



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:10 PM UTC

PDB ID : 5LHD / pdb_00005lhd
Title : Structure of glycosylated human aminopeptidase N
Authors : Recacha, R.; Mudgal, G.; Santiago, C.; Casasnovas, J.M.
Deposited on : 2016-07-11
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

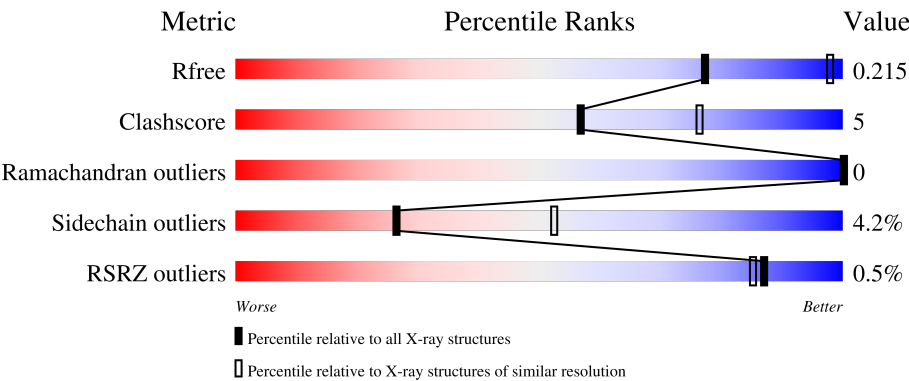
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



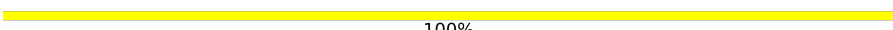
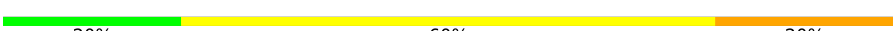
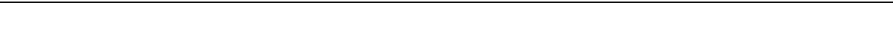
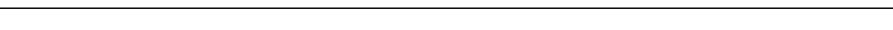
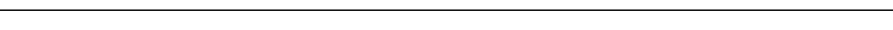
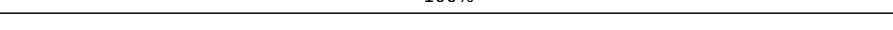
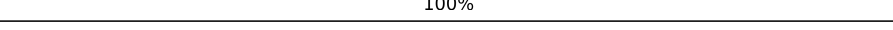
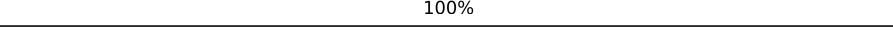
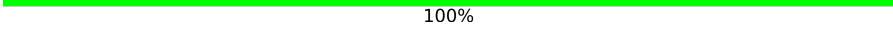
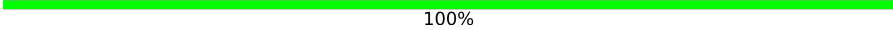
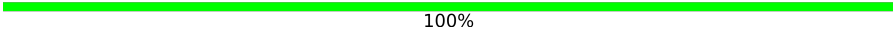
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	950	83%11%• 5%
1	B	950	% 82%12%• 5%
1	C	950	80%14%• 5%
1	D	950	83%11%• 5%
2	E	4	100%

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Mol	Chain	Length	Quality of chain
2	J	4	 50% 50%
2	K	4	 50% 25% 25%
2	R	4	 100%
3	F	5	 80% 20%
3	L	5	 20% 60% 20%
3	S	5	 100%
4	G	2	 50% 50%
4	I	2	 100%
4	M	2	 100%
4	N	2	 100%
4	P	2	 50% 50%
4	Q	2	 100%
4	V	2	 50% 50%
4	X	2	 100%
4	d	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 100%
4	g	2	 50% 50%
5	H	3	 100%
5	O	3	 67% 33%
5	U	3	 67% 33%
5	Z	3	 100%
5	b	3	 100%
5	c	3	 100%
6	T	4	 50% 50%

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Mol	Chain	Length	Quality of chain
7	W	6	
7	a	6	
8	Y	6	

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	J	1	X	-	-	-
4	NAG	Q	1	X	-	-	-
4	NAG	V	1	X	-	-	-
4	NAG	X	1	X	-	-	-
4	NAG	d	1	X	-	-	-
4	NAG	f	1	X	-	-	-
4	NAG	g	1	X	-	-	-
8	NAG	Y	1	X	-	-	-
9	NAG	A	1015	X	-	-	-
9	NAG	C	1117	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7285	4647	1226	1388	24			
1	B	904	Total	C	N	O	S	0	1	0
			7302	4656	1232	1390	24			
1	C	905	Total	C	N	O	S	0	0	0
			7300	4654	1231	1391	24			
1	D	904	Total	C	N	O	S	0	0	0
			7295	4651	1230	1390	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	TYR	-	expression tag	UNP P15144
A	19	PRO	-	expression tag	UNP P15144
A	20	TYR	-	expression tag	UNP P15144
A	21	ASP	-	expression tag	UNP P15144
A	22	VAL	-	expression tag	UNP P15144
A	23	PRO	-	expression tag	UNP P15144
A	24	ASP	-	expression tag	UNP P15144
A	25	TYR	-	expression tag	UNP P15144
A	26	ALA	-	expression tag	UNP P15144
A	27	GLY	-	expression tag	UNP P15144
A	28	ALA	-	expression tag	UNP P15144
A	29	GLN	-	expression tag	UNP P15144
A	30	PRO	-	expression tag	UNP P15144
A	31	ALA	-	expression tag	UNP P15144
A	32	ARG	-	expression tag	UNP P15144
A	33	SER	-	expression tag	UNP P15144
A	34	PRO	-	expression tag	UNP P15144
A	35	GLY	-	expression tag	UNP P15144
B	18	TYR	-	expression tag	UNP P15144
B	19	PRO	-	expression tag	UNP P15144
B	20	TYR	-	expression tag	UNP P15144

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP P15144
B	22	VAL	-	expression tag	UNP P15144
B	23	PRO	-	expression tag	UNP P15144
B	24	ASP	-	expression tag	UNP P15144
B	25	TYR	-	expression tag	UNP P15144
B	26	ALA	-	expression tag	UNP P15144
B	27	GLY	-	expression tag	UNP P15144
B	28	ALA	-	expression tag	UNP P15144
B	29	GLN	-	expression tag	UNP P15144
B	30	PRO	-	expression tag	UNP P15144
B	31	ALA	-	expression tag	UNP P15144
B	32	ARG	-	expression tag	UNP P15144
B	33	SER	-	expression tag	UNP P15144
B	34	PRO	-	expression tag	UNP P15144
B	35	GLY	-	expression tag	UNP P15144
C	18	TYR	-	expression tag	UNP P15144
C	19	PRO	-	expression tag	UNP P15144
C	20	TYR	-	expression tag	UNP P15144
C	21	ASP	-	expression tag	UNP P15144
C	22	VAL	-	expression tag	UNP P15144
C	23	PRO	-	expression tag	UNP P15144
C	24	ASP	-	expression tag	UNP P15144
C	25	TYR	-	expression tag	UNP P15144
C	26	ALA	-	expression tag	UNP P15144
C	27	GLY	-	expression tag	UNP P15144
C	28	ALA	-	expression tag	UNP P15144
C	29	GLN	-	expression tag	UNP P15144
C	30	PRO	-	expression tag	UNP P15144
C	31	ALA	-	expression tag	UNP P15144
C	32	ARG	-	expression tag	UNP P15144
C	33	SER	-	expression tag	UNP P15144
C	34	PRO	-	expression tag	UNP P15144
C	35	GLY	-	expression tag	UNP P15144
D	18	TYR	-	expression tag	UNP P15144
D	19	PRO	-	expression tag	UNP P15144
D	20	TYR	-	expression tag	UNP P15144
D	21	ASP	-	expression tag	UNP P15144
D	22	VAL	-	expression tag	UNP P15144
D	23	PRO	-	expression tag	UNP P15144
D	24	ASP	-	expression tag	UNP P15144
D	25	TYR	-	expression tag	UNP P15144
D	26	ALA	-	expression tag	UNP P15144

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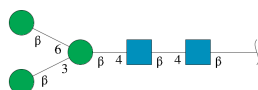
Chain	Residue	Modelled	Actual	Comment	Reference
D	27	GLY	-	expression tag	UNP P15144
D	28	ALA	-	expression tag	UNP P15144
D	29	GLN	-	expression tag	UNP P15144
D	30	PRO	-	expression tag	UNP P15144
D	31	ALA	-	expression tag	UNP P15144
D	32	ARG	-	expression tag	UNP P15144
D	33	SER	-	expression tag	UNP P15144
D	34	PRO	-	expression tag	UNP P15144
D	35	GLY	-	expression tag	UNP P15144

- Molecule 2 is an oligosaccharide called beta-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				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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.



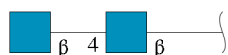
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

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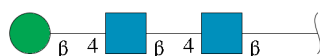
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



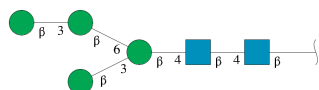
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called beta-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.



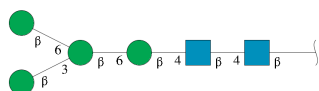
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-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.



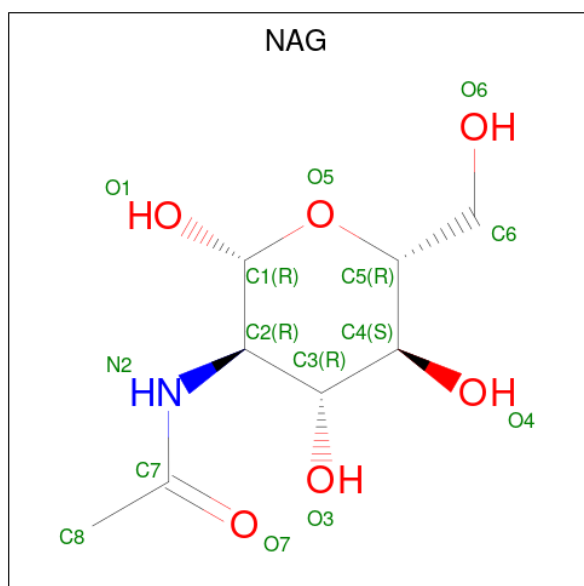
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	W	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	a	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-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				ZeroOcc	AltConf	Trace
8	Y	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

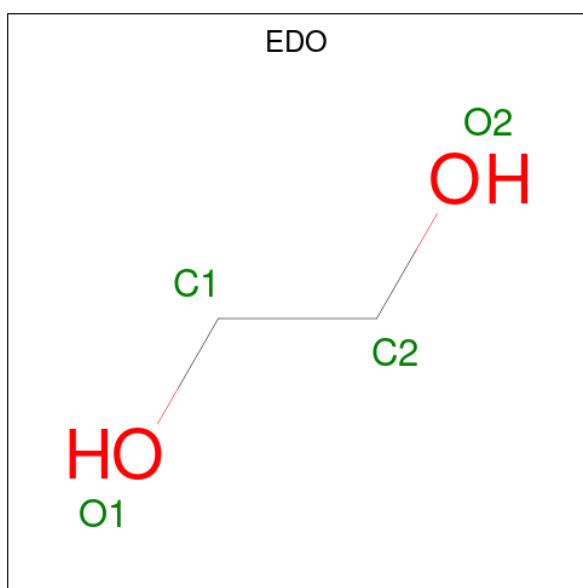


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Zn 1 1	0	0
10	B	1	Total Zn 1 1	0	0
10	C	1	Total Zn 1 1	0	0
10	D	1	Total Zn 1 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	A	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0
11	B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	157	Total O 157 157	0	0
12	B	186	Total O 186 186	0	0

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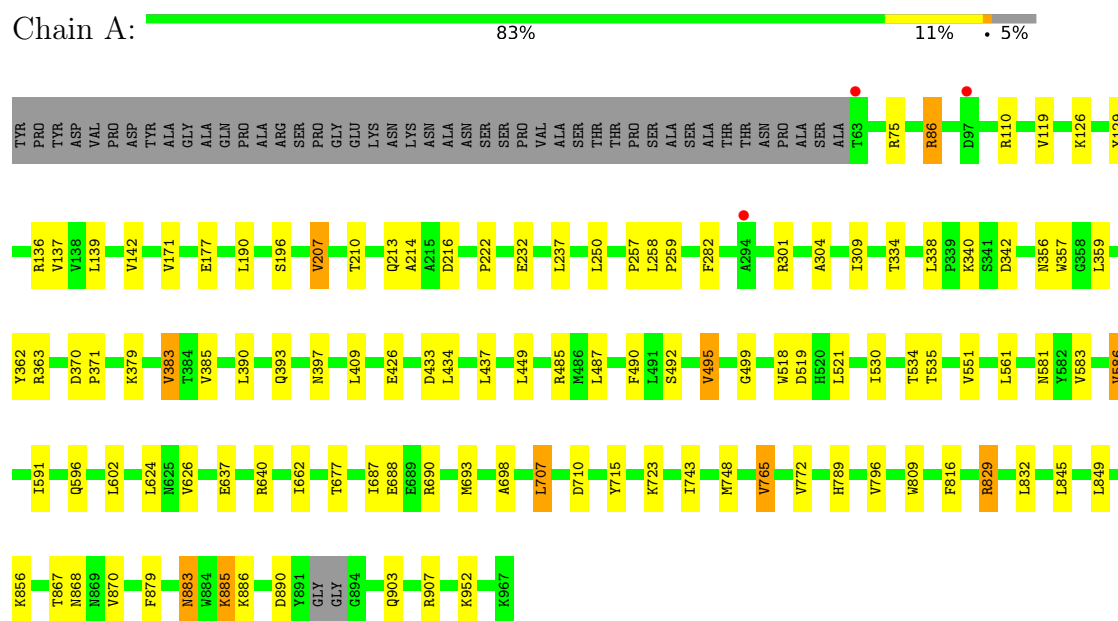
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	154	Total 154	O 154	0	0
12	D	168	Total 168	O 168	0	0

3 Residue-property plots [i](#)

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

• Molecule 1: Aminopeptidase N



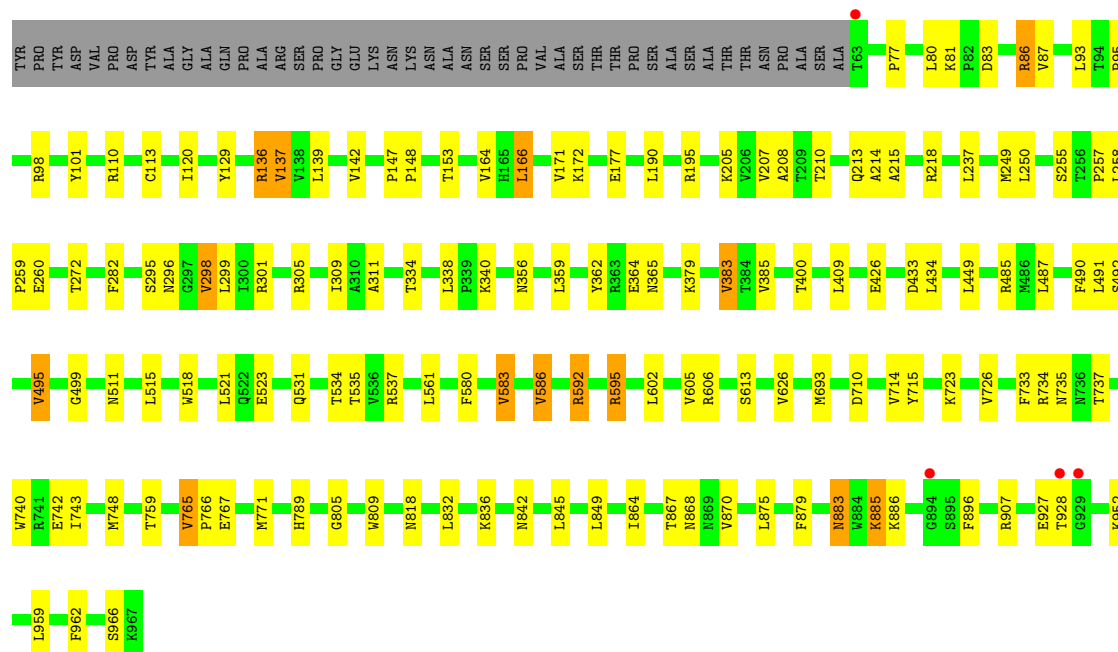
• Molecule 1: Aminopeptidase N





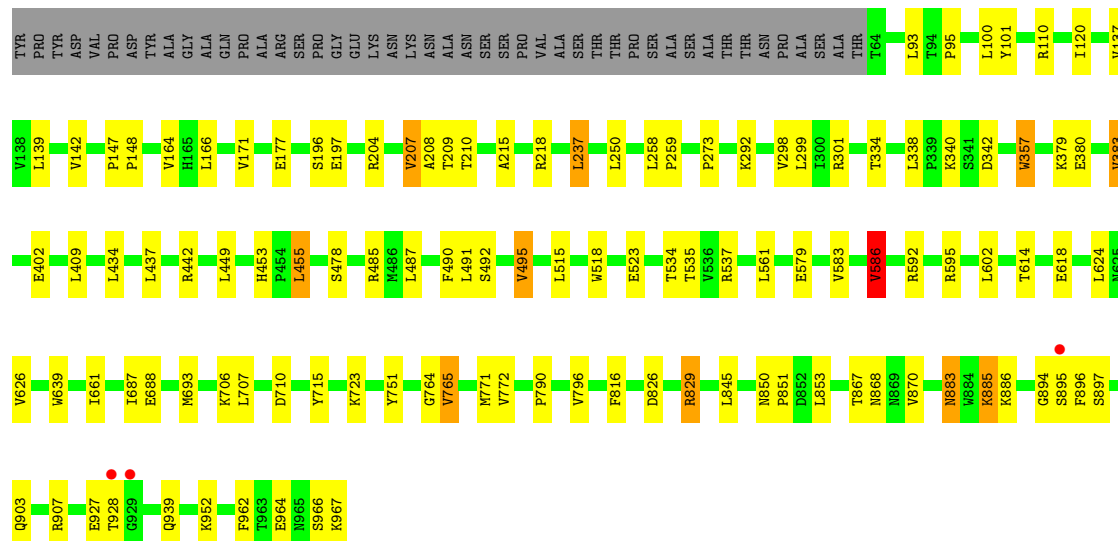
• Molecule 1: Aminopeptidase N

Chain C: 80% 14% 5%



• Molecule 1: Aminopeptidase N

Chain D: 83% 11% 5%



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

Chain E:  100%

NAG1
NAG2
BMA3
BMA4

- Molecule 2: beta-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 J:  50% 50%

NAG1
NAG2
BMA3
BMA4

- Molecule 2: beta-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 K:  50% 25% 25%

NAG1
NAG2
BMA3
BMA4

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

Chain R:  100%

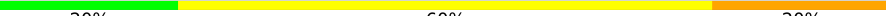
NAG1
NAG2
BMA3
BMA4

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

Chain F:  80% 20%

NAG1
NAG2
BMA3
BMA4
BMA5

- Molecule 3: beta-D-mannopyranose-(1-3)-[beta-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 L:  20% 60% 20%

NAG1
NAG2
BMA3
BMA4
BMA5

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

Chain S:  100%



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

Chain G:



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

Chain I:



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

Chain M:



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

Chain N:



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

Chain P:



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

Chain Q:



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

Chain V:  50% 50%



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

Chain X:  100%



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

Chain d:  50% 50%

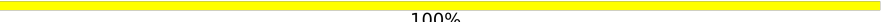


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%



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

Chain f:  100%



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

Chain g:  50% 50%



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

Chain H:  100%



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

Chain O: 67% 33%



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

Chain U: 67% 33%



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

Chain Z: 100%



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

Chain b: 100%



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

Chain c: 100%



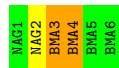
- Molecule 6: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 50% 50%



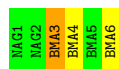
- Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 17% 33%



- Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-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:  50% 33% 17%



- Molecule 8: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-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 Y:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.09Å 168.86Å 244.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.97-2.60) 99.5 (19.97-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.60Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.181 , 0.214 0.182 , 0.215	Depositor DCC
R_{free} test set	8073 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtrriage
Anisotropy	0.392	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31338	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0639e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/7472	0.68	0/10179
1	B	0.30	0/7494	0.70	1/10208 (0.0%)
1	C	0.29	0/7488	0.68	1/10200 (0.0%)
1	D	0.29	0/7483	0.69	4/10193 (0.0%)
All	All	0.29	0/29937	0.69	6/40780 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	491	LEU	N-CA-C	-5.30	101.89	110.32
1	D	586	VAL	N-CA-C	5.13	113.71	107.61
1	D	764	GLY	CA-C-N	-5.09	118.93	122.59
1	D	764	GLY	C-N-CA	-5.09	118.93	122.59
1	C	491	LEU	N-CA-C	-5.01	103.32	110.59
1	B	898	PHE	N-CA-C	-5.00	106.69	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7285	0	7037	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7302	0	7062	79	0
1	C	7300	0	7056	81	0
1	D	7295	0	7054	56	0
2	E	50	0	43	0	0
2	J	50	0	43	0	0
2	K	50	0	43	1	0
2	R	50	0	43	2	0
3	F	61	0	52	0	0
3	L	61	0	52	1	0
3	S	61	0	52	0	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
4	X	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
5	H	39	0	34	0	0
5	O	39	0	34	0	0
5	U	39	0	34	0	0
5	Z	39	0	34	0	0
5	b	39	0	34	0	0
5	c	39	0	34	0	0
6	T	50	0	43	1	0
7	W	72	0	61	2	0
7	a	72	0	61	2	0
8	Y	72	0	61	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
9	C	14	0	13	0	0
9	D	28	0	26	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	68	0	102	6	0
11	B	48	0	72	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	48	0	72	3	0
11	D	20	0	30	0	0
12	A	157	0	0	8	1
12	B	186	0	0	17	0
12	C	154	0	0	11	1
12	D	168	0	0	6	0
All	All	31338	0	29621	277	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (277) 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:232:GLU:OE1	12:A:1101:HOH:O	1.81	0.96
1:C:77:PRO:O	12:C:1201:HOH:O	1.87	0.93
1:A:710:ASP:OD1	12:A:1102:HOH:O	1.95	0.84
1:A:530:ILE:O	12:A:1103:HOH:O	1.97	0.81
1:B:213:GLN:NE2	12:B:1105:HOH:O	2.13	0.81
1:C:426:GLU:O	12:C:1202:HOH:O	1.97	0.80
1:B:73:ARG:NH1	12:B:1106:HOH:O	2.15	0.80
1:A:222:PRO:HG2	11:A:1040:EDO:H11	1.62	0.79
1:B:737:THR:HG23	1:B:740:TRP:H	1.48	0.78
1:A:126:LYS:H	11:A:1032:EDO:H22	1.47	0.77
1:C:737:THR:HG23	1:C:740:TRP:H	1.49	0.77
1:A:581:ASN:ND2	1:B:65:LEU:O	2.18	0.76
1:A:119:VAL:HG13	11:A:1029:EDO:H12	1.69	0.75
1:C:137:VAL:O	12:C:1203:HOH:O	2.04	0.75
1:B:198:TYR:OH	12:B:1101:HOH:O	2.03	0.75
1:A:492:SER:HB3	1:A:495:VAL:HG13	1.70	0.73
1:B:77:PRO:O	12:B:1102:HOH:O	2.07	0.72
1:B:724:LYS:O	12:B:1103:HOH:O	2.08	0.71
1:C:723:LYS:HG3	1:C:765:VAL:HG12	1.73	0.70
1:B:723:LYS:HG3	1:B:765:VAL:HG12	1.75	0.68
1:D:790:PRO:O	12:D:1101:HOH:O	2.11	0.68
1:C:485:ARG:NH2	1:C:626:VAL:O	2.26	0.68
1:A:426:GLU:O	12:A:1104:HOH:O	2.12	0.67
1:C:492:SER:HB2	1:C:495:VAL:HG13	1.77	0.67
1:B:110:ARG:NH1	1:B:177:GLU:OE2	2.27	0.66
1:C:805:GLY:HA2	11:C:1146:EDO:H11	1.78	0.66
1:B:216:ASP:OD2	12:B:1104:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:A:177:GLU:OE2	2.28	0.66
1:C:531:GLN:NE2	12:C:1214:HOH:O	2.30	0.65
1:A:119:VAL:O	11:A:1029:EDO:O2	2.13	0.65
1:C:110:ARG:NH1	1:C:177:GLU:OE2	2.31	0.64
1:B:737:THR:OG1	1:B:742:GLU:O	2.15	0.64
1:B:185:GLU:OE2	12:B:1107:HOH:O	2.15	0.64
1:D:292:LYS:NZ	12:D:1104:HOH:O	2.29	0.64
1:D:485:ARG:NH2	1:D:626:VAL:O	2.31	0.64
1:A:883:ASN:OD1	1:A:883:ASN:N	2.30	0.64
1:B:433:ASP:HB3	1:B:693:MET:HE1	1.79	0.64
1:B:81:LYS:NZ	12:B:1114:HOH:O	2.27	0.63
1:A:723:LYS:HG3	1:A:765:VAL:HG12	1.80	0.63
1:A:363:ARG:NH1	12:A:1108:HOH:O	2.22	0.62
1:B:434:LEU:HD11	1:B:748:MET:HE1	1.80	0.62
1:B:98:ARG:NH1	12:B:1118:HOH:O	2.32	0.62
1:B:348:ASP:OD1	1:B:857:GLN:NE2	2.33	0.62
1:B:136:ARG:NH2	1:C:295:SER:O	2.34	0.61
1:C:733:PHE:O	1:C:737:THR:HG22	2.00	0.61
7:W:2:NAG:O3	7:W:4:BMA:O2	2.18	0.61
1:A:499:GLY:HA3	1:A:521:LEU:HD23	1.83	0.60
1:C:734:ARG:NH1	1:C:767:GLU:OE1	2.35	0.60
1:B:883:ASN:OD1	1:B:883:ASN:N	2.35	0.60
1:D:723:LYS:HG3	1:D:765:VAL:HG12	1.85	0.59
1:B:499:GLY:HA3	1:B:521:LEU:HD23	1.85	0.59
1:A:868:ASN:OD1	1:A:907:ARG:NH2	2.36	0.58
1:A:586:VAL:HG13	1:A:602:LEU:HB3	1.85	0.58
1:B:895:SER:HA	1:B:896:PHE:C	2.28	0.58
1:C:305:ARG:NH1	1:C:364:GLU:OE1	2.29	0.58
1:B:586:VAL:HG13	1:B:602:LEU:HB3	1.86	0.58
1:C:885:LYS:HD2	1:C:886:LYS:H	1.69	0.58
1:B:172:LYS:H	11:B:1034:EDO:H12	1.67	0.58
1:C:95:PRO:HG3	1:C:101:TYR:CZ	2.38	0.58
11:B:1027:EDO:H22	1:C:296:ASN:HB2	1.86	0.57
1:B:569:ASP:HB3	1:B:572:SER:HB3	1.86	0.57
1:D:196:SER:HB3	1:D:207:VAL:HG13	1.86	0.57
1:C:586:VAL:HG13	1:C:602:LEU:HB3	1.86	0.57
1:B:250:LEU:HG	1:B:340:LYS:HG2	1.87	0.57
1:A:257:PRO:HG3	4:G:1:NAG:H62	1.87	0.56
1:C:311:ALA:O	12:C:1204:HOH:O	2.17	0.56
1:A:485:ARG:NH2	1:A:626:VAL:O	2.38	0.56
1:D:868:ASN:OD1	1:D:907:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:LYS:HD2	1:D:886:LYS:H	1.71	0.56
1:B:205:LYS:NZ	12:B:1125:HOH:O	2.38	0.55
1:C:737:THR:OG1	1:C:742:GLU:O	2.23	0.55
1:B:896:PHE:N	1:B:897:SER:HB3	2.21	0.55
1:A:196:SER:HB3	1:A:207:VAL:HG13	1.89	0.55
1:A:433:ASP:HB3	1:A:693:MET:HE1	1.89	0.55
1:B:75:ARG:NH2	12:B:1127:HOH:O	2.41	0.54
1:B:525:VAL:HG13	1:B:530:ILE:HB	1.89	0.54
1:D:120:ILE:HG13	1:D:166:LEU:HD21	1.89	0.54
1:D:883:ASN:OD1	1:D:883:ASN:N	2.40	0.54
1:B:363:ARG:NH2	12:B:1123:HOH:O	2.35	0.54
1:D:437:LEU:HD11	1:D:693:MET:HG3	1.89	0.54
1:D:586:VAL:HG13	1:D:602:LEU:HB3	1.89	0.54
1:A:885:LYS:HD2	1:A:886:LYS:N	2.23	0.54
1:B:849:LEU:HD11	1:B:879:PHE:HZ	1.73	0.54
1:C:98:ARG:HH12	2:R:4:BMA:H62	1.72	0.54
1:C:365:ASN:O	12:C:1206:HOH:O	2.18	0.54
1:C:818:ASN:OD1	12:C:1205:HOH:O	2.18	0.54
1:C:250:LEU:HG	1:C:340:LYS:HG2	1.90	0.54
1:D:442:ARG:NH1	1:D:478:SER:OG	2.42	0.53
1:D:110:ARG:NH1	1:D:177:GLU:OE2	2.41	0.53
1:B:171:VAL:HA	11:B:1034:EDO:H12	1.91	0.53
1:B:305:ARG:NE	1:B:364:GLU:OE1	2.37	0.53
1:B:485:ARG:NH2	1:B:626:VAL:O	2.41	0.53
1:C:195:ARG:NH1	12:C:1228:HOH:O	2.42	0.53
1:C:120:ILE:HG13	1:C:166:LEU:HD21	1.92	0.52
1:D:93:LEU:HD21	1:D:208:ALA:HB2	1.92	0.52
1:D:258:LEU:HD12	1:D:259:PRO:HD2	1.91	0.52
1:A:86:ARG:NH1	12:A:1123:HOH:O	2.42	0.52
1:A:885:LYS:HD2	1:A:886:LYS:H	1.75	0.52
1:C:129:TYR:HB2	1:C:136:ARG:HG3	1.92	0.52
1:B:816:PHE:CE1	1:B:829:ARG:HG3	2.45	0.52
1:D:197:GLU:OE1	1:D:204:ARG:NH2	2.34	0.52
1:B:492:SER:HB2	1:B:495:VAL:HG13	1.92	0.51
1:C:842:ASN:HA	1:C:875:LEU:HD21	1.91	0.51
1:C:515:LEU:HD13	1:C:537:ARG:HH21	1.75	0.51
1:A:662:ILE:HD13	1:A:698:ALA:HB2	1.92	0.51
1:C:883:ASN:OD1	1:C:883:ASN:N	2.43	0.51
1:A:903:GLN:O	1:A:907:ARG:HG3	2.12	0.50
1:B:838:LEU:HD21	1:B:875:LEU:HD21	1.93	0.50
1:B:437:LEU:HD11	1:B:693:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:LYS:HD2	1:B:886:LYS:N	2.26	0.50
1:B:432:LYS:NZ	12:B:1111:HOH:O	2.23	0.50
1:C:499:GLY:HA3	1:C:521:LEU:HD23	1.93	0.50
1:A:849:LEU:HD11	1:A:879:PHE:HZ	1.77	0.49
1:C:172:LYS:HB3	7:a:6:BMA:H62	1.94	0.49
1:B:378:ASN:HD22	1:B:381:ARG:HH12	1.61	0.49
1:C:592:ARG:NH1	1:C:613:SER:O	2.45	0.49
1:D:455:LEU:HB2	12:D:1124:HOH:O	2.12	0.49
1:C:93:LEU:HD21	1:C:208:ALA:HB2	1.94	0.49
1:B:97:ASP:OD2	1:C:255:SER:N	2.33	0.49
1:B:710:ASP:HA	1:B:715:TYR:CG	2.48	0.49
1:D:579:GLU:HG3	12:D:1127:HOH:O	2.13	0.48
1:B:390:LEU:HA	1:B:393:GLN:HG2	1.95	0.48
1:B:733:PHE:O	1:B:737:THR:HG22	2.12	0.48
1:D:534:THR:OG1	1:D:535:THR:N	2.46	0.48
1:D:772:VAL:HG12	1:D:796:VAL:HG22	1.95	0.48
1:A:75:ARG:NH2	11:A:1028:EDO:H22	2.29	0.48
1:D:639:TRP:HZ3	1:D:661:ILE:HG23	1.76	0.48
1:D:816:PHE:CE1	1:D:829:ARG:HG3	2.49	0.48
1:C:258:LEU:HD12	1:C:259:PRO:HD2	1.96	0.48
1:C:299:LEU:HD21	1:C:301:ARG:HD3	1.95	0.48
1:C:534:THR:OG1	1:C:535:THR:N	2.46	0.48
1:C:433:ASP:HB3	1:C:693:MET:HE1	1.94	0.48
1:B:868:ASN:OD1	1:B:907:ARG:NH2	2.47	0.48
1:A:519:ASP:OD2	12:A:1106:HOH:O	2.20	0.48
1:D:927:GLU:HG2	1:D:928:THR:HG23	1.96	0.47
1:C:81:LYS:HG2	12:C:1280:HOH:O	2.14	0.47
1:C:693:MET:HE3	1:C:693:MET:HB2	1.77	0.47
1:D:895:SER:HA	1:D:896:PHE:C	2.39	0.47
1:A:772:VAL:HG12	1:A:796:VAL:HG22	1.97	0.47
1:C:362:TYR:HE2	1:C:385:VAL:HG12	1.79	0.47
1:C:868:ASN:OD1	1:C:907:ARG:NH2	2.47	0.47
1:A:258:LEU:HD12	1:A:259:PRO:HD2	1.96	0.47
1:B:356:ASN:HB2	1:B:359:LEU:O	2.14	0.47
1:C:592:ARG:O	1:C:595:ARG:HG3	2.15	0.47
1:C:849:LEU:HD11	1:C:879:PHE:HZ	1.79	0.47
1:A:213:GLN:HA	1:A:214:ALA:HA	1.56	0.47
1:B:120:ILE:HB	1:B:164:VAL:HB	1.95	0.47
1:A:304:ALA:HB3	1:A:309:ILE:HG13	1.97	0.47
1:D:453:HIS:O	12:D:1102:HOH:O	2.20	0.47
1:D:710:ASP:HA	1:D:715:TYR:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ALA:HB1	1:D:218:ARG:CZ	2.45	0.46
1:D:380:GLU:OE1	1:D:751:TYR:OH	2.26	0.46
1:C:83:ASP:OD1	12:C:1207:HOH:O	2.21	0.46
1:A:687:ILE:HG23	1:A:688:GLU:HG3	1.98	0.46
1:A:816:PHE:CE1	1:A:829:ARG:HG3	2.51	0.46
1:C:885:LYS:HD2	1:C:886:LYS:N	2.30	0.46
1:A:250:LEU:HG	1:A:340:LYS:HG2	1.98	0.46
1:C:379:LYS:O	1:C:383:VAL:HG23	2.15	0.46
1:B:664:ASP:OD2	11:B:1031:EDO:O1	2.34	0.46
1:C:487:LEU:HA	1:C:490:PHE:CE2	2.51	0.46
1:B:153:THR:HG23	11:B:1027:EDO:H12	1.98	0.46
1:B:395:PHE:CZ	11:B:1025:EDO:H21	2.51	0.46
1:D:896:PHE:N	1:D:897:SER:HB3	2.31	0.46
1:B:883:ASN:HA	1:B:885:LYS:HE3	1.97	0.46
1:A:710:ASP:HA	1:A:715:TYR:CG	2.51	0.46
1:B:232:GLU:OE2	12:B:1108:HOH:O	2.21	0.45
1:D:120:ILE:HB	1:D:164:VAL:HB	1.98	0.45
1:D:250:LEU:HG	1:D:340:LYS:HG2	1.97	0.45
1:A:743:ILE:HD13	1:A:789:HIS:CE1	2.52	0.45
1:C:580:PHE:O	1:C:583:VAL:HG13	2.17	0.45
7:W:3:BMA:H61	7:W:4:BMA:H2	1.61	0.45
1:C:726:VAL:HG21	1:C:759:THR:HB	1.99	0.45
1:D:402:GLU:HG2	3:L:5:BMA:H62	1.99	0.45
1:A:362:TYR:HE2	1:A:385:VAL:HG12	1.82	0.45
1:B:555:ASP:HB3	1:B:560:THR:HG22	1.99	0.45
1:C:864:ILE:HA	1:C:867:THR:HG22	1.99	0.45
1:C:356:ASN:HB2	1:C:359:LEU:O	2.17	0.44
1:D:273:PRO:HG2	1:D:357:TRP:CZ3	2.53	0.44
1:D:962:PHE:O	1:D:966:SER:OG	2.25	0.44
1:D:894:GLY:HA2	1:D:896:PHE:O	2.17	0.44
1:C:710:ASP:HA	1:C:715:TYR:CG	2.52	0.44
1:B:213:GLN:HA	1:B:214:ALA:HA	1.59	0.44
1:C:743:ILE:HD13	1:C:789:HIS:CE1	2.53	0.44
1:D:95:PRO:HG3	1:D:101:TYR:CZ	2.52	0.44
1:B:99:GLY:O	12:B:1110:HOH:O	2.21	0.44
1:B:232:GLU:OE1	12:B:1109:HOH:O	2.21	0.44
1:B:693:MET:HE3	1:B:693:MET:HB2	1.88	0.44
2:R:3:BMA:H61	2:R:4:BMA:H2	1.75	0.43
1:B:363:ARG:NE	12:B:1123:HOH:O	2.49	0.43
1:B:580:PHE:O	1:B:583:VAL:HG13	2.18	0.43
1:C:765:VAL:HA	1:C:766:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:LYS:HE2	1:C:886:LYS:HB3	1.84	0.43
1:A:591:ILE:HG22	1:A:596:GLN:HA	2.01	0.43
1:C:213:GLN:HA	1:C:214:ALA:HA	1.60	0.43
1:C:305:ARG:HD3	1:C:364:GLU:OE1	2.17	0.43
1:D:209:THR:OG1	1:D:210:THR:N	2.51	0.43
1:D:964:GLU:HA	1:D:967:LYS:HE3	2.00	0.43
1:A:129:TYR:CB	1:A:136:ARG:HG3	2.49	0.43
1:A:216:ASP:OD2	12:A:1107:HOH:O	2.21	0.43
1:C:296:ASN:OD1	1:C:298:VAL:HG12	2.18	0.43
1:B:885:LYS:HD2	1:B:886:LYS:H	1.83	0.43
1:B:637:GLU:OE1	1:B:640:ARG:NH1	2.51	0.43
1:A:809:TRP:CE2	1:A:832:LEU:HD22	2.53	0.43
1:B:174:SER:OG	1:D:523:GLU:OE2	2.26	0.43
1:A:390:LEU:HA	1:A:393:GLN:HG2	1.99	0.43
1:A:437:LEU:HD11	1:A:693:MET:HG3	2.01	0.43
1:B:258:LEU:HD12	1:B:259:PRO:HD2	2.01	0.43
1:C:400:THR:O	1:C:511:ASN:HA	2.19	0.42
1:C:962:PHE:O	1:C:966:SER:OG	2.17	0.42
1:D:903:GLN:O	1:D:907:ARG:HG3	2.18	0.42
1:C:927:GLU:HG2	1:C:928:THR:HG23	2.01	0.42
1:B:743:ILE:HD13	1:B:789:HIS:NE2	2.35	0.42
1:C:836:LYS:HE2	1:C:836:LYS:HB3	1.90	0.42
1:A:356:ASN:HB2	1:A:359:LEU:O	2.20	0.42
1:C:249:MET:HG2	1:C:272:THR:HG22	2.01	0.42
1:D:147:PRO:HA	1:D:148:PRO:HD3	1.94	0.42
1:D:237:LEU:HD12	1:D:237:LEU:HA	1.90	0.42
1:D:614:THR:HB	1:D:618:GLU:HG3	2.00	0.42
1:D:487:LEU:HA	1:D:490:PHE:CE2	2.55	0.42
1:A:379:LYS:O	1:A:383:VAL:HG23	2.20	0.42
1:C:434:LEU:HD11	1:C:748:MET:HE1	2.02	0.42
1:C:215:ALA:HB1	1:C:218:ARG:CZ	2.49	0.42
1:A:301:ARG:HB2	1:A:342:ASP:OD1	2.19	0.42
1:B:228:ALA:HB3	11:B:1028:EDO:H21	2.01	0.42
1:B:737:THR:HG21	1:B:740:TRP:CE3	2.55	0.42
1:D:895:SER:HA	1:D:896:PHE:O	2.19	0.42
1:A:210:THR:HG21	1:A:282:PHE:CD1	2.55	0.42
1:A:357:TRP:CD1	1:A:397:ASN:HD22	2.38	0.42
1:D:434:LEU:HD23	1:D:693:MET:HE2	2.02	0.42
1:A:707:LEU:HD12	1:A:707:LEU:HA	1.86	0.41
1:D:885:LYS:HD2	1:D:886:LYS:N	2.33	0.41
1:A:75:ARG:HH21	11:A:1028:EDO:H22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HB	1:C:164:VAL:HB	2.01	0.41
1:A:434:LEU:HD11	1:A:748:MET:HE1	2.01	0.41
1:C:356:ASN:OD1	12:C:1208:HOH:O	2.22	0.41
1:C:362:TYR:CE2	1:C:385:VAL:HG12	2.55	0.41
1:D:299:LEU:HD21	1:D:301:ARG:HD3	2.02	0.41
4:P:1:NAG:H62	4:P:2:NAG:N2	2.35	0.41
1:A:487:LEU:HA	1:A:490:PHE:CE2	2.55	0.41
1:B:777:LYS:O	1:B:781:GLU:HG2	2.21	0.41
1:B:910:SER:HB2	1:B:951:VAL:HG21	2.03	0.41
1:C:809:TRP:CE2	1:C:832:LEU:HD22	2.55	0.41
1:D:515:LEU:HD13	1:D:537:ARG:NH2	2.36	0.41
1:D:826:ASP:OD1	1:D:829:ARG:NH2	2.48	0.41
1:D:687:ILE:HG23	1:D:688:GLU:HG3	2.02	0.41
1:B:723:LYS:HE3	1:B:765:VAL:HA	2.02	0.41
1:C:86:ARG:NH1	1:C:87:VAL:O	2.53	0.41
1:D:379:LYS:O	1:D:383:VAL:HG23	2.20	0.41
1:D:850:ASN:HA	1:D:851:PRO:HD3	1.94	0.41
1:A:370:ASP:HA	1:A:371:PRO:HD2	1.94	0.41
1:B:65:LEU:HB3	1:B:66:ASP:H	1.71	0.41
1:B:101:TYR:HB3	1:B:186:LEU:HB3	2.02	0.41
1:B:894:GLY:HA2	1:B:896:PHE:O	2.20	0.41
1:C:147:PRO:HA	1:C:148:PRO:HD3	1.91	0.41
1:C:210:THR:HG21	1:C:282:PHE:CD1	2.55	0.41
1:C:714:VAL:HA	1:C:959:LEU:HD13	2.02	0.41
1:B:129:TYR:CB	1:B:136:ARG:HG3	2.51	0.41
1:B:952:LYS:HE2	1:B:952:LYS:HB2	1.80	0.41
1:B:135:HIS:HA	11:B:1027:EDO:H21	2.03	0.40
1:C:153:THR:HG1	11:C:1139:EDO:HO2	1.61	0.40
1:C:605:VAL:HG12	1:C:606:ARG:HG3	2.03	0.40
1:A:637:GLU:OE1	1:A:640:ARG:NH2	2.52	0.40
1:A:849:LEU:HD11	1:A:879:PHE:CZ	2.56	0.40
1:C:129:TYR:CB	1:C:136:ARG:HG3	2.51	0.40
1:D:706:LYS:NZ	12:D:1110:HOH:O	2.39	0.40
7:a:3:BMA:H3	7:a:6:BMA:H2	1.76	0.40
1:A:362:TYR:CE2	1:A:385:VAL:HG12	2.55	0.40
1:A:534:THR:OG1	1:A:535:THR:N	2.54	0.40
1:B:836:LYS:HB3	1:B:836:LYS:HE2	1.92	0.40
1:B:903:GLN:O	1:B:907:ARG:HG3	2.21	0.40
1:C:80:LEU:HD23	1:C:113:CYS:HA	2.03	0.40
1:D:492:SER:OG	1:D:495:VAL:HG13	2.20	0.40
2:K:3:BMA:H61	2:K:4:BMA:O2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:SER:OG	1:B:265:ASN:HB3	2.22	0.40
1:C:205:LYS:HA	11:C:1141:EDO:H22	2.03	0.40
1:C:257:PRO:HG3	6:T:1:NAG:H62	2.04	0.40
1:D:301:ARG:HB2	1:D:342:ASP:OD1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1171:HOH:O	12:C:1310:HOH:O[3_555]	2.15	0.05

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 X-ray entries followed by that with respect to entries of similar resolution.

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	899/950 (95%)	868 (97%)	31 (3%)	0	100	100
1	B	903/950 (95%)	870 (96%)	33 (4%)	0	100	100
1	C	903/950 (95%)	874 (97%)	29 (3%)	0	100	100
1	D	902/950 (95%)	873 (97%)	29 (3%)	0	100	100
All	All	3607/3800 (95%)	3485 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	800/837 (96%)	767 (96%)	33 (4%)	27	54
1	B	803/837 (96%)	771 (96%)	32 (4%)	28	55
1	C	802/837 (96%)	767 (96%)	35 (4%)	25	50
1	D	802/837 (96%)	767 (96%)	35 (4%)	25	50
All	All	3207/3348 (96%)	3072 (96%)	135 (4%)	26	52

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	137	VAL
1	A	139	LEU
1	A	142	VAL
1	A	171	VAL
1	A	190	LEU
1	A	207	VAL
1	A	237	LEU
1	A	334	THR
1	A	338	LEU
1	A	383	VAL
1	A	409	LEU
1	A	449	LEU
1	A	495	VAL
1	A	518	TRP
1	A	551	VAL
1	A	561	LEU
1	A	583	VAL
1	A	586	VAL
1	A	624	LEU
1	A	677	THR
1	A	690	ARG
1	A	707	LEU
1	A	765	VAL
1	A	829	ARG
1	A	845	LEU
1	A	856	LYS
1	A	867	THR
1	A	870	VAL
1	A	883	ASN
1	A	885	LYS
1	A	890	ASP
1	A	952	LYS

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Mol	Chain	Res	Type
1	B	65	LEU
1	B	75	ARG
1	B	137	VAL
1	B	139	LEU
1	B	142	VAL
1	B	171	VAL
1	B	190	LEU
1	B	207	VAL
1	B	237	LEU
1	B	309	ILE
1	B	334	THR
1	B	383	VAL
1	B	409	LEU
1	B	449	LEU
1	B	495	VAL
1	B	518	TRP
1	B	551	VAL
1	B	561	LEU
1	B	583	VAL
1	B	586	VAL
1	B	592	ARG
1	B	765	VAL
1	B	822	VAL
1	B	829	ARG
1	B	845	LEU
1	B	853	LEU
1	B	867	THR
1	B	870	VAL
1	B	883	ASN
1	B	885	LYS
1	B	896	PHE
1	B	952	LYS
1	C	86	ARG
1	C	136	ARG
1	C	137	VAL
1	C	139	LEU
1	C	142	VAL
1	C	166	LEU
1	C	171	VAL
1	C	190	LEU
1	C	207	VAL
1	C	237	LEU

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Mol	Chain	Res	Type
1	C	260	GLU
1	C	298	VAL
1	C	309	ILE
1	C	334	THR
1	C	338	LEU
1	C	383	VAL
1	C	409	LEU
1	C	449	LEU
1	C	495	VAL
1	C	518	TRP
1	C	523	GLU
1	C	561	LEU
1	C	583	VAL
1	C	586	VAL
1	C	592	ARG
1	C	595	ARG
1	C	735	ASN
1	C	765	VAL
1	C	771	MET
1	C	845	LEU
1	C	870	VAL
1	C	883	ASN
1	C	885	LYS
1	C	896	PHE
1	C	952	LYS
1	D	100	LEU
1	D	137	VAL
1	D	139	LEU
1	D	142	VAL
1	D	171	VAL
1	D	207	VAL
1	D	237	LEU
1	D	298	VAL
1	D	334	THR
1	D	338	LEU
1	D	357	TRP
1	D	383	VAL
1	D	409	LEU
1	D	449	LEU
1	D	455	LEU
1	D	495	VAL
1	D	518	TRP

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Mol	Chain	Res	Type
1	D	561	LEU
1	D	583	VAL
1	D	586	VAL
1	D	592	ARG
1	D	595	ARG
1	D	624	LEU
1	D	707	LEU
1	D	765	VAL
1	D	771	MET
1	D	829	ARG
1	D	845	LEU
1	D	853	LEU
1	D	867	THR
1	D	870	VAL
1	D	883	ASN
1	D	885	LYS
1	D	939	GLN
1	D	952	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	ASN
1	A	650	HIS
1	A	815	GLN
1	A	857	GLN
1	B	650	HIS
1	B	881	GLN
1	C	410	ASN
1	C	463	ASN
1	D	135	HIS
1	D	463	ASN
1	D	510	GLN
1	D	739	ASN
1	D	815	GLN
1	D	881	GLN
1	D	920	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 ⓘ

95 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	E	1	2,1	14,14,15	0.53	0	17,19,21	0.66	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.77	0
2	BMA	E	3	2	11,11,12	0.56	0	15,15,17	1.01	0
2	BMA	E	4	2	11,11,12	0.68	0	15,15,17	0.46	0
3	NAG	F	1	3,1	14,14,15	0.53	0	17,19,21	0.67	0
3	NAG	F	2	3	14,14,15	0.55	0	17,19,21	0.66	0
3	BMA	F	3	3	11,11,12	0.52	0	15,15,17	1.02	2 (13%)
3	BMA	F	4	3	11,11,12	0.58	0	15,15,17	0.52	0
3	BMA	F	5	3	11,11,12	0.57	0	15,15,17	0.74	0
4	NAG	G	1	4,1	14,14,15	0.49	0	17,19,21	0.74	0
4	NAG	G	2	4	14,14,15	0.57	0	17,19,21	0.72	0
5	NAG	H	1	5,1	14,14,15	0.58	0	17,19,21	0.72	0
5	NAG	H	2	5	14,14,15	0.58	0	17,19,21	0.88	0
5	BMA	H	3	5	11,11,12	0.62	0	15,15,17	0.63	0
4	NAG	I	1	4,1	14,14,15	0.57	0	17,19,21	0.72	0
4	NAG	I	2	4	14,14,15	0.50	0	17,19,21	0.62	0
2	NAG	J	1	2,1	14,14,15	0.52	0	17,19,21	0.75	0
2	NAG	J	2	2	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
2	BMA	J	3	2	11,11,12	0.53	0	15,15,17	0.75	1 (6%)
2	BMA	J	4	2	11,11,12	0.65	0	15,15,17	0.50	0
2	NAG	K	1	2,1	14,14,15	0.61	0	17,19,21	0.81	0
2	NAG	K	2	2	14,14,15	0.55	0	17,19,21	0.57	0
2	BMA	K	3	2	11,11,12	0.67	0	15,15,17	0.85	0
2	BMA	K	4	2	11,11,12	0.83	1 (9%)	15,15,17	1.30	3 (20%)
3	NAG	L	1	3,1	14,14,15	0.56	0	17,19,21	0.69	0
3	NAG	L	2	3	14,14,15	0.44	0	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	L	3	3	11,11,12	0.58	0	15,15,17	1.36	1 (6%)
3	BMA	L	4	3	11,11,12	0.53	0	15,15,17	1.31	1 (6%)
3	BMA	L	5	3	11,11,12	0.55	0	15,15,17	1.05	1 (6%)
4	NAG	M	1	4,1	14,14,15	0.60	0	17,19,21	0.77	0
4	NAG	M	2	4	14,14,15	0.56	0	17,19,21	0.59	0
4	NAG	N	1	4,1	14,14,15	0.59	0	17,19,21	0.68	0
4	NAG	N	2	4	14,14,15	0.50	0	17,19,21	0.74	0
5	NAG	O	1	5,1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
5	NAG	O	2	5	14,14,15	0.58	0	17,19,21	0.65	0
5	BMA	O	3	5	11,11,12	0.55	0	15,15,17	0.81	0
4	NAG	P	1	4,1	14,14,15	0.55	0	17,19,21	0.70	0
4	NAG	P	2	4	14,14,15	0.54	0	17,19,21	1.28	2 (11%)
4	NAG	Q	1	4,1	14,14,15	0.54	0	17,19,21	0.93	0
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.75	0
2	NAG	R	1	2,1	14,14,15	0.67	0	17,19,21	1.55	3 (17%)
2	NAG	R	2	2	14,14,15	0.59	0	17,19,21	0.96	1 (5%)
2	BMA	R	3	2	11,11,12	0.61	0	15,15,17	0.73	0
2	BMA	R	4	2	11,11,12	0.61	0	15,15,17	0.44	0
3	NAG	S	1	3,1	14,14,15	0.54	0	17,19,21	0.60	0
3	NAG	S	2	3	14,14,15	0.54	0	17,19,21	0.74	0
3	BMA	S	3	3	11,11,12	0.74	0	15,15,17	0.71	0
3	BMA	S	4	3	11,11,12	0.64	0	15,15,17	0.49	0
3	BMA	S	5	3	11,11,12	0.64	0	15,15,17	0.82	0
6	NAG	T	1	6,1	14,14,15	0.58	0	17,19,21	0.80	0
6	NAG	T	2	6	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
6	BMA	T	3	6	11,11,12	0.59	0	15,15,17	0.62	0
6	BMA	T	4	6	11,11,12	0.60	0	15,15,17	0.86	0
5	NAG	U	1	5,1	14,14,15	0.55	0	17,19,21	0.60	0
5	NAG	U	2	5	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
5	BMA	U	3	5	11,11,12	0.64	0	15,15,17	0.64	0
4	NAG	V	1	4,1	14,14,15	0.57	0	17,19,21	0.98	1 (5%)
4	NAG	V	2	4	14,14,15	0.49	0	17,19,21	0.65	0
7	NAG	W	1	7,1	14,14,15	0.58	0	17,19,21	0.70	0
7	NAG	W	2	7	14,14,15	0.53	0	17,19,21	0.60	0
7	BMA	W	3	7	11,11,12	0.49	0	15,15,17	0.92	1 (6%)
7	BMA	W	4	7	11,11,12	0.61	0	15,15,17	1.68	4 (26%)
7	BMA	W	5	7	11,11,12	0.59	0	15,15,17	0.74	0
7	BMA	W	6	7	11,11,12	0.60	0	15,15,17	0.84	0
4	NAG	X	1	4,1	14,14,15	0.56	0	17,19,21	0.72	0
4	NAG	X	2	4	14,14,15	0.53	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	Y	1	8,1	14,14,15	0.50	0	17,19,21	0.74	0
8	NAG	Y	2	8	14,14,15	0.60	0	17,19,21	0.75	1 (5%)
8	BMA	Y	3	8	11,11,12	0.61	0	15,15,17	0.83	1 (6%)
8	BMA	Y	4	8	11,11,12	0.66	0	15,15,17	0.51	0
8	BMA	Y	5	8	11,11,12	0.63	0	15,15,17	0.55	0
8	BMA	Y	6	8	11,11,12	0.65	0	15,15,17	0.51	0
5	NAG	Z	1	5,1	14,14,15	0.53	0	17,19,21	0.61	0
5	NAG	Z	2	5	14,14,15	0.50	0	17,19,21	0.69	0
5	BMA	Z	3	5	11,11,12	0.62	0	15,15,17	0.89	0
7	NAG	a	1	7,1	14,14,15	0.57	0	17,19,21	0.57	0
7	NAG	a	2	7	14,14,15	0.53	0	17,19,21	0.68	0
7	BMA	a	3	7	11,11,12	0.62	0	15,15,17	1.16	1 (6%)
7	BMA	a	4	7	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
7	BMA	a	5	7	11,11,12	0.57	0	15,15,17	0.94	0
7	BMA	a	6	7	11,11,12	0.82	0	15,15,17	0.63	0
5	NAG	b	1	5,1	14,14,15	0.48	0	17,19,21	0.92	0
5	NAG	b	2	5	14,14,15	0.58	0	17,19,21	0.68	0
5	BMA	b	3	5	11,11,12	0.55	0	15,15,17	0.91	0
5	NAG	c	1	5,1	14,14,15	0.56	0	17,19,21	0.55	0
5	NAG	c	2	5	14,14,15	0.50	0	17,19,21	0.52	0
5	BMA	c	3	5	11,11,12	0.62	0	15,15,17	0.57	0
4	NAG	d	1	4,1	14,14,15	0.53	0	17,19,21	0.80	0
4	NAG	d	2	4	14,14,15	0.52	0	17,19,21	1.20	1 (5%)
4	NAG	e	1	4,1	14,14,15	0.58	0	17,19,21	0.95	2 (11%)
4	NAG	e	2	4	14,14,15	0.45	0	17,19,21	0.76	0
4	NAG	f	1	4,1	14,14,15	0.62	0	17,19,21	1.27	2 (11%)
4	NAG	f	2	4	14,14,15	0.50	0	17,19,21	1.09	1 (5%)
4	NAG	g	1	4,1	14,14,15	0.48	0	17,19,21	0.66	0
4	NAG	g	2	4	14,14,15	0.54	0	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	BMA	E	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	BMA	F	4	3	-	1/2/19/22	0/1/1/1
3	BMA	F	5	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
2	NAG	J	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	1/1/1/1
2	BMA	J	4	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	BMA	K	3	2	-	1/2/19/22	0/1/1/1
2	BMA	K	4	2	-	2/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	BMA	L	4	3	-	1/2/19/22	1/1/1/1
3	BMA	L	5	3	-	2/2/19/22	1/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	a	6	7	-	2/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
4	NAG	d	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	d	2	4	-	3/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	3/6/23/26	0/1/1/1
4	NAG	f	1	4,1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	BMA	O5-C1	-2.01	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4	BMA	C1-O5-C5	4.11	117.69	112.19
2	R	1	NAG	C4-C3-C2	3.85	116.67	111.02
7	W	4	BMA	O3-C3-C2	-3.79	102.32	110.05
2	R	1	NAG	C3-C4-C5	3.67	116.88	110.23
3	L	3	BMA	C1-O5-C5	3.64	117.07	112.19
3	L	5	BMA	C1-O5-C5	3.58	116.98	112.19
3	L	2	NAG	C1-O5-C5	3.57	116.97	112.19
4	d	2	NAG	C1-O5-C5	3.40	116.74	112.19
7	W	4	BMA	C1-C2-C3	3.28	114.43	109.64
7	a	4	BMA	C1-O5-C5	3.07	116.30	112.19
4	f	1	NAG	O5-C1-C2	3.02	115.96	111.29
2	K	4	BMA	O5-C1-C2	-2.90	103.87	110.79
4	V	1	NAG	O5-C1-C2	-2.89	106.82	111.29
7	a	3	BMA	C1-C2-C3	2.85	113.79	109.64
4	g	2	NAG	C1-O5-C5	2.80	115.94	112.19
7	W	3	BMA	O5-C5-C6	2.69	112.89	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	O3-C3-C2	2.55	115.26	110.05
4	P	2	NAG	O5-C1-C2	-2.47	107.46	111.29
4	P	2	NAG	C3-C4-C5	2.46	114.69	110.23
5	U	2	NAG	C4-C3-C2	2.45	114.61	111.02
4	f	1	NAG	C1-O5-C5	2.42	115.42	112.19
2	J	2	NAG	C1-O5-C5	2.31	115.28	112.19
7	W	4	BMA	C3-C4-C5	2.31	114.41	110.23
2	R	1	NAG	O5-C1-C2	-2.27	107.78	111.29
3	L	2	NAG	O4-C4-C5	2.25	114.87	109.32
2	K	4	BMA	O5-C5-C6	2.25	112.05	107.66
4	e	1	NAG	O4-C4-C3	-2.24	105.08	110.38
4	f	2	NAG	C1-O5-C5	2.24	115.19	112.19
2	J	3	BMA	O5-C5-C6	2.22	111.98	107.66
6	T	2	NAG	C1-O5-C5	2.20	115.14	112.19
5	O	1	NAG	O5-C1-C2	-2.15	107.96	111.29
2	R	2	NAG	C1-O5-C5	-2.13	109.33	112.19
2	K	4	BMA	C2-C3-C4	-2.10	107.16	110.86
8	Y	2	NAG	C4-C3-C2	2.08	114.06	111.02
3	F	3	BMA	O5-C5-C6	2.08	111.70	107.66
4	e	1	NAG	C4-C3-C2	2.07	114.06	111.02
7	W	4	BMA	O6-C6-C5	-2.06	104.31	111.33
8	Y	3	BMA	O5-C5-C6	2.01	111.57	107.66

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	J	1	NAG	C1
4	Q	1	NAG	C1
4	V	1	NAG	C1
4	X	1	NAG	C1
4	d	1	NAG	C1
4	f	1	NAG	C1
4	g	1	NAG	C1
8	Y	1	NAG	C1

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	f	2	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C1-C2-N2-C7
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	f	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
2	R	3	BMA	O5-C5-C6-O6
7	W	4	BMA	C4-C5-C6-O6
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
5	c	2	NAG	C8-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
2	R	3	BMA	C4-C5-C6-O6
7	W	4	BMA	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C8-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
2	K	4	BMA	O5-C5-C6-O6
4	N	1	NAG	O7-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
7	a	6	BMA	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	L	4	BMA	O5-C5-C6-O6
2	K	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	g	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
3	L	3	BMA	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
8	Y	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C8-C7-N2-C2
5	c	3	BMA	O5-C5-C6-O6
4	I	2	NAG	O7-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2
4	g	2	NAG	O7-C7-N2-C2
7	a	4	BMA	O5-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
2	R	4	BMA	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	3	BMA	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
3	L	5	BMA	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	e	2	NAG	C8-C7-N2-C2
4	e	1	NAG	C8-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
8	Y	5	BMA	C4-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
8	Y	5	BMA	O5-C5-C6-O6
4	e	2	NAG	O7-C7-N2-C2
4	e	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C4-C5-C6-O6
7	a	6	BMA	C4-C5-C6-O6
2	K	4	BMA	C4-C5-C6-O6
3	L	5	BMA	O5-C5-C6-O6
5	U	2	NAG	C1-C2-N2-C7
4	d	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C3-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
4	X	2	NAG	C8-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O7-C7-N2-C2
2	J	3	BMA	O5-C5-C6-O6

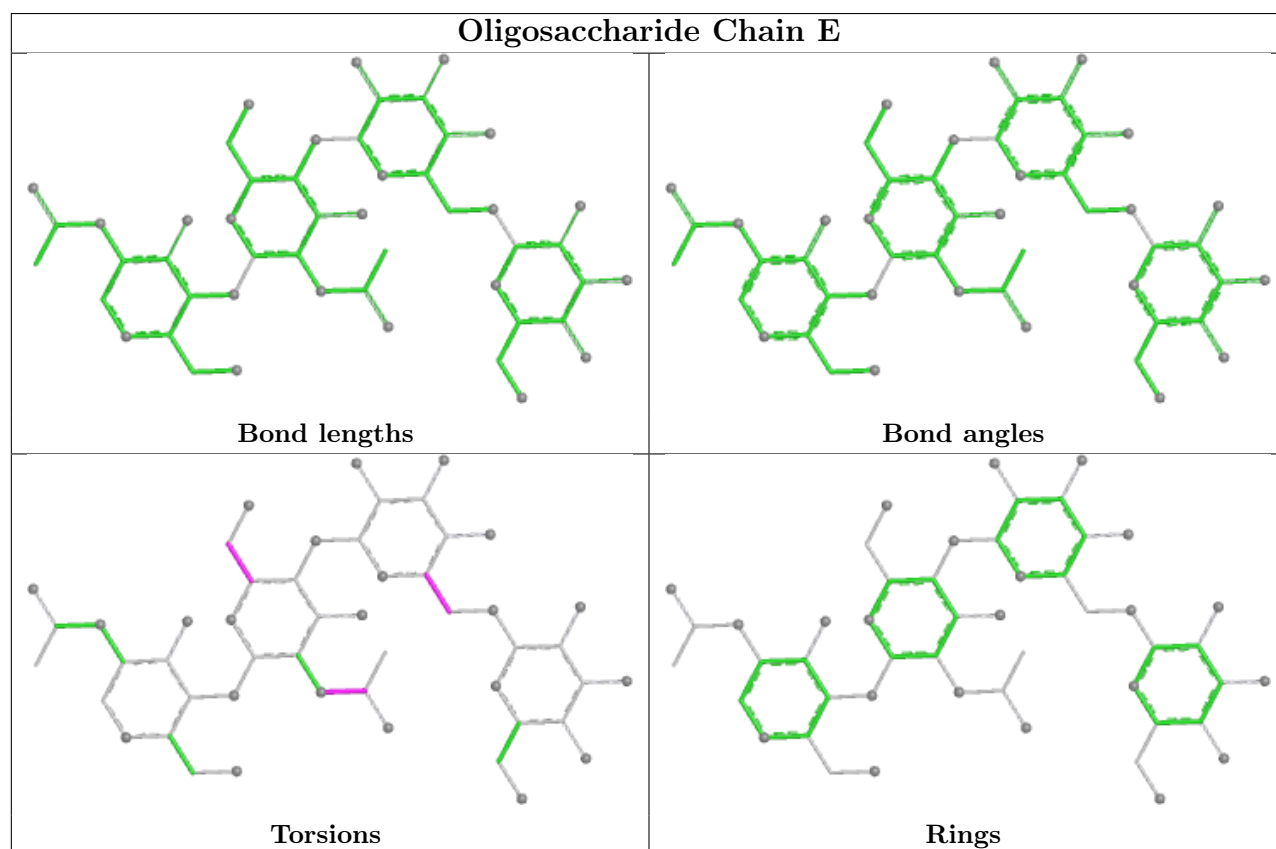
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	5	BMA	C1-C2-C3-C4-C5-O5
2	J	3	BMA	C1-C2-C3-C4-C5-O5
3	L	4	BMA	C1-C2-C3-C4-C5-O5

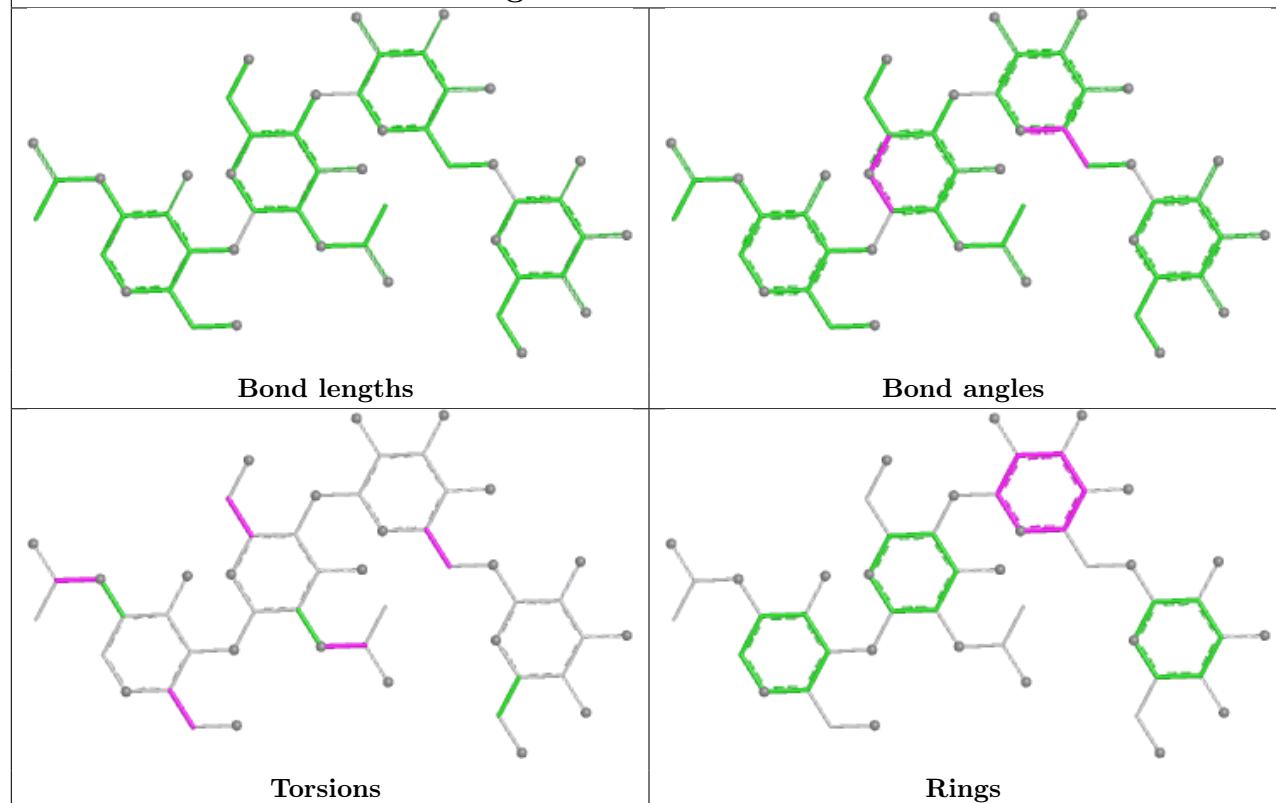
14 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	a	6	BMA	2	0
2	K	3	BMA	1	0
7	a	3	BMA	1	0
2	R	3	BMA	1	0
7	W	4	BMA	2	0
7	W	3	BMA	1	0
4	P	2	NAG	1	0
2	R	4	BMA	2	0
4	G	1	NAG	1	0
3	L	5	BMA	1	0
4	P	1	NAG	1	0
2	K	4	BMA	1	0
6	T	1	NAG	1	0
7	W	2	NAG	1	0

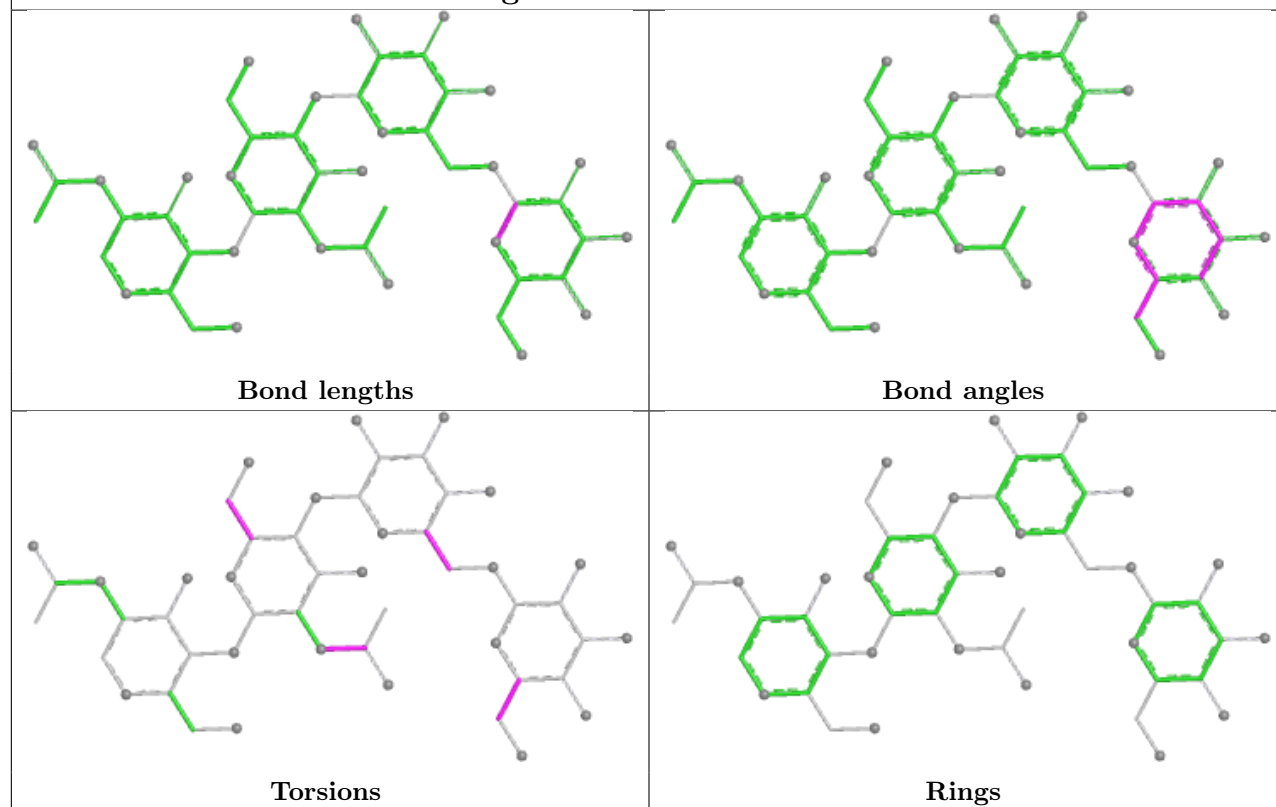
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

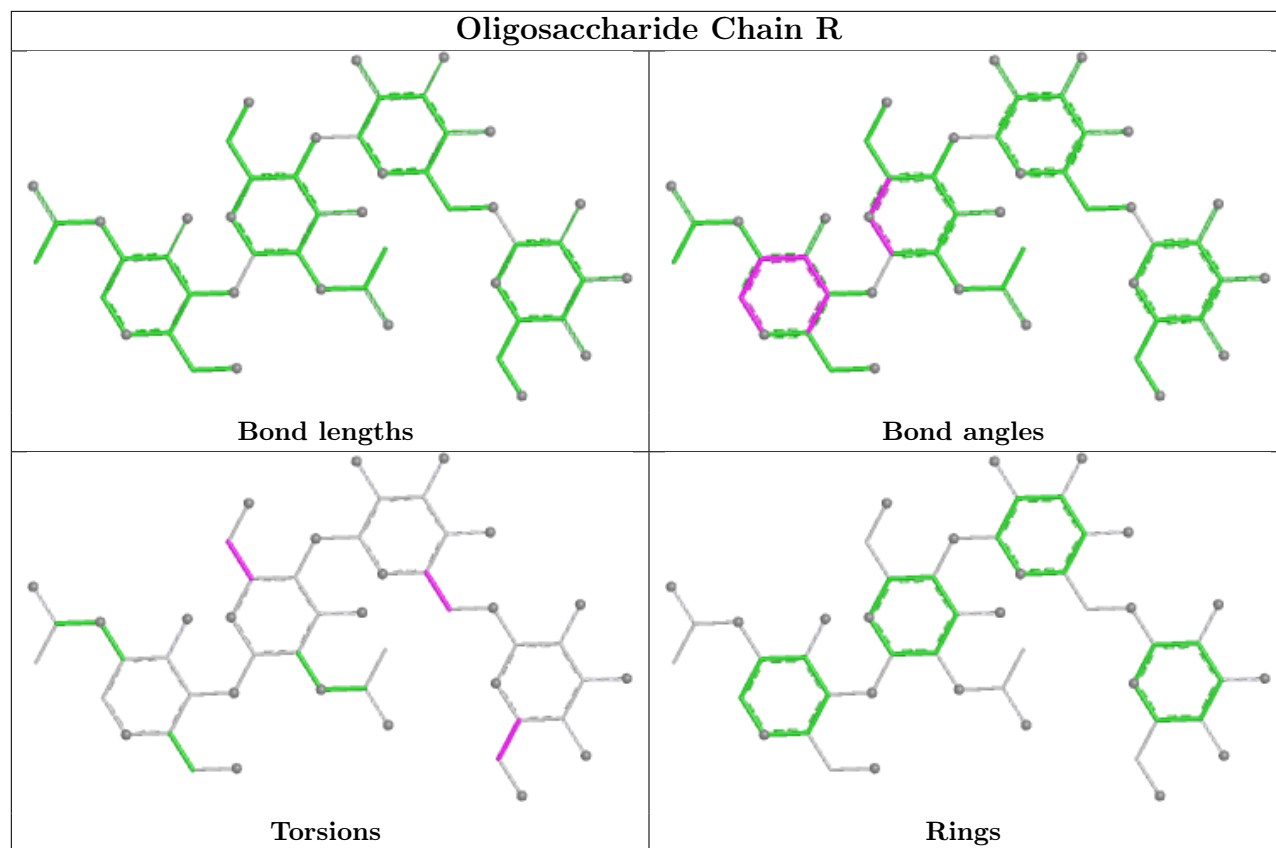


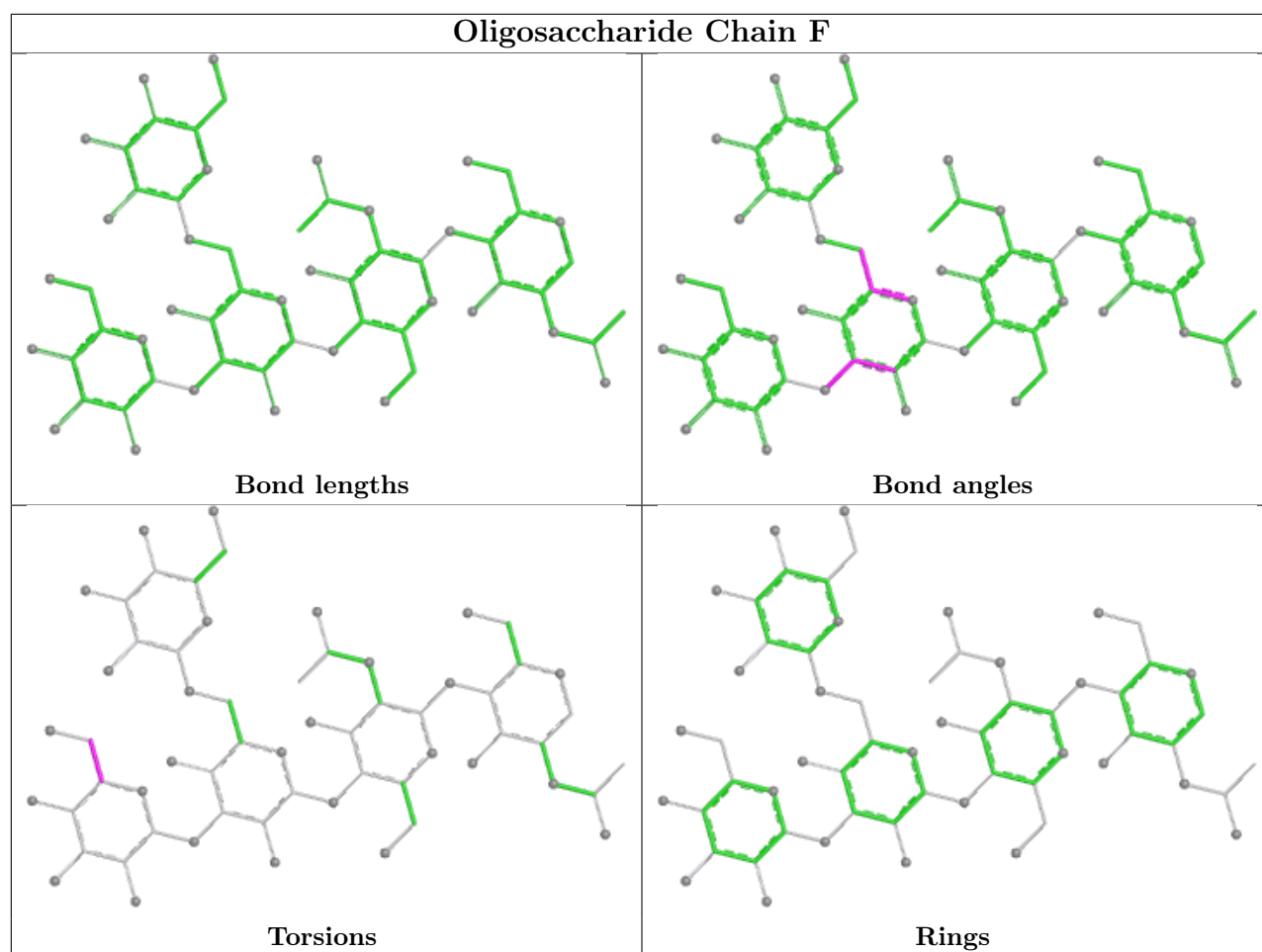
Oligosaccharide Chain J

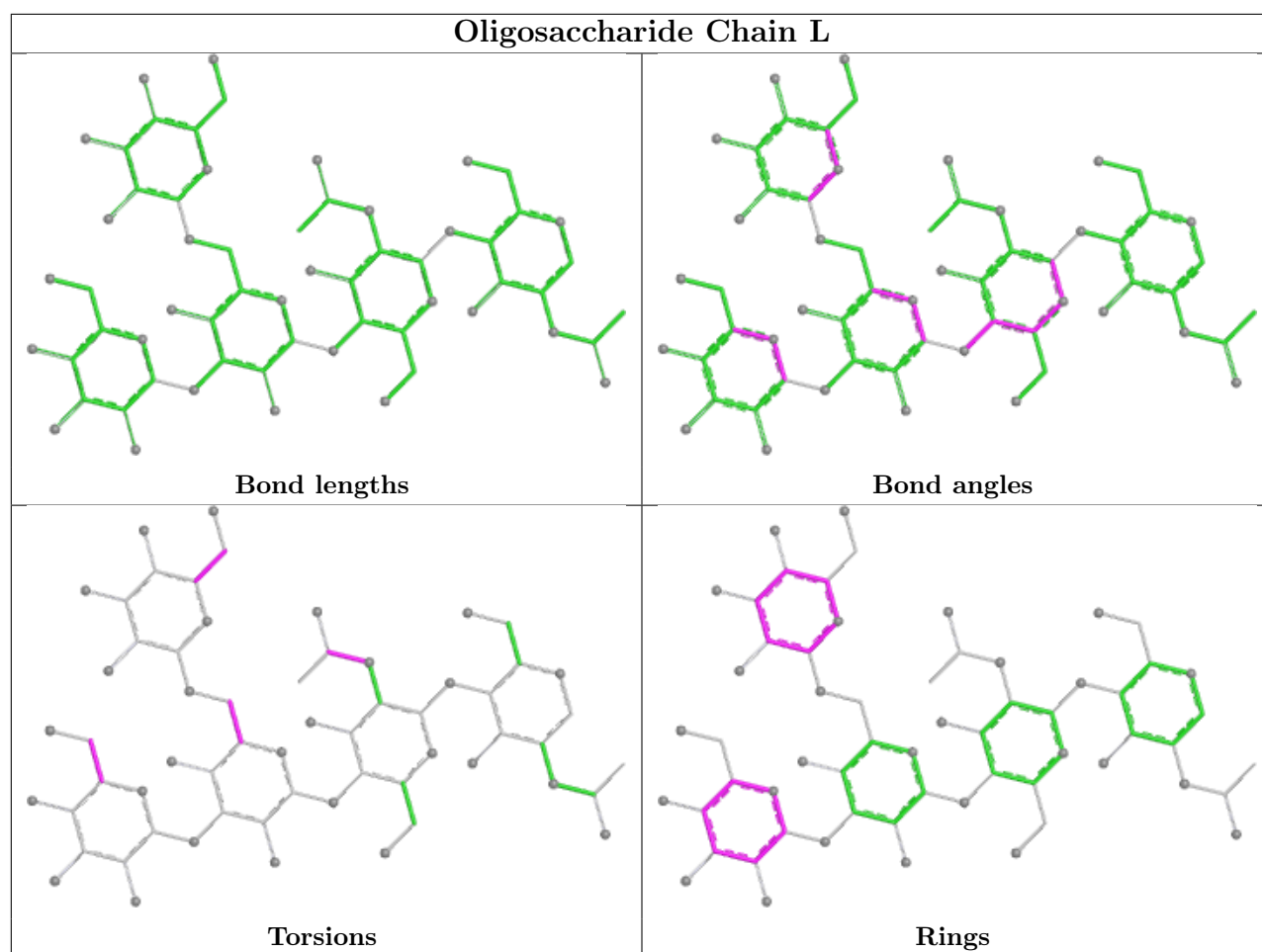


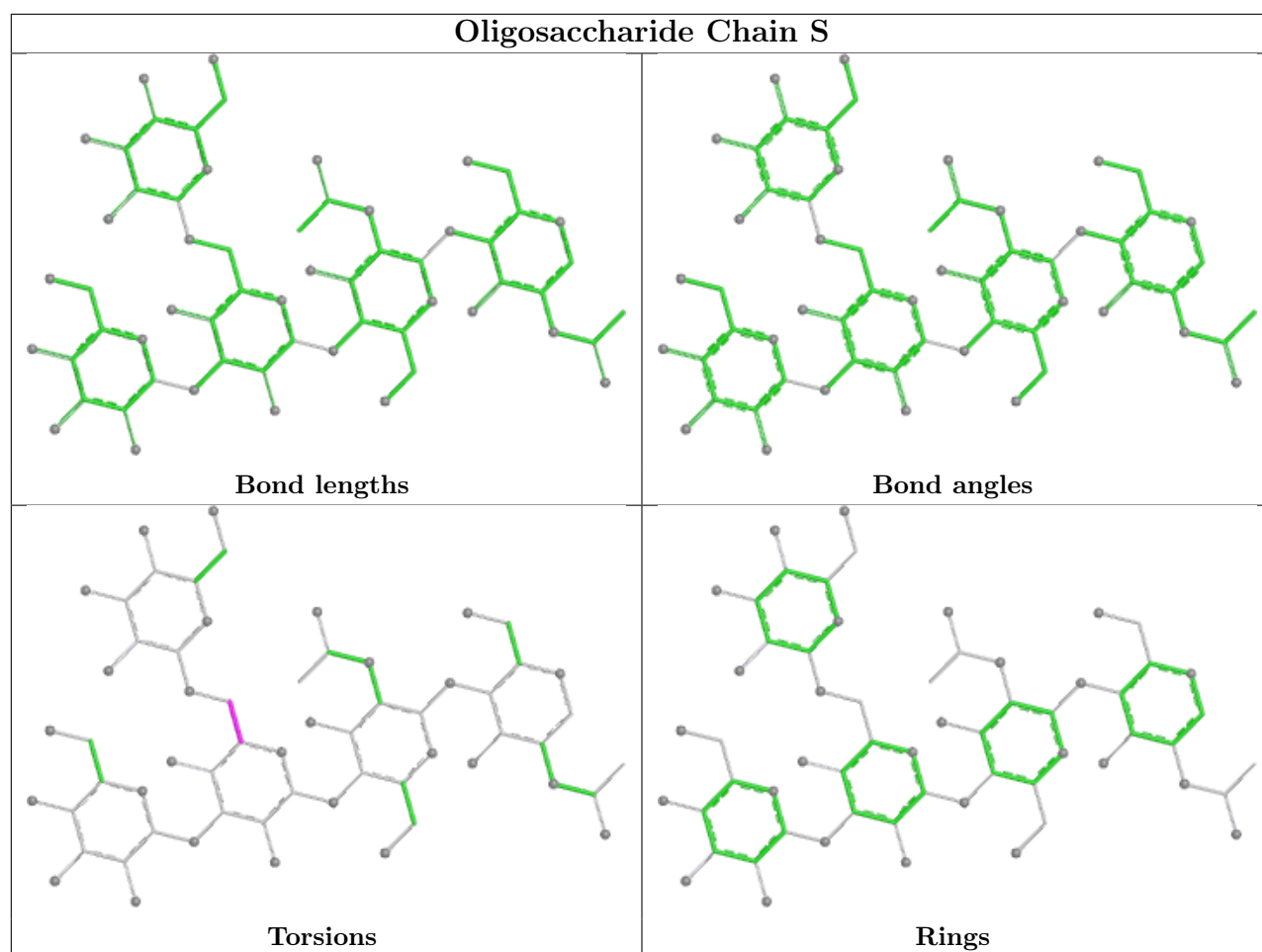
Oligosaccharide Chain K

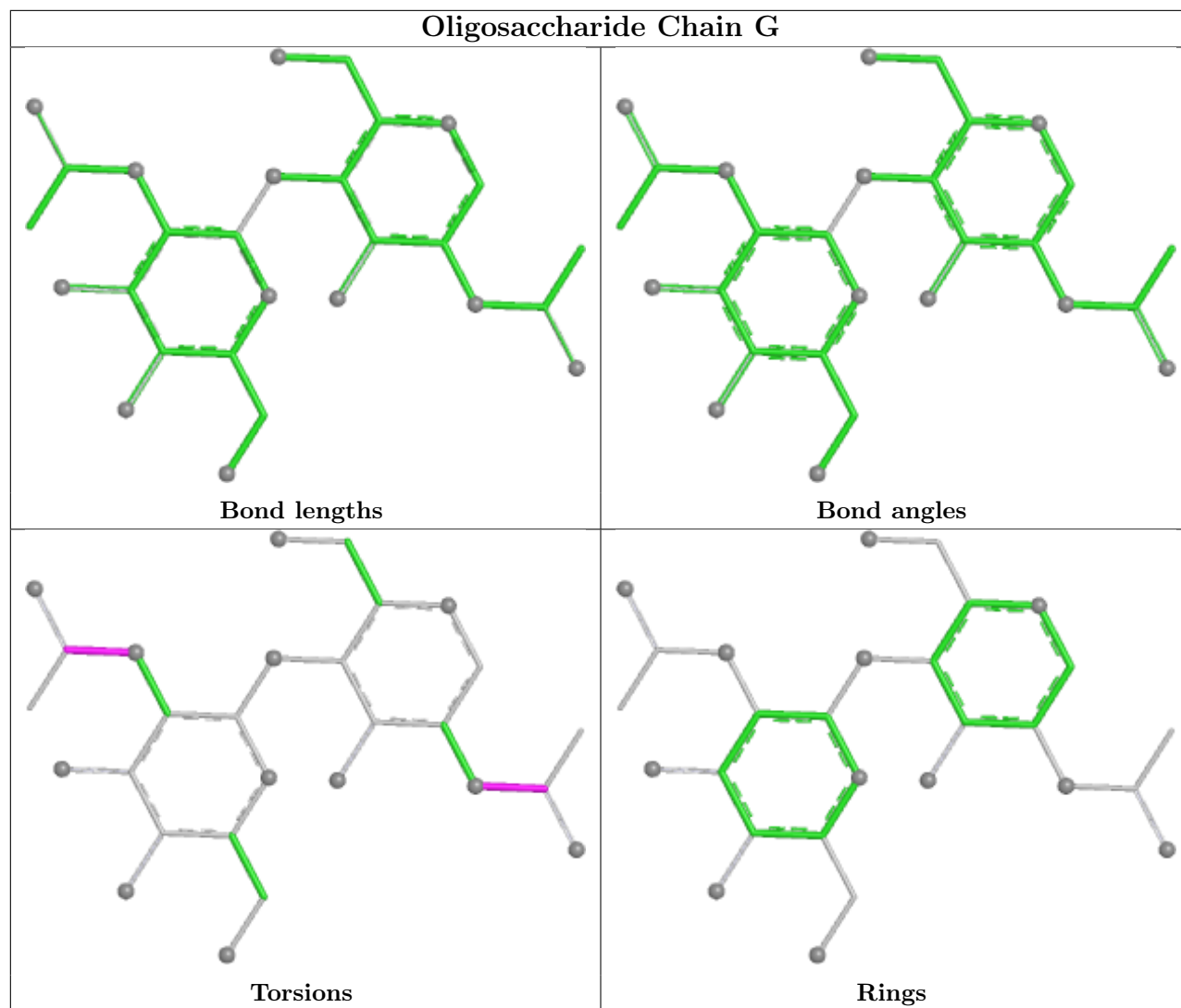


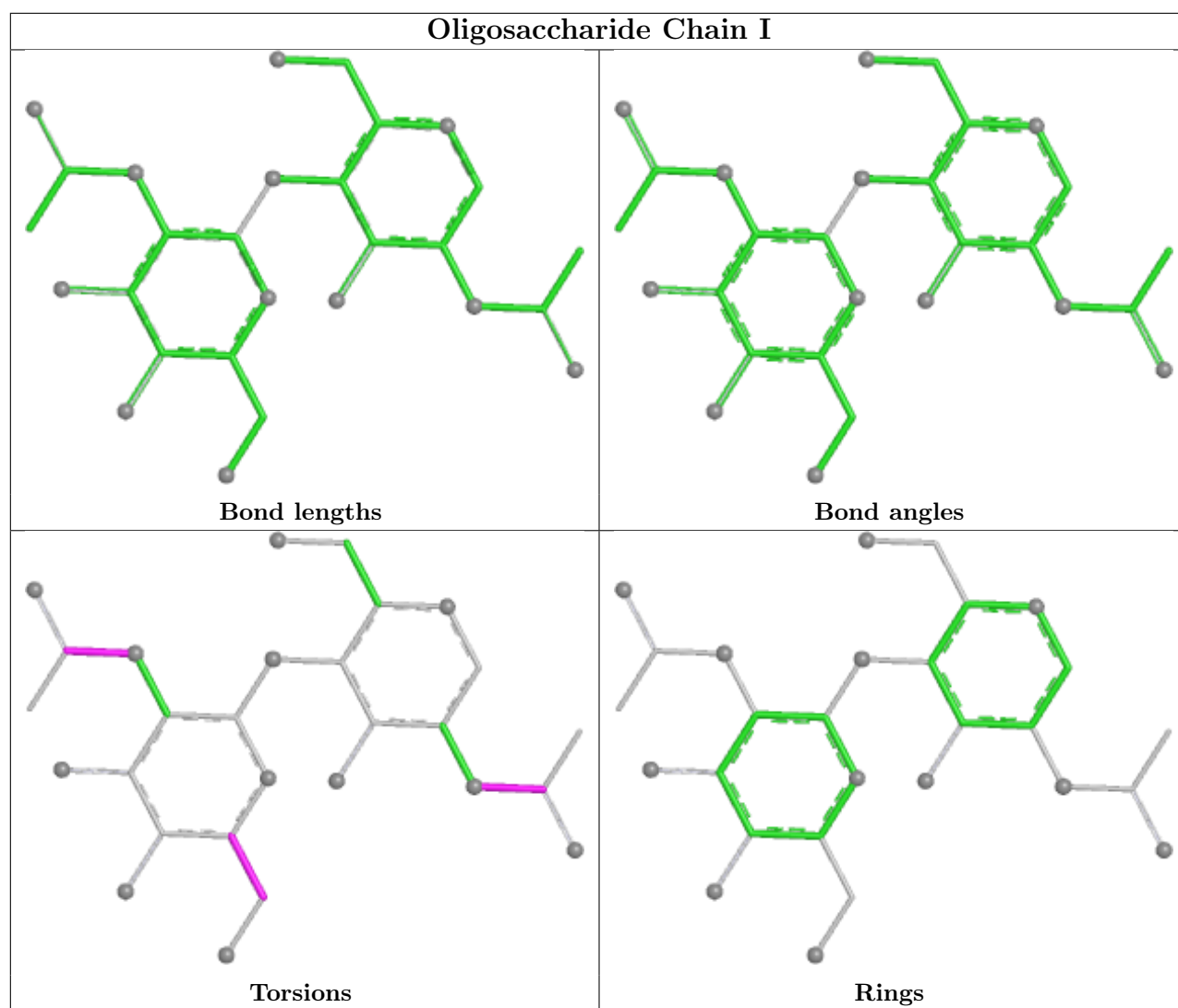


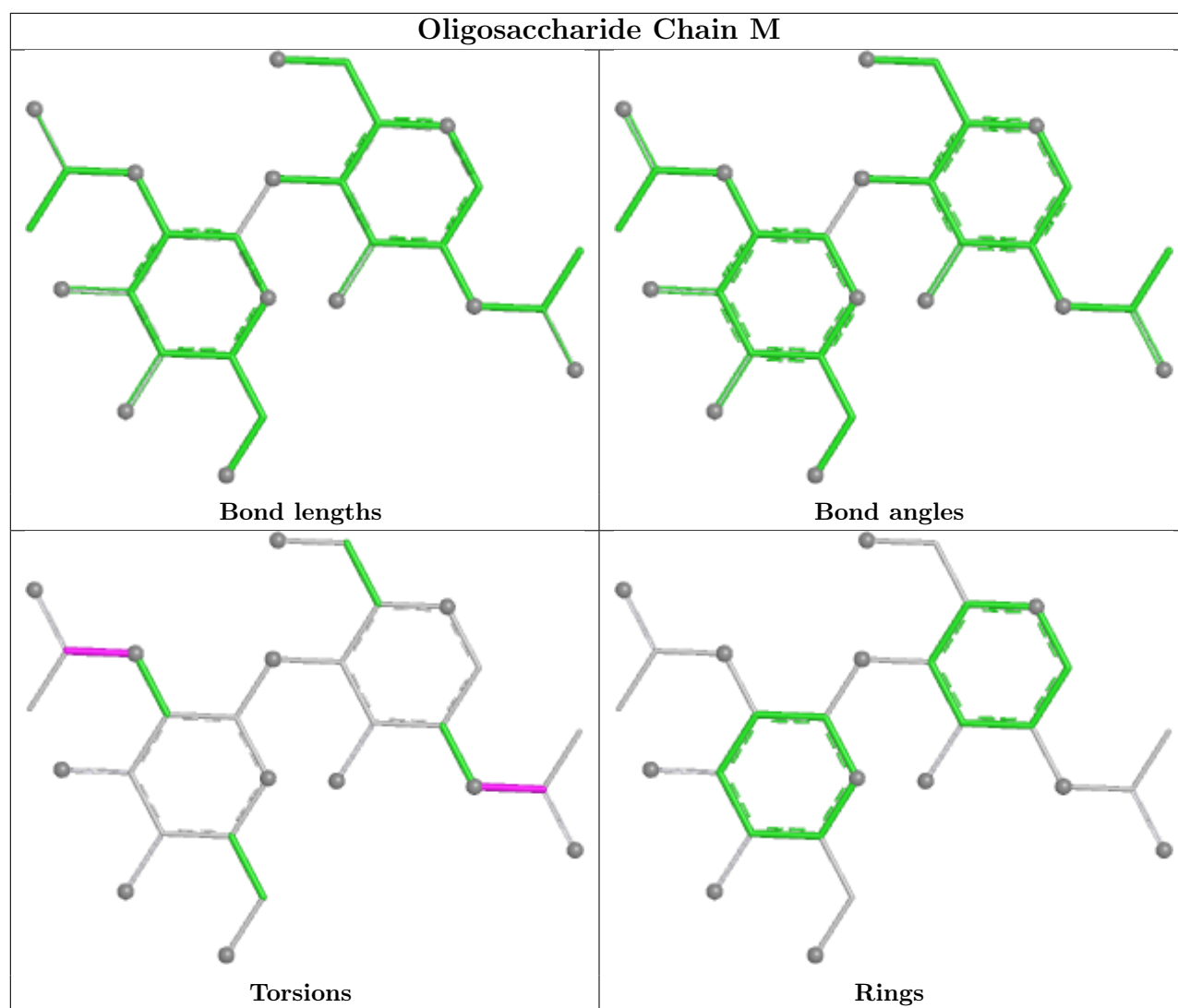


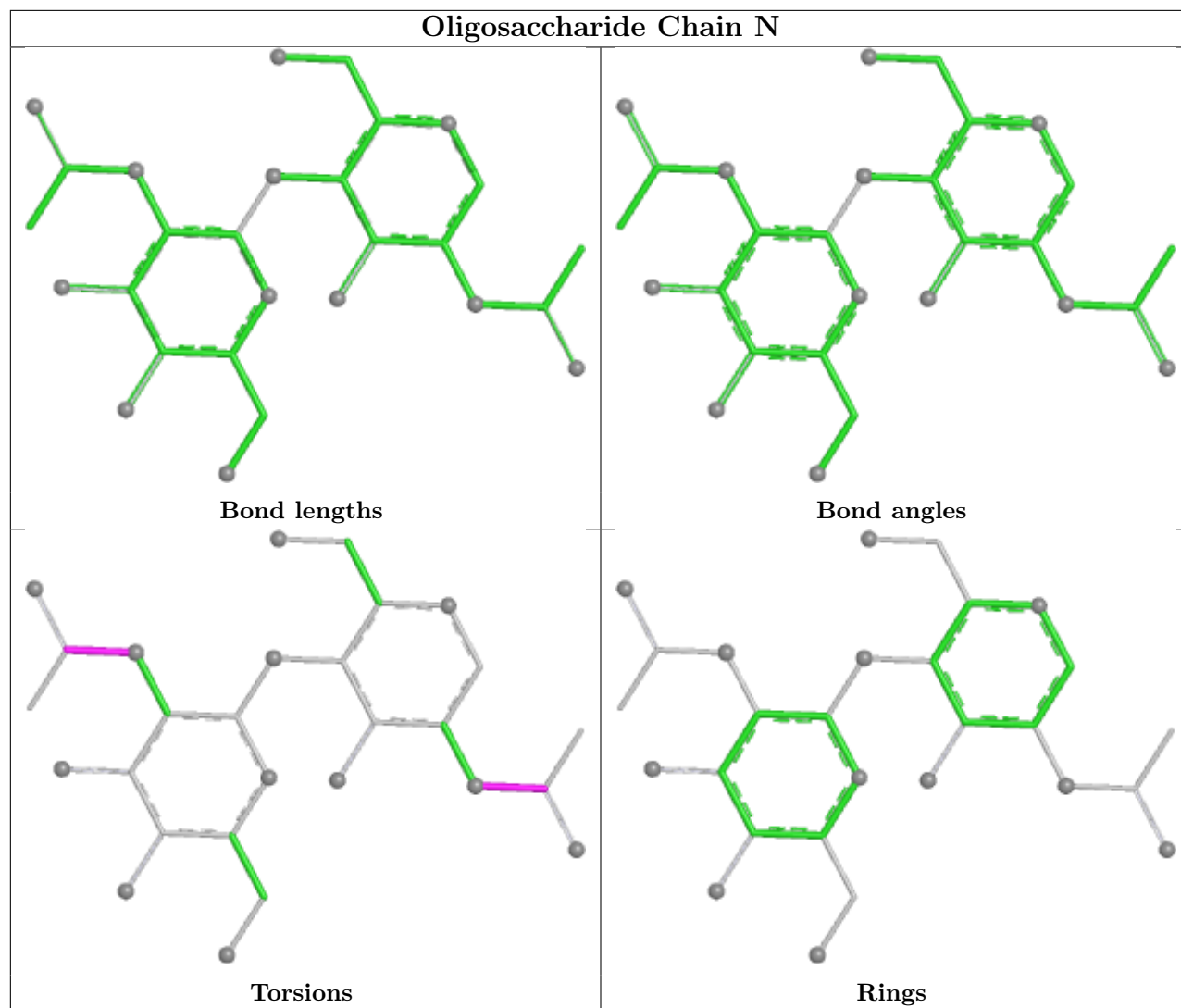


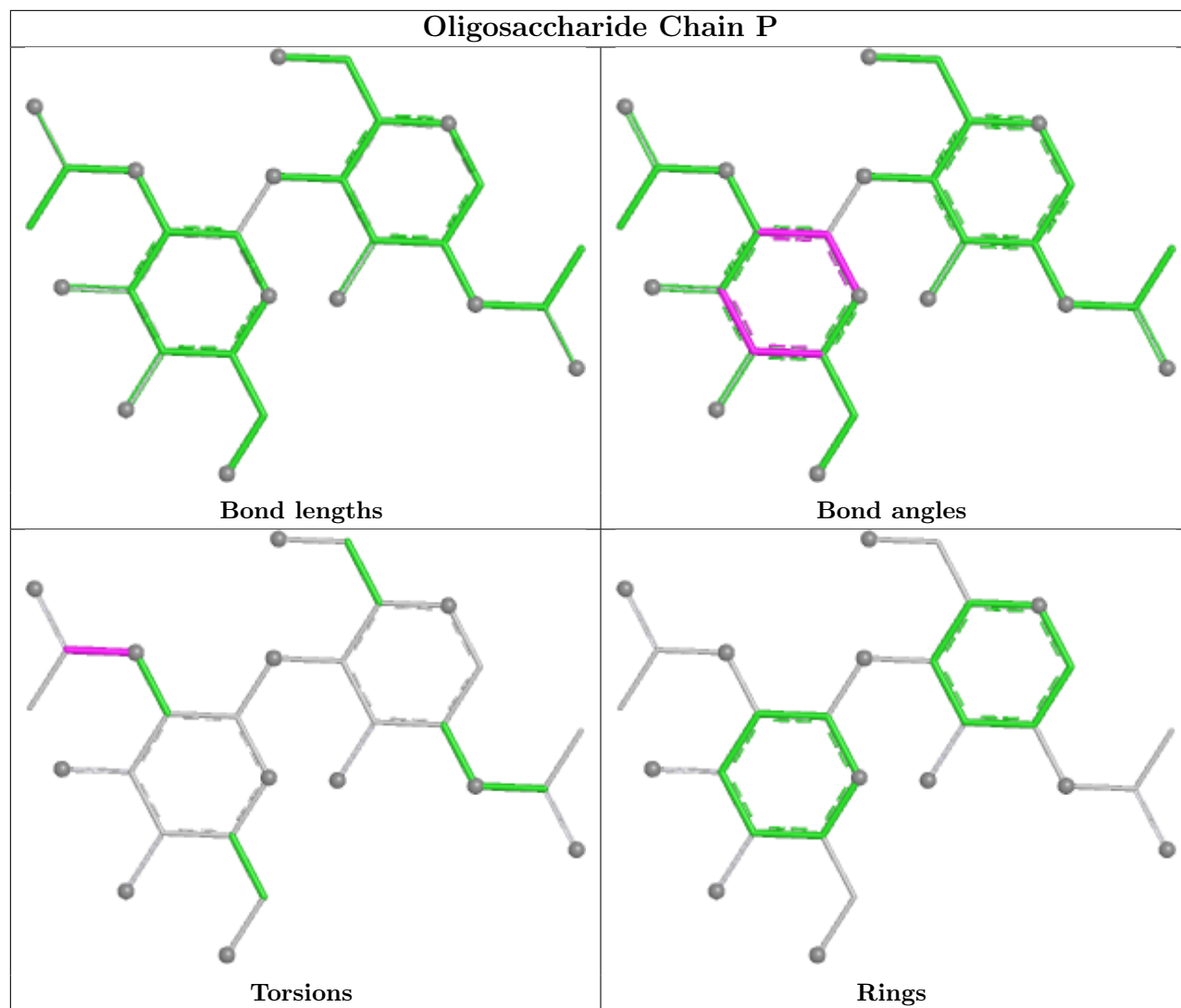


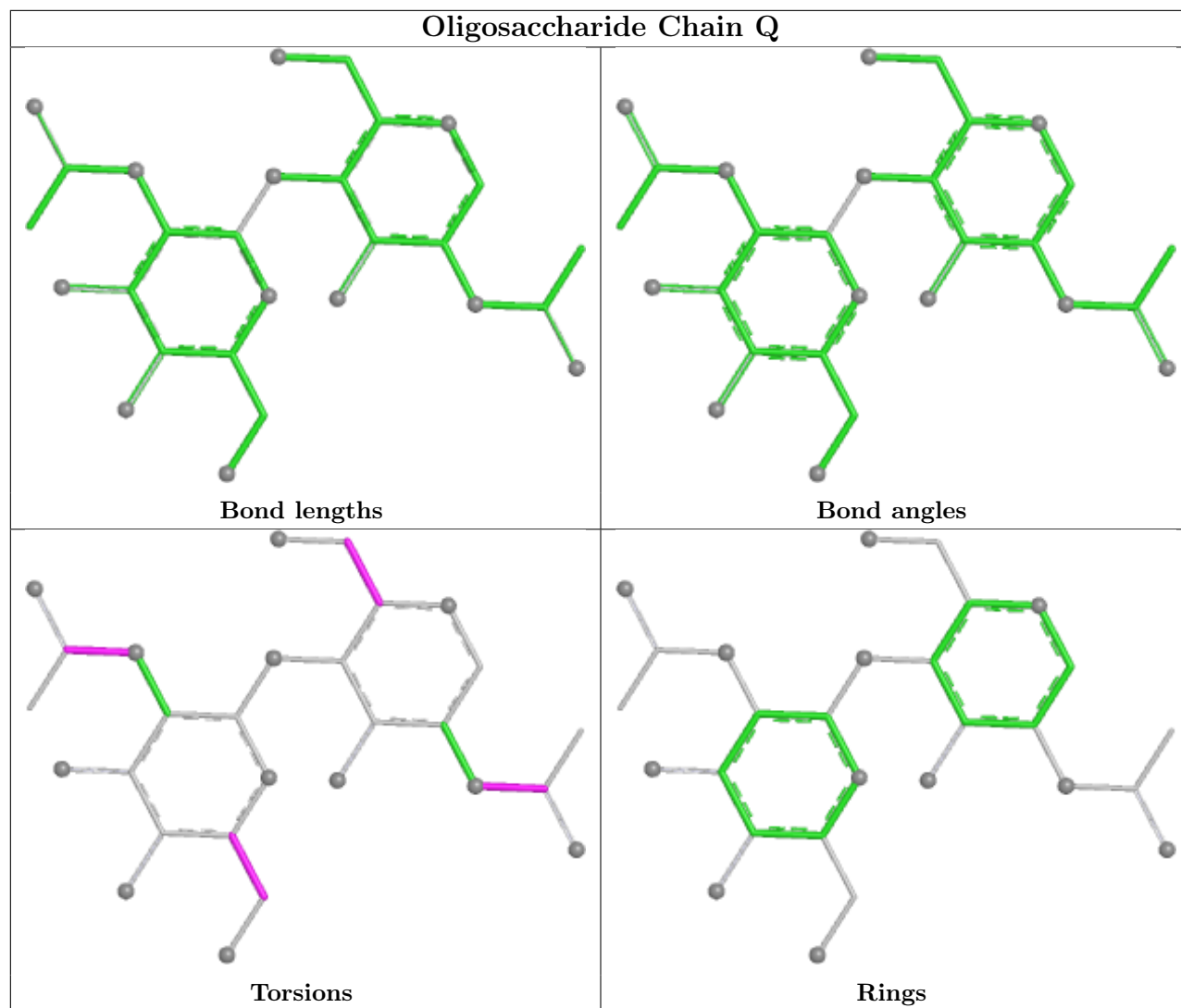


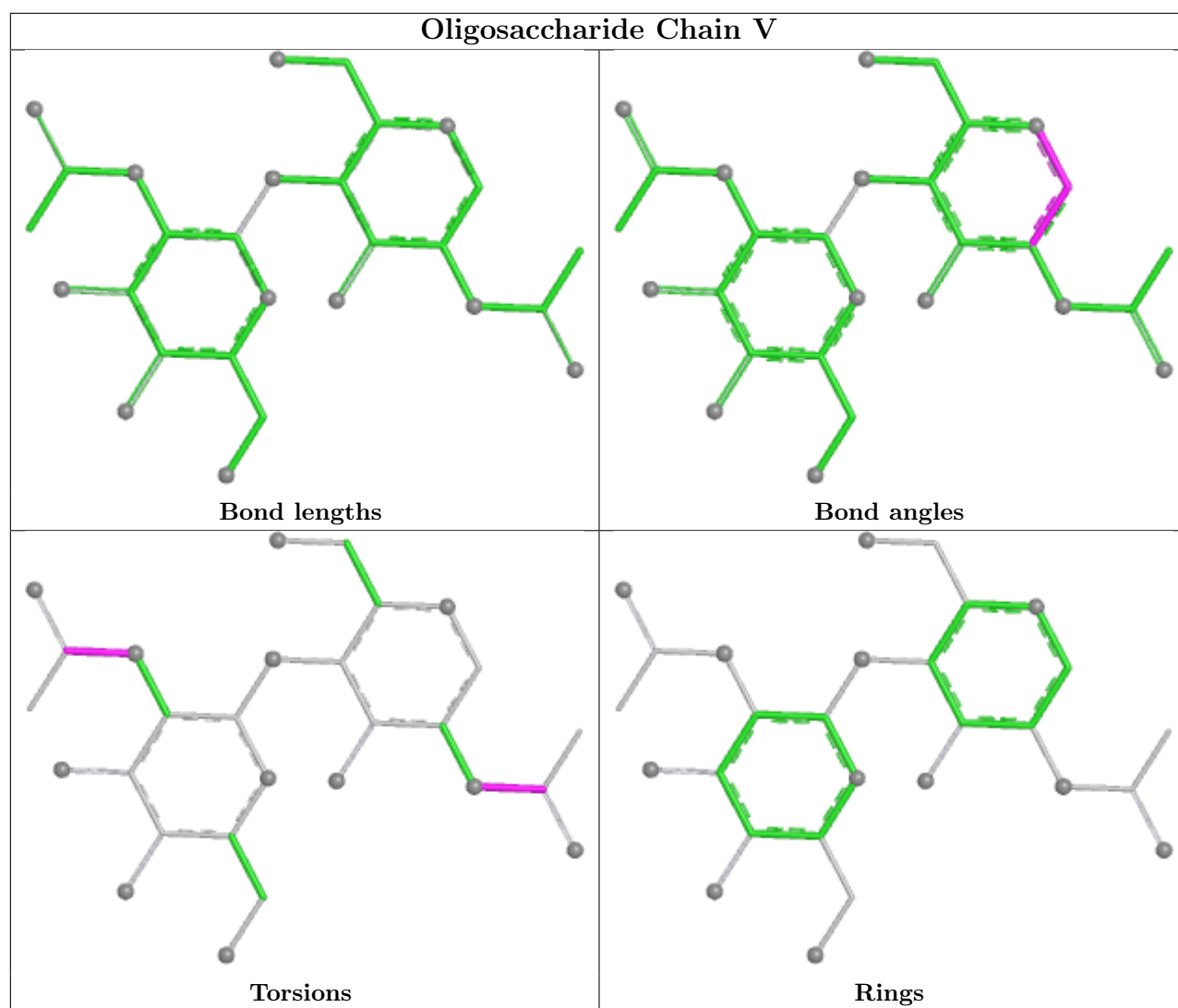


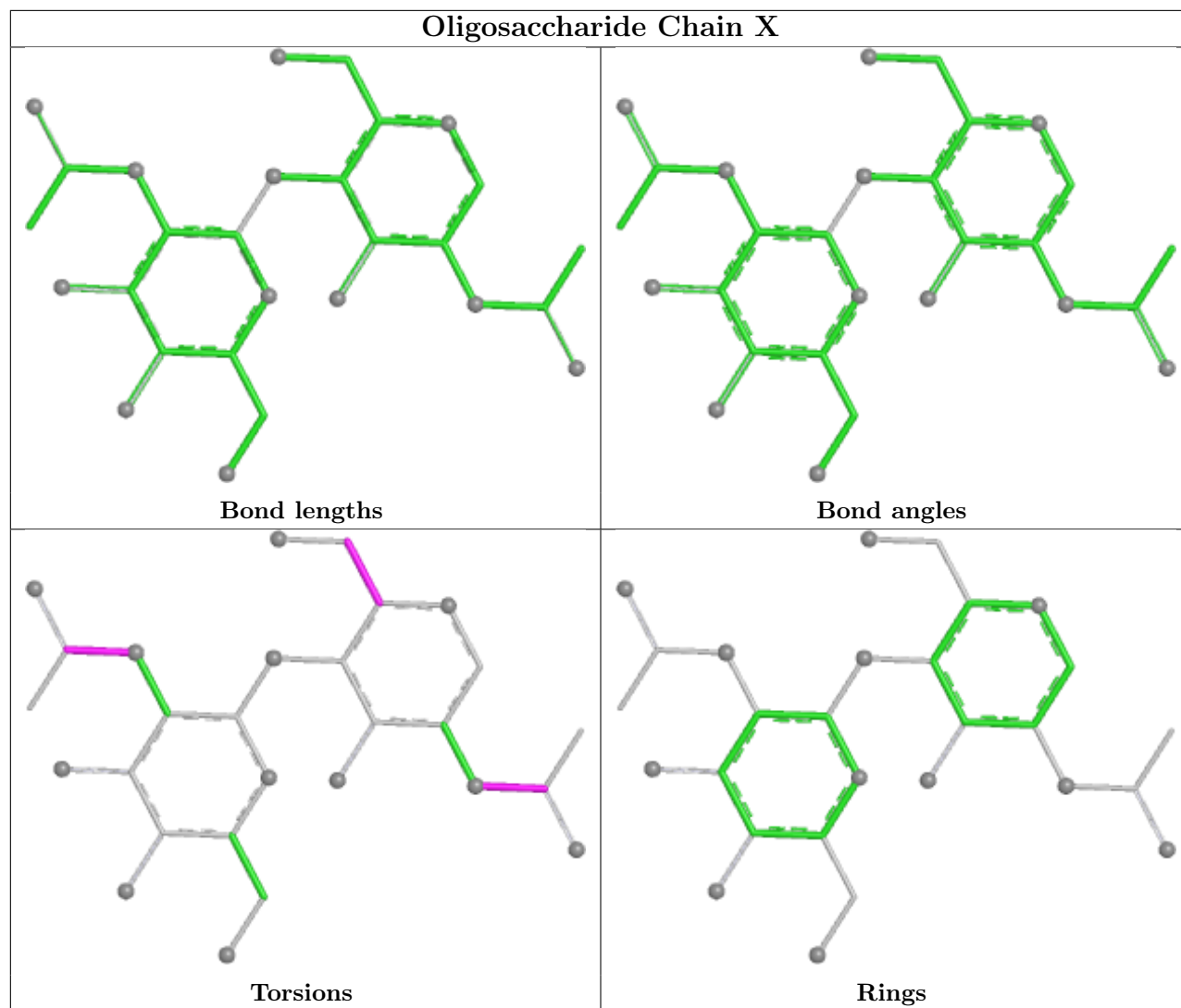


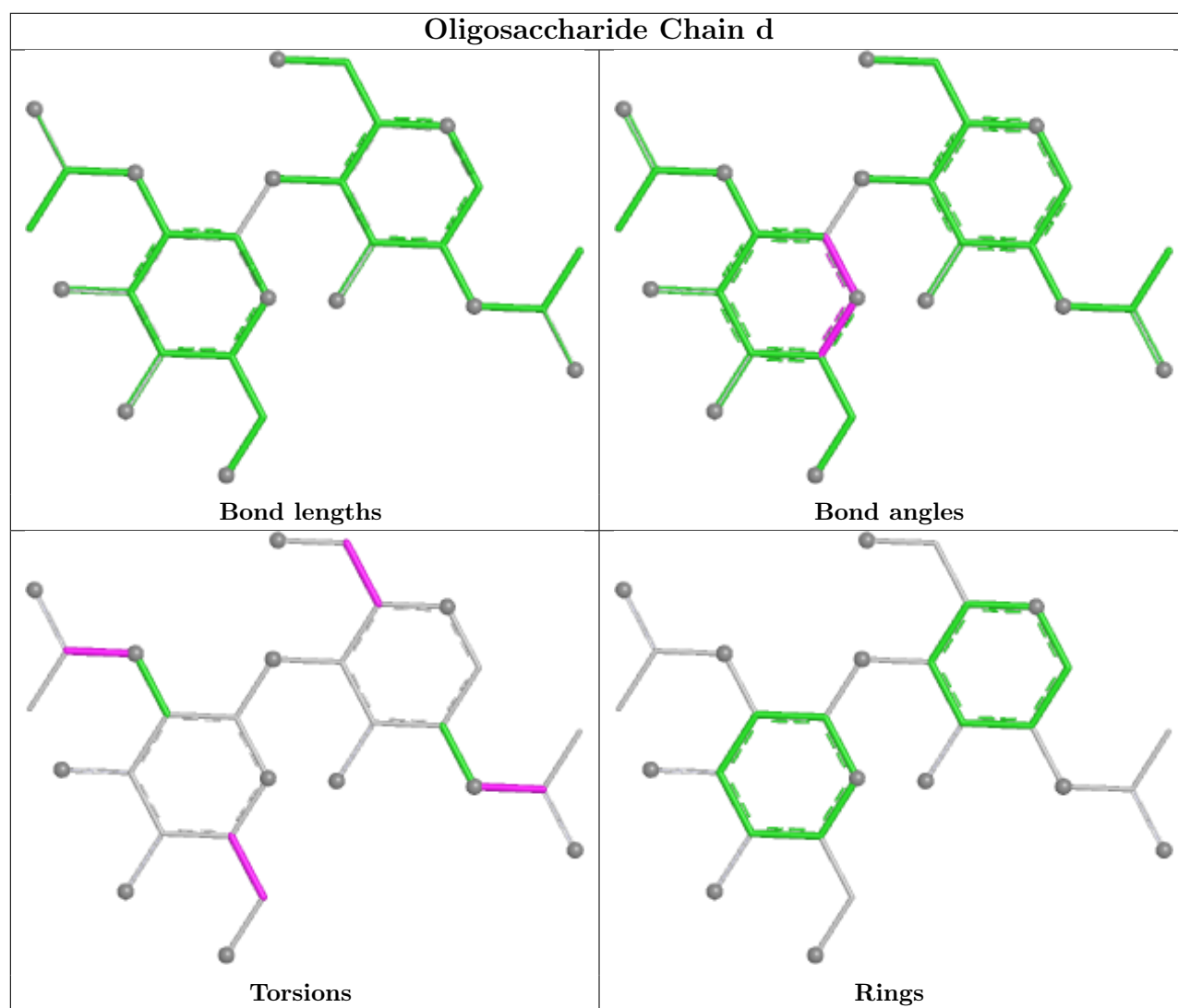


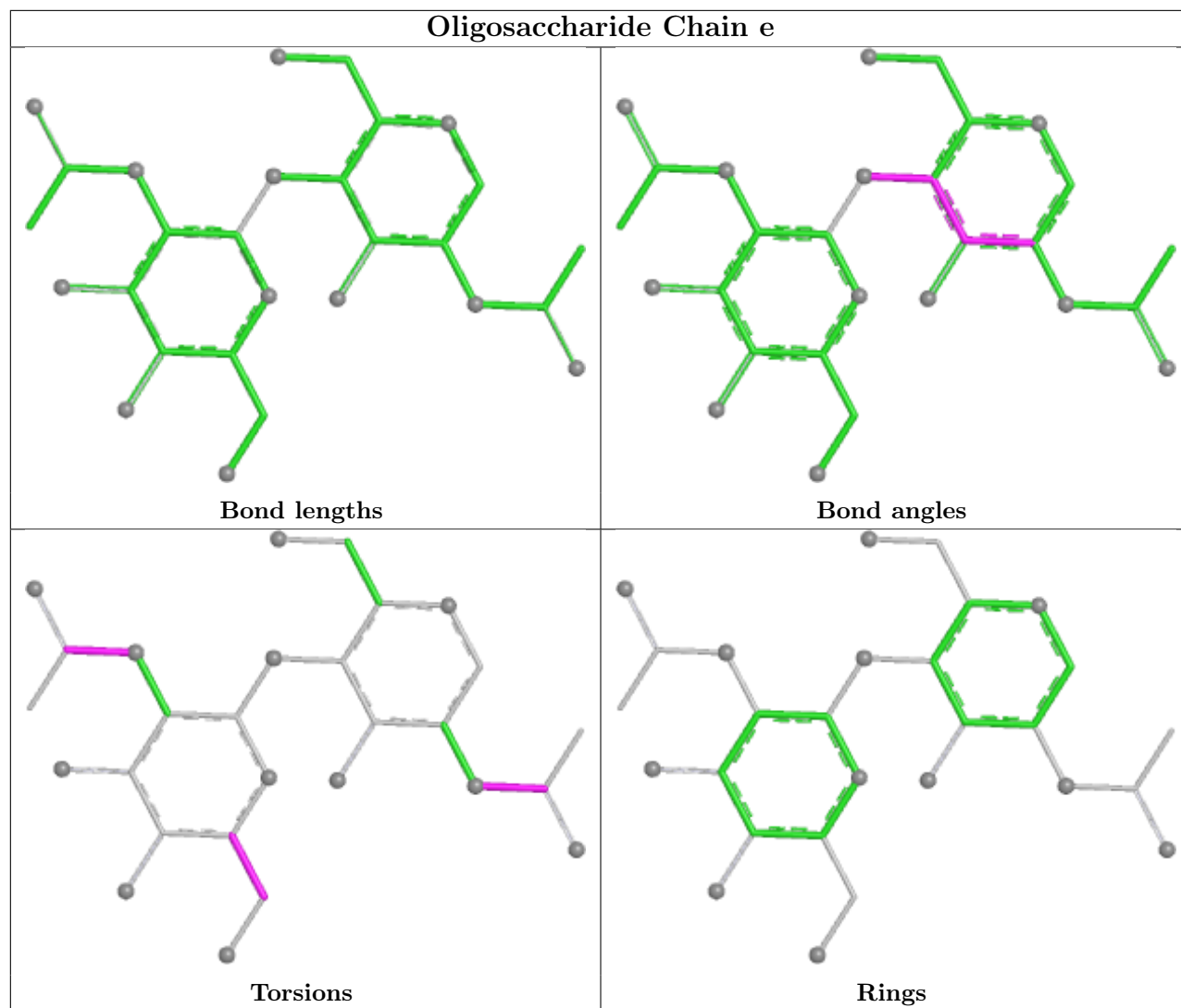


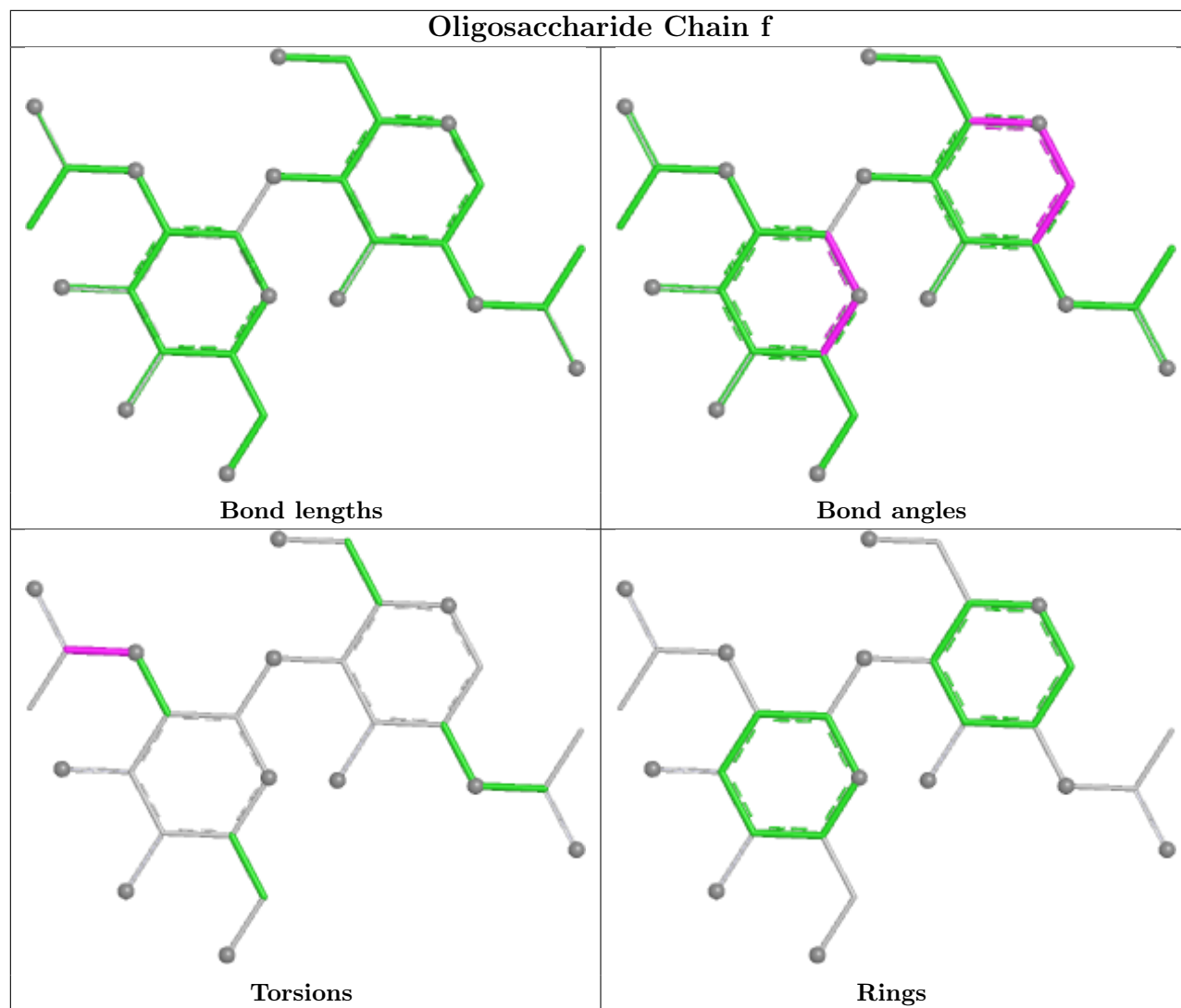


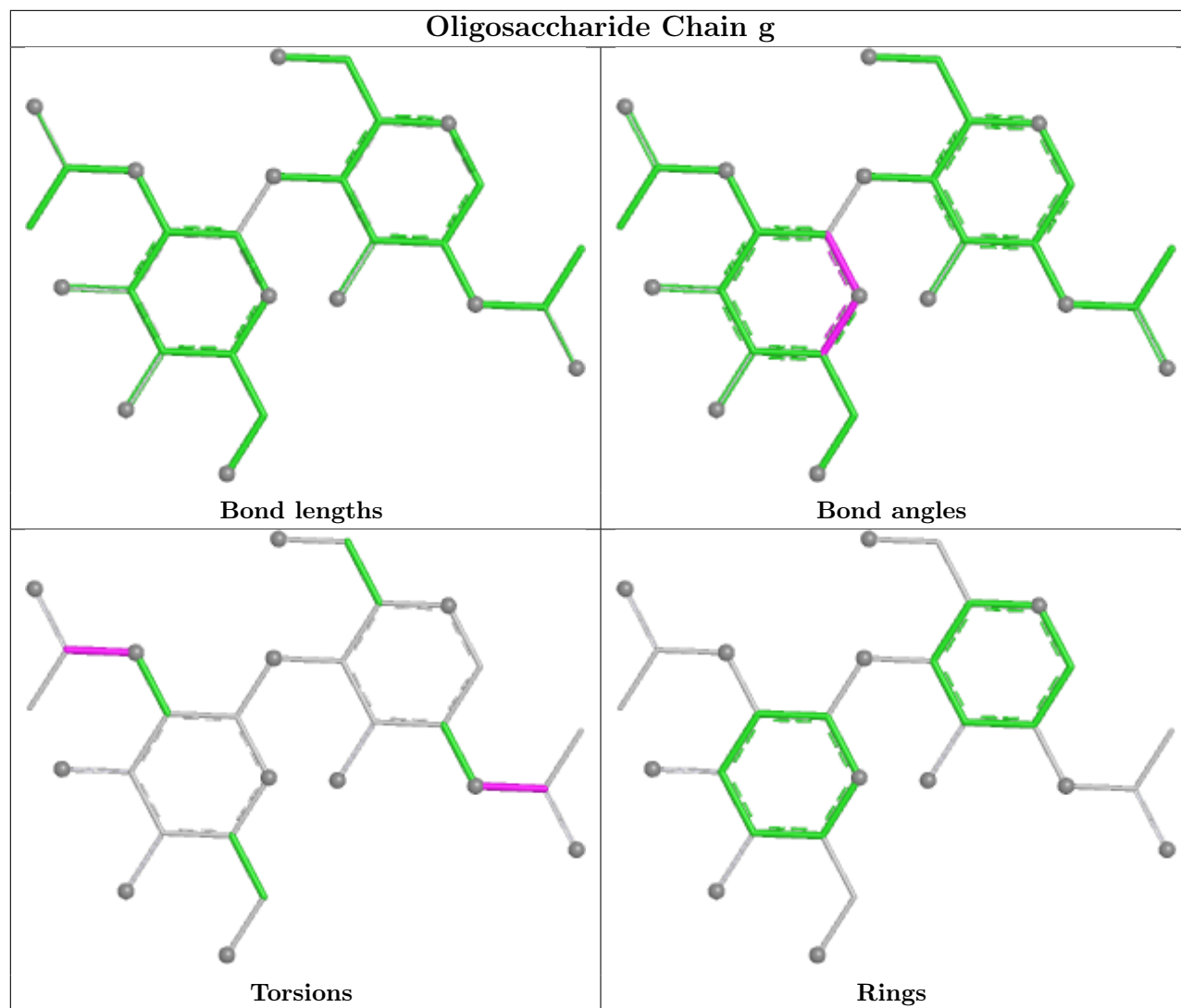




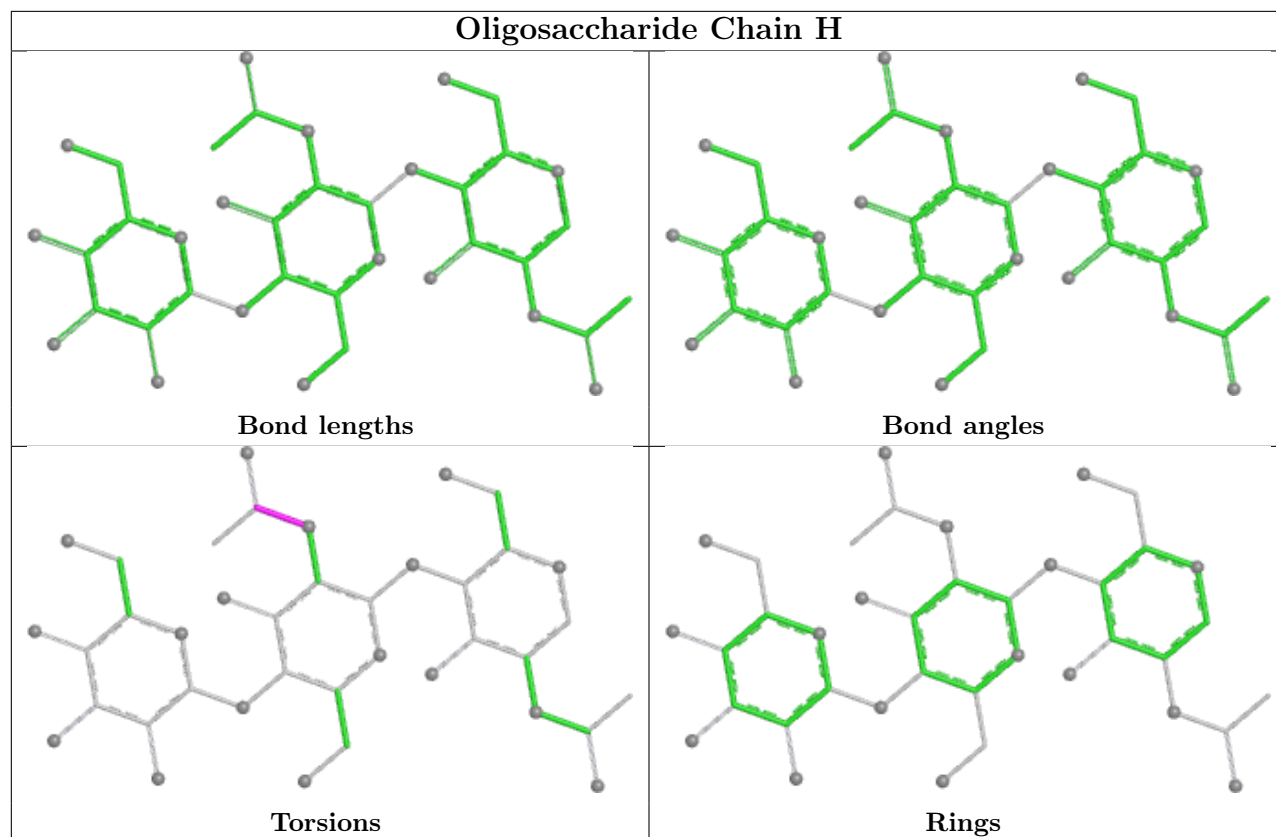




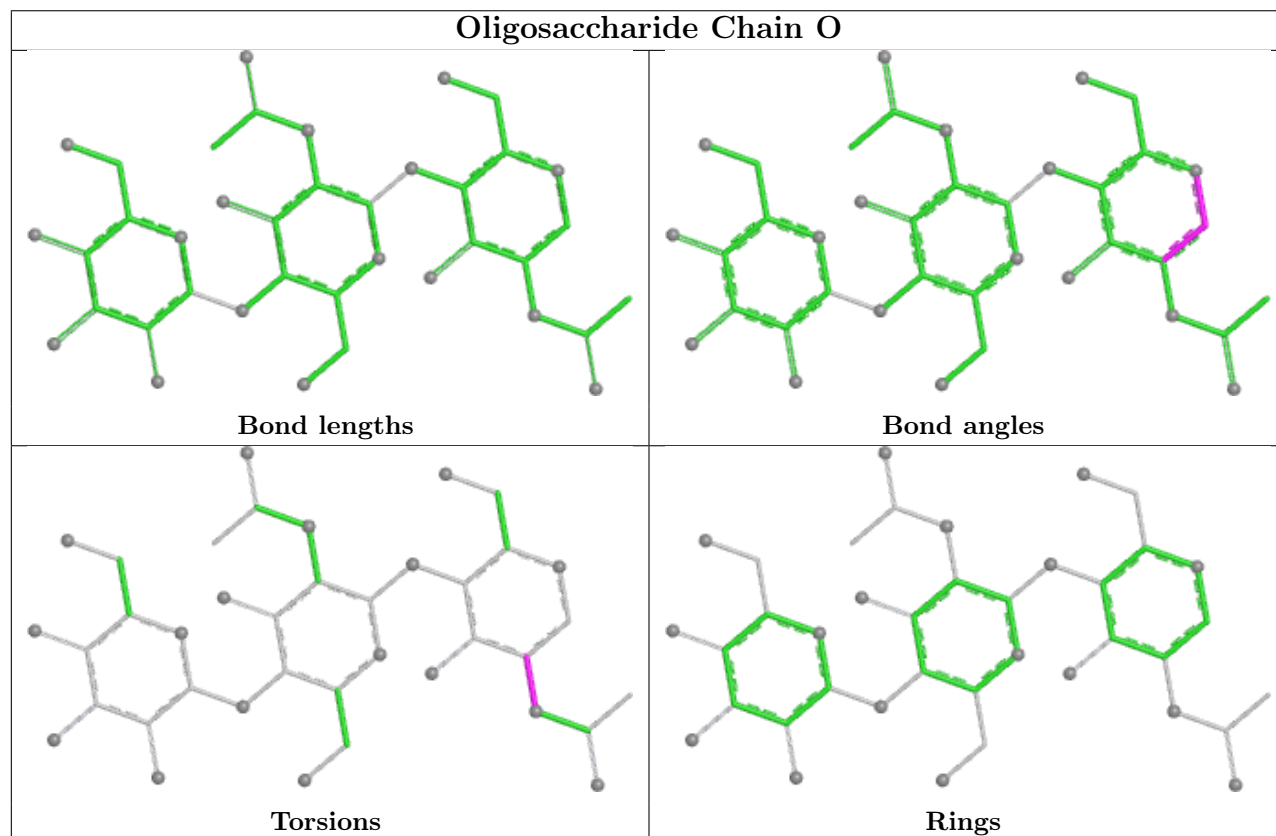


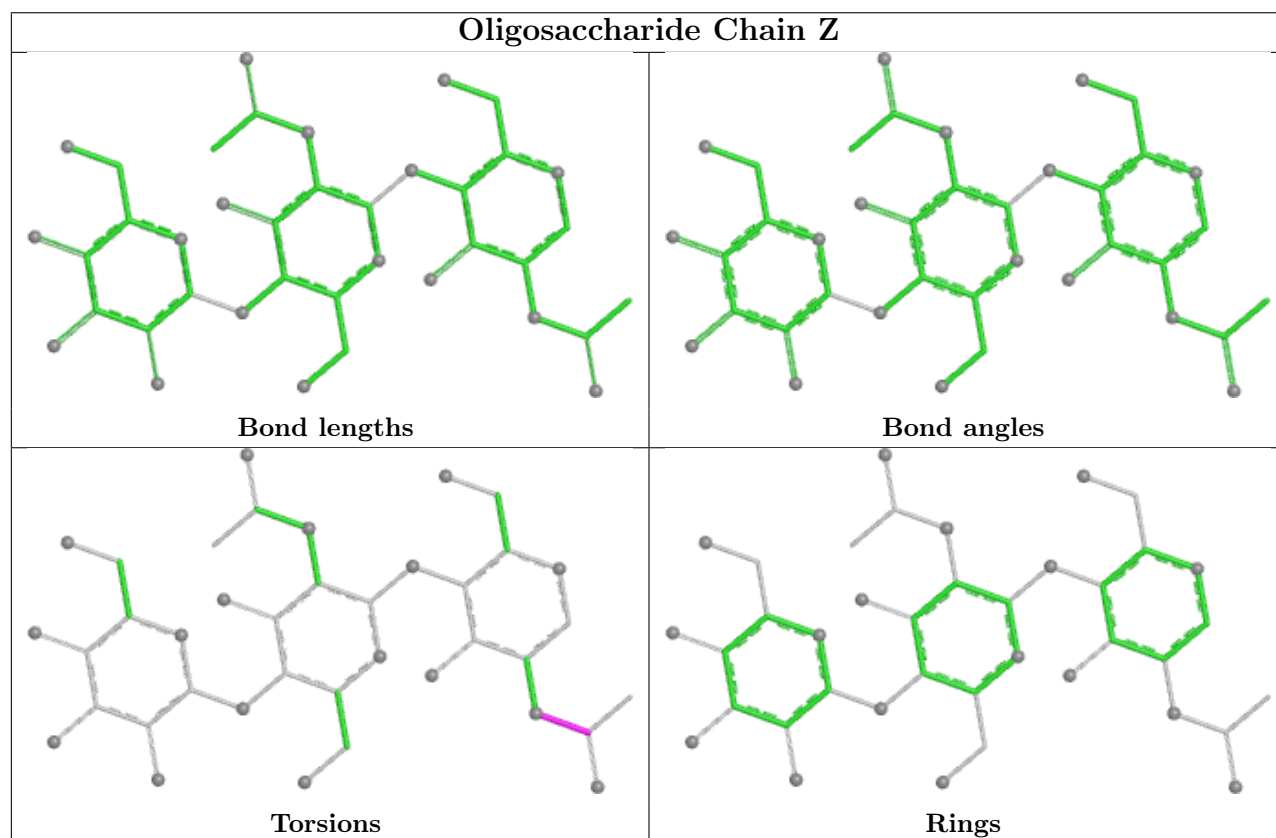
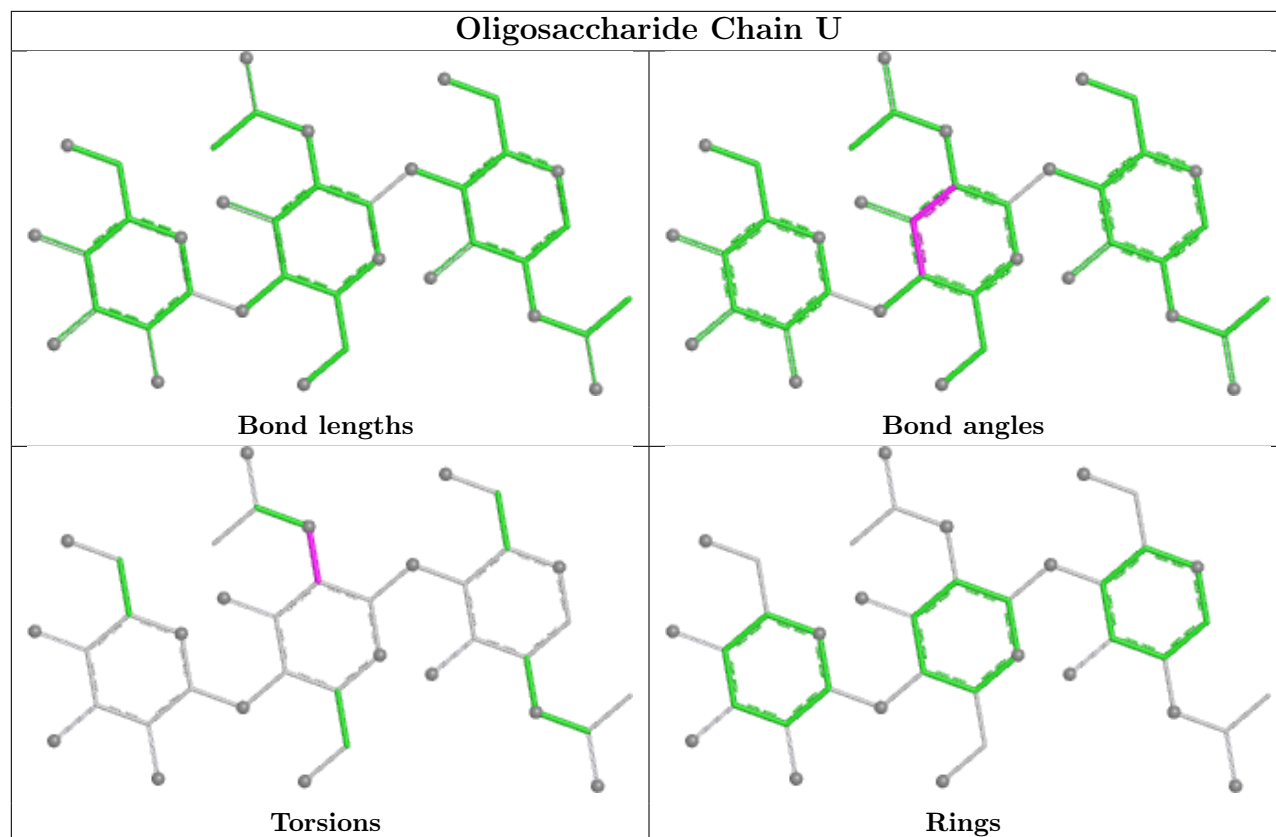


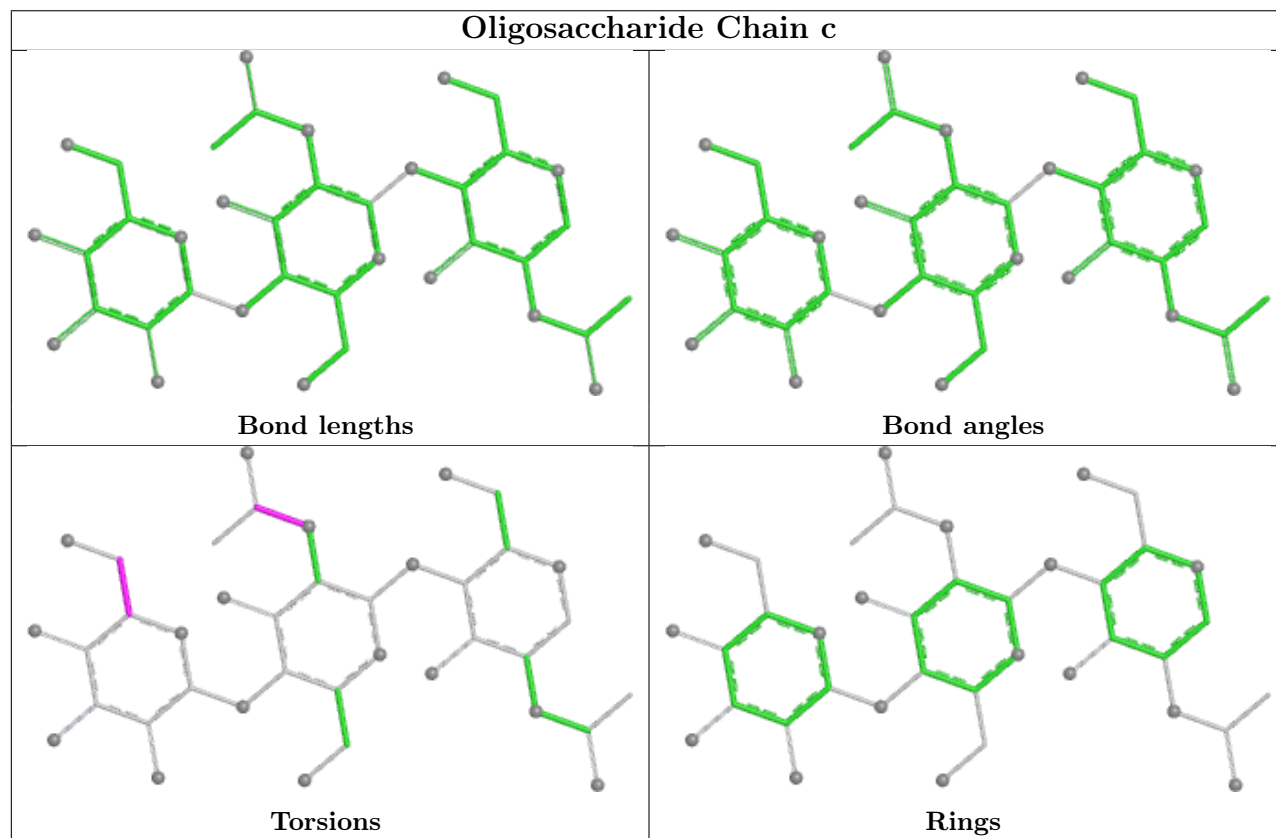
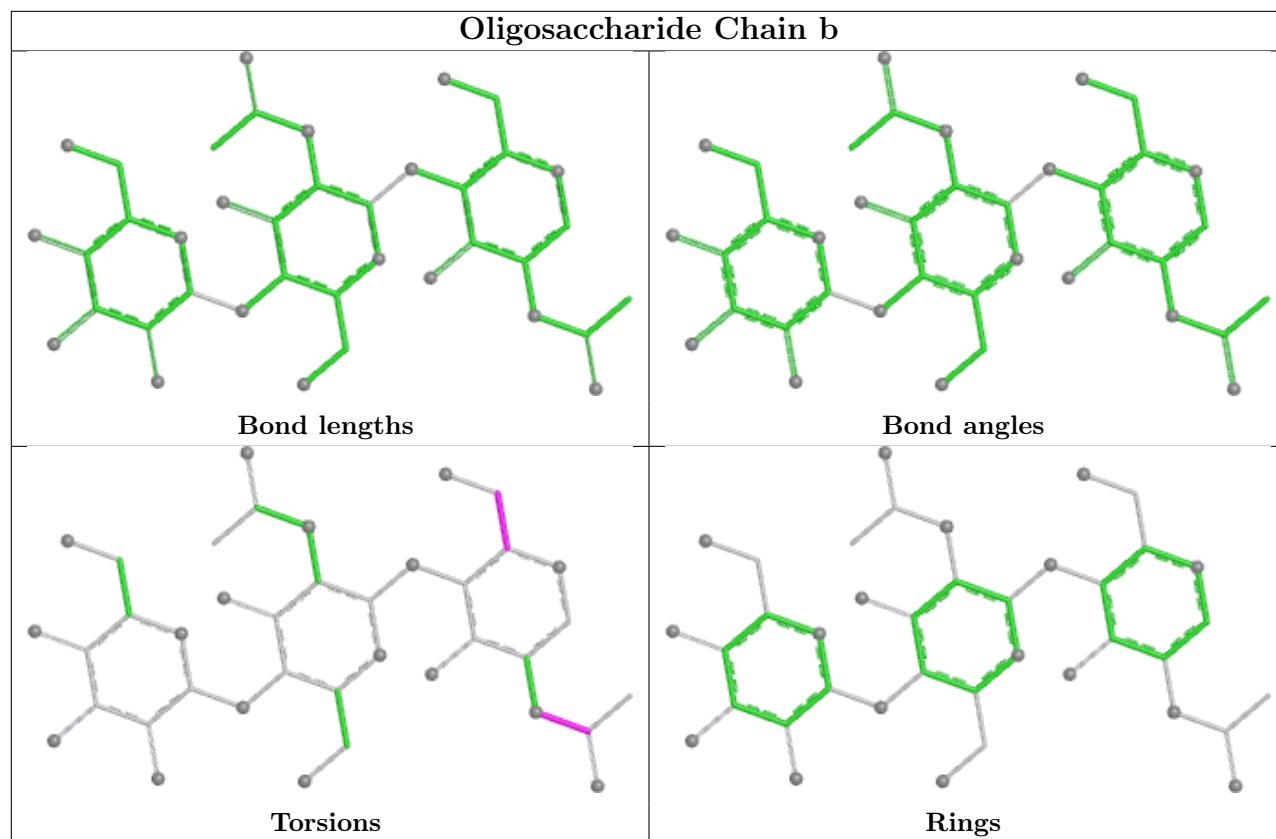
Oligosaccharide Chain H

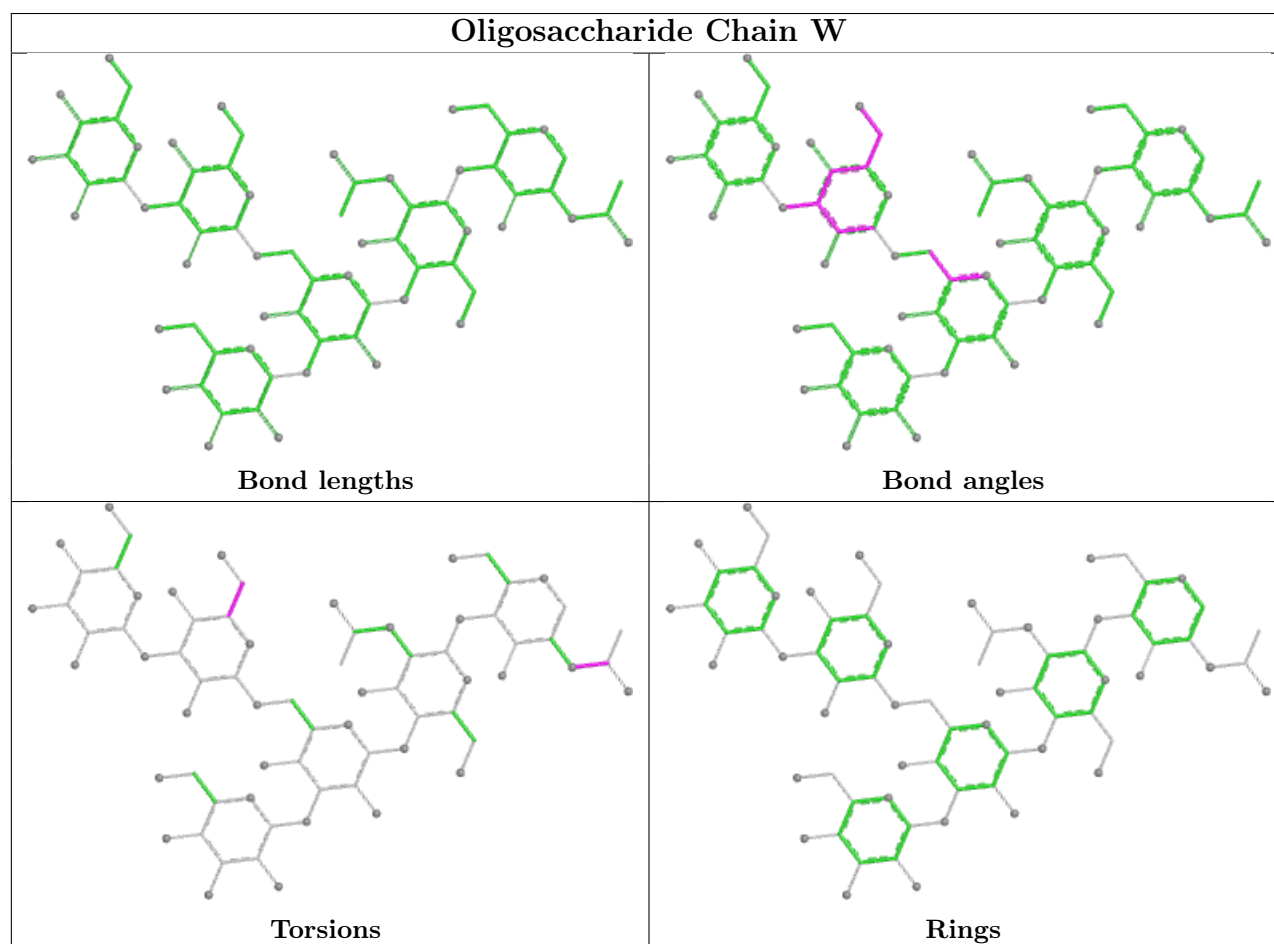
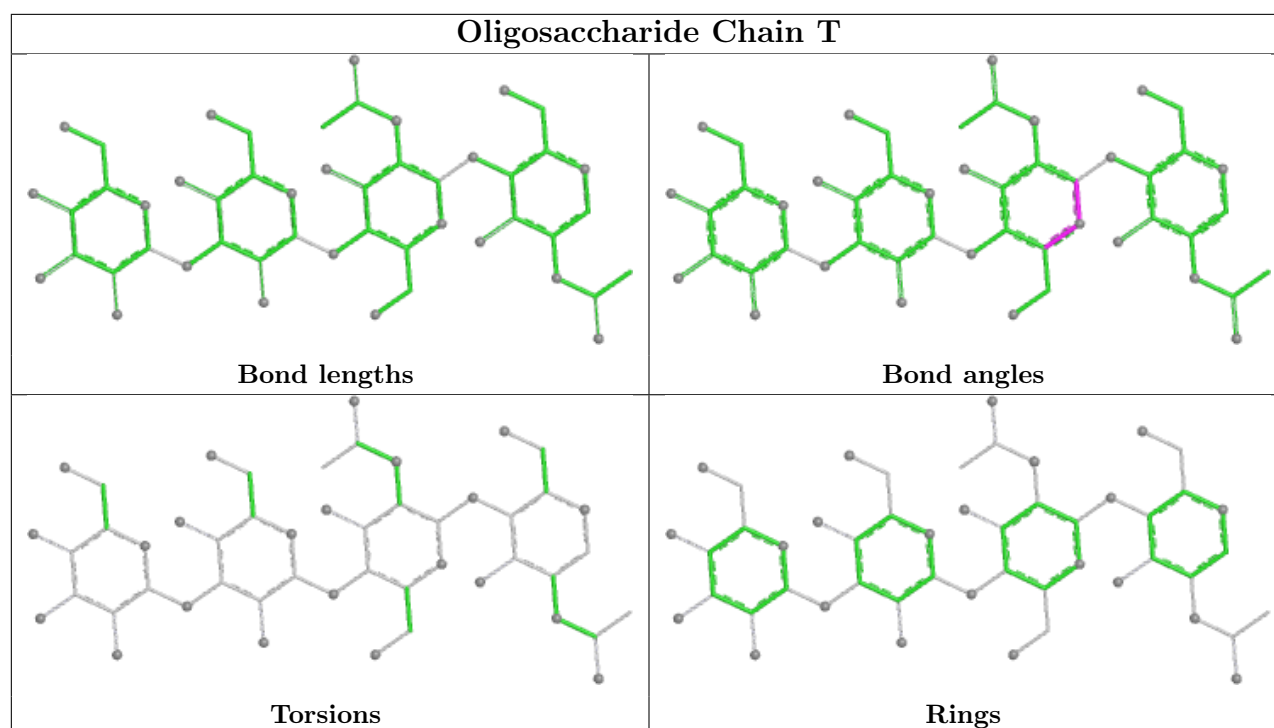


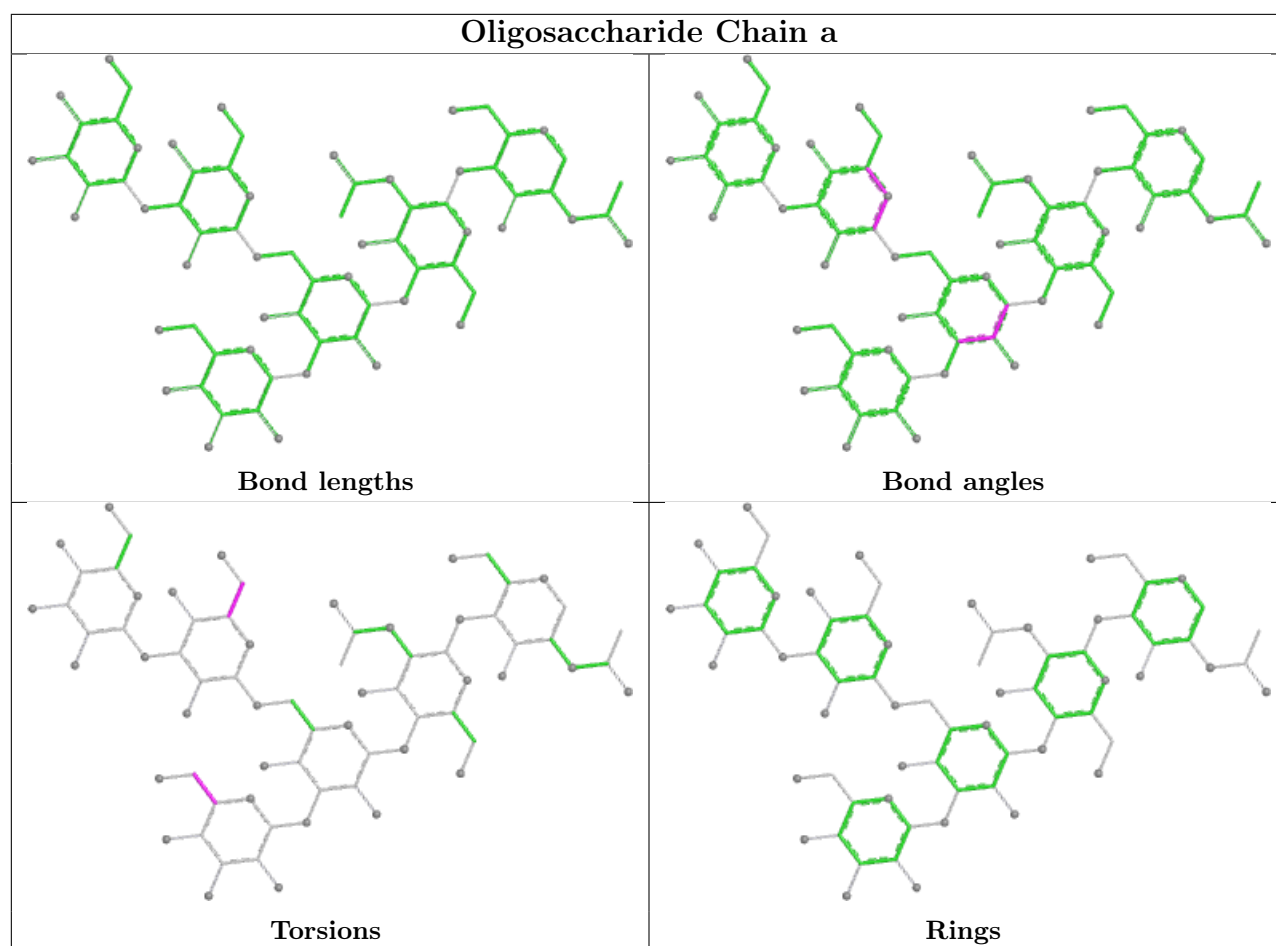
Oligosaccharide Chain O

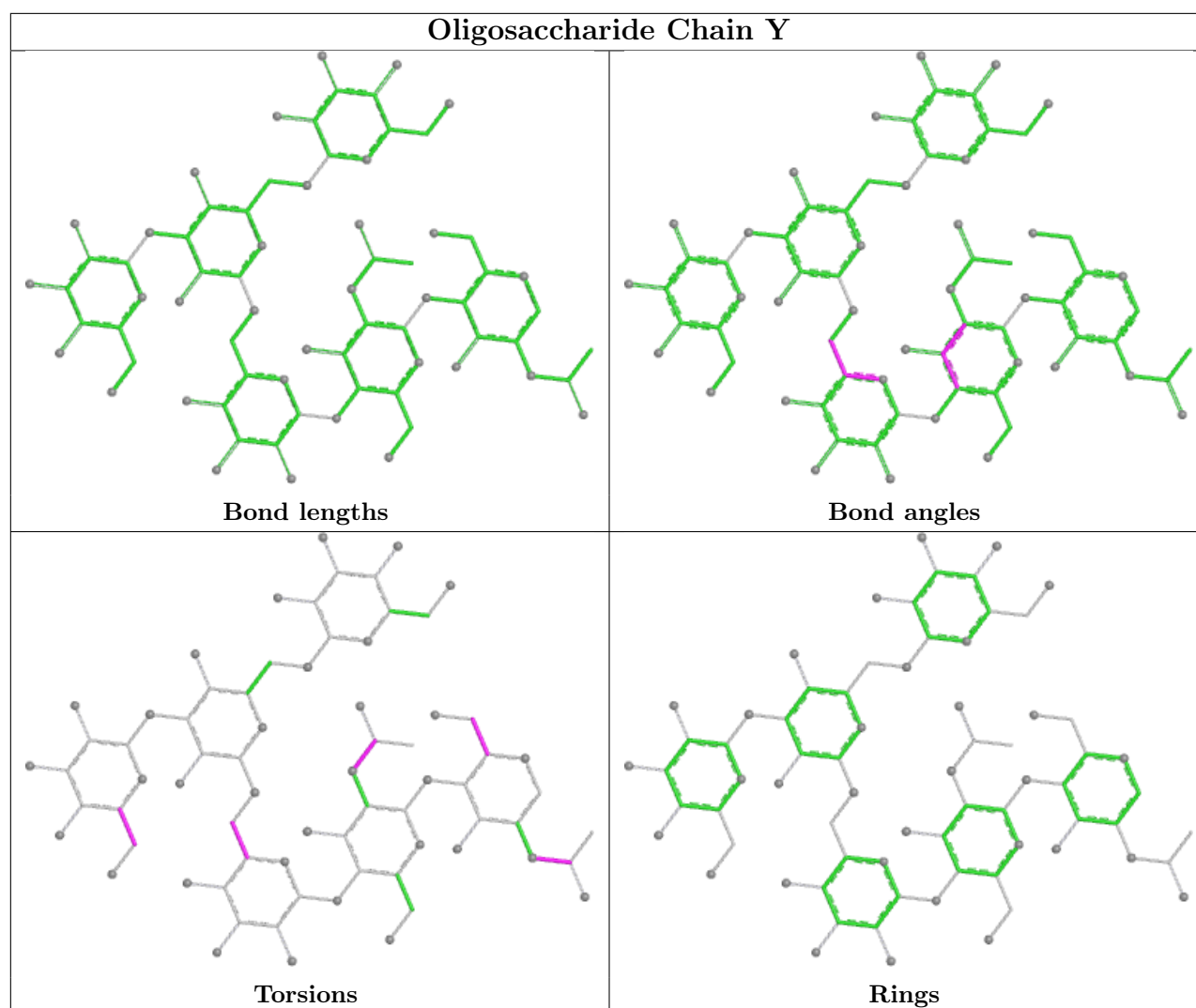












5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 4 are monoatomic - leaving 52 for Mogul analysis.

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	$\# Z > 2$
11	EDO	B	1029	-	3,3,3	0.44	0	2,2,2	0.33	0
9	NAG	A	1022	1	14,14,15	0.47	0	17,19,21	0.73	0
11	EDO	C	1136	-	3,3,3	0.42	0	2,2,2	0.39	0
11	EDO	A	1024	-	3,3,3	0.44	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EDO	C	1141	-	3,3,3	0.43	0	2,2,2	0.40	0
11	EDO	C	1137	-	3,3,3	0.43	0	2,2,2	0.39	0
11	EDO	B	1031	-	3,3,3	0.45	0	2,2,2	0.29	0
11	EDO	C	1135	-	3,3,3	0.42	0	2,2,2	0.40	0
11	EDO	A	1034	-	3,3,3	0.45	0	2,2,2	0.30	0
11	EDO	B	1025	-	3,3,3	0.39	0	2,2,2	0.52	0
11	EDO	B	1028	-	3,3,3	0.45	0	2,2,2	0.35	0
11	EDO	B	1034	-	3,3,3	0.46	0	2,2,2	0.26	0
11	EDO	A	1040	-	3,3,3	0.40	0	2,2,2	0.32	0
11	EDO	A	1030	-	3,3,3	0.42	0	2,2,2	0.40	0
9	NAG	D	1025	1	14,14,15	0.53	0	17,19,21	0.59	0
11	EDO	A	1025	-	3,3,3	0.44	0	2,2,2	0.35	0
11	EDO	C	1139	-	3,3,3	0.42	0	2,2,2	0.40	0
11	EDO	A	1028	-	3,3,3	0.45	0	2,2,2	0.31	0
11	EDO	D	1029	-	3,3,3	0.42	0	2,2,2	0.37	0
11	EDO	A	1029	-	3,3,3	0.42	0	2,2,2	0.23	0
11	EDO	D	1031	-	3,3,3	0.45	0	2,2,2	0.31	0
11	EDO	C	1144	-	3,3,3	0.43	0	2,2,2	0.40	0
11	EDO	A	1037	-	3,3,3	0.42	0	2,2,2	0.40	0
11	EDO	A	1039	-	3,3,3	0.41	0	2,2,2	0.40	0
11	EDO	C	1145	-	3,3,3	0.44	0	2,2,2	0.39	0
11	EDO	A	1038	-	3,3,3	0.43	0	2,2,2	0.38	0
11	EDO	A	1032	-	3,3,3	0.43	0	2,2,2	0.36	0
9	NAG	B	1021	1	14,14,15	0.56	0	17,19,21	0.88	0
11	EDO	A	1035	-	3,3,3	0.43	0	2,2,2	0.43	0
11	EDO	B	1024	-	3,3,3	0.42	0	2,2,2	0.39	0
11	EDO	A	1036	-	3,3,3	0.43	0	2,2,2	0.37	0
11	EDO	B	1027	-	3,3,3	0.39	0	2,2,2	0.43	0
11	EDO	B	1033	-	3,3,3	0.43	0	2,2,2	0.38	0
11	EDO	C	1140	-	3,3,3	0.48	0	2,2,2	0.25	0
11	EDO	B	1032	-	3,3,3	0.43	0	2,2,2	0.39	0
11	EDO	C	1138	-	3,3,3	0.43	0	2,2,2	0.39	0
11	EDO	D	1028	-	3,3,3	0.43	0	2,2,2	0.41	0
11	EDO	C	1146	-	3,3,3	0.46	0	2,2,2	0.26	0
11	EDO	B	1026	-	3,3,3	0.43	0	2,2,2	0.44	0
9	NAG	C	1117	1	14,14,15	0.51	0	17,19,21	0.74	0
9	NAG	D	1016	1	14,14,15	0.46	0	17,19,21	0.74	1 (5%)
11	EDO	C	1143	-	3,3,3	0.43	0	2,2,2	0.36	0
11	EDO	D	1027	-	3,3,3	0.41	0	2,2,2	0.42	0
9	NAG	A	1015	1	14,14,15	0.53	0	17,19,21	0.63	0
11	EDO	B	1023	-	3,3,3	0.41	0	2,2,2	0.41	0
11	EDO	B	1030	-	3,3,3	0.46	0	2,2,2	0.32	0
11	EDO	A	1031	-	3,3,3	0.45	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EDO	A	1026	-	3,3,3	0.43	0	2,2,2	0.39	0
11	EDO	A	1027	-	3,3,3	0.42	0	2,2,2	0.44	0
11	EDO	A	1033	-	3,3,3	0.42	0	2,2,2	0.36	0
11	EDO	D	1030	-	3,3,3	0.44	0	2,2,2	0.27	0
11	EDO	C	1142	-	3,3,3	0.43	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	B	1029	-	-	0/1/1/1	-
9	NAG	A	1022	1	-	2/6/23/26	0/1/1/1
11	EDO	C	1136	-	-	0/1/1/1	-
11	EDO	A	1024	-	-	0/1/1/1	-
11	EDO	C	1141	-	-	0/1/1/1	-
11	EDO	C	1137	-	-	0/1/1/1	-
11	EDO	B	1031	-	-	0/1/1/1	-
11	EDO	C	1135	-	-	0/1/1/1	-
11	EDO	A	1034	-	-	0/1/1/1	-
11	EDO	B	1025	-	-	0/1/1/1	-
11	EDO	B	1028	-	-	1/1/1/1	-
11	EDO	B	1034	-	-	1/1/1/1	-
11	EDO	A	1040	-	-	0/1/1/1	-
11	EDO	A	1030	-	-	0/1/1/1	-
9	NAG	D	1025	1	-	2/6/23/26	0/1/1/1
11	EDO	A	1025	-	-	0/1/1/1	-
11	EDO	C	1139	-	-	0/1/1/1	-
11	EDO	A	1028	-	-	0/1/1/1	-
11	EDO	D	1029	-	-	0/1/1/1	-
11	EDO	A	1029	-	-	0/1/1/1	-
11	EDO	D	1031	-	-	0/1/1/1	-
11	EDO	C	1144	-	-	0/1/1/1	-
11	EDO	A	1037	-	-	0/1/1/1	-
11	EDO	A	1039	-	-	0/1/1/1	-
11	EDO	C	1145	-	-	0/1/1/1	-
11	EDO	A	1038	-	-	0/1/1/1	-
11	EDO	A	1032	-	-	0/1/1/1	-
9	NAG	B	1021	1	-	2/6/23/26	0/1/1/1
11	EDO	A	1035	-	-	0/1/1/1	-
11	EDO	B	1024	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	A	1036	-	-	0/1/1/1	-
11	EDO	B	1027	-	-	0/1/1/1	-
11	EDO	B	1033	-	-	0/1/1/1	-
11	EDO	C	1140	-	-	0/1/1/1	-
11	EDO	B	1032	-	-	0/1/1/1	-
11	EDO	C	1138	-	-	0/1/1/1	-
11	EDO	D	1028	-	-	0/1/1/1	-
11	EDO	C	1146	-	-	0/1/1/1	-
11	EDO	B	1026	-	-	0/1/1/1	-
9	NAG	C	1117	1	1/1/5/7	2/6/23/26	0/1/1/1
9	NAG	D	1016	1	-	2/6/23/26	0/1/1/1
11	EDO	C	1143	-	-	0/1/1/1	-
11	EDO	D	1027	-	-	0/1/1/1	-
9	NAG	A	1015	1	1/1/5/7	3/6/23/26	0/1/1/1
11	EDO	B	1023	-	-	0/1/1/1	-
11	EDO	B	1030	-	-	0/1/1/1	-
11	EDO	A	1031	-	-	1/1/1/1	-
11	EDO	A	1026	-	-	0/1/1/1	-
11	EDO	A	1027	-	-	1/1/1/1	-
11	EDO	A	1033	-	-	0/1/1/1	-
11	EDO	D	1030	-	-	0/1/1/1	-
11	EDO	C	1142	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1016	NAG	C1-O5-C5	2.01	114.89	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1015	NAG	C1
9	C	1117	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1015	NAG	C1-C2-N2-C7
9	A	1015	NAG	C8-C7-N2-C2
9	A	1015	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	A	1022	NAG	C8-C7-N2-C2
9	A	1022	NAG	O7-C7-N2-C2
9	B	1021	NAG	C8-C7-N2-C2
9	B	1021	NAG	O7-C7-N2-C2
9	C	1117	NAG	C8-C7-N2-C2
9	C	1117	NAG	O7-C7-N2-C2
9	D	1016	NAG	C8-C7-N2-C2
9	D	1016	NAG	O7-C7-N2-C2
9	D	1025	NAG	C8-C7-N2-C2
9	D	1025	NAG	O7-C7-N2-C2
11	B	1034	EDO	O1-C1-C2-O2
11	A	1031	EDO	O1-C1-C2-O2
11	B	1028	EDO	O1-C1-C2-O2
11	A	1027	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1141	EDO	1	0
11	B	1031	EDO	1	0
11	B	1025	EDO	1	0
11	B	1028	EDO	1	0
11	B	1034	EDO	2	0
11	A	1040	EDO	1	0
11	C	1139	EDO	1	0
11	A	1028	EDO	2	0
11	A	1029	EDO	2	0
11	A	1032	EDO	1	0
11	B	1027	EDO	3	0
11	C	1146	EDO	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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	903/950 (95%)	-0.46	3 (0%) 90 88	31, 54, 87, 120	0
1	B	904/950 (95%)	-0.49	8 (0%) 81 78	31, 51, 83, 124	1 (0%)
1	C	905/950 (95%)	-0.47	4 (0%) 88 86	34, 53, 85, 126	0
1	D	904/950 (95%)	-0.47	3 (0%) 90 88	33, 55, 85, 123	0
All	All	3616/3800 (95%)	-0.47	18 (0%) 87 85	31, 53, 85, 126	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	LEU	4.4
1	C	894	GLY	3.1
1	B	895	SER	3.1
1	A	63	THR	3.1
1	B	331[A]	HIS	3.0
1	D	895	SER	2.6
1	D	928	THR	2.6
1	C	929	GLY	2.5
1	B	395	PHE	2.3
1	C	928	THR	2.3
1	D	929	GLY	2.2
1	B	894	GLY	2.2
1	A	294	ALA	2.2
1	B	332	TYR	2.2
1	C	63	THR	2.1
1	A	97	ASP	2.0
1	B	492	SER	2.0
1	B	64	THR	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BMA	W	4	11/12	0.03	0.17	138,140,141,142	0
5	BMA	U	3	11/12	0.15	0.15	123,126,129,132	0
5	BMA	O	3	11/12	0.18	0.18	105,108,114,116	0
2	BMA	R	3	11/12	0.23	0.15	134,138,146,147	0
4	NAG	V	1	14/15	0.24	0.18	149,151,153,156	0
7	BMA	W	5	11/12	0.27	0.18	131,138,142,143	0
2	BMA	K	4	11/12	0.32	0.18	132,138,143,143	0
5	BMA	H	3	11/12	0.34	0.15	120,127,130,133	0
7	BMA	W	3	11/12	0.37	0.14	121,129,136,138	0
2	BMA	R	4	11/12	0.42	0.14	146,150,152,153	0
2	NAG	R	2	14/15	0.43	0.17	126,131,133,133	0
3	BMA	F	5	11/12	0.44	0.15	103,109,113,115	0
7	BMA	W	6	11/12	0.44	0.16	122,126,128,129	0
6	BMA	T	3	11/12	0.46	0.16	113,124,129,131	0
2	BMA	E	3	11/12	0.47	0.14	106,108,111,114	0
8	BMA	Y	6	11/12	0.49	0.17	133,143,147,148	0
6	BMA	T	4	11/12	0.50	0.14	127,134,137,138	0
5	NAG	Z	2	14/15	0.50	0.20	121,128,134,134	0
3	BMA	S	5	11/12	0.51	0.15	103,105,114,114	0
4	NAG	G	2	14/15	0.51	0.16	110,115,121,122	0
4	NAG	V	2	14/15	0.52	0.16	139,156,163,163	0
2	BMA	K	3	11/12	0.52	0.14	129,131,133,137	0
3	BMA	L	4	11/12	0.53	0.18	104,108,110,111	0
4	NAG	Q	2	14/15	0.55	0.18	118,123,130,132	0
2	NAG	J	2	14/15	0.55	0.15	109,114,120,122	0
5	BMA	Z	3	11/12	0.56	0.16	131,136,139,141	0
8	BMA	Y	3	11/12	0.57	0.17	138,144,148,148	0
4	NAG	N	2	14/15	0.57	0.15	108,121,126,126	0
8	BMA	Y	5	11/12	0.58	0.14	138,141,145,145	0
8	NAG	Y	1	14/15	0.60	0.15	114,122,126,127	0
2	BMA	J	4	11/12	0.61	0.13	120,125,128,129	0
5	NAG	O	2	14/15	0.61	0.14	95,99,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	L	3	11/12	0.64	0.16	94,96,102,106	0
4	NAG	M	2	14/15	0.66	0.14	112,116,121,122	0
5	NAG	U	2	14/15	0.67	0.12	99,109,115,118	0
3	BMA	F	4	11/12	0.68	0.12	98,100,102,102	0
2	BMA	J	3	11/12	0.68	0.14	126,128,132,134	0
2	NAG	K	2	14/15	0.69	0.14	99,105,115,124	0
4	NAG	X	2	14/15	0.69	0.13	123,127,133,135	0
8	NAG	Y	2	14/15	0.69	0.13	124,128,135,135	0
8	BMA	Y	4	11/12	0.71	0.15	134,143,145,146	0
5	NAG	O	1	14/15	0.71	0.14	87,89,94,95	0
4	NAG	N	1	14/15	0.71	0.16	92,102,108,113	0
2	BMA	E	4	11/12	0.73	0.13	100,107,109,110	0
2	NAG	J	1	14/15	0.73	0.16	86,97,102,106	0
4	NAG	Q	1	14/15	0.73	0.17	100,107,113,116	0
4	NAG	P	2	14/15	0.75	0.13	80,87,99,102	0
4	NAG	d	1	14/15	-	-	131,138,145,147	0
4	NAG	d	2	14/15	-	-	148,153,158,158	0
4	NAG	e	1	14/15	-	-	73,75,79,88	0
4	NAG	e	2	14/15	-	-	94,97,101,102	0
4	NAG	f	1	14/15	-	-	103,108,115,117	0
4	NAG	f	2	14/15	-	-	115,120,124,125	0
4	NAG	g	1	14/15	-	-	128,131,133,134	0
4	NAG	g	2	14/15	-	-	126,131,135,136	0
4	NAG	I	2	14/15	0.77	0.11	87,94,99,101	0
4	NAG	G	1	14/15	0.77	0.12	84,92,98,105	0
3	BMA	L	5	11/12	0.78	0.12	99,102,107,108	0
7	NAG	W	2	14/15	0.78	0.14	88,94,104,112	0
3	BMA	S	3	11/12	0.78	0.12	85,92,98,99	0
4	NAG	M	1	14/15	0.79	0.13	81,100,109,109	0
4	NAG	X	1	14/15	0.79	0.15	106,117,122,125	0
5	NAG	H	2	14/15	0.80	0.10	100,105,112,115	0
3	BMA	F	3	11/12	0.81	0.11	85,92,98,102	0
3	BMA	S	4	11/12	0.82	0.13	95,103,106,108	0
2	NAG	R	1	14/15	0.82	0.13	92,112,119,123	0
5	NAG	U	1	14/15	0.83	0.11	84,96,100,105	0
5	NAG	b	1	14/15	-	-	67,78,79,85	0
5	NAG	b	2	14/15	-	-	90,93,100,100	0
5	BMA	b	3	11/12	-	-	103,107,110,113	0
5	NAG	c	1	14/15	-	-	81,95,105,112	0
5	NAG	c	2	14/15	-	-	115,122,129,133	0
5	BMA	c	3	11/12	-	-	138,142,145,148	0
7	NAG	W	1	14/15	0.84	0.11	77,85,87,90	0

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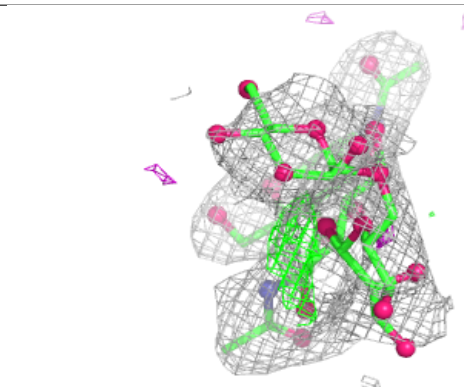
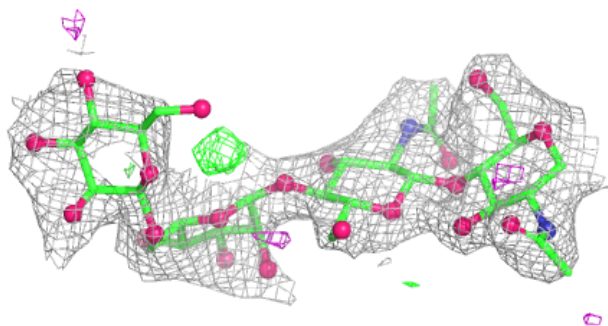
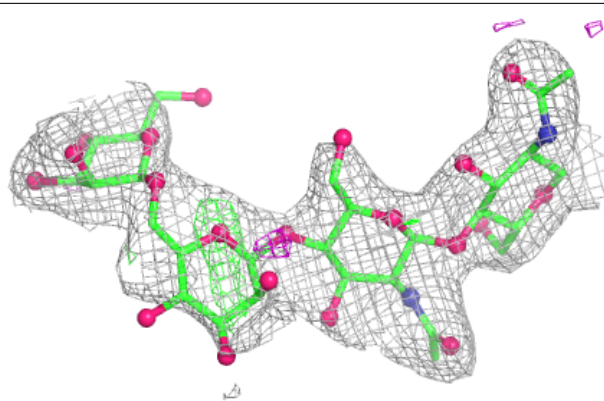
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.84	0.10	80,88,95,102	0
5	NAG	Z	1	14/15	0.85	0.12	106,114,117,120	0
6	NAG	T	2	14/15	0.86	0.11	86,91,97,104	0
5	NAG	H	1	14/15	0.88	0.10	76,90,95,99	0
2	NAG	K	1	14/15	0.88	0.12	80,88,93,98	0
3	NAG	L	2	14/15	0.88	0.10	67,70,79,85	0
3	NAG	F	2	14/15	0.90	0.09	63,71,74,80	0
3	NAG	F	1	14/15	0.90	0.10	49,55,60,61	0
4	NAG	I	1	14/15	0.92	0.07	67,70,74,81	0
7	NAG	a	1	14/15	-	-	59,63,65,65	0
7	NAG	a	2	14/15	-	-	61,70,74,80	0
7	BMA	a	3	11/12	-	-	87,94,100,103	0
7	BMA	a	4	11/12	-	-	104,106,109,112	0
7	BMA	a	5	11/12	-	-	115,117,121,122	0
7	BMA	a	6	11/12	-	-	107,113,116,117	0
4	NAG	P	1	14/15	0.92	0.07	68,72,79,82	0
3	NAG	S	2	14/15	0.93	0.07	59,64,72,78	0
3	NAG	L	1	14/15	0.93	0.09	58,59,67,68	0
6	NAG	T	1	14/15	0.93	0.09	67,76,81,86	0
2	NAG	E	1	14/15	0.95	0.07	59,65,69,76	0
3	NAG	S	1	14/15	0.96	0.07	58,61,64,66	0

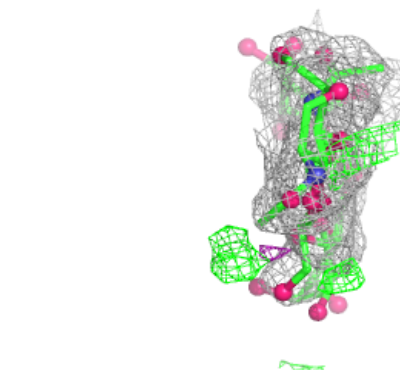
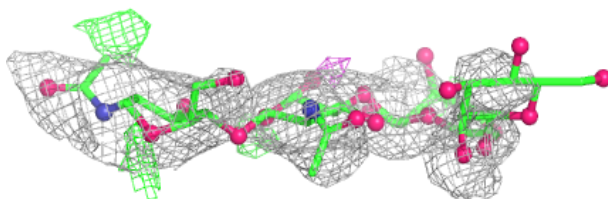
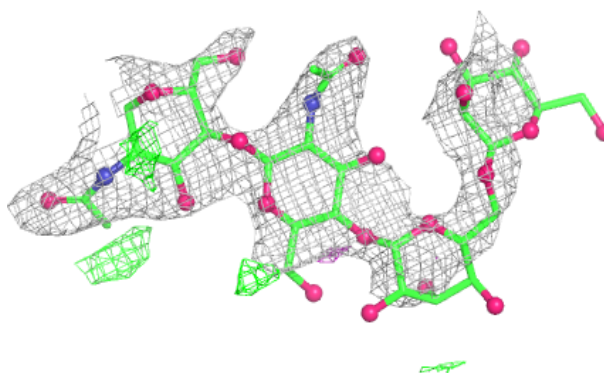
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

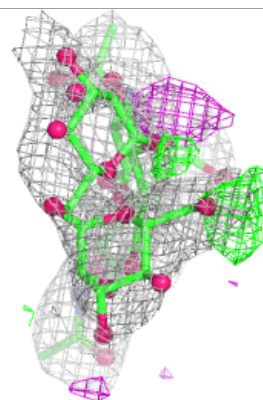
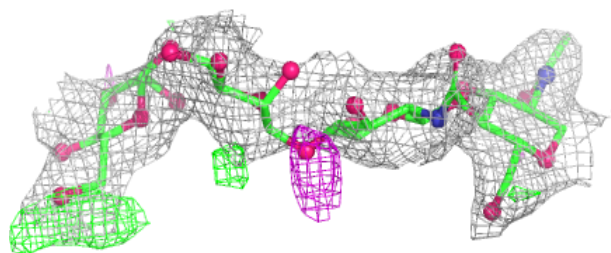
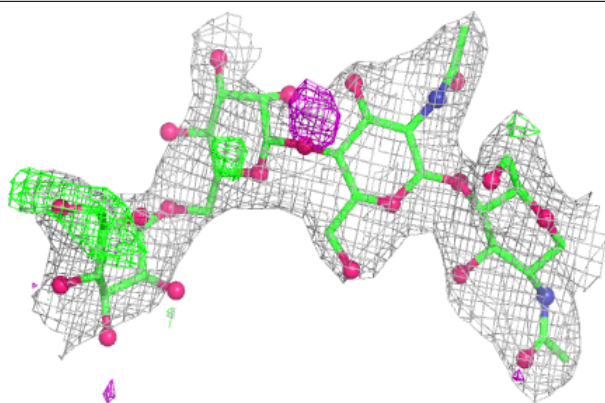
**Electron density around Chain J:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

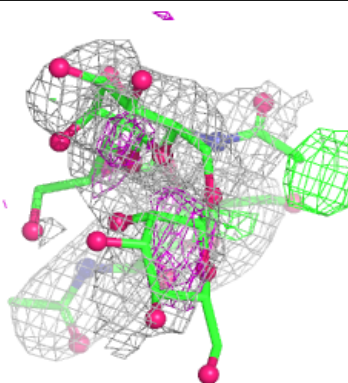
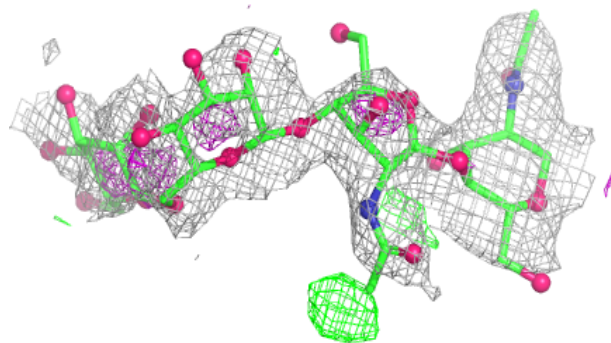
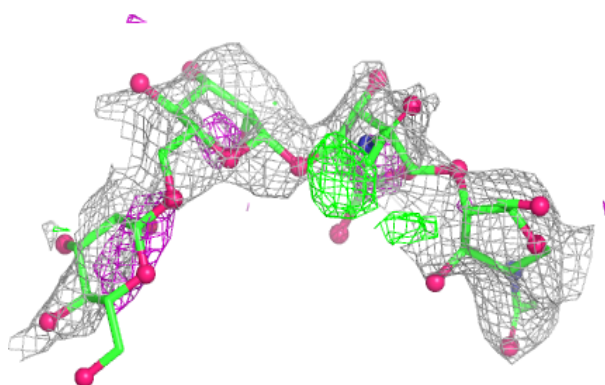


Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

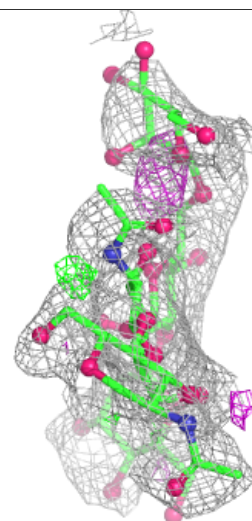
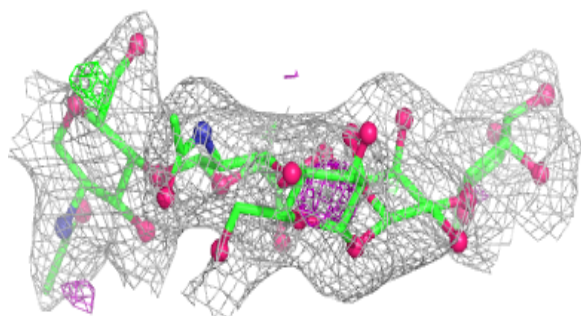
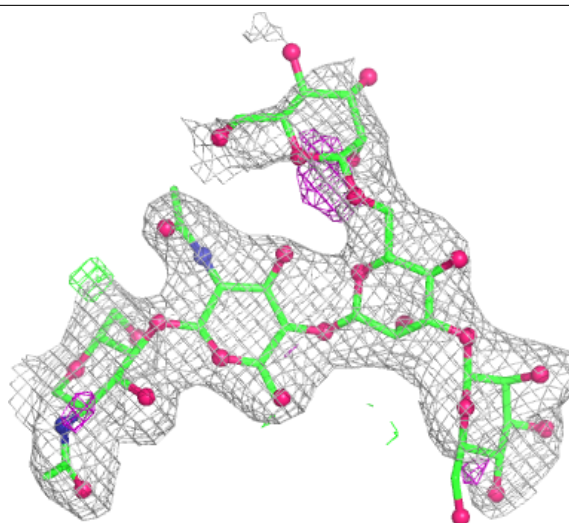
**Electron density around Chain R:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



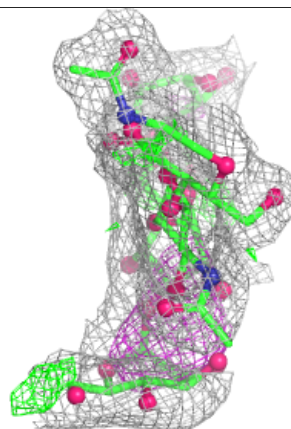
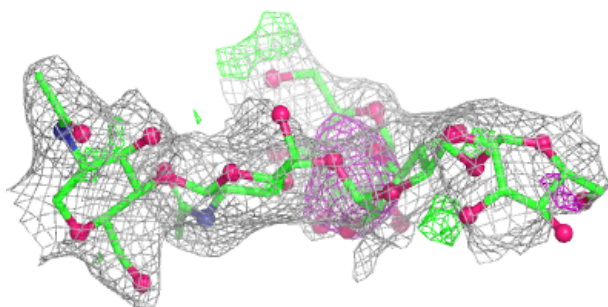
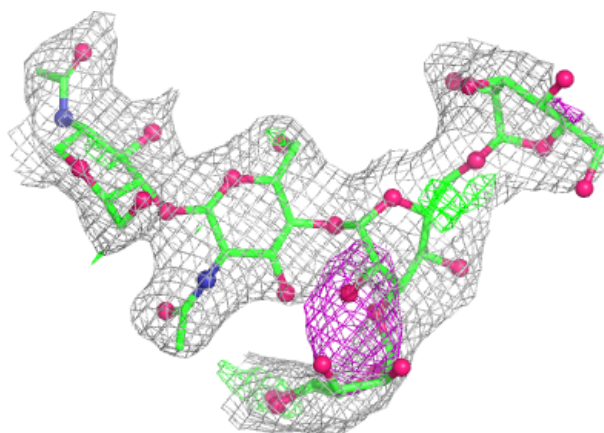
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

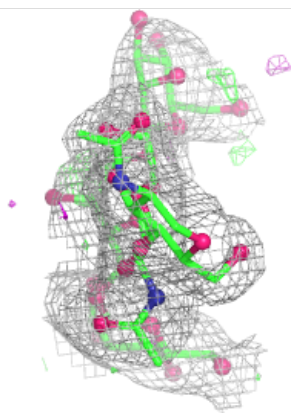
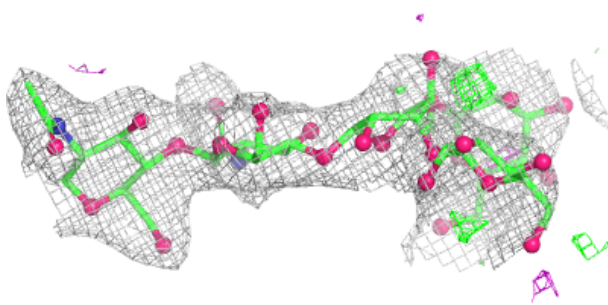
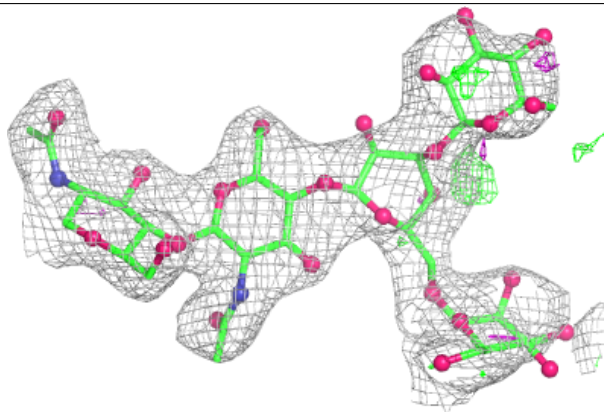


Electron density around Chain L:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

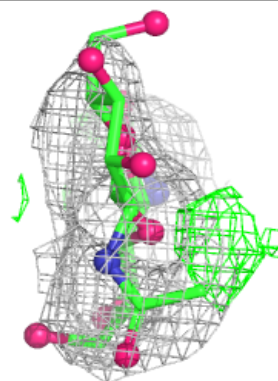
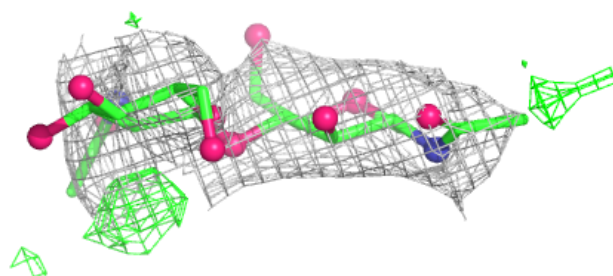
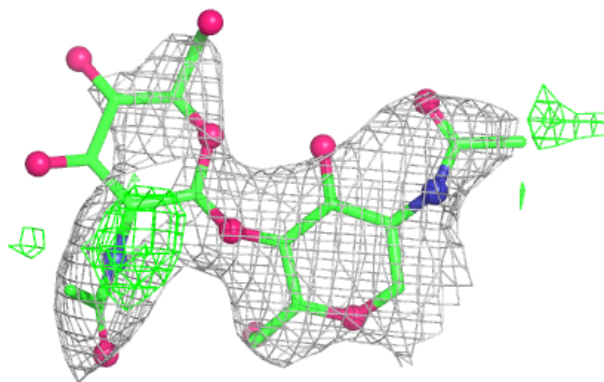
**Electron density around Chain S:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



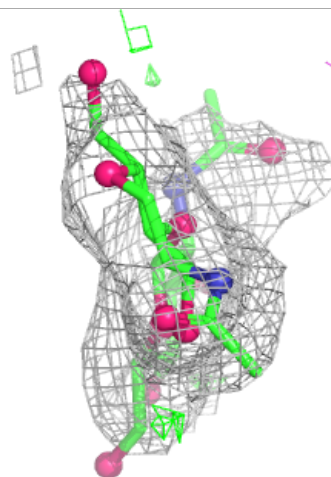
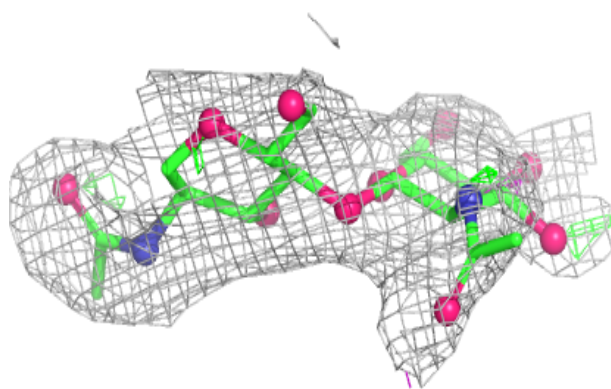
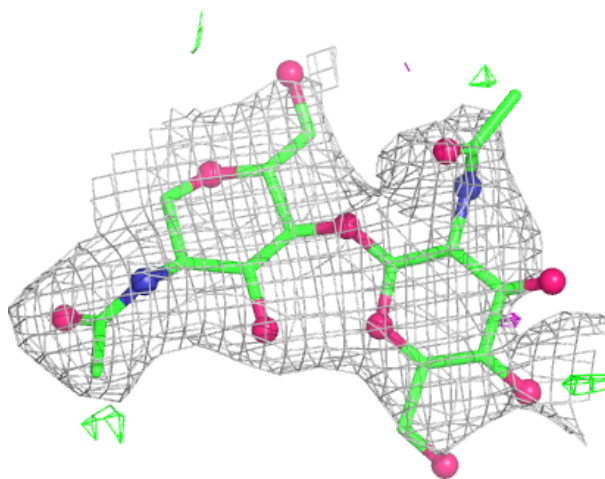
Electron density around Chain G:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



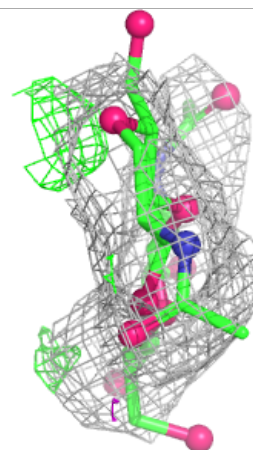
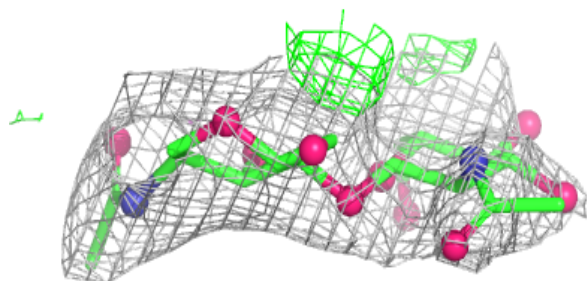
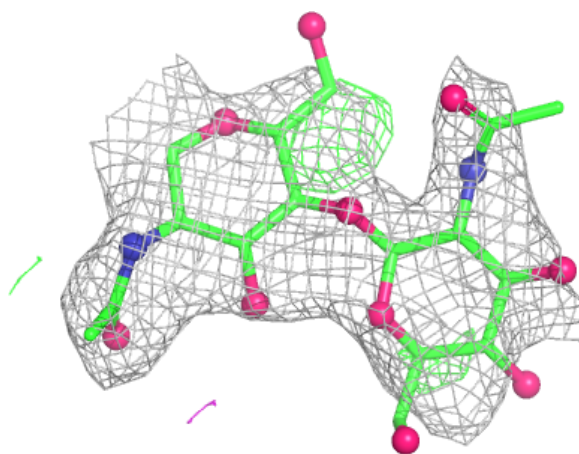
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



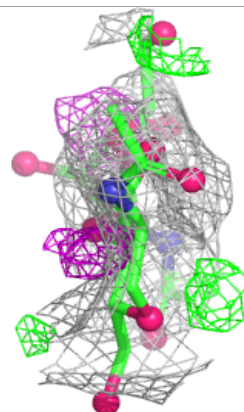
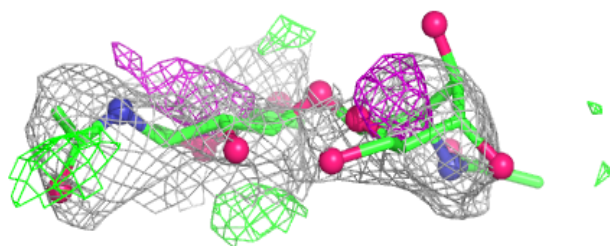
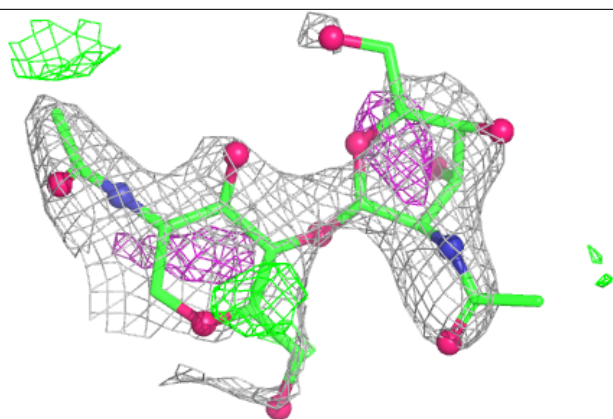
Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

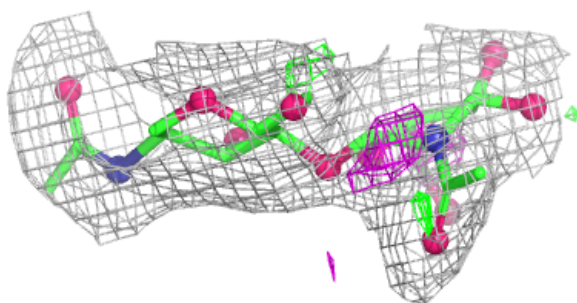
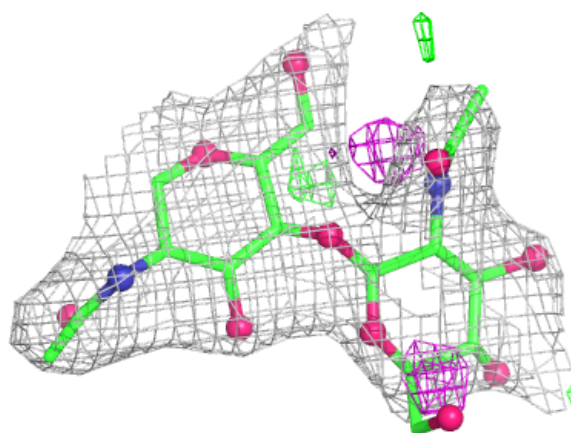


Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

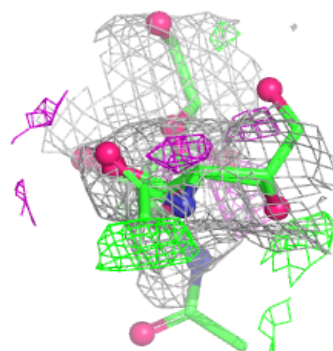
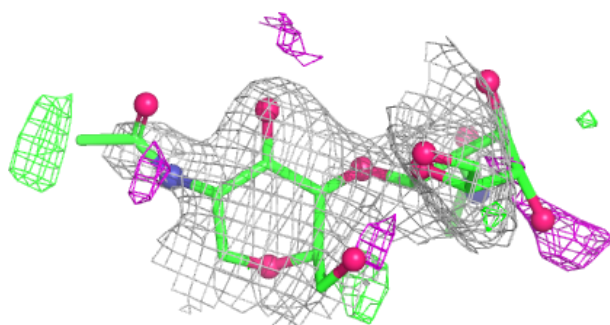
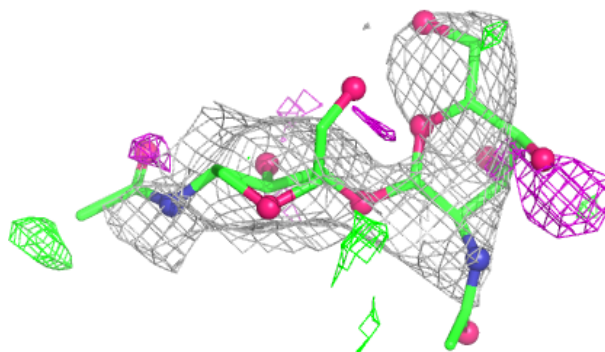
**Electron density around Chain P:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

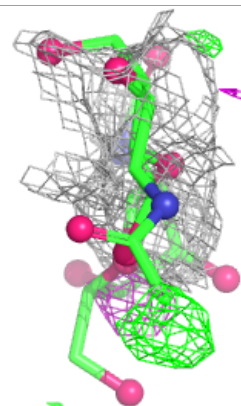
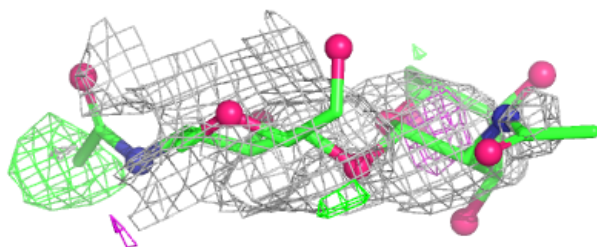
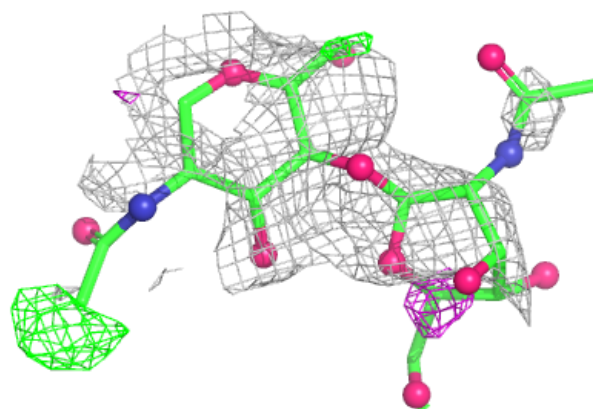


Electron density around Chain Q:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

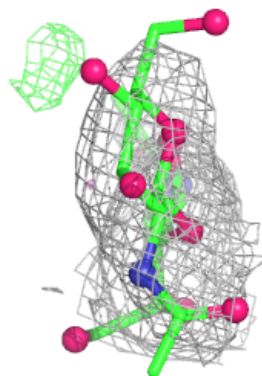
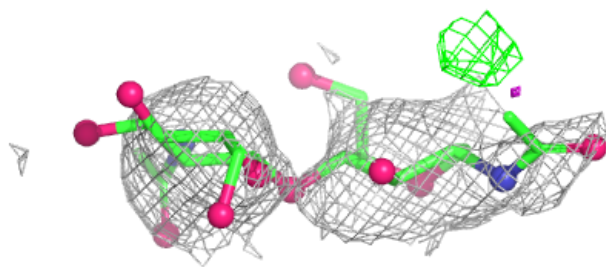
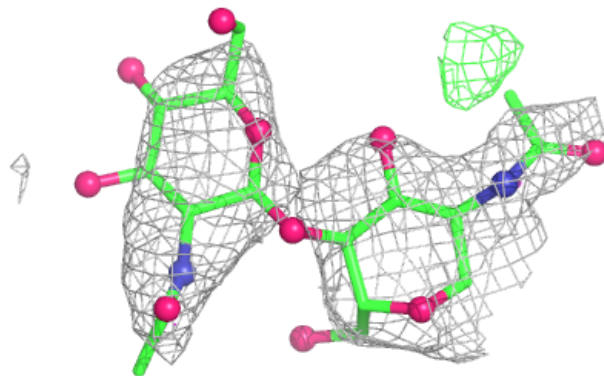
**Electron density around Chain V:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

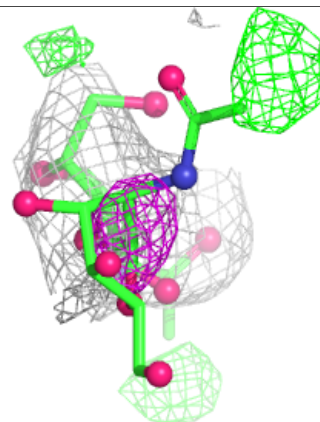
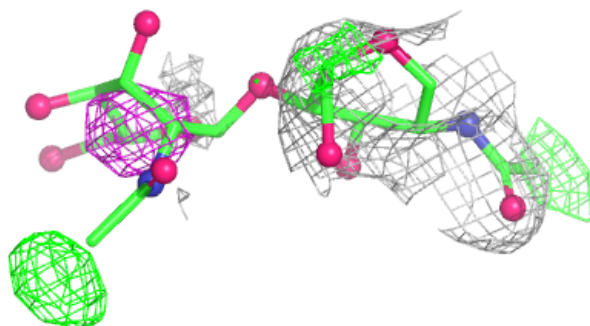
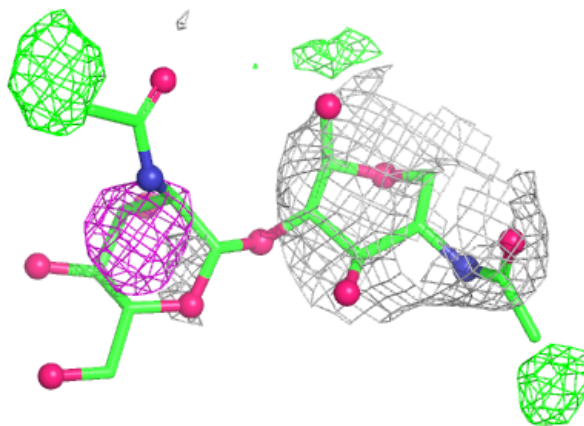


Electron density around Chain X:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

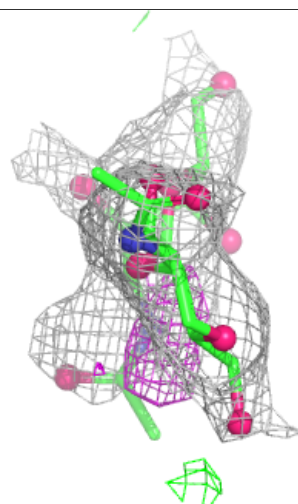
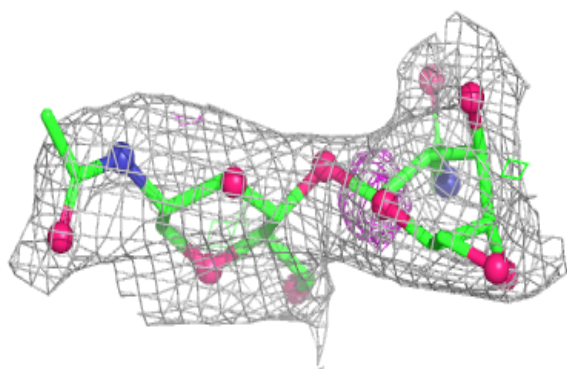
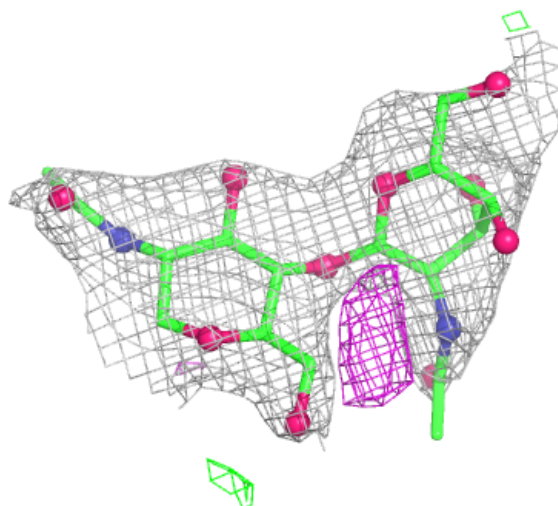
**Electron density around Chain d:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



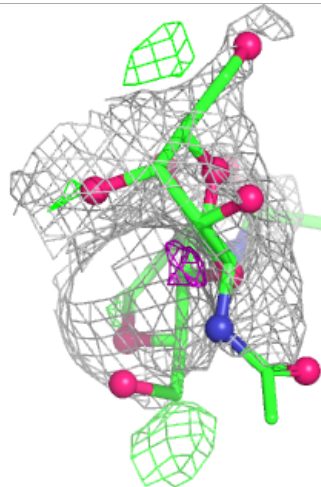
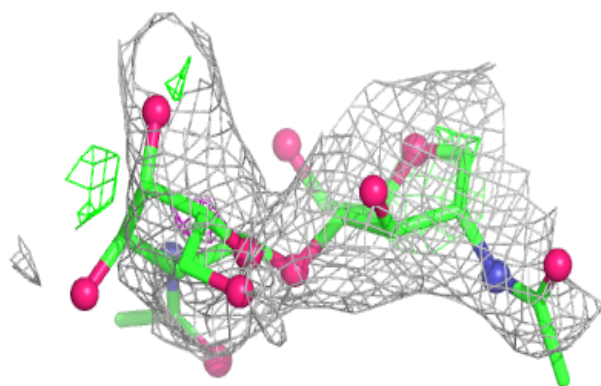
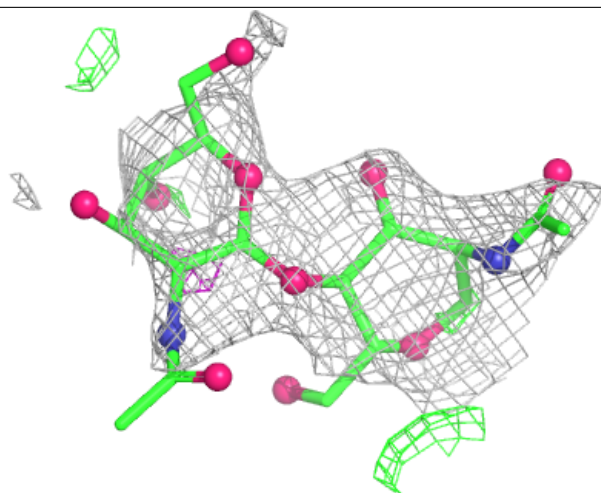
Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



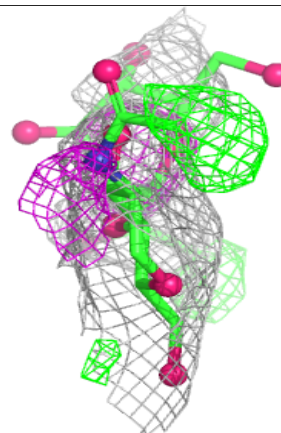
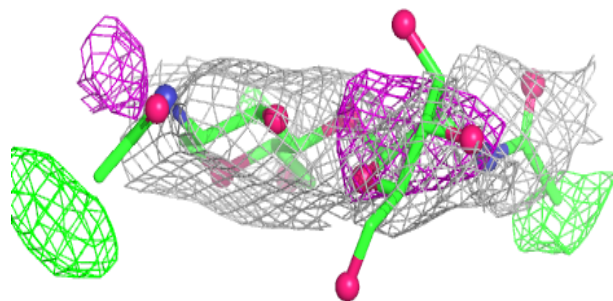
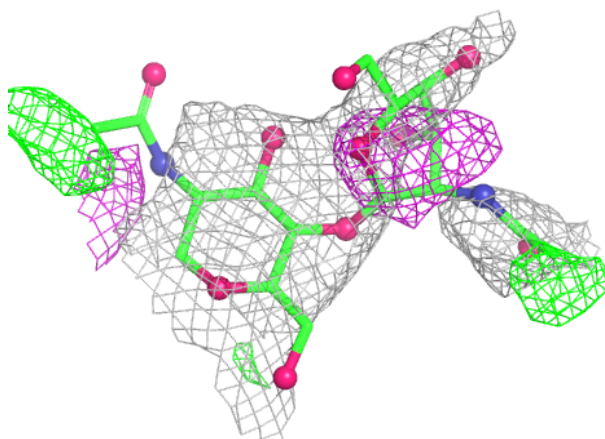
Electron density around Chain f:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

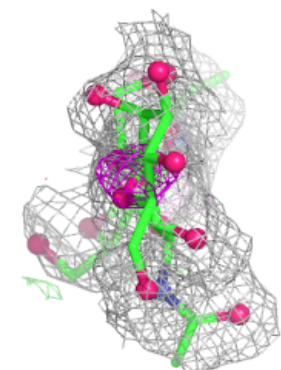
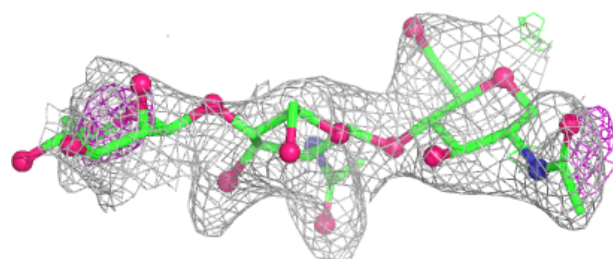
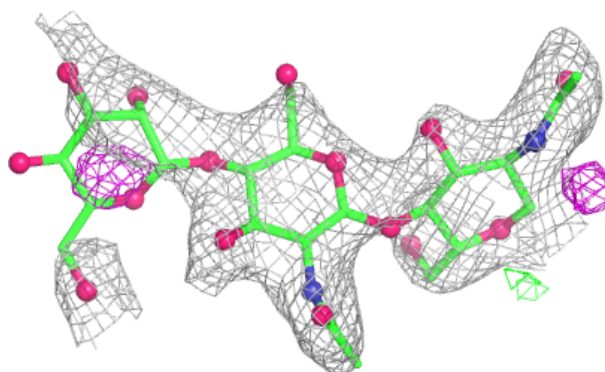


Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

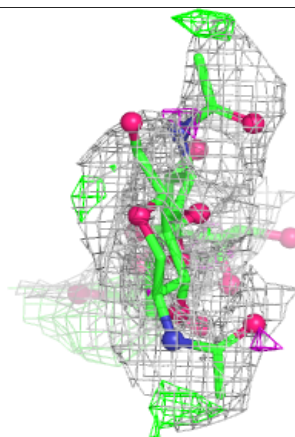
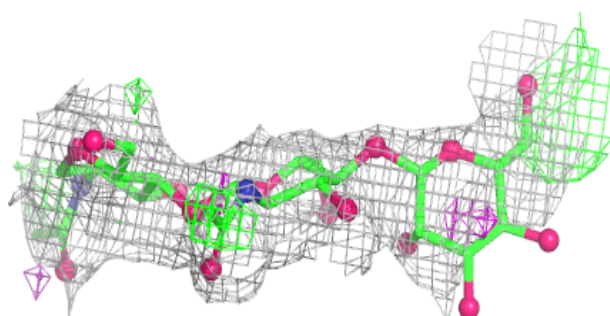
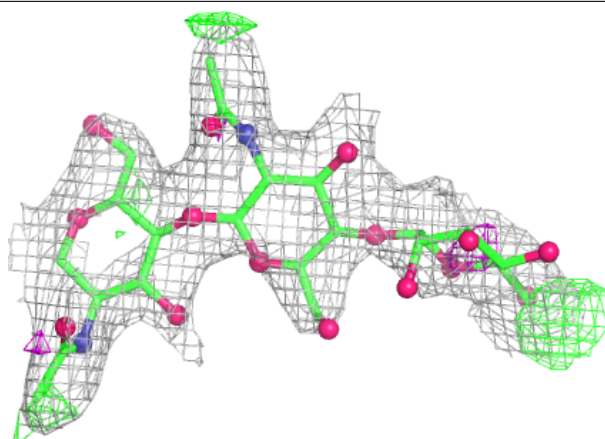
**Electron density around Chain H:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

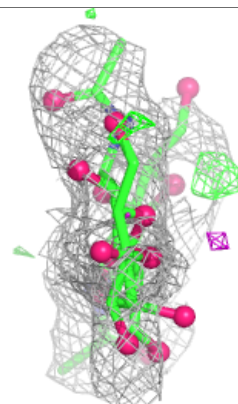
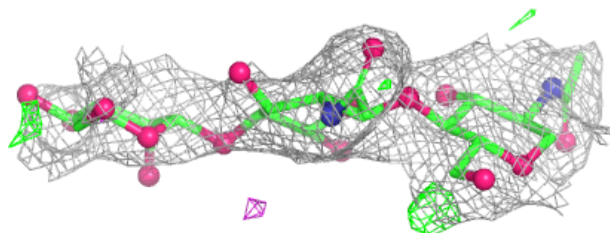
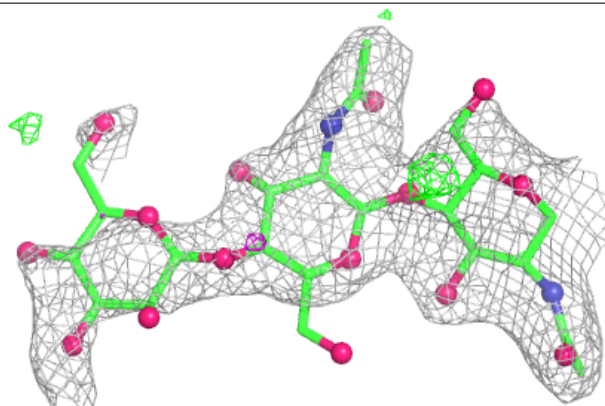


Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

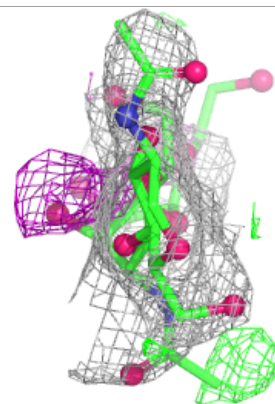
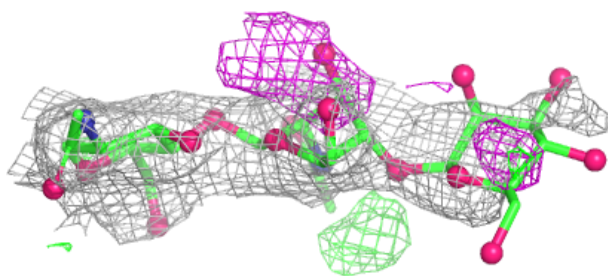
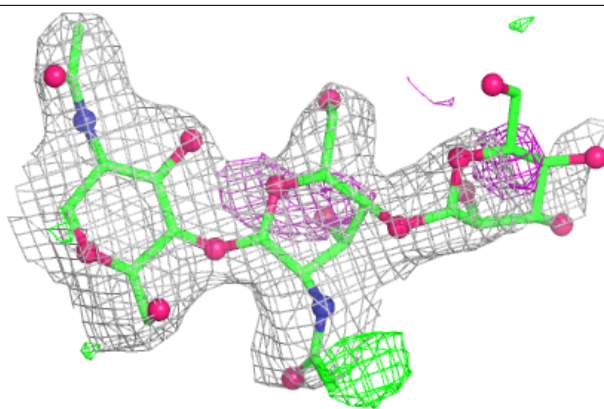
**Electron density around Chain U:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



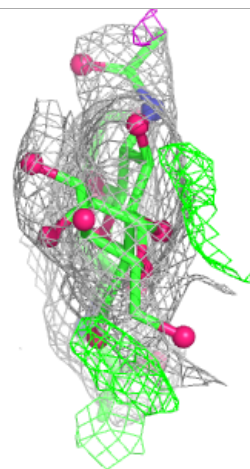
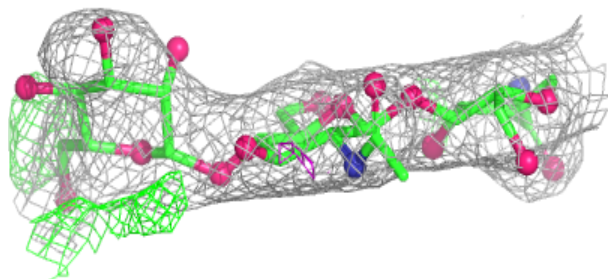
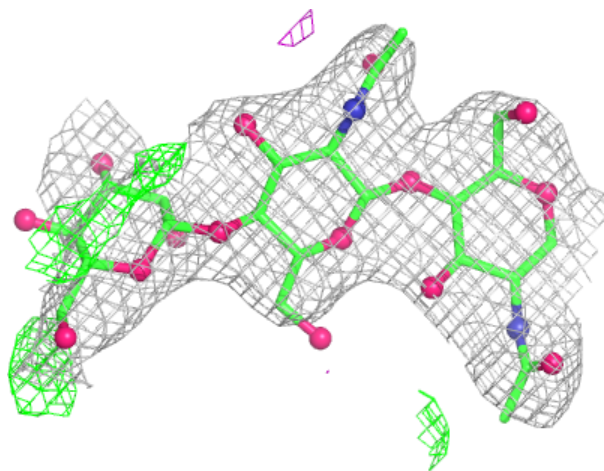
Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



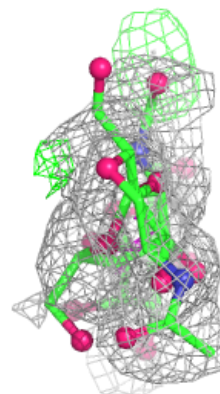
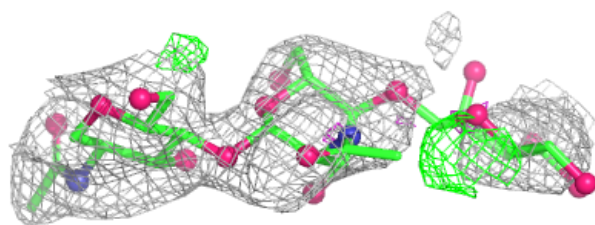
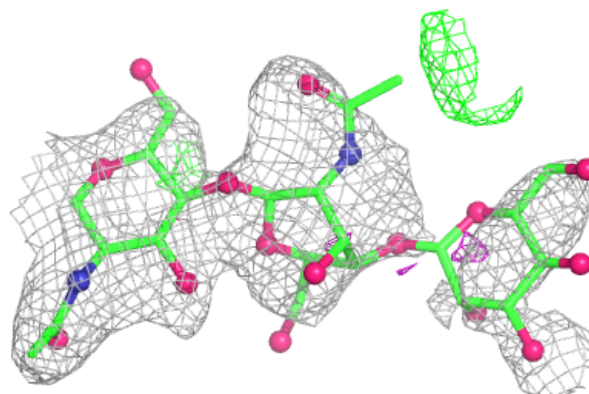
Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

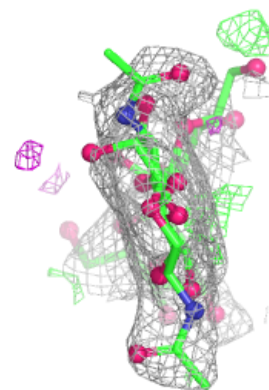
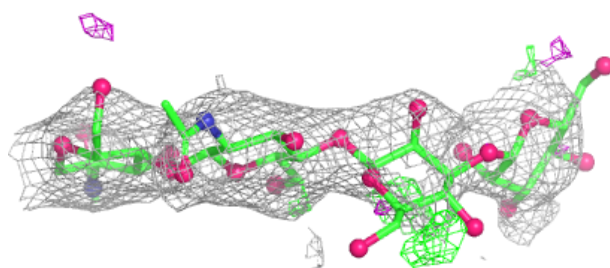
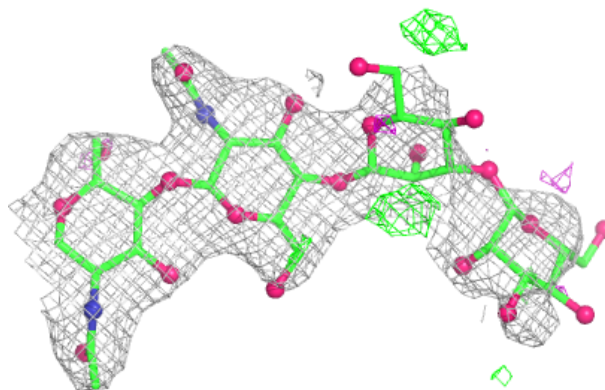


Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

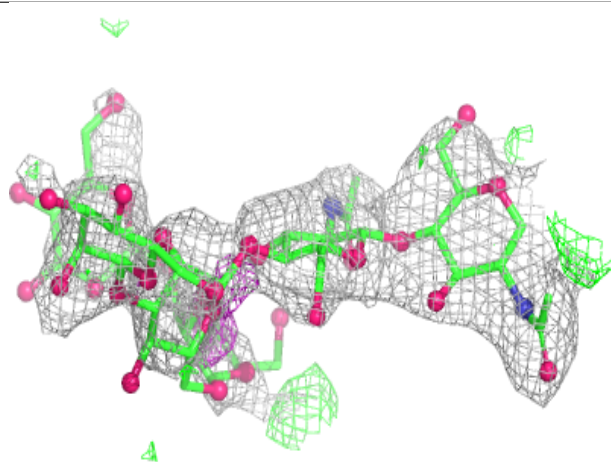
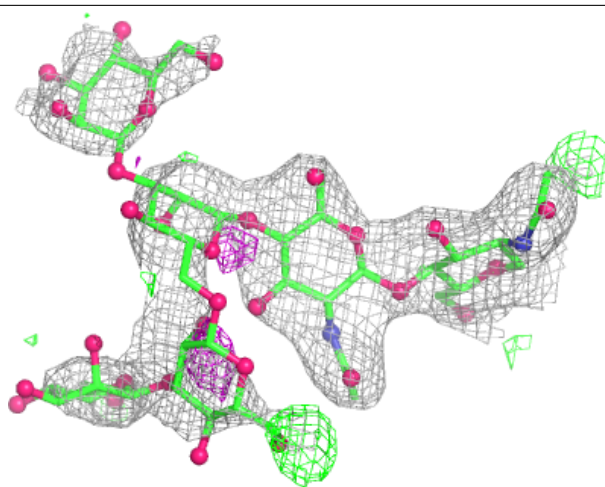
**Electron density around Chain T:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



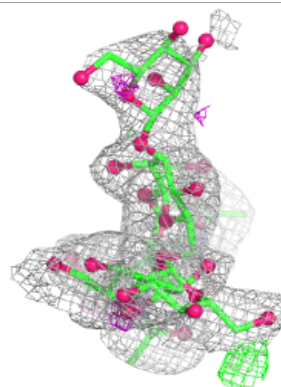
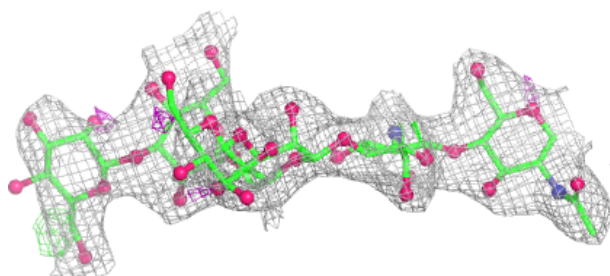
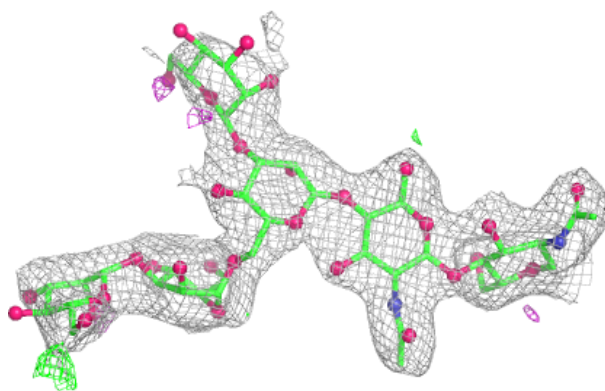
Electron density around Chain W:

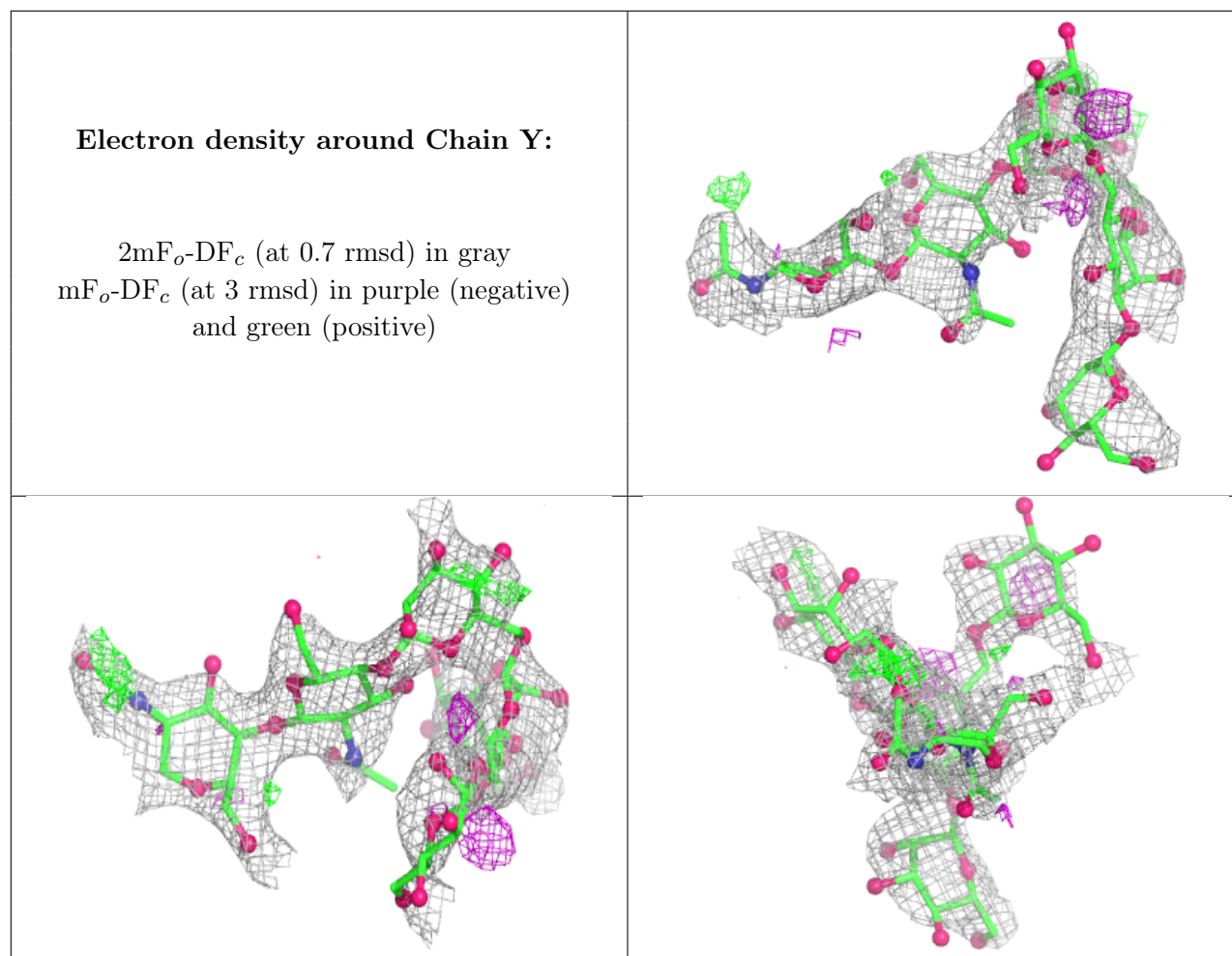
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain a:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	D	1025	14/15	0.45	0.15	134,144,148,151	0
9	NAG	B	1021	14/15	0.53	0.17	129,142,145,148	0
9	NAG	D	1016	14/15	0.56	0.17	85,97,99,102	0
9	NAG	A	1022	14/15	0.56	0.14	136,139,145,147	0
9	NAG	A	1015	14/15	0.60	0.15	97,107,115,116	0
9	NAG	C	1117	14/15	0.65	0.17	94,100,106,107	0
11	EDO	B	1023	4/4	0.69	0.17	65,66,69,70	0
11	EDO	A	1036	4/4	0.71	0.16	73,74,76,77	0
11	EDO	D	1030	4/4	0.72	0.16	65,68,71,72	0
11	EDO	B	1030	4/4	0.73	0.18	69,70,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	EDO	C	1141	4/4	0.74	0.15	79,80,82,84	0
11	EDO	A	1035	4/4	0.75	0.23	90,90,91,92	0
11	EDO	A	1037	4/4	0.76	0.24	77,80,82,84	0
11	EDO	B	1029	4/4	0.77	0.16	68,70,70,71	0
11	EDO	A	1031	4/4	0.77	0.24	57,62,63,67	0
11	EDO	B	1034	4/4	0.78	0.21	63,66,66,66	0
11	EDO	C	1143	4/4	0.79	0.18	65,68,69,71	0
11	EDO	B	1032	4/4	0.81	0.18	81,81,82,82	0
11	EDO	A	1032	4/4	0.82	0.17	61,62,64,64	0
11	EDO	A	1029	4/4	0.82	0.23	59,63,65,68	0
11	EDO	C	1136	4/4	0.83	0.13	67,67,68,71	0
11	EDO	C	1140	4/4	0.83	0.17	68,70,71,71	0
11	EDO	A	1027	4/4	0.83	0.17	73,73,75,75	0
11	EDO	C	1142	4/4	0.83	0.14	73,75,77,77	0
11	EDO	A	1034	4/4	0.83	0.18	65,69,69,70	0
11	EDO	C	1135	4/4	0.83	0.13	67,69,71,71	0
11	EDO	B	1026	4/4	0.84	0.14	67,68,68,68	0
11	EDO	C	1138	4/4	0.85	0.20	77,78,79,79	0
11	EDO	A	1028	4/4	0.85	0.20	63,66,66,69	0
11	EDO	C	1137	4/4	0.85	0.11	75,75,76,76	0
11	EDO	A	1026	4/4	0.86	0.16	81,82,82,83	0
11	EDO	B	1024	4/4	0.87	0.09	60,61,64,67	0
11	EDO	A	1039	4/4	0.88	0.15	81,82,82,83	0
11	EDO	C	1146	4/4	0.88	0.17	72,73,74,74	0
11	EDO	D	1028	4/4	0.88	0.16	61,62,64,65	0
11	EDO	D	1029	4/4	0.88	0.12	58,58,58,58	0
11	EDO	B	1025	4/4	0.88	0.26	79,79,80,81	0
11	EDO	A	1030	4/4	0.89	0.14	73,76,77,78	0
11	EDO	C	1145	4/4	0.89	0.09	58,58,60,62	0
11	EDO	B	1027	4/4	0.90	0.15	57,59,63,66	0
11	EDO	A	1033	4/4	0.90	0.17	71,72,75,76	0
11	EDO	D	1031	4/4	0.90	0.11	64,64,65,66	0
11	EDO	B	1028	4/4	0.91	0.17	54,55,56,57	0
11	EDO	C	1144	4/4	0.91	0.12	62,63,63,64	0
11	EDO	A	1024	4/4	0.92	0.10	71,71,72,73	0
11	EDO	A	1025	4/4	0.92	0.10	63,65,67,68	0
11	EDO	B	1033	4/4	0.92	0.12	69,69,69,70	0
11	EDO	D	1027	4/4	0.92	0.11	69,69,70,71	0
11	EDO	B	1031	4/4	0.93	0.21	58,62,63,63	0
11	EDO	A	1038	4/4	0.93	0.10	72,73,75,77	0
11	EDO	A	1040	4/4	0.94	0.19	54,56,59,61	0
11	EDO	C	1139	4/4	0.95	0.08	62,63,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ZN	A	1023	1/1	0.99	0.02	43,43,43,43	0
10	ZN	D	1026	1/1	0.99	0.02	43,43,43,43	0
10	ZN	C	1134	1/1	1.00	0.01	41,41,41,41	0
10	ZN	B	1022	1/1	1.00	0.01	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.