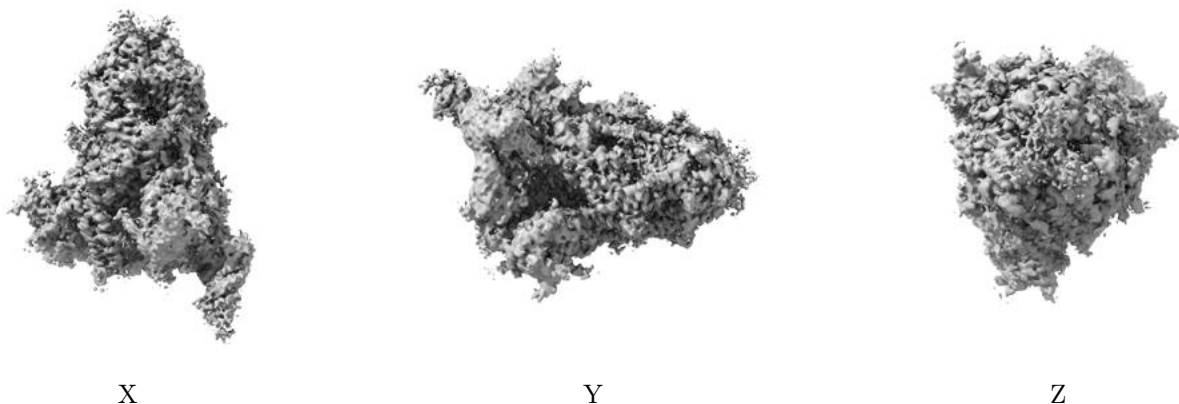


Z

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.

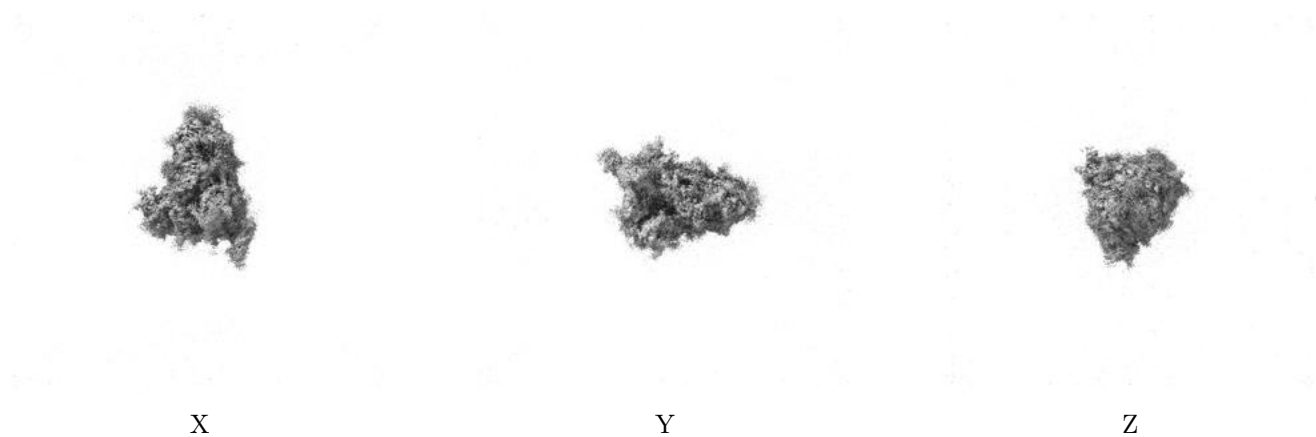
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

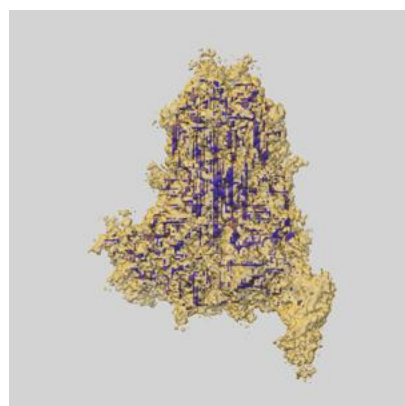
## 6.6 Mask visualisation [i](#)

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

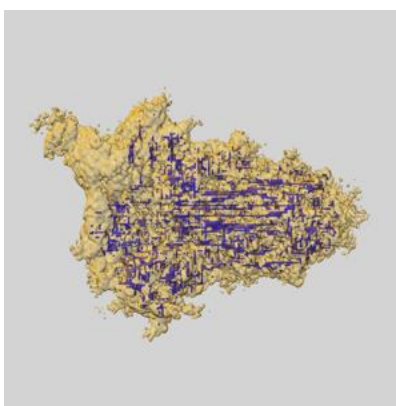
A mask typically either:

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

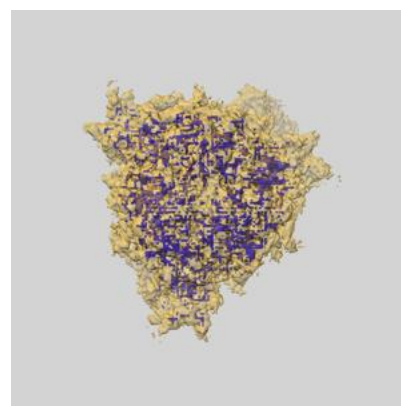
### 6.6.1 emd\_44876\_msk\_1.map [i](#)



X



Y

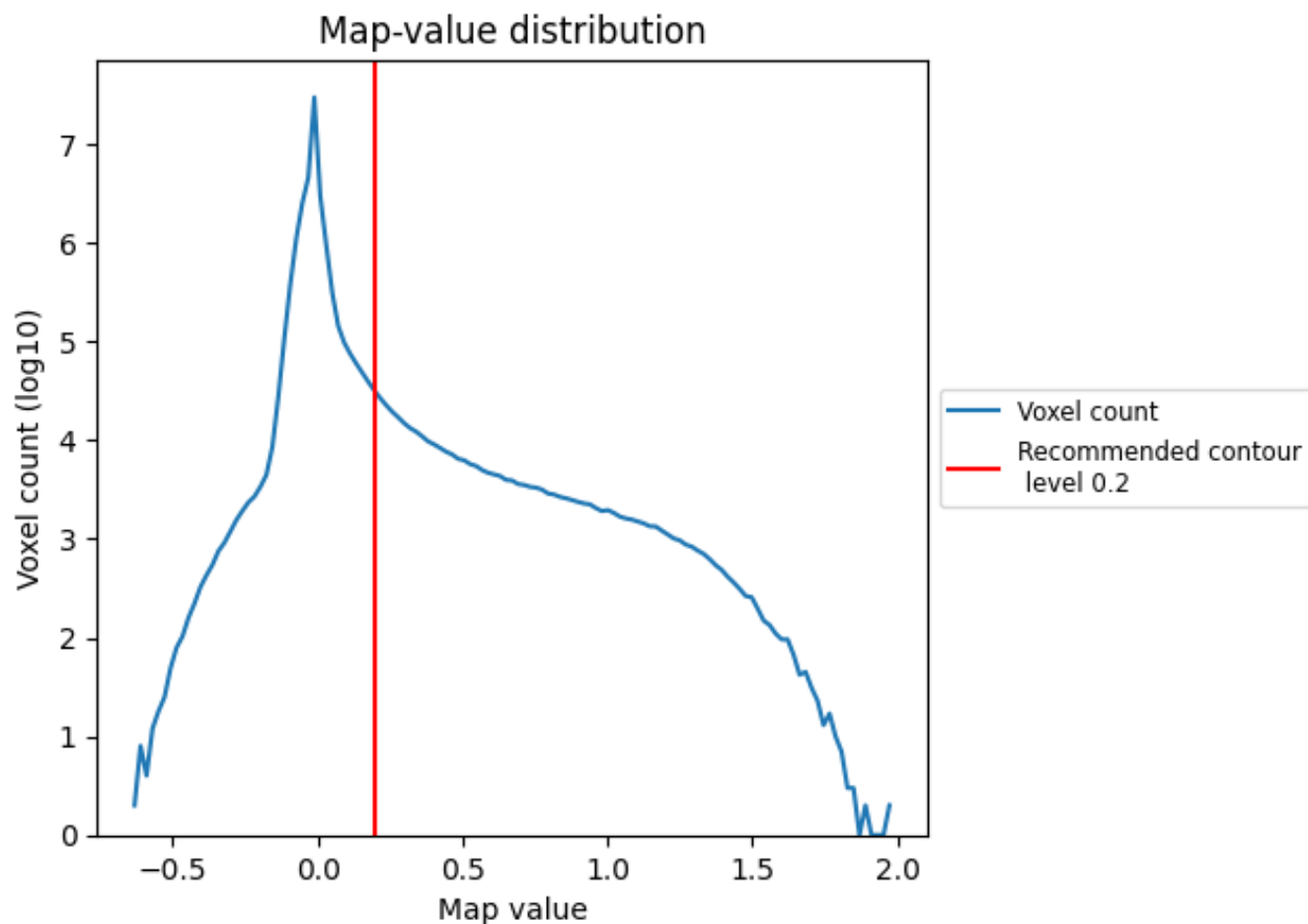


Z

## 7 Map analysis [i](#)

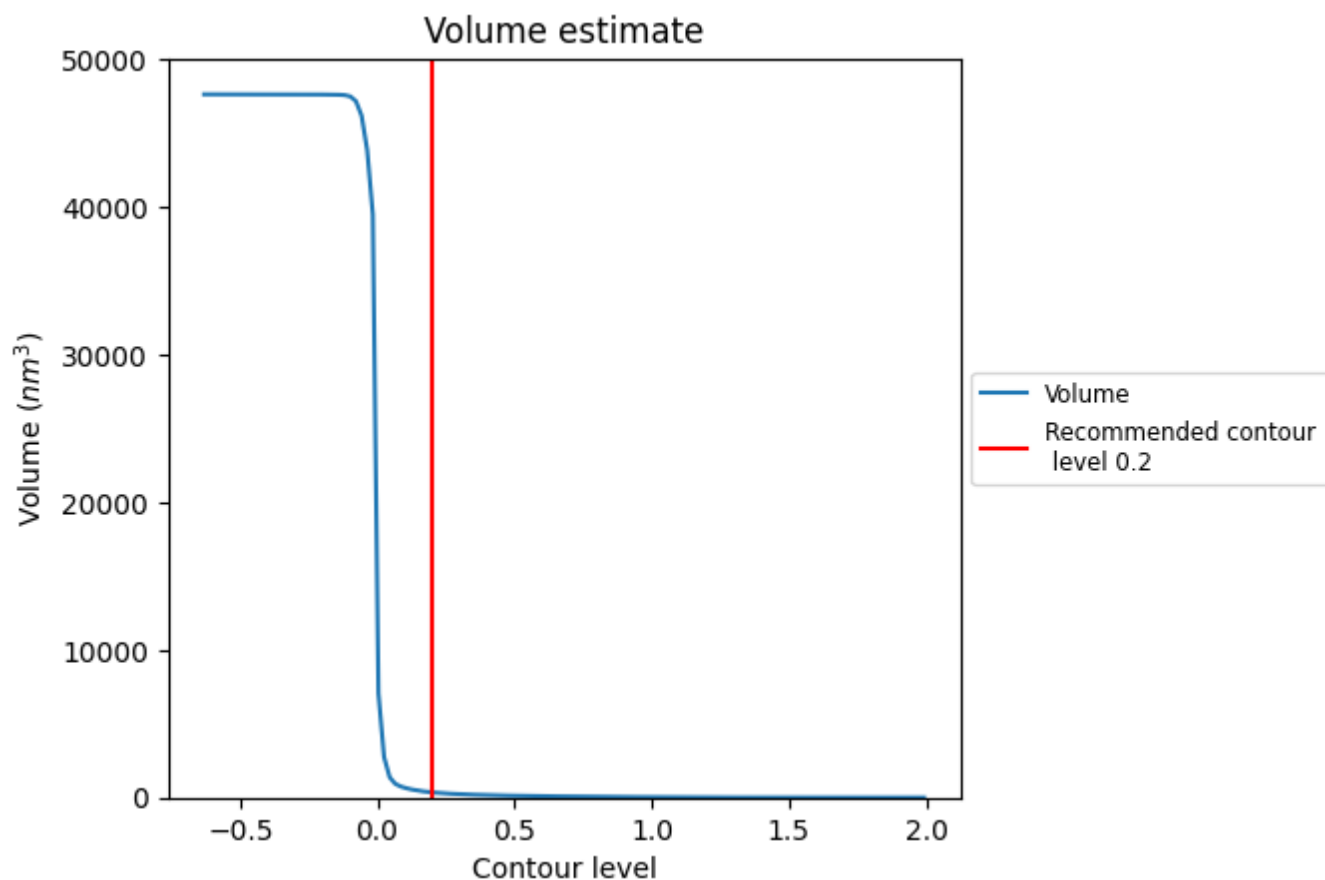
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

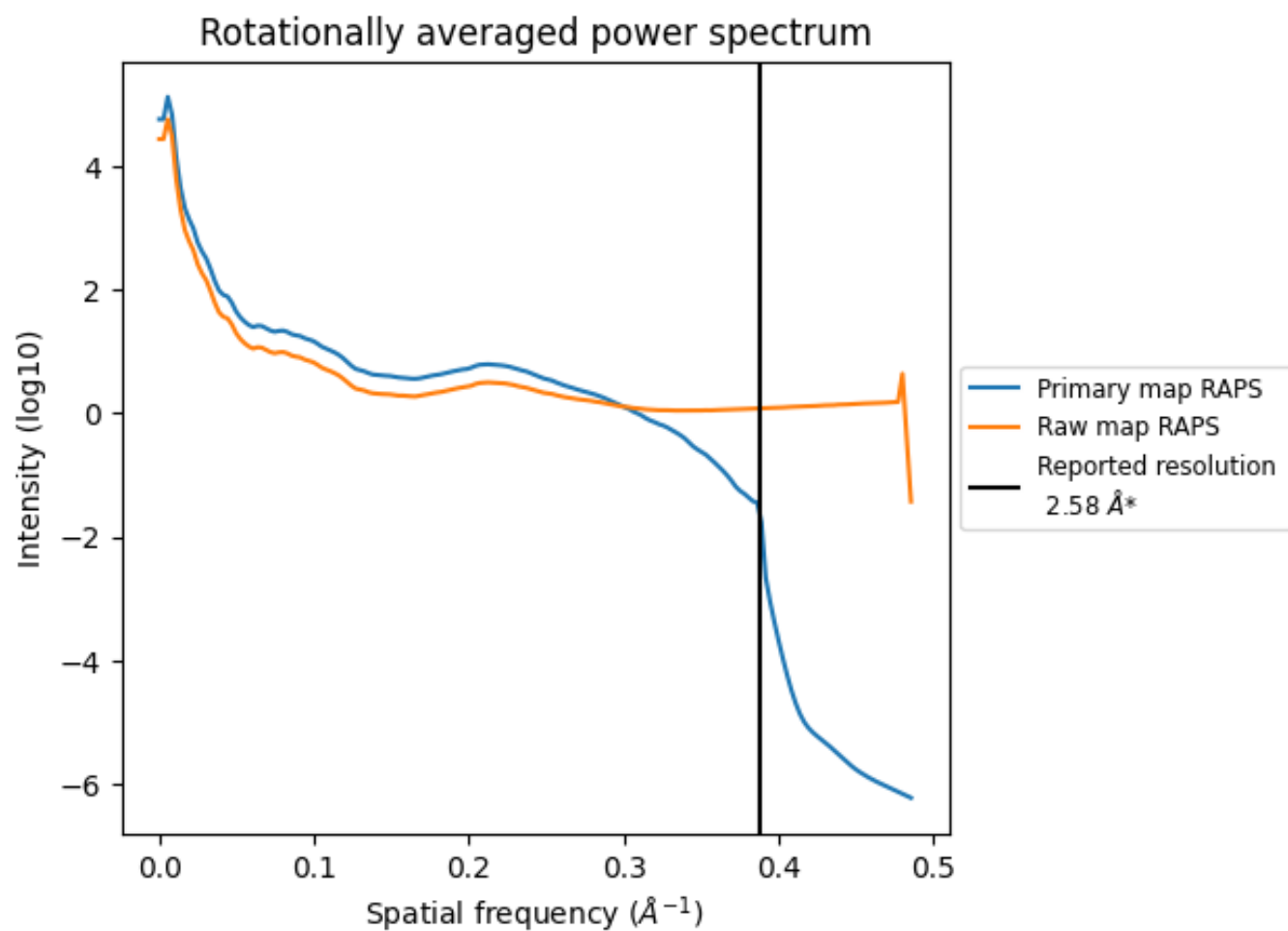
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm<sup>3</sup>; this corresponds to an approximate mass of 318 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 ⓘ

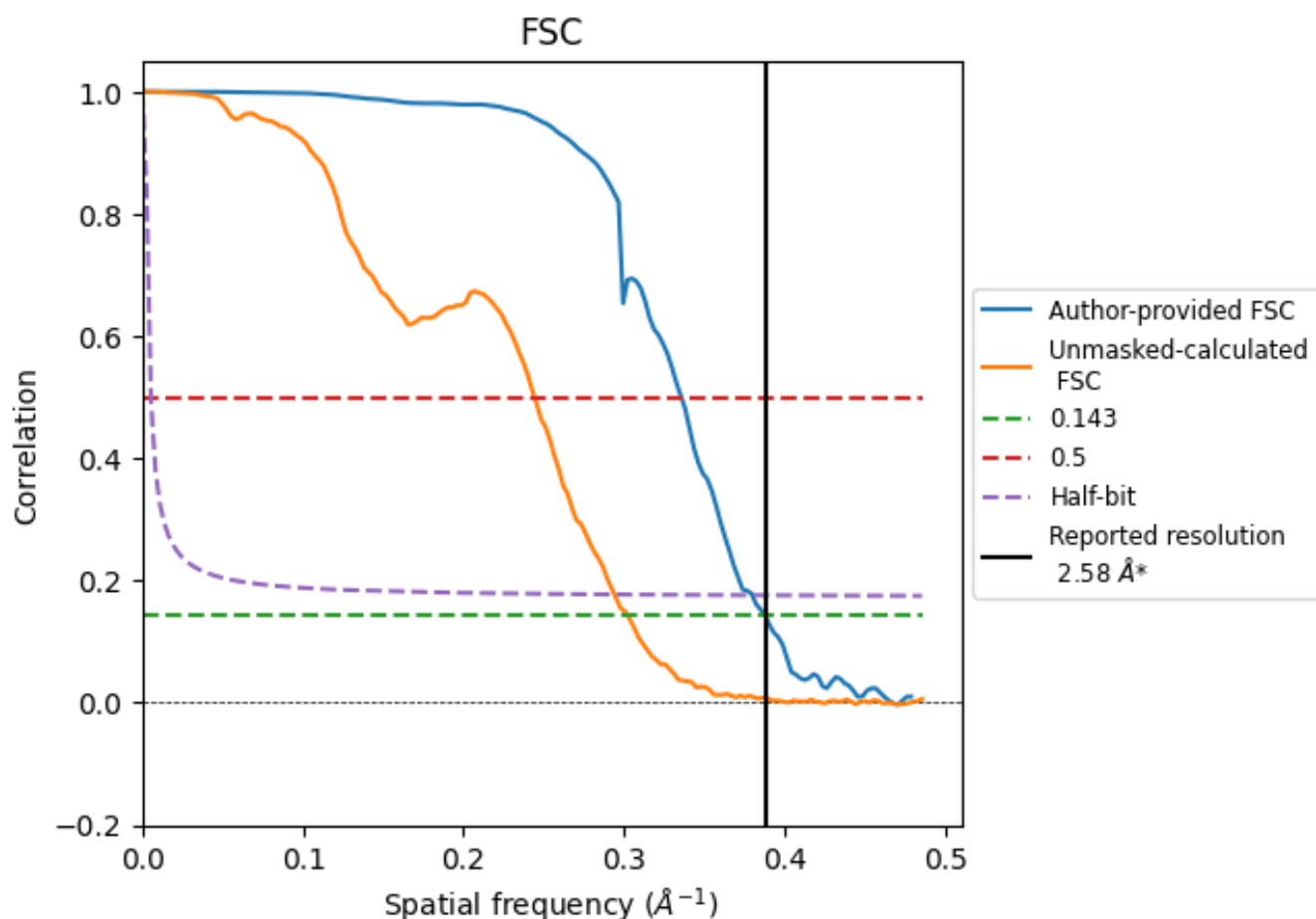


\*Reported resolution corresponds to spatial frequency of 0.388 Å<sup>-1</sup>

## 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 0.388  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.98	2.63
Unmasked-calculated*	3.31	4.10	3.40

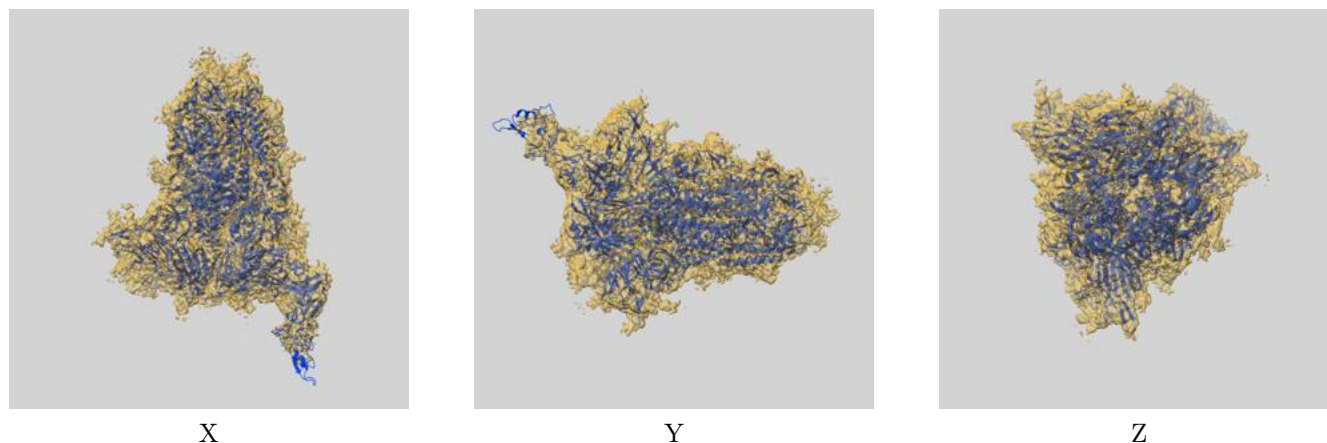
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.58 by more than 10 %



## 9 Map-model fit [i](#)

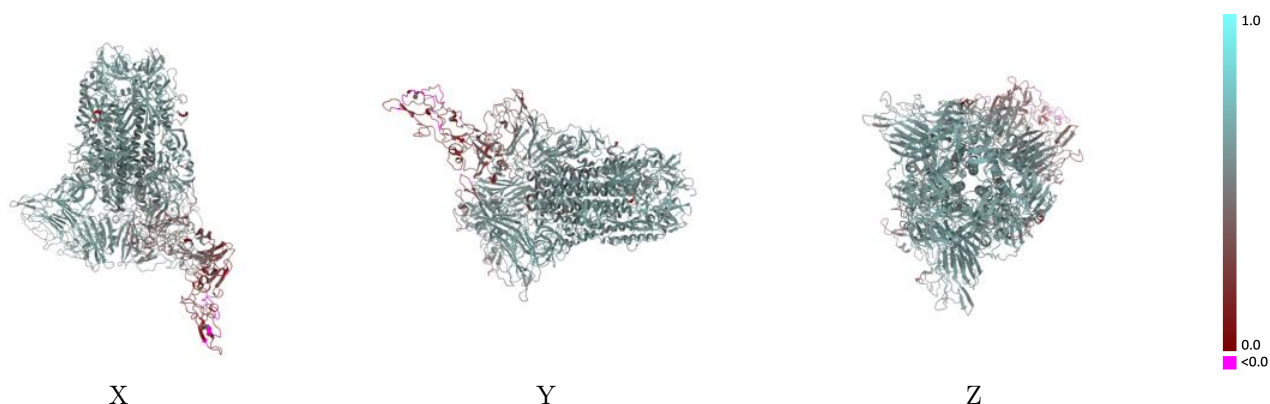
This section contains information regarding the fit between EMDB map EMD-44876 and PDB model 9BSY. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

### 9.1 Map-model overlay [i](#)



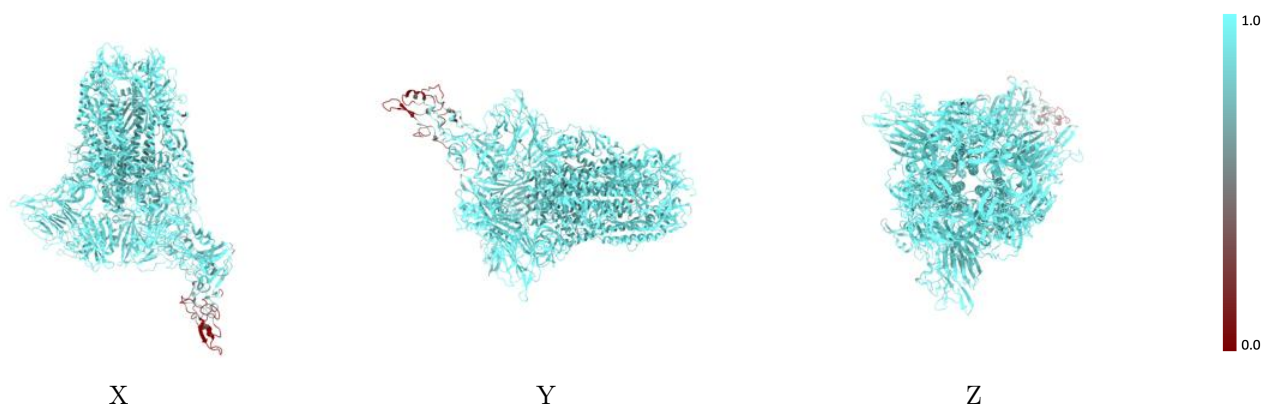
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



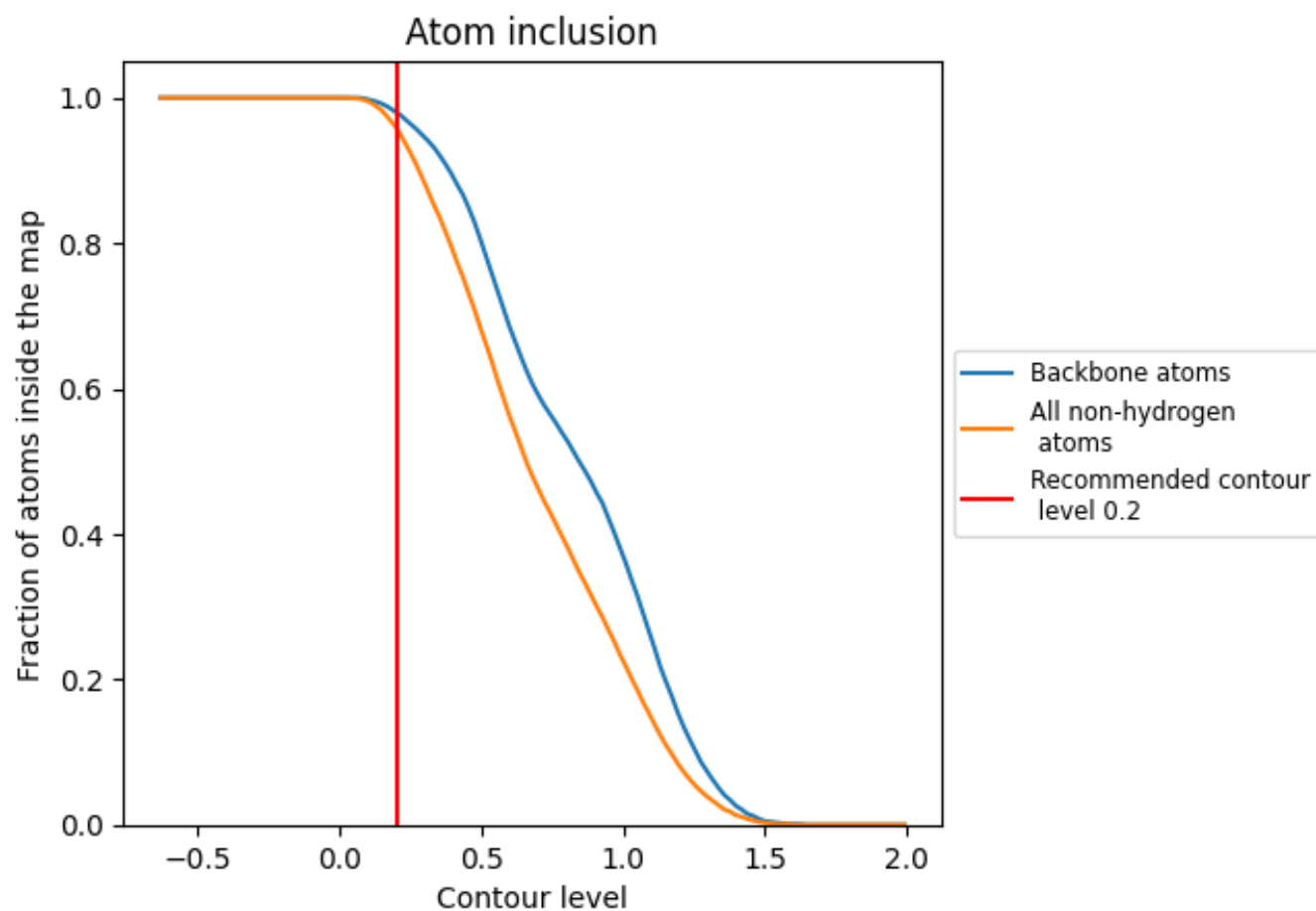
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.5310
A	 0.9160	 0.4960
B	 0.9800	 0.5360
C	 0.9820	 0.5660
D	 0.9640	 0.4710
E	 0.8570	 0.4150
F	 1.0000	 0.4500
G	 0.9290	 0.4640
H	 0.9640	 0.4950
I	 0.9290	 0.4620
J	 0.8570	 0.4000
K	 0.8210	 0.2790
L	 0.9290	 0.3860
M	 0.9640	 0.4530
N	 0.9290	 0.3940
O	 0.9290	 0.4380
P	 0.8970	 0.4660
Q	 1.0000	 0.5000
R	 0.9740	 0.4920
S	 0.8930	 0.4430
T	 0.9290	 0.4460
U	 0.8930	 0.4820
V	 0.9490	 0.4380

