



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:06 AM UTC

PDB ID : 9BBK / pdb_00009bbk
EMDB ID : EMD-44420
Title : SARS-CoV-2 full-length spike protein with His1271Lys substitution in the coatomer binding motif, 2RBD-up conformation (SPIKE-KxK)
Authors : Singh, S.; Hasan, S.S.
Deposited on : 2024-04-06
Resolution : 2.95 Å(reported)
Based on initial model : 7KRR

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

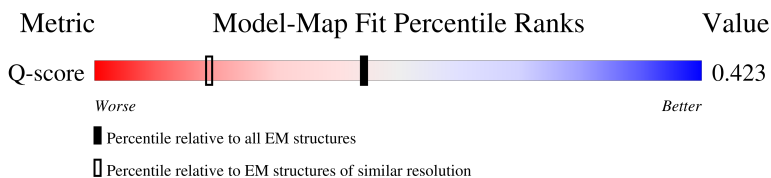
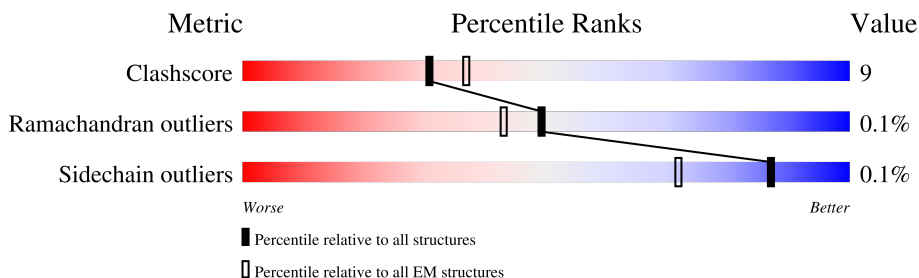
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	 6% 68% 11% 22%
1	B	1312	 70% 11% 19%
1	C	1312	 70% 10% 20%
2	D	2	 100%

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

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Mol	Chain	Length	Quality of chain
7	a	4	 100%
7	b	4	 25% 25% 50%
8	d	5	 20% 80%

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	Y	1	-	-	X	-
2	NAG	Y	2	-	-	X	-
3	NAG	K	1	-	-	X	-
3	NAG	U	2	-	-	X	-
3	NAG	e	1	-	-	X	-
3	NAG	e	2	-	-	X	-
9	NAG	A	1308	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 49671 atoms, of which 23756 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	1028	Total	C	H	N	O	S	0	0
			15750	5106	7751	1334	1523	36		
1	B	1064	Total	C	H	N	O	S	0	0
			16335	5302	8027	1386	1583	37		
1	C	1052	Total	C	H	N	O	S	0	0
			16143	5239	7944	1365	1559	36		

There are 138 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

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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	1271	LYS	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
B	-1	GLY	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1271	LYS	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
C	-6	GLY	-	insertion	UNP P0DTC2
C	-5	GLY	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1271	LYS	HIS	engineered mutation	UNP P0DTC2

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



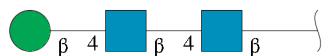
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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.



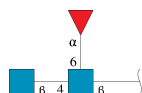
Mol	Chain	Residues	Atoms				AltConf	Trace	
3	E	3	Total 39	C 22	N 2	O 15	0	0	
3	F	3	Total 39	C 22	N 2	O 15	0	0	
3	G	3	Total 39	C 22	N 2	O 15	0	0	
3	I	3	Total 39	C 22	N 2	O 15	0	0	
3	J	3	Total 39	C 22	N 2	O 15	0	0	
3	K	3	Total 39	C 22	N 2	O 15	0	0	
3	T	3	Total 39	C 22	N 2	O 15	0	0	
3	U	3	Total 39	C 22	N 2	O 15	0	0	
3	W	3	Total 72	C 21	H 34	N 2	O 15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	e	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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.



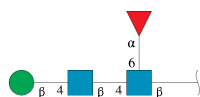
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	3	Total	C	N	O	0	0
			38	22	2	14		
4	c	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 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
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		

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



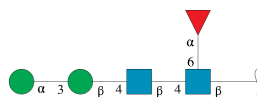
Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	4	Total	C	N	O	0	0
			49	28	2	19		

- 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.



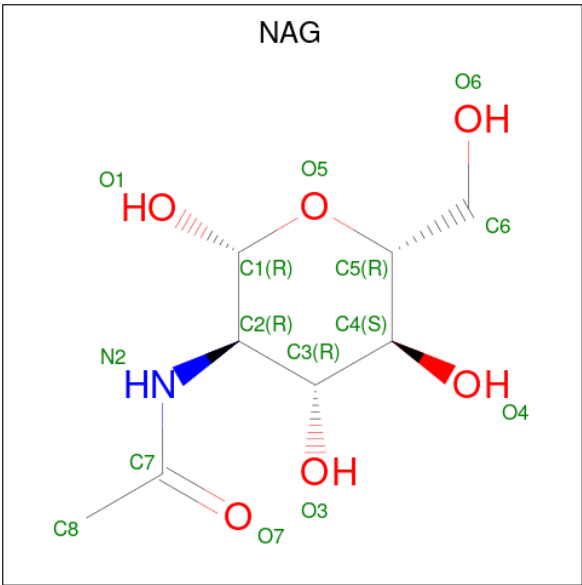
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	4	Total	C	N	O	0	0
			50	28	2	20		
7	a	4	Total	C	N	O	0	0
			50	28	2	20		
7	b	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-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
8	d	5	Total	C	N	O	0	0
			60	34	2	24		

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



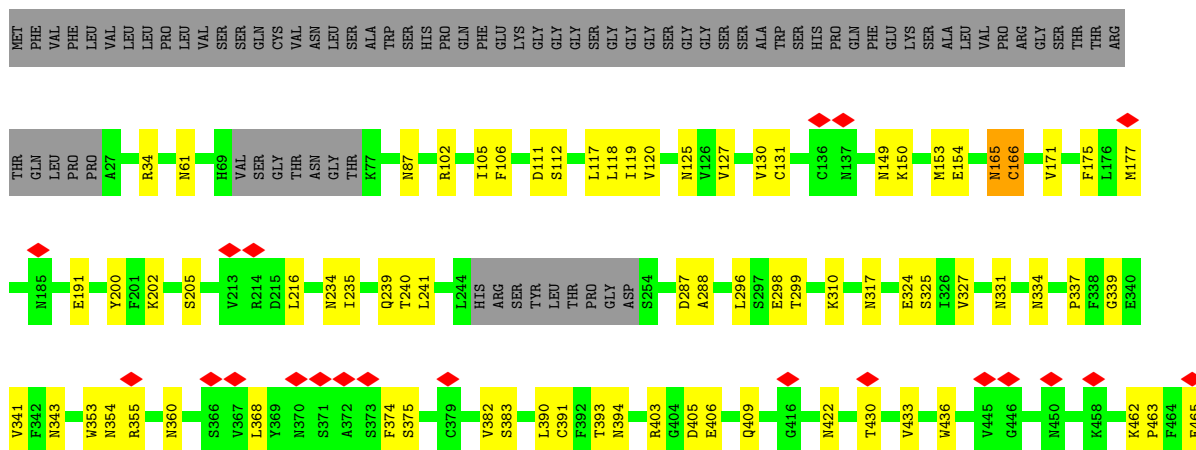
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9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

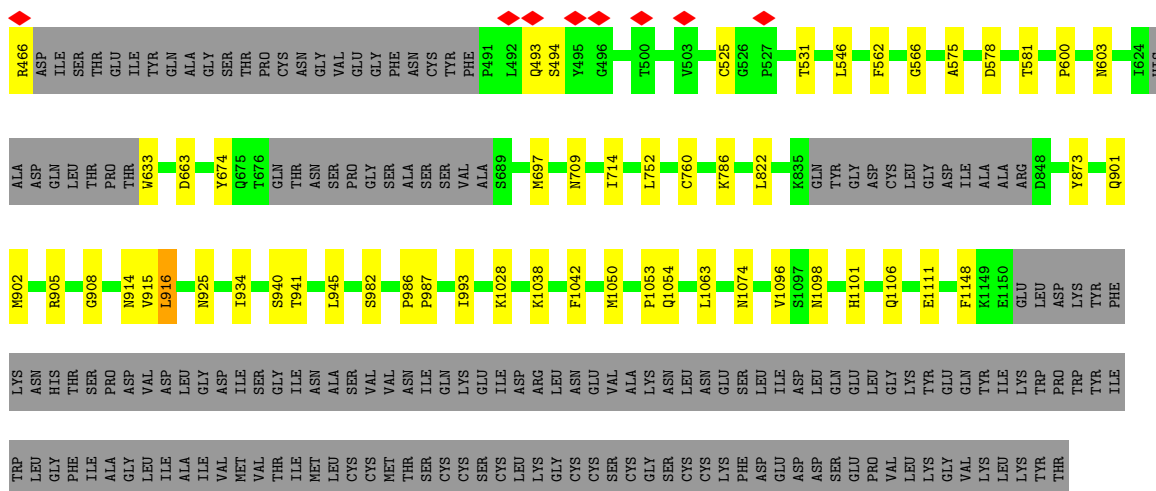
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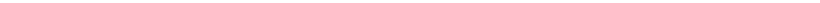
Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	

Chain B: 70% 11% 19%





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

Chain D:  100%



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

Chain L: 100%



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

Chain M: 100%



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

Chain N: 100%



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

Chain V: 100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

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

Chain E:  33% 67%

MAG1
MAG2
BNA3

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

Chain F:  33% 67%

MAG1
MAG2
BNA3

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

Chain G:  33% 67%

MAG1
MAG2
BMA3

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

Chain I:  33% 67%

MAG1
MAG2
BMA3

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

Chain J:  33% 67%

MAG1
MAG2
BMA3

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

Chain K:  33% 67%

MAG1
MAG2
BMA3

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

Chain T:  33% 67%

MAG1
MAG2
BMA3

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

Chain W:  33% 67%



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

Chain X:



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

Chain e:



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

Chain H:



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

Chain c:



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

Chain P:



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

Chain Q:



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

Chain R:  25% 100%



- 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

Chain S:  25% 75%



- 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

Chain a:  100%



- 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

Chain b:  25% 25% 50%



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  20% 80%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87816	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.482	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	304.8, 304.8, 304.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9525, 0.9525, 0.9525	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, 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	0/8175	0.31	2/11118 (0.0%)
1	B	0.13	0/8502	0.32	1/11569 (0.0%)
1	C	0.13	0/8387	0.30	2/11410 (0.0%)
All	All	0.13	0/25064	0.31	5/34097 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ASN	CA-C-N	9.56	139.80	121.54
1	C	165	ASN	C-N-CA	9.56	139.80	121.54
1	B	234	ASN	CB-CA-C	6.44	119.18	110.94
1	A	61	ASN	CA-C-N	6.03	132.82	121.97
1	A	61	ASN	C-N-CA	6.03	132.82	121.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	ASN	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	7999	7751	7795	123	0
1	B	8308	8027	8056	109	0
1	C	8199	7944	7975	98	0
2	D	28	0	25	6	0
2	L	28	0	25	1	0
2	M	28	0	25	5	0
2	N	28	0	25	6	0
2	V	28	0	25	0	0
2	Y	28	0	25	8	0
2	Z	28	0	25	6	0
2	f	28	0	25	7	0
2	g	28	0	25	5	0
3	E	39	0	34	7	0
3	F	39	0	34	6	0
3	G	39	0	34	3	0
3	I	39	0	34	5	0
3	J	39	0	34	5	0
3	K	39	0	34	8	0
3	T	39	0	34	4	0
3	U	39	0	34	8	0
3	W	38	34	33	2	0
3	X	39	0	34	0	0
3	e	39	0	34	9	0
4	H	38	0	34	2	0
4	c	38	0	34	6	0
5	P	50	0	43	2	0
5	Q	50	0	43	6	0
6	R	49	0	43	7	0
7	S	50	0	43	7	0
7	a	50	0	43	9	0
7	b	50	0	43	6	0
8	d	60	0	52	11	0
9	A	112	0	104	28	0
9	B	112	0	103	13	0
9	C	70	0	65	6	0
All	All	25915	23756	25074	454	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 9.

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD21	9:A:1308:NAG:H81	1.31	1.07
1:C:1074:ASN:HD21	4:c:1:NAG:H61	1.29	0.94
2:Z:1:NAG:H61	2:Z:2:NAG:H82	1.49	0.94
1:C:234:ASN:OD1	2:Y:1:NAG:N2	2.06	0.89
1:A:32:PHE:O	9:A:1308:NAG:H3	1.75	0.87
1:B:122:ASN:OD1	1:B:123:ALA:N	2.08	0.86
3:U:2:NAG:H3	3:U:3:BMA:H2	1.57	0.86
5:P:2:NAG:O6	5:P:3:BMA:O2	1.96	0.84
5:Q:2:NAG:O4	5:Q:3:BMA:O6	1.96	0.83
7:S:3:BMA:H3	7:S:4:MAN:H5	1.58	0.83
7:a:3:BMA:O2	7:a:4:MAN:O5	1.98	0.82
1:A:985:ASP:OD1	1:A:986:PRO:HD2	1.79	0.81
3:U:2:NAG:H83	3:U:3:BMA:H2	1.64	0.80
1:B:493:GLN:NE2	1:B:494:SER:O	2.15	0.79
1:B:408:ARG:NH1	1:B:414:GLN:OE1	2.16	0.79
1:A:884:SER:OG	1:A:887:THR:OG1	1.99	0.79
1:A:234:ASN:HB3	9:A:1302:NAG:N2	1.98	0.79
6:R:2:NAG:H62	6:R:3:BMA:O2	1.83	0.79
1:A:331:ASN:OD1	3:E:1:NAG:N2	2.16	0.78
9:B:1302:NAG:H83	9:B:1302:NAG:H3	1.65	0.78
2:f:1:NAG:O3	2:f:2:NAG:O5	2.01	0.78
1:A:142:GLY:O	1:A:155:SER:OG	2.03	0.77
3:U:2:NAG:H3	3:U:2:NAG:H83	1.67	0.77
8:d:1:NAG:O3	8:d:2:NAG:N2	2.17	0.77
7:a:1:NAG:O3	7:a:2:NAG:O5	2.01	0.77
4:H:2:NAG:H3	4:H:2:NAG:H83	1.67	0.76
5:Q:2:NAG:H4	5:Q:4:MAN:H5	1.67	0.76
1:A:603:ASN:OD1	1:A:604:THR:N	2.19	0.76
2:N:1:NAG:H3	2:N:1:NAG:H83	1.68	0.76
1:A:233:ILE:HA	9:A:1302:NAG:H81	1.68	0.76
1:B:178:ASP:OD1	1:B:190:ARG:NH2	2.20	0.75
3:e:1:NAG:H4	3:e:2:NAG:C7	2.17	0.75
1:A:41:LYS:HG3	1:C:562:PHE:O	1.86	0.75
1:B:145:TYR:O	1:B:146:HIS:ND1	2.19	0.74
1:A:902:MET:HE1	1:A:1050:MET:CE	2.17	0.74
4:c:2:NAG:H3	4:c:2:NAG:H83	1.69	0.74
1:A:919:ASN:O	1:A:923:ILE:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:ND2	1:C:360:ASN:O	2.22	0.73
1:A:59:PHE:CE1	9:A:1308:NAG:H62	2.23	0.73
9:B:1308:NAG:H3	9:B:1308:NAG:H83	1.70	0.73
1:C:111:ASP:O	1:C:112:SER:OG	2.07	0.72
1:C:1101:HIS:ND1	8:d:1:NAG:H5	2.04	0.72
3:K:1:NAG:H4	3:K:2:NAG:C7	2.19	0.72
2:Z:2:NAG:H3	2:Z:2:NAG:H83	1.70	0.72
3:e:2:NAG:H3	3:e:3:BMA:H2	1.72	0.72
3:e:1:NAG:H82	3:e:2:NAG:H82	1.71	0.72
3:T:2:NAG:H83	3:T:2:NAG:H3	1.72	0.72
1:A:31:SER:N	1:A:61:ASN:OD1	2.23	0.71
1:C:403:ARG:NH1	1:C:494:SER:OG	2.22	0.71
2:f:1:NAG:O6	2:f:2:NAG:O7	2.08	0.71
6:R:2:NAG:O4	6:R:3:BMA:O6	2.07	0.71
7:S:3:BMA:H3	7:S:4:MAN:C5	2.20	0.71
1:C:1074:ASN:ND2	4:c:1:NAG:H61	1.99	0.70
1:B:657:ASN:OD1	9:B:1305:NAG:N2	2.25	0.70
1:A:902:MET:HE1	1:A:1050:MET:HE1	1.73	0.70
9:A:1304:NAG:O7	1:C:466:ARG:NH2	2.25	0.70
1:A:109:THR:OG1	1:A:114:THR:OG1	2.08	0.69
1:A:580:GLN:O	3:E:2:NAG:H81	1.92	0.69
7:S:3:BMA:H3	7:S:4:MAN:H3	1.73	0.69
1:B:155:SER:OG	1:B:156:GLU:OE1	2.08	0.69
1:B:1092:GLU:OE1	1:B:1092:GLU:N	2.26	0.69
1:C:165:ASN:OD1	9:C:1303:NAG:N2	2.27	0.68
1:B:424:LYS:HG2	1:B:461:LEU:HD13	1.76	0.68
1:B:340:GLU:OE2	1:B:356:LYS:NZ	2.27	0.67
1:C:1074:ASN:OD1	4:c:3:FUC:H61	1.93	0.67
1:A:436:TRP:NE1	1:A:509:ARG:O	2.26	0.67
7:b:1:NAG:H83	7:b:2:NAG:C8	2.24	0.67
1:B:987:PRO:HG2	1:B:988:GLU:OE1	1.93	0.67
1:C:324:GLU:OE1	1:C:325:SER:N	2.28	0.67
3:e:1:NAG:O6	3:e:2:NAG:H2	1.95	0.67
1:A:32:PHE:HA	9:A:1308:NAG:H5	1.77	0.67
1:A:580:GLN:C	3:E:2:NAG:H81	2.19	0.66
1:C:578:ASP:OD1	1:C:581:THR:N	2.28	0.66
1:A:717:ASN:OD1	1:A:718:PHE:N	2.29	0.66
1:B:378:LYS:NZ	1:B:380:TYR:OH	2.29	0.66
1:A:56:LEU:HD21	9:A:1308:NAG:C8	2.20	0.65
2:f:1:NAG:H3	2:f:2:NAG:O3	1.95	0.65
1:B:160:TYR:OH	2:M:2:NAG:H3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:CZ	9:A:1308:NAG:H62	2.32	0.65
1:A:563:GLN:NE2	1:B:42:VAL:O	2.30	0.65
3:J:1:NAG:O6	3:J:2:NAG:H2	1.97	0.65
9:A:1308:NAG:O7	9:A:1308:NAG:O3	2.10	0.64
2:Y:1:NAG:H62	2:Y:2:NAG:H2	1.79	0.64
1:A:717:ASN:HD22	3:F:1:NAG:H83	1.61	0.64
3:W:1:NAG:O3	3:W:2:NAG:O5	2.13	0.64
2:N:1:NAG:H62	2:N:2:NAG:H2	1.80	0.64
1:A:341:VAL:HG21	1:A:397:ALA:HB1	1.78	0.64
1:A:581:THR:HG22	3:E:2:NAG:H83	1.78	0.64
3:F:2:NAG:H3	3:F:2:NAG:H83	1.78	0.64
1:A:99:ASN:O	1:A:102:ARG:NH1	2.30	0.64
3:G:1:NAG:H62	3:G:2:NAG:C1	2.28	0.64
1:A:986:PRO:N	1:A:987:PRO:HD2	2.13	0.63
7:a:1:NAG:H83	7:a:1:NAG:H3	1.80	0.63
1:A:151:SER:OG	1:A:153:MET:HE1	1.97	0.63
1:A:442:ASP:OD1	1:A:509:ARG:NE	2.30	0.63
1:C:1106:GLN:NE2	1:C:1111:GLU:OE2	2.32	0.63
1:A:153:MET:HE3	1:A:153:MET:H	1.63	0.62
1:A:657:ASN:HB2	9:A:1307:NAG:H2	1.81	0.62
1:A:737:ASP:OD2	1:C:317:ASN:ND2	2.32	0.62
9:A:1304:NAG:H2	1:C:466:ARG:HH22	1.64	0.62
1:B:578:ASP:OD1	1:B:581:THR:N	2.31	0.62
4:c:1:NAG:H5	4:c:2:NAG:C7	2.29	0.62
1:C:603:ASN:HB3	9:C:1304:NAG:H83	1.82	0.62
3:I:2:NAG:H3	3:I:3:BMA:O5	1.98	0.62
1:B:457:ARG:NH1	1:B:460:ASN:O	2.32	0.61
1:B:657:ASN:OD1	9:B:1305:NAG:C2	2.47	0.61
7:S:3:BMA:H3	7:S:4:MAN:C3	2.31	0.61
1:C:546:LEU:HD12	1:C:546:LEU:O	2.00	0.61
1:B:96:GLU:OE1	1:B:100:ILE:N	2.33	0.60
9:B:1307:NAG:H83	9:B:1307:NAG:H3	1.81	0.60
8:d:3:BMA:O6	8:d:4:MAN:H3	2.02	0.60
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.32	0.60
1:B:62:VAL:HG23	1:B:268:GLY:CA	2.31	0.60
1:A:315:THR:HG22	1:A:316:SER:H	1.66	0.60
2:Z:1:NAG:H61	2:Z:2:NAG:C1	2.31	0.60
1:A:581:THR:OG1	1:A:583:GLU:OE2	2.16	0.60
1:B:985:ASP:HB2	1:B:986:PRO:HD2	1.83	0.60
1:A:68:ILE:O	1:A:77:LYS:N	2.34	0.59
1:B:1074:ASN:ND2	6:R:1:NAG:O6	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:NAG:O6	3:F:3:BMA:O2	2.16	0.59
1:A:357:ARG:NH2	1:B:166:CYS:O	2.34	0.59
9:B:1302:NAG:H3	9:B:1302:NAG:C8	2.33	0.59
1:A:157:PHE:CZ	9:A:1301:NAG:H62	2.38	0.59
1:B:580:GLN:O	9:B:1306:NAG:H3	2.03	0.59
3:J:1:NAG:H4	3:J:2:NAG:C7	2.33	0.59
1:A:363:ALA:N	1:A:525:CYS:O	2.33	0.59
1:C:403:ARG:NE	1:C:405:ASP:OD1	2.35	0.59
1:C:786:LYS:NZ	1:C:873:TYR:OH	2.36	0.59
1:B:403:ARG:NH1	1:B:505:TYR:O	2.35	0.58
1:C:149:ASN:OD1	1:C:150:LYS:N	2.36	0.58
1:B:618:THR:OG1	9:B:1308:NAG:H61	2.02	0.58
8:d:1:NAG:H4	8:d:5:FUC:H5	1.85	0.58
4:H:2:NAG:H3	4:H:2:NAG:C8	2.34	0.58
1:B:160:TYR:OH	2:M:2:NAG:H83	2.04	0.58
5:Q:1:NAG:O3	5:Q:2:NAG:N2	2.37	0.58
1:A:902:MET:HE1	1:A:1050:MET:HE2	1.86	0.58
1:C:331:ASN:ND2	3:W:1:NAG:O5	2.34	0.58
3:I:1:NAG:C6	3:I:2:NAG:H2	2.34	0.57
3:I:1:NAG:H4	3:I:2:NAG:C7	2.35	0.57
1:A:66:HIS:ND1	1:A:263:ALA:O	2.37	0.57
1:B:149:ASN:OD1	9:B:1302:NAG:N2	2.37	0.57
2:g:1:NAG:O6	2:g:2:NAG:H2	2.04	0.57
3:G:2:NAG:O7	3:G:2:NAG:H3	2.03	0.57
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.37	0.57
1:C:127:VAL:HG21	9:C:1301:NAG:H62	1.87	0.57
1:B:159:VAL:HG23	1:B:160:TYR:CD1	2.40	0.57
1:C:118:LEU:HD11	1:C:120:VAL:HB	1.87	0.57
1:C:986:PRO:N	1:C:987:PRO:HD2	2.20	0.56
1:A:1077:THR:OG1	1:B:900:MET:HE1	2.06	0.56
3:e:1:NAG:H4	3:e:2:NAG:O7	2.04	0.56
3:K:1:NAG:H2	3:K:2:NAG:C7	2.36	0.56
3:U:2:NAG:H3	3:U:2:NAG:C8	2.35	0.56
1:B:393:THR:O	1:B:523:THR:HG22	2.05	0.56
1:A:62:VAL:HG23	1:A:267:VAL:C	2.31	0.56
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.36	0.56
1:C:390:LEU:HD23	1:C:391:CYS:N	2.20	0.56
2:D:1:NAG:H4	2:D:2:NAG:C7	2.36	0.56
1:B:796:ASP:OD2	3:K:1:NAG:N2	2.39	0.56
7:b:1:NAG:O4	7:b:1:NAG:N2	2.38	0.56
3:E:1:NAG:O3	3:E:2:NAG:H2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:1:NAG:H83	7:b:2:NAG:H82	1.89	0.55
1:B:532:ASN:OD1	1:B:533:LEU:N	2.39	0.55
2:N:1:NAG:H3	2:N:1:NAG:C8	2.36	0.55
1:C:119:ILE:HG22	1:C:119:ILE:O	2.06	0.55
1:C:200:TYR:HB2	1:C:202:LYS:HZ2	1.72	0.54
2:D:1:NAG:H61	2:D:2:NAG:O5	2.07	0.54
9:B:1308:NAG:H3	9:B:1308:NAG:C8	2.37	0.54
1:C:34:ARG:HG3	1:C:216:LEU:HD21	1.88	0.54
2:g:1:NAG:H4	2:g:2:NAG:C7	2.37	0.54
1:A:59:PHE:H	9:A:1308:NAG:H2	1.72	0.54
9:A:1303:NAG:H83	9:A:1303:NAG:H3	1.89	0.54
1:A:234:ASN:HB3	9:A:1302:NAG:C7	2.38	0.54
1:C:382:VAL:HG23	1:C:383:SER:H	1.72	0.54
6:R:2:NAG:O3	6:R:2:NAG:H82	2.08	0.54
3:E:1:NAG:H3	3:E:1:NAG:O7	2.08	0.54
3:J:1:NAG:H4	3:J:2:NAG:N2	2.17	0.54
4:c:2:NAG:H3	4:c:2:NAG:C8	2.37	0.54
1:A:327:VAL:O	1:A:531:THR:OG1	2.25	0.53
1:B:287:ASP:OD1	1:B:288:ALA:N	2.41	0.53
1:C:131:CYS:HA	1:C:166:CYS:CB	2.38	0.53
1:A:287:ASP:OD1	1:A:288:ALA:N	2.40	0.53
1:B:165:ASN:OD1	1:B:166:CYS:N	2.42	0.53
3:K:1:NAG:H4	3:K:2:NAG:O7	2.07	0.53
2:g:1:NAG:H61	2:g:2:NAG:O5	2.09	0.53
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.41	0.53
1:B:567:ARG:NH1	1:B:571:ASP:OD1	2.42	0.53
7:a:3:BMA:H4	7:a:4:MAN:O5	2.09	0.53
1:B:34:ARG:HG3	1:B:216:LEU:HD21	1.89	0.52
1:B:612:TYR:CD2	1:B:620:VAL:HG21	2.44	0.52
3:e:1:NAG:H4	3:e:2:NAG:N2	2.09	0.52
2:Y:1:NAG:O6	2:Y:2:NAG:O5	2.19	0.52
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.91	0.52
1:B:519:HIS:ND1	1:B:519:HIS:O	2.43	0.52
1:C:1098:ASN:ND2	8:d:5:FUC:H61	2.24	0.52
2:N:1:NAG:H4	2:N:2:NAG:N2	2.22	0.52
1:A:33:THR:OG1	1:A:219:GLY:O	2.12	0.52
1:A:166:CYS:SG	1:A:167:THR:N	2.82	0.52
1:C:327:VAL:HG11	1:C:531:THR:HG23	1.92	0.52
1:C:177:MET:SD	1:C:177:MET:N	2.84	0.52
1:B:827:THR:O	1:B:949:GLN:NE2	2.43	0.51
1:C:310:LYS:NZ	1:C:663:ASP:OD1	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ASN:OD1	1:C:355:ARG:N	2.43	0.51
1:C:391:CYS:SG	1:C:525:CYS:N	2.83	0.51
1:A:869:MET:HE1	1:C:697:MET:HG2	1.92	0.51
3:I:1:NAG:H4	3:I:2:NAG:O7	2.11	0.51
1:B:984:LEU:HD12	1:B:988:GLU:CB	2.41	0.51
1:B:516:GLU:OE1	1:B:516:GLU:N	2.42	0.51
1:A:191:GLU:N	1:A:191:GLU:OE1	2.44	0.51
9:C:1304:NAG:H61	9:C:1304:NAG:O3	2.10	0.51
3:T:2:NAG:H3	3:T:2:NAG:C8	2.40	0.50
7:b:1:NAG:N2	7:b:2:NAG:O7	2.45	0.50
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.44	0.50
1:B:239:GLN:OE1	1:B:240:THR:N	2.43	0.50
1:A:233:ILE:HA	9:A:1302:NAG:C8	2.40	0.50
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.44	0.50
1:A:931:ILE:O	1:A:934:ILE:HG22	2.12	0.50
3:K:1:NAG:H4	3:K:2:NAG:N2	2.19	0.50
1:C:353:TRP:NE1	1:C:465:GLU:OE2	2.44	0.50
1:B:66:HIS:NE2	1:B:261:GLY:O	2.43	0.50
2:Z:2:NAG:H3	2:Z:2:NAG:C8	2.39	0.50
1:A:267:VAL:HG12	1:A:267:VAL:O	2.11	0.50
1:C:339:GLY:HA3	2:f:1:NAG:H62	1.94	0.50
2:D:1:NAG:H61	2:D:2:NAG:C1	2.42	0.50
1:A:149:ASN:HD21	1:A:152:TRP:CB	2.25	0.50
1:B:878:LEU:O	1:B:882:ILE:HG23	2.12	0.50
2:Z:1:NAG:C6	2:Z:2:NAG:H82	2.32	0.50
1:A:620:VAL:N	1:A:621:PRO:CD	2.75	0.49
2:L:1:NAG:O3	2:L:2:NAG:H2	2.11	0.49
1:A:153:MET:HE3	1:A:153:MET:N	2.26	0.49
1:A:1002:GLN:OE1	1:B:1002:GLN:NE2	2.45	0.49
1:C:117:LEU:HG	1:C:130:VAL:HG22	1.95	0.49
2:N:1:NAG:H4	2:N:2:NAG:C7	2.42	0.49
1:B:601:GLY:O	1:B:604:THR:HG22	2.12	0.49
3:U:1:NAG:O3	3:U:2:NAG:H2	2.11	0.49
3:K:2:NAG:H3	3:K:3:BMA:O5	2.06	0.49
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.94	0.49
1:A:38:TYR:OH	1:A:284:THR:OG1	2.22	0.49
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.45	0.49
1:C:374:PHE:HA	2:f:2:NAG:H62	1.93	0.49
1:A:796:ASP:OD2	1:C:709:ASN:ND2	2.46	0.49
1:A:603:ASN:OD1	1:A:603:ASN:C	2.56	0.49
1:C:287:ASP:OD1	1:C:288:ALA:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:HB2	9:A:1303:NAG:C2	2.42	0.48
1:A:172:SER:OG	1:A:173:GLN:N	2.46	0.48
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	1.94	0.48
1:B:62:VAL:HG23	1:B:268:GLY:N	2.29	0.48
1:B:801:ASN:HD22	5:Q:1:NAG:H62	1.79	0.48
6:R:1:NAG:O3	6:R:2:NAG:O5	2.21	0.48
1:B:119:ILE:HG22	1:B:119:ILE:O	2.13	0.48
8:d:1:NAG:HO3	8:d:2:NAG:HN2	1.58	0.48
3:U:2:NAG:H3	3:U:3:BMA:C2	2.35	0.48
8:d:2:NAG:O4	8:d:3:BMA:H62	2.14	0.48
1:B:234:ASN:HB3	9:B:1304:NAG:C7	2.44	0.48
1:B:530:SER:O	1:B:531:THR:HG23	2.13	0.48
1:A:87:ASN:OD1	1:A:87:ASN:N	2.44	0.48
1:C:902:MET:HG3	1:C:916:LEU:HD13	1.95	0.48
7:b:1:NAG:H83	7:b:2:NAG:H81	1.95	0.47
2:f:1:NAG:C3	2:f:2:NAG:O5	2.62	0.47
9:A:1304:NAG:O3	1:C:355:ARG:NH2	2.46	0.47
1:B:359:SER:HB2	1:B:523:THR:HG21	1.96	0.47
1:C:165:ASN:OD1	9:C:1303:NAG:C7	2.62	0.47
8:d:2:NAG:O7	8:d:2:NAG:H3	2.13	0.47
1:A:32:PHE:CA	9:A:1308:NAG:H5	2.42	0.47
1:B:1074:ASN:ND2	6:R:1:NAG:C6	2.77	0.47
2:Y:1:NAG:H4	2:Y:2:NAG:H2	1.45	0.47
1:B:945:LEU:HD12	1:B:945:LEU:N	2.29	0.47
1:A:59:PHE:N	9:A:1308:NAG:H2	2.28	0.47
1:A:111:ASP:OD1	1:A:111:ASP:N	2.47	0.47
1:B:427:ASP:OD1	1:B:427:ASP:N	2.47	0.47
1:C:200:TYR:CB	1:C:202:LYS:HZ2	2.28	0.47
1:A:359:SER:HB3	1:A:523:THR:HG21	1.97	0.47
1:A:902:MET:HB3	1:A:916:LEU:HD21	1.96	0.47
1:B:724:THR:HB	1:B:934:ILE:HD11	1.97	0.47
1:C:239:GLN:NE2	1:C:240:THR:O	2.48	0.47
1:B:473:TYR:CD1	1:B:474:GLN:N	2.84	0.46
1:B:916:LEU:HD12	1:B:923:ILE:HD13	1.96	0.46
7:S:2:NAG:O7	7:S:2:NAG:H3	2.15	0.46
2:Z:1:NAG:H82	2:Z:1:NAG:O3	2.15	0.46
1:A:615:VAL:HG12	1:A:616:ASN:O	2.14	0.46
1:A:709:ASN:HD22	3:K:1:NAG:C7	2.28	0.46
1:A:326:ILE:HG23	1:A:541:PHE:HA	1.97	0.46
1:B:454:ARG:NH2	1:B:467:ASP:O	2.47	0.46
1:C:125:ASN:ND2	1:C:171:VAL:HG13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:2:NAG:C4	5:Q:4:MAN:H5	2.43	0.46
8:d:2:NAG:H2	8:d:5:FUC:H3	1.98	0.46
1:A:801:ASN:OD1	3:G:1:NAG:N2	2.48	0.46
1:B:546:LEU:HD23	1:B:546:LEU:O	2.16	0.46
1:B:985:ASP:O	1:B:986:PRO:C	2.58	0.46
1:C:405:ASP:OD2	1:C:493:GLN:NE2	2.49	0.46
1:B:33:THR:O	1:B:34:ARG:C	2.58	0.46
7:a:3:BMA:HO2	7:a:4:MAN:C1	2.18	0.46
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.48	0.46
1:A:234:ASN:CB	9:A:1302:NAG:N2	2.76	0.46
1:B:33:THR:HG22	1:B:58:PHE:CD2	2.50	0.46
1:B:496:GLY:O	1:B:501:ASN:ND2	2.47	0.46
1:B:625:HIS:ND1	1:B:632:THR:HG23	2.30	0.46
2:D:1:NAG:H2	2:D:2:NAG:O7	2.16	0.46
3:T:1:NAG:C6	3:T:2:NAG:H82	2.45	0.46
1:B:166:CYS:SG	1:B:167:THR:N	2.89	0.46
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.97	0.46
1:A:338:PHE:HE1	1:A:358:ILE:HD13	1.81	0.45
1:A:1134:ASN:OD1	3:J:1:NAG:O5	2.32	0.45
1:B:1074:ASN:OD1	6:R:4:FUC:H3	2.16	0.45
1:B:124:THR:OG1	2:M:1:NAG:H83	2.16	0.45
3:K:1:NAG:H2	3:K:2:NAG:C8	2.46	0.45
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.97	0.45
1:A:149:ASN:HB2	9:A:1303:NAG:H2	1.98	0.45
1:A:409:GLN:N	1:A:409:GLN:OE1	2.50	0.45
1:A:1132:ILE:HG23	3:J:1:NAG:H82	1.99	0.45
1:C:102:ARG:N	1:C:241:LEU:O	2.49	0.45
1:C:934:ILE:CD1	1:C:1063:LEU:HD22	2.46	0.45
1:B:455:LEU:HD21	1:B:493:GLN:HB2	1.97	0.45
1:C:393:THR:OG1	1:C:394:ASN:N	2.49	0.45
3:F:2:NAG:C4	3:F:3:BMA:HO2	2.29	0.45
8:d:1:NAG:H4	8:d:2:NAG:H2	1.52	0.45
1:C:430:THR:HG22	1:C:430:THR:O	2.17	0.45
1:A:391:CYS:HA	1:A:525:CYS:HA	1.99	0.45
1:A:657:ASN:HB2	9:A:1307:NAG:C2	2.47	0.45
2:M:2:NAG:C1	2:M:2:NAG:C8	2.94	0.45
1:B:410:ILE:HG21	1:B:433:VAL:HG11	1.99	0.45
1:B:717:ASN:HB3	1:B:1070:ALA:HB3	1.99	0.45
7:b:1:NAG:O4	7:b:2:NAG:O7	2.35	0.45
1:A:96:GLU:OE2	1:A:99:ASN:ND2	2.42	0.44
1:B:40:ASP:OD1	1:B:40:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG23	1:C:383:SER:N	2.33	0.44
1:C:1074:ASN:OD1	1:C:1074:ASN:C	2.59	0.44
1:A:106:PHE:CD2	1:A:117:LEU:HD22	2.52	0.44
1:C:409:GLN:OE1	1:C:422:ASN:ND2	2.51	0.44
2:M:2:NAG:C1	2:M:2:NAG:H82	2.47	0.44
1:A:108:THR:HB	1:A:234:ASN:O	2.16	0.44
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.50	0.44
1:C:406:GLU:O	1:C:409:GLN:HG3	2.17	0.44
1:B:407:VAL:O	1:B:410:ILE:HG22	2.17	0.44
8:d:1:NAG:H2	8:d:5:FUC:C6	2.48	0.44
1:C:982:SER:O	1:C:982:SER:OG	2.33	0.44
2:g:1:NAG:H4	2:g:2:NAG:H2	1.44	0.44
1:A:708:SER:OG	1:A:709:ASN:N	2.50	0.44
1:B:358:ILE:HB	1:B:395:VAL:CG2	2.48	0.44
1:B:804:GLN:CD	5:Q:1:NAG:H61	2.43	0.44
1:A:1079:PRO:HA	1:B:900:MET:HE2	2.00	0.44
1:C:175:PHE:HB3	1:C:177:MET:HE1	2.00	0.44
3:e:2:NAG:H3	3:e:3:BMA:C2	2.45	0.44
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	2.00	0.44
2:N:1:NAG:C6	2:N:2:NAG:H2	2.47	0.44
3:e:1:NAG:C6	3:e:2:NAG:H2	2.47	0.44
2:Y:1:NAG:H4	2:Y:2:NAG:C7	2.48	0.43
9:A:1304:NAG:H83	1:C:355:ARG:HD3	2.00	0.43
1:B:689:SER:OG	1:B:690:GLN:N	2.50	0.43
1:B:901:GLN:O	1:B:905:ARG:HG2	2.18	0.43
1:C:914:ASN:OD1	1:C:915:VAL:N	2.51	0.43
1:B:36:VAL:HG23	1:B:55:PHE:CE2	2.53	0.43
1:B:231:ILE:HG22	1:B:233:ILE:HG23	2.00	0.43
1:C:368:LEU:HD11	1:C:374:PHE:CE2	2.53	0.43
7:S:3:BMA:C3	7:S:4:MAN:H5	2.39	0.43
2:g:1:NAG:H4	2:g:2:NAG:O7	2.18	0.43
1:A:986:PRO:N	1:A:987:PRO:CD	2.80	0.43
1:C:375:SER:HB2	1:C:436:TRP:CB	2.48	0.43
1:C:752:LEU:HD12	1:C:993:ILE:HG21	2.00	0.43
1:B:36:VAL:HG23	1:B:55:PHE:CD2	2.54	0.43
1:B:736:VAL:HG13	1:B:858:LEU:HD23	2.01	0.43
1:C:925:ASN:HB3	7:a:2:NAG:H81	2.00	0.43
1:B:320:VAL:HG22	1:B:623:ALA:CB	2.49	0.43
1:C:296:LEU:O	1:C:299:THR:OG1	2.28	0.43
1:C:339:GLY:O	1:C:343:ASN:ND2	2.47	0.43
3:F:2:NAG:H3	3:F:2:NAG:C8	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:1:NAG:HO3	7:a:2:NAG:C5	2.26	0.43
1:A:62:VAL:HG22	1:A:63:THR:O	2.19	0.43
1:C:940:SER:OG	1:C:941:THR:N	2.50	0.43
1:A:1148:PHE:CE2	1:C:1148:PHE:CE2	3.07	0.43
1:B:124:THR:O	1:B:175:PHE:N	2.52	0.43
1:B:616:ASN:OD1	1:B:616:ASN:C	2.61	0.43
2:Y:1:NAG:O3	2:Y:2:NAG:C7	2.66	0.43
7:a:2:NAG:O3	7:a:3:BMA:H2	2.19	0.43
2:D:1:NAG:H4	2:D:2:NAG:N2	2.17	0.43
1:A:62:VAL:CG2	1:A:267:VAL:C	2.92	0.42
1:A:641:ASN:ND2	1:A:654:GLU:OE1	2.48	0.42
1:B:42:VAL:HG21	1:B:44:ARG:CZ	2.49	0.42
5:P:2:NAG:H4	5:P:3:BMA:H2	1.46	0.42
1:B:173:GLN:O	1:B:175:PHE:N	2.52	0.42
2:D:1:NAG:H4	2:D:2:NAG:O7	2.19	0.42
1:B:759:PHE:HD2	1:B:1001:LEU:HD21	1.84	0.42
1:A:234:ASN:HB3	9:A:1302:NAG:C2	2.49	0.42
1:C:153:MET:HE3	1:C:154:GLU:H	1.85	0.42
3:F:2:NAG:O3	3:F:3:BMA:C1	2.68	0.42
1:A:30:ASN:CG	1:A:61:ASN:OD1	2.63	0.42
1:A:35:GLY:HA3	1:A:56:LEU:HD23	2.00	0.42
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.53	0.42
1:B:342:PHE:HB2	3:U:1:NAG:H82	2.01	0.42
1:B:914:ASN:OD1	1:B:915:VAL:N	2.53	0.42
2:Y:1:NAG:H4	2:Y:2:NAG:O7	2.18	0.42
3:I:1:NAG:H61	3:I:2:NAG:H2	2.02	0.42
3:T:1:NAG:H62	3:T:2:NAG:H82	2.01	0.42
1:B:37:TYR:O	1:B:38:TYR:CD2	2.72	0.42
1:B:42:VAL:HG21	1:B:44:ARG:NH2	2.35	0.42
1:B:214:ARG:HG3	1:B:215:ASP:H	1.85	0.42
1:B:461:LEU:HD12	1:B:461:LEU:C	2.45	0.42
1:C:61:ASN:CB	9:C:1302:NAG:H2	2.49	0.42
1:C:105:ILE:HG23	1:C:241:LEU:HD11	2.01	0.42
1:C:327:VAL:HG13	1:C:531:THR:H	1.85	0.42
7:a:1:NAG:H3	7:a:1:NAG:C8	2.48	0.42
1:A:901:GLN:O	1:A:905:ARG:HG2	2.20	0.41
1:A:919:ASN:HB2	1:A:923:ILE:HD11	2.01	0.41
1:B:205:SER:OG	1:B:206:LYS:N	2.52	0.41
1:B:657:ASN:OD1	9:B:1305:NAG:C7	2.67	0.41
1:C:433:VAL:O	1:C:433:VAL:HG13	2.19	0.41
1:A:581:THR:HG22	3:E:2:NAG:C8	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:CD1	1:B:37:TYR:N	2.88	0.41
1:B:612:TYR:CG	1:B:620:VAL:HG21	2.55	0.41
9:B:1307:NAG:H3	9:B:1307:NAG:C8	2.50	0.41
1:A:358:ILE:HB	1:A:395:VAL:HB	2.01	0.41
1:A:985:ASP:C	1:A:987:PRO:HD2	2.44	0.41
2:f:1:NAG:H5	2:f:2:NAG:H2	2.02	0.41
1:A:33:THR:HA	9:A:1308:NAG:O4	2.20	0.41
1:B:865:LEU:HD23	1:B:869:MET:CE	2.51	0.41
1:C:87:ASN:OD1	1:C:87:ASN:N	2.52	0.41
1:B:331:ASN:HD21	1:B:580:GLN:HA	1.85	0.41
1:A:813:SER:O	1:A:815:ARG:N	2.54	0.41
1:C:298:GLU:OE1	1:C:633:TRP:NE1	2.48	0.41
1:C:902:MET:HE1	1:C:1050:MET:CE	2.51	0.41
2:Y:1:NAG:HO6	2:Y:2:NAG:C5	2.32	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HG23	2.03	0.41
1:C:131:CYS:HA	1:C:166:CYS:HB3	2.02	0.41
1:A:294:ASP:N	1:A:294:ASP:OD1	2.54	0.41
1:A:326:ILE:HD11	1:A:533:LEU:HA	2.03	0.41
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.56	0.41
1:A:560:LEU:O	1:A:577:ARG:NH1	2.48	0.41
1:B:1103:PHE:HZ	7:S:1:NAG:H5	1.86	0.41
1:C:566:GLY:N	1:C:575:ALA:O	2.53	0.41
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.03	0.41
1:C:901:GLN:O	1:C:905:ARG:HG2	2.21	0.41
1:C:986:PRO:CD	1:C:987:PRO:HD2	2.51	0.41
3:U:1:NAG:HO6	3:U:2:NAG:HO6	1.65	0.41
3:e:1:NAG:H4	3:e:2:NAG:H2	1.66	0.41
1:A:81:ASN:O	1:A:239:GLN:NE2	2.53	0.41
1:A:337:PRO:HD2	1:A:358:ILE:HG23	2.03	0.41
1:A:656:VAL:HG12	1:A:658:ASN:H	1.84	0.41
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.33	0.41
1:B:461:LEU:HD12	1:B:461:LEU:O	2.20	0.40
1:C:117:LEU:CD2	1:C:119:ILE:HD11	2.51	0.40
1:C:191:GLU:O	1:C:205:SER:HA	2.21	0.40
1:C:1074:ASN:OD1	1:C:1074:ASN:O	2.39	0.40
1:A:728:PRO:O	1:A:1021:SER:OG	2.35	0.40
1:B:1048:HIS:HA	1:B:1066:THR:HG22	2.02	0.40
1:A:350:VAL:HG13	1:A:351:TYR:N	2.37	0.40
1:A:452:LEU:H	1:A:452:LEU:HD23	1.86	0.40
1:C:337:PRO:O	1:C:341:VAL:HG23	2.21	0.40
1:C:462:LYS:HB3	1:C:463:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:NZ	1:C:562:PHE:O	2.55	0.40
1:B:331:ASN:OD1	1:B:331:ASN:N	2.52	0.40
1:C:131:CYS:HA	1:C:166:CYS:HB2	2.02	0.40
1:C:360:ASN:O	1:C:360:ASN:ND2	2.55	0.40
1:A:32:PHE:C	9:A:1308:NAG:H5	2.46	0.40
1:A:724:THR:HB	1:A:934:ILE:HD11	2.02	0.40
1:B:620:VAL:N	1:B:621:PRO:HD2	2.36	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	1010/1312 (77%)	967 (96%)	43 (4%)	0	100	100
1	B	1052/1312 (80%)	977 (93%)	73 (7%)	2 (0%)	43	66
1	C	1038/1312 (79%)	959 (92%)	78 (8%)	1 (0%)	48	72
All	All	3100/3936 (79%)	2903 (94%)	194 (6%)	3 (0%)	49	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ILE
1	C	166	CYS
1	B	34	ARG

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	890/1137 (78%)	889 (100%)	1 (0%)	88	95
1	B	923/1137 (81%)	922 (100%)	1 (0%)	88	95
1	C	909/1137 (80%)	907 (100%)	2 (0%)	87	94
All	All	2722/3411 (80%)	2718 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	B	616	ASN
1	C	760	CYS
1	C	916	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	173	GLN
1	A	563	GLN
1	A	564	GLN
1	A	919	ASN
1	B	321	GLN
1	B	764	ASN
1	B	955	ASN
1	B	1010	GLN
1	B	1058	HIS
1	C	146	HIS
1	C	183	GLN
1	C	370	ASN
1	C	655	HIS
1	C	949	GLN
1	C	1011	GLN
1	C	1088	HIS
1	C	1142	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 ⓘ

86 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2,1	14,14,15	2.08	4 (28%)	17,19,21	1.18	3 (17%)
2	NAG	D	2	2	14,14,15	2.06	4 (28%)	17,19,21	1.27	3 (17%)
3	NAG	E	1	3,1	14,14,15	1.99	4 (28%)	17,19,21	1.44	4 (23%)
3	NAG	E	2	3	14,14,15	1.96	5 (35%)	17,19,21	1.52	3 (17%)
3	BMA	E	3	3	11,11,12	0.56	0	15,15,17	0.72	0
3	NAG	F	1	3,1	14,14,15	1.88	3 (21%)	17,19,21	1.49	4 (23%)
3	NAG	F	2	3	14,14,15	1.97	4 (28%)	17,19,21	1.30	1 (5%)
3	BMA	F	3	3	11,11,12	0.87	0	15,15,17	0.87	0
3	NAG	G	1	3,1	14,14,15	1.73	3 (21%)	17,19,21	2.54	5 (29%)
3	NAG	G	2	3	14,14,15	1.99	3 (21%)	17,19,21	0.92	1 (5%)
3	BMA	G	3	3	11,11,12	0.55	0	15,15,17	0.67	0
4	NAG	H	1	4,1	14,14,15	2.13	4 (28%)	17,19,21	2.21	4 (23%)
4	NAG	H	2	4	14,14,15	2.09	4 (28%)	17,19,21	1.16	2 (11%)
4	FUC	H	3	4	10,10,11	0.64	0	14,14,16	0.67	0
3	NAG	I	1	3,1	14,14,15	1.96	4 (28%)	17,19,21	1.28	2 (11%)
3	NAG	I	2	3	14,14,15	1.97	3 (21%)	17,19,21	1.28	3 (17%)
3	BMA	I	3	3	11,11,12	0.67	0	15,15,17	0.70	0
3	NAG	J	1	3,1	14,14,15	1.99	4 (28%)	17,19,21	1.09	1 (5%)
3	NAG	J	2	3	14,14,15	2.01	4 (28%)	17,19,21	1.21	2 (11%)
3	BMA	J	3	3	11,11,12	0.56	0	15,15,17	0.70	0
3	NAG	K	1	3,1	14,14,15	2.03	5 (35%)	17,19,21	1.54	3 (17%)
3	NAG	K	2	3	14,14,15	2.06	3 (21%)	17,19,21	1.40	3 (17%)
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	1	2,1	14,14,15	1.95	4 (28%)	17,19,21	1.22	2 (11%)
2	NAG	L	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.03	1 (5%)
2	NAG	M	1	2,1	14,14,15	1.99	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	M	2	2	14,14,15	2.08	4 (28%)	17,19,21	1.54	4 (23%)
2	NAG	N	1	2,1	14,14,15	2.02	4 (28%)	17,19,21	1.36	2 (11%)
2	NAG	N	2	2	14,14,15	1.99	4 (28%)	17,19,21	1.13	3 (17%)
5	NAG	P	1	5,1	14,14,15	1.83	3 (21%)	17,19,21	1.48	4 (23%)
5	NAG	P	2	5	14,14,15	1.98	3 (21%)	17,19,21	1.27	3 (17%)
5	BMA	P	3	5	11,11,12	0.65	0	15,15,17	0.68	0
5	MAN	P	4	5	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
5	NAG	Q	1	5,1	14,14,15	1.94	4 (28%)	17,19,21	1.64	5 (29%)
5	NAG	Q	2	5	14,14,15	2.09	5 (35%)	17,19,21	1.59	4 (23%)
5	BMA	Q	3	5	11,11,12	0.83	0	15,15,17	1.23	1 (6%)
5	MAN	Q	4	5	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
6	NAG	R	1	6,1	14,14,15	2.16	4 (28%)	17,19,21	2.31	6 (35%)
6	NAG	R	2	6	14,14,15	2.10	4 (28%)	17,19,21	1.25	2 (11%)
6	BMA	R	3	6	11,11,12	0.82	0	15,15,17	1.15	1 (6%)
6	FUC	R	4	6	10,10,11	1.06	1 (10%)	14,14,16	1.13	1 (7%)
7	NAG	S	1	7,1	14,14,15	1.99	4 (28%)	17,19,21	1.52	3 (17%)
7	NAG	S	2	7	14,14,15	2.01	4 (28%)	17,19,21	1.11	2 (11%)
7	BMA	S	3	7	11,11,12	0.51	0	15,15,17	0.78	0
7	MAN	S	4	7	11,11,12	1.09	1 (9%)	15,15,17	1.49	3 (20%)
3	NAG	T	1	3,1	14,14,15	1.96	4 (28%)	17,19,21	1.12	2 (11%)
3	NAG	T	2	3	14,14,15	2.00	4 (28%)	17,19,21	1.18	1 (5%)
3	BMA	T	3	3	11,11,12	0.54	0	15,15,17	0.71	0
3	NAG	U	1	3,1	14,14,15	1.97	4 (28%)	17,19,21	1.12	2 (11%)
3	NAG	U	2	3	14,14,15	2.02	4 (28%)	17,19,21	1.18	1 (5%)
3	BMA	U	3	3	11,11,12	0.51	0	15,15,17	0.73	0
2	NAG	V	1	2,1	14,14,15	1.97	4 (28%)	17,19,21	1.15	2 (11%)
2	NAG	V	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.12	2 (11%)
3	NAG	W	1	3	12,12,15	1.99	2 (16%)	15,15,21	1.17	1 (6%)
3	NAG	W	2	3	14,14,15	2.03	4 (28%)	17,19,21	0.89	1 (5%)
3	BMA	W	3	3	11,11,12	0.82	0	15,15,17	0.80	0
3	NAG	X	1	3,1	14,14,15	2.01	4 (28%)	17,19,21	1.05	2 (11%)
3	NAG	X	2	3	14,14,15	2.00	4 (28%)	17,19,21	1.08	2 (11%)
3	BMA	X	3	3	11,11,12	0.55	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Y	1	2,1	14,14,15	1.95	4 (28%)	17,19,21	2.33	4 (23%)
2	NAG	Y	2	2	14,14,15	2.06	4 (28%)	17,19,21	1.13	2 (11%)
2	NAG	Z	1	2,1	14,14,15	1.95	4 (28%)	17,19,21	1.28	2 (11%)
2	NAG	Z	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.25	1 (5%)
7	NAG	a	1	7,1	14,14,15	1.99	5 (35%)	17,19,21	1.19	1 (5%)
7	NAG	a	2	7	14,14,15	2.04	3 (21%)	17,19,21	1.52	3 (17%)
7	BMA	a	3	7	11,11,12	0.87	1 (9%)	15,15,17	0.90	0
7	MAN	a	4	7	11,11,12	0.61	0	15,15,17	1.05	2 (13%)
7	NAG	b	1	7,1	14,14,15	2.03	5 (35%)	17,19,21	1.72	4 (23%)
7	NAG	b	2	7	14,14,15	1.99	4 (28%)	17,19,21	1.31	2 (11%)
7	BMA	b	3	7	11,11,12	0.64	0	15,15,17	0.71	0
7	MAN	b	4	7	11,11,12	0.77	0	15,15,17	1.11	2 (13%)
4	NAG	c	1	4,1	14,14,15	1.98	3 (21%)	17,19,21	1.84	4 (23%)
4	NAG	c	2	4	14,14,15	2.02	4 (28%)	17,19,21	1.15	1 (5%)
4	FUC	c	3	4	10,10,11	0.53	0	14,14,16	0.79	0
8	NAG	d	1	8,1	14,14,15	2.00	4 (28%)	17,19,21	1.49	3 (17%)
8	NAG	d	2	8	14,14,15	1.96	4 (28%)	17,19,21	1.49	3 (17%)
8	BMA	d	3	8	11,11,12	0.75	0	15,15,17	1.03	1 (6%)
8	MAN	d	4	8	11,11,12	0.68	0	15,15,17	0.85	1 (6%)
8	FUC	d	5	8	10,10,11	0.72	0	14,14,16	0.63	0
3	NAG	e	1	3,1	14,14,15	1.98	5 (35%)	17,19,21	1.21	1 (5%)
3	NAG	e	2	3	14,14,15	1.97	3 (21%)	17,19,21	1.37	3 (17%)
3	BMA	e	3	3	11,11,12	0.58	0	15,15,17	0.68	0
2	NAG	f	1	2,1	14,14,15	2.07	4 (28%)	17,19,21	1.38	3 (17%)
2	NAG	f	2	2	14,14,15	2.11	4 (28%)	17,19,21	0.92	1 (5%)
2	NAG	g	1	2,1	14,14,15	2.00	4 (28%)	17,19,21	1.13	2 (11%)
2	NAG	g	2	2	14,14,15	2.02	4 (28%)	17,19,21	1.12	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	S	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	4/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	5/6/23/26	0/1/1/1
3	BMA	T	3	3	-	1/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	6/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
2	NAG	V	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3	-	2/15/15/26	-
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	4/6/23/26	0/1/1/1
3	BMA	X	3	3	-	1/2/19/22	0/1/1/1
2	NAG	Y	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	6/6/23/26	0/1/1/1
7	NAG	a	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	BMA	a	3	7	-	1/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	1/1/1/1
7	NAG	b	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	MAN	b	4	7	-	0/2/19/22	0/1/1/1
4	NAG	c	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	c	2	4	-	6/6/23/26	0/1/1/1
4	FUC	c	3	4	-	-	0/1/1/1
8	NAG	d	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	4/6/23/26	0/1/1/1
8	BMA	d	3	8	-	1/2/19/22	0/1/1/1
8	MAN	d	4	8	-	1/2/19/22	0/1/1/1
8	FUC	d	5	8	-	-	0/1/1/1

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

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	4.97	1.52	1.43
2	f	2	NAG	O5-C1	4.86	1.51	1.43
2	D	1	NAG	O5-C1	4.81	1.51	1.43
6	R	1	NAG	O5-C1	4.80	1.51	1.43
3	W	1	NAG	C7-N2	4.73	1.46	1.34
2	D	2	NAG	O5-C1	4.70	1.51	1.43
2	Y	2	NAG	O5-C1	4.70	1.51	1.43
2	f	1	NAG	O5-C1	4.65	1.51	1.43
7	a	2	NAG	O5-C1	4.59	1.51	1.43
3	K	2	NAG	O5-C1	4.58	1.51	1.43
6	R	2	NAG	O5-C1	4.57	1.51	1.43
3	J	1	NAG	O5-C1	4.50	1.51	1.43
4	H	2	NAG	O5-C1	4.49	1.51	1.43
7	S	2	NAG	O5-C1	4.48	1.51	1.43
5	Q	2	NAG	O5-C1	4.45	1.51	1.43
2	N	2	NAG	O5-C1	4.44	1.51	1.43
2	g	2	NAG	O5-C1	4.40	1.51	1.43
7	b	1	NAG	O5-C1	4.37	1.51	1.43
3	I	2	NAG	O5-C1	4.37	1.51	1.43
3	J	2	NAG	O5-C1	4.36	1.51	1.43
4	c	2	NAG	O5-C1	4.35	1.51	1.43
8	d	1	NAG	O5-C1	4.35	1.51	1.43
3	X	2	NAG	O5-C1	4.34	1.51	1.43
2	g	1	NAG	O5-C1	4.34	1.51	1.43
5	P	2	NAG	O5-C1	4.33	1.51	1.43
3	W	2	NAG	O5-C1	4.33	1.51	1.43
2	N	1	NAG	O5-C1	4.32	1.51	1.43
2	M	1	NAG	O5-C1	4.32	1.50	1.43
4	c	1	NAG	O5-C1	4.31	1.50	1.43
3	K	1	NAG	O5-C1	4.30	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1	NAG	O5-C1	4.29	1.50	1.43
3	U	2	NAG	O5-C1	4.28	1.50	1.43
2	L	2	NAG	O5-C1	4.28	1.50	1.43
7	b	2	NAG	O5-C1	4.26	1.50	1.43
2	V	2	NAG	O5-C1	4.25	1.50	1.43
3	e	1	NAG	O5-C1	4.25	1.50	1.43
2	Z	2	NAG	O5-C1	4.24	1.50	1.43
3	e	2	NAG	O5-C1	4.24	1.50	1.43
2	M	2	NAG	O5-C1	4.23	1.50	1.43
8	d	2	NAG	O5-C1	4.23	1.50	1.43
2	V	1	NAG	O5-C1	4.22	1.50	1.43
3	U	1	NAG	O5-C1	4.20	1.50	1.43
3	T	1	NAG	O5-C1	4.20	1.50	1.43
3	I	1	NAG	O5-C1	4.18	1.50	1.43
3	T	2	NAG	O5-C1	4.18	1.50	1.43
2	L	1	NAG	O5-C1	4.16	1.50	1.43
7	a	1	NAG	O5-C1	4.16	1.50	1.43
7	S	1	NAG	O5-C1	4.16	1.50	1.43
3	E	2	NAG	O5-C1	4.15	1.50	1.43
3	E	1	NAG	O5-C1	4.12	1.50	1.43
2	M	2	NAG	C7-N2	4.12	1.47	1.34
3	G	2	NAG	O5-C1	4.11	1.50	1.43
2	Z	1	NAG	O5-C1	4.08	1.50	1.43
5	Q	1	NAG	O5-C1	4.02	1.50	1.43
6	R	1	NAG	C7-N2	4.00	1.47	1.34
3	G	2	NAG	C7-N2	4.00	1.47	1.34
4	H	2	NAG	C7-N2	3.98	1.47	1.34
2	N	1	NAG	C7-N2	3.97	1.47	1.34
3	U	2	NAG	C7-N2	3.97	1.47	1.34
3	F	2	NAG	O5-C1	3.96	1.50	1.43
2	Y	1	NAG	C7-N2	3.96	1.47	1.34
4	c	2	NAG	C7-N2	3.96	1.47	1.34
6	R	2	NAG	C7-N2	3.95	1.47	1.34
2	Z	2	NAG	C7-N2	3.94	1.47	1.34
5	P	1	NAG	O5-C1	3.94	1.50	1.43
3	T	2	NAG	C7-N2	3.93	1.47	1.34
2	f	2	NAG	C7-N2	3.93	1.47	1.34
3	F	2	NAG	C7-N2	3.92	1.47	1.34
3	E	1	NAG	C7-N2	3.92	1.47	1.34
3	W	2	NAG	C7-N2	3.92	1.47	1.34
2	Y	1	NAG	O5-C1	3.91	1.50	1.43
3	J	2	NAG	C7-N2	3.91	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	d	2	NAG	C7-N2	3.90	1.46	1.34
5	Q	2	NAG	C7-N2	3.90	1.46	1.34
4	c	1	NAG	C7-N2	3.90	1.46	1.34
2	g	2	NAG	C7-N2	3.90	1.46	1.34
3	K	2	NAG	C7-N2	3.90	1.46	1.34
3	e	2	NAG	C7-N2	3.89	1.46	1.34
3	F	1	NAG	O5-C1	3.88	1.50	1.43
2	f	1	NAG	C7-N2	3.88	1.46	1.34
2	M	1	NAG	C7-N2	3.87	1.46	1.34
3	X	2	NAG	C7-N2	3.87	1.46	1.34
4	H	1	NAG	C7-N2	3.87	1.46	1.34
2	Z	1	NAG	C7-N2	3.87	1.46	1.34
3	U	1	NAG	C7-N2	3.87	1.46	1.34
2	L	2	NAG	C7-N2	3.86	1.46	1.34
7	S	2	NAG	C7-N2	3.86	1.46	1.34
2	D	2	NAG	C7-N2	3.85	1.46	1.34
2	V	2	NAG	C7-N2	3.85	1.46	1.34
2	Y	2	NAG	C7-N2	3.85	1.46	1.34
3	G	1	NAG	C7-N2	3.85	1.46	1.34
7	a	2	NAG	C7-N2	3.84	1.46	1.34
7	b	2	NAG	C7-N2	3.84	1.46	1.34
2	N	2	NAG	C7-N2	3.84	1.46	1.34
5	P	2	NAG	C7-N2	3.84	1.46	1.34
7	a	1	NAG	C7-N2	3.84	1.46	1.34
3	K	1	NAG	C7-N2	3.82	1.46	1.34
3	X	1	NAG	C7-N2	3.82	1.46	1.34
5	P	1	NAG	C7-N2	3.82	1.46	1.34
3	I	2	NAG	C7-N2	3.82	1.46	1.34
2	L	1	NAG	C7-N2	3.82	1.46	1.34
2	V	1	NAG	C7-N2	3.82	1.46	1.34
3	T	1	NAG	C7-N2	3.82	1.46	1.34
3	e	1	NAG	C7-N2	3.82	1.46	1.34
7	b	1	NAG	C7-N2	3.81	1.46	1.34
7	S	1	NAG	C7-N2	3.81	1.46	1.34
3	F	1	NAG	C7-N2	3.80	1.46	1.34
3	I	1	NAG	C7-N2	3.79	1.46	1.34
2	g	1	NAG	C7-N2	3.79	1.46	1.34
5	Q	1	NAG	C7-N2	3.79	1.46	1.34
8	d	1	NAG	C7-N2	3.79	1.46	1.34
2	D	1	NAG	C7-N2	3.78	1.46	1.34
3	E	2	NAG	C7-N2	3.75	1.46	1.34
3	J	1	NAG	C7-N2	3.75	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	3.30	1.49	1.43
6	R	1	NAG	O5-C5	3.30	1.49	1.43
7	S	4	MAN	C1-C2	3.10	1.59	1.52
2	M	2	NAG	C2-N2	2.97	1.51	1.46
3	W	1	NAG	C2-C3	-2.91	1.49	1.52
4	H	1	NAG	O5-C5	2.78	1.48	1.43
4	H	2	NAG	C2-N2	2.75	1.50	1.46
3	G	2	NAG	C2-N2	2.68	1.50	1.46
3	K	2	NAG	C2-N2	2.67	1.50	1.46
3	F	2	NAG	C2-N2	2.66	1.50	1.46
3	E	1	NAG	C2-N2	2.66	1.50	1.46
6	R	2	NAG	C2-N2	2.64	1.50	1.46
3	U	2	NAG	C2-N2	2.63	1.50	1.46
5	Q	2	NAG	O5-C5	2.63	1.48	1.43
4	c	2	NAG	C2-N2	2.62	1.50	1.46
6	R	4	FUC	C1-C2	2.60	1.58	1.52
3	W	2	NAG	C2-N2	2.59	1.50	1.46
2	N	1	NAG	C2-N2	2.58	1.50	1.46
3	T	2	NAG	C2-N2	2.58	1.50	1.46
2	Z	2	NAG	C2-N2	2.58	1.50	1.46
5	Q	2	NAG	C2-N2	2.58	1.50	1.46
3	e	2	NAG	C2-N2	2.56	1.50	1.46
2	f	2	NAG	C2-N2	2.55	1.50	1.46
7	S	1	NAG	O5-C5	2.55	1.48	1.43
4	c	1	NAG	C2-N2	2.54	1.50	1.46
7	a	1	NAG	C2-N2	2.54	1.50	1.46
2	g	2	NAG	C2-N2	2.54	1.50	1.46
3	J	2	NAG	C2-N2	2.53	1.50	1.46
2	f	1	NAG	C2-N2	2.53	1.50	1.46
2	D	2	NAG	C2-N2	2.52	1.50	1.46
2	M	1	NAG	C2-N2	2.49	1.50	1.46
2	L	2	NAG	C2-N2	2.48	1.50	1.46
7	a	2	NAG	C2-N2	2.48	1.50	1.46
3	E	2	NAG	O5-C5	2.48	1.48	1.43
2	Y	2	NAG	C2-N2	2.47	1.50	1.46
6	R	1	NAG	C2-N2	2.46	1.50	1.46
5	P	2	NAG	C2-N2	2.46	1.50	1.46
3	X	2	NAG	C2-N2	2.45	1.50	1.46
4	H	2	NAG	O5-C5	2.45	1.48	1.43
8	d	2	NAG	C2-N2	2.44	1.50	1.46
7	b	1	NAG	O5-C5	2.44	1.48	1.43
2	V	2	NAG	C2-N2	2.42	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	C2-N2	2.42	1.50	1.46
7	b	2	NAG	C2-N2	2.42	1.50	1.46
8	d	1	NAG	O5-C5	2.41	1.48	1.43
3	I	2	NAG	C2-N2	2.41	1.50	1.46
3	X	1	NAG	C2-N2	2.41	1.50	1.46
3	K	1	NAG	O5-C5	2.40	1.48	1.43
2	N	2	NAG	C2-N2	2.40	1.50	1.46
2	Z	1	NAG	C2-N2	2.39	1.50	1.46
2	V	1	NAG	C2-N2	2.37	1.50	1.46
3	e	1	NAG	C2-N2	2.37	1.50	1.46
3	X	1	NAG	O5-C5	2.37	1.48	1.43
2	Y	1	NAG	O5-C5	2.36	1.48	1.43
2	L	1	NAG	C2-N2	2.36	1.50	1.46
2	D	2	NAG	O5-C5	2.35	1.48	1.43
3	K	1	NAG	C2-N2	2.35	1.50	1.46
2	D	1	NAG	C2-N2	2.34	1.50	1.46
7	S	1	NAG	C2-N2	2.32	1.50	1.46
7	S	2	NAG	C2-N2	2.32	1.50	1.46
7	b	2	NAG	O5-C5	2.32	1.48	1.43
2	Y	1	NAG	C2-N2	2.31	1.50	1.46
2	g	1	NAG	O5-C5	2.30	1.47	1.43
3	T	1	NAG	C2-N2	2.30	1.50	1.46
8	d	1	NAG	C2-N2	2.30	1.50	1.46
3	I	1	NAG	C2-N2	2.30	1.50	1.46
7	b	1	NAG	C2-N2	2.28	1.50	1.46
3	I	1	NAG	O5-C5	2.28	1.47	1.43
3	F	1	NAG	C2-N2	2.27	1.50	1.46
2	g	1	NAG	C2-N2	2.25	1.50	1.46
5	P	1	NAG	C2-N2	2.24	1.50	1.46
2	M	2	NAG	O5-C5	2.24	1.47	1.43
5	Q	1	NAG	C2-N2	2.24	1.50	1.46
3	T	2	NAG	O5-C5	2.23	1.47	1.43
3	W	2	NAG	O5-C5	2.23	1.47	1.43
7	a	1	NAG	O5-C5	2.23	1.47	1.43
2	Y	2	NAG	O5-C5	2.23	1.47	1.43
6	R	2	NAG	O5-C5	2.22	1.47	1.43
2	V	2	NAG	O5-C5	2.22	1.47	1.43
2	N	1	NAG	O5-C5	2.22	1.47	1.43
3	J	1	NAG	O5-C5	2.20	1.47	1.43
3	X	2	NAG	O5-C5	2.19	1.47	1.43
2	Z	2	NAG	O5-C5	2.19	1.47	1.43
7	S	2	NAG	O5-C5	2.19	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C5	2.18	1.47	1.43
2	L	1	NAG	O5-C5	2.16	1.47	1.43
2	f	2	NAG	O5-C5	2.15	1.47	1.43
3	E	1	NAG	O5-C5	2.15	1.47	1.43
3	U	2	NAG	O5-C5	2.15	1.47	1.43
2	Z	1	NAG	O5-C5	2.14	1.47	1.43
4	c	2	NAG	O5-C5	2.14	1.47	1.43
3	F	2	NAG	O5-C5	2.13	1.47	1.43
2	V	1	NAG	O5-C5	2.13	1.47	1.43
3	T	1	NAG	O5-C5	2.13	1.47	1.43
3	G	1	NAG	C2-N2	2.13	1.49	1.46
2	M	1	NAG	O5-C5	2.12	1.47	1.43
2	f	1	NAG	O5-C5	2.11	1.47	1.43
3	E	2	NAG	C2-N2	2.11	1.49	1.46
2	L	2	NAG	O5-C5	2.10	1.47	1.43
3	e	1	NAG	O5-C5	2.10	1.47	1.43
5	Q	1	NAG	O5-C5	2.10	1.47	1.43
2	g	2	NAG	O5-C5	2.09	1.47	1.43
3	K	1	NAG	C3-C2	-2.09	1.48	1.52
4	H	1	NAG	C2-N2	2.09	1.49	1.46
3	J	1	NAG	C2-N2	2.08	1.49	1.46
2	N	2	NAG	O5-C5	2.06	1.47	1.43
2	D	1	NAG	O5-C5	2.05	1.47	1.43
3	E	2	NAG	C3-C2	-2.05	1.48	1.52
8	d	2	NAG	O5-C5	2.05	1.47	1.43
7	a	3	BMA	C2-C3	2.04	1.55	1.52
7	a	1	NAG	C3-C2	-2.04	1.48	1.52
3	J	2	NAG	O5-C5	2.04	1.47	1.43
7	b	1	NAG	C3-C2	-2.03	1.48	1.52
3	e	1	NAG	C3-C2	-2.02	1.48	1.52
5	Q	2	NAG	C3-C2	-2.02	1.48	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	-8.44	100.87	112.19
2	Y	1	NAG	C1-O5-C5	-7.60	102.00	112.19
4	H	1	NAG	C1-O5-C5	7.15	121.76	112.19
6	R	1	NAG	C2-N2-C7	5.42	130.17	122.90
4	c	1	NAG	C4-C3-C2	5.06	118.43	111.02
2	M	2	NAG	C8-C7-N2	4.26	123.18	116.12
7	S	4	MAN	C1-O5-C5	4.17	117.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	1	NAG	C1-O5-C5	4.11	117.70	112.19
6	R	1	NAG	C8-C7-N2	3.83	122.48	116.12
5	P	1	NAG	C4-C3-C2	3.69	116.42	111.02
3	G	1	NAG	C4-C3-C2	3.64	116.35	111.02
3	K	1	NAG	C2-N2-C7	-3.60	118.08	122.90
7	a	2	NAG	O5-C1-C2	3.58	116.83	111.29
5	Q	1	NAG	C2-N2-C7	-3.52	118.18	122.90
3	E	2	NAG	C2-N2-C7	-3.48	118.24	122.90
5	Q	3	BMA	C1-O5-C5	3.35	116.67	112.19
6	R	1	NAG	O5-C5-C6	3.26	114.01	107.66
8	d	2	NAG	C4-C3-C2	3.25	115.78	111.02
6	R	1	NAG	O5-C1-C2	-3.21	106.33	111.29
5	Q	2	NAG	C2-N2-C7	-3.15	118.68	122.90
2	N	1	NAG	C8-C7-N2	3.13	121.31	116.12
8	d	3	BMA	C1-O5-C5	3.10	116.34	112.19
6	R	3	BMA	C1-O5-C5	3.09	116.33	112.19
4	c	2	NAG	C8-C7-N2	3.09	121.24	116.12
7	b	1	NAG	C1-C2-N2	-3.09	105.56	110.43
3	U	2	NAG	C8-C7-N2	3.09	121.23	116.12
4	H	2	NAG	C8-C7-N2	3.06	121.20	116.12
3	F	2	NAG	C8-C7-N2	3.06	121.19	116.12
3	T	2	NAG	C8-C7-N2	3.06	121.19	116.12
2	Z	2	NAG	C8-C7-N2	3.03	121.15	116.12
3	e	2	NAG	C4-C3-C2	2.98	115.39	111.02
3	K	2	NAG	C4-C3-C2	2.98	115.39	111.02
8	d	1	NAG	C2-N2-C7	-2.98	118.91	122.90
2	D	1	NAG	C1-O5-C5	2.96	116.16	112.19
7	a	1	NAG	C8-C7-N2	2.96	121.03	116.12
7	a	4	MAN	C1-O5-C5	2.92	116.11	112.19
7	S	1	NAG	C2-N2-C7	-2.91	119.00	122.90
8	d	1	NAG	C8-C7-N2	2.85	120.85	116.12
3	K	1	NAG	C8-C7-N2	2.84	120.82	116.12
2	Z	1	NAG	C1-O5-C5	-2.83	108.39	112.19
5	Q	2	NAG	C3-C4-C5	2.81	115.33	110.23
2	D	2	NAG	C2-N2-C7	-2.73	119.25	122.90
5	Q	2	NAG	C8-C7-N2	2.72	120.62	116.12
2	g	1	NAG	C2-N2-C7	-2.72	119.26	122.90
7	b	4	MAN	C1-O5-C5	2.71	115.81	112.19
5	P	2	NAG	C2-N2-C7	-2.69	119.29	122.90
2	Y	1	NAG	C1-C2-N2	2.68	114.66	110.43
3	G	1	NAG	C8-C7-N2	2.64	120.50	116.12
6	R	2	NAG	C8-C7-N2	2.60	120.43	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	NAG	C1-O5-C5	2.60	115.67	112.19
3	K	1	NAG	C4-C3-C2	-2.59	107.22	111.02
4	c	1	NAG	C2-N2-C7	-2.58	119.44	122.90
5	Q	1	NAG	C8-C7-N2	2.58	120.40	116.12
6	R	1	NAG	C4-C3-C2	2.57	114.79	111.02
7	S	2	NAG	C2-N2-C7	-2.55	119.48	122.90
3	F	1	NAG	C3-C4-C5	2.54	114.84	110.23
2	g	2	NAG	C2-N2-C7	-2.50	119.55	122.90
2	Z	1	NAG	C8-C7-N2	2.50	120.26	116.12
3	I	2	NAG	C4-C3-C2	2.49	114.67	111.02
2	M	2	NAG	C2-N2-C7	2.49	126.24	122.90
3	F	1	NAG	C2-N2-C7	-2.47	119.59	122.90
2	V	1	NAG	C2-N2-C7	-2.46	119.60	122.90
2	M	1	NAG	C8-C7-N2	2.46	120.19	116.12
3	T	1	NAG	C2-N2-C7	-2.45	119.61	122.90
3	J	2	NAG	C2-N2-C7	-2.45	119.61	122.90
3	E	1	NAG	C4-C3-C2	2.45	114.61	111.02
6	R	4	FUC	C1-O5-C5	2.45	118.74	112.97
5	P	2	NAG	C8-C7-N2	2.44	120.16	116.12
7	a	2	NAG	C8-C7-N2	2.44	120.16	116.12
4	c	1	NAG	C8-C7-N2	2.43	120.14	116.12
4	H	1	NAG	C2-N2-C7	-2.42	119.65	122.90
3	J	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	f	1	NAG	C8-C7-N2	2.41	120.11	116.12
7	S	1	NAG	C8-C7-N2	2.41	120.11	116.12
3	e	2	NAG	C8-C7-N2	2.40	120.10	116.12
2	f	1	NAG	O5-C1-C2	2.40	115.00	111.29
3	I	1	NAG	C8-C7-N2	2.38	120.06	116.12
2	V	1	NAG	C8-C7-N2	2.38	120.06	116.12
2	g	2	NAG	C8-C7-N2	2.38	120.06	116.12
3	I	1	NAG	C2-N2-C7	-2.37	119.72	122.90
3	e	1	NAG	C8-C7-N2	2.37	120.04	116.12
7	b	1	NAG	C8-C7-N2	2.36	120.04	116.12
8	d	2	NAG	C8-C7-N2	2.36	120.03	116.12
3	K	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	Y	1	NAG	C3-C4-C5	2.35	114.49	110.23
8	d	2	NAG	C2-N2-C7	-2.34	119.76	122.90
2	V	2	NAG	C2-N2-C7	-2.34	119.76	122.90
7	a	2	NAG	C2-N2-C7	-2.34	119.76	122.90
2	L	1	NAG	C8-C7-N2	2.34	119.99	116.12
4	H	1	NAG	O5-C5-C4	2.34	116.51	110.83
3	U	1	NAG	C8-C7-N2	2.33	119.99	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	4	MAN	C1-C2-C3	2.32	113.03	109.64
2	V	2	NAG	C8-C7-N2	2.32	119.97	116.12
3	X	2	NAG	C8-C7-N2	2.32	119.96	116.12
7	b	2	NAG	C8-C7-N2	2.32	119.96	116.12
2	D	1	NAG	C8-C7-N2	2.31	119.96	116.12
7	S	2	NAG	C8-C7-N2	2.31	119.96	116.12
5	Q	1	NAG	O3-C3-C2	-2.31	104.59	109.40
2	g	1	NAG	C8-C7-N2	2.31	119.95	116.12
3	T	1	NAG	C8-C7-N2	2.31	119.95	116.12
2	L	1	NAG	C2-N2-C7	-2.31	119.81	122.90
3	I	2	NAG	C8-C7-N2	2.30	119.94	116.12
2	Y	2	NAG	C2-N2-C7	-2.30	119.81	122.90
2	L	2	NAG	C8-C7-N2	2.30	119.93	116.12
3	G	1	NAG	C2-N2-C7	-2.30	119.82	122.90
3	F	1	NAG	C4-C3-C2	2.28	114.37	111.02
2	Y	1	NAG	C8-C7-N2	2.28	119.91	116.12
3	G	1	NAG	C3-C4-C5	2.28	114.36	110.23
2	f	1	NAG	O4-C4-C3	2.26	115.71	110.38
3	K	2	NAG	O5-C1-C2	2.26	114.79	111.29
3	I	2	NAG	C2-N2-C7	-2.26	119.88	122.90
2	Y	2	NAG	C8-C7-N2	2.25	119.86	116.12
3	F	1	NAG	C8-C7-N2	2.25	119.85	116.12
2	N	1	NAG	C4-C3-C2	2.25	114.31	111.02
2	D	2	NAG	C8-C7-N2	2.25	119.84	116.12
3	U	1	NAG	C2-N2-C7	-2.23	119.91	122.90
7	b	4	MAN	O2-C2-C3	-2.22	105.55	110.15
3	X	1	NAG	C8-C7-N2	2.21	119.79	116.12
7	S	4	MAN	O2-C2-C3	-2.21	105.57	110.15
3	G	2	NAG	C8-C7-N2	2.21	119.78	116.12
7	b	2	NAG	C2-N2-C7	-2.21	119.94	122.90
3	J	1	NAG	C6-C5-C4	-2.21	107.60	113.02
3	E	2	NAG	C3-C4-C5	2.20	114.23	110.23
4	H	1	NAG	C8-C7-N2	2.20	119.76	116.12
5	P	4	MAN	O2-C2-C3	-2.19	105.61	110.15
5	Q	4	MAN	O2-C2-C3	-2.18	105.63	110.15
3	W	1	NAG	C8-C7-N2	2.18	119.85	116.12
5	P	1	NAG	C8-C7-N2	2.18	119.74	116.12
5	P	4	MAN	C1-O5-C5	2.18	115.11	112.19
8	d	4	MAN	O2-C2-C3	-2.17	105.66	110.15
3	E	1	NAG	C3-C4-C5	2.17	114.16	110.23
5	Q	4	MAN	C1-O5-C5	2.16	115.08	112.19
5	Q	1	NAG	C6-C5-C4	-2.14	107.75	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	2	NAG	C8-C7-N2	2.14	119.67	116.12
6	R	2	NAG	C1-O5-C5	2.14	115.05	112.19
3	X	2	NAG	C2-N2-C7	-2.12	120.05	122.90
3	W	2	NAG	C8-C7-N2	2.10	119.61	116.12
4	c	1	NAG	C6-C5-C4	-2.10	107.86	113.02
3	E	2	NAG	C8-C7-N2	2.10	119.60	116.12
3	E	1	NAG	C6-C5-C4	-2.10	107.87	113.02
4	H	2	NAG	C6-C5-C4	-2.10	107.87	113.02
7	S	1	NAG	O5-C5-C4	2.10	115.92	110.83
6	R	1	NAG	O7-C7-N2	-2.09	118.28	121.98
2	N	2	NAG	C4-C3-C2	2.09	114.08	111.02
7	b	1	NAG	O5-C5-C4	2.09	115.90	110.83
3	X	1	NAG	C2-N2-C7	-2.08	120.11	122.90
7	a	4	MAN	O2-C2-C3	-2.07	105.86	110.15
2	N	2	NAG	C8-C7-N2	2.07	119.55	116.12
2	M	2	NAG	O7-C7-C8	-2.06	118.39	122.05
2	D	2	NAG	C4-C3-C2	2.06	114.03	111.02
5	P	1	NAG	C3-C4-C5	2.05	113.95	110.23
3	E	1	NAG	C8-C7-N2	2.05	119.51	116.12
2	N	2	NAG	C2-N2-C7	-2.05	120.16	122.90
3	e	2	NAG	C2-N2-C7	-2.02	120.19	122.90
5	P	1	NAG	C6-C5-C4	-2.01	108.09	113.02
5	P	2	NAG	O5-C1-C2	2.01	114.40	111.29
8	d	1	NAG	C4-C3-C2	2.01	113.96	111.02
2	M	2	NAG	O7-C7-N2	-2.01	118.44	121.98
2	D	1	NAG	C6-C5-C4	-2.00	108.10	113.02
5	Q	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (172) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C1-C2-N2-C7
2	f	2	NAG	C1-C2-N2-C7
3	W	2	NAG	C1-C2-N2-C7
4	H	1	NAG	C1-C2-N2-C7
5	Q	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Y	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	M	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	Y	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	Z	2	NAG	O7-C7-N2-C2
2	f	1	NAG	C8-C7-N2-C2
2	f	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	c	1	NAG	C8-C7-N2-C2
4	c	1	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	e	3	BMA	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
8	d	4	MAN	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	T	3	BMA	O5-C5-C6-O6
8	d	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
3	X	3	BMA	O5-C5-C6-O6
7	a	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	T	2	NAG	C1-C2-N2-C7
3	X	1	NAG	C1-C2-N2-C7
3	X	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	P	2	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
3	W	1	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
3	X	1	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7
4	c	2	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
7	S	2	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
8	d	2	NAG	C3-C2-N2-C7
3	I	1	NAG	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C1-C2-N2-C7
3	U	2	NAG	C1-C2-N2-C7
4	H	2	NAG	C1-C2-N2-C7
4	c	2	NAG	C1-C2-N2-C7
7	S	2	NAG	C1-C2-N2-C7
8	d	2	NAG	C1-C2-N2-C7
2	Z	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
4	c	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	a	4	MAN	C1-C2-C3-C4-C5-O5

70 monomers are involved in 157 short contacts:

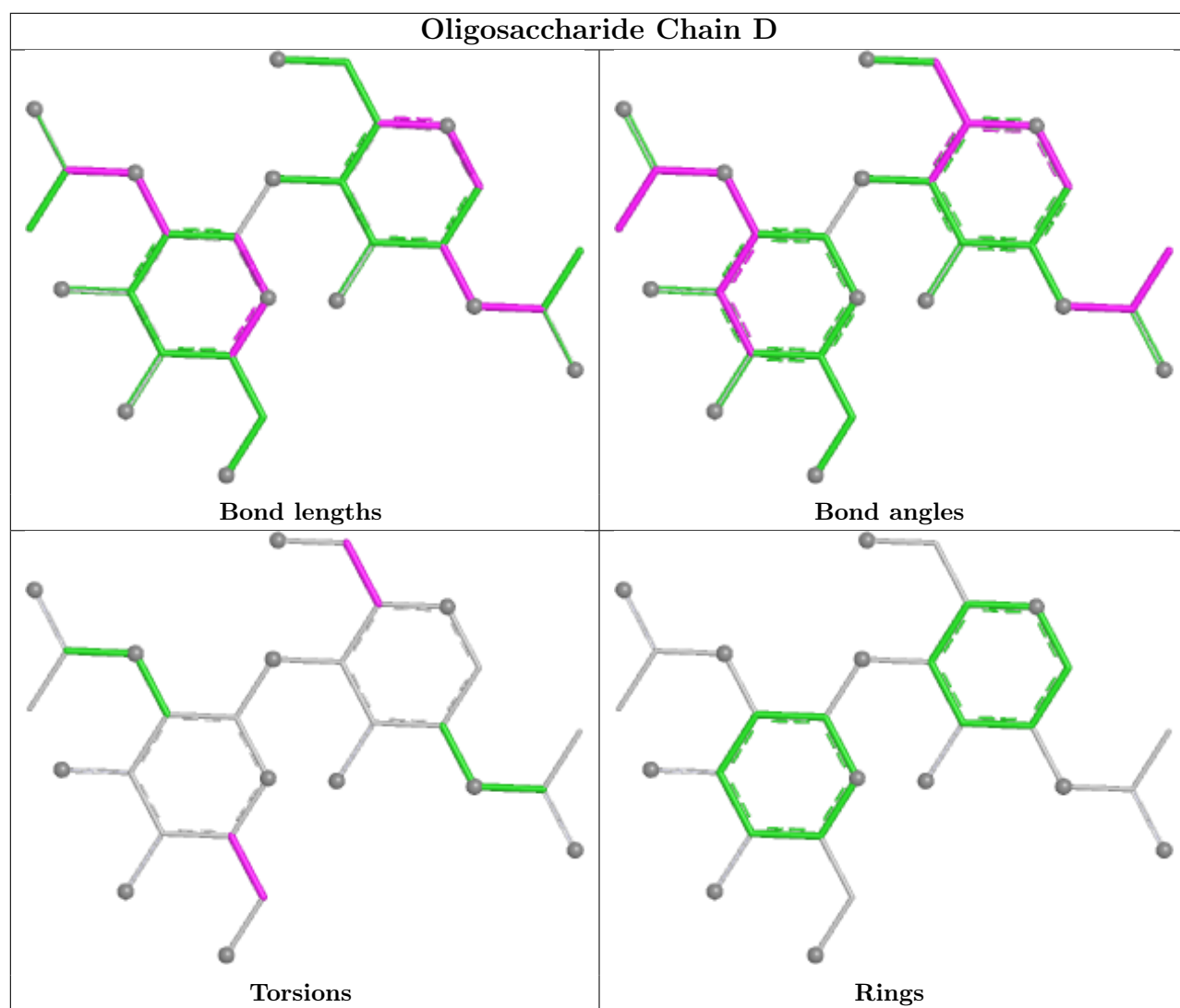
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	BMA	1	0
2	M	1	NAG	1	0
7	a	4	MAN	3	0
5	Q	2	NAG	4	0
3	F	3	BMA	3	0
2	N	2	NAG	4	0
3	F	2	NAG	5	0
6	R	4	FUC	1	0
3	J	1	NAG	5	0
3	U	3	BMA	3	0
3	K	2	NAG	6	0
2	Z	1	NAG	4	0
6	R	2	NAG	4	0
2	g	1	NAG	5	0
4	c	3	FUC	1	0
2	Y	1	NAG	8	0
3	U	1	NAG	3	0
3	e	3	BMA	2	0
3	U	2	NAG	7	0
7	S	4	MAN	5	0
8	d	4	MAN	1	0
5	P	3	BMA	2	0
5	P	2	NAG	2	0
4	H	2	NAG	2	0
7	a	3	BMA	4	0
2	L	1	NAG	1	0
7	S	2	NAG	1	0
8	d	2	NAG	6	0
7	a	2	NAG	4	0
2	f	1	NAG	6	0
3	e	1	NAG	7	0
5	Q	3	BMA	1	0
3	K	3	BMA	1	0
8	d	5	FUC	4	0
7	a	1	NAG	4	0
2	g	2	NAG	5	0
8	d	3	BMA	2	0
4	c	2	NAG	3	0
3	T	1	NAG	2	0
6	R	3	BMA	2	0
3	F	1	NAG	1	0
7	b	1	NAG	6	0
3	I	2	NAG	5	0

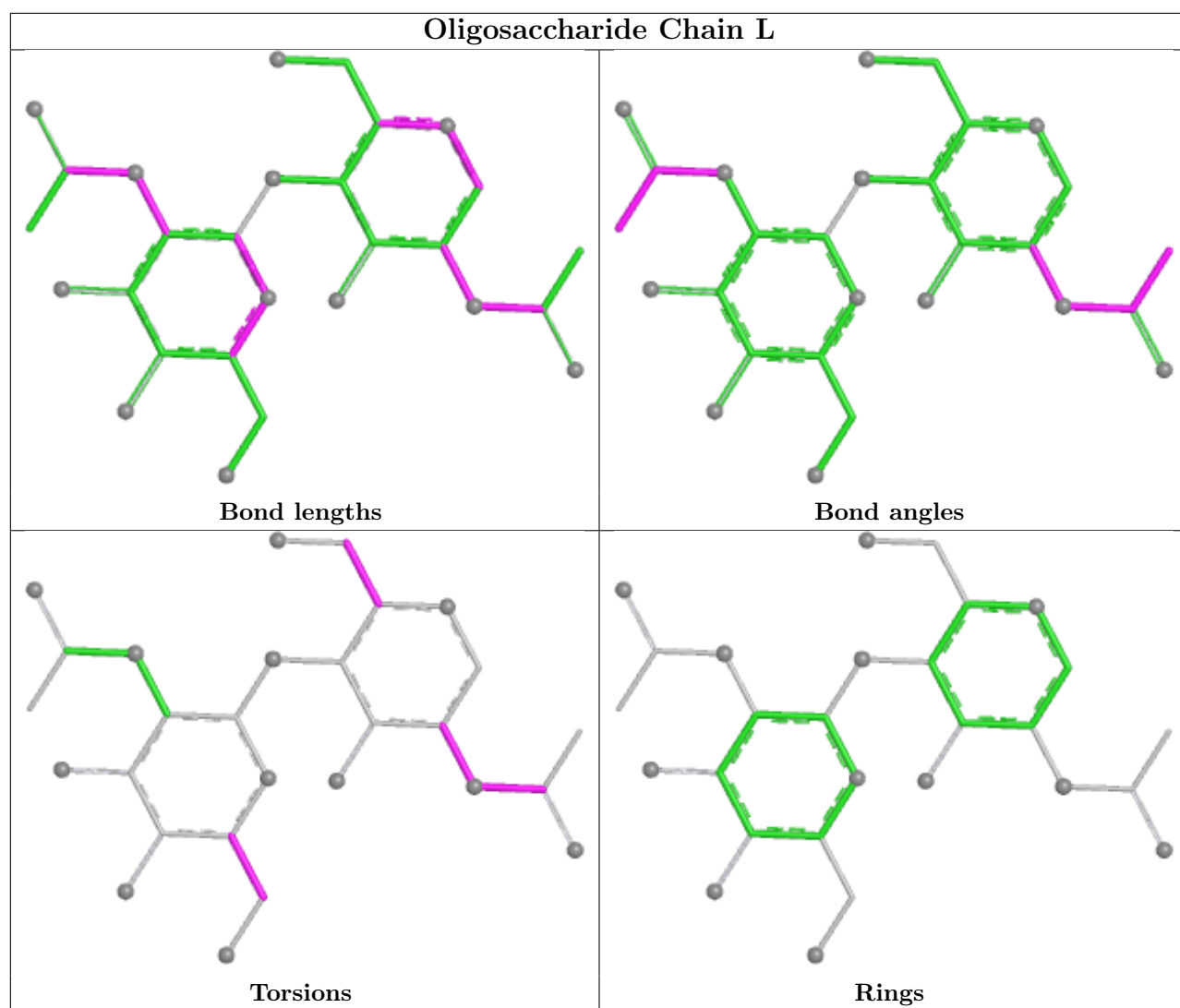
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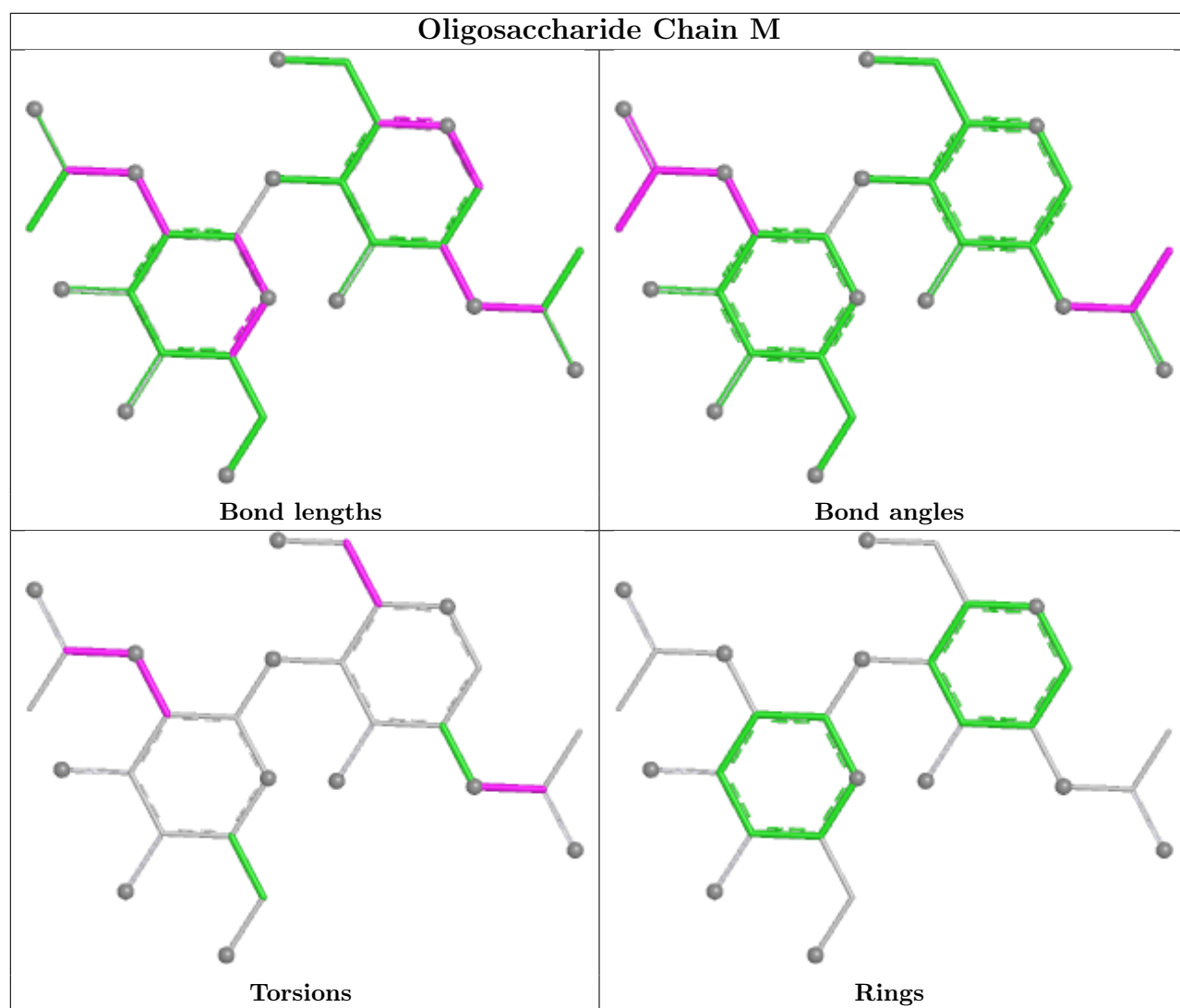
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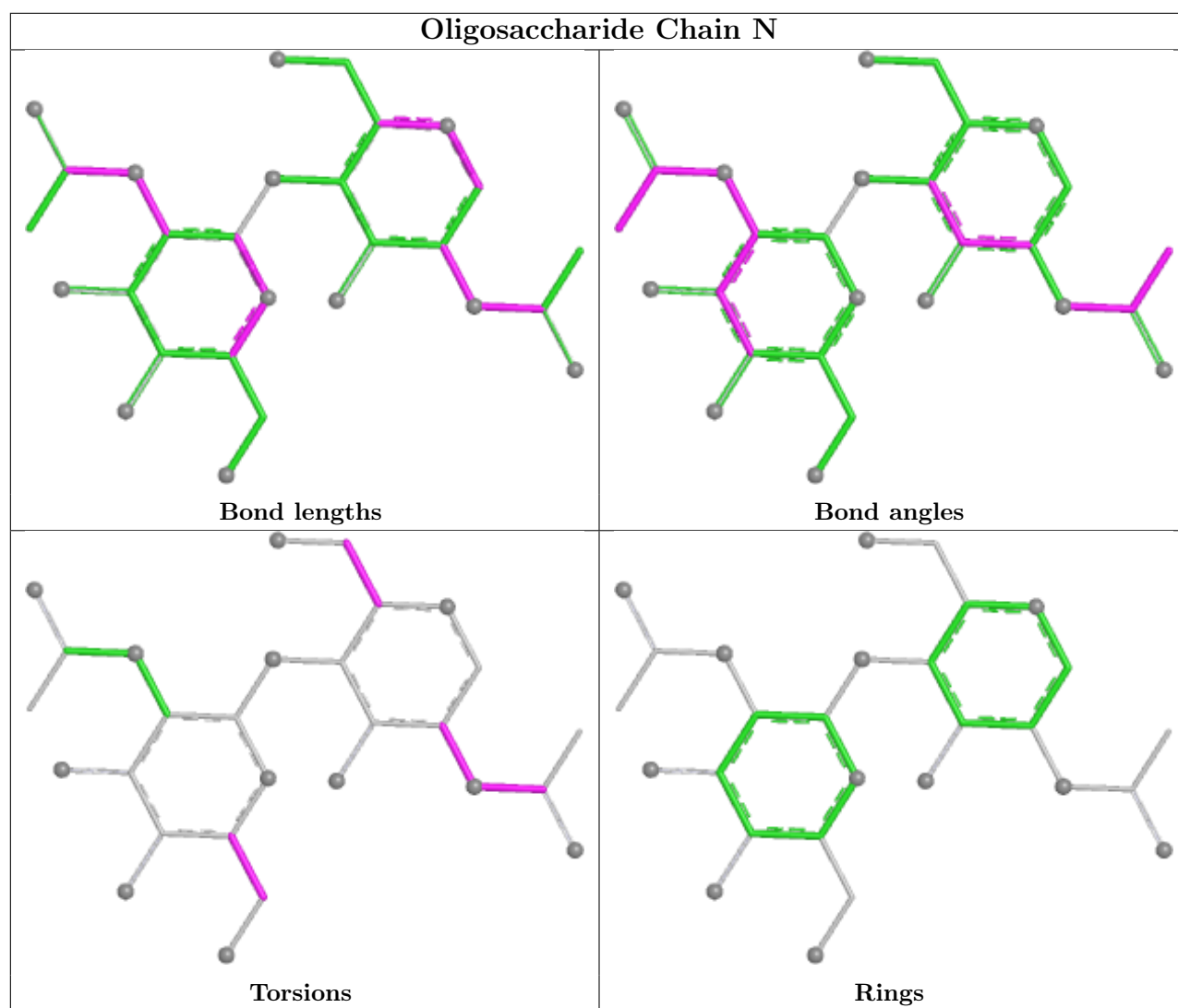
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	1	NAG	1	0
8	d	1	NAG	6	0
2	M	2	NAG	4	0
3	K	1	NAG	7	0
3	e	2	NAG	9	0
3	J	2	NAG	3	0
3	G	1	NAG	2	0
3	G	2	NAG	2	0
2	D	2	NAG	6	0
3	E	2	NAG	5	0
2	L	2	NAG	1	0
3	W	2	NAG	1	0
7	S	3	BMA	5	0
5	Q	1	NAG	3	0
2	N	1	NAG	6	0
2	f	2	NAG	6	0
5	Q	4	MAN	2	0
3	I	1	NAG	4	0
3	T	2	NAG	4	0
2	Y	2	NAG	7	0
7	b	2	NAG	5	0
2	D	1	NAG	6	0
2	Z	2	NAG	5	0
3	E	1	NAG	3	0
6	R	1	NAG	3	0
4	c	1	NAG	3	0
3	W	1	NAG	2	0

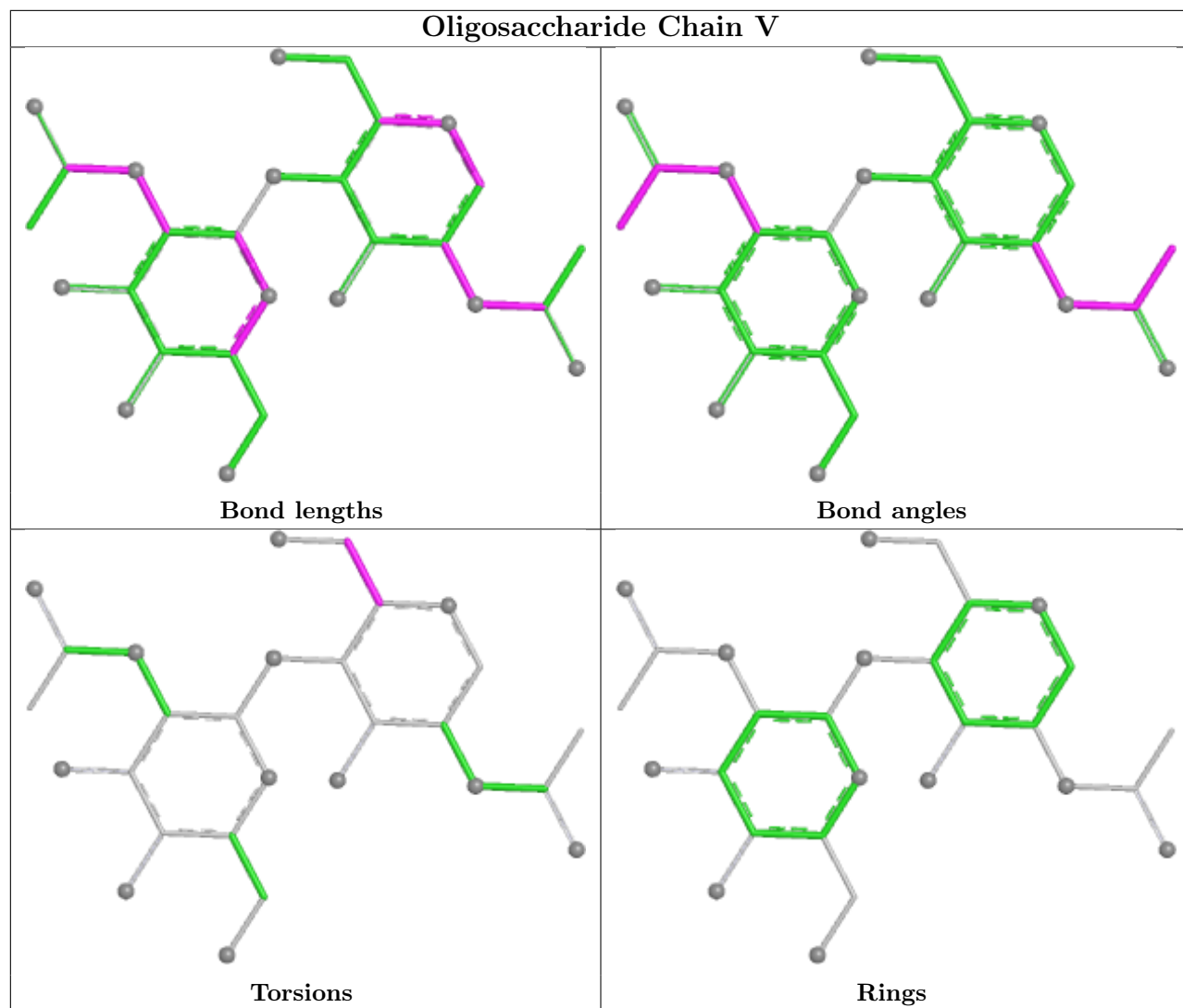
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

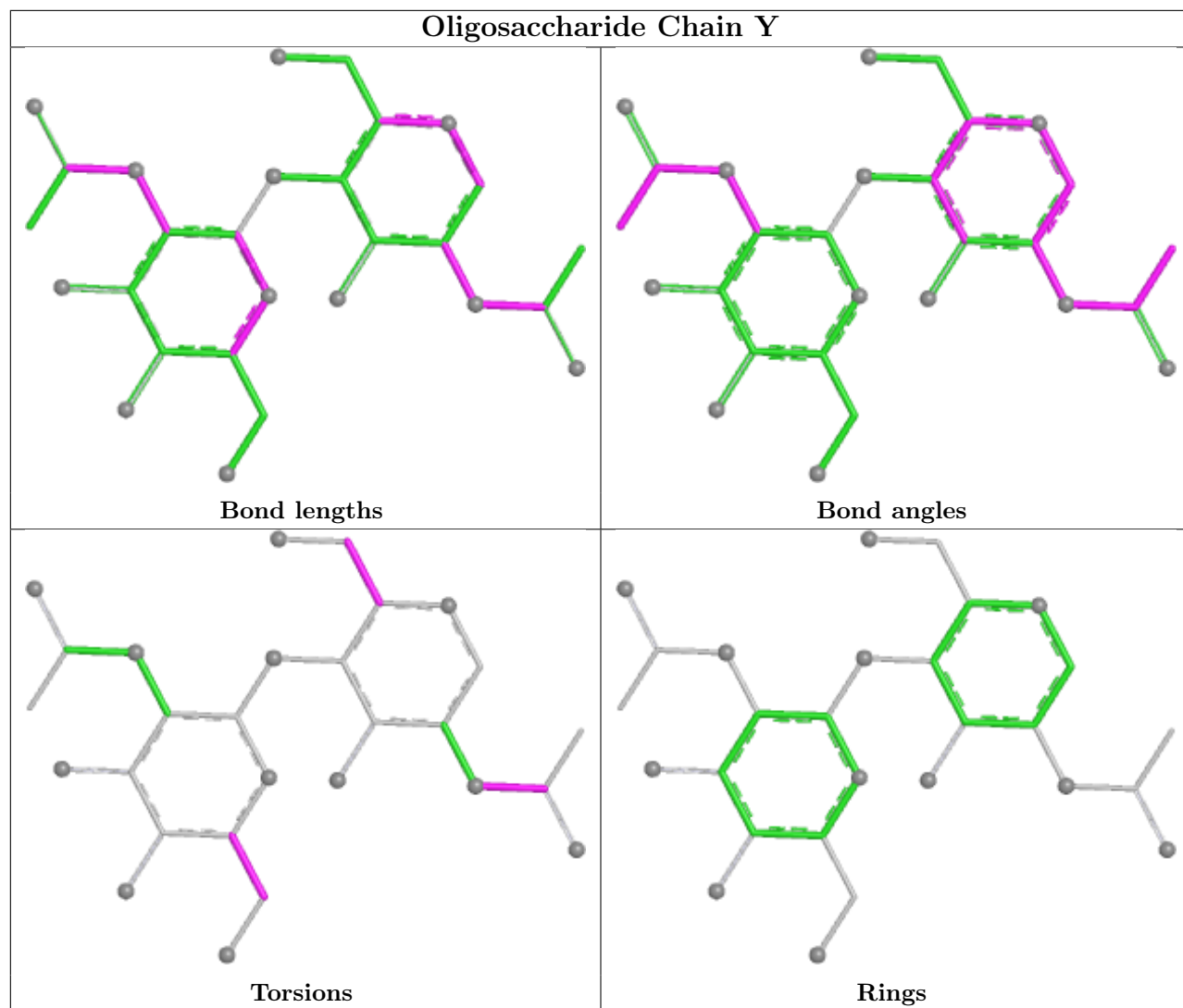


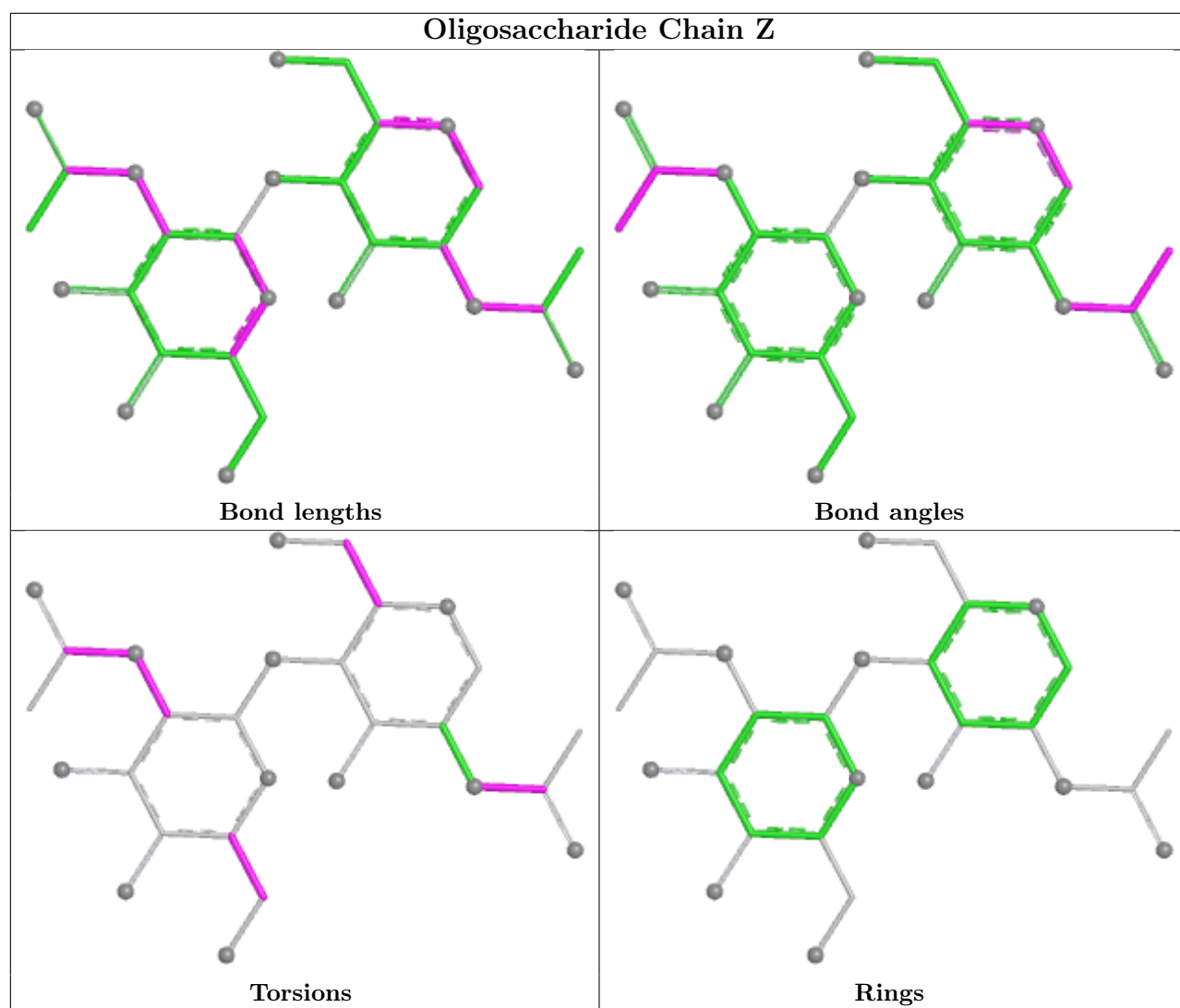


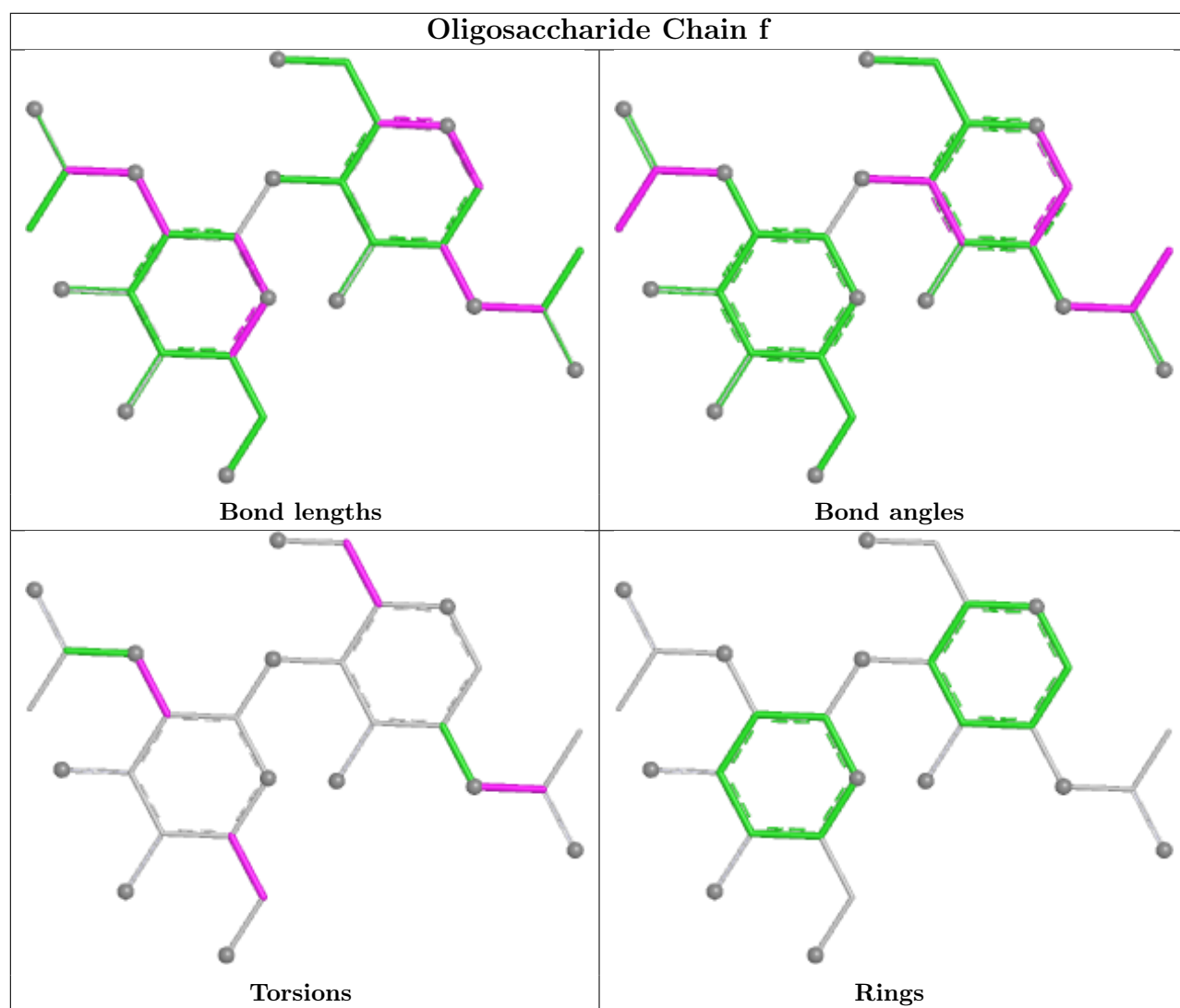


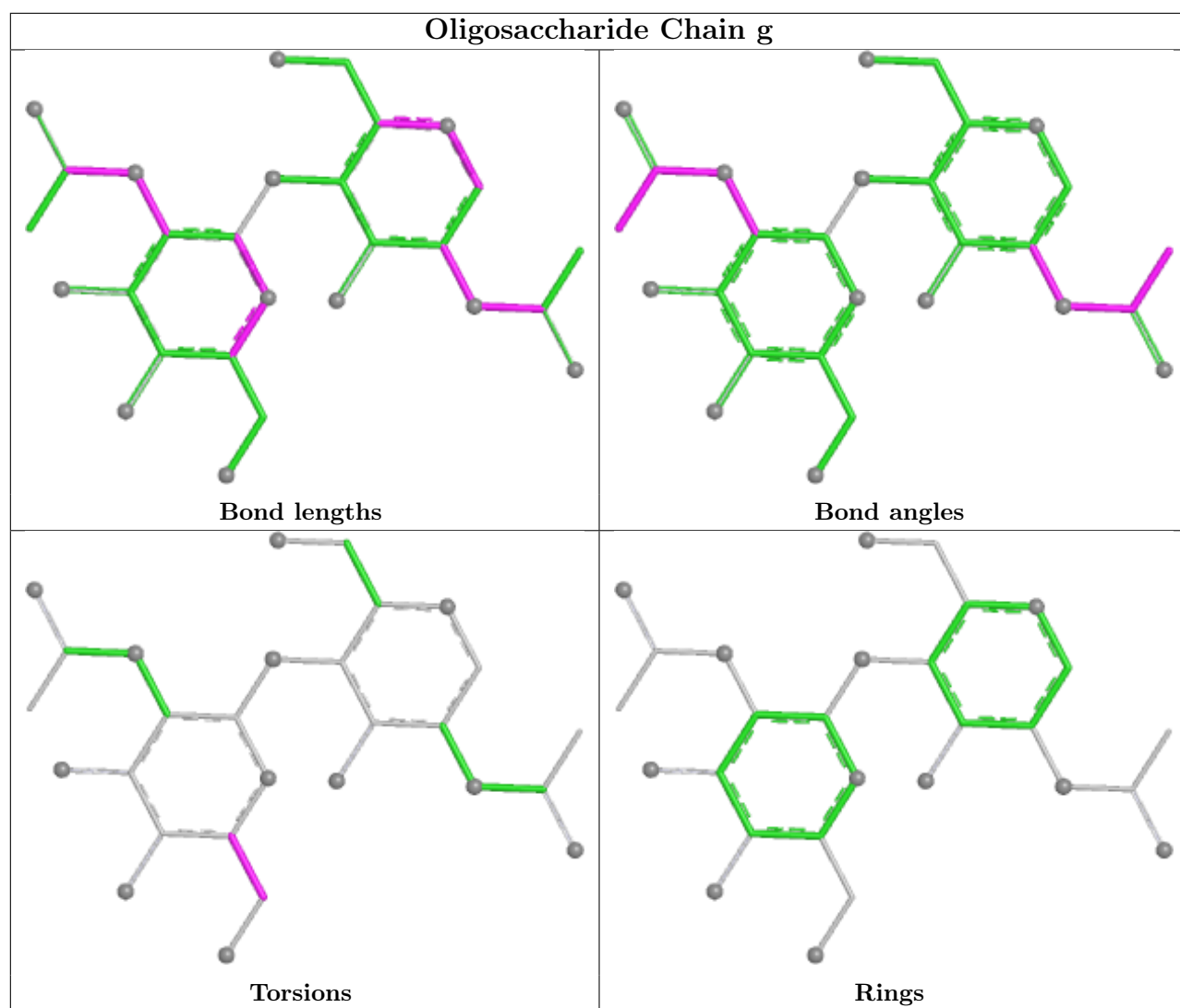


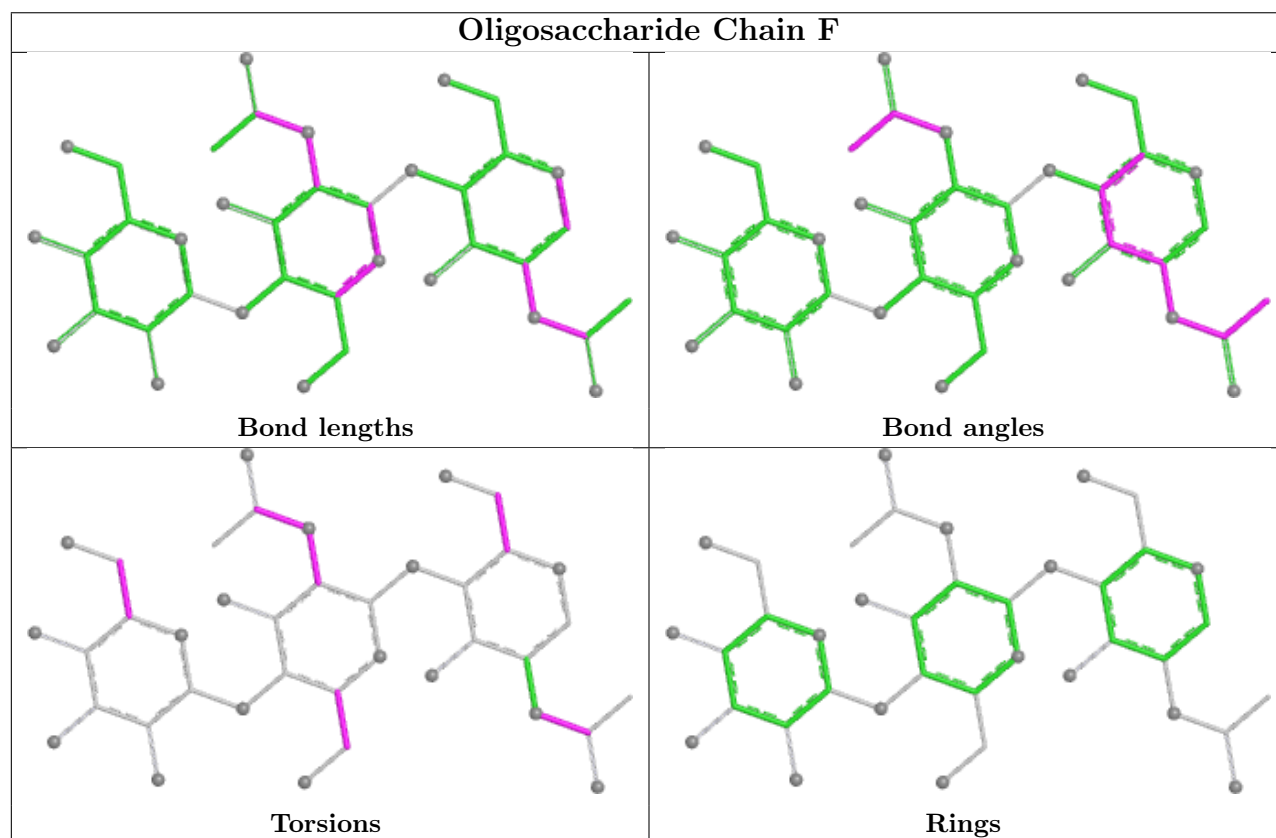
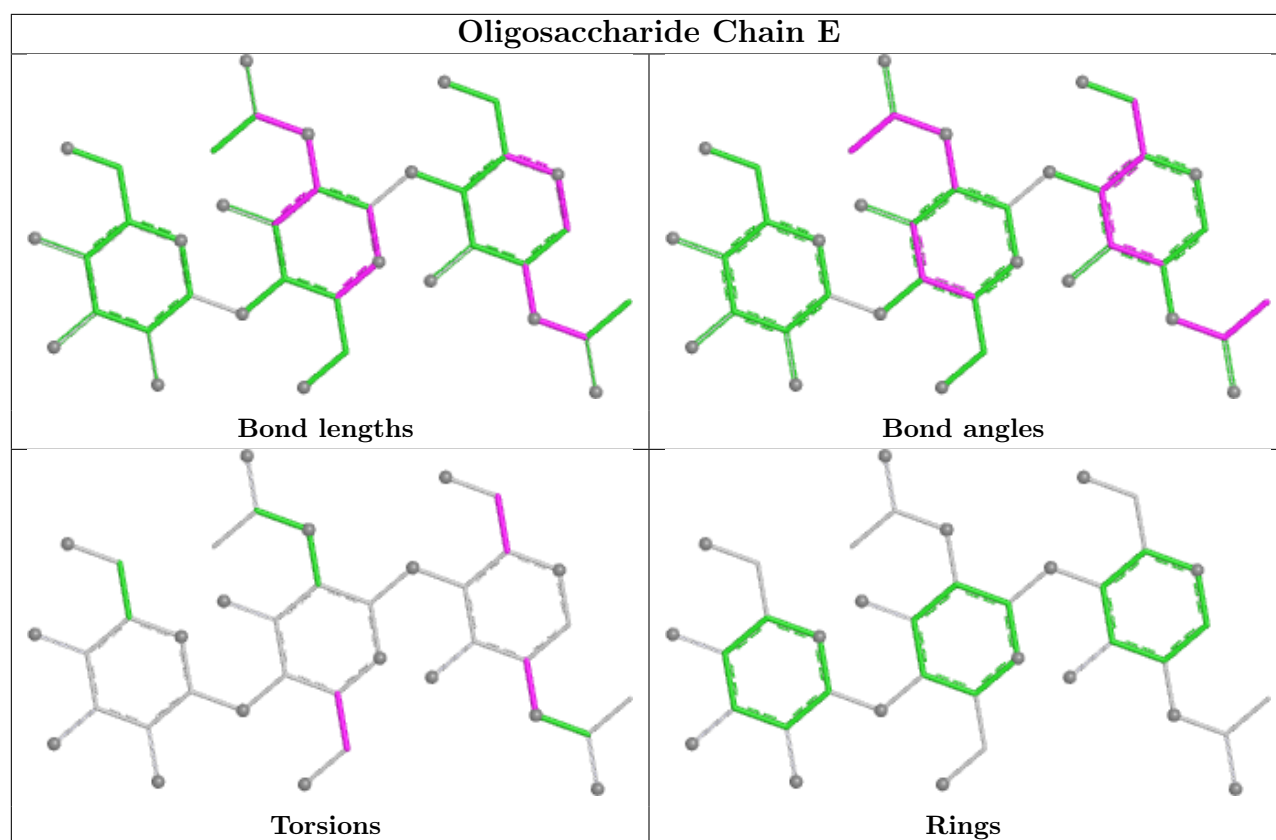


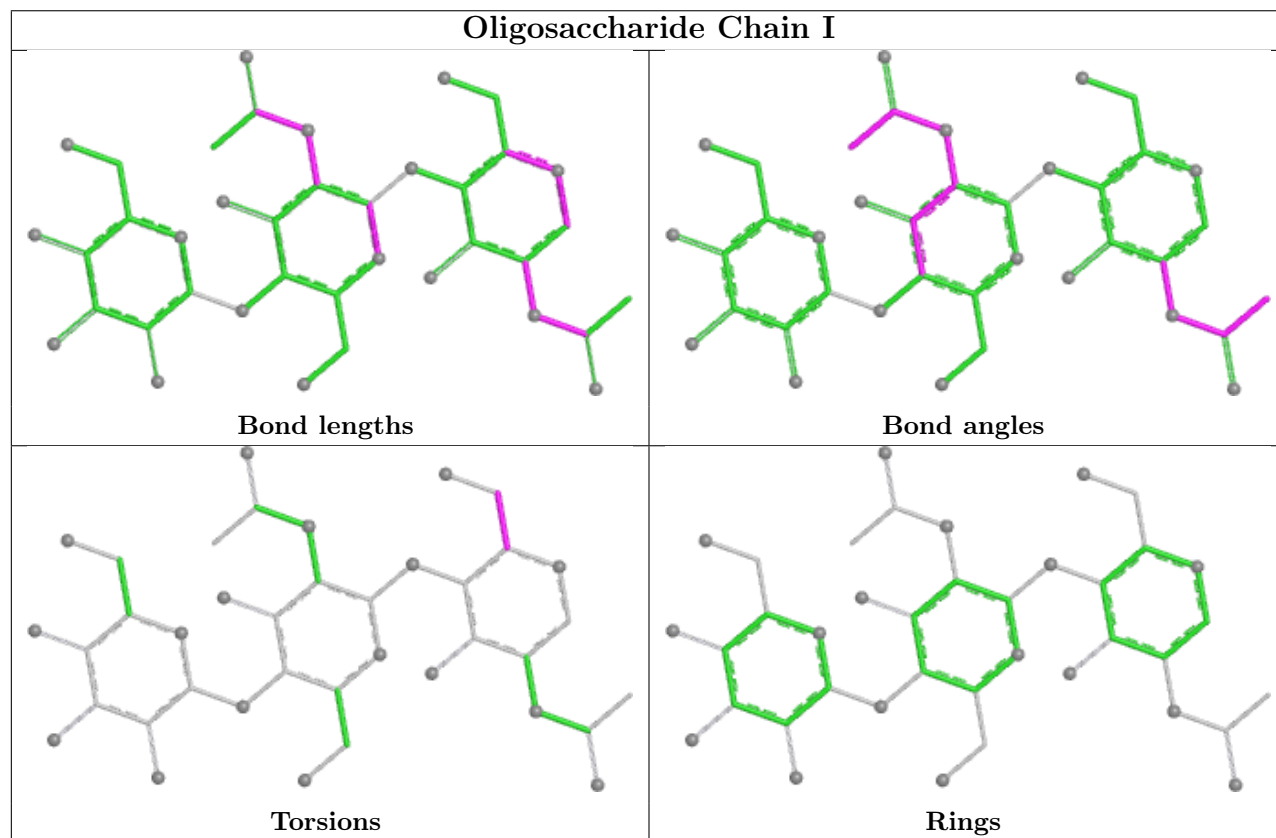
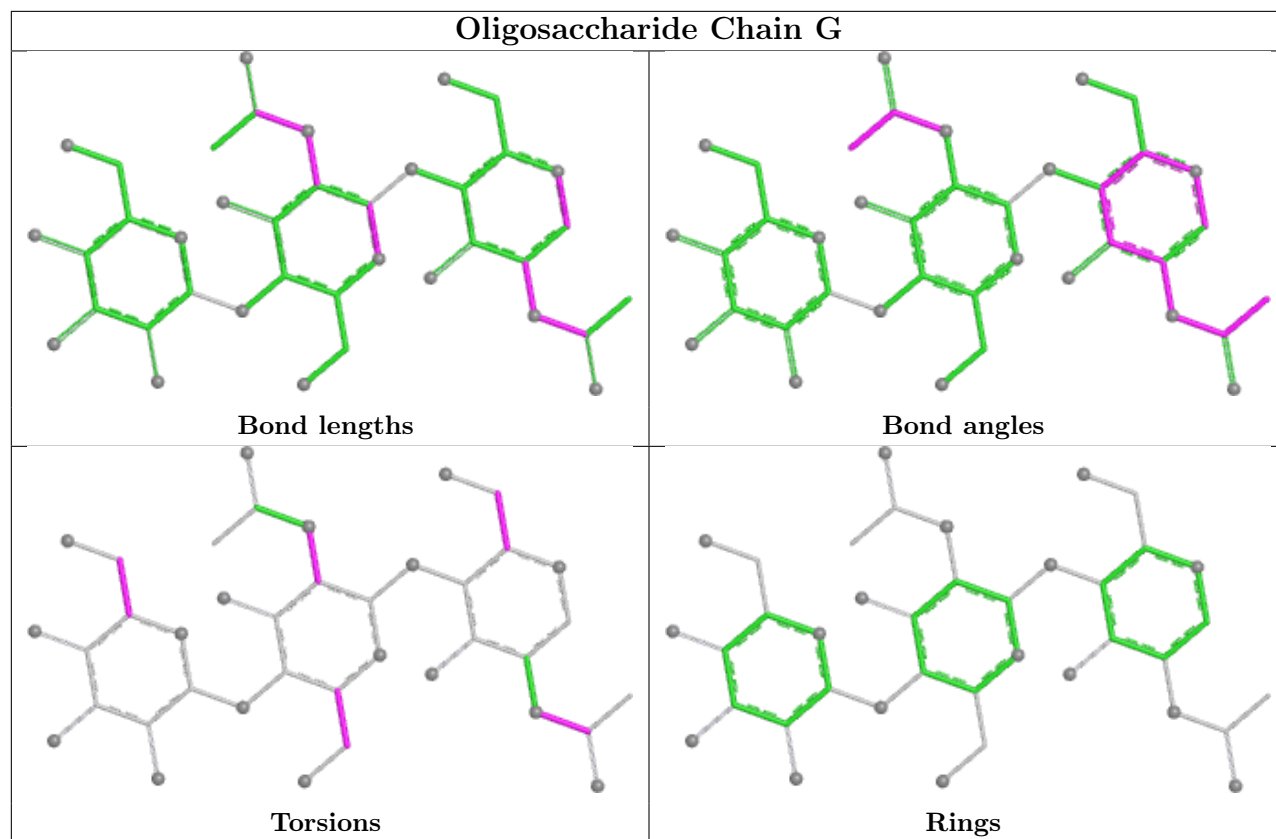


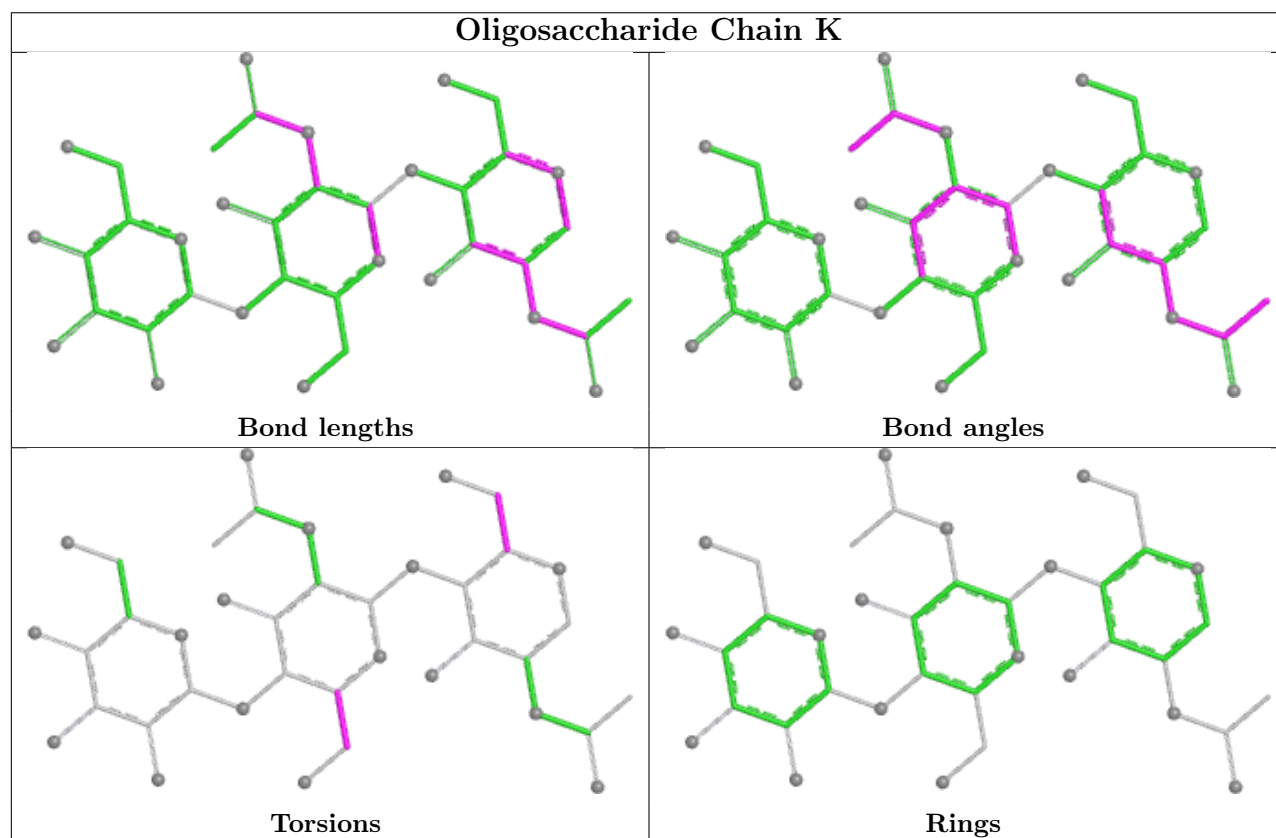
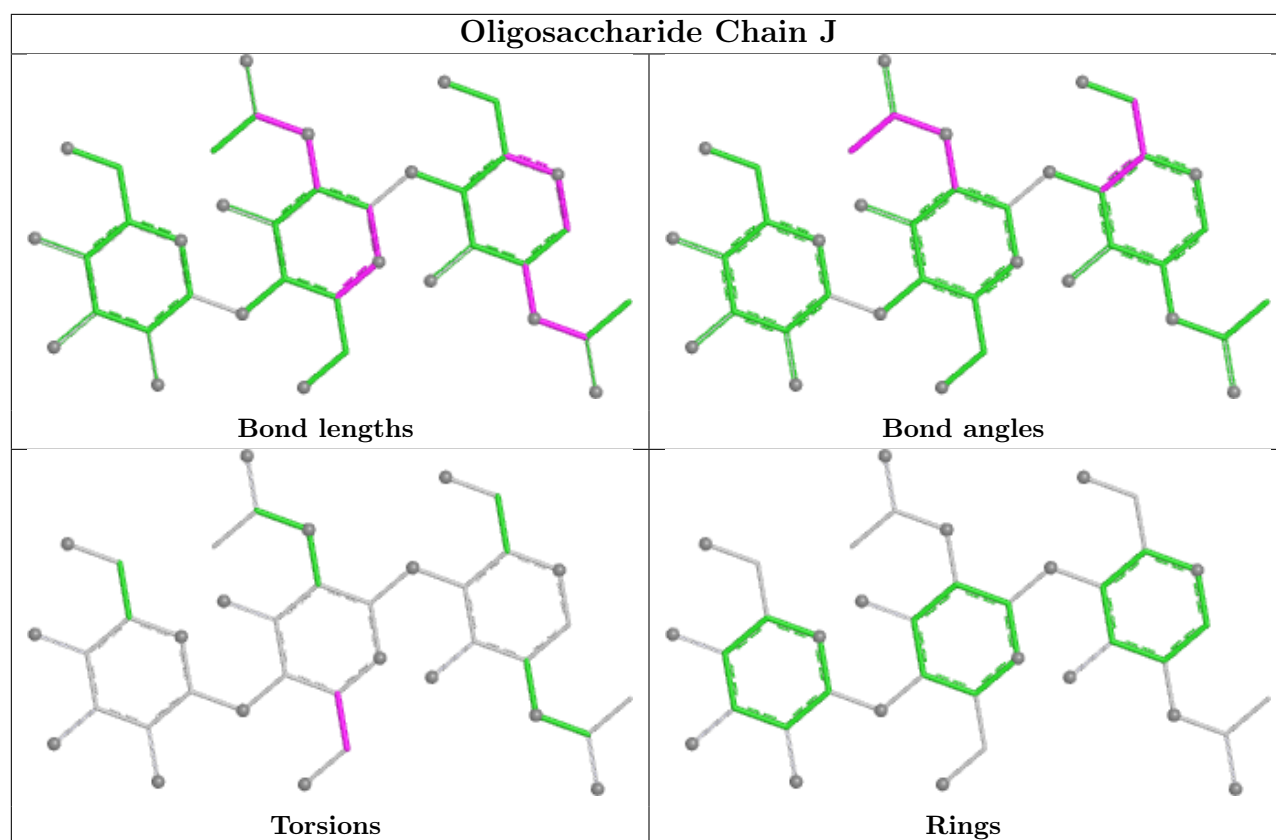


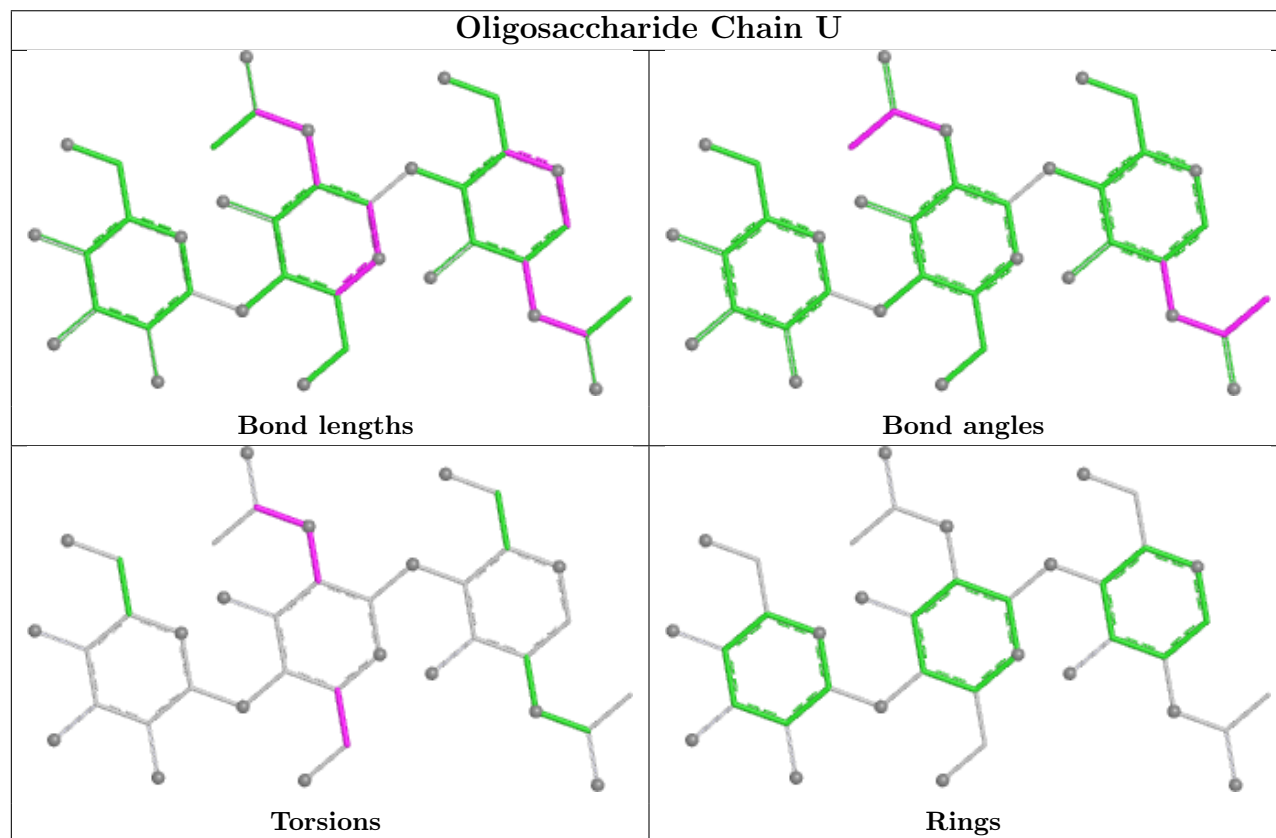
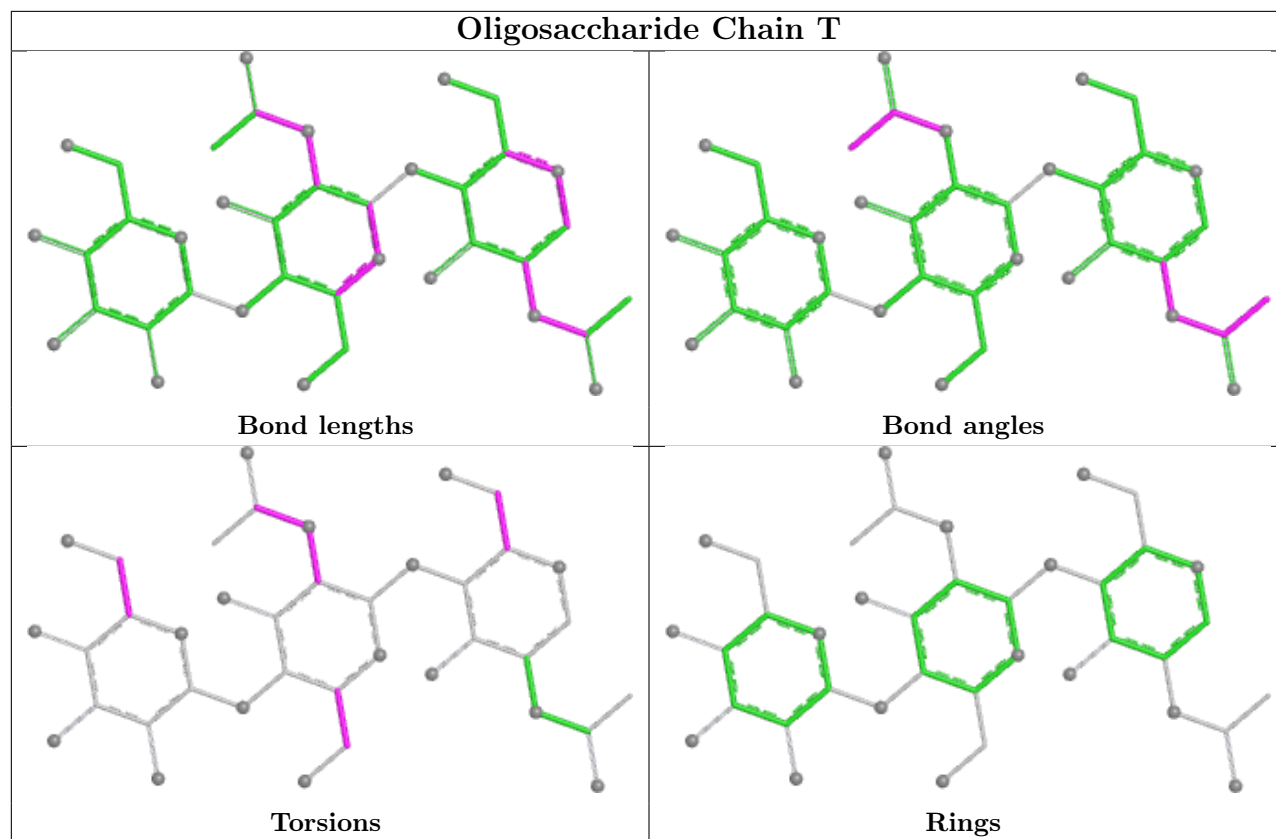


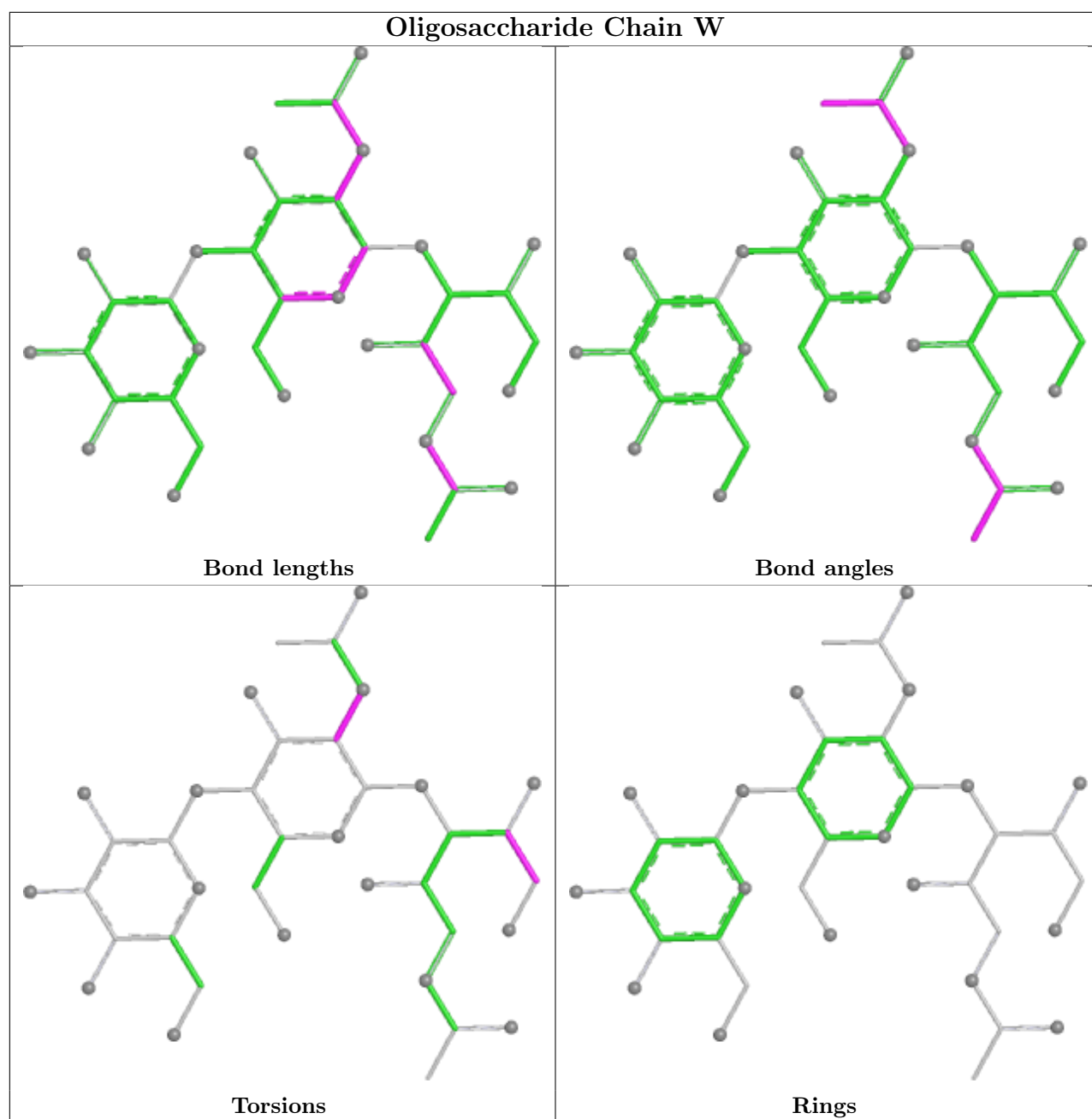


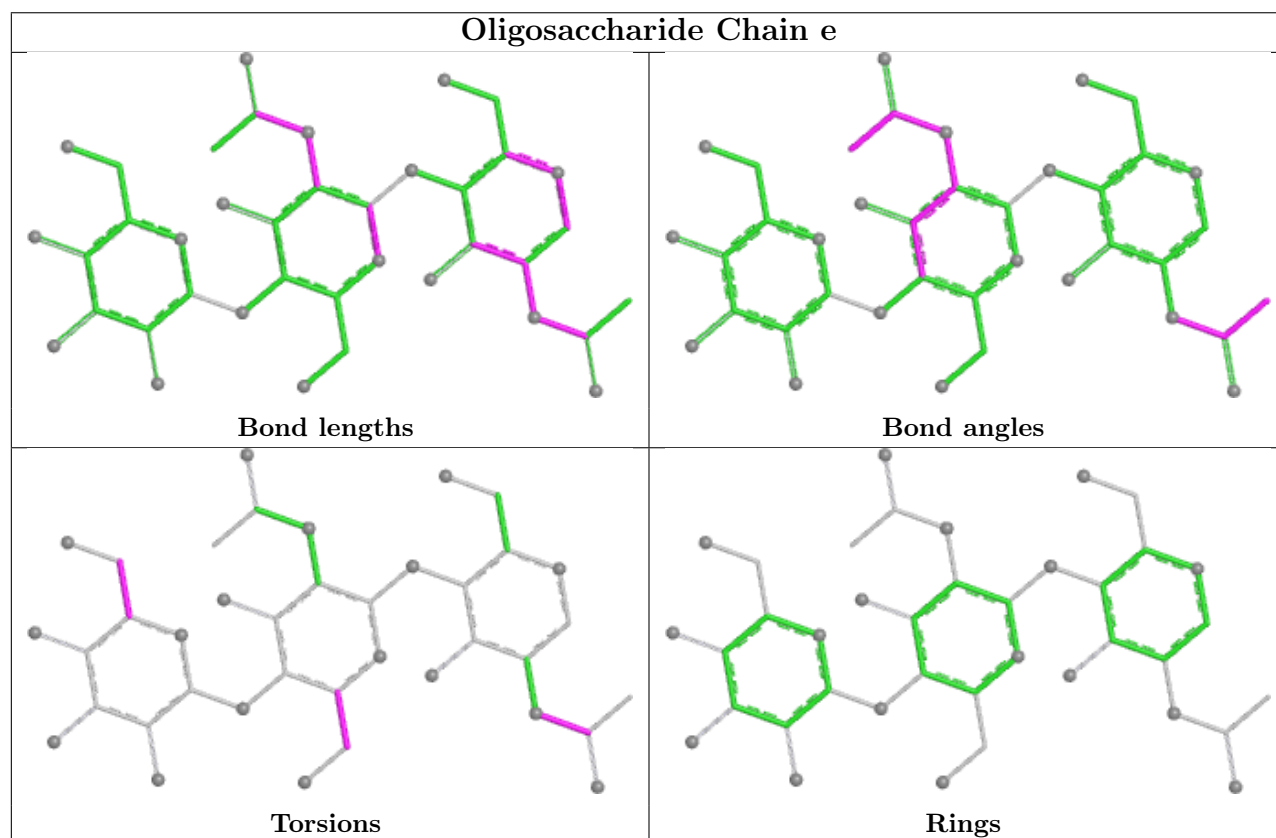
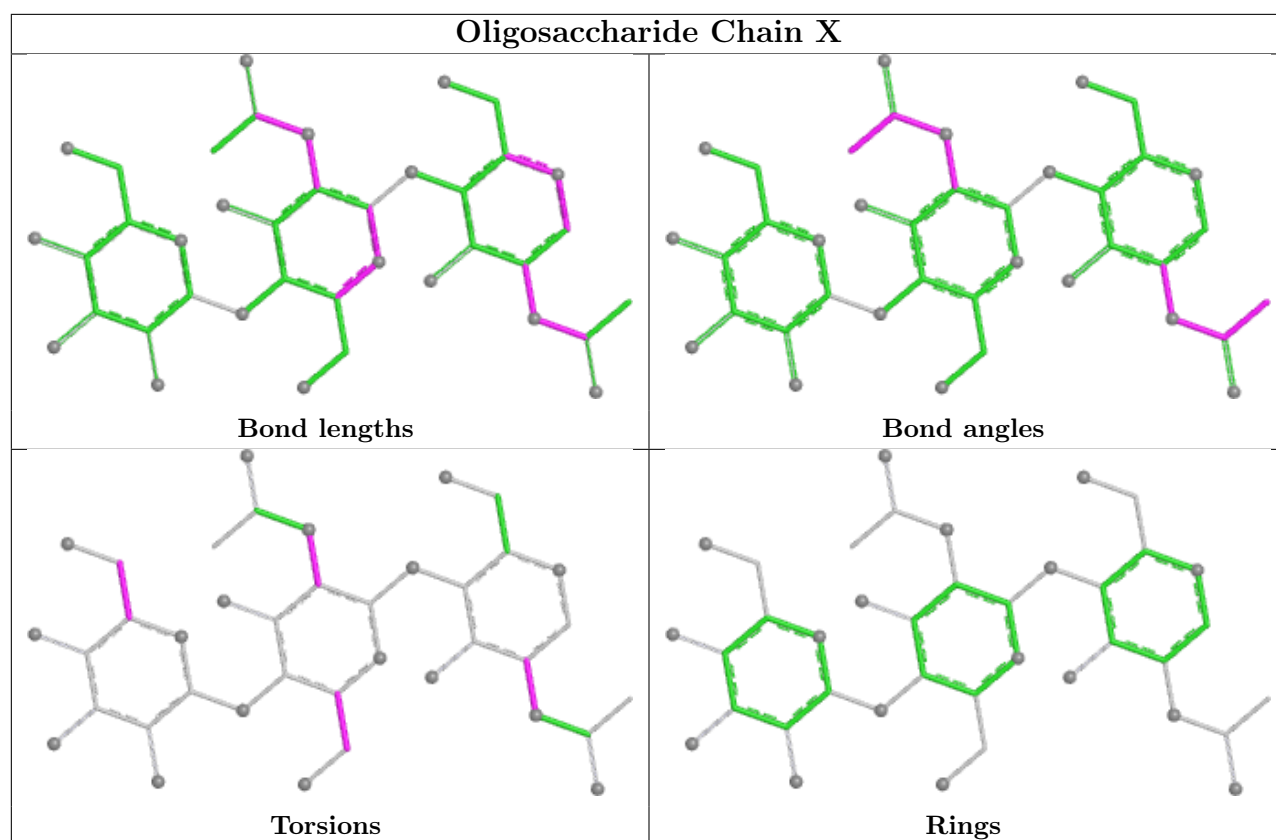


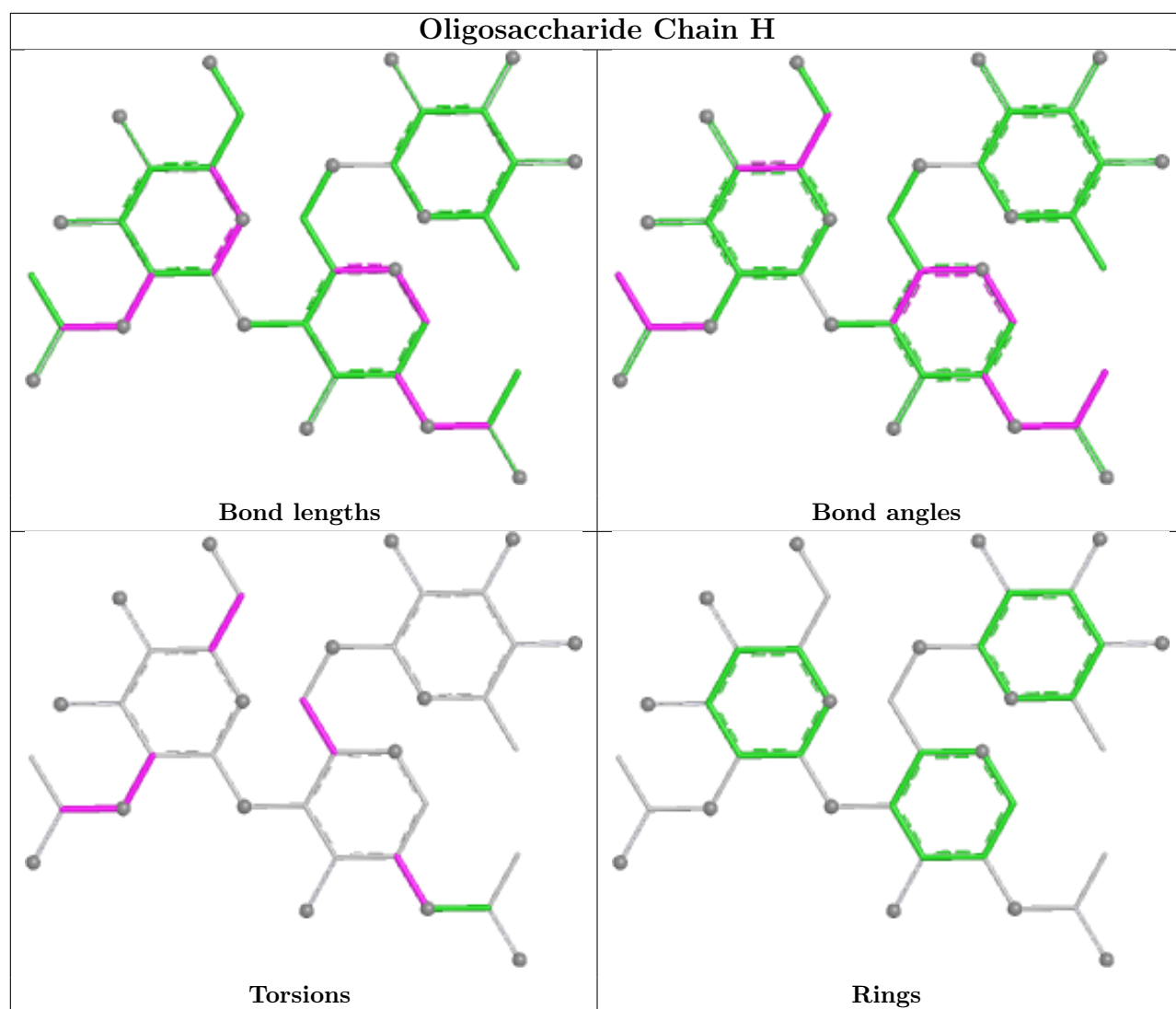


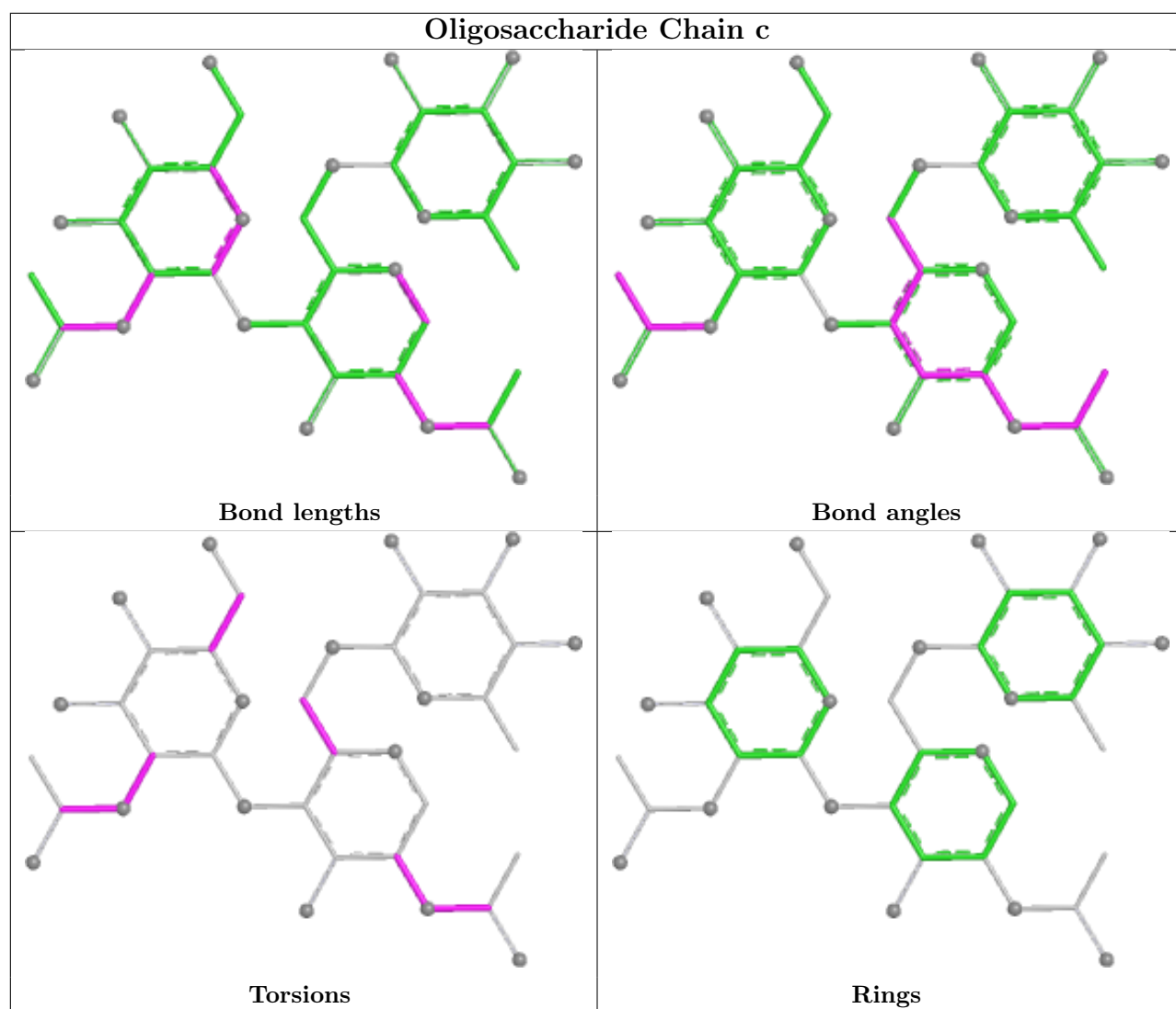


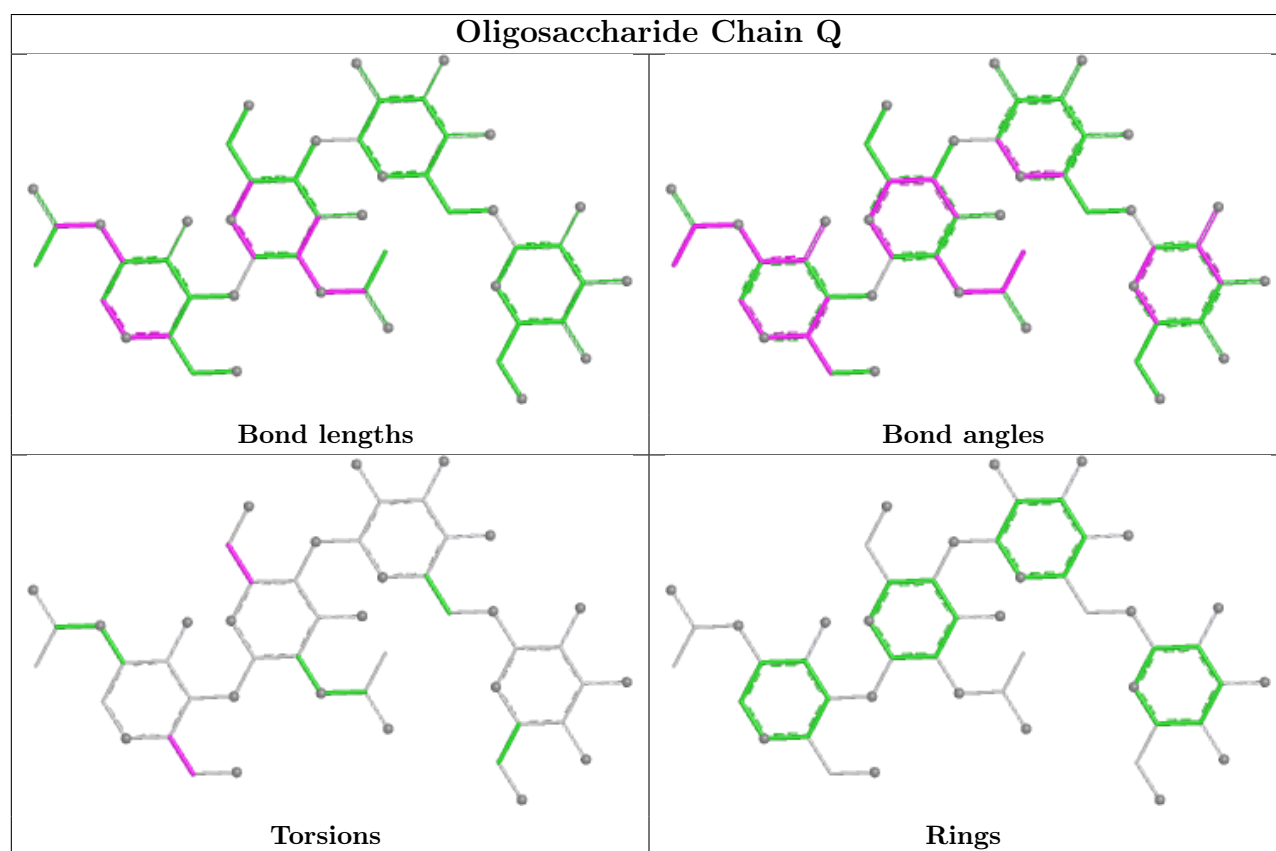
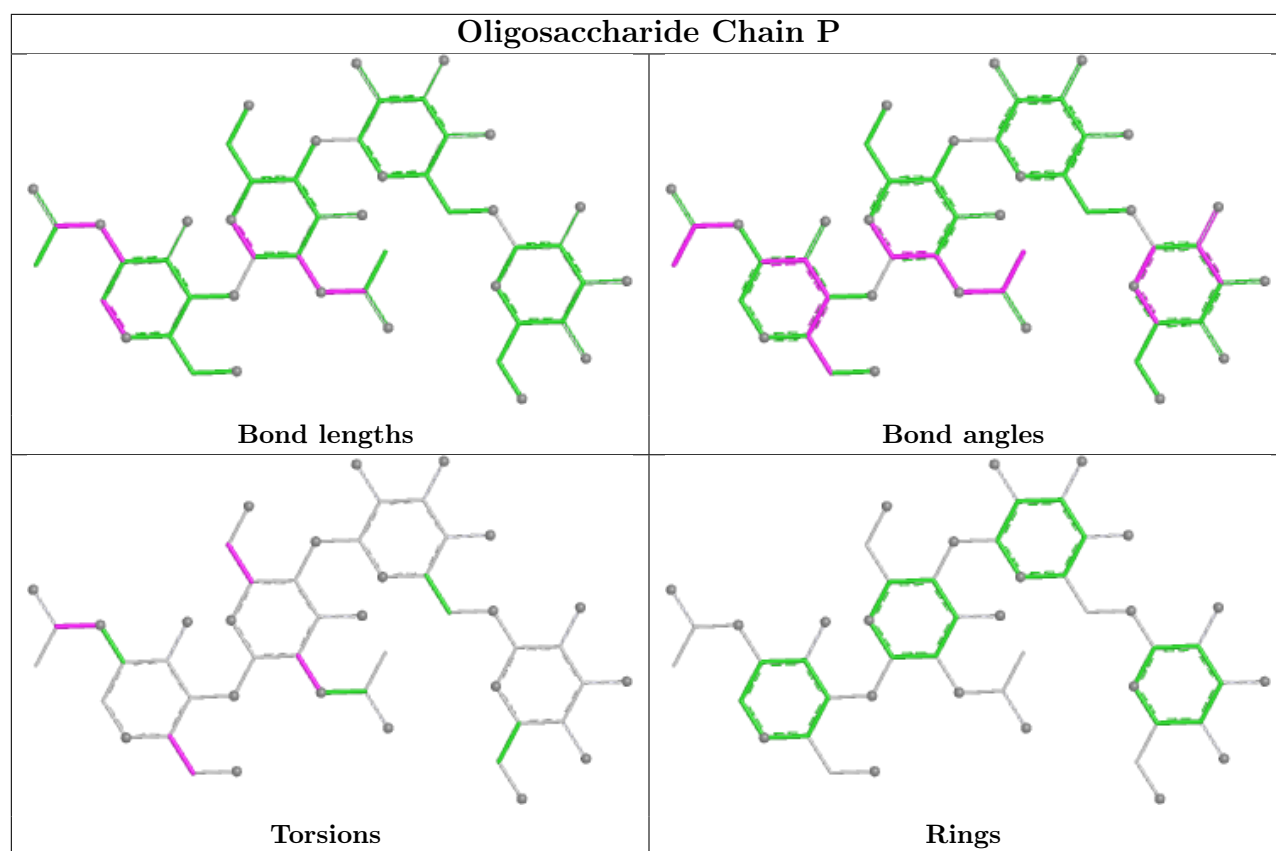


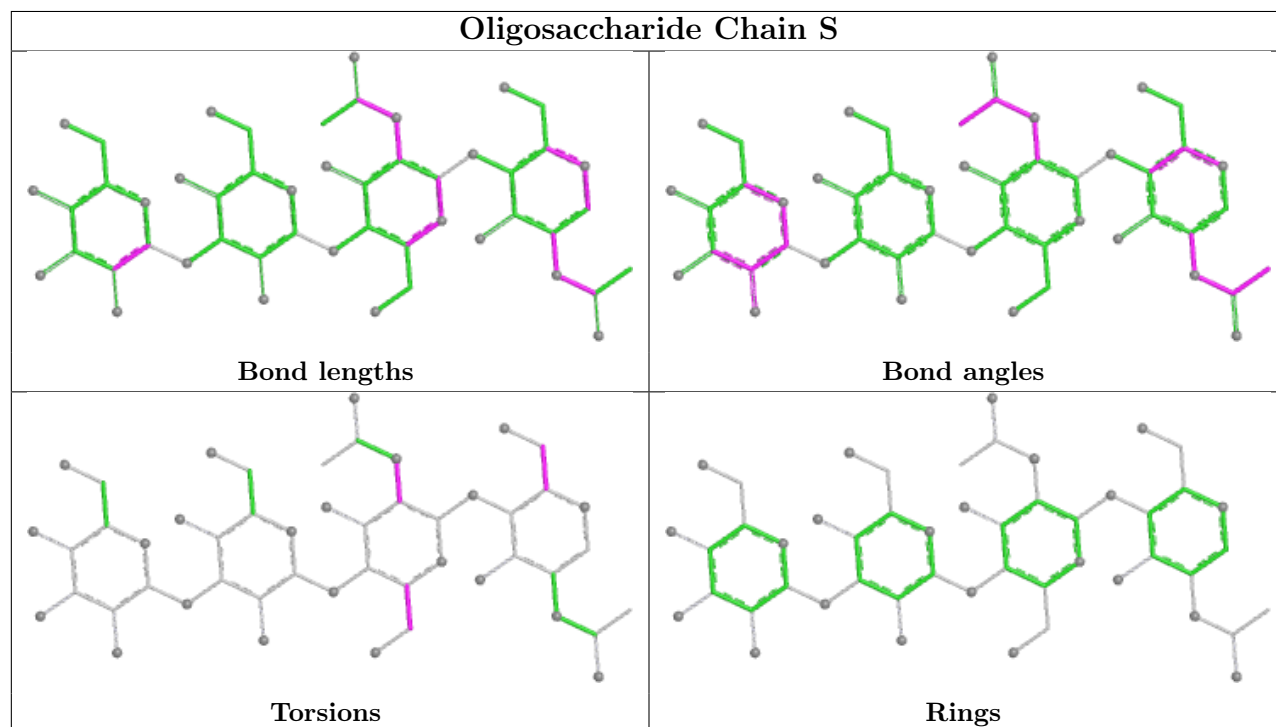
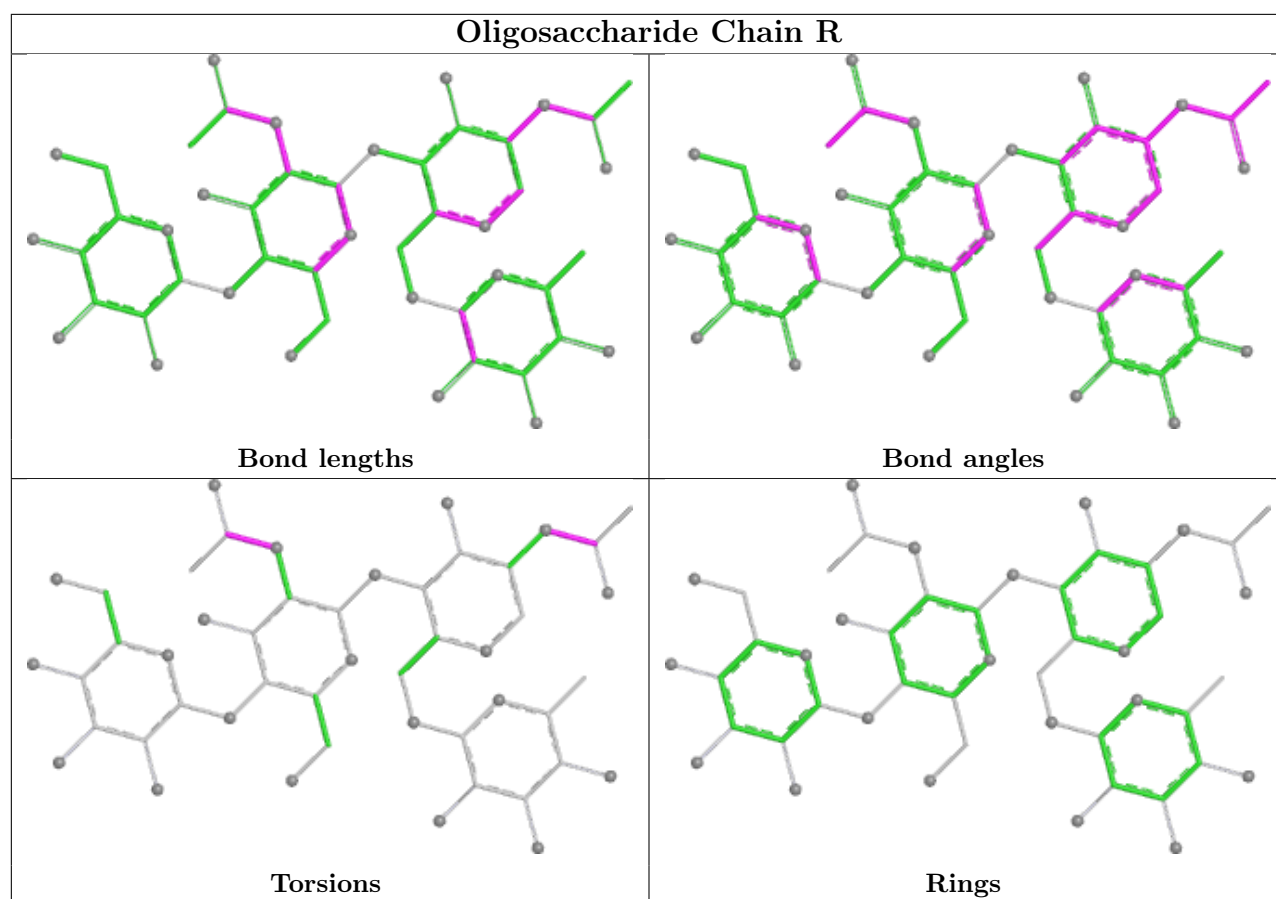


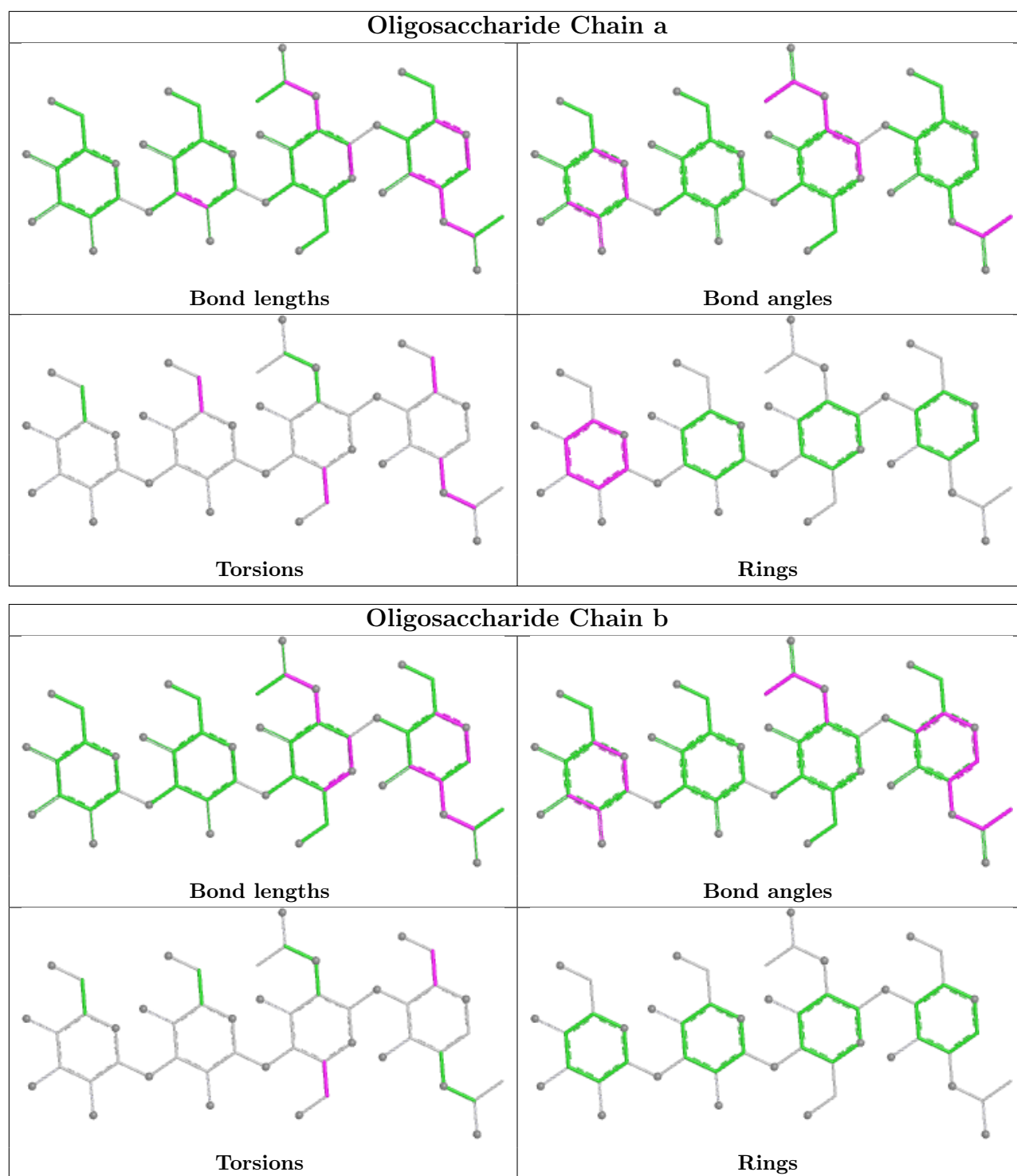


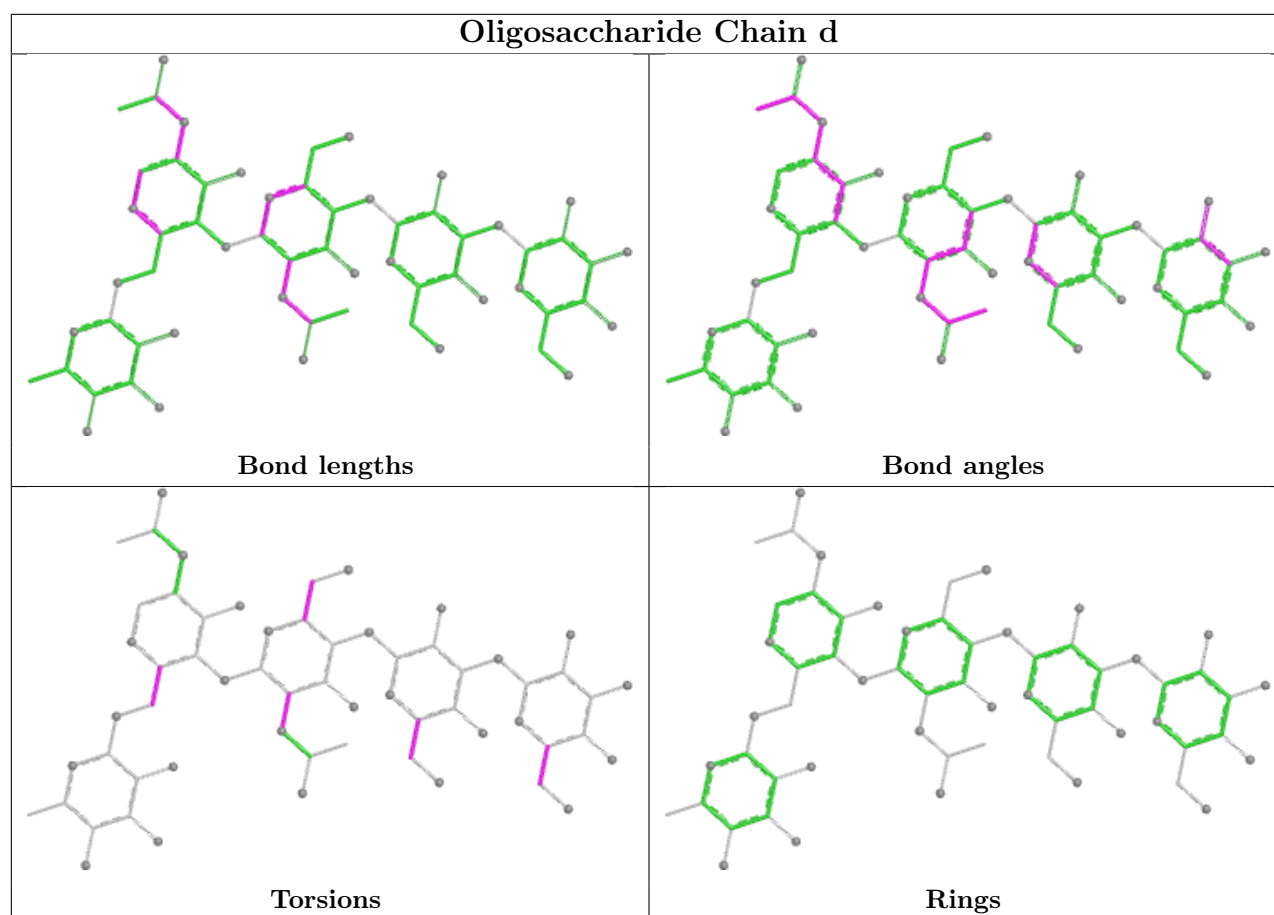












5.6 Ligand geometry [i](#)

21 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	1302	1	14,14,15	2.01	4 (28%)	17,19,21	1.09	1 (5%)
9	NAG	B	1302	1	14,14,15	2.07	4 (28%)	17,19,21	1.23	1 (5%)
9	NAG	C	1301	1	14,14,15	2.08	3 (21%)	17,19,21	1.57	2 (11%)
9	NAG	A	1302	1	14,14,15	2.11	5 (35%)	17,19,21	2.77	4 (23%)
9	NAG	A	1306	1	14,14,15	1.99	4 (28%)	17,19,21	1.21	2 (11%)
9	NAG	C	1303	1	14,14,15	2.02	3 (21%)	17,19,21	1.76	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	1303	1	14,14,15	2.02	4 (28%)	17,19,21	1.40	3 (17%)
9	NAG	B	1304	1	14,14,15	2.22	6 (42%)	17,19,21	3.44	7 (41%)
9	NAG	B	1303	1	14,14,15	1.98	4 (28%)	17,19,21	1.09	1 (5%)
9	NAG	B	1308	1	14,14,15	2.01	4 (28%)	17,19,21	2.00	3 (17%)
9	NAG	C	1304	1	14,14,15	2.04	4 (28%)	17,19,21	1.24	2 (11%)
9	NAG	A	1308	1	14,14,15	2.03	4 (28%)	17,19,21	1.61	4 (23%)
9	NAG	C	1305	1	14,14,15	2.02	4 (28%)	17,19,21	1.07	2 (11%)
9	NAG	B	1305	1	14,14,15	1.96	4 (28%)	17,19,21	1.27	3 (17%)
9	NAG	A	1304	1	14,14,15	2.00	4 (28%)	17,19,21	1.06	2 (11%)
9	NAG	B	1306	1	14,14,15	1.80	2 (14%)	17,19,21	1.83	4 (23%)
9	NAG	B	1307	1	14,14,15	2.03	4 (28%)	17,19,21	1.15	1 (5%)
9	NAG	A	1307	1	14,14,15	1.98	4 (28%)	17,19,21	1.43	3 (17%)
9	NAG	A	1305	1	14,14,15	1.96	4 (28%)	17,19,21	1.47	3 (17%)
9	NAG	B	1301	1	14,14,15	2.01	4 (28%)	17,19,21	1.11	2 (11%)
9	NAG	A	1301	1	14,14,15	2.01	4 (28%)	17,19,21	1.29	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1302	1	-	6/6/23/26	0/1/1/1
9	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1303	1	-	5/6/23/26	0/1/1/1
9	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1308	1	-	6/6/23/26	0/1/1/1
9	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
9	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
9	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1307	1	-	5/6/23/26	0/1/1/1
9	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1301	NAG	O5-C1	4.70	1.51	1.43
9	A	1302	NAG	O5-C1	4.67	1.51	1.43
9	B	1302	NAG	O5-C1	4.50	1.51	1.43
9	C	1303	NAG	O5-C1	4.48	1.51	1.43
9	C	1304	NAG	O5-C1	4.47	1.51	1.43
9	A	1301	NAG	O5-C1	4.39	1.51	1.43
9	B	1301	NAG	O5-C1	4.37	1.51	1.43
9	C	1302	NAG	O5-C1	4.37	1.51	1.43
9	C	1305	NAG	O5-C1	4.35	1.51	1.43
9	B	1303	NAG	O5-C1	4.33	1.51	1.43
9	A	1304	NAG	O5-C1	4.31	1.50	1.43
9	B	1307	NAG	O5-C1	4.24	1.50	1.43
9	A	1306	NAG	O5-C1	4.23	1.50	1.43
9	A	1307	NAG	O5-C1	4.17	1.50	1.43
9	A	1303	NAG	O5-C1	4.16	1.50	1.43
9	A	1308	NAG	O5-C1	4.12	1.50	1.43
9	B	1308	NAG	O5-C1	4.08	1.50	1.43
9	A	1305	NAG	O5-C1	4.06	1.50	1.43
9	B	1304	NAG	C7-N2	4.03	1.47	1.34
9	B	1308	NAG	C7-N2	4.01	1.47	1.34
9	B	1302	NAG	C7-N2	3.99	1.47	1.34
9	B	1306	NAG	O5-C1	3.97	1.50	1.43
9	B	1305	NAG	C7-N2	3.96	1.47	1.34
9	B	1305	NAG	O5-C1	3.94	1.50	1.43
9	B	1304	NAG	O5-C1	3.93	1.50	1.43
9	B	1307	NAG	C7-N2	3.93	1.47	1.34
9	A	1302	NAG	C7-N2	3.91	1.47	1.34
9	C	1302	NAG	C7-N2	3.90	1.46	1.34
9	A	1307	NAG	C7-N2	3.89	1.46	1.34
9	A	1304	NAG	C7-N2	3.89	1.46	1.34
9	C	1305	NAG	C7-N2	3.88	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1301	NAG	C7-N2	3.87	1.46	1.34
9	B	1301	NAG	C7-N2	3.87	1.46	1.34
9	A	1306	NAG	C7-N2	3.86	1.46	1.34
9	C	1303	NAG	C7-N2	3.86	1.46	1.34
9	A	1303	NAG	C7-N2	3.86	1.46	1.34
9	C	1304	NAG	C7-N2	3.85	1.46	1.34
9	A	1305	NAG	C7-N2	3.85	1.46	1.34
9	B	1303	NAG	C7-N2	3.85	1.46	1.34
9	A	1308	NAG	C7-N2	3.83	1.46	1.34
9	A	1301	NAG	C7-N2	3.79	1.46	1.34
9	B	1306	NAG	C7-N2	3.74	1.46	1.34
9	B	1304	NAG	C1-C2	3.12	1.56	1.52
9	B	1304	NAG	O5-C5	2.95	1.49	1.43
9	A	1308	NAG	C2-N2	2.71	1.50	1.46
9	B	1302	NAG	C2-N2	2.70	1.50	1.46
9	B	1307	NAG	C2-N2	2.68	1.50	1.46
9	A	1303	NAG	C2-N2	2.66	1.50	1.46
9	C	1301	NAG	C2-N2	2.59	1.50	1.46
9	C	1303	NAG	C2-N2	2.52	1.50	1.46
9	C	1302	NAG	C2-N2	2.50	1.50	1.46
9	A	1304	NAG	C2-N2	2.49	1.50	1.46
9	C	1305	NAG	C2-N2	2.49	1.50	1.46
9	A	1306	NAG	C2-N2	2.47	1.50	1.46
9	B	1308	NAG	C2-N2	2.46	1.50	1.46
9	B	1301	NAG	C2-N2	2.46	1.50	1.46
9	A	1303	NAG	O5-C5	2.45	1.48	1.43
9	C	1304	NAG	O5-C5	2.45	1.48	1.43
9	A	1308	NAG	O5-C5	2.45	1.48	1.43
9	B	1303	NAG	C2-N2	2.43	1.50	1.46
9	A	1302	NAG	C1-C2	2.42	1.55	1.52
9	A	1307	NAG	C2-N2	2.42	1.50	1.46
9	C	1304	NAG	C2-N2	2.41	1.50	1.46
9	B	1308	NAG	O5-C5	2.41	1.48	1.43
9	A	1301	NAG	C2-N2	2.40	1.50	1.46
9	B	1305	NAG	C2-N2	2.40	1.50	1.46
9	A	1305	NAG	C2-N2	2.38	1.50	1.46
9	B	1307	NAG	O5-C5	2.34	1.48	1.43
9	A	1305	NAG	O5-C5	2.28	1.47	1.43
9	C	1305	NAG	O5-C5	2.27	1.47	1.43
9	A	1307	NAG	O5-C5	2.25	1.47	1.43
9	A	1306	NAG	O5-C5	2.23	1.47	1.43
9	B	1304	NAG	C2-N2	2.22	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1304	NAG	O5-C5	2.21	1.47	1.43
9	C	1302	NAG	O5-C5	2.19	1.47	1.43
9	A	1302	NAG	O5-C5	2.19	1.47	1.43
9	B	1301	NAG	O5-C5	2.18	1.47	1.43
9	A	1302	NAG	C2-N2	2.15	1.49	1.46
9	A	1301	NAG	O5-C5	2.14	1.47	1.43
9	B	1302	NAG	O5-C5	2.09	1.47	1.43
9	B	1303	NAG	O5-C5	2.04	1.47	1.43
9	B	1305	NAG	O5-C5	2.02	1.47	1.43
9	B	1304	NAG	C4-C3	-2.01	1.47	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1304	NAG	C2-N2-C7	-10.66	108.61	122.90
9	A	1302	NAG	C1-O5-C5	-8.66	100.58	112.19
9	B	1308	NAG	C1-O5-C5	-6.13	103.97	112.19
9	A	1302	NAG	O5-C5-C6	4.97	117.34	107.66
9	C	1303	NAG	C4-C3-C2	4.45	117.53	111.02
9	B	1304	NAG	C1-C2-N2	4.42	117.40	110.43
9	A	1308	NAG	C1-O5-C5	-4.33	106.39	112.19
9	B	1306	NAG	C1-O5-C5	-4.22	106.53	112.19
9	B	1304	NAG	C8-C7-N2	4.18	123.05	116.12
9	C	1301	NAG	O5-C1-C2	3.93	117.36	111.29
9	A	1302	NAG	C4-C3-C2	3.86	116.68	111.02
9	B	1304	NAG	O5-C5-C6	3.78	115.01	107.66
9	B	1306	NAG	C3-C4-C5	3.71	116.95	110.23
9	B	1306	NAG	C2-N2-C7	-3.37	118.38	122.90
9	B	1304	NAG	C3-C4-C5	-3.32	104.22	110.23
9	B	1308	NAG	C8-C7-N2	3.26	121.52	116.12
9	B	1302	NAG	C8-C7-N2	3.05	121.18	116.12
9	B	1307	NAG	C8-C7-N2	3.01	121.11	116.12
9	C	1303	NAG	C1-O5-C5	-3.00	108.16	112.19
9	B	1304	NAG	O7-C7-N2	-3.00	116.69	121.98
9	A	1303	NAG	C8-C7-N2	2.95	121.02	116.12
9	A	1307	NAG	C2-N2-C7	-2.82	119.13	122.90
9	A	1308	NAG	C1-C2-N2	-2.75	106.10	110.43
9	A	1305	NAG	C3-C4-C5	2.75	115.22	110.23
9	A	1307	NAG	C1-O5-C5	-2.70	108.57	112.19
9	B	1305	NAG	C8-C7-N2	2.67	120.54	116.12
9	A	1305	NAG	C2-N2-C7	-2.66	119.34	122.90
9	A	1301	NAG	C2-N2-C7	-2.63	119.37	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1303	NAG	C1-C2-N2	-2.60	106.34	110.43
9	B	1305	NAG	C2-N2-C7	-2.59	119.42	122.90
9	A	1307	NAG	C8-C7-N2	2.45	120.19	116.12
9	A	1305	NAG	C8-C7-N2	2.40	120.11	116.12
9	A	1306	NAG	C8-C7-N2	2.39	120.08	116.12
9	C	1305	NAG	C8-C7-N2	2.39	120.08	116.12
9	C	1304	NAG	C8-C7-N2	2.37	120.04	116.12
9	A	1304	NAG	C8-C7-N2	2.36	120.03	116.12
9	A	1303	NAG	C1-O5-C5	-2.35	109.03	112.19
9	B	1301	NAG	C8-C7-N2	2.32	119.97	116.12
9	A	1303	NAG	C3-C4-C5	2.32	114.43	110.23
9	A	1302	NAG	C3-C4-C5	2.28	114.36	110.23
9	C	1301	NAG	C8-C7-N2	2.28	119.90	116.12
9	A	1301	NAG	C8-C7-N2	2.27	119.89	116.12
9	C	1304	NAG	C2-N2-C7	-2.27	119.86	122.90
9	B	1308	NAG	C3-C4-C5	2.27	114.34	110.23
9	A	1306	NAG	C2-N2-C7	-2.26	119.87	122.90
9	B	1306	NAG	O5-C5-C6	2.26	112.05	107.66
9	B	1304	NAG	C6-C5-C4	-2.24	107.51	113.02
9	C	1305	NAG	C2-N2-C7	-2.24	119.89	122.90
9	B	1303	NAG	C8-C7-N2	2.23	119.82	116.12
9	C	1302	NAG	C8-C7-N2	2.23	119.81	116.12
9	B	1301	NAG	C2-N2-C7	-2.14	120.03	122.90
9	B	1305	NAG	C6-C5-C4	-2.09	107.89	113.02
9	C	1303	NAG	O5-C5-C6	2.06	111.67	107.66
9	A	1308	NAG	C4-C3-C2	-2.06	108.01	111.02
9	A	1308	NAG	C6-C5-C4	-2.06	107.97	113.02
9	A	1304	NAG	C2-N2-C7	-2.03	120.18	122.90

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1308	NAG	C3-C2-N2-C7
9	C	1301	NAG	C4-C5-C6-O6
9	A	1302	NAG	O5-C5-C6-O6
9	C	1301	NAG	O5-C5-C6-O6
9	A	1308	NAG	C4-C5-C6-O6
9	B	1301	NAG	C4-C5-C6-O6
9	A	1308	NAG	O5-C5-C6-O6
9	B	1304	NAG	O5-C5-C6-O6
9	A	1302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	1302	NAG	O5-C5-C6-O6
9	A	1305	NAG	O5-C5-C6-O6
9	B	1308	NAG	O5-C5-C6-O6
9	B	1301	NAG	O5-C5-C6-O6
9	B	1304	NAG	C4-C5-C6-O6
9	A	1305	NAG	C4-C5-C6-O6
9	A	1301	NAG	C8-C7-N2-C2
9	A	1301	NAG	O7-C7-N2-C2
9	A	1303	NAG	C8-C7-N2-C2
9	A	1303	NAG	O7-C7-N2-C2
9	B	1302	NAG	C8-C7-N2-C2
9	B	1302	NAG	O7-C7-N2-C2
9	B	1307	NAG	C8-C7-N2-C2
9	B	1307	NAG	O7-C7-N2-C2
9	B	1308	NAG	C8-C7-N2-C2
9	B	1308	NAG	O7-C7-N2-C2
9	C	1304	NAG	C8-C7-N2-C2
9	C	1304	NAG	O7-C7-N2-C2
9	B	1302	NAG	C4-C5-C6-O6
9	C	1304	NAG	O5-C5-C6-O6
9	B	1303	NAG	O5-C5-C6-O6
9	B	1303	NAG	C4-C5-C6-O6
9	A	1306	NAG	O5-C5-C6-O6
9	A	1303	NAG	O5-C5-C6-O6
9	C	1302	NAG	O5-C5-C6-O6
9	C	1302	NAG	C3-C2-N2-C7
9	A	1307	NAG	O5-C5-C6-O6
9	B	1308	NAG	C4-C5-C6-O6
9	A	1303	NAG	C1-C2-N2-C7
9	B	1307	NAG	C1-C2-N2-C7
9	B	1308	NAG	C1-C2-N2-C7
9	B	1306	NAG	C4-C5-C6-O6
9	B	1302	NAG	C3-C2-N2-C7
9	B	1308	NAG	C3-C2-N2-C7
9	B	1306	NAG	O5-C5-C6-O6
9	B	1307	NAG	C4-C5-C6-O6
9	B	1302	NAG	C1-C2-N2-C7
9	A	1303	NAG	C3-C2-N2-C7
9	B	1307	NAG	C3-C2-N2-C7
9	C	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1302	NAG	1	0
9	B	1302	NAG	3	0
9	C	1301	NAG	1	0
9	A	1302	NAG	6	0
9	C	1303	NAG	2	0
9	A	1303	NAG	3	0
9	B	1304	NAG	1	0
9	B	1308	NAG	3	0
9	C	1304	NAG	2	0
9	A	1308	NAG	12	0
9	B	1305	NAG	3	0
9	A	1304	NAG	4	0
9	B	1306	NAG	1	0
9	B	1307	NAG	2	0
9	A	1307	NAG	2	0
9	A	1301	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.

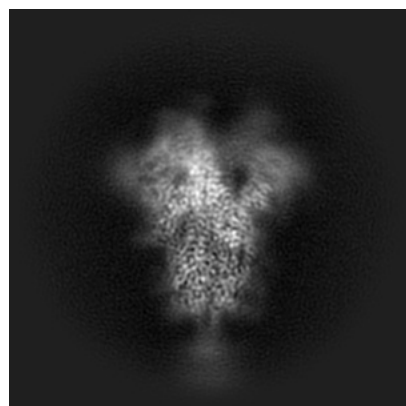
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44420. These allow visual inspection of the internal detail of the map and identification of artifacts.

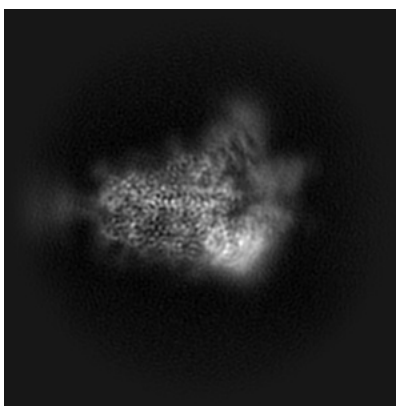
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

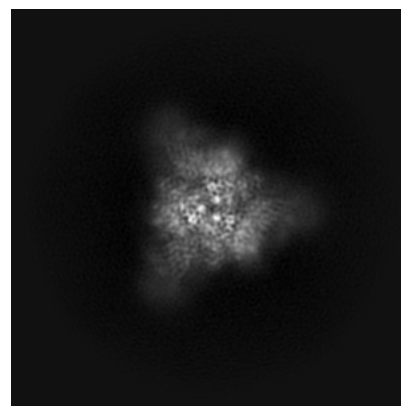
6.1.1 Primary map



X

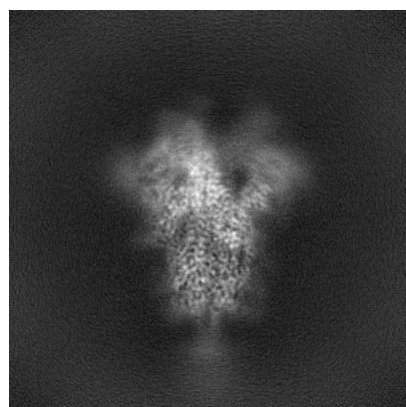


Y

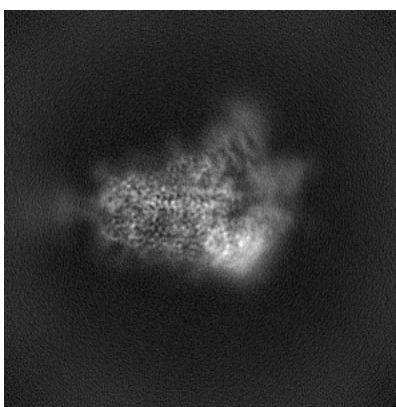


Z

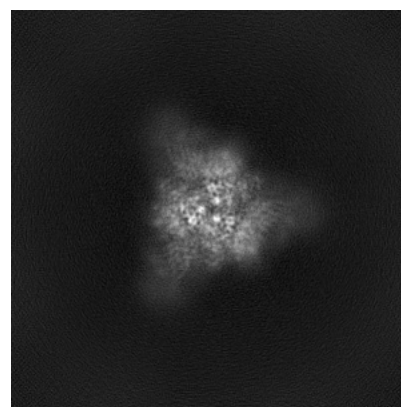
6.1.2 Raw map



X



Y

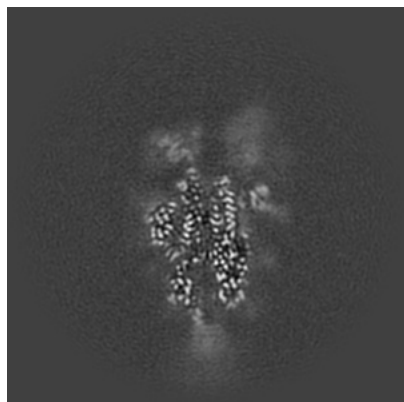


Z

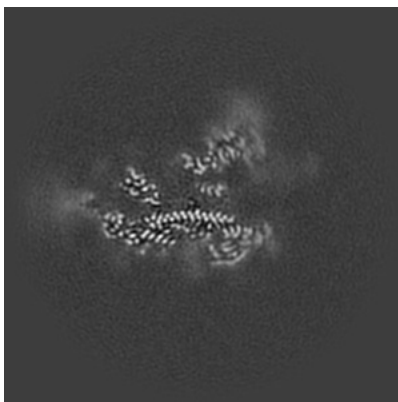
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

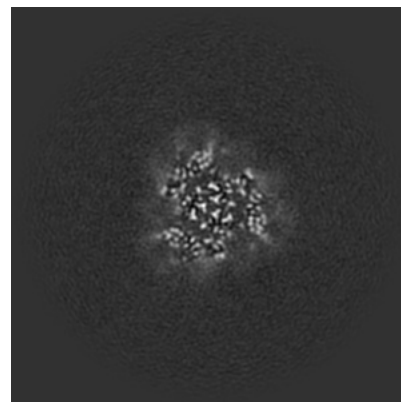
6.2.1 Primary map



X Index: 160

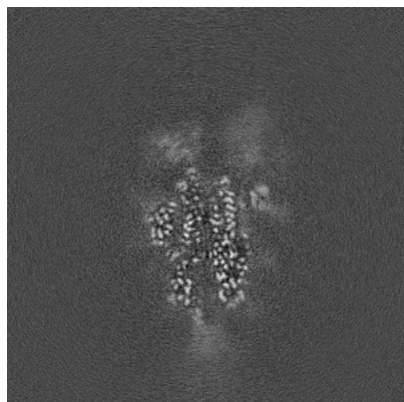


Y Index: 160

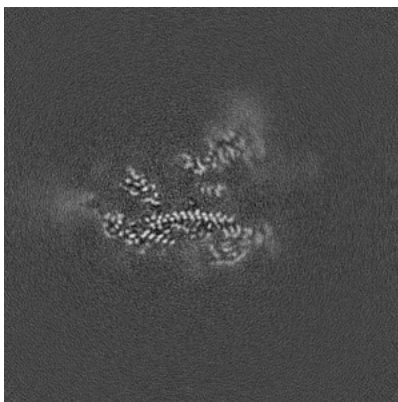


Z Index: 160

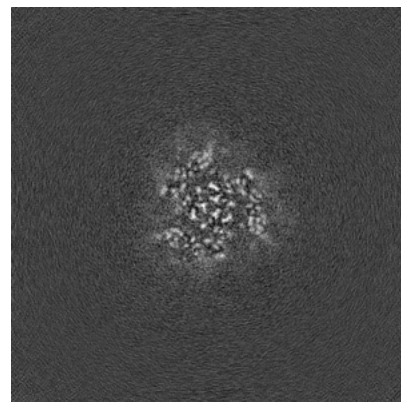
6.2.2 Raw map



X Index: 160



Y Index: 160

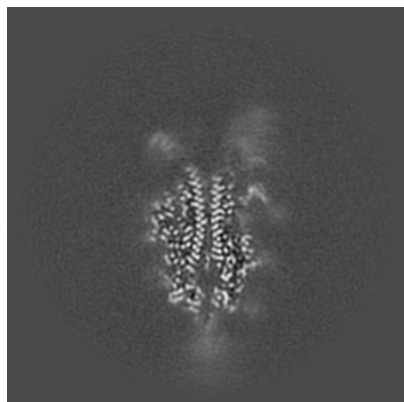


Z Index: 160

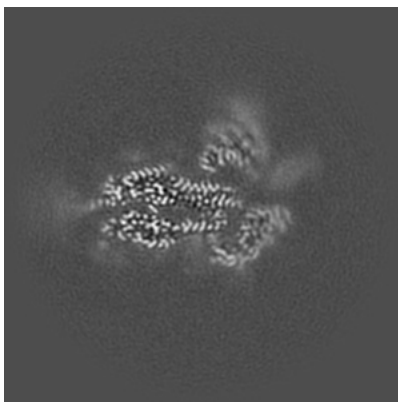
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

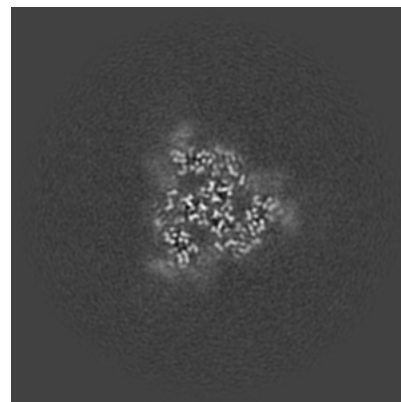
6.3.1 Primary map



X Index: 164

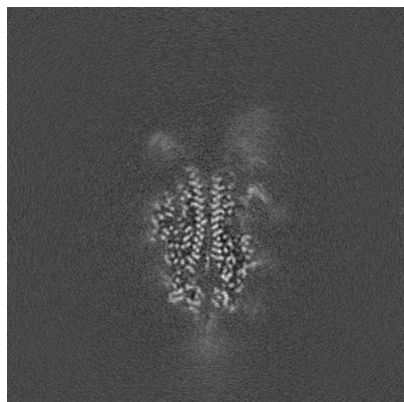


Y Index: 150

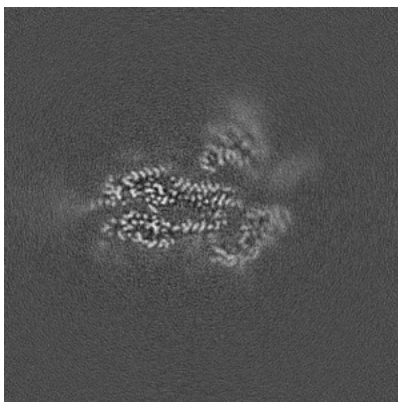


Z Index: 165

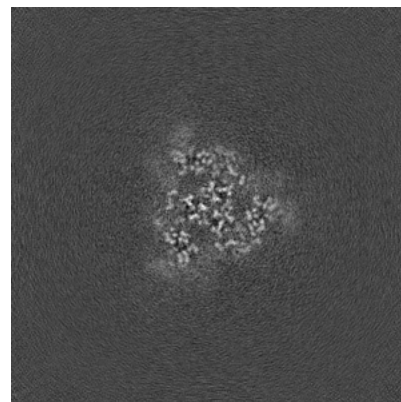
6.3.2 Raw map



X Index: 164



Y Index: 150



Z Index: 165

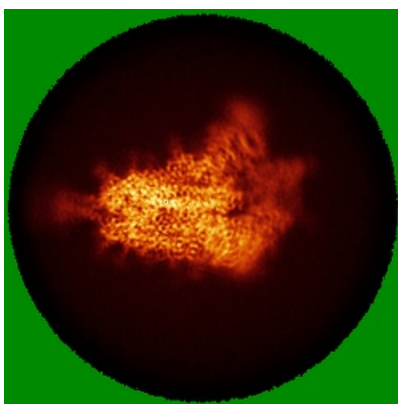
The images above show the largest variance slices of the map in three orthogonal directions.

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

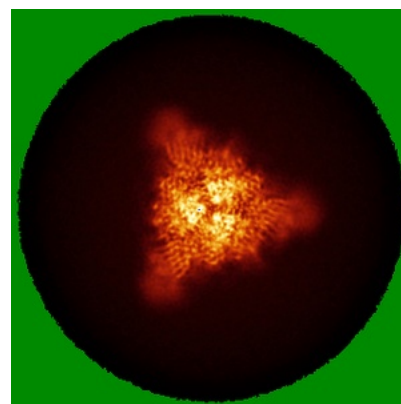
6.4.1 Primary map



X

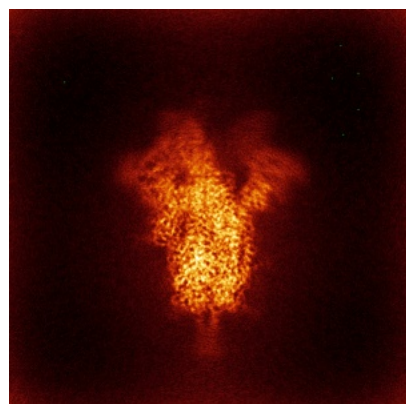


Y

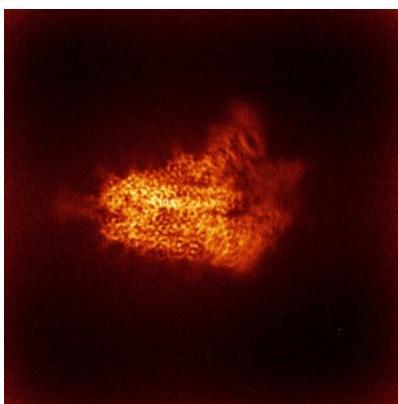


Z

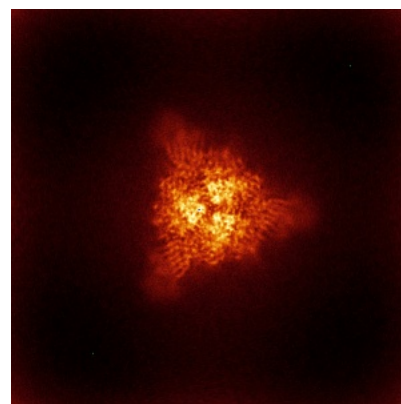
6.4.2 Raw map



X



Y

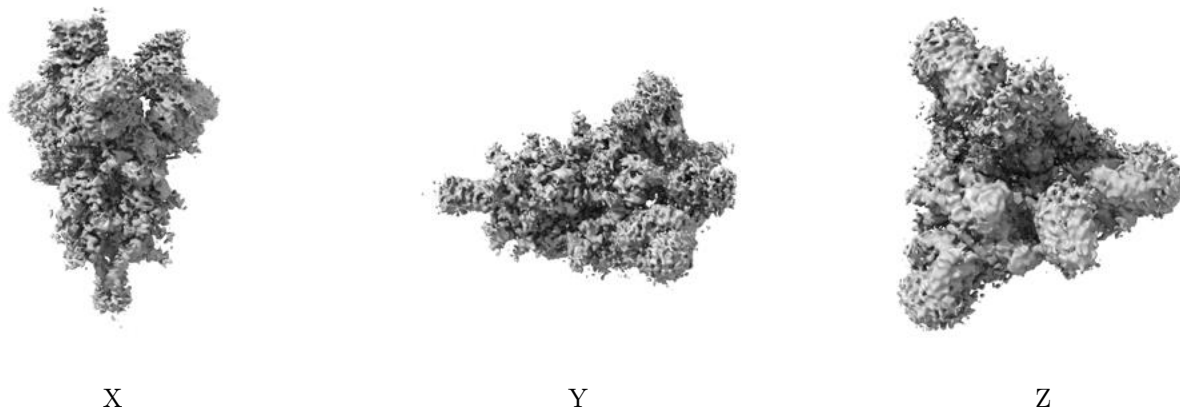


Z

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.

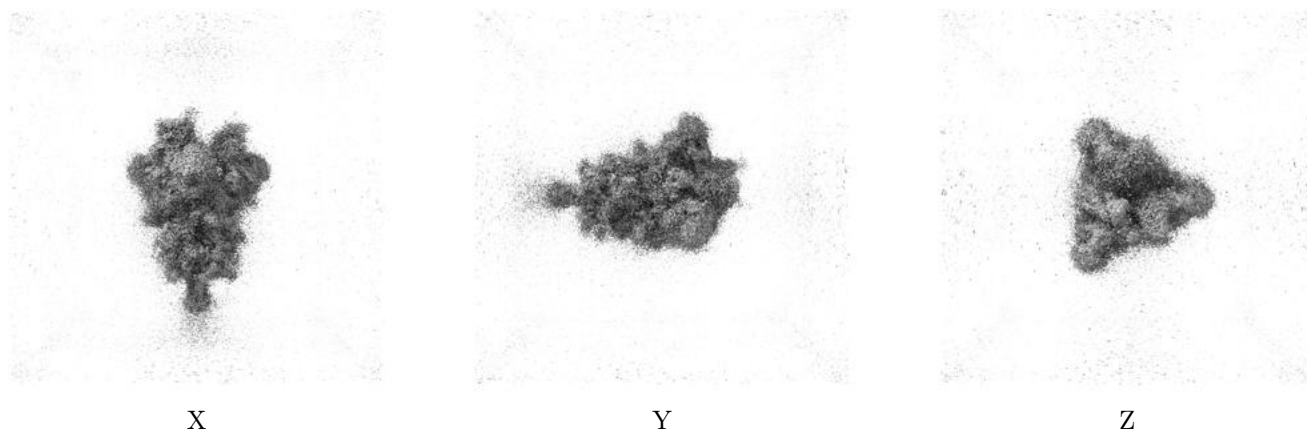
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. 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.

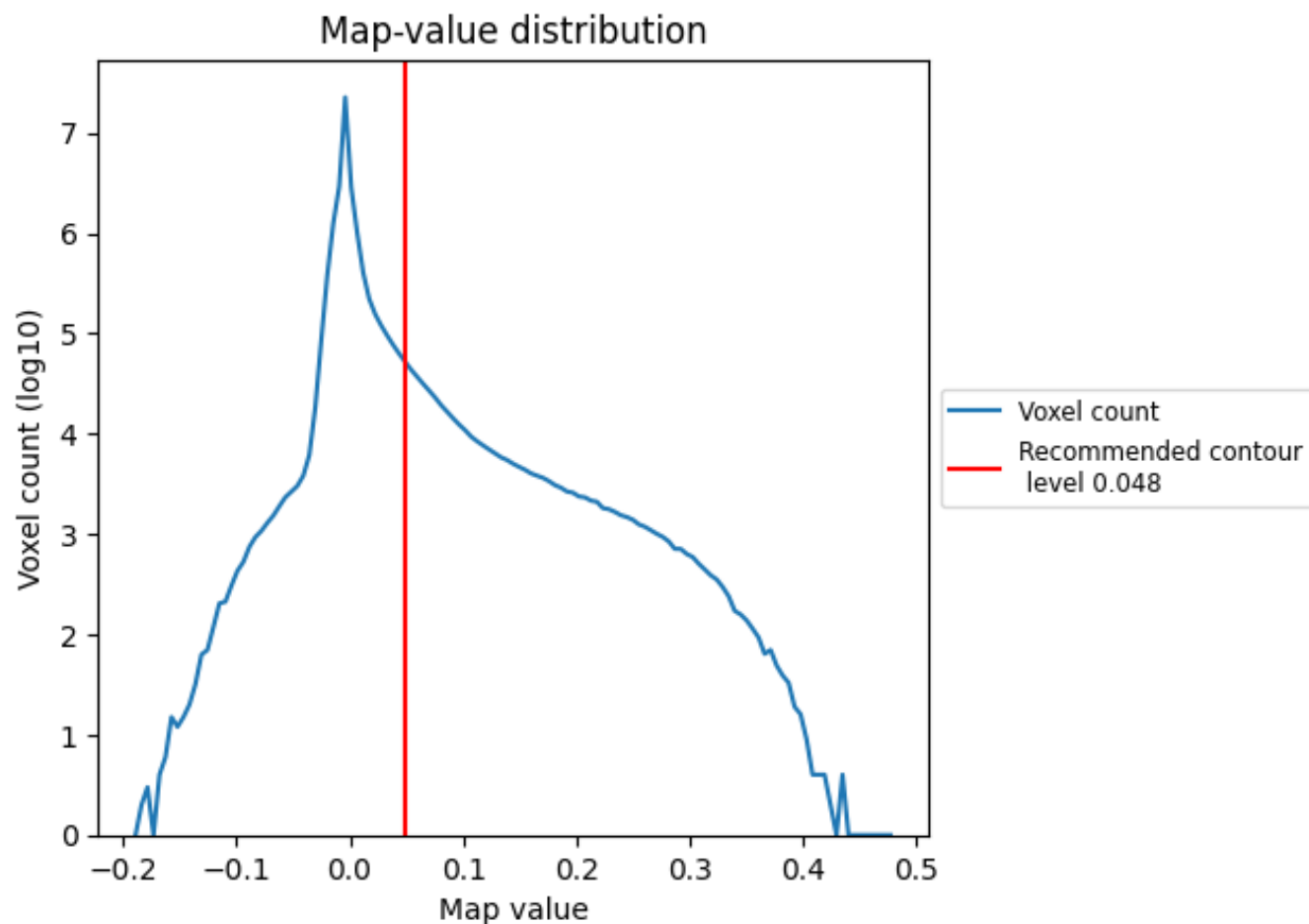
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

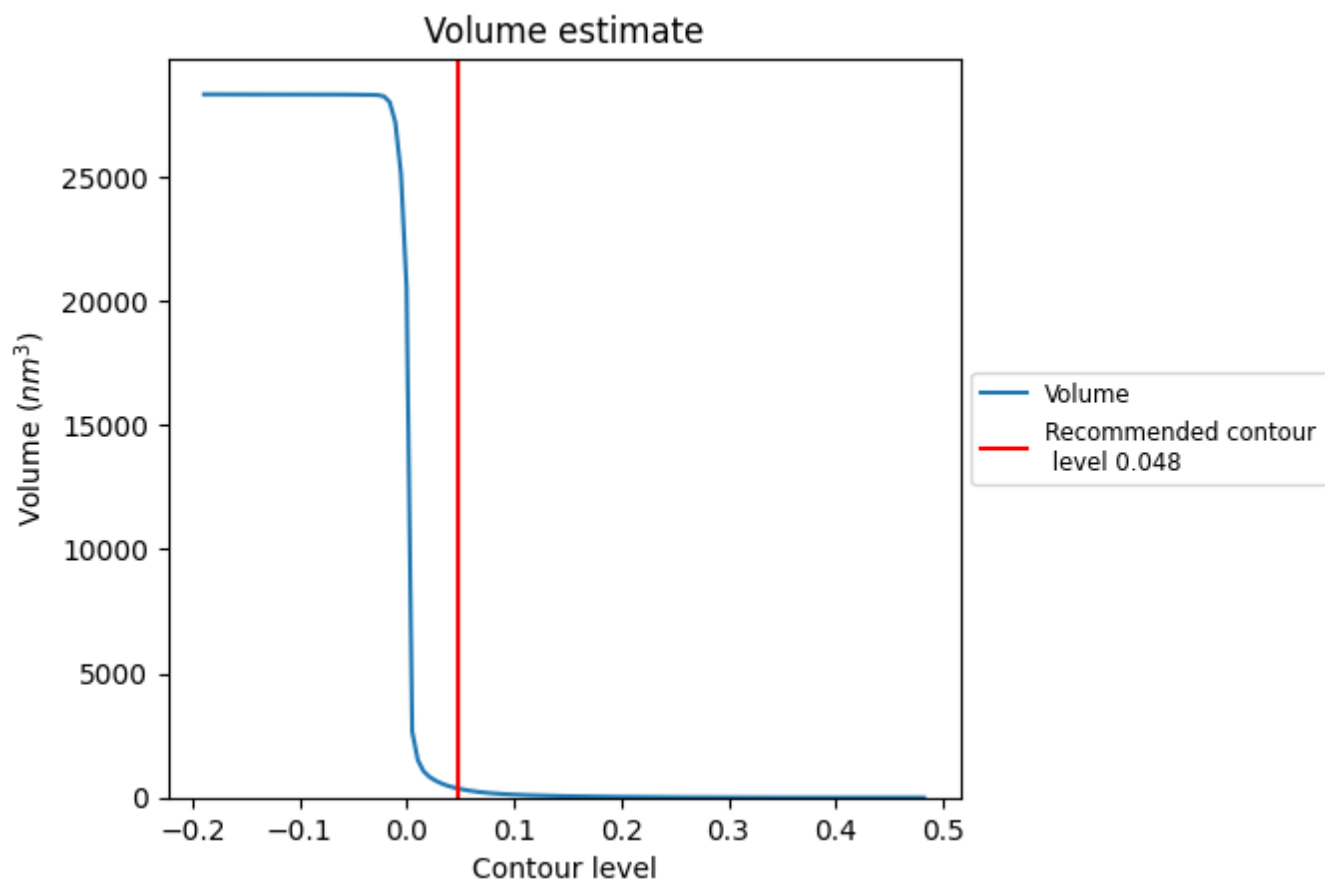
This section contains the results of statistical analysis of the map.

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.

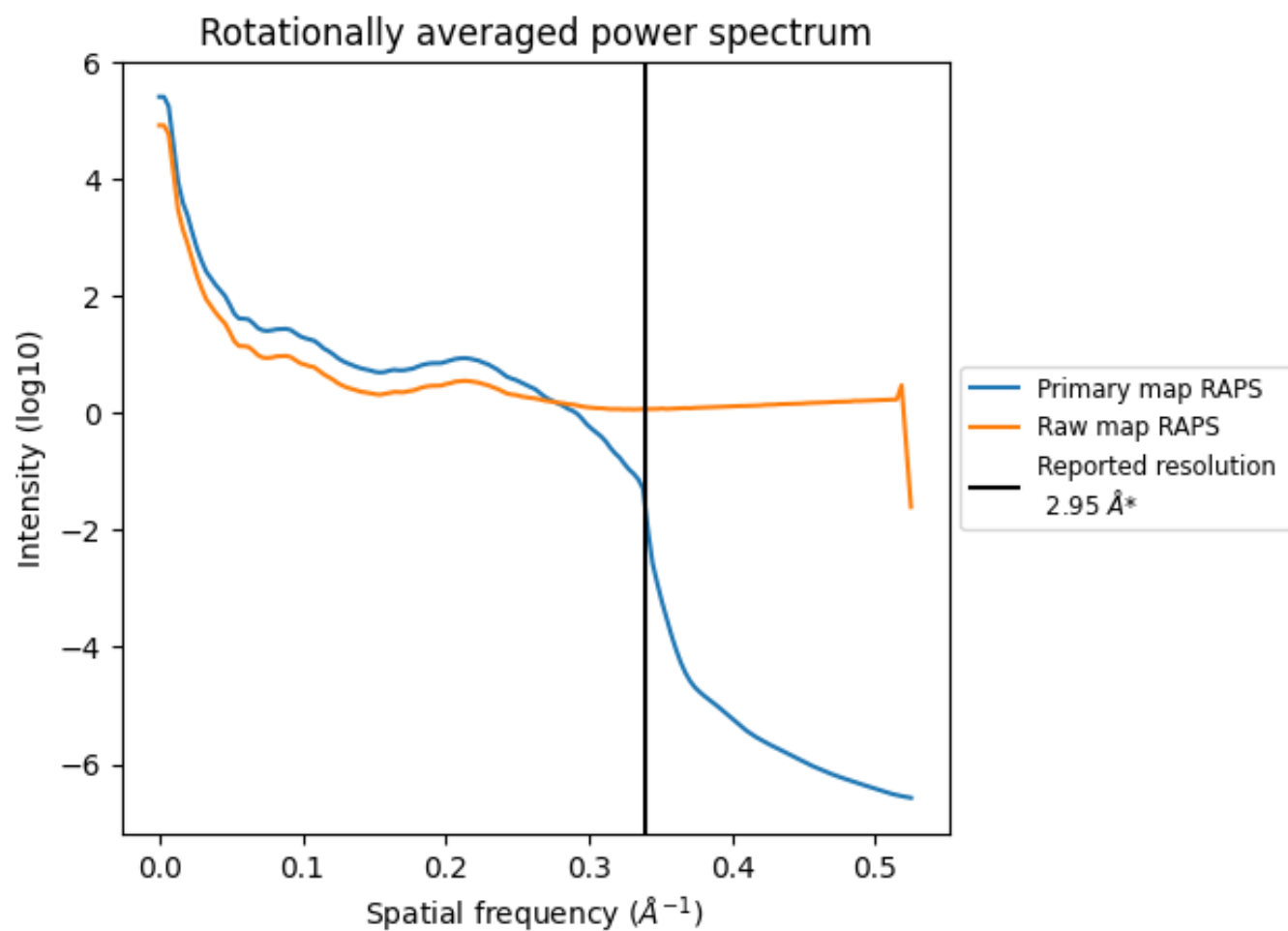
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 328 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 ⓘ

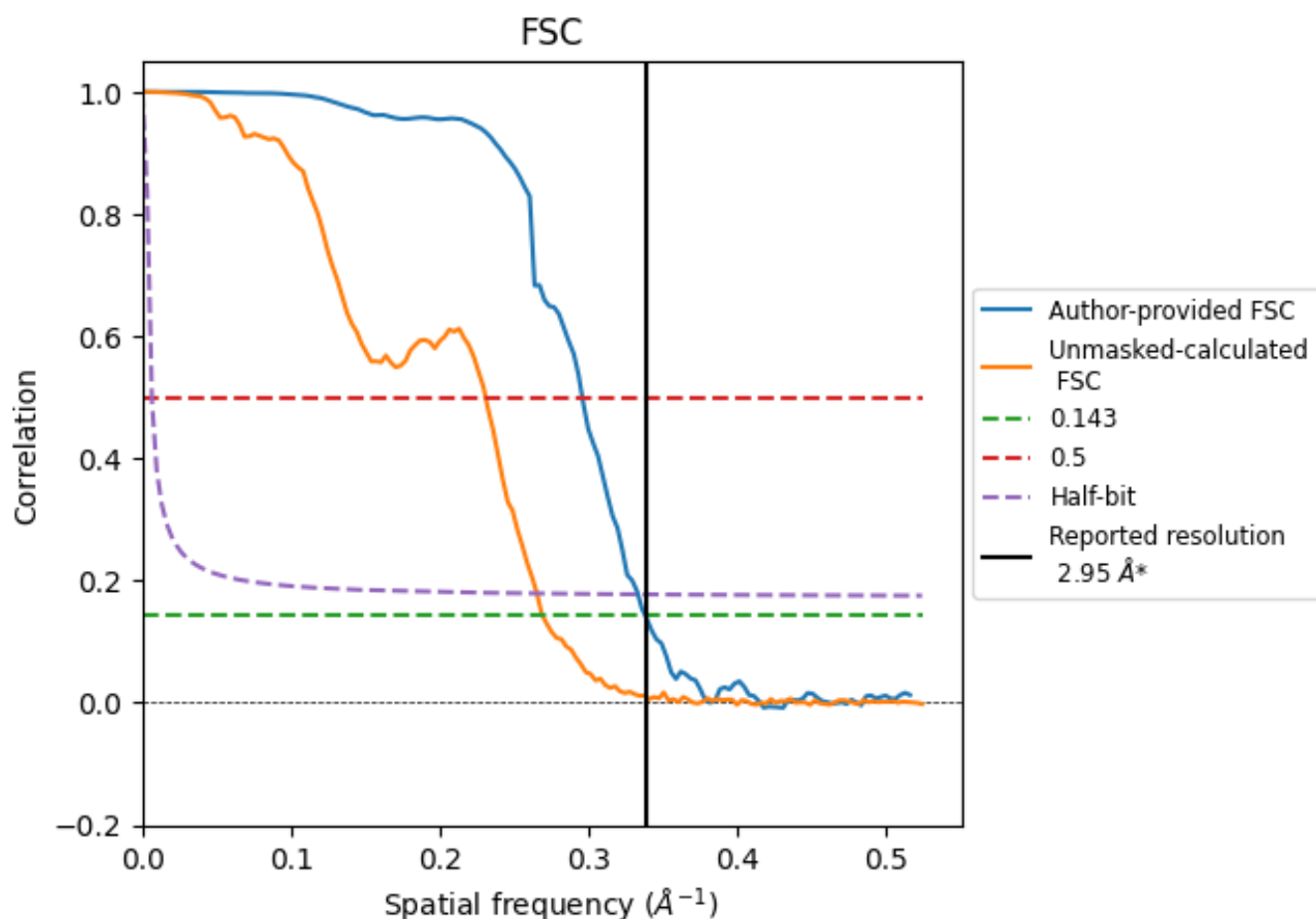


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

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 0.339 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

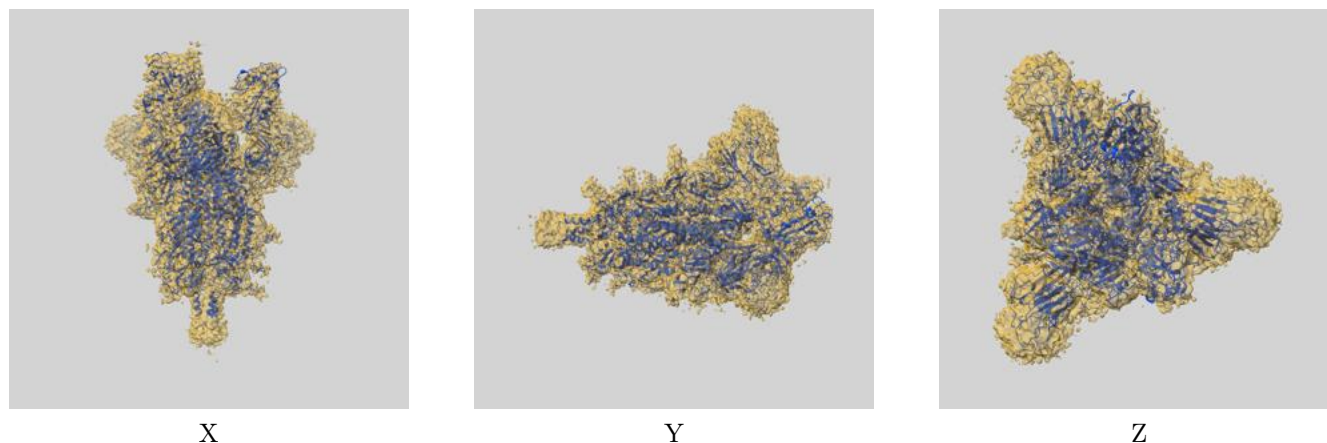
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.38	3.00
Unmasked-calculated*	3.71	4.33	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

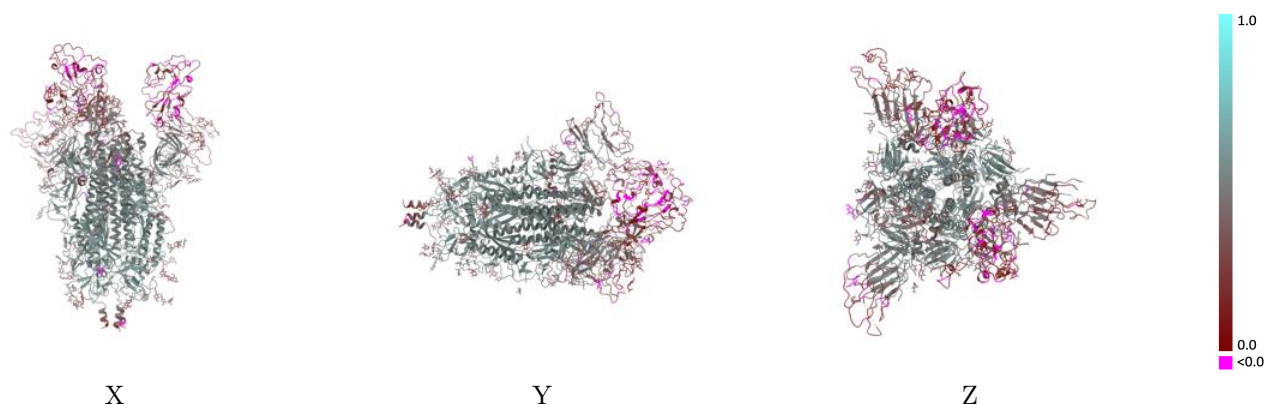
This section contains information regarding the fit between EMDB map EMD-44420 and PDB model 9BBK. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



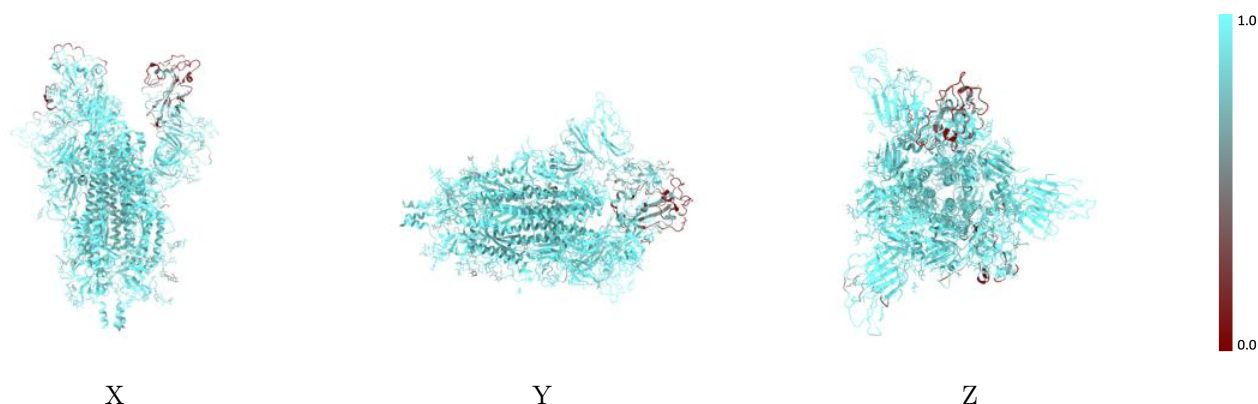
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



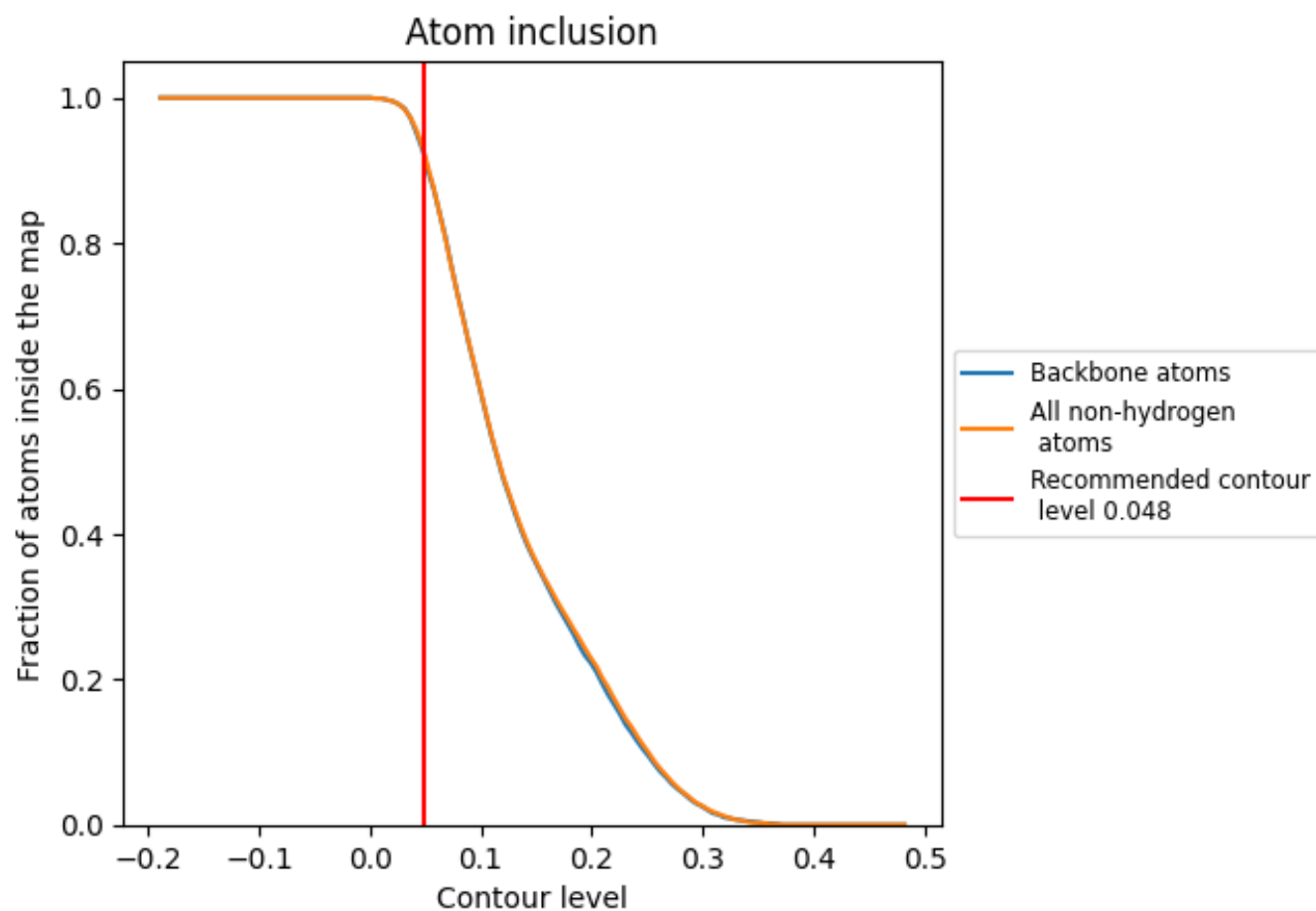
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.048).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.4230
A	 0.8890	 0.4100
B	 0.9660	 0.4490
C	 0.9390	 0.4230
D	 0.9640	 0.3040
E	 0.8210	 0.2740
F	 0.8210	 0.3360
G	 0.9490	 0.3980
H	 0.6840	 0.3560
I	 0.9740	 0.3040
J	 0.8460	 0.2670
K	 0.5900	 0.2110
L	 0.8210	 0.3680
M	 0.7860	 0.1930
N	 0.7860	 0.1870
P	 0.8400	 0.3660
Q	 0.8000	 0.2780
R	 0.7350	 0.3910
S	 0.8800	 0.2940
T	 1.0000	 0.4720
U	 0.8970	 0.2600
V	 0.9290	 0.4710
W	 0.7890	 0.1690
X	 0.8970	 0.3750
Y	 0.8210	 0.3280
Z	 0.9640	 0.4040
a	 0.7600	 0.3290
b	 0.8000	 0.3300
c	 0.8680	 0.3580
d	 0.7830	 0.3180
e	 0.8970	 0.2600
f	 0.7500	 0.1070
g	 0.8930	 0.3280

