



## wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 01:03 PM UTC

PDB ID : 6NB7 / pdb\_00006nb7  
EMDB ID : EMD-0404  
Title : SARS-CoV complex with human neutralizing S230 antibody Fab fragment (state 2)  
Authors : Walls, A.C.; Xiong, X.; Park, Y.J.; Tortorici, M.A.; Snijder, S.; Quispe, J.; Cameroni, E.; Gopal, R.; Mian, D.; Lanzavecchia, A.; Zambon, M.; Rey, F.A.; Corti, D.; Veessler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2018-12-06  
Resolution : 4.50 Å(reported)

This is a wwPDB EM Validation Summary 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:

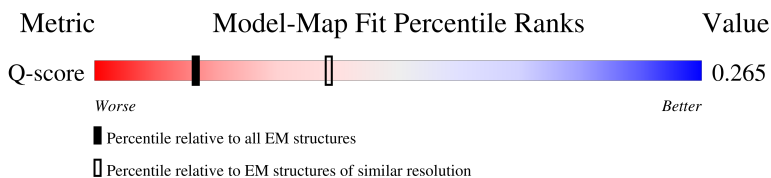
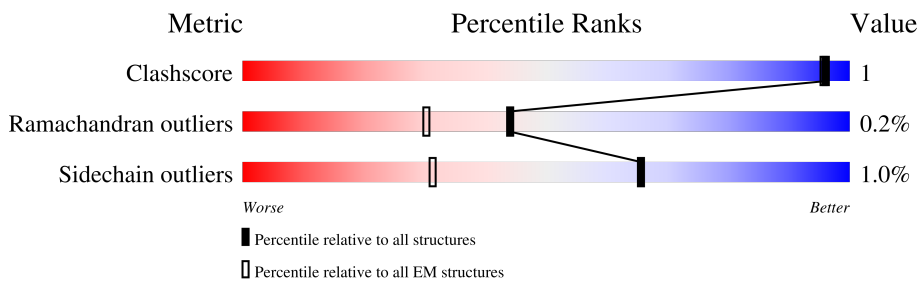
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 4.50 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	2937 ( 4.00 - 5.00 )

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	1263	
1	B	1263	
1	C	1263	

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Mol	Chain	Length	Quality of chain	
2	D	127	26%	95%
2	G	127	24%	95%
2	H	127	17%	94%
3	E	112	40%	95%
3	I	112	42%	96%
3	L	112	38%	95%
4	F	3	67%	100%
4	J	3	33%	100%
4	K	3		100%
4	M	3	33%	100%
4	N	3	67%	100%
4	O	3	33%	100%
4	Q	3	33%	100%
4	V	3		100%
4	X	3		100%
4	Y	3		100%
4	Z	3	67%	100%
4	a	3	33%	100%
4	c	3		100%
4	e	3	67%	100%
4	h	3	67%	100%
4	j	3		100%
4	l	3	33%	100%
4	m	3	33%	100%
4	n	3	33%	100%

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Mol	Chain	Length	Quality of chain
4	r	3	100%
4	t	3	67%
5	P	5	60%
5	R	5	40%
5	S	5	80%
5	U	5	80%
5	d	5	20%
5	q	5	40%
6	T	4	25%
6	s	4	75%
7	W	2	50%
7	b	2	50%
7	i	2	100%
7	k	2	100%
7	o	2	100%
7	p	2	100%
8	f	4	25%
8	g	4	50%

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 24718 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
			Total	C	N	O	S		
1	A	1049	6609	4147	1200	1223	39	0	0
1	B	1032	6428	4027	1171	1191	39	0	0
1	C	1048	6394	4018	1167	1172	37	0	0

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P59594
A	-17	GLY	-	expression tag	UNP P59594
A	-16	ILE	-	expression tag	UNP P59594
A	-15	LEU	-	expression tag	UNP P59594
A	-14	PRO	-	expression tag	UNP P59594
A	-13	SER	-	expression tag	UNP P59594
A	-12	PRO	-	expression tag	UNP P59594
A	-11	GLY	-	expression tag	UNP P59594
A	-10	MET	-	expression tag	UNP P59594
A	-9	PRO	-	expression tag	UNP P59594
A	-8	ALA	-	expression tag	UNP P59594
A	-7	LEU	-	expression tag	UNP P59594
A	-6	LEU	-	expression tag	UNP P59594
A	-5	SER	-	expression tag	UNP P59594
A	-4	LEU	-	expression tag	UNP P59594
A	-3	VAL	-	expression tag	UNP P59594
A	-2	SER	-	expression tag	UNP P59594
A	-1	LEU	-	expression tag	UNP P59594
A	0	LEU	-	expression tag	UNP P59594
A	1	SER	-	expression tag	UNP P59594
A	2	VAL	-	expression tag	UNP P59594
A	3	LEU	-	expression tag	UNP P59594
A	4	LEU	-	expression tag	UNP P59594
A	5	MET	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P59594
A	7	CYS	-	expression tag	UNP P59594
A	8	VAL	-	expression tag	UNP P59594
A	9	ALA	-	expression tag	UNP P59594
A	10	GLU	-	expression tag	UNP P59594
A	11	THR	-	expression tag	UNP P59594
A	12	GLY	-	expression tag	UNP P59594
A	13	THR	-	expression tag	UNP P59594
A	77	ASP	GLY	conflict	UNP P59594
A	244	THR	ILE	conflict	UNP P59594
A	968	PRO	LYS	conflict	UNP P59594
A	969	PRO	VAL	conflict	UNP P59594
A	1194	GLY	-	expression tag	UNP P59594
A	1195	SER	-	expression tag	UNP P59594
A	1196	GLY	-	expression tag	UNP P59594
A	1197	ARG	-	expression tag	UNP P59594
A	1198	GLU	-	expression tag	UNP P59594
A	1199	ASN	-	expression tag	UNP P59594
A	1200	LEU	-	expression tag	UNP P59594
A	1201	TYR	-	expression tag	UNP P59594
A	1202	PHE	-	expression tag	UNP P59594
A	1203	GLN	-	expression tag	UNP P59594
A	1204	GLY	-	expression tag	UNP P59594
A	1205	GLY	-	expression tag	UNP P59594
A	1206	GLY	-	expression tag	UNP P59594
A	1207	GLY	-	expression tag	UNP P59594
A	1208	SER	-	expression tag	UNP P59594
A	1209	GLY	-	expression tag	UNP P59594
A	1210	TYR	-	expression tag	UNP P59594
A	1211	ILE	-	expression tag	UNP P59594
A	1212	PRO	-	expression tag	UNP P59594
A	1213	GLU	-	expression tag	UNP P59594
A	1214	ALA	-	expression tag	UNP P59594
A	1215	PRO	-	expression tag	UNP P59594
A	1216	ARG	-	expression tag	UNP P59594
A	1217	ASP	-	expression tag	UNP P59594
A	1218	GLY	-	expression tag	UNP P59594
A	1219	GLN	-	expression tag	UNP P59594
A	1220	ALA	-	expression tag	UNP P59594
A	1221	TYR	-	expression tag	UNP P59594
A	1222	VAL	-	expression tag	UNP P59594
A	1223	ARG	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	LYS	-	expression tag	UNP P59594
A	1225	ASP	-	expression tag	UNP P59594
A	1226	GLY	-	expression tag	UNP P59594
A	1227	GLU	-	expression tag	UNP P59594
A	1228	TRP	-	expression tag	UNP P59594
A	1229	VAL	-	expression tag	UNP P59594
A	1230	LEU	-	expression tag	UNP P59594
A	1231	LEU	-	expression tag	UNP P59594
A	1232	SER	-	expression tag	UNP P59594
A	1233	THR	-	expression tag	UNP P59594
A	1234	PHE	-	expression tag	UNP P59594
A	1235	LEU	-	expression tag	UNP P59594
A	1236	GLY	-	expression tag	UNP P59594
A	1237	HIS	-	expression tag	UNP P59594
A	1238	HIS	-	expression tag	UNP P59594
A	1239	HIS	-	expression tag	UNP P59594
A	1240	HIS	-	expression tag	UNP P59594
A	1241	HIS	-	expression tag	UNP P59594
A	1242	HIS	-	expression tag	UNP P59594
A	1243	HIS	-	expression tag	UNP P59594
A	1244	HIS	-	expression tag	UNP P59594
B	-18	MET	-	initiating methionine	UNP P59594
B	-17	GLY	-	expression tag	UNP P59594
B	-16	ILE	-	expression tag	UNP P59594
B	-15	LEU	-	expression tag	UNP P59594
B	-14	PRO	-	expression tag	UNP P59594
B	-13	SER	-	expression tag	UNP P59594
B	-12	PRO	-	expression tag	UNP P59594
B	-11	GLY	-	expression tag	UNP P59594
B	-10	MET	-	expression tag	UNP P59594
B	-9	PRO	-	expression tag	UNP P59594
B	-8	ALA	-	expression tag	UNP P59594
B	-7	LEU	-	expression tag	UNP P59594
B	-6	LEU	-	expression tag	UNP P59594
B	-5	SER	-	expression tag	UNP P59594
B	-4	LEU	-	expression tag	UNP P59594
B	-3	VAL	-	expression tag	UNP P59594
B	-2	SER	-	expression tag	UNP P59594
B	-1	LEU	-	expression tag	UNP P59594
B	0	LEU	-	expression tag	UNP P59594
B	1	SER	-	expression tag	UNP P59594
B	2	VAL	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP P59594
B	4	LEU	-	expression tag	UNP P59594
B	5	MET	-	expression tag	UNP P59594
B	6	GLY	-	expression tag	UNP P59594
B	7	CYS	-	expression tag	UNP P59594
B	8	VAL	-	expression tag	UNP P59594
B	9	ALA	-	expression tag	UNP P59594
B	10	GLU	-	expression tag	UNP P59594
B	11	THR	-	expression tag	UNP P59594
B	12	GLY	-	expression tag	UNP P59594
B	13	THR	-	expression tag	UNP P59594
B	77	ASP	GLY	conflict	UNP P59594
B	244	THR	ILE	conflict	UNP P59594
B	968	PRO	LYS	conflict	UNP P59594
B	969	PRO	VAL	conflict	UNP P59594
B	1194	GLY	-	expression tag	UNP P59594
B	1195	SER	-	expression tag	UNP P59594
B	1196	GLY	-	expression tag	UNP P59594
B	1197	ARG	-	expression tag	UNP P59594
B	1198	GLU	-	expression tag	UNP P59594
B	1199	ASN	-	expression tag	UNP P59594
B	1200	LEU	-	expression tag	UNP P59594
B	1201	TYR	-	expression tag	UNP P59594
B	1202	PHE	-	expression tag	UNP P59594
B	1203	GLN	-	expression tag	UNP P59594
B	1204	GLY	-	expression tag	UNP P59594
B	1205	GLY	-	expression tag	UNP P59594
B	1206	GLY	-	expression tag	UNP P59594
B	1207	GLY	-	expression tag	UNP P59594
B	1208	SER	-	expression tag	UNP P59594
B	1209	GLY	-	expression tag	UNP P59594
B	1210	TYR	-	expression tag	UNP P59594
B	1211	ILE	-	expression tag	UNP P59594
B	1212	PRO	-	expression tag	UNP P59594
B	1213	GLU	-	expression tag	UNP P59594
B	1214	ALA	-	expression tag	UNP P59594
B	1215	PRO	-	expression tag	UNP P59594
B	1216	ARG	-	expression tag	UNP P59594
B	1217	ASP	-	expression tag	UNP P59594
B	1218	GLY	-	expression tag	UNP P59594
B	1219	GLN	-	expression tag	UNP P59594
B	1220	ALA	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1221	TYR	-	expression tag	UNP P59594
B	1222	VAL	-	expression tag	UNP P59594
B	1223	ARG	-	expression tag	UNP P59594
B	1224	LYS	-	expression tag	UNP P59594
B	1225	ASP	-	expression tag	UNP P59594
B	1226	GLY	-	expression tag	UNP P59594
B	1227	GLU	-	expression tag	UNP P59594
B	1228	TRP	-	expression tag	UNP P59594
B	1229	VAL	-	expression tag	UNP P59594
B	1230	LEU	-	expression tag	UNP P59594
B	1231	LEU	-	expression tag	UNP P59594
B	1232	SER	-	expression tag	UNP P59594
B	1233	THR	-	expression tag	UNP P59594
B	1234	PHE	-	expression tag	UNP P59594
B	1235	LEU	-	expression tag	UNP P59594
B	1236	GLY	-	expression tag	UNP P59594
B	1237	HIS	-	expression tag	UNP P59594
B	1238	HIS	-	expression tag	UNP P59594
B	1239	HIS	-	expression tag	UNP P59594
B	1240	HIS	-	expression tag	UNP P59594
B	1241	HIS	-	expression tag	UNP P59594
B	1242	HIS	-	expression tag	UNP P59594
B	1243	HIS	-	expression tag	UNP P59594
B	1244	HIS	-	expression tag	UNP P59594
C	-18	MET	-	initiating methionine	UNP P59594
C	-17	GLY	-	expression tag	UNP P59594
C	-16	ILE	-	expression tag	UNP P59594
C	-15	LEU	-	expression tag	UNP P59594
C	-14	PRO	-	expression tag	UNP P59594
C	-13	SER	-	expression tag	UNP P59594
C	-12	PRO	-	expression tag	UNP P59594
C	-11	GLY	-	expression tag	UNP P59594
C	-10	MET	-	expression tag	UNP P59594
C	-9	PRO	-	expression tag	UNP P59594
C	-8	ALA	-	expression tag	UNP P59594
C	-7	LEU	-	expression tag	UNP P59594
C	-6	LEU	-	expression tag	UNP P59594
C	-5	SER	-	expression tag	UNP P59594
C	-4	LEU	-	expression tag	UNP P59594
C	-3	VAL	-	expression tag	UNP P59594
C	-2	SER	-	expression tag	UNP P59594
C	-1	LEU	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	LEU	-	expression tag	UNP P59594
C	1	SER	-	expression tag	UNP P59594
C	2	VAL	-	expression tag	UNP P59594
C	3	LEU	-	expression tag	UNP P59594
C	4	LEU	-	expression tag	UNP P59594
C	5	MET	-	expression tag	UNP P59594
C	6	GLY	-	expression tag	UNP P59594
C	7	CYS	-	expression tag	UNP P59594
C	8	VAL	-	expression tag	UNP P59594
C	9	ALA	-	expression tag	UNP P59594
C	10	GLU	-	expression tag	UNP P59594
C	11	THR	-	expression tag	UNP P59594
C	12	GLY	-	expression tag	UNP P59594
C	13	THR	-	expression tag	UNP P59594
C	77	ASP	GLY	conflict	UNP P59594
C	244	THR	ILE	conflict	UNP P59594
C	968	PRO	LYS	conflict	UNP P59594
C	969	PRO	VAL	conflict	UNP P59594
C	1194	GLY	-	expression tag	UNP P59594
C	1195	SER	-	expression tag	UNP P59594
C	1196	GLY	-	expression tag	UNP P59594
C	1197	ARG	-	expression tag	UNP P59594
C	1198	GLU	-	expression tag	UNP P59594
C	1199	ASN	-	expression tag	UNP P59594
C	1200	LEU	-	expression tag	UNP P59594
C	1201	TYR	-	expression tag	UNP P59594
C	1202	PHE	-	expression tag	UNP P59594
C	1203	GLN	-	expression tag	UNP P59594
C	1204	GLY	-	expression tag	UNP P59594
C	1205	GLY	-	expression tag	UNP P59594
C	1206	GLY	-	expression tag	UNP P59594
C	1207	GLY	-	expression tag	UNP P59594
C	1208	SER	-	expression tag	UNP P59594
C	1209	GLY	-	expression tag	UNP P59594
C	1210	TYR	-	expression tag	UNP P59594
C	1211	ILE	-	expression tag	UNP P59594
C	1212	PRO	-	expression tag	UNP P59594
C	1213	GLU	-	expression tag	UNP P59594
C	1214	ALA	-	expression tag	UNP P59594
C	1215	PRO	-	expression tag	UNP P59594
C	1216	ARG	-	expression tag	UNP P59594
C	1217	ASP	-	expression tag	UNP P59594

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	GLY	-	expression tag	UNP P59594
C	1219	GLN	-	expression tag	UNP P59594
C	1220	ALA	-	expression tag	UNP P59594
C	1221	TYR	-	expression tag	UNP P59594
C	1222	VAL	-	expression tag	UNP P59594
C	1223	ARG	-	expression tag	UNP P59594
C	1224	LYS	-	expression tag	UNP P59594
C	1225	ASP	-	expression tag	UNP P59594
C	1226	GLY	-	expression tag	UNP P59594
C	1227	GLU	-	expression tag	UNP P59594
C	1228	TRP	-	expression tag	UNP P59594
C	1229	VAL	-	expression tag	UNP P59594
C	1230	LEU	-	expression tag	UNP P59594
C	1231	LEU	-	expression tag	UNP P59594
C	1232	SER	-	expression tag	UNP P59594
C	1233	THR	-	expression tag	UNP P59594
C	1234	PHE	-	expression tag	UNP P59594
C	1235	LEU	-	expression tag	UNP P59594
C	1236	GLY	-	expression tag	UNP P59594
C	1237	HIS	-	expression tag	UNP P59594
C	1238	HIS	-	expression tag	UNP P59594
C	1239	HIS	-	expression tag	UNP P59594
C	1240	HIS	-	expression tag	UNP P59594
C	1241	HIS	-	expression tag	UNP P59594
C	1242	HIS	-	expression tag	UNP P59594
C	1243	HIS	-	expression tag	UNP P59594
C	1244	HIS	-	expression tag	UNP P59594

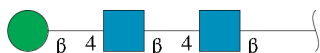
- Molecule 2 is a protein called S230 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	123	Total	C	N	O	S	0	0
			613	365	123	123	2		
2	G	123	Total	C	N	O	S	0	0
			613	365	123	123	2		
2	H	123	Total	C	N	O	S	0	0
			613	365	123	123	2		

- Molecule 3 is a protein called S230 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	110	Total	C	N	O	S	0	0
			557	335	110	110	2		
3	I	110	Total	C	N	O	S	0	0
			557	335	110	110	2		
3	L	110	Total	C	N	O	S	0	0
			557	335	110	110	2		

- 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.



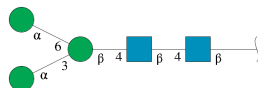
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	O	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	3	Total	C	N	O	0	0
			39	22	2	15		
4	X	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	Z	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		
4	c	3	Total	C	N	O	0	0
			39	22	2	15		
4	e	3	Total	C	N	O	0	0
			39	22	2	15		

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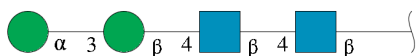
Mol	Chain	Residues	Atoms				AltConf	Trace
4	h	3	Total	C	N	O	0	0
			39	22	2	15		
4	j	3	Total	C	N	O	0	0
			39	22	2	15		
4	l	3	Total	C	N	O	0	0
			39	22	2	15		
4	m	3	Total	C	N	O	0	0
			39	22	2	15		
4	n	3	Total	C	N	O	0	0
			39	22	2	15		
4	r	3	Total	C	N	O	0	0
			39	22	2	15		
4	t	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		
5	S	5	Total	C	N	O	0	0
			61	34	2	25		
5	U	5	Total	C	N	O	0	0
			61	34	2	25		
5	d	5	Total	C	N	O	0	0
			61	34	2	25		
5	q	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	T	4	50	28	2	20	0	0
6	s	4	50	28	2	20	0	0

- Molecule 7 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
			Total	C	N	O		
7	W	2	28	16	2	10	0	0
7	b	2	28	16	2	10	0	0
7	i	2	28	16	2	10	0	0
7	k	2	28	16	2	10	0	0
7	o	2	28	16	2	10	0	0
7	p	2	28	16	2	10	0	0

- Molecule 8 is an oligosaccharide called 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.



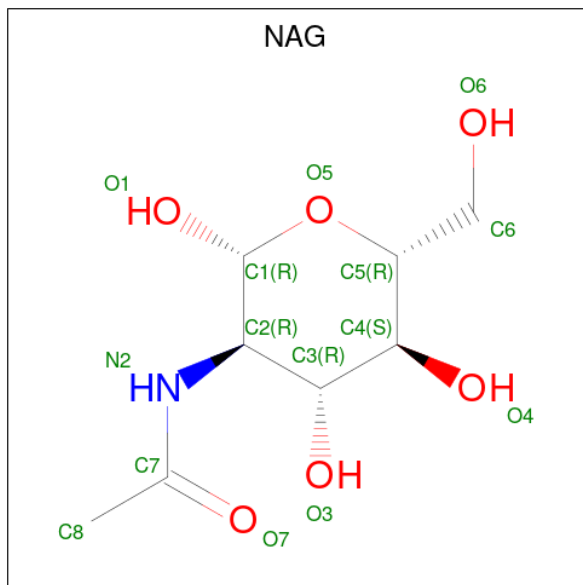
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	f	4	50	28	2	20	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	g	4	50	28	2	20	0	0

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



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

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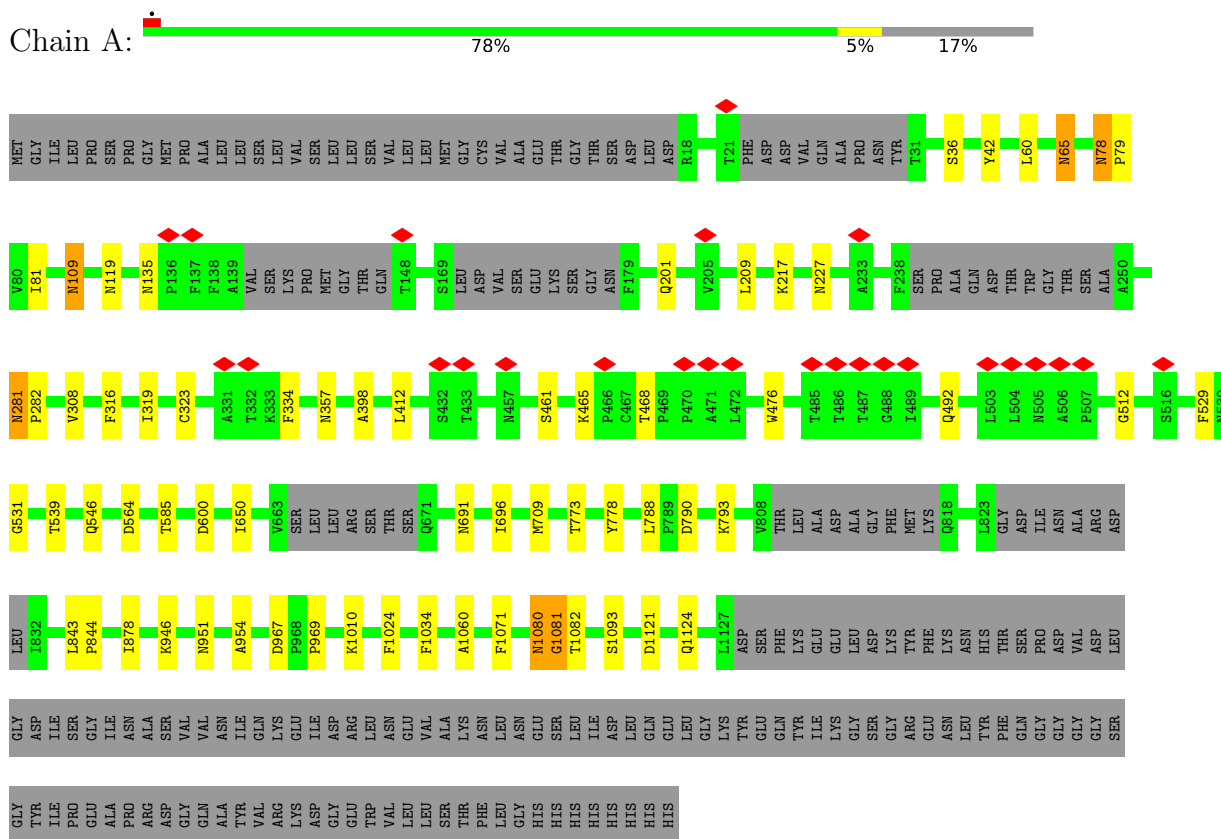
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	Total 14	8	1	5	0
9	B	1	Total 14	8	1	5	0
9	C	1	Total 14	8	1	5	0
9	C	1	Total 14	8	1	5	0
9	C	1	Total 14	8	1	5	0
9	C	1	Total 14	8	1	5	0

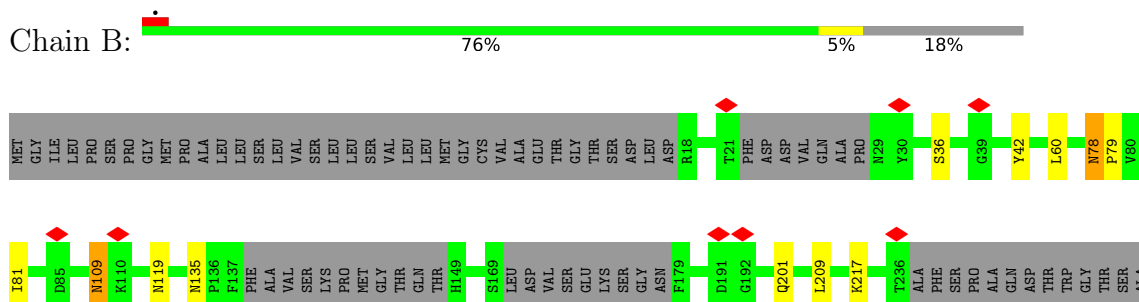
### 3 Residue-property plots

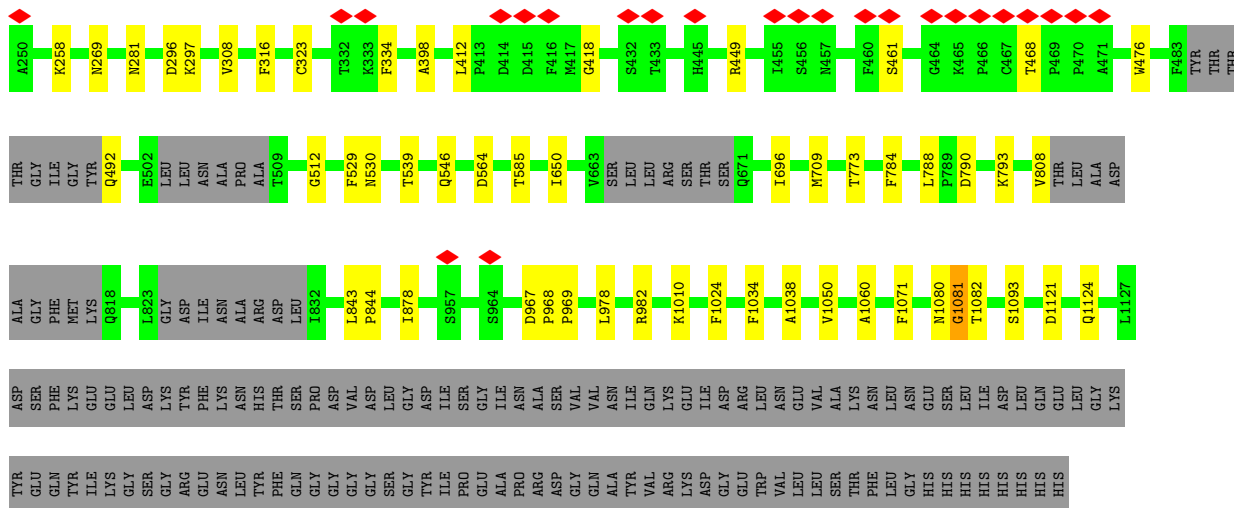
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike glycoprotein

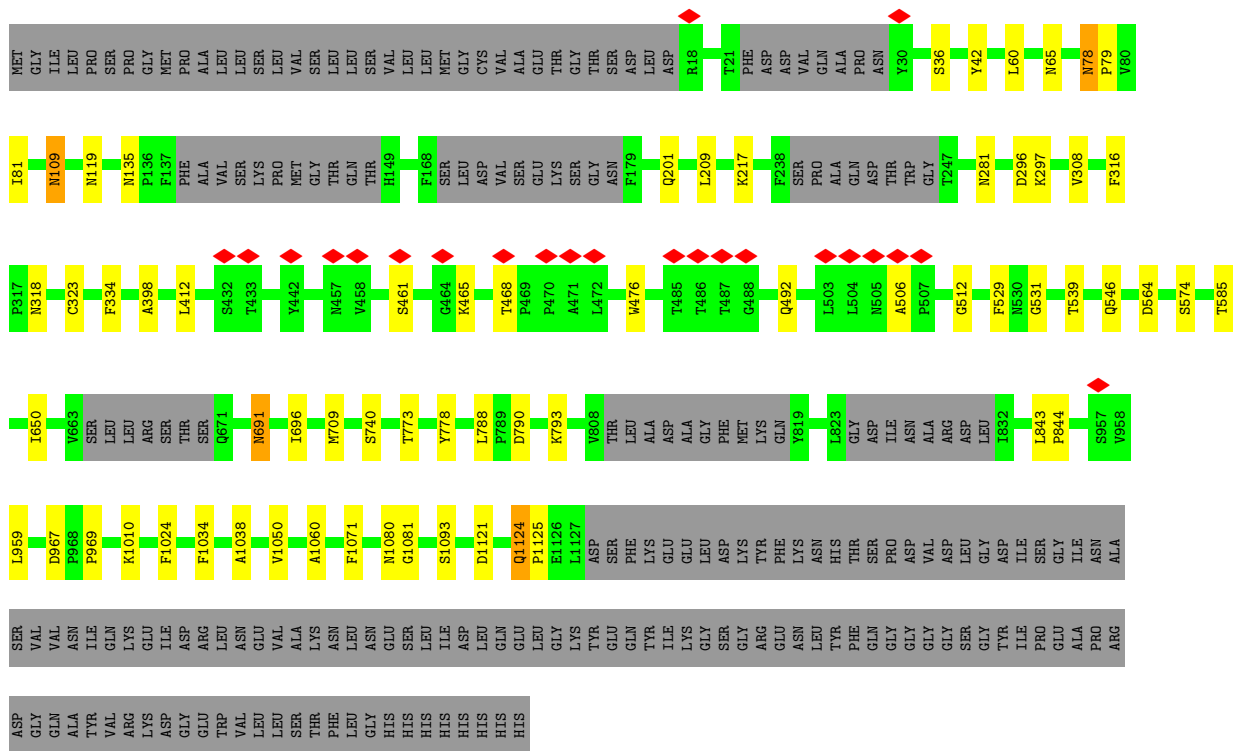
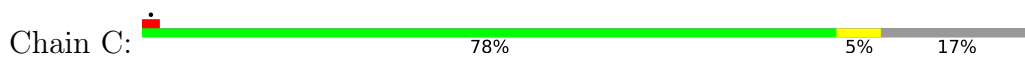


- Molecule 1: Spike glycoprotein

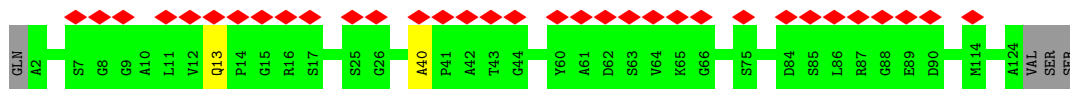




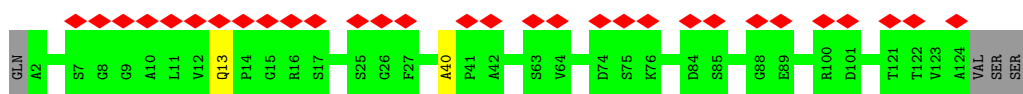
• Molecule 1: Spike glycoprotein



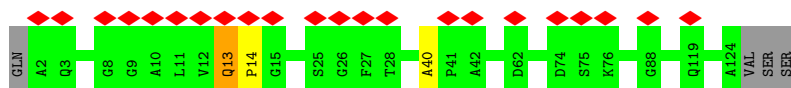
• Molecule 2: S230 heavy chain



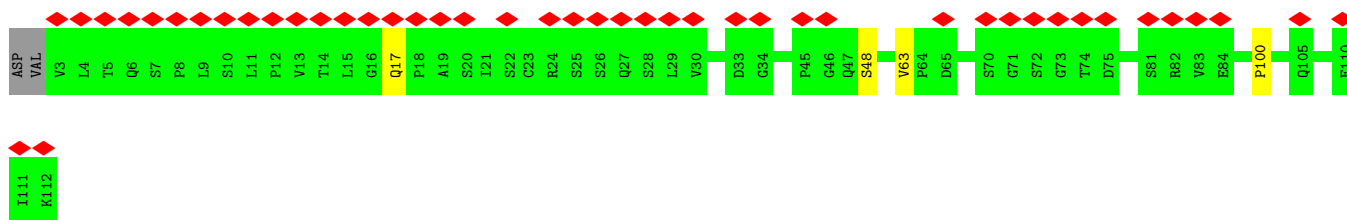
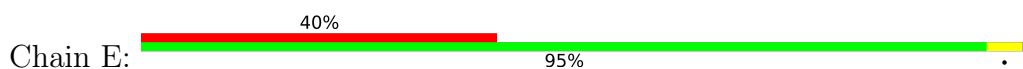
• Molecule 2: S230 heavy chain



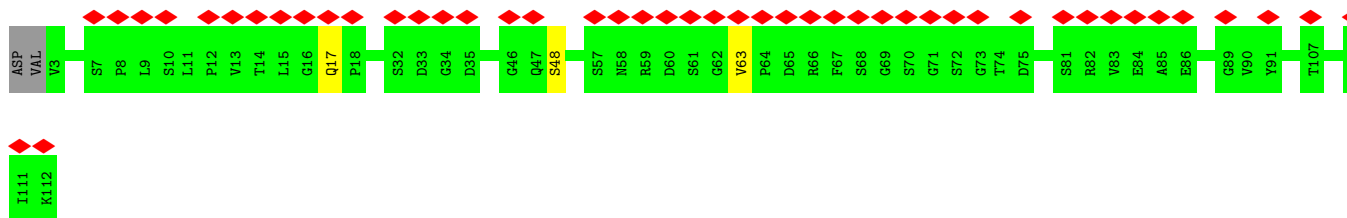
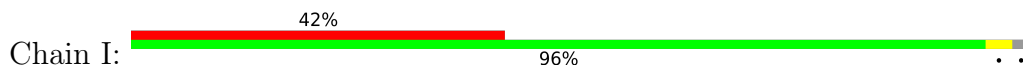
- Molecule 2: S230 heavy chain



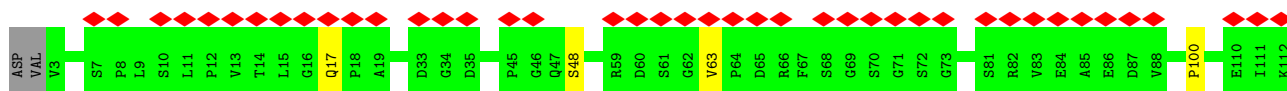
- Molecule 3: S230 light chain



- Molecule 3: S230 light chain



- Molecule 3: S230 light chain



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

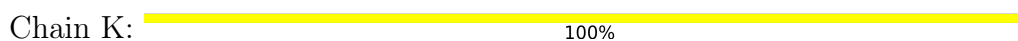




- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



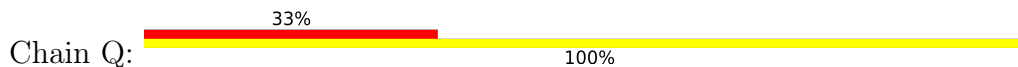
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

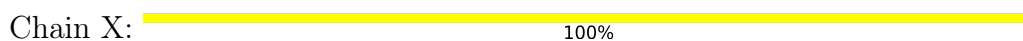




- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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 e: 

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 h: 

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 j: 

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 l: 

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 m: 

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 n: 



- 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%



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

Chain t: 67%  
100%



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

Chain P: 60%  
100%



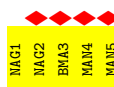
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 40%  
80% 20%



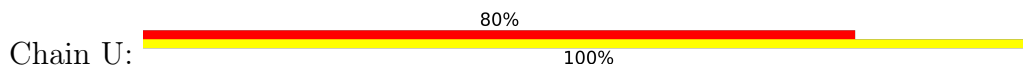
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 80%  
100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose

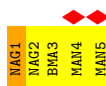
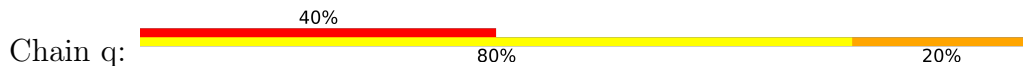
se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



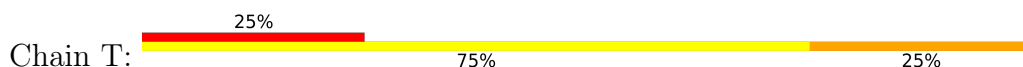
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

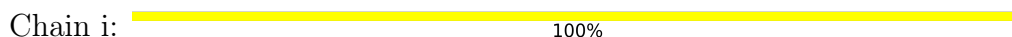




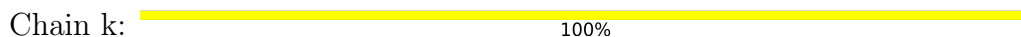
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



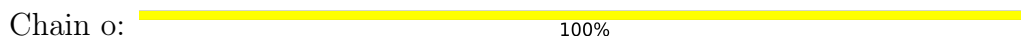
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



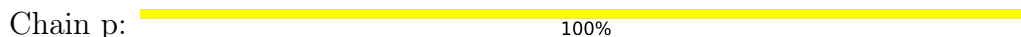
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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





- Molecule 8: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.611	Depositor
Minimum map value	-3.199	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	526.08, 526.08, 526.08	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7536, 1.7536, 1.7536	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: MAN, 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	0.64	0/6733	1.03	85/9274 (0.9%)
1	B	0.63	0/6542	1.06	94/9007 (1.0%)
1	C	0.63	0/6522	1.05	91/9002 (1.0%)
2	D	0.52	0/615	0.98	4/855 (0.5%)
2	G	0.52	0/615	0.99	4/855 (0.5%)
2	H	0.52	0/615	0.99	4/855 (0.5%)
3	E	0.58	0/564	1.09	8/787 (1.0%)
3	I	0.57	0/564	1.08	6/787 (0.8%)
3	L	0.57	0/564	1.09	8/787 (1.0%)
All	All	0.62	0/23334	1.04	304/32209 (0.9%)

There are no bond length outliers.

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	784	PHE	N-CA-CB	-9.72	95.17	111.20
1	B	808	VAL	CG1-CB-CG2	9.00	130.59	110.80
1	B	784	PHE	N-CA-C	-8.96	100.76	112.41
1	C	468	THR	CA-C-N	8.69	126.00	119.66
1	C	468	THR	C-N-CA	8.69	126.00	119.66

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	6609	0	5040	15	0
1	B	6428	0	4821	10	0
1	C	6394	0	4494	12	0
2	D	613	0	307	0	0
2	G	613	0	307	0	0
2	H	613	0	307	1	0
3	E	557	0	280	0	0
3	I	557	0	280	0	0
3	L	557	0	280	0	0
4	F	39	0	33	0	0
4	J	39	0	33	0	0
4	K	39	0	33	0	0
4	M	39	0	33	0	0
4	N	39	0	33	0	0
4	O	39	0	33	0	0
4	Q	39	0	33	0	0
4	V	39	0	33	0	0
4	X	39	0	33	0	0
4	Y	39	0	33	0	0
4	Z	39	0	33	0	0
4	a	39	0	33	0	0
4	c	39	0	33	0	0
4	e	39	0	33	0	0
4	h	39	0	33	0	0
4	j	39	0	33	0	0
4	l	39	0	33	0	0
4	m	39	0	33	0	0
4	n	39	0	33	0	0
4	r	39	0	33	0	0
4	t	39	0	33	0	0
5	P	61	0	49	0	0
5	R	61	0	49	1	0
5	S	61	0	49	0	0
5	U	61	0	49	0	0
5	d	61	0	49	0	0
5	q	61	0	49	1	0
6	T	50	0	41	1	0
6	s	50	0	41	0	0
7	W	28	0	25	0	0
7	b	28	0	25	0	0
7	i	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	k	28	0	25	0	0
7	o	28	0	25	0	0
7	p	28	0	25	0	0
8	f	50	0	41	0	0
8	g	50	0	41	0	0
9	A	84	0	78	0	0
9	B	84	0	78	0	0
9	C	56	0	52	0	0
All	All	24718	0	17625	37	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.

The worst 5 of 37 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:TYR:HB2	5:q:1:NAG:H81	1.82	0.61
1:B:1080:ASN:CG	1:B:1081:GLY:N	2.63	0.54
1:C:78:ASN:N	1:C:79:PRO:CD	2.69	0.54
1:A:1080:ASN:CG	1:A:1081:GLY:N	2.66	0.54
1:B:78:ASN:N	1:B:79:PRO:CD	2.71	0.53

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1033/1263 (82%)	990 (96%)	39 (4%)	4 (0%)	30 67
1	B	1012/1263 (80%)	973 (96%)	37 (4%)	2 (0%)	43 77
1	C	1032/1263 (82%)	996 (96%)	34 (3%)	2 (0%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
2	G	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
2	H	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
3	E	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
3	I	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
3	L	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
All	All	3764/4506 (84%)	3635 (97%)	121 (3%)	8 (0%)	44	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ASP
1	A	1081	GLY
1	C	318	ASN
1	B	1081	GLY
1	A	319	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/1092 (40%)	433 (99%)	5 (1%)	65	74
1	B	410/1092 (38%)	407 (99%)	3 (1%)	76	79
1	C	350/1092 (32%)	346 (99%)	4 (1%)	65	74
2	D	5/106 (5%)	5 (100%)	0	100	100
2	G	5/106 (5%)	5 (100%)	0	100	100
2	H	5/106 (5%)	5 (100%)	0	100	100
3	E	10/99 (10%)	10 (100%)	0	100	100
3	I	10/99 (10%)	10 (100%)	0	100	100
3	L	10/99 (10%)	10 (100%)	0	100	100
All	All	1243/3891 (32%)	1231 (99%)	12 (1%)	65	76

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	269	ASN
1	C	65	ASN
1	C	691	ASN
1	C	109	ASN
1	A	357	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	786	GLN
1	C	737	GLN
1	C	661	HIS
1	B	1046	HIS
1	C	721	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

121 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	F	1	1,4	14,14,15	2.08	4 (28%)	17,19,21	1.02	1 (5%)
4	NAG	F	2	4	14,14,15	2.19	4 (28%)	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	F	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	J	1	1,4	14,14,15	2.06	4 (28%)	17,19,21	1.15	3 (17%)
4	NAG	J	2	4	14,14,15	2.19	5 (35%)	17,19,21	1.14	1 (5%)
4	BMA	J	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.95	1 (6%)
4	NAG	K	1	1,4	14,14,15	2.12	4 (28%)	17,19,21	1.22	1 (5%)
4	NAG	K	2	4	14,14,15	2.23	4 (28%)	17,19,21	1.09	1 (5%)
4	BMA	K	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.87	0
4	NAG	M	1	1,4	14,14,15	1.77	3 (21%)	17,19,21	1.69	3 (17%)
4	NAG	M	2	4	14,14,15	2.12	3 (21%)	17,19,21	1.64	5 (29%)
4	BMA	M	3	4	11,11,12	1.82	2 (18%)	15,15,17	0.92	0
4	NAG	N	1	1,4	14,14,15	2.02	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	N	2	4	14,14,15	2.17	4 (28%)	17,19,21	1.37	2 (11%)
4	BMA	N	3	4	11,11,12	1.82	2 (18%)	15,15,17	1.06	1 (6%)
4	NAG	O	1	1,4	14,14,15	1.97	3 (21%)	17,19,21	0.91	1 (5%)
4	NAG	O	2	4	14,14,15	2.24	4 (28%)	17,19,21	1.45	5 (29%)
4	BMA	O	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.85	0
5	NAG	P	1	1,5	14,14,15	2.00	3 (21%)	17,19,21	1.15	1 (5%)
5	NAG	P	2	5	14,14,15	2.24	5 (35%)	17,19,21	1.29	3 (17%)
5	BMA	P	3	5	11,11,12	1.74	1 (9%)	15,15,17	0.85	0
5	MAN	P	4	5	11,11,12	1.83	2 (18%)	15,15,17	1.30	2 (13%)
5	MAN	P	5	5	11,11,12	1.82	2 (18%)	15,15,17	1.05	2 (13%)
4	NAG	Q	1	1,4	14,14,15	2.10	2 (14%)	17,19,21	1.09	2 (11%)
4	NAG	Q	2	4	14,14,15	2.19	5 (35%)	17,19,21	1.87	5 (29%)
4	BMA	Q	3	4	11,11,12	1.79	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	R	1	1,5	14,14,15	2.04	3 (21%)	17,19,21	1.15	2 (11%)
5	NAG	R	2	5	14,14,15	2.18	5 (35%)	17,19,21	1.33	3 (17%)
5	BMA	R	3	5	11,11,12	1.74	2 (18%)	15,15,17	1.09	1 (6%)
5	MAN	R	4	5	11,11,12	1.82	1 (9%)	15,15,17	1.19	2 (13%)
5	MAN	R	5	5	11,11,12	1.82	2 (18%)	15,15,17	1.24	2 (13%)
5	NAG	S	1	1,5	14,14,15	1.94	1 (7%)	17,19,21	1.38	3 (17%)
5	NAG	S	2	5	14,14,15	2.07	3 (21%)	17,19,21	1.38	3 (17%)
5	BMA	S	3	5	11,11,12	1.80	2 (18%)	15,15,17	1.14	2 (13%)
5	MAN	S	4	5	11,11,12	1.82	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	S	5	5	11,11,12	1.84	2 (18%)	15,15,17	1.07	1 (6%)
6	NAG	T	1	1,6	14,14,15	2.06	2 (14%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	T	2	6	14,14,15	2.17	4 (28%)	17,19,21	1.14	2 (11%)
6	BMA	T	3	6	11,11,12	1.79	2 (18%)	15,15,17	0.93	1 (6%)
6	MAN	T	4	6	11,11,12	1.83	2 (18%)	15,15,17	1.01	0
5	NAG	U	1	1,5	14,14,15	2.04	3 (21%)	17,19,21	0.85	1 (5%)
5	NAG	U	2	5	14,14,15	2.16	4 (28%)	17,19,21	1.10	2 (11%)
5	BMA	U	3	5	11,11,12	1.86	3 (27%)	15,15,17	0.92	1 (6%)
5	MAN	U	4	5	11,11,12	1.76	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	U	5	5	11,11,12	1.81	2 (18%)	15,15,17	1.03	1 (6%)
4	NAG	V	1	1,4	14,14,15	2.19	3 (21%)	17,19,21	0.96	0
4	NAG	V	2	4	14,14,15	2.19	5 (35%)	17,19,21	1.20	2 (11%)
4	BMA	V	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.94	1 (6%)
7	NAG	W	1	1,7	14,14,15	2.11	3 (21%)	17,19,21	1.16	2 (11%)
7	NAG	W	2	7	14,14,15	2.20	4 (28%)	17,19,21	1.05	1 (5%)
4	NAG	X	1	1,4	14,14,15	2.05	3 (21%)	17,19,21	1.40	2 (11%)
4	NAG	X	2	4	14,14,15	2.26	5 (35%)	17,19,21	1.56	3 (17%)
4	BMA	X	3	4	11,11,12	1.83	2 (18%)	15,15,17	0.98	1 (6%)
4	NAG	Y	1	1,4	14,14,15	2.05	2 (14%)	17,19,21	0.85	0
4	NAG	Y	2	4	14,14,15	2.22	5 (35%)	17,19,21	1.72	3 (17%)
4	BMA	Y	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.95	1 (6%)
4	NAG	Z	1	1,4	14,14,15	2.28	3 (21%)	17,19,21	0.96	1 (5%)
4	NAG	Z	2	4	14,14,15	2.25	5 (35%)	17,19,21	1.27	2 (11%)
4	BMA	Z	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.92	1 (6%)
4	NAG	a	1	1,4	14,14,15	2.07	3 (21%)	17,19,21	1.12	1 (5%)
4	NAG	a	2	4	14,14,15	2.18	4 (28%)	17,19,21	1.80	5 (29%)
4	BMA	a	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.99	1 (6%)
7	NAG	b	1	1,7	14,14,15	2.03	3 (21%)	17,19,21	1.23	1 (5%)
7	NAG	b	2	7	14,14,15	2.12	2 (14%)	17,19,21	1.24	2 (11%)
4	NAG	c	1	1,4	14,14,15	2.09	1 (7%)	17,19,21	0.68	0
4	NAG	c	2	4	14,14,15	2.11	2 (14%)	17,19,21	0.87	0
4	BMA	c	3	4	11,11,12	1.84	2 (18%)	15,15,17	0.94	1 (6%)
5	NAG	d	1	1,5	14,14,15	1.94	2 (14%)	17,19,21	0.79	0
5	NAG	d	2	5	14,14,15	2.13	5 (35%)	17,19,21	1.42	2 (11%)
5	BMA	d	3	5	11,11,12	1.67	2 (18%)	15,15,17	1.00	1 (6%)
5	MAN	d	4	5	11,11,12	1.89	3 (27%)	15,15,17	1.23	2 (13%)
5	MAN	d	5	5	11,11,12	1.85	2 (18%)	15,15,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	e	1	1,4	14,14,15	2.06	3 (21%)	17,19,21	0.82	1 (5%)
4	NAG	e	2	4	14,14,15	2.13	4 (28%)	17,19,21	1.41	4 (23%)
4	BMA	e	3	4	11,11,12	1.83	2 (18%)	15,15,17	0.97	1 (6%)
8	NAG	f	1	1,8	14,14,15	2.01	3 (21%)	17,19,21	1.03	2 (11%)
8	NAG	f	2	8	14,14,15	2.08	3 (21%)	17,19,21	0.89	0
8	BMA	f	3	8	11,11,12	1.88	2 (18%)	15,15,17	0.97	0
8	MAN	f	4	8	11,11,12	1.84	2 (18%)	15,15,17	1.15	2 (13%)
8	NAG	g	1	1,8	14,14,15	2.06	4 (28%)	17,19,21	0.87	0
8	NAG	g	2	8	14,14,15	2.17	4 (28%)	17,19,21	1.48	3 (17%)
8	BMA	g	3	8	11,11,12	1.80	3 (27%)	15,15,17	0.78	0
8	MAN	g	4	8	11,11,12	1.81	2 (18%)	15,15,17	1.05	1 (6%)
4	NAG	h	1	1,4	14,14,15	2.10	4 (28%)	17,19,21	1.21	1 (5%)
4	NAG	h	2	4	14,14,15	2.18	4 (28%)	17,19,21	1.82	4 (23%)
4	BMA	h	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.85	1 (6%)
7	NAG	i	1	1,7	14,14,15	1.95	1 (7%)	17,19,21	1.19	2 (11%)
7	NAG	i	2	7	14,14,15	2.17	3 (21%)	17,19,21	0.77	0
4	NAG	j	1	1,4	14,14,15	2.05	4 (28%)	17,19,21	0.87	1 (5%)
4	NAG	j	2	4	14,14,15	2.18	3 (21%)	17,19,21	1.70	4 (23%)
4	BMA	j	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.97	1 (6%)
7	NAG	k	1	1,7	14,14,15	2.12	3 (21%)	17,19,21	2.11	2 (11%)
7	NAG	k	2	7	14,14,15	2.18	3 (21%)	17,19,21	1.25	2 (11%)
4	NAG	l	1	1,4	14,14,15	1.99	4 (28%)	17,19,21	1.06	1 (5%)
4	NAG	l	2	4	14,14,15	2.07	4 (28%)	17,19,21	1.46	3 (17%)
4	BMA	l	3	4	11,11,12	1.84	2 (18%)	15,15,17	1.08	1 (6%)
4	NAG	m	1	1,4	14,14,15	2.04	3 (21%)	17,19,21	1.11	3 (17%)
4	NAG	m	2	4	14,14,15	2.18	4 (28%)	17,19,21	1.10	2 (11%)
4	BMA	m	3	4	11,11,12	1.82	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	n	1	1,4	14,14,15	2.06	3 (21%)	17,19,21	0.88	0
4	NAG	n	2	4	14,14,15	2.20	4 (28%)	17,19,21	1.10	2 (11%)
4	BMA	n	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.92	1 (6%)
7	NAG	o	1	1,7	14,14,15	2.10	2 (14%)	17,19,21	0.92	1 (5%)
7	NAG	o	2	7	14,14,15	2.09	3 (21%)	17,19,21	1.14	1 (5%)
7	NAG	p	1	1,7	14,14,15	2.04	3 (21%)	17,19,21	0.90	1 (5%)
7	NAG	p	2	7	14,14,15	2.17	3 (21%)	17,19,21	1.22	2 (11%)
5	NAG	q	1	1,5	14,14,15	2.09	3 (21%)	17,19,21	1.09	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	q	2	5	14,14,15	2.17	2 (14%)	17,19,21	1.50	3 (17%)
5	BMA	q	3	5	11,11,12	1.62	2 (18%)	15,15,17	1.33	3 (20%)
5	MAN	q	4	5	11,11,12	1.80	3 (27%)	15,15,17	1.03	1 (6%)
5	MAN	q	5	5	11,11,12	1.86	2 (18%)	15,15,17	1.05	1 (6%)
4	NAG	r	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	0.81	1 (5%)
4	NAG	r	2	4	14,14,15	2.13	3 (21%)	17,19,21	1.41	2 (11%)
4	BMA	r	3	4	11,11,12	1.84	2 (18%)	15,15,17	1.00	1 (6%)
6	NAG	s	1	1,6	14,14,15	2.14	4 (28%)	17,19,21	0.96	1 (5%)
6	NAG	s	2	6	14,14,15	2.10	4 (28%)	17,19,21	1.38	2 (11%)
6	BMA	s	3	6	11,11,12	1.70	1 (9%)	15,15,17	1.04	1 (6%)
6	MAN	s	4	6	11,11,12	1.83	2 (18%)	15,15,17	1.13	2 (13%)
4	NAG	t	1	1,4	14,14,15	2.08	2 (14%)	17,19,21	0.93	1 (5%)
4	NAG	t	2	4	14,14,15	2.18	5 (35%)	17,19,21	1.13	1 (5%)
4	BMA	t	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.96	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	BMA	M	3	4	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	O	3	4	-	1/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	1/2/19/22	0/1/1/1
5	MAN	P	5	5	-	1/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	2/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	1/2/19/22	0/1/1/1
5	MAN	R	5	5	-	1/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	BMA	S	3	5	-	2/2/19/22	0/1/1/1
5	MAN	S	4	5	-	1/2/19/22	0/1/1/1
5	MAN	S	5	5	-	1/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1
6	MAN	T	4	6	-	1/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	MAN	U	4	5	-	1/2/19/22	0/1/1/1
5	MAN	U	5	5	-	1/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	1/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	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	BMA	X	3	4	-	1/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	BMA	l	3	4	-	1/2/19/22	0/1/1/1
4	NAG	m	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
4	BMA	m	3	4	-	1/2/19/22	0/1/1/1
4	NAG	n	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	0/6/23/26	0/1/1/1
4	BMA	n	3	4	-	1/2/19/22	0/1/1/1
7	NAG	o	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	1/6/23/26	0/1/1/1
7	NAG	p	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	p	2	7	-	0/6/23/26	0/1/1/1
5	NAG	q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	q	3	5	-	1/2/19/22	0/1/1/1
5	MAN	q	4	5	-	1/2/19/22	0/1/1/1
5	MAN	q	5	5	-	1/2/19/22	0/1/1/1
4	NAG	r	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	r	2	4	-	0/6/23/26	0/1/1/1
4	BMA	r	3	4	-	1/2/19/22	0/1/1/1
6	NAG	s	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	0/6/23/26	0/1/1/1
6	BMA	s	3	6	-	2/2/19/22	0/1/1/1
6	MAN	s	4	6	-	2/2/19/22	0/1/1/1
4	NAG	t	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	t	2	4	-	0/6/23/26	0/1/1/1
4	BMA	t	3	4	-	1/2/19/22	0/1/1/1

The worst 5 of 342 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	1	NAG	O5-C1	7.28	1.55	1.43
4	K	2	NAG	O5-C1	7.04	1.55	1.43
4	O	2	NAG	O5-C1	7.01	1.55	1.43
4	Z	2	NAG	O5-C1	6.97	1.55	1.43
4	X	2	NAG	O5-C1	6.93	1.55	1.43

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	k	1	NAG	C1-O5-C5	-6.69	103.22	112.19
4	Q	2	NAG	C4-C3-C2	-5.41	103.09	111.02
4	Y	2	NAG	C4-C3-C2	-4.78	104.02	111.02
4	X	2	NAG	C4-C3-C2	-4.67	104.17	111.02
7	k	1	NAG	C4-C3-C2	-4.23	104.83	111.02

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

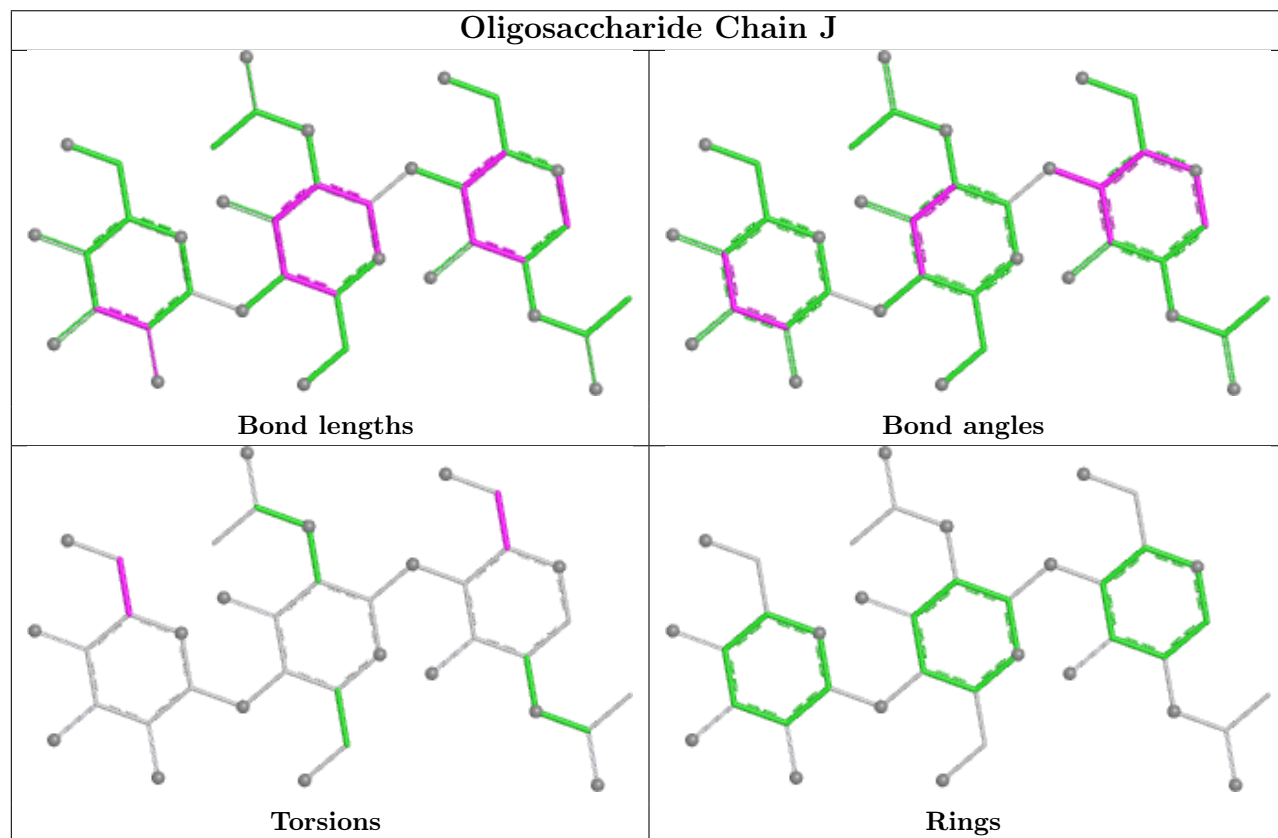
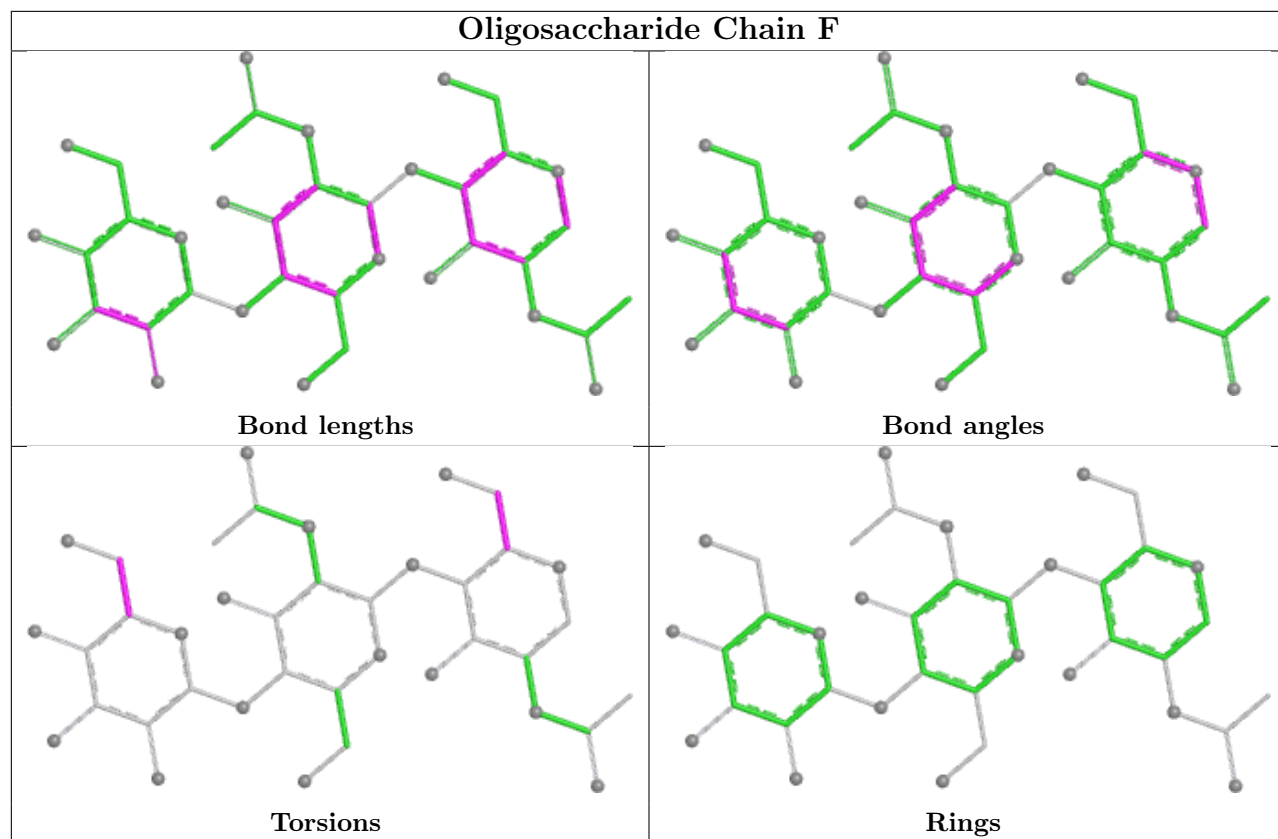
Mol	Chain	Res	Type	Atoms
6	s	3	BMA	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
6	s	3	BMA	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6

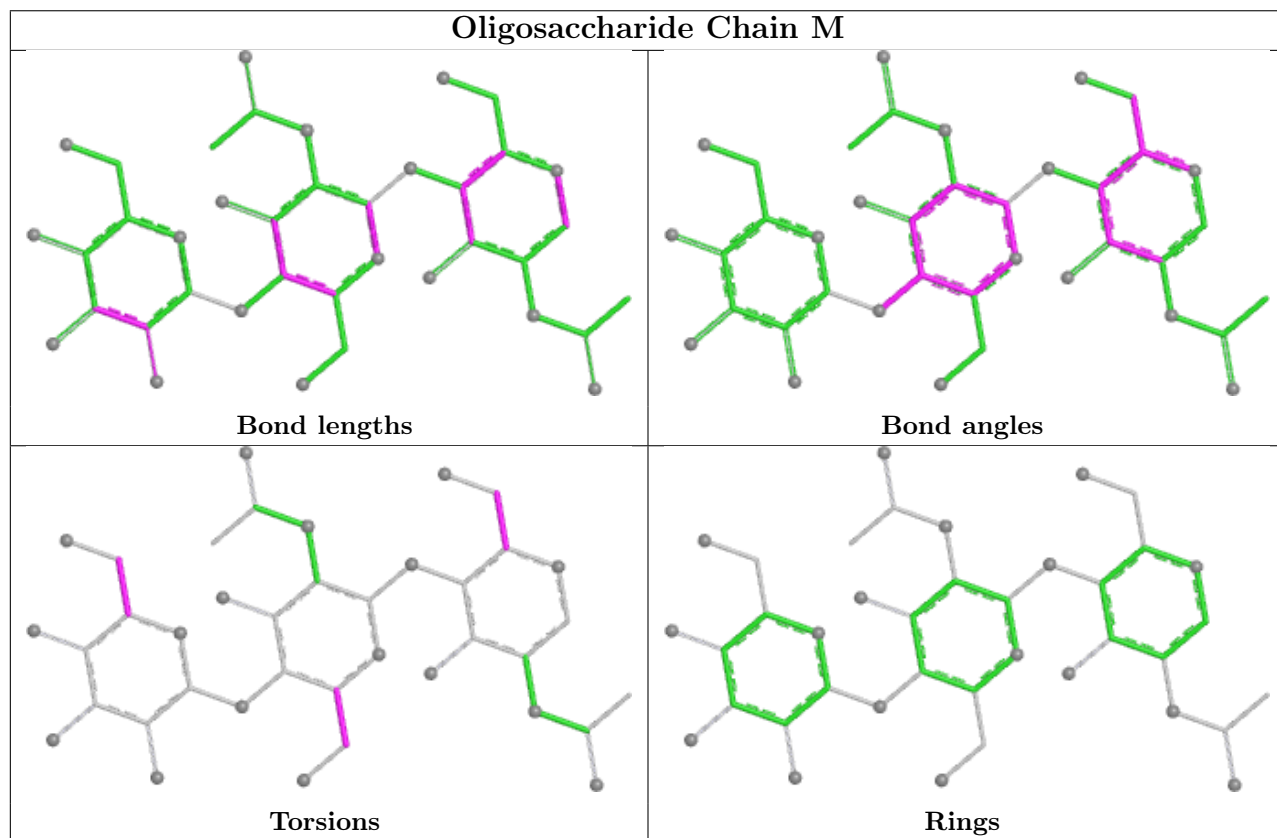
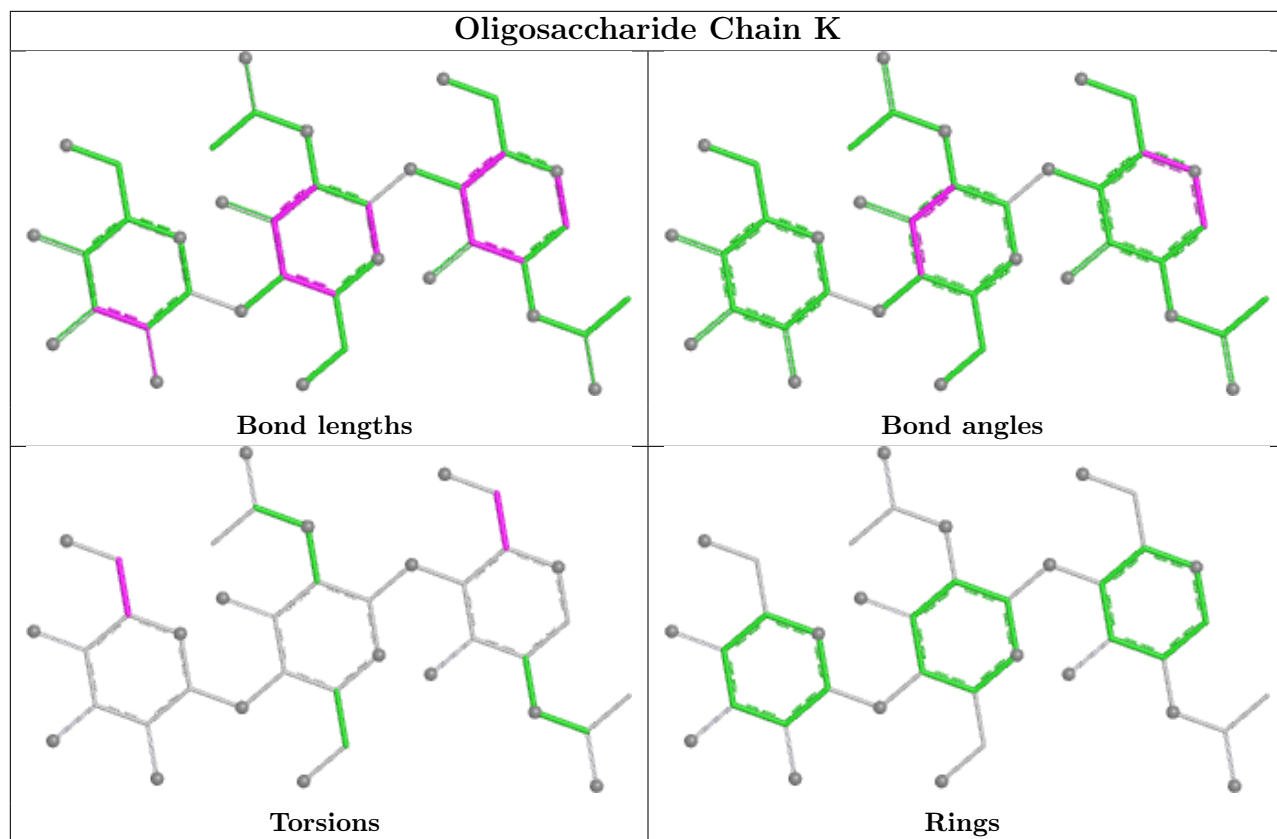
There are no ring outliers.

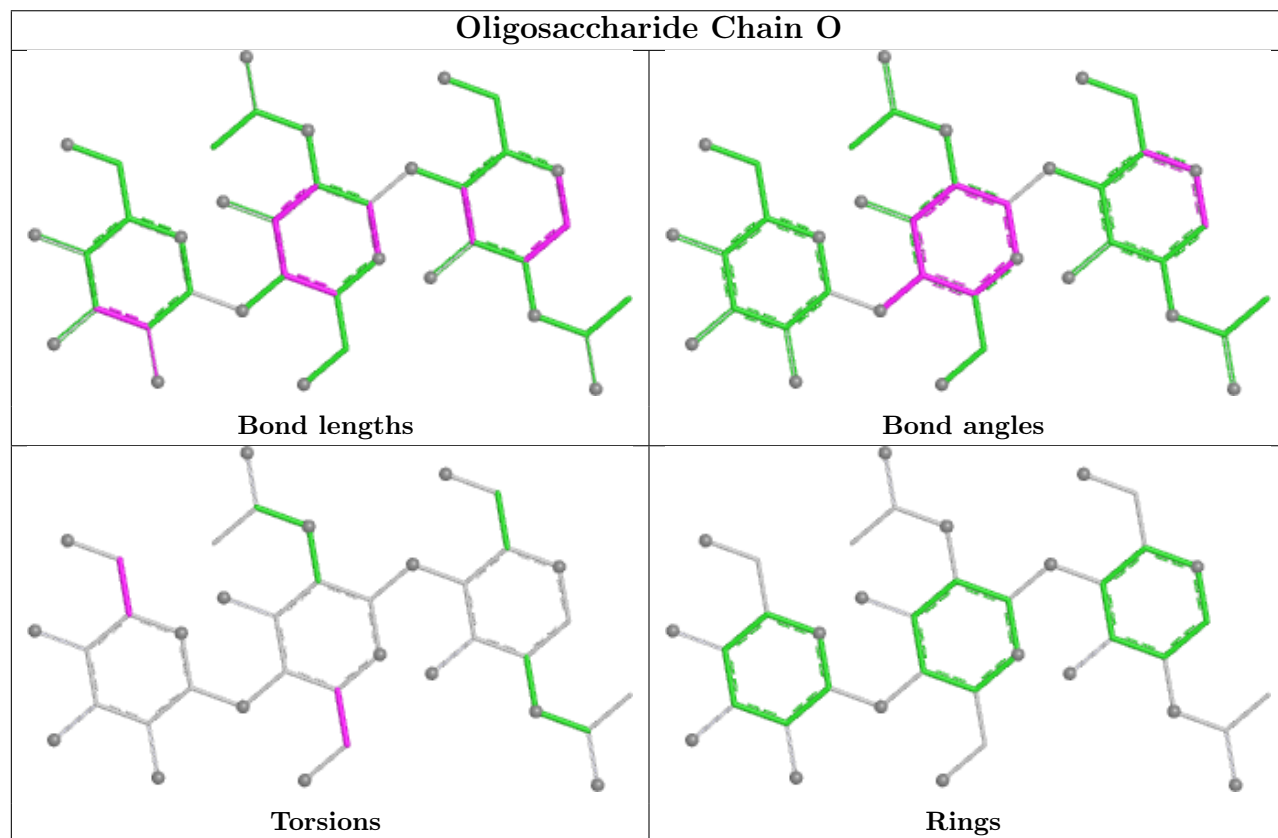
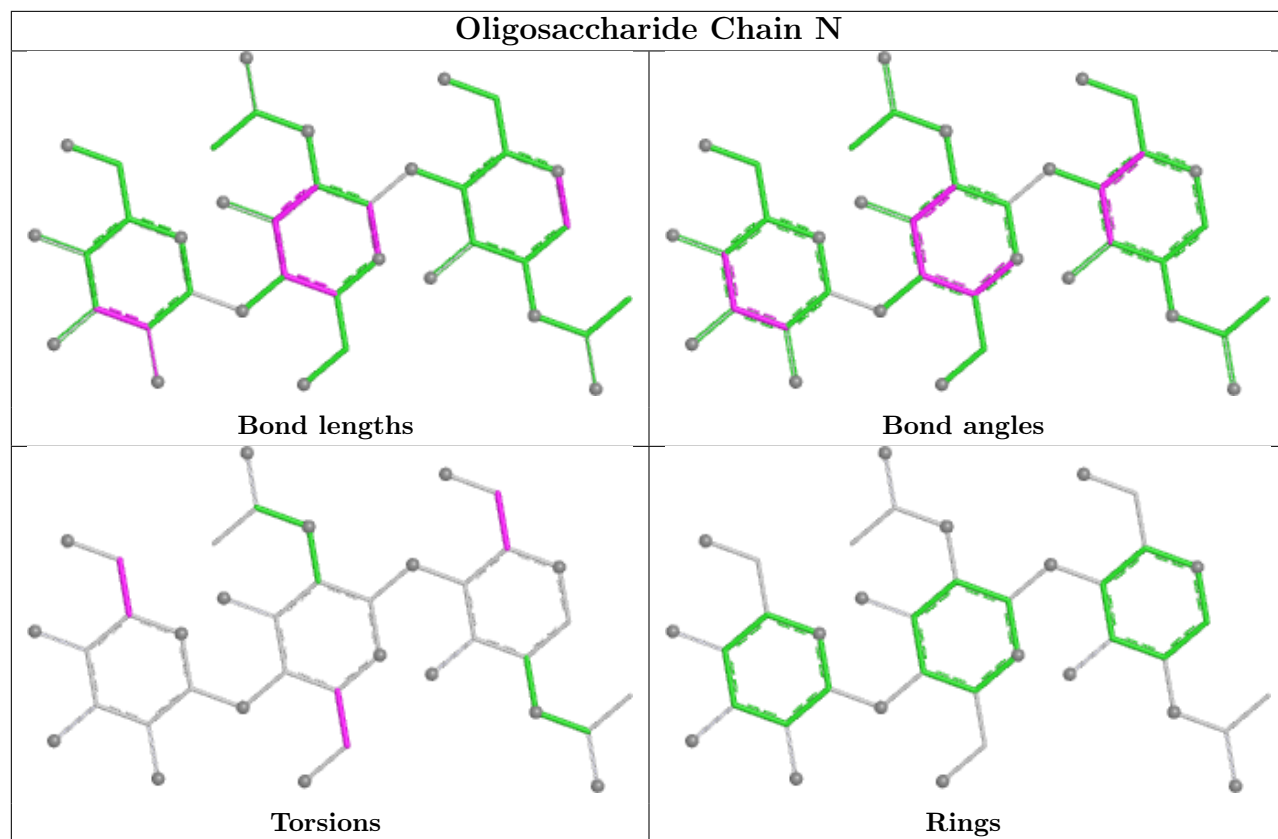
3 monomers are involved in 3 short contacts:

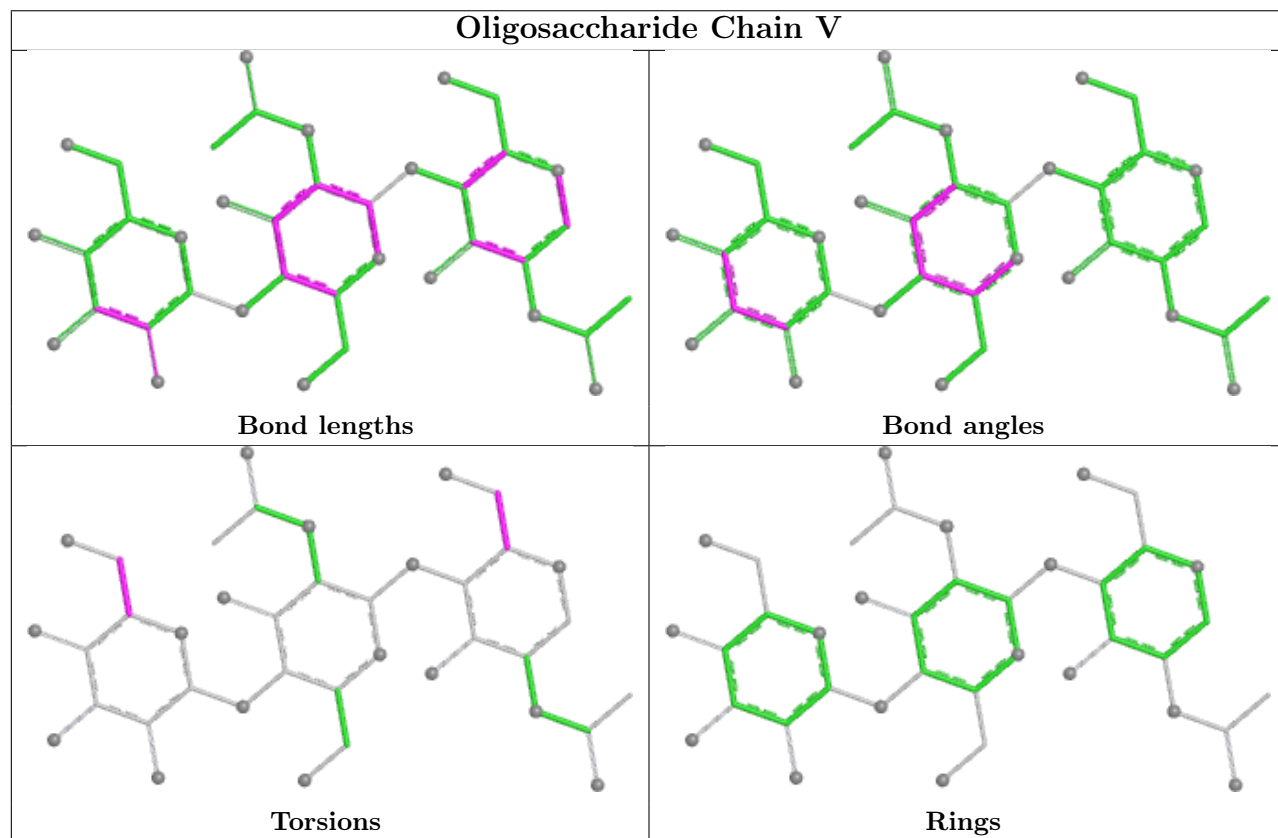
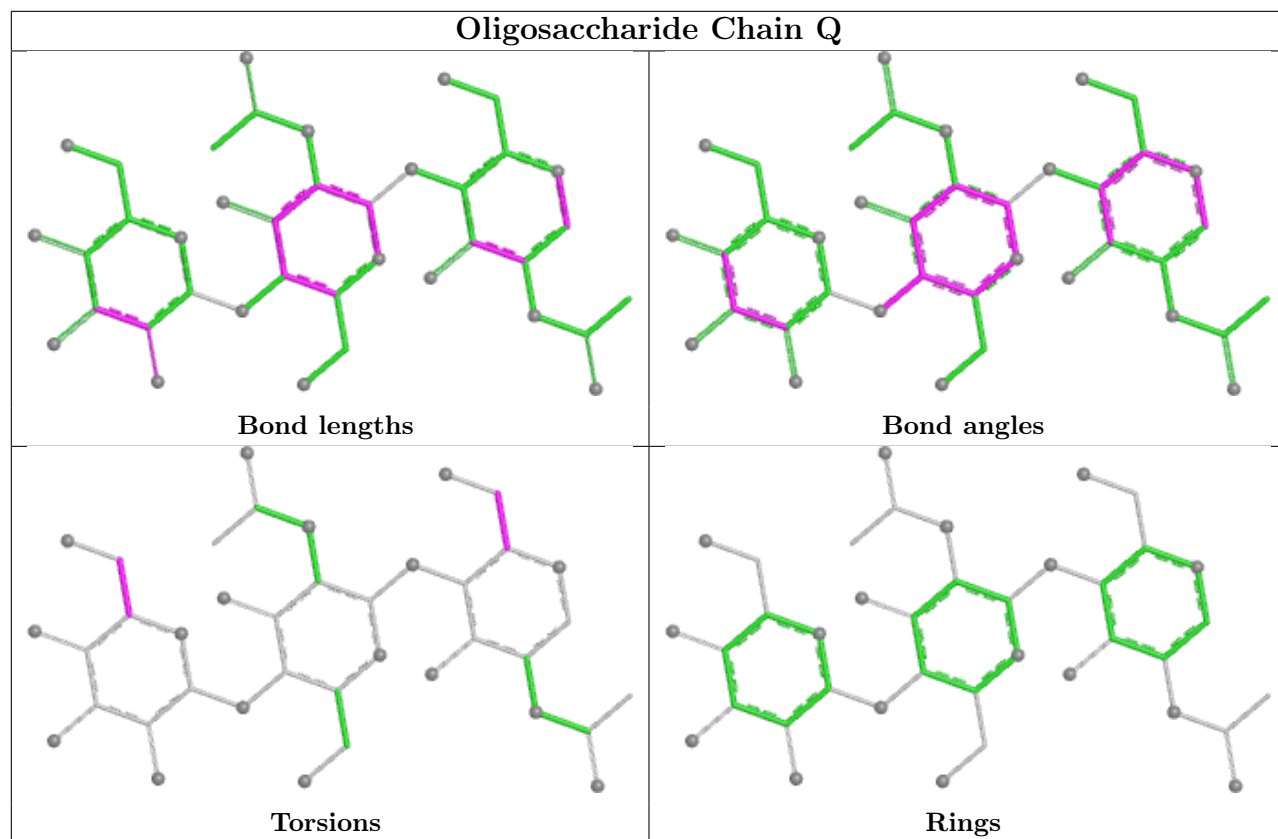
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	q	1	NAG	1	0
5	R	1	NAG	1	0
6	T	1	NAG	1	0

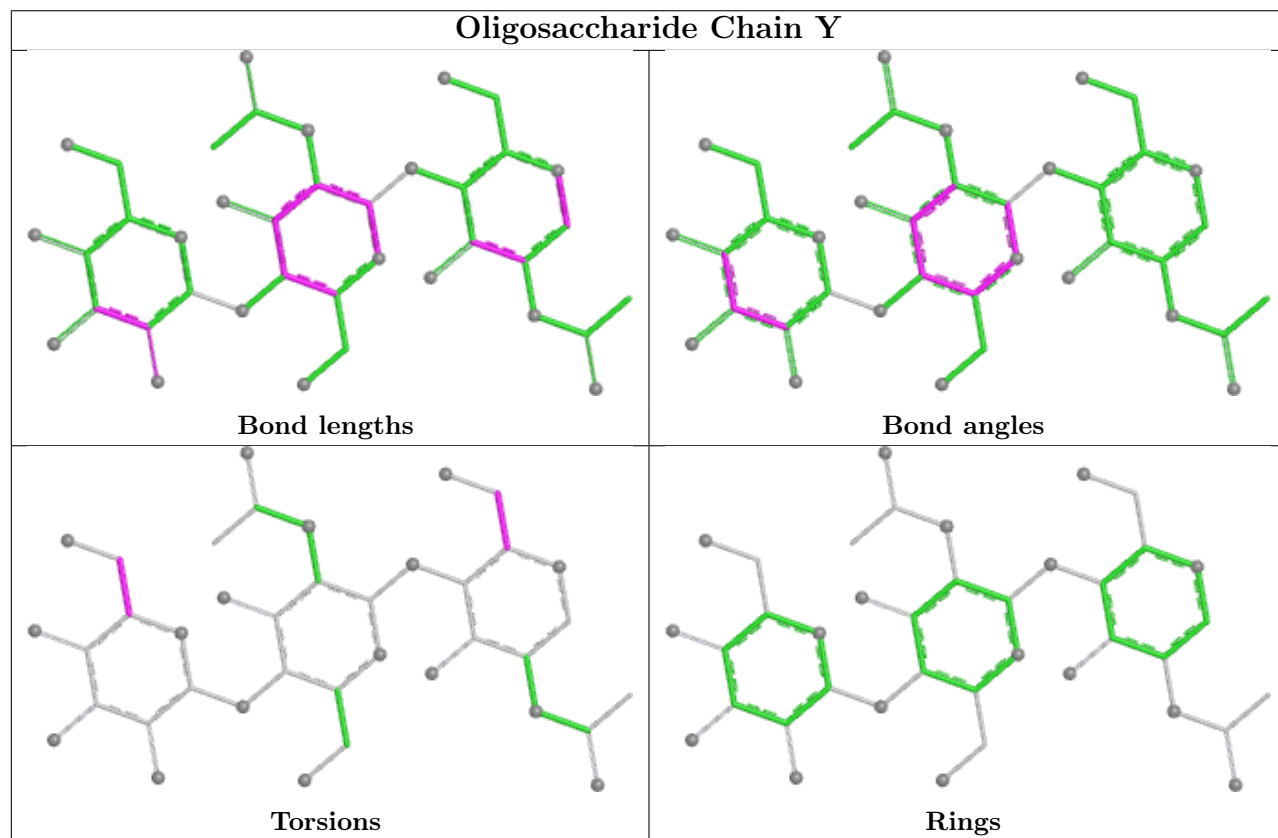
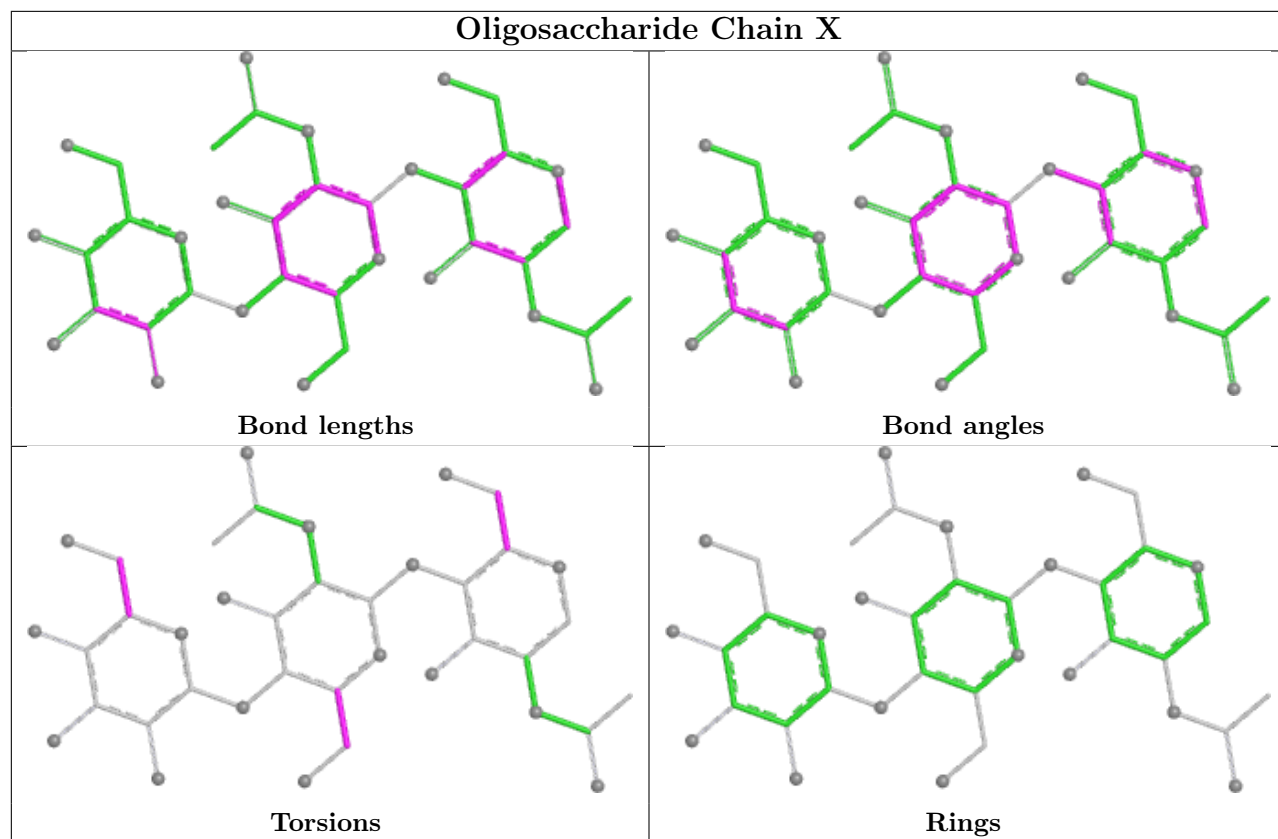
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

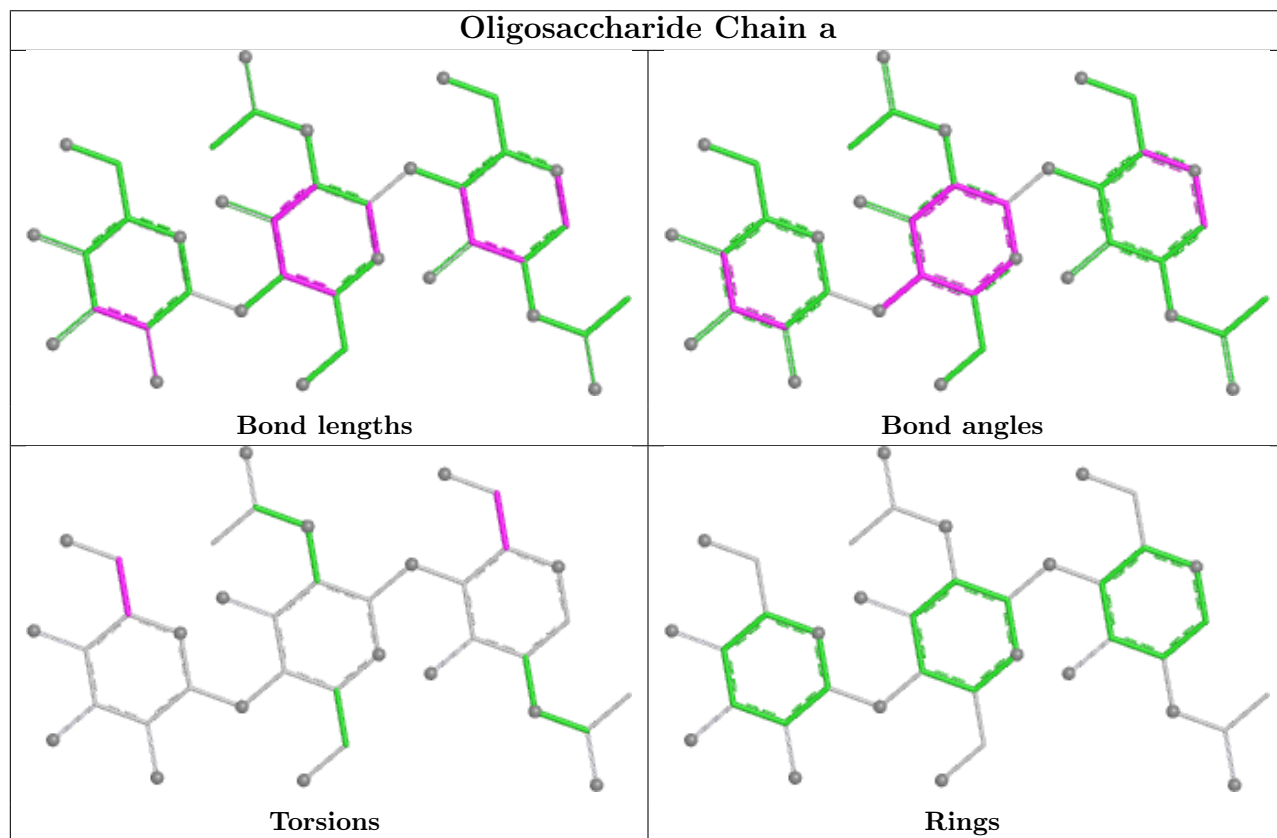
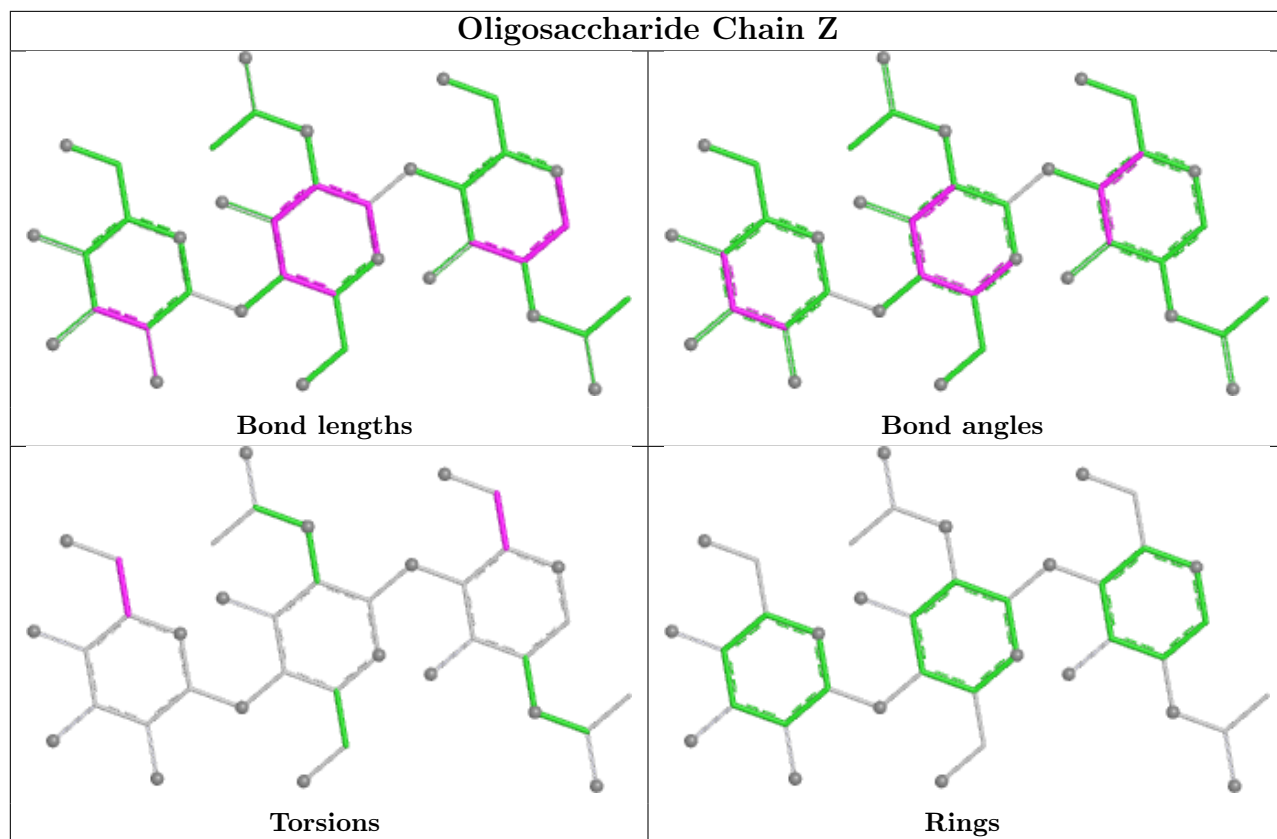


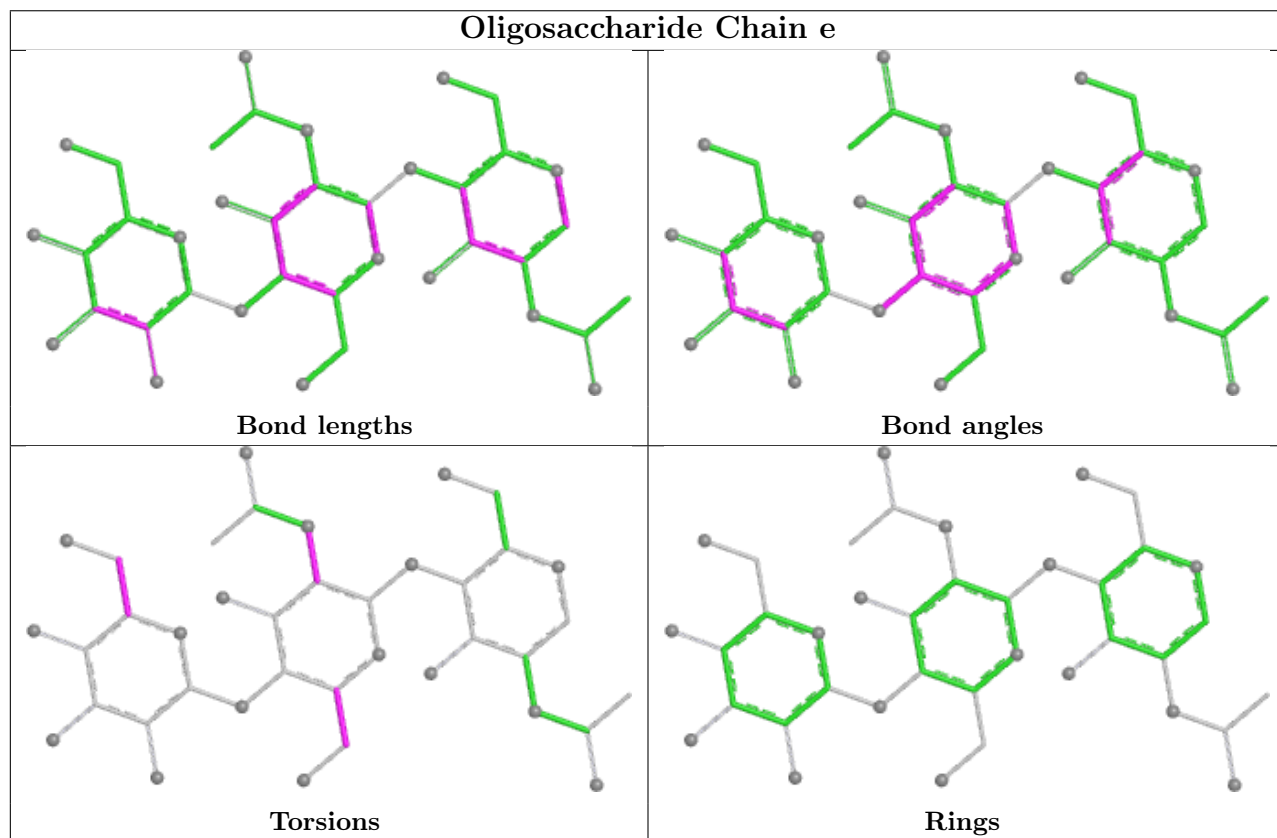
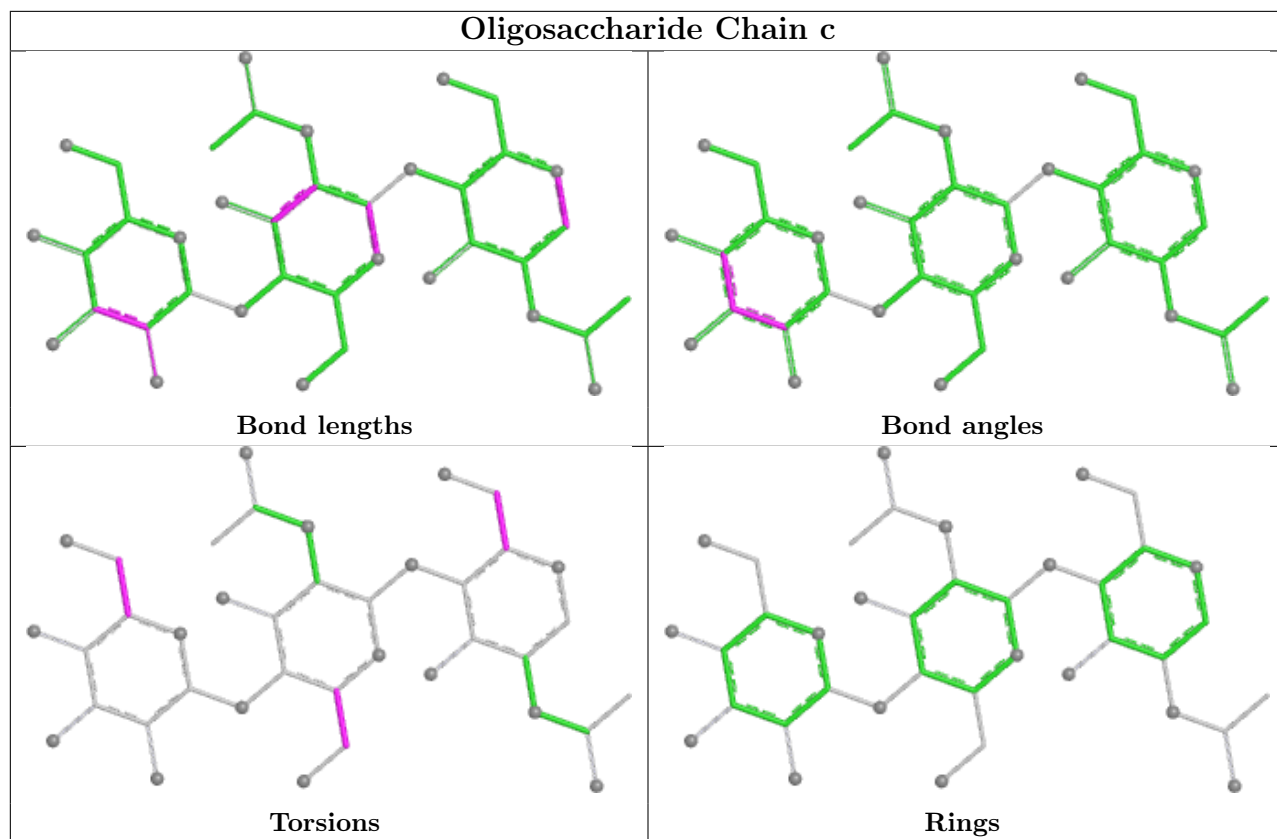


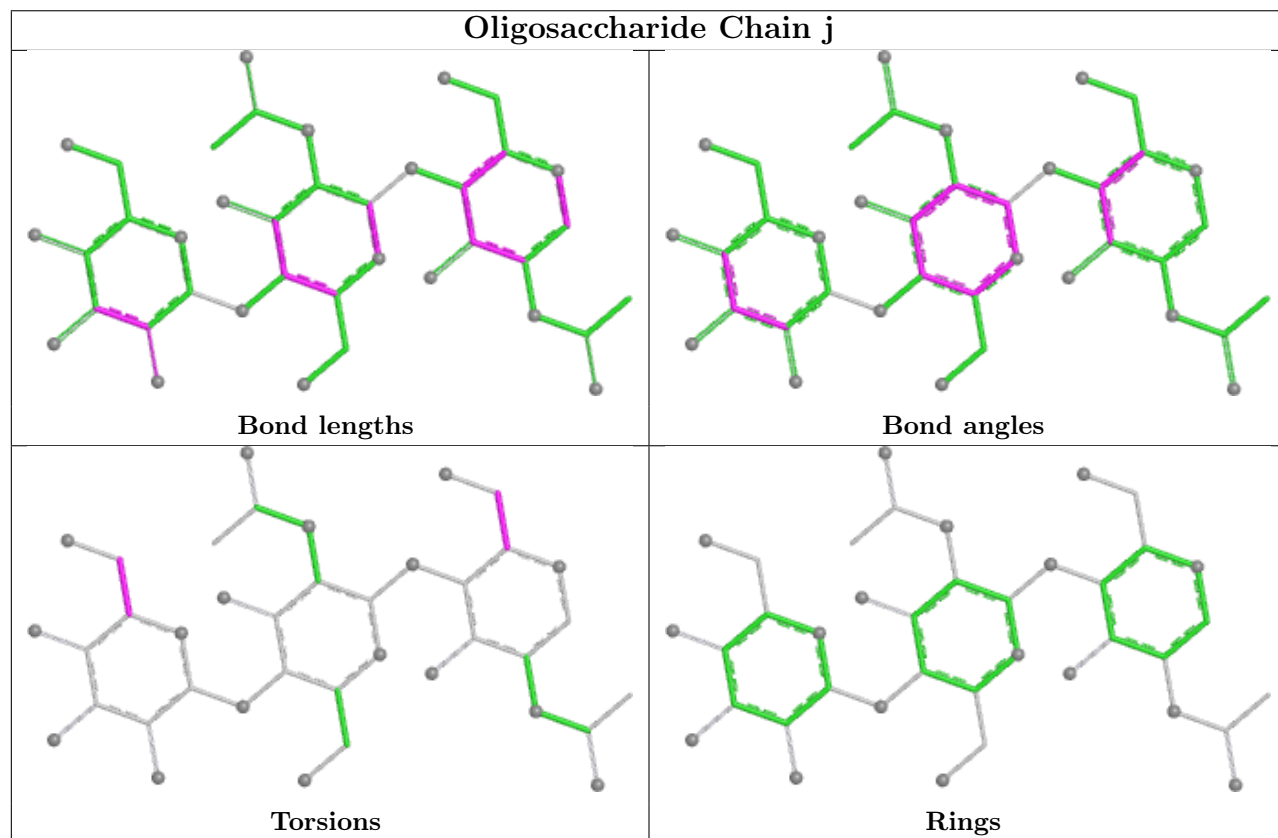
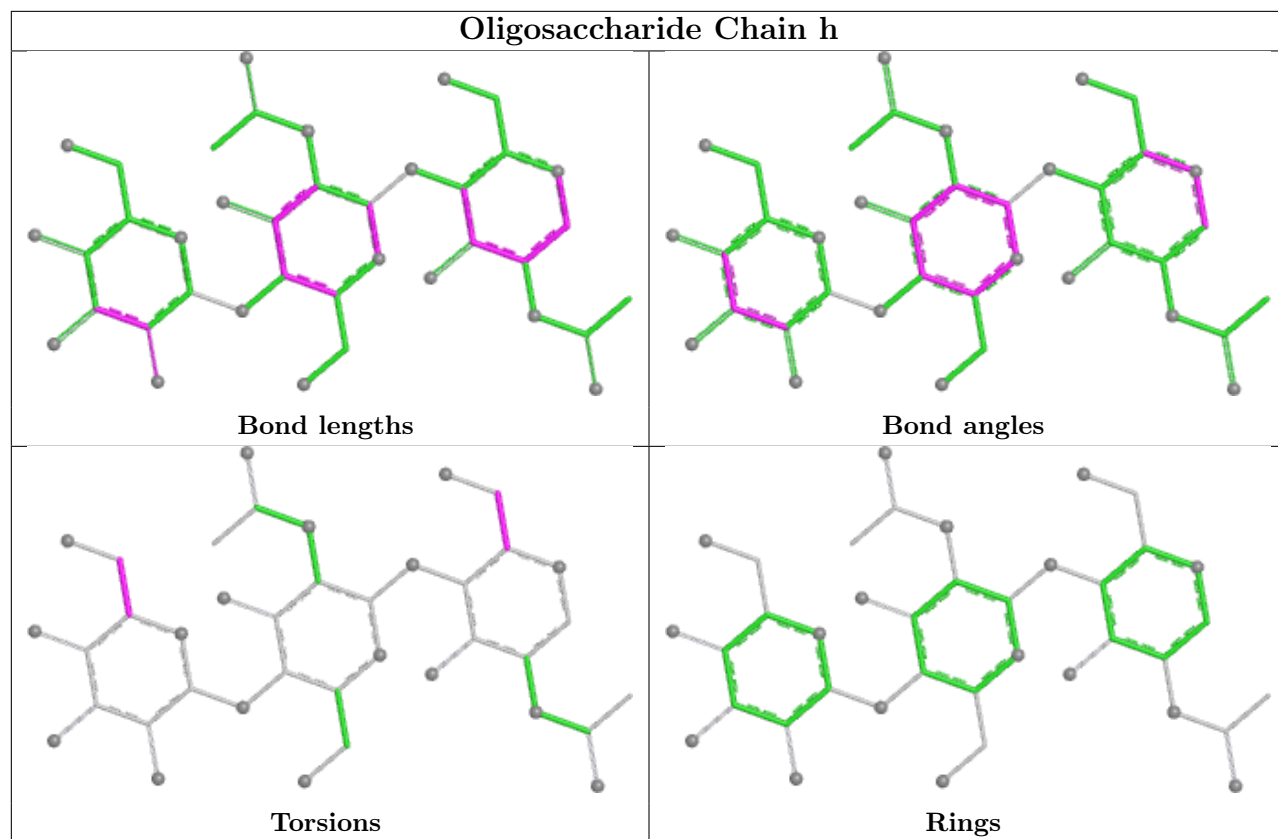


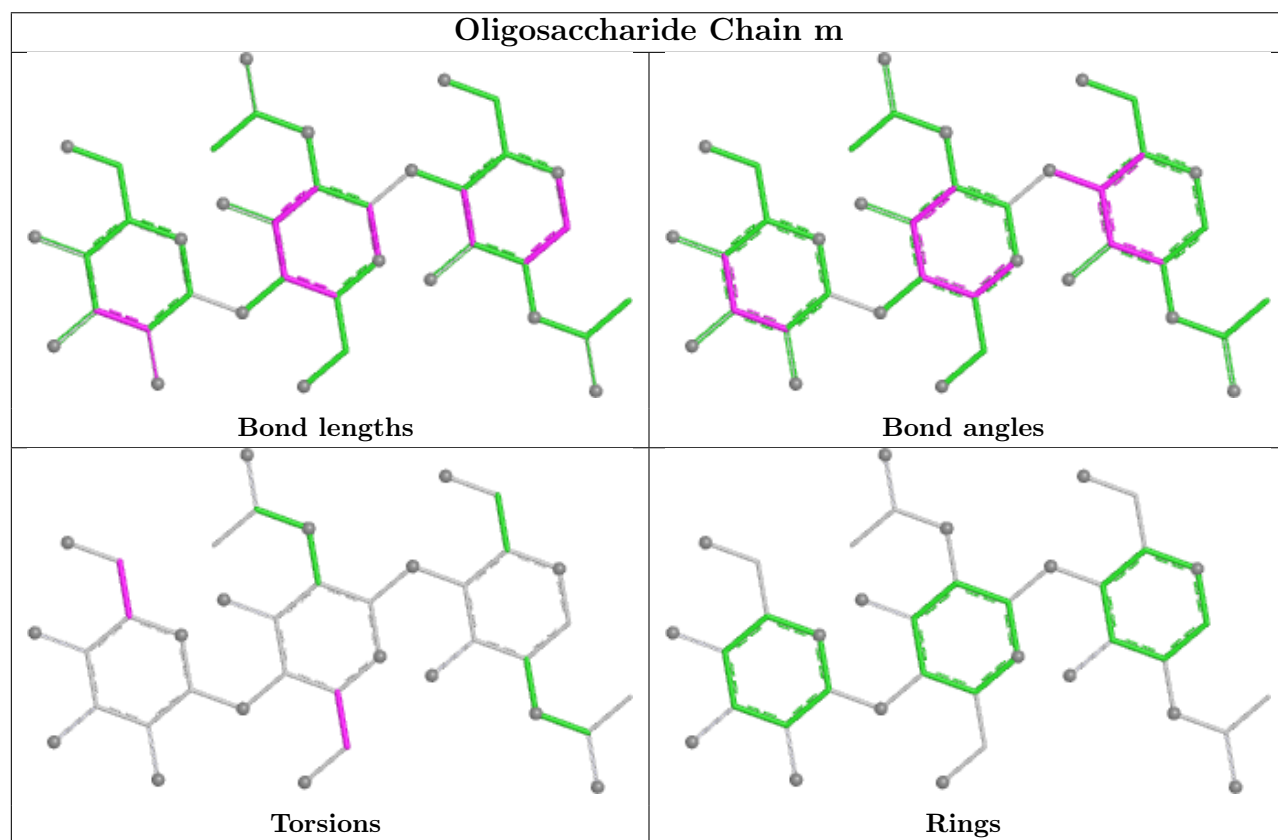
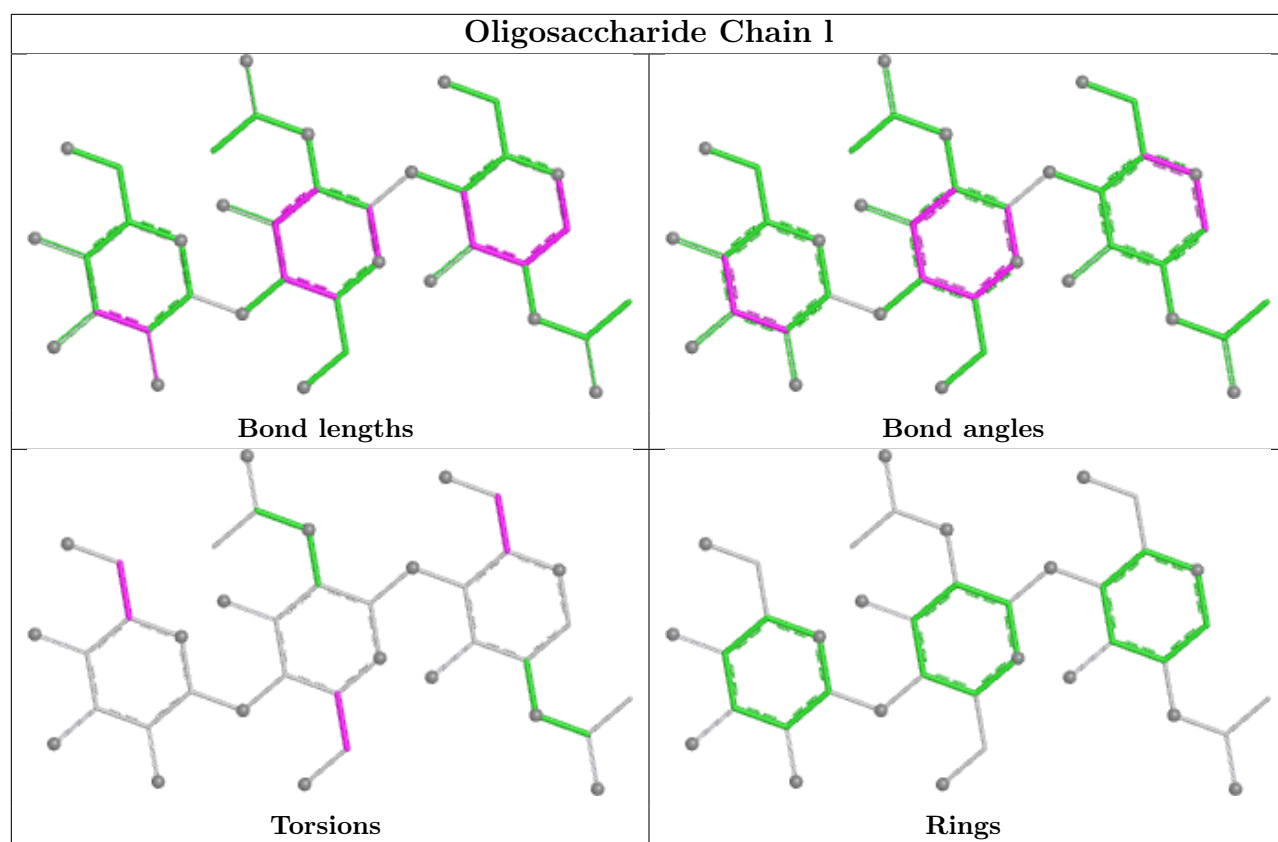


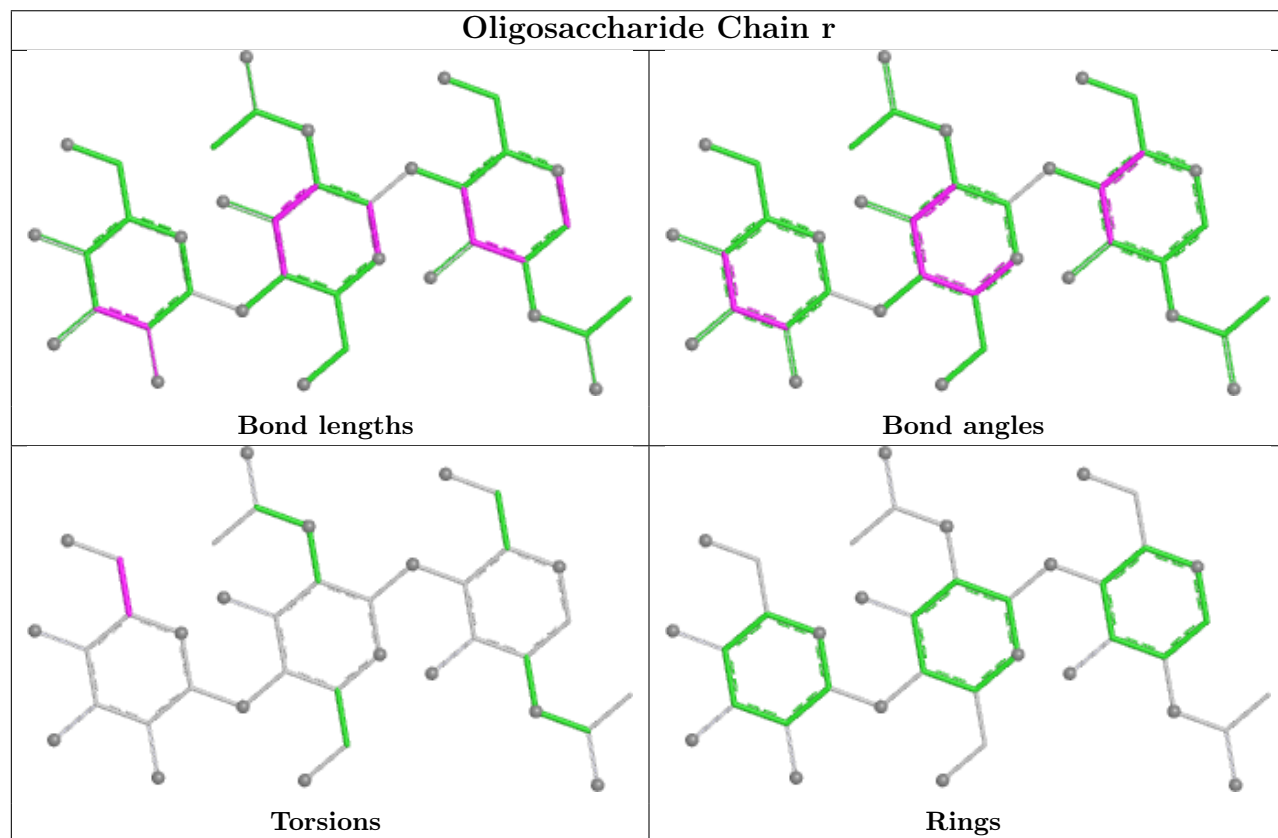
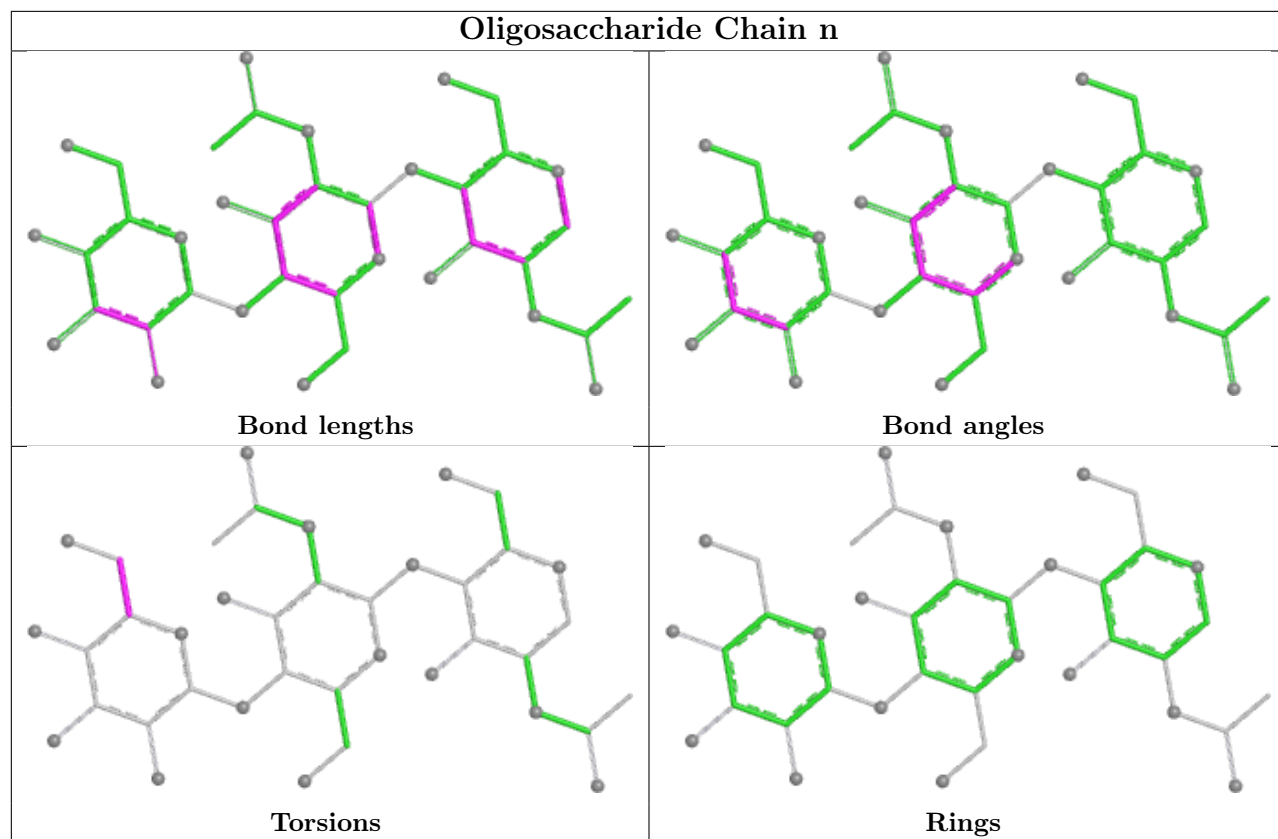


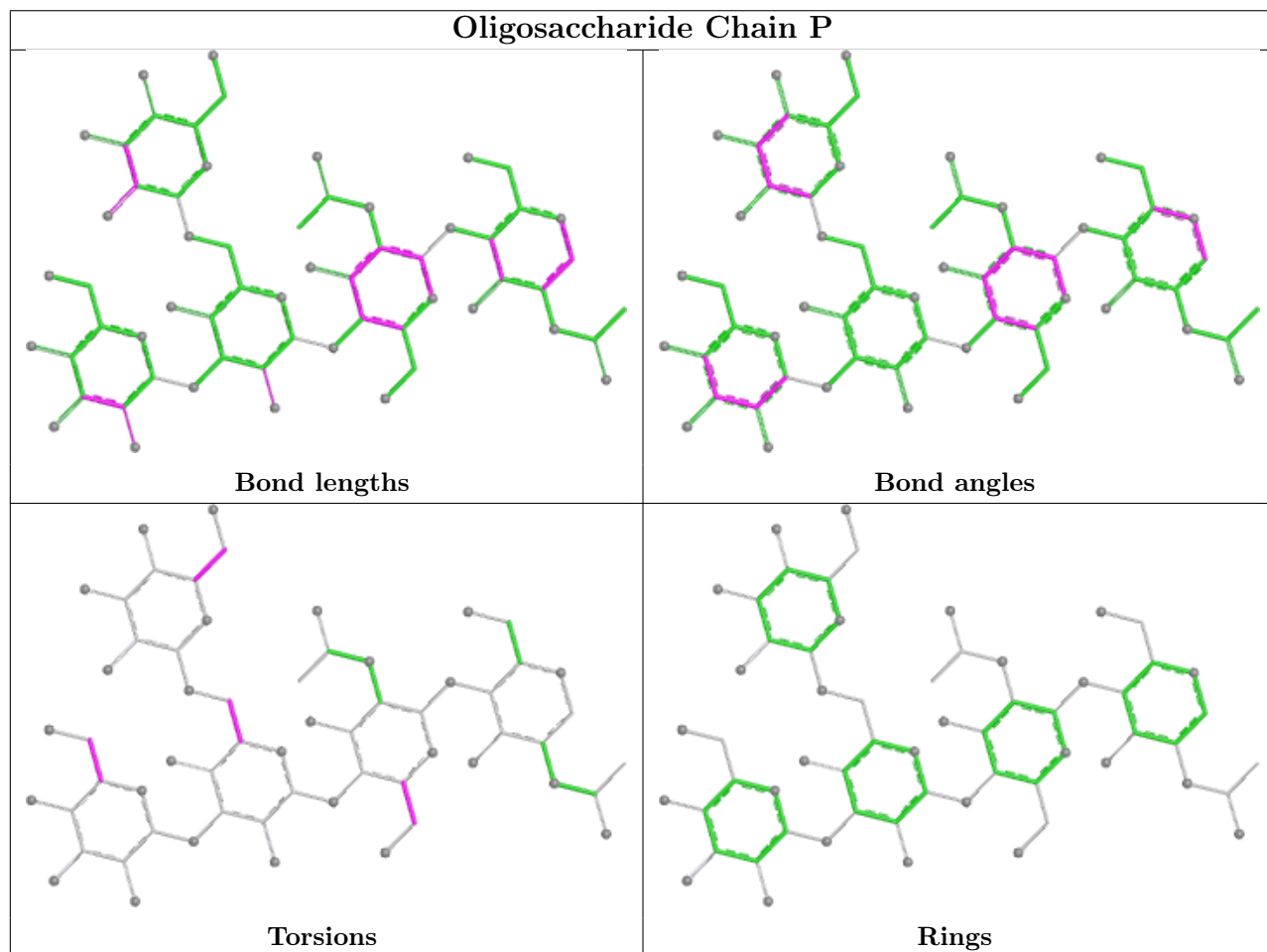
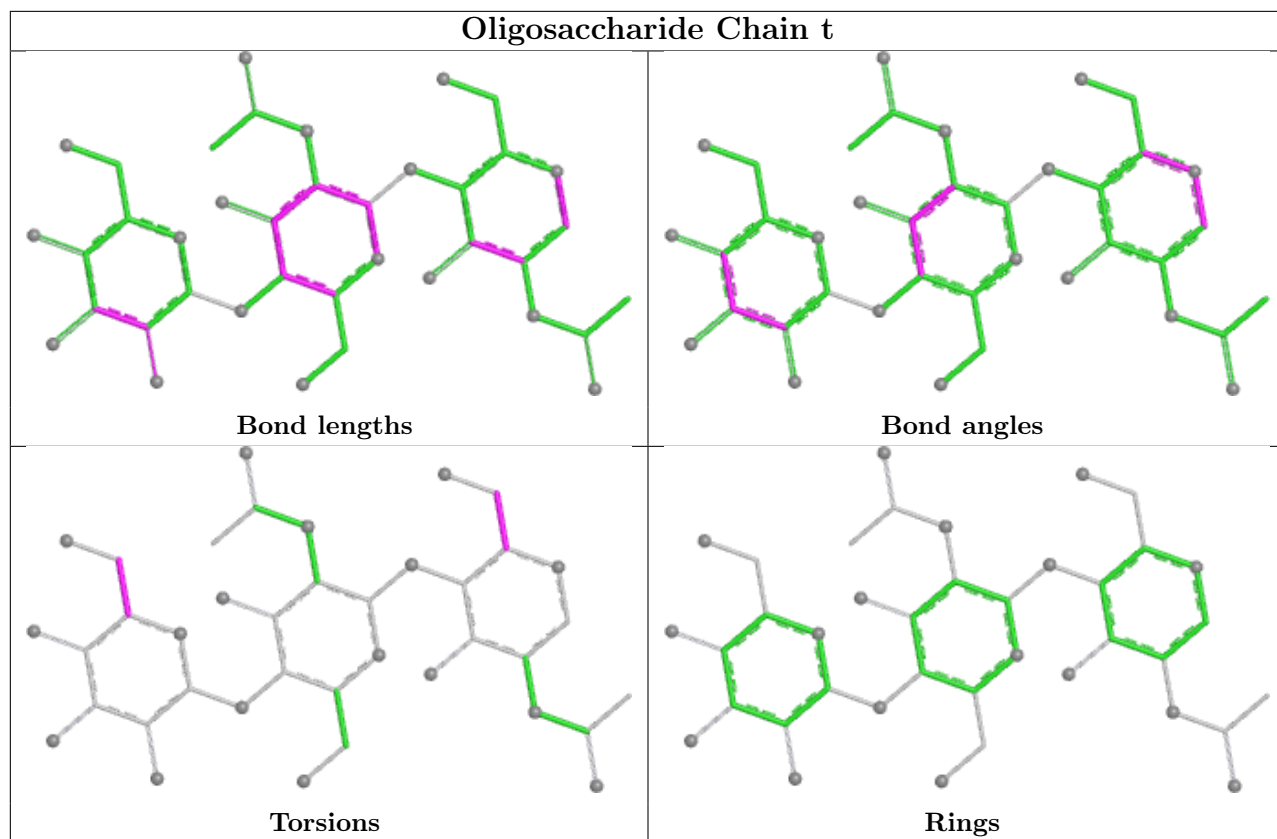


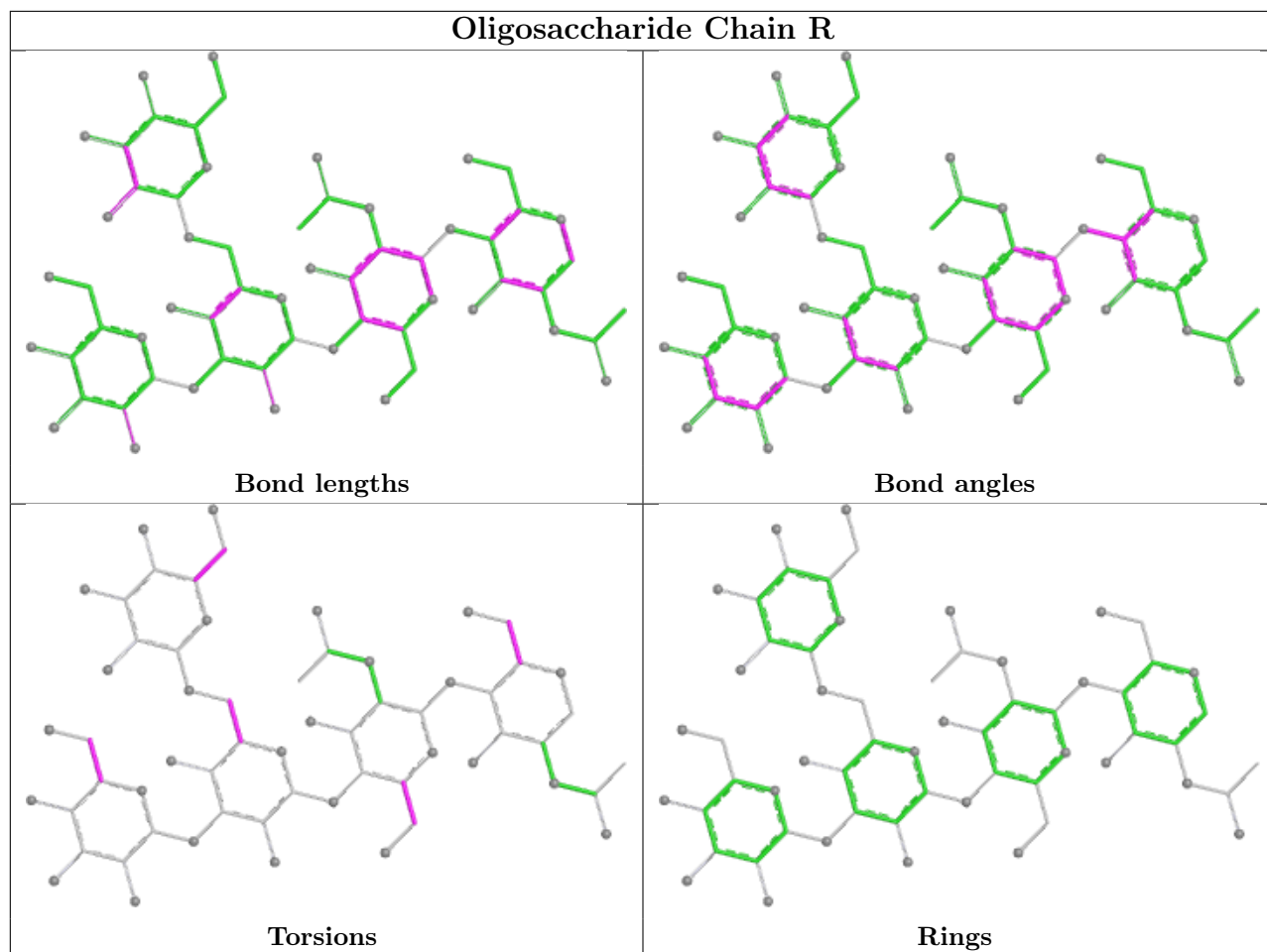


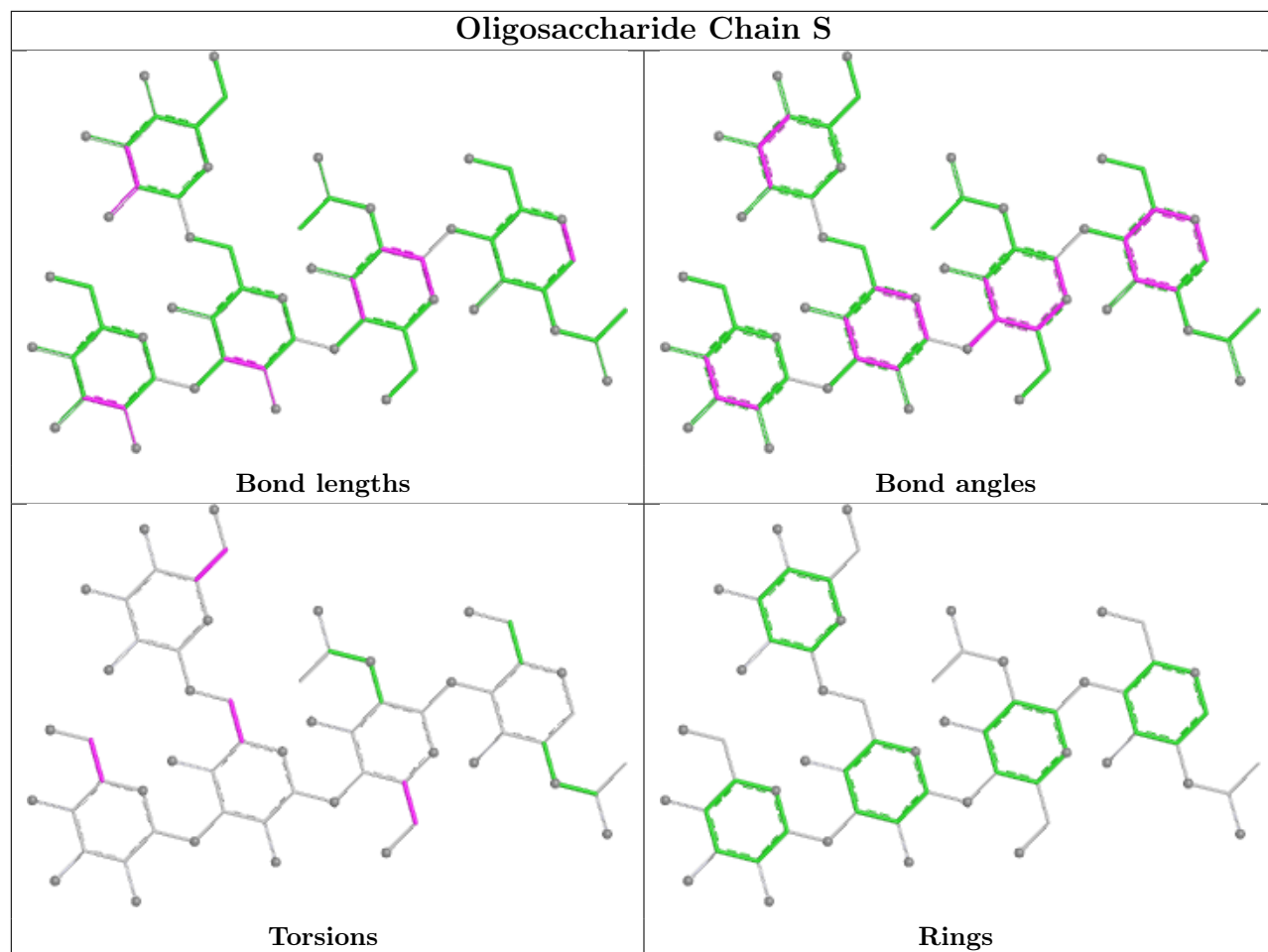


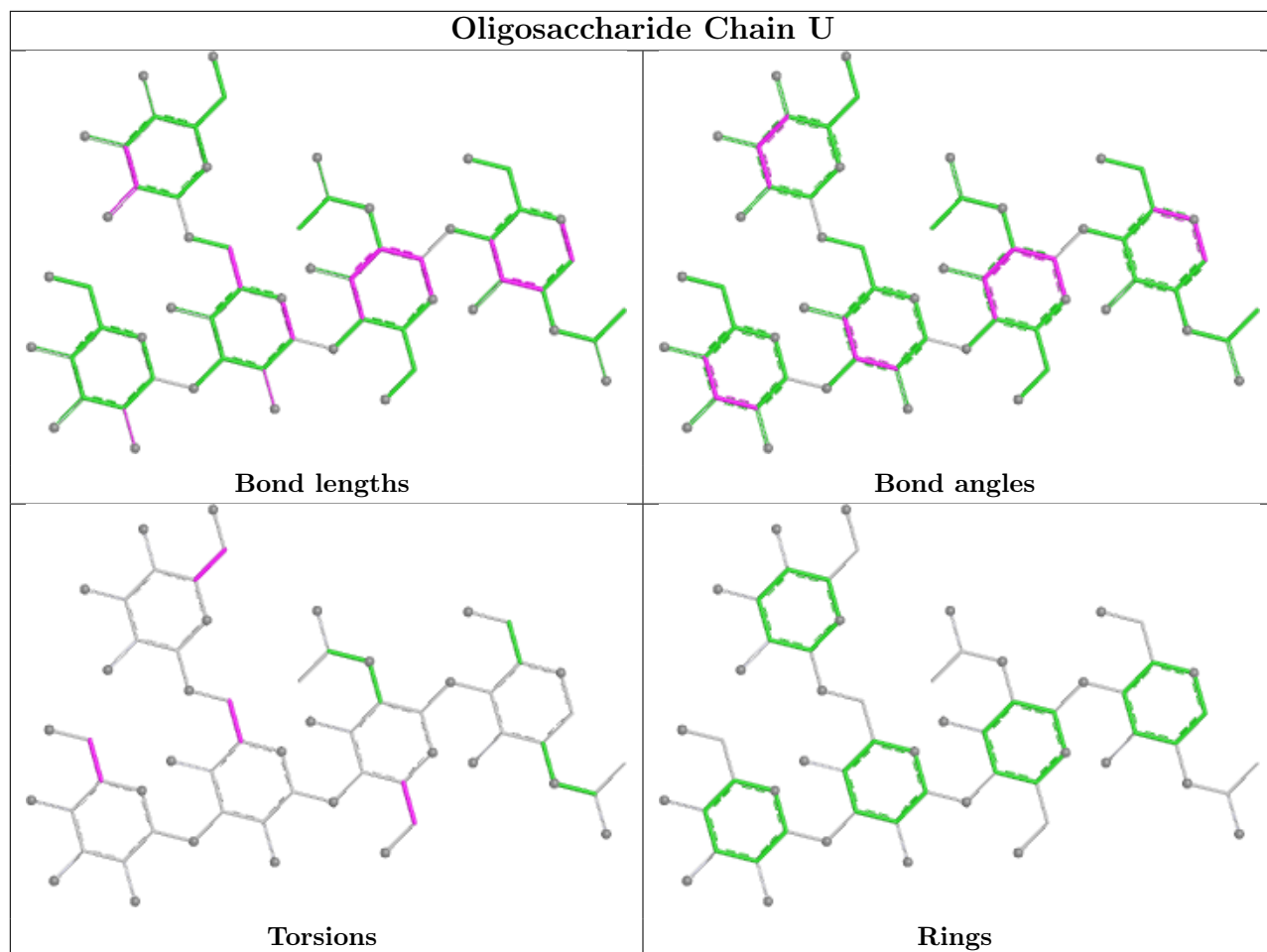


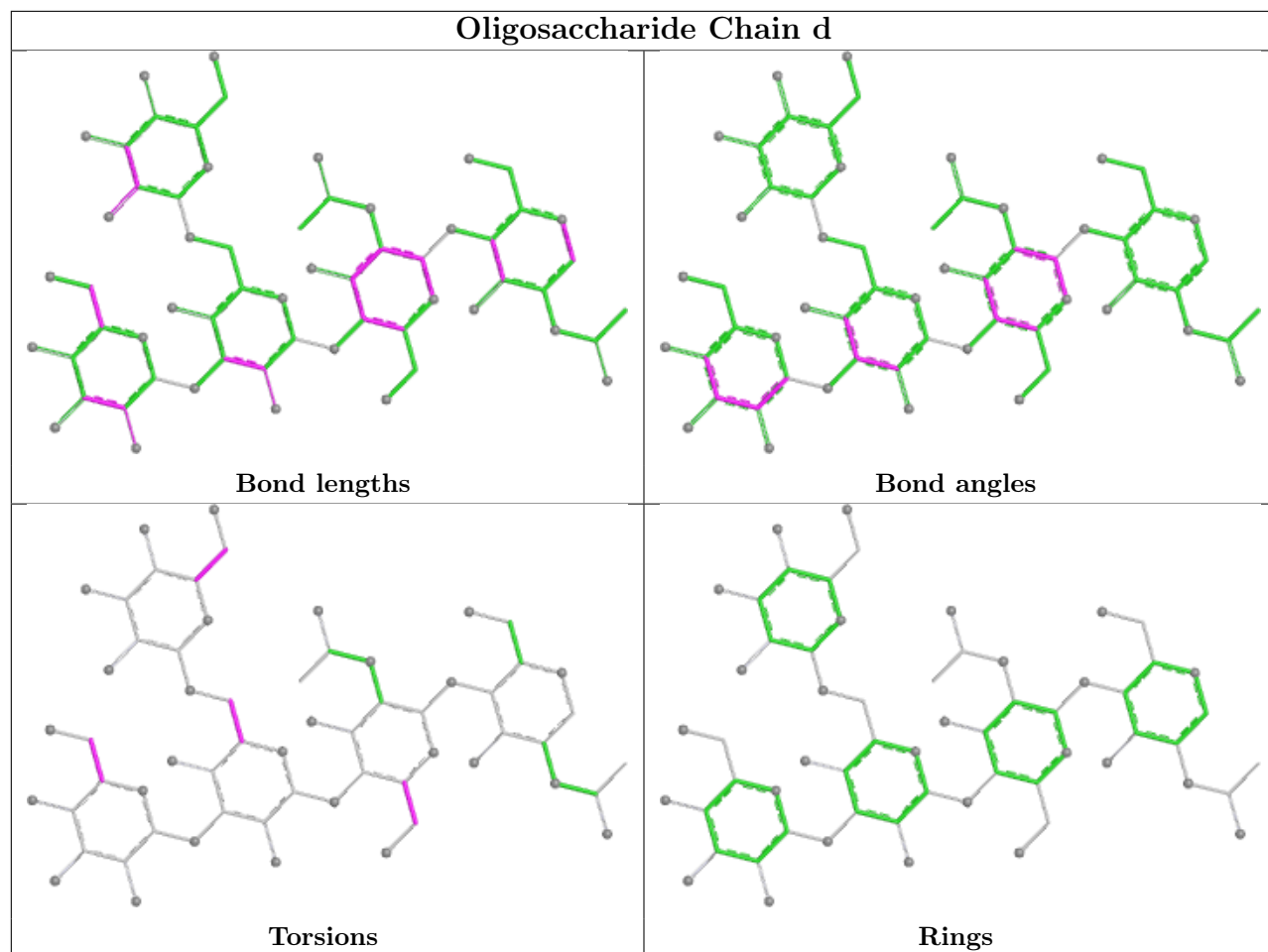


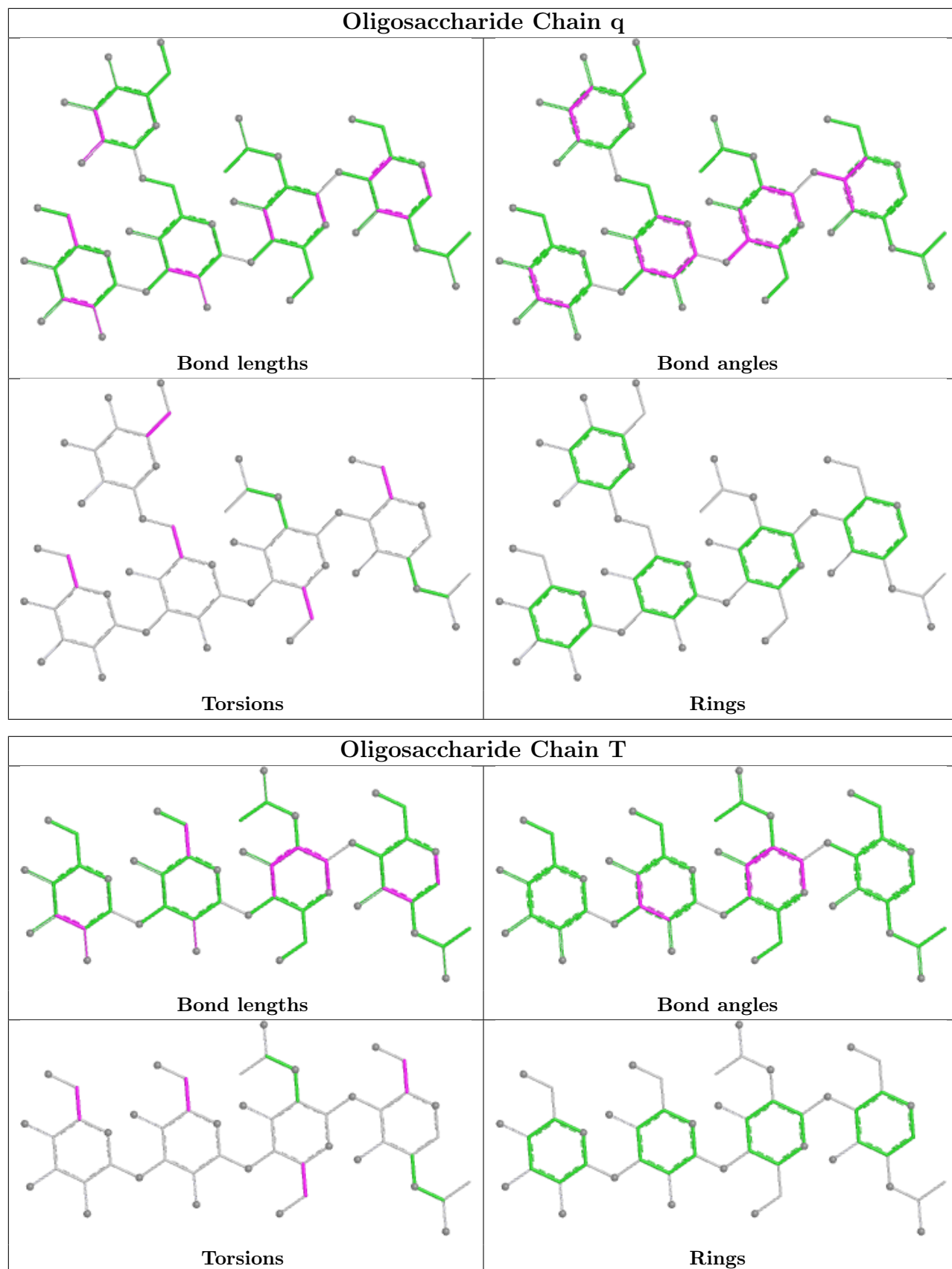


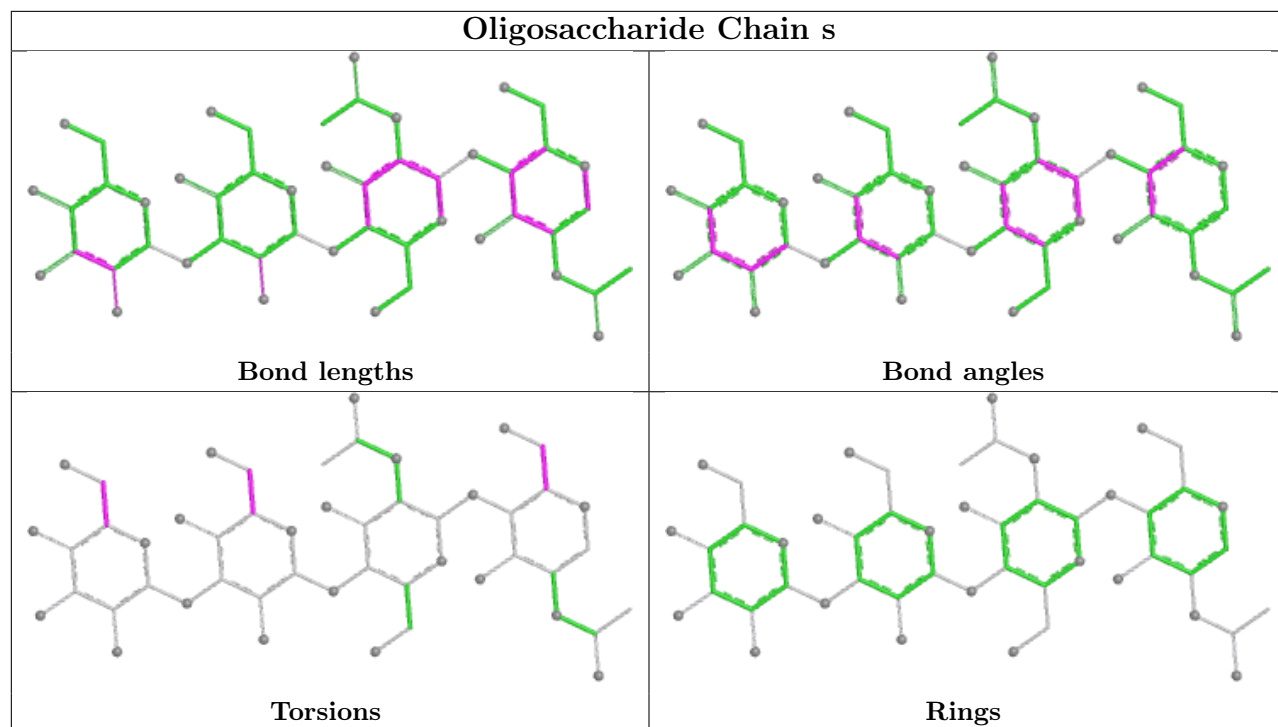


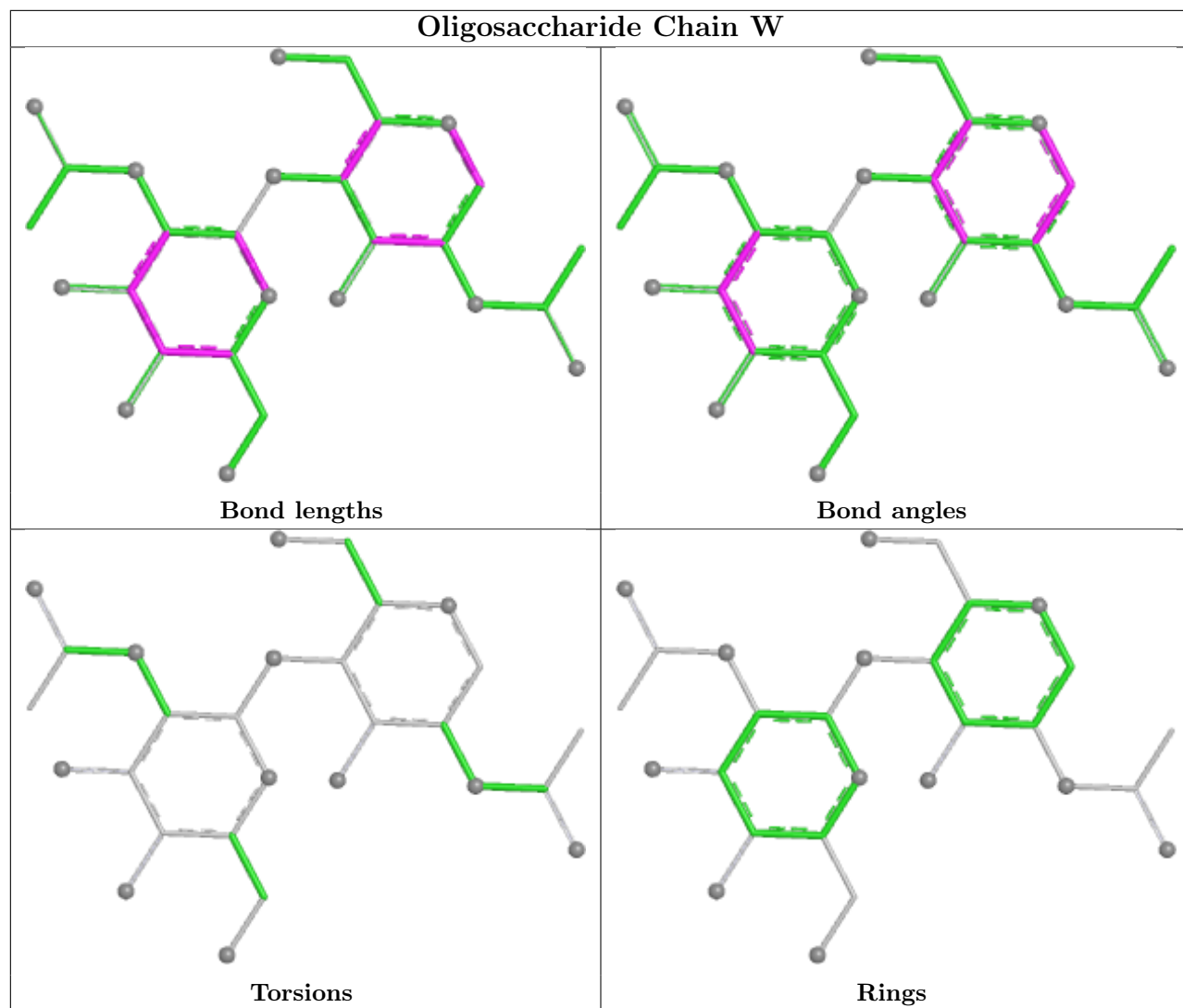


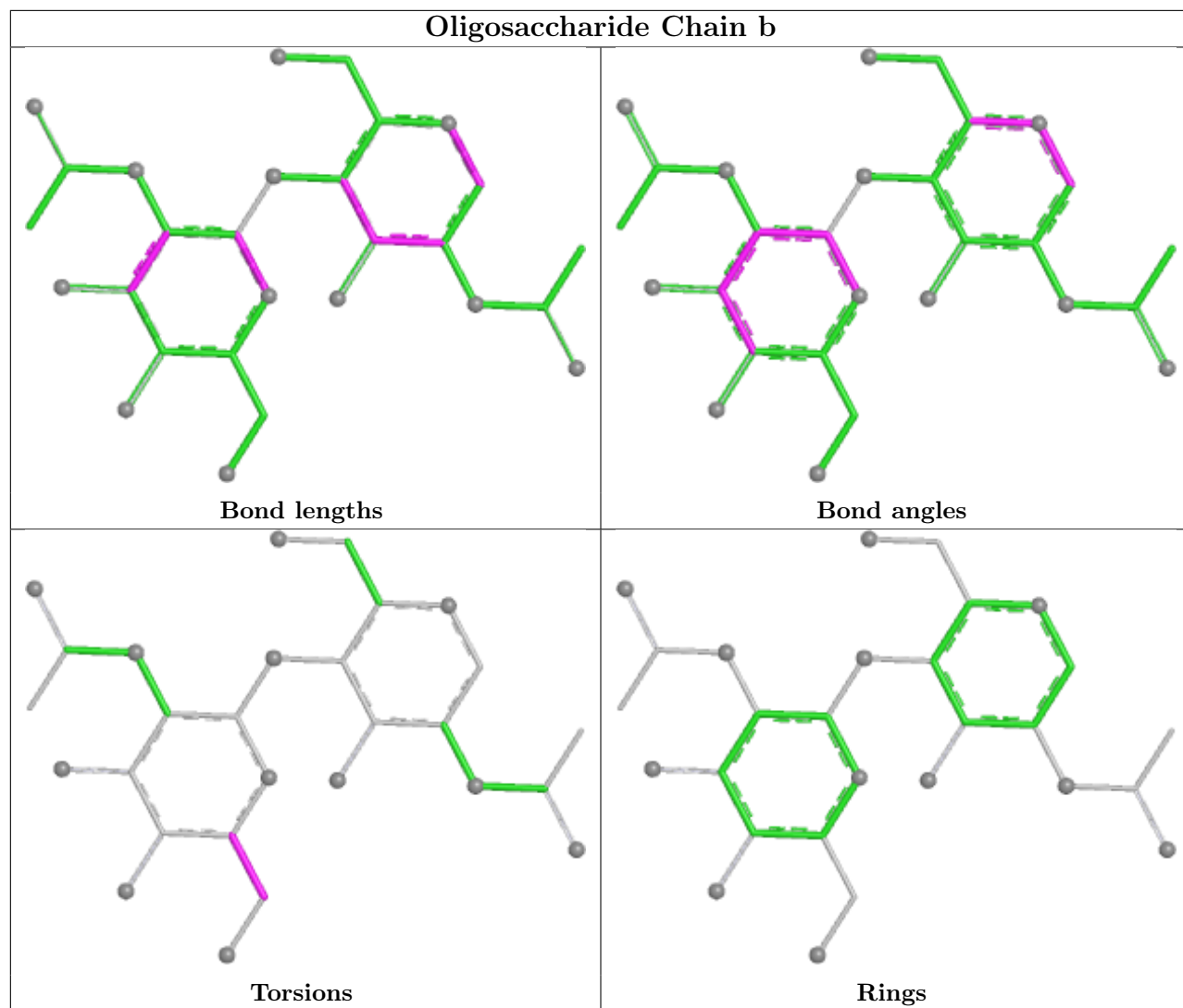


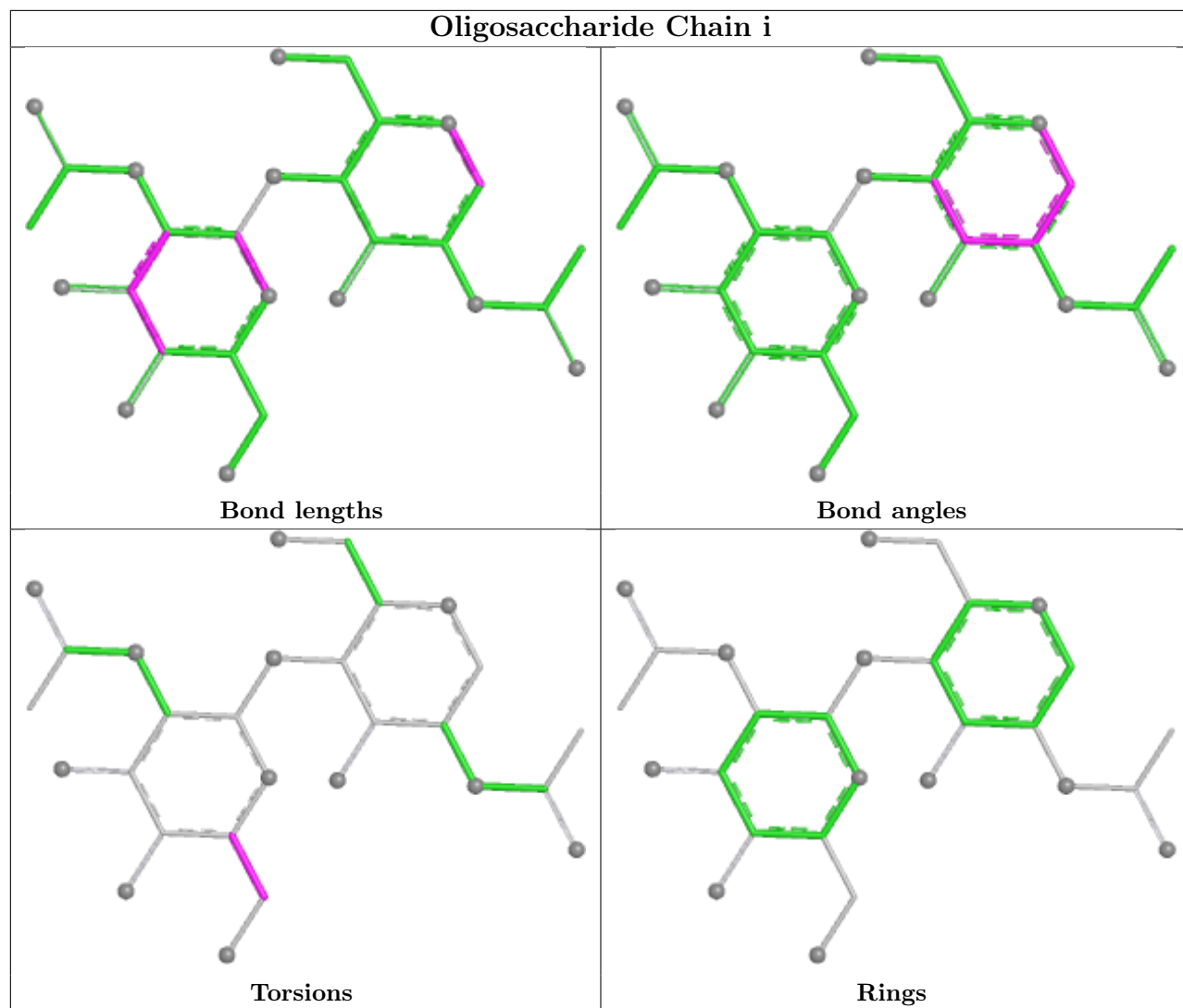


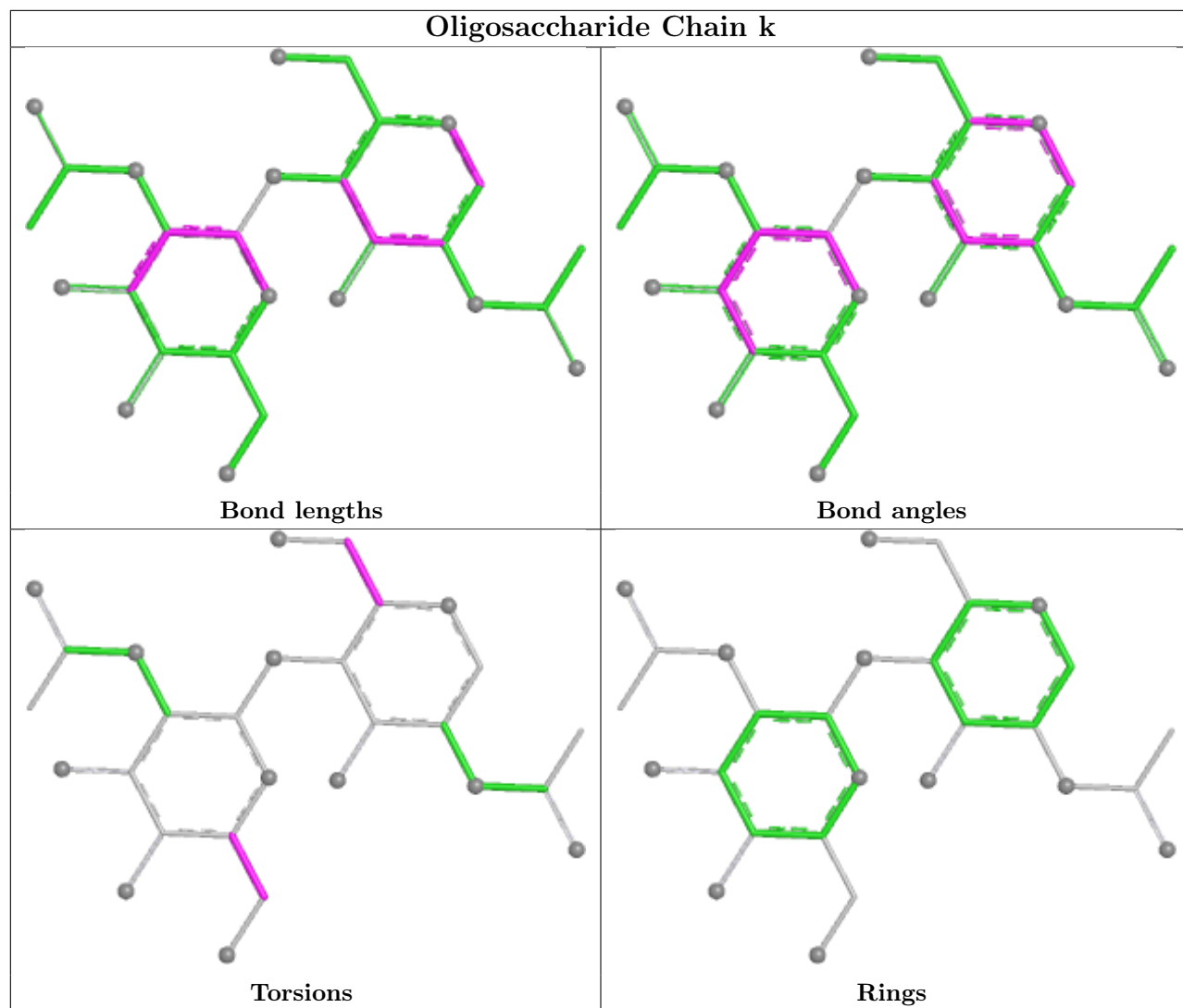


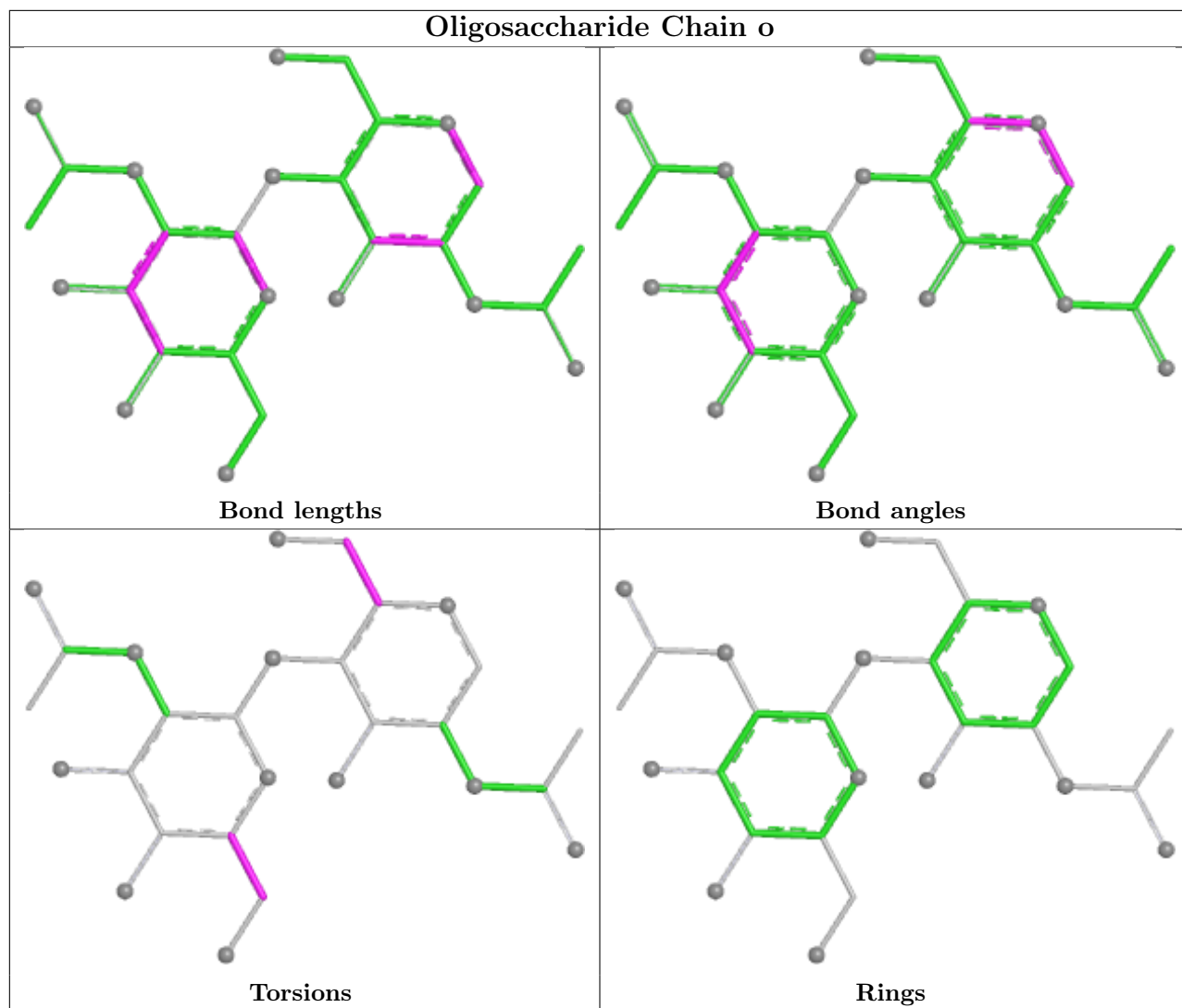


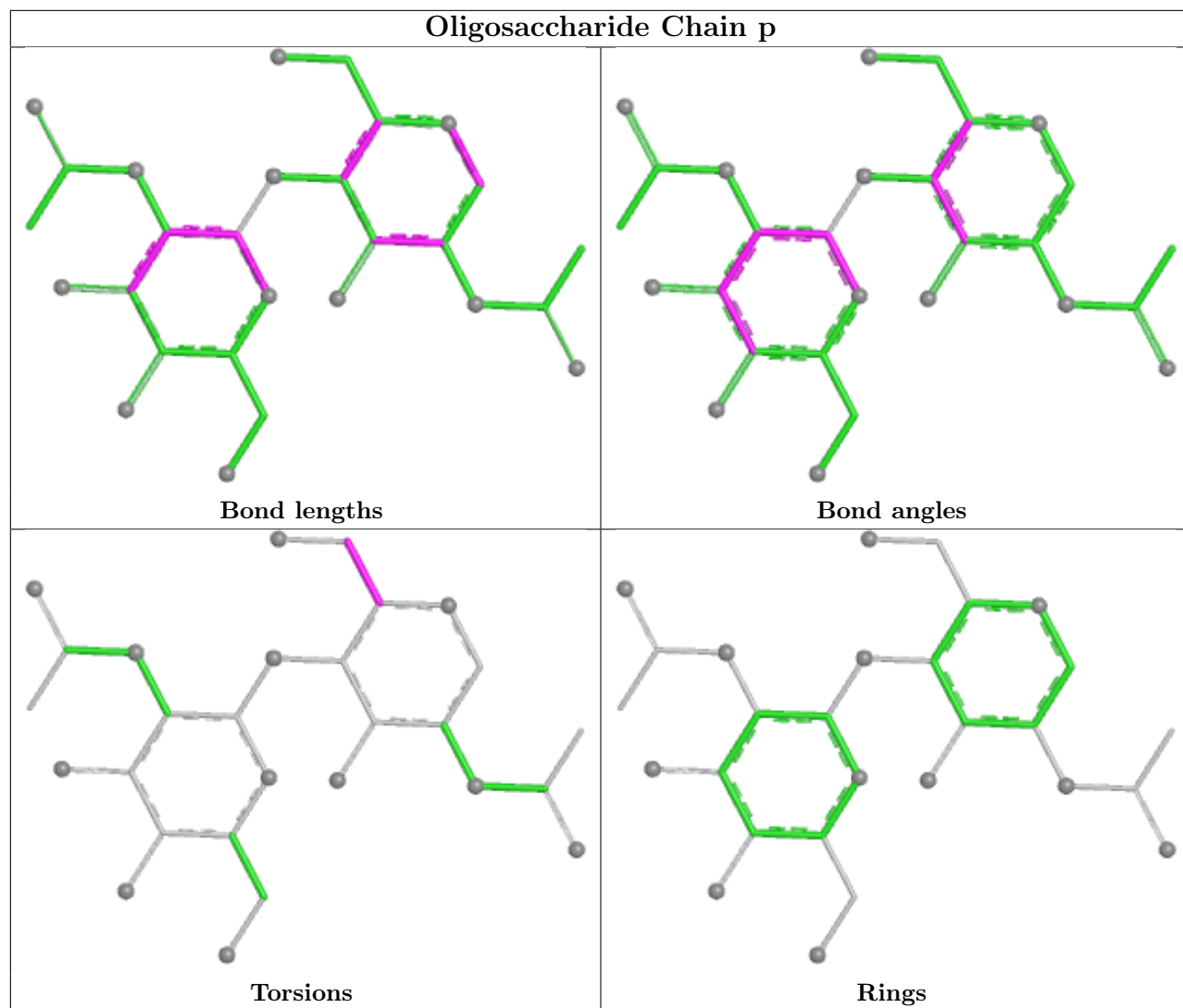


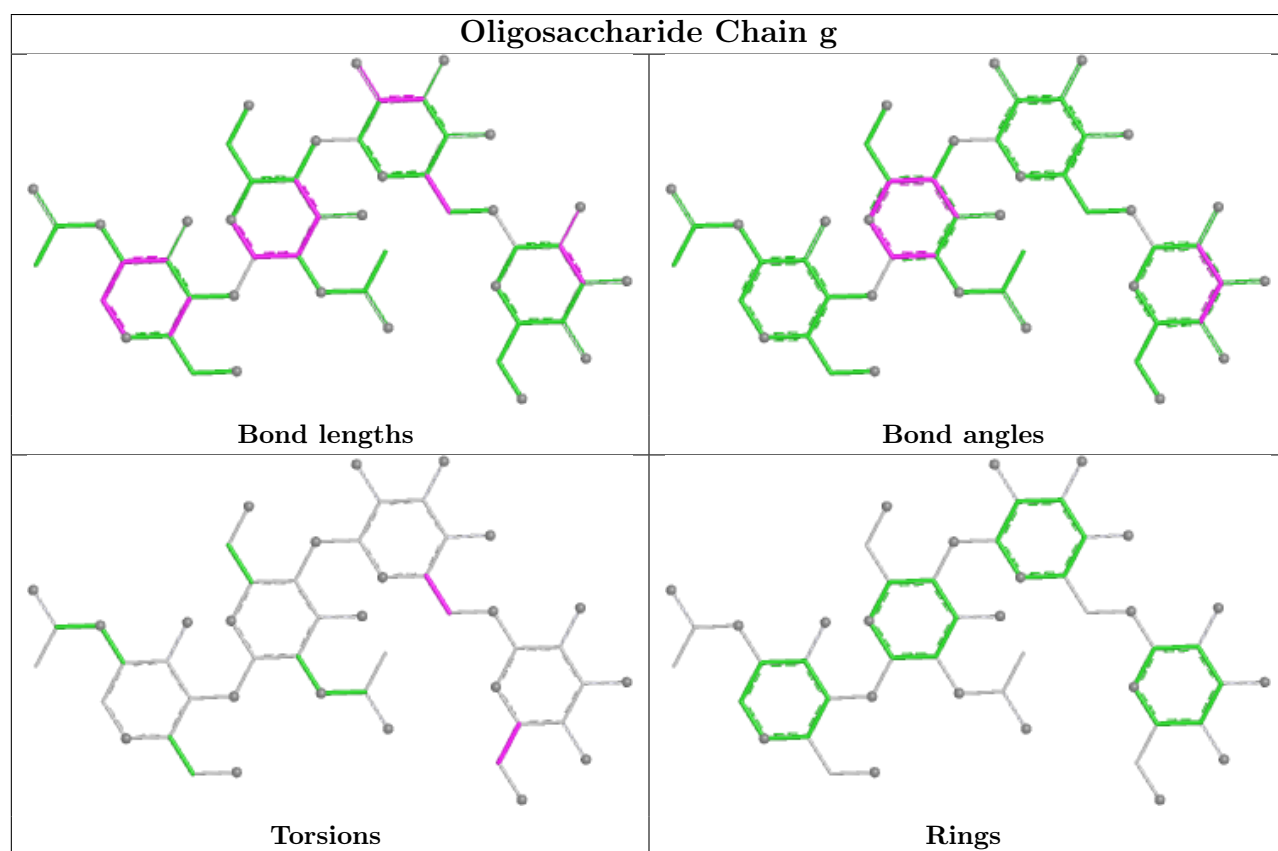
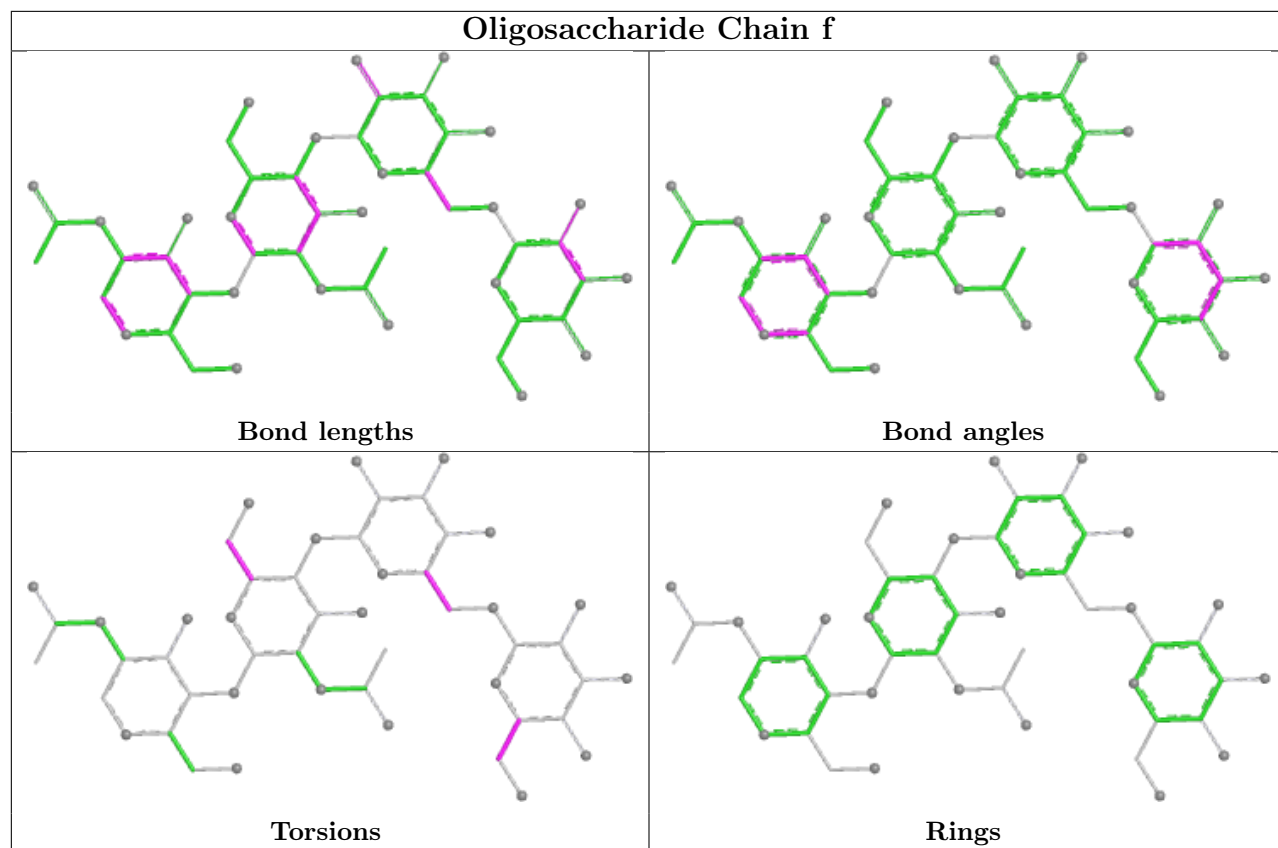












## 5.6 Ligand geometry

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	1301	1	14,14,15	2.06	2 (14%)	17,19,21	1.10	1 (5%)
9	NAG	A	1310	1	14,14,15	2.07	2 (14%)	17,19,21	0.78	0
9	NAG	B	1309	1	14,14,15	2.11	2 (14%)	17,19,21	0.91	1 (5%)
9	NAG	B	1320	1	14,14,15	2.13	2 (14%)	17,19,21	0.81	1 (5%)
9	NAG	A	1321	1	14,14,15	2.11	1 (7%)	17,19,21	0.75	0
9	NAG	C	1301	1	14,14,15	2.19	2 (14%)	17,19,21	1.31	2 (11%)
9	NAG	B	1310	1	14,14,15	2.10	2 (14%)	17,19,21	0.80	1 (5%)
9	NAG	C	1302	1	14,14,15	2.07	4 (28%)	17,19,21	0.99	1 (5%)
9	NAG	C	1303	1	14,14,15	1.77	3 (21%)	17,19,21	0.94	1 (5%)
9	NAG	A	1311	1	14,14,15	2.13	2 (14%)	17,19,21	0.93	1 (5%)
9	NAG	A	1303	1	14,14,15	2.10	2 (14%)	17,19,21	0.93	1 (5%)
9	NAG	A	1302	1	14,14,15	2.02	1 (7%)	17,19,21	0.74	0
9	NAG	C	1320	1	14,14,15	2.10	2 (14%)	17,19,21	0.98	1 (5%)
9	NAG	B	1302	1	14,14,15	2.09	1 (7%)	17,19,21	0.78	1 (5%)
9	NAG	B	1303	1	14,14,15	2.07	2 (14%)	17,19,21	0.75	0
9	NAG	B	1301	1	14,14,15	1.98	2 (14%)	17,19,21	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1320	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1321	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1320	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1301	1	-	1/6/23/26	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1301	NAG	O5-C1	7.16	1.55	1.43
9	A	1321	NAG	O5-C1	6.85	1.55	1.43
9	B	1310	NAG	O5-C1	6.85	1.55	1.43
9	A	1303	NAG	O5-C1	6.81	1.55	1.43
9	B	1320	NAG	O5-C1	6.81	1.55	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1301	NAG	C4-C3-C2	-3.26	106.24	111.02
9	C	1301	NAG	C4-C3-C2	-3.23	106.28	111.02
9	C	1302	NAG	C4-C3-C2	-3.20	106.33	111.02
9	C	1320	NAG	C4-C3-C2	-2.94	106.71	111.02
9	B	1301	NAG	C4-C3-C2	-2.79	106.93	111.02

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1301	NAG	O5-C5-C6-O6
9	A	1321	NAG	O5-C5-C6-O6
9	C	1320	NAG	O5-C5-C6-O6
9	A	1310	NAG	O5-C5-C6-O6
9	B	1310	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

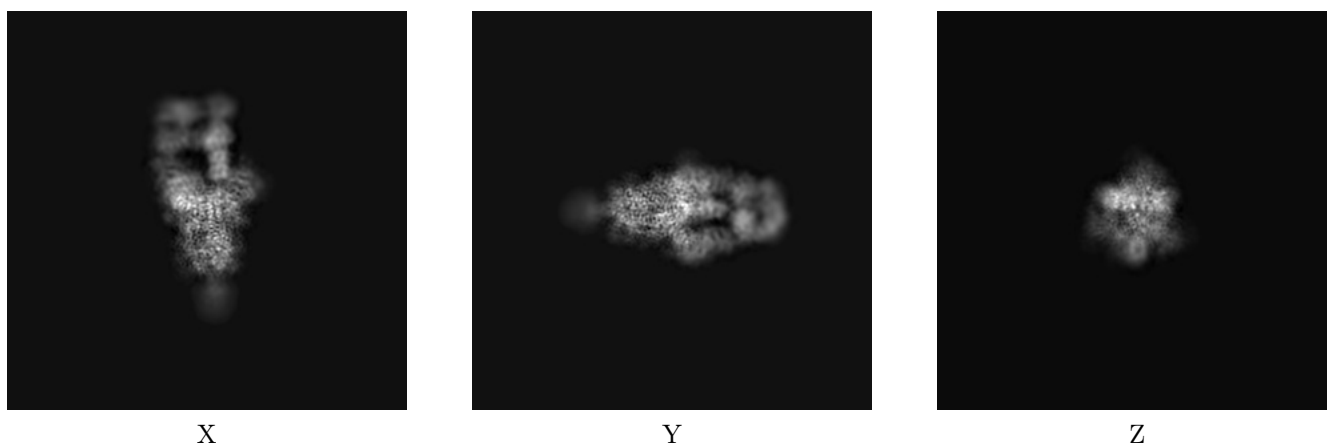
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0404. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

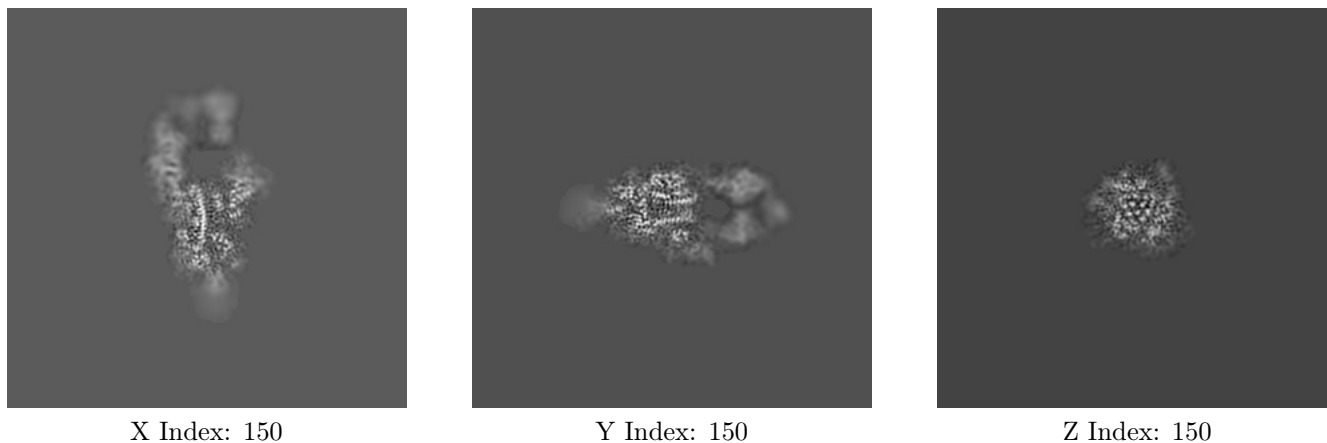
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

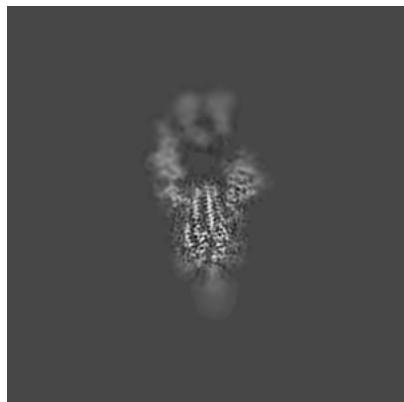
#### 6.2.1 Primary map



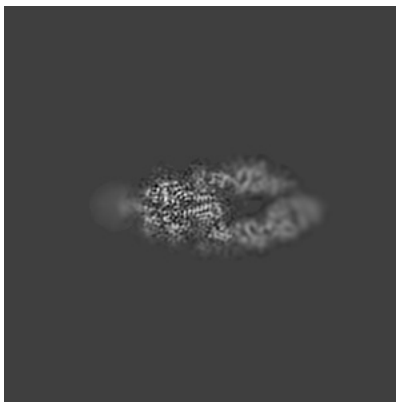
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 154



Y Index: 158

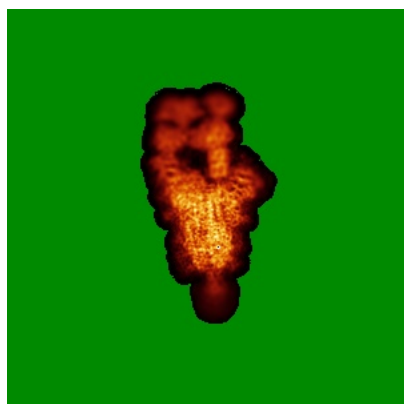


Z Index: 154

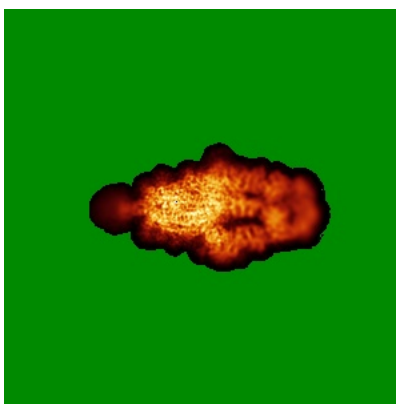
The images above show the largest variance slices of the map in three orthogonal directions.

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

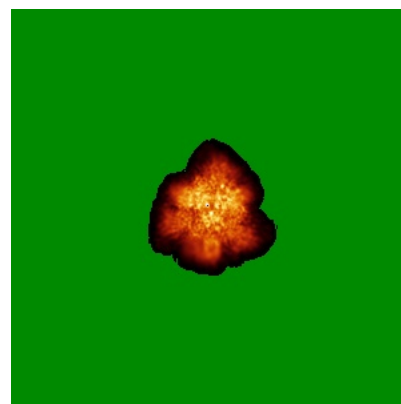
### 6.4.1 Primary map



X



Y



Z

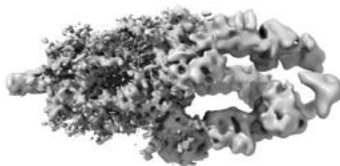
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

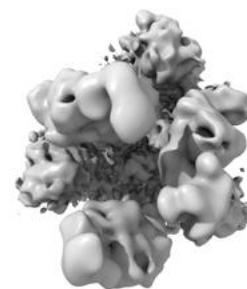
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

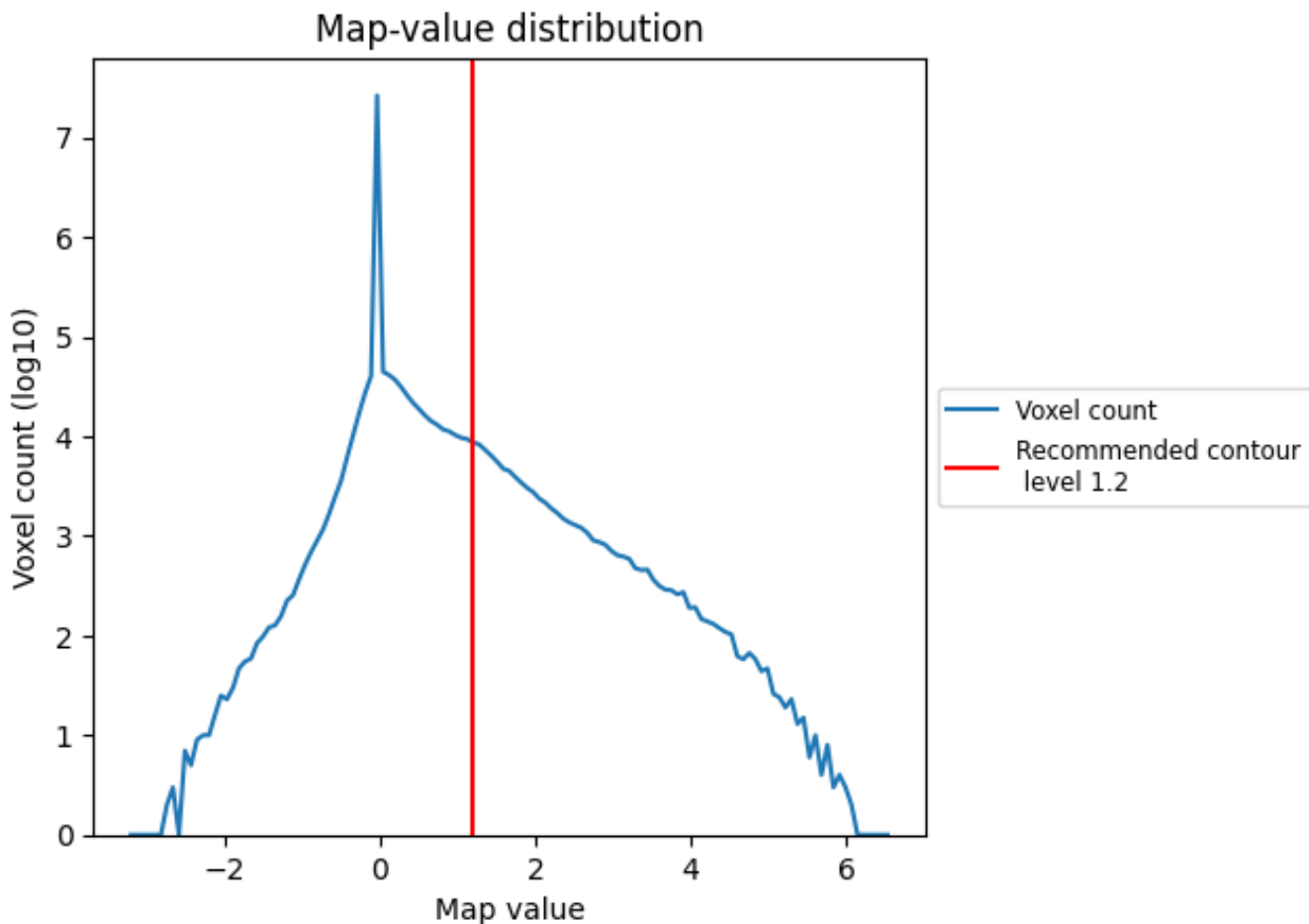
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

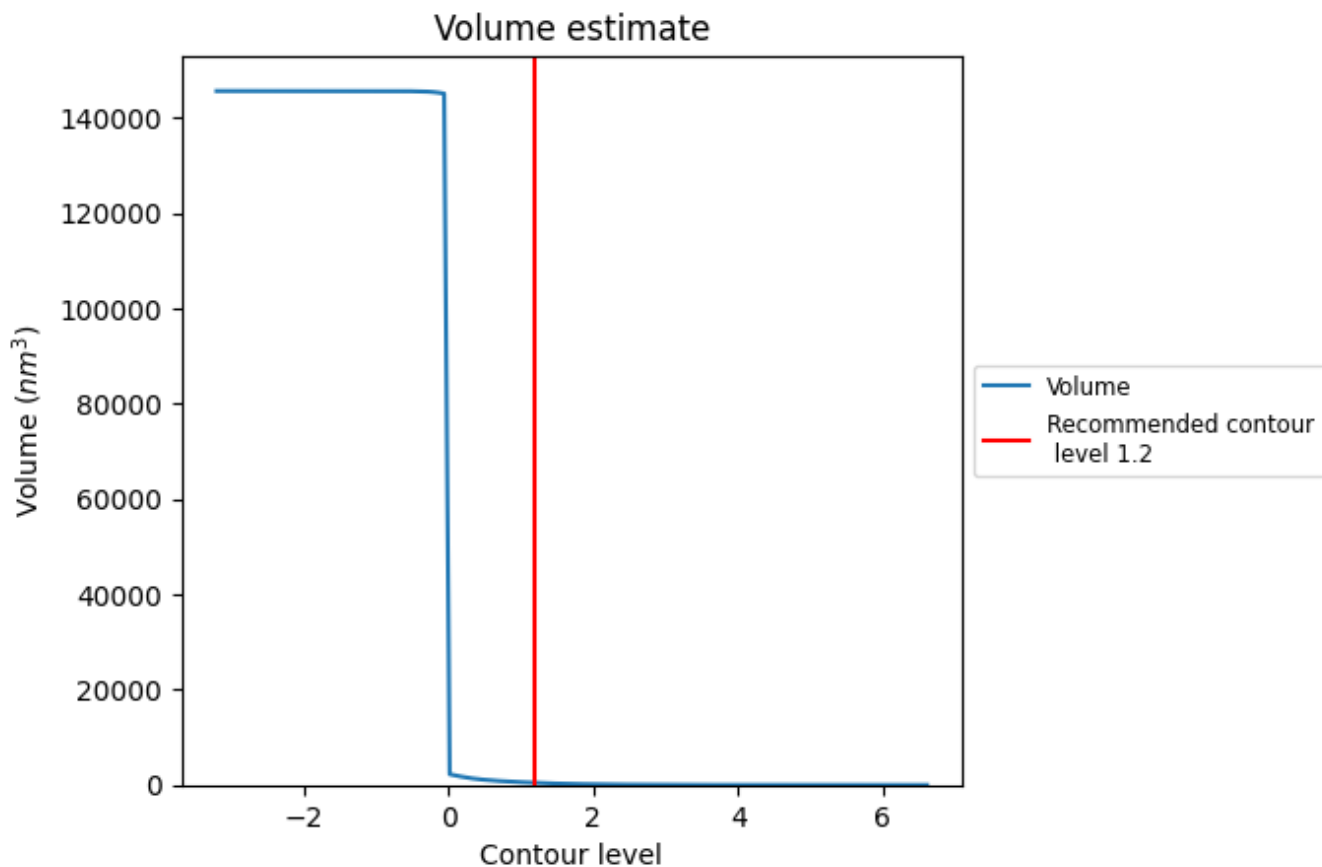
This section contains the results of statistical analysis of the map.

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



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

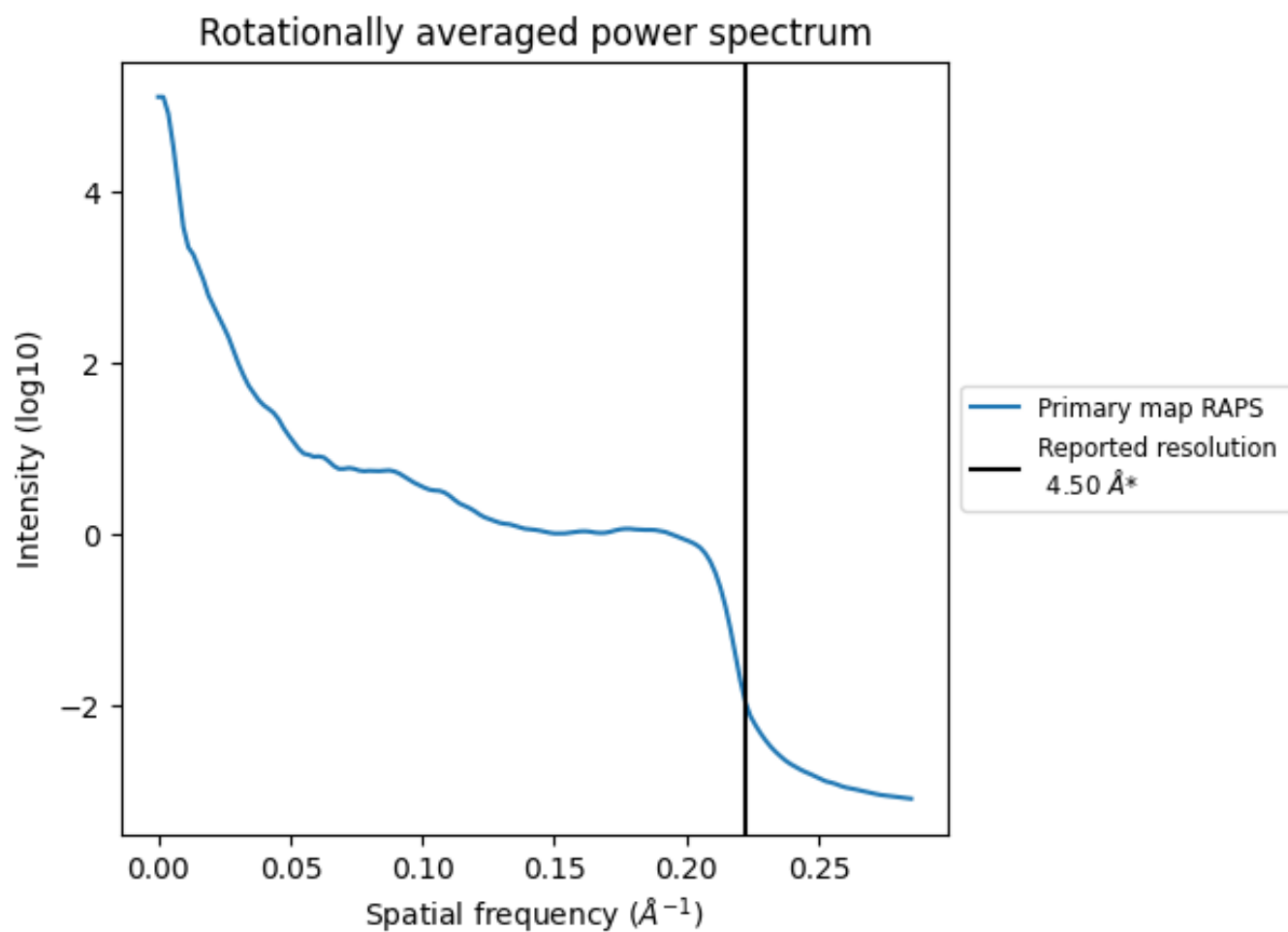
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm<sup>3</sup>; this corresponds to an approximate mass of 408 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.222 \text{\AA}^{-1}$

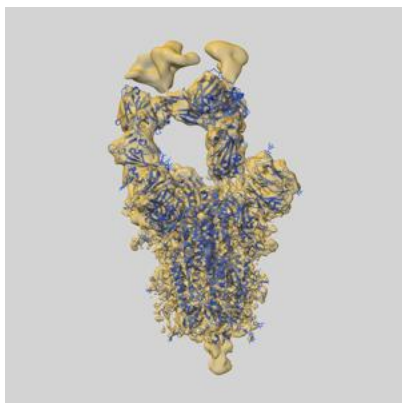
## 8 Fourier-Shell correlation

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

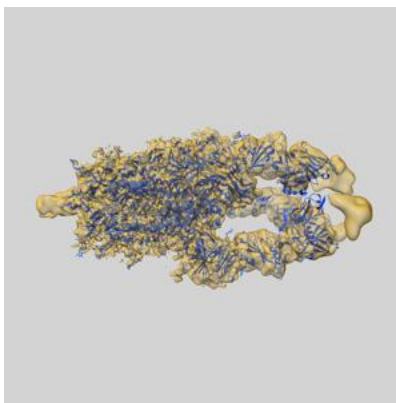
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0404 and PDB model 6NB7. Per-residue inclusion information can be found in section 3 on page 17.

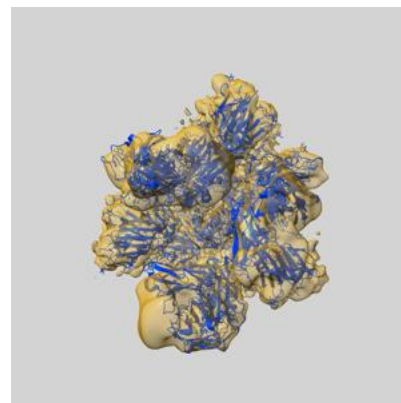
### 9.1 Map-model overlay [i](#)



X



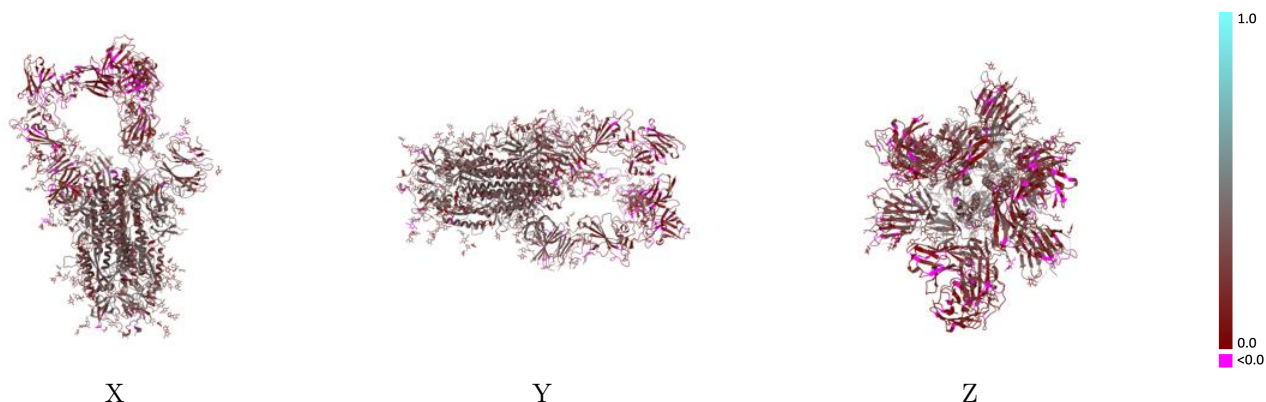
Y



Z

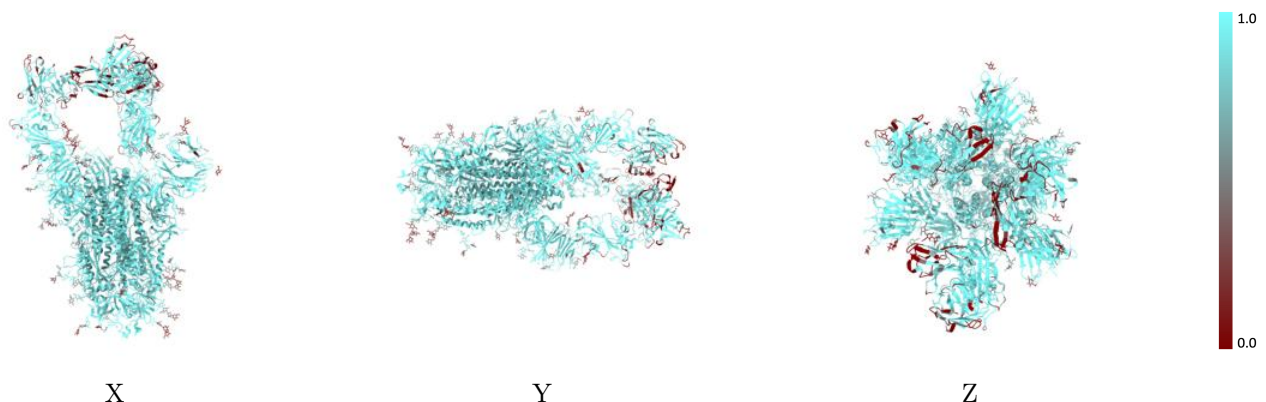
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



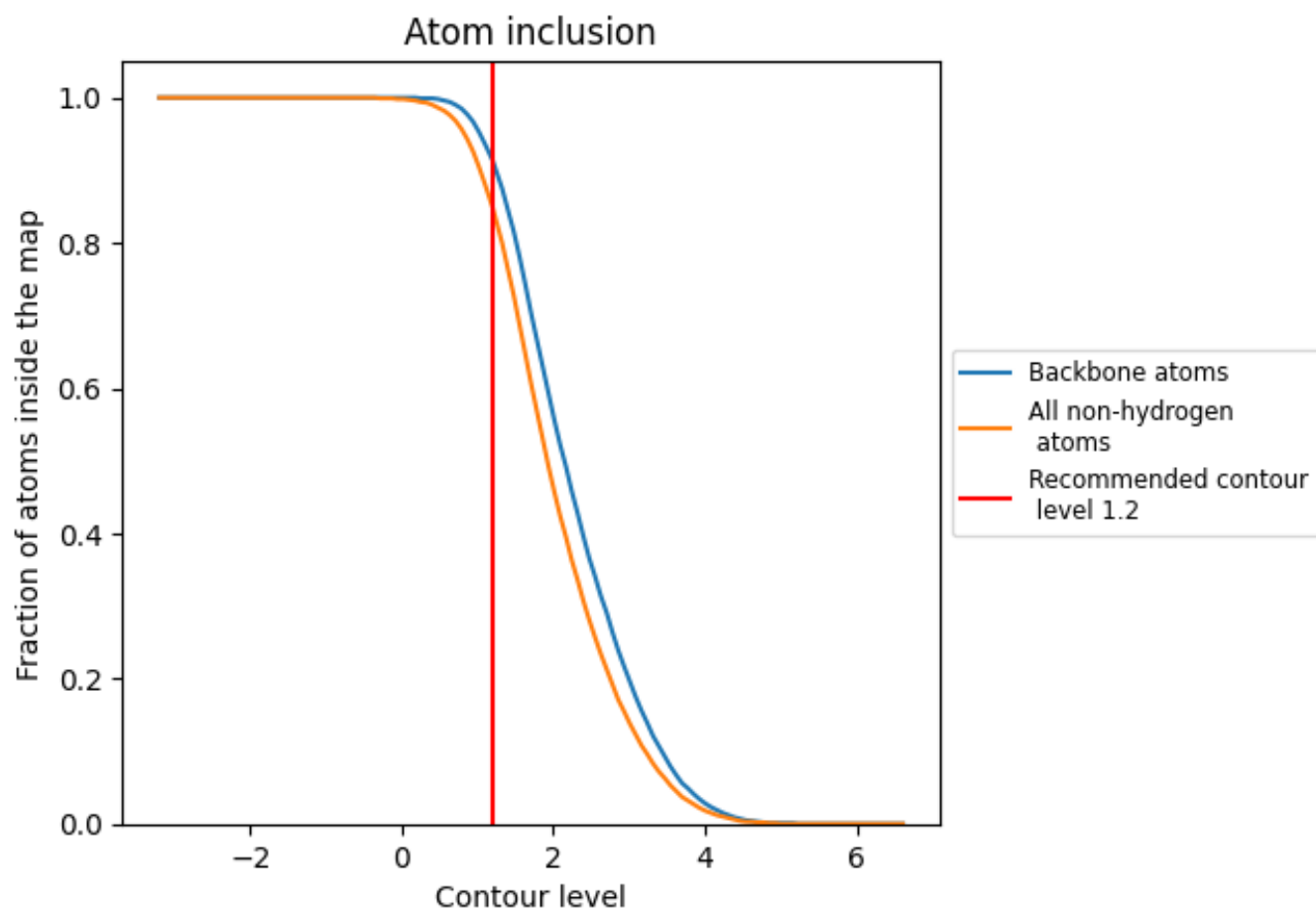
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

























The table lists the average atom inclusion at the recommended contour level (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.2650
A	 0.9050	 0.2960
B	 0.8970	 0.2870
C	 0.9160	 0.2970
D	 0.7230	 0.1270
E	 0.5570	 0.1230
F	 0.1790	 0.0760
G	 0.7490	 0.1150
H	 0.7900	 0.1570
I	 0.5660	 0.0950
J	 0.5900	 0.2220
K	 0.6920	 0.2620
L	 0.6100	 0.1320
M	 0.6410	 0.2810
N	 0.3590	 0.1520
O	 0.5900	 0.2320
P	 0.3930	 0.2460
Q	 0.5640	 0.2630
R	 0.6230	 0.2360
S	 0.2950	 0.1640
T	 0.5200	 0.2260
U	 0.3110	 0.1090
V	 0.1280	 0.1890
W	 0.6070	 0.1900
X	 0.5640	 0.0670
Y	 0.7690	 0.3330
Z	 0.4360	 0.1500
a	 0.6410	 0.1590
b	 0.5000	 0.1370
c	 0.7440	 0.2840
d	 0.6720	 0.2600
e	 0.4620	 0.2460
f	 0.7000	 0.2310
g	 0.4200	 0.2660
h	 0.3080	 0.0820



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Chain	Atom inclusion	Q-score
i	 0.6790	 0.2110
j	 0.1280	 0.2010
k	 0.7140	 0.2440
l	 0.6670	 0.2770
m	 0.5900	 0.1960
n	 0.5130	 0.2110
o	 0.6070	 0.1900
p	 0.7140	 0.3160
q	 0.6560	 0.2760
r	 0.5900	 0.2280
s	 0.6000	 0.2900
t	 0.5380	 0.2710