



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:10 AM UTC

PDB ID : 9B8F / pdb_00009b8f
EMDB ID : EMD-44344
Title : SARS CoV-2 full-length spike protein with Lys1269Ala and His1271Ala substitutions in the coatomer binding motif, 2RBD-up conformation (SPIKE-AXA)
Authors : Singh, S.; Hasan, S.S.
Deposited on : 2024-03-29
Resolution : 4.15 Å(reported)
Based on initial model : 7KRQ

This is a wwPDB EM Validation Summary 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:

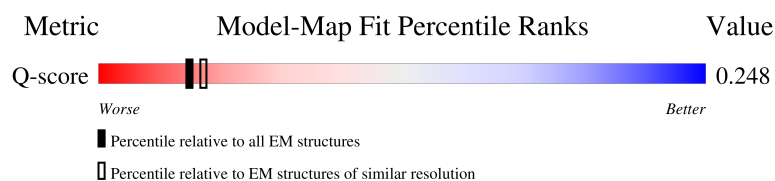
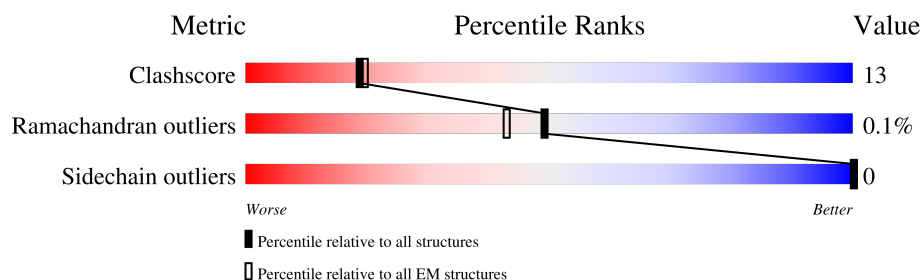
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

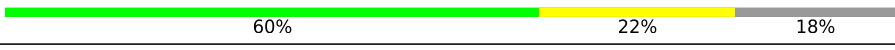
The reported resolution of this entry is 4.15 Å.

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.



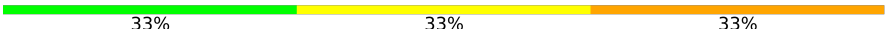
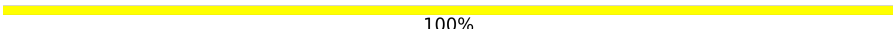
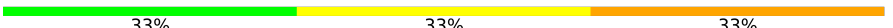
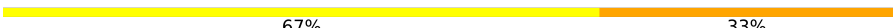
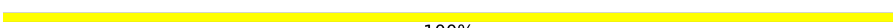
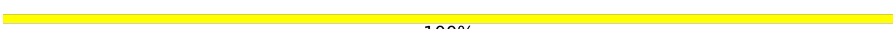
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5475 (3.66 - 4.65)

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	1312	
1	B	1312	
1	C	1312	
2	D	3	

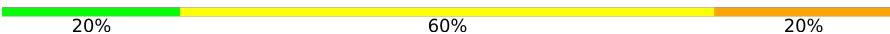
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	3	 33% 67%
2	M	3	 33% 33% 33%
2	N	3	 33% 67%
2	P	3	 100%
2	R	3	 33% 67%
2	S	3	 33% 67%
2	U	3	 33% 67%
2	V	3	 33% 33% 33%
2	W	3	 67% 33%
2	X	3	 33% 67%
2	b	3	 33% 67%
3	E	4	 25% 75%
3	F	4	 25% 75%
4	G	2	 100%
4	I	2	 100%
4	K	2	 50% 50%
4	O	2	 100%
4	Q	2	 100%
4	T	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 100%
5	H	4	 50% 50%
6	J	4	 100%
6	Z	4	 25% 75%
7	Y	3	 33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	a	5	 20% 80%
8	d	5	 20% 60% 20%
9	c	4	 25% 25% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	-	-	X	-
2	BMA	D	3	-	-	X	-
3	NAG	E	1	-	-	X	-
3	BMA	E	3	-	-	X	-
3	MAN	E	4	-	-	X	-
3	NAG	F	1	-	-	X	-
3	NAG	F	2	-	-	X	-
3	MAN	F	4	-	-	X	-
9	NAG	c	1	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 51495 atoms, of which 25203 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	1044	Total	C	H	N	O	S	0	0
			16045	5197	7909	1356	1547	36		
1	B	1076	Total	C	H	N	O	S	0	0
			16504	5360	8106	1399	1601	38		
1	C	1073	Total	C	H	N	O	S	0	0
			16425	5333	8070	1392	1594	36		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	insertion	UNP P0DTC2
A	-19	ALA	-	insertion	UNP P0DTC2
A	-18	TRP	-	insertion	UNP P0DTC2
A	-17	SER	-	insertion	UNP P0DTC2
A	-16	HIS	-	insertion	UNP P0DTC2
A	-15	PRO	-	insertion	UNP P0DTC2
A	-14	GLN	-	insertion	UNP P0DTC2
A	-13	PHE	-	insertion	UNP P0DTC2
A	-12	GLU	-	insertion	UNP P0DTC2
A	-11	LYS	-	insertion	UNP P0DTC2
A	-10	GLY	-	insertion	UNP P0DTC2
A	-9	GLY	-	insertion	UNP P0DTC2
A	-8	GLY	-	insertion	UNP P0DTC2
A	-7	SER	-	insertion	UNP P0DTC2
A	-6	GLY	-	insertion	UNP P0DTC2
A	-5	GLY	-	insertion	UNP P0DTC2
A	-4	GLY	-	insertion	UNP P0DTC2
A	-3	SER	-	insertion	UNP P0DTC2
A	-2	GLY	-	insertion	UNP P0DTC2
A	-1	GLY	-	insertion	UNP P0DTC2
A	0	SER	-	insertion	UNP P0DTC2
A	1	SER	-	insertion	UNP P0DTC2
A	2	ALA	-	insertion	UNP P0DTC2
A	3	TRP	-	insertion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	insertion	UNP P0DTC2
A	5	HIS	-	insertion	UNP P0DTC2
A	6	PRO	-	insertion	UNP P0DTC2
A	7	GLN	-	insertion	UNP P0DTC2
A	8	PHE	-	insertion	UNP P0DTC2
A	9	GLU	-	insertion	UNP P0DTC2
A	10	LYS	-	insertion	UNP P0DTC2
A	11	SER	-	insertion	UNP P0DTC2
A	12	ALA	-	insertion	UNP P0DTC2
A	13	LEU	-	insertion	UNP P0DTC2
A	14	VAL	-	insertion	UNP P0DTC2
A	15	PRO	-	insertion	UNP P0DTC2
A	16	ARG	-	insertion	UNP P0DTC2
A	17	GLY	-	insertion	UNP P0DTC2
A	18	SER	-	insertion	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1269	ALA	LYS	engineered mutation	UNP P0DTC2
A	1271	ALA	HIS	engineered mutation	UNP P0DTC2
B	-20	SER	-	insertion	UNP P0DTC2
B	-19	ALA	-	insertion	UNP P0DTC2
B	-18	TRP	-	insertion	UNP P0DTC2
B	-17	SER	-	insertion	UNP P0DTC2
B	-16	HIS	-	insertion	UNP P0DTC2
B	-15	PRO	-	insertion	UNP P0DTC2
B	-14	GLN	-	insertion	UNP P0DTC2
B	-13	PHE	-	insertion	UNP P0DTC2
B	-12	GLU	-	insertion	UNP P0DTC2
B	-11	LYS	-	insertion	UNP P0DTC2
B	-10	GLY	-	insertion	UNP P0DTC2
B	-9	GLY	-	insertion	UNP P0DTC2
B	-8	GLY	-	insertion	UNP P0DTC2
B	-7	SER	-	insertion	UNP P0DTC2
B	-6	GLY	-	insertion	UNP P0DTC2
B	-5	GLY	-	insertion	UNP P0DTC2
B	-4	GLY	-	insertion	UNP P0DTC2
B	-3	SER	-	insertion	UNP P0DTC2
B	-2	GLY	-	insertion	UNP P0DTC2

Continued on next page...

Continued from previous page...

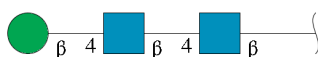
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	insertion	UNP P0DTC2
B	0	SER	-	insertion	UNP P0DTC2
B	1	SER	-	insertion	UNP P0DTC2
B	2	ALA	-	insertion	UNP P0DTC2
B	3	TRP	-	insertion	UNP P0DTC2
B	4	SER	-	insertion	UNP P0DTC2
B	5	HIS	-	insertion	UNP P0DTC2
B	6	PRO	-	insertion	UNP P0DTC2
B	7	GLN	-	insertion	UNP P0DTC2
B	8	PHE	-	insertion	UNP P0DTC2
B	9	GLU	-	insertion	UNP P0DTC2
B	10	LYS	-	insertion	UNP P0DTC2
B	11	SER	-	insertion	UNP P0DTC2
B	12	ALA	-	insertion	UNP P0DTC2
B	13	LEU	-	insertion	UNP P0DTC2
B	14	VAL	-	insertion	UNP P0DTC2
B	15	PRO	-	insertion	UNP P0DTC2
B	16	ARG	-	insertion	UNP P0DTC2
B	17	GLY	-	insertion	UNP P0DTC2
B	18	SER	-	insertion	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1269	ALA	LYS	engineered mutation	UNP P0DTC2
B	1271	ALA	HIS	engineered mutation	UNP P0DTC2
C	-20	SER	-	insertion	UNP P0DTC2
C	-19	ALA	-	insertion	UNP P0DTC2
C	-18	TRP	-	insertion	UNP P0DTC2
C	-17	SER	-	insertion	UNP P0DTC2
C	-16	HIS	-	insertion	UNP P0DTC2
C	-15	PRO	-	insertion	UNP P0DTC2
C	-14	GLN	-	insertion	UNP P0DTC2
C	-13	PHE	-	insertion	UNP P0DTC2
C	-12	GLU	-	insertion	UNP P0DTC2
C	-11	LYS	-	insertion	UNP P0DTC2
C	-10	GLY	-	insertion	UNP P0DTC2
C	-9	GLY	-	insertion	UNP P0DTC2
C	-8	GLY	-	insertion	UNP P0DTC2
C	-7	SER	-	insertion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	insertion	UNP P0DTC2
C	-5	GLY	-	insertion	UNP P0DTC2
C	-4	GLY	-	insertion	UNP P0DTC2
C	-3	SER	-	insertion	UNP P0DTC2
C	-2	GLY	-	insertion	UNP P0DTC2
C	-1	GLY	-	insertion	UNP P0DTC2
C	0	SER	-	insertion	UNP P0DTC2
C	1	SER	-	insertion	UNP P0DTC2
C	2	ALA	-	insertion	UNP P0DTC2
C	3	TRP	-	insertion	UNP P0DTC2
C	4	SER	-	insertion	UNP P0DTC2
C	5	HIS	-	insertion	UNP P0DTC2
C	6	PRO	-	insertion	UNP P0DTC2
C	7	GLN	-	insertion	UNP P0DTC2
C	8	PHE	-	insertion	UNP P0DTC2
C	9	GLU	-	insertion	UNP P0DTC2
C	10	LYS	-	insertion	UNP P0DTC2
C	11	SER	-	insertion	UNP P0DTC2
C	12	ALA	-	insertion	UNP P0DTC2
C	13	LEU	-	insertion	UNP P0DTC2
C	14	VAL	-	insertion	UNP P0DTC2
C	15	PRO	-	insertion	UNP P0DTC2
C	16	ARG	-	insertion	UNP P0DTC2
C	17	GLY	-	insertion	UNP P0DTC2
C	18	SER	-	insertion	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1269	ALA	LYS	engineered mutation	UNP P0DTC2
C	1271	ALA	HIS	engineered mutation	UNP P0DTC2

- Molecule 2 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.



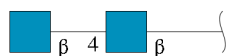
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	H	N	0	0
			73	22	34	2		
2	M	3	Total	C	H	N	0	0
			73	22	34	2		
2	N	3	Total	C	H	N	0	0
			73	22	34	2		
2	P	3	Total	C	H	N	0	0
			73	22	34	2		
2	R	3	Total	C	H	N	0	0
			73	22	34	2		
2	S	3	Total	C	H	N	0	0
			73	22	34	2		
2	U	3	Total	C	H	N	0	0
			73	22	34	2		
2	V	3	Total	C	H	N	0	0
			73	22	34	2		
2	W	3	Total	C	H	N	0	0
			73	22	34	2		
2	X	3	Total	C	H	N	0	0
			73	22	34	2		
2	b	3	Total	C	H	N	0	0
			73	22	34	2		

- Molecule 3 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.



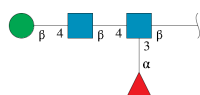
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		
3	F	4	Total	C	N	O	0	0
			50	28	2	20		

- 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	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	e	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	f	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

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



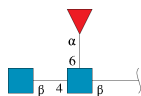
Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	4	Total	C	H	N	O	0	0
			92	28	43	2	19		

- 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.



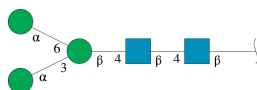
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	4	Total	C	H	N	O	0	0
			93	28	43	2	20		
6	Z	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	3	Total	C	H	N	O	0	0
			72	22	34	2	14		

- Molecule 8 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.



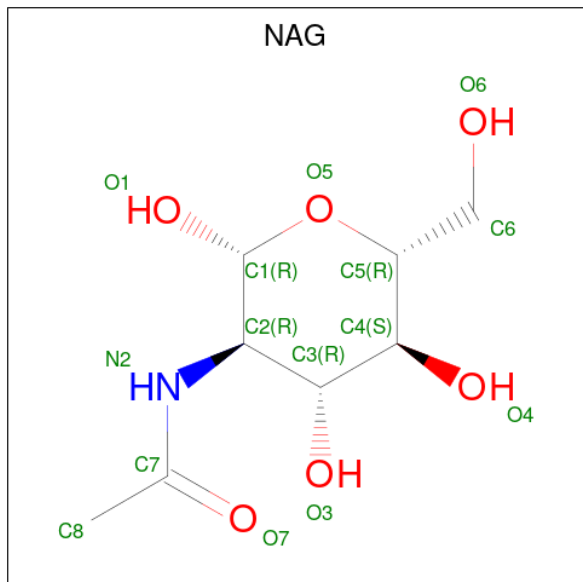
Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	5	Total	C	H	N	O	0	0
			113	34	52	2	25		
8	d	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

[illegible]

- Molecule 1: Spike glycoprotein



MET	PHE	VAL	VAL	PHE	LEU	VAL	LEU	LEU	LEU	PRO	PRO	VAL	SER	SER	GLN	CYS	GLY	VAL	VAL	ASN	ASN	LEU	SER	SER	ALA	ALA	TRP	TRP	HIS	HIS	PRO	PRO	GLN	PHE	GLU	GLY	LYS	GLY	GLY	GLY	SER	SER	GLY	GLY	GLY	GLY	SER	SER	ALA	ALA	TRP	TRP	SER	HIS	HIS	PRO	GLN	GLN	PHE	PHE	GLU	LYS	SER	SER	ALA	ALA	VAL	VAL	PRO	PRO	ARG	GLY	GLY	SER	SER	THR	THR	ARG	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	GLN	LEU	PRO	PRO	A27	S31	R34	D40	K41	V42	F43	S46	D53	L54	F59	S60	N61	F65	H66	A67	I68	H69	VAL	SER	GLY	THR	THR	ASN	GLY	THR	K77	D80	E86	I101	G107	I108	T109	L110	D111	S112	L117	L118	L119	V120	N125	I126
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------

F136	K136	N137	D138	P139	K140	N141	K142	N143	K144	N145	K146	N147	K148	N149	K150	N151	W152	M153	Y150	S161	V171	F175	L176	M177	D178	L179	E180	G181	K187	V193	F194	K195	Y204	I210	L216	P217	E224	P225	L226	V227	D228	L229	P230	I231	G232	D233	N234	L235	T236	R237	F238	Q239	T240	L241	L242	A243	L244
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	S254	Y265	R273	Y279	N280	T284	D287	A288	Y289	D290	C291	S314	T315	S316	T323	T326	Y327	R328	N331	N334	P337	F338	G339	E340	N343	A348	A352	W353	N354	R355	L358	S359	N360	Y365	S366
-----	-----	-----	-----	-----	-----	-----	-----	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------	-------------

L368	L369	L370	L371	S375	T376	T377	K378	K379	V382	S383	P384	T385	T393	N394	V395	D398	R403	G404	D405	E406	Q409	T415	G416	N422	Y423	C432	V433	W436	E465	R466	ASP	ILE	SER	THR	GLU	ILE	TYR	GLN	ALA	GLY	SER	THR	PRO	CYS	ASN	GLY
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------

E726	N731	D737	C738	T739	L742	L743	G744	C749	S750	L753	L763	A766	I770	O774	D775	K776	E780	D796	F817	L821	D830	D836	T836	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	D848	L849	I850	L865	T866	M869	L870	A871
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------

T874	L878	A893	L894	Q901	R905	T912	Q913	L914	V915	L916	V917	R918	N919	Q920	K921	L922	L923	A924	N925	Q926			S929	K933	P986	E990	L996	1997	T1006	V1007	V1008	T1009	L1012	A1015	T1018	K1028	F1042	L1049	V1060	V1061	H1064	1065
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--	--	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------

TI066	EL072	TI073	FI075	TI076	TI077	TI081	CI082	HI088	RI091	SI097	GI098	GI099	TI100	HI101	HI102	TI116	TI117	DI118	TI119	TI120	FI121	VI122	MI126	CI127	DI128	VI128	VI129	GI131	HI132	VI133	MI134	QI142	DI146	SI147	FI148	LI152	DI153	FI162	ASP	VAL	ASP	ASP	LEU	GLY	ASP	ASP	TLE	FER
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY	ILE	ASN	ALA	SER	VAL	VAL	ASN	ASN	ILE	GLN	LYS	GLU	GLU	ILE	ILE	ARG	LEU	ASN	ASN	ASN	GLU	SER	LEU	LEU	GLN	GLY	LYS	TYR	GLU	GLN	TYR	TRP	TRP	TRP	TRP	ILE	ILE	GLY	LEU	ILE	ALA	ILE	VAL	MET	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

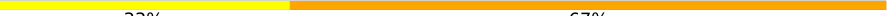
THR	ILE	MET	LEU	CYS	CYS	MET	THR	SER	SER	CYS	CYS	SER	SER	CYS	GLY	CYS	CYS	SER	SER	CYS	GLY	SER	SER	CYS	CYS	LYS	PHE	ASP	GLU	ASP	ASP	ASP	SER	SER	GLU	PRO	VAL	LEU	LYS	GLY	VAL	ALA	LEU	ALA	ALA	TYR	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain D:  100%

NAG1
NAG2
BMA3

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

Chain L:  33% 67%

NAG1
NAG2
BMA3

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

Chain M:  33% 33% 33%

NAG1
NAG2
BMA3

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

Chain N:  33% 67%

NAG1
NAG2
BMA3

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

Chain P:  100%

NAG1
NAG2
BMA3

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

Chain R:  33% 67%

NAG1
NAG2
BMA3

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

Chain S:  33% 67%

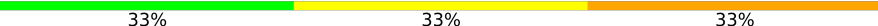
NAG1
NAG2
BMA3

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

Chain U:  33% 67%

MAG1
MAG2
BMA3

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

Chain V:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain W:  67% 33%

MAG1
MAG2
BMA3

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

Chain X:  33% 67%

MAG1
MAG2
BMA3

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

Chain b:  33% 67%

MAG1
MAG2
BMA3

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

Chain E:  25% 75%

MAG1
MAG2
BMA3
MAN4

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

Chain F:  25% 75%



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

Chain G:  100%



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

Chain I:  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:  100%



- 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 T:  50% 50%

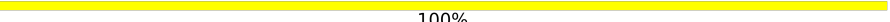


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain H:  50% 50%

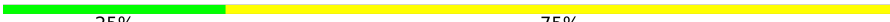
MAG1
MAG2
BMA3
FUC4

- 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

Chain J:  100%

MAG1
MAG2
BMA3
MAN4

- 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

Chain Z:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 67%

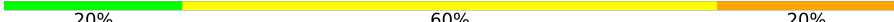
MAG1
MAG2
FUC3

- Molecule 8: 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 a:  20% 80%

MAG1
MAG2
BGA3
MAN4
MAN5

- Molecule 8: 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 d:  20% 60% 20%

MAG1
MAG2
BGA3
MAN4
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  25% 25% 50%

MAG1
MAG2
BGA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59137	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.19	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0607	Depositor
Map size (Å)	332.112, 332.112, 332.112	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.221, 1.221, 1.221	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/8318	0.32	1/11312 (0.0%)
1	B	0.13	0/8594	0.33	2/11694 (0.0%)
1	C	0.13	0/8549	0.32	0/11638
All	All	0.13	0/25461	0.32	3/34644 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASN	CB-CA-C	-5.75	101.18	114.41
1	B	165	ASN	N-CA-CB	5.46	120.63	110.86
1	A	1134	ASN	N-CA-CB	-5.36	102.05	110.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1133	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	165	ASN	Peptide
1	C	233	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8136	7909	7934	200	0
1	B	8398	8106	8135	221	0
1	C	8355	8070	8099	192	0
2	D	39	0	34	12	0
2	L	39	34	34	2	0
2	M	39	34	34	3	0
2	N	39	34	34	6	0
2	P	39	34	34	0	0
2	R	39	34	34	4	0
2	S	39	34	34	1	0
2	U	39	34	34	2	0
2	V	39	34	34	1	0
2	W	39	34	34	1	0
2	X	39	34	34	0	0
2	b	39	34	34	3	0
3	E	50	0	43	13	0
3	F	50	0	43	30	0
4	G	28	25	25	3	0
4	I	28	25	25	2	0
4	K	28	25	25	3	0
4	O	28	25	25	1	0
4	Q	28	25	25	0	0
4	T	28	25	25	1	0
4	e	28	25	25	1	0
4	f	28	25	25	0	0
5	H	49	43	43	3	0
6	J	50	43	43	6	0
6	Z	50	43	43	0	0
7	Y	38	34	34	4	0
8	a	61	52	52	3	0
8	d	61	52	52	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	c	50	43	43	12	0
10	A	84	78	78	6	0
10	B	98	91	91	9	0
10	C	70	65	65	3	0
All	All	26292	25203	25406	669	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 13.

The worst 5 of 669 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)
3:F:3:BMA:H4	3:F:4:MAN:H5	1.27	1.14
3:E:3:BMA:H4	3:E:4:MAN:H5	1.39	1.02
1:B:1075:PHE:HD1	1:B:1098:ASN:HB3	1.25	1.01
3:F:1:NAG:H4	3:F:2:NAG:C7	1.99	0.92
1:A:142:GLY:O	1:A:155:SER:OG	1.89	0.89

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	1028/1312 (78%)	950 (92%)	78 (8%)	0	100	100
1	B	1064/1312 (81%)	968 (91%)	95 (9%)	1 (0%)	48	82
1	C	1061/1312 (81%)	941 (89%)	117 (11%)	3 (0%)	36	70
All	All	3153/3936 (80%)	2859 (91%)	290 (9%)	4 (0%)	49	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	LYS
1	C	327	VAL
1	C	234	ASN
1	B	332	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	905/1135 (80%)	905 (100%)	0	100	100
1	B	931/1135 (82%)	931 (100%)	0	100	100
1	C	925/1135 (82%)	925 (100%)	0	100	100
All	All	2761/3405 (81%)	2761 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1106	GLN
1	C	925	ASN
1	B	928	ASN
1	C	928	ASN
1	C	448	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 ⓘ

89 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	1.99	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	D	2	2	14,14,15	2.05	4 (28%)	17,19,21	1.43	2 (11%)
2	BMA	D	3	2	11,11,12	0.90	1 (9%)	15,15,17	0.92	1 (6%)
3	NAG	E	1	1,3	14,14,15	2.05	5 (35%)	17,19,21	1.03	2 (11%)
3	NAG	E	2	3	14,14,15	2.01	3 (21%)	17,19,21	1.14	2 (11%)
3	BMA	E	3	3	11,11,12	0.46	0	15,15,17	0.71	0
3	MAN	E	4	3	11,11,12	0.86	0	15,15,17	1.49	2 (13%)
3	NAG	F	1	1,3	14,14,15	2.30	4 (28%)	17,19,21	1.96	4 (23%)
3	NAG	F	2	3	14,14,15	2.14	4 (28%)	17,19,21	1.45	3 (17%)
3	BMA	F	3	3	11,11,12	0.66	0	15,15,17	0.84	0
3	MAN	F	4	3	11,11,12	0.89	1 (9%)	15,15,17	1.57	2 (13%)
4	NAG	G	1	1,4	14,14,15	2.42	5 (35%)	17,19,21	2.58	8 (47%)
4	NAG	G	2	4	14,14,15	2.02	4 (28%)	17,19,21	1.25	1 (5%)
5	NAG	H	1	1,5	14,14,15	2.14	4 (28%)	17,19,21	1.56	3 (17%)
5	NAG	H	2	5	14,14,15	1.95	3 (21%)	17,19,21	1.97	5 (29%)
5	BMA	H	3	5	11,11,12	0.54	0	15,15,17	0.66	0
5	FUC	H	4	5	10,10,11	0.76	0	14,14,16	0.65	0
4	NAG	I	1	1,4	14,14,15	2.09	5 (35%)	17,19,21	1.32	1 (5%)
4	NAG	I	2	4	14,14,15	2.09	4 (28%)	17,19,21	1.12	1 (5%)
6	NAG	J	1	1,6	14,14,15	2.07	5 (35%)	17,19,21	1.28	2 (11%)
6	NAG	J	2	6	14,14,15	2.03	5 (35%)	17,19,21	1.18	2 (11%)
6	BMA	J	3	6	11,11,12	1.12	1 (9%)	15,15,17	0.87	0
6	MAN	J	4	6	11,11,12	1.28	3 (27%)	15,15,17	2.39	3 (20%)
4	NAG	K	1	1,4	14,14,15	2.07	4 (28%)	17,19,21	1.71	4 (23%)
4	NAG	K	2	4	14,14,15	1.94	4 (28%)	17,19,21	1.11	2 (11%)
2	NAG	L	1	1,2	14,14,15	2.16	4 (28%)	17,19,21	1.48	2 (11%)
2	NAG	L	2	2	14,14,15	1.95	4 (28%)	17,19,21	1.30	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	L	3	2	11,11,12	0.95	1 (9%)	15,15,17	0.84	0
2	NAG	M	1	1,2	14,14,15	2.28	6 (42%)	17,19,21	2.38	8 (47%)
2	NAG	M	2	2	14,14,15	1.96	4 (28%)	17,19,21	1.57	3 (17%)
2	BMA	M	3	2	11,11,12	0.46	0	15,15,17	0.74	0
2	NAG	N	1	1,2	14,14,15	2.05	4 (28%)	17,19,21	1.55	3 (17%)
2	NAG	N	2	2	14,14,15	1.92	4 (28%)	17,19,21	1.23	1 (5%)
2	BMA	N	3	2	11,11,12	0.68	0	15,15,17	0.72	0
4	NAG	O	1	4	14,14,15	1.95	5 (35%)	17,19,21	1.33	2 (11%)
4	NAG	O	2	4	14,14,15	1.99	4 (28%)	17,19,21	1.09	2 (11%)
2	NAG	P	1	1,2	14,14,15	2.03	4 (28%)	17,19,21	1.39	3 (17%)
2	NAG	P	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.41	3 (17%)
2	BMA	P	3	2	11,11,12	0.64	0	15,15,17	0.86	1 (6%)
4	NAG	Q	1	1,4	14,14,15	2.05	4 (28%)	17,19,21	1.21	2 (11%)
4	NAG	Q	2	4	14,14,15	2.07	4 (28%)	17,19,21	1.44	3 (17%)
2	NAG	R	1	1,2	14,14,15	2.07	4 (28%)	17,19,21	1.28	2 (11%)
2	NAG	R	2	2	14,14,15	2.26	5 (35%)	17,19,21	2.22	5 (29%)
2	BMA	R	3	2	11,11,12	0.62	0	15,15,17	0.77	0
2	NAG	S	1	1,2	14,14,15	2.09	4 (28%)	17,19,21	2.04	6 (35%)
2	NAG	S	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.31	2 (11%)
2	BMA	S	3	2	11,11,12	0.55	0	15,15,17	0.75	0
4	NAG	T	1	1,4	14,14,15	1.98	3 (21%)	17,19,21	1.28	1 (5%)
4	NAG	T	2	4	14,14,15	1.97	4 (28%)	17,19,21	1.29	2 (11%)
2	NAG	U	1	1,2	14,14,15	2.05	4 (28%)	17,19,21	1.60	4 (23%)
2	NAG	U	2	2	14,14,15	2.05	4 (28%)	17,19,21	1.26	2 (11%)
2	BMA	U	3	2	11,11,12	0.65	0	15,15,17	0.69	0
2	NAG	V	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	2.14	4 (23%)
2	NAG	V	2	2	14,14,15	1.94	3 (21%)	17,19,21	1.22	2 (11%)
2	BMA	V	3	2	11,11,12	0.72	0	15,15,17	0.69	0
2	NAG	W	1	1,2	14,14,15	1.88	3 (21%)	17,19,21	2.13	7 (41%)
2	NAG	W	2	2	14,14,15	1.92	3 (21%)	17,19,21	1.36	3 (17%)
2	BMA	W	3	2	11,11,12	0.57	0	15,15,17	0.68	0
2	NAG	X	1	1,2	14,14,15	2.00	4 (28%)	17,19,21	1.35	2 (11%)
2	NAG	X	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.47	2 (11%)
2	BMA	X	3	2	11,11,12	0.59	0	15,15,17	0.68	0
7	NAG	Y	1	7	14,14,15	1.97	5 (35%)	17,19,21	1.31	2 (11%)
7	NAG	Y	2	7	14,14,15	2.06	3 (21%)	17,19,21	1.42	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FUC	Y	3	7	10,10,11	0.60	0	14,14,16	0.73	0
6	NAG	Z	1	1,6	14,14,15	1.94	5 (35%)	17,19,21	1.26	2 (11%)
6	NAG	Z	2	6	14,14,15	1.95	3 (21%)	17,19,21	1.00	1 (5%)
6	BMA	Z	3	6	11,11,12	0.53	0	15,15,17	0.86	0
6	MAN	Z	4	6	11,11,12	0.59	0	15,15,17	0.99	2 (13%)
8	NAG	a	1	8,1	14,14,15	2.04	5 (35%)	17,19,21	1.16	2 (11%)
8	NAG	a	2	8	14,14,15	2.15	4 (28%)	17,19,21	1.62	4 (23%)
8	BMA	a	3	8	11,11,12	0.58	0	15,15,17	0.71	0
8	MAN	a	4	8	11,11,12	0.76	0	15,15,17	1.41	3 (20%)
8	MAN	a	5	8	11,11,12	0.64	0	15,15,17	1.32	1 (6%)
2	NAG	b	1	2	14,14,15	2.04	5 (35%)	17,19,21	1.40	3 (17%)
2	NAG	b	2	2	14,14,15	2.08	4 (28%)	17,19,21	1.20	2 (11%)
2	BMA	b	3	2	11,11,12	0.63	0	15,15,17	0.68	0
9	NAG	c	1	1,9	14,14,15	1.83	5 (35%)	17,19,21	2.29	6 (35%)
9	NAG	c	2	9	14,14,15	1.90	3 (21%)	17,19,21	2.06	4 (23%)
9	BMA	c	3	9	11,11,12	0.82	0	15,15,17	0.81	0
9	MAN	c	4	9	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
8	NAG	d	1	8	14,14,15	2.02	4 (28%)	17,19,21	1.46	2 (11%)
8	NAG	d	2	8	14,14,15	1.94	3 (21%)	17,19,21	1.20	2 (11%)
8	BMA	d	3	8	11,11,12	0.81	0	15,15,17	0.79	0
8	MAN	d	4	8	11,11,12	0.75	0	15,15,17	1.18	2 (13%)
8	MAN	d	5	8	11,11,12	0.67	0	15,15,17	0.84	1 (6%)
4	NAG	e	1	1,4	14,14,15	1.94	4 (28%)	17,19,21	1.29	2 (11%)
4	NAG	e	2	4	14,14,15	2.00	4 (28%)	17,19,21	1.08	1 (5%)
4	NAG	f	1	1,4	14,14,15	2.08	5 (35%)	17,19,21	1.25	2 (11%)
4	NAG	f	2	4	14,14,15	2.06	4 (28%)	17,19,21	1.32	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
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	0/2/19/22	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	BMA	S	3	2	-	0/2/19/22	0/1/1/1
4	NAG	T	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	BMA	U	3	2	-	0/2/19/22	0/1/1/1
2	NAG	V	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	BMA	V	3	2	-	0/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	BMA	W	3	2	-	0/2/19/22	0/1/1/1
2	NAG	X	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	X	2	2	-	5/6/23/26	0/1/1/1
2	BMA	X	3	2	-	0/2/19/22	0/1/1/1
7	NAG	Y	1	7	-	0/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	0/6/23/26	0/1/1/1
7	FUC	Y	3	7	-	-	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	6/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	1/1/1/1
8	MAN	a	4	8	-	0/2/19/22	0/1/1/1
8	MAN	a	5	8	-	1/2/19/22	1/1/1/1
2	NAG	b	1	2	-	1/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	BMA	b	3	2	-	2/2/19/22	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	1/6/23/26	0/1/1/1
9	BMA	c	3	9	-	2/2/19/22	0/1/1/1
9	MAN	c	4	9	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	d	1	8	-	5/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	BMA	d	3	8	-	2/2/19/22	0/1/1/1
8	MAN	d	4	8	-	1/2/19/22	0/1/1/1
8	MAN	d	5	8	-	0/2/19/22	0/1/1/1
4	NAG	e	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	5.60	1.53	1.43
2	R	2	NAG	O5-C1	5.34	1.52	1.43
3	F	2	NAG	O5-C1	4.86	1.51	1.43
2	S	1	NAG	O5-C1	4.73	1.51	1.43
3	F	1	NAG	C7-N2	4.71	1.49	1.34

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	4	MAN	C1-O5-C5	8.12	123.07	112.19
4	G	1	NAG	C1-O5-C5	6.81	121.31	112.19
2	V	1	NAG	C1-O5-C5	-6.64	103.28	112.19
3	F	1	NAG	C1-O5-C5	-6.36	103.67	112.19
2	R	2	NAG	C1-O5-C5	5.69	119.81	112.19

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7
2	V	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	e	1	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	a	3	BMA	C1-C2-C3-C4-C5-O5
8	a	5	MAN	C1-C2-C3-C4-C5-O5

56 monomers are involved in 118 short contacts:

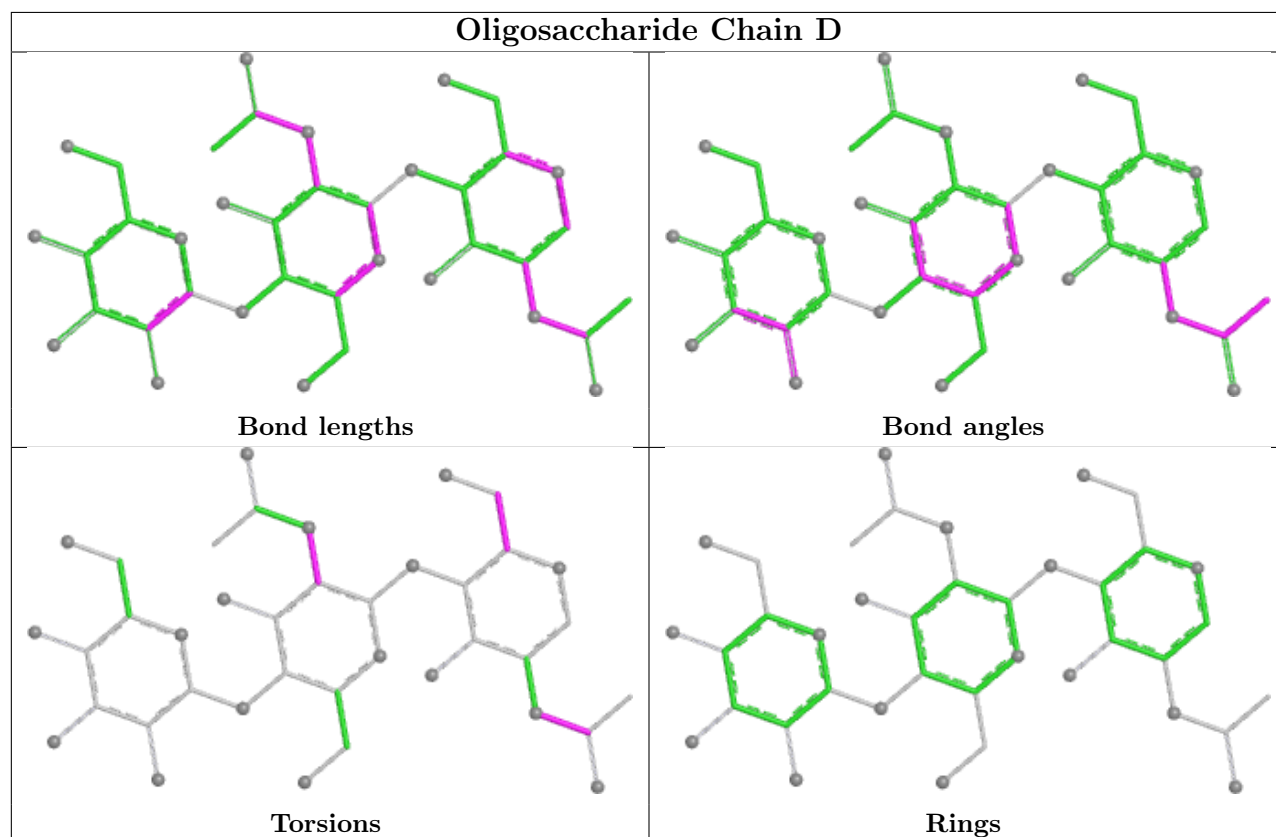
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	G	1	NAG	3	0
2	V	1	NAG	1	0
8	d	1	NAG	1	0
3	F	4	MAN	8	0
2	N	1	NAG	5	0
2	U	3	BMA	1	0
2	D	3	BMA	6	0
3	E	2	NAG	5	0
8	a	3	BMA	1	0
8	a	1	NAG	1	0
4	K	1	NAG	3	0
2	U	2	NAG	1	0
2	L	2	NAG	1	0
3	E	1	NAG	7	0
2	b	2	NAG	3	0
4	T	1	NAG	1	0
2	U	1	NAG	1	0
5	H	1	NAG	2	0
9	c	1	NAG	12	0
6	J	4	MAN	2	0
2	D	1	NAG	5	0
2	N	3	BMA	1	0
3	E	3	BMA	6	0
3	F	1	NAG	19	0
2	S	1	NAG	1	0
8	a	5	MAN	1	0
3	F	3	BMA	5	0
8	a	4	MAN	1	0
2	R	1	NAG	3	0
6	J	2	NAG	2	0
8	a	2	NAG	2	0
2	D	2	NAG	11	0
4	O	2	NAG	1	0
2	M	1	NAG	3	0
2	W	3	BMA	1	0
4	O	1	NAG	1	0
7	Y	1	NAG	2	0

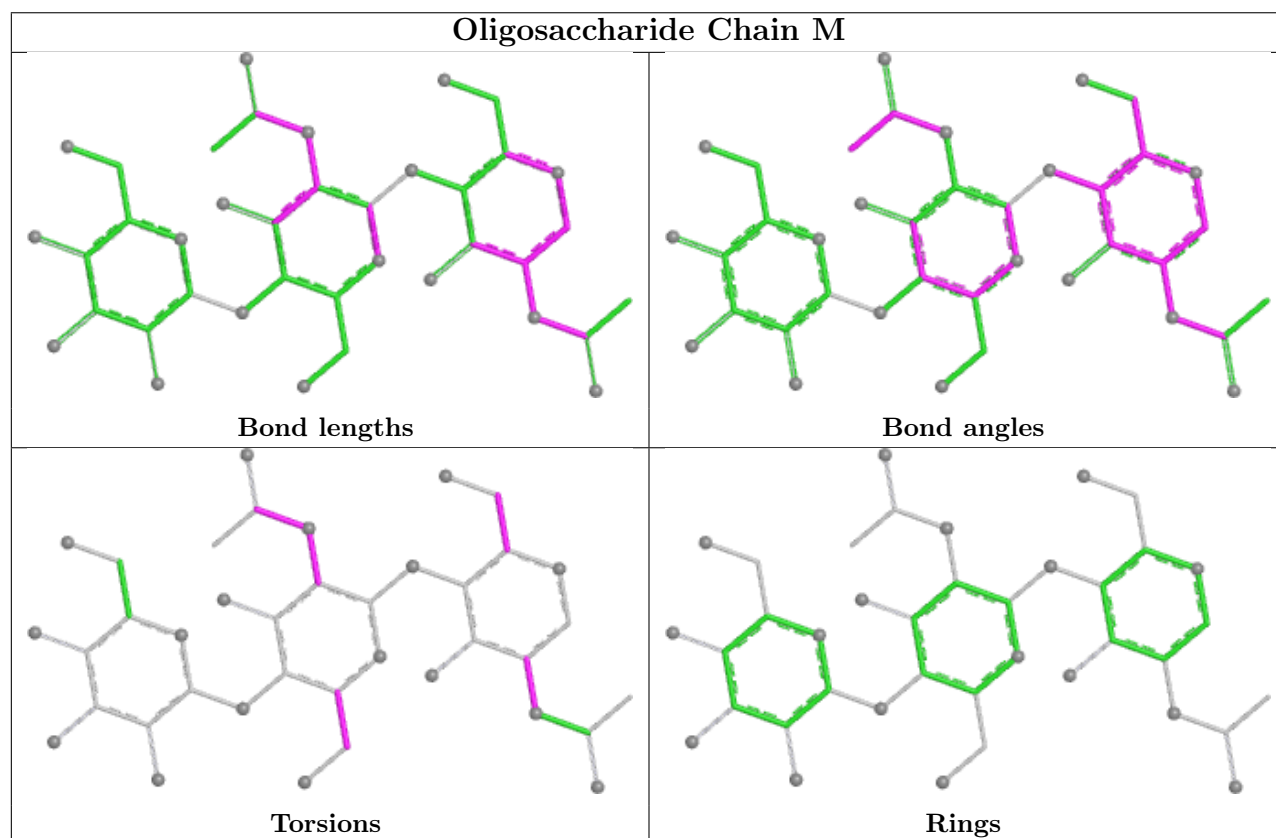
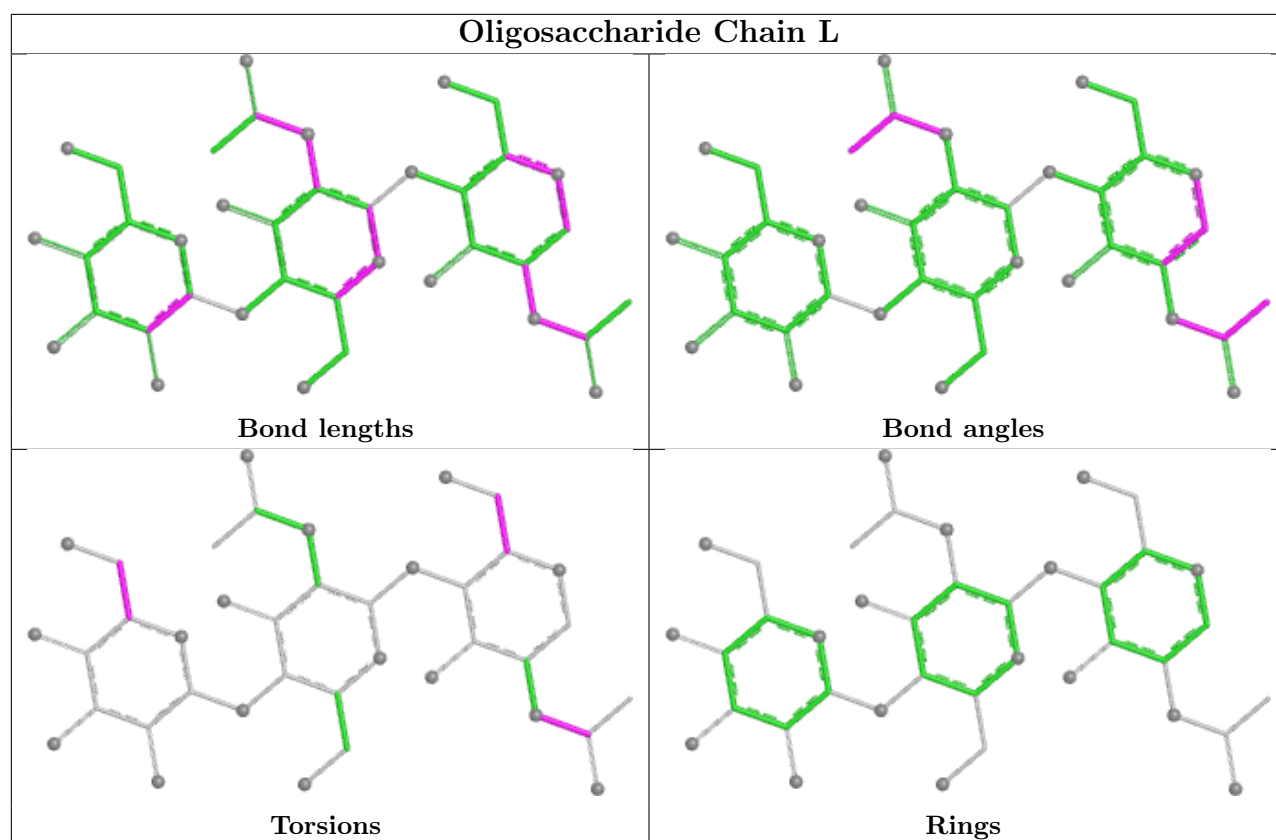
Continued on next page...

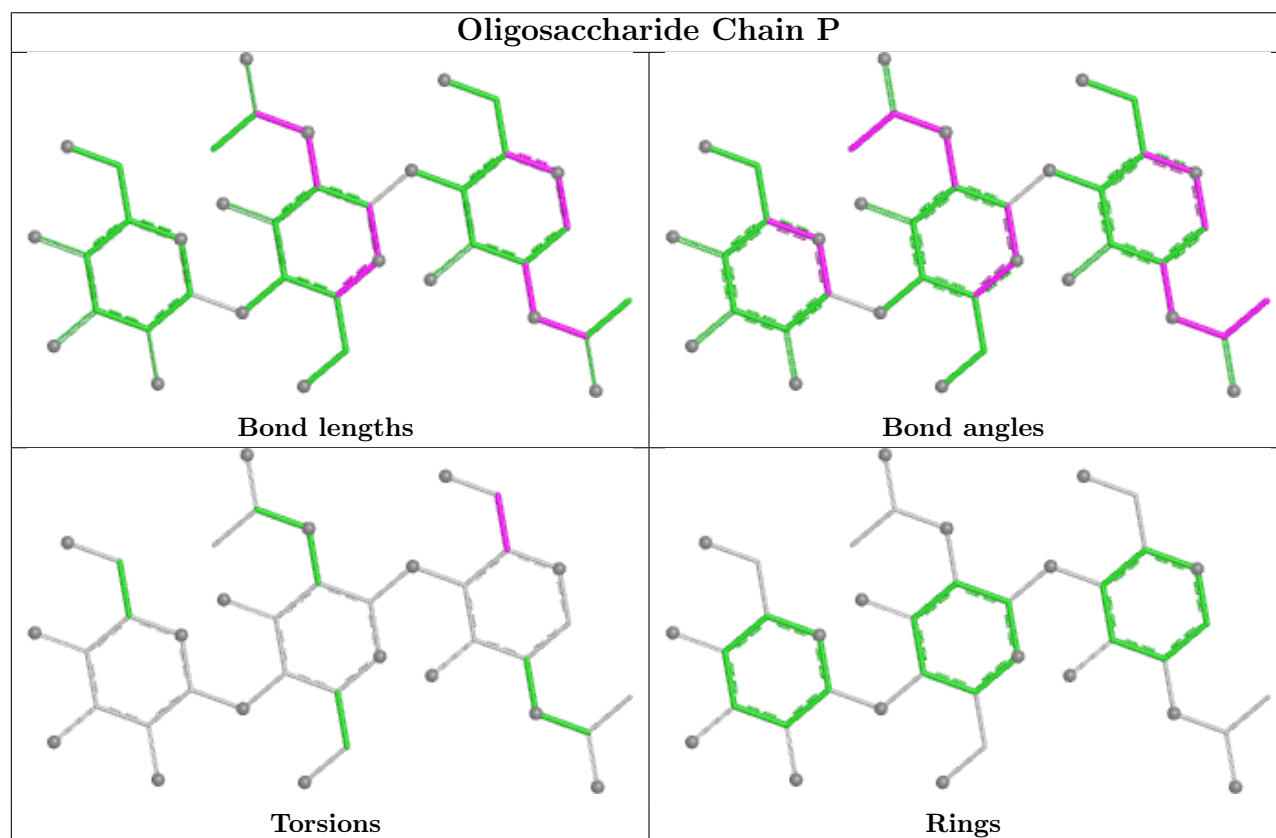
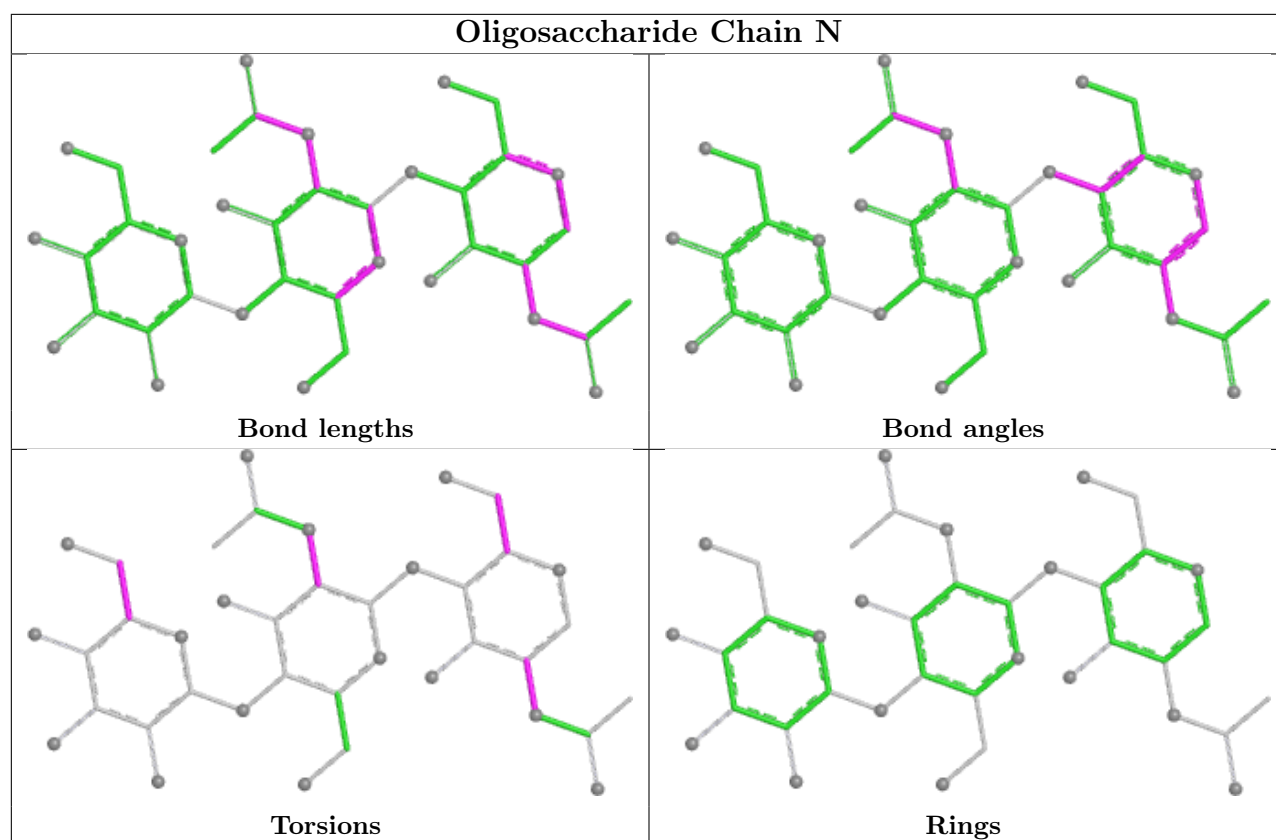
Continued from previous page...

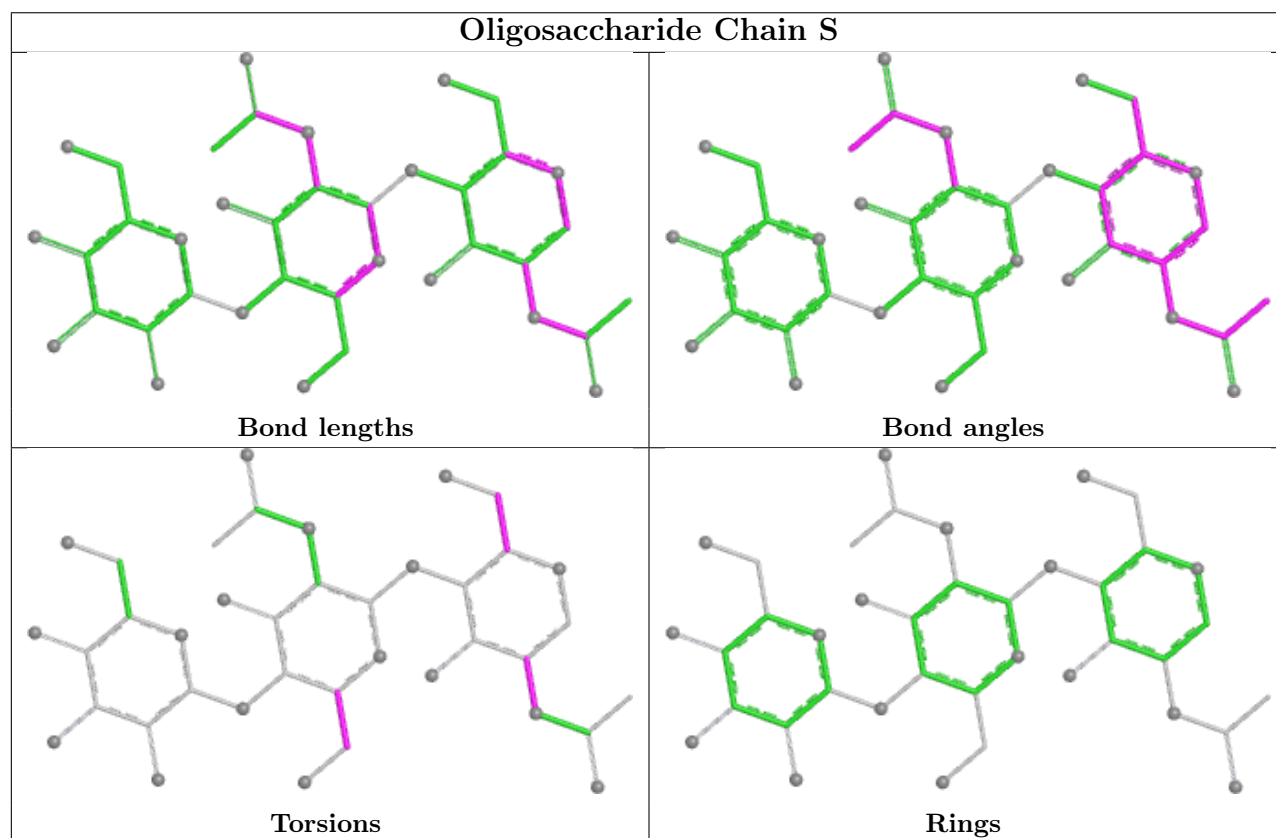
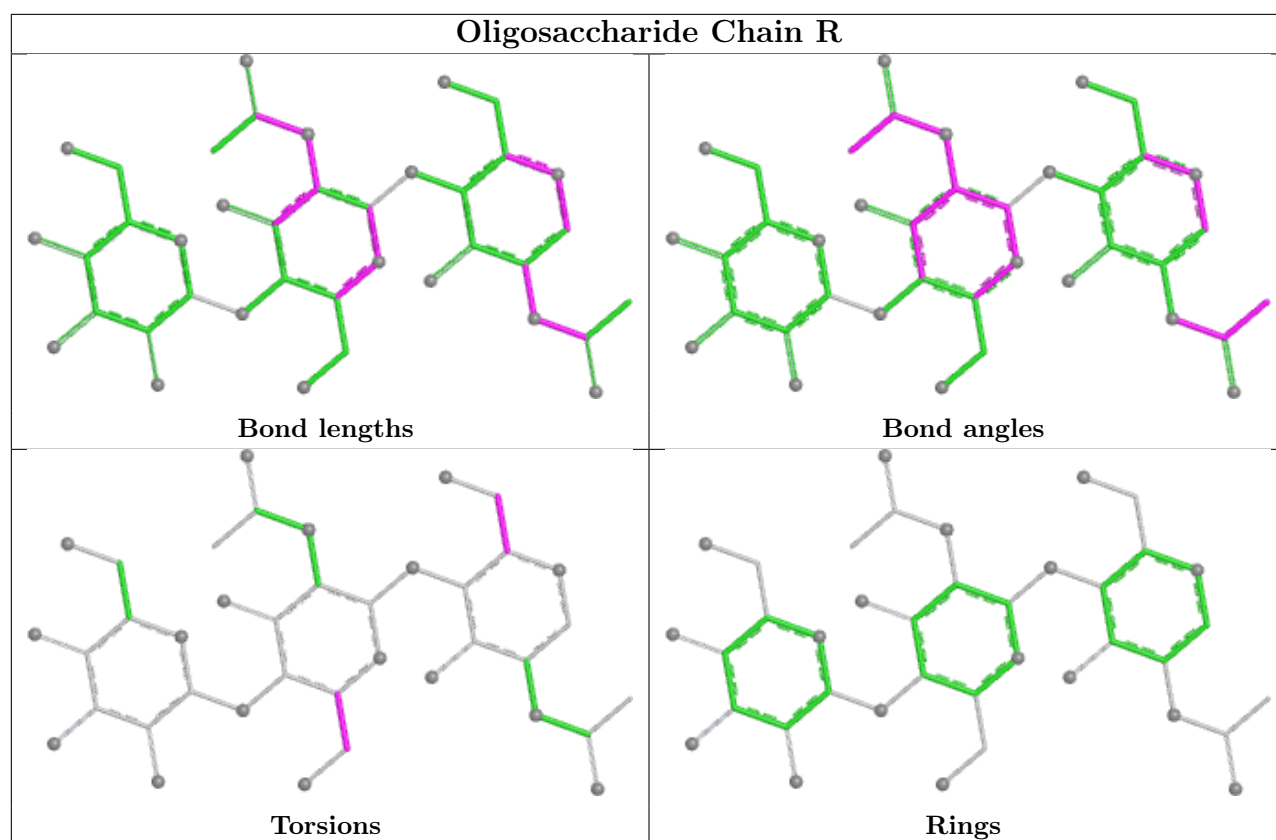
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
7	Y	2	NAG	2	0
2	b	1	NAG	2	0
5	H	2	NAG	2	0
9	c	2	NAG	3	0
2	N	2	NAG	2	0
2	W	2	NAG	1	0
2	L	1	NAG	1	0
4	I	2	NAG	1	0
4	e	1	NAG	1	0
2	R	2	NAG	1	0
3	E	4	MAN	6	0
7	Y	3	FUC	2	0
3	F	2	NAG	14	0
2	R	3	BMA	1	0
6	J	3	BMA	2	0
6	J	1	NAG	2	0
2	S	2	NAG	1	0

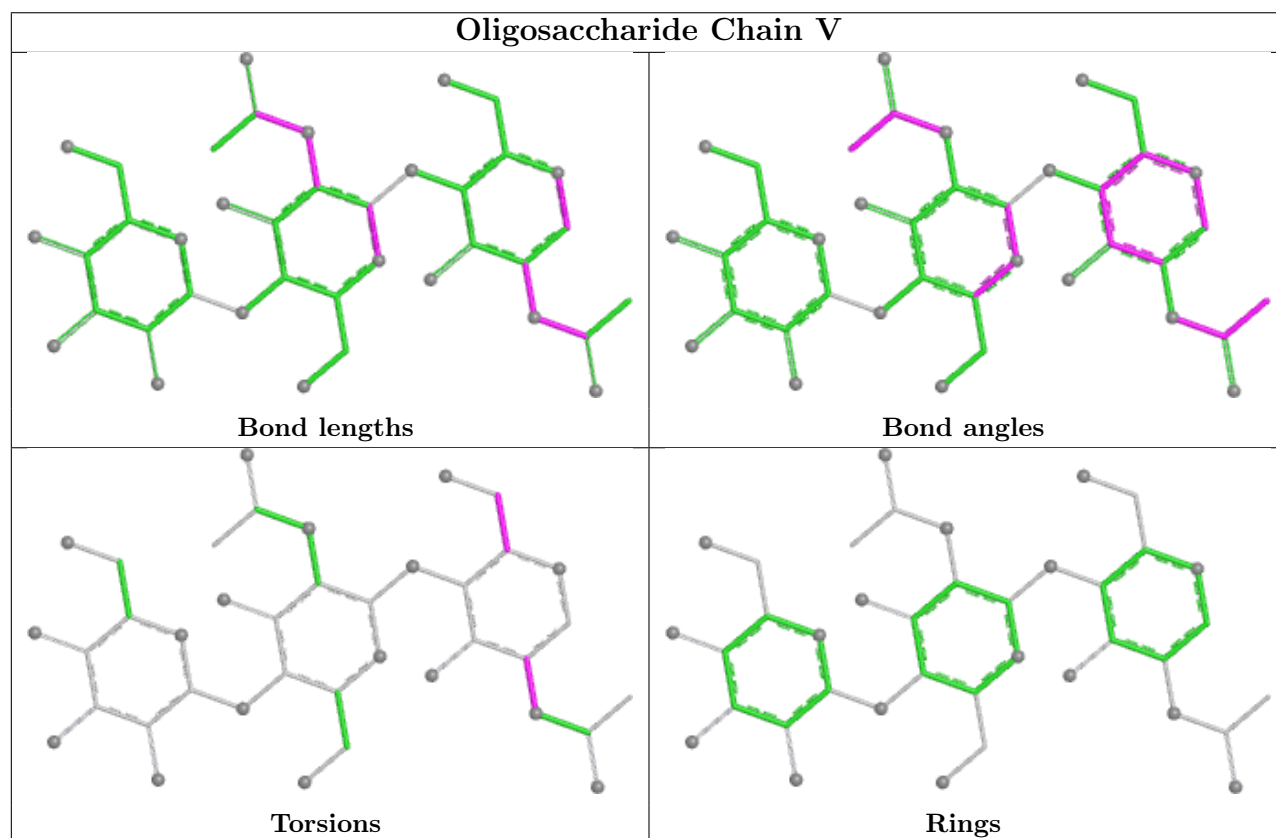
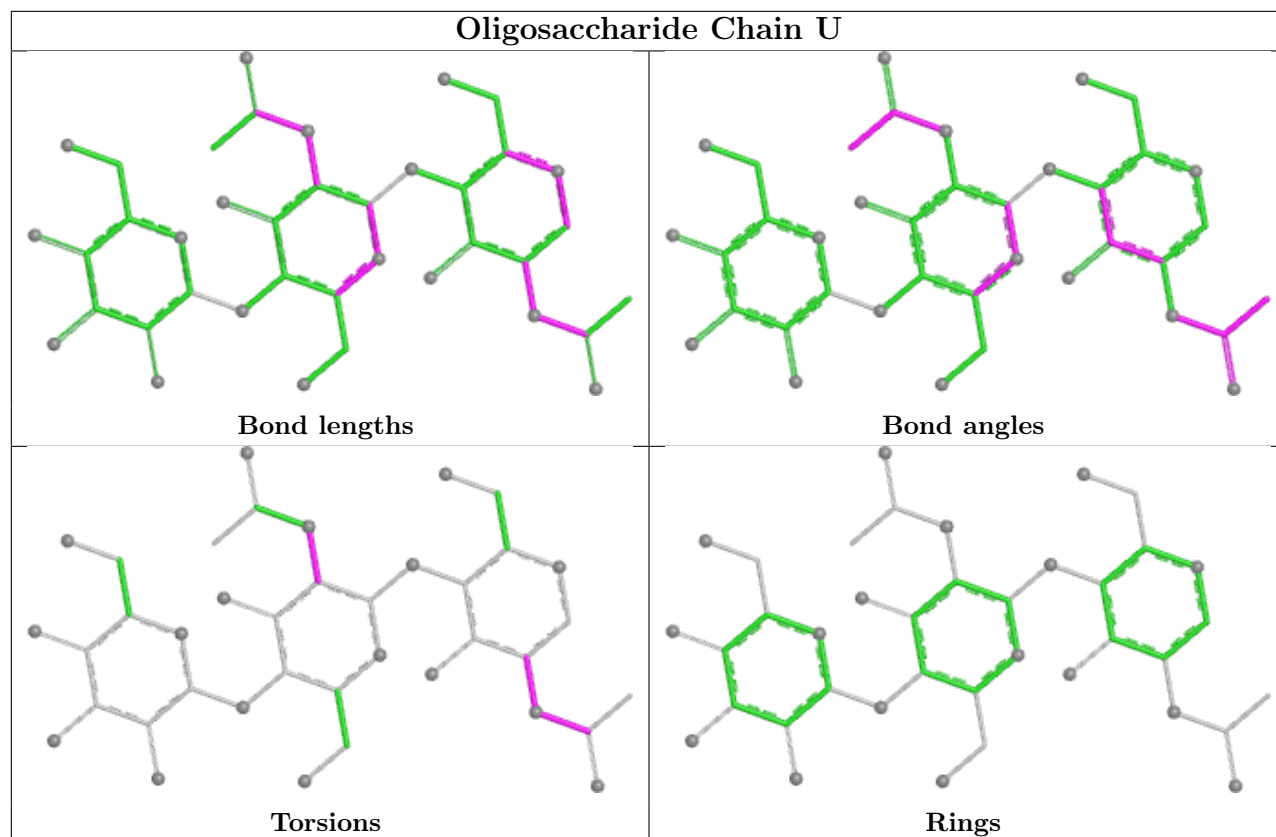
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

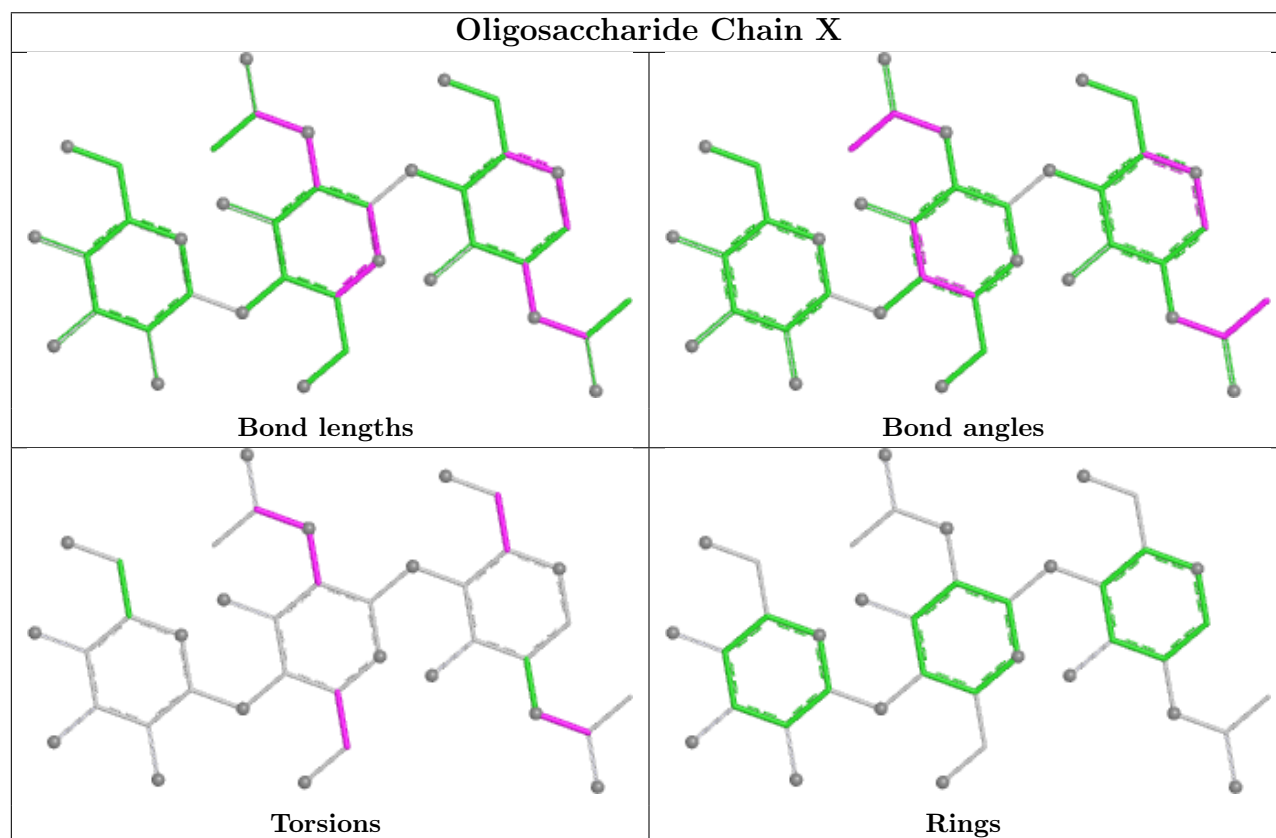
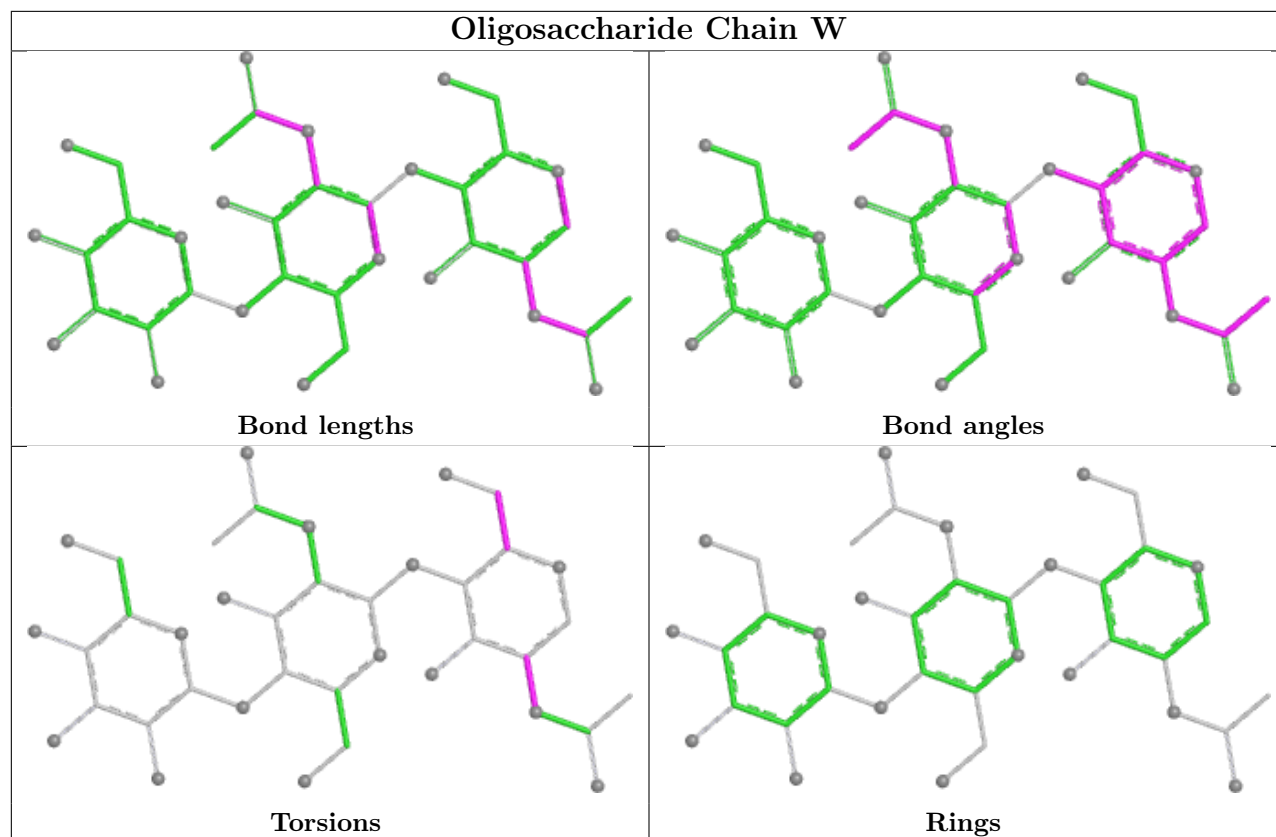


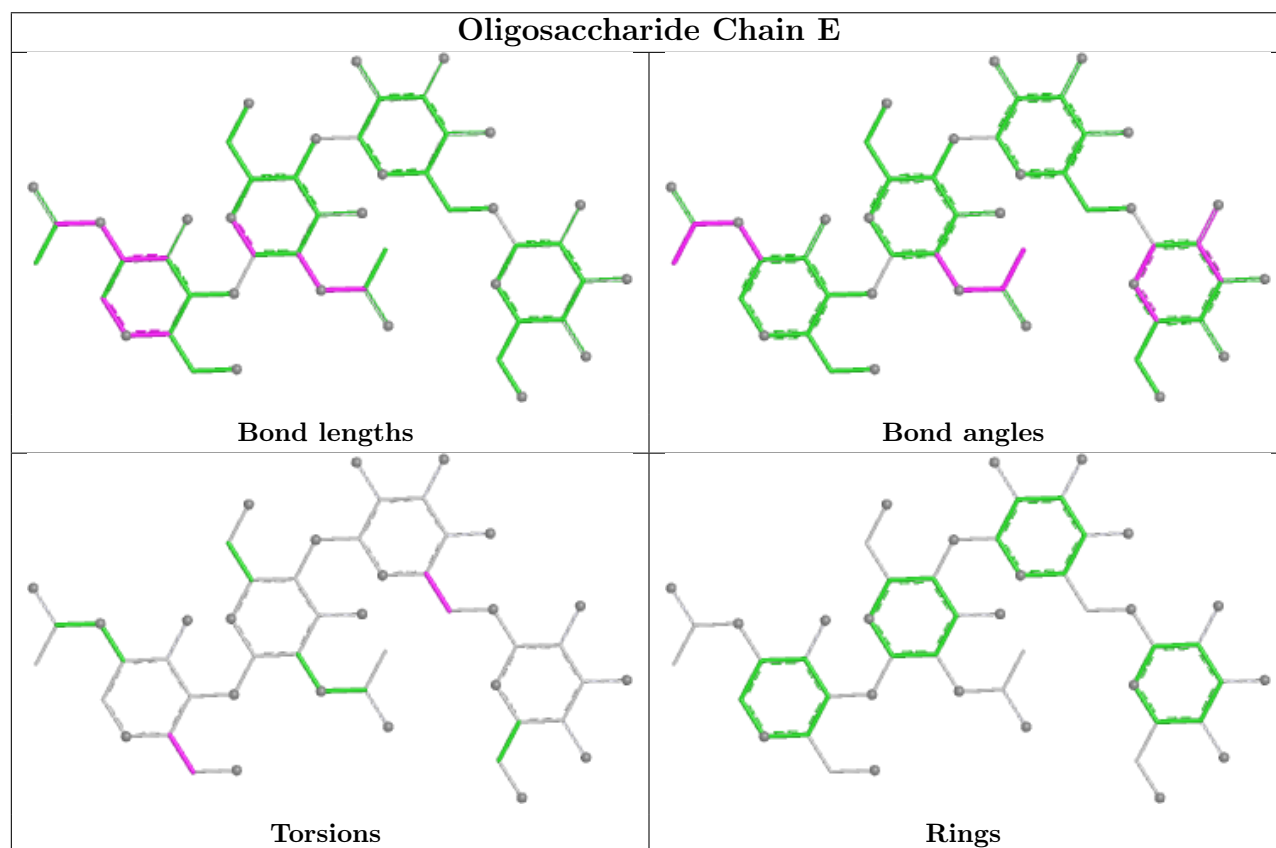
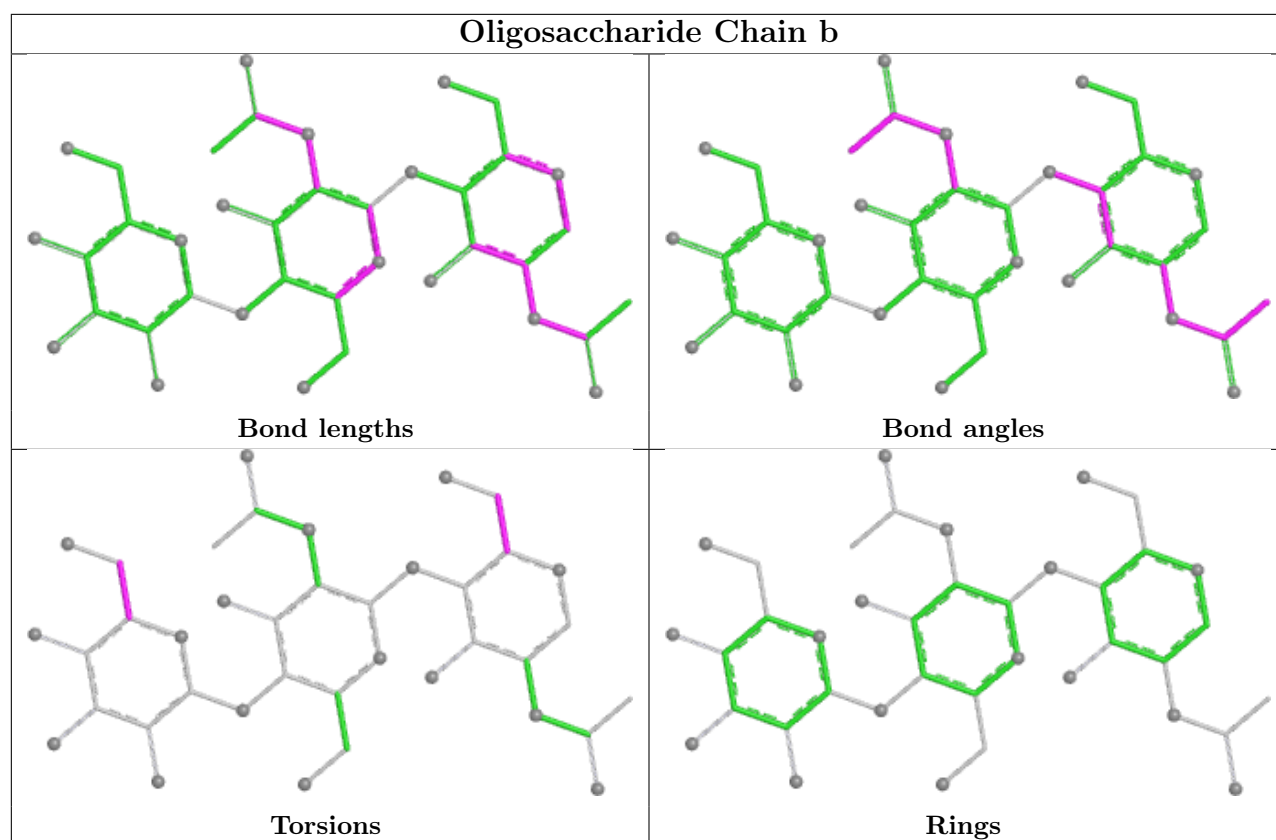


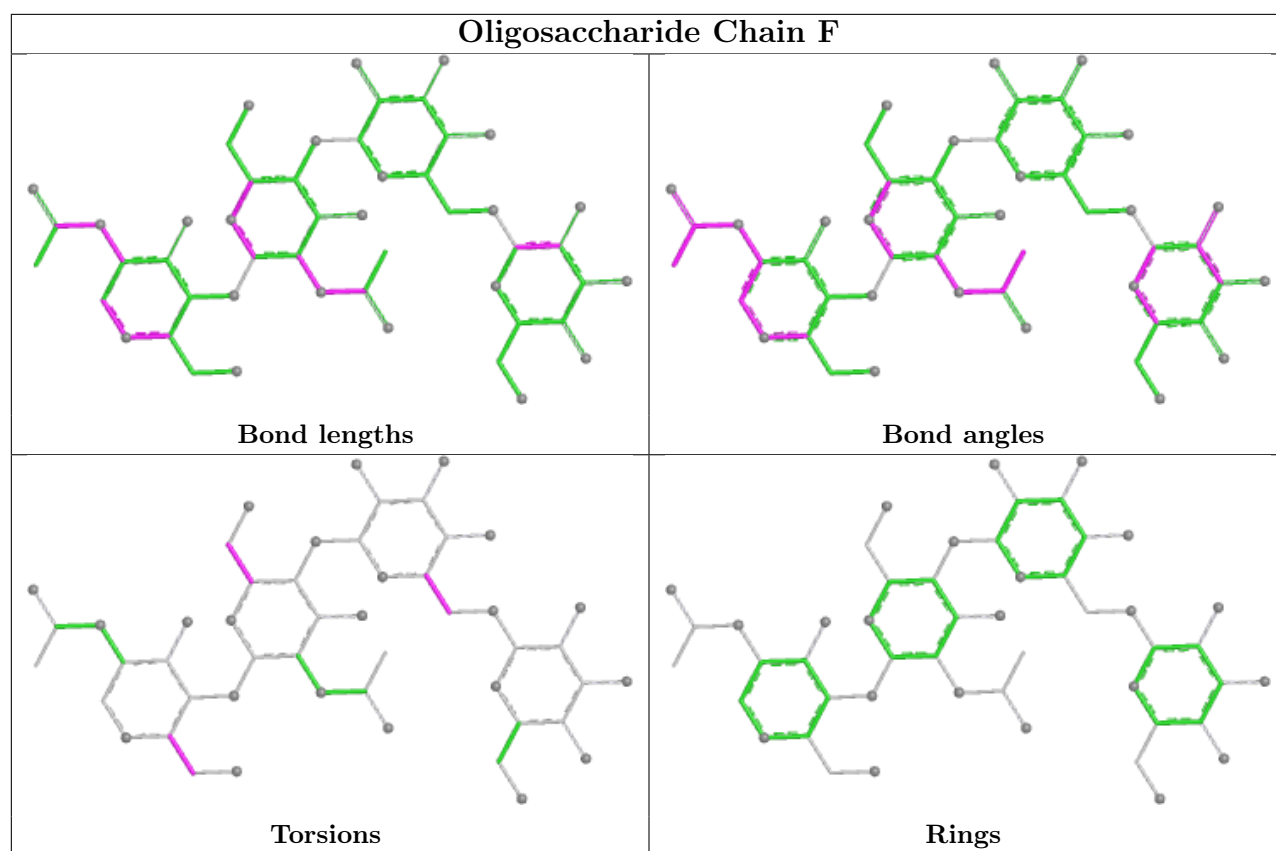


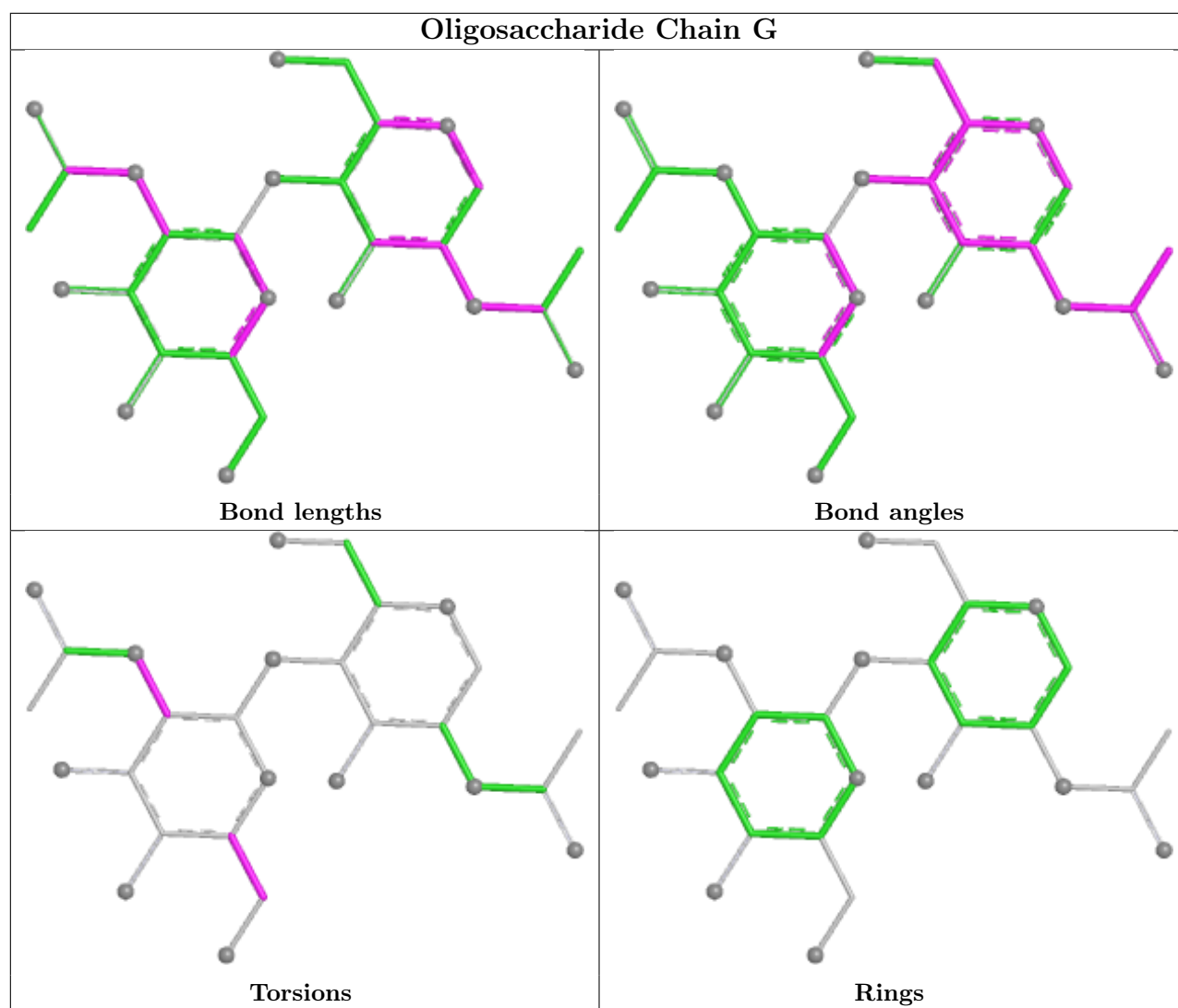


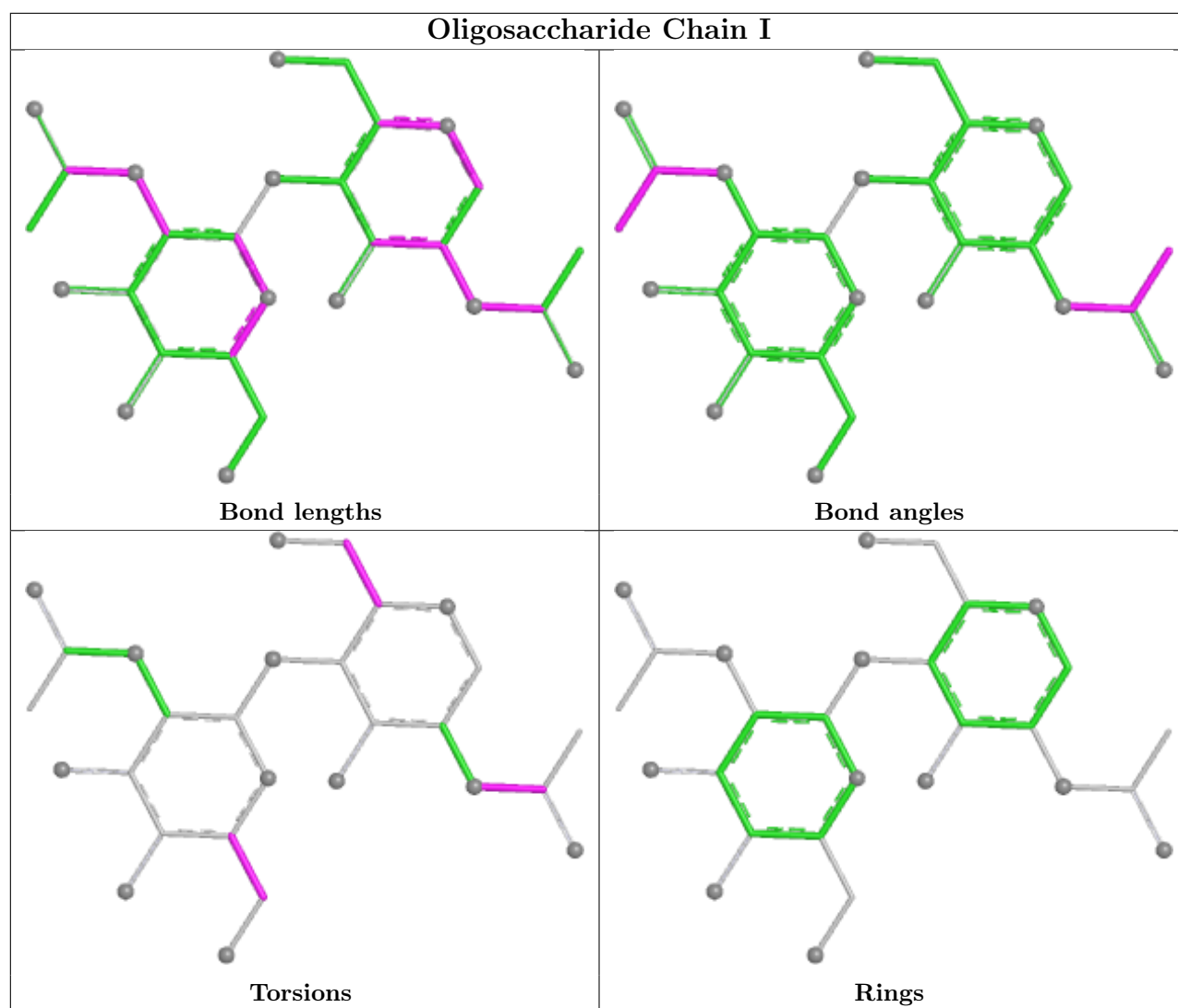


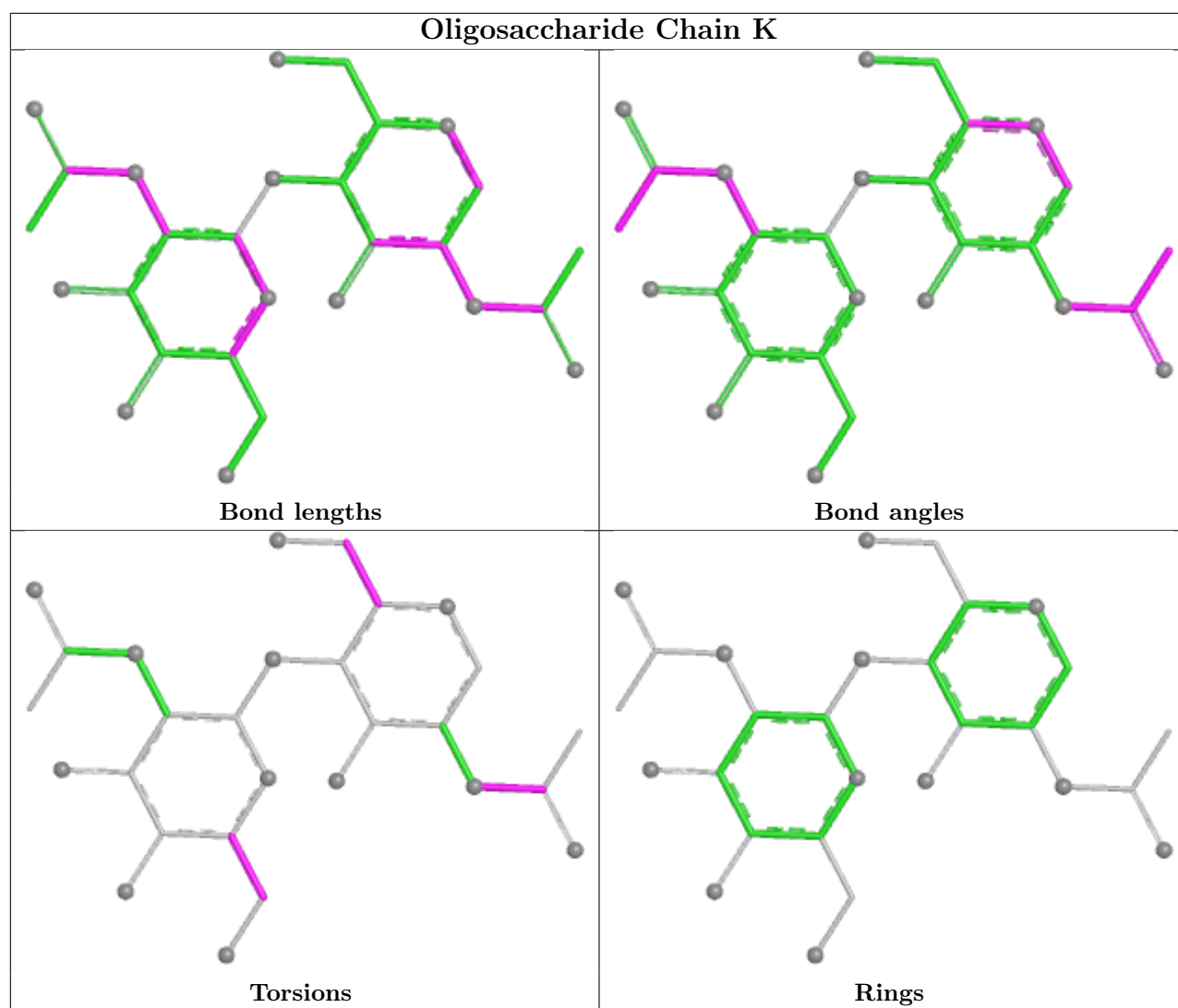


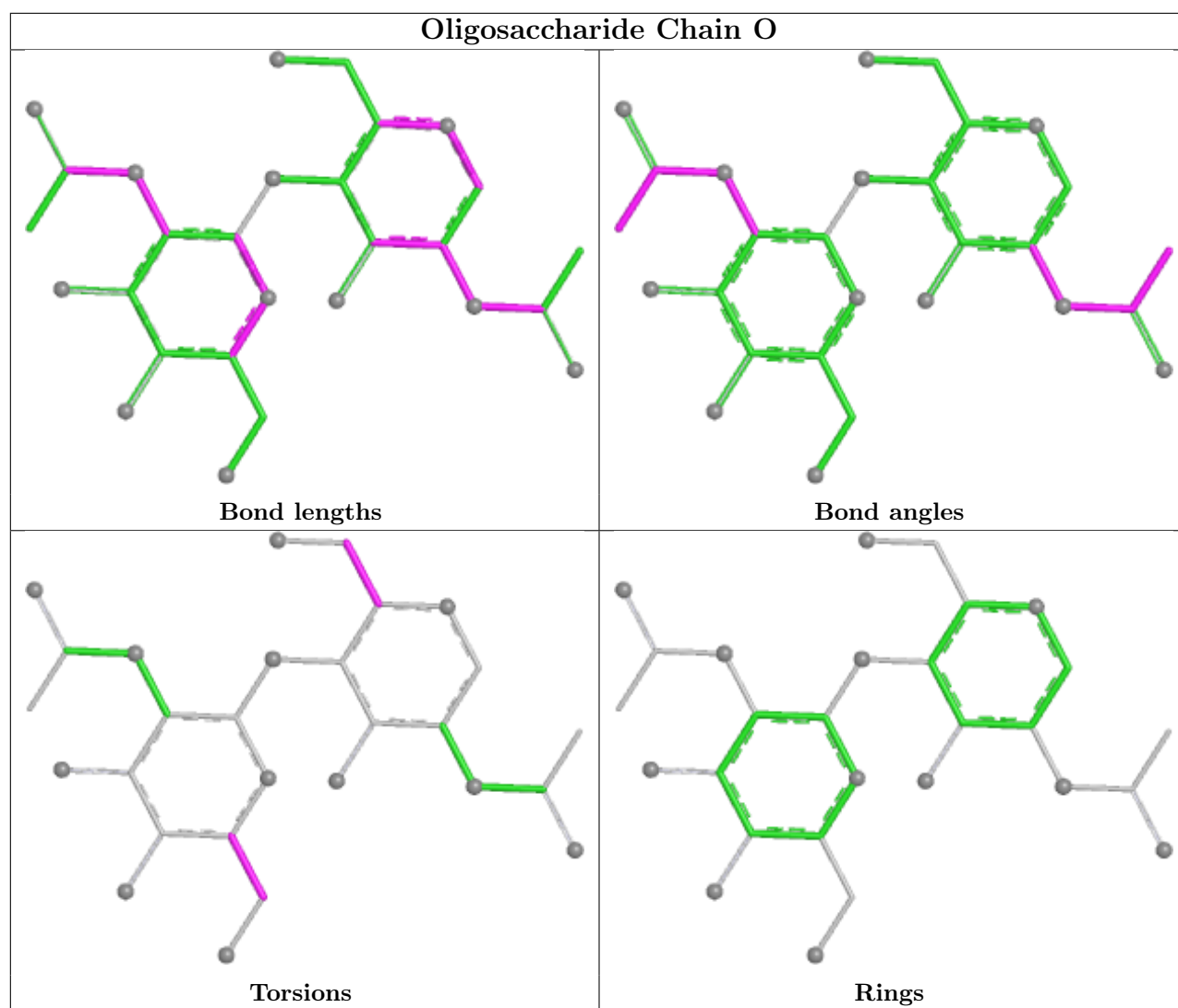


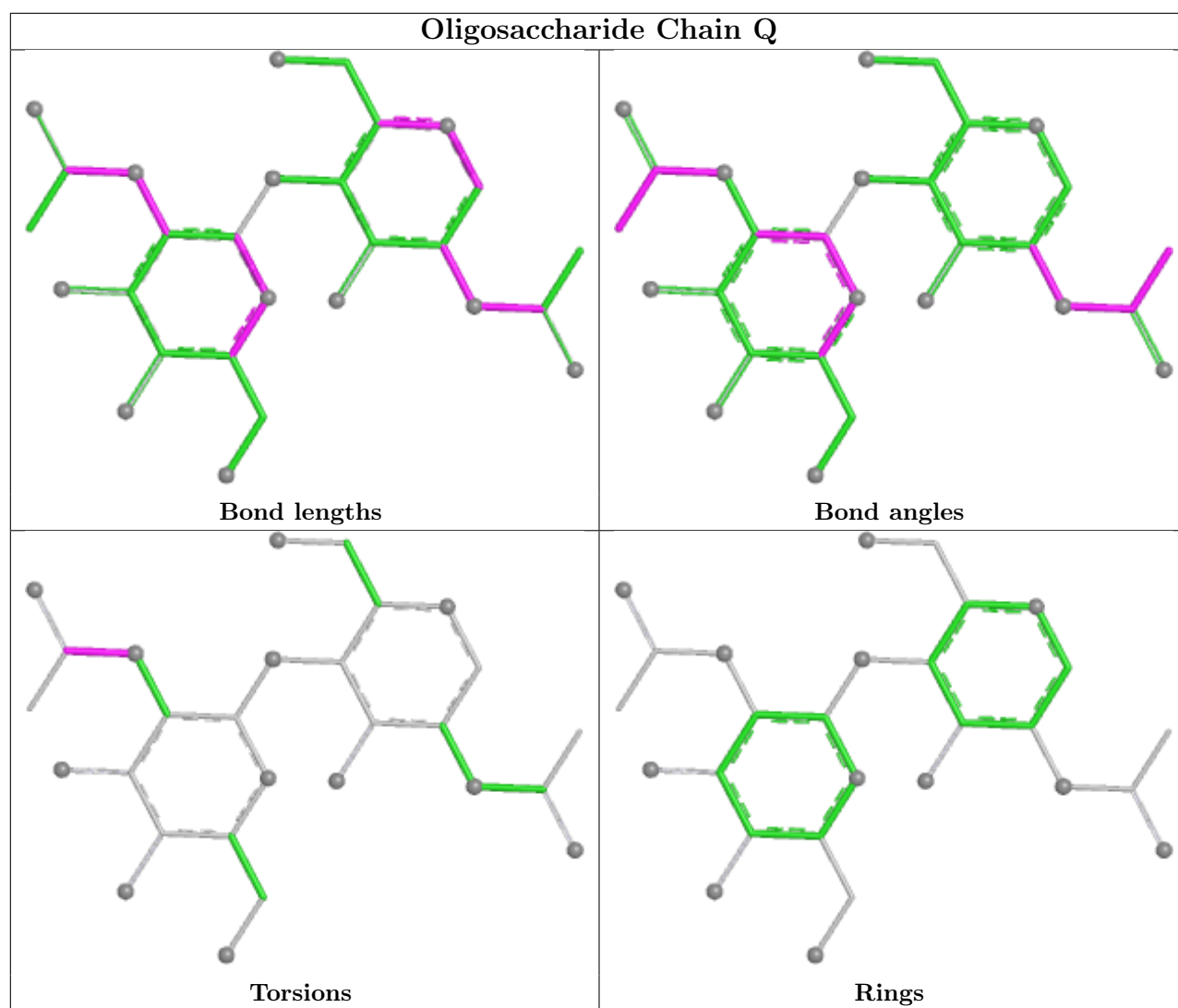


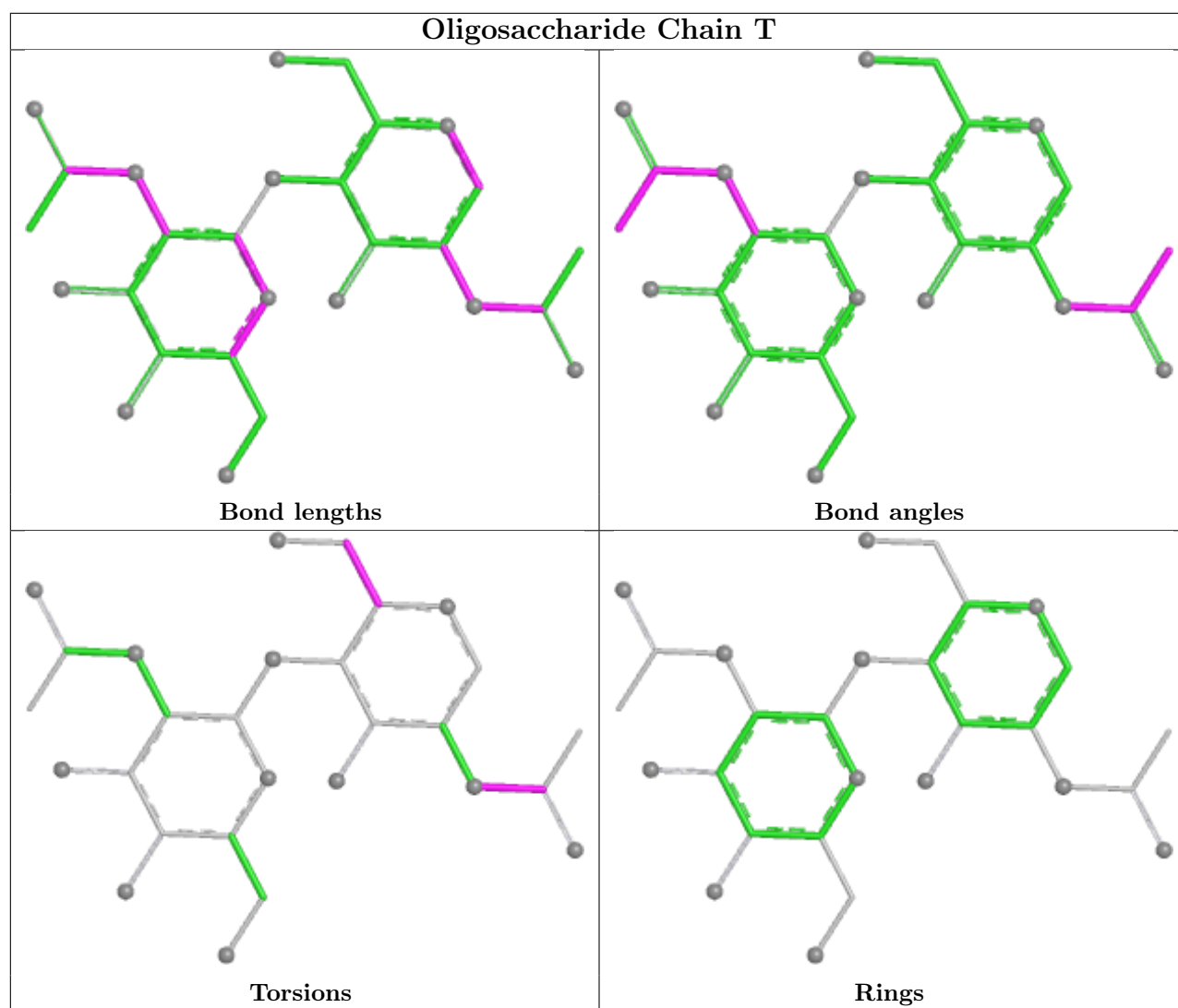


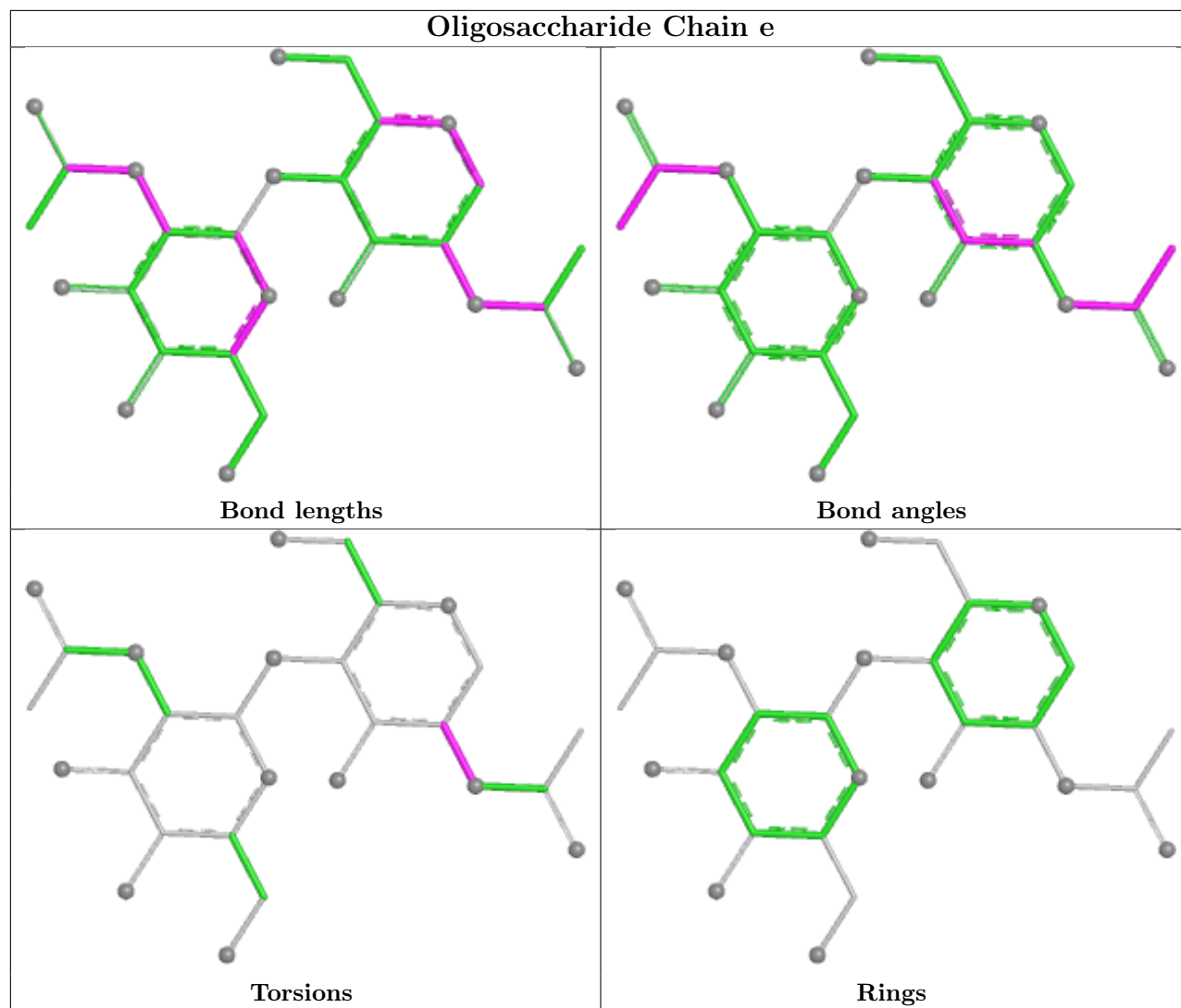


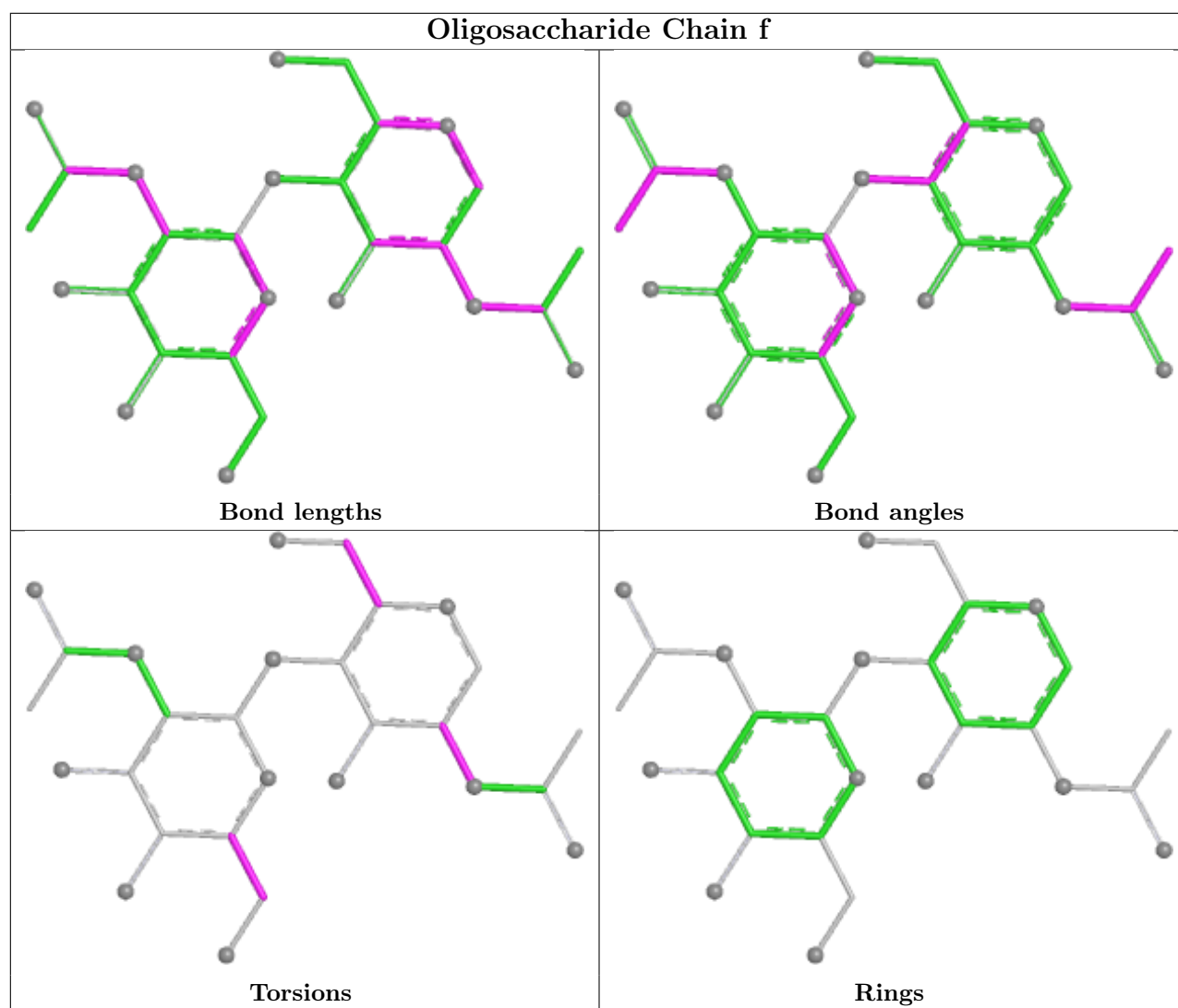


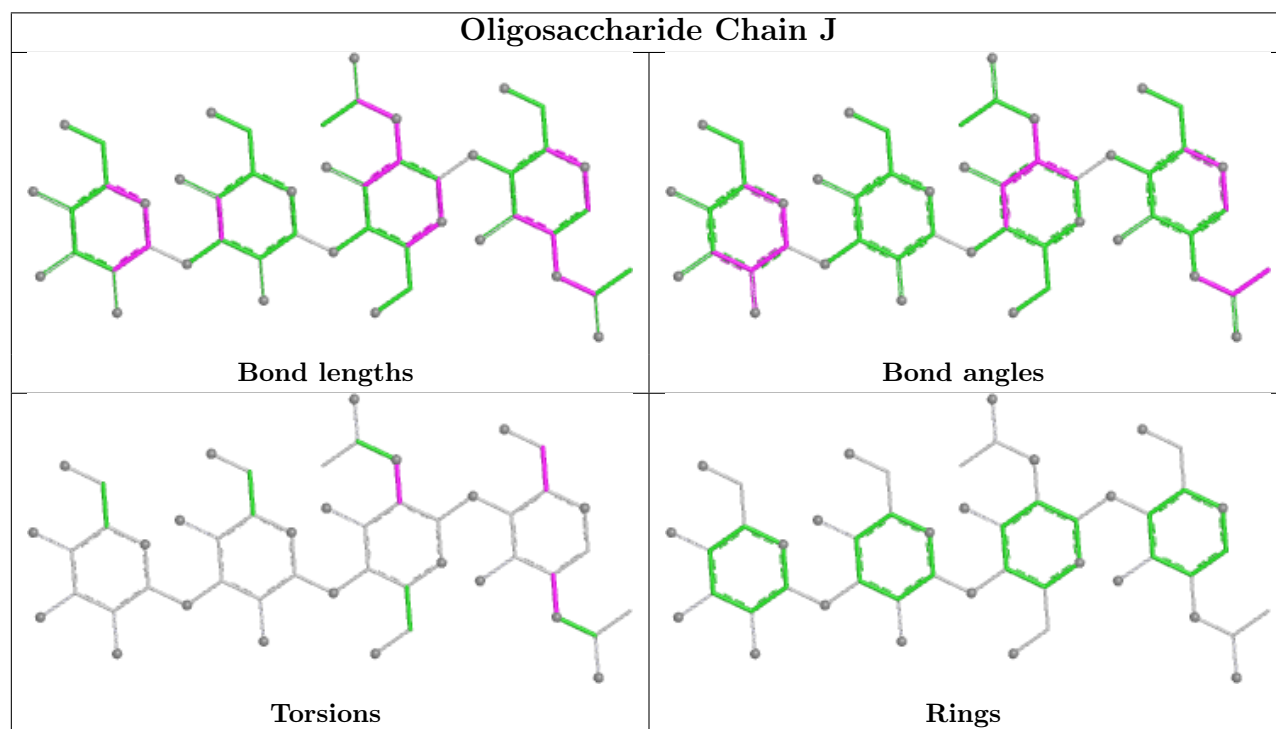
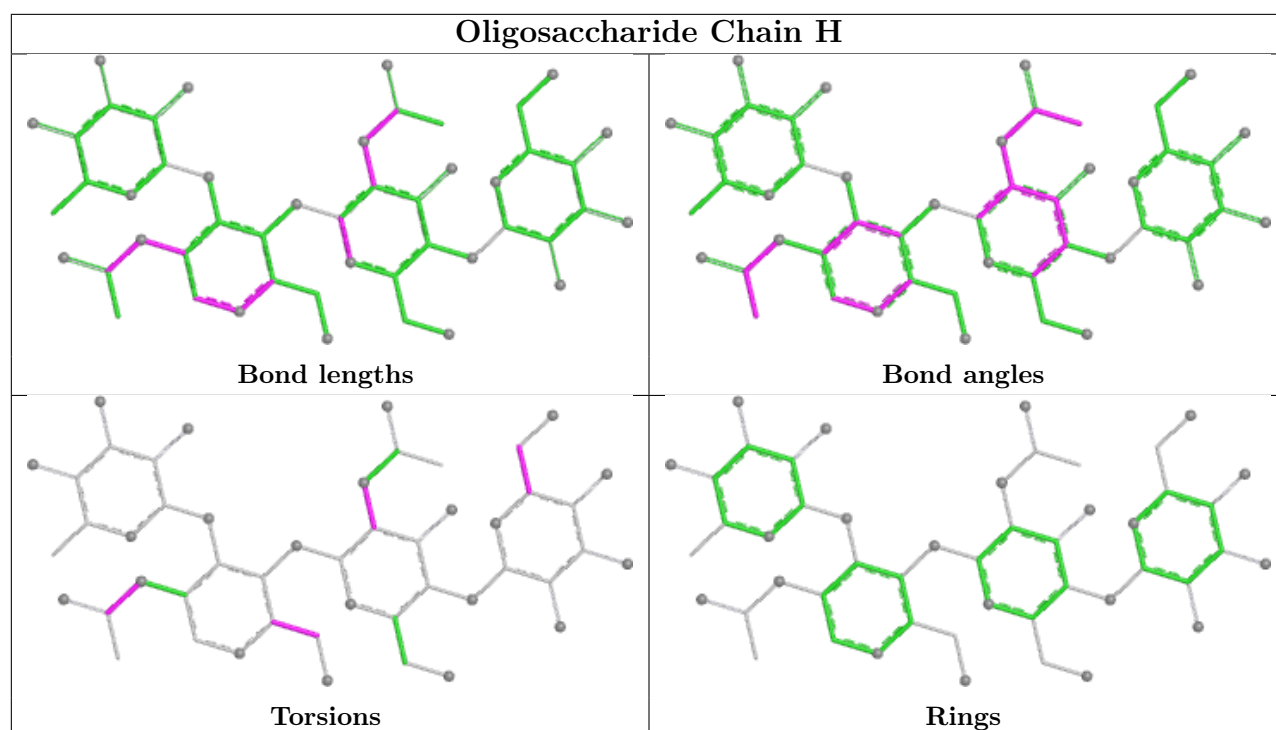


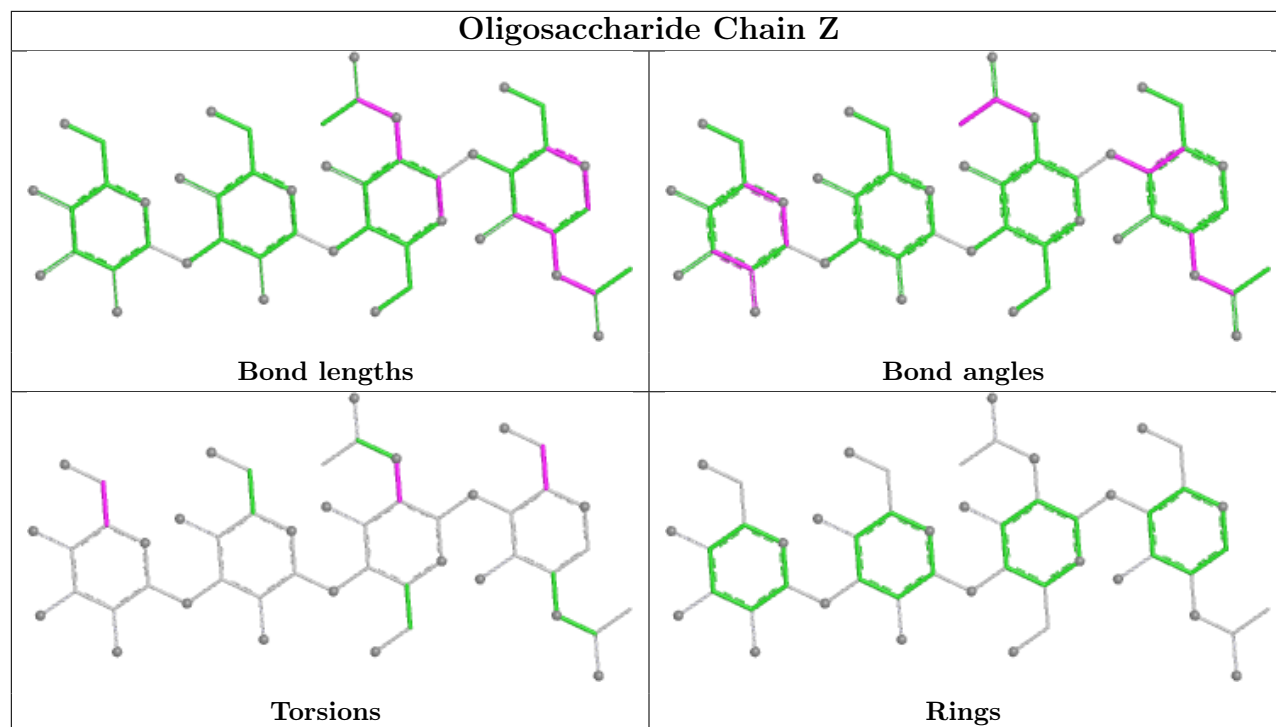


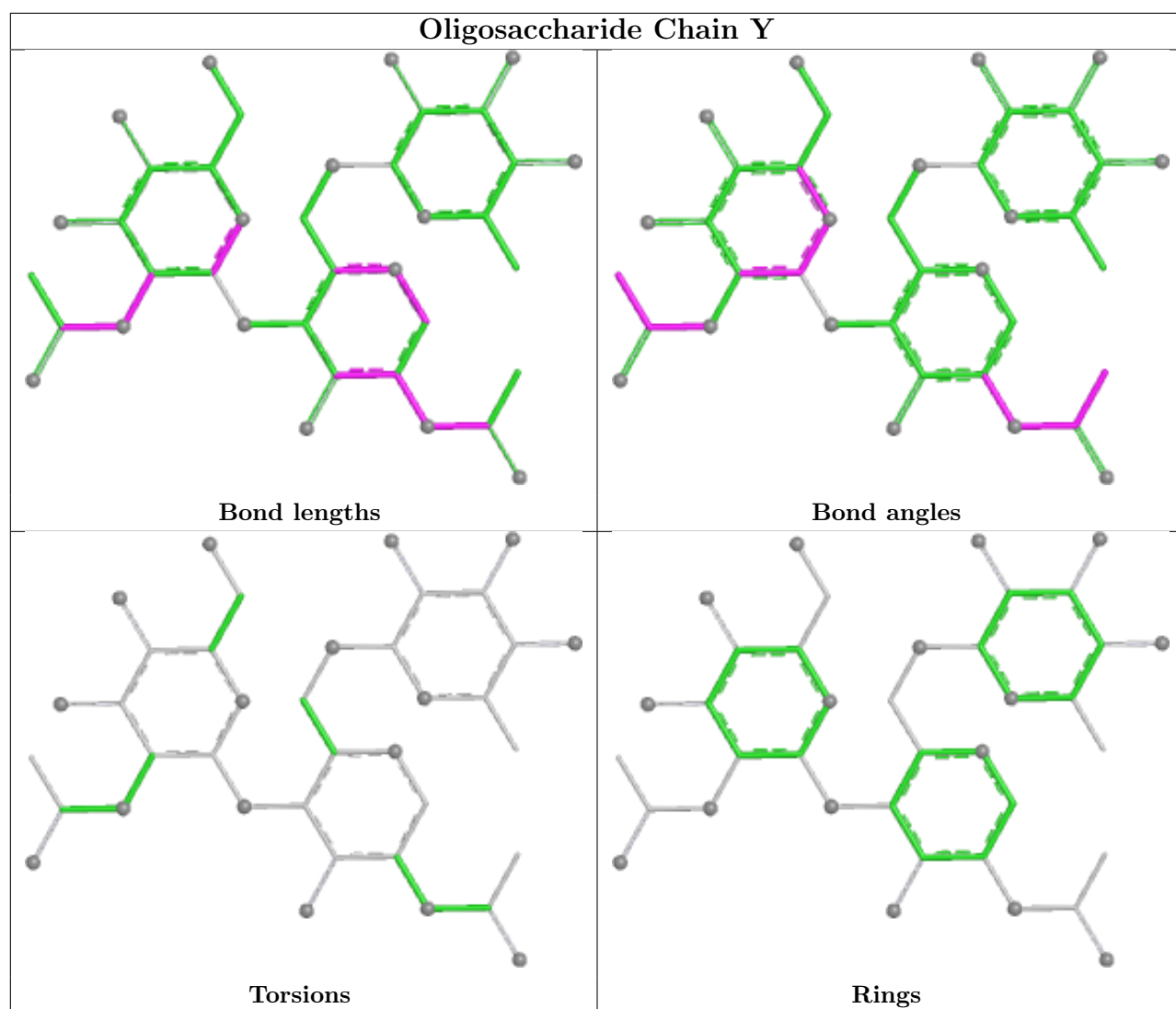


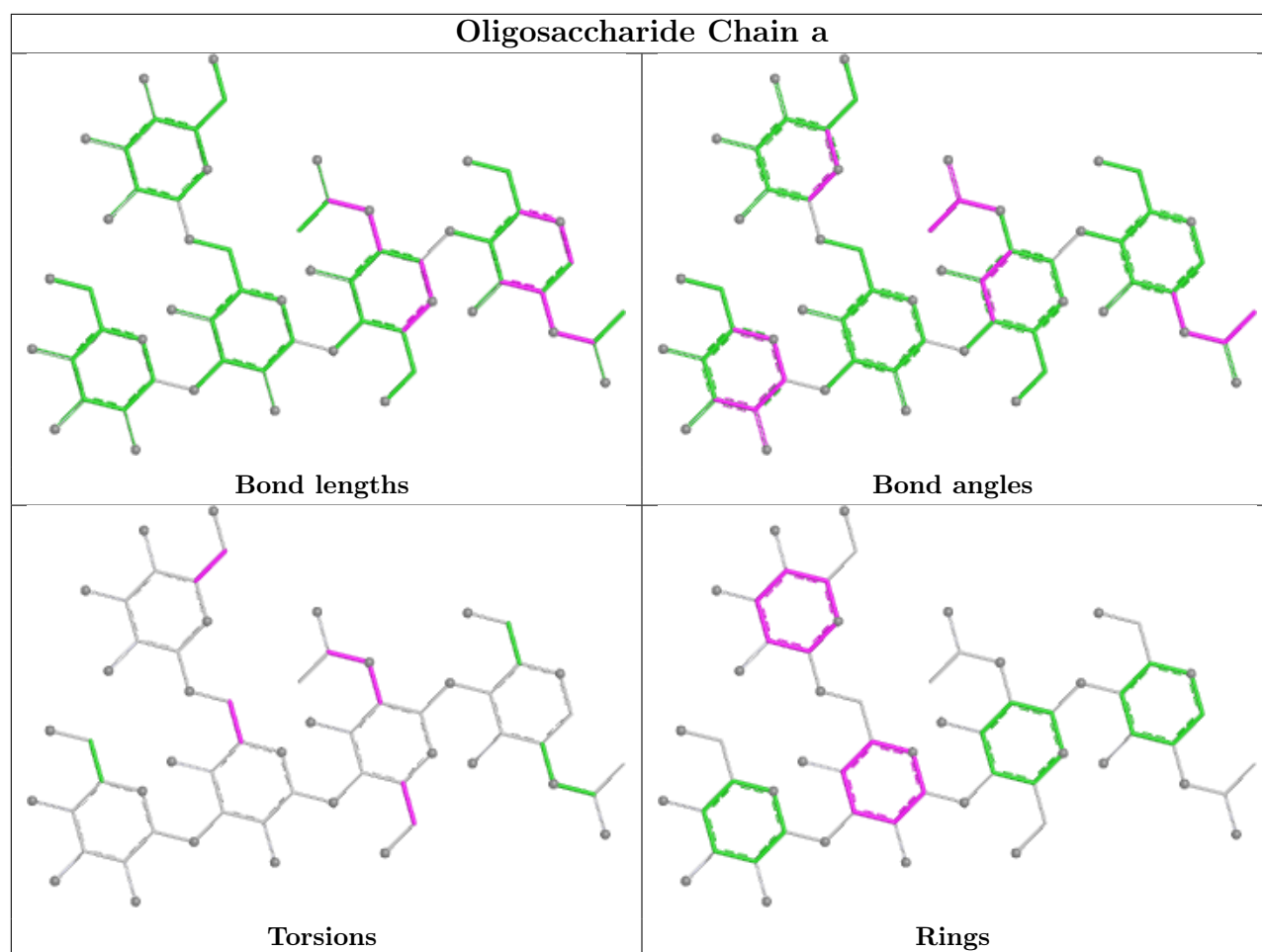


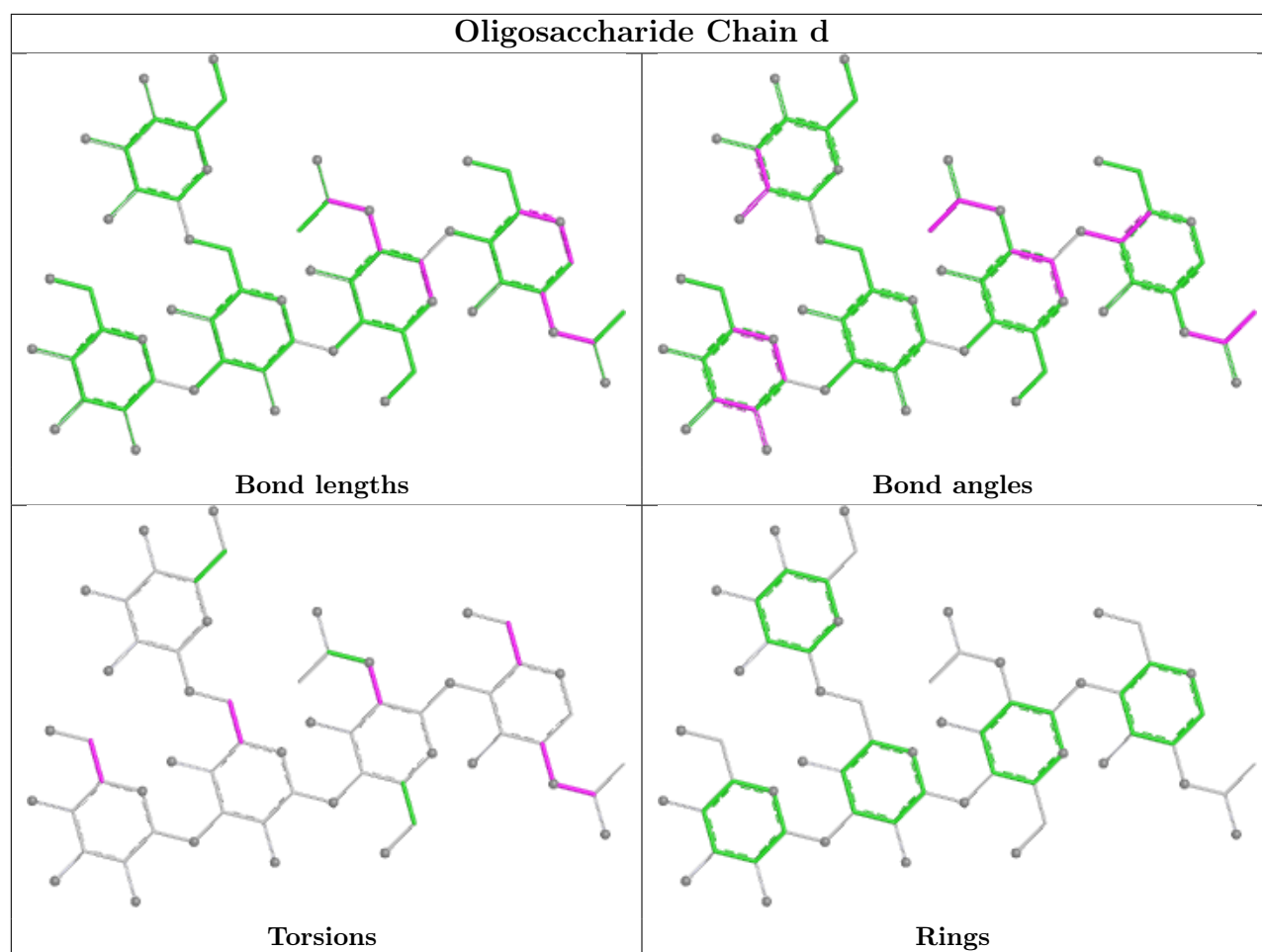


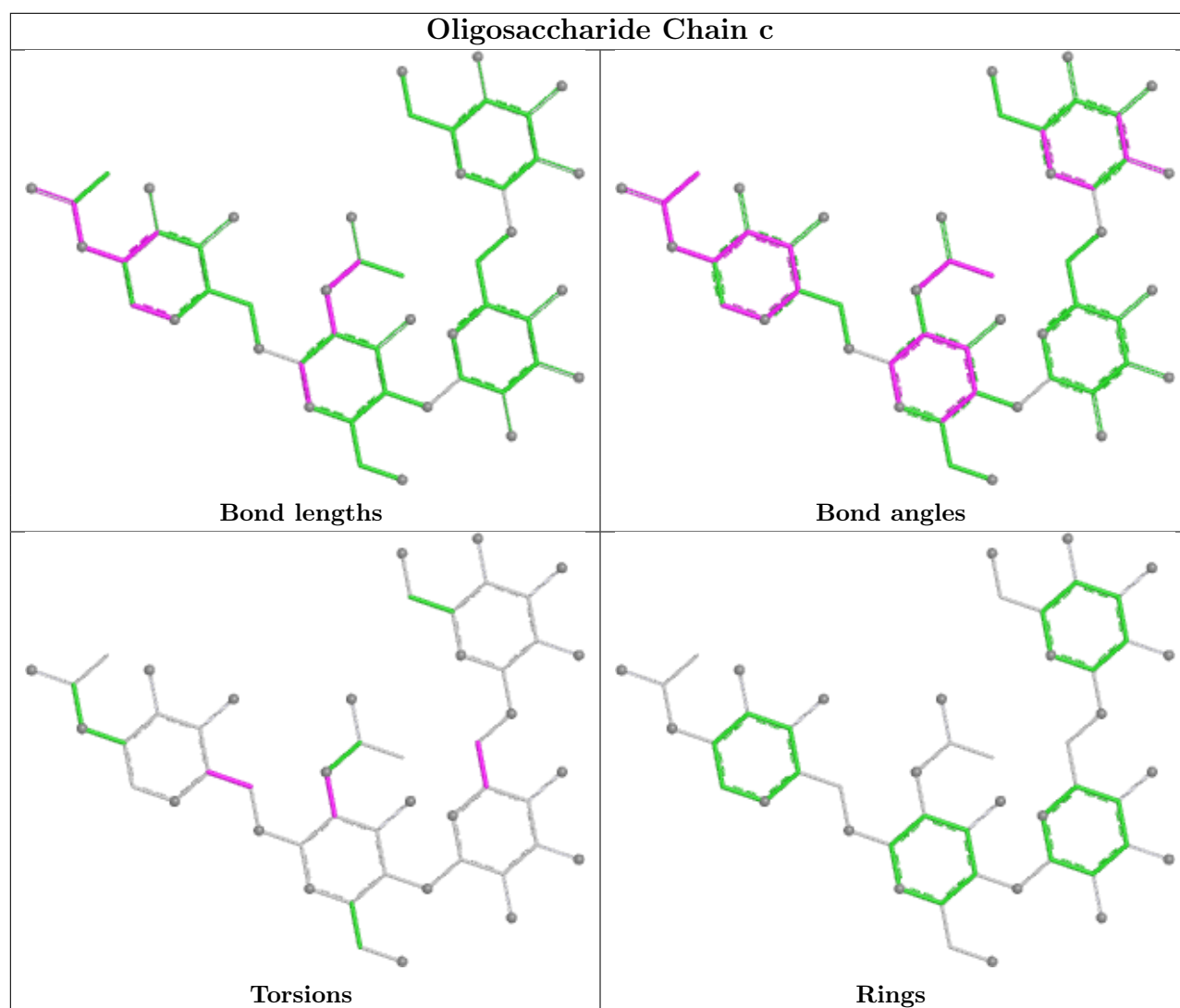












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	NAG	C	1403	1	14,14,15	1.93	3 (21%)	17,19,21	1.91	2 (11%)
10	NAG	B	1406	1	14,14,15	2.09	4 (28%)	17,19,21	2.62	7 (41%)
10	NAG	B	1407	1	14,14,15	2.36	5 (35%)	17,19,21	1.46	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	C	1405	1	14,14,15	2.02	4 (28%)	17,19,21	0.99	1 (5%)
10	NAG	B	1403	1	14,14,15	2.05	4 (28%)	17,19,21	1.37	4 (23%)
10	NAG	B	1402	1	14,14,15	2.05	4 (28%)	17,19,21	1.26	2 (11%)
10	NAG	C	1401	1	14,14,15	2.03	3 (21%)	17,19,21	1.50	2 (11%)
10	NAG	A	1305	1	14,14,15	2.21	4 (28%)	17,19,21	1.72	5 (29%)
10	NAG	B	1405	1	14,14,15	1.96	4 (28%)	17,19,21	1.18	2 (11%)
10	NAG	A	1303	1	14,14,15	1.99	4 (28%)	17,19,21	1.04	2 (11%)
10	NAG	A	1301	1	14,14,15	2.01	4 (28%)	17,19,21	1.08	2 (11%)
10	NAG	C	1404	1	14,14,15	2.01	4 (28%)	17,19,21	1.60	5 (29%)
10	NAG	A	1302	1	14,14,15	2.02	4 (28%)	17,19,21	1.19	2 (11%)
10	NAG	A	1306	1	14,14,15	2.04	3 (21%)	17,19,21	1.48	3 (17%)
10	NAG	C	1402	1	14,14,15	2.02	4 (28%)	17,19,21	1.21	1 (5%)
10	NAG	B	1404	1	14,14,15	1.99	4 (28%)	17,19,21	1.17	2 (11%)
10	NAG	B	1401	1	14,14,15	2.04	4 (28%)	17,19,21	1.20	1 (5%)
10	NAG	A	1304	1	14,14,15	2.16	4 (28%)	17,19,21	2.13	3 (17%)

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
10	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
10	NAG	B	1406	1	-	5/6/23/26	0/1/1/1
10	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1403	1	-	3/6/23/26	0/1/1/1
10	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
10	NAG	C	1401	1	-	4/6/23/26	0/1/1/1
10	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1402	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	1404	1	-	3/6/23/26	0/1/1/1
10	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1304	1	-	3/6/23/26	0/1/1/1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1305	NAG	O5-C1	4.84	1.51	1.43
10	A	1304	NAG	O5-C1	4.80	1.51	1.43
10	B	1407	NAG	O5-C1	4.69	1.51	1.43
10	B	1403	NAG	O5-C1	4.53	1.51	1.43
10	B	1401	NAG	O5-C1	4.41	1.51	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1403	NAG	C1-O5-C5	6.13	120.40	112.19
10	B	1406	NAG	C1-O5-C5	4.91	118.77	112.19
10	B	1406	NAG	C4-C3-C2	4.90	118.20	111.02
10	A	1305	NAG	C8-C7-N2	4.75	124.00	116.12
10	A	1304	NAG	O5-C1-C2	4.72	118.60	111.29

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1304	NAG	C1-C2-N2-C7
10	B	1407	NAG	C3-C2-N2-C7
10	C	1405	NAG	C1-C2-N2-C7
10	B	1402	NAG	O5-C5-C6-O6
10	B	1404	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1406	NAG	4	0
10	B	1407	NAG	4	0
10	C	1401	NAG	2	0
10	A	1305	NAG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1404	NAG	1	0
10	A	1302	NAG	1	0
10	B	1404	NAG	1	0
10	A	1304	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.

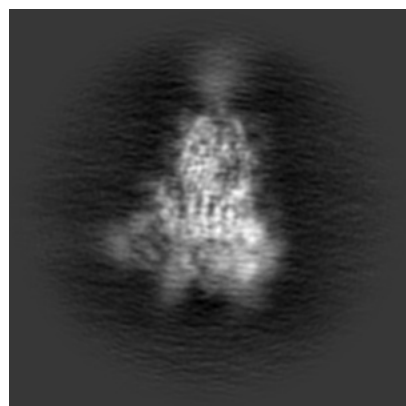
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44344. These allow visual inspection of the internal detail of the map and identification of artifacts.

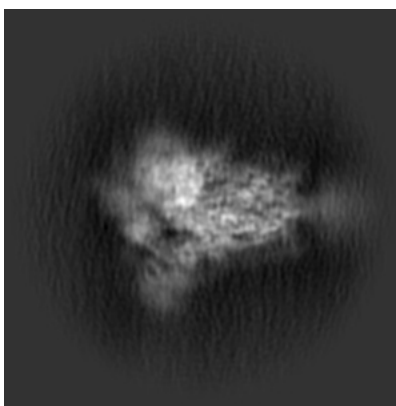
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

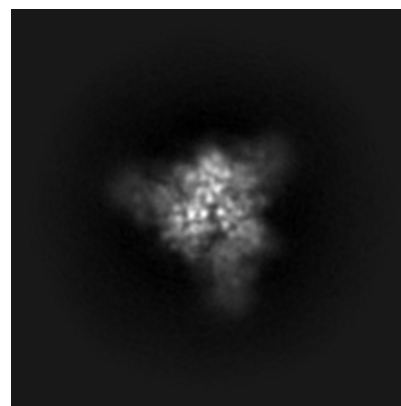
6.1.1 Primary map



X

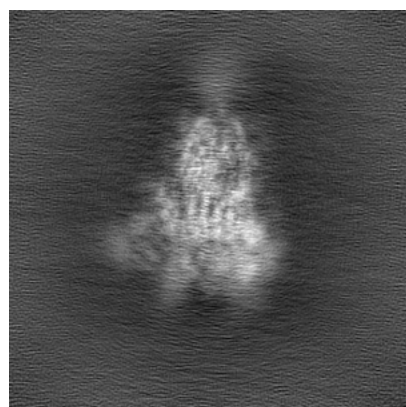


Y

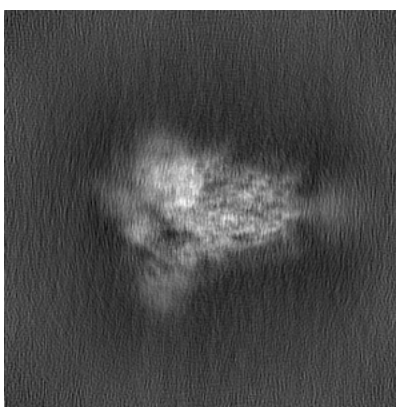


Z

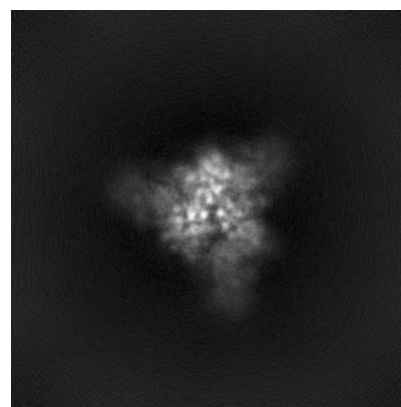
6.1.2 Raw map



X



Y

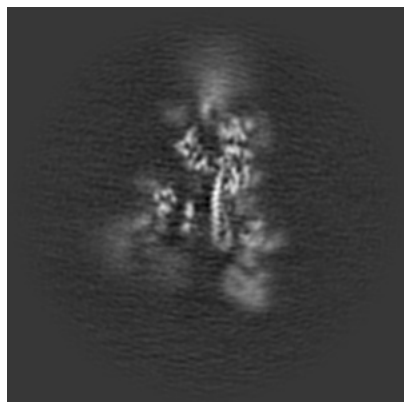


Z

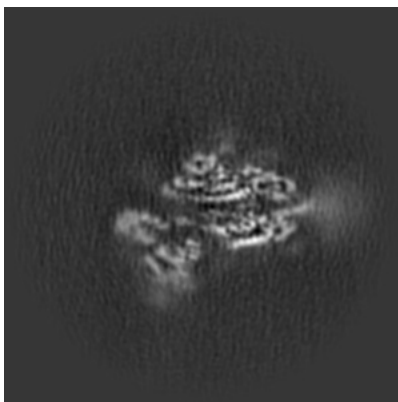
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

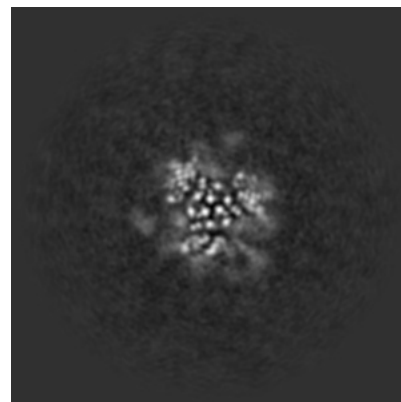
6.2.1 Primary map



X Index: 136

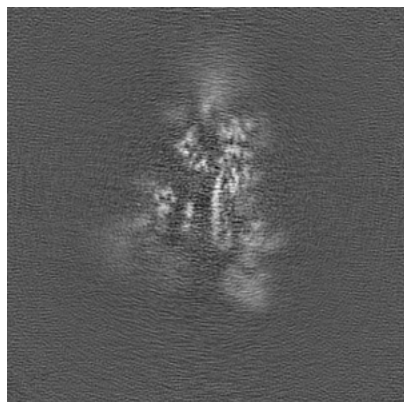


Y Index: 136

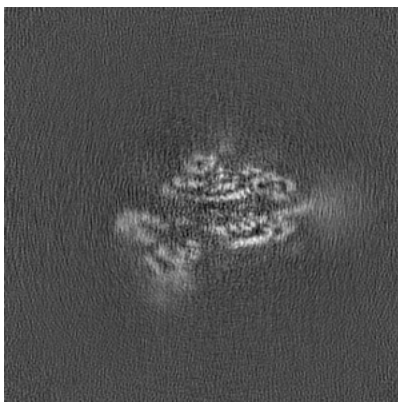


Z Index: 136

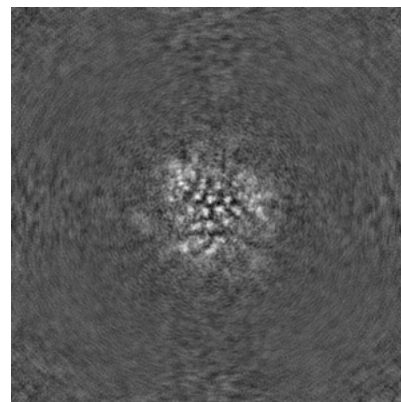
6.2.2 Raw map



X Index: 136



Y Index: 136

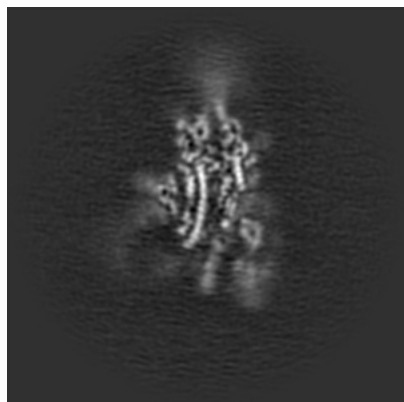


Z Index: 136

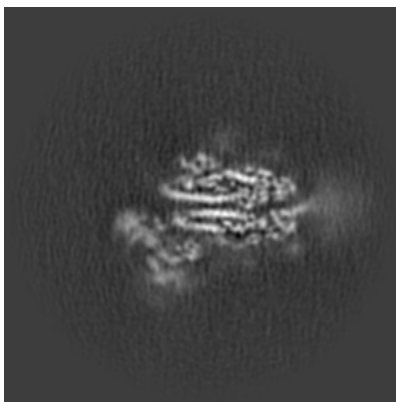
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

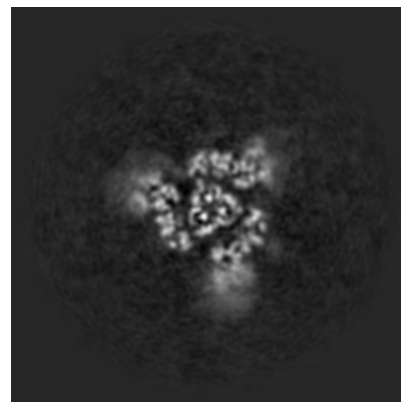
6.3.1 Primary map



X Index: 130

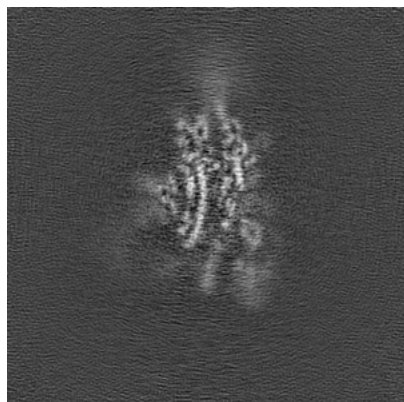


Y Index: 133

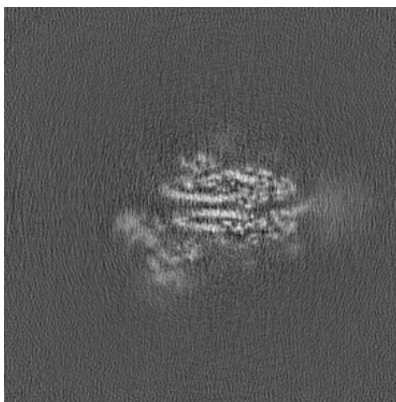


Z Index: 121

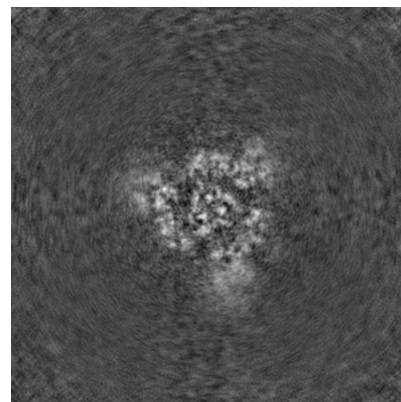
6.3.2 Raw map



X Index: 130



Y Index: 133

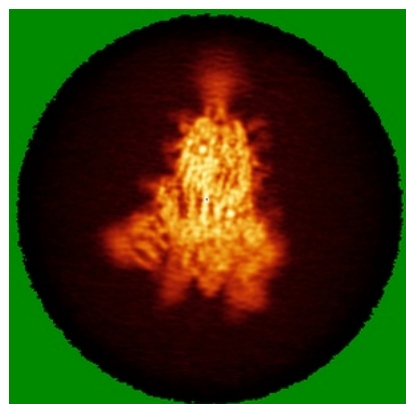


Z Index: 121

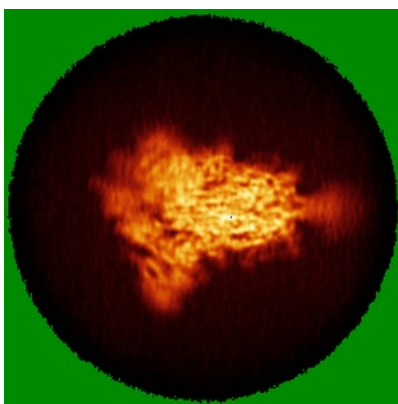
The images above show the largest variance slices of the map in three orthogonal directions.

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

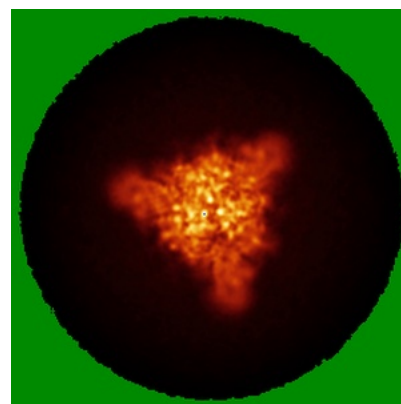
6.4.1 Primary map



X

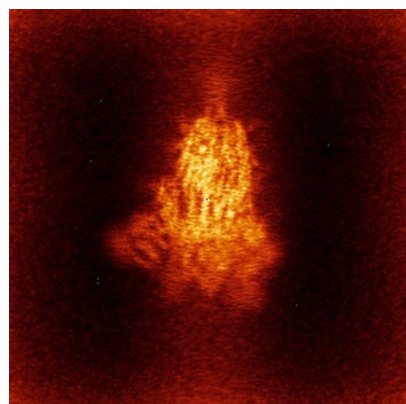


Y

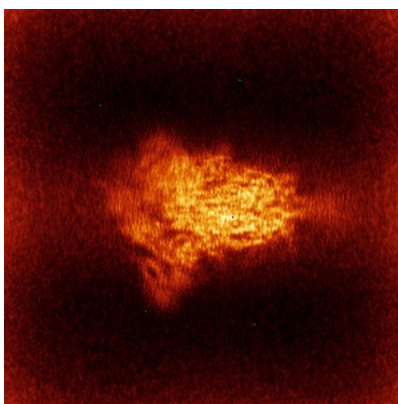


Z

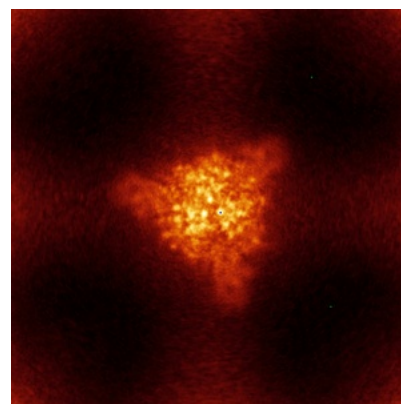
6.4.2 Raw map



X



Y

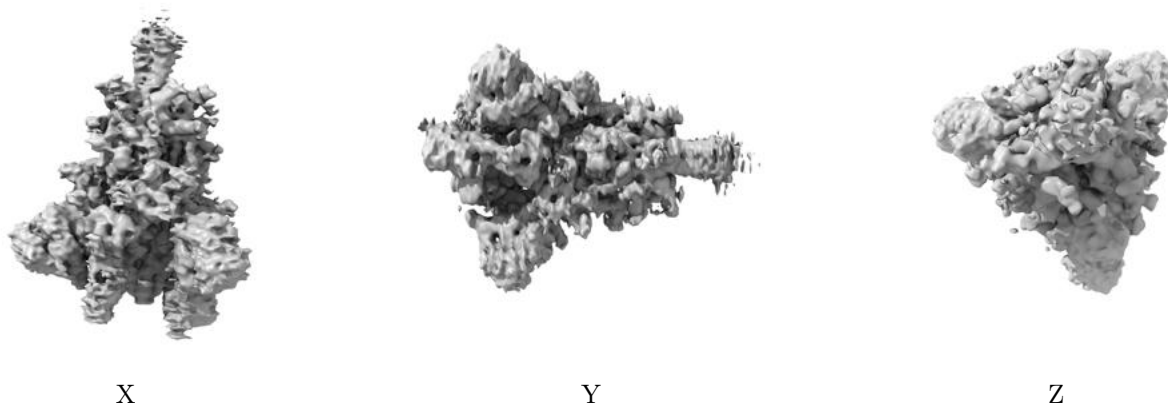


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0607. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

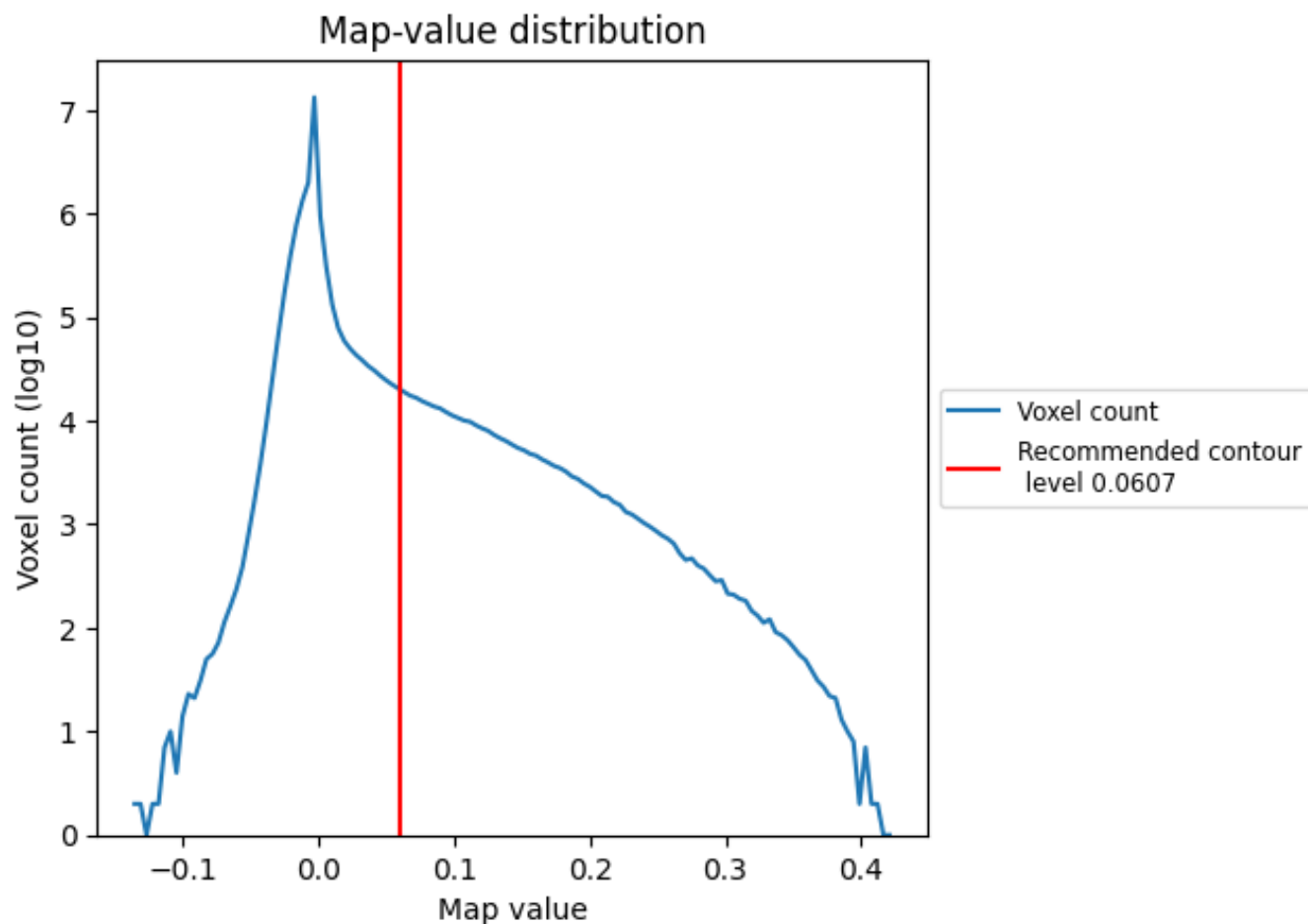
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

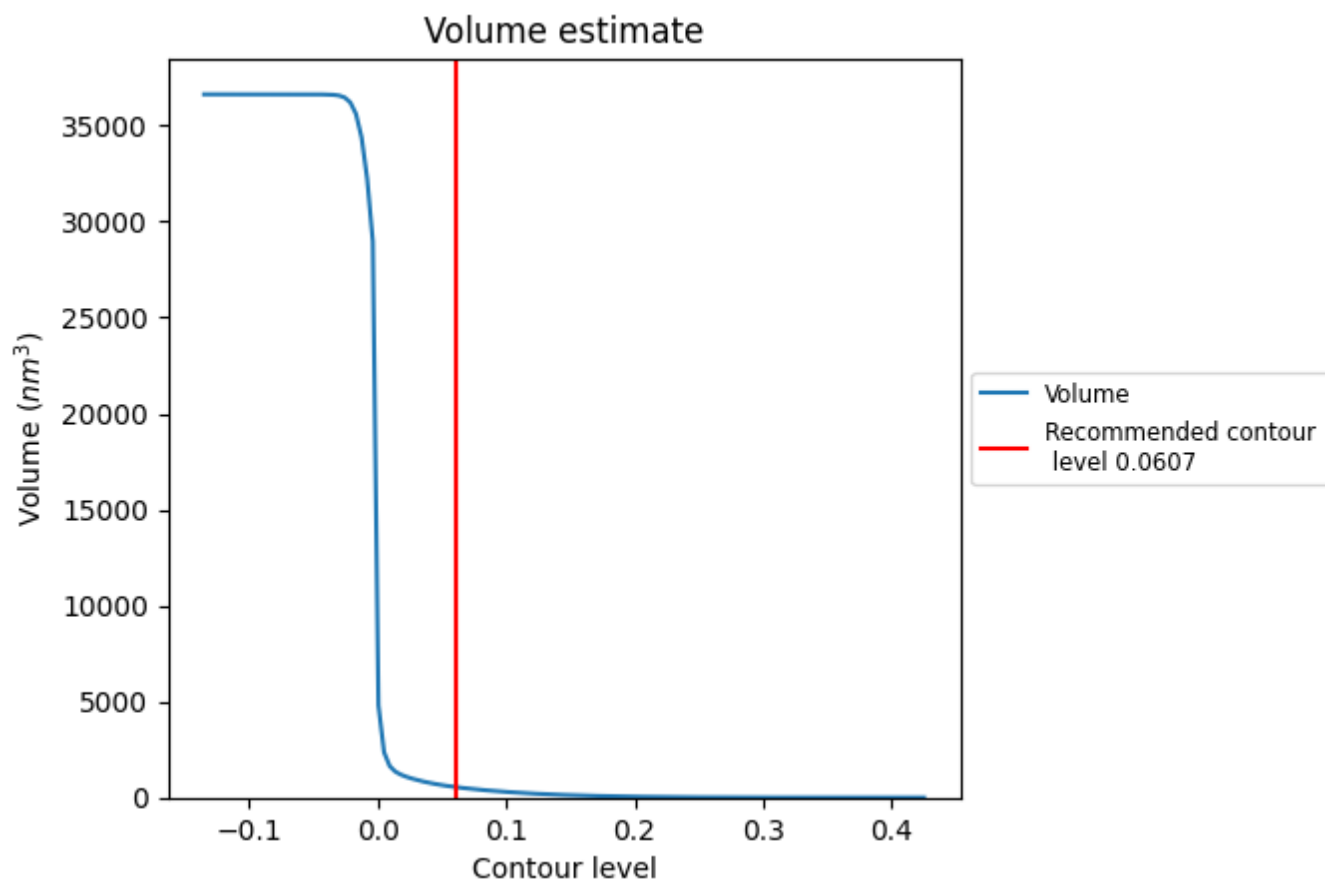
This section contains the results of statistical analysis of the map.

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.

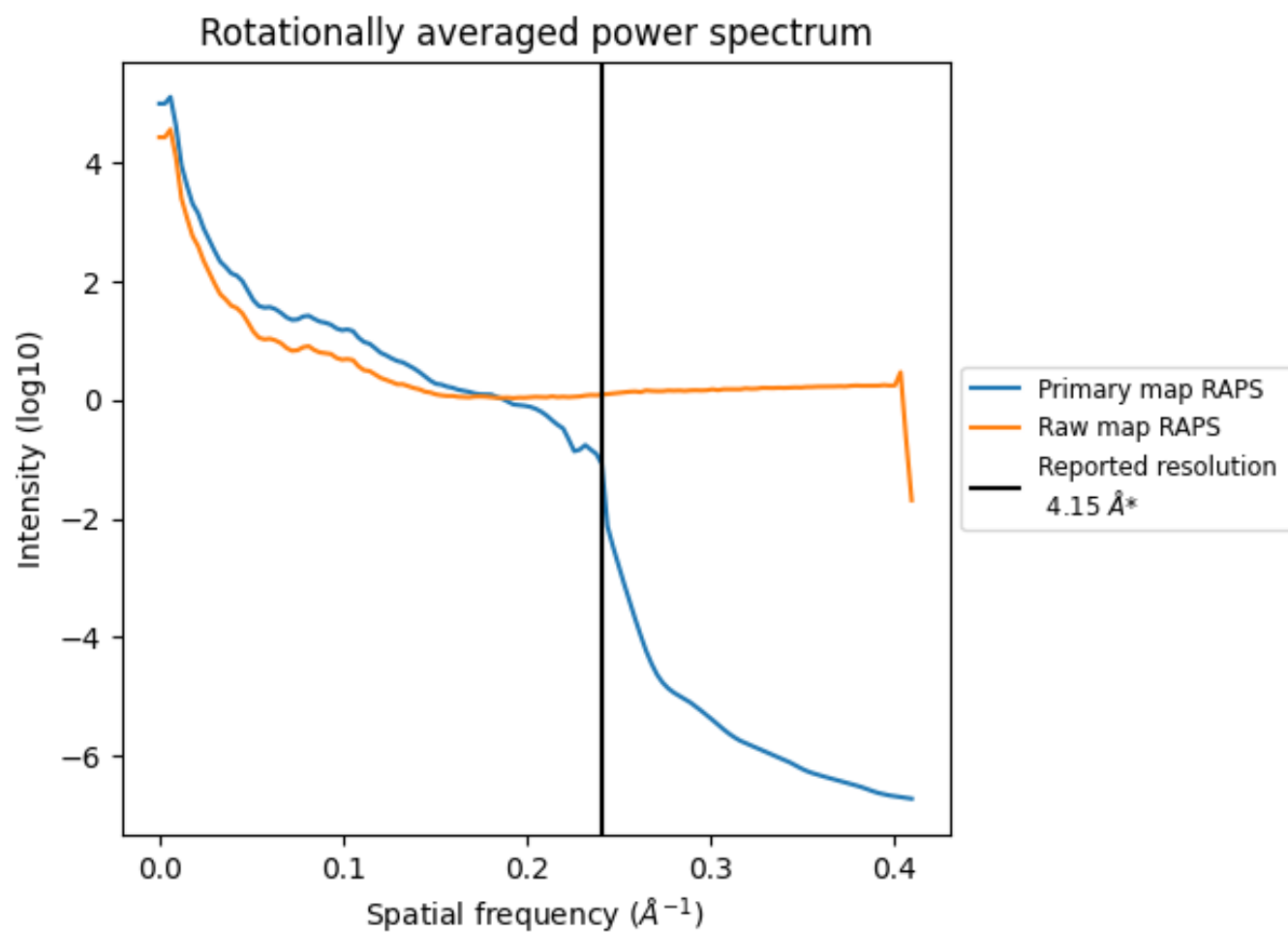
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 ⓘ

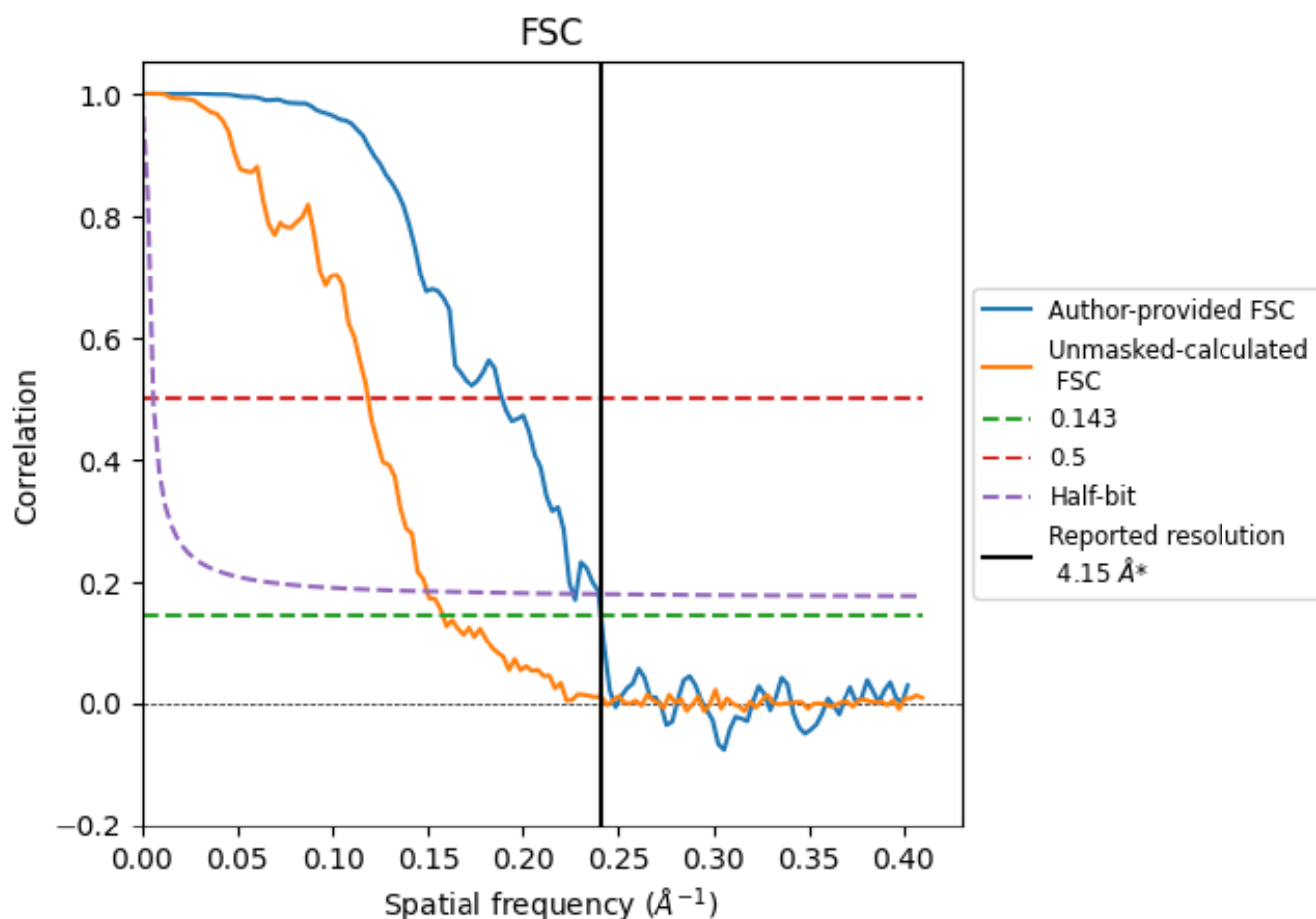


*Reported resolution corresponds to spatial frequency of $0.241 \text{ \AA}^{-1}$

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 0.241 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

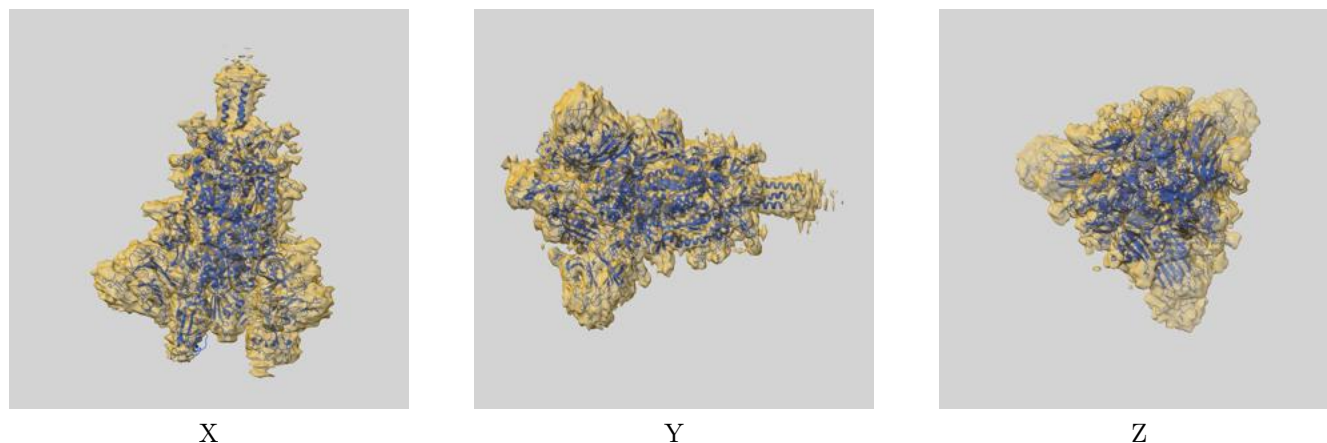
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	4.15	5.29	4.42
Unmasked-calculated*	6.34	8.43	6.69

*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 6.34 differs from the reported value 4.15 by more than 10 %

9 Map-model fit [i](#)

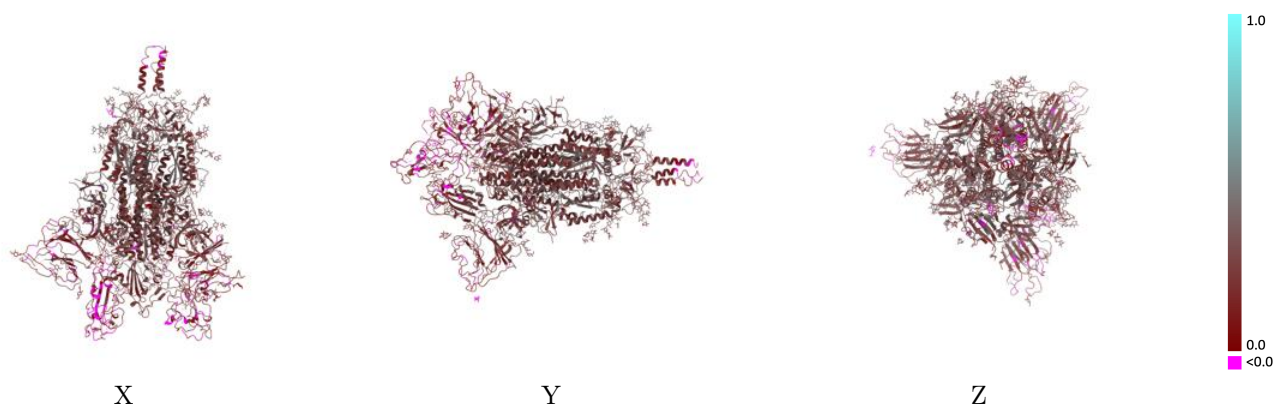
This section contains information regarding the fit between EMDB map EMD-44344 and PDB model 9B8F. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



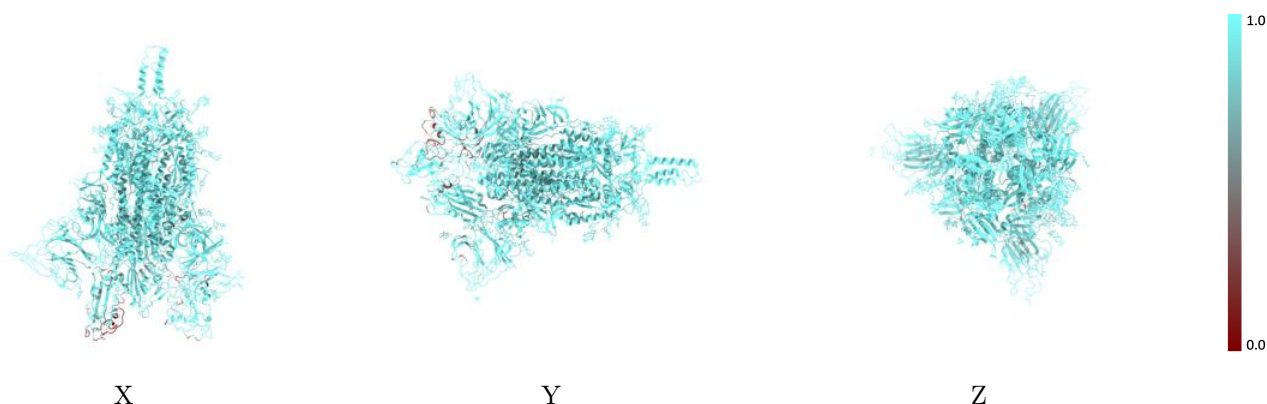
The images above show the 3D surface view of the map at the recommended contour level 0.0607 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



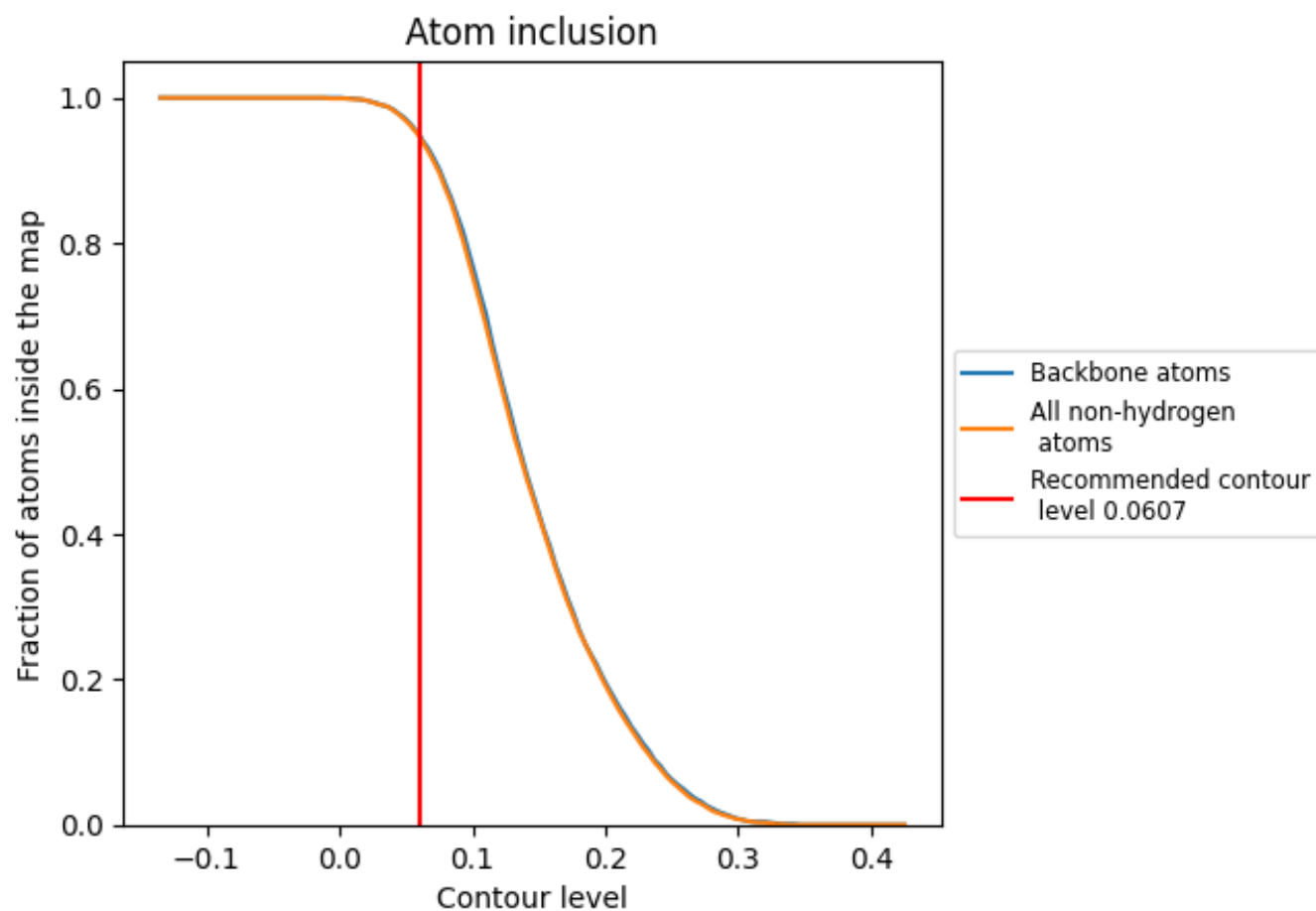
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0607).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0607) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.2480
A	 0.9190	 0.2350
B	 0.9670	 0.2570
C	 0.9520	 0.2460
D	 0.9490	 0.2530
E	 1.0000	 0.3320
F	 0.9400	 0.1930
G	 0.8570	 0.2910
H	 0.9390	 0.1380
I	 0.8930	 0.2210
J	 0.9600	 0.2600
K	 1.0000	 0.3920
L	 1.0000	 0.3700
M	 1.0000	 0.3540
N	 0.9740	 0.2790
O	 0.9640	 0.2820
P	 0.9490	 0.3520
Q	 0.9640	 0.3040
R	 0.8720	 0.2020
S	 0.9740	 0.3720
T	 1.0000	 0.2710
U	 1.0000	 0.3120
V	 1.0000	 0.2850
W	 0.9740	 0.2400
X	 0.9740	 0.2470
Y	 0.9740	 0.2210
Z	 0.9400	 0.3100
a	 0.9840	 0.2990
b	 0.9740	 0.2760
c	 0.9800	 0.3100
d	 1.0000	 0.2700
e	 1.0000	 0.3960
f	 0.7860	 0.1960

