



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 03:51 AM UTC

PDB ID : 7KML / pdb_00007kml
EMDB ID : EMD-22926
Title : cryo-EM structure of SARS-CoV-2 spike in complex with Fab 15033-7, three RBDs bound
Authors : Li, Z.; Rini, J.M.
Deposited on : 2020-11-03
Resolution : 3.80 Å (reported)
Based on initial models : 7KLH, 6VXX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

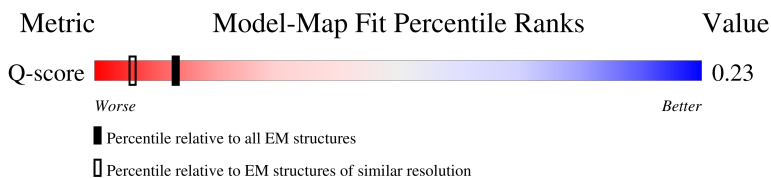
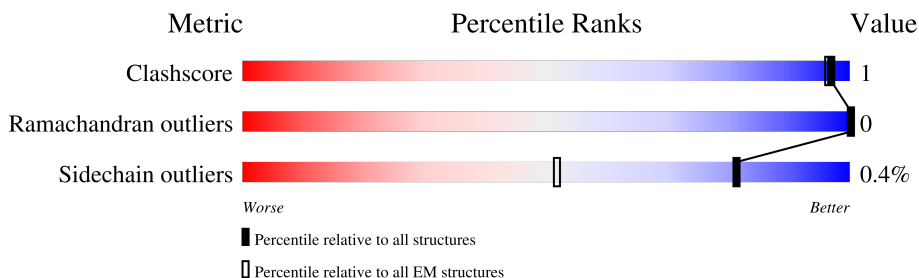
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



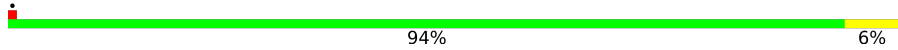
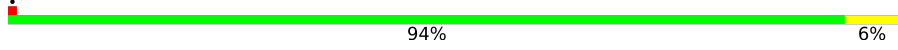
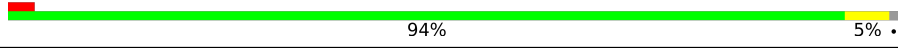
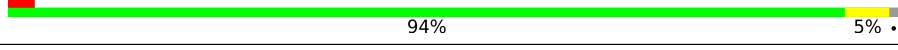
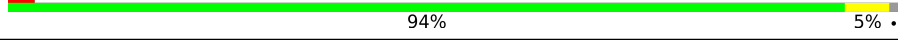
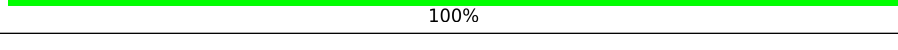
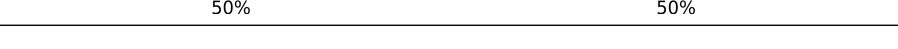
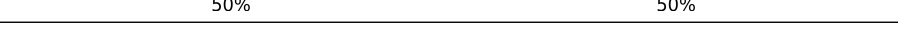
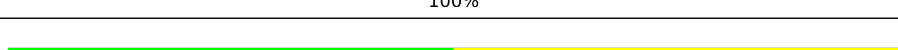
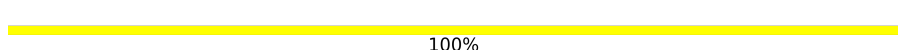
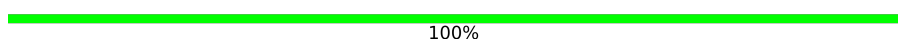
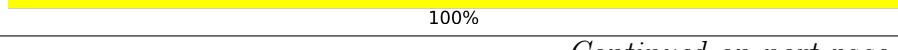
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1274	 74% 7% 19%
1	B	1274	 74% 7% 19%
1	C	1274	 75% 6% 19%
2	L	214	 94% 6%

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Mol	Chain	Length	Quality of chain
2	M	214	
2	N	214	
3	H	225	
3	I	225	
3	J	225	
4	D	2	
4	E	2	
4	K	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	
4	f	2	
4	g	2	
4	h	2	
4	i	2	

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Mol	Chain	Length	Quality of chain
4	j	2	50% 50%
5	F	3	100%
5	G	3	100%
5	U	3	100%
5	V	3	100%
5	d	3	100%
5	e	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35136 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	1034	Total	C	N	O	S	0	0
			8078	5154	1347	1539	38		
1	B	1034	Total	C	N	O	S	0	0
			8078	5154	1347	1539	38		
1	C	1034	Total	C	N	O	S	0	0
			8078	5154	1347	1539	38		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	SER	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	ASN	-	expression tag	UNP P0DTC2
A	1242	SER	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	ARG	-	expression tag	UNP P0DTC2
A	1245	ALA	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	ALA	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	LEU	-	expression tag	UNP P0DTC2
A	1257	ASN	-	expression tag	UNP P0DTC2
A	1258	ASP	-	expression tag	UNP P0DTC2
A	1259	ILE	-	expression tag	UNP P0DTC2
A	1260	PHE	-	expression tag	UNP P0DTC2
A	1261	GLU	-	expression tag	UNP P0DTC2
A	1262	ALA	-	expression tag	UNP P0DTC2
A	1263	GLN	-	expression tag	UNP P0DTC2
A	1264	LYS	-	expression tag	UNP P0DTC2
A	1265	ILE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	TRP	-	expression tag	UNP P0DTC2
A	1268	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLU	-	expression tag	UNP P0DTC2
A	1270	ASP	-	expression tag	UNP P0DTC2
A	1271	THR	-	expression tag	UNP P0DTC2
A	1272	ALA	-	expression tag	UNP P0DTC2
A	1273	ALA	-	expression tag	UNP P0DTC2
A	1274	ALA	-	expression tag	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	ASN	-	expression tag	UNP P0DTC2
B	1242	SER	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	ARG	-	expression tag	UNP P0DTC2
B	1245	ALA	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	ALA	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	LEU	-	expression tag	UNP P0DTC2
B	1257	ASN	-	expression tag	UNP P0DTC2
B	1258	ASP	-	expression tag	UNP P0DTC2
B	1259	ILE	-	expression tag	UNP P0DTC2
B	1260	PHE	-	expression tag	UNP P0DTC2
B	1261	GLU	-	expression tag	UNP P0DTC2
B	1262	ALA	-	expression tag	UNP P0DTC2
B	1263	GLN	-	expression tag	UNP P0DTC2
B	1264	LYS	-	expression tag	UNP P0DTC2
B	1265	ILE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	TRP	-	expression tag	UNP P0DTC2
B	1268	HIS	-	expression tag	UNP P0DTC2
B	1269	GLU	-	expression tag	UNP P0DTC2
B	1270	ASP	-	expression tag	UNP P0DTC2
B	1271	THR	-	expression tag	UNP P0DTC2
B	1272	ALA	-	expression tag	UNP P0DTC2
B	1273	ALA	-	expression tag	UNP P0DTC2
B	1274	ALA	-	expression tag	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	ASN	-	expression tag	UNP P0DTC2
C	1242	SER	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	ARG	-	expression tag	UNP P0DTC2
C	1245	ALA	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	ALA	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	GLY	-	expression tag	UNP P0DTC2
C	1256	LEU	-	expression tag	UNP P0DTC2
C	1257	ASN	-	expression tag	UNP P0DTC2
C	1258	ASP	-	expression tag	UNP P0DTC2
C	1259	ILE	-	expression tag	UNP P0DTC2
C	1260	PHE	-	expression tag	UNP P0DTC2
C	1261	GLU	-	expression tag	UNP P0DTC2
C	1262	ALA	-	expression tag	UNP P0DTC2
C	1263	GLN	-	expression tag	UNP P0DTC2
C	1264	LYS	-	expression tag	UNP P0DTC2
C	1265	ILE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	TRP	-	expression tag	UNP P0DTC2
C	1268	HIS	-	expression tag	UNP P0DTC2
C	1269	GLU	-	expression tag	UNP P0DTC2
C	1270	ASP	-	expression tag	UNP P0DTC2
C	1271	THR	-	expression tag	UNP P0DTC2
C	1272	ALA	-	expression tag	UNP P0DTC2
C	1273	ALA	-	expression tag	UNP P0DTC2
C	1274	ALA	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab 15033-7 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	214	Total	C	N	O	S	0	0
			1641	1024	276	335	6		
2	M	214	Total	C	N	O	S	0	0
			1641	1024	276	335	6		
2	N	214	Total	C	N	O	S	0	0
			1641	1024	276	335	6		

- Molecule 3 is a protein called Fab 15033-7 heavy chain.

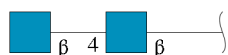
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	223	Total	C	N	O	S	0	0
			1635	1031	272	324	8		
3	I	223	Total	C	N	O	S	0	0
			1635	1031	272	324	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	223	Total	C	N	O	S	0	0
			1635	1031	272	324	8		

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



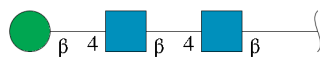
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	N	O		0	0
			28	16	2	10			
4	E	2	Total	C	N	O		0	0
			28	16	2	10			
4	K	2	Total	C	N	O		0	0
			28	16	2	10			
4	O	2	Total	C	N	O		0	0
			28	16	2	10			
4	P	2	Total	C	N	O		0	0
			28	16	2	10			
4	Q	2	Total	C	N	O		0	0
			28	16	2	10			
4	R	2	Total	C	N	O		0	0
			28	16	2	10			
4	S	2	Total	C	N	O		0	0
			28	16	2	10			
4	T	2	Total	C	N	O		0	0
			28	16	2	10			
4	W	2	Total	C	N	O		0	0
			28	16	2	10			
4	X	2	Total	C	N	O		0	0
			28	16	2	10			
4	Y	2	Total	C	N	O		0	0
			28	16	2	10			
4	Z	2	Total	C	N	O		0	0
			28	16	2	10			
4	a	2	Total	C	N	O		0	0
			28	16	2	10			
4	b	2	Total	C	N	O		0	0
			28	16	2	10			
4	c	2	Total	C	N	O		0	0
			28	16	2	10			

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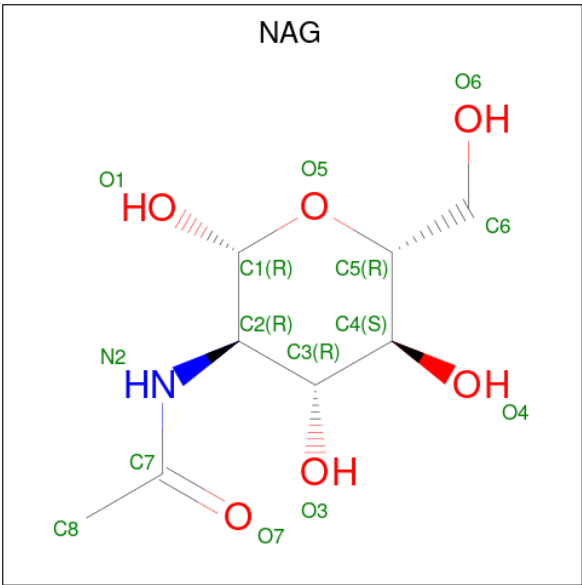
Mol	Chain	Residues	Atoms				AltConf	Trace
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	U	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	d	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

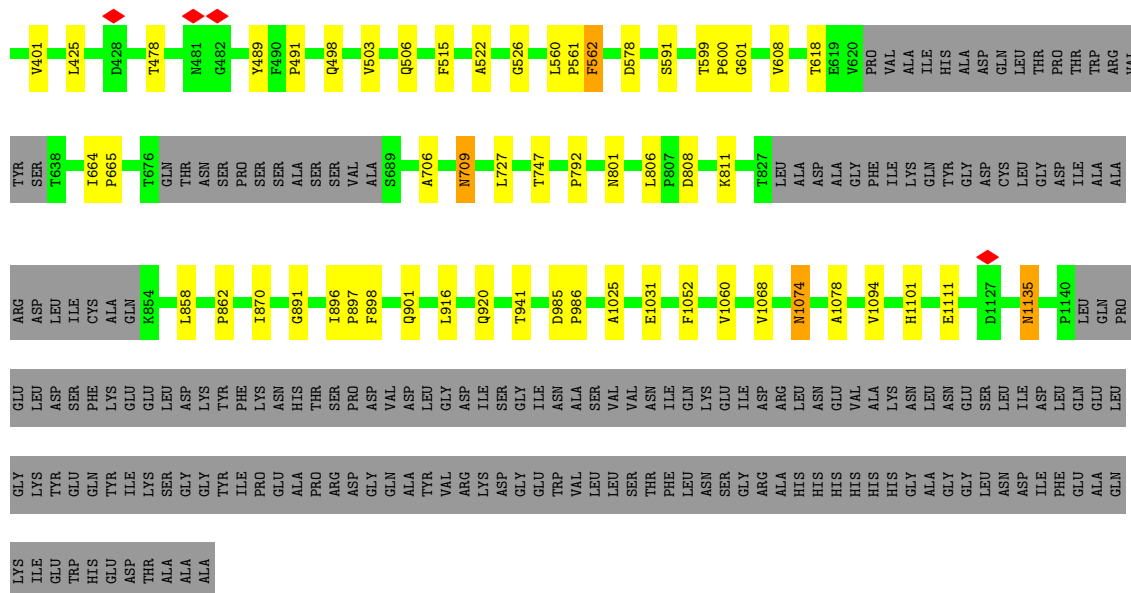


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	C	1	14	8	1	5	0

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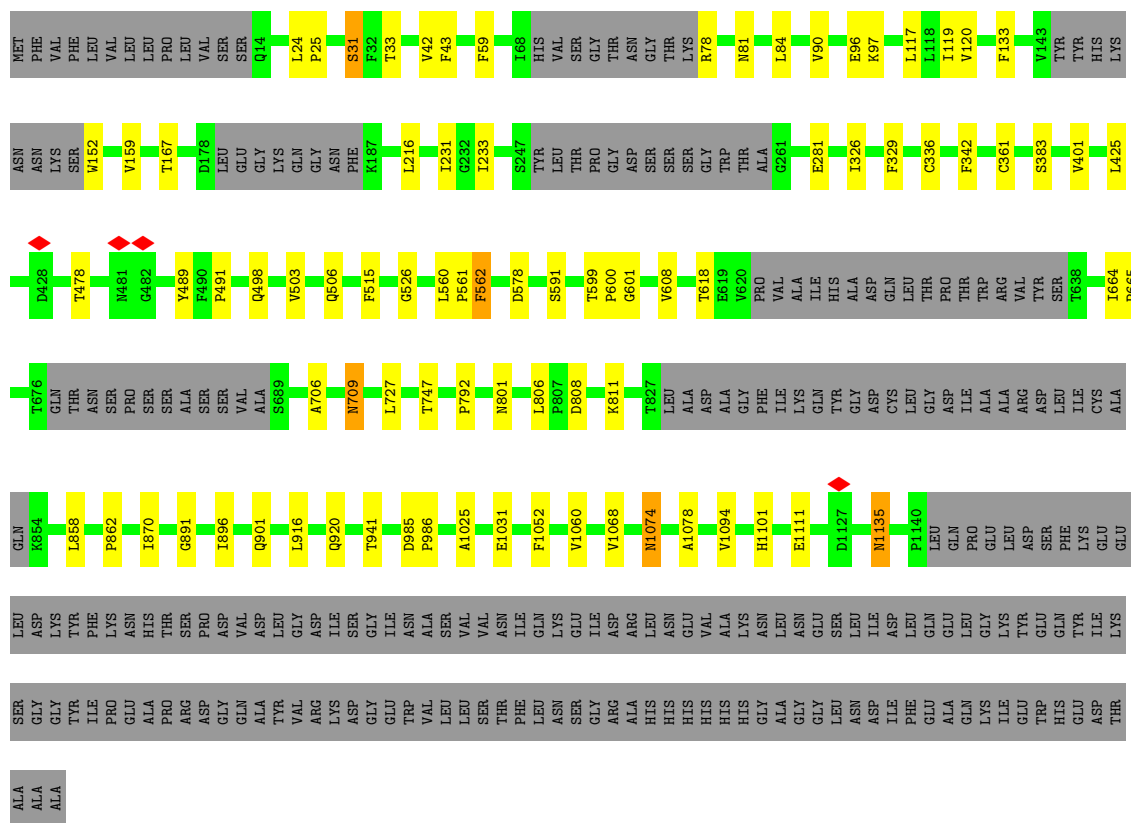
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	



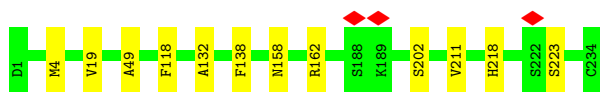
• Molecule 1: Spike glycoprotein

Chain C: 75% 6% 19%

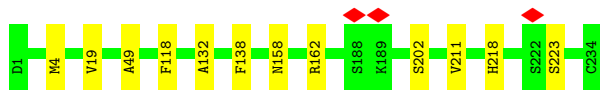


• Molecule 2: Fab 15033-7 light chain

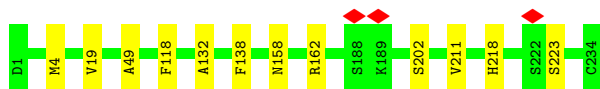
Chain L: 94% 6%



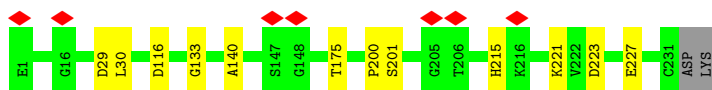
- Molecule 2: Fab 15033-7 light chain



- Molecule 2: Fab 15033-7 light chain



- Molecule 3: Fab 15033-7 heavy chain



- Molecule 3: Fab 15033-7 heavy chain



- Molecule 3: Fab 15033-7 heavy chain



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



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

Chain E:  100%



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

Chain K:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  100%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  50% 50%



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

Chain Z:  100%



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

Chain a:  50% 50%



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

Chain b:  50% 50%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain f:  50% 50%

MAG1
MAG2

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

Chain g:  50% 50%

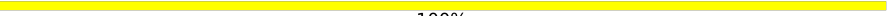
MAG1
MAG2

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

Chain h:  50% 50%

MAG1
MAG2

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

Chain i:  100%

MAG1
MAG2

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

Chain j:  50% 50%



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

Chain F:  100%



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

Chain G:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain d:  100%



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

Chain e:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	93853	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 ($e^-/\text{\AA}^2$)	38.08	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.895	Depositor
Minimum map value	-0.768	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	412.0, 412.0, 412.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	3/8263 (0.0%)	1.38	104/11247 (0.9%)
1	B	0.96	3/8263 (0.0%)	1.38	104/11247 (0.9%)
1	C	0.96	3/8263 (0.0%)	1.38	104/11247 (0.9%)
2	L	0.90	0/1676	1.34	16/2276 (0.7%)
2	M	0.90	0/1676	1.34	16/2276 (0.7%)
2	N	0.90	0/1676	1.34	16/2276 (0.7%)
3	H	0.89	1/1675 (0.1%)	1.29	12/2280 (0.5%)
3	I	0.89	1/1675 (0.1%)	1.29	12/2280 (0.5%)
3	J	0.89	1/1675 (0.1%)	1.29	12/2280 (0.5%)
All	All	0.94	12/34842 (0.0%)	1.36	396/47409 (0.8%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ARG	NE-CZ	6.74	1.40	1.33
1	C	78	ARG	NE-CZ	6.71	1.40	1.33
1	A	78	ARG	NE-CZ	6.71	1.40	1.33
3	H	215	HIS	CB-CG	-6.36	1.41	1.50
3	J	215	HIS	CB-CG	-6.36	1.41	1.50
3	I	215	HIS	CB-CG	-6.32	1.41	1.50
1	B	152	TRP	CZ2-CH2	6.19	1.49	1.37
1	A	152	TRP	CZ2-CH2	6.18	1.49	1.37
1	C	152	TRP	CZ2-CH2	6.15	1.49	1.37
1	B	152	TRP	CD2-CE3	5.62	1.49	1.40
1	A	152	TRP	CD2-CE3	5.58	1.49	1.40
1	C	152	TRP	CD2-CE3	5.57	1.49	1.40

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	LYS	N-CA-C	-9.68	102.04	114.04
1	C	97	LYS	N-CA-C	-9.68	102.04	114.04
1	B	97	LYS	N-CA-C	-9.66	102.06	114.04
1	A	336	CYS	CA-C-N	8.78	128.42	119.82
1	A	336	CYS	C-N-CA	8.78	128.42	119.82
1	C	336	CYS	CA-C-N	8.77	128.41	119.82
1	C	336	CYS	C-N-CA	8.77	128.41	119.82
1	B	336	CYS	CA-C-N	8.76	128.41	119.82
1	B	336	CYS	C-N-CA	8.76	128.41	119.82
1	A	42	VAL	N-CA-C	8.16	119.54	108.11
1	C	42	VAL	N-CA-C	8.16	119.54	108.11
1	B	42	VAL	N-CA-C	8.15	119.52	108.11
1	B	618	THR	N-CA-C	-8.08	104.29	114.56
1	A	618	THR	N-CA-C	-8.08	104.30	114.56
1	C	618	THR	N-CA-C	-8.08	104.30	114.56
1	C	231	ILE	N-CA-C	7.98	118.87	111.45
1	A	231	ILE	N-CA-C	7.96	118.85	111.45
1	B	600	PRO	CA-C-N	-7.94	112.30	119.92
1	B	600	PRO	C-N-CA	-7.94	112.30	119.92
1	A	600	PRO	CA-C-N	-7.92	112.31	119.92
1	A	600	PRO	C-N-CA	-7.92	112.31	119.92
1	C	600	PRO	CA-C-N	-7.92	112.32	119.92
1	C	600	PRO	C-N-CA	-7.92	112.32	119.92
2	N	138	PHE	CA-C-N	7.86	125.40	119.66
2	N	138	PHE	C-N-CA	7.86	125.40	119.66
1	A	561	PRO	CA-C-N	7.81	130.60	120.44
1	A	561	PRO	C-N-CA	7.81	130.60	120.44
1	B	561	PRO	CA-C-N	7.81	130.59	120.44
1	B	561	PRO	C-N-CA	7.81	130.59	120.44
1	C	561	PRO	CA-C-N	7.81	130.59	120.44
1	C	561	PRO	C-N-CA	7.81	130.59	120.44
2	L	138	PHE	CA-C-N	7.78	125.34	119.66
2	L	138	PHE	C-N-CA	7.78	125.34	119.66
2	M	138	PHE	CA-C-N	7.75	125.31	119.66
2	M	138	PHE	C-N-CA	7.75	125.31	119.66
1	A	747	THR	N-CA-C	7.68	119.65	111.28
1	C	747	THR	N-CA-C	7.68	119.65	111.28
1	B	747	THR	N-CA-C	7.65	119.61	111.28
1	B	329	PHE	CA-C-N	7.55	128.00	119.92
1	B	329	PHE	C-N-CA	7.55	128.00	119.92
1	A	329	PHE	CA-C-N	7.54	127.99	119.92
1	A	329	PHE	C-N-CA	7.54	127.99	119.92
1	C	329	PHE	CA-C-N	7.54	127.99	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	PHE	C-N-CA	7.54	127.99	119.92
1	C	664	ILE	CA-C-N	7.48	127.91	119.83
1	C	664	ILE	C-N-CA	7.48	127.91	119.83
1	B	664	ILE	CA-C-N	7.42	127.84	119.83
1	B	664	ILE	C-N-CA	7.42	127.84	119.83
1	A	664	ILE	CA-C-N	7.41	127.83	119.83
1	A	664	ILE	C-N-CA	7.41	127.83	119.83
3	I	175	THR	N-CA-C	-7.32	105.26	114.56
3	J	175	THR	N-CA-C	-7.32	105.26	114.56
3	H	175	THR	N-CA-C	-7.31	105.27	114.56
1	B	133	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	133	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	498	GLN	CA-C-N	7.16	126.86	119.56
1	A	498	GLN	C-N-CA	7.16	126.86	119.56
1	C	133	PHE	CA-CB-CG	7.15	120.95	113.80
1	C	498	GLN	CA-C-N	7.14	126.84	119.56
1	C	498	GLN	C-N-CA	7.14	126.84	119.56
1	B	498	GLN	CA-C-N	7.13	126.83	119.56
1	B	498	GLN	C-N-CA	7.13	126.83	119.56
1	A	342	PHE	N-CA-C	-7.03	98.58	109.76
1	C	342	PHE	N-CA-C	-7.02	98.59	109.76
1	B	342	PHE	N-CA-C	-7.01	98.61	109.76
1	A	808	ASP	CA-C-N	6.96	126.66	119.56
1	A	808	ASP	C-N-CA	6.96	126.66	119.56
1	B	808	ASP	CA-C-N	6.96	126.66	119.56
1	B	808	ASP	C-N-CA	6.96	126.66	119.56
1	C	808	ASP	CA-C-N	6.96	126.65	119.56
1	C	808	ASP	C-N-CA	6.96	126.65	119.56
2	L	132	ALA	CA-C-N	6.89	126.81	119.85
2	L	132	ALA	C-N-CA	6.89	126.81	119.85
1	A	1078	ALA	CA-C-N	6.89	126.52	119.56
1	A	1078	ALA	C-N-CA	6.89	126.52	119.56
1	B	1078	ALA	CA-C-N	6.89	126.52	119.56
1	B	1078	ALA	C-N-CA	6.89	126.52	119.56
1	B	231	ILE	N-CA-C	6.88	118.87	111.58
2	M	132	ALA	CA-C-N	6.87	126.79	119.85
2	M	132	ALA	C-N-CA	6.87	126.79	119.85
1	C	1078	ALA	CA-C-N	6.87	126.50	119.56
1	C	1078	ALA	C-N-CA	6.87	126.50	119.56
2	N	132	ALA	CA-C-N	6.87	126.79	119.85
2	N	132	ALA	C-N-CA	6.87	126.79	119.85
3	J	133	GLY	CA-C-N	6.86	127.03	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	133	GLY	C-N-CA	6.86	127.03	120.31
3	H	133	GLY	CA-C-N	6.84	127.01	120.31
3	H	133	GLY	C-N-CA	6.84	127.01	120.31
3	I	133	GLY	CA-C-N	6.84	127.01	120.31
3	I	133	GLY	C-N-CA	6.84	127.01	120.31
1	B	425	LEU	CA-C-N	6.70	126.66	120.03
1	B	425	LEU	C-N-CA	6.70	126.66	120.03
1	B	601	GLY	N-CA-C	-6.70	103.52	111.36
1	C	601	GLY	N-CA-C	-6.70	103.53	111.36
1	A	601	GLY	N-CA-C	-6.70	103.53	111.36
1	C	159	VAL	N-CA-C	-6.68	105.82	111.56
1	B	159	VAL	N-CA-C	-6.67	105.82	111.56
1	A	425	LEU	CA-C-N	6.67	126.63	120.03
1	A	425	LEU	C-N-CA	6.67	126.63	120.03
1	A	159	VAL	N-CA-C	-6.67	105.83	111.56
1	B	599	THR	CA-C-N	6.67	127.12	120.52
1	B	599	THR	C-N-CA	6.67	127.12	120.52
1	A	599	THR	CA-C-N	6.66	127.11	120.52
1	A	599	THR	C-N-CA	6.66	127.11	120.52
1	C	425	LEU	CA-C-N	6.66	126.62	120.03
1	C	425	LEU	C-N-CA	6.66	126.62	120.03
1	C	599	THR	CA-C-N	6.66	127.11	120.52
1	C	599	THR	C-N-CA	6.66	127.11	120.52
3	J	227	GLU	CA-C-N	6.59	126.54	119.76
3	J	227	GLU	C-N-CA	6.59	126.54	119.76
3	I	227	GLU	CA-C-N	6.55	126.51	119.76
3	I	227	GLU	C-N-CA	6.55	126.51	119.76
3	H	227	GLU	CA-C-N	6.54	126.49	119.76
3	H	227	GLU	C-N-CA	6.54	126.49	119.76
1	A	43	PHE	CA-CB-CG	6.52	120.32	113.80
1	C	43	PHE	CA-CB-CG	6.52	120.32	113.80
1	B	43	PHE	CA-CB-CG	6.52	120.32	113.80
1	A	90	VAL	N-CA-C	6.46	118.08	108.46
1	B	90	VAL	N-CA-C	6.45	118.08	108.46
1	B	43	PHE	CB-CA-C	-6.44	102.12	111.91
1	A	43	PHE	CB-CA-C	-6.44	102.12	111.91
1	C	43	PHE	CB-CA-C	-6.44	102.13	111.91
1	C	90	VAL	N-CA-C	6.43	118.04	108.46
1	A	81	ASN	CA-C-N	6.41	126.38	120.03
1	A	81	ASN	C-N-CA	6.41	126.38	120.03
1	B	81	ASN	CA-C-N	6.41	126.38	120.03
1	B	81	ASN	C-N-CA	6.41	126.38	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	19	VAL	N-CA-C	6.40	117.07	108.11
2	M	19	VAL	N-CA-C	6.40	117.07	108.11
2	N	19	VAL	N-CA-C	6.40	117.07	108.11
1	C	81	ASN	CA-C-N	6.39	126.36	120.03
1	C	81	ASN	C-N-CA	6.39	126.36	120.03
2	N	223	SER	CA-C-N	6.35	126.32	119.78
2	N	223	SER	C-N-CA	6.35	126.32	119.78
2	M	223	SER	CA-C-N	6.34	126.31	119.78
2	M	223	SER	C-N-CA	6.34	126.31	119.78
1	C	862	PRO	CA-C-N	6.33	126.24	119.85
1	C	862	PRO	C-N-CA	6.33	126.24	119.85
2	L	223	SER	CA-C-N	6.33	126.30	119.78
2	L	223	SER	C-N-CA	6.33	126.30	119.78
1	A	862	PRO	CA-C-N	6.33	126.24	119.85
1	A	862	PRO	C-N-CA	6.33	126.24	119.85
3	H	29	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	862	PRO	CA-C-N	6.32	126.23	119.85
1	B	862	PRO	C-N-CA	6.32	126.23	119.85
3	J	29	ASP	CA-CB-CG	6.32	118.92	112.60
3	I	29	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	96	GLU	N-CA-C	6.31	119.38	110.23
1	B	96	GLU	N-CA-C	6.30	119.37	110.23
1	C	96	GLU	N-CA-C	6.29	119.35	110.23
1	C	342	PHE	CB-CA-C	6.27	120.07	109.84
1	B	342	PHE	CB-CA-C	6.27	120.06	109.84
2	M	162	ARG	N-CA-C	6.26	118.92	111.71
1	A	342	PHE	CB-CA-C	6.25	120.03	109.84
2	L	162	ARG	N-CA-C	6.24	118.89	111.71
2	N	162	ARG	N-CA-C	6.23	118.87	111.71
1	B	1111	GLU	CA-C-N	6.21	125.97	119.76
1	B	1111	GLU	C-N-CA	6.21	125.97	119.76
1	C	1111	GLU	CA-C-N	6.20	125.96	119.76
1	C	1111	GLU	C-N-CA	6.20	125.96	119.76
3	I	30	LEU	N-CA-C	-6.19	105.86	113.41
3	J	30	LEU	N-CA-C	-6.19	105.86	113.41
3	H	30	LEU	N-CA-C	-6.18	105.86	113.41
1	C	361	CYS	N-CA-C	6.18	116.72	108.38
1	A	811	LYS	CA-C-N	6.17	126.62	119.47
1	A	811	LYS	C-N-CA	6.17	126.62	119.47
1	A	1111	GLU	CA-C-N	6.17	125.92	119.76
1	A	1111	GLU	C-N-CA	6.17	125.92	119.76
1	B	361	CYS	N-CA-C	6.16	116.69	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	811	LYS	CA-C-N	6.15	126.60	119.47
1	B	811	LYS	C-N-CA	6.15	126.60	119.47
1	C	811	LYS	CA-C-N	6.15	126.60	119.47
1	C	811	LYS	C-N-CA	6.15	126.60	119.47
1	A	361	CYS	N-CA-C	6.14	116.68	108.38
2	L	158	ASN	N-CA-C	6.12	119.84	111.39
2	M	158	ASN	N-CA-C	6.12	119.84	111.39
1	A	560	LEU	CA-C-N	6.12	126.57	119.47
1	A	560	LEU	C-N-CA	6.12	126.57	119.47
2	N	158	ASN	N-CA-C	6.11	119.82	111.39
1	C	560	LEU	CA-C-N	6.10	126.55	119.47
1	C	560	LEU	C-N-CA	6.10	126.55	119.47
1	B	560	LEU	CA-C-N	6.09	126.54	119.47
1	B	560	LEU	C-N-CA	6.09	126.54	119.47
3	H	116	ASP	CA-CB-CG	6.01	118.61	112.60
3	I	116	ASP	CA-CB-CG	6.00	118.60	112.60
3	J	116	ASP	CA-CB-CG	6.00	118.60	112.60
3	I	200	PRO	N-CA-C	-5.99	101.68	111.15
3	J	200	PRO	N-CA-C	-5.99	101.69	111.15
3	H	200	PRO	N-CA-C	-5.98	101.70	111.15
1	B	24	LEU	CB-CA-C	-5.95	106.98	111.20
1	C	24	LEU	CB-CA-C	-5.95	106.98	111.20
1	A	24	LEU	CB-CA-C	-5.89	107.02	111.20
1	A	727	LEU	CA-C-N	5.86	125.80	119.76
1	A	727	LEU	C-N-CA	5.86	125.80	119.76
1	C	727	LEU	CA-C-N	5.84	125.78	119.76
1	C	727	LEU	C-N-CA	5.84	125.78	119.76
1	B	727	LEU	CA-C-N	5.84	125.77	119.76
1	B	727	LEU	C-N-CA	5.84	125.77	119.76
1	C	383	SER	CA-C-N	5.84	125.97	119.32
1	C	383	SER	C-N-CA	5.84	125.97	119.32
1	B	383	SER	CA-C-N	5.83	125.97	119.32
1	B	383	SER	C-N-CA	5.83	125.97	119.32
1	B	1068	VAL	CA-C-N	5.83	125.77	119.76
1	B	1068	VAL	C-N-CA	5.83	125.77	119.76
1	B	792	PRO	CA-C-N	5.82	126.22	119.47
1	B	792	PRO	C-N-CA	5.82	126.22	119.47
1	C	792	PRO	CA-C-N	5.82	126.22	119.47
1	C	792	PRO	C-N-CA	5.82	126.22	119.47
1	A	792	PRO	CA-C-N	5.81	126.21	119.47
1	A	792	PRO	C-N-CA	5.81	126.21	119.47
1	C	1068	VAL	CA-C-N	5.81	125.74	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1068	VAL	C-N-CA	5.81	125.74	119.76
1	A	1068	VAL	CA-C-N	5.81	125.74	119.76
1	A	1068	VAL	C-N-CA	5.81	125.74	119.76
1	A	383	SER	CA-C-N	5.80	125.93	119.32
1	A	383	SER	C-N-CA	5.80	125.93	119.32
1	C	1052	PHE	CA-C-N	5.79	125.77	120.03
1	C	1052	PHE	C-N-CA	5.79	125.77	120.03
1	A	1052	PHE	CA-C-N	5.78	125.75	120.03
1	A	1052	PHE	C-N-CA	5.78	125.75	120.03
1	A	503	VAL	N-CA-C	5.77	116.51	110.62
1	B	1031	GLU	N-CA-C	5.76	117.64	111.36
1	C	1031	GLU	N-CA-C	5.75	117.63	111.36
1	C	1094	VAL	N-CA-C	5.75	116.96	108.45
1	A	489	TYR	N-CA-C	5.75	118.58	109.50
1	B	503	VAL	N-CA-C	5.75	116.48	110.62
1	C	503	VAL	N-CA-C	5.75	116.48	110.62
1	A	1031	GLU	N-CA-C	5.75	117.62	111.36
1	B	1052	PHE	CA-C-N	5.75	125.72	120.03
1	B	1052	PHE	C-N-CA	5.75	125.72	120.03
1	A	1094	VAL	N-CA-C	5.74	116.95	108.45
1	B	1094	VAL	N-CA-C	5.74	116.95	108.45
1	C	489	TYR	N-CA-C	5.74	118.57	109.50
1	A	985	ASP	CA-C-N	5.74	126.29	120.38
1	A	985	ASP	C-N-CA	5.74	126.29	120.38
1	B	489	TYR	N-CA-C	5.74	118.56	109.50
1	B	985	ASP	CA-C-N	5.73	126.28	120.38
1	B	985	ASP	C-N-CA	5.73	126.28	120.38
1	A	117	LEU	N-CA-C	5.73	117.86	108.52
1	C	117	LEU	N-CA-C	5.73	117.85	108.52
1	C	985	ASP	CA-C-N	5.72	126.27	120.38
1	C	985	ASP	C-N-CA	5.72	126.27	120.38
1	B	117	LEU	N-CA-C	5.71	117.83	108.52
1	B	120	VAL	N-CA-C	5.69	116.08	108.11
1	A	120	VAL	N-CA-C	5.68	116.06	108.11
1	C	120	VAL	N-CA-C	5.68	116.06	108.11
1	B	806	LEU	CA-C-N	5.64	125.55	119.85
1	B	806	LEU	C-N-CA	5.64	125.55	119.85
1	C	806	LEU	CA-C-N	5.64	125.55	119.85
1	C	806	LEU	C-N-CA	5.64	125.55	119.85
1	A	1135	ASN	CA-CB-CG	-5.61	106.99	112.60
1	B	1135	ASN	CA-CB-CG	-5.61	106.99	112.60
1	C	1135	ASN	CA-CB-CG	-5.61	106.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	806	LEU	CA-C-N	5.60	125.51	119.85
1	A	806	LEU	C-N-CA	5.60	125.51	119.85
1	A	526	GLY	CA-C-N	5.60	125.50	119.85
1	A	526	GLY	C-N-CA	5.60	125.50	119.85
1	C	526	GLY	CA-C-N	5.59	125.49	119.85
1	C	526	GLY	C-N-CA	5.59	125.49	119.85
1	B	526	GLY	CA-C-N	5.58	125.48	119.85
1	B	526	GLY	C-N-CA	5.58	125.48	119.85
1	B	665	PRO	N-CA-C	5.55	119.58	111.03
1	A	578	ASP	CA-C-N	5.55	125.22	119.56
1	A	578	ASP	C-N-CA	5.55	125.22	119.56
1	A	665	PRO	N-CA-C	5.53	119.55	111.03
1	C	578	ASP	CA-C-N	5.53	125.20	119.56
1	C	578	ASP	C-N-CA	5.53	125.20	119.56
1	C	665	PRO	N-CA-C	5.53	119.55	111.03
1	B	578	ASP	CA-C-N	5.52	125.19	119.56
1	B	578	ASP	C-N-CA	5.52	125.19	119.56
1	A	31	SER	N-CA-C	5.46	120.00	113.23
1	C	216	LEU	CA-C-N	5.46	125.36	119.85
1	C	216	LEU	C-N-CA	5.46	125.36	119.85
1	A	216	LEU	CA-C-N	5.46	125.36	119.85
1	A	216	LEU	C-N-CA	5.46	125.36	119.85
1	B	31	SER	N-CA-C	5.45	119.99	113.23
1	B	216	LEU	CA-C-N	5.45	125.36	119.85
1	B	216	LEU	C-N-CA	5.45	125.36	119.85
2	N	218	HIS	CA-CB-CG	5.45	119.25	113.80
1	C	31	SER	N-CA-C	5.44	119.98	113.23
1	A	591	SER	N-CA-C	5.44	118.12	110.23
1	C	591	SER	N-CA-C	5.43	118.11	110.23
1	B	591	SER	N-CA-C	5.43	118.11	110.23
2	L	218	HIS	CA-CB-CG	5.43	119.23	113.80
1	C	941	THR	CA-C-N	5.43	125.09	119.56
1	C	941	THR	C-N-CA	5.43	125.09	119.56
2	M	218	HIS	CA-CB-CG	5.42	119.22	113.80
1	B	941	THR	CA-C-N	5.38	125.05	119.56
1	B	941	THR	C-N-CA	5.38	125.05	119.56
1	A	941	THR	CA-C-N	5.38	125.04	119.56
1	A	941	THR	C-N-CA	5.38	125.04	119.56
2	L	49	ALA	CA-C-N	5.35	125.29	119.78
2	L	49	ALA	C-N-CA	5.35	125.29	119.78
2	N	202	SER	N-CA-C	-5.34	103.34	110.55
2	N	49	ALA	CA-C-N	5.34	125.28	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	49	ALA	C-N-CA	5.34	125.28	119.78
2	L	202	SER	N-CA-C	-5.34	103.34	110.55
2	M	202	SER	N-CA-C	-5.34	103.35	110.55
1	C	84	LEU	CA-C-N	5.32	125.26	119.78
1	C	84	LEU	C-N-CA	5.32	125.26	119.78
2	M	49	ALA	CA-C-N	5.31	125.25	119.78
2	M	49	ALA	C-N-CA	5.31	125.25	119.78
1	B	84	LEU	CA-C-N	5.28	125.22	119.78
1	B	84	LEU	C-N-CA	5.28	125.22	119.78
1	A	896	ILE	CA-C-N	5.28	125.29	119.90
1	A	896	ILE	C-N-CA	5.28	125.29	119.90
1	B	896	ILE	CA-C-N	5.28	125.28	119.90
1	B	896	ILE	C-N-CA	5.28	125.28	119.90
1	A	858	LEU	N-CA-C	5.27	117.34	108.96
1	C	896	ILE	CA-C-N	5.27	125.28	119.90
1	C	896	ILE	C-N-CA	5.27	125.28	119.90
1	A	84	LEU	CA-C-N	5.26	125.20	119.78
1	A	84	LEU	C-N-CA	5.26	125.20	119.78
1	C	858	LEU	N-CA-C	5.26	117.32	108.96
1	B	858	LEU	N-CA-C	5.25	117.31	108.96
1	B	515	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	25	PRO	CA-C-N	5.25	125.19	119.78
1	C	25	PRO	C-N-CA	5.25	125.19	119.78
1	B	986	PRO	N-CA-C	5.25	117.11	110.70
1	C	986	PRO	N-CA-C	5.25	117.10	110.70
1	A	25	PRO	CA-C-N	5.24	125.18	119.78
1	A	25	PRO	C-N-CA	5.24	125.18	119.78
1	B	25	PRO	CA-C-N	5.24	125.17	119.78
1	B	25	PRO	C-N-CA	5.24	125.17	119.78
1	C	515	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	901	GLN	N-CA-C	-5.23	105.66	111.36
1	A	986	PRO	N-CA-C	5.22	117.07	110.70
1	C	901	GLN	N-CA-C	-5.21	105.68	111.36
1	A	515	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	901	GLN	N-CA-C	-5.21	105.68	111.36
2	M	4	MET	N-CA-C	5.20	117.97	109.59
2	N	4	MET	N-CA-C	5.19	117.95	109.59
2	N	211	VAL	N-CA-C	5.19	115.38	108.11
2	M	211	VAL	N-CA-C	5.18	115.37	108.11
2	L	4	MET	N-CA-C	5.18	117.94	109.59
1	A	342	PHE	CA-CB-CG	-5.17	108.63	113.80
2	L	211	VAL	N-CA-C	5.16	115.33	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	PRO	N-CA-C	5.16	120.31	113.86
1	B	342	PHE	CA-CB-CG	-5.15	108.65	113.80
1	C	491	PRO	N-CA-C	5.15	120.30	113.86
1	C	119	ILE	CB-CA-C	-5.14	104.84	111.53
3	I	140	ALA	CA-C-N	5.14	125.59	120.14
3	I	140	ALA	C-N-CA	5.14	125.59	120.14
1	A	119	ILE	CB-CA-C	-5.14	104.85	111.53
1	B	119	ILE	CB-CA-C	-5.14	104.85	111.53
3	J	140	ALA	CA-C-N	5.13	125.58	120.14
3	J	140	ALA	C-N-CA	5.13	125.58	120.14
1	B	870	ILE	N-CA-C	-5.13	105.54	110.72
1	C	342	PHE	CA-CB-CG	-5.12	108.68	113.80
3	H	140	ALA	CA-C-N	5.12	125.57	120.14
3	H	140	ALA	C-N-CA	5.12	125.57	120.14
1	A	491	PRO	N-CA-C	5.12	120.26	113.86
1	C	608	VAL	N-CA-C	5.12	115.27	108.11
1	A	608	VAL	N-CA-C	5.11	115.27	108.11
1	A	281	GLU	CA-C-N	5.11	131.30	121.54
1	A	281	GLU	C-N-CA	5.11	131.30	121.54
1	C	281	GLU	CA-C-N	5.11	131.30	121.54
1	C	281	GLU	C-N-CA	5.11	131.30	121.54
2	M	118	PHE	CA-CB-CG	5.11	118.91	113.80
2	N	118	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	281	GLU	CA-C-N	5.10	131.28	121.54
1	B	281	GLU	C-N-CA	5.10	131.28	121.54
1	A	891	GLY	CA-C-N	5.10	125.01	119.76
1	A	891	GLY	C-N-CA	5.10	125.01	119.76
1	C	870	ILE	N-CA-C	-5.10	105.57	110.72
1	C	891	GLY	CA-C-N	5.10	125.01	119.76
1	C	891	GLY	C-N-CA	5.10	125.01	119.76
1	A	506	GLN	CA-C-N	5.10	125.00	119.85
1	A	506	GLN	C-N-CA	5.10	125.00	119.85
2	L	118	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	506	GLN	CA-C-N	5.08	124.98	119.85
1	C	506	GLN	C-N-CA	5.08	124.98	119.85
1	B	401	VAL	N-CA-C	5.08	115.17	107.80
1	C	401	VAL	N-CA-C	5.08	115.17	107.80
3	H	201	SER	N-CA-C	5.08	117.56	111.71
3	I	201	SER	N-CA-C	5.08	117.56	111.71
1	A	401	VAL	N-CA-C	5.08	115.17	107.80
1	B	506	GLN	CA-C-N	5.08	124.98	119.85
1	B	506	GLN	C-N-CA	5.08	124.98	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	608	VAL	N-CA-C	5.08	115.22	108.11
3	J	201	SER	N-CA-C	5.08	117.55	111.71
1	A	870	ILE	N-CA-C	-5.07	105.60	110.72
1	B	891	GLY	CA-C-N	5.06	124.97	119.76
1	B	891	GLY	C-N-CA	5.06	124.97	119.76
1	C	326	ILE	N-CA-C	5.06	115.14	107.75
1	A	478	THR	CA-C-N	5.05	124.98	119.78
1	A	478	THR	C-N-CA	5.05	124.98	119.78
1	B	326	ILE	N-CA-C	5.05	115.12	107.75
1	A	326	ILE	N-CA-C	5.05	115.12	107.75
1	B	478	THR	CA-C-N	5.03	124.96	119.78
1	B	478	THR	C-N-CA	5.03	124.96	119.78
1	C	478	THR	CA-C-N	5.03	124.97	119.78
1	C	478	THR	C-N-CA	5.03	124.97	119.78
1	A	233	ILE	N-CA-C	5.02	115.20	108.17
1	C	233	ILE	N-CA-C	5.02	115.19	108.17
1	B	233	ILE	N-CA-C	5.01	115.19	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8078	0	7873	15	0
1	B	8078	0	7873	15	0
1	C	8078	0	7873	12	0
2	L	1641	0	1594	0	0
2	M	1641	0	1594	0	0
2	N	1641	0	1594	0	0
3	H	1635	0	1586	1	0
3	I	1635	0	1586	1	0
3	J	1635	0	1586	1	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	K	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	1	0
4	R	28	0	25	2	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	2	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	i	28	0	25	1	0
4	j	28	0	25	2	0
5	F	39	0	34	0	0
5	G	39	0	34	0	0
5	U	39	0	34	0	0
5	V	39	0	34	0	0
5	d	39	0	34	0	0
5	e	39	0	34	0	0
6	A	84	0	78	1	0
6	B	84	0	78	1	0
6	C	84	0	78	1	0
All	All	35136	0	34122	45	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 (45) 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:709:ASN:C	1:A:709:ASN:HD22	2.05	0.65
1:B:709:ASN:HD22	1:B:709:ASN:C	2.05	0.64
1:C:709:ASN:C	1:C:709:ASN:HD22	2.05	0.62
3:I:221:LYS:NZ	3:I:223:ASP:OD2	2.42	0.53
3:H:221:LYS:NZ	3:H:223:ASP:OD2	2.42	0.53
3:J:221:LYS:NZ	3:J:223:ASP:OD2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:ASN:OD1	1:A:1074:ASN:N	2.45	0.50
1:B:1074:ASN:N	1:B:1074:ASN:OD1	2.45	0.50
1:B:167:THR:OG1	6:B:1302:NAG:H62	2.12	0.50
1:A:167:THR:OG1	6:A:1302:NAG:H62	2.12	0.49
1:C:1074:ASN:N	1:C:1074:ASN:OD1	2.45	0.49
1:C:167:THR:OG1	6:C:1302:NAG:H62	2.12	0.49
1:A:33:THR:HG23	1:A:59:PHE:CZ	2.48	0.48
1:B:33:THR:HG23	1:B:59:PHE:CZ	2.48	0.48
1:B:31:SER:O	1:B:59:PHE:HA	2.13	0.48
1:B:1101:HIS:HD2	4:a:1:NAG:H5	1.79	0.48
1:C:1101:HIS:HD2	4:j:1:NAG:H5	1.79	0.48
1:A:1101:HIS:HD2	4:R:1:NAG:H5	1.79	0.48
1:C:31:SER:O	1:C:59:PHE:HA	2.13	0.48
1:C:33:THR:HG23	1:C:59:PHE:CZ	2.48	0.47
1:A:31:SER:O	1:A:59:PHE:HA	2.13	0.47
1:C:916:LEU:O	1:C:920:GLN:N	2.49	0.46
1:B:916:LEU:O	1:B:920:GLN:N	2.49	0.46
1:A:916:LEU:O	1:A:920:GLN:N	2.49	0.45
1:A:706:ALA:H	4:Q:1:NAG:H62	1.82	0.45
1:B:706:ALA:H	4:Z:1:NAG:H62	1.82	0.44
1:C:706:ALA:H	4:i:1:NAG:H62	1.82	0.44
1:A:1101:HIS:CD2	4:R:1:NAG:H5	2.55	0.42
1:A:220:PHE:CD2	1:A:220:PHE:C	2.98	0.42
1:B:562:PHE:CD1	1:B:562:PHE:C	2.98	0.42
1:C:562:PHE:CD1	1:C:562:PHE:C	2.98	0.42
1:B:1101:HIS:CD2	4:a:1:NAG:H5	2.55	0.41
1:C:1101:HIS:CD2	4:j:1:NAG:H5	2.55	0.41
1:B:709:ASN:C	1:B:709:ASN:ND2	2.77	0.41
1:B:1025:ALA:HB1	1:B:1060:VAL:HG11	2.02	0.41
1:C:1025:ALA:HB1	1:C:1060:VAL:HG11	2.02	0.41
1:A:562:PHE:CD1	1:A:562:PHE:C	2.98	0.41
1:A:1025:ALA:HB1	1:A:1060:VAL:HG11	2.02	0.41
1:A:393:THR:HA	1:A:522:ALA:HA	2.03	0.41
1:B:165:ASN:O	1:B:165:ASN:ND2	2.54	0.41
1:B:393:THR:HA	1:B:522:ALA:HA	2.03	0.41
1:C:709:ASN:C	1:C:709:ASN:ND2	2.77	0.41
1:A:897:PRO:O	1:A:898:PHE:C	2.63	0.40
1:A:165:ASN:ND2	1:A:165:ASN:O	2.54	0.40
1:B:897:PRO:O	1:B:898:PHE:C	2.63	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	1018/1274 (80%)	998 (98%)	20 (2%)	0	100	100
1	B	1018/1274 (80%)	998 (98%)	20 (2%)	0	100	100
1	C	1018/1274 (80%)	998 (98%)	20 (2%)	0	100	100
2	L	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
2	M	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
2	N	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
3	H	221/225 (98%)	216 (98%)	5 (2%)	0	100	100
3	I	221/225 (98%)	216 (98%)	5 (2%)	0	100	100
3	J	221/225 (98%)	216 (98%)	5 (2%)	0	100	100
All	All	4353/5139 (85%)	4272 (98%)	81 (2%)	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	907/1107 (82%)	902 (99%)	5 (1%)	78	79
1	B	907/1107 (82%)	902 (99%)	5 (1%)	78	79
1	C	907/1107 (82%)	902 (99%)	5 (1%)	78	79
2	L	189/189 (100%)	189 (100%)	0	100	100
2	M	189/189 (100%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	189/189 (100%)	189 (100%)	0	100	100
3	H	177/179 (99%)	177 (100%)	0	100	100
3	I	177/179 (99%)	177 (100%)	0	100	100
3	J	177/179 (99%)	177 (100%)	0	100	100
All	All	3819/4425 (86%)	3804 (100%)	15 (0%)	81	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	562	PHE
1	A	709	ASN
1	A	801	ASN
1	A	1074	ASN
1	A	1135	ASN
1	B	562	PHE
1	B	709	ASN
1	B	801	ASN
1	B	1074	ASN
1	B	1135	ASN
1	C	562	PHE
1	C	709	ASN
1	C	801	ASN
1	C	1074	ASN
1	C	1135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	239	GLN
1	A	360	ASN
1	A	762	GLN
1	A	955	ASN
1	A	965	GLN
1	A	1011	GLN
1	A	1101	HIS
1	B	49	HIS
1	B	360	ASN
1	B	762	GLN
1	B	955	ASN

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Mol	Chain	Res	Type
1	B	965	GLN
1	B	1011	GLN
1	B	1101	HIS
1	C	49	HIS
1	C	360	ASN
1	C	450	ASN
1	C	762	GLN
1	C	955	ASN
1	C	965	GLN
1	C	1011	GLN
1	C	1101	HIS
2	L	44	GLN
3	H	44	GLN
2	M	44	GLN
3	I	44	GLN

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 ⓘ

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.39	0	17,19,21	1.43	1 (5%)
4	NAG	D	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	NAG	E	1	1,4	14,14,15	0.43	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.61	0
5	NAG	F	1	1,5	14,14,15	0.39	0	17,19,21	0.60	0
5	NAG	F	2	5	14,14,15	0.34	0	17,19,21	0.77	0
5	BMA	F	3	5	11,11,12	0.26	0	15,15,17	0.63	0
5	NAG	G	1	1,5	14,14,15	0.28	0	17,19,21	0.73	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.54	0
5	BMA	G	3	5	11,11,12	0.29	0	15,15,17	0.57	0
4	NAG	K	1	1,4	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.69	0
4	NAG	O	1	1,4	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
4	NAG	O	2	4	14,14,15	0.33	0	17,19,21	0.62	0
4	NAG	P	1	1,4	14,14,15	0.34	0	17,19,21	0.76	0
4	NAG	P	2	4	14,14,15	0.39	0	17,19,21	2.17	2 (11%)
4	NAG	Q	1	1,4	14,14,15	0.34	0	17,19,21	0.82	0
4	NAG	Q	2	4	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
4	NAG	R	1	1,4	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	R	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	S	1	1,4	14,14,15	0.39	0	17,19,21	1.43	1 (5%)
4	NAG	S	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	NAG	T	1	1,4	14,14,15	0.43	0	17,19,21	0.71	0
4	NAG	T	2	4	14,14,15	0.32	0	17,19,21	0.61	0
5	NAG	U	1	1,5	14,14,15	0.39	0	17,19,21	0.60	0
5	NAG	U	2	5	14,14,15	0.34	0	17,19,21	0.77	0
5	BMA	U	3	5	11,11,12	0.26	0	15,15,17	0.63	0
5	NAG	V	1	1,5	14,14,15	0.28	0	17,19,21	0.73	0
5	NAG	V	2	5	14,14,15	0.31	0	17,19,21	0.54	0
5	BMA	V	3	5	11,11,12	0.29	0	15,15,17	0.57	0
4	NAG	W	1	1,4	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
4	NAG	W	2	4	14,14,15	0.31	0	17,19,21	0.68	0
4	NAG	X	1	1,4	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
4	NAG	X	2	4	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	Y	1	1,4	14,14,15	0.35	0	17,19,21	0.76	0
4	NAG	Y	2	4	14,14,15	0.39	0	17,19,21	2.17	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.34	0	17,19,21	0.82	0
4	NAG	Z	2	4	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
4	NAG	a	1	1,4	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	a	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	b	1	1,4	14,14,15	0.39	0	17,19,21	1.43	1 (5%)
4	NAG	b	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	NAG	c	1	1,4	14,14,15	0.42	0	17,19,21	0.71	0
4	NAG	c	2	4	14,14,15	0.34	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	d	1	1,5	14,14,15	0.39	0	17,19,21	0.60	0
5	NAG	d	2	5	14,14,15	0.34	0	17,19,21	0.77	0
5	BMA	d	3	5	11,11,12	0.27	0	15,15,17	0.63	0
5	NAG	e	1	1,5	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	e	2	5	14,14,15	0.31	0	17,19,21	0.54	0
5	BMA	e	3	5	11,11,12	0.29	0	15,15,17	0.57	0
4	NAG	f	1	1,4	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
4	NAG	f	2	4	14,14,15	0.30	0	17,19,21	0.69	0
4	NAG	g	1	1,4	14,14,15	0.32	0	17,19,21	0.97	1 (5%)
4	NAG	g	2	4	14,14,15	0.32	0	17,19,21	0.63	0
4	NAG	h	1	1,4	14,14,15	0.34	0	17,19,21	0.76	0
4	NAG	h	2	4	14,14,15	0.39	0	17,19,21	2.17	2 (11%)
4	NAG	i	1	1,4	14,14,15	0.35	0	17,19,21	0.81	0
4	NAG	i	2	4	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
4	NAG	j	1	1,4	14,14,15	0.29	0	17,19,21	0.60	0
4	NAG	j	2	4	14,14,15	0.31	0	17,19,21	0.64	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
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	6/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	h	2	4	-	6/6/23/26	0/1/1/1
4	NAG	i	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
4	NAG	j	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	2	NAG	C2-N2-C7	7.32	132.72	122.90
4	h	2	NAG	C2-N2-C7	7.32	132.71	122.90
4	Y	2	NAG	C2-N2-C7	7.32	132.71	122.90
4	h	2	NAG	C8-C7-N2	3.64	122.15	116.12
4	P	2	NAG	C8-C7-N2	3.63	122.13	116.12
4	Y	2	NAG	C8-C7-N2	3.62	122.13	116.12
4	b	1	NAG	C2-N2-C7	3.21	127.21	122.90
4	S	1	NAG	C2-N2-C7	3.20	127.19	122.90
4	D	1	NAG	C2-N2-C7	3.20	127.19	122.90
4	g	1	NAG	O5-C1-C2	-2.77	107.00	111.29
4	O	1	NAG	O5-C1-C2	-2.77	107.01	111.29
4	X	1	NAG	O5-C1-C2	-2.76	107.03	111.29
4	f	1	NAG	C1-O5-C5	-2.42	108.94	112.19
4	K	1	NAG	C1-O5-C5	-2.40	108.97	112.19
4	W	1	NAG	C1-O5-C5	-2.39	108.98	112.19
4	Q	2	NAG	C1-O5-C5	2.32	115.30	112.19
4	i	2	NAG	C1-O5-C5	2.32	115.29	112.19
4	Z	2	NAG	C1-O5-C5	2.31	115.28	112.19

There are no chirality outliers.

All (126) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	i	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	i	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
5	d	3	BMA	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
5	U	3	BMA	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	V	3	BMA	C4-C5-C6-O6
5	e	3	BMA	C4-C5-C6-O6
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	h	1	NAG	C8-C7-N2-C2
4	h	1	NAG	O7-C7-N2-C2
4	h	2	NAG	C8-C7-N2-C2
4	h	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6

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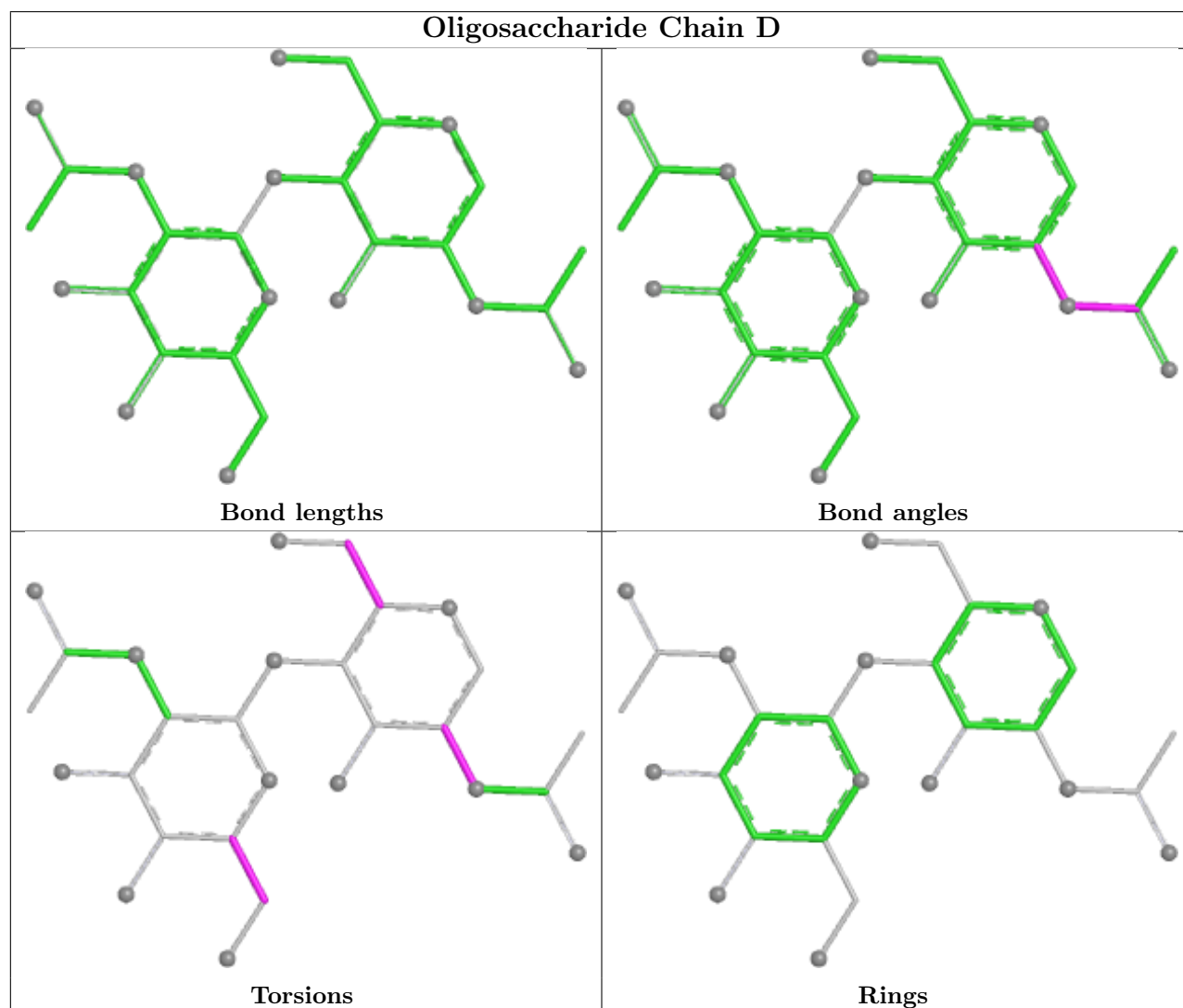
Mol	Chain	Res	Type	Atoms
4	g	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
5	e	2	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
4	R	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
4	S	1	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
4	b	1	NAG	C1-C2-N2-C7
4	h	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	h	2	NAG	C3-C2-N2-C7

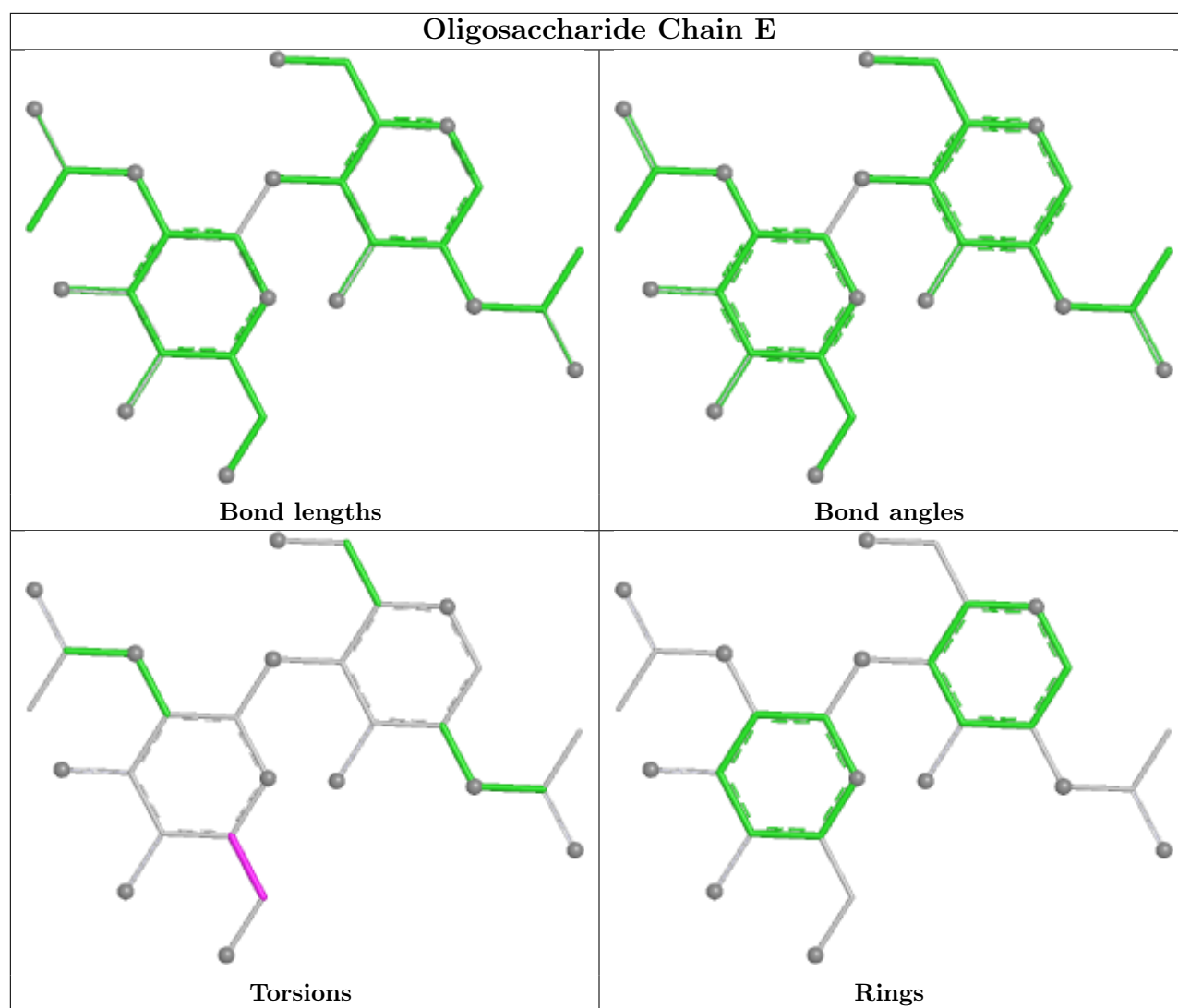
There are no ring outliers.

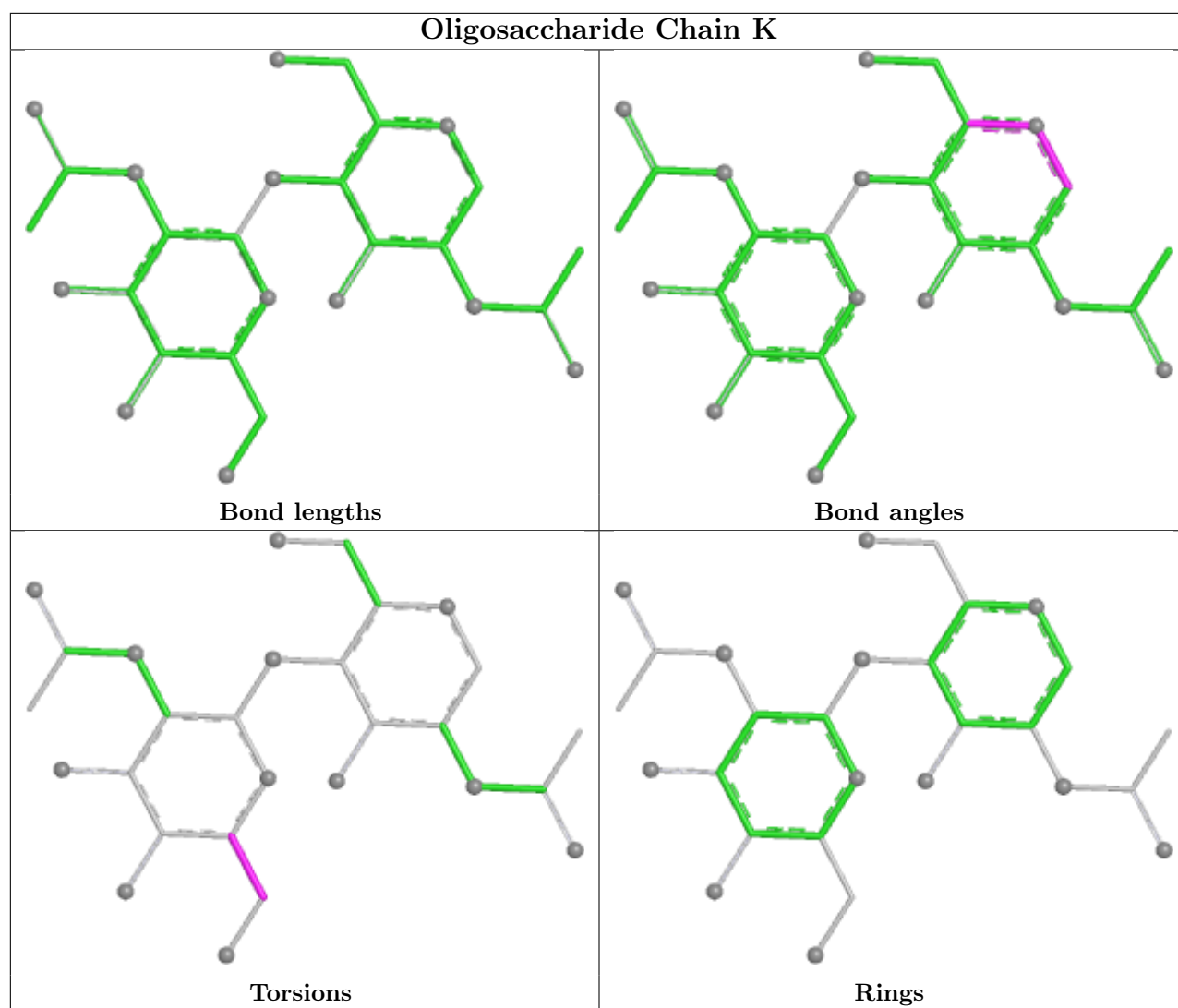
6 monomers are involved in 9 short contacts:

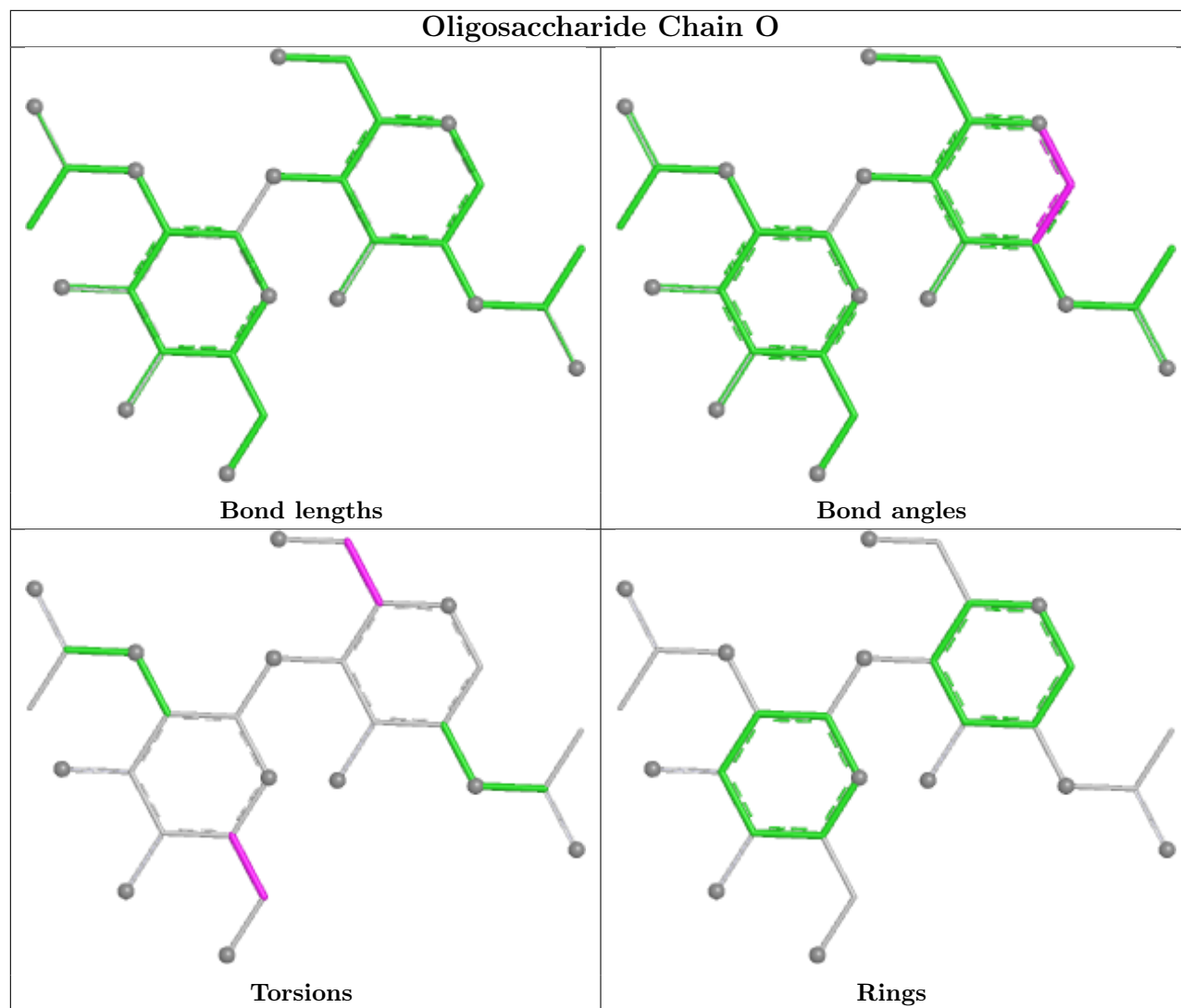
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	1	NAG	1	0
4	Q	1	NAG	1	0
4	R	1	NAG	2	0
4	a	1	NAG	2	0
4	i	1	NAG	1	0
4	j	1	NAG	2	0

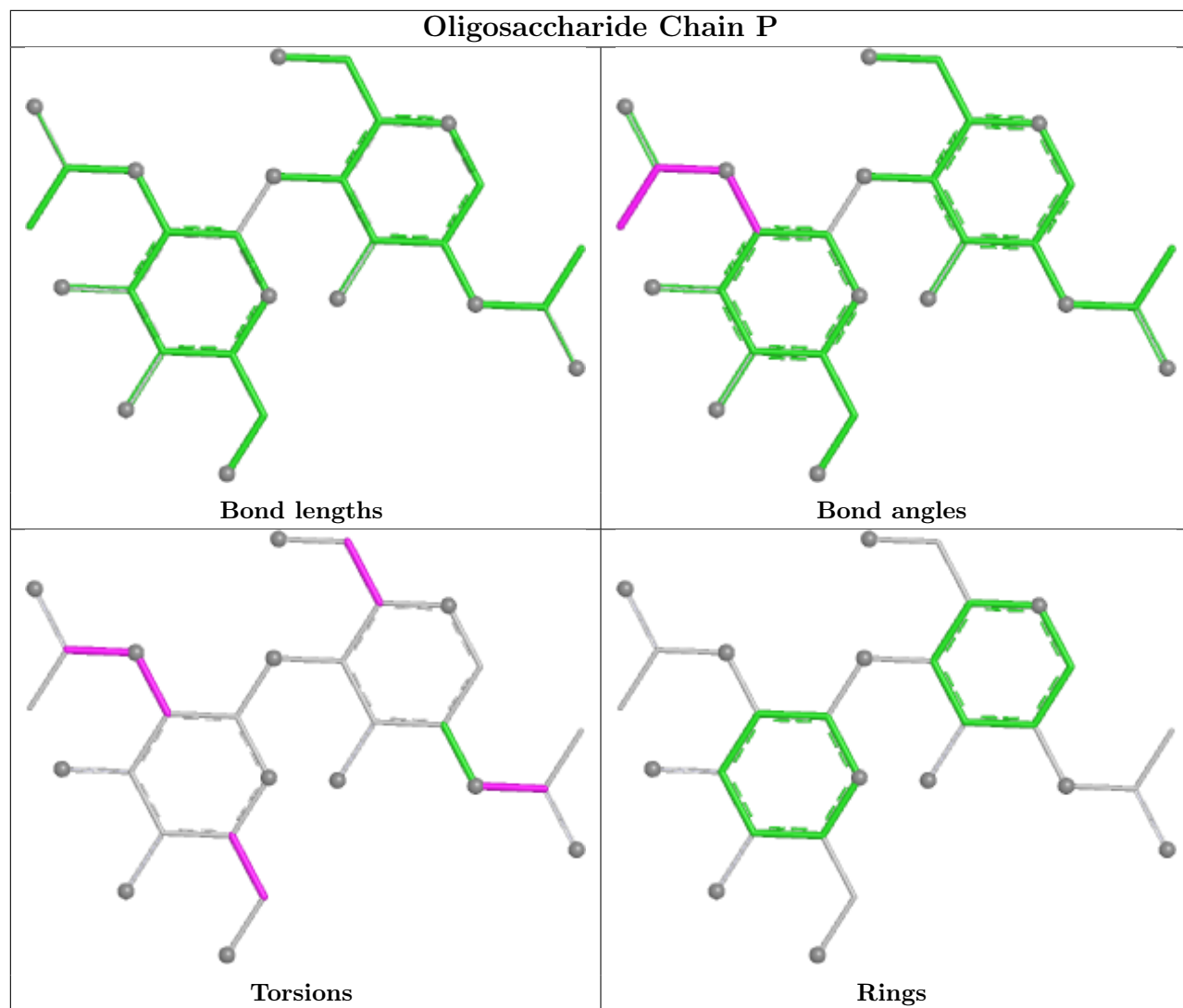
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

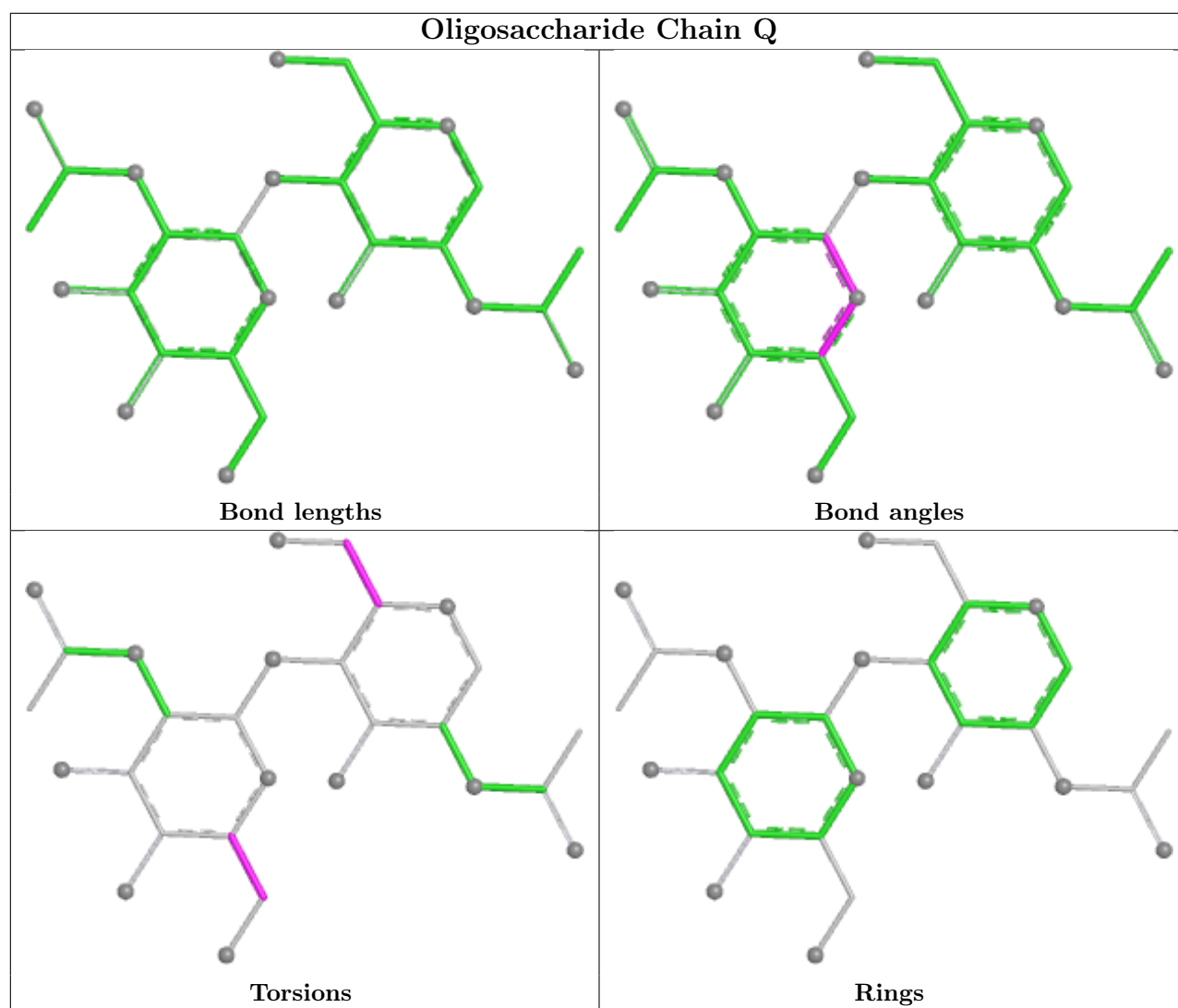


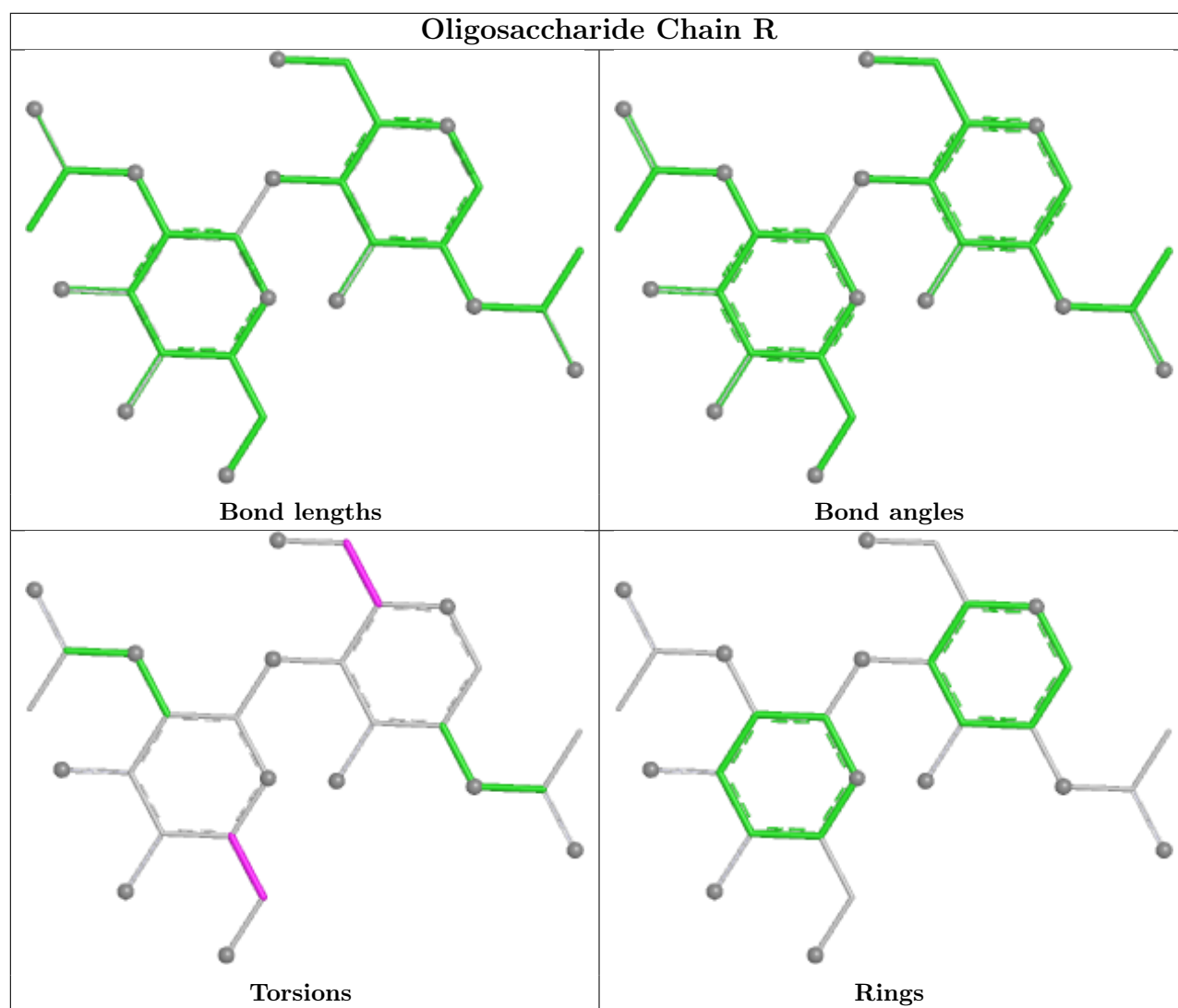


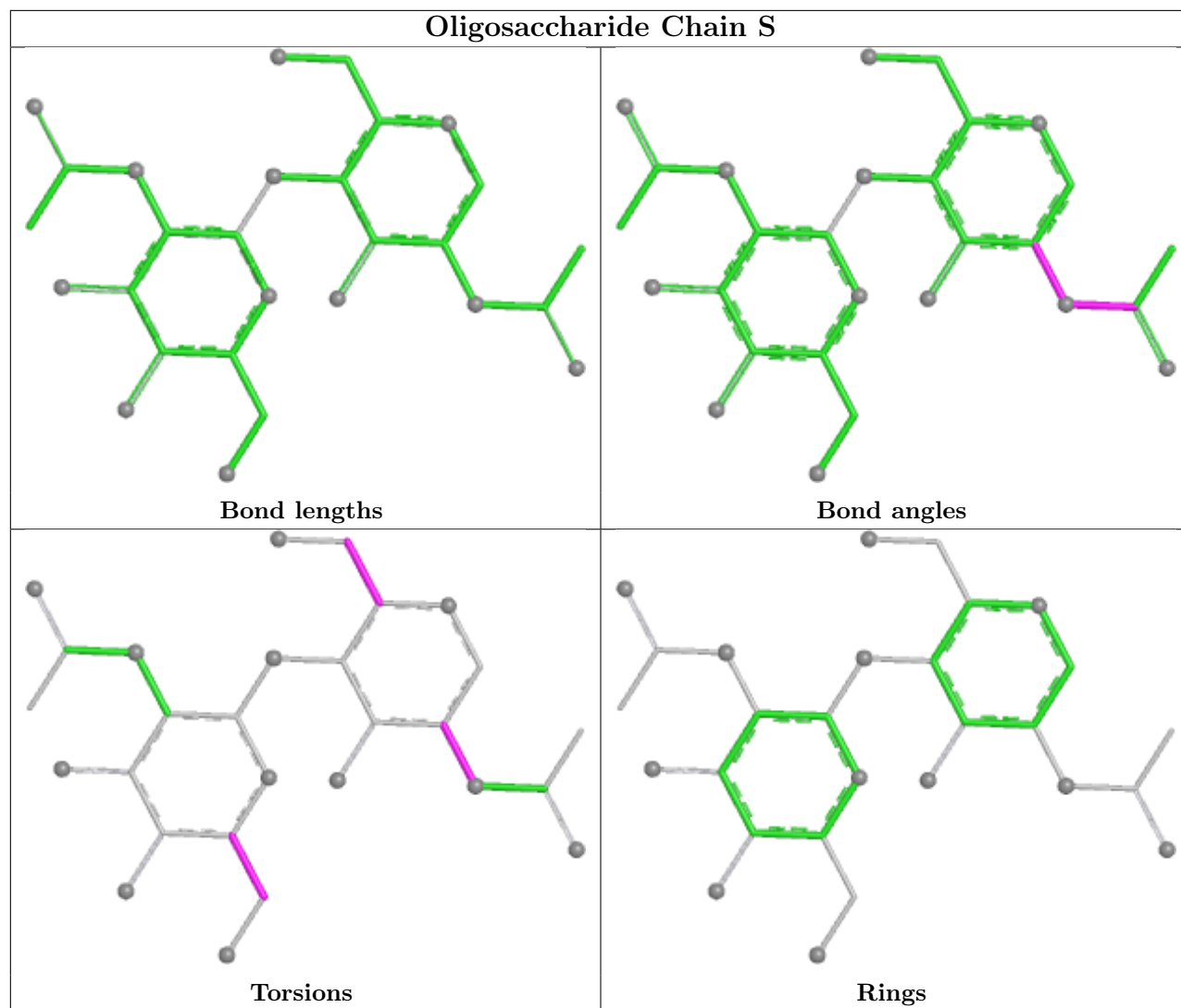


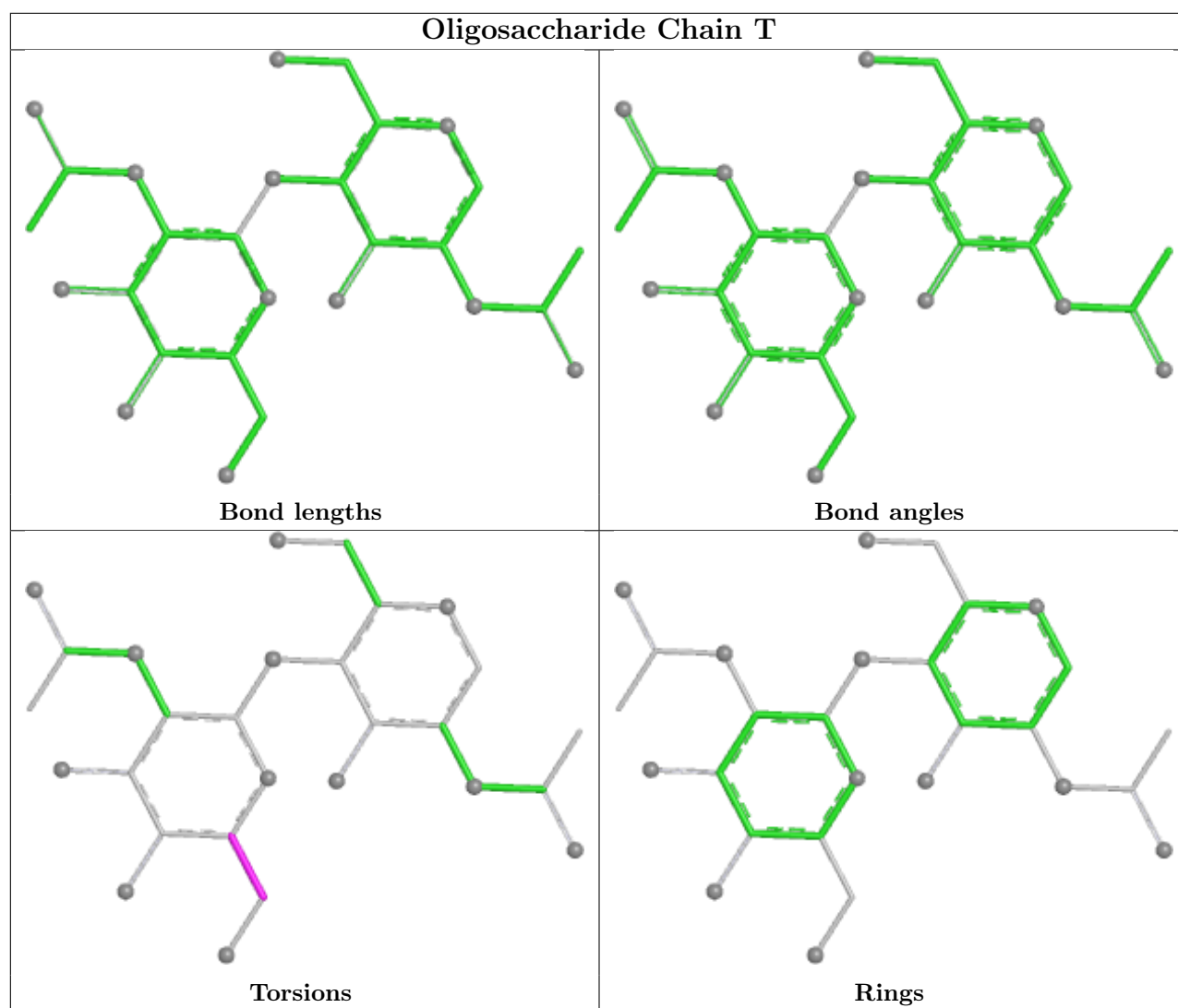


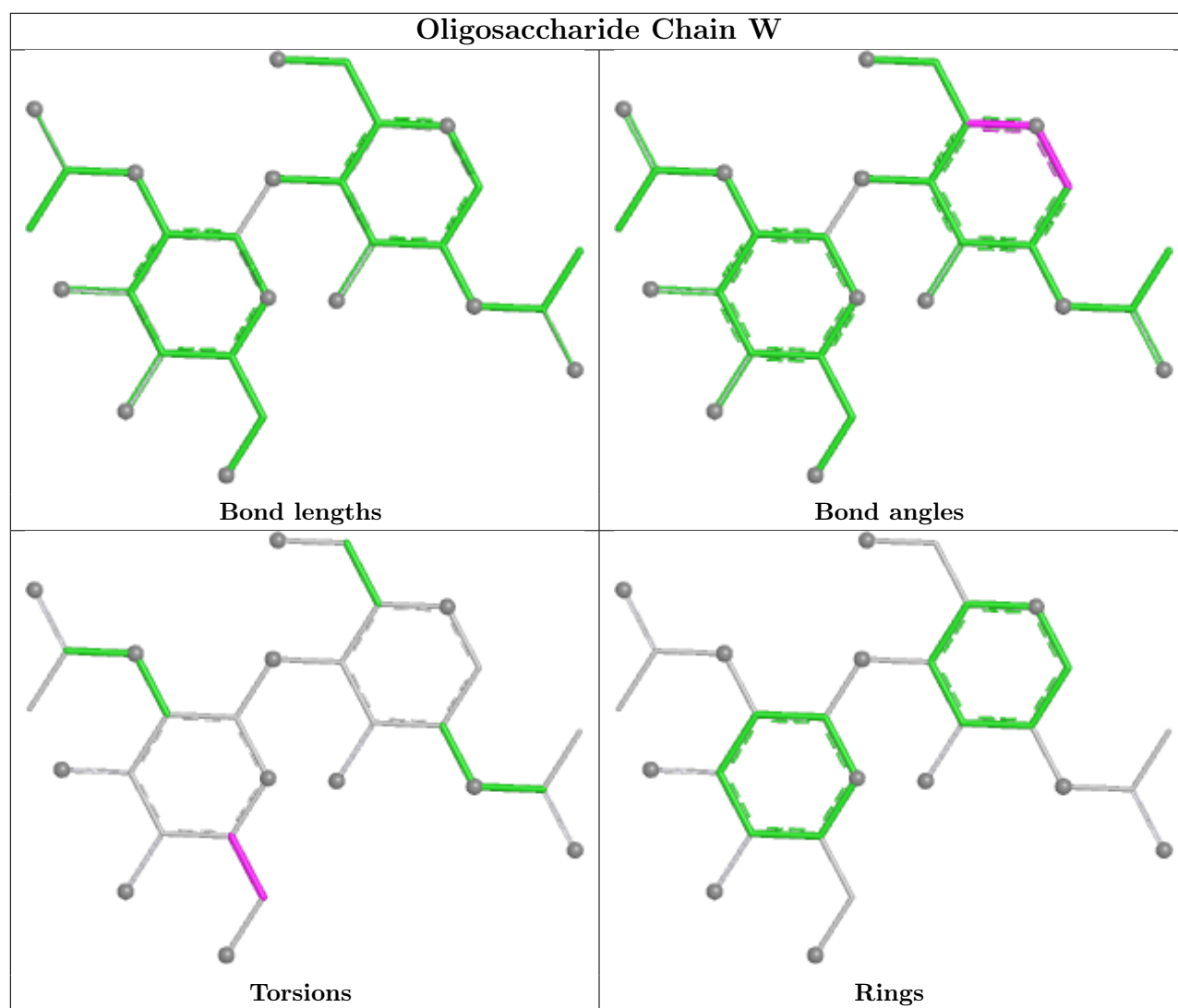


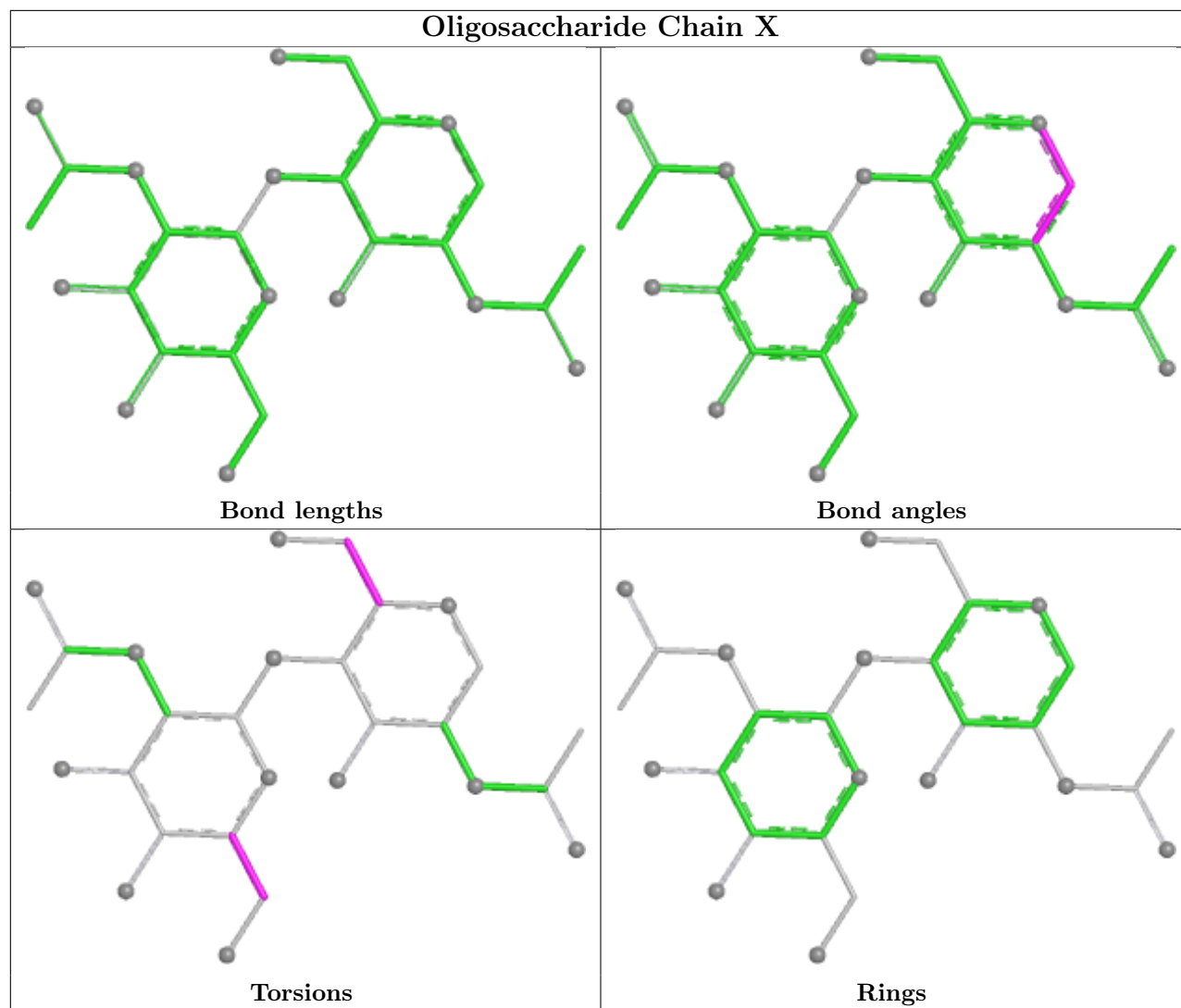


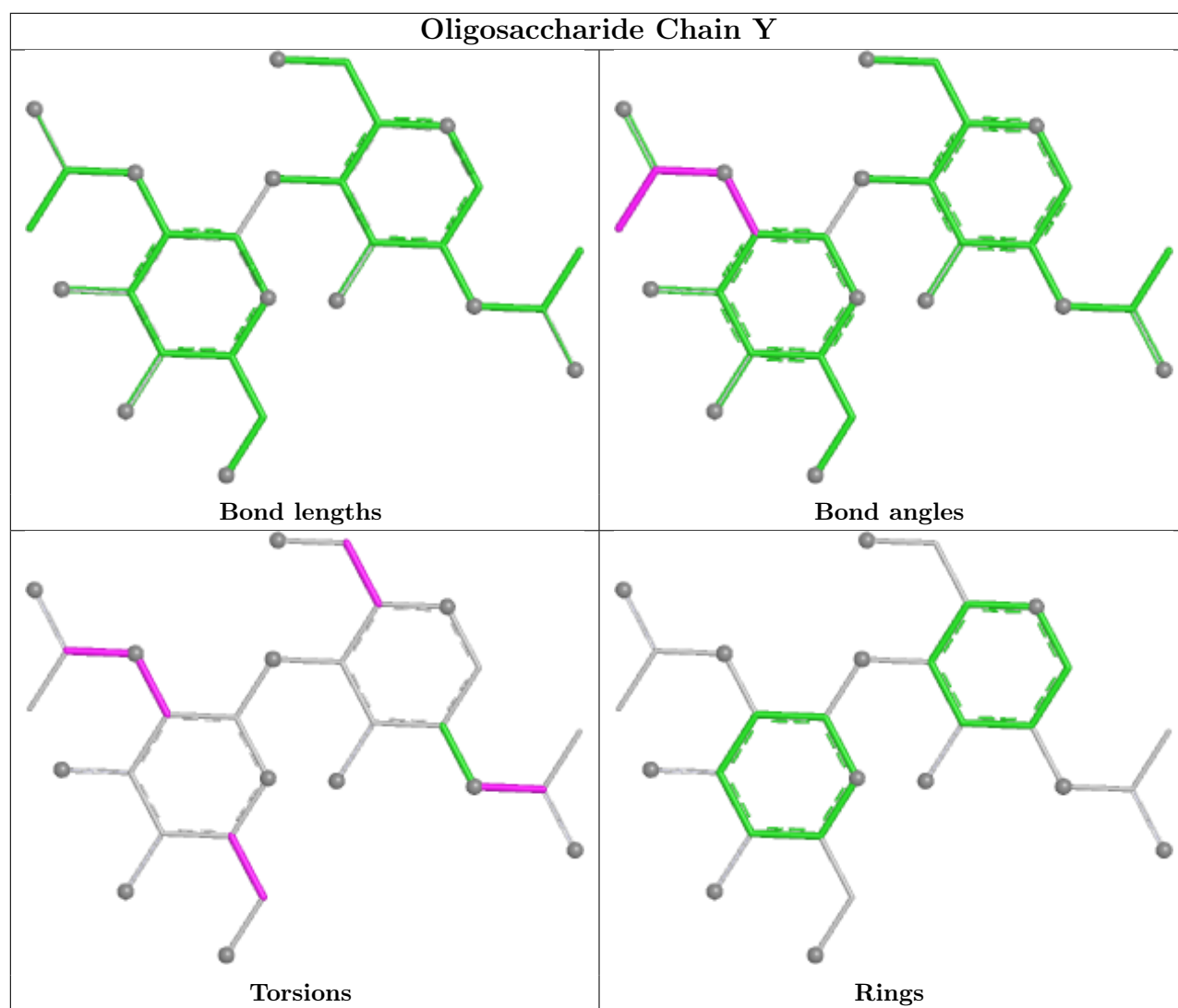


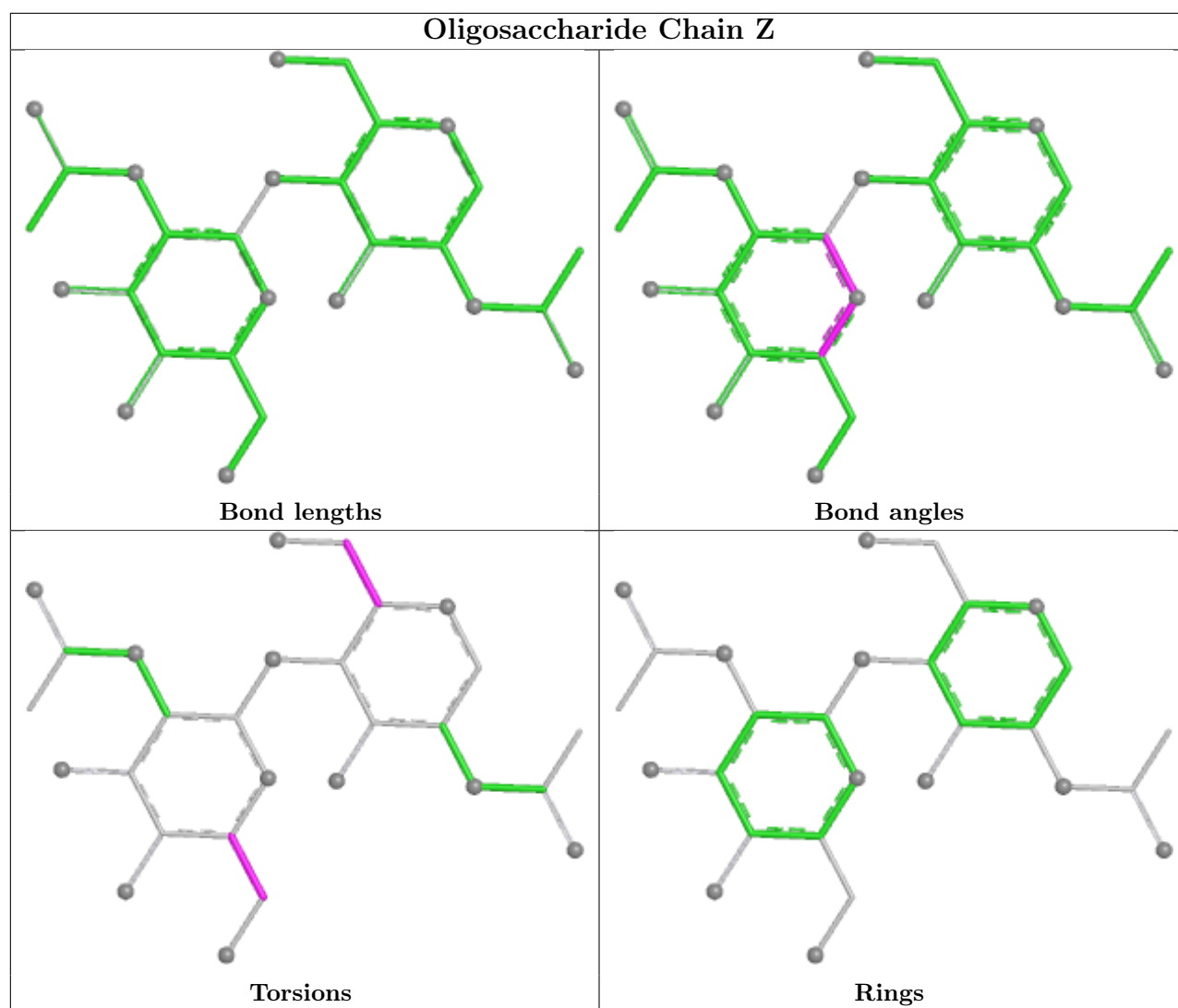


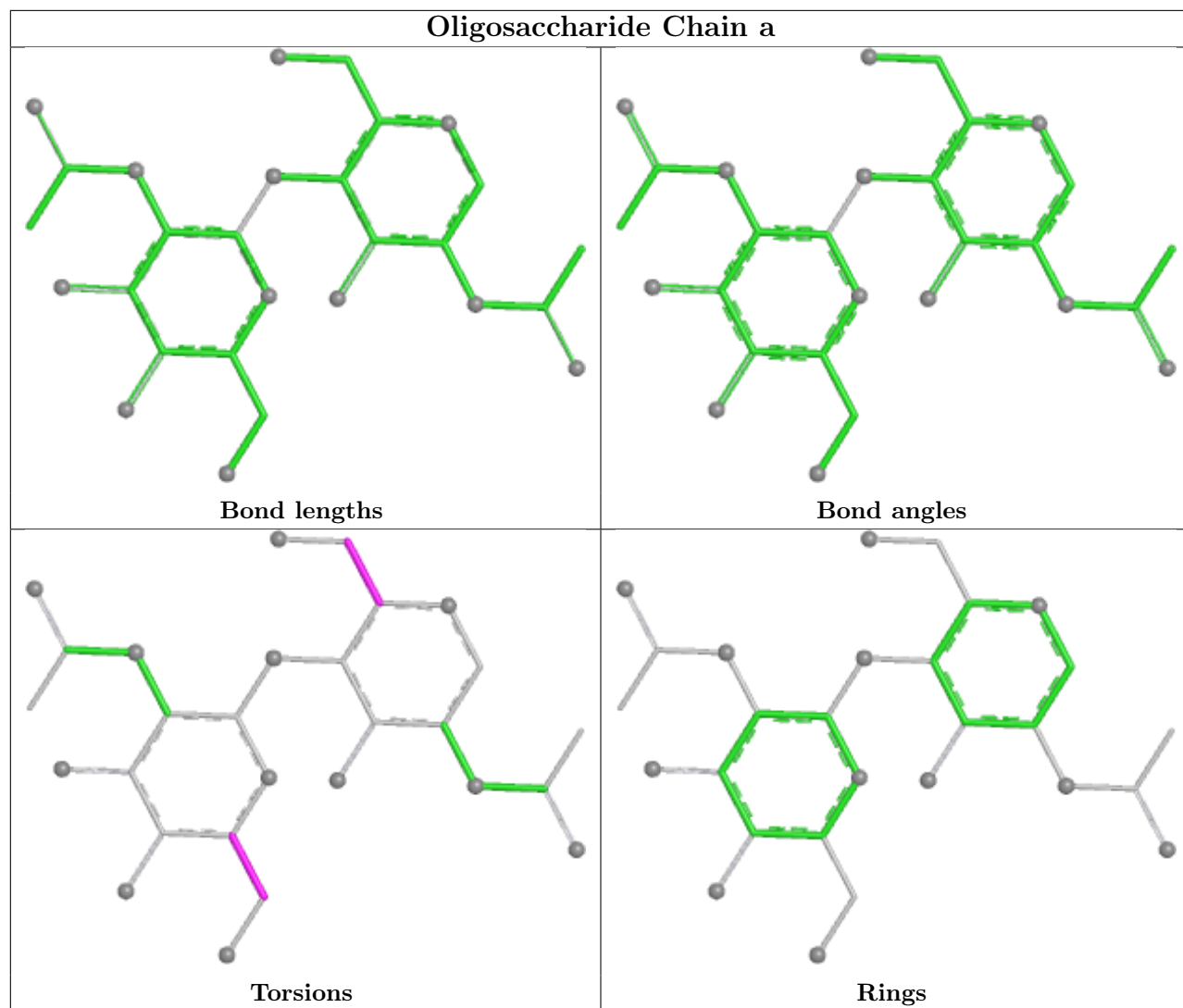


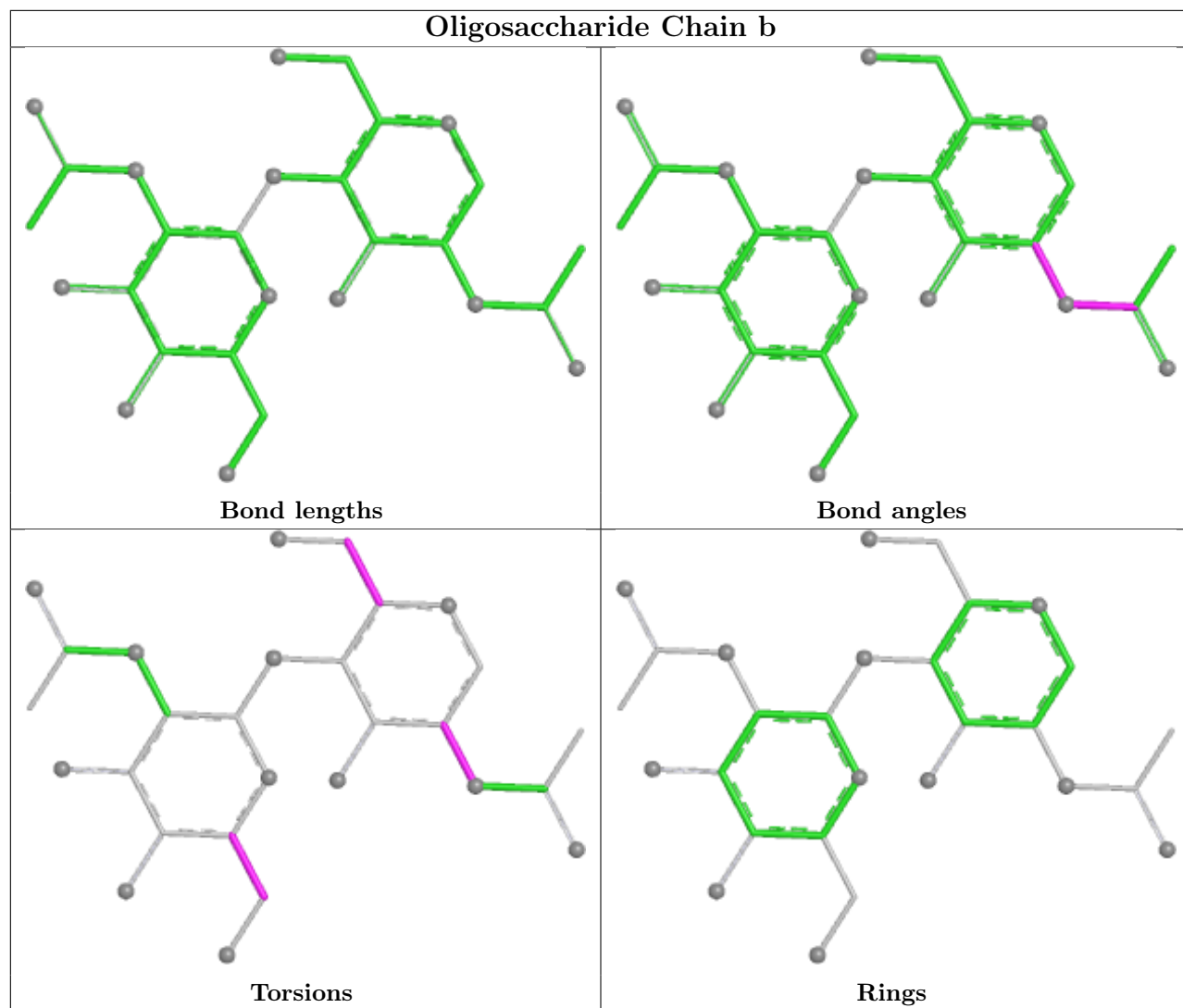


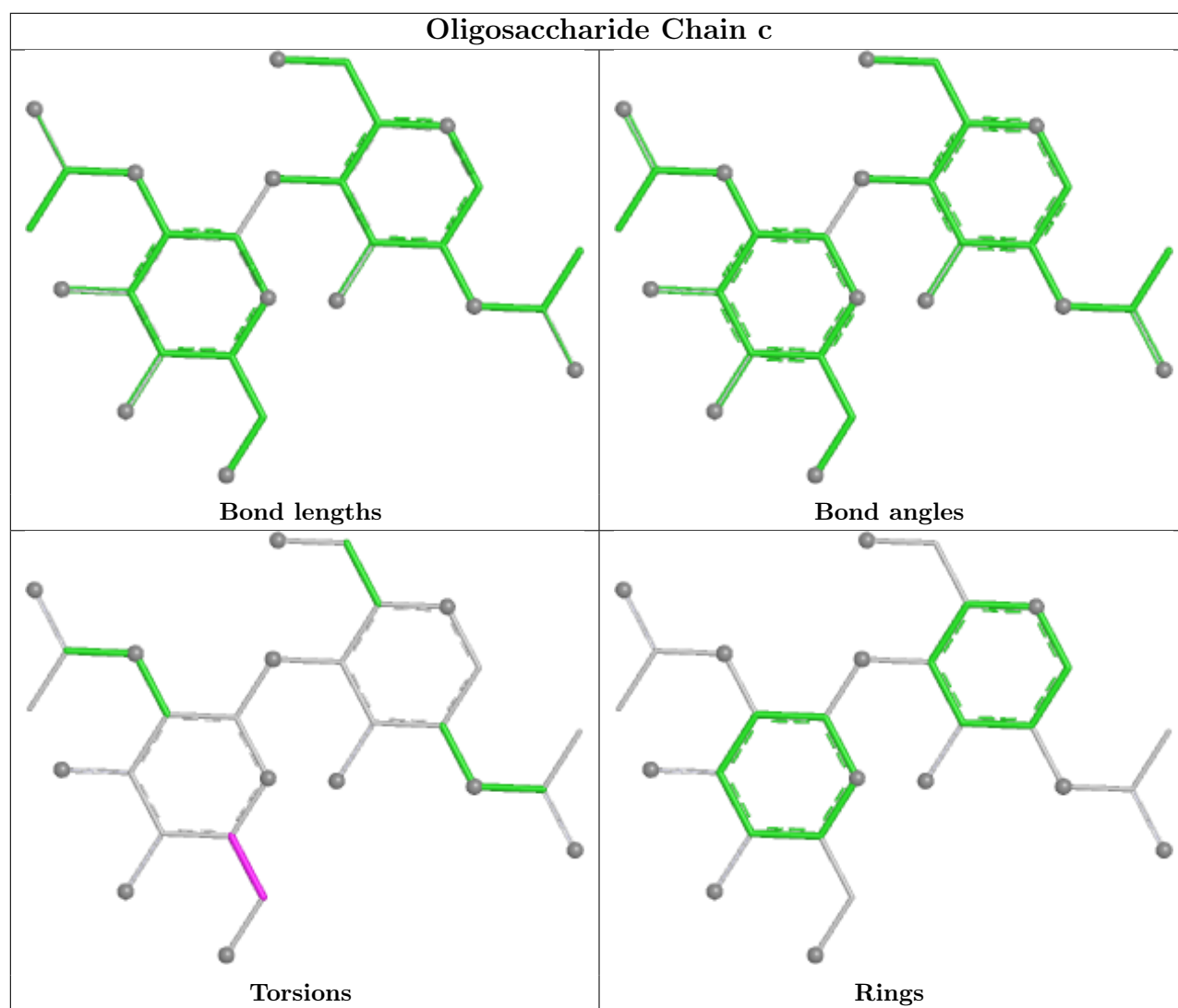


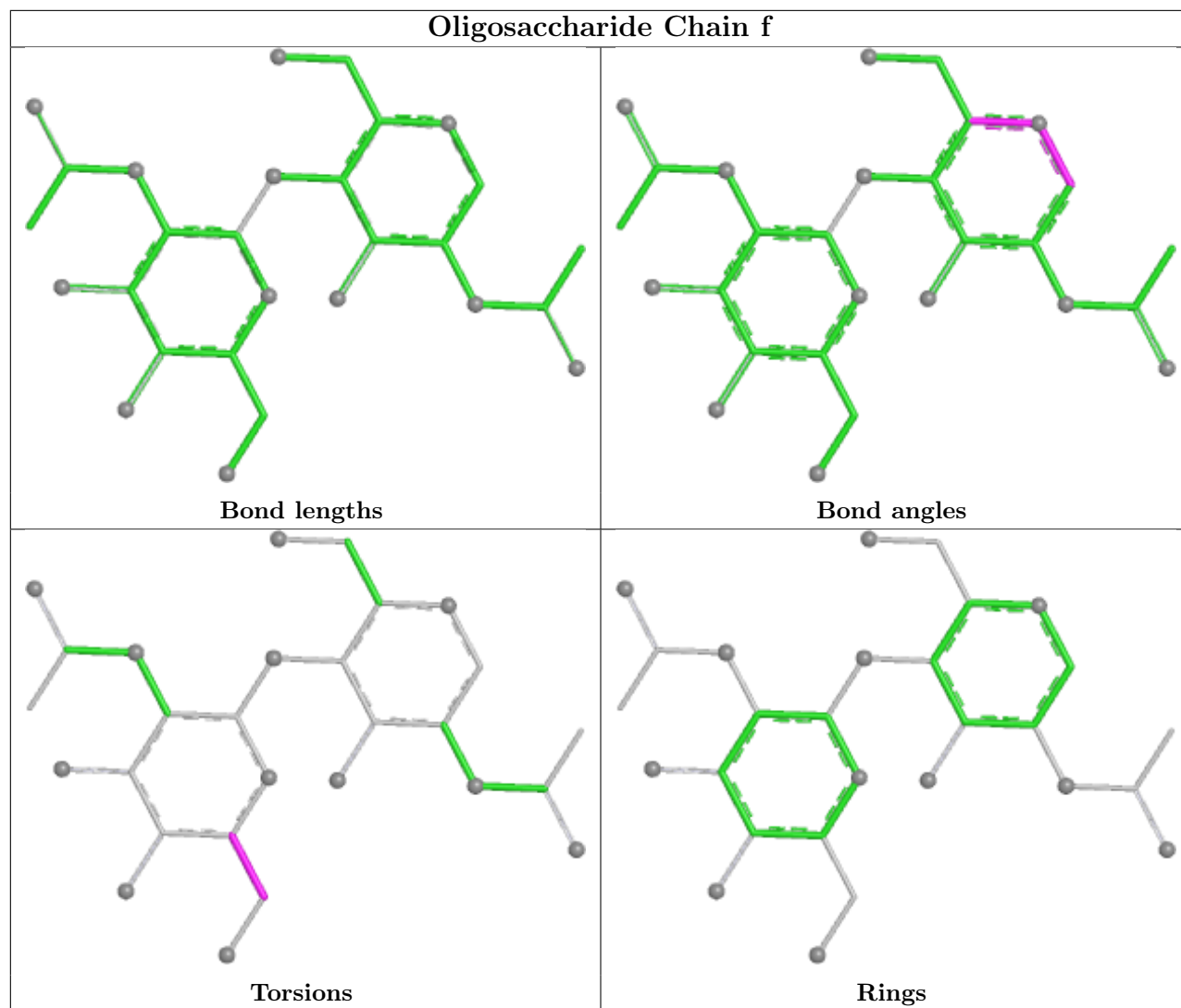


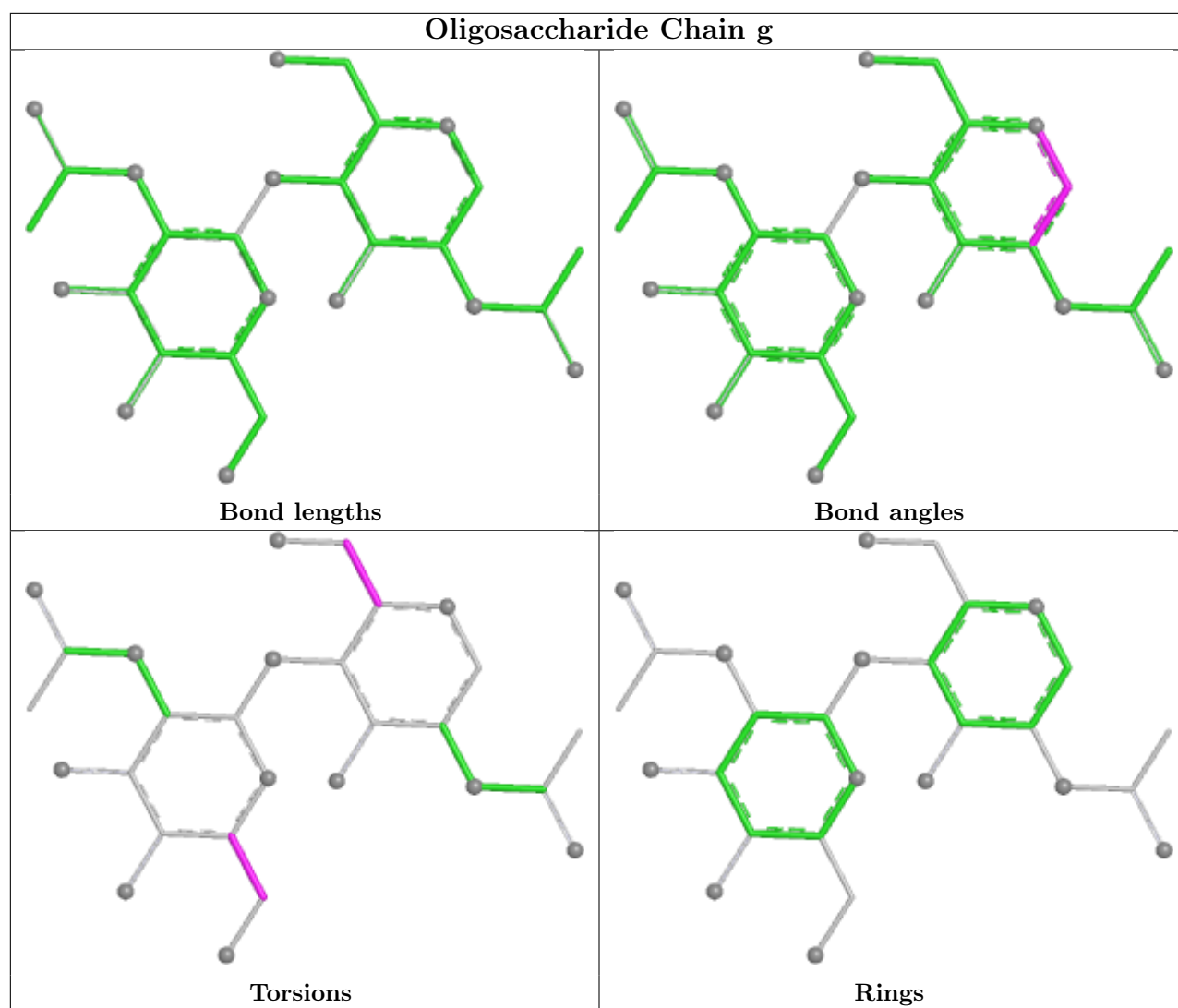


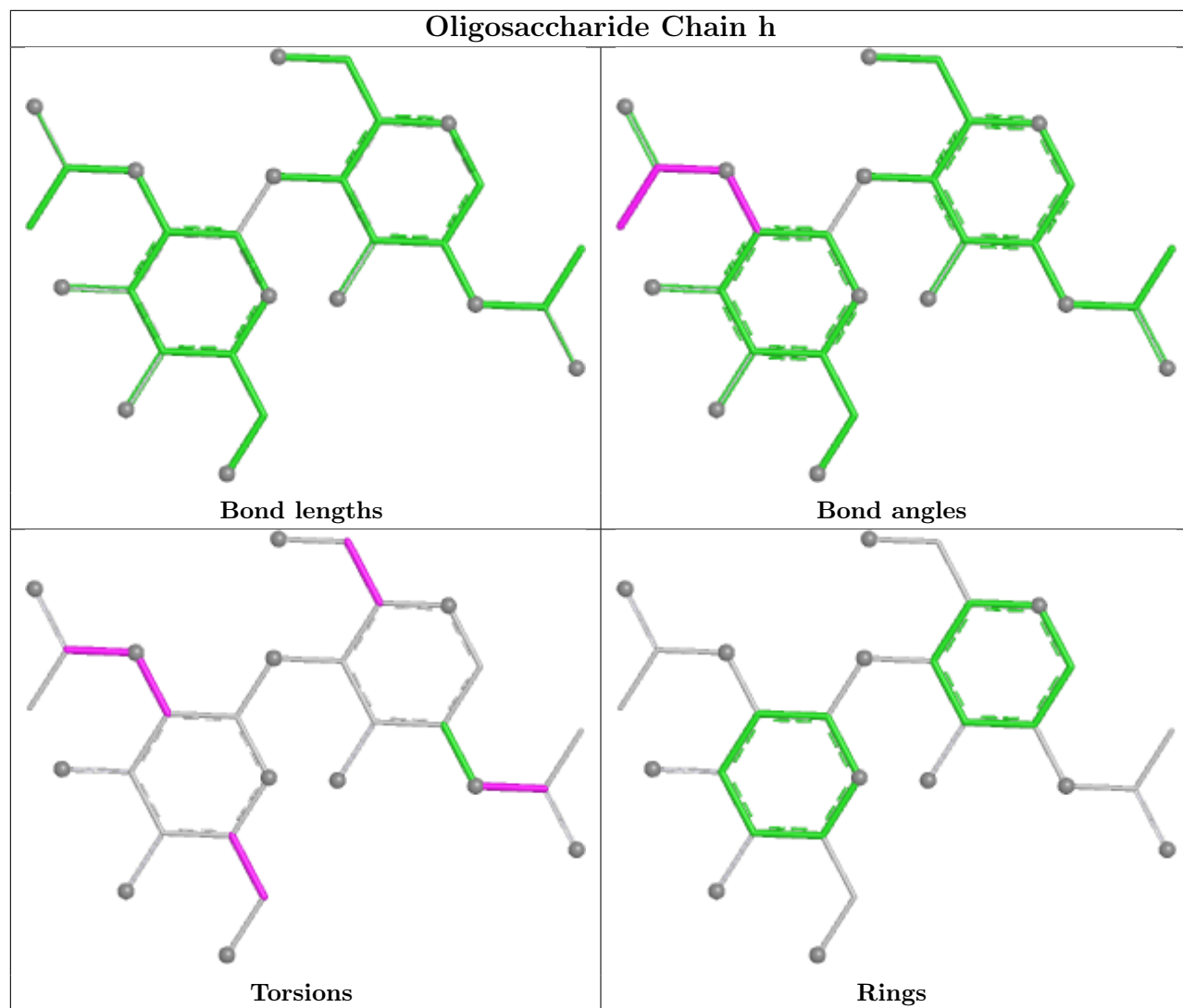


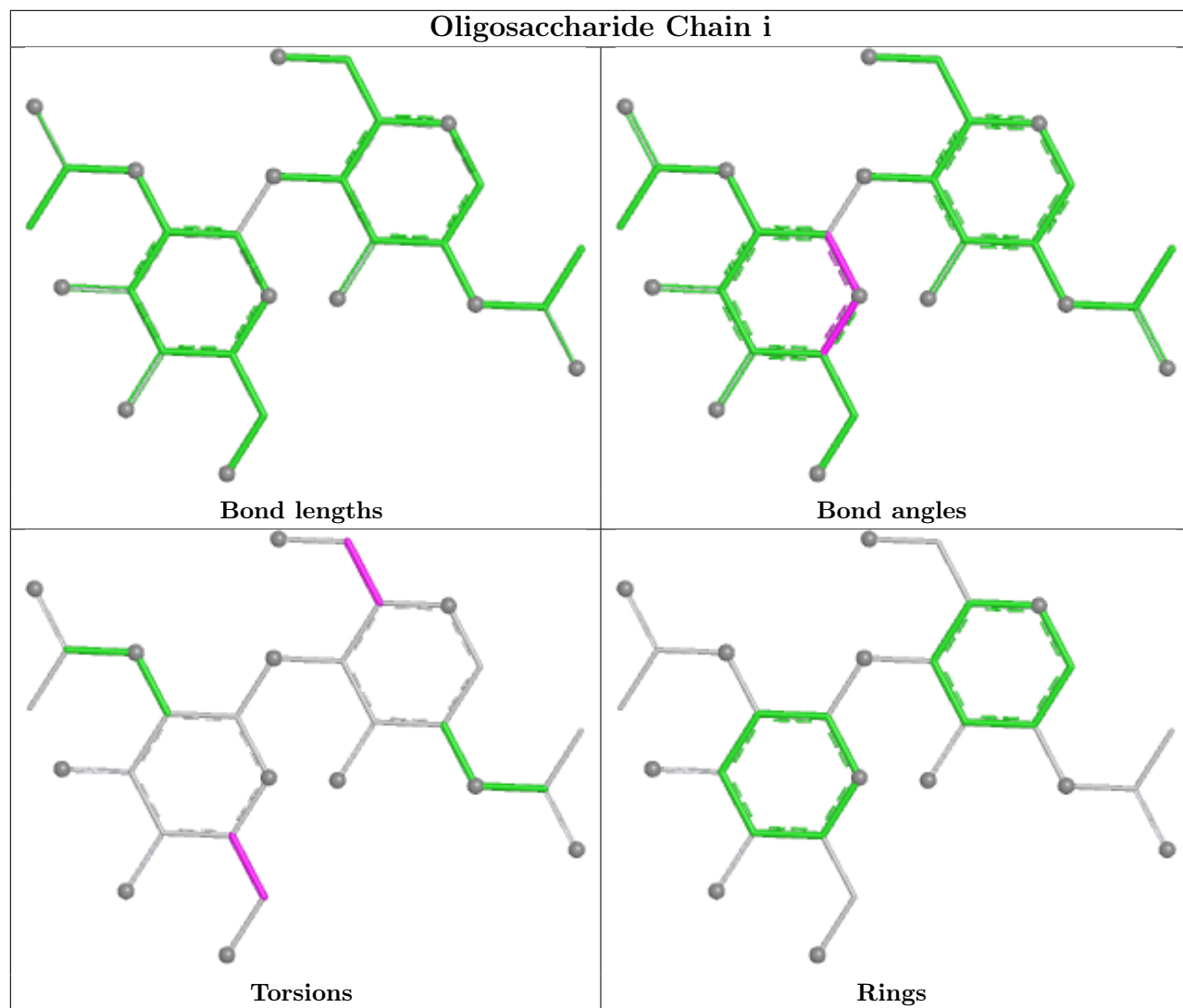


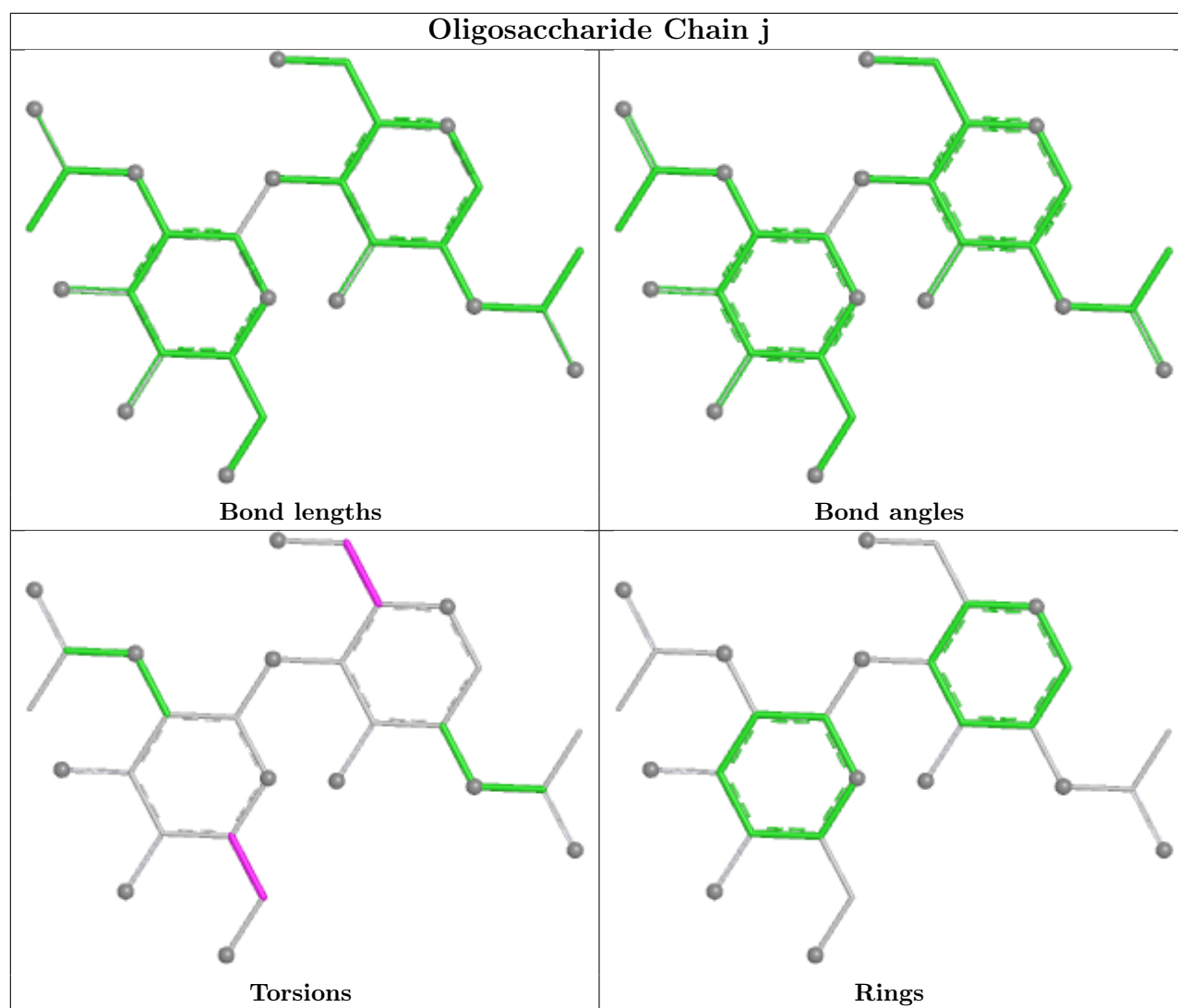


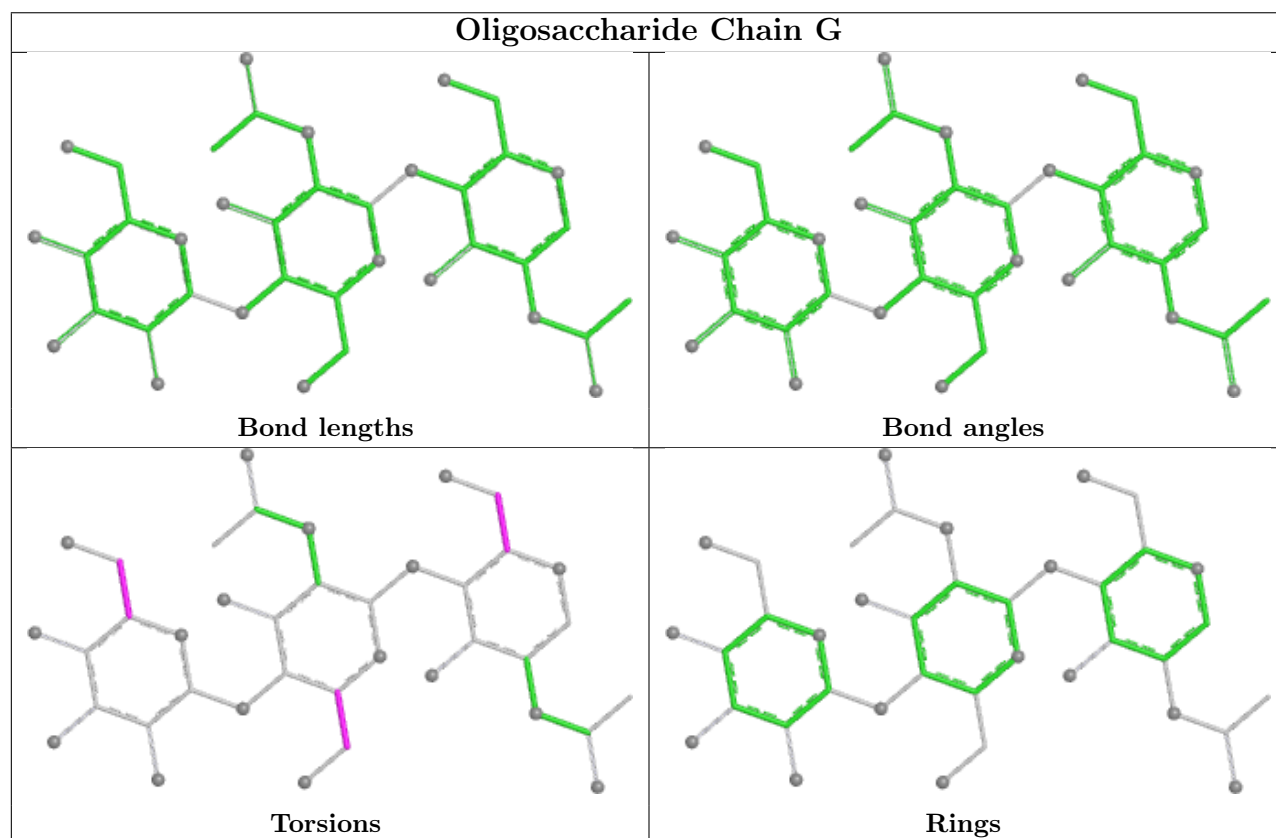
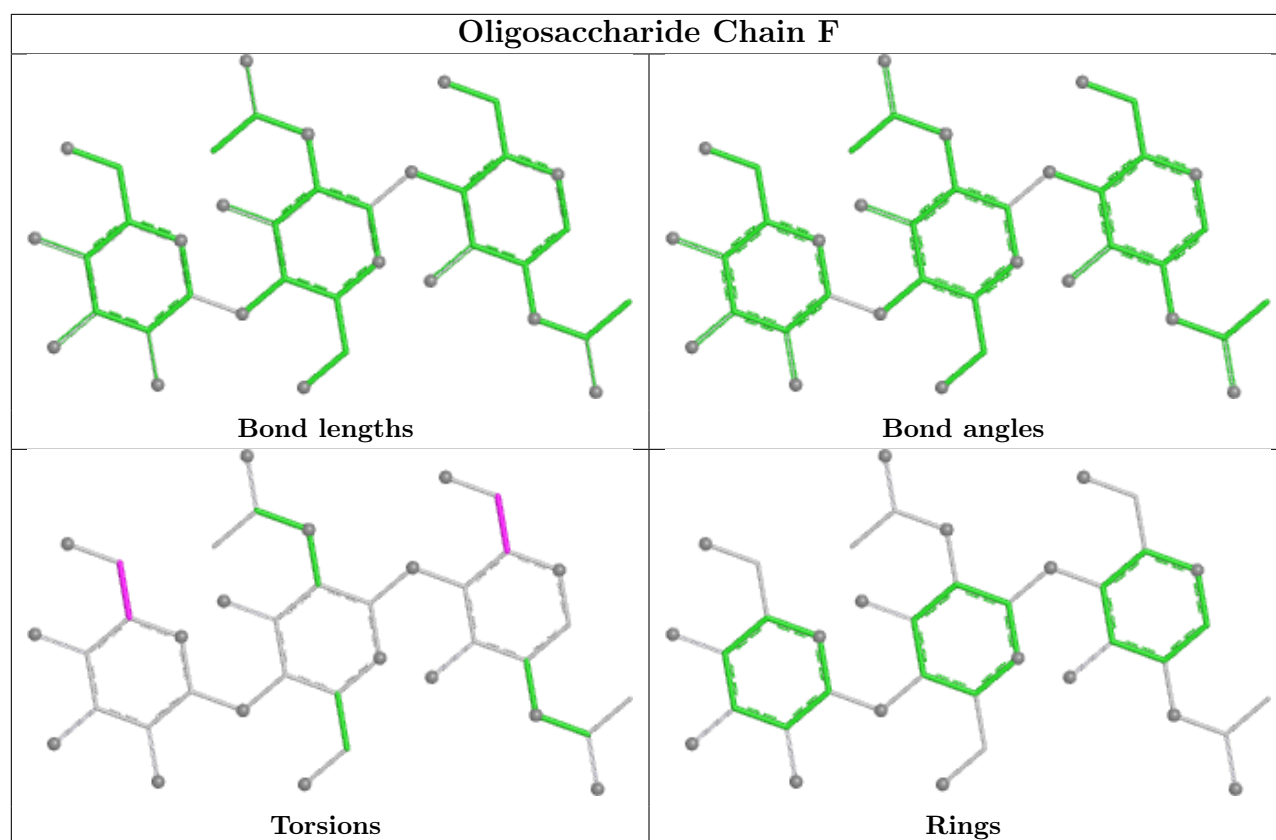


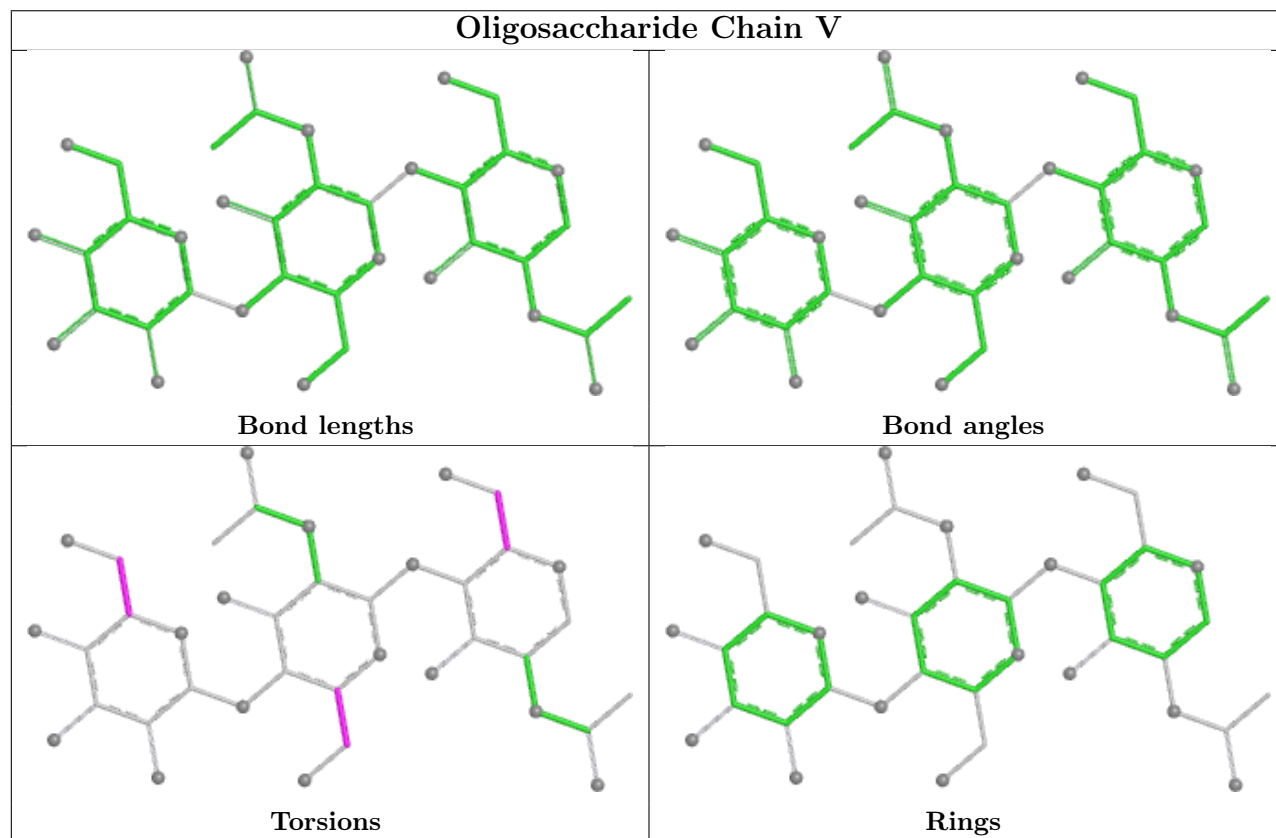
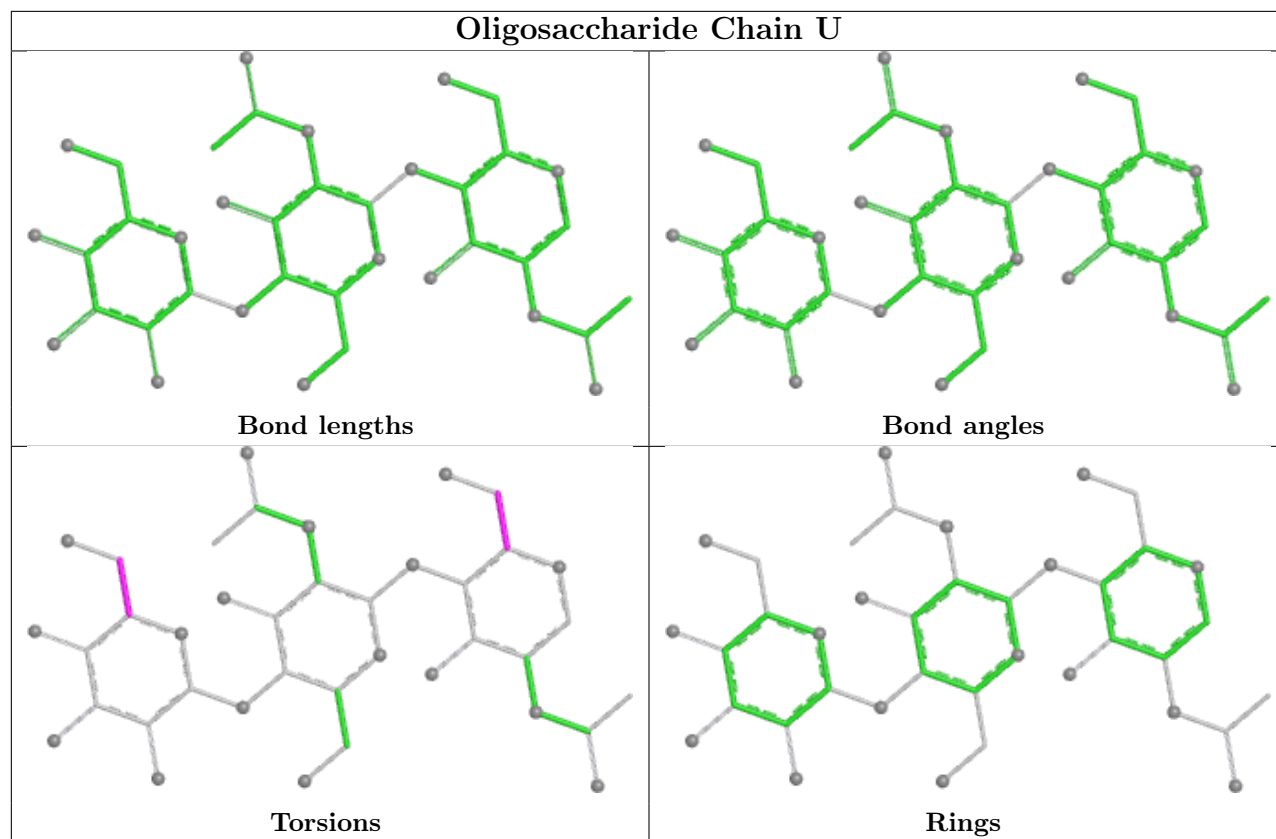


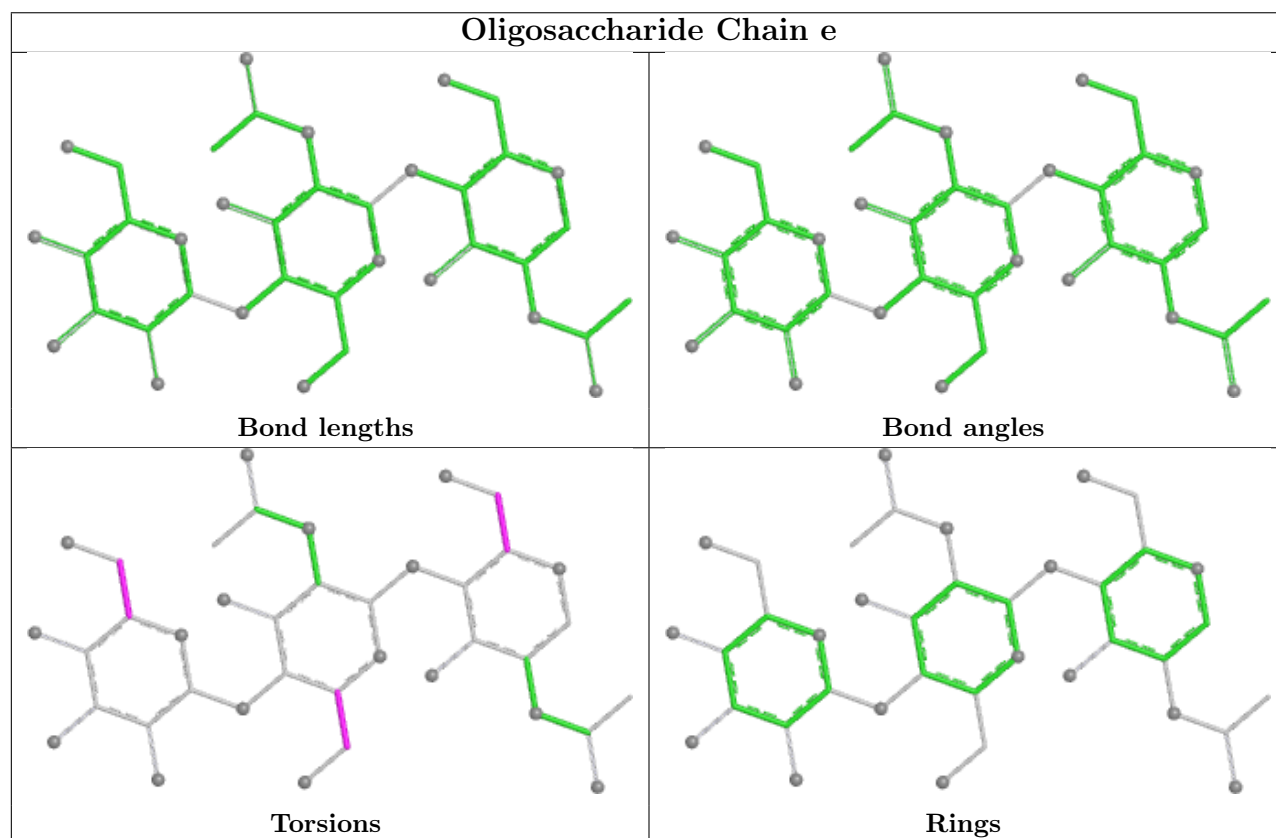
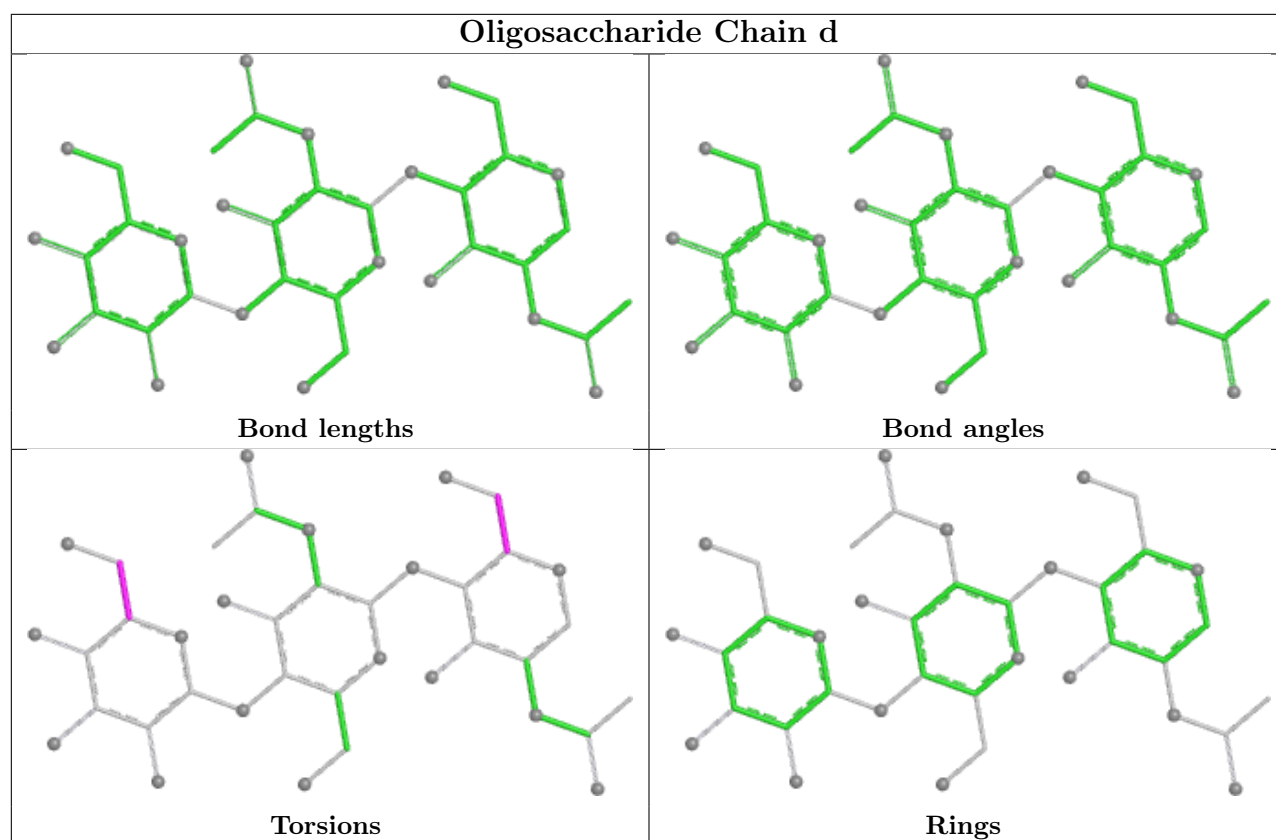












5.6 Ligand geometry

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	1303	1	14,14,15	0.34	0	17,19,21	0.51	0
6	NAG	C	1304	1	14,14,15	0.32	0	17,19,21	0.64	0
6	NAG	B	1304	1	14,14,15	0.32	0	17,19,21	0.65	0
6	NAG	A	1304	1	14,14,15	0.32	0	17,19,21	0.65	0
6	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.64	0
6	NAG	B	1306	1	14,14,15	0.29	0	17,19,21	0.64	0
6	NAG	C	1303	1	14,14,15	0.35	0	17,19,21	0.51	0
6	NAG	B	1303	1	14,14,15	0.34	0	17,19,21	0.51	0
6	NAG	A	1301	1	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
6	NAG	C	1302	1	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
6	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
6	NAG	A	1305	1	14,14,15	0.31	0	17,19,21	0.54	0
6	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
6	NAG	C	1305	1	14,14,15	0.32	0	17,19,21	0.54	0
6	NAG	C	1306	1	14,14,15	0.29	0	17,19,21	0.64	0
6	NAG	B	1302	1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
6	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
6	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.55	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
6	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1301	NAG	C1-O5-C5	-2.85	108.37	112.19
6	B	1301	NAG	C1-O5-C5	-2.85	108.37	112.19
6	A	1301	NAG	C1-O5-C5	-2.83	108.39	112.19
6	B	1302	NAG	O5-C1-C2	-2.13	107.99	111.29
6	A	1302	NAG	O5-C1-C2	-2.13	108.00	111.29
6	C	1302	NAG	O5-C1-C2	-2.13	108.00	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1306	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1304	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1302	NAG	1	0
6	A	1302	NAG	1	0
6	B	1302	NAG	1	0

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.

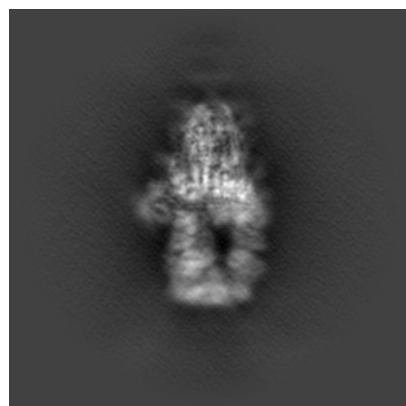
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22926. These allow visual inspection of the internal detail of the map and identification of artifacts.

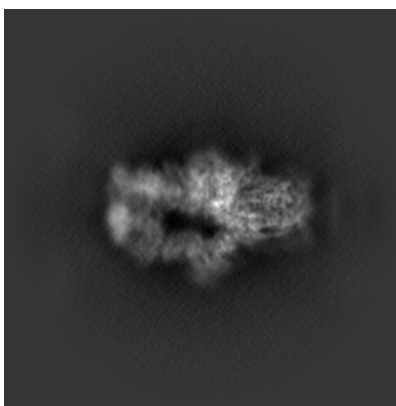
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

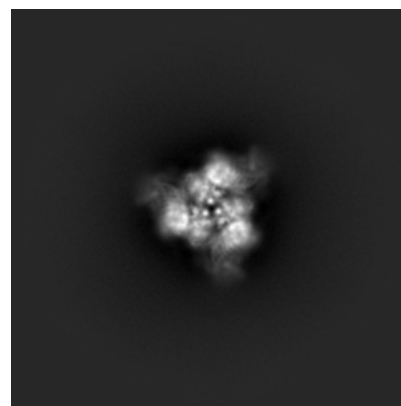
6.1.1 Primary map



X

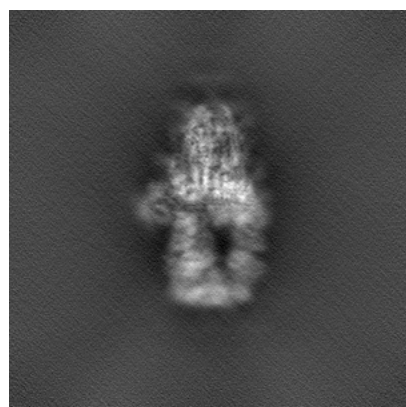


Y

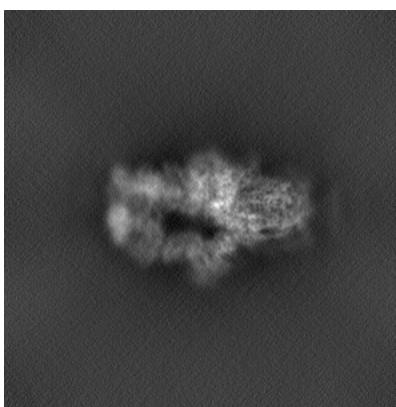


Z

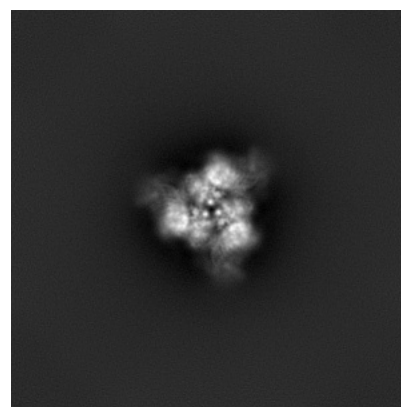
6.1.2 Raw map



X



Y

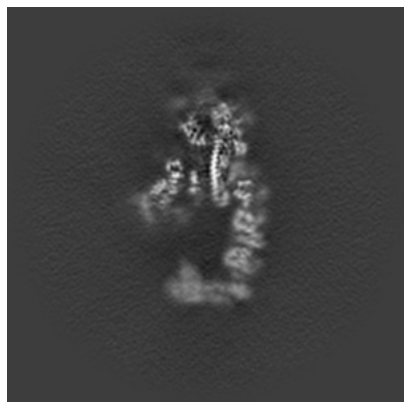


Z

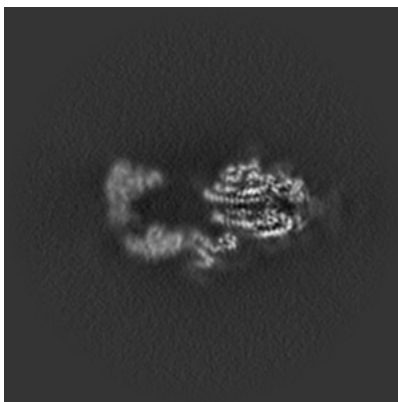
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

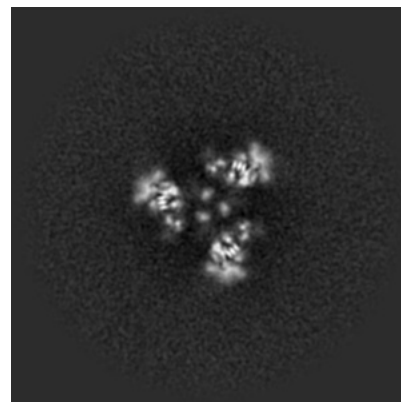
6.2.1 Primary map



X Index: 200

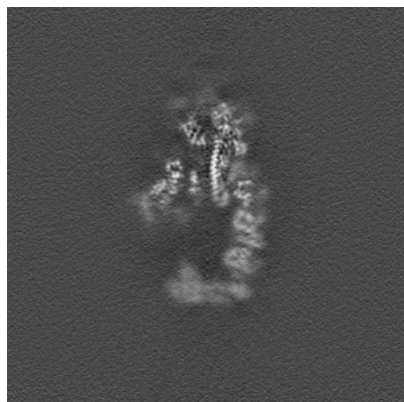


Y Index: 200

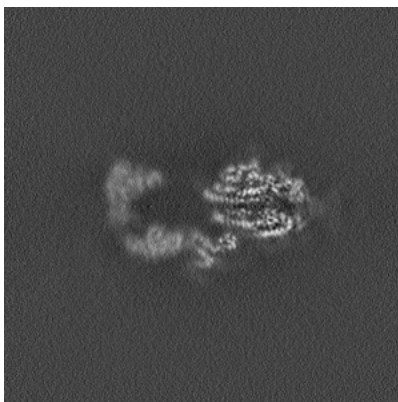


Z Index: 200

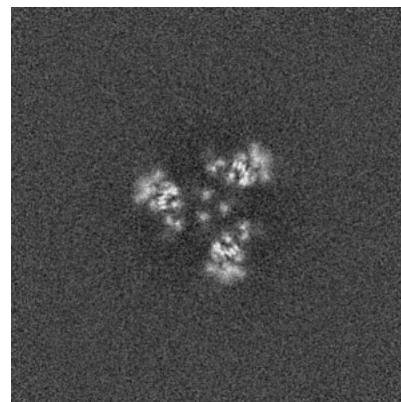
6.2.2 Raw map



X Index: 200



Y Index: 200

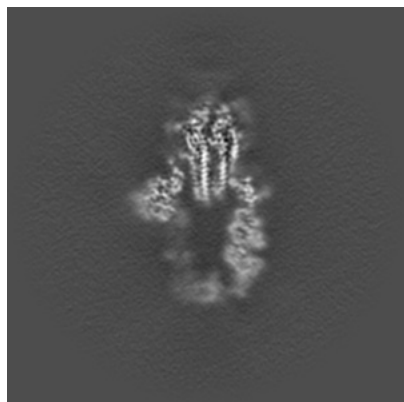


Z Index: 200

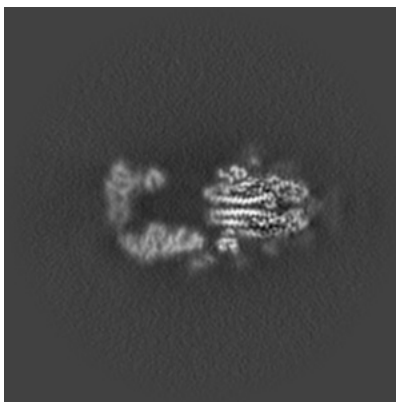
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

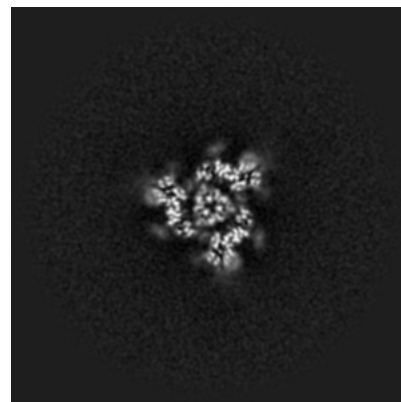
6.3.1 Primary map



X Index: 207

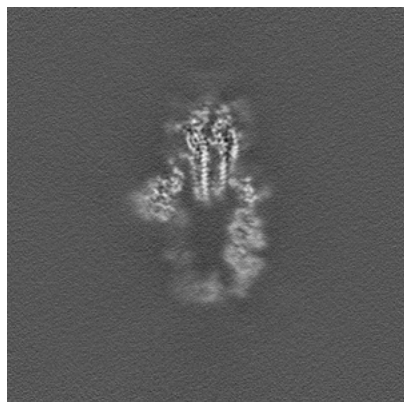


Y Index: 196

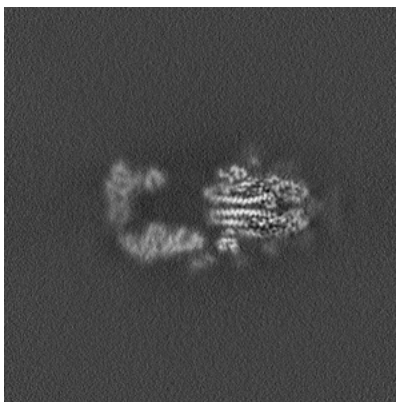


Z Index: 217

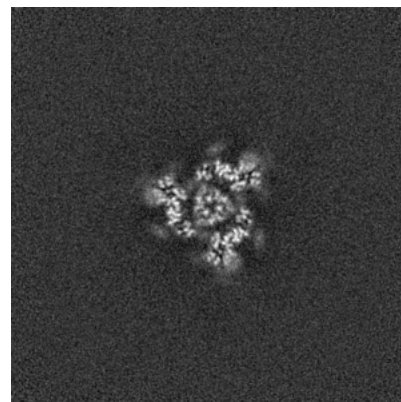
6.3.2 Raw map



X Index: 207



Y Index: 196

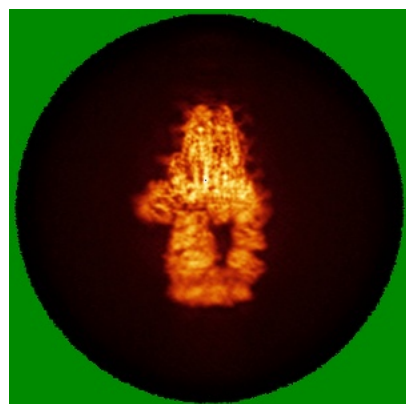


Z Index: 217

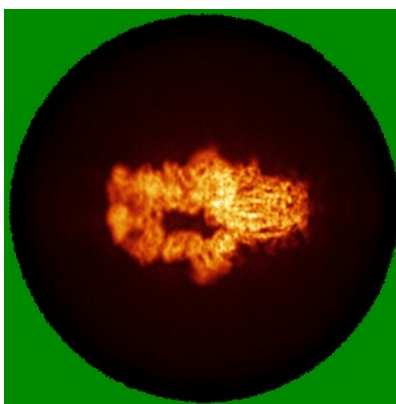
The images above show the largest variance slices of the map in three orthogonal directions.

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

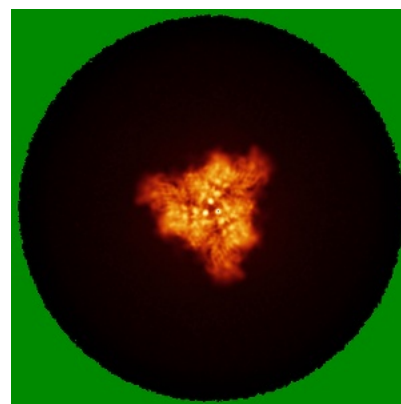
6.4.1 Primary map



X

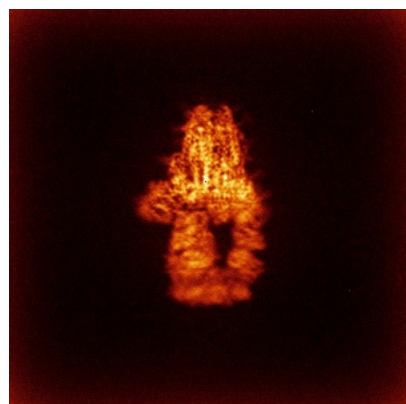


Y

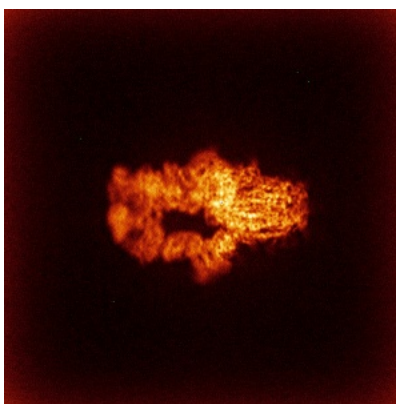


Z

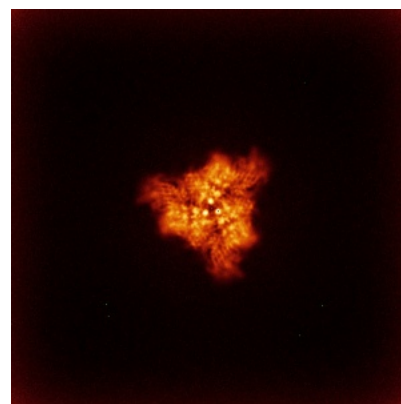
6.4.2 Raw map



X



Y



Z

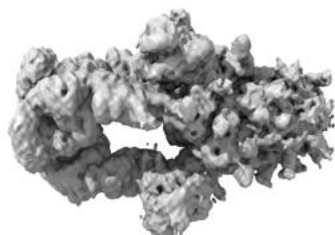
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

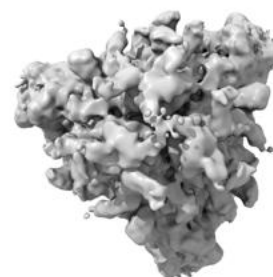
6.5.1 Primary map



X



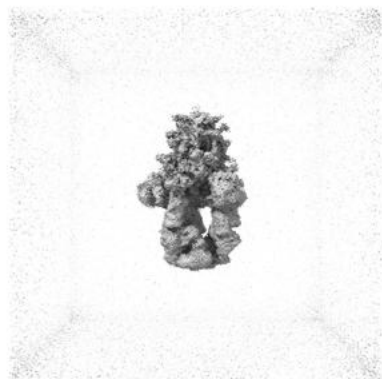
Y



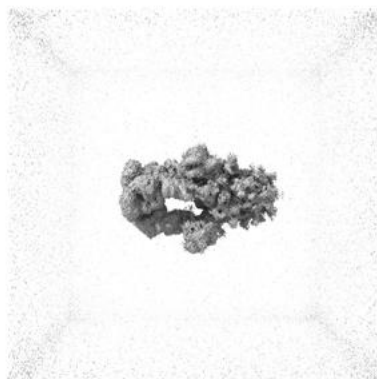
Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

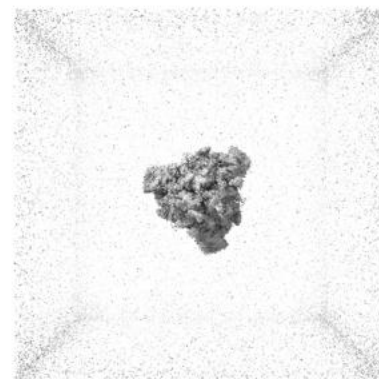
6.5.2 Raw map



X



Y



Z

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.

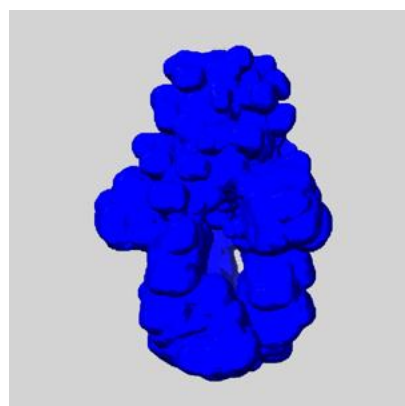
6.6 Mask visualisation [i](#)

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

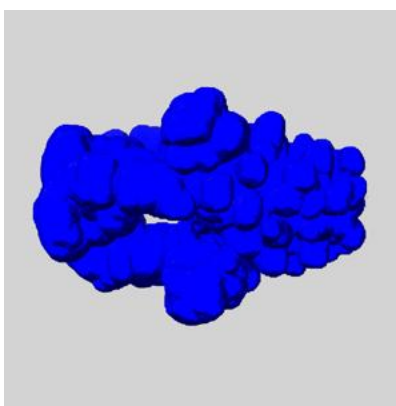
A mask typically either:

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

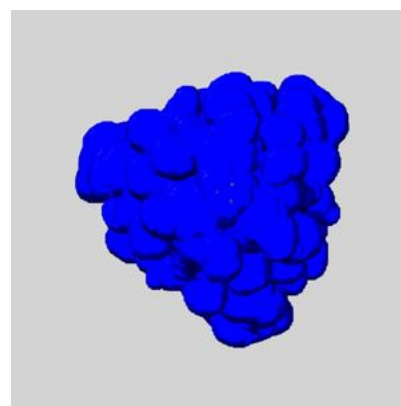
6.6.1 emd_22926_msk_1.map [i](#)



X



Y

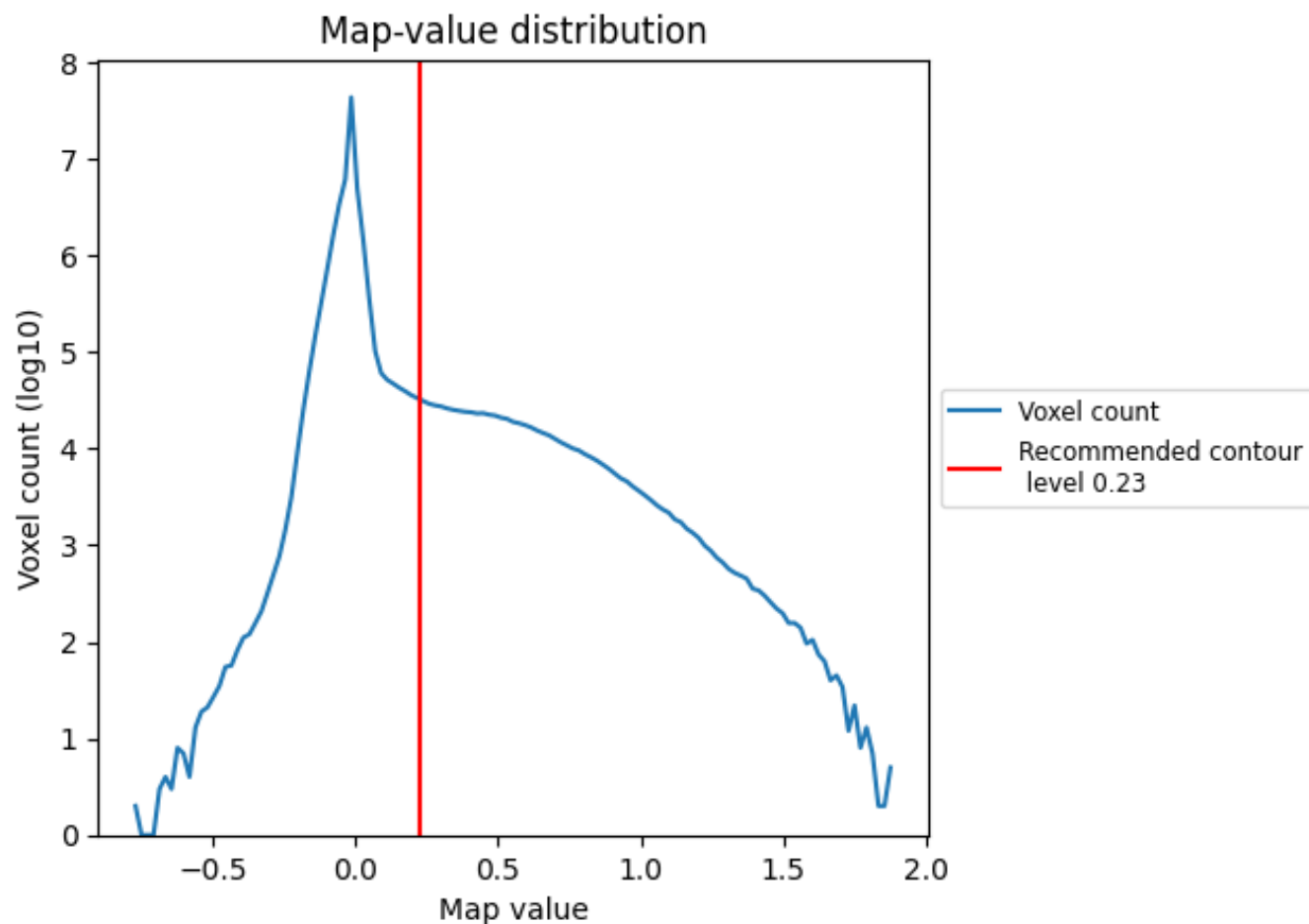


Z

7 Map analysis [i](#)

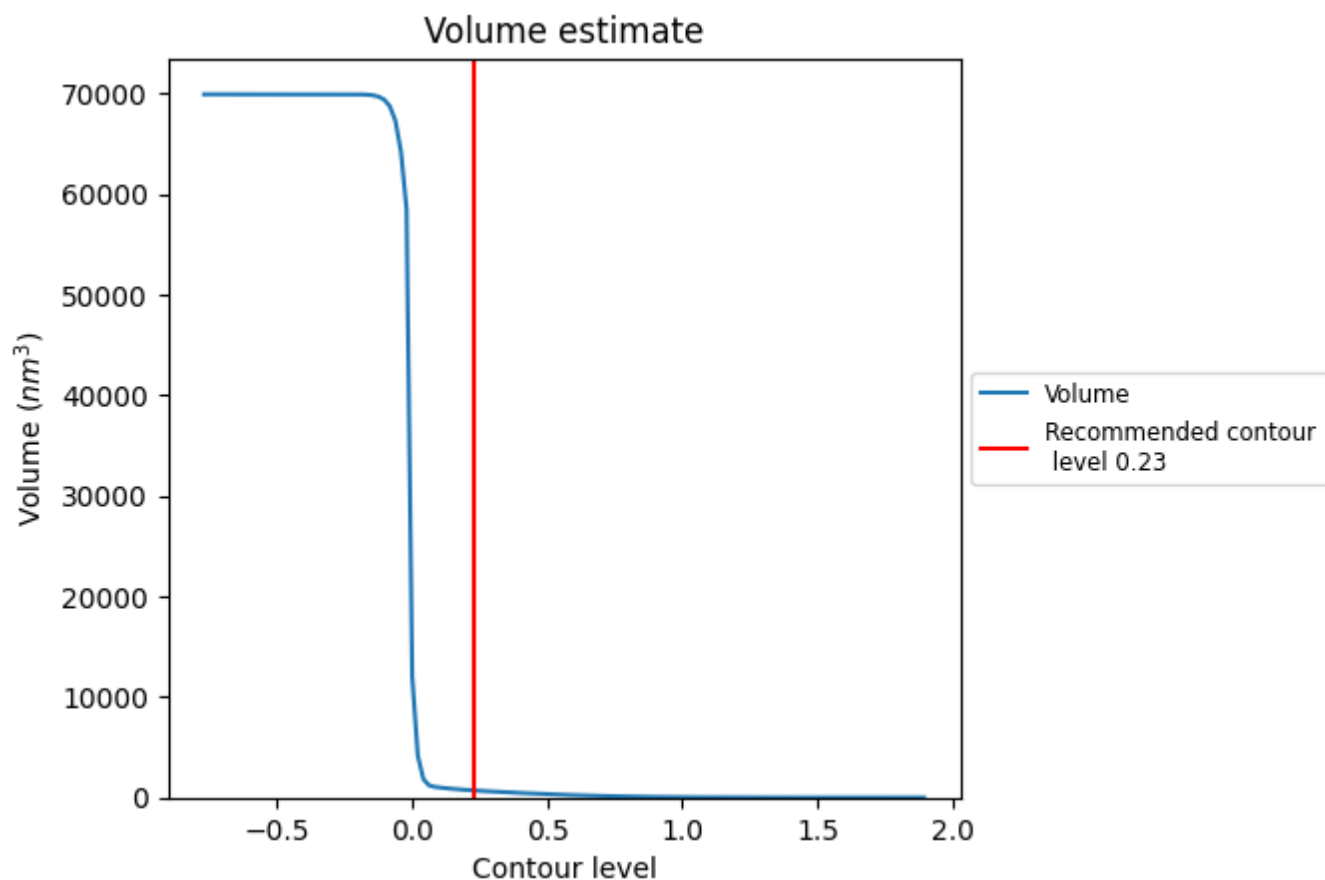
This section contains the results of statistical analysis of the map.

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.

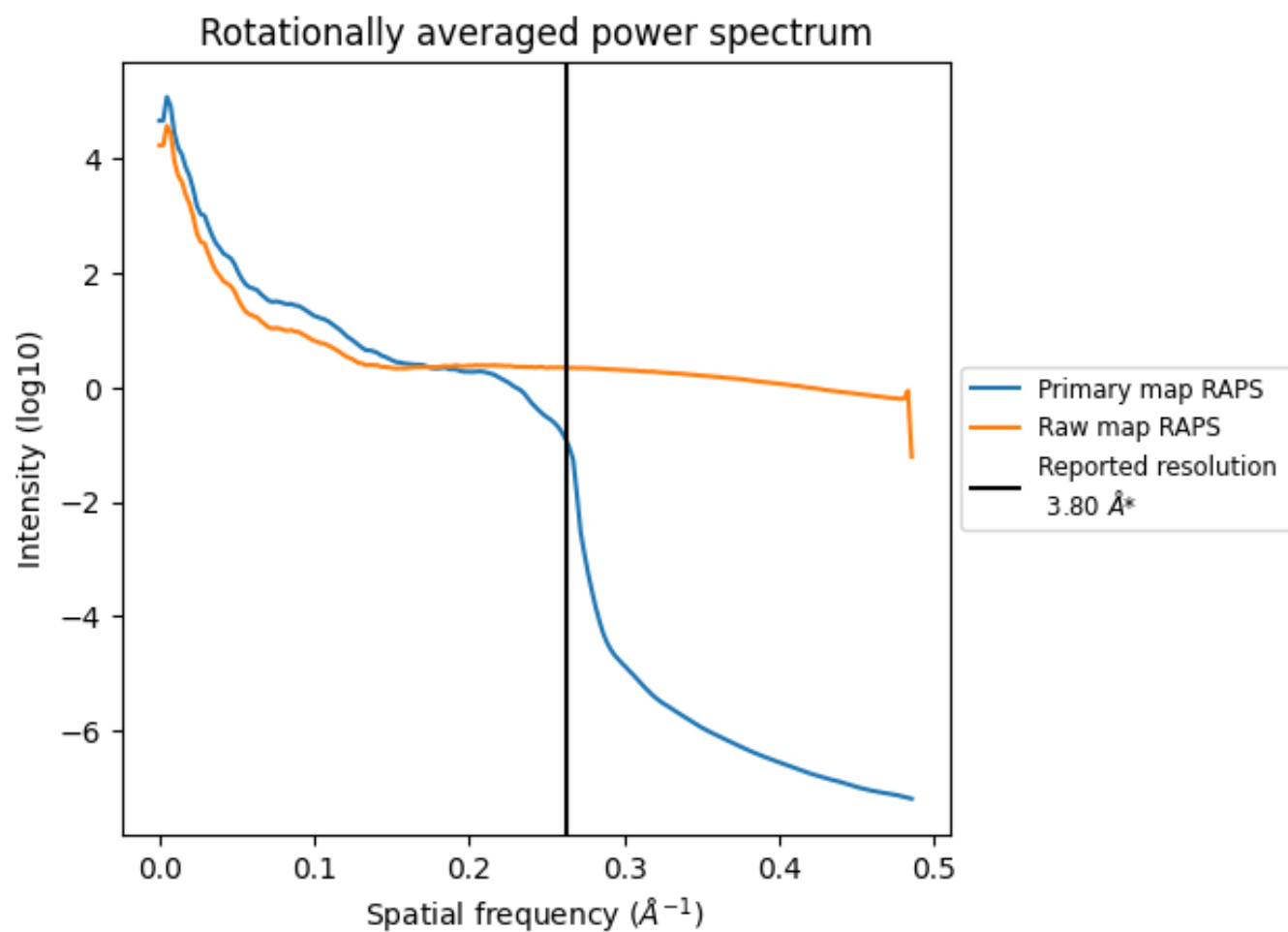
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 706 nm³; this corresponds to an approximate mass of 637 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 ⓘ

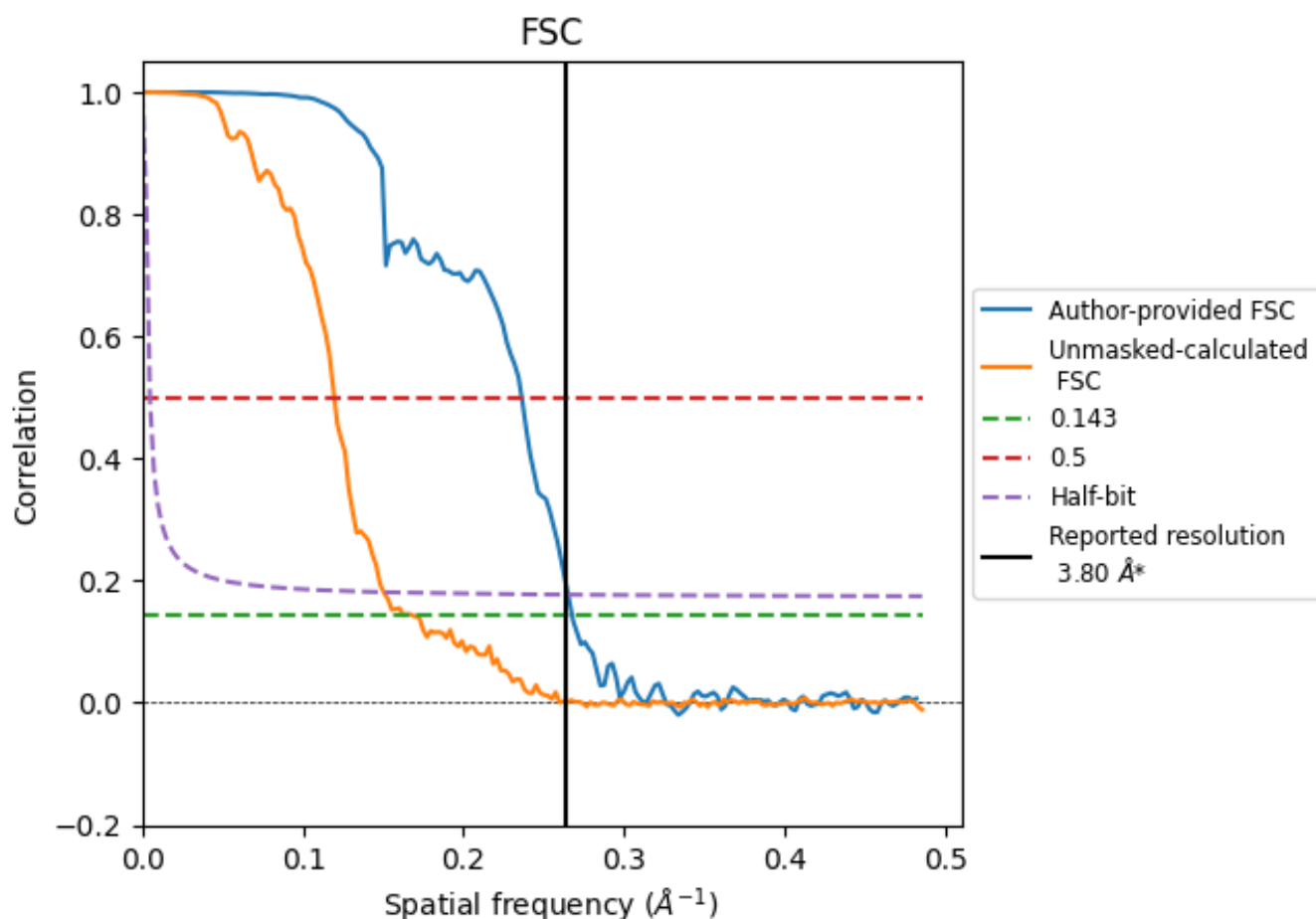


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

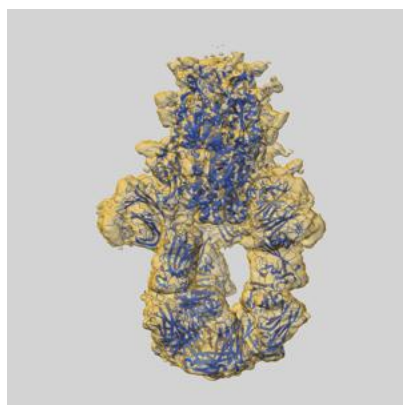
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.23	3.77
Unmasked-calculated*	6.15	8.36	6.65

*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 6.15 differs from the reported value 3.8 by more than 10 %

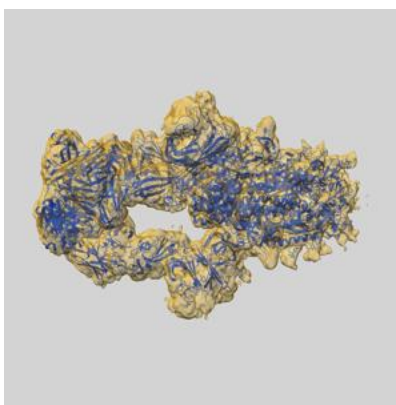
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22926 and PDB model 7KML. Per-residue inclusion information can be found in section [3](#) on page [15](#).

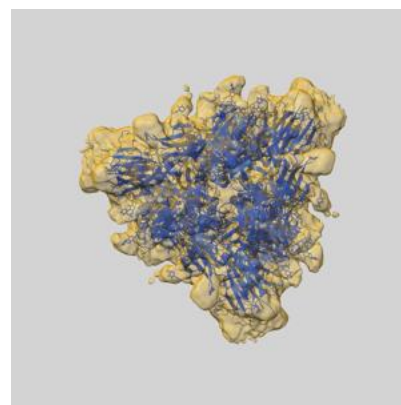
9.1 Map-model overlay [i](#)



X



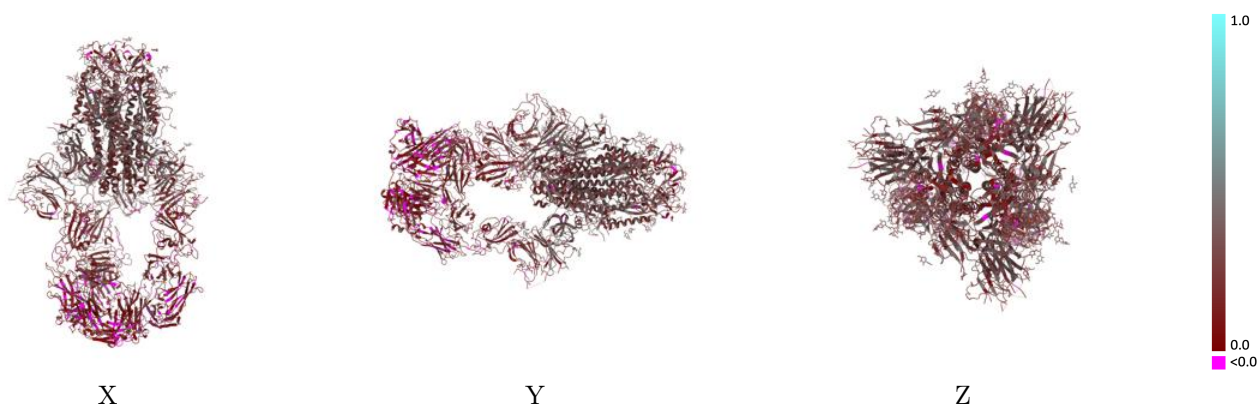
Y



Z

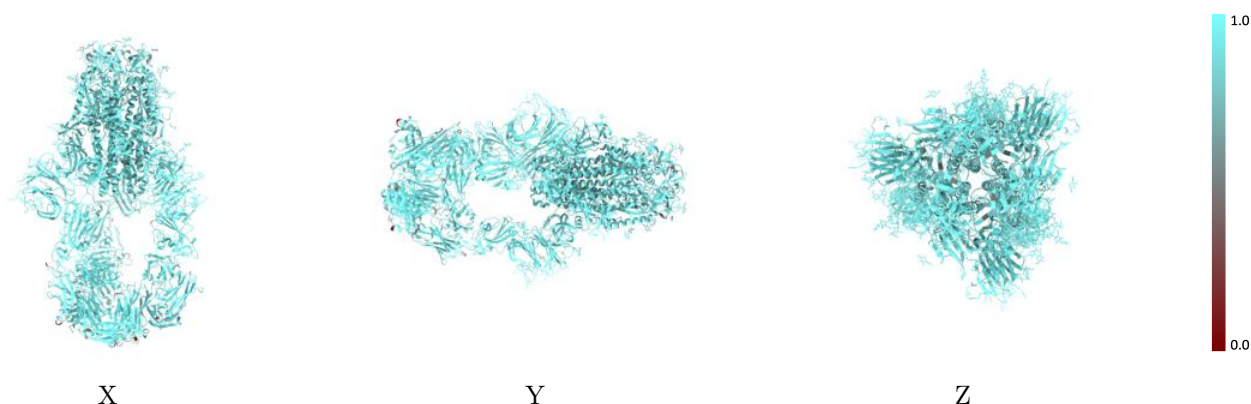
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



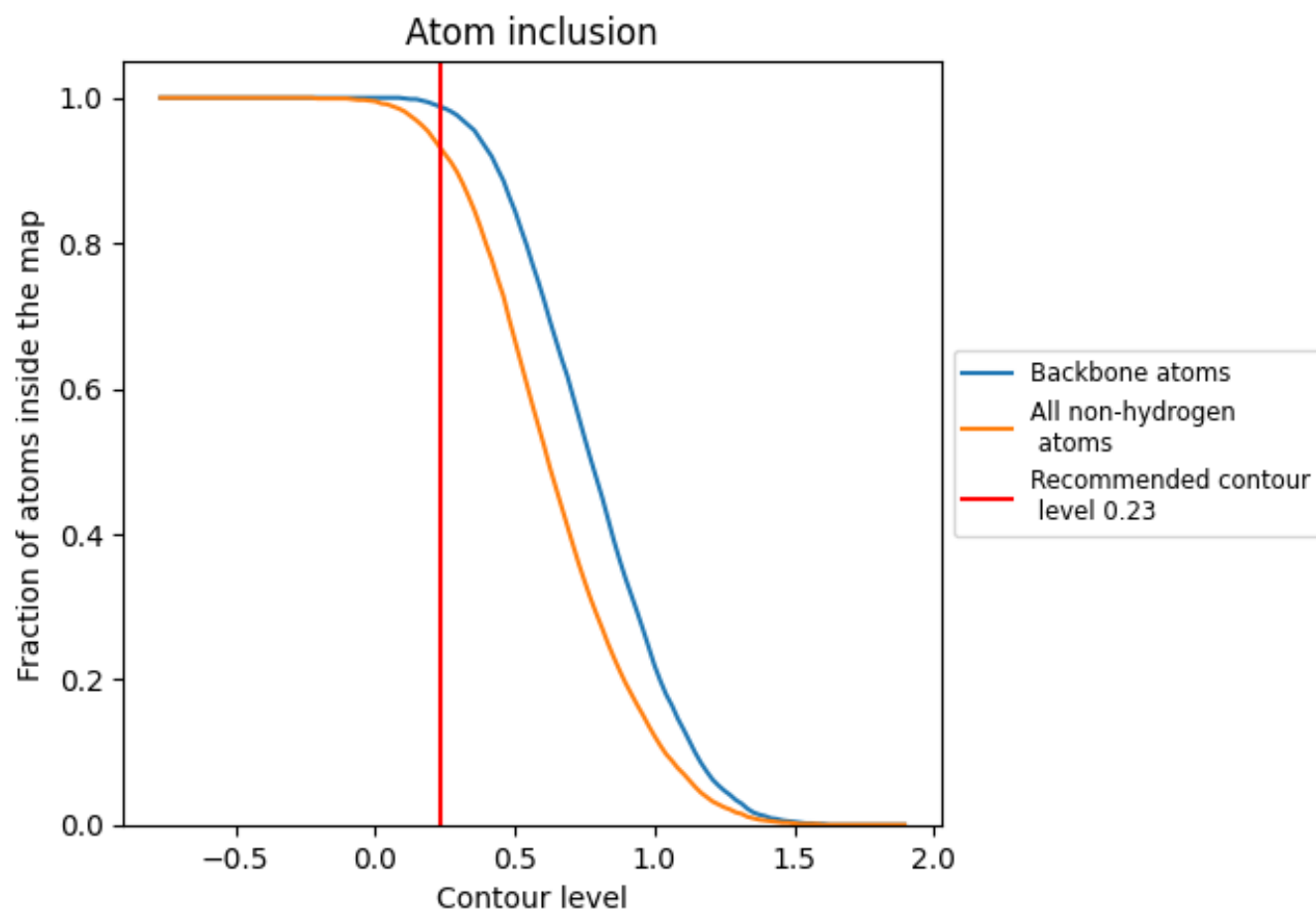
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.2300
A	 0.9310	 0.2630
B	 0.9320	 0.2640
C	 0.9310	 0.2640
D	 1.0000	 0.2380
E	 0.9640	 0.3160
F	 1.0000	 0.3790
G	 1.0000	 0.1880
H	 0.9230	 0.1270
I	 0.9230	 0.1260
J	 0.9230	 0.1240
K	 0.7860	 0.2720
L	 0.9550	 0.1560
M	 0.9550	 0.1600
N	 0.9550	 0.1600
O	 0.8570	 0.3130
P	 0.9290	 0.3370
Q	 0.7860	 0.3090
R	 0.8570	 0.2050
S	 1.0000	 0.2270
T	 0.9640	 0.3320
U	 1.0000	 0.3670
V	 1.0000	 0.1890
W	 0.7860	 0.2700
X	 0.8570	 0.3080
Y	 0.9290	 0.3470
Z	 0.7860	 0.3040
a	 0.8570	 0.2130
b	 1.0000	 0.2280
c	 0.9640	 0.3360
d	 1.0000	 0.3720
e	 1.0000	 0.1890
f	 0.8210	 0.2780
g	 0.8570	 0.3320
h	 0.9290	 0.3620



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Chain	Atom inclusion	Q-score
i	 0.7860	 0.3030
j	 0.8570	 0.2000