



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:44 AM UTC

PDB ID : 7AUW / pdb_00007auw
Title : Inhibitory complex of human meprin beta with mouse fetuin-B.
Authors : Eckhard, U.; Gomis-Ruth, F.X.
Deposited on : 2020-11-03
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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

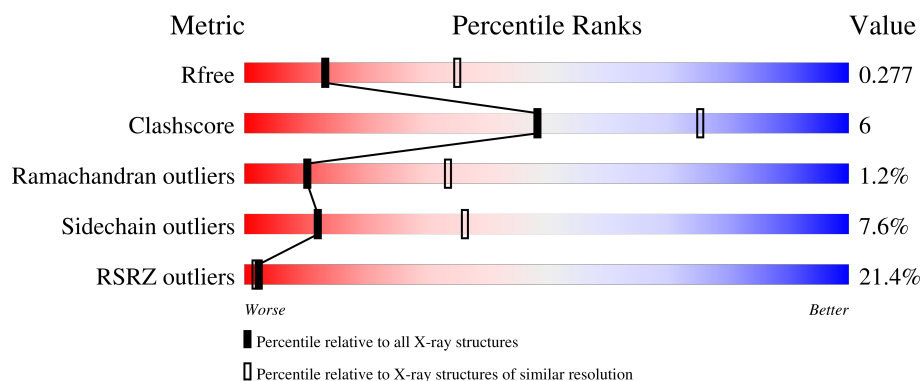
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



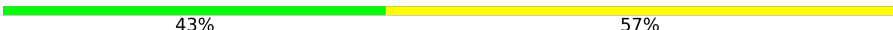
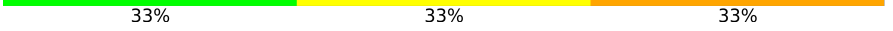
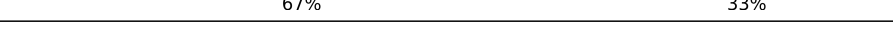
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	550	12% 81% 14% ..
1	C	550	17% 78% 17% ...
2	B	394	24% 68% 10% 20%
2	D	394	27% 64% 10% 24%
3	E	7	43% 57%

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Mol	Chain	Length	Quality of chain
3	G	7	 43% 57%
3	M	7	 43% 57%
3	O	7	 43% 57%
4	F	3	 33% 67%
4	N	3	 33% 67%
4	T	3	 33% 67%
5	H	6	 33% 33% 33%
5	P	6	 50% 50%
6	I	3	 33% 67%
6	Q	3	 33% 67%
7	J	12	 8% 67% 25%
7	R	12	 8% 67% 25%
8	K	3	 67% 33%
8	S	3	 67% 33%
9	L	4	 25% 75%
10	U	3	 33% 67%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 13918 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 Meprin A subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4260	2679	740	820	21			
1	C	532	Total	C	N	O	S	0	0	0
			4260	2679	740	820	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	609	PRO	-	expression tag	UNP Q16820
A	610	SER	-	expression tag	UNP Q16820
A	611	LYS	-	expression tag	UNP Q16820
C	609	PRO	-	expression tag	UNP Q16820
C	610	SER	-	expression tag	UNP Q16820
C	611	LYS	-	expression tag	UNP Q16820

- Molecule 2 is a protein called Fetuin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2129	1314	365	434	16			
2	D	298	Total	C	N	O	S	0	0	0
			1979	1219	346	399	15			

There are 12 discrepancies between the modelled and reference sequences:

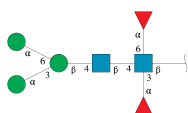
Chain	Residue	Modelled	Actual	Comment	Reference
B	389	HIS	-	expression tag	UNP Q9QXC1
B	390	HIS	-	expression tag	UNP Q9QXC1
B	391	HIS	-	expression tag	UNP Q9QXC1
B	392	HIS	-	expression tag	UNP Q9QXC1
B	393	HIS	-	expression tag	UNP Q9QXC1
B	394	HIS	-	expression tag	UNP Q9QXC1

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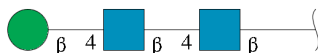
Chain	Residue	Modelled	Actual	Comment	Reference
D	389	HIS	-	expression tag	UNP Q9QXC1
D	390	HIS	-	expression tag	UNP Q9QXC1
D	391	HIS	-	expression tag	UNP Q9QXC1
D	392	HIS	-	expression tag	UNP Q9QXC1
D	393	HIS	-	expression tag	UNP Q9QXC1
D	394	HIS	-	expression tag	UNP Q9QXC1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	0	0	0
			81	46	2	33			
3	G	7	Total	C	N	O	0	0	0
			81	46	2	33			
3	M	7	Total	C	N	O	0	0	0
			81	46	2	33			
3	O	7	Total	C	N	O	0	0	0
			81	46	2	33			

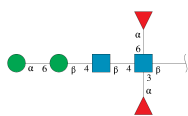
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

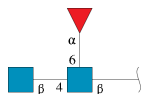
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



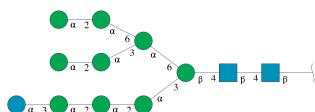
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			70	40	2	28			
5	P	6	Total	C	N	O	0	0	0
			70	40	2	28			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	Q	3	Total	C	N	O	0	0	0
			38	22	2	14			

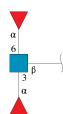
- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	12	Total	C	N	O	0	0	0
			138	76	2	60			
7	R	12	Total	C	N	O	0	0	0
			138	76	2	60			

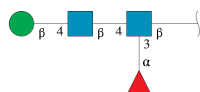
- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1

-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



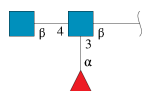
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	3	Total	C	N	O	0	0	0
			34	20	1	13			
8	S	3	Total	C	N	O	0	0	0
			34	20	1	13			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	U	3	Total	C	N	O	0	0	0
			38	22	2	14			

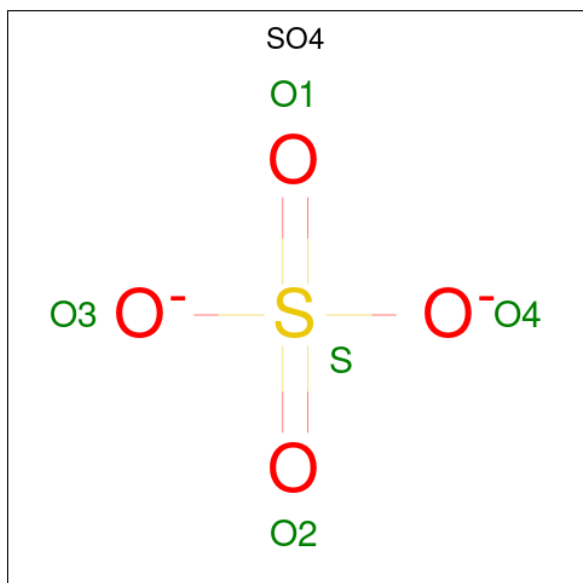
- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Na	0	0
			1	1		
11	C	1	Total	Na	0	0
			1	1		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Zn	0	0
			1	1		
12	C	1	Total	Zn	0	0
			1	1		

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

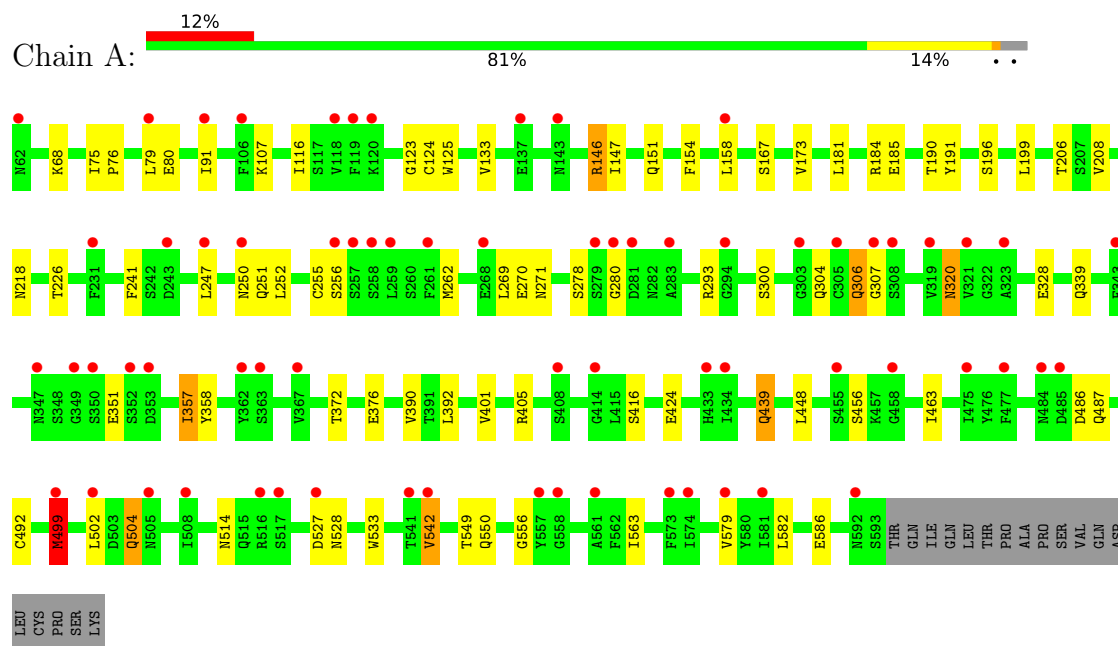
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	85	Total	O	0	0
			85	85		
15	B	2	Total	O	0	0
			2	2		
15	C	86	Total	O	0	0
			86	86		
15	D	1	Total	O	0	0
			1	1		

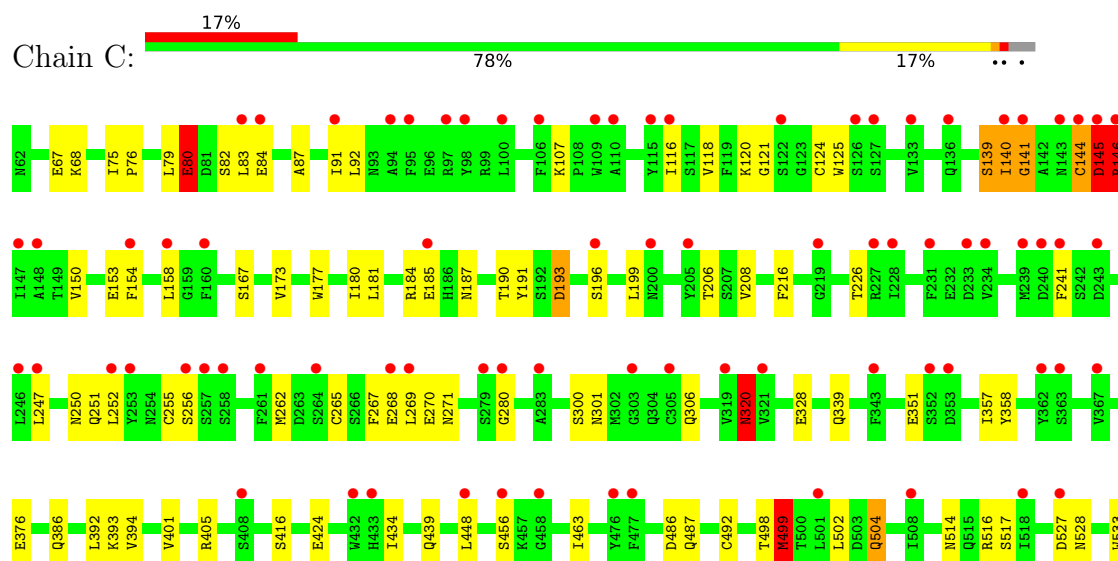
3 Residue-property plots [i](#)

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: Meprin A subunit beta

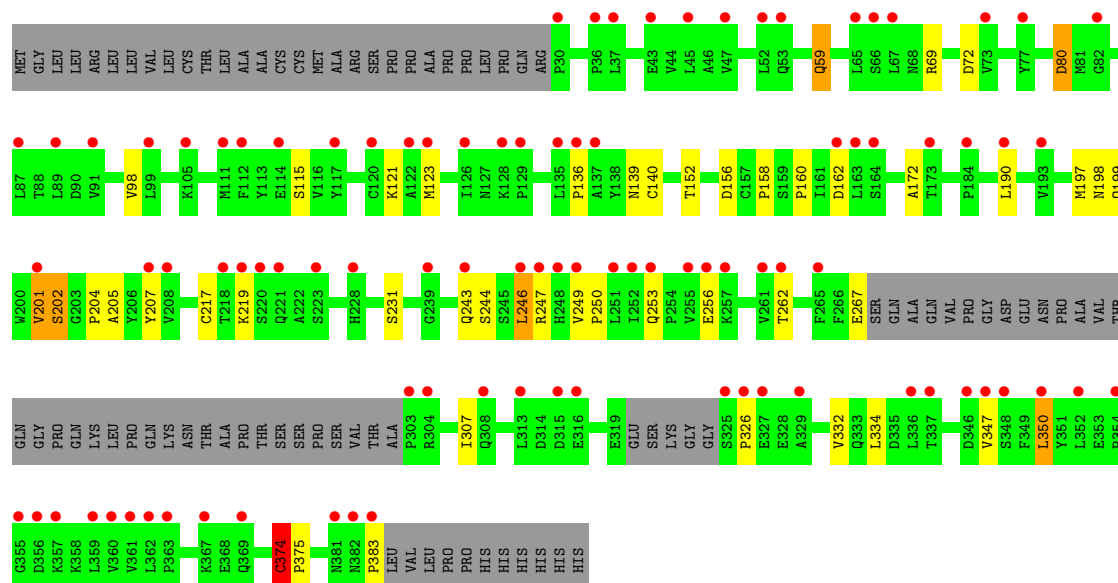


• Molecule 1: Meprin A subunit beta

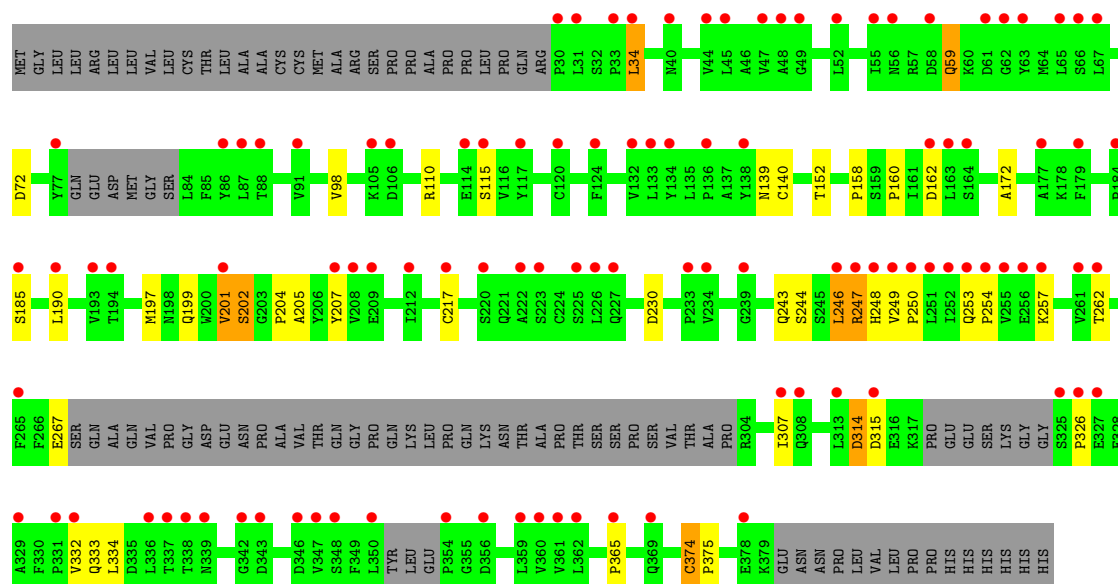




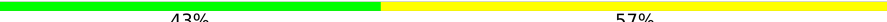
• Molecule 2: Fetuin-B



• Molecule 2: Fetuin-B



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

Chain E:  43% 57%

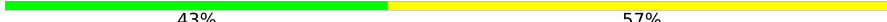


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  43% 57%

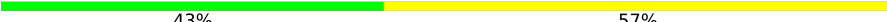


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  43% 57%

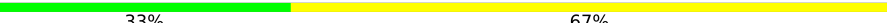


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  43% 57%

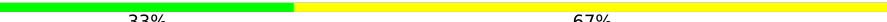


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

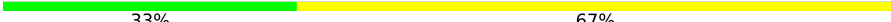


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%



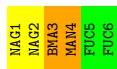
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 67%



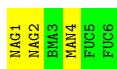
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%



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

Chain P:  50% 50%



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

Chain I:  33% 67%



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

Chain Q:  33% 67%

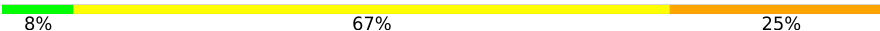


- Molecule 7: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  8% 67% 25%



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

Chain R:  8% 67% 25%



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

Chain K:  67% 33%



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

Chain S:  67% 33%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  25% 75%



- Molecule 10: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.66Å 88.24Å 156.66Å 90.00° 113.82° 90.00°	Depositor
Resolution (Å)	76.26 – 2.80 76.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (76.26-2.80) 93.7 (76.26-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.236 , 0.261 0.257 , 0.277	Depositor DCC
R_{free} test set	744 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 129.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13918	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, NA, FUC, BMA, ZN, MAN, GLC

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	0.76	2/4368 (0.0%)	1.06	8/5920 (0.1%)
1	C	0.87	7/4368 (0.2%)	1.10	13/5920 (0.2%)
2	B	0.69	0/2177	0.97	3/2997 (0.1%)
2	D	0.69	0/2020	0.94	3/2777 (0.1%)
All	All	0.78	9/12933 (0.1%)	1.04	27/17614 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	ASP	CA-C	10.44	1.66	1.52
1	C	140	ILE	CA-CB	5.92	1.62	1.54
1	C	146	ARG	N-CA	-5.66	1.39	1.45
1	C	499	MET	SD-CE	-5.64	1.65	1.79
1	A	499	MET	SD-CE	-5.58	1.65	1.79

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASN	CA-CB-CG	8.55	121.15	112.60
1	C	140	ILE	N-CA-CB	8.22	124.79	111.23
1	A	241	PHE	CA-CB-CG	8.19	121.99	113.80
1	C	241	PHE	CA-CB-CG	8.18	121.98	113.80
2	B	80	ASP	CA-CB-CG	7.24	119.84	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4260	0	4019	35	0
1	C	4260	0	4019	65	0
2	B	2129	0	1741	29	0
2	D	1979	0	1587	28	0
3	E	81	0	70	0	0
3	G	81	0	70	0	0
3	M	81	0	70	0	0
3	O	81	0	70	0	0
4	F	39	0	34	0	0
4	N	39	0	34	0	0
4	T	39	0	34	0	0
5	H	70	0	61	1	0
5	P	70	0	61	0	0
6	I	38	0	34	1	0
6	Q	38	0	34	1	0
7	J	138	0	115	2	0
7	R	138	0	115	2	0
8	K	34	0	31	0	0
8	S	34	0	31	0	0
9	L	49	0	43	0	0
10	U	38	0	34	2	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
12	A	1	0	0	0	0
12	C	1	0	0	0	0
13	A	5	0	0	0	0
13	C	5	0	0	0	0
14	B	14	0	13	0	0
15	A	85	0	0	0	0
15	B	2	0	0	0	0
15	C	86	0	0	1	0
15	D	1	0	0	0	0
All	All	13918	0	12320	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 144 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)
2:B:121:LYS:HE3	2:B:332:VAL:HB	1.08	1.03
1:C:140:ILE:HG23	1:C:144:CYS:HB2	1.39	1.00
1:C:146:ARG:HE	2:D:246:LEU:HD13	1.26	1.00
1:C:84:GLU:HG3	1:C:120:LYS:HZ2	1.40	0.86
1:C:146:ARG:NE	2:D:246:LEU:HD13	1.93	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	530/550 (96%)	493 (93%)	35 (7%)	2 (0%)	30	60
1	C	530/550 (96%)	489 (92%)	38 (7%)	3 (1%)	21	51
2	B	308/394 (78%)	280 (91%)	21 (7%)	7 (2%)	5	18
2	D	288/394 (73%)	259 (90%)	21 (7%)	8 (3%)	4	14
All	All	1656/1888 (88%)	1521 (92%)	115 (7%)	20 (1%)	10	34

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	326	PRO
2	D	247	ARG
2	D	326	PRO
2	B	202	SER
2	B	231	SER

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	471/489 (96%)	435 (92%)	36 (8%)	12	36
1	C	471/489 (96%)	433 (92%)	38 (8%)	11	33
2	B	196/352 (56%)	183 (93%)	13 (7%)	15	43
2	D	173/352 (49%)	160 (92%)	13 (8%)	12	37
All	All	1311/1682 (78%)	1211 (92%)	100 (8%)	12	36

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	GLU
1	C	376	GLU
2	D	374	CYS
1	C	206	THR
1	C	300	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	510	GLN
1	C	514	ASN
2	D	68	ASN
2	B	78	GLN
2	B	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

92 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	2.08	4 (23%)
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
3	BMA	E	3	3	11,11,12	0.30	0	15,15,17	0.77	0
3	MAN	E	4	3	11,11,12	0.43	0	15,15,17	0.94	1 (6%)
3	MAN	E	5	3	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
3	FUC	E	6	3	10,10,11	0.34	0	14,14,16	0.57	0
3	FUC	E	7	3	10,10,11	0.40	0	14,14,16	0.68	0
4	NAG	F	1	1,4	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
4	NAG	F	2	4	14,14,15	0.40	0	17,19,21	1.30	1 (5%)
4	BMA	F	3	4	11,11,12	0.32	0	15,15,17	0.59	0
3	NAG	G	1	3,1	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.64	0
3	BMA	G	3	3	11,11,12	0.25	0	15,15,17	0.90	1 (6%)
3	MAN	G	4	3	11,11,12	0.34	0	15,15,17	0.67	1 (6%)
3	MAN	G	5	3	11,11,12	0.44	0	15,15,17	1.59	2 (13%)
3	FUC	G	6	3	10,10,11	0.33	0	14,14,16	0.86	0
3	FUC	G	7	3	10,10,11	0.34	0	14,14,16	0.55	0
5	NAG	H	1	5,1	14,14,15	0.29	0	17,19,21	0.97	1 (5%)
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
5	BMA	H	3	5	11,11,12	0.63	0	15,15,17	1.69	3 (20%)
5	MAN	H	4	5	11,11,12	0.44	0	15,15,17	1.19	2 (13%)
5	FUC	H	5	5	10,10,11	0.37	0	14,14,16	0.55	0
5	FUC	H	6	5	10,10,11	0.46	0	14,14,16	0.73	0
6	NAG	I	1	1,6	14,14,15	0.52	0	17,19,21	2.08	4 (23%)
6	NAG	I	2	6	14,14,15	0.39	0	17,19,21	1.05	2 (11%)
6	FUC	I	3	6	10,10,11	0.53	0	14,14,16	0.90	1 (7%)
7	NAG	J	1	7,1	14,14,15	0.25	0	17,19,21	0.96	1 (5%)
7	MAN	J	10	7	11,11,12	0.34	0	15,15,17	1.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	J	11	7	11,11,12	0.28	0	15,15,17	0.93	1 (6%)
7	MAN	J	12	7	11,11,12	0.25	0	15,15,17	0.68	1 (6%)
7	NAG	J	2	7	14,14,15	0.34	0	17,19,21	0.93	1 (5%)
7	BMA	J	3	7	11,11,12	0.25	0	15,15,17	0.54	0
7	MAN	J	4	7	11,11,12	0.22	0	15,15,17	0.86	1 (6%)
7	MAN	J	5	7	11,11,12	0.29	0	15,15,17	0.87	1 (6%)
7	MAN	J	6	7	11,11,12	0.33	0	15,15,17	1.03	1 (6%)
7	GLC	J	7	7	11,11,12	0.49	0	15,15,17	0.83	1 (6%)
7	MAN	J	8	7	11,11,12	0.28	0	15,15,17	1.13	1 (6%)
7	MAN	J	9	7	11,11,12	0.32	0	15,15,17	1.31	2 (13%)
8	NAG	K	1	8,1	14,14,15	0.41	0	17,19,21	1.40	4 (23%)
8	FUC	K	2	8	10,10,11	0.45	0	14,14,16	0.57	0
8	FUC	K	3	8	10,10,11	0.45	0	14,14,16	0.61	0
9	NAG	L	1	2,9	14,14,15	0.36	0	17,19,21	0.93	2 (11%)
9	NAG	L	2	9	14,14,15	0.32	0	17,19,21	0.95	1 (5%)
9	BMA	L	3	9	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
9	FUC	L	4	9	10,10,11	0.43	0	14,14,16	0.73	0
3	NAG	M	1	3,1	14,14,15	0.40	0	17,19,21	2.11	4 (23%)
3	NAG	M	2	3	14,14,15	0.34	0	17,19,21	0.77	1 (5%)
3	BMA	M	3	3	11,11,12	0.27	0	15,15,17	0.60	0
3	MAN	M	4	3	11,11,12	0.39	0	15,15,17	0.93	1 (6%)
3	MAN	M	5	3	11,11,12	0.38	0	15,15,17	0.86	1 (6%)
3	FUC	M	6	3	10,10,11	0.29	0	14,14,16	0.57	0
3	FUC	M	7	3	10,10,11	0.42	0	14,14,16	0.73	0
4	NAG	N	1	1,4	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	N	2	4	14,14,15	0.38	0	17,19,21	1.16	1 (5%)
4	BMA	N	3	4	11,11,12	0.31	0	15,15,17	0.65	0
3	NAG	O	1	3,1	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
3	NAG	O	2	3	14,14,15	0.28	0	17,19,21	0.73	0
3	BMA	O	3	3	11,11,12	0.28	0	15,15,17	0.87	1 (6%)
3	MAN	O	4	3	11,11,12	0.31	0	15,15,17	0.66	1 (6%)
3	MAN	O	5	3	11,11,12	0.42	0	15,15,17	1.62	2 (13%)
3	FUC	O	6	3	10,10,11	0.37	0	14,14,16	0.84	0
3	FUC	O	7	3	10,10,11	0.38	0	14,14,16	0.56	0
5	NAG	P	1	5,1	14,14,15	0.29	0	17,19,21	1.01	2 (11%)
5	NAG	P	2	5	14,14,15	0.30	0	17,19,21	0.92	1 (5%)
5	BMA	P	3	5	11,11,12	0.40	0	15,15,17	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	P	4	5	11,11,12	0.44	0	15,15,17	1.01	1 (6%)
5	FUC	P	5	5	10,10,11	0.40	0	14,14,16	0.58	0
5	FUC	P	6	5	10,10,11	0.44	0	14,14,16	0.72	0
6	NAG	Q	1	1,6	14,14,15	0.52	0	17,19,21	2.07	4 (23%)
6	NAG	Q	2	6	14,14,15	0.39	0	17,19,21	1.04	2 (11%)
6	FUC	Q	3	6	10,10,11	0.52	0	14,14,16	0.92	1 (7%)
7	NAG	R	1	7,1	14,14,15	0.25	0	17,19,21	0.95	1 (5%)
7	MAN	R	10	7	11,11,12	0.35	0	15,15,17	1.15	1 (6%)
7	MAN	R	11	7	11,11,12	0.26	0	15,15,17	0.92	1 (6%)
7	MAN	R	12	7	11,11,12	0.26	0	15,15,17	0.70	1 (6%)
7	NAG	R	2	7	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
7	BMA	R	3	7	11,11,12	0.25	0	15,15,17	0.51	0
7	MAN	R	4	7	11,11,12	0.26	0	15,15,17	0.80	1 (6%)
7	MAN	R	5	7	11,11,12	0.33	0	15,15,17	0.87	1 (6%)
7	MAN	R	6	7	11,11,12	0.30	0	15,15,17	1.09	1 (6%)
7	GLC	R	7	7	11,11,12	0.51	0	15,15,17	0.93	1 (6%)
7	MAN	R	8	7	11,11,12	0.31	0	15,15,17	1.09	1 (6%)
7	MAN	R	9	7	11,11,12	0.30	0	15,15,17	1.31	2 (13%)
8	NAG	S	1	8,1	14,14,15	0.41	0	17,19,21	1.43	3 (17%)
8	FUC	S	2	8	10,10,11	0.43	0	14,14,16	0.56	0
8	FUC	S	3	8	10,10,11	0.45	0	14,14,16	0.61	0
4	NAG	T	1	2,4	14,14,15	0.34	0	17,19,21	0.79	1 (5%)
4	NAG	T	2	4	14,14,15	0.36	0	17,19,21	1.29	1 (5%)
4	BMA	T	3	4	11,11,12	0.26	0	15,15,17	0.38	0
10	NAG	U	1	2,10	14,14,15	0.35	0	17,19,21	0.98	2 (11%)
10	FUC	U	2	10	10,10,11	0.51	0	14,14,16	0.90	1 (7%)
10	NAG	U	3	10	14,14,15	0.32	0	17,19,21	0.73	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
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	5	3	-	1/2/19/22	0/1/1/1
3	FUC	E	6	3	-	-	0/1/1/1
3	FUC	E	7	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1
3	FUC	G	6	3	-	-	0/1/1/1
3	FUC	G	7	3	-	-	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	1/1/1/1
5	FUC	H	5	5	-	-	0/1/1/1
5	FUC	H	6	5	-	-	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	FUC	I	3	6	-	-	0/1/1/1
7	NAG	J	1	7,1	-	0/6/23/26	0/1/1/1
7	MAN	J	10	7	-	0/2/19/22	0/1/1/1
7	MAN	J	11	7	-	0/2/19/22	0/1/1/1
7	MAN	J	12	7	-	0/2/19/22	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
7	MAN	J	5	7	-	0/2/19/22	0/1/1/1
7	MAN	J	6	7	-	0/2/19/22	0/1/1/1
7	GLC	J	7	7	-	2/2/19/22	0/1/1/1
7	MAN	J	8	7	-	0/2/19/22	0/1/1/1
7	MAN	J	9	7	-	2/2/19/22	0/1/1/1
8	NAG	K	1	8,1	-	2/6/23/26	0/1/1/1
8	FUC	K	2	8	-	-	0/1/1/1
8	FUC	K	3	8	-	-	0/1/1/1
9	NAG	L	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	L	2	9	-	0/6/23/26	0/1/1/1
9	BMA	L	3	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUC	L	4	9	-	-	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	MAN	M	4	3	-	0/2/19/22	0/1/1/1
3	MAN	M	5	3	-	1/2/19/22	0/1/1/1
3	FUC	M	6	3	-	-	0/1/1/1
3	FUC	M	7	3	-	-	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	1/2/19/22	0/1/1/1
3	MAN	O	5	3	-	2/2/19/22	0/1/1/1
3	FUC	O	6	3	-	-	0/1/1/1
3	FUC	O	7	3	-	-	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	1/1/1/1
5	FUC	P	5	5	-	-	0/1/1/1
5	FUC	P	6	5	-	-	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	FUC	Q	3	6	-	-	0/1/1/1
7	NAG	R	1	7,1	-	0/6/23/26	0/1/1/1
7	MAN	R	10	7	-	0/2/19/22	0/1/1/1
7	MAN	R	11	7	-	0/2/19/22	0/1/1/1
7	MAN	R	12	7	-	0/2/19/22	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
7	MAN	R	4	7	-	2/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
7	MAN	R	6	7	-	0/2/19/22	0/1/1/1
7	GLC	R	7	7	-	2/2/19/22	0/1/1/1
7	MAN	R	8	7	-	0/2/19/22	0/1/1/1
7	MAN	R	9	7	-	1/2/19/22	0/1/1/1
8	NAG	S	1	8,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FUC	S	2	8	-	-	0/1/1/1
8	FUC	S	3	8	-	-	0/1/1/1
4	NAG	T	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
10	NAG	U	1	2,10	-	0/6/23/26	0/1/1/1
10	FUC	U	2	10	-	-	0/1/1/1
10	NAG	U	3	10	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C1-O5-C5	6.25	120.57	112.19
6	Q	1	NAG	C1-O5-C5	6.22	120.52	112.19
3	M	1	NAG	C1-O5-C5	5.50	119.56	112.19
3	E	1	NAG	C1-O5-C5	5.42	119.45	112.19
5	H	3	BMA	C1-O5-C5	5.14	119.07	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7
7	J	2	NAG	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	4	MAN	C1-C2-C3-C4-C5-O5
5	H	4	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 9 short contacts:

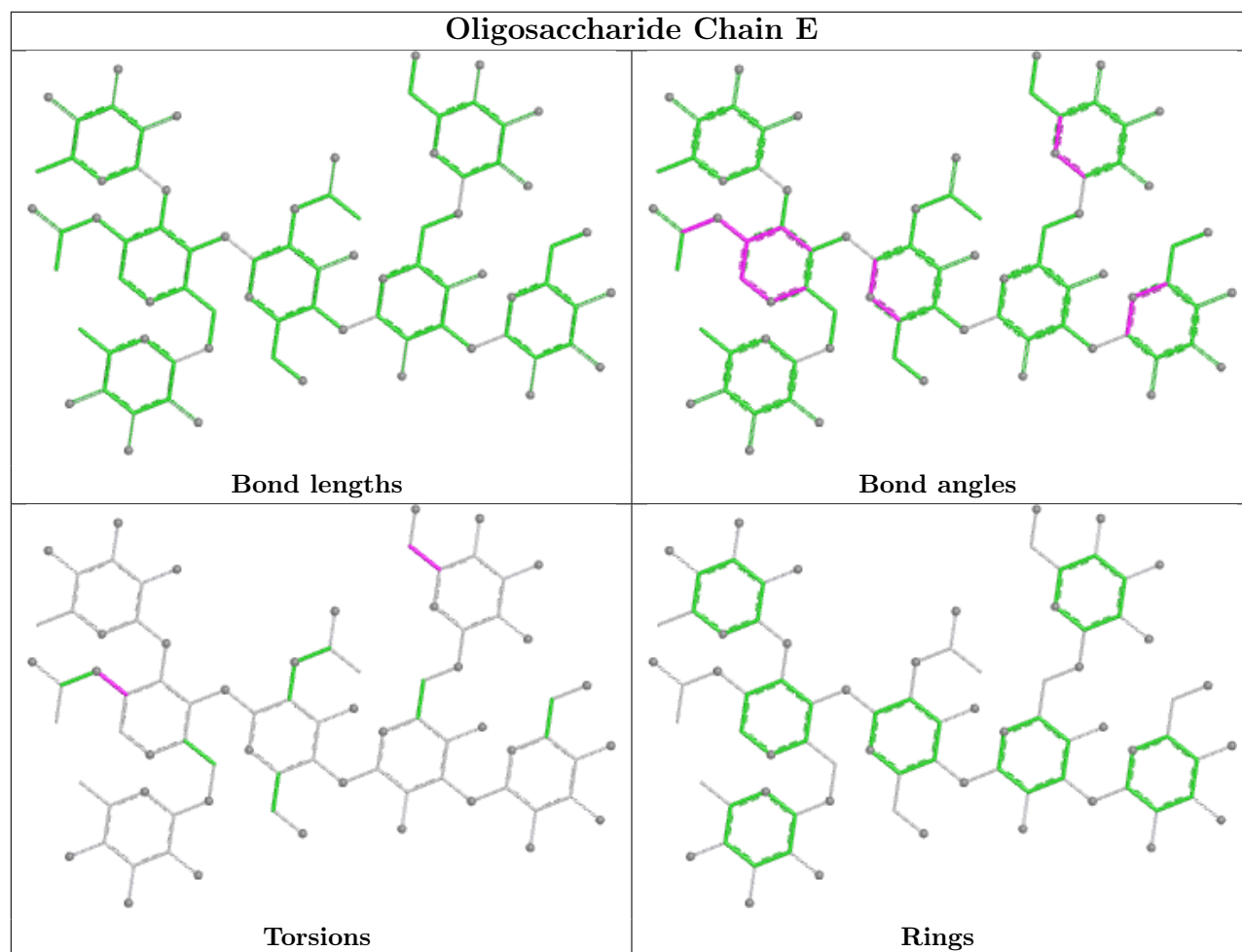
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	4	MAN	1	0
6	Q	1	NAG	1	0
6	Q	3	FUC	1	0

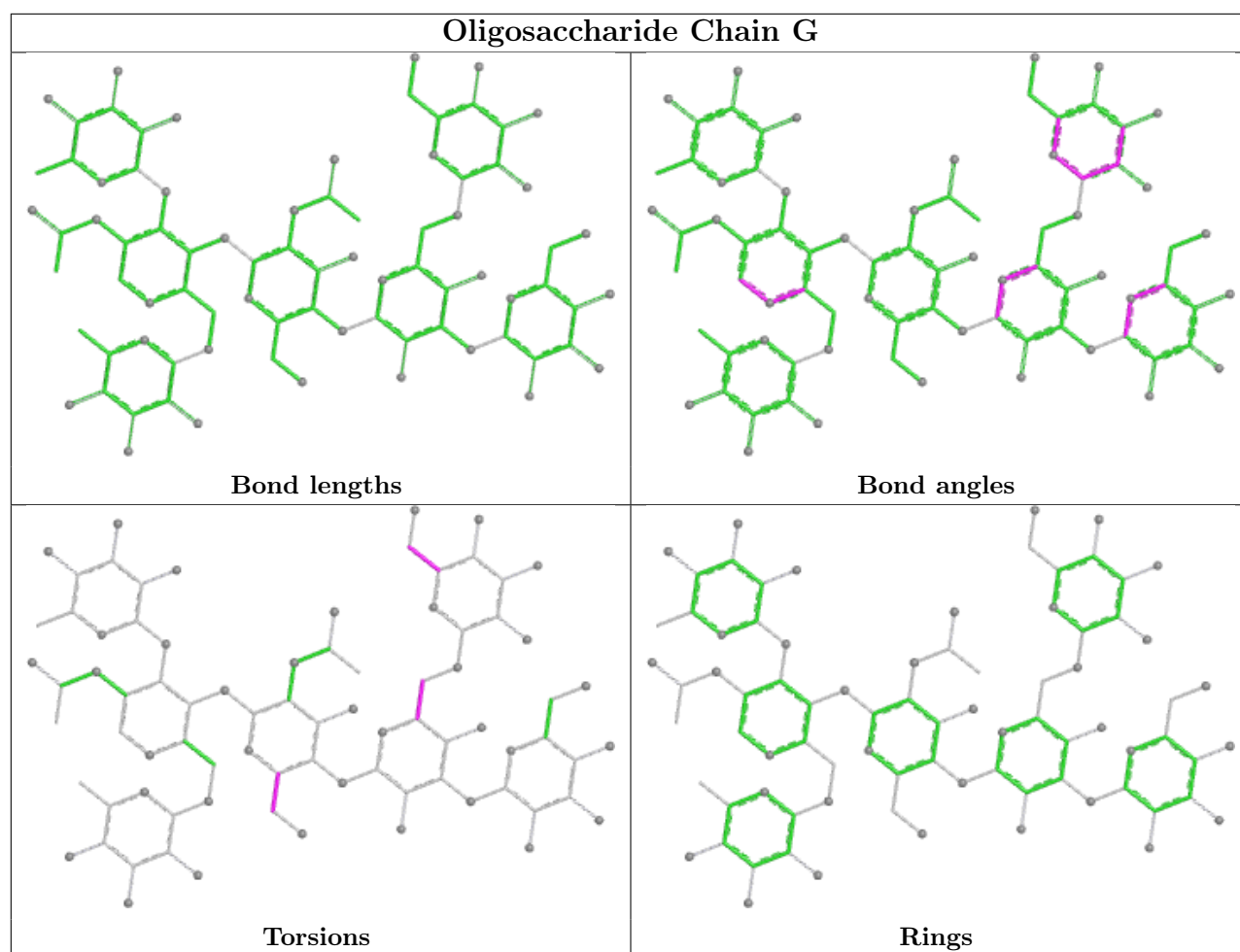
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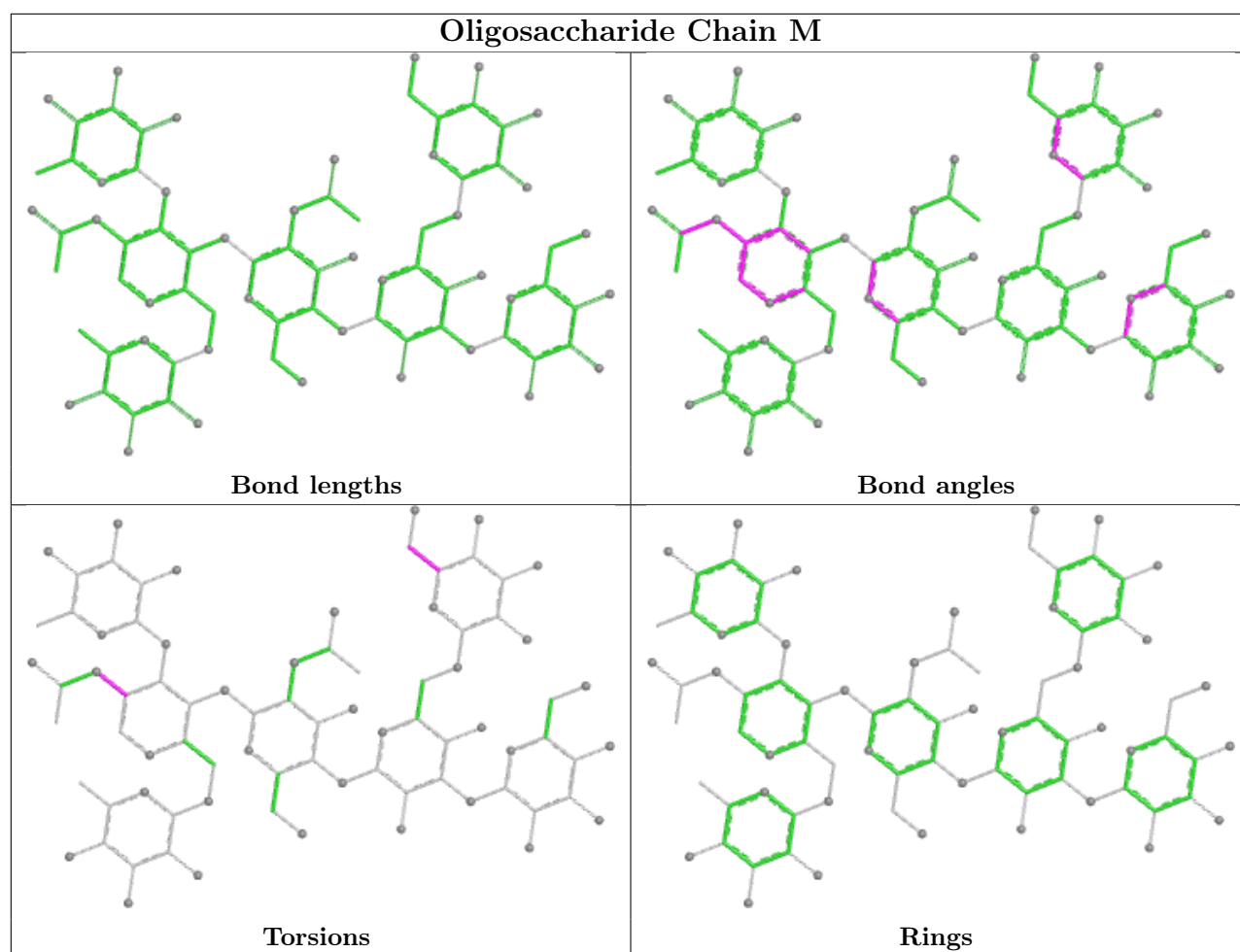
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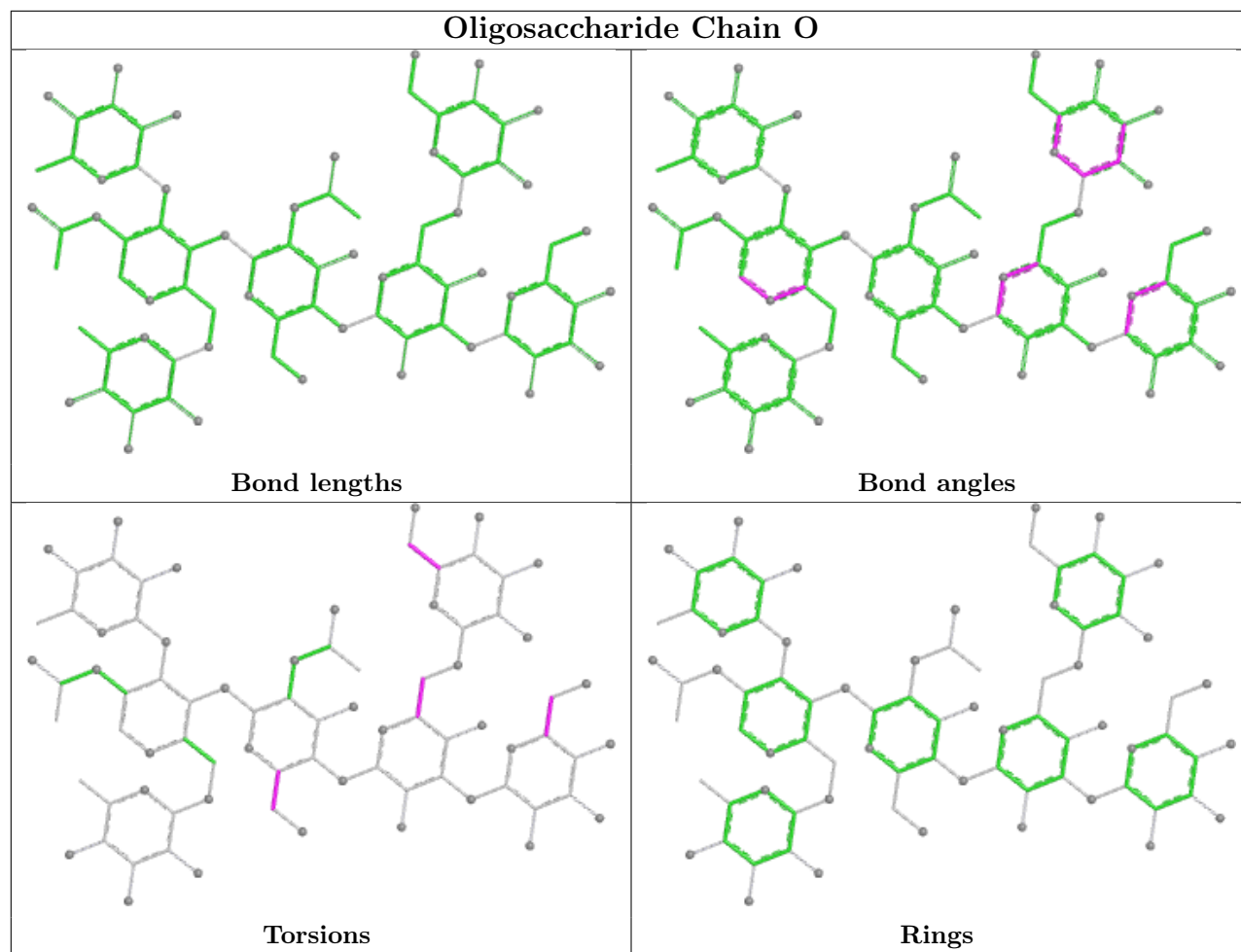
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	6	MAN	1	0
6	I	3	FUC	1	0
7	J	12	MAN	1	0
7	R	12	MAN	1	0
7	J	6	MAN	1	0
6	I	1	NAG	1	0
10	U	2	FUC	2	0
5	H	3	BMA	1	0
7	J	7	GLC	1	0
7	R	7	GLC	1	0
10	U	1	NAG	2	0

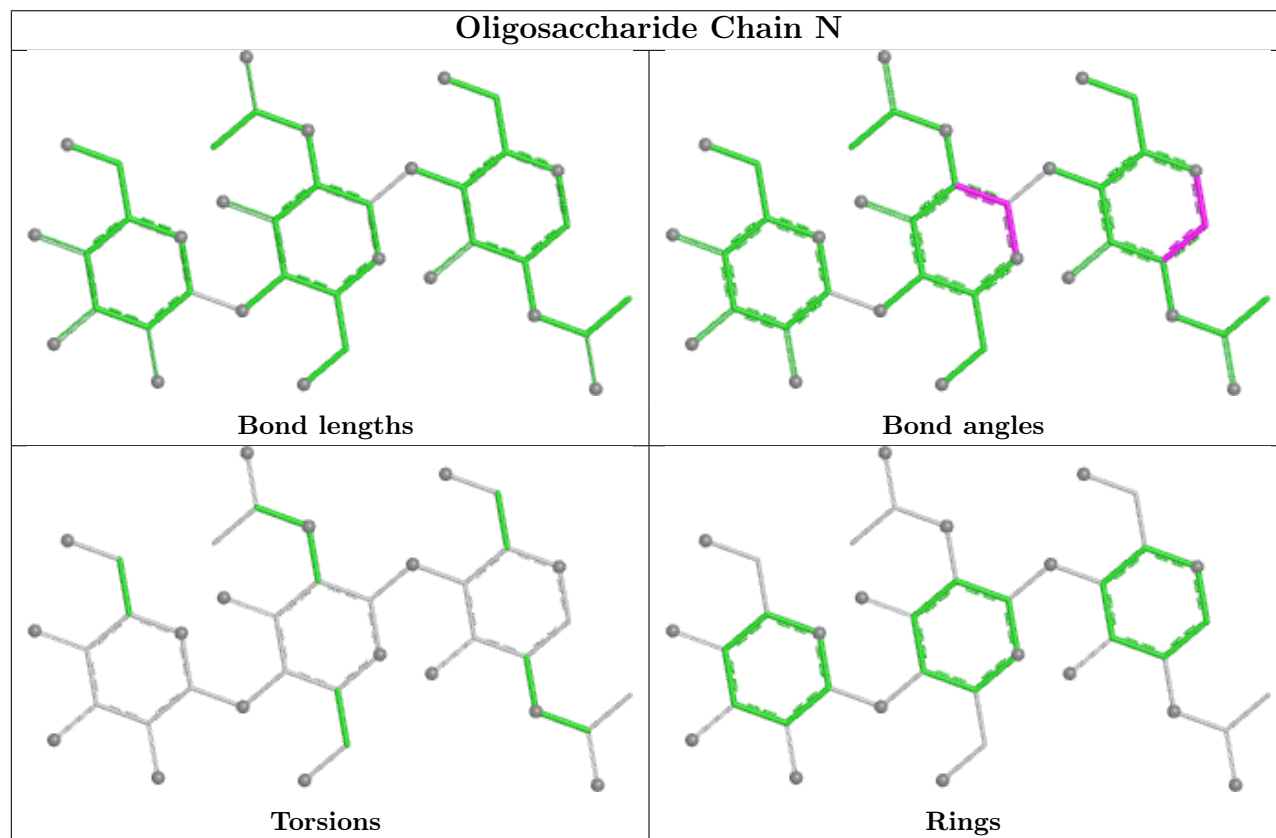
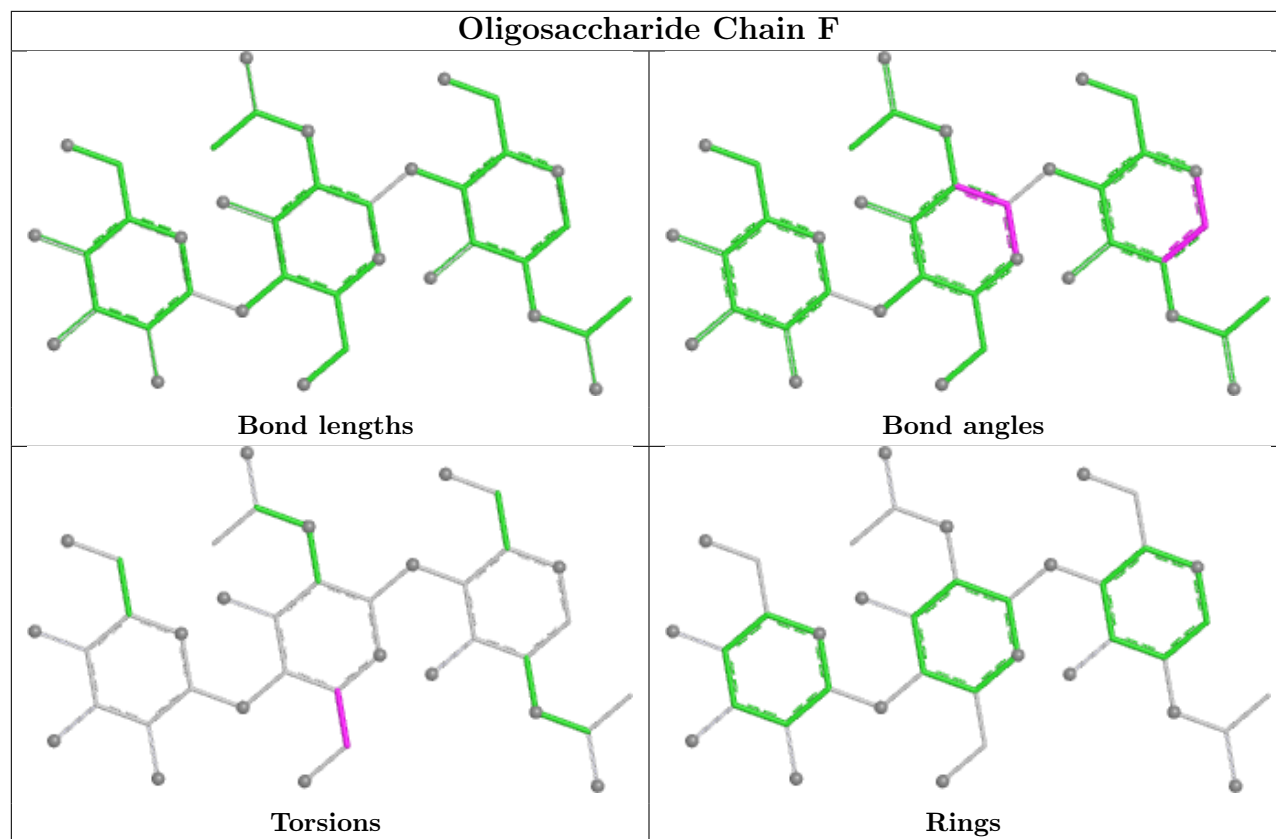
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

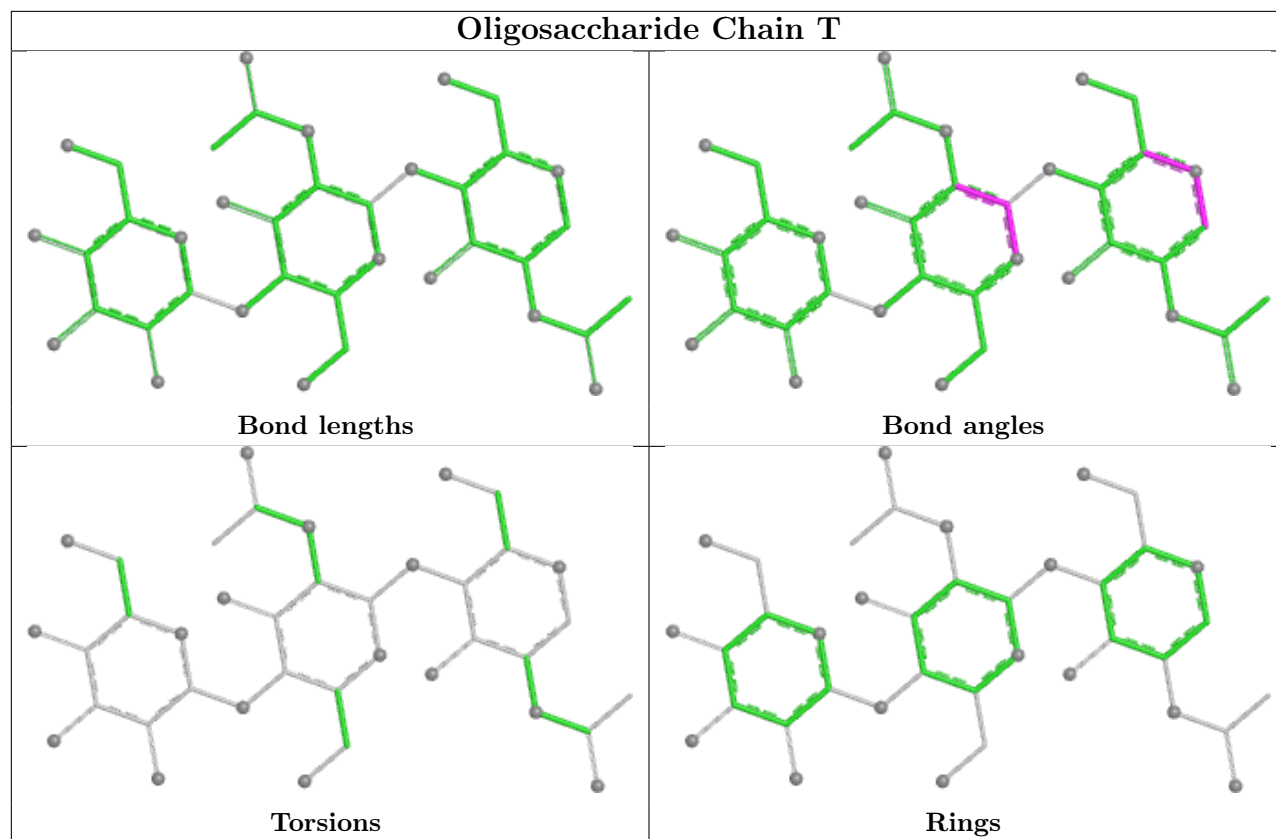


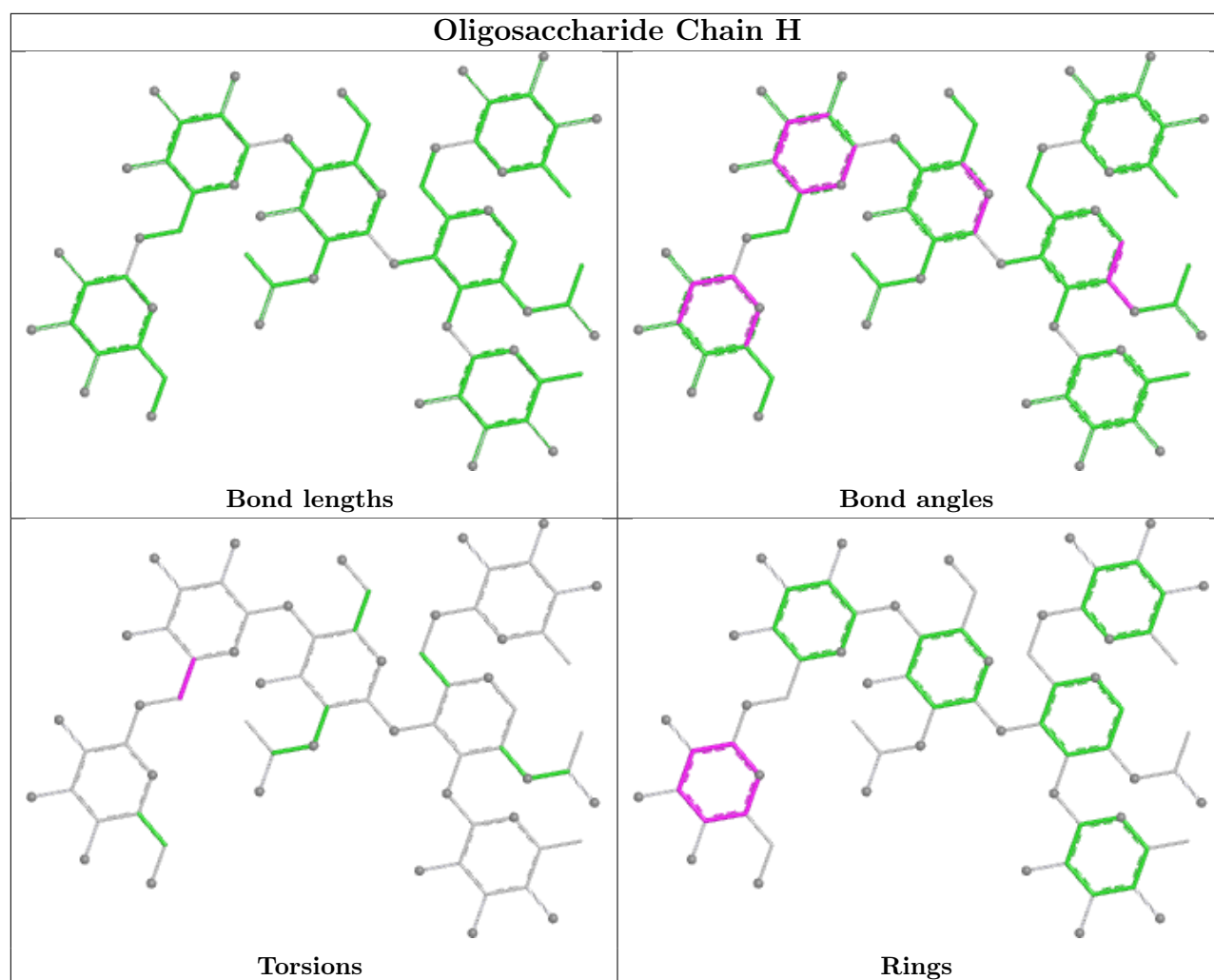


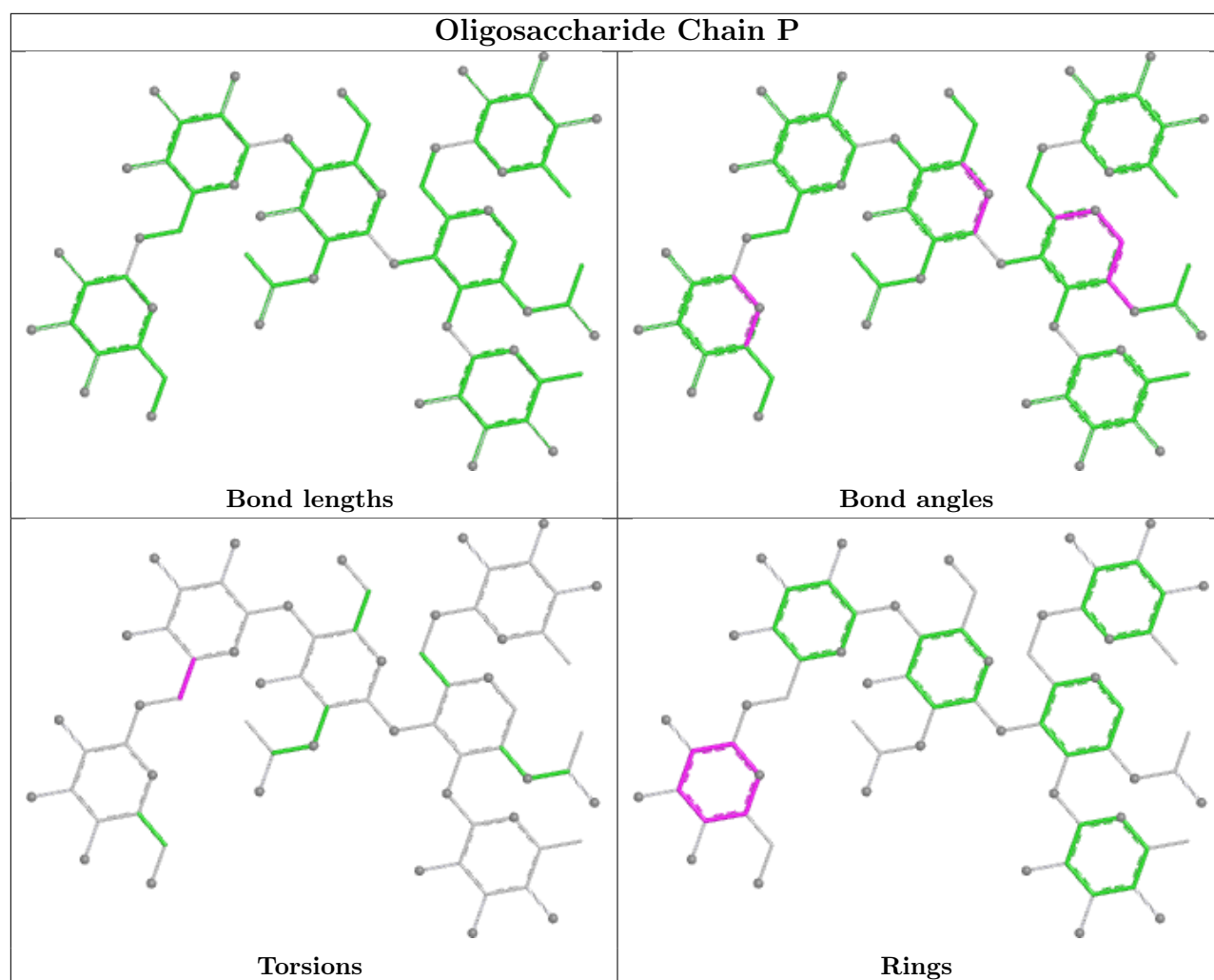


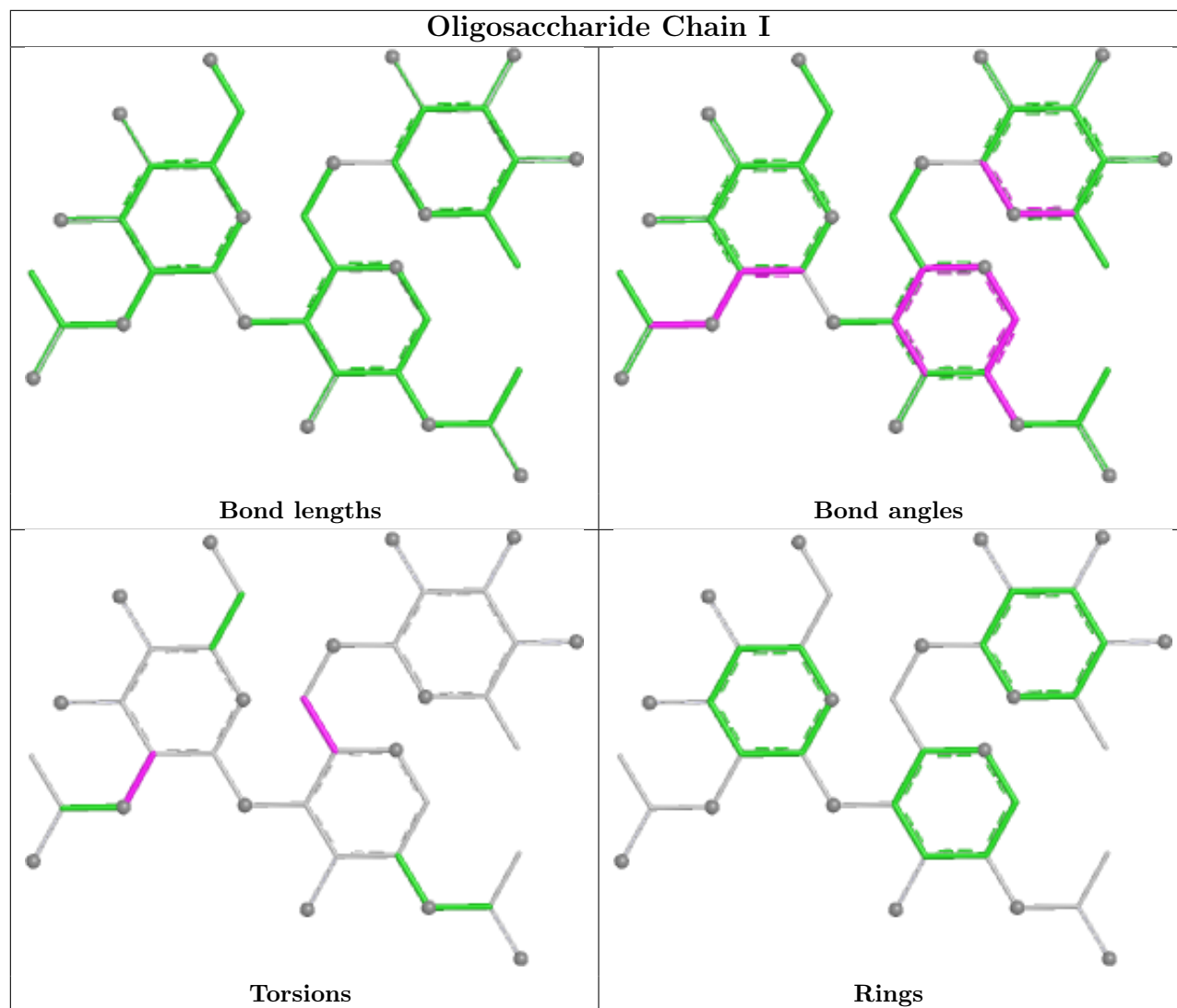


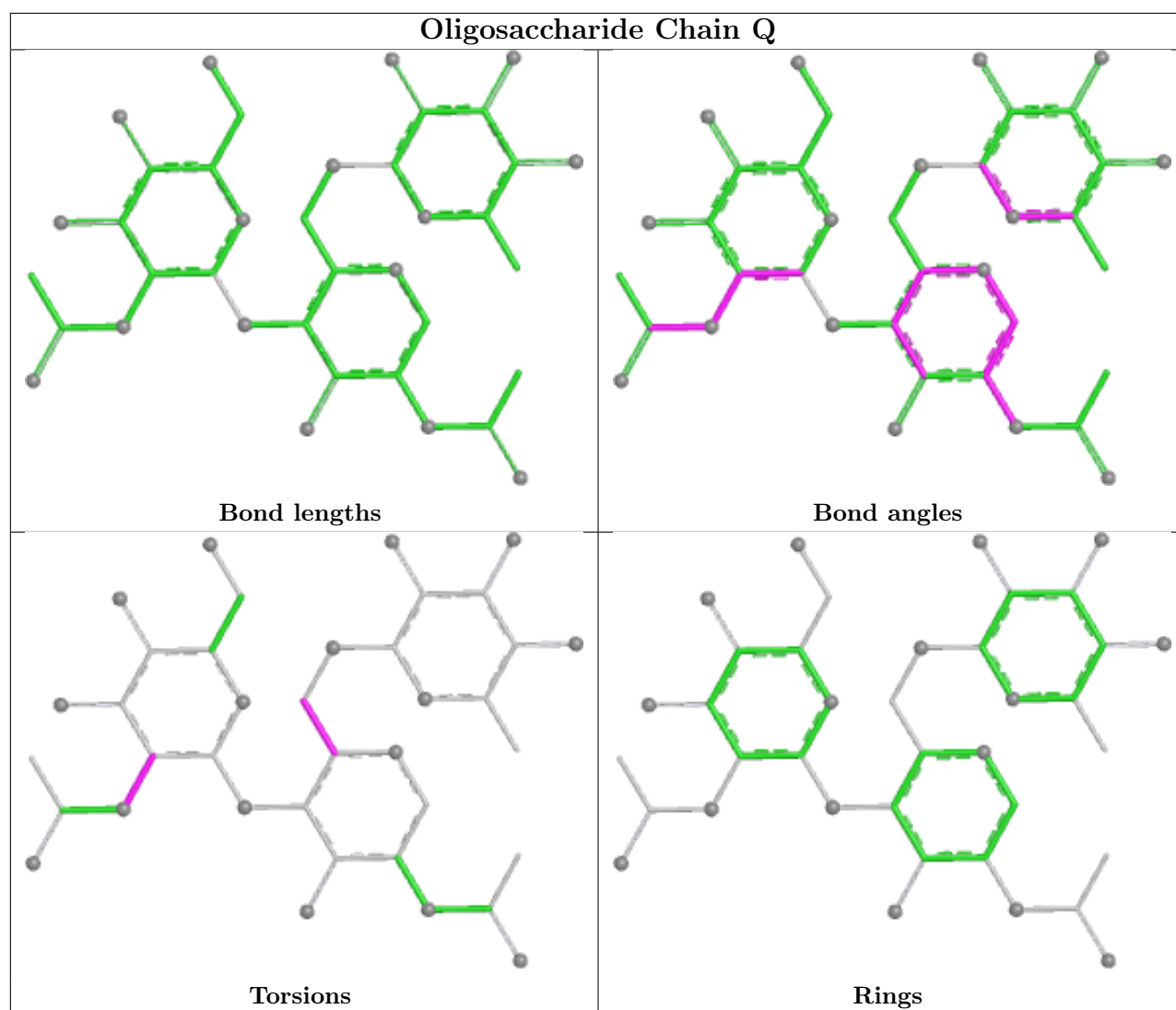




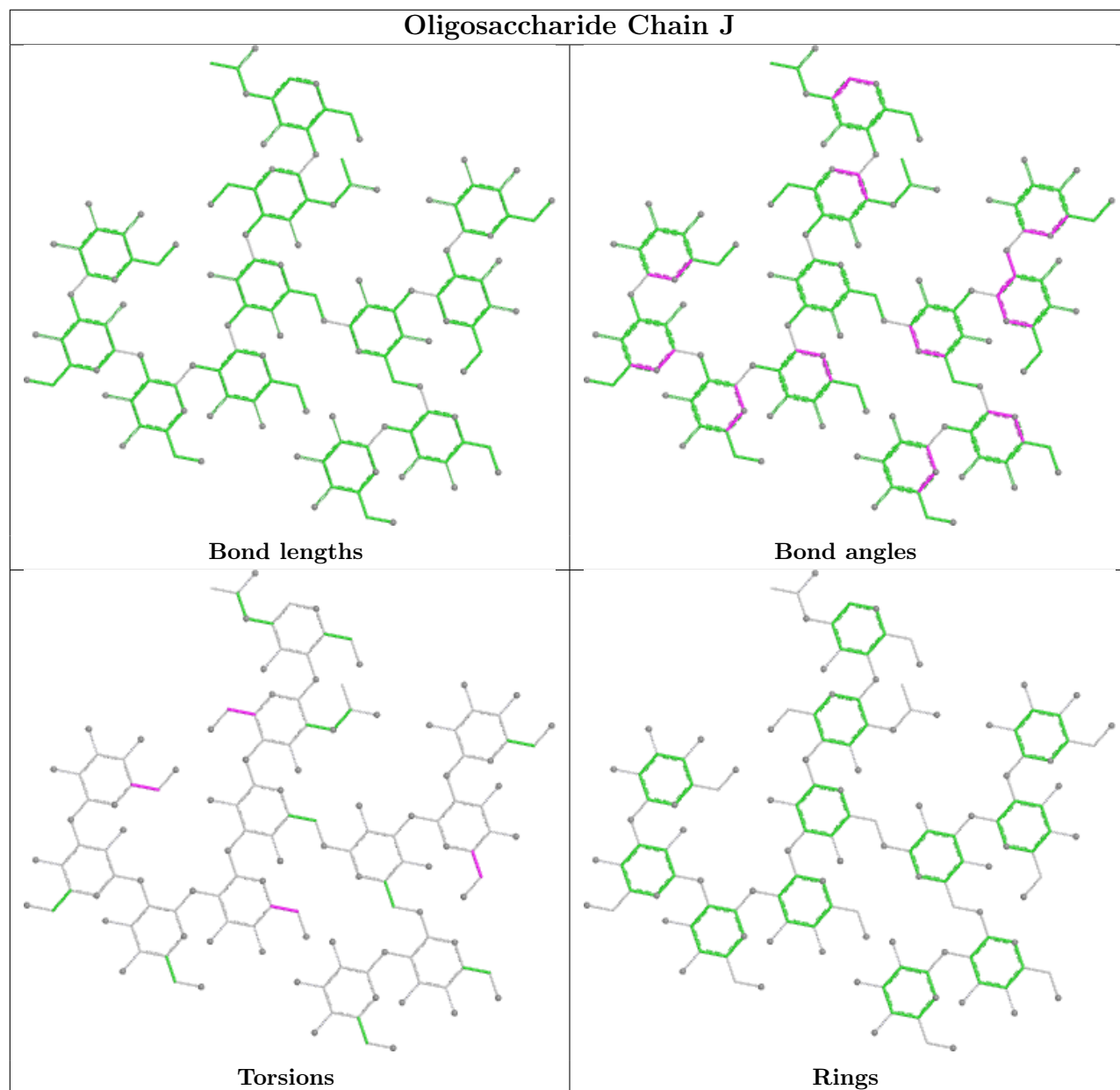


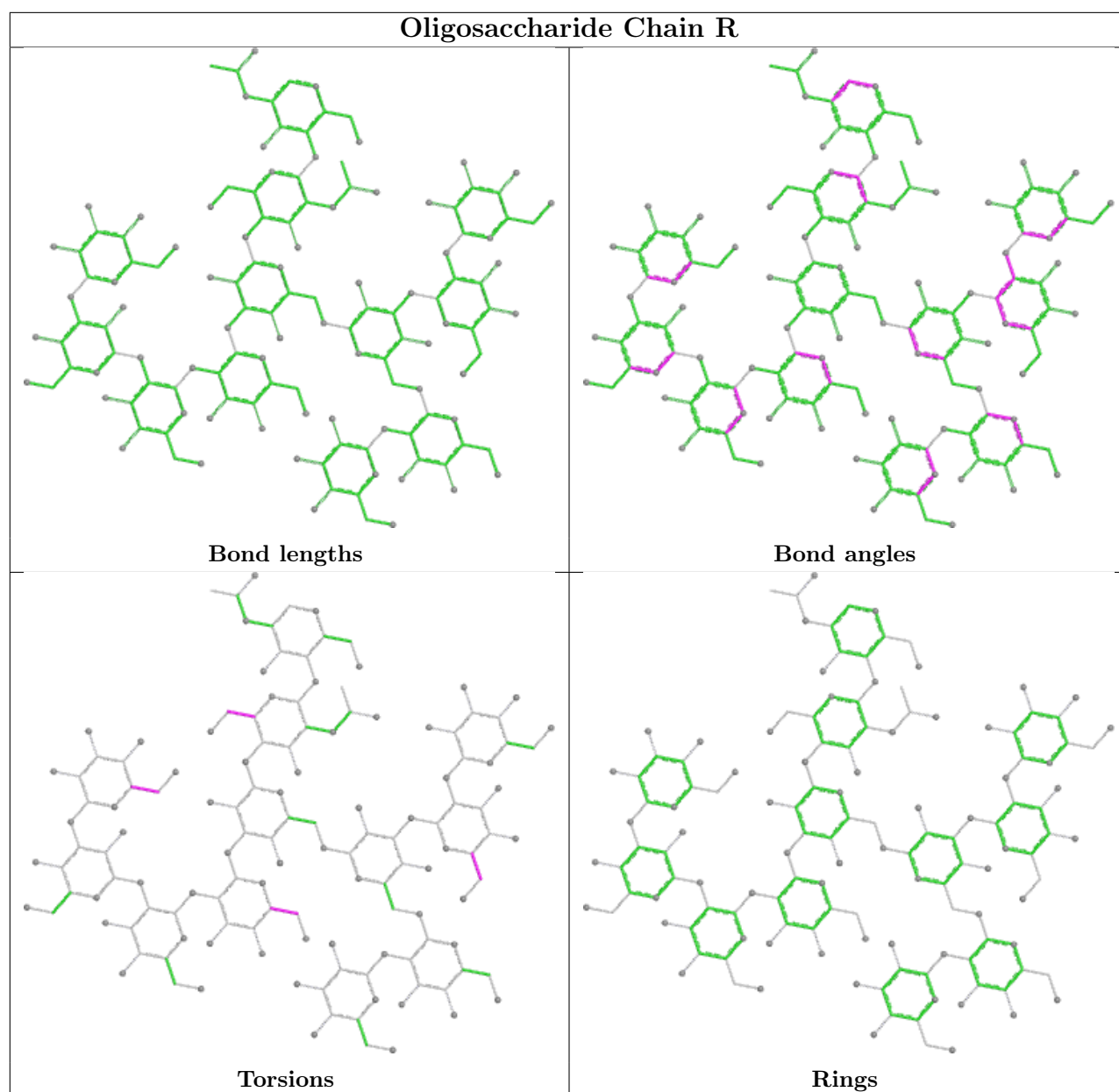


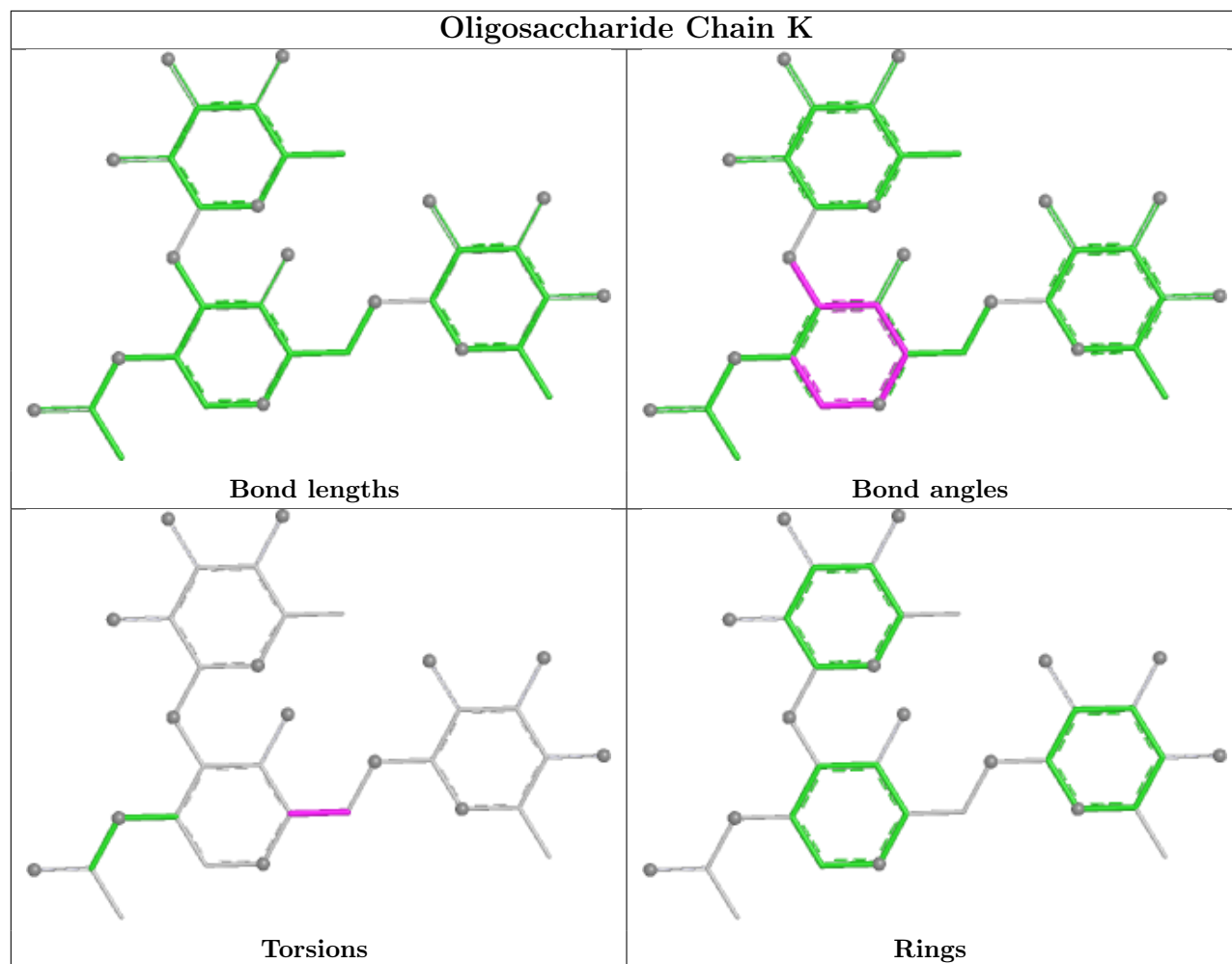


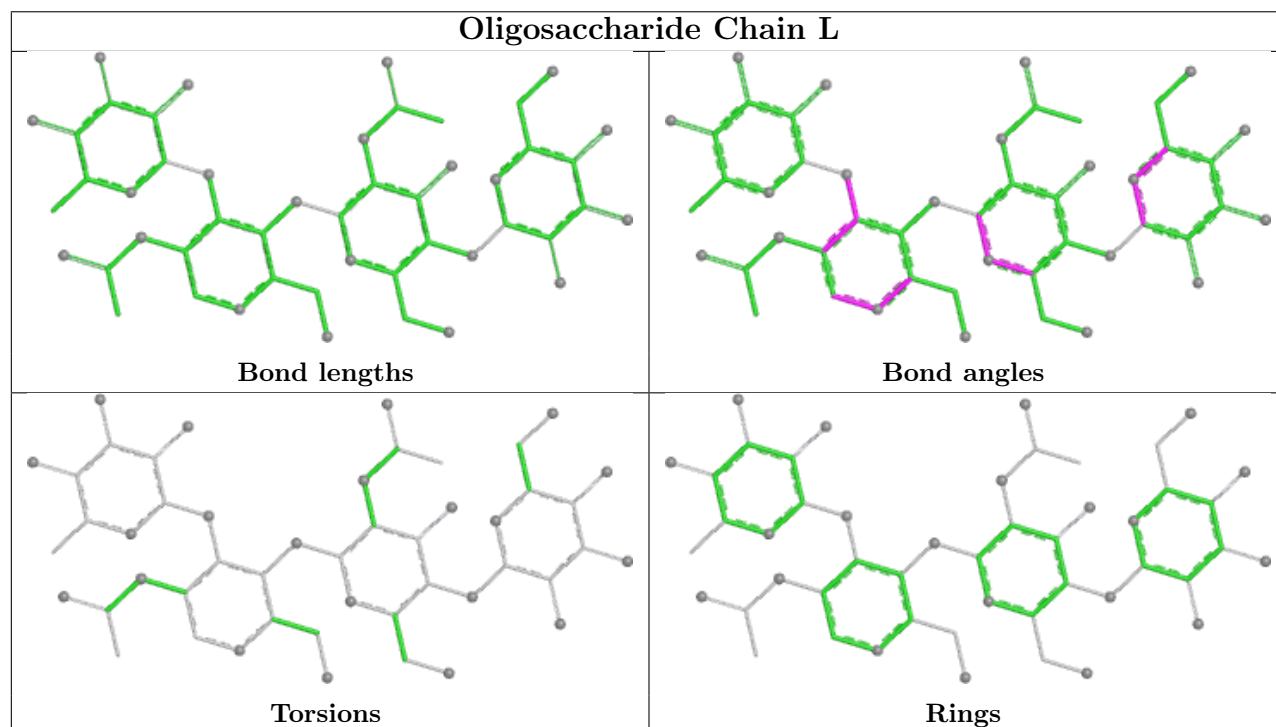
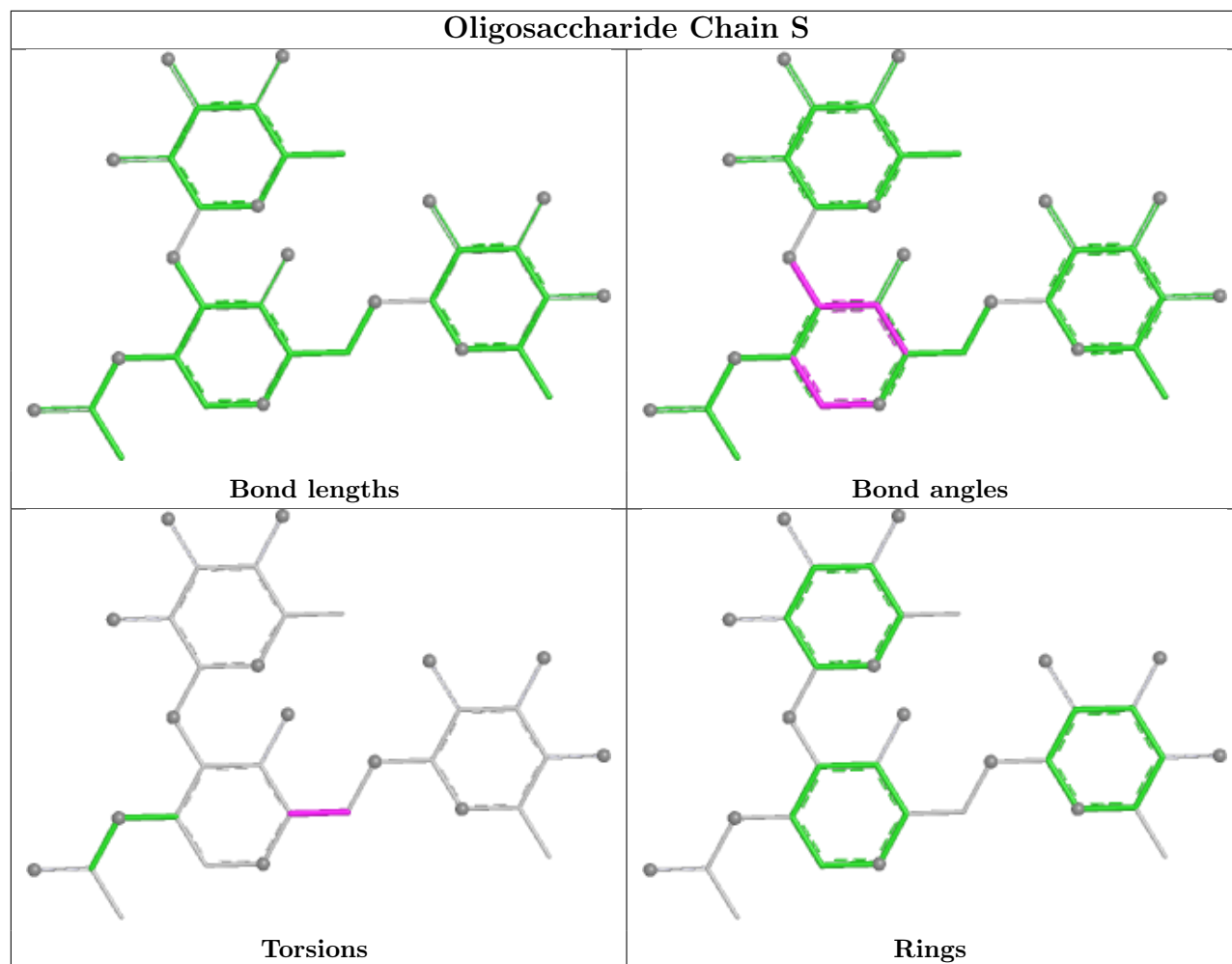


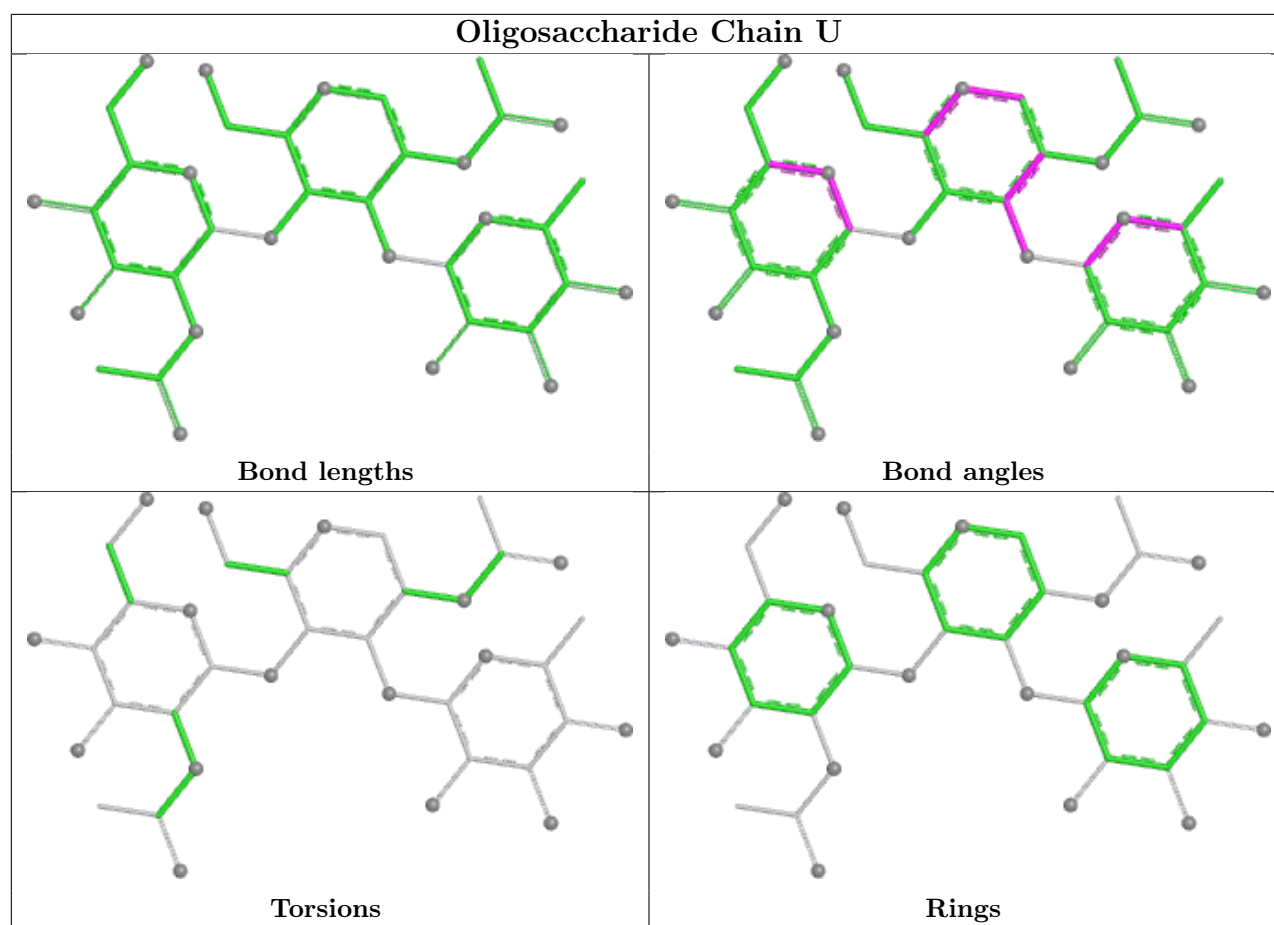
Oligosaccharide Chain J











5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
13	SO4	A	703	-	4,4,4	0.26	0	6,6,6	0.15	0
13	SO4	C	703	-	4,4,4	0.30	0	6,6,6	0.09	0
14	NAG	B	701	2	14,14,15	0.35	0	17,19,21	0.71	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
14	NAG	B	701	2	-	1/6/23/26	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(°)
14	B	701	NAG	C1-O5-C5	2.57	115.63	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	532/550 (96%)	1.01	68 (12%) 7 6	84, 101, 129, 156	0
1	C	532/550 (96%)	1.23	91 (17%) 4 3	38, 102, 128, 156	0
2	B	314/394 (79%)	1.63	94 (29%) 1 1	99, 155, 210, 217	0
2	D	298/394 (75%)	1.69	106 (35%) 1 0	101, 160, 227, 231	0
All	All	1676/1888 (88%)	1.32	359 (21%) 2 2	38, 109, 207, 231	0

The worst 5 of 359 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	252	ILE	5.7
2	B	362	LEU	5.6
1	C	408	SER	5.4
2	B	221	GLN	5.1
2	B	354	PRO	5.0

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

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

6.3 Carbohydrates [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(Å ²)	Q<0.9
4	NAG	N	2	14/15	0.20	0.16	161,163,165,166	0
5	BMA	H	3	11/12	0.22	0.17	155,157,158,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	O	4	11/12	0.23	0.18	168,168,169,169	0
4	BMA	F	3	11/12	0.23	0.15	157,158,159,160	0
4	NAG	T	2	14/15	0.24	0.15	233,233,234,234	0
5	BMA	P	3	11/12	0.29	0.18	159,160,163,164	0
10	FUC	U	2	10/11	0.29	0.18	195,195,195,195	0
8	FUC	S	2	10/11	0.33	0.19	155,156,156,156	0
9	BMA	L	3	11/12	0.33	0.18	195,196,196,196	0
4	BMA	T	3	11/12	0.33	0.12	234,234,234,234	0
5	NAG	P	2	14/15	0.34	0.17	149,151,154,156	0
3	MAN	O	5	11/12	0.35	0.22	168,168,169,169	0
9	FUC	L	4	10/11	0.36	0.20	185,185,186,186	0
5	MAN	H	4	11/12	0.37	0.19	160,160,161,161	0
8	FUC	K	3	10/11	0.37	0.20	163,163,163,163	0
8	FUC	K	2	10/11	0.39	0.20	162,162,162,162	0
4	NAG	F	2	14/15	0.39	0.16	150,152,154,156	0
6	NAG	Q	2	14/15	0.39	0.16	153,154,155,155	0
5	MAN	P	4	11/12	0.40	0.17	166,166,167,167	0
3	MAN	G	4	11/12	0.43	0.17	168,169,169,169	0
4	BMA	N	3	11/12	0.43	0.15	168,170,170,170	0
6	FUC	I	3	10/11	0.45	0.17	155,156,156,156	0
6	NAG	Q	1	14/15	0.46	0.18	148,151,153,155	0
6	NAG	I	2	14/15	0.46	0.14	153,154,154,154	0
6	FUC	Q	3	10/11	0.48	0.15	156,157,157,157	0
6	NAG	I	1	14/15	0.50	0.19	148,150,153,154	0
3	BMA	O	3	11/12	0.52	0.16	164,166,167,167	0
3	MAN	G	5	11/12	0.57	0.17	168,169,170,170	0
5	FUC	P	6	10/11	0.57	0.20	144,144,144,144	0
8	FUC	S	3	10/11	0.58	0.17	155,155,156,156	0
10	NAG	U	3	14/15	0.58	0.16	195,196,196,196	0
5	NAG	H	2	14/15	0.59	0.14	145,147,150,153	0
9	NAG	L	2	14/15	0.59	0.16	189,191,192,193	0
5	FUC	P	5	10/11	0.62	0.14	144,144,145,145	0
3	MAN	M	5	11/12	0.64	0.18	154,155,156,156	0
10	NAG	U	1	14/15	0.66	0.16	192,193,194,194	0
4	NAG	T	1	14/15	0.67	0.14	232,232,233,233	0
5	FUC	H	5	10/11	0.68	0.13	140,140,140,141	0
3	BMA	E	3	11/12	0.68	0.14	149,152,155,157	0
3	MAN	M	4	11/12	0.70	0.15	149,150,150,150	0
8	NAG	S	1	14/15	0.70	0.19	151,153,155,155	0
3	MAN	E	5	11/12	0.71	0.17	157,157,159,159	0
9	NAG	L	1	14/15	0.71	0.15	182,183,185,187	0
3	FUC	G	6	10/11	0.71	0.17	148,149,149,150	0

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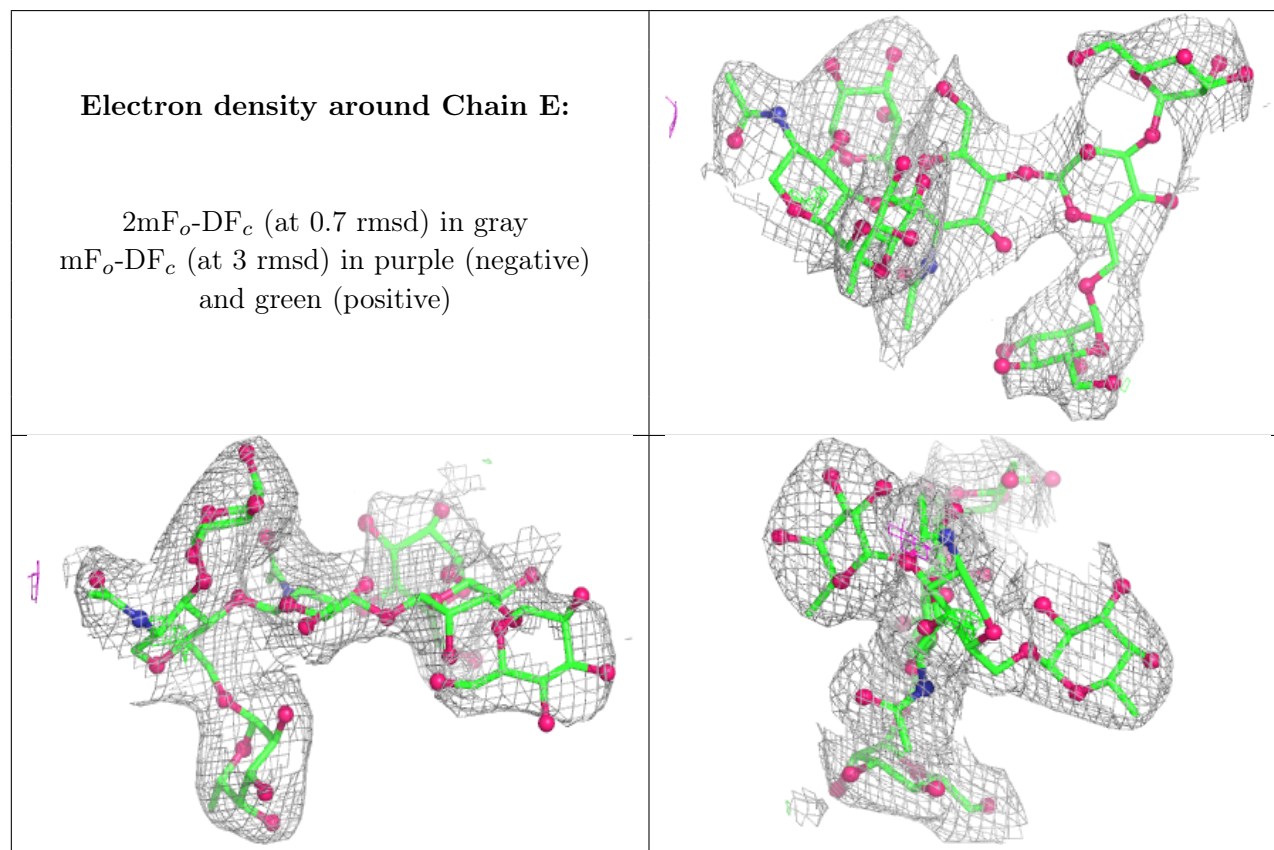
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	E	4	11/12	0.71	0.15	153,154,154,155	0
5	FUC	H	6	10/11	0.72	0.17	139,140,140,140	0
3	FUC	O	6	10/11	0.72	0.15	148,149,149,149	0
7	GLC	R	7	11/12	0.73	0.20	150,151,151,151	0
7	MAN	R	10	11/12	0.73	0.19	128,130,131,131	0
8	NAG	K	1	14/15	0.73	0.18	157,159,161,162	0
3	BMA	M	3	11/12	0.75	0.13	143,147,150,152	0
4	NAG	F	1	14/15	0.75	0.15	139,142,144,147	0
7	MAN	R	6	11/12	0.76	0.17	142,145,146,148	0
7	MAN	J	10	11/12	0.76	0.19	125,126,126,127	0
7	GLC	J	7	11/12	0.77	0.18	145,146,146,146	0
4	NAG	N	1	14/15	0.78	0.15	149,152,155,158	0
3	BMA	G	3	11/12	0.80	0.09	164,166,167,167	0
7	MAN	J	6	11/12	0.82	0.18	139,142,143,143	0
5	NAG	P	1	14/15	0.83	0.11	138,140,144,146	0
3	NAG	G	2	14/15	0.84	0.15	153,155,158,161	0
3	NAG	M	2	14/15	0.84	0.16	130,132,136,140	0
3	NAG	O	2	14/15	0.85	0.16	154,155,158,161	0
7	MAN	R	4	11/12	0.85	0.13	123,123,126,129	0
7	MAN	J	9	11/12	0.85	0.13	116,117,119,122	0
7	MAN	J	4	11/12	0.86	0.13	121,122,123,127	0
3	NAG	O	1	14/15	0.86	0.13	143,146,148,151	0
7	MAN	R	9	11/12	0.87	0.12	117,118,121,125	0
5	NAG	H	1	14/15	0.87	0.11	134,135,139,142	0
7	MAN	R	12	11/12	0.87	0.16	114,115,116,116	0
3	FUC	O	7	10/11	0.87	0.20	140,141,142,142	0
7	MAN	J	12	11/12	0.88	0.16	113,113,114,114	0
3	NAG	G	1	14/15	0.88	0.12	142,146,148,150	0
3	FUC	M	7	10/11	0.89	0.15	126,126,126,127	0
3	NAG	E	2	14/15	0.90	0.13	136,138,142,145	0
7	MAN	R	11	11/12	0.90	0.11	116,117,118,118	0
7	NAG	R	1	14/15	0.90	0.24	109,110,112,112	0
7	MAN	J	5	11/12	0.90	0.14	130,133,133,136	0
7	NAG	J	1	14/15	0.91	0.26	104,106,110,111	0
7	MAN	J	11	11/12	0.91	0.12	112,113,114,114	0
3	FUC	M	6	10/11	0.91	0.17	124,124,125,125	0
7	MAN	R	5	11/12	0.92	0.13	132,134,136,139	0
3	FUC	E	6	10/11	0.92	0.14	126,126,127,127	0
3	FUC	E	7	10/11	0.92	0.12	132,132,132,132	0
3	FUC	G	7	10/11	0.92	0.20	139,139,140,140	0
7	NAG	R	2	14/15	0.93	0.18	108,111,112,113	0
3	NAG	E	1	14/15	0.93	0.13	125,127,131,133	0

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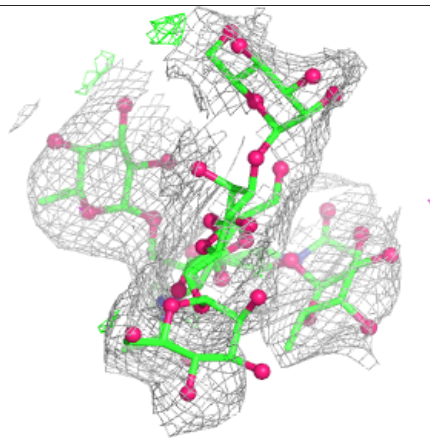
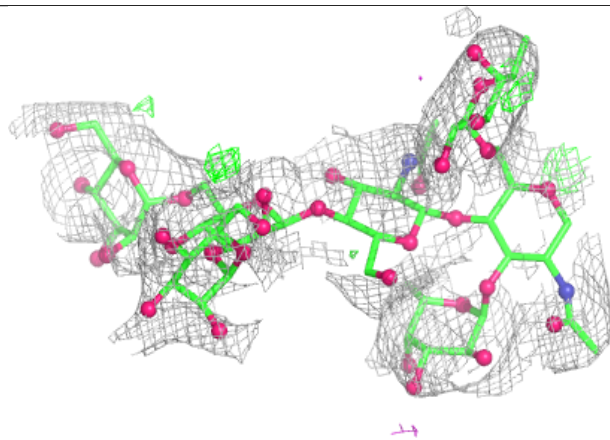
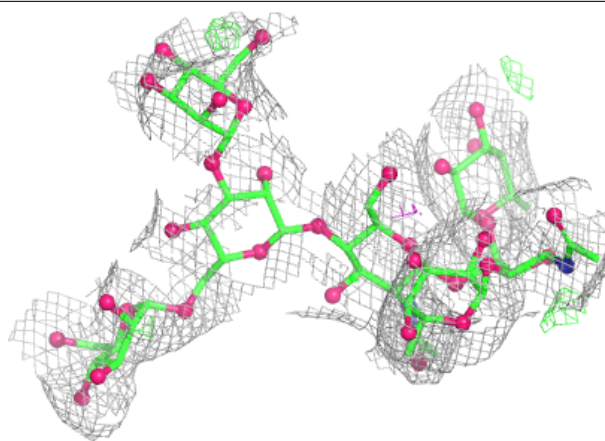
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	R	8	11/12	0.93	0.12	114,116,117,118	0
3	NAG	M	1	14/15	0.93	0.13	121,123,125,128	0
7	MAN	J	8	11/12	0.94	0.11	111,112,114,116	0
7	BMA	R	3	11/12	0.94	0.12	115,116,118,121	0
7	NAG	J	2	14/15	0.95	0.18	104,106,107,109	0
7	BMA	J	3	11/12	0.97	0.10	110,112,114,118	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.



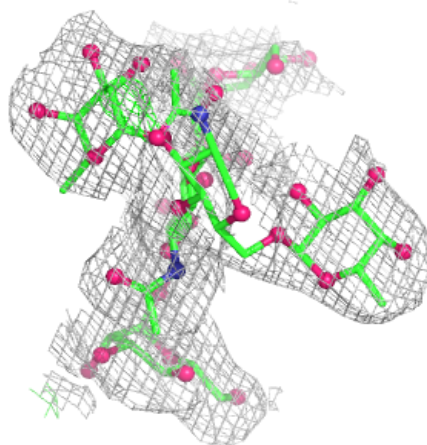
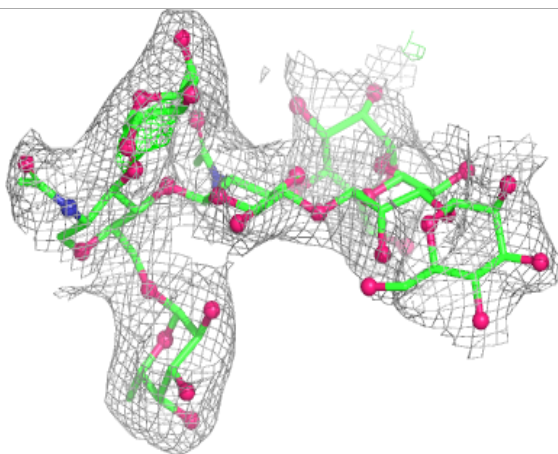
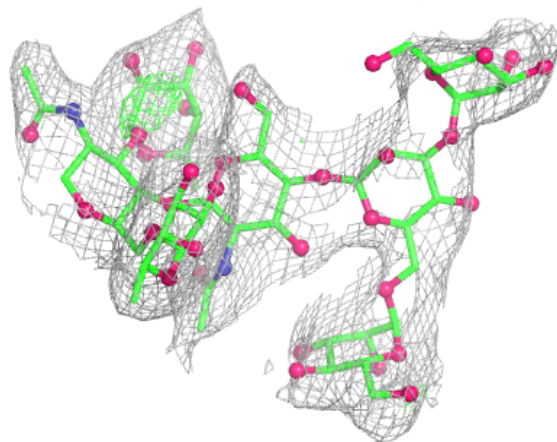
Electron density around Chain G:

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



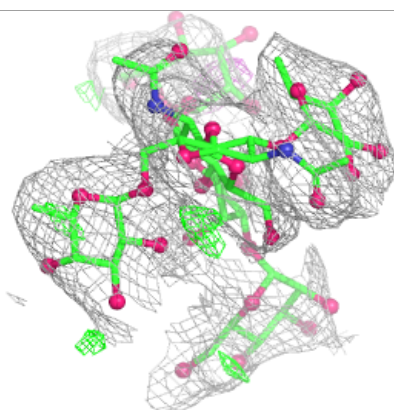
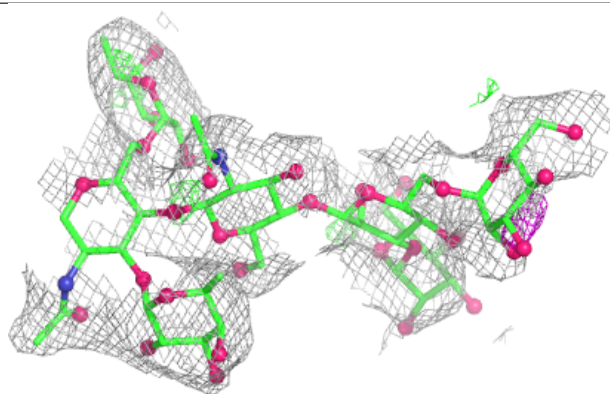
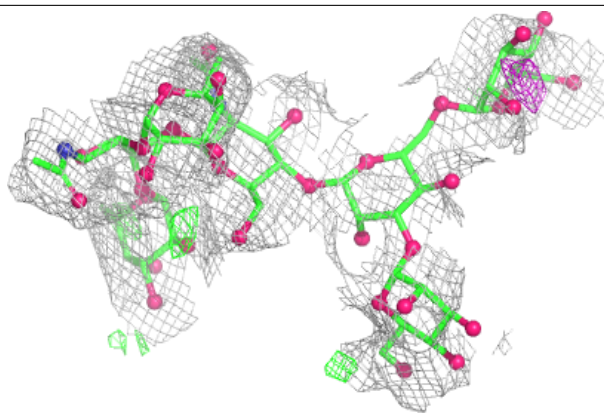
Electron density around Chain M:

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

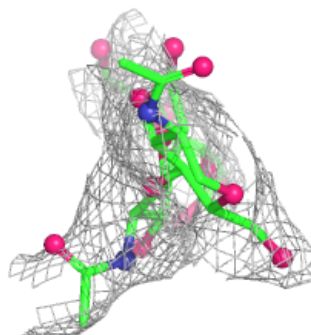
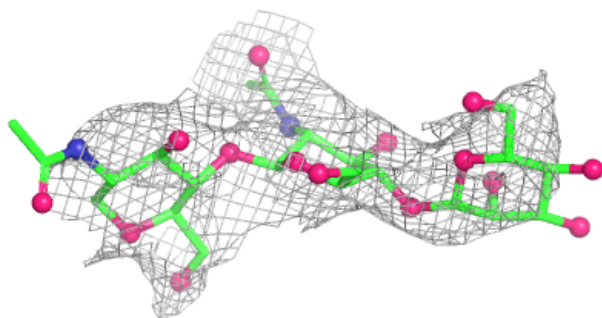
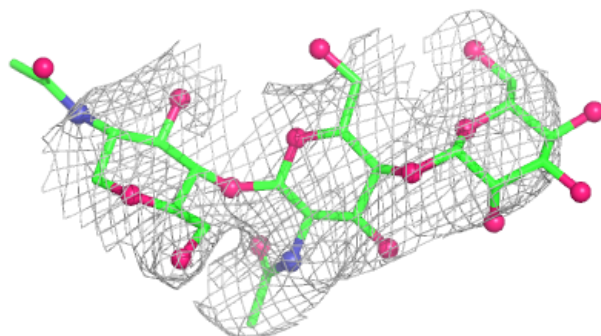


Electron density around Chain O:

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

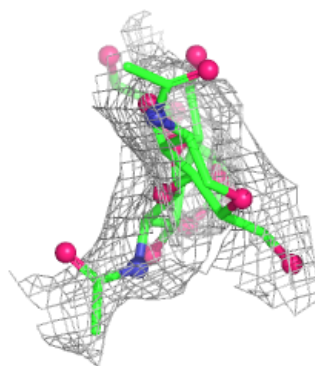
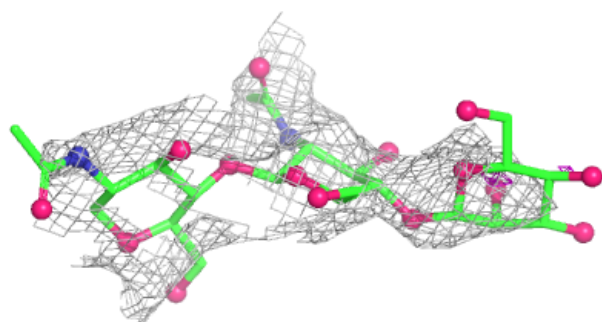
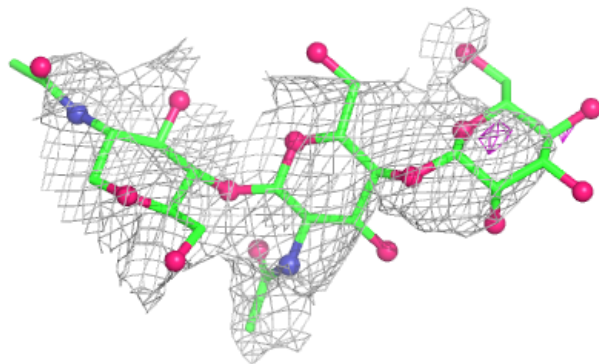
**Electron density around Chain F:**

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

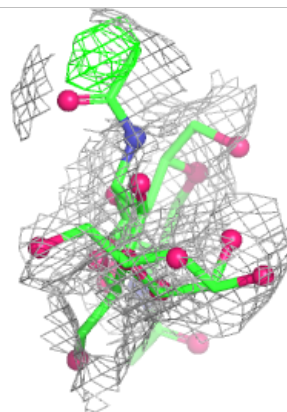
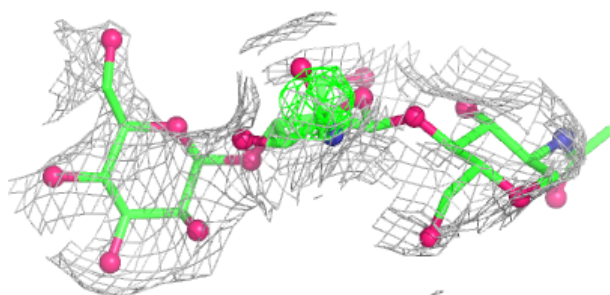
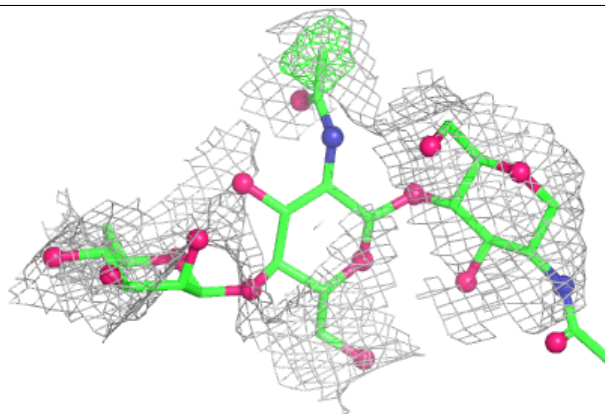


Electron density around Chain N:

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

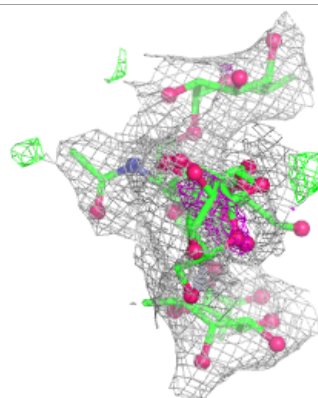
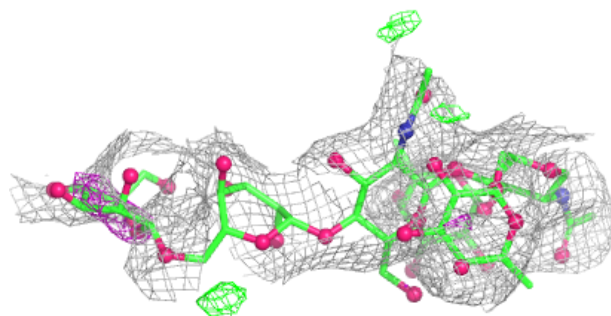
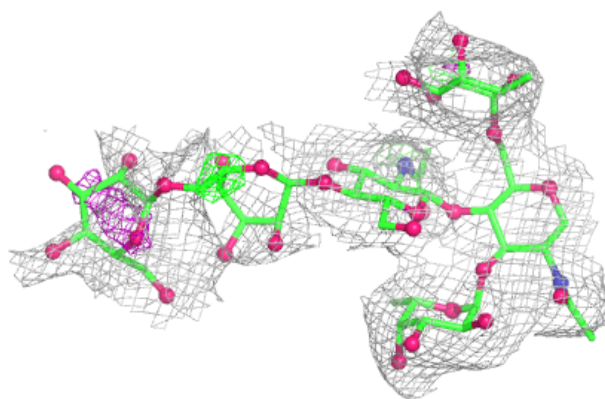
**Electron density around Chain T:**

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

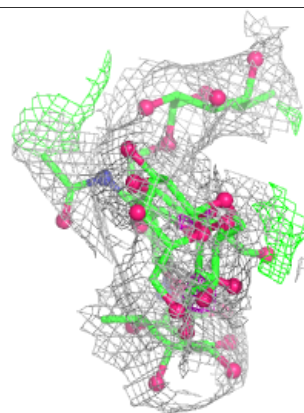
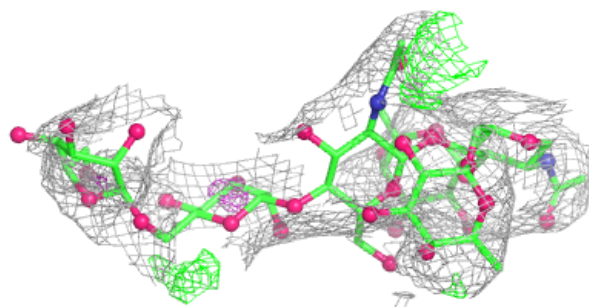
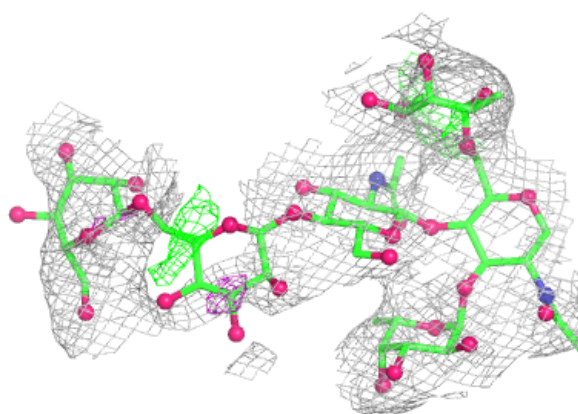


Electron density around Chain H:

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

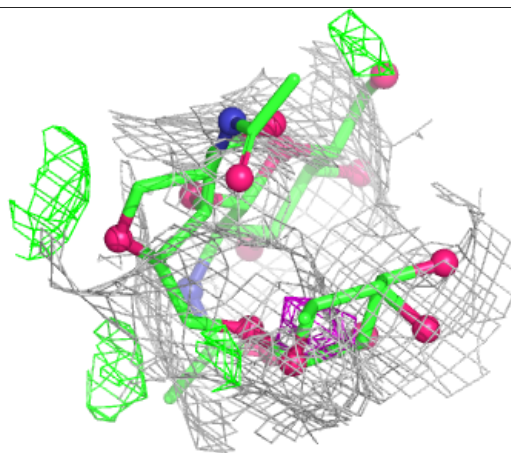
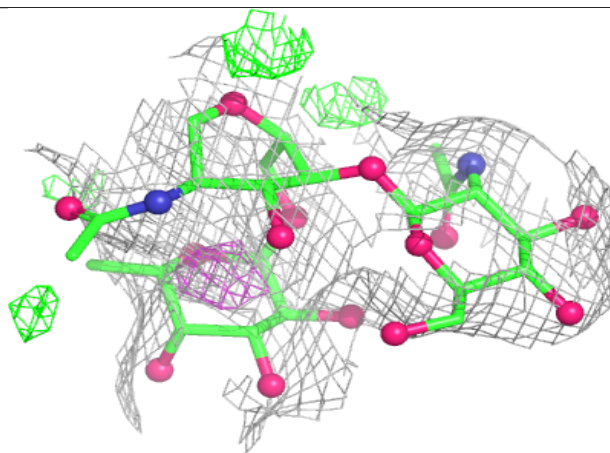
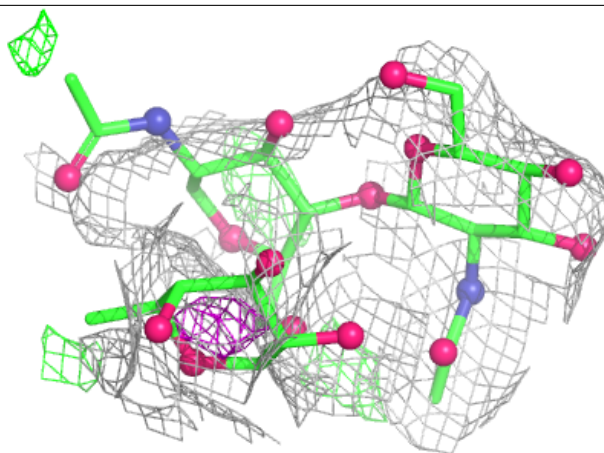
**Electron density around Chain P:**

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



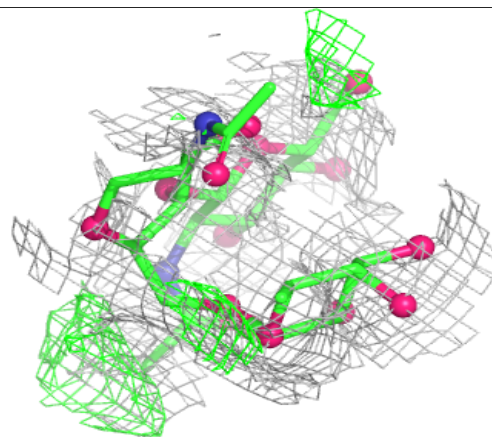
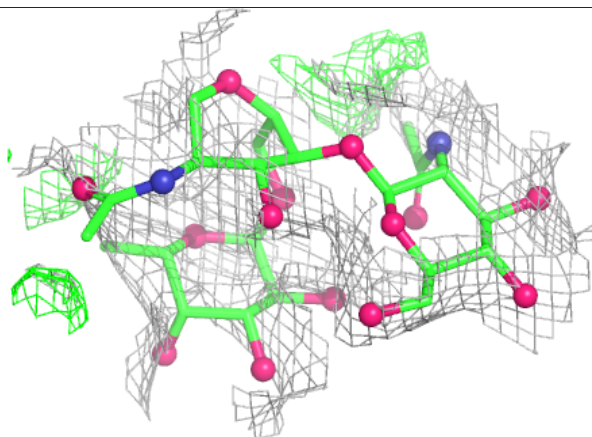
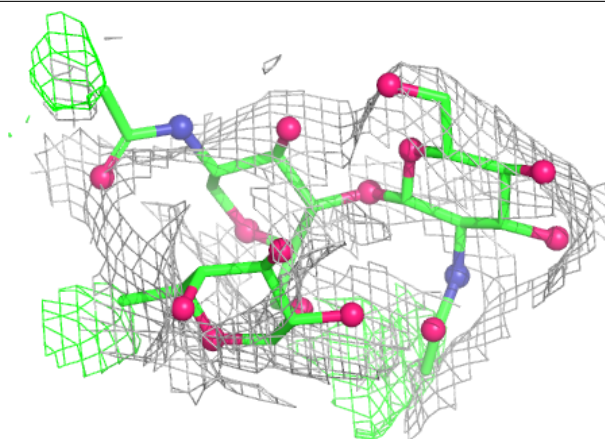
Electron density around Chain I:

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

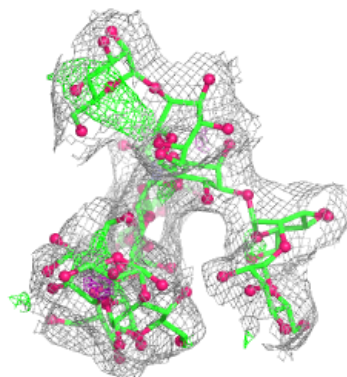
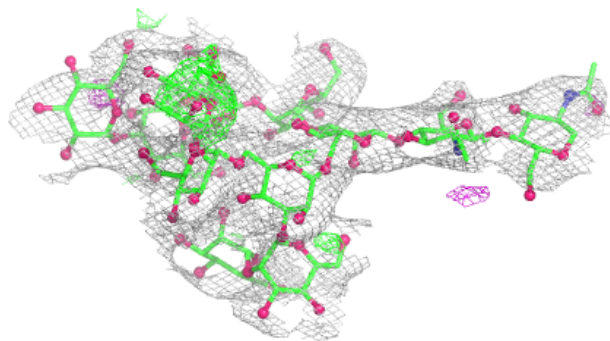
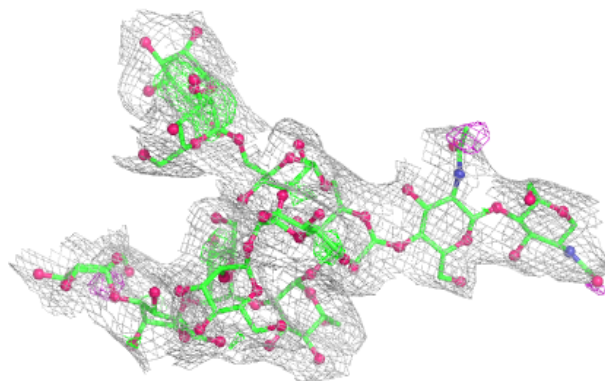


Electron density around Chain Q:

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

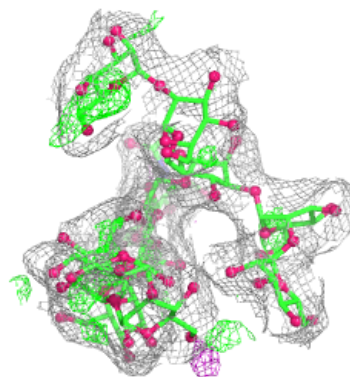
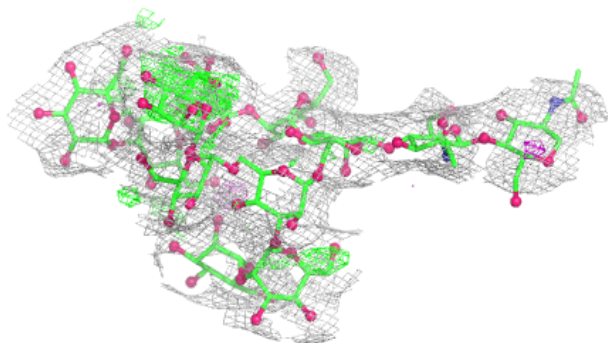
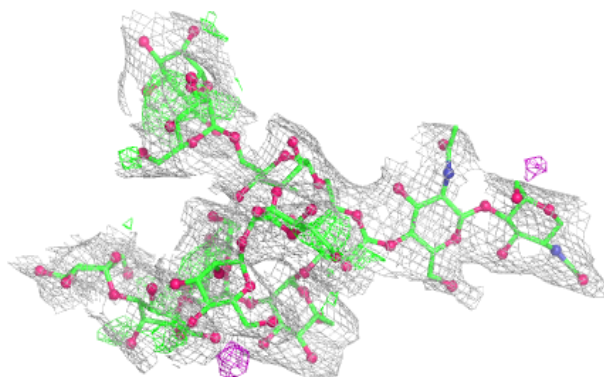
**Electron density around Chain J:**

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

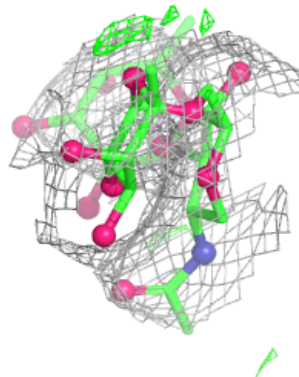
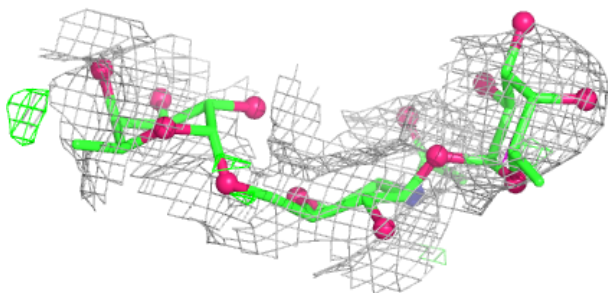
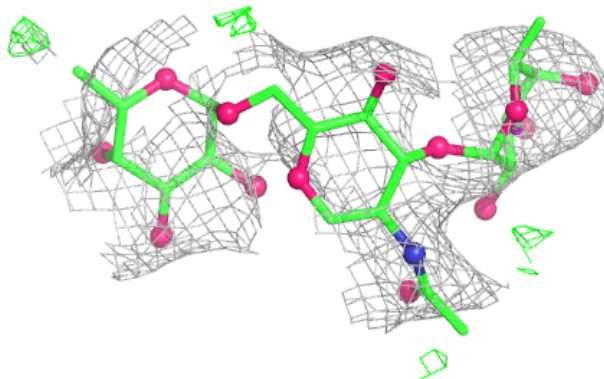


Electron density around Chain R:

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

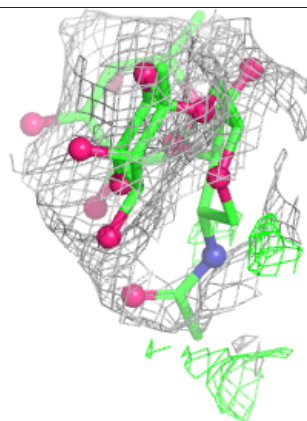
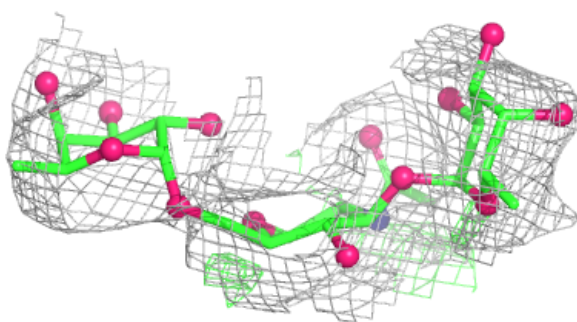
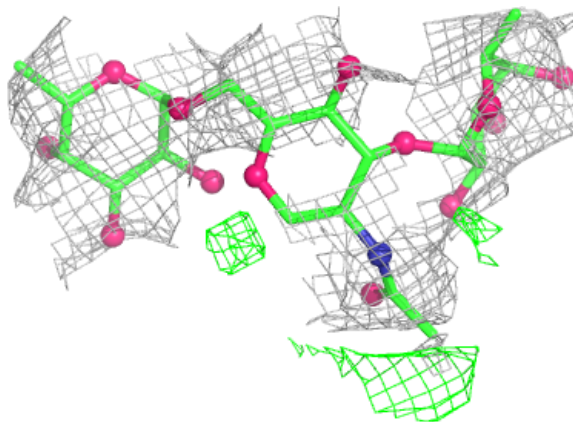
**Electron density around Chain K:**

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

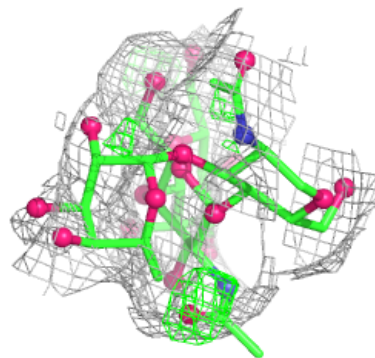
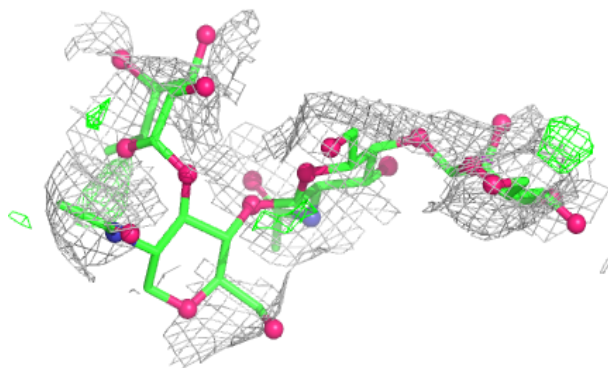
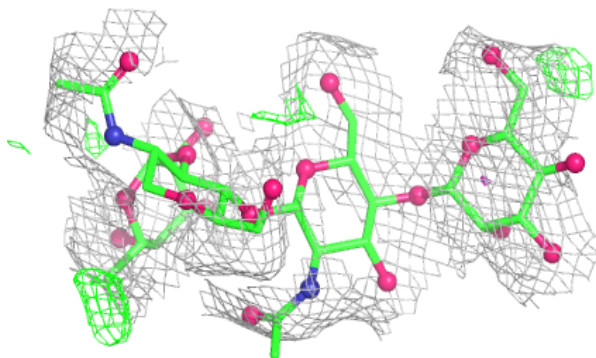


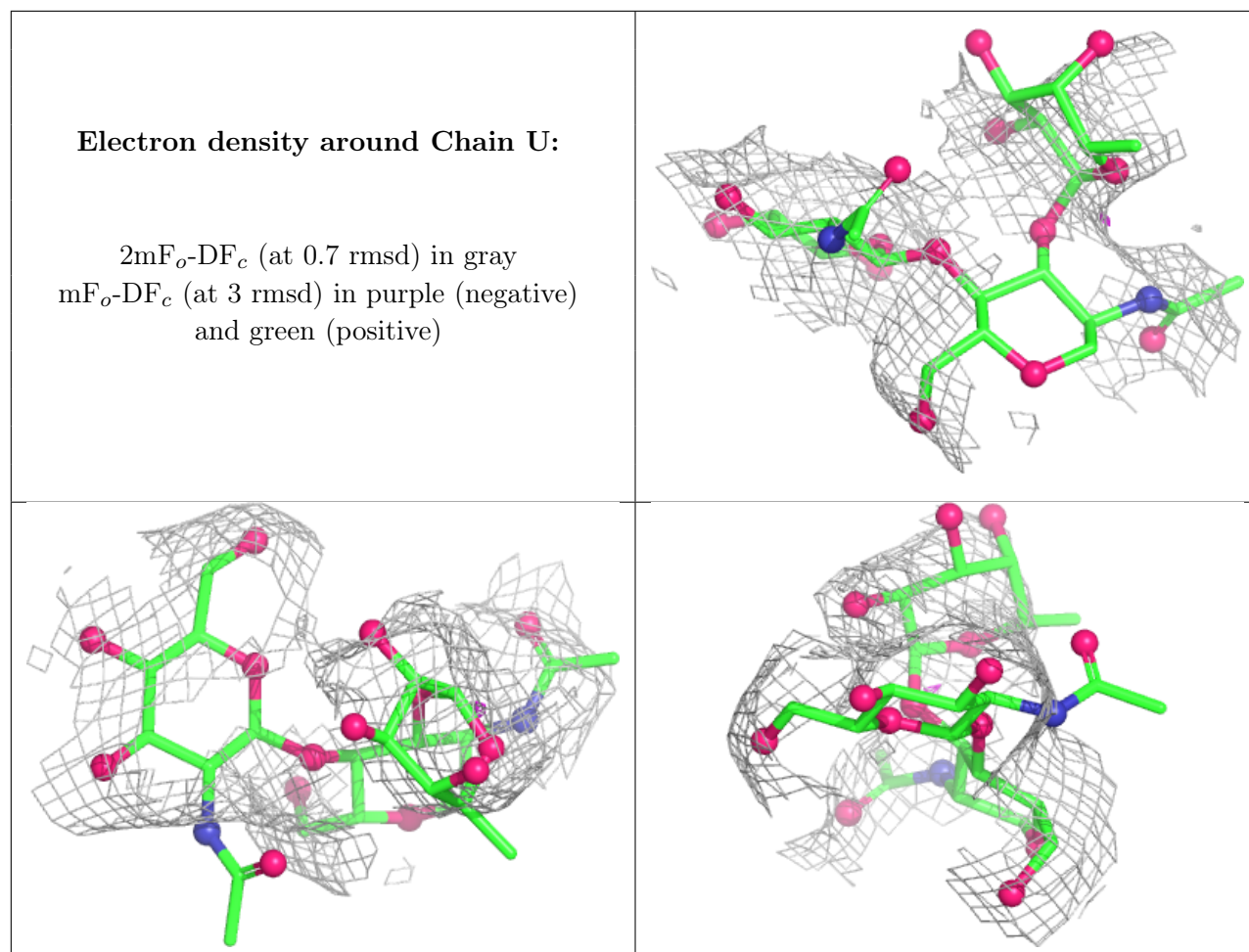
Electron density around Chain S:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
14	NAG	B	701	14/15	0.59	0.15	204,204,204,204	0
13	SO4	C	703	5/5	0.83	0.18	170,170,170,170	0
13	SO4	A	703	5/5	0.89	0.13	160,160,160,160	0
11	NA	C	701	1/1	0.96	0.07	97,97,97,97	0
11	NA	A	701	1/1	0.99	0.03	92,92,92,92	0
12	ZN	A	702	1/1	0.99	0.04	97,97,97,97	0
12	ZN	C	702	1/1	0.99	0.03	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.