



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:08 AM UTC

PDB ID : 9ZRU / pdb_00009zru
EMDB ID : EMD-74650
Title : Cryo-EM structure of Croatia 2023 H3N2 Influenza A hemagglutinin (HA) trimer
Authors : Kanai, T.; Gorman, J.
Deposited on : 2025-12-21
Resolution : 3.55 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

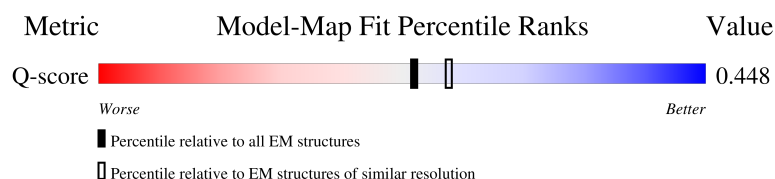
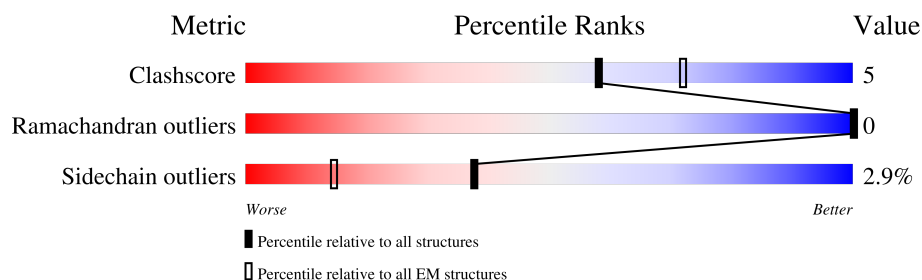
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.55 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	12819 (3.05 - 4.05)

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	334	
1	B	334	
1	C	334	
2	a	238	

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Mol	Chain	Length	Quality of chain
2	b	238	
2	c	238	
3	D	2	
3	G	2	
3	I	2	
3	N	2	
3	Q	2	
3	S	2	
3	X	2	
3	d	2	
3	f	2	
4	E	4	
4	O	4	
4	Y	4	
5	F	5	
5	P	5	
5	Z	5	
6	H	3	
6	J	3	
6	L	3	
6	R	3	
6	T	3	
6	V	3	
6	e	3	
6	g	3	

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Mol	Chain	Length	Quality of chain
6	i	3	67% 100%
7	K	4	25% 50% 50%
7	U	4	50% 50% 50%
7	h	4	25% 50% 50%
8	M	7	14% 86%
8	W	7	14% 86%
8	j	7	14% 86%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13209 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 HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	323	Total	C	N	O	S	0	0
			2503	1558	451	482	12		
1	B	323	Total	C	N	O	S	0	0
			2503	1558	451	482	12		
1	C	323	Total	C	N	O	S	0	0
			2503	1558	451	482	12		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASN	ASP	conflict	UNP A0A8K2AP79
A	96	SER	ASN	conflict	UNP A0A8K2AP79
A	122	ASP	ASN	conflict	UNP A0A8K2AP79
A	140	LYS	ILE	conflict	UNP A0A8K2AP79
A	145	ASN	SER	conflict	UNP A0A8K2AP79
A	156	SER	HIS	conflict	UNP A0A8K2AP79
A	186	ALA	ASP	conflict	UNP A0A8K2AP79
A	192	PHE	ILE	conflict	UNP A0A8K2AP79
A	223	VAL	ILE	conflict	UNP A0A8K2AP79
A	276	GLU	LYS	conflict	UNP A0A8K2AP79
A	330	ARG	-	expression tag	UNP A0A8K2AP79
A	331	ARG	-	expression tag	UNP A0A8K2AP79
A	332	ARG	-	expression tag	UNP A0A8K2AP79
A	333	ARG	-	expression tag	UNP A0A8K2AP79
A	334	ARG	-	expression tag	UNP A0A8K2AP79
B	53	ASN	ASP	conflict	UNP A0A8K2AP79
B	96	SER	ASN	conflict	UNP A0A8K2AP79
B	122	ASP	ASN	conflict	UNP A0A8K2AP79
B	140	LYS	ILE	conflict	UNP A0A8K2AP79
B	145	ASN	SER	conflict	UNP A0A8K2AP79
B	156	SER	HIS	conflict	UNP A0A8K2AP79
B	186	ALA	ASP	conflict	UNP A0A8K2AP79
B	192	PHE	ILE	conflict	UNP A0A8K2AP79
B	223	VAL	ILE	conflict	UNP A0A8K2AP79

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Chain	Residue	Modelled	Actual	Comment	Reference
B	276	GLU	LYS	conflict	UNP A0A8K2AP79
B	330	ARG	-	expression tag	UNP A0A8K2AP79
B	331	ARG	-	expression tag	UNP A0A8K2AP79
B	332	ARG	-	expression tag	UNP A0A8K2AP79
B	333	ARG	-	expression tag	UNP A0A8K2AP79
B	334	ARG	-	expression tag	UNP A0A8K2AP79
C	53	ASN	ASP	conflict	UNP A0A8K2AP79
C	96	SER	ASN	conflict	UNP A0A8K2AP79
C	122	ASP	ASN	conflict	UNP A0A8K2AP79
C	140	LYS	ILE	conflict	UNP A0A8K2AP79
C	145	ASN	SER	conflict	UNP A0A8K2AP79
C	156	SER	HIS	conflict	UNP A0A8K2AP79
C	186	ALA	ASP	conflict	UNP A0A8K2AP79
C	192	PHE	ILE	conflict	UNP A0A8K2AP79
C	223	VAL	ILE	conflict	UNP A0A8K2AP79
C	276	GLU	LYS	conflict	UNP A0A8K2AP79
C	330	ARG	-	expression tag	UNP A0A8K2AP79
C	331	ARG	-	expression tag	UNP A0A8K2AP79
C	332	ARG	-	expression tag	UNP A0A8K2AP79
C	333	ARG	-	expression tag	UNP A0A8K2AP79
C	334	ARG	-	expression tag	UNP A0A8K2AP79

- Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	177	Total	C	N	O	S	0	0
			1427	888	251	282	6		
2	b	177	Total	C	N	O	S	0	0
			1427	888	251	282	6		
2	c	177	Total	C	N	O	S	0	0
			1427	888	251	282	6		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	185	GLY	-	expression tag	UNP A0A5B8WI41
a	186	SER	-	expression tag	UNP A0A5B8WI41
a	187	GLY	-	expression tag	UNP A0A5B8WI41
a	188	LEU	-	expression tag	UNP A0A5B8WI41
a	189	VAL	-	expression tag	UNP A0A5B8WI41
a	190	PRO	-	expression tag	UNP A0A5B8WI41
a	191	ARG	-	expression tag	UNP A0A5B8WI41

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Chain	Residue	Modelled	Actual	Comment	Reference
a	192	GLY	-	expression tag	UNP A0A5B8WI41
a	193	SER	-	expression tag	UNP A0A5B8WI41
a	194	GLY	-	expression tag	UNP A0A5B8WI41
a	195	LEU	-	expression tag	UNP A0A5B8WI41
a	196	GLU	-	expression tag	UNP A0A5B8WI41
a	197	VAL	-	expression tag	UNP A0A5B8WI41
a	198	LEU	-	expression tag	UNP A0A5B8WI41
a	199	PHE	-	expression tag	UNP A0A5B8WI41
a	200	GLN	-	expression tag	UNP A0A5B8WI41
a	201	GLY	-	expression tag	UNP A0A5B8WI41
a	202	PRO	-	expression tag	UNP A0A5B8WI41
a	203	GLY	-	expression tag	UNP A0A5B8WI41
a	204	SER	-	expression tag	UNP A0A5B8WI41
a	205	GLY	-	expression tag	UNP A0A5B8WI41
a	206	TYR	-	expression tag	UNP A0A5B8WI41
a	207	ILE	-	expression tag	UNP A0A5B8WI41
a	208	PRO	-	expression tag	UNP A0A5B8WI41
a	209	GLU	-	expression tag	UNP A0A5B8WI41
a	210	ALA	-	expression tag	UNP A0A5B8WI41
a	211	PRO	-	expression tag	UNP A0A5B8WI41
a	212	ARG	-	expression tag	UNP A0A5B8WI41
a	213	ASP	-	expression tag	UNP A0A5B8WI41
a	214	GLY	-	expression tag	UNP A0A5B8WI41
a	215	GLN	-	expression tag	UNP A0A5B8WI41
a	216	ALA	-	expression tag	UNP A0A5B8WI41
a	217	TYR	-	expression tag	UNP A0A5B8WI41
a	218	VAL	-	expression tag	UNP A0A5B8WI41
a	219	ARG	-	expression tag	UNP A0A5B8WI41
a	220	LYS	-	expression tag	UNP A0A5B8WI41
a	221	ASP	-	expression tag	UNP A0A5B8WI41
a	222	GLY	-	expression tag	UNP A0A5B8WI41
a	223	GLU	-	expression tag	UNP A0A5B8WI41
a	224	TRP	-	expression tag	UNP A0A5B8WI41
a	225	VAL	-	expression tag	UNP A0A5B8WI41
a	226	LEU	-	expression tag	UNP A0A5B8WI41
a	227	LEU	-	expression tag	UNP A0A5B8WI41
a	228	SER	-	expression tag	UNP A0A5B8WI41
a	229	THR	-	expression tag	UNP A0A5B8WI41
a	230	PHE	-	expression tag	UNP A0A5B8WI41
a	231	LEU	-	expression tag	UNP A0A5B8WI41
a	232	GLY	-	expression tag	UNP A0A5B8WI41
a	233	HIS	-	expression tag	UNP A0A5B8WI41

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Chain	Residue	Modelled	Actual	Comment	Reference
a	234	HIS	-	expression tag	UNP A0A5B8WI41
a	235	HIS	-	expression tag	UNP A0A5B8WI41
a	236	HIS	-	expression tag	UNP A0A5B8WI41
a	237	HIS	-	expression tag	UNP A0A5B8WI41
a	238	HIS	-	expression tag	UNP A0A5B8WI41
b	185	GLY	-	expression tag	UNP A0A5B8WI41
b	186	SER	-	expression tag	UNP A0A5B8WI41
b	187	GLY	-	expression tag	UNP A0A5B8WI41
b	188	LEU	-	expression tag	UNP A0A5B8WI41
b	189	VAL	-	expression tag	UNP A0A5B8WI41
b	190	PRO	-	expression tag	UNP A0A5B8WI41
b	191	ARG	-	expression tag	UNP A0A5B8WI41
b	192	GLY	-	expression tag	UNP A0A5B8WI41
b	193	SER	-	expression tag	UNP A0A5B8WI41
b	194	GLY	-	expression tag	UNP A0A5B8WI41
b	195	LEU	-	expression tag	UNP A0A5B8WI41
b	196	GLU	-	expression tag	UNP A0A5B8WI41
b	197	VAL	-	expression tag	UNP A0A5B8WI41
b	198	LEU	-	expression tag	UNP A0A5B8WI41
b	199	PHE	-	expression tag	UNP A0A5B8WI41
b	200	GLN	-	expression tag	UNP A0A5B8WI41
b	201	GLY	-	expression tag	UNP A0A5B8WI41
b	202	PRO	-	expression tag	UNP A0A5B8WI41
b	203	GLY	-	expression tag	UNP A0A5B8WI41
b	204	SER	-	expression tag	UNP A0A5B8WI41
b	205	GLY	-	expression tag	UNP A0A5B8WI41
b	206	TYR	-	expression tag	UNP A0A5B8WI41
b	207	ILE	-	expression tag	UNP A0A5B8WI41
b	208	PRO	-	expression tag	UNP A0A5B8WI41
b	209	GLU	-	expression tag	UNP A0A5B8WI41
b	210	ALA	-	expression tag	UNP A0A5B8WI41
b	211	PRO	-	expression tag	UNP A0A5B8WI41
b	212	ARG	-	expression tag	UNP A0A5B8WI41
b	213	ASP	-	expression tag	UNP A0A5B8WI41
b	214	GLY	-	expression tag	UNP A0A5B8WI41
b	215	GLN	-	expression tag	UNP A0A5B8WI41
b	216	ALA	-	expression tag	UNP A0A5B8WI41
b	217	TYR	-	expression tag	UNP A0A5B8WI41
b	218	VAL	-	expression tag	UNP A0A5B8WI41
b	219	ARG	-	expression tag	UNP A0A5B8WI41
b	220	LYS	-	expression tag	UNP A0A5B8WI41
b	221	ASP	-	expression tag	UNP A0A5B8WI41

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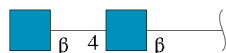
Chain	Residue	Modelled	Actual	Comment	Reference
b	222	GLY	-	expression tag	UNP A0A5B8WI41
b	223	GLU	-	expression tag	UNP A0A5B8WI41
b	224	TRP	-	expression tag	UNP A0A5B8WI41
b	225	VAL	-	expression tag	UNP A0A5B8WI41
b	226	LEU	-	expression tag	UNP A0A5B8WI41
b	227	LEU	-	expression tag	UNP A0A5B8WI41
b	228	SER	-	expression tag	UNP A0A5B8WI41
b	229	THR	-	expression tag	UNP A0A5B8WI41
b	230	PHE	-	expression tag	UNP A0A5B8WI41
b	231	LEU	-	expression tag	UNP A0A5B8WI41
b	232	GLY	-	expression tag	UNP A0A5B8WI41
b	233	HIS	-	expression tag	UNP A0A5B8WI41
b	234	HIS	-	expression tag	UNP A0A5B8WI41
b	235	HIS	-	expression tag	UNP A0A5B8WI41
b	236	HIS	-	expression tag	UNP A0A5B8WI41
b	237	HIS	-	expression tag	UNP A0A5B8WI41
b	238	HIS	-	expression tag	UNP A0A5B8WI41
c	185	GLY	-	expression tag	UNP A0A5B8WI41
c	186	SER	-	expression tag	UNP A0A5B8WI41
c	187	GLY	-	expression tag	UNP A0A5B8WI41
c	188	LEU	-	expression tag	UNP A0A5B8WI41
c	189	VAL	-	expression tag	UNP A0A5B8WI41
c	190	PRO	-	expression tag	UNP A0A5B8WI41
c	191	ARG	-	expression tag	UNP A0A5B8WI41
c	192	GLY	-	expression tag	UNP A0A5B8WI41
c	193	SER	-	expression tag	UNP A0A5B8WI41
c	194	GLY	-	expression tag	UNP A0A5B8WI41
c	195	LEU	-	expression tag	UNP A0A5B8WI41
c	196	GLU	-	expression tag	UNP A0A5B8WI41
c	197	VAL	-	expression tag	UNP A0A5B8WI41
c	198	LEU	-	expression tag	UNP A0A5B8WI41
c	199	PHE	-	expression tag	UNP A0A5B8WI41
c	200	GLN	-	expression tag	UNP A0A5B8WI41
c	201	GLY	-	expression tag	UNP A0A5B8WI41
c	202	PRO	-	expression tag	UNP A0A5B8WI41
c	203	GLY	-	expression tag	UNP A0A5B8WI41
c	204	SER	-	expression tag	UNP A0A5B8WI41
c	205	GLY	-	expression tag	UNP A0A5B8WI41
c	206	TYR	-	expression tag	UNP A0A5B8WI41
c	207	ILE	-	expression tag	UNP A0A5B8WI41
c	208	PRO	-	expression tag	UNP A0A5B8WI41
c	209	GLU	-	expression tag	UNP A0A5B8WI41

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Chain	Residue	Modelled	Actual	Comment	Reference
c	210	ALA	-	expression tag	UNP A0A5B8WI41
c	211	PRO	-	expression tag	UNP A0A5B8WI41
c	212	ARG	-	expression tag	UNP A0A5B8WI41
c	213	ASP	-	expression tag	UNP A0A5B8WI41
c	214	GLY	-	expression tag	UNP A0A5B8WI41
c	215	GLN	-	expression tag	UNP A0A5B8WI41
c	216	ALA	-	expression tag	UNP A0A5B8WI41
c	217	TYR	-	expression tag	UNP A0A5B8WI41
c	218	VAL	-	expression tag	UNP A0A5B8WI41
c	219	ARG	-	expression tag	UNP A0A5B8WI41
c	220	LYS	-	expression tag	UNP A0A5B8WI41
c	221	ASP	-	expression tag	UNP A0A5B8WI41
c	222	GLY	-	expression tag	UNP A0A5B8WI41
c	223	GLU	-	expression tag	UNP A0A5B8WI41
c	224	TRP	-	expression tag	UNP A0A5B8WI41
c	225	VAL	-	expression tag	UNP A0A5B8WI41
c	226	LEU	-	expression tag	UNP A0A5B8WI41
c	227	LEU	-	expression tag	UNP A0A5B8WI41
c	228	SER	-	expression tag	UNP A0A5B8WI41
c	229	THR	-	expression tag	UNP A0A5B8WI41
c	230	PHE	-	expression tag	UNP A0A5B8WI41
c	231	LEU	-	expression tag	UNP A0A5B8WI41
c	232	GLY	-	expression tag	UNP A0A5B8WI41
c	233	HIS	-	expression tag	UNP A0A5B8WI41
c	234	HIS	-	expression tag	UNP A0A5B8WI41
c	235	HIS	-	expression tag	UNP A0A5B8WI41
c	236	HIS	-	expression tag	UNP A0A5B8WI41
c	237	HIS	-	expression tag	UNP A0A5B8WI41
c	238	HIS	-	expression tag	UNP A0A5B8WI41

- Molecule 3 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
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

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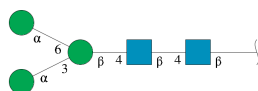
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	E	4	Total	C	N	O	0	0
			50	28	2	20		
4	O	4	Total	C	N	O	0	0
			50	28	2	20		
4	Y	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



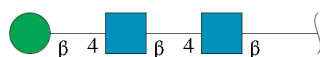
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	5	Total	C	N	O	0	0
			61	34	2	25		
5	Z	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 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.



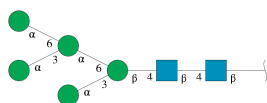
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	3	Total	C	N	O	0	0
			39	22	2	15		
6	J	3	Total	C	N	O	0	0
			39	22	2	15		
6	L	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	T	3	Total	C	N	O	0	0
			39	22	2	15		
6	V	3	Total	C	N	O	0	0
			39	22	2	15		
6	e	3	Total	C	N	O	0	0
			39	22	2	15		
6	g	3	Total	C	N	O	0	0
			39	22	2	15		
6	i	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 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.



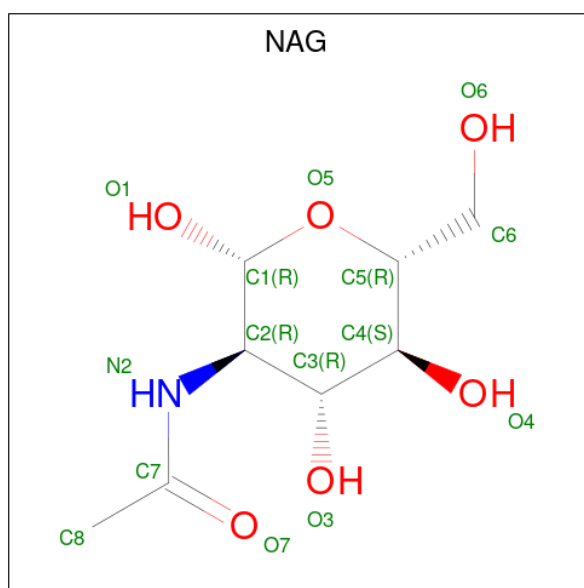
Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	4	Total	C	N	O	0	0
			50	28	2	20		
7	U	4	Total	C	N	O	0	0
			50	28	2	20		
7	h	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	7	Total	C	N	O	0	0
			83	46	2	35		
8	W	7	Total	C	N	O	0	0
			83	46	2	35		
8	j	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

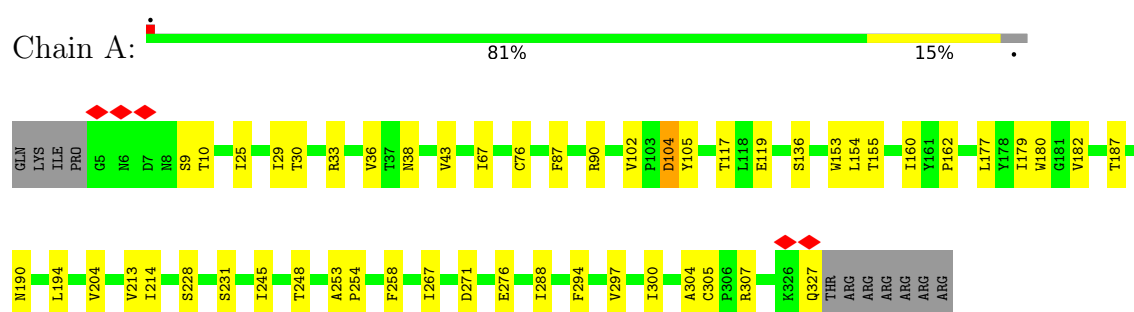


Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	

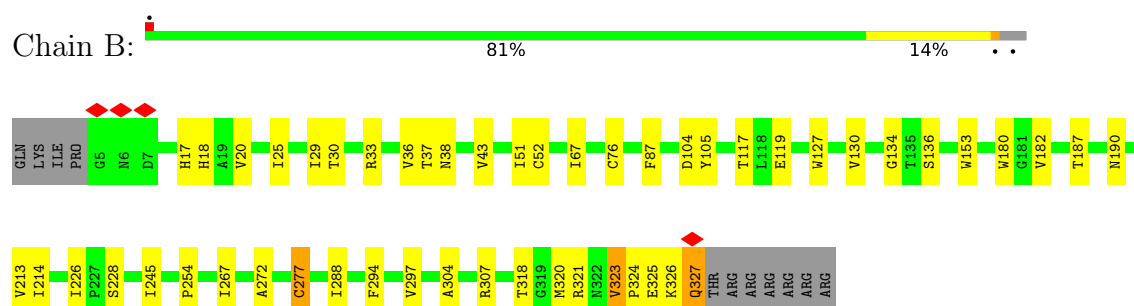
3 Residue-property plots

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.

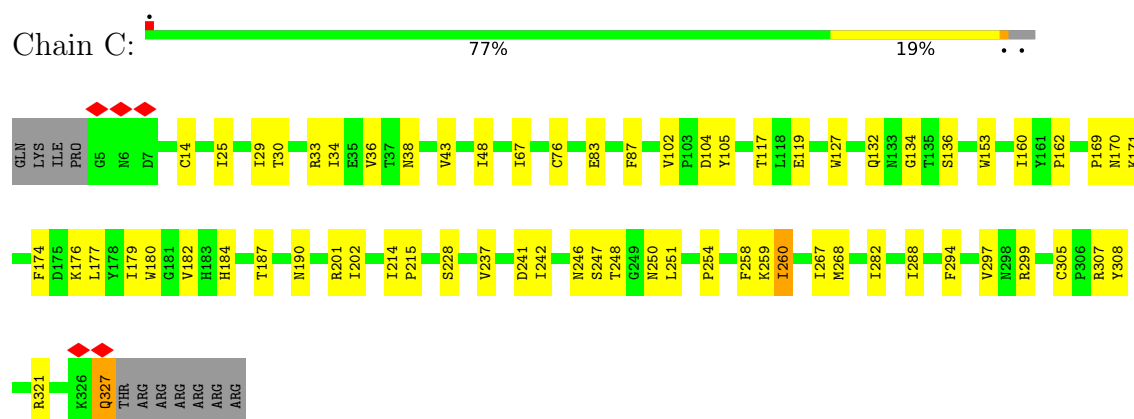
• Molecule 1: HA1



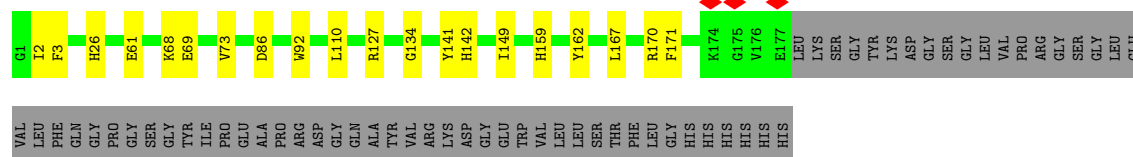
• Molecule 1: HA1



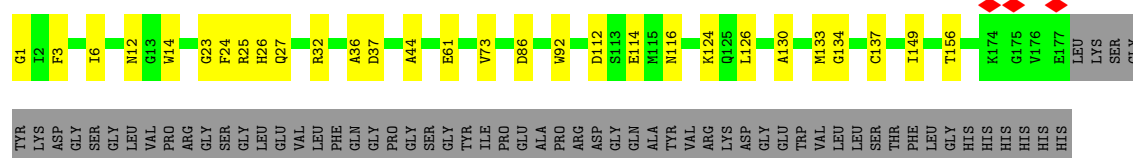
• Molecule 1: HA1



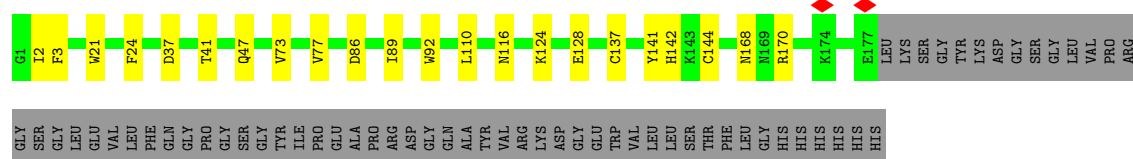
• Molecule 2: HA2



- Molecule 2: HA2



- Molecule 2: HA2



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



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



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





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



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



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



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



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



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





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



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



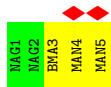
- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



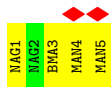
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose





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



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



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



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



- Molecule 7: 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: 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



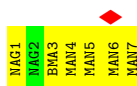
- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	44300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TUNDRA	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	4.267	Depositor
Minimum map value	-2.658	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/2556	0.34	0/3469
1	B	0.12	0/2556	0.32	0/3469
1	C	0.11	0/2556	0.33	0/3469
2	a	0.11	0/1451	0.34	0/1947
2	b	0.11	0/1451	0.31	0/1947
2	c	0.12	0/1451	0.30	0/1947
All	All	0.11	0/12021	0.33	0/16248

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9	SER	Peptide

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	2503	0	2452	26	0
1	B	2503	0	2452	28	0
1	C	2503	0	2452	36	0
2	a	1427	0	1360	14	0
2	b	1427	0	1360	18	0
2	c	1427	0	1360	14	0
3	D	28	0	25	0	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	N	28	0	25	0	0
3	Q	28	0	25	0	0
3	S	28	0	25	0	0
3	X	28	0	25	0	0
3	d	28	0	25	0	0
3	f	28	0	25	0	0
4	E	50	0	43	0	0
4	O	50	0	43	0	0
4	Y	50	0	43	0	0
5	F	61	0	52	0	0
5	P	61	0	52	0	0
5	Z	61	0	52	1	0
6	H	39	0	34	1	0
6	J	39	0	34	0	0
6	L	39	0	34	0	0
6	R	39	0	34	0	0
6	T	39	0	34	0	0
6	V	39	0	34	0	0
6	e	39	0	34	0	0
6	g	39	0	34	0	0
6	i	39	0	34	0	0
7	K	50	0	43	0	0
7	U	50	0	43	0	0
7	h	50	0	43	0	0
8	M	83	0	70	0	0
8	W	83	0	70	0	0
8	j	83	0	70	0	0
9	A	28	0	26	0	0
9	B	28	0	26	0	0
9	C	28	0	26	0	0
All	All	13209	0	12669	121	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 5.

All (121) 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:B:52:CYS:HB2	1:B:277:CYS:H	1.53	0.74
1:C:182:VAL:HG22	1:C:202:ILE:HD12	1.71	0.73
1:C:87:PHE:HB3	1:C:267:ILE:HG13	1.76	0.66
2:a:110:LEU:HA	2:c:2:ILE:HD11	1.79	0.64
1:B:304:ALA:HB2	2:b:61:GLU:HG2	1.79	0.62
2:c:3:PHE:HB3	2:c:116:ASN:HD22	1.64	0.62
1:C:34:ILE:HD11	1:C:321:ARG:HH11	1.66	0.61
1:B:51:ILE:HG12	1:B:272:ALA:HB3	1.84	0.60
1:B:180:TRP:HB3	1:B:254:PRO:HD3	1.84	0.59
2:b:134:GLY:HA2	2:c:124:LYS:HD3	1.85	0.59
1:A:25:ILE:HD11	1:A:33:ARG:HG3	1.85	0.59
1:C:25:ILE:HD11	1:C:33:ARG:HG3	1.84	0.59
1:A:10:THR:HB	2:a:141:TYR:HA	1.84	0.59
1:B:87:PHE:HB3	1:B:267:ILE:HG13	1.83	0.58
1:B:43:VAL:HG12	1:B:294:PHE:HB2	1.86	0.57
1:A:304:ALA:HB2	2:a:61:GLU:HG2	1.84	0.57
1:C:67:ILE:HG13	1:C:105:TYR:HE1	1.69	0.57
2:c:142:HIS:CD2	2:c:144:CYS:HB2	2.40	0.56
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.87	0.56
1:A:204:VAL:HG22	1:A:245:ILE:HG12	1.88	0.56
2:a:141:TYR:HE1	2:a:170:ARG:HD2	1.71	0.56
1:B:288:ILE:HG21	1:B:297:VAL:HG21	1.88	0.56
2:b:133:MET:HE2	2:b:137:CYS:HB3	1.89	0.55
1:A:182:VAL:HG11	1:A:213:VAL:HG11	1.89	0.55
1:B:134:GLY:HA3	1:B:153:TRP:HB3	1.88	0.54
1:B:67:ILE:HG13	1:B:105:TYR:HE2	1.72	0.54
1:A:67:ILE:HG13	1:A:105:TYR:HE2	1.73	0.54
1:A:155:THR:HG23	1:A:194:LEU:HB3	1.91	0.53
2:b:3:PHE:HB3	2:b:116:ASN:HD22	1.74	0.51
1:C:136:SER:HB2	1:C:153:TRP:HZ3	1.74	0.51
1:C:43:VAL:HG12	1:C:294:PHE:HB2	1.92	0.51
1:C:180:TRP:HB3	1:C:254:PRO:HD3	1.92	0.51
2:b:24:PHE:HE1	2:b:37:ASP:HB2	1.76	0.51
1:A:43:VAL:HG12	1:A:294:PHE:HB2	1.93	0.50
1:C:169:PRO:HB3	1:C:242:ILE:HD12	1.92	0.50
2:c:141:TYR:HE2	2:c:170:ARG:HG3	1.76	0.50
1:B:136:SER:HB2	1:B:153:TRP:HZ3	1.77	0.50
1:B:52:CYS:HB2	1:B:277:CYS:N	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:SER:HB2	1:C:251:LEU:HD22	1.95	0.49
2:c:142:HIS:HD2	2:c:144:CYS:HB2	1.78	0.49
1:A:190:ASN:O	1:A:194:LEU:HD12	2.13	0.48
2:b:23:GLY:HA2	2:b:36:ALA:HA	1.95	0.48
1:B:29:ILE:HG23	1:B:30:THR:HG23	1.95	0.48
2:c:24:PHE:HE1	2:c:37:ASP:HB2	1.78	0.48
1:C:160:ILE:HG22	1:C:162:PRO:HD3	1.95	0.47
1:C:14:CYS:HA	2:c:137:CYS:HA	1.97	0.47
1:C:215:PRO:HG3	1:C:250:ASN:HD22	1.78	0.47
1:C:36:VAL:HG12	1:C:38:ASN:H	1.80	0.47
1:A:29:ILE:HG23	1:A:30:THR:HG23	1.95	0.47
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.97	0.47
1:A:300:ILE:HG12	2:a:68:LYS:HB2	1.96	0.47
2:b:14:TRP:CH2	2:b:25:ARG:HG3	2.50	0.47
2:a:134:GLY:HA2	2:b:124:LYS:HD3	1.96	0.47
1:B:25:ILE:HD11	1:B:33:ARG:HG3	1.96	0.47
1:C:169:PRO:HG2	1:C:171:LYS:NZ	2.29	0.46
1:C:29:ILE:HG23	1:C:30:THR:HG23	1.97	0.46
1:C:288:ILE:HG21	1:C:297:VAL:HG21	1.98	0.46
1:A:187:THR:HG23	1:A:190:ASN:H	1.80	0.46
1:B:325:GLU:HG2	2:b:12:ASN:HD22	1.81	0.46
2:b:44:ALA:HB2	2:b:114:GLU:HG2	1.98	0.45
2:b:27:GLN:NE2	2:b:32:ARG:HH21	2.14	0.45
1:C:307:ARG:HD2	2:c:92:TRP:CE2	2.52	0.45
1:B:127:TRP:HH2	1:B:245:ILE:HG21	1.81	0.45
1:C:237:VAL:HG13	1:C:241:ASP:HB3	1.98	0.45
1:A:180:TRP:HB3	1:A:254:PRO:HD3	1.98	0.45
1:B:127:TRP:CH2	1:B:245:ILE:HG21	2.51	0.45
1:C:184:HIS:O	1:C:228:SER:HB2	2.17	0.45
1:A:136:SER:HB2	1:A:153:TRP:HZ3	1.82	0.45
2:b:149:ILE:HD13	2:b:149:ILE:HA	1.89	0.45
1:C:177:LEU:HD23	1:C:258:PHE:HB2	1.98	0.45
1:A:177:LEU:HD23	1:A:258:PHE:HB2	1.99	0.44
1:A:90:ARG:HD2	1:A:90:ARG:N	2.32	0.44
1:B:117:THR:HG22	1:B:119:GLU:H	1.83	0.44
1:C:308:TYR:HD1	2:c:89:ILE:HG12	1.83	0.44
1:A:160:ILE:HG22	1:A:162:PRO:HD3	1.99	0.44
1:C:187:THR:HG23	1:C:190:ASN:H	1.84	0.43
1:A:90:ARG:HH21	1:A:271:ASP:HA	1.84	0.43
2:a:127:ARG:HG3	2:a:159:HIS:CD2	2.54	0.43
2:b:26:HIS:CG	2:b:149:ILE:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG12	1:A:38:ASN:H	1.84	0.43
2:a:142:HIS:HB2	2:a:162:TYR:HB3	2.01	0.43
1:B:182:VAL:HG11	1:B:213:VAL:HG11	2.01	0.43
1:C:25:ILE:HD12	1:C:25:ILE:HA	1.90	0.43
2:a:141:TYR:CE1	2:a:170:ARG:HD2	2.52	0.42
1:C:268:MET:HE1	1:C:282:ILE:HG22	2.00	0.42
1:C:127:TRP:HD1	1:C:132:GLN:HE21	1.67	0.42
1:C:299:ARG:HH21	2:c:89:ILE:HD13	1.84	0.42
1:A:288:ILE:HG21	1:A:297:VAL:HG21	2.01	0.42
1:B:307:ARG:HD2	2:b:92:TRP:CE2	2.54	0.42
1:C:117:THR:HG22	1:C:119:GLU:H	1.84	0.42
2:c:128:GLU:HB2	2:c:170:ARG:NH1	2.34	0.42
1:A:154:LEU:HD11	1:A:253:ALA:HB2	2.01	0.42
2:a:167:LEU:HD22	2:a:171:PHE:HE2	1.85	0.42
1:C:327:GLN:HE21	1:C:327:GLN:HB3	1.66	0.42
1:C:174:PHE:CZ	1:C:259:LYS:HE2	2.55	0.42
6:H:1:NAG:H61	6:H:2:NAG:H82	2.02	0.42
2:b:126:LEU:HD23	2:b:130:ALA:HB3	2.02	0.42
2:c:47:GLN:OE1	2:c:110:LEU:HD11	2.20	0.42
1:A:10:THR:CB	2:a:141:TYR:HA	2.49	0.42
2:c:21:TRP:HB2	2:c:41:THR:HB	2.01	0.42
1:A:102:VAL:HG12	1:A:104:ASP:H	1.85	0.41
1:A:117:THR:HG22	1:A:119:GLU:H	1.85	0.41
2:b:1:GLY:HA2	2:b:112:ASP:OD2	2.21	0.41
1:A:307:ARG:HD2	2:a:92:TRP:CE2	2.55	0.41
1:B:36:VAL:HG12	1:B:38:ASN:H	1.85	0.41
1:B:37:THR:HG22	1:B:320:MET:H	1.84	0.41
1:C:177:LEU:HB2	1:C:260:ILE:HD12	2.02	0.41
1:C:48:ILE:H	1:C:48:ILE:HG13	1.63	0.41
1:C:201:ARG:HD2	5:Z:1:NAG:H83	2.02	0.41
1:B:321:ARG:HB3	2:b:6:ILE:HG21	2.02	0.41
1:C:102:VAL:HG12	1:C:104:ASP:H	1.86	0.41
1:C:170:ASN:ND2	1:C:176:LYS:HG3	2.35	0.41
2:a:26:HIS:CG	2:a:149:ILE:HG21	2.55	0.41
1:B:187:THR:HG23	1:B:190:ASN:H	1.85	0.41
1:B:318:THR:HG22	1:B:318:THR:O	2.21	0.41
2:b:156:THR:HG23	2:b:156:THR:O	2.22	0.40
1:B:226:ILE:HD13	1:B:226:ILE:HA	1.99	0.40
1:B:323:VAL:HA	1:B:324:PRO:HD3	1.90	0.40
1:B:326:LYS:HG3	1:B:327:GLN:H	1.87	0.40
2:a:2:ILE:HG23	2:a:3:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:HIS:HE1	1:B:323:VAL:HG13	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/334 (96%)	310 (97%)	11 (3%)	0	100	100
1	B	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	C	321/334 (96%)	312 (97%)	9 (3%)	0	100	100
2	a	175/238 (74%)	168 (96%)	7 (4%)	0	100	100
2	b	175/238 (74%)	168 (96%)	7 (4%)	0	100	100
2	c	175/238 (74%)	167 (95%)	8 (5%)	0	100	100
All	All	1488/1716 (87%)	1436 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/295 (96%)	274 (96%)	10 (4%)	32	56
1	B	284/295 (96%)	274 (96%)	10 (4%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	284/295 (96%)	275 (97%)	9 (3%)	34	58
2	a	150/198 (76%)	147 (98%)	3 (2%)	48	66
2	b	150/198 (76%)	148 (99%)	2 (1%)	61	72
2	c	150/198 (76%)	146 (97%)	4 (3%)	39	61
All	All	1302/1479 (88%)	1264 (97%)	38 (3%)	38	60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	CYS
1	A	104	ASP
1	A	179	ILE
1	A	214	ILE
1	A	228	SER
1	A	231	SER
1	A	248	THR
1	A	276	GLU
1	A	305	CYS
1	A	327	GLN
2	a	69	GLU
2	a	73	VAL
2	a	86	ASP
1	B	18	HIS
1	B	20	VAL
1	B	76	CYS
1	B	104	ASP
1	B	130	VAL
1	B	214	ILE
1	B	228	SER
1	B	277	CYS
1	B	323	VAL
1	B	327	GLN
2	b	73	VAL
2	b	86	ASP
1	C	76	CYS
1	C	83	GLU
1	C	179	ILE
1	C	214	ILE
1	C	246	ASN
1	C	248	THR
1	C	260	ILE

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Mol	Chain	Res	Type
1	C	305	CYS
1	C	327	GLN
2	c	73	VAL
2	c	77	VAL
2	c	86	ASP
2	c	168	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	31	ASN
1	A	56	HIS
1	A	132	GLN
1	A	158	ASN
1	A	211	GLN
1	A	327	GLN
2	a	27	GLN
2	a	65	GLN
1	B	31	ASN
1	B	132	GLN
1	B	190	ASN
1	B	250	ASN
1	B	290	ASN
1	B	327	GLN
2	b	27	GLN
2	b	47	GLN
2	b	65	GLN
2	b	116	ASN
1	C	6	ASN
1	C	18	HIS
1	C	31	ASN
1	C	132	GLN
1	C	190	ASN
1	C	250	ASN
1	C	327	GLN
2	c	27	GLN
2	c	78	GLN
2	c	116	ASN
2	c	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

105 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	$\# Z > 2$
3	NAG	D	1	2,3	14,14,15	0.72	0	17,19,21	1.64	3 (17%)
3	NAG	D	2	3	14,14,15	0.74	0	17,19,21	0.89	0
4	NAG	E	1	1,4	14,14,15	0.73	0	17,19,21	1.23	2 (11%)
4	NAG	E	2	4	14,14,15	0.70	0	17,19,21	1.32	1 (5%)
4	BMA	E	3	4	11,11,12	0.85	0	15,15,17	2.27	3 (20%)
4	MAN	E	4	4	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
5	NAG	F	1	5,1	14,14,15	0.79	0	17,19,21	1.24	4 (23%)
5	NAG	F	2	5	14,14,15	0.71	0	17,19,21	0.87	0
5	BMA	F	3	5	11,11,12	0.81	0	15,15,17	2.07	4 (26%)
5	MAN	F	4	5	11,11,12	0.66	0	15,15,17	1.32	1 (6%)
5	MAN	F	5	5	11,11,12	0.72	0	15,15,17	1.09	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.72	0	17,19,21	1.18	1 (5%)
3	NAG	G	2	3	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
6	NAG	H	1	6,1	14,14,15	0.76	0	17,19,21	1.53	3 (17%)
6	NAG	H	2	6	14,14,15	0.73	0	17,19,21	0.95	0
6	BMA	H	3	6	11,11,12	0.84	0	15,15,17	2.11	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.72	0	17,19,21	0.76	0
3	NAG	I	2	3	14,14,15	0.72	0	17,19,21	0.86	0
6	NAG	J	1	6,1	14,14,15	0.74	0	17,19,21	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	J	2	6	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
6	BMA	J	3	6	11,11,12	0.83	0	15,15,17	2.12	3 (20%)
7	NAG	K	1	7,1	14,14,15	0.73	0	17,19,21	0.84	0
7	NAG	K	2	7	14,14,15	0.72	0	17,19,21	0.89	0
7	BMA	K	3	7	11,11,12	0.83	0	15,15,17	1.99	2 (13%)
7	MAN	K	4	7	11,11,12	0.73	0	15,15,17	1.02	1 (6%)
6	NAG	L	1	6,1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
6	NAG	L	2	6	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
6	BMA	L	3	6	11,11,12	0.84	0	15,15,17	2.13	3 (20%)
8	NAG	M	1	1,8	14,14,15	0.70	0	17,19,21	1.21	2 (11%)
8	NAG	M	2	8	14,14,15	0.74	0	17,19,21	0.99	0
8	BMA	M	3	8	11,11,12	0.83	0	15,15,17	2.00	4 (26%)
8	MAN	M	4	8	11,11,12	0.63	0	15,15,17	1.44	1 (6%)
8	MAN	M	5	8	11,11,12	0.73	0	15,15,17	1.01	1 (6%)
8	MAN	M	6	8	11,11,12	0.69	0	15,15,17	1.16	1 (6%)
8	MAN	M	7	8	11,11,12	0.63	0	15,15,17	1.38	1 (6%)
3	NAG	N	1	2,3	14,14,15	0.68	0	17,19,21	1.01	1 (5%)
3	NAG	N	2	3	14,14,15	0.74	0	17,19,21	0.88	0
4	NAG	O	1	1,4	14,14,15	0.73	0	17,19,21	1.24	2 (11%)
4	NAG	O	2	4	14,14,15	0.70	0	17,19,21	1.33	1 (5%)
4	BMA	O	3	4	11,11,12	0.85	0	15,15,17	2.25	3 (20%)
4	MAN	O	4	4	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
5	NAG	P	1	5,1	14,14,15	0.72	0	17,19,21	0.85	0
5	NAG	P	2	5	14,14,15	0.72	0	17,19,21	0.86	0
5	BMA	P	3	5	11,11,12	0.81	0	15,15,17	2.04	4 (26%)
5	MAN	P	4	5	11,11,12	0.67	0	15,15,17	1.28	1 (6%)
5	MAN	P	5	5	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
3	NAG	Q	1	3,1	14,14,15	0.72	0	17,19,21	1.18	1 (5%)
3	NAG	Q	2	3	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
6	NAG	R	1	6,1	14,14,15	0.69	0	17,19,21	1.32	1 (5%)
6	NAG	R	2	6	14,14,15	0.72	0	17,19,21	0.91	0
6	BMA	R	3	6	11,11,12	0.84	0	15,15,17	2.12	3 (20%)
3	NAG	S	1	3,1	14,14,15	0.72	0	17,19,21	0.76	0
3	NAG	S	2	3	14,14,15	0.72	0	17,19,21	0.86	0
6	NAG	T	1	6,1	14,14,15	0.72	0	17,19,21	0.98	0
6	NAG	T	2	6	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
6	BMA	T	3	6	11,11,12	0.84	0	15,15,17	2.12	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	U	1	7,1	14,14,15	0.72	0	17,19,21	0.87	0
7	NAG	U	2	7	14,14,15	0.72	0	17,19,21	0.88	0
7	BMA	U	3	7	11,11,12	0.83	0	15,15,17	1.99	2 (13%)
7	MAN	U	4	7	11,11,12	0.73	0	15,15,17	1.02	1 (6%)
6	NAG	V	1	6,1	14,14,15	0.70	0	17,19,21	1.29	2 (11%)
6	NAG	V	2	6	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
6	BMA	V	3	6	11,11,12	0.84	0	15,15,17	2.14	3 (20%)
8	NAG	W	1	1,8	14,14,15	0.70	0	17,19,21	1.20	2 (11%)
8	NAG	W	2	8	14,14,15	0.76	0	17,19,21	1.00	0
8	BMA	W	3	8	11,11,12	0.83	0	15,15,17	2.00	4 (26%)
8	MAN	W	4	8	11,11,12	0.64	0	15,15,17	1.45	1 (6%)
8	MAN	W	5	8	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
8	MAN	W	6	8	11,11,12	0.68	0	15,15,17	1.17	1 (6%)
8	MAN	W	7	8	11,11,12	0.64	0	15,15,17	1.37	1 (6%)
3	NAG	X	1	2,3	14,14,15	0.68	0	17,19,21	0.91	1 (5%)
3	NAG	X	2	3	14,14,15	0.73	0	17,19,21	0.84	0
4	NAG	Y	1	1,4	14,14,15	0.72	0	17,19,21	1.23	2 (11%)
4	NAG	Y	2	4	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
4	BMA	Y	3	4	11,11,12	0.85	0	15,15,17	2.26	3 (20%)
4	MAN	Y	4	4	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
5	NAG	Z	1	5,1	14,14,15	0.71	0	17,19,21	0.85	0
5	NAG	Z	2	5	14,14,15	0.71	0	17,19,21	0.86	0
5	BMA	Z	3	5	11,11,12	0.81	0	15,15,17	2.04	4 (26%)
5	MAN	Z	4	5	11,11,12	0.67	0	15,15,17	1.28	1 (6%)
5	MAN	Z	5	5	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
3	NAG	d	1	3,1	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
3	NAG	d	2	3	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.69	0	17,19,21	1.52	3 (17%)
6	NAG	e	2	6	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
6	BMA	e	3	6	11,11,12	0.84	0	15,15,17	2.17	3 (20%)
3	NAG	f	1	3,1	14,14,15	0.72	0	17,19,21	0.76	0
3	NAG	f	2	3	14,14,15	0.72	0	17,19,21	0.85	0
6	NAG	g	1	6,1	14,14,15	0.73	0	17,19,21	0.98	0
6	NAG	g	2	6	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
6	BMA	g	3	6	11,11,12	0.84	0	15,15,17	2.12	3 (20%)
7	NAG	h	1	7,1	14,14,15	0.73	0	17,19,21	0.83	0
7	NAG	h	2	7	14,14,15	0.72	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	h	3	7	11,11,12	0.83	0	15,15,17	1.99	3 (20%)
7	MAN	h	4	7	11,11,12	0.73	0	15,15,17	1.02	1 (6%)
6	NAG	i	1	6,1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
6	NAG	i	2	6	14,14,15	0.70	0	17,19,21	0.86	1 (5%)
6	BMA	i	3	6	11,11,12	0.84	0	15,15,17	2.13	3 (20%)
8	NAG	j	1	1,8	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
8	NAG	j	2	8	14,14,15	0.75	0	17,19,21	1.01	0
8	BMA	j	3	8	11,11,12	0.83	0	15,15,17	1.99	4 (26%)
8	MAN	j	4	8	11,11,12	0.63	0	15,15,17	1.43	1 (6%)
8	MAN	j	5	8	11,11,12	0.73	0	15,15,17	1.01	1 (6%)
8	MAN	j	6	8	11,11,12	0.68	0	15,15,17	1.16	1 (6%)
8	MAN	j	7	8	11,11,12	0.63	0	15,15,17	1.40	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. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	1/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	1/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
8	NAG	M	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	1/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1
8	MAN	M	5	8	-	0/2/19/22	0/1/1/1
8	MAN	M	6	8	-	0/2/19/22	0/1/1/1
8	MAN	M	7	8	-	0/2/19/22	0/1/1/1
3	NAG	N	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	0/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	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
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
6	BMA	R	3	6	-	1/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	1/2/19/22	0/1/1/1
7	NAG	U	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	BMA	U	3	7	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	2/2/19/22	0/1/1/1
8	MAN	j	4	8	-	0/2/19/22	0/1/1/1
8	MAN	j	5	8	-	0/2/19/22	0/1/1/1
8	MAN	j	6	8	-	0/2/19/22	0/1/1/1
8	MAN	j	7	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C1-O5-C5	7.24	121.89	112.19
4	Y	3	BMA	C1-O5-C5	7.20	121.83	112.19
4	O	3	BMA	C1-O5-C5	7.19	121.82	112.19
6	e	3	BMA	C1-O5-C5	6.76	121.25	112.19
6	V	3	BMA	C1-O5-C5	6.65	121.10	112.19
6	L	3	BMA	C1-O5-C5	6.63	121.08	112.19
6	i	3	BMA	C1-O5-C5	6.62	121.05	112.19
6	R	3	BMA	C1-O5-C5	6.59	121.01	112.19
6	g	3	BMA	C1-O5-C5	6.58	121.00	112.19
6	T	3	BMA	C1-O5-C5	6.57	121.00	112.19
6	J	3	BMA	C1-O5-C5	6.57	120.99	112.19
6	H	3	BMA	C1-O5-C5	6.51	120.91	112.19
5	F	3	BMA	C1-O5-C5	6.04	120.28	112.19
7	U	3	BMA	C1-O5-C5	5.97	120.19	112.19
7	K	3	BMA	C1-O5-C5	5.97	120.18	112.19
7	h	3	BMA	C1-O5-C5	5.97	120.18	112.19
5	Z	3	BMA	C1-O5-C5	5.90	120.09	112.19
5	P	3	BMA	C1-O5-C5	5.89	120.08	112.19
8	j	7	MAN	C1-O5-C5	4.53	118.26	112.19
8	M	3	BMA	C1-O5-C5	4.52	118.25	112.19
8	j	3	BMA	C1-O5-C5	4.52	118.24	112.19
8	W	3	BMA	C1-O5-C5	4.49	118.21	112.19
8	j	4	MAN	C1-O5-C5	4.49	118.21	112.19
8	M	4	MAN	C1-O5-C5	4.47	118.17	112.19
8	M	7	MAN	C1-O5-C5	4.44	118.13	112.19
8	W	4	MAN	C1-O5-C5	4.41	118.10	112.19
8	W	7	MAN	C1-O5-C5	4.35	118.02	112.19
5	F	4	MAN	C1-O5-C5	4.23	117.85	112.19
5	Z	4	MAN	C1-O5-C5	4.07	117.64	112.19
5	P	4	MAN	C1-O5-C5	4.07	117.64	112.19
6	e	1	NAG	C2-N2-C7	3.96	128.21	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O5-C1-C2	-3.82	105.38	111.29
6	R	1	NAG	C2-N2-C7	3.65	127.79	122.90
8	W	6	MAN	C1-O5-C5	3.52	116.90	112.19
6	H	1	NAG	C1-O5-C5	3.52	116.90	112.19
8	j	6	MAN	C1-O5-C5	3.49	116.86	112.19
8	M	6	MAN	C1-O5-C5	3.48	116.85	112.19
6	i	1	NAG	C2-N2-C7	3.47	127.54	122.90
6	L	1	NAG	C2-N2-C7	3.46	127.54	122.90
6	V	1	NAG	C2-N2-C7	3.42	127.49	122.90
3	D	1	NAG	C1-C2-N2	3.40	115.78	110.43
4	O	1	NAG	C2-N2-C7	3.39	127.44	122.90
4	Y	1	NAG	C2-N2-C7	3.38	127.44	122.90
4	E	1	NAG	C2-N2-C7	3.37	127.42	122.90
8	W	3	BMA	C3-C4-C5	3.36	116.32	110.23
8	M	3	BMA	C3-C4-C5	3.31	116.24	110.23
4	O	2	NAG	C2-N2-C7	3.28	127.30	122.90
8	j	3	BMA	C3-C4-C5	3.27	116.16	110.23
4	E	2	NAG	C2-N2-C7	3.25	127.26	122.90
8	j	1	NAG	C2-N2-C7	3.25	127.26	122.90
3	G	1	NAG	C2-N2-C7	3.24	127.24	122.90
3	Q	1	NAG	C2-N2-C7	3.24	127.24	122.90
4	Y	2	NAG	C2-N2-C7	3.24	127.24	122.90
3	d	1	NAG	C2-N2-C7	3.22	127.22	122.90
3	d	2	NAG	C2-N2-C7	3.21	127.21	122.90
3	Q	2	NAG	C2-N2-C7	3.21	127.21	122.90
3	G	2	NAG	C2-N2-C7	3.21	127.20	122.90
8	W	1	NAG	C2-N2-C7	3.18	127.16	122.90
5	Z	5	MAN	C1-O5-C5	3.17	116.44	112.19
5	P	5	MAN	C1-O5-C5	3.17	116.44	112.19
8	M	1	NAG	C2-N2-C7	3.12	127.08	122.90
5	F	5	MAN	C1-O5-C5	3.08	116.32	112.19
4	O	4	MAN	C1-O5-C5	3.02	116.23	112.19
4	Y	4	MAN	C1-O5-C5	2.94	116.13	112.19
4	E	4	MAN	C1-O5-C5	2.92	116.10	112.19
6	H	1	NAG	C2-N2-C7	2.87	126.75	122.90
6	H	1	NAG	C3-C4-C5	-2.83	105.10	110.23
3	D	1	NAG	C1-O5-C5	2.79	115.92	112.19
8	j	5	MAN	C1-O5-C5	2.77	115.89	112.19
8	M	5	MAN	C1-O5-C5	2.75	115.87	112.19
3	N	1	NAG	O5-C1-C2	-2.70	107.11	111.29
8	W	5	MAN	C1-O5-C5	2.70	115.80	112.19
7	h	4	MAN	C1-O5-C5	2.68	115.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	4	MAN	C1-O5-C5	2.67	115.77	112.19
7	U	4	MAN	C1-O5-C5	2.67	115.76	112.19
6	e	1	NAG	C1-O5-C5	-2.60	108.70	112.19
6	L	1	NAG	O5-C1-C2	-2.56	107.32	111.29
6	i	1	NAG	O5-C1-C2	-2.56	107.33	111.29
6	V	1	NAG	O5-C1-C2	-2.52	107.39	111.29
3	X	1	NAG	O5-C1-C2	-2.50	107.42	111.29
8	M	3	BMA	C2-C3-C4	2.38	115.05	110.86
5	F	1	NAG	O5-C1-C2	-2.36	107.64	111.29
8	W	3	BMA	O4-C4-C3	-2.36	104.82	110.38
8	j	3	BMA	C2-C3-C4	2.35	115.00	110.86
8	W	3	BMA	C2-C3-C4	2.35	115.00	110.86
6	g	2	NAG	O5-C1-C2	-2.34	107.67	111.29
4	E	3	BMA	C2-C3-C4	2.33	114.96	110.86
4	Y	3	BMA	C2-C3-C4	2.33	114.96	110.86
4	O	3	BMA	C2-C3-C4	2.32	114.94	110.86
8	M	3	BMA	O4-C4-C3	-2.32	104.92	110.38
6	T	2	NAG	O5-C1-C2	-2.31	107.71	111.29
6	J	2	NAG	O5-C1-C2	-2.31	107.72	111.29
4	O	1	NAG	O5-C1-C2	-2.29	107.75	111.29
8	j	3	BMA	O4-C4-C3	-2.29	104.98	110.38
5	F	1	NAG	C2-N2-C7	2.28	125.96	122.90
7	h	3	BMA	C3-C4-C5	2.28	114.36	110.23
5	F	3	BMA	O3-C3-C2	-2.28	105.41	110.05
7	K	3	BMA	C3-C4-C5	2.27	114.35	110.23
6	e	3	BMA	C2-C3-C4	2.27	114.86	110.86
7	U	3	BMA	C3-C4-C5	2.27	114.34	110.23
6	V	3	BMA	C2-C3-C4	2.26	114.83	110.86
6	R	3	BMA	C2-C3-C4	2.25	114.83	110.86
6	L	3	BMA	C2-C3-C4	2.25	114.82	110.86
6	i	3	BMA	C2-C3-C4	2.25	114.82	110.86
5	Z	3	BMA	O3-C3-C2	-2.24	105.48	110.05
6	H	3	BMA	C2-C3-C4	2.23	114.78	110.86
5	P	3	BMA	O3-C3-C2	-2.23	105.51	110.05
6	g	3	BMA	C2-C3-C4	2.22	114.77	110.86
6	J	3	BMA	C2-C3-C4	2.22	114.76	110.86
5	P	3	BMA	C3-C4-C5	2.22	114.25	110.23
6	T	3	BMA	C2-C3-C4	2.22	114.76	110.86
5	Z	3	BMA	C3-C4-C5	2.21	114.24	110.23
6	e	3	BMA	C3-C4-C5	2.21	114.24	110.23
5	F	3	BMA	C3-C4-C5	2.21	114.23	110.23
5	Z	3	BMA	C2-C3-C4	2.20	114.72	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	3	BMA	C3-C4-C5	2.20	114.21	110.23
6	e	2	NAG	O5-C1-C2	-2.19	107.90	111.29
6	V	3	BMA	C3-C4-C5	2.19	114.21	110.23
6	i	3	BMA	C3-C4-C5	2.19	114.21	110.23
4	Y	3	BMA	C3-C4-C5	2.19	114.21	110.23
4	E	3	BMA	C3-C4-C5	2.19	114.20	110.23
5	P	3	BMA	C2-C3-C4	2.19	114.71	110.86
6	H	3	BMA	C3-C4-C5	2.19	114.20	110.23
5	F	3	BMA	C2-C3-C4	2.19	114.71	110.86
6	R	3	BMA	C3-C4-C5	2.19	114.20	110.23
6	T	3	BMA	C3-C4-C5	2.19	114.20	110.23
4	O	3	BMA	C3-C4-C5	2.19	114.19	110.23
6	J	3	BMA	C3-C4-C5	2.18	114.19	110.23
6	g	3	BMA	C3-C4-C5	2.18	114.19	110.23
6	V	2	NAG	O5-C1-C2	-2.18	107.92	111.29
6	L	2	NAG	O5-C1-C2	-2.14	107.98	111.29
6	i	2	NAG	O5-C1-C2	-2.14	107.98	111.29
8	W	1	NAG	O5-C1-C2	-2.13	107.99	111.29
4	Y	1	NAG	O5-C1-C2	-2.12	108.02	111.29
5	F	1	NAG	O4-C4-C3	-2.11	105.41	110.38
5	F	1	NAG	C1-O5-C5	2.09	114.99	112.19
8	M	1	NAG	O5-C1-C2	-2.05	108.12	111.29
4	E	1	NAG	O5-C1-C2	-2.03	108.14	111.29
6	e	1	NAG	O5-C1-C2	-2.03	108.15	111.29
8	j	1	NAG	O5-C1-C2	-2.01	108.18	111.29
7	h	3	BMA	C2-C3-C4	2.00	114.38	110.86

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C1-C2-N2-C7
4	E	3	BMA	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
4	Y	3	BMA	O5-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	Y	3	BMA	C4-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
8	j	3	BMA	C4-C5-C6-O6
8	W	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
8	j	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
8	M	3	BMA	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
5	P	5	MAN	O5-C5-C6-O6
5	Z	5	MAN	O5-C5-C6-O6
5	F	5	MAN	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6
7	h	4	MAN	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	Q	1	NAG	C1-C2-N2-C7
3	d	1	NAG	C1-C2-N2-C7
3	d	2	NAG	C1-C2-N2-C7
4	E	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
6	L	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C1-C2-N2-C7
6	i	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C4-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

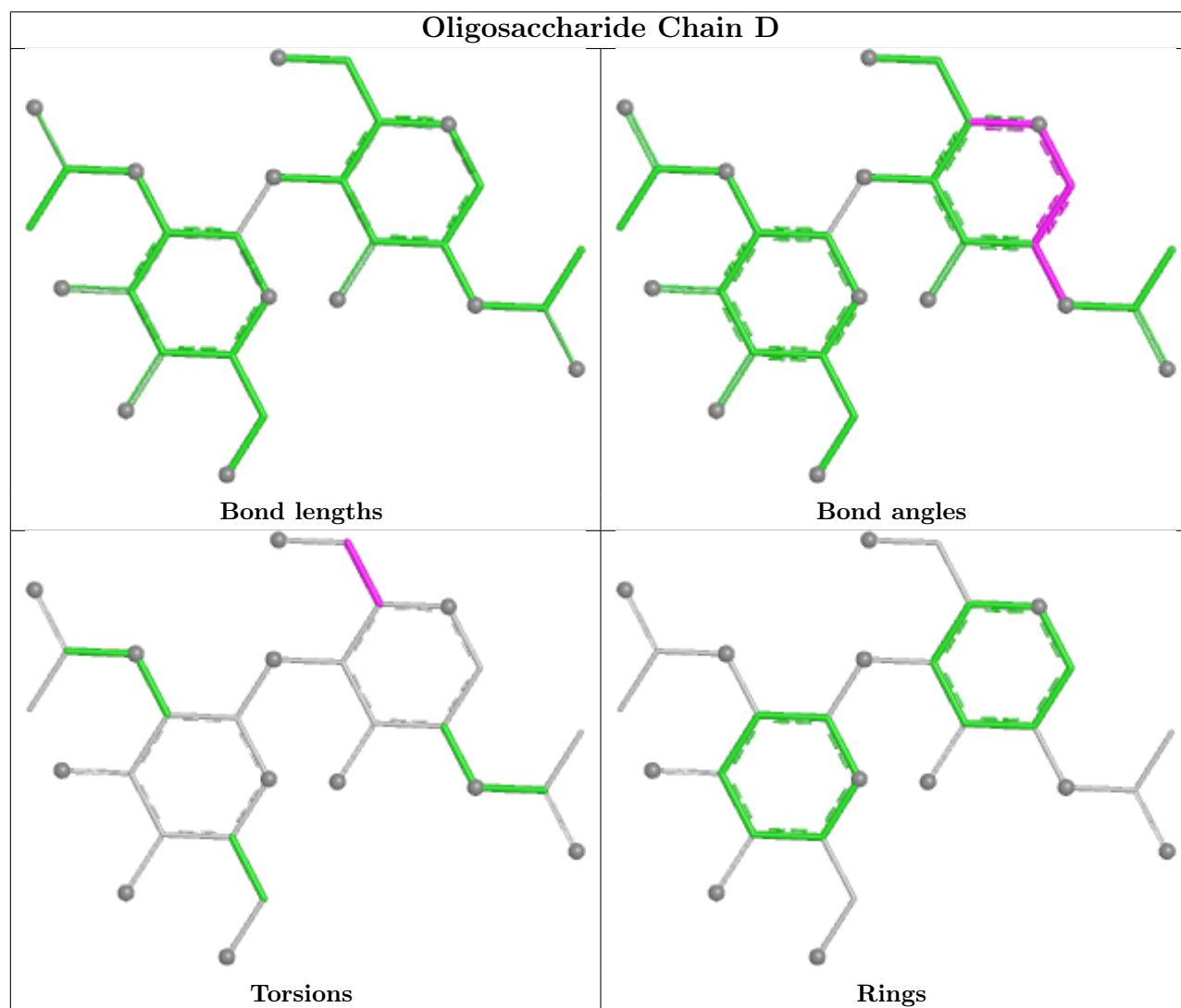
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C3-C2-N2-C7
4	O	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
6	e	1	NAG	C3-C2-N2-C7
8	M	1	NAG	C3-C2-N2-C7
8	W	1	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
6	L	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	i	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	O	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
6	H	1	NAG	C1-C2-N2-C7
8	M	1	NAG	C1-C2-N2-C7
8	M	2	NAG	C1-C2-N2-C7
8	W	1	NAG	C1-C2-N2-C7
8	j	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	Q	1	NAG	C3-C2-N2-C7
3	d	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
6	H	1	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	i	1	NAG	C3-C2-N2-C7
4	O	1	NAG	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6

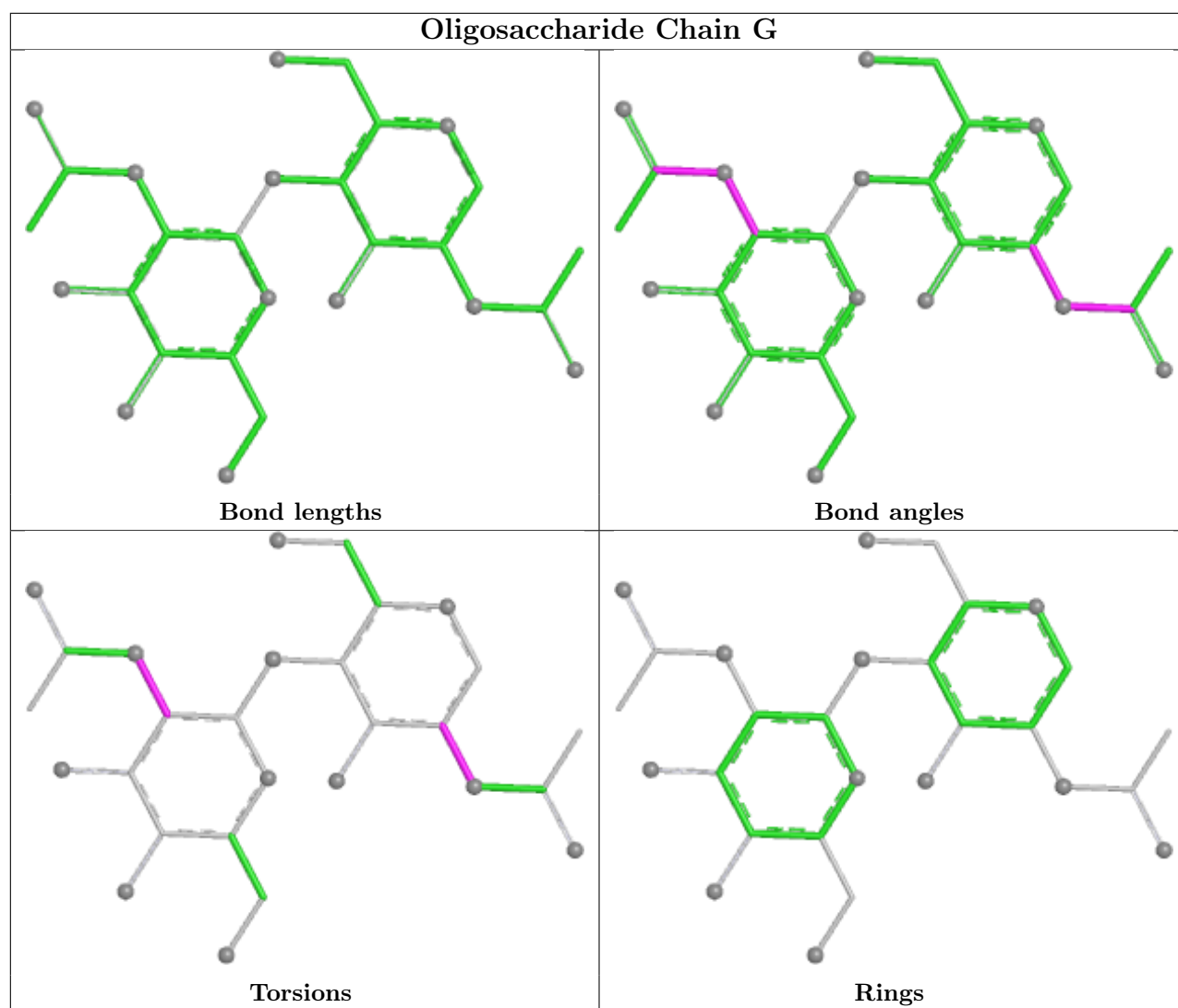
There are no ring outliers.

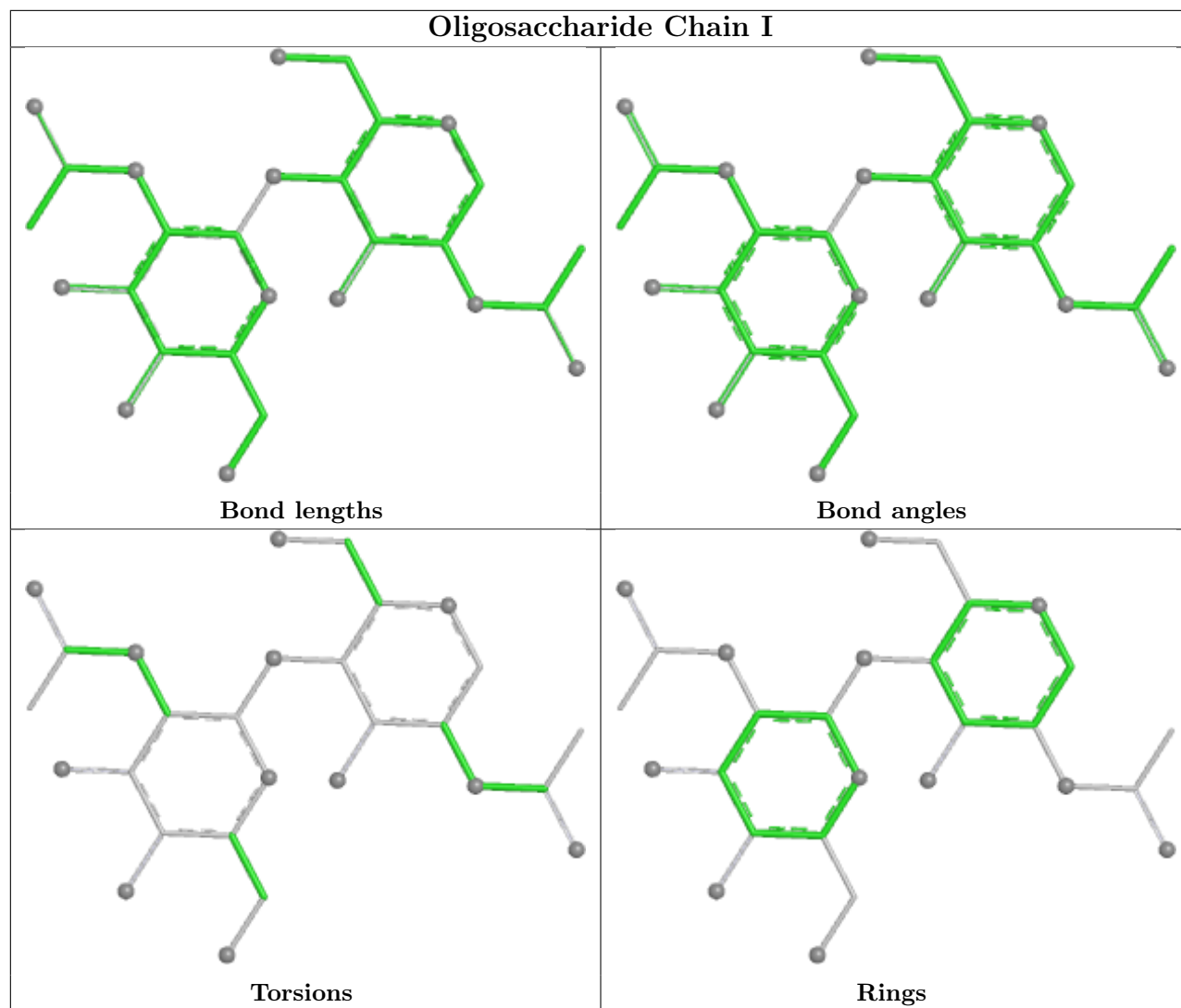
3 monomers are involved in 2 short contacts:

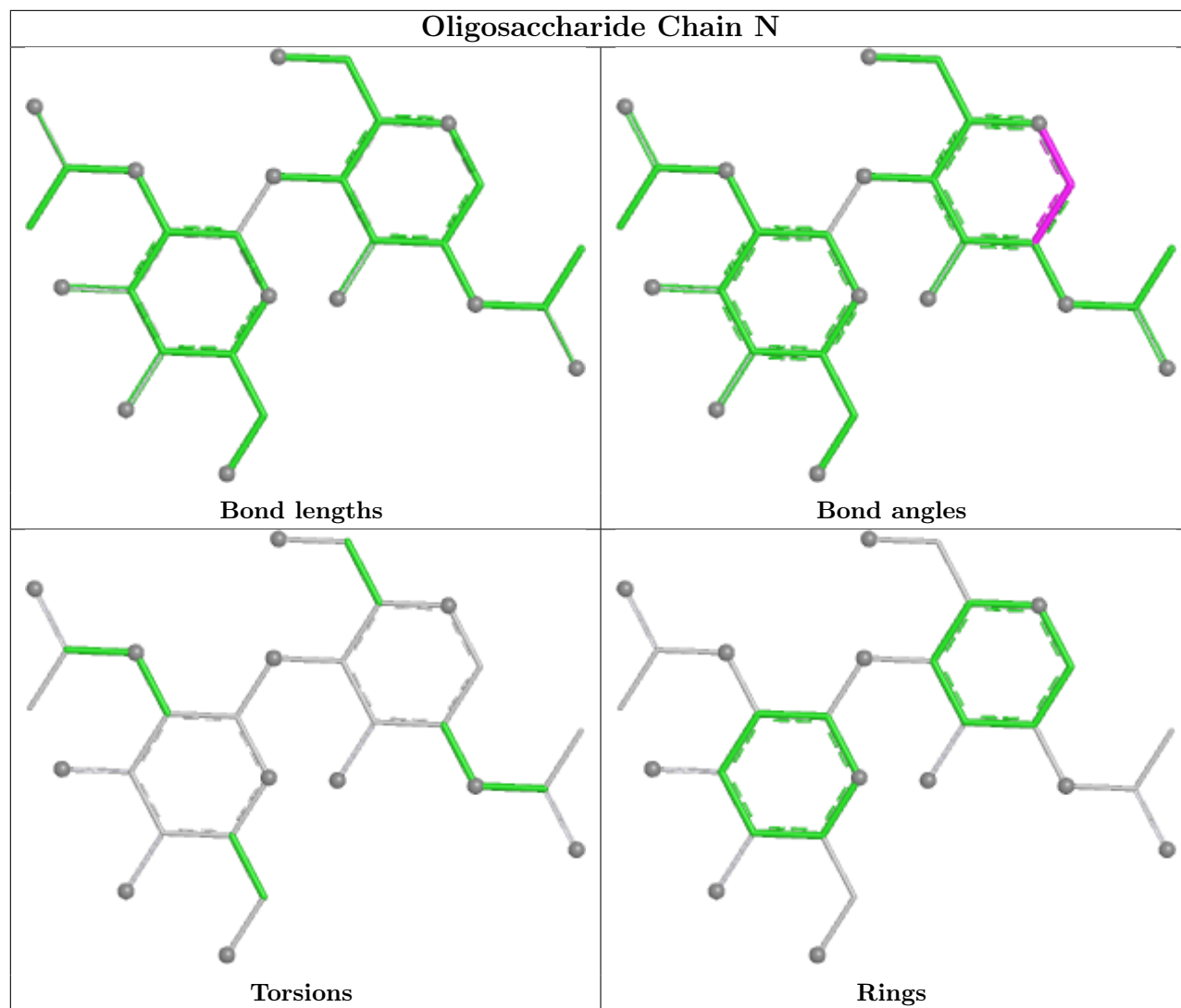
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0
6	H	2	NAG	1	0
5	Z	1	NAG	1	0

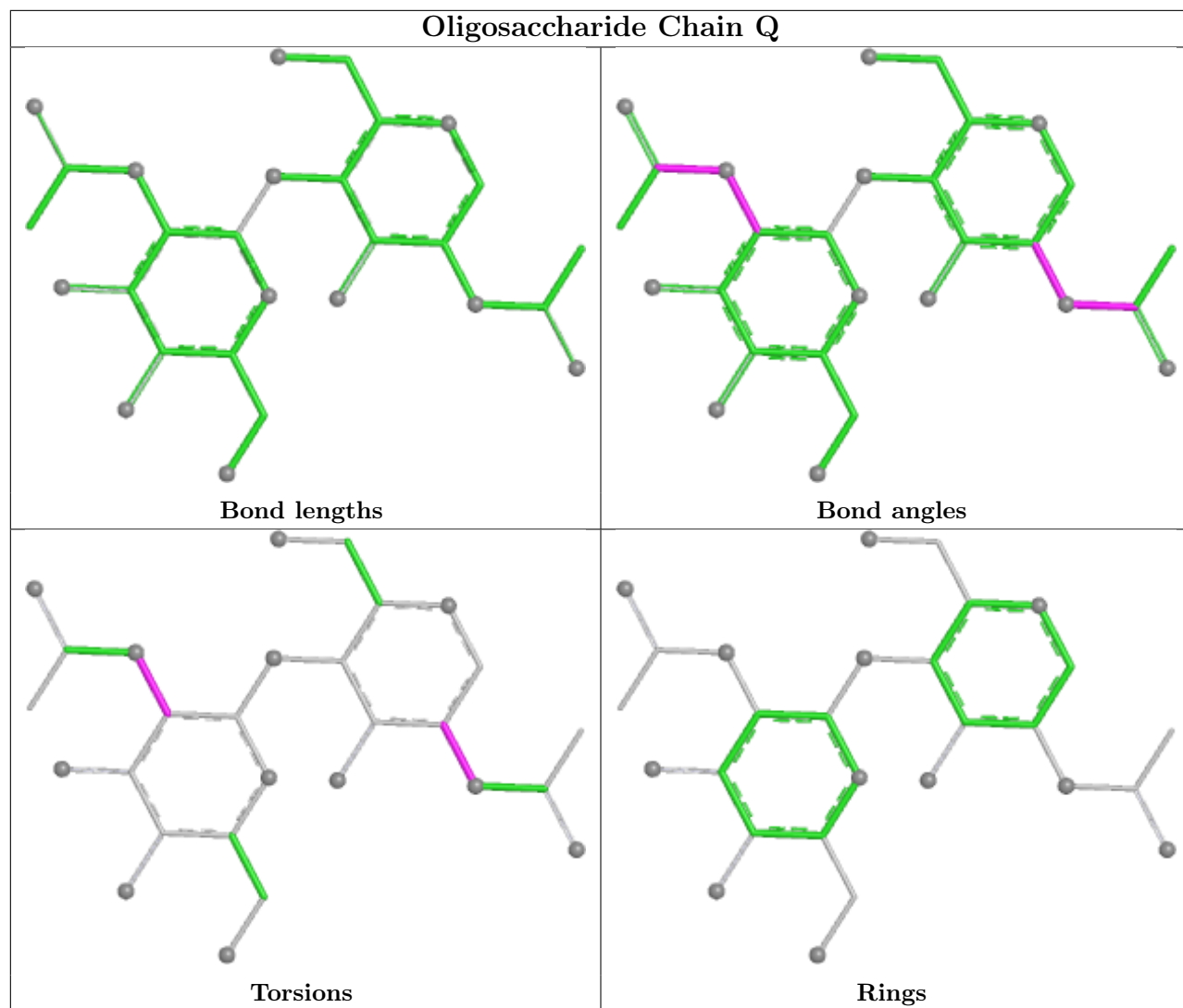
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

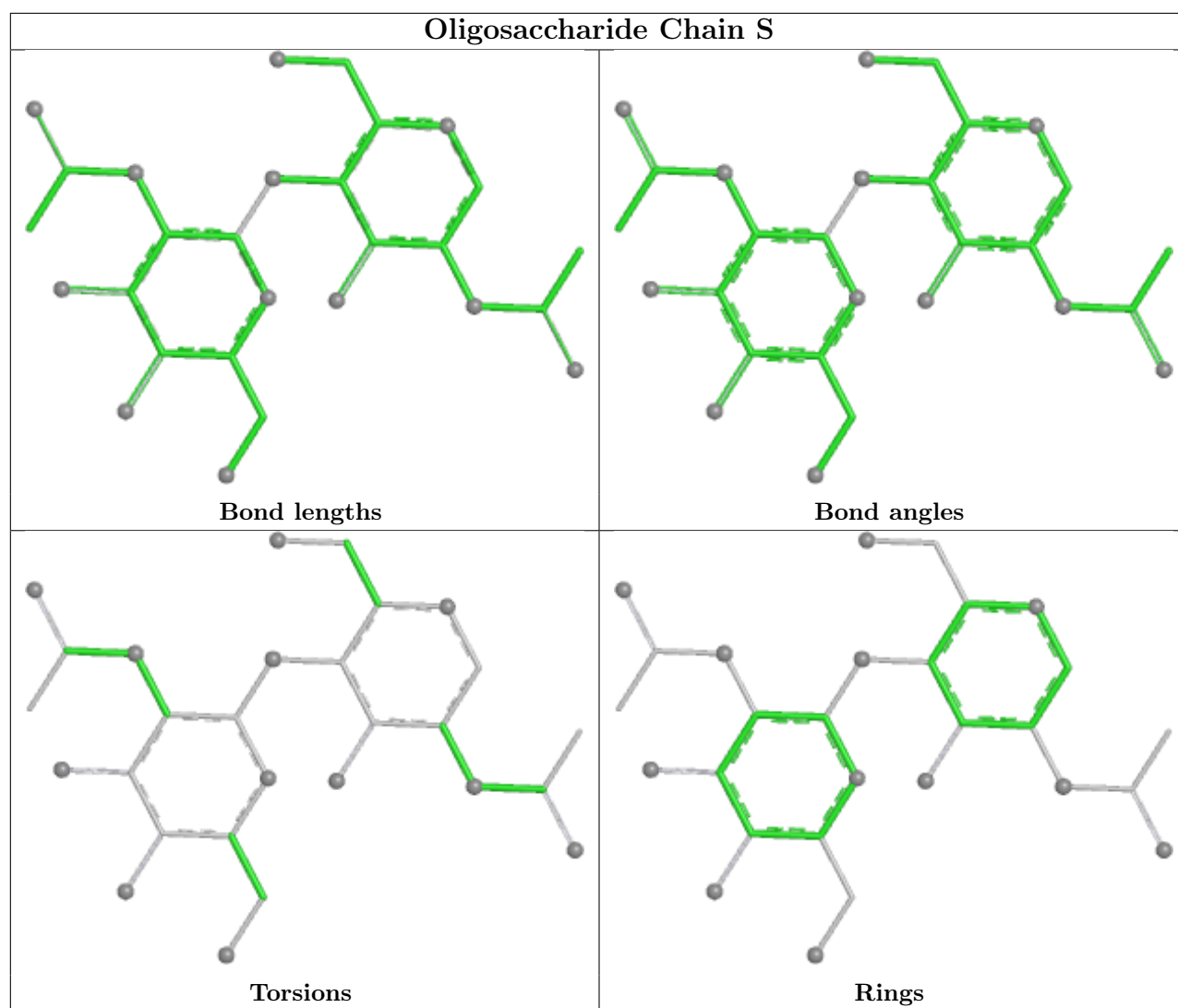


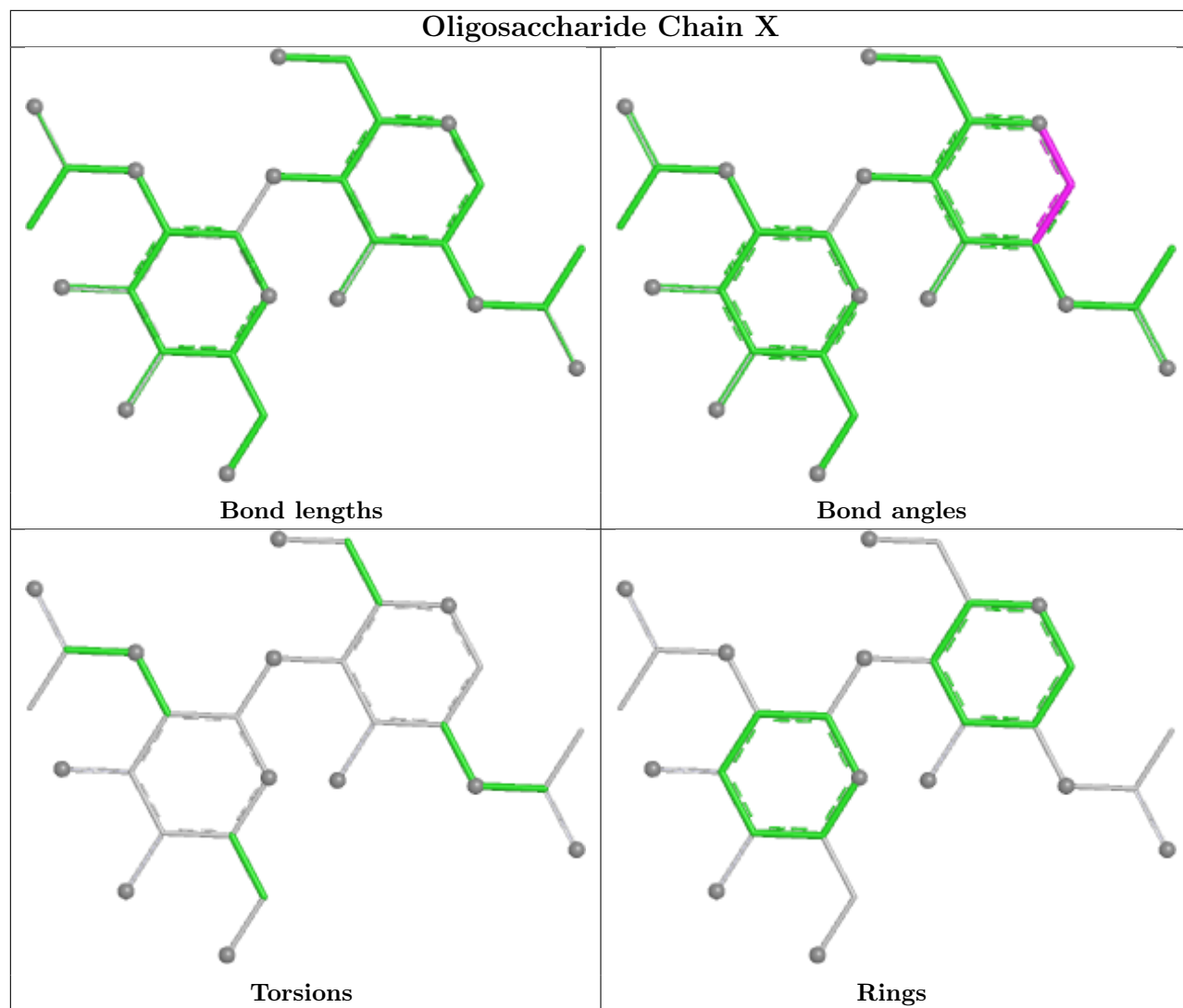


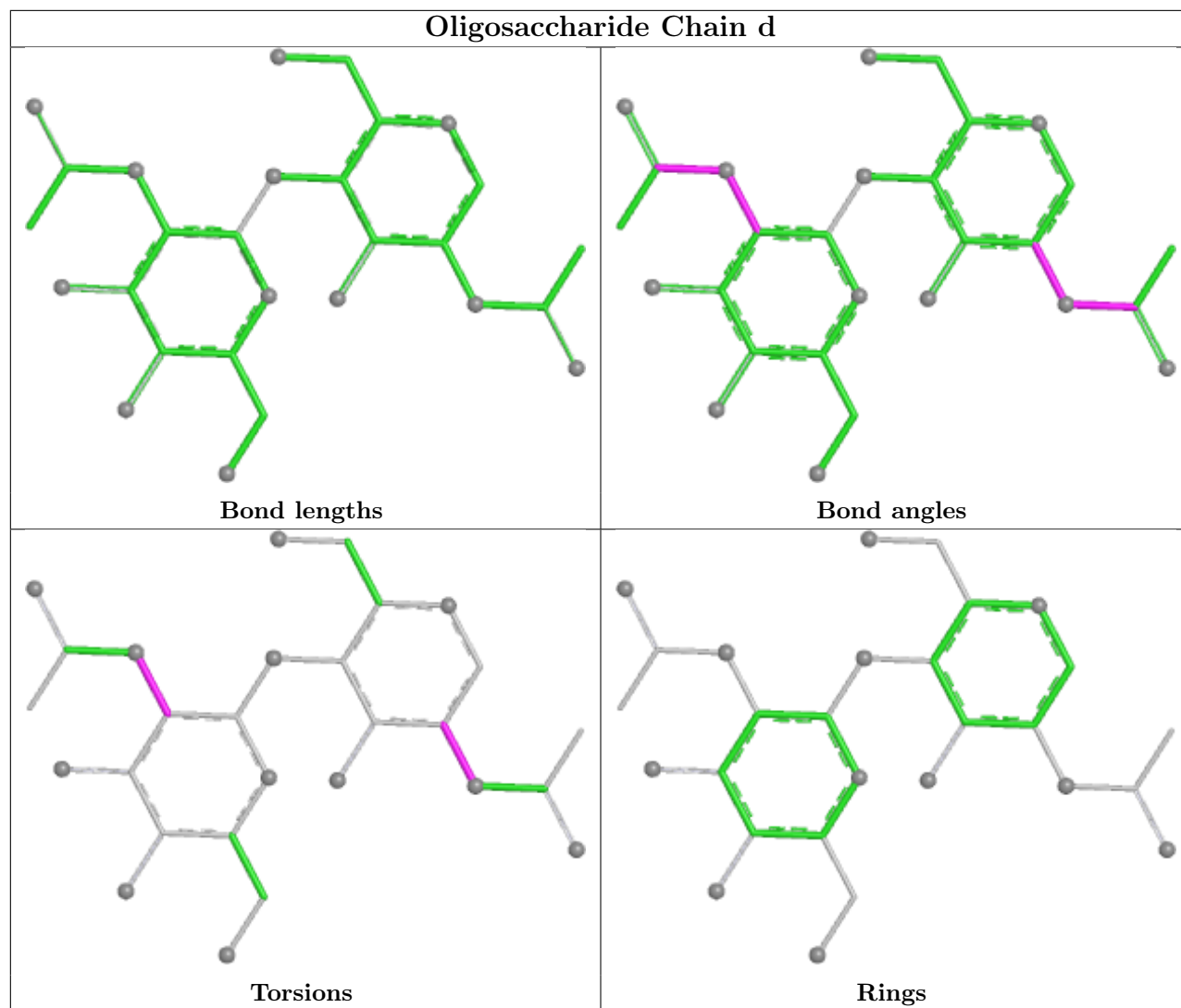


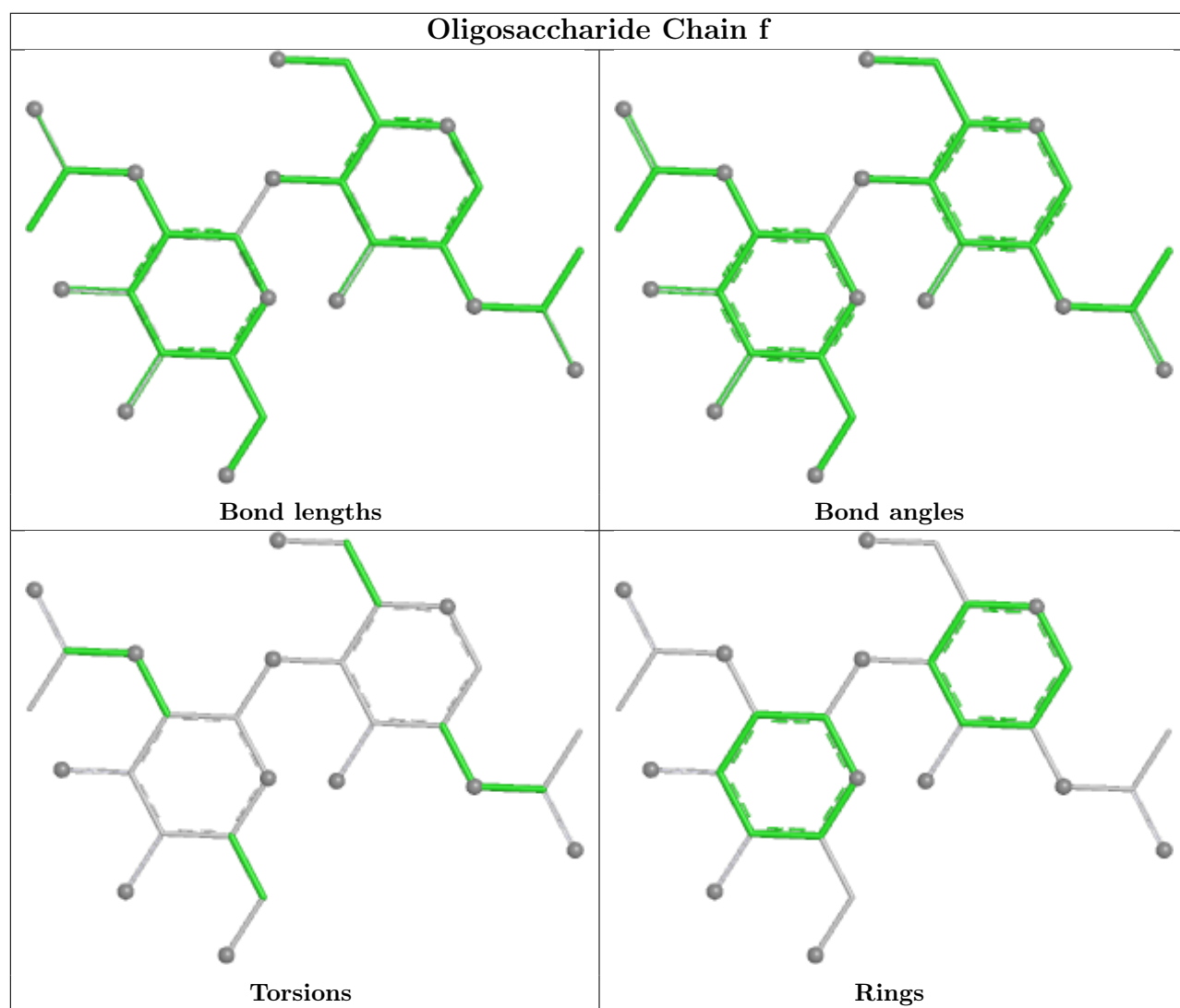


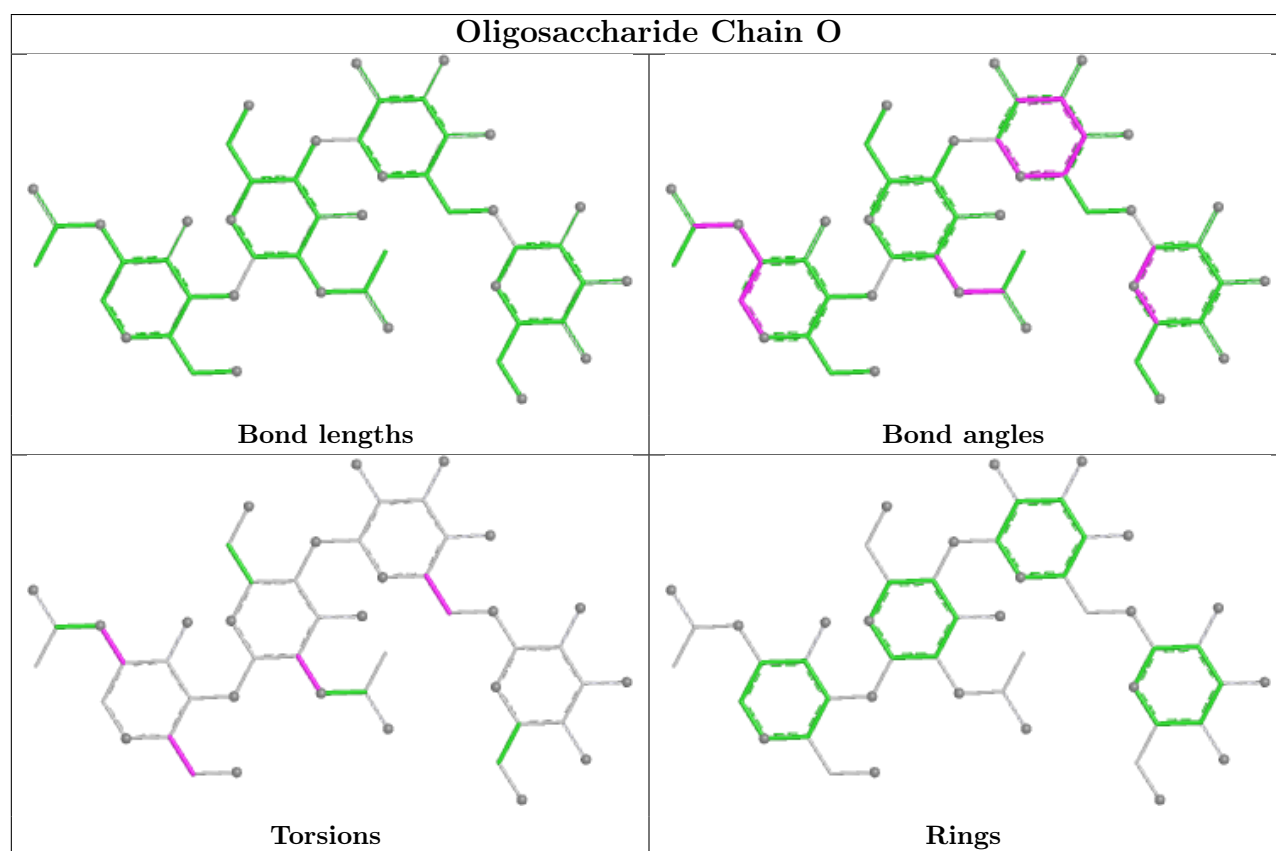
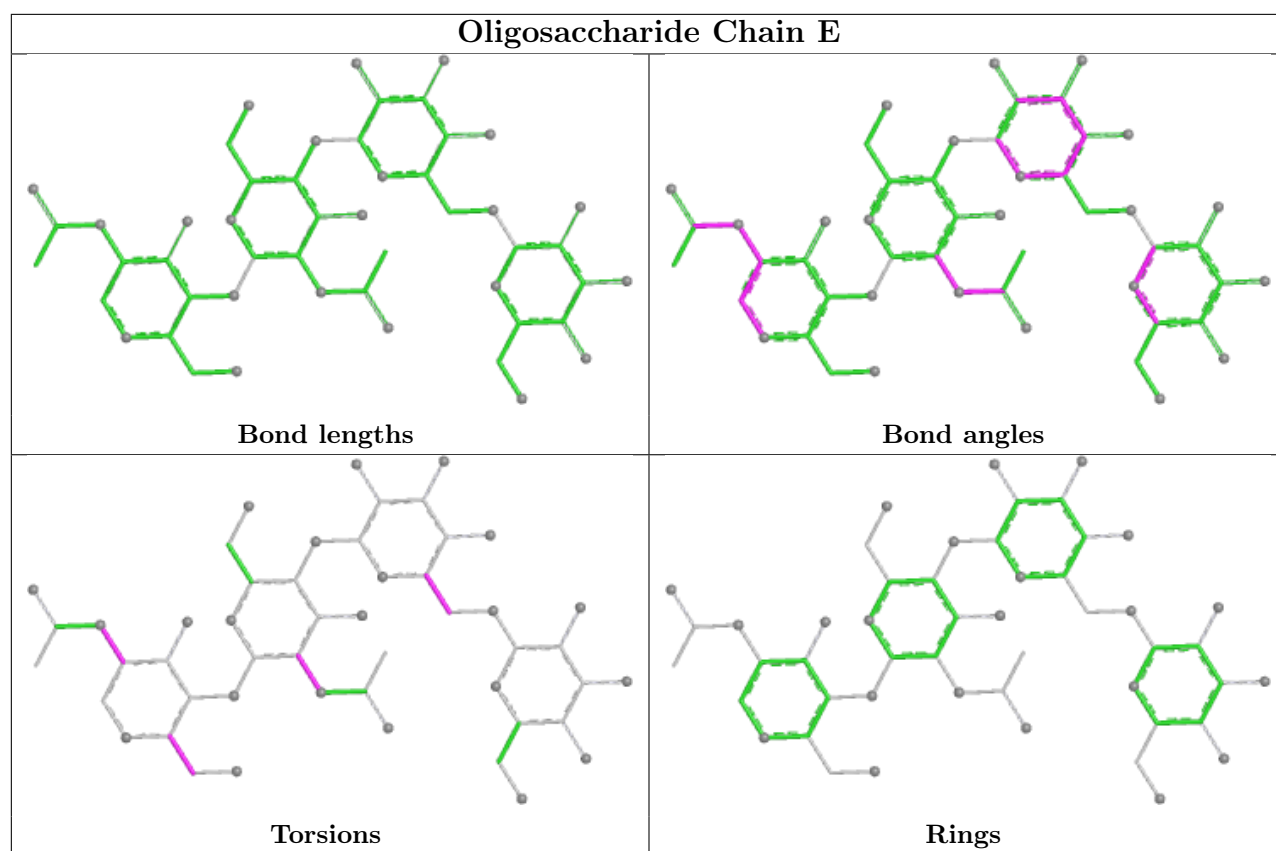


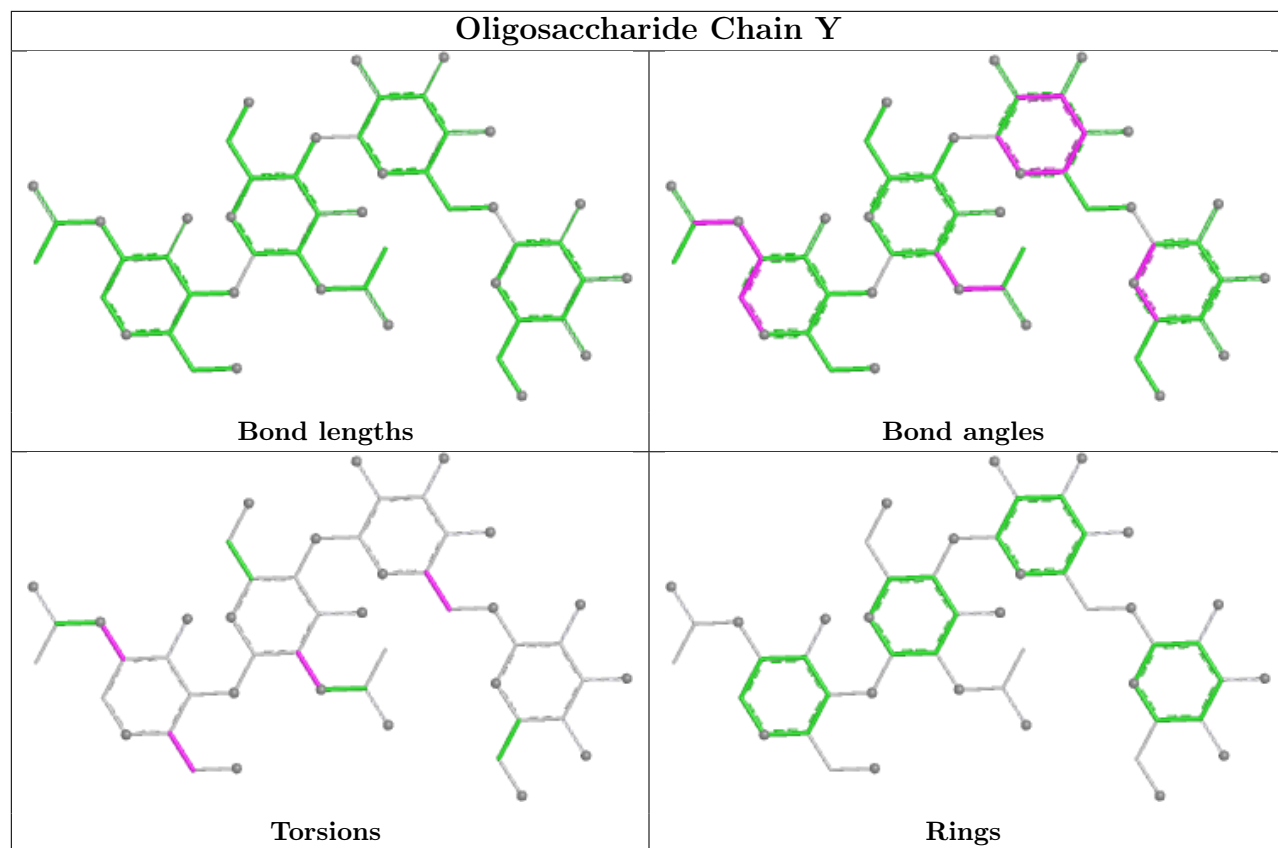


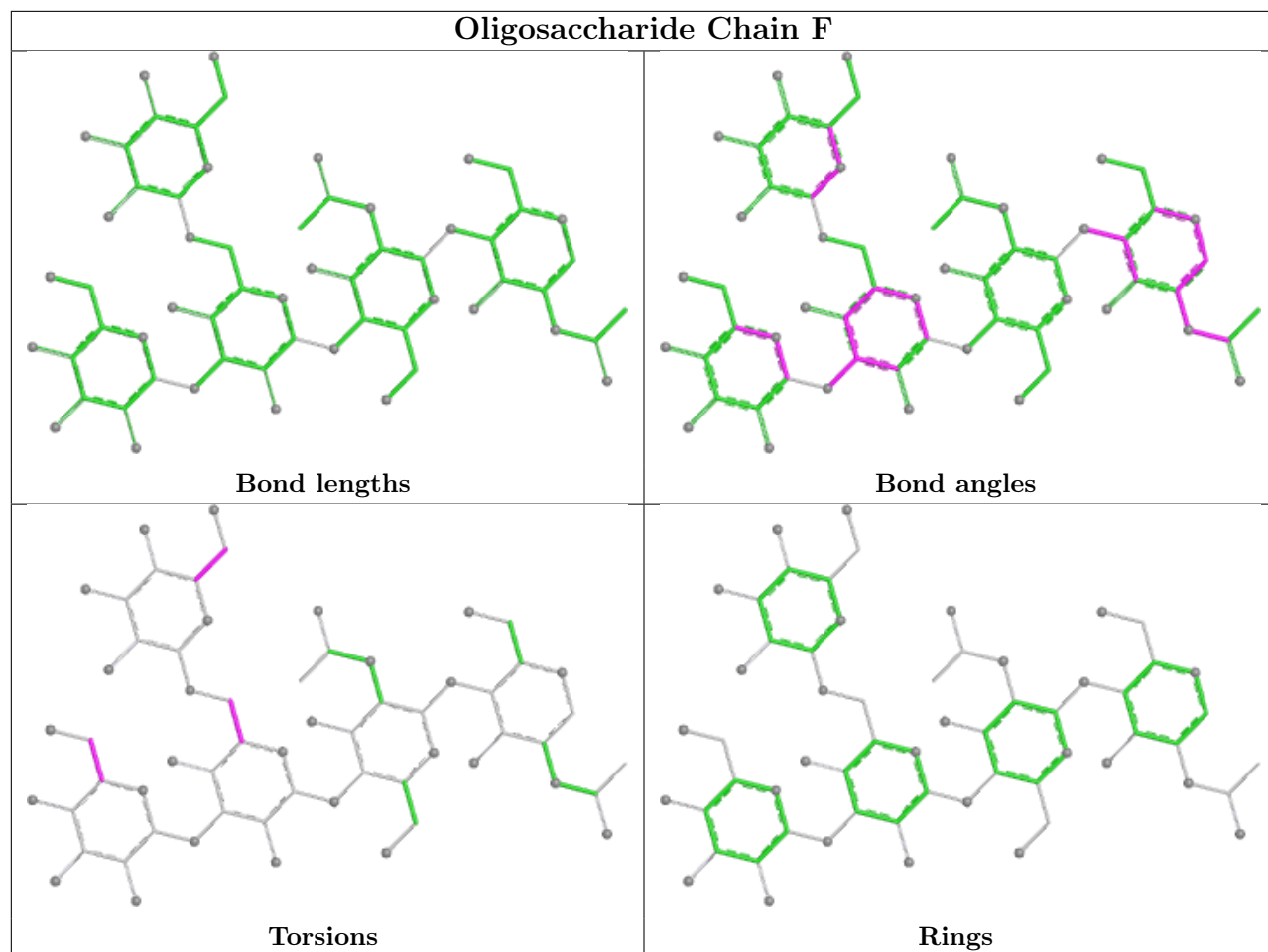


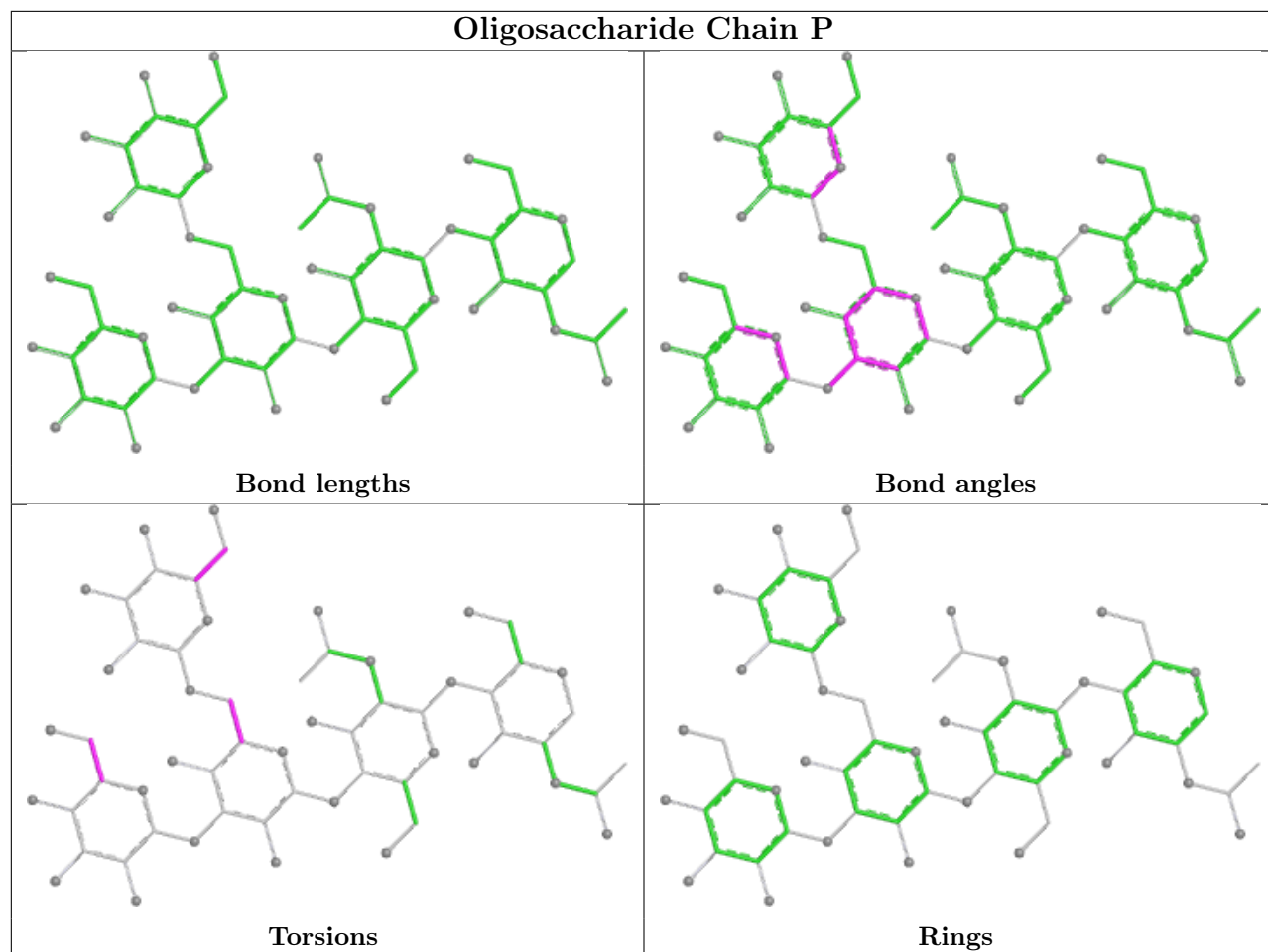


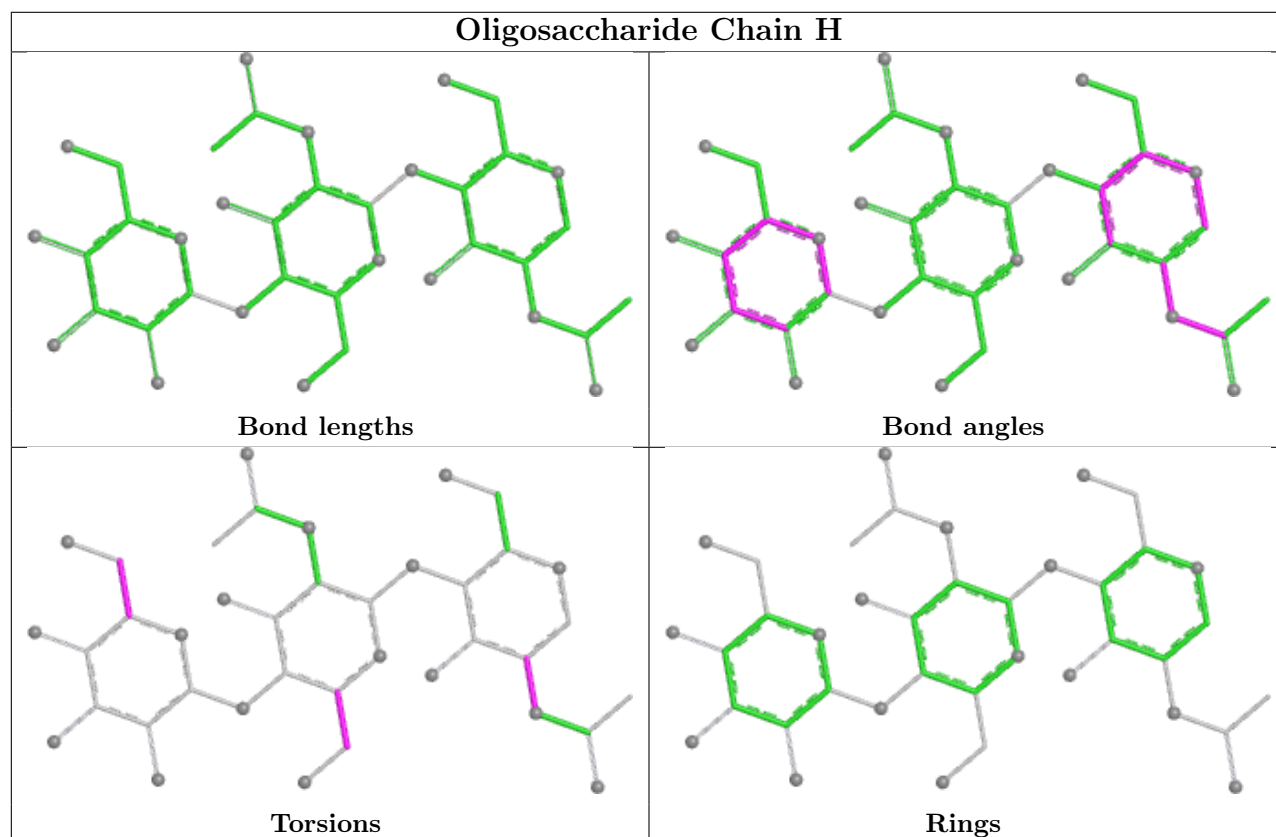
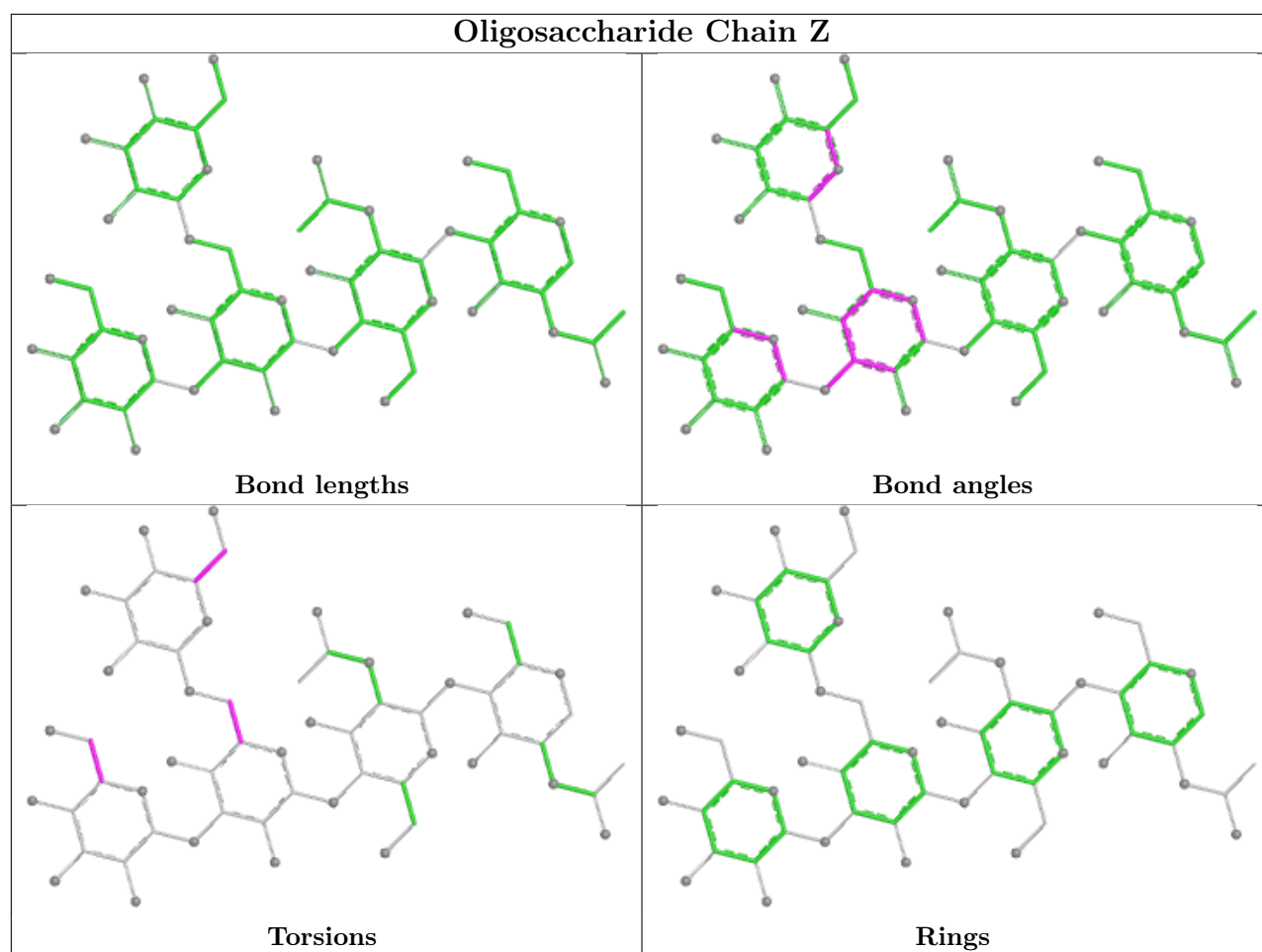


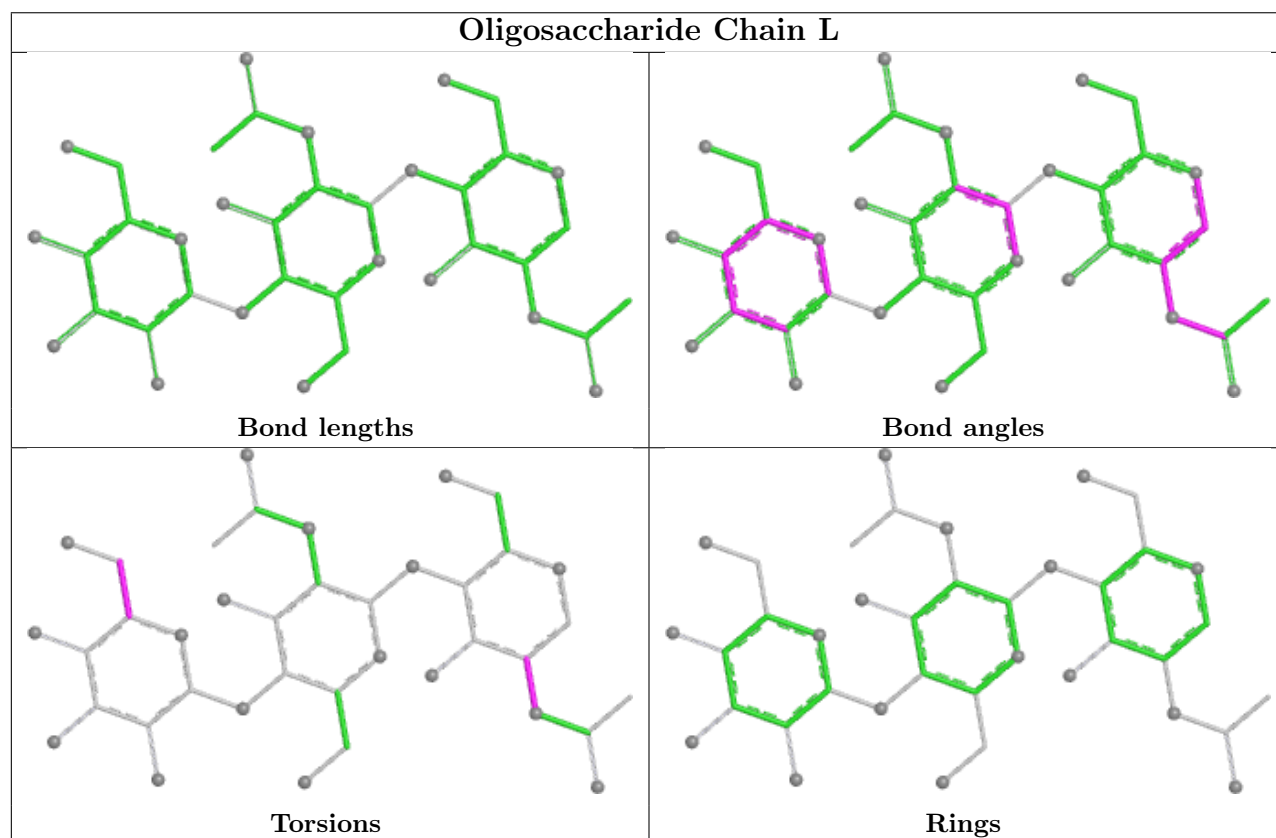
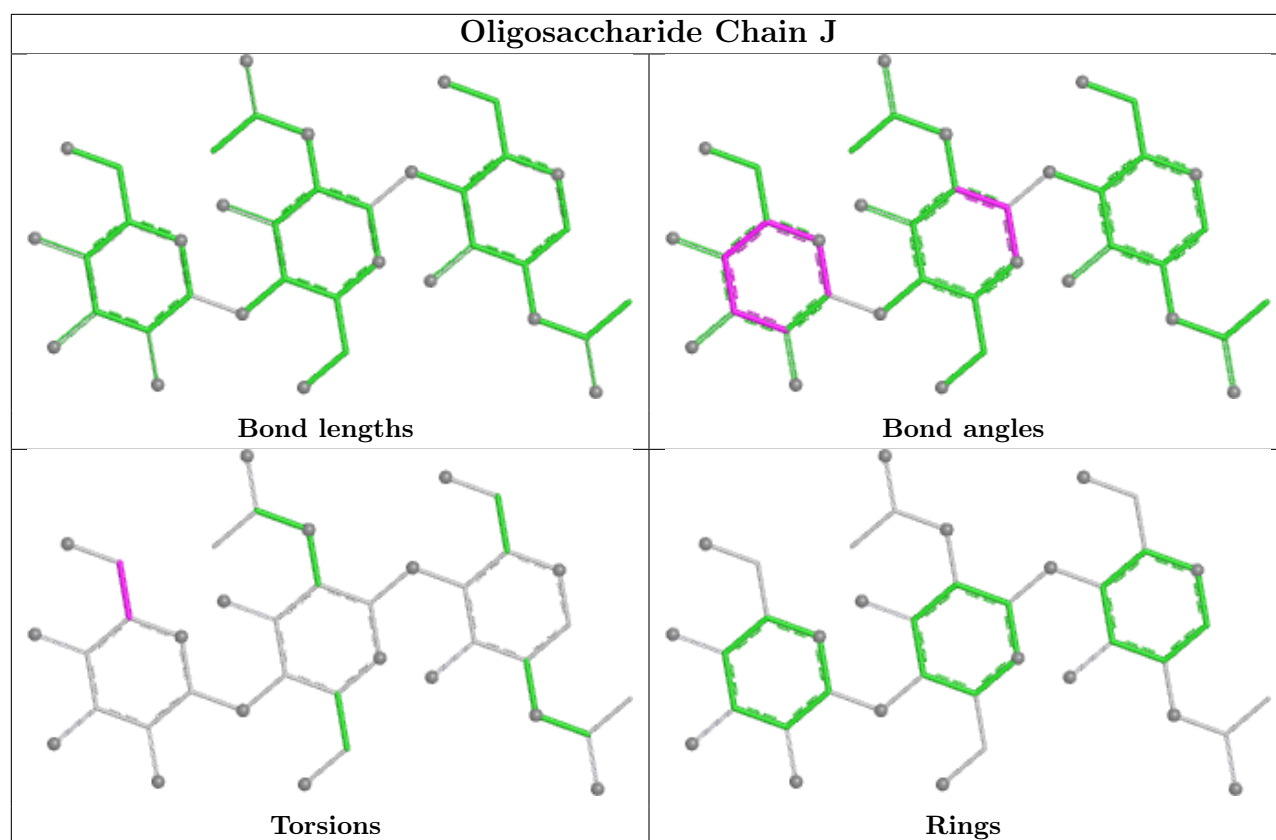


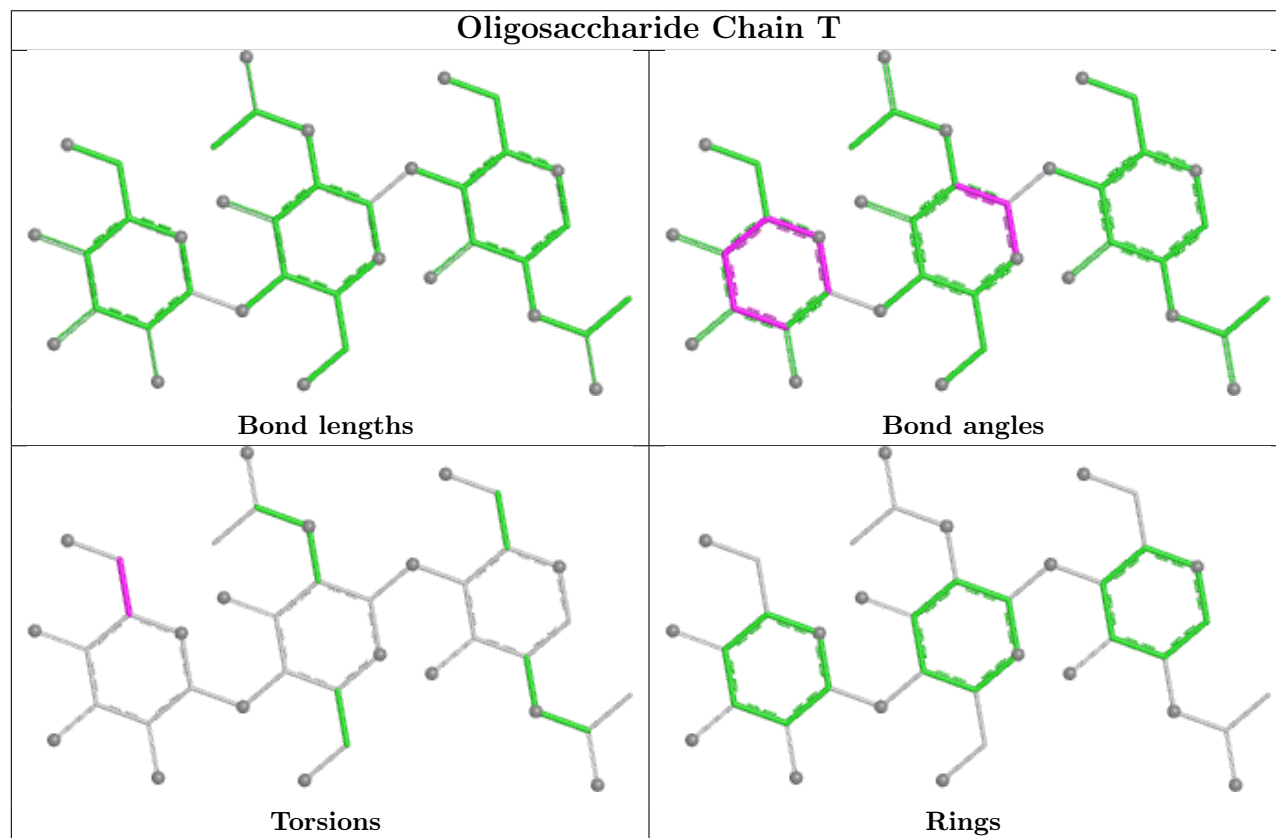
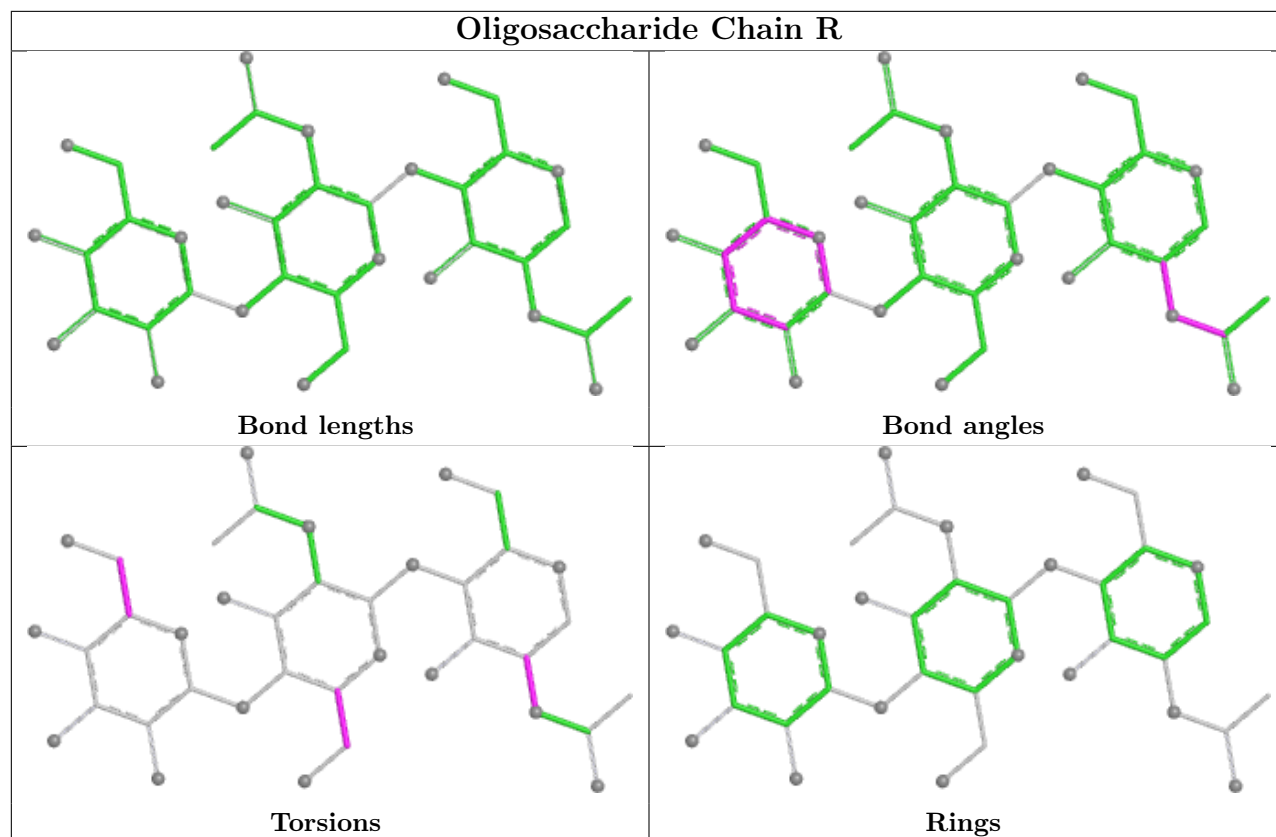


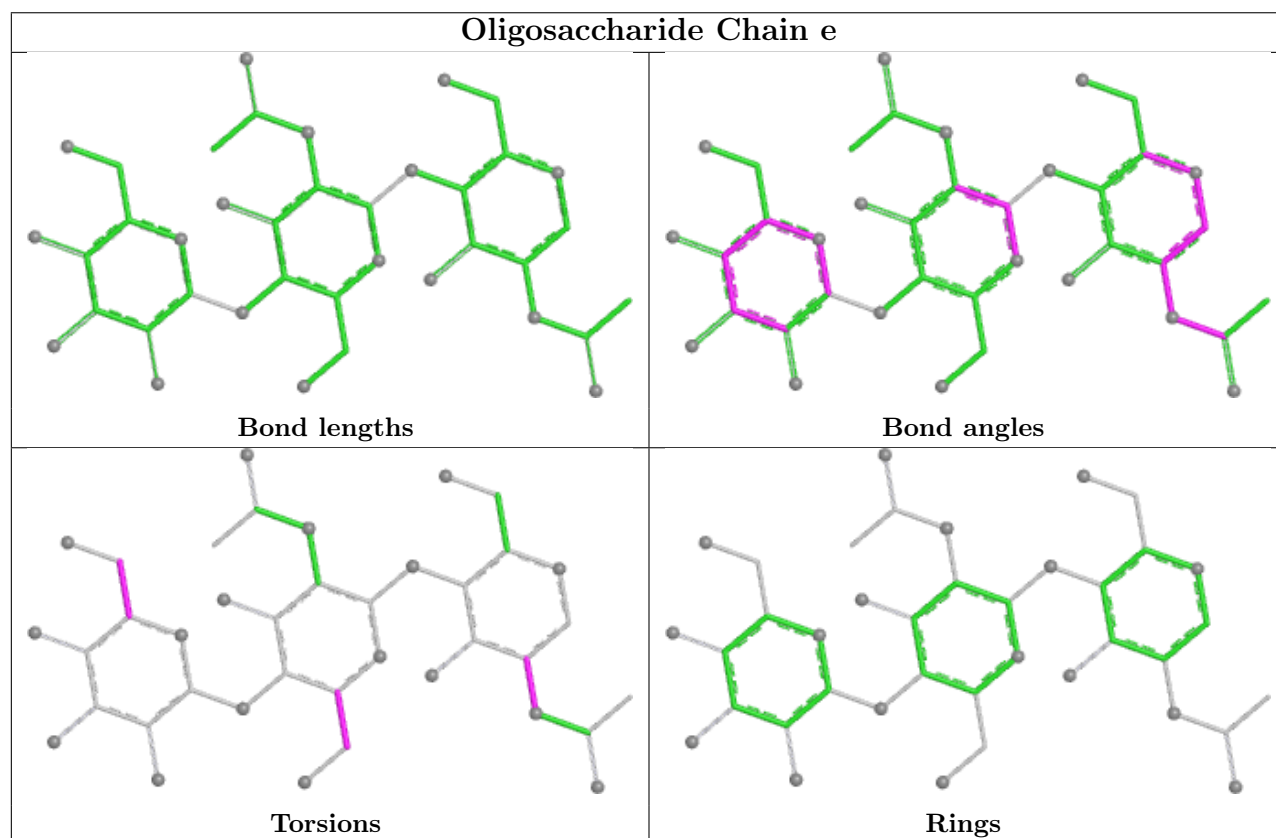
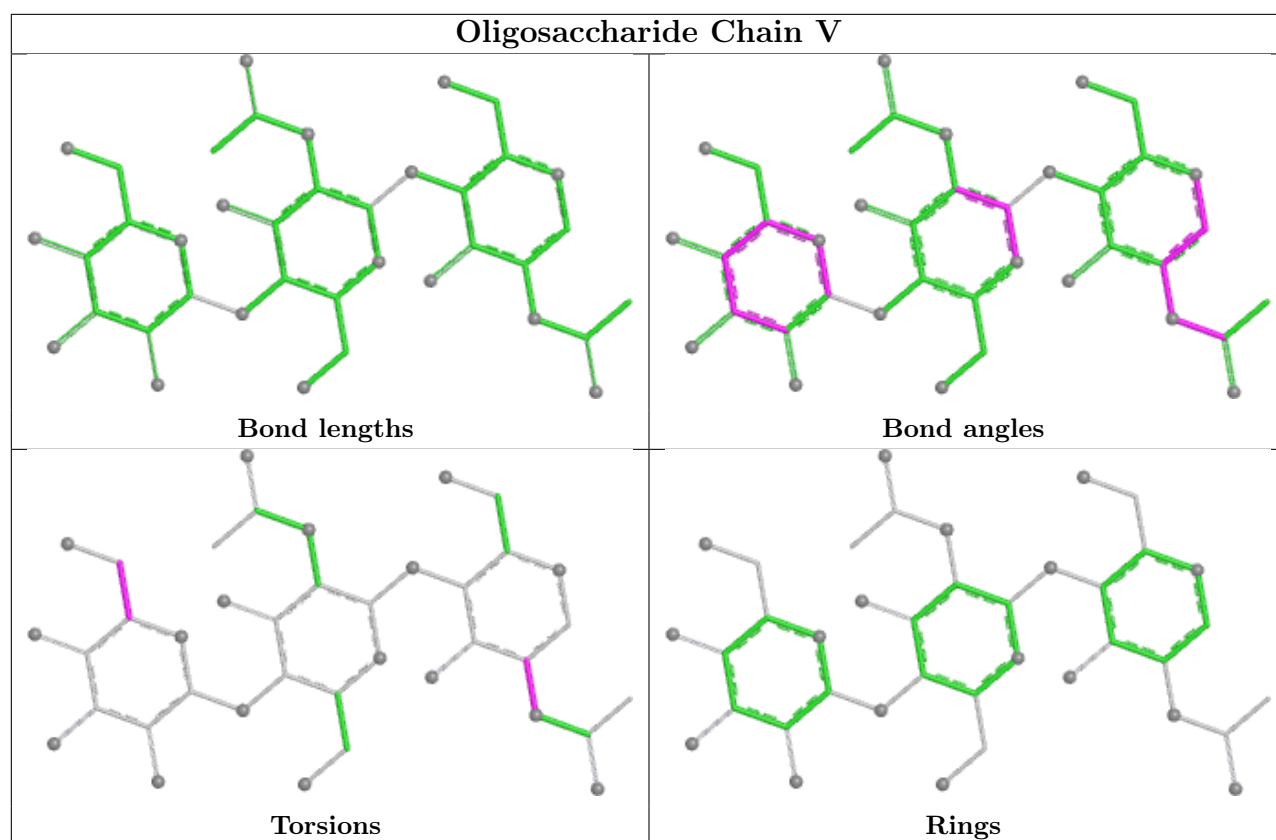


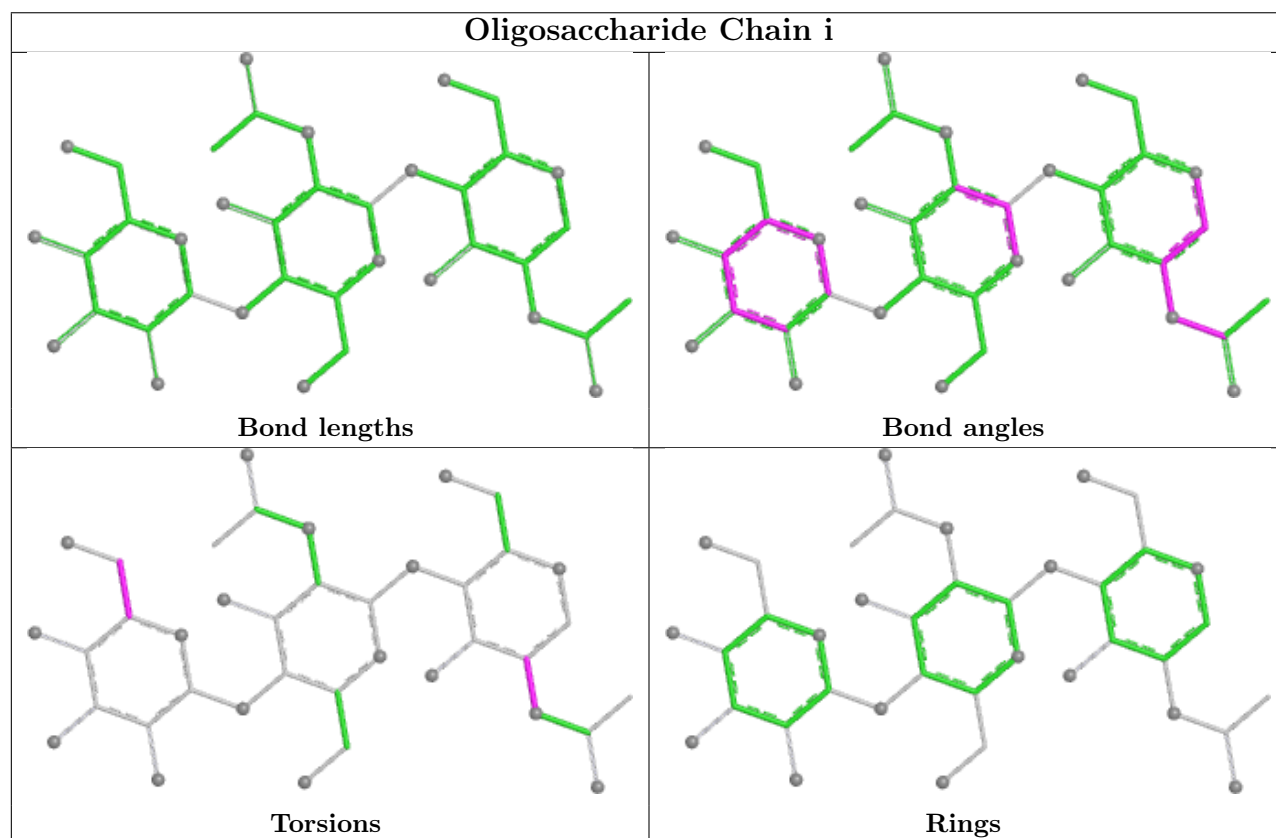
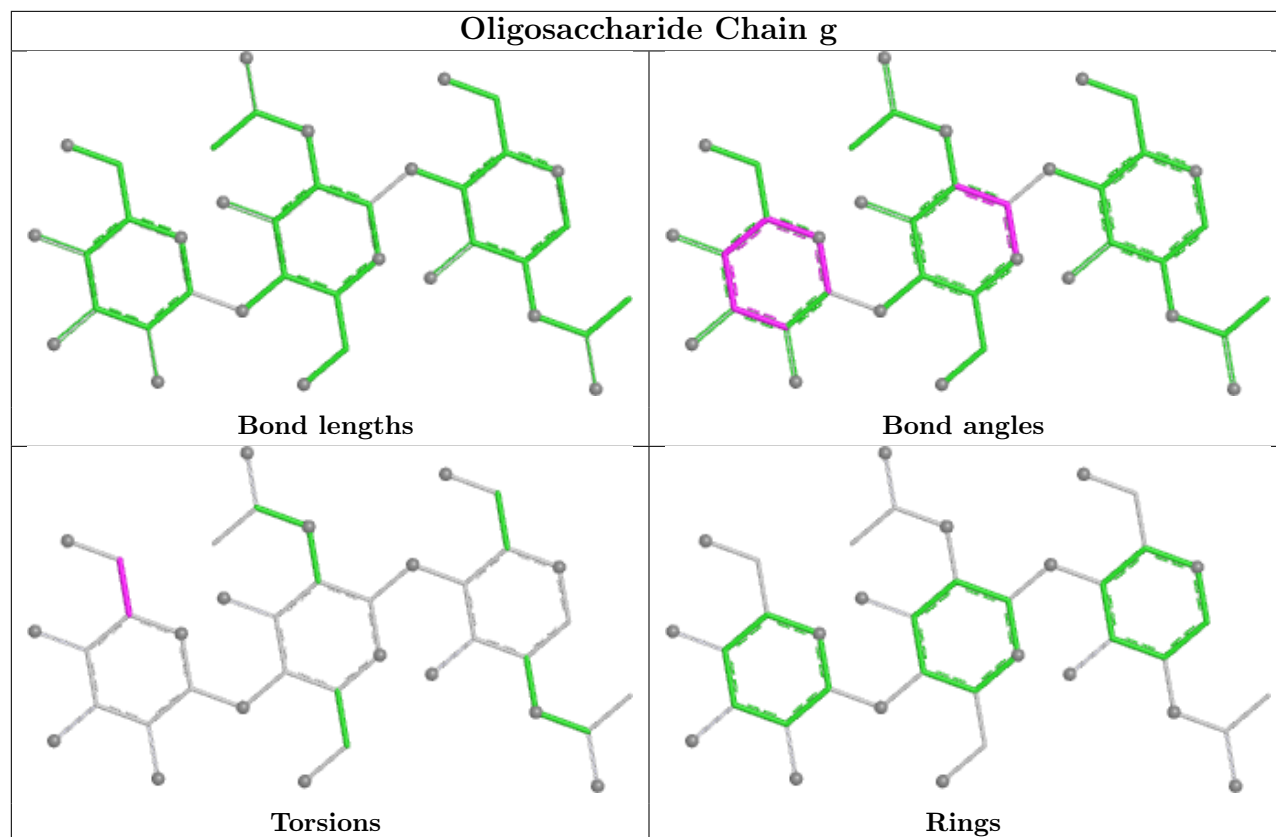


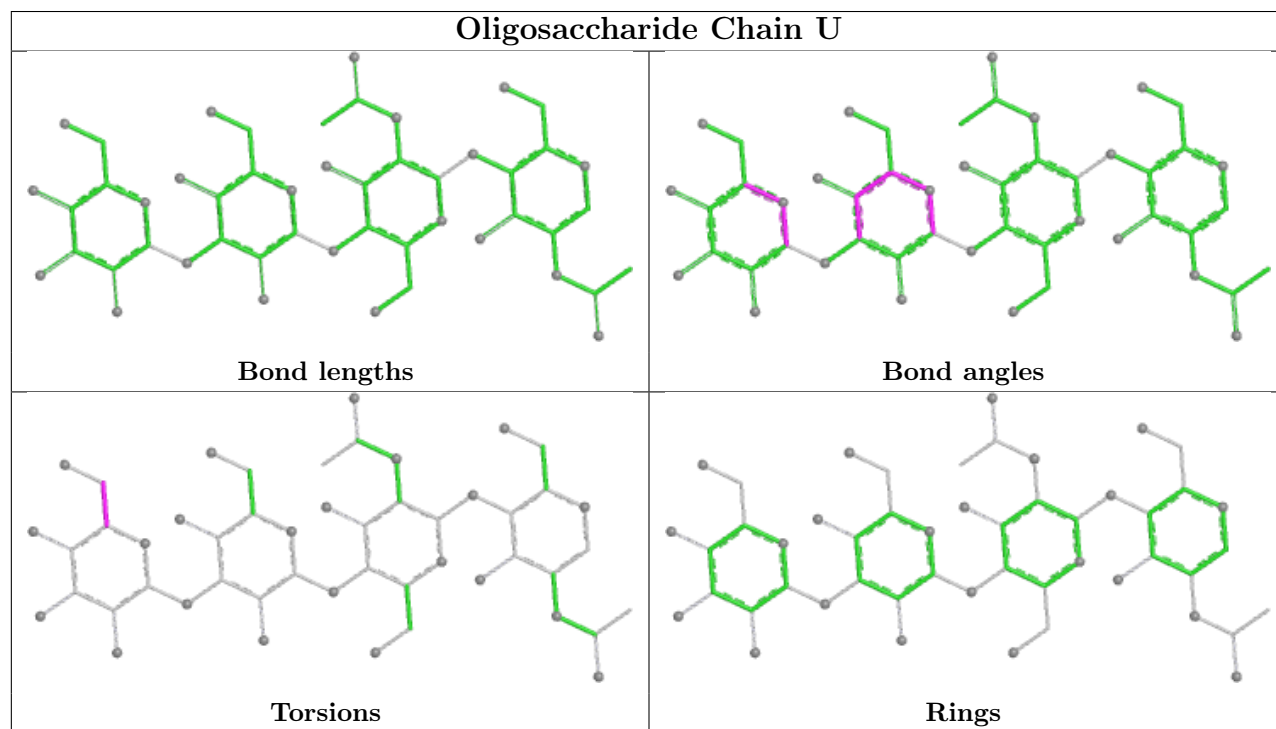
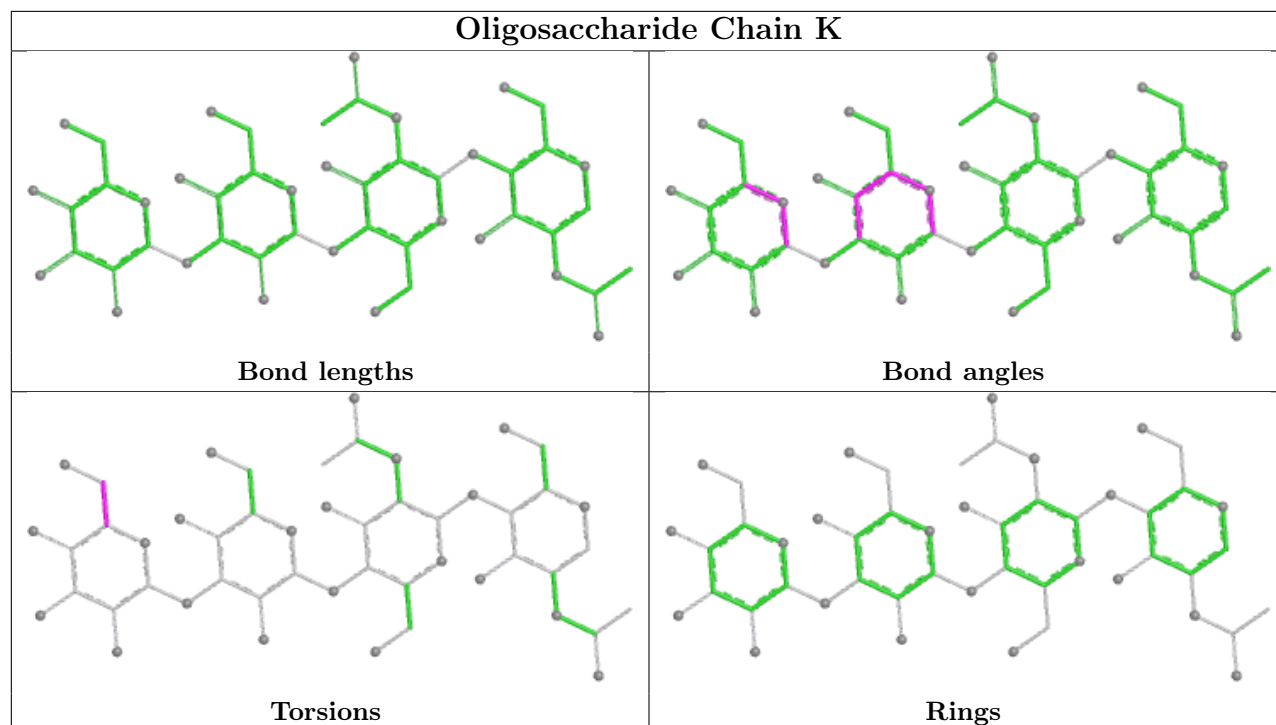


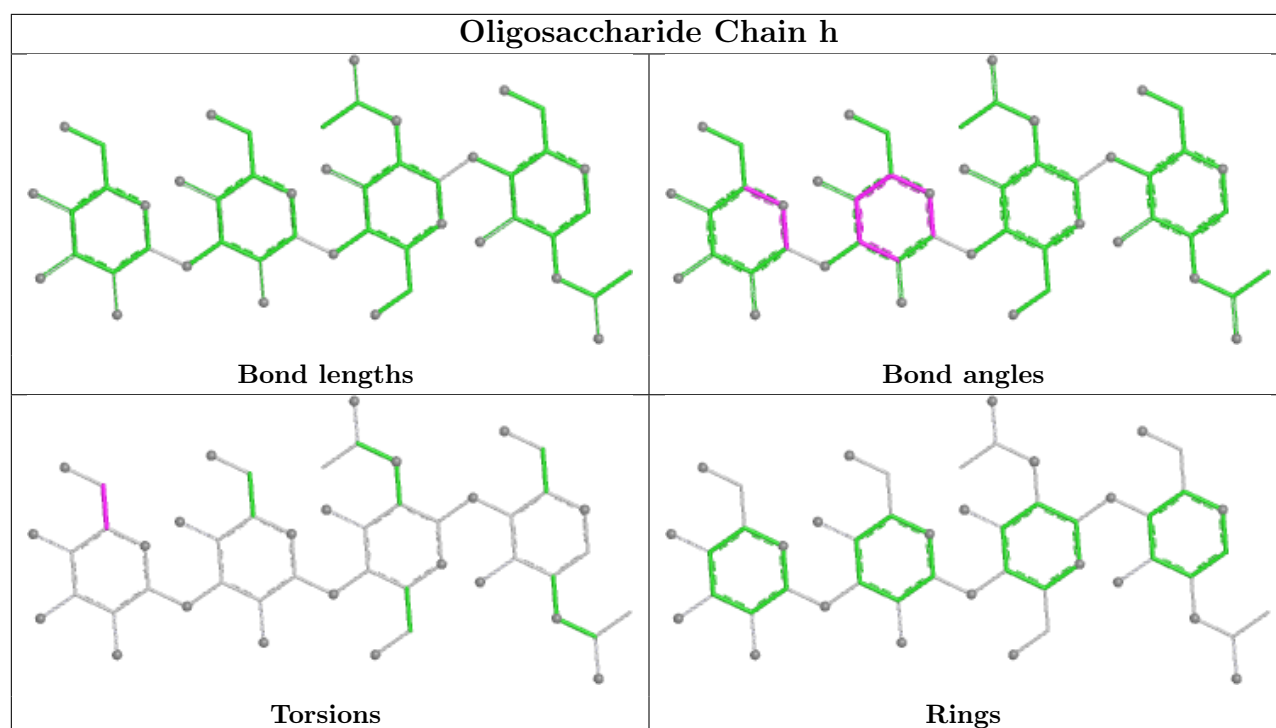


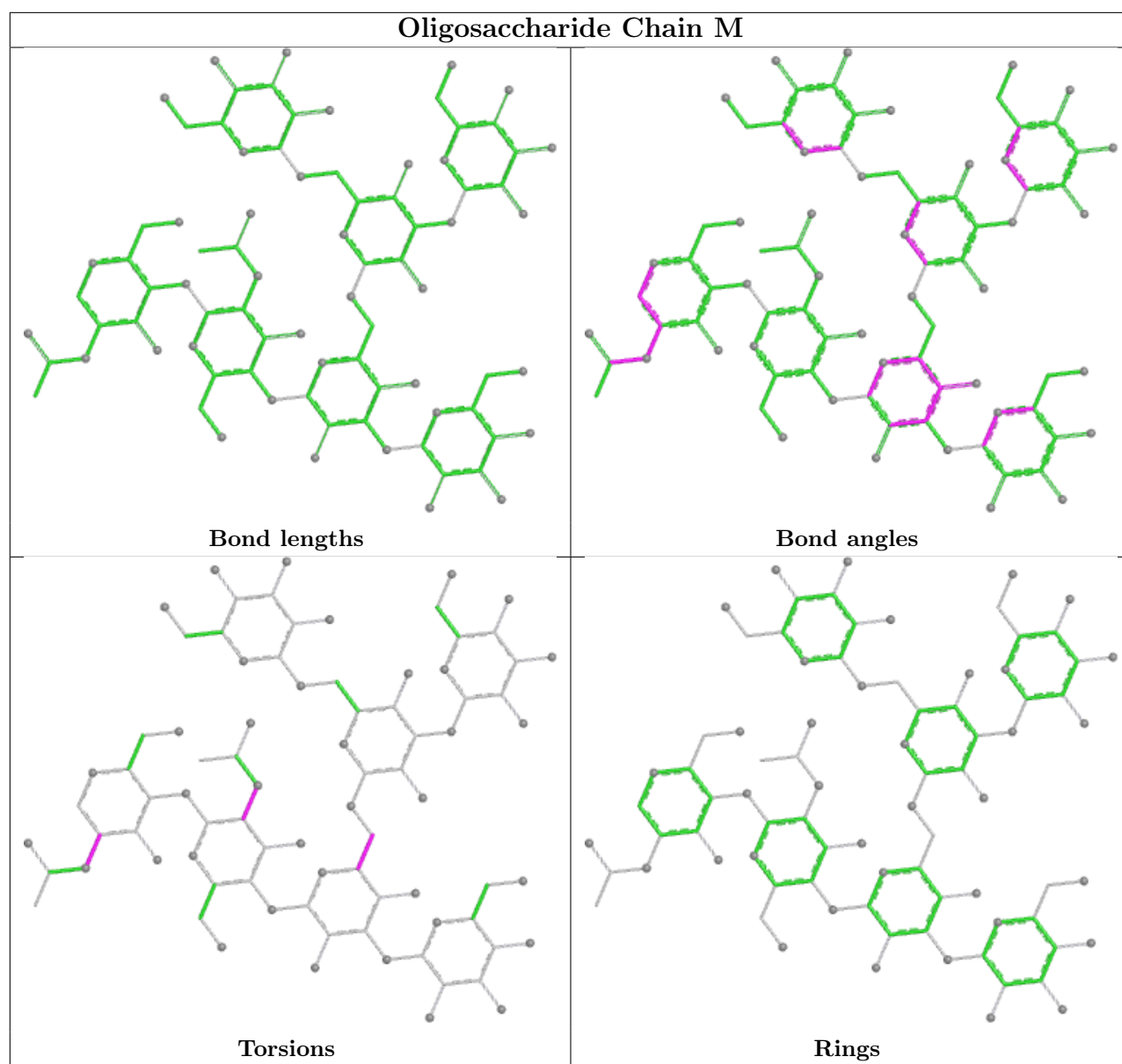


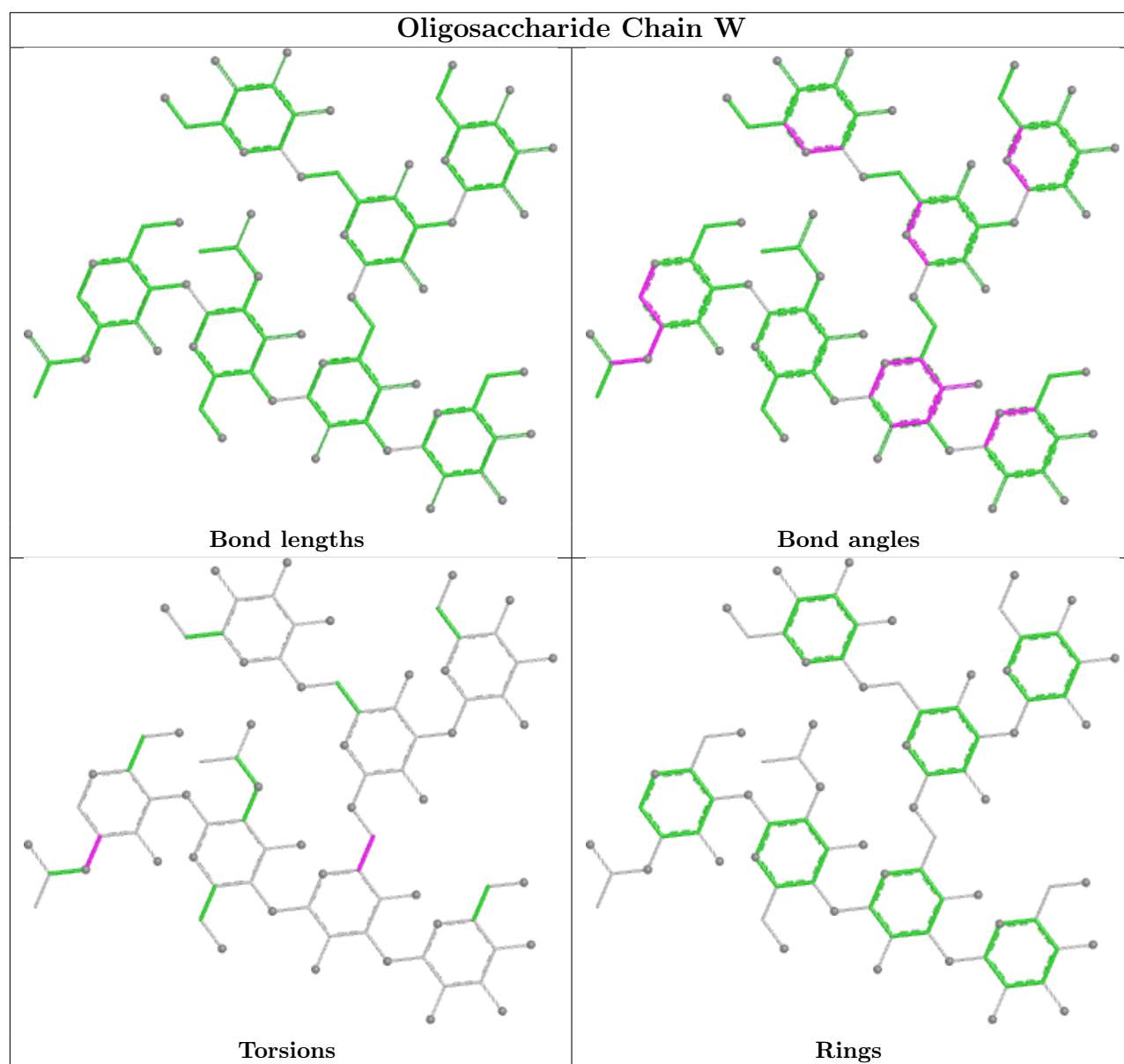


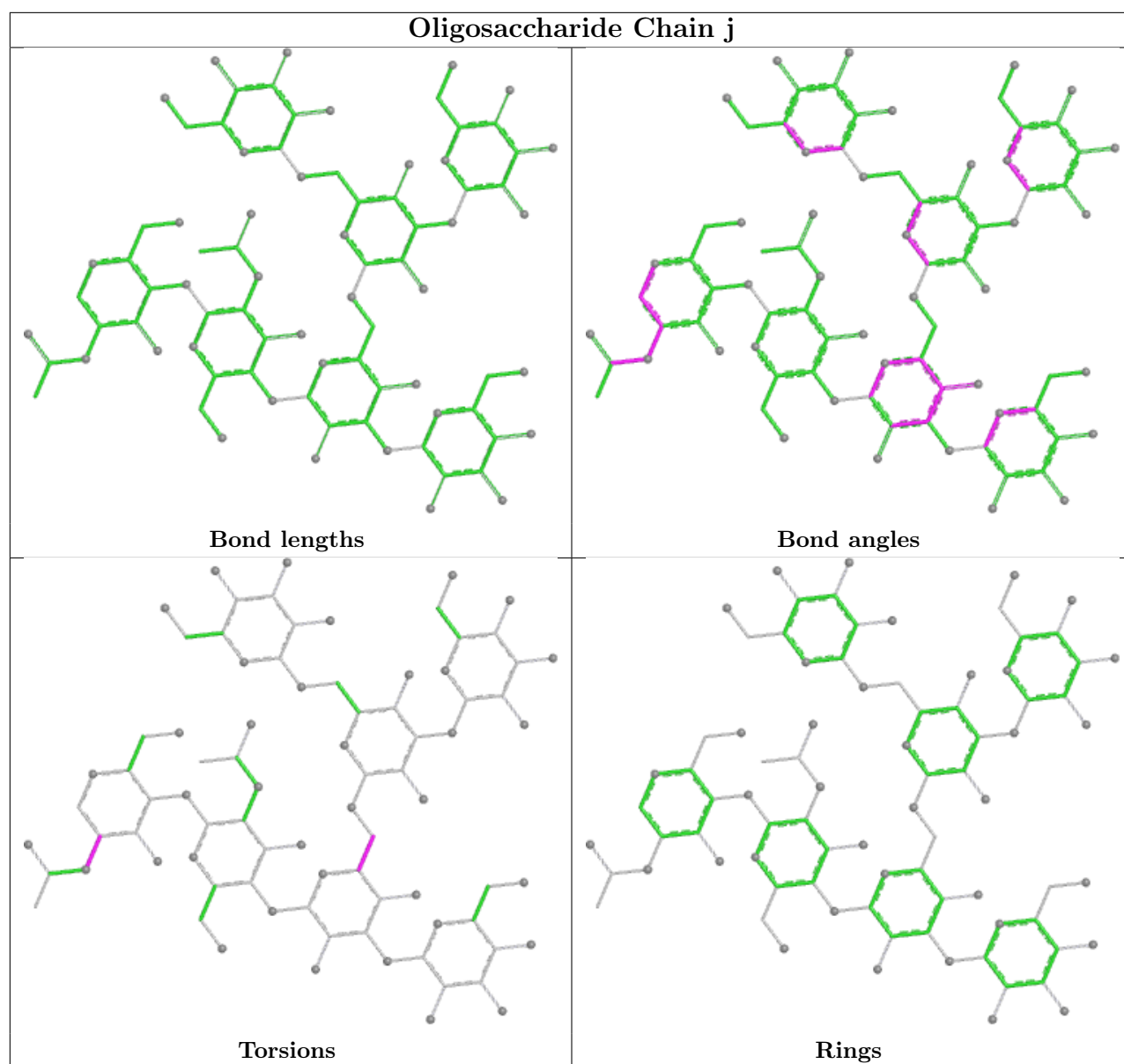












5.6 Ligand geometry [i](#)

6 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	C	401	1	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
9	NAG	A	402	1	14,14,15	0.71	0	17,19,21	0.78	0
9	NAG	B	402	1	14,14,15	0.71	0	17,19,21	0.78	0
9	NAG	C	402	1	14,14,15	0.70	0	17,19,21	0.82	0
9	NAG	A	401	1	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
9	NAG	B	401	1	14,14,15	0.72	0	17,19,21	1.16	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	401	1	-	2/6/23/26	0/1/1/1
9	NAG	A	402	1	-	0/6/23/26	0/1/1/1
9	NAG	B	402	1	-	0/6/23/26	0/1/1/1
9	NAG	C	402	1	-	0/6/23/26	0/1/1/1
9	NAG	A	401	1	-	2/6/23/26	0/1/1/1
9	NAG	B	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	401	NAG	C2-N2-C7	3.13	127.10	122.90
9	B	401	NAG	C2-N2-C7	3.11	127.07	122.90
9	A	401	NAG	C2-N2-C7	3.11	127.07	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	401	NAG	C3-C2-N2-C7
9	B	401	NAG	C3-C2-N2-C7
9	C	401	NAG	C3-C2-N2-C7
9	A	401	NAG	C1-C2-N2-C7
9	B	401	NAG	C1-C2-N2-C7
9	C	401	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

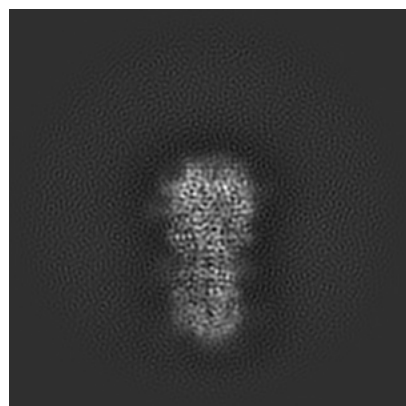
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74650. These allow visual inspection of the internal detail of the map and identification of artifacts.

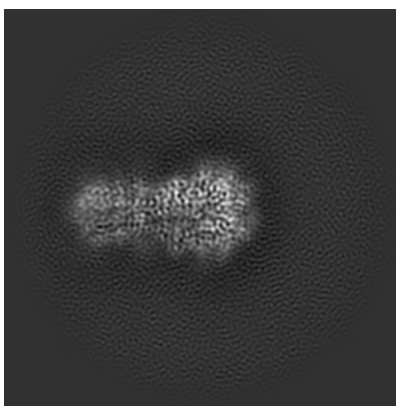
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

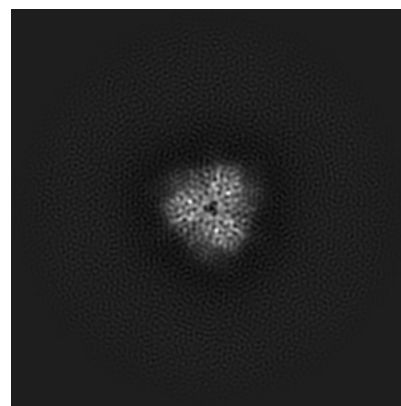
6.1.1 Primary map



X

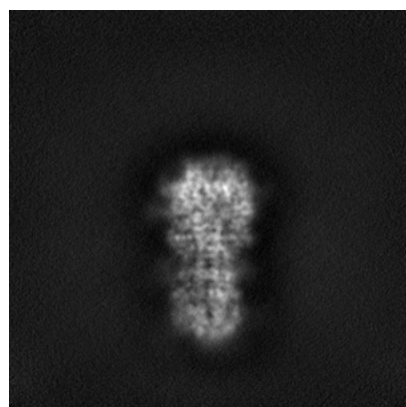


Y

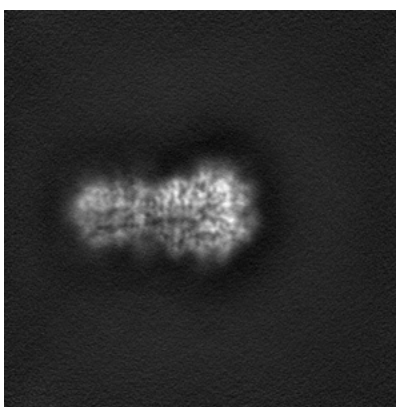


Z

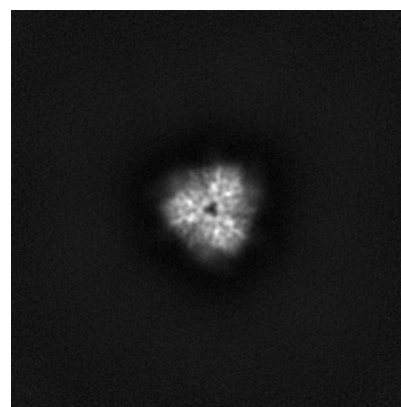
6.1.2 Raw map



X



Y

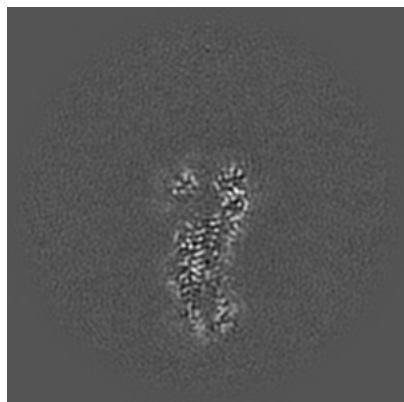


Z

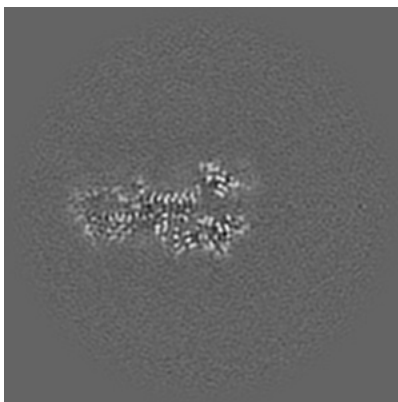
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

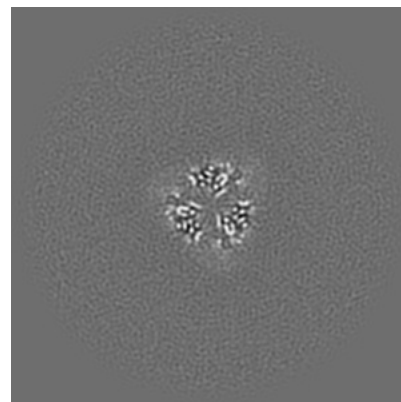
6.2.1 Primary map



X Index: 160

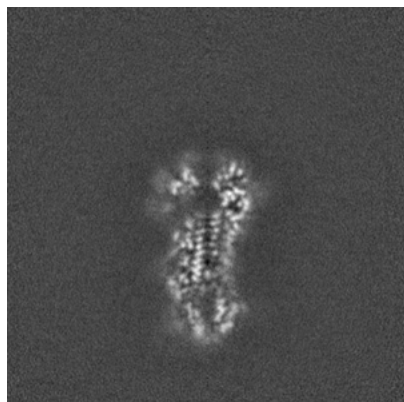


Y Index: 160

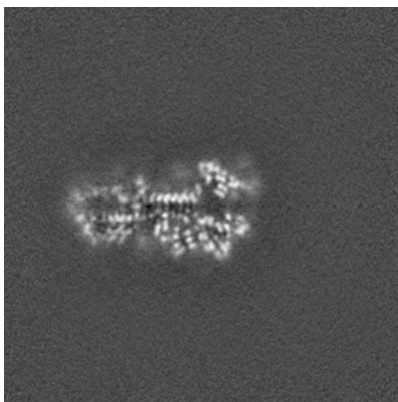


Z Index: 160

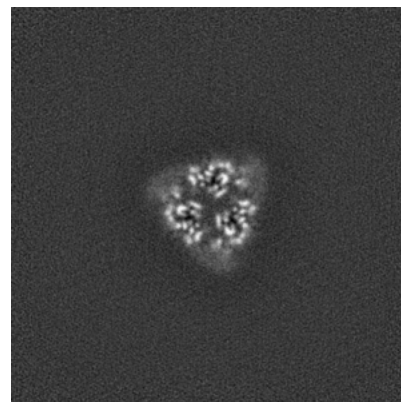
6.2.2 Raw map



X Index: 160



Y Index: 160

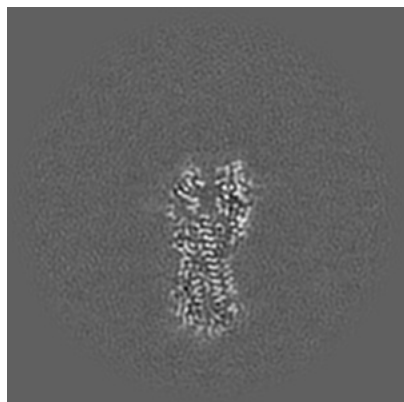


Z Index: 160

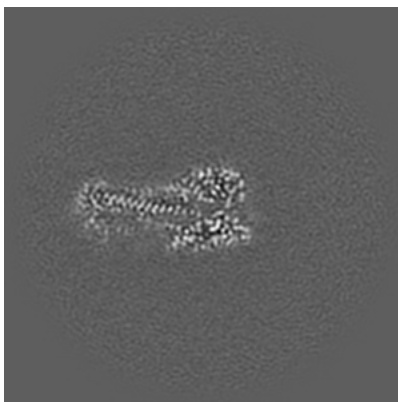
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

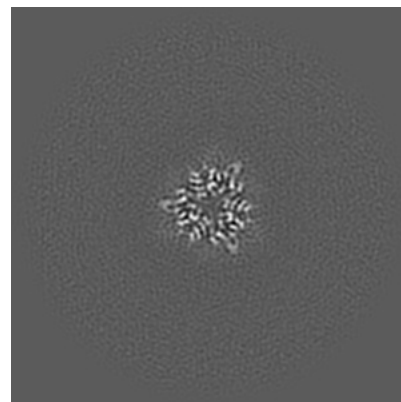
6.3.1 Primary map



X Index: 165

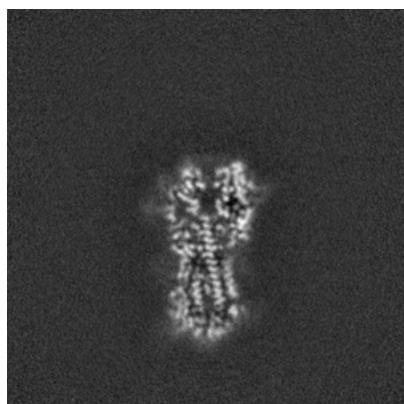


Y Index: 151

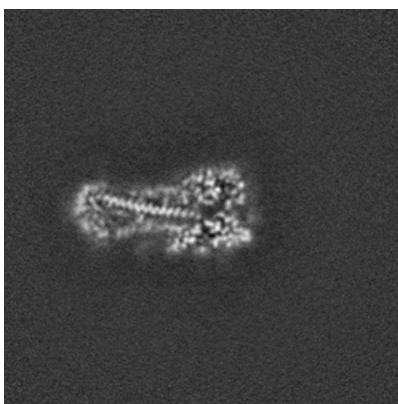


Z Index: 171

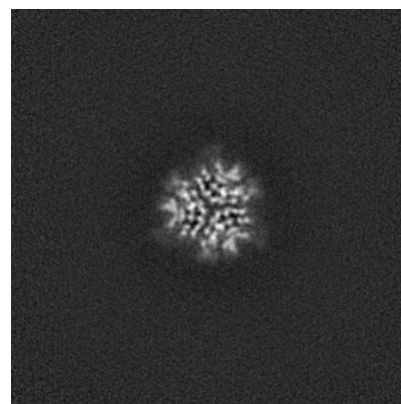
6.3.2 Raw map



X Index: 165



Y Index: 152

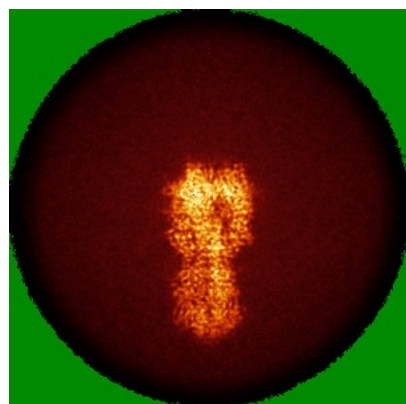


Z Index: 178

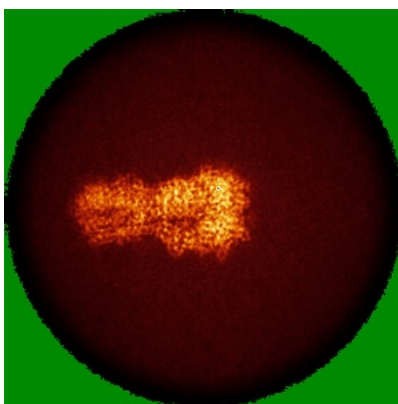
The images above show the largest variance slices of the map in three orthogonal directions.

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

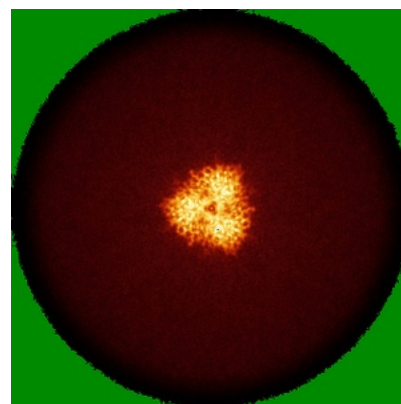
6.4.1 Primary map



X

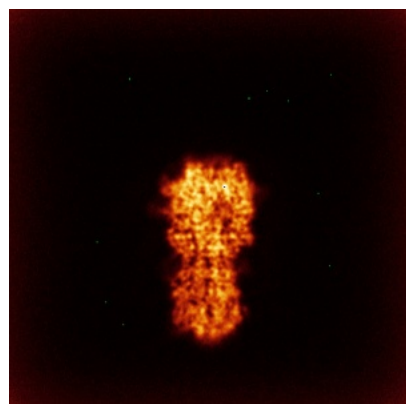


Y

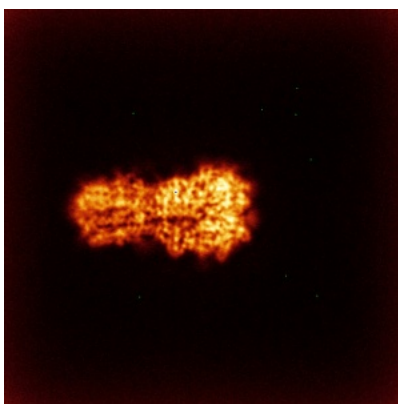


Z

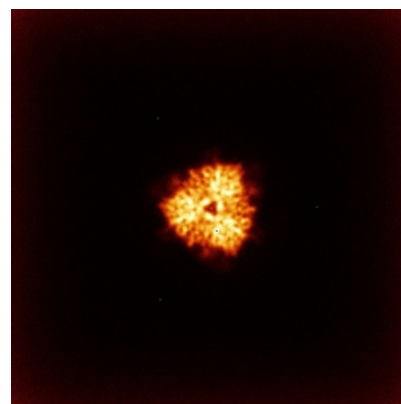
6.4.2 Raw map



X



Y

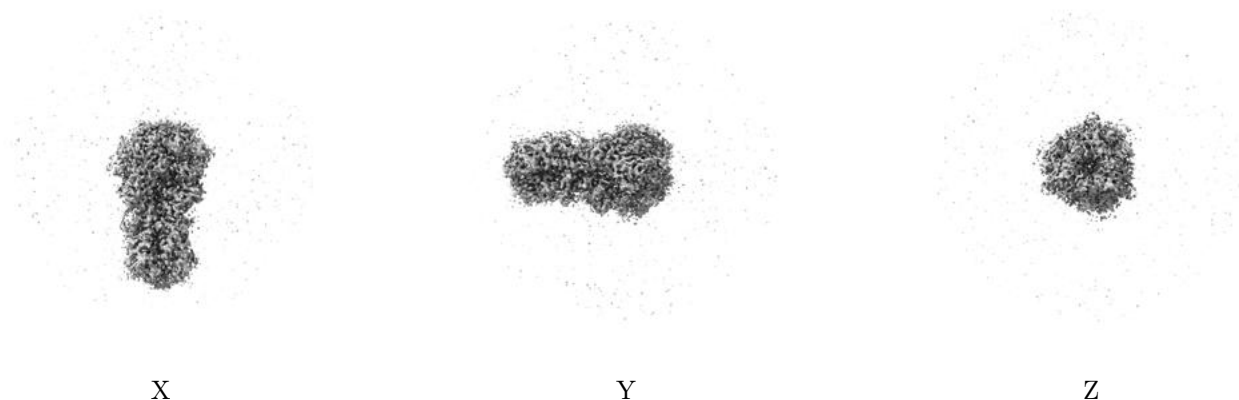


Z

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.

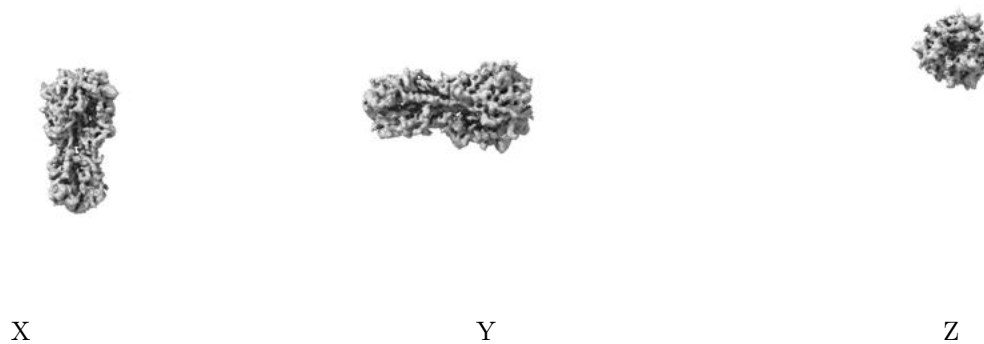
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

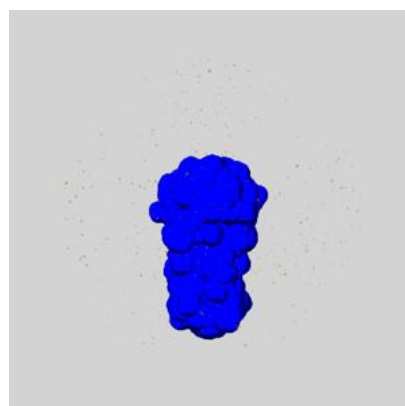
6.6 Mask visualisation [i](#)

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

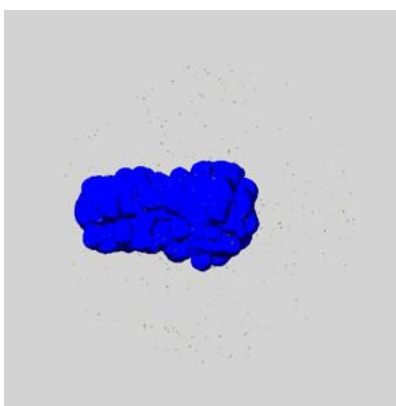
A mask typically either:

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

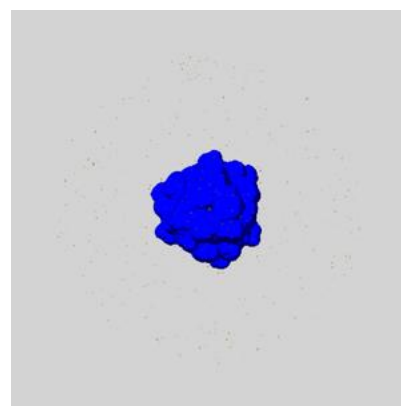
6.6.1 emd_74650_msk_1.map [i](#)



X



Y

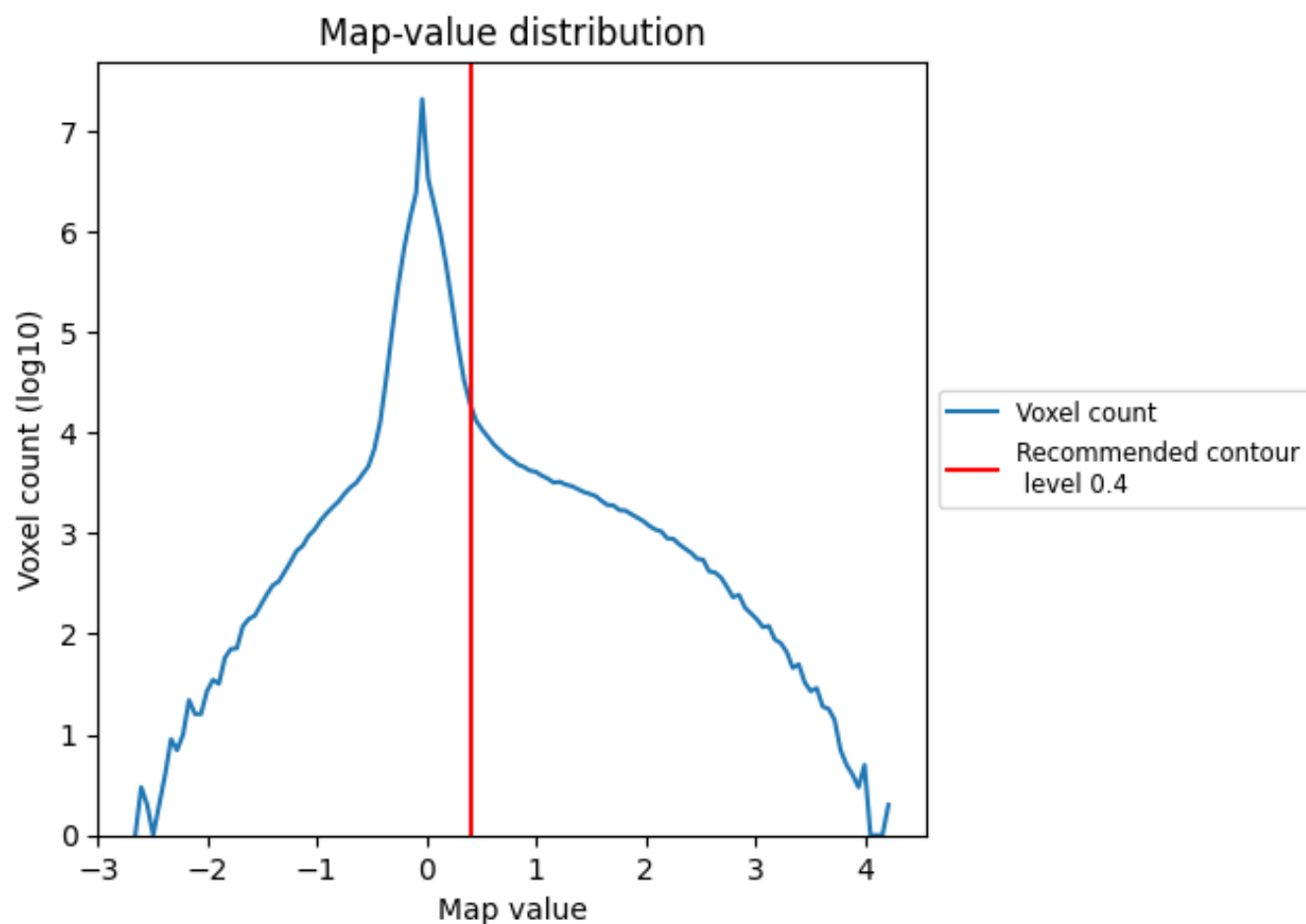


Z

7 Map analysis [i](#)

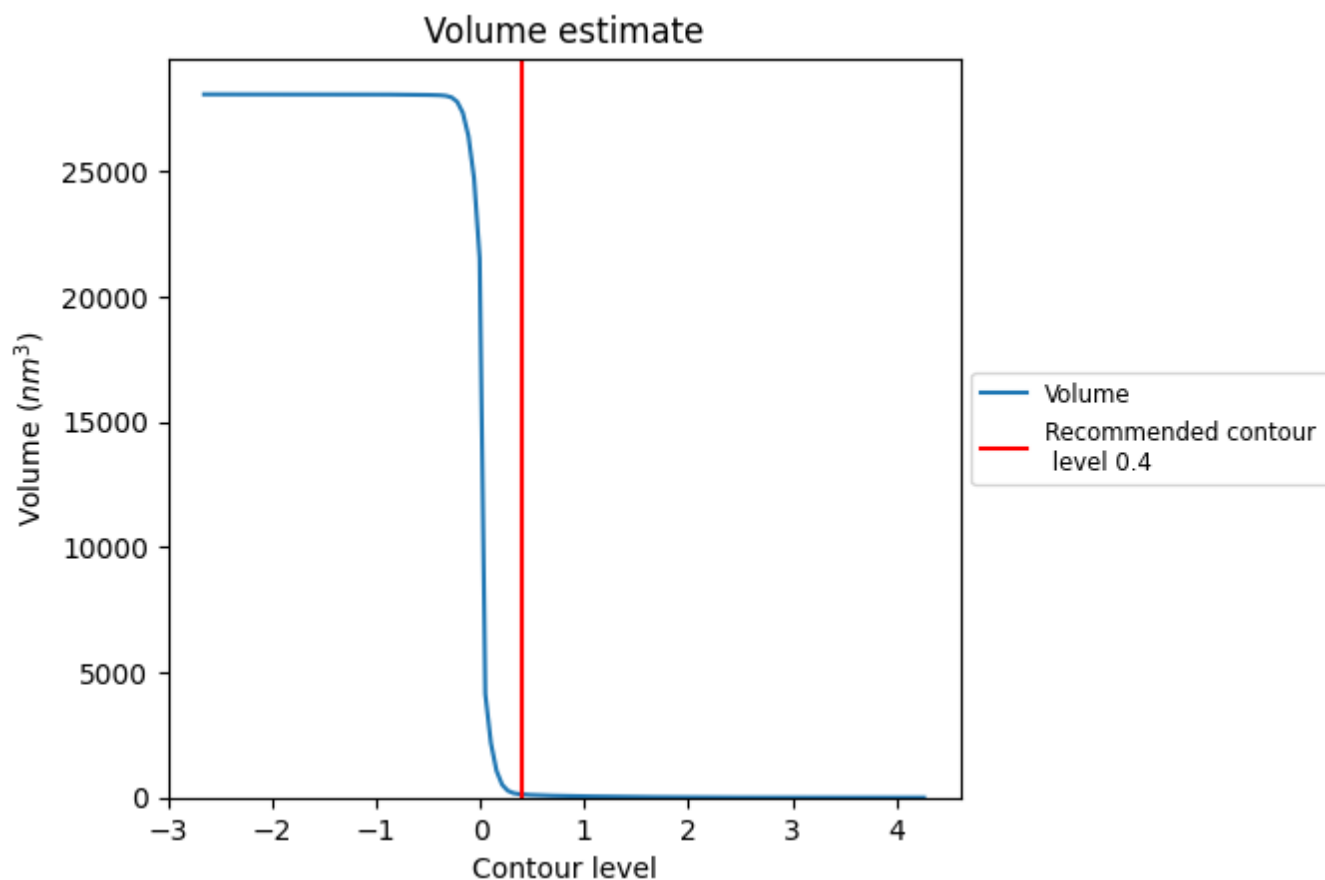
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

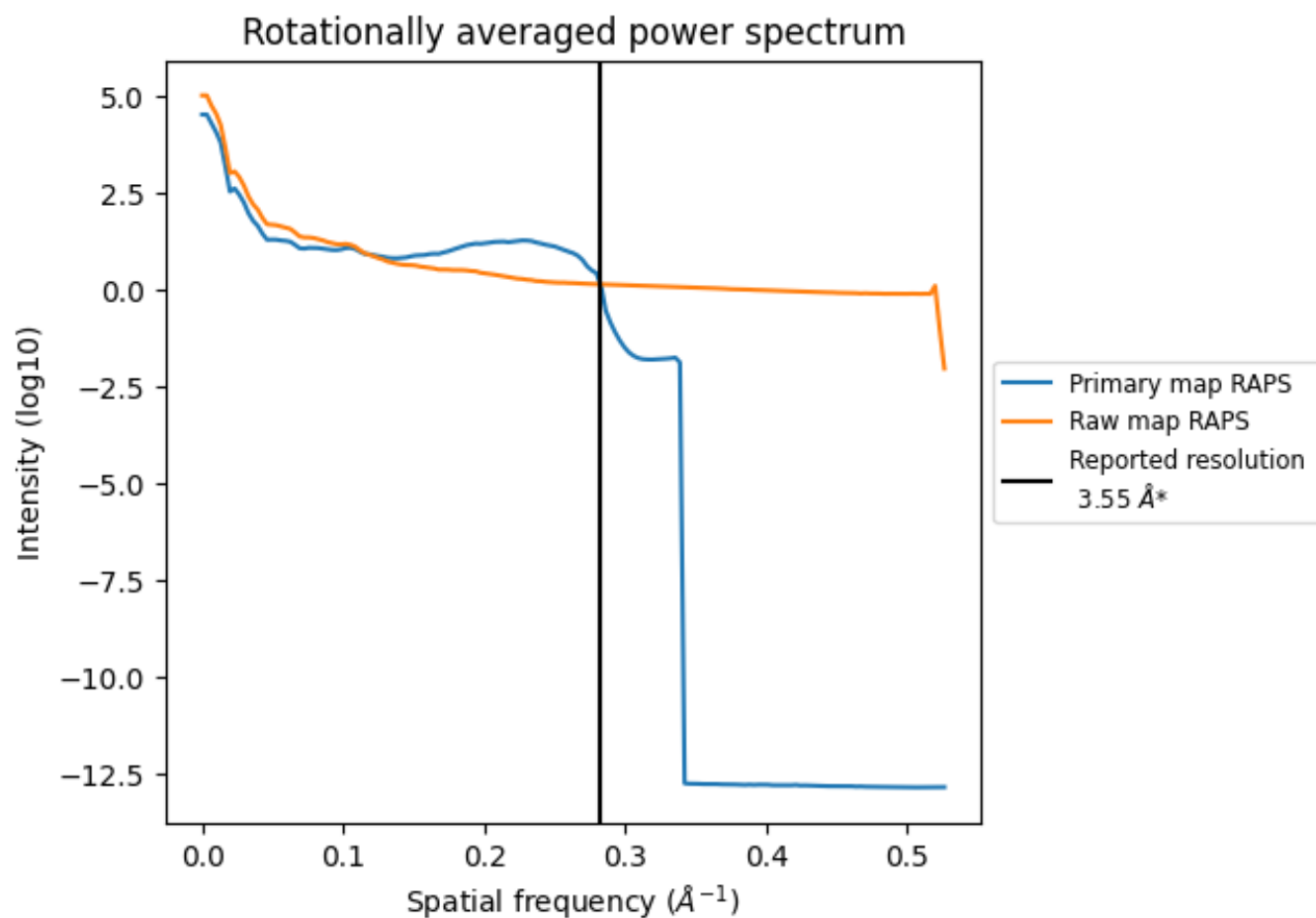
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm^3 ; this corresponds to an approximate mass of 117 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 ⓘ

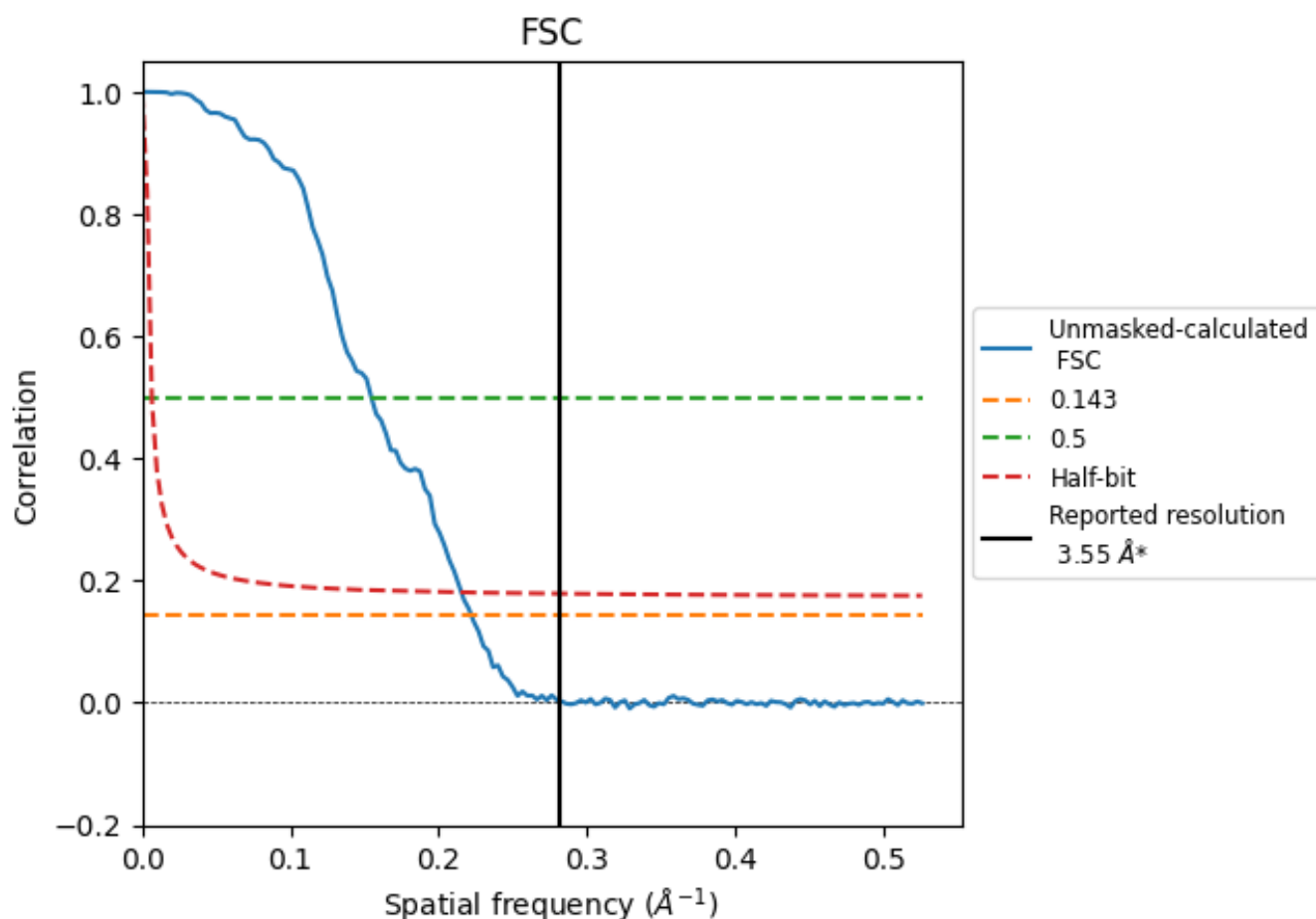


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

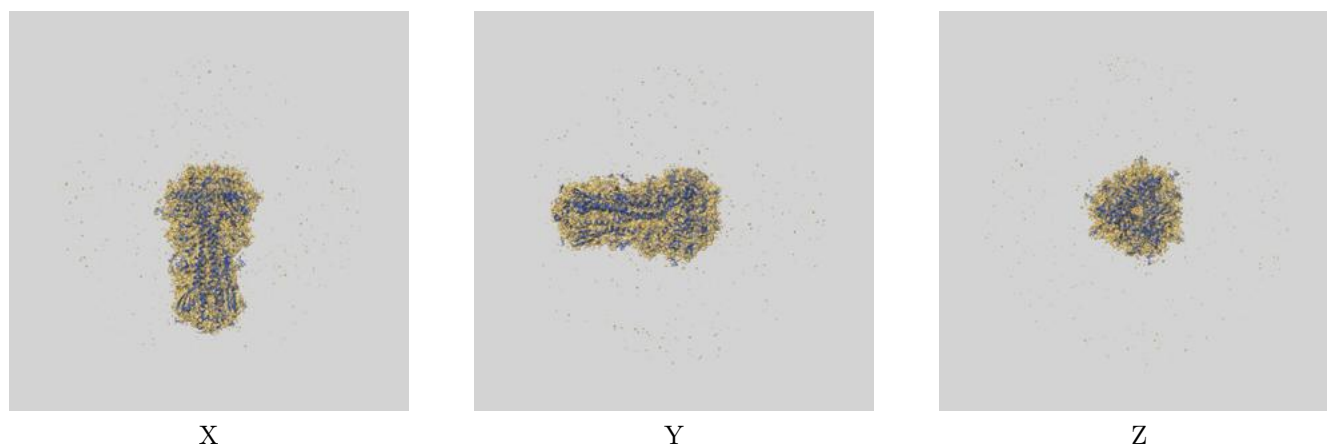
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	6.47	4.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.55 by more than 10 %

9 Map-model fit [i](#)

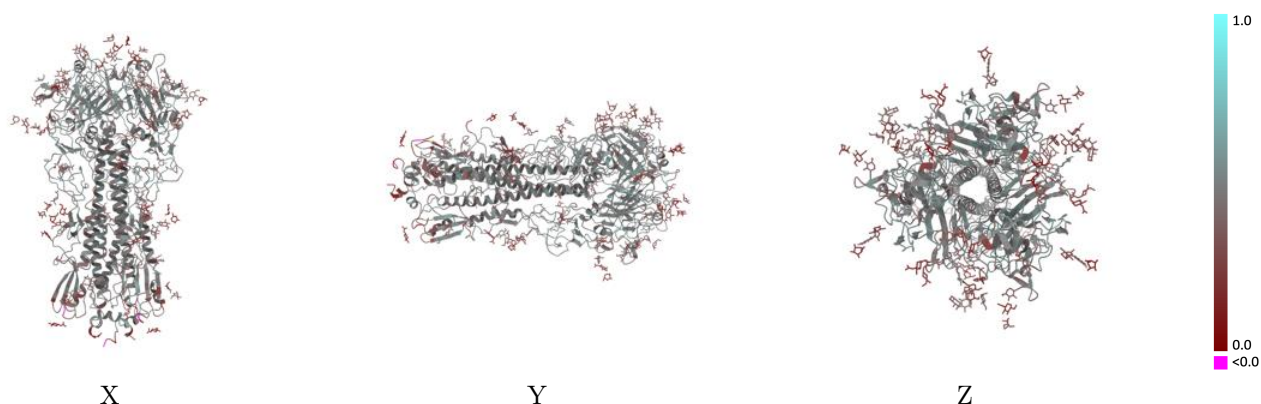
This section contains information regarding the fit between EMDB map EMD-74650 and PDB model 9ZRU. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



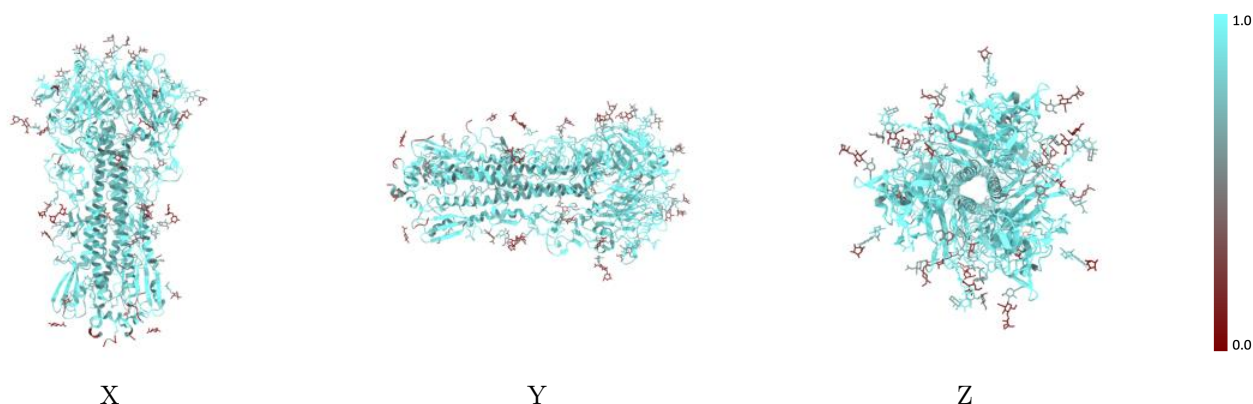
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



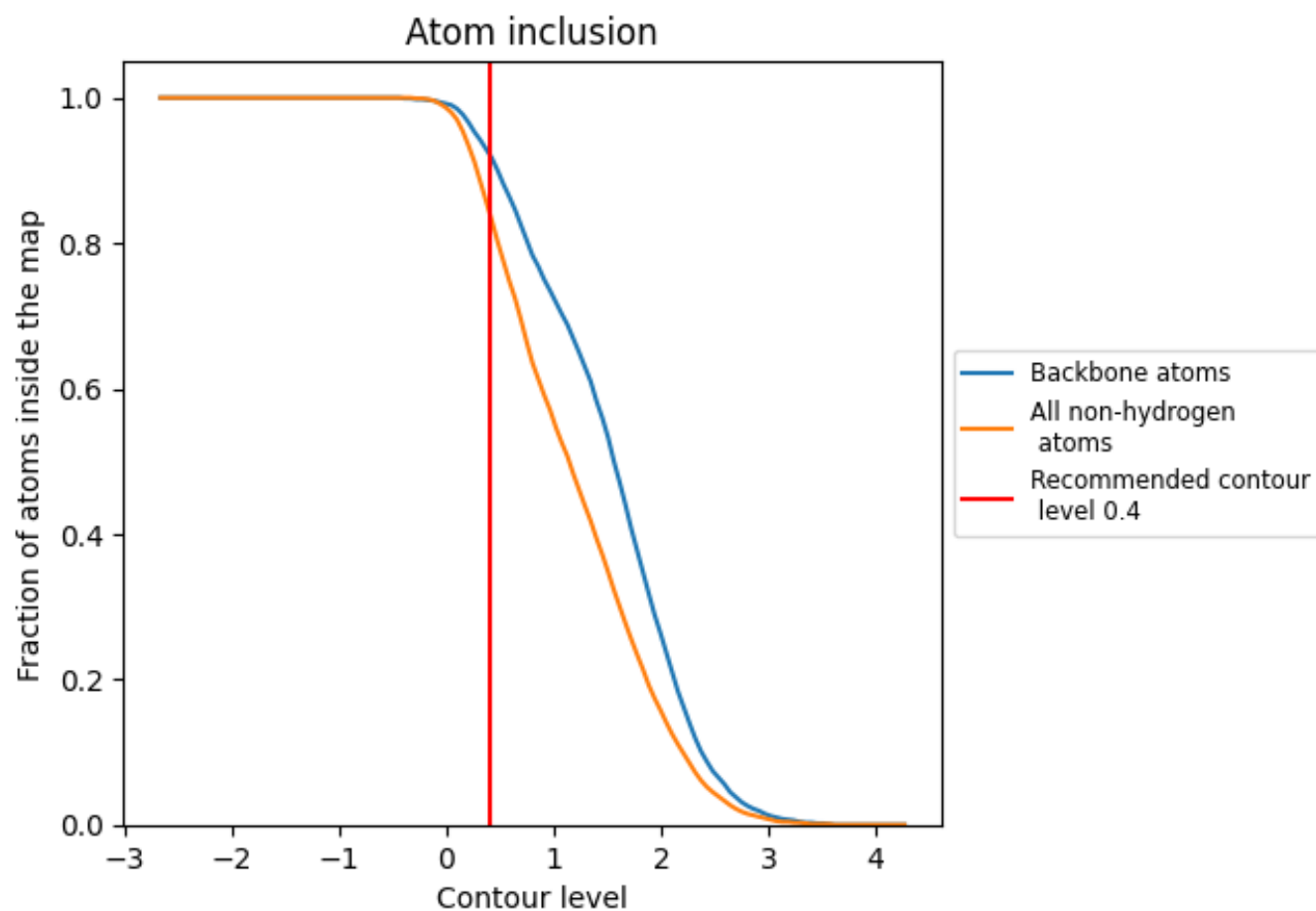
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.4480
A	 0.8960	 0.4770
B	 0.8950	 0.4760
C	 0.9030	 0.4800
D	 0.5360	 0.3260
E	 0.3800	 0.2410
F	 0.6560	 0.2940
G	 0.4290	 0.1790
H	 0.6410	 0.2910
I	 0.3570	 0.2110
J	 0.3590	 0.2710
K	 0.5600	 0.3520
L	 0.3590	 0.2640
M	 0.8070	 0.3830
N	 0.5000	 0.2900
O	 0.3800	 0.2130
P	 0.6890	 0.2700
Q	 0.5000	 0.2310
R	 0.5380	 0.2290
S	 0.3210	 0.1880
T	 0.3330	 0.2650
U	 0.5400	 0.3430
V	 0.3850	 0.2440
W	 0.7350	 0.3430
X	 0.6070	 0.3230
Y	 0.4000	 0.2710
Z	 0.6560	 0.3350
a	 0.8380	 0.4360
b	 0.8460	 0.4460
c	 0.8550	 0.4510
d	 0.4290	 0.1880
e	 0.5640	 0.2760
f	 0.2860	 0.2140
g	 0.3080	 0.2540
h	 0.5600	 0.3650



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Chain	Atom inclusion	Q-score
i	 0.3850	 0.3040
j	 0.8190	 0.3890