



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 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 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

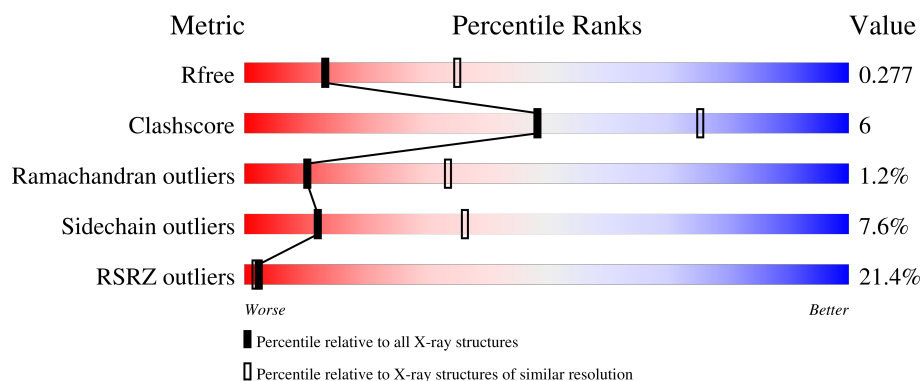
1 Overall quality at a glance

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.



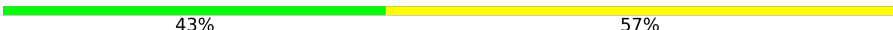
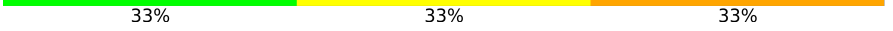
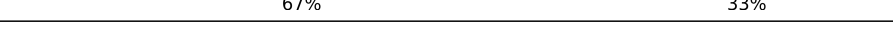
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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:

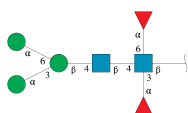
Chain	Residue	Modelled	Actual	Comment	Reference
B	389	HIS	-	expression tag	UNP Q9QXC1
B	390	HIS	-	expression tag	UNP Q9QXC1
B	391	HIS	-	expression tag	UNP Q9QXC1
B	392	HIS	-	expression tag	UNP Q9QXC1
B	393	HIS	-	expression tag	UNP Q9QXC1
B	394	HIS	-	expression tag	UNP Q9QXC1

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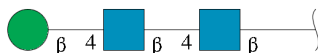
Chain	Residue	Modelled	Actual	Comment	Reference
D	389	HIS	-	expression tag	UNP Q9QXC1
D	390	HIS	-	expression tag	UNP Q9QXC1
D	391	HIS	-	expression tag	UNP Q9QXC1
D	392	HIS	-	expression tag	UNP Q9QXC1
D	393	HIS	-	expression tag	UNP Q9QXC1
D	394	HIS	-	expression tag	UNP Q9QXC1

- 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			

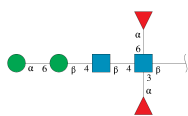
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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			

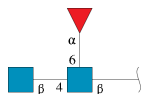
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

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.



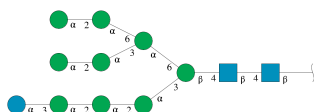
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			70	40	2	28			
5	P	6	Total	C	N	O	0	0	0
			70	40	2	28			

- 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			

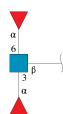
- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-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

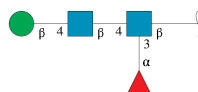
- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1

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



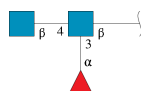
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	3	Total	C	N	O	0	0	0
			34	20	1	13			
8	S	3	Total	C	N	O	0	0	0
			34	20	1	13			

- 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			

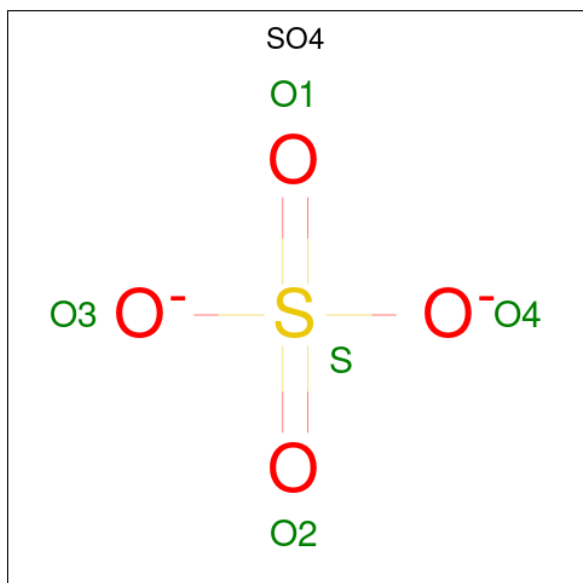
- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

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).

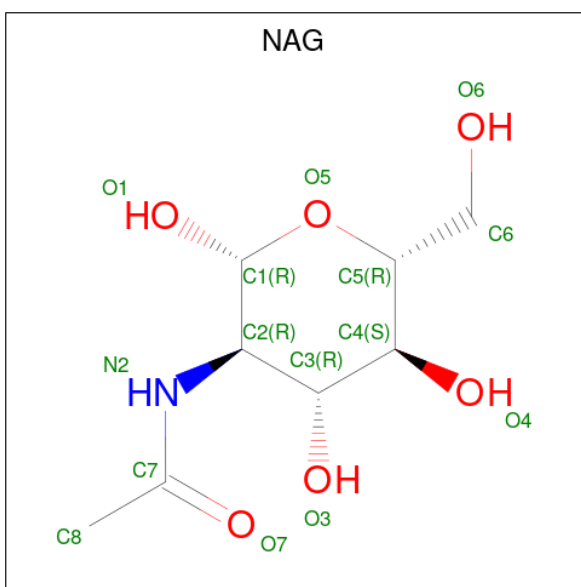
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Zn	0	0
			1	1		
12	C	1	Total	Zn	0	0
			1	1		

- 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		

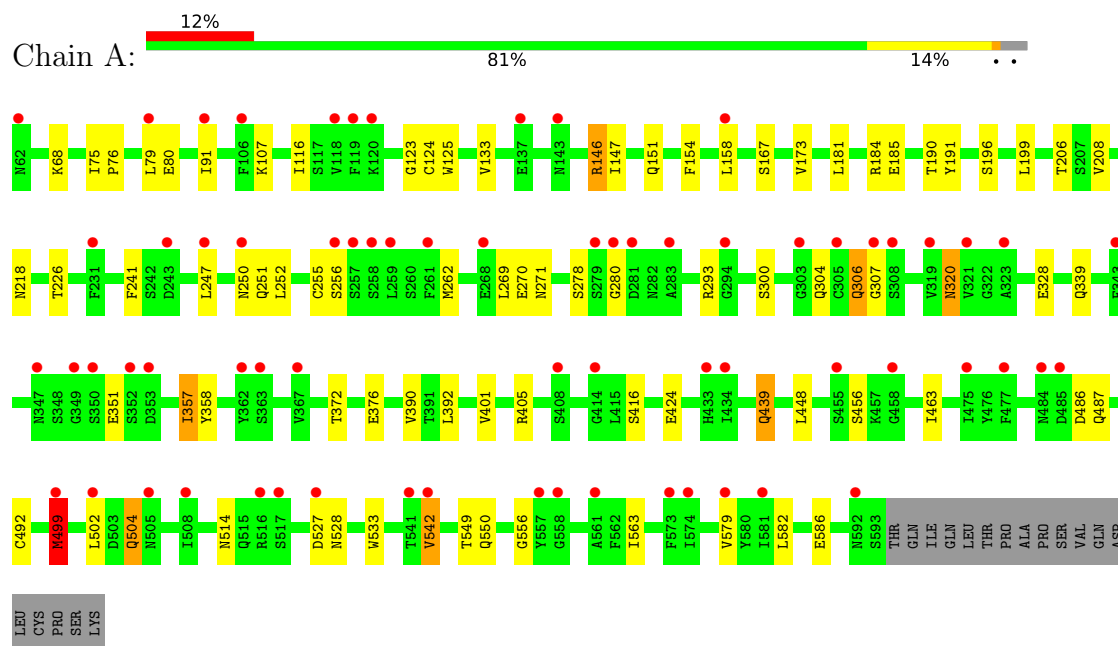
- Molecule 15 is water.

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		

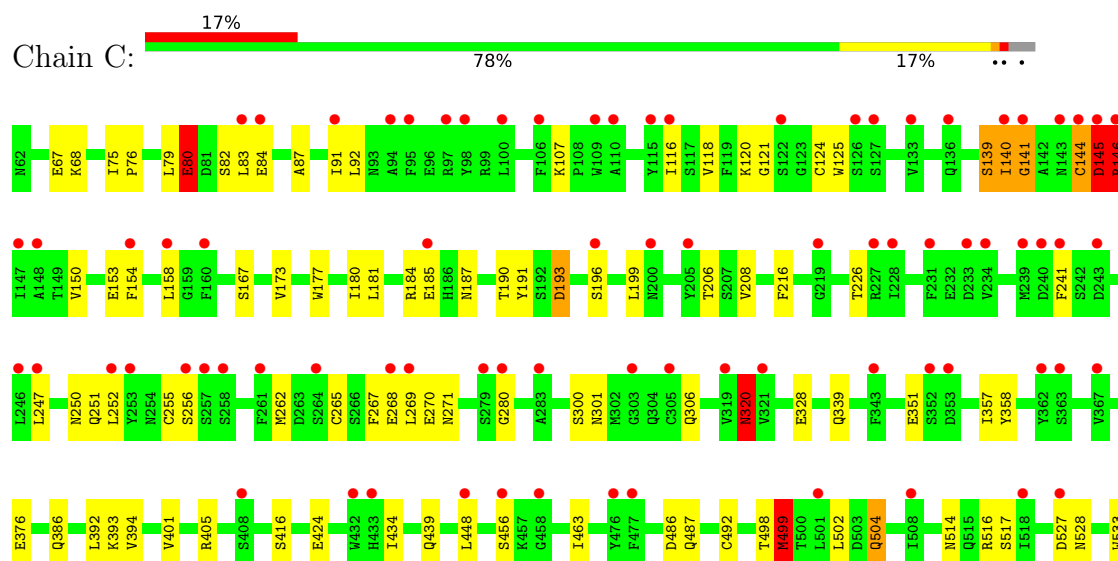
3 Residue-property plots

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

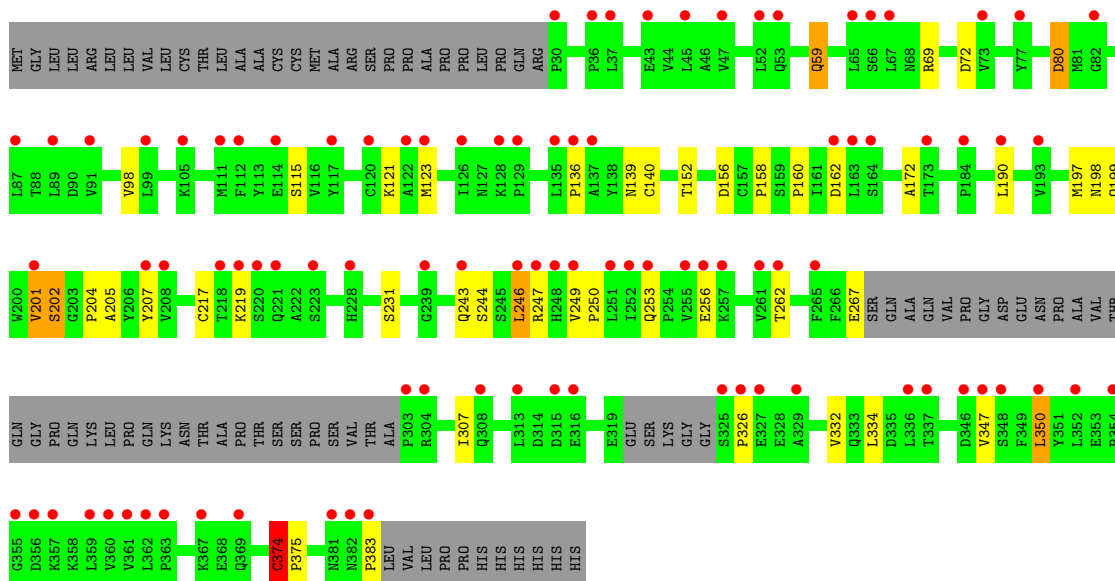


• Molecule 1: Meprin A subunit beta

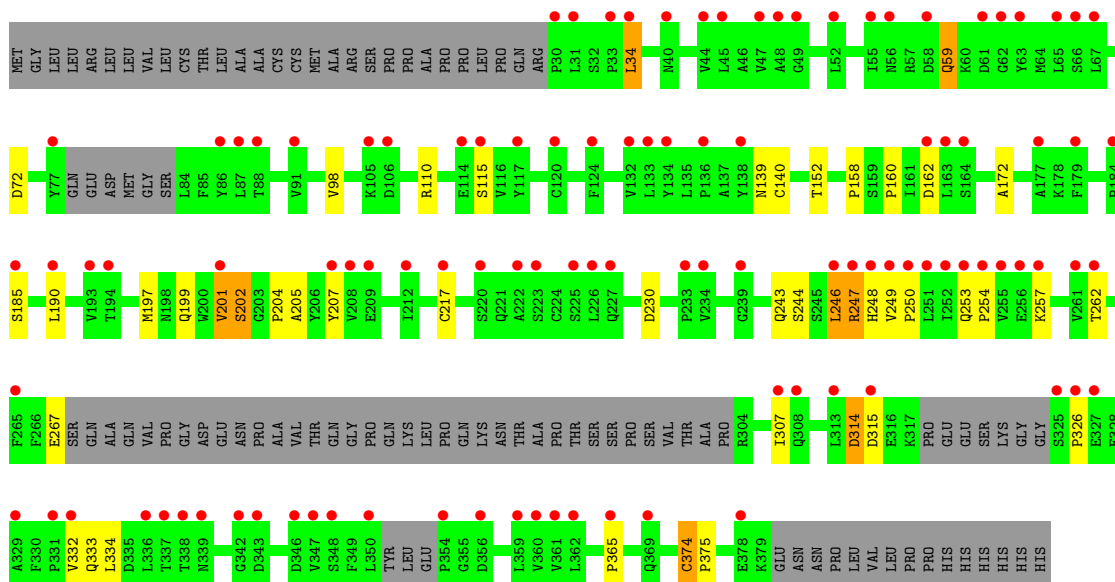




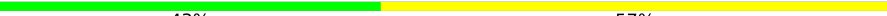
• Molecule 2: Fetuin-B



• 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%

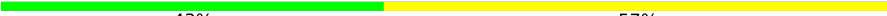


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

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%

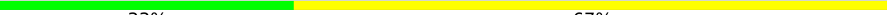


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

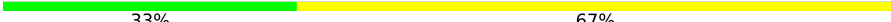


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%



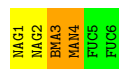
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%

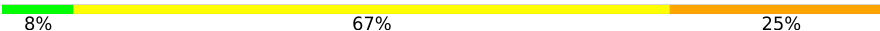


- Molecule 7: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 [i](#)

5.1 Standard geometry [i](#)

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%)

All (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
1	A	357	ILE	CG1-CD1	-5.34	1.30	1.51
1	C	92	LEU	CA-C	-5.16	1.46	1.52
1	C	92	LEU	CB-CG	5.07	1.63	1.53
1	C	141	GLY	C-O	5.00	1.28	1.23

All (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
1	C	144	CYS	N-CA-C	-6.18	107.57	114.62
2	B	246	LEU	CA-C-N	5.95	132.91	121.54
2	B	246	LEU	C-N-CA	5.95	132.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	PHE	CA-CB-CG	-5.80	108.00	113.80
1	C	154	PHE	CA-CB-CG	-5.72	108.08	113.80
1	C	271	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	271	ASN	CA-CB-CG	5.51	118.11	112.60
1	C	542	VAL	N-CA-CB	5.40	116.41	110.53
1	C	320	ASN	CA-CB-CG	5.39	117.99	112.60
1	A	271	ASN	CA-C-N	5.38	131.66	121.97
1	A	271	ASN	C-N-CA	5.38	131.66	121.97
1	C	271	ASN	CA-C-N	5.33	131.57	121.97
1	C	271	ASN	C-N-CA	5.33	131.57	121.97
2	D	246	LEU	CA-C-N	5.27	131.61	121.54
2	D	246	LEU	C-N-CA	5.27	131.61	121.54
1	A	542	VAL	N-CA-CB	5.24	116.25	110.53
1	C	193	ASP	CA-C-N	5.24	128.28	120.31
1	C	193	ASP	C-N-CA	5.24	128.28	120.31
1	A	218	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	80	GLU	CA-C-N	5.08	127.79	120.38
1	C	80	GLU	C-N-CA	5.08	127.79	120.38
2	D	314	ASP	CA-CB-CG	5.06	117.66	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:C:120:LYS:HG3	1:C:141:GLY:HA2	1.61	0.82
5:H:3:BMA:H4	5:H:4:MAN:C1	2.09	0.82
1:A:251:GLN:HA	1:C:256:SER:HB2	1.66	0.75
2:B:121:LYS:CE	2:B:332:VAL:HB	2.03	0.75
1:A:256:SER:HB2	1:C:251:GLN:HA	1.68	0.75
1:C:84:GLU:HG3	1:C:120:LYS:NZ	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:HG23	1:C:144:CYS:CB	2.16	0.74
1:C:121:GLY:HA3	1:C:139:SER:OG	1.89	0.72
6:I:1:NAG:H2	6:I:3:FUC:H5	1.75	0.69
6:Q:1:NAG:H2	6:Q:3:FUC:H5	1.75	0.68
1:C:556:GLY:O	2:D:250:PRO:HD3	1.94	0.67
1:C:393:LYS:NZ	15:C:801:HOH:O	2.30	0.65
1:A:556:GLY:O	2:B:250:PRO:HD3	1.98	0.64
1:C:141:GLY:O	1:C:144:CYS:SG	2.57	0.62
1:A:181:LEU:HB2	1:A:184:ARG:HG3	1.82	0.62
1:C:191:TYR:HE2	2:D:152:THR:HG22	1.64	0.62
1:A:191:TYR:HE2	2:B:152:THR:HG22	1.63	0.62
1:C:498:THR:HG22	1:C:517:SER:OG	2.01	0.60
2:D:204:PRO:HG2	2:D:243:GLN:HB3	1.85	0.58
1:C:80:GLU:O	1:C:83:LEU:HD12	2.03	0.58
1:C:146:ARG:HE	2:D:246:LEU:CD1	2.09	0.58
2:B:204:PRO:HG2	2:B:243:GLN:HB3	1.85	0.57
1:A:328:GLU:HG3	1:A:401:VAL:HG22	1.86	0.57
2:D:249:VAL:HB	2:D:250:PRO:HD2	1.85	0.57
2:B:249:VAL:HB	2:B:250:PRO:HD2	1.87	0.56
1:A:339:GLN:HG3	1:A:424:GLU:HG2	1.87	0.56
2:B:158:PRO:HA	2:B:199:GLN:HB3	1.88	0.56
1:C:339:GLN:HG3	1:C:424:GLU:HG2	1.88	0.56
10:U:1:NAG:H3	10:U:2:FUC:H5	1.87	0.56
2:B:201:VAL:HG22	2:B:205:ALA:HB2	1.87	0.55
1:C:516:ARG:HH22	2:D:246:LEU:HD22	1.71	0.55
2:D:158:PRO:HA	2:D:199:GLN:HB3	1.88	0.55
1:C:181:LEU:HB2	1:C:184:ARG:HG3	1.87	0.55
1:C:125:TRP:CE2	1:C:139:SER:HB2	2.41	0.55
2:D:201:VAL:HG22	2:D:205:ALA:HB2	1.89	0.55
2:B:374:CYS:N	2:B:375:PRO:HD3	2.22	0.55
1:C:328:GLU:HG3	1:C:401:VAL:HG22	1.88	0.54
1:C:199:LEU:HD11	1:C:252:LEU:HD13	1.89	0.54
10:U:1:NAG:H3	10:U:2:FUC:C5	2.39	0.53
1:A:146:ARG:NH1	2:B:246:LEU:CB	2.72	0.52
1:A:199:LEU:HD11	1:A:252:LEU:HD13	1.90	0.52
1:C:320:ASN:HD22	1:C:320:ASN:H	1.56	0.52
1:C:358:TYR:HB2	1:C:401:VAL:HB	1.92	0.52
2:D:248:HIS:ND1	2:D:254:PRO:HB3	2.25	0.51
1:A:79:LEU:HD11	1:A:91:ILE:HG21	1.92	0.51
1:C:120:LYS:HA	1:C:141:GLY:HA2	1.92	0.51
1:A:358:TYR:HB2	1:A:401:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ALA:HB1	2:B:190:LEU:HD11	1.93	0.50
1:C:120:LYS:CG	1:C:141:GLY:HA2	2.38	0.50
1:A:147:ILE:O	1:A:151:GLN:HG3	2.11	0.50
1:A:184:ARG:HD2	2:B:198:ASN:OD1	2.11	0.49
1:A:339:GLN:HB2	1:A:392:LEU:HB2	1.93	0.49
1:C:502:LEU:HD13	1:C:582:LEU:HD11	1.94	0.49
1:A:262:MET:HE2	1:A:339:GLN:HG2	1.94	0.49
1:C:79:LEU:HD11	1:C:91:ILE:HG21	1.93	0.49
1:C:339:GLN:HB2	1:C:392:LEU:HB2	1.94	0.49
1:C:84:GLU:CG	1:C:120:LYS:NZ	2.74	0.49
1:A:502:LEU:HD13	1:A:582:LEU:HD11	1.94	0.49
2:D:140:CYS:HB2	2:D:307:ILE:HG12	1.93	0.49
2:D:172:ALA:HB1	2:D:190:LEU:HD11	1.94	0.48
1:C:184:ARG:NE	1:C:216:PHE:CE1	2.79	0.48
1:A:173:VAL:HG12	1:A:226:THR:HG22	1.95	0.48
1:C:125:TRP:HA	1:C:153:GLU:OE1	2.14	0.48
1:C:320:ASN:HD22	1:C:320:ASN:N	2.12	0.48
1:A:357:ILE:HD12	1:A:390:VAL:HG21	1.97	0.47
1:C:262:MET:HE2	1:C:339:GLN:HG2	1.95	0.47
2:B:123:MET:O	2:B:136:PRO:HD2	2.14	0.47
1:C:83:LEU:HD21	1:C:118:VAL:HG12	1.97	0.47
1:C:463:ILE:HG23	1:C:499:MET:HE2	1.97	0.47
1:C:144:CYS:C	1:C:146:ARG:H	2.22	0.47
1:C:140:ILE:CD1	1:C:144:CYS:HB3	2.45	0.46
2:D:374:CYS:N	2:D:375:PRO:HD3	2.31	0.46
1:A:463:ILE:HG23	1:A:499:MET:HE2	1.98	0.46
1:C:173:VAL:HG12	1:C:226:THR:HG22	1.96	0.46
2:B:202:SER:HB3	2:B:244:SER:OG	2.16	0.46
7:R:6:MAN:H2	7:R:7:GLC:H5	1.98	0.45
1:A:123:GLY:HA3	2:B:199:GLN:OE1	2.15	0.45
1:A:306:GLN:HG2	1:A:307:GLY:H	1.82	0.45
2:D:202:SER:HB3	2:D:244:SER:OG	2.17	0.45
1:C:516:ARG:HH12	2:D:247:ARG:H	1.65	0.45
2:B:160:PRO:HA	2:B:197:MET:HA	1.99	0.45
7:J:6:MAN:H2	7:J:7:GLC:H5	1.99	0.45
1:A:125:TRP:HA	2:B:156:ASP:HB2	1.98	0.45
2:D:249:VAL:HB	2:D:250:PRO:CD	2.46	0.45
2:B:249:VAL:HB	2:B:250:PRO:CD	2.47	0.44
1:C:140:ILE:HD13	1:C:144:CYS:HB3	1.98	0.44
2:D:34:LEU:HD13	2:D:365:PRO:HB3	2.00	0.44
2:B:139:ASN:HB2	2:B:334:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLN:HG3	7:J:12:MAN:H61	2.00	0.44
1:A:514:ASN:HD22	1:A:563:ILE:HD12	1.82	0.44
1:A:133:VAL:HG12	2:B:383:PRO:HA	1.99	0.44
1:C:75:ILE:HD11	1:C:158:LEU:HD21	2.00	0.44
2:D:197:MET:HB3	2:D:207:TYR:HB2	2.00	0.44
1:A:439:GLN:HE21	1:A:439:GLN:HB2	1.69	0.43
1:C:120:LYS:HG3	1:C:141:GLY:CA	2.42	0.43
2:B:121:LYS:HB2	2:B:332:VAL:HG11	2.00	0.43
1:C:502:LEU:HD23	1:C:504:GLN:HG2	2.00	0.43
1:A:75:ILE:HD11	1:A:158:LEU:HD21	2.00	0.43
2:B:347:VAL:O	2:B:350:LEU:HB2	2.18	0.43
1:C:434:ILE:HG21	1:C:448:LEU:HD13	2.00	0.43
2:D:139:ASN:HB2	2:D:334:LEU:HD13	2.00	0.43
1:A:502:LEU:HD23	1:A:504:GLN:HG2	2.00	0.43
2:B:140:CYS:HB2	2:B:307:ILE:HG22	2.00	0.43
1:C:121:GLY:CA	1:C:139:SER:OG	2.63	0.43
1:C:514:ASN:HD22	1:C:563:ILE:HD12	1.82	0.43
1:C:184:ARG:NH2	1:C:187:ASN:HD21	2.16	0.43
1:A:75:ILE:HG21	1:A:116:ILE:HD12	2.01	0.43
1:C:487:GLN:HG3	7:R:12:MAN:H61	1.99	0.43
2:D:160:PRO:HA	2:D:197:MET:HA	1.99	0.43
1:C:191:TYR:CE2	2:D:152:THR:HG22	2.50	0.43
2:B:197:MET:HB3	2:B:207:TYR:HB2	2.00	0.42
1:C:556:GLY:O	2:D:250:PRO:CD	2.66	0.42
2:D:199:GLN:HG2	2:D:207:TYR:HE1	1.85	0.42
1:A:191:TYR:CE2	2:B:152:THR:HG22	2.47	0.42
1:C:250:ASN:HB3	1:C:255:CYS:HB2	2.01	0.42
2:B:197:MET:HE3	2:B:197:MET:HB2	1.93	0.42
1:C:516:ARG:NH1	2:D:247:ARG:H	2.18	0.42
1:C:76:PRO:HA	1:C:107:LYS:O	2.20	0.41
2:D:197:MET:HE3	2:D:197:MET:HB2	1.92	0.41
1:A:76:PRO:HA	1:A:107:LYS:O	2.20	0.41
1:A:463:ILE:HD12	1:A:499:MET:HE3	2.03	0.41
2:B:199:GLN:HG2	2:B:207:TYR:HE1	1.85	0.41
1:C:463:ILE:HD12	1:C:499:MET:HE3	2.03	0.41
1:A:250:ASN:HB3	1:A:255:CYS:HB2	2.02	0.41
2:D:59:GLN:HB3	2:D:98:VAL:HG11	2.03	0.41
1:C:146:ARG:HB2	1:C:146:ARG:NH2	2.35	0.41
1:C:492:CYS:HB3	1:C:533:TRP:HB3	2.03	0.41
2:D:243:GLN:NE2	2:D:257:LYS:NZ	2.69	0.41
1:A:492:CYS:HB3	1:A:533:TRP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:GLN:HB3	2:B:98:VAL:HG11	2.03	0.41
1:C:193:ASP:HA	1:C:196:SER:O	2.21	0.41
1:C:75:ILE:HG21	1:C:116:ILE:HD12	2.02	0.41
1:C:265:CYS:SG	1:C:267:PHE:CE2	3.14	0.41
2:B:307:ILE:O	2:B:307:ILE:HG13	2.21	0.40
1:C:177:TRP:HA	1:C:180:ILE:HD12	2.02	0.40
1:C:87:ALA:HA	1:C:145:ASP:HB3	2.03	0.40
1:A:75:ILE:HA	1:A:76:PRO:HD3	1.94	0.40
1:C:146:ARG:O	1:C:150:VAL:HG23	2.21	0.40
1:C:140:ILE:CG2	1:C:144:CYS:HB2	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

All (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

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Mol	Chain	Res	Type
2	B	247	ARG
1	C	280	GLY
2	D	202	SER
2	D	230	ASP
2	B	219	LYS
2	D	217	CYS
2	D	315	ASP
1	A	280	GLY
1	A	504	GLN
2	B	253	GLN
1	C	145	ASP
1	C	504	GLN
2	D	253	GLN
2	D	185	SER
2	B	374	CYS

5.3.2 Protein sidechains ⓘ

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

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	80	GLU
1	A	124	CYS
1	A	146	ARG
1	A	167	SER
1	A	185	GLU

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Mol	Chain	Res	Type
1	A	190	THR
1	A	196	SER
1	A	206	THR
1	A	208	VAL
1	A	247	LEU
1	A	269	LEU
1	A	270	GLU
1	A	278	SER
1	A	293	ARG
1	A	300	SER
1	A	304	GLN
1	A	306	GLN
1	A	320	ASN
1	A	351	GLU
1	A	372	THR
1	A	376	GLU
1	A	405	ARG
1	A	416	SER
1	A	439	GLN
1	A	448	LEU
1	A	456	SER
1	A	486	ASP
1	A	499	MET
1	A	527	ASP
1	A	528	ASN
1	A	542	VAL
1	A	549	THR
1	A	550	GLN
1	A	579	VAL
1	A	586	GLU
2	B	59	GLN
2	B	69	ARG
2	B	72	ASP
2	B	80	ASP
2	B	115	SER
2	B	162	ASP
2	B	201	VAL
2	B	217	CYS
2	B	256	GLU
2	B	262	THR
2	B	267	GLU
2	B	350	LEU

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Mol	Chain	Res	Type
2	B	374	CYS
1	C	67	GLU
1	C	68	LYS
1	C	80	GLU
1	C	82	SER
1	C	124	CYS
1	C	139	SER
1	C	146	ARG
1	C	167	SER
1	C	185	GLU
1	C	190	THR
1	C	206	THR
1	C	208	VAL
1	C	247	LEU
1	C	268	GLU
1	C	269	LEU
1	C	270	GLU
1	C	300	SER
1	C	301	ASN
1	C	306	GLN
1	C	320	ASN
1	C	351	GLU
1	C	357	ILE
1	C	376	GLU
1	C	386	GLN
1	C	394	VAL
1	C	405	ARG
1	C	416	SER
1	C	439	GLN
1	C	456	SER
1	C	486	ASP
1	C	499	MET
1	C	527	ASP
1	C	528	ASN
1	C	542	VAL
1	C	549	THR
1	C	550	GLN
1	C	579	VAL
1	C	586	GLU
2	D	34	LEU
2	D	59	GLN
2	D	72	ASP

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Mol	Chain	Res	Type
2	D	110	ARG
2	D	115	SER
2	D	162	ASP
2	D	201	VAL
2	D	262	THR
2	D	267	GLU
2	D	314	ASP
2	D	332	VAL
2	D	333	GLN
2	D	374	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
1	A	271	ASN
1	A	282	ASN
1	A	313	HIS
1	A	386	GLN
1	A	429	HIS
1	A	439	GLN
1	A	466	ASN
1	A	510	GLN
1	A	514	ASN
1	A	550	GLN
2	B	59	GLN
2	B	78	GLN
2	B	243	GLN
1	C	62	ASN
1	C	86	ASN
1	C	186	HIS
1	C	187	ASN
1	C	271	ASN
1	C	282	ASN
1	C	306	GLN
1	C	313	HIS
1	C	320	ASN
1	C	356	ASN
1	C	386	GLN
1	C	429	HIS
1	C	439	GLN
1	C	496	GLN

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Mol	Chain	Res	Type
1	C	510	GLN
1	C	514	ASN
1	C	550	GLN
2	D	59	GLN
2	D	68	ASN
2	D	119	GLN
2	D	243	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 ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

All (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
3	O	5	MAN	C1-O5-C5	5.10	119.02	112.19
3	M	1	NAG	C1-C2-N2	5.02	118.34	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-C2-N2	4.95	118.23	110.43
3	G	5	MAN	C1-O5-C5	4.89	118.74	112.19
4	T	2	NAG	O5-C1-C2	-4.40	104.48	111.29
6	Q	1	NAG	C1-C2-N2	4.12	116.93	110.43
6	I	1	NAG	C1-C2-N2	4.10	116.90	110.43
4	F	2	NAG	O5-C1-C2	-4.01	105.09	111.29
7	J	8	MAN	C1-O5-C5	3.96	117.50	112.19
7	J	10	MAN	C1-O5-C5	3.95	117.48	112.19
7	R	8	MAN	C1-O5-C5	3.82	117.30	112.19
4	N	2	NAG	O5-C1-C2	-3.80	105.40	111.29
7	R	10	MAN	C1-O5-C5	3.65	117.08	112.19
8	S	1	NAG	C3-C4-C5	3.34	116.29	110.23
5	H	4	MAN	C1-O5-C5	3.34	116.66	112.19
8	K	1	NAG	C3-C4-C5	3.23	116.09	110.23
3	O	1	NAG	C1-O5-C5	3.23	116.52	112.19
5	P	1	NAG	C1-C2-N2	-3.23	105.35	110.43
7	R	9	MAN	C1-O5-C5	3.20	116.47	112.19
8	S	1	NAG	O5-C1-C2	-3.20	106.35	111.29
5	H	1	NAG	C1-C2-N2	-3.16	105.46	110.43
9	L	3	BMA	C1-O5-C5	3.11	116.36	112.19
7	J	9	MAN	C1-O5-C5	3.11	116.35	112.19
7	R	6	MAN	C1-O5-C5	3.04	116.26	112.19
3	G	5	MAN	C1-C2-C3	2.99	114.00	109.64
3	M	1	NAG	C2-N2-C7	2.97	126.88	122.90
7	J	6	MAN	C1-O5-C5	2.95	116.14	112.19
3	E	1	NAG	C2-N2-C7	2.94	126.84	122.90
7	R	11	MAN	C1-O5-C5	2.93	116.12	112.19
7	J	11	MAN	C1-O5-C5	2.93	116.11	112.19
3	G	1	NAG	C1-O5-C5	2.92	116.10	112.19
4	F	1	NAG	O5-C1-C2	-2.91	106.80	111.29
3	O	5	MAN	C1-C2-C3	2.90	113.87	109.64
6	I	1	NAG	C3-C4-C5	2.89	115.47	110.23
7	J	4	MAN	C1-O5-C5	2.86	116.02	112.19
9	L	2	NAG	C1-O5-C5	2.86	116.02	112.19
8	K	1	NAG	O5-C1-C2	-2.84	106.89	111.29
6	Q	1	NAG	C3-C4-C5	2.83	115.36	110.23
7	J	9	MAN	O2-C2-C1	2.81	115.65	109.22
7	R	9	MAN	O2-C2-C1	2.76	115.53	109.22
4	N	1	NAG	O5-C1-C2	-2.76	107.03	111.29
3	M	5	MAN	C1-O5-C5	2.71	115.81	112.19
5	H	2	NAG	C1-O5-C5	2.69	115.80	112.19
7	R	4	MAN	C1-O5-C5	2.66	115.75	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	2	NAG	C1-O5-C5	2.66	115.75	112.19
10	U	3	NAG	C1-O5-C5	2.64	115.72	112.19
3	G	3	BMA	C1-O5-C5	2.63	115.71	112.19
5	P	4	MAN	C1-O5-C5	2.63	115.70	112.19
10	U	1	NAG	C1-O5-C5	2.61	115.68	112.19
6	Q	2	NAG	C2-N2-C7	2.55	126.32	122.90
4	T	1	NAG	C1-O5-C5	2.53	115.58	112.19
7	R	5	MAN	C1-O5-C5	2.52	115.57	112.19
7	J	5	MAN	C1-O5-C5	2.47	115.50	112.19
6	I	2	NAG	C2-N2-C7	2.47	126.21	122.90
9	L	1	NAG	O3-C3-C2	2.41	114.40	109.40
10	U	2	FUC	C1-O5-C5	2.40	118.63	112.97
7	R	12	MAN	C1-O5-C5	2.38	115.38	112.19
3	M	2	NAG	C1-O5-C5	2.35	115.34	112.19
3	E	4	MAN	C1-O5-C5	2.33	115.31	112.19
7	J	7	GLC	C1-O5-C5	2.33	115.30	112.19
7	R	7	GLC	C1-O5-C5	2.32	115.30	112.19
6	I	3	FUC	C1-O5-C5	2.31	118.42	112.97
10	U	1	NAG	O3-C3-C2	2.31	114.20	109.40
6	Q	3	FUC	C1-O5-C5	2.29	118.36	112.97
7	J	12	MAN	C1-O5-C5	2.28	115.25	112.19
5	H	3	BMA	C3-C4-C5	2.27	114.35	110.23
3	M	1	NAG	C4-C3-C2	-2.27	107.69	111.02
3	O	4	MAN	C1-O5-C5	2.26	115.22	112.19
3	E	1	NAG	C4-C3-C2	-2.26	107.71	111.02
3	E	5	MAN	C1-O5-C5	2.26	115.21	112.19
3	O	3	BMA	C1-O5-C5	2.25	115.21	112.19
6	Q	1	NAG	O5-C1-C2	2.24	114.76	111.29
3	E	2	NAG	C1-O5-C5	2.24	115.19	112.19
8	S	1	NAG	O3-C3-C4	-2.24	105.09	110.38
8	K	1	NAG	O3-C3-C4	-2.24	105.10	110.38
7	R	2	NAG	O5-C1-C2	-2.24	107.83	111.29
7	R	1	NAG	O5-C1-C2	2.24	114.75	111.29
3	M	4	MAN	C1-O5-C5	2.24	115.18	112.19
5	H	3	BMA	C2-C3-C4	2.23	114.78	110.86
9	L	1	NAG	C1-O5-C5	2.23	115.17	112.19
3	G	4	MAN	C1-O5-C5	2.21	115.15	112.19
6	I	1	NAG	O5-C1-C2	2.20	114.69	111.29
5	H	4	MAN	C1-C2-C3	2.18	112.81	109.64
7	J	2	NAG	O5-C1-C2	-2.17	107.94	111.29
6	I	2	NAG	C1-C2-N2	2.16	113.84	110.43
7	J	1	NAG	O5-C1-C2	2.16	114.64	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1	NAG	C1-O5-C5	2.14	115.05	112.19
6	Q	2	NAG	C1-C2-N2	2.12	113.78	110.43
8	K	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (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
5	P	3	BMA	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
7	J	7	GLC	O5-C5-C6-O6
7	R	7	GLC	O5-C5-C6-O6
8	K	1	NAG	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
7	J	7	GLC	C4-C5-C6-O6
7	R	7	GLC	C4-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
7	R	4	MAN	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
7	R	4	MAN	O5-C5-C6-O6
7	J	9	MAN	O5-C5-C6-O6
7	R	9	MAN	O5-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
3	M	5	MAN	O5-C5-C6-O6
3	O	5	MAN	C4-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	J	4	MAN	O5-C5-C6-O6
6	I	2	NAG	C1-C2-N2-C7
3	E	5	MAN	O5-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	O	5	MAN	O5-C5-C6-O6
6	Q	2	NAG	C1-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
3	O	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
7	J	9	MAN	C4-C5-C6-O6

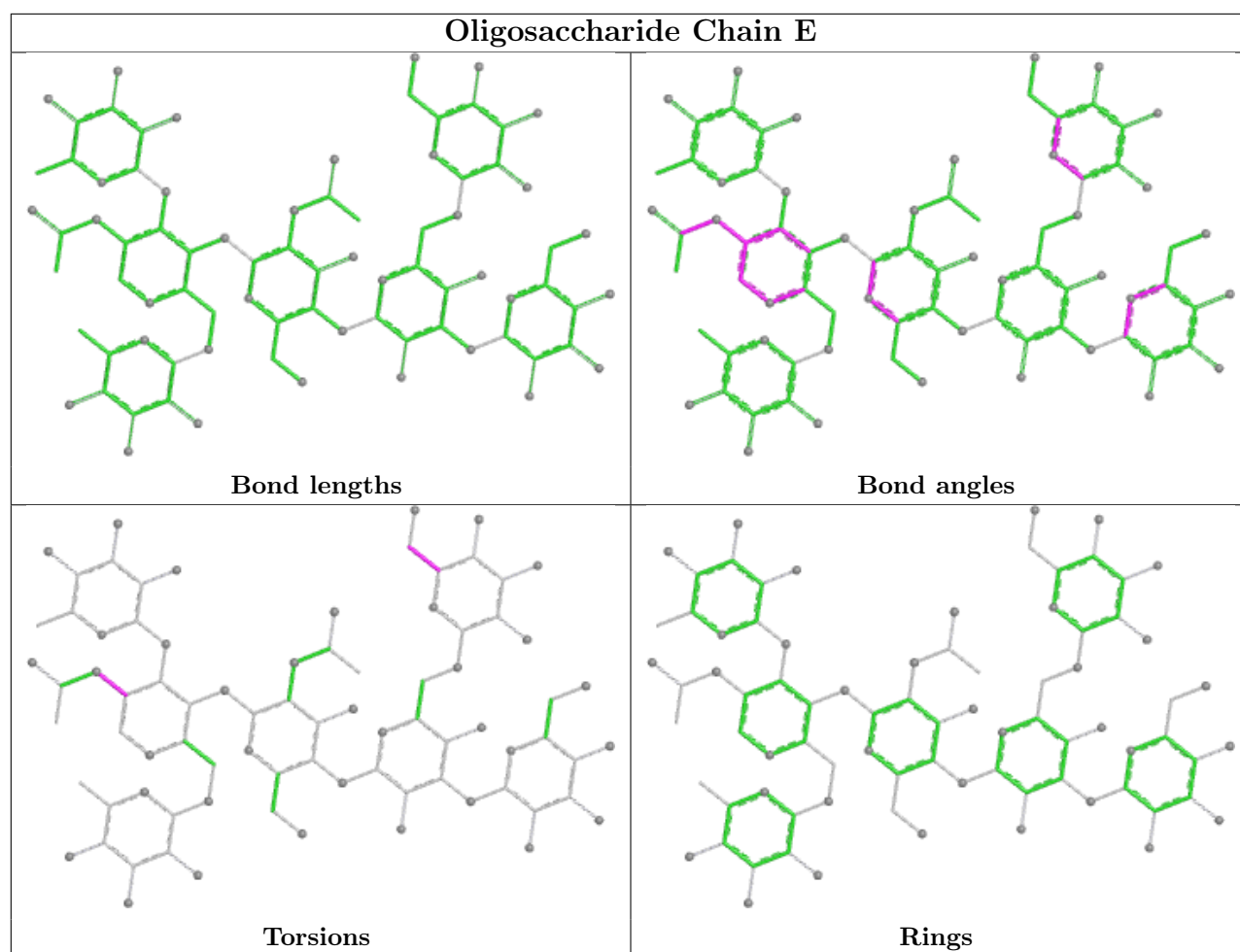
All (2) ring outliers are listed below:

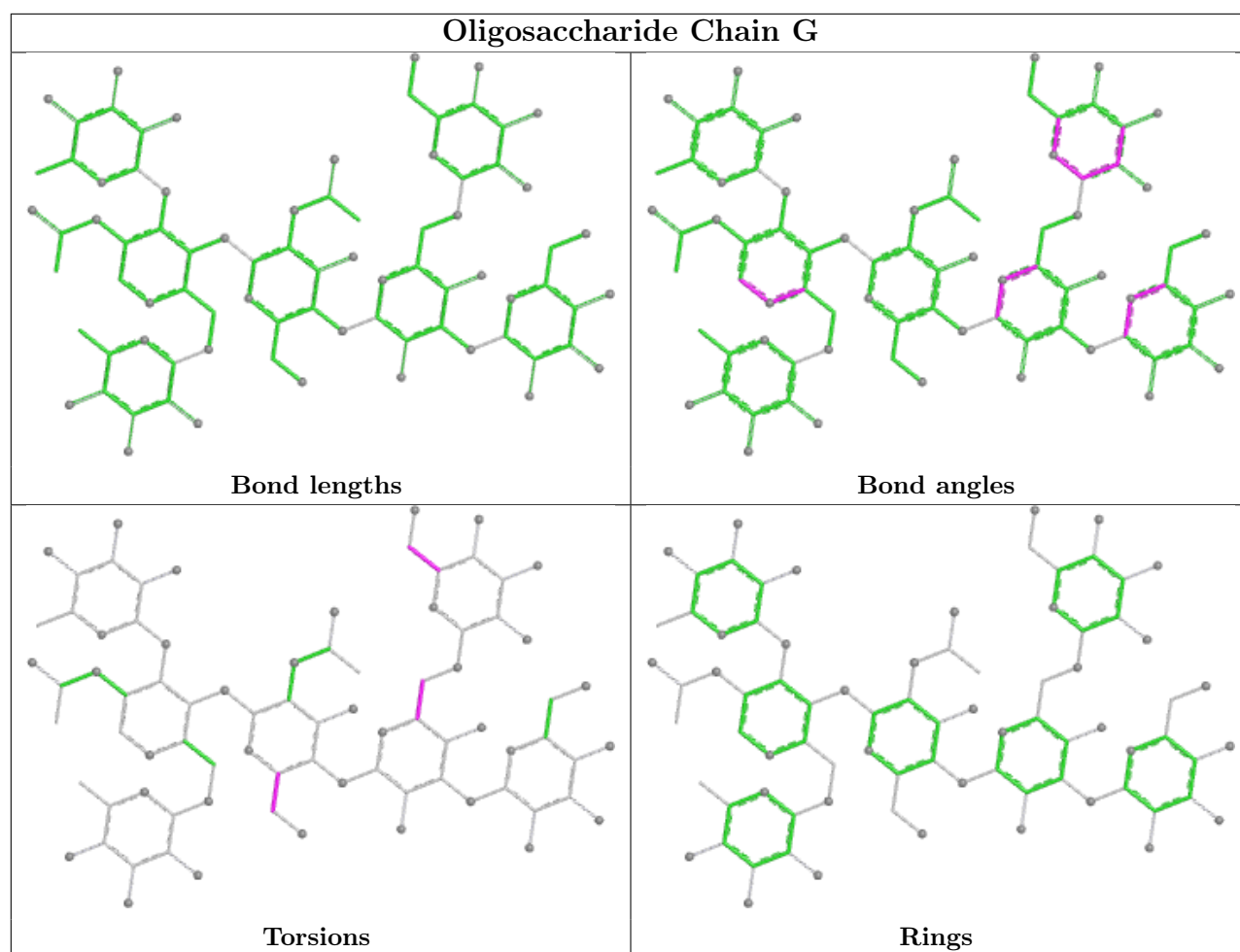
Mol	Chain	Res	Type	Atoms
5	P	4	MAN	C1-C2-C3-C4-C5-O5
5	H	4	MAN	C1-C2-C3-C4-C5-O5

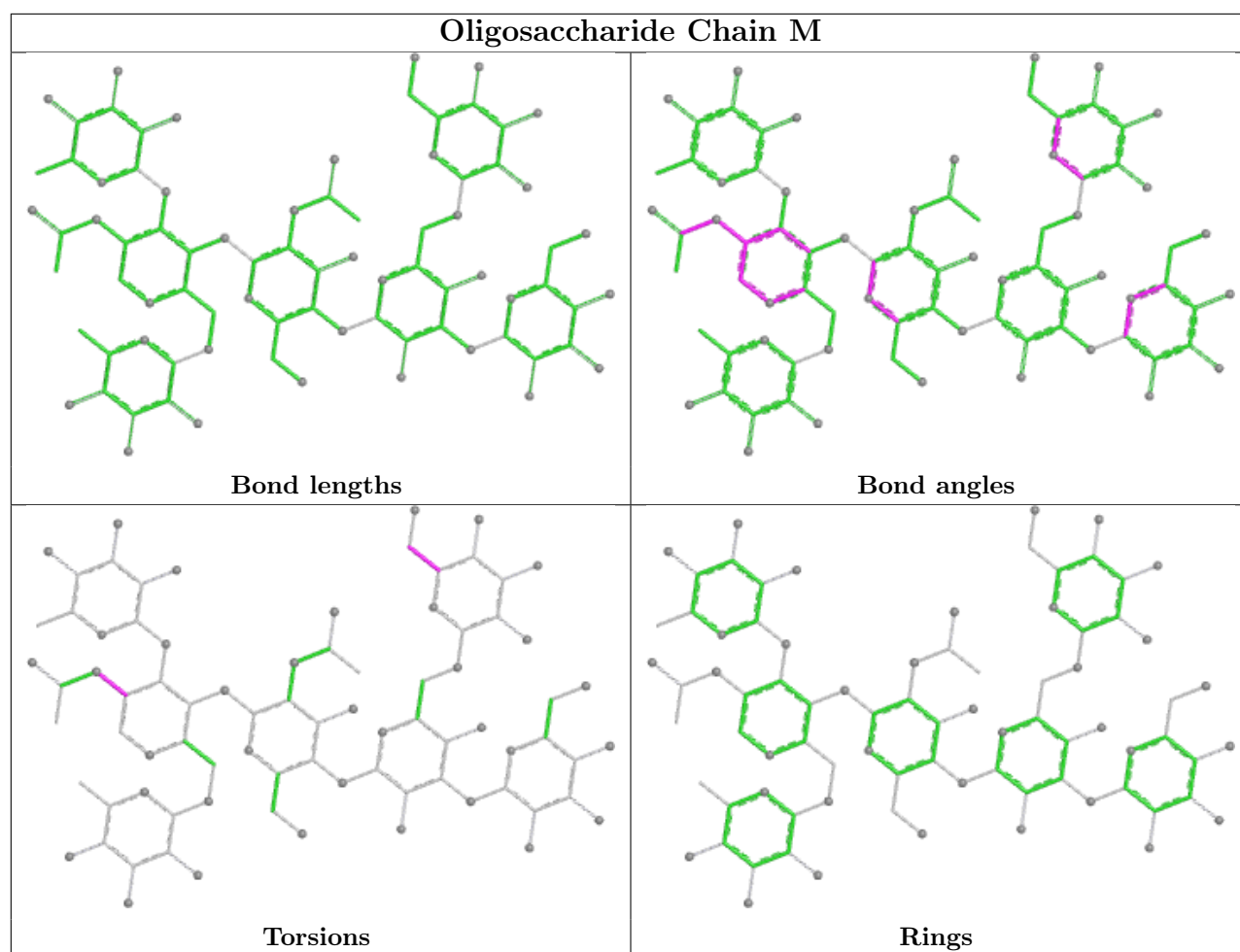
14 monomers are involved in 9 short contacts:

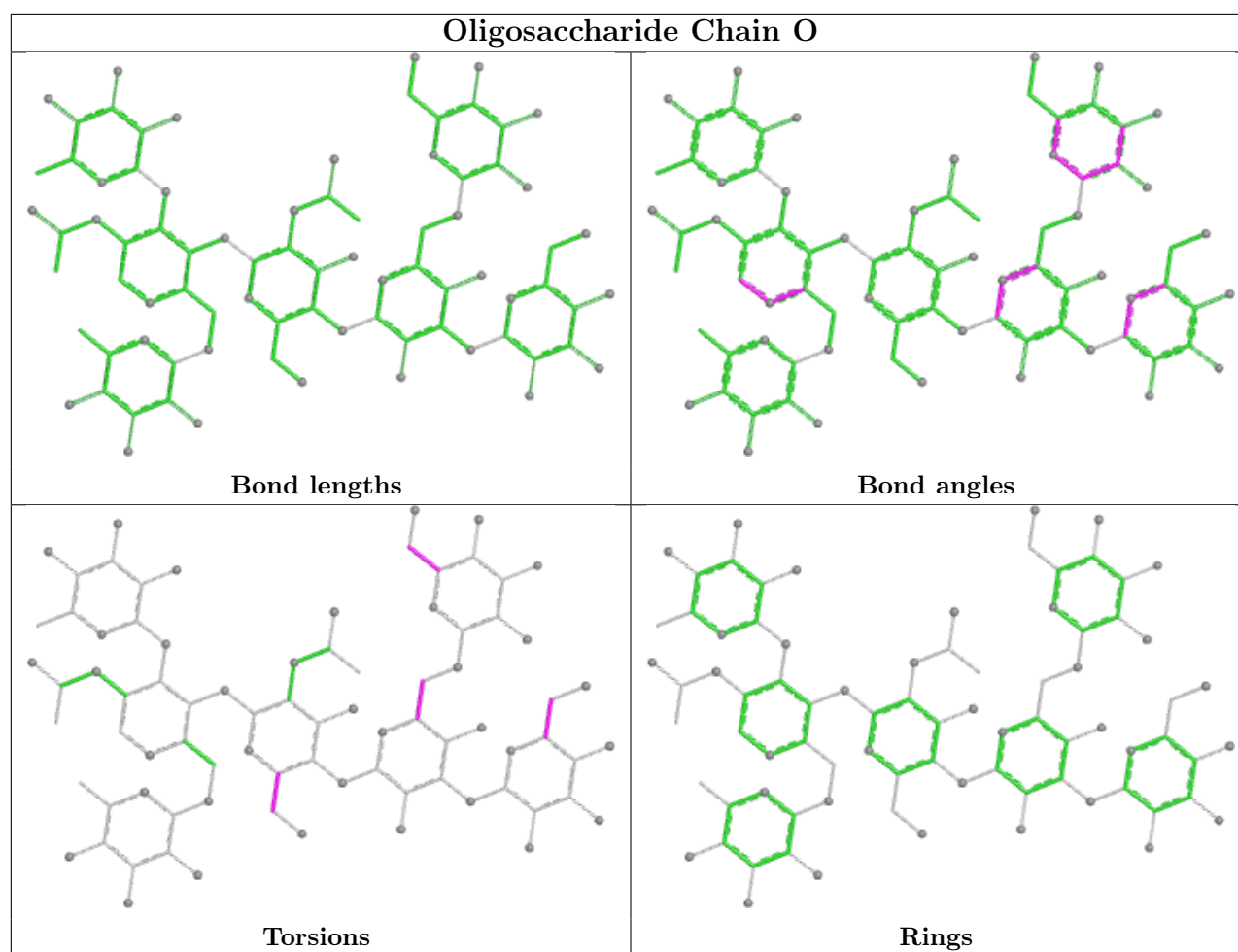
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	4	MAN	1	0
6	Q	1	NAG	1	0
6	Q	3	FUC	1	0
7	R	6	MAN	1	0
6	I	3	FUC	1	0
7	J	12	MAN	1	0
7	R	12	MAN	1	0
7	J	6	MAN	1	0
6	I	1	NAG	1	0
10	U	2	FUC	2	0
5	H	3	BMA	1	0
7	J	7	GLC	1	0
7	R	7	GLC	1	0
10	U	1	NAG	2	0

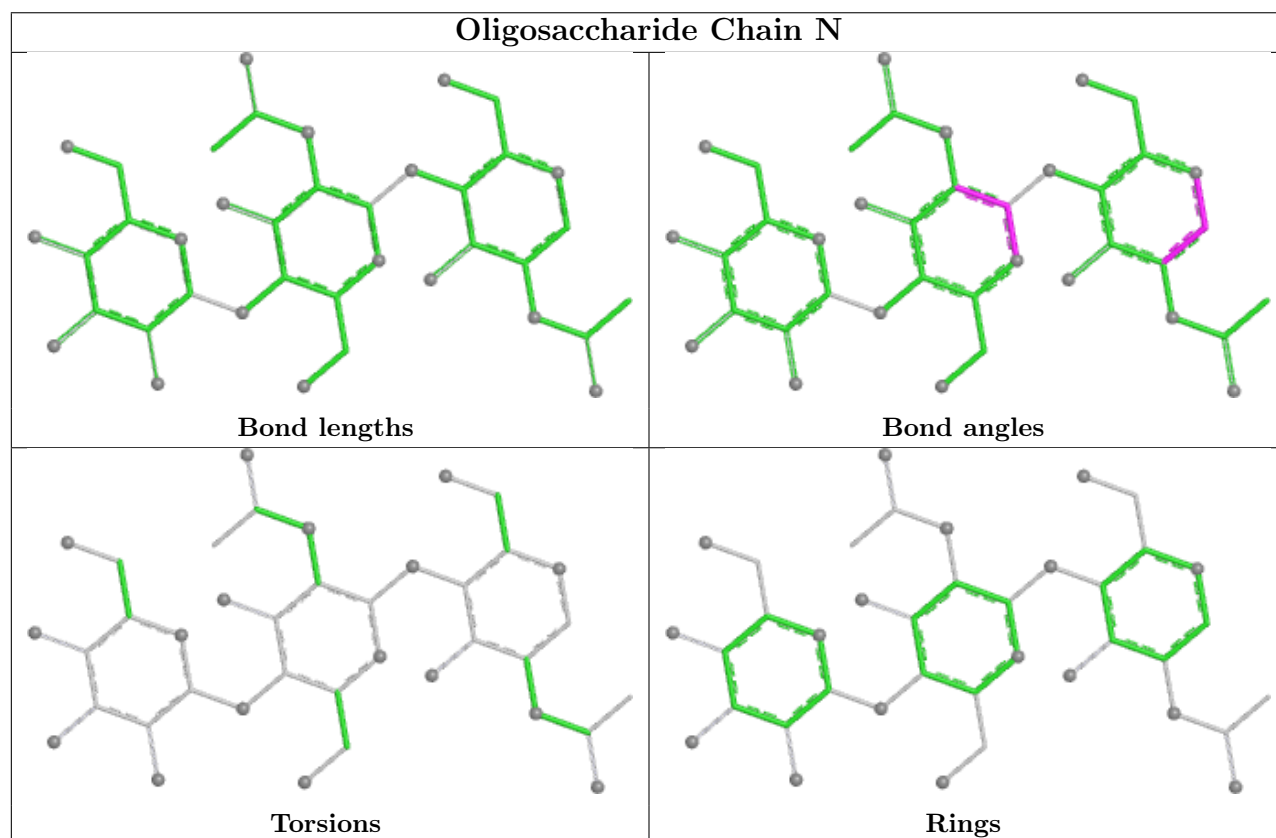
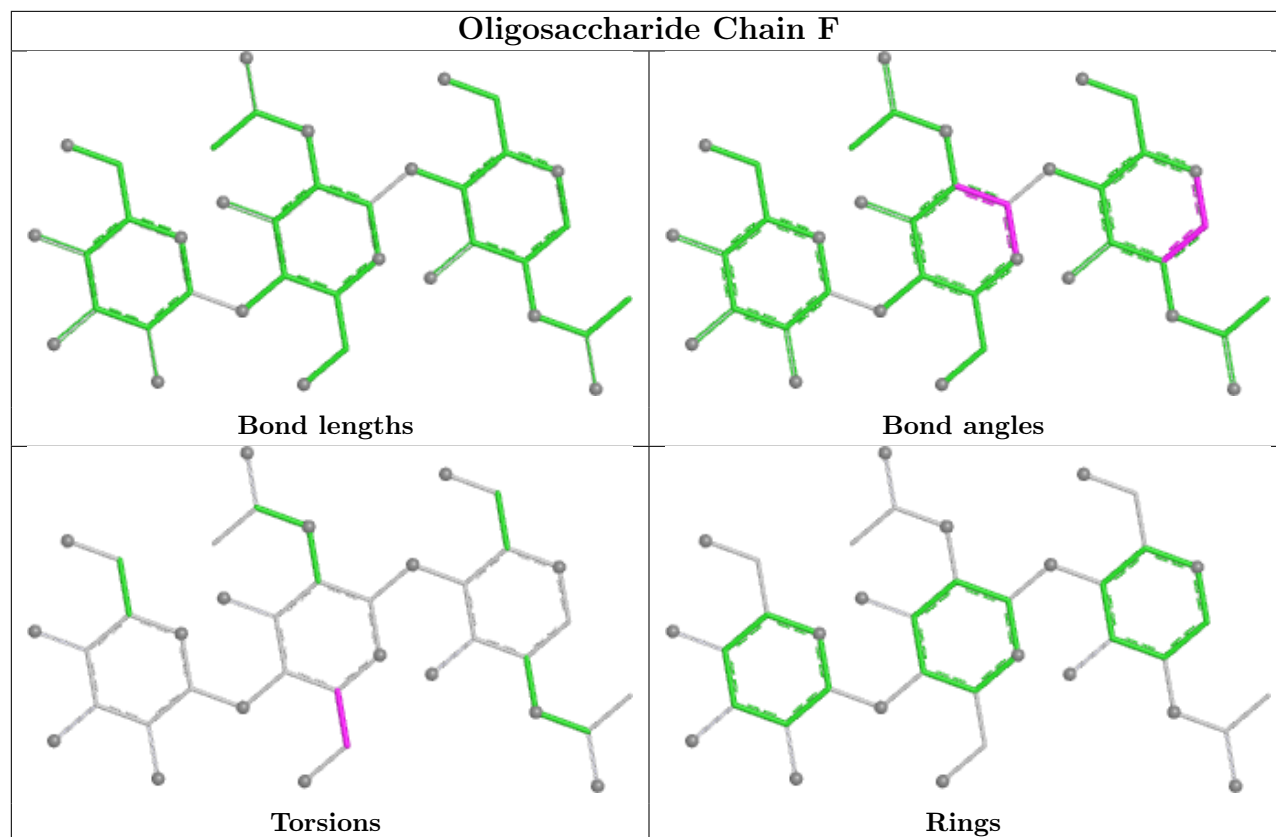
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

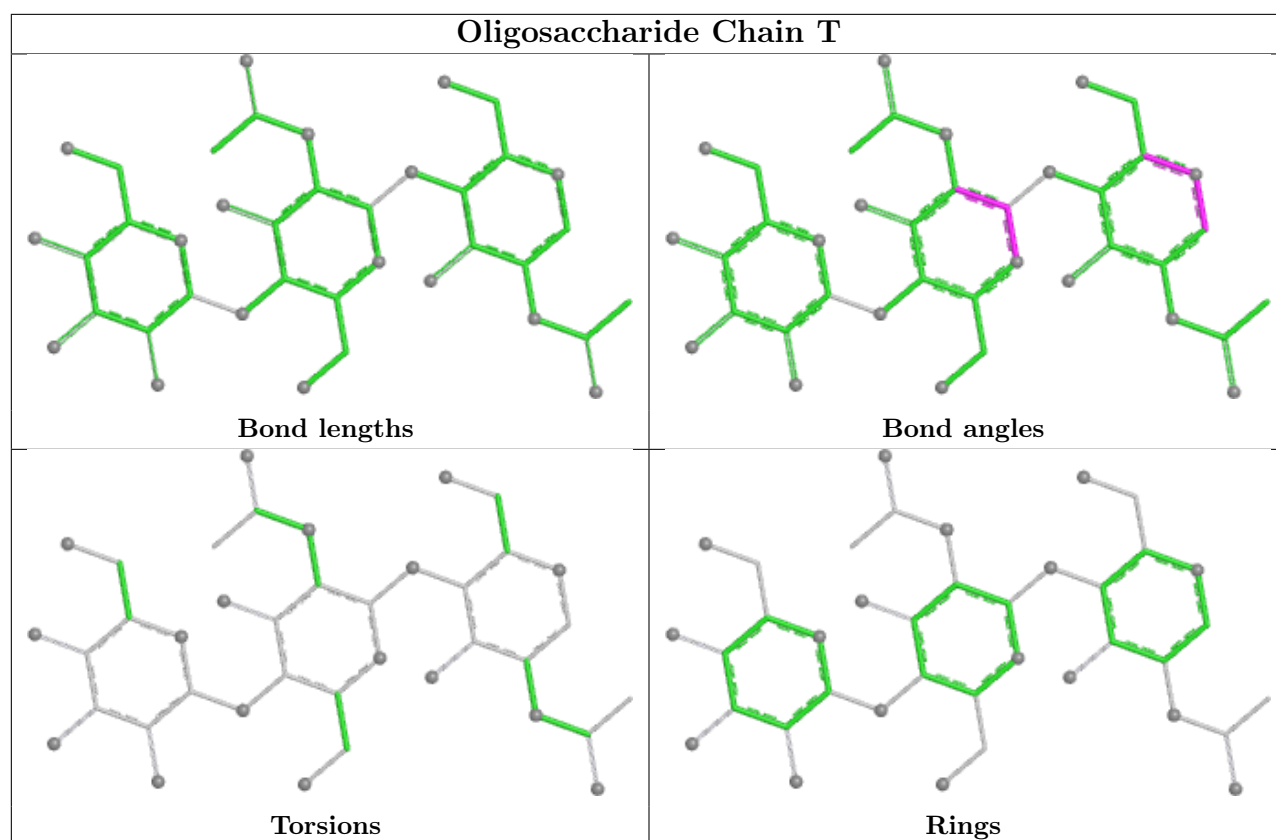


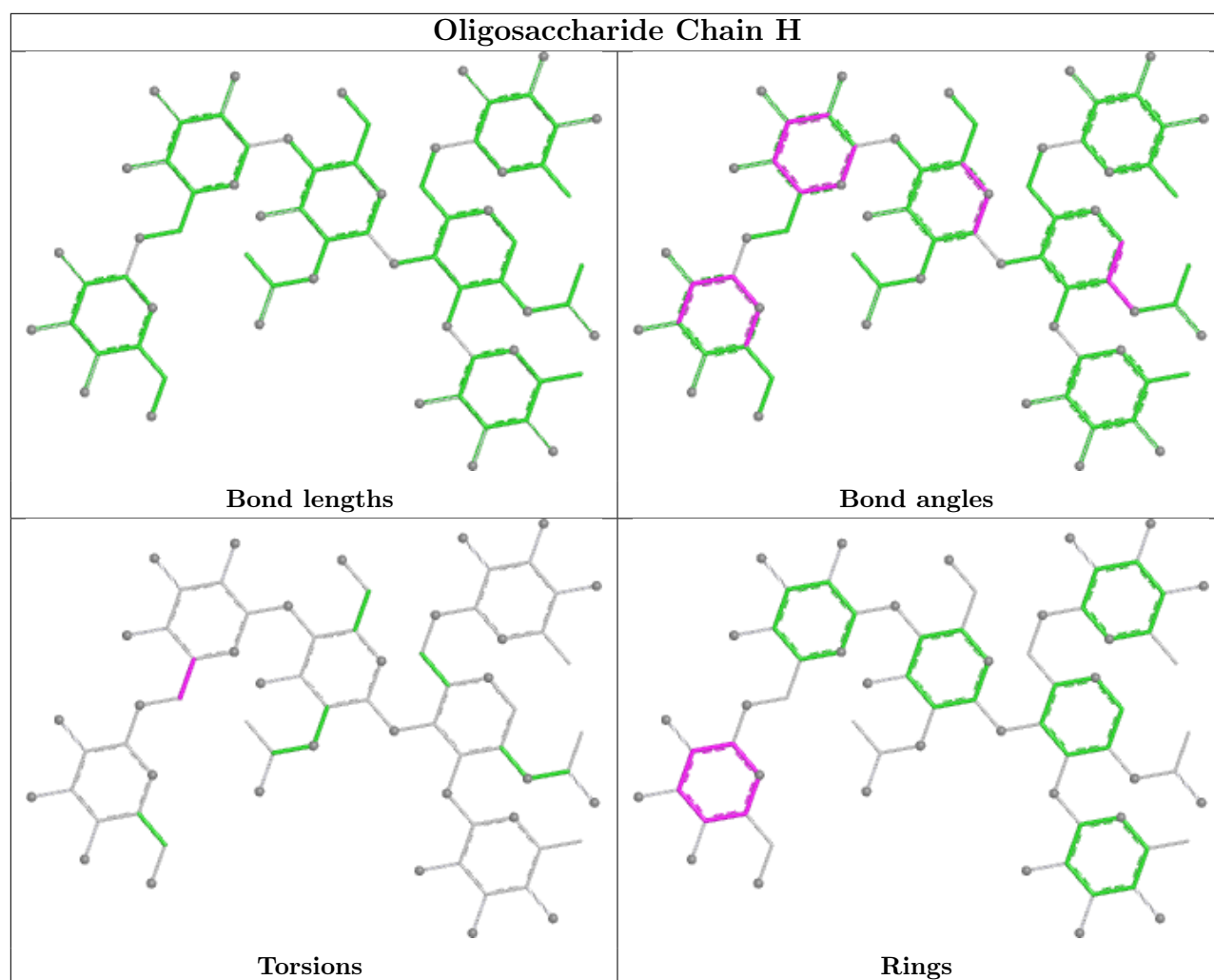


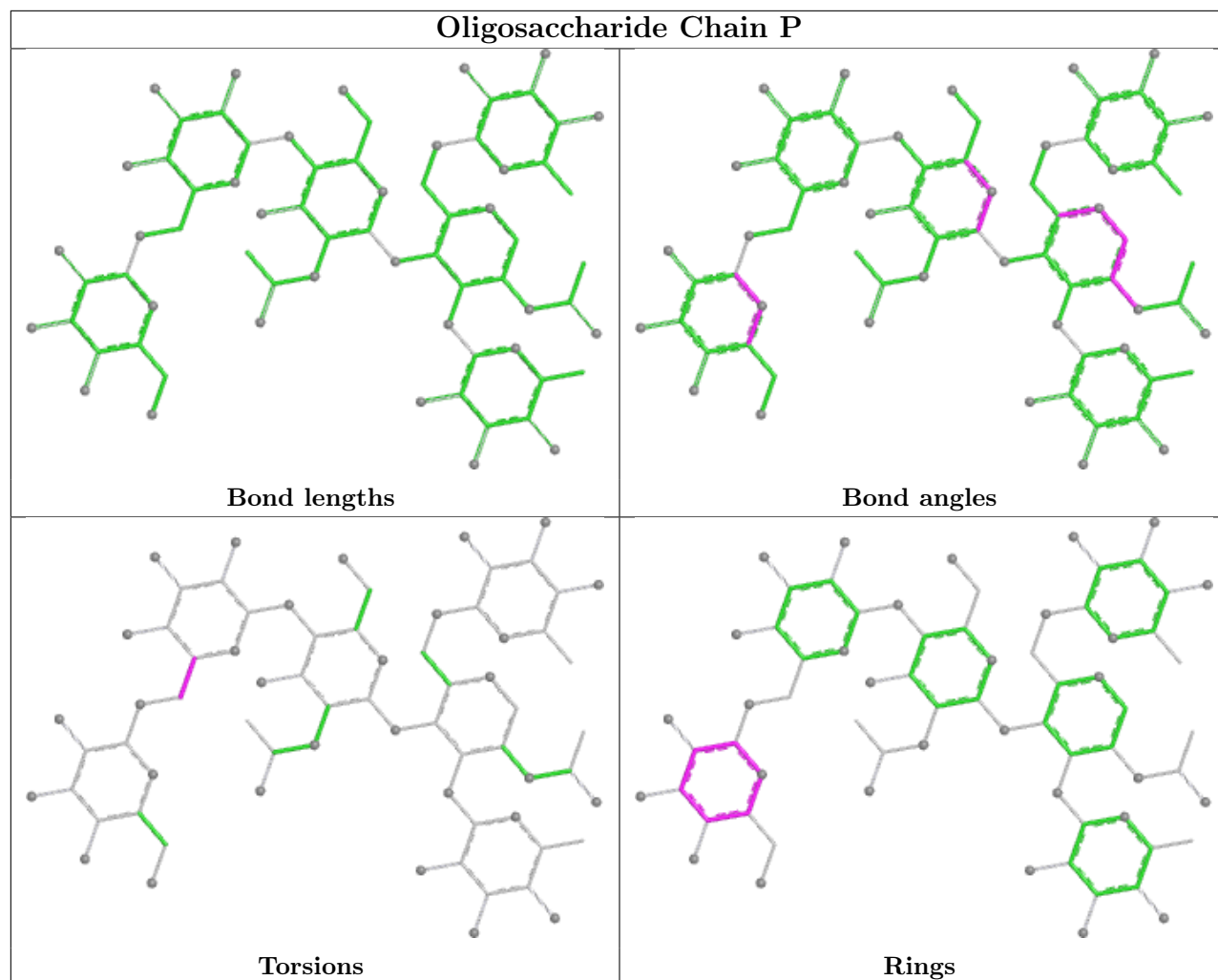


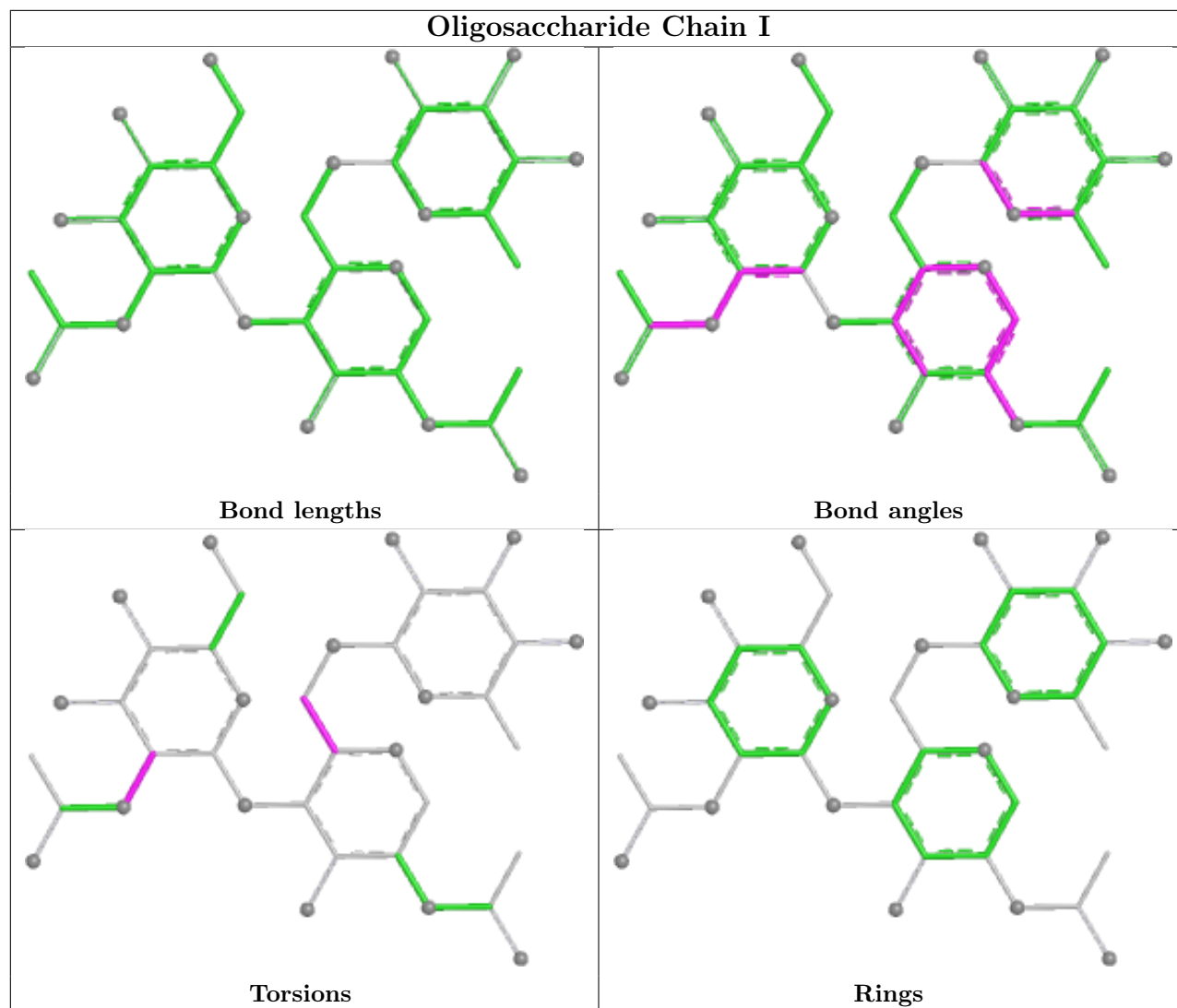


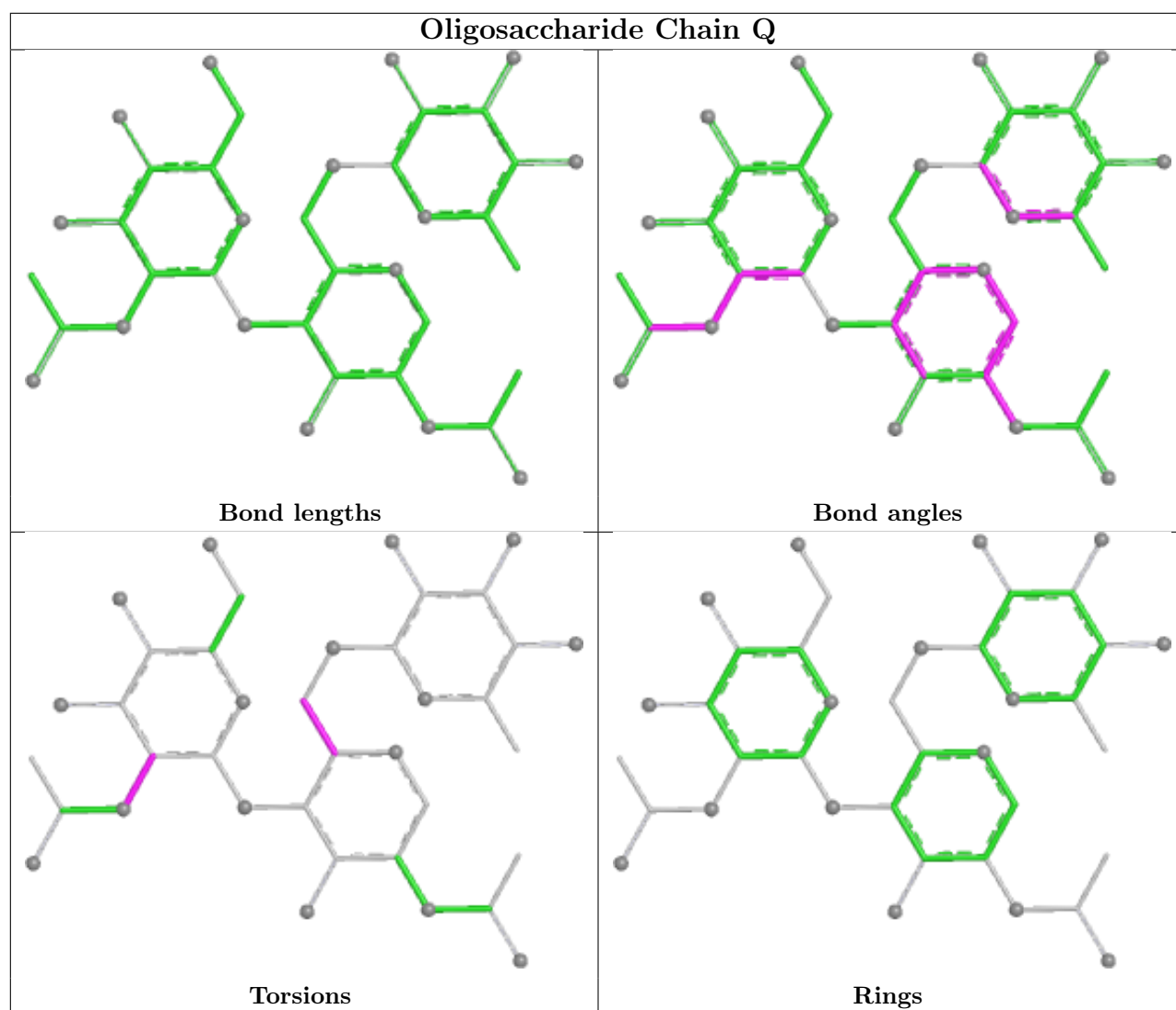


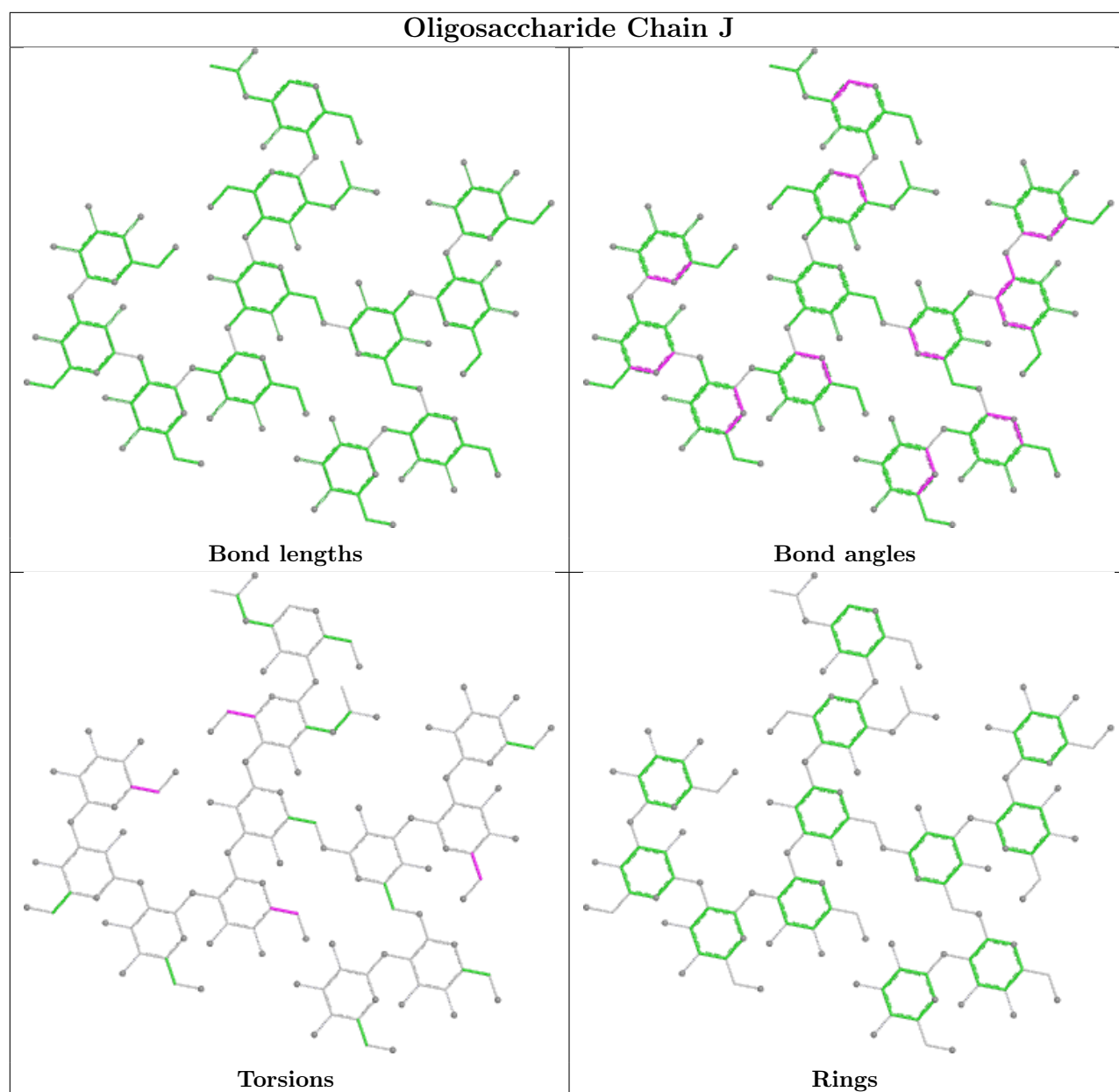


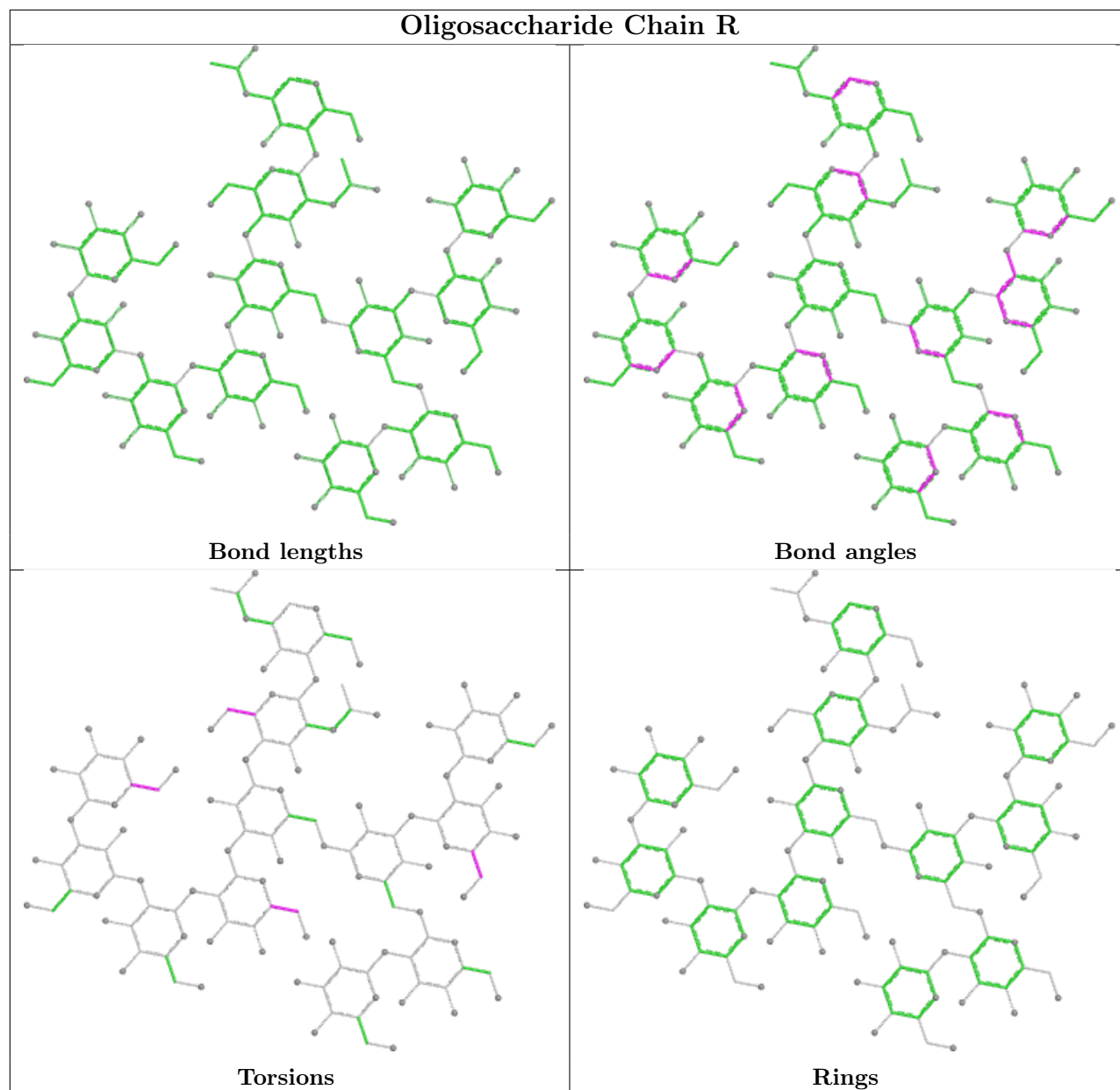


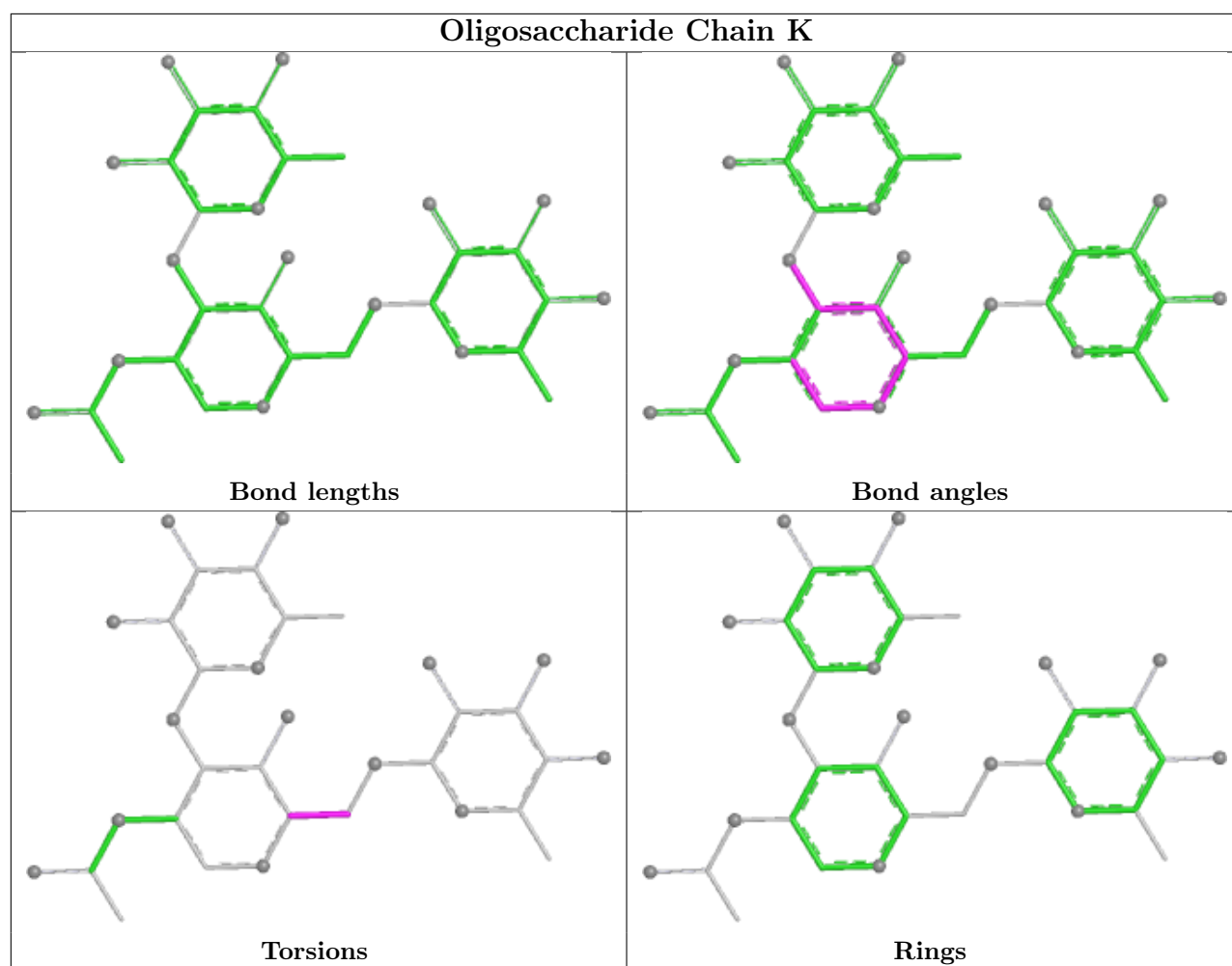




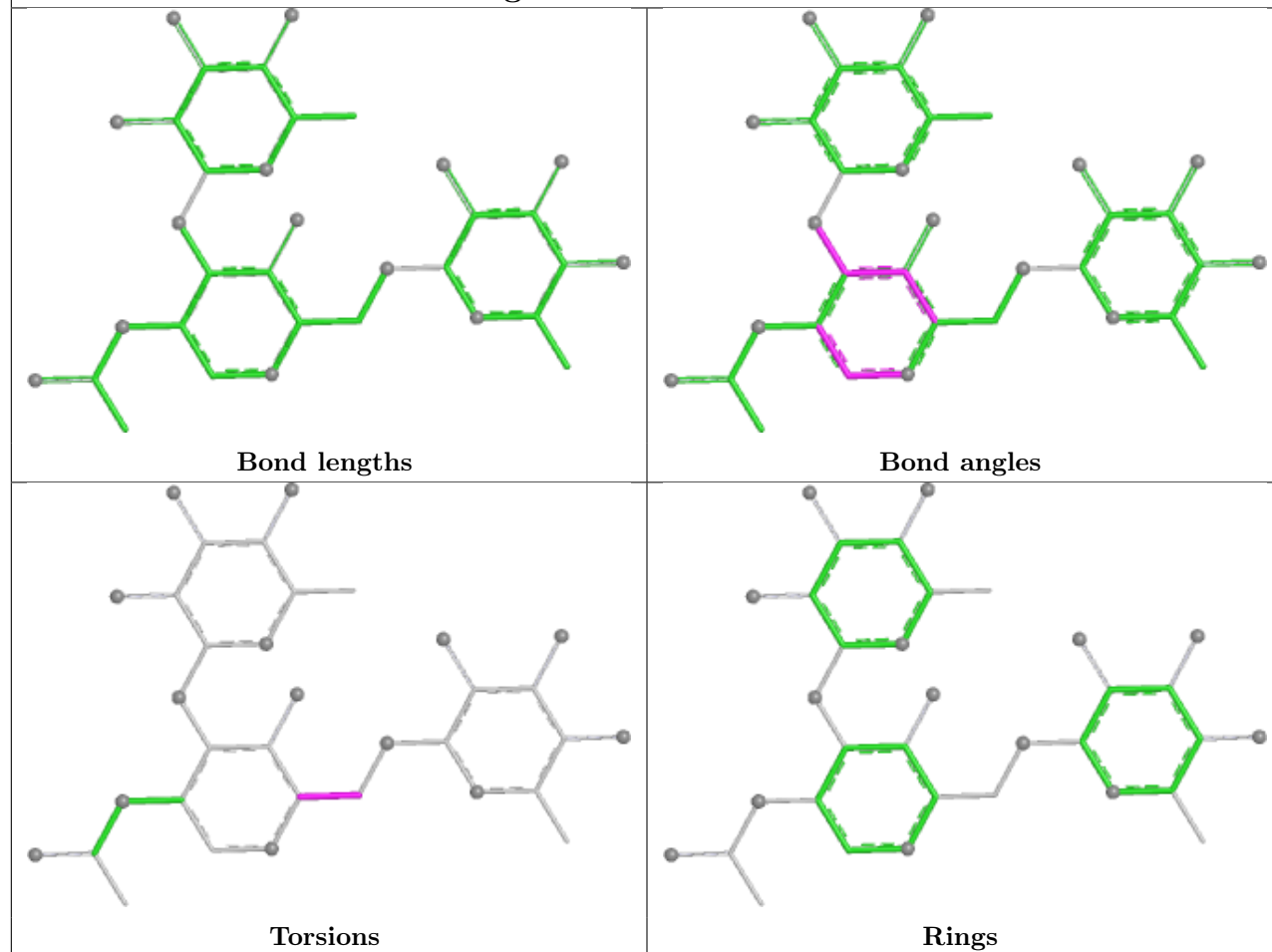




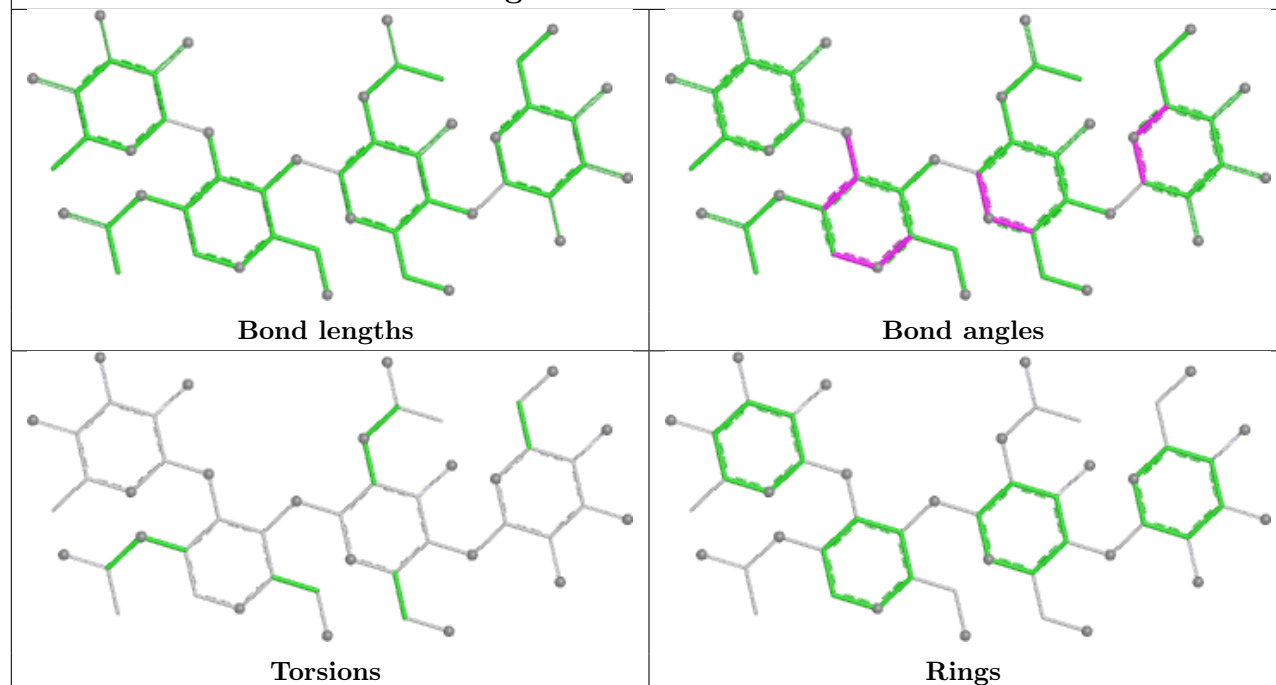


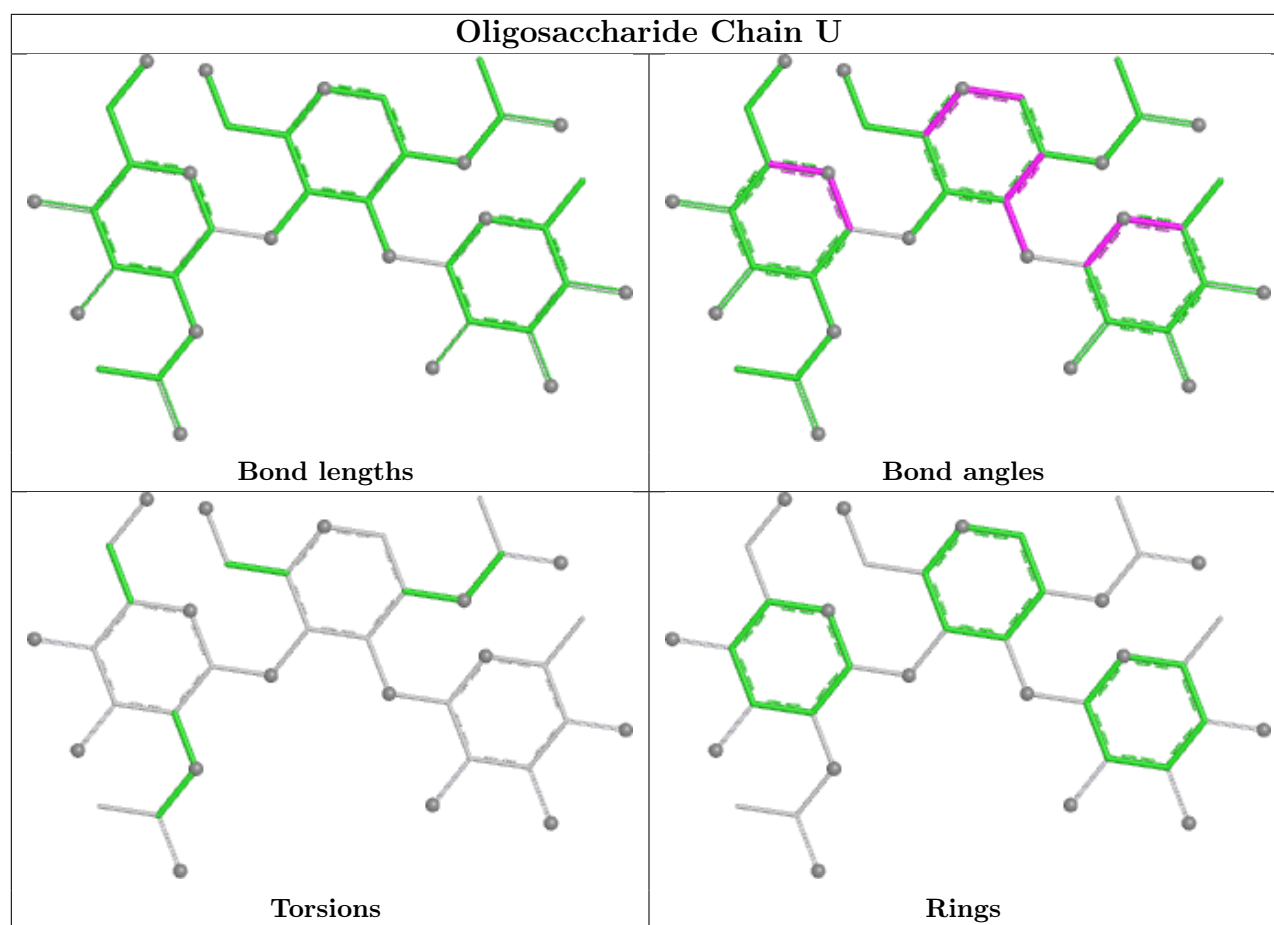


Oligosaccharide Chain S



Oligosaccharide Chain L





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

6.1 Protein, DNA and RNA chains

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

All (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
2	D	77	TYR	5.0
1	C	243	ASP	4.9
2	B	382	ASN	4.9
2	B	252	ILE	4.9
2	B	117	TYR	4.7
1	C	240	ASP	4.7
2	D	362	LEU	4.6
2	D	337	THR	4.6
2	B	256	GLU	4.6
2	D	208	VAL	4.6
2	D	339	ASN	4.4
2	D	261	VAL	4.4
2	D	56	ASN	4.2
1	C	283	ALA	4.2
1	A	508	ILE	4.2
2	B	162	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	67	LEU	4.1
2	B	220	SER	4.1
2	B	383	PRO	4.1
2	D	117	TYR	4.1
1	C	508	ILE	4.1
2	D	248	HIS	4.0
2	B	350	LEU	4.0
2	D	257	LYS	4.0
1	C	247	LEU	4.0
1	C	592	ASN	4.0
2	D	66	SER	4.0
2	D	201	VAL	3.9
2	D	61	ASP	3.9
1	A	261	PHE	3.9
2	B	123	MET	3.9
2	B	129	PRO	3.9
2	B	249	VAL	3.8
2	D	30	PRO	3.8
1	A	581	ILE	3.8
2	B	248	HIS	3.8
2	D	63	TYR	3.8
2	D	48	ALA	3.8
1	C	280	GLY	3.8
2	D	255	VAL	3.8
1	C	158	LEU	3.8
2	B	251	LEU	3.8
1	C	558	GLY	3.7
2	B	255	VAL	3.7
2	B	82	GLY	3.7
1	A	573	PHE	3.7
2	D	350	LEU	3.6
2	D	361	VAL	3.6
1	C	231	PHE	3.6
2	D	31	LEU	3.6
1	A	558	GLY	3.6
1	A	579	VAL	3.6
2	D	220	SER	3.6
2	D	193	VAL	3.6
2	D	246	LEU	3.6
1	A	349	GLY	3.5
2	D	347	VAL	3.5
2	B	45	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	336	LEU	3.5
2	D	253	GLN	3.5
2	D	65	LEU	3.5
2	D	256	GLU	3.5
2	D	249	VAL	3.4
1	C	140	ILE	3.4
1	C	477	PHE	3.4
1	A	319	VAL	3.4
1	C	239	MET	3.4
1	C	98	TYR	3.4
1	C	154	PHE	3.4
2	B	265	PHE	3.4
2	D	124	PHE	3.4
2	B	352	LEU	3.3
2	B	315	ASP	3.3
2	D	120	CYS	3.3
2	D	163	LEU	3.3
1	C	353	ASP	3.3
2	D	86	TYR	3.3
2	B	36	PRO	3.3
2	B	126	ILE	3.3
1	A	516	ARG	3.3
2	B	361	VAL	3.3
1	C	573	PHE	3.2
1	C	579	VAL	3.2
2	D	343	ASP	3.2
1	C	160	PHE	3.2
2	B	218	THR	3.2
2	D	250	PRO	3.2
2	D	162	ASP	3.1
2	D	329	ALA	3.1
2	B	201	VAL	3.1
2	B	190	LEU	3.1
2	B	120	CYS	3.1
2	B	356	ASP	3.1
1	C	234	VAL	3.1
2	B	262	THR	3.1
2	D	247	ARG	3.1
1	C	94	ALA	3.1
2	B	329	ALA	3.1
1	A	119	PHE	3.1
1	A	256	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	353	ASP	3.1
1	A	280	GLY	3.1
1	C	136	GLN	3.1
1	C	95	PHE	3.0
2	B	261	VAL	3.0
1	A	408	SER	3.0
2	D	239	GLY	3.0
2	D	45	LEU	3.0
1	A	561	ALA	3.0
1	C	141	GLY	3.0
1	C	144	CYS	3.0
2	D	251	LEU	3.0
1	C	433	HIS	3.0
1	A	303	GLY	3.0
1	C	146	ARG	3.0
1	C	303	GLY	3.0
2	B	89	LEU	3.0
2	D	222	ALA	3.0
2	B	228	HIS	3.0
2	D	133	LEU	3.0
2	B	363	PRO	2.9
1	C	541	THR	2.9
1	A	574	ILE	2.9
2	B	246	LEU	2.9
1	A	137	GLU	2.9
1	C	115	TYR	2.9
2	B	308	GLN	2.9
2	B	30	PRO	2.9
2	D	40	ASN	2.9
1	C	264	SER	2.9
1	A	477	PHE	2.9
1	C	100	LEU	2.9
2	D	360	VAL	2.9
2	D	227	GLN	2.8
1	C	557	TYR	2.8
1	C	561	ALA	2.8
2	D	47	VAL	2.8
1	A	458	GLY	2.8
1	A	367	VAL	2.8
1	C	97	ARG	2.8
1	A	143	ASN	2.8
1	A	484	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	369	GLN	2.8
1	A	247	LEU	2.8
2	D	62	GLY	2.8
2	B	253	GLN	2.8
1	A	268	GLU	2.8
2	D	234	VAL	2.8
1	C	106	PHE	2.8
1	C	127	SER	2.8
2	B	184	PRO	2.8
1	A	243	ASP	2.7
1	C	352	SER	2.7
2	B	348	SER	2.7
2	D	164	SER	2.7
2	D	325	SER	2.7
2	D	209	GLU	2.7
2	B	193	VAL	2.7
1	A	283	ALA	2.7
2	B	257	LYS	2.7
1	C	145	ASP	2.7
2	B	223	SER	2.7
2	B	47	VAL	2.7
2	D	327	GLU	2.7
1	C	269	LEU	2.7
1	A	250	ASN	2.7
2	D	194	THR	2.7
1	A	279	SER	2.7
1	C	363	SER	2.7
2	B	347	VAL	2.6
2	B	359	LEU	2.6
1	C	147	ILE	2.6
2	B	66	SER	2.6
1	C	253	TYR	2.6
2	B	304	ARG	2.6
2	B	173	THR	2.6
1	A	502	LEU	2.6
2	D	307	ILE	2.6
1	C	148	ALA	2.6
1	C	343	PHE	2.6
1	C	279	SER	2.6
2	D	207	TYR	2.6
1	A	120	LYS	2.6
2	D	332	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	164	SER	2.6
1	C	109	TRP	2.6
1	A	362	TYR	2.6
1	C	581	ILE	2.6
1	C	233	ASP	2.6
1	A	350	SER	2.5
2	D	115	SER	2.5
2	B	326	PRO	2.5
2	D	315	ASP	2.5
2	B	336	LEU	2.5
2	D	184	PRO	2.5
2	D	34	LEU	2.5
1	A	307	GLY	2.5
1	A	485	ASP	2.5
1	C	527	ASP	2.5
2	B	346	ASP	2.5
2	D	359	LEU	2.5
1	A	257	SER	2.5
1	C	116	ILE	2.5
1	C	122	SER	2.5
1	C	133	VAL	2.5
2	B	208	VAL	2.5
1	C	268	GLU	2.5
2	D	33	PRO	2.4
2	D	136	PRO	2.4
2	D	185	SER	2.4
2	B	316	GLU	2.4
2	B	357	LYS	2.4
2	D	338	THR	2.4
2	B	65	LEU	2.4
2	D	179	PHE	2.4
1	C	319	VAL	2.4
2	B	355	GLY	2.4
2	B	128	LYS	2.4
1	C	241	PHE	2.4
2	B	87	LEU	2.4
2	D	190	LEU	2.4
2	B	381	ASN	2.4
2	B	43	GLU	2.4
2	B	325	SER	2.4
2	D	49	GLY	2.3
1	A	231	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	305	CYS	2.3
2	D	348	SER	2.3
2	B	37	LEU	2.3
2	D	52	LEU	2.3
1	A	118	VAL	2.3
1	C	367	VAL	2.3
2	B	327	GLU	2.3
2	D	106	ASP	2.3
1	C	126	SER	2.3
1	C	257	SER	2.3
1	C	456	SER	2.3
1	A	475	ILE	2.3
1	C	476	TYR	2.3
2	D	88	THR	2.3
2	D	138	TYR	2.3
1	A	542	VAL	2.3
2	B	360	VAL	2.3
2	D	91	VAL	2.3
1	A	505	ASN	2.3
1	C	185	GLU	2.3
1	C	252	LEU	2.3
1	A	434	ILE	2.3
2	B	303	PRO	2.3
2	D	233	PRO	2.3
2	B	239	GLY	2.3
1	C	261	PHE	2.3
1	C	110	ALA	2.3
2	B	99	LEU	2.3
2	D	58	ASP	2.3
1	A	352	SER	2.3
1	A	363	SER	2.3
2	B	337	THR	2.3
2	D	225	SER	2.3
1	A	557	TYR	2.3
2	B	207	TYR	2.3
2	D	44	VAL	2.3
2	D	326	PRO	2.3
2	D	265	PHE	2.2
2	B	105	LYS	2.2
2	B	243	GLN	2.2
1	A	433	HIS	2.2
1	A	321	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	455	SER	2.2
1	C	258	SER	2.2
1	A	347	ASN	2.2
1	C	83	LEU	2.2
2	B	52	LEU	2.2
2	D	67	LEU	2.2
1	C	518	ILE	2.2
2	B	91	VAL	2.2
2	D	262	THR	2.2
2	D	354	PRO	2.2
2	B	112	PHE	2.2
1	C	501	LEU	2.2
2	B	137	ALA	2.2
2	B	163	LEU	2.2
1	C	228	ILE	2.2
1	A	414	GLY	2.2
1	C	219	GLY	2.2
1	C	256	SER	2.2
1	C	458	GLY	2.2
2	D	134	TYR	2.2
2	B	219	LYS	2.2
1	C	571	ARG	2.2
2	D	212	ILE	2.2
1	A	281	ASP	2.2
2	D	346	ASP	2.2
1	A	294	GLY	2.2
1	C	205	TYR	2.2
1	A	323	ALA	2.2
2	B	114	GLU	2.2
2	B	122	ALA	2.2
1	A	91	ILE	2.1
1	A	62	ASN	2.1
2	B	136	PRO	2.1
2	D	365	PRO	2.1
1	A	499	MET	2.1
2	D	105	LYS	2.1
2	B	247	ARG	2.1
1	C	91	ILE	2.1
2	D	308	GLN	2.1
1	C	143	ASN	2.1
2	B	367	LYS	2.1
1	A	541	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	2.1
1	C	246	LEU	2.1
2	D	226	LEU	2.1
1	C	362	TYR	2.1
1	C	537	SER	2.1
2	D	378	GLU	2.1
1	C	542	VAL	2.1
2	D	331	PRO	2.1
1	A	106	PHE	2.1
1	A	527	ASP	2.1
1	C	227	ARG	2.1
1	A	258	SER	2.1
1	C	305	CYS	2.1
2	D	217	CYS	2.1
1	C	321	VAL	2.1
2	B	73	VAL	2.1
2	D	254	PRO	2.1
1	C	448	LEU	2.1
2	B	135	LEU	2.1
2	D	87	LEU	2.1
1	A	343	PHE	2.1
2	D	356	ASP	2.1
2	D	177	ALA	2.1
2	B	77	TYR	2.1
1	A	308	SER	2.0
1	A	517	SER	2.0
2	B	53	GLN	2.0
2	B	111	MET	2.0
1	A	158	LEU	2.0
2	B	313	LEU	2.0
2	D	342	GLY	2.0
2	D	55	ILE	2.0
1	C	84	GLU	2.0
1	C	432	TRP	2.0
2	D	114	GLU	2.0
1	C	196	SER	2.0
2	B	369	GLN	2.0
2	D	132	VAL	2.0
2	D	223	SER	2.0
1	A	259	LEU	2.0
2	D	313	LEU	2.0
1	A	592	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	200	ASN	2.0
1	C	548	GLY	2.0

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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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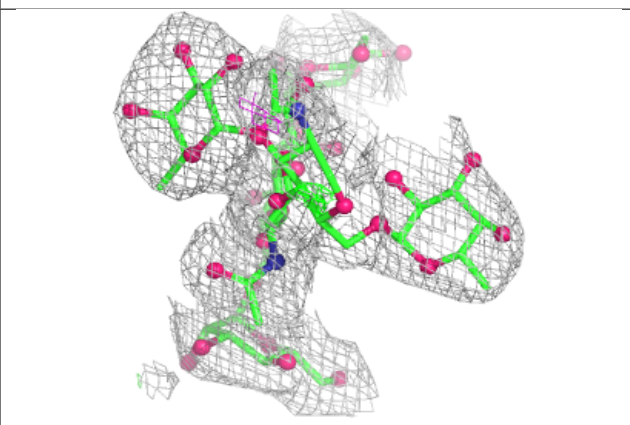
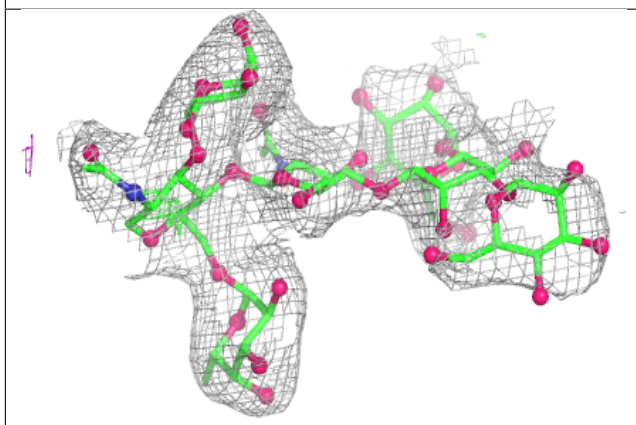
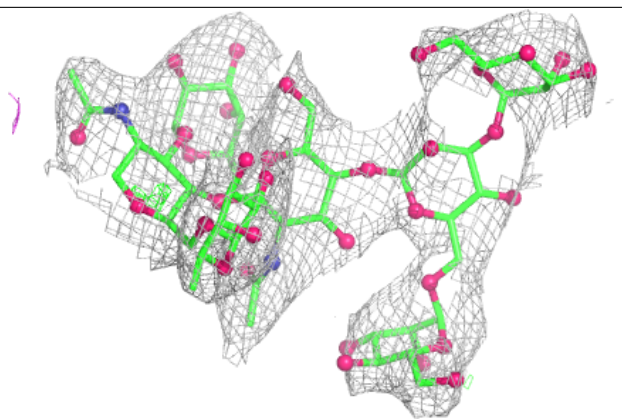
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	R	12	11/12	0.87	0.16	114,115,116,116	0
3	FUC	O	7	10/11	0.87	0.20	140,141,142,142	0
7	MAN	J	12	11/12	0.88	0.16	113,113,114,114	0
3	NAG	G	1	14/15	0.88	0.12	142,146,148,150	0
3	FUC	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
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

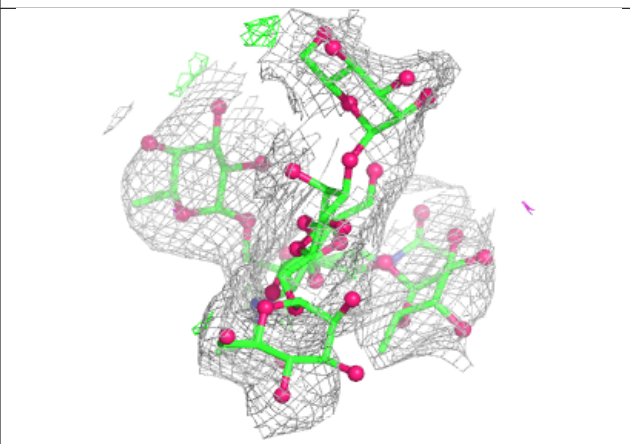
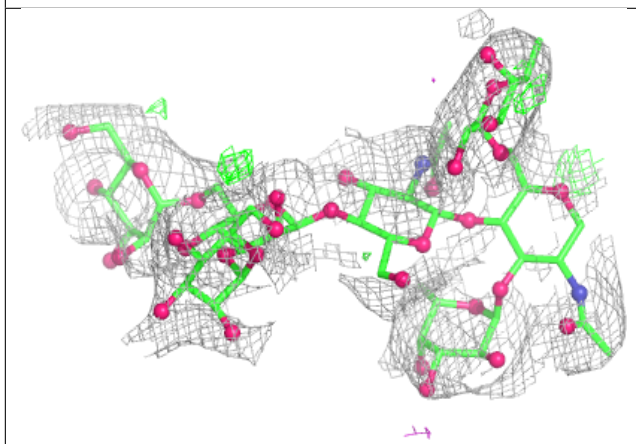
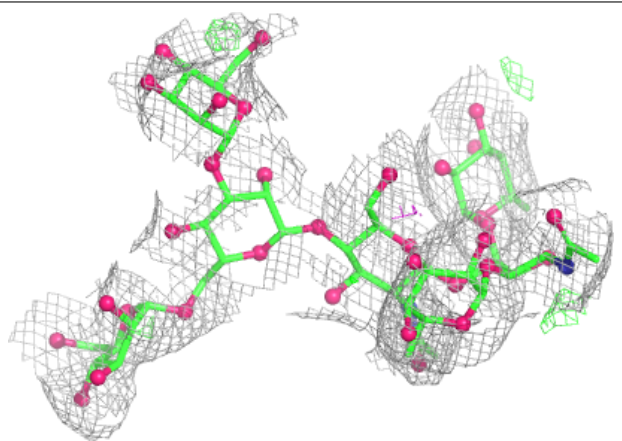
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

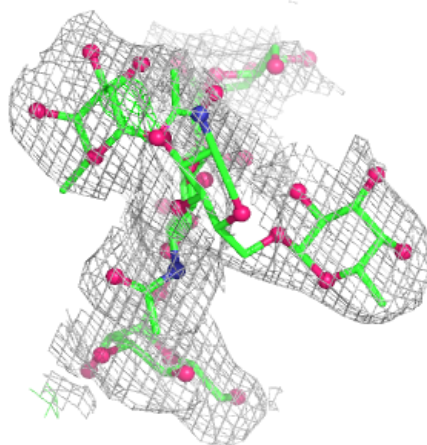
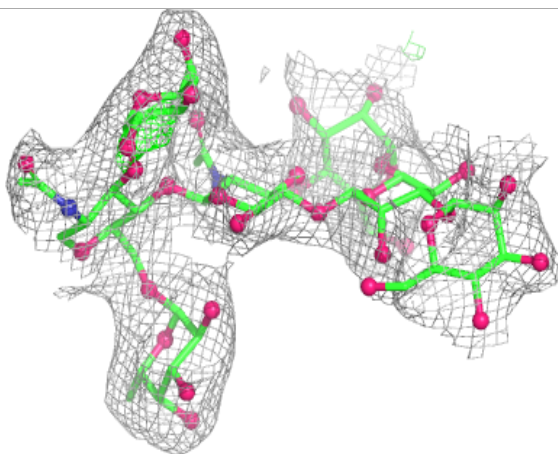
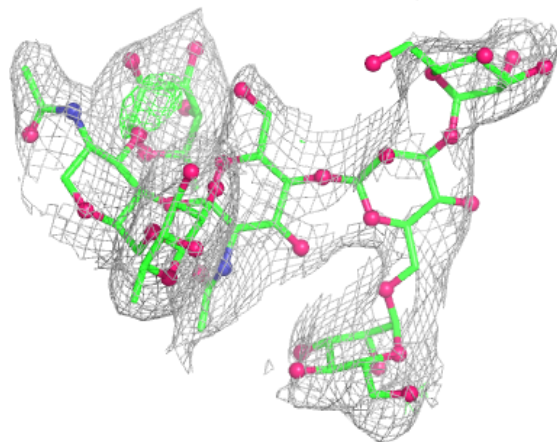
**Electron density around Chain G:**

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



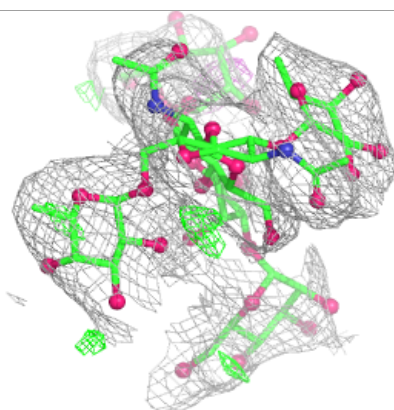
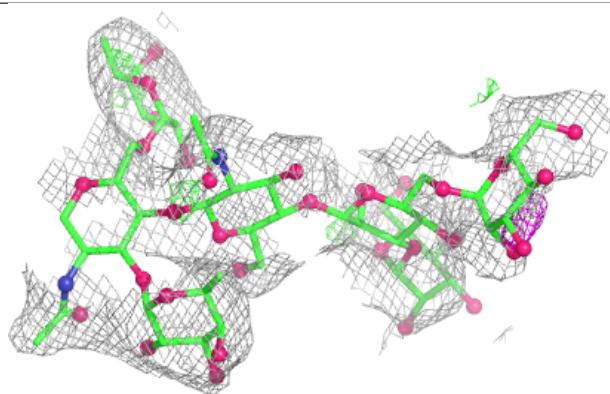
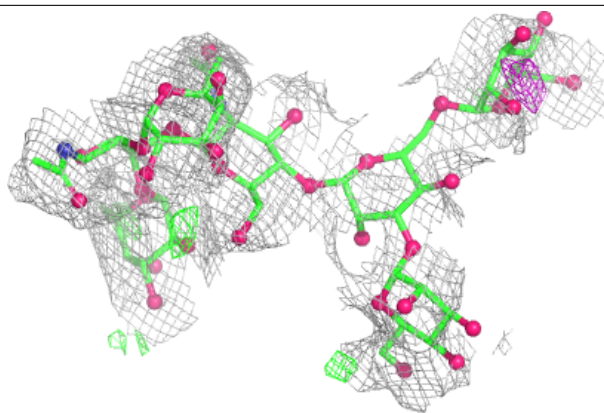
Electron density around Chain M:

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

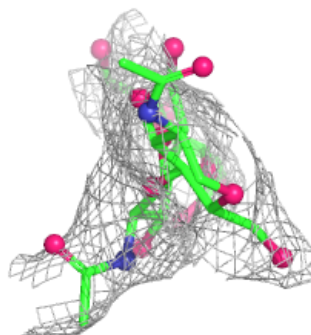
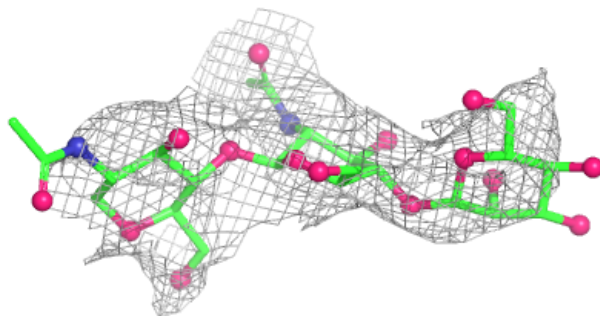
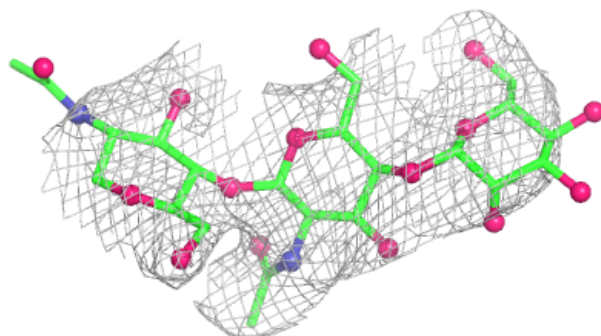


Electron density around Chain O:

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

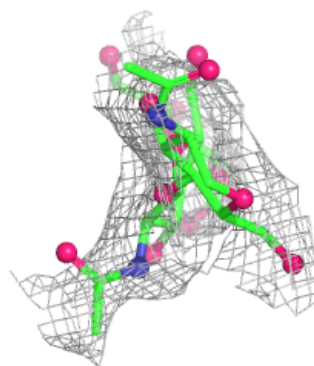
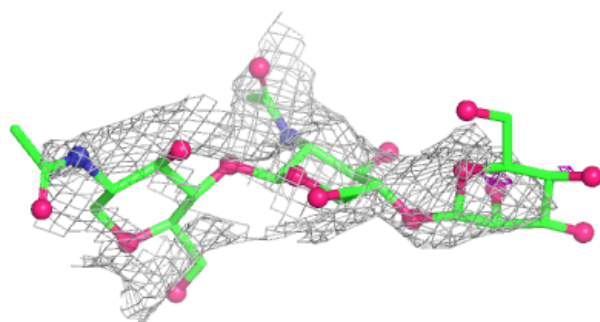
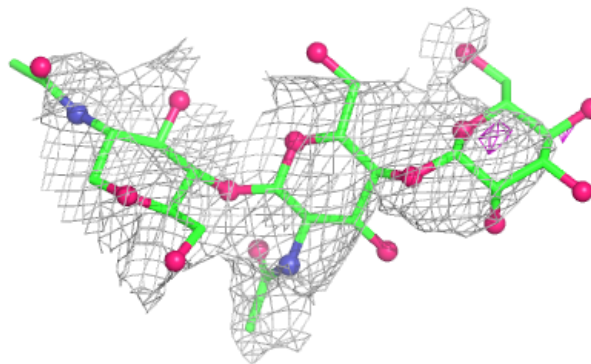
**Electron density around Chain F:**

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

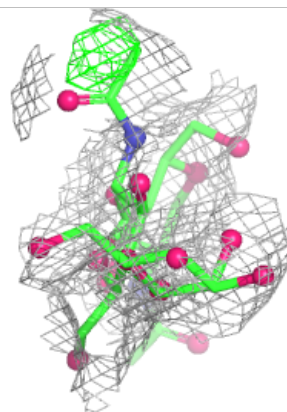
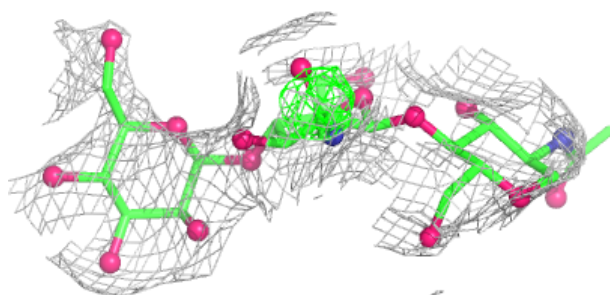
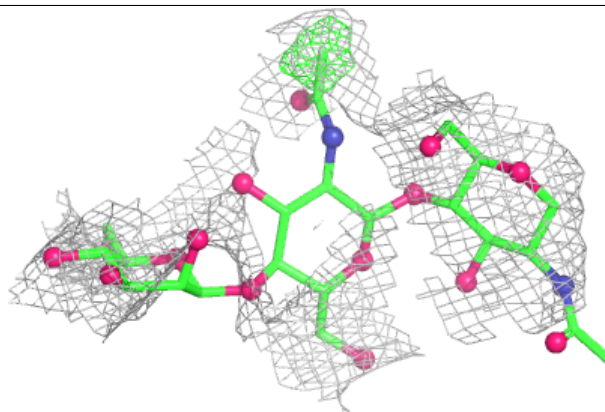


Electron density around Chain N:

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

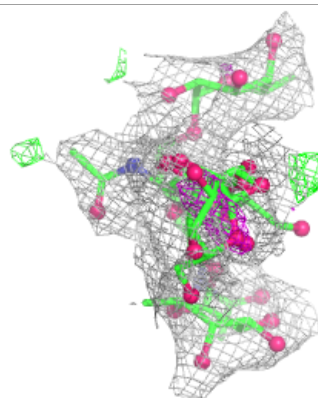
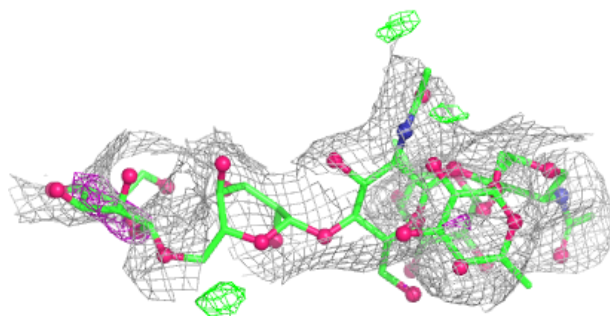
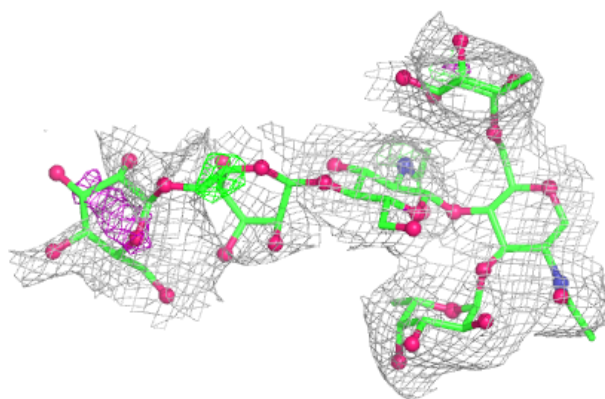
**Electron density around Chain T:**

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

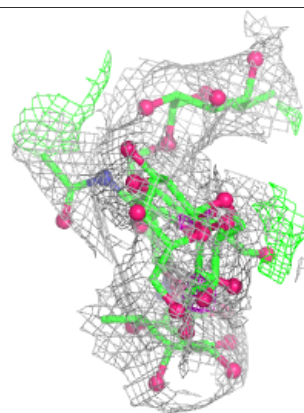
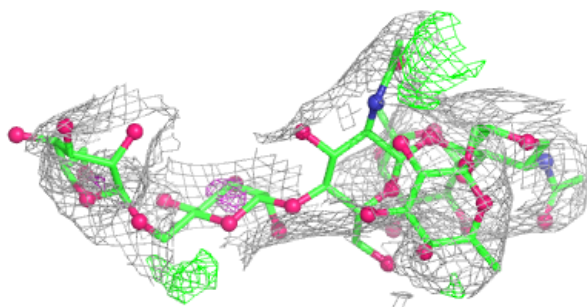
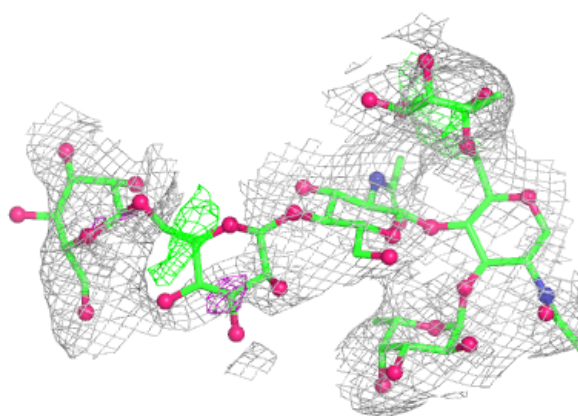


Electron density around Chain H:

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

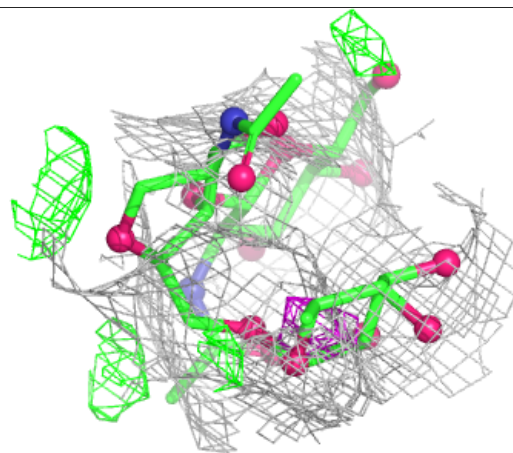
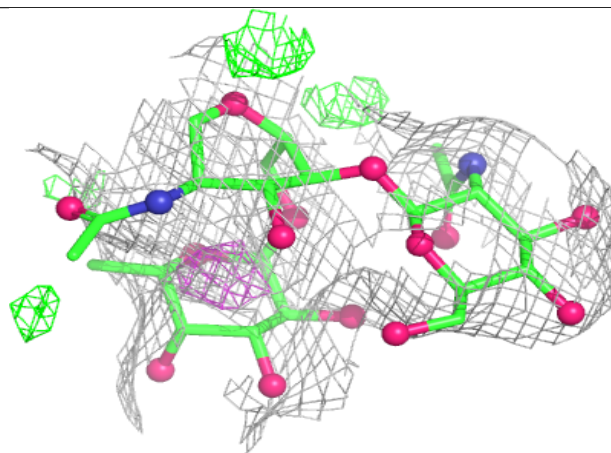
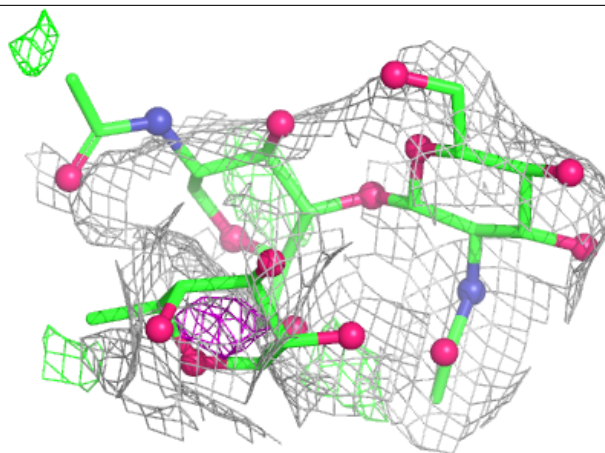
**Electron density around Chain P:**

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



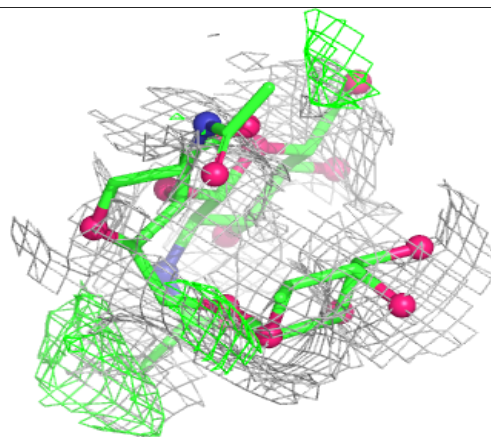
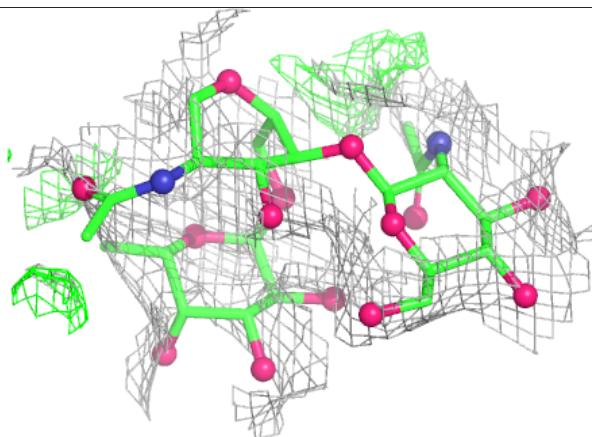
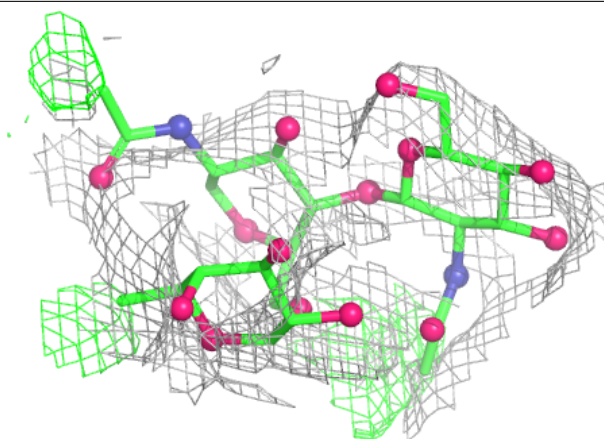
Electron density around Chain I:

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

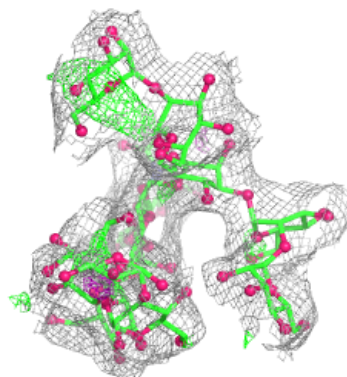
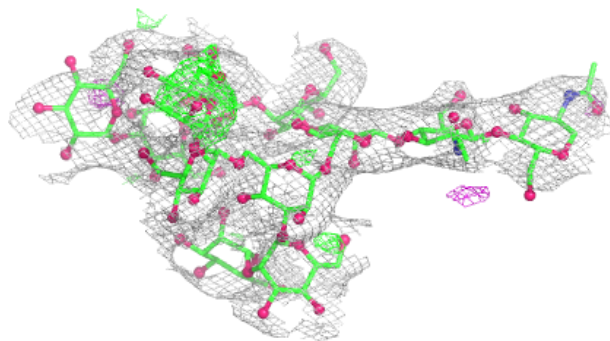
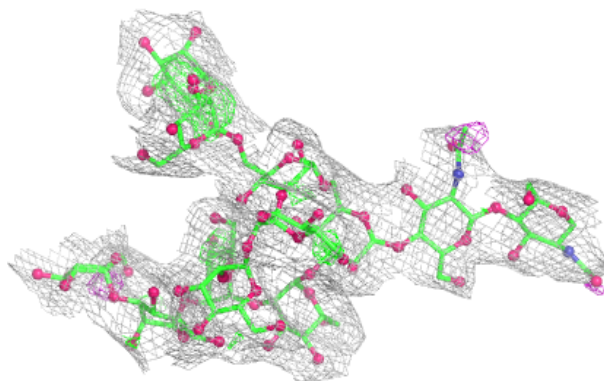


Electron density around Chain Q:

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

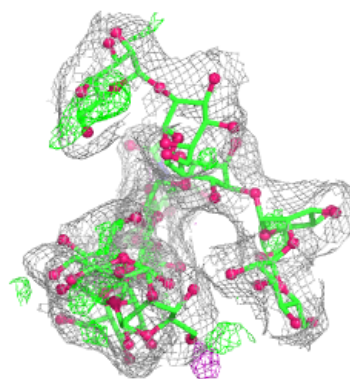
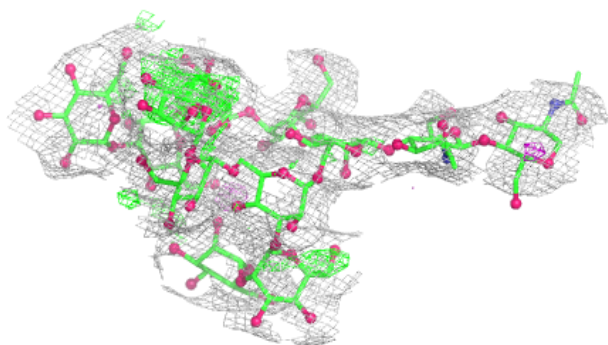
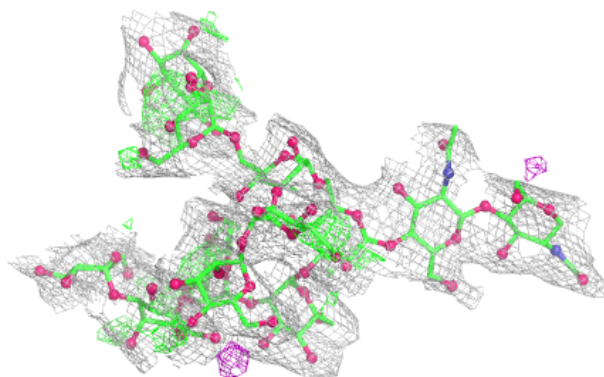
**Electron density around Chain J:**

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

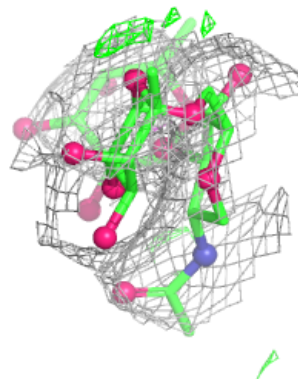
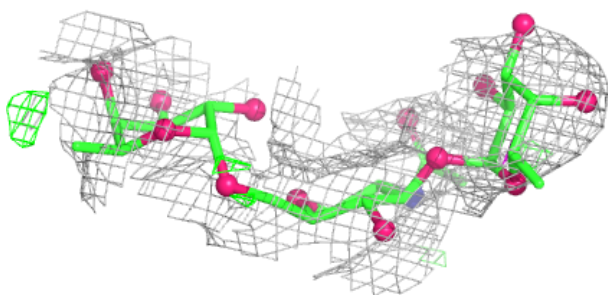
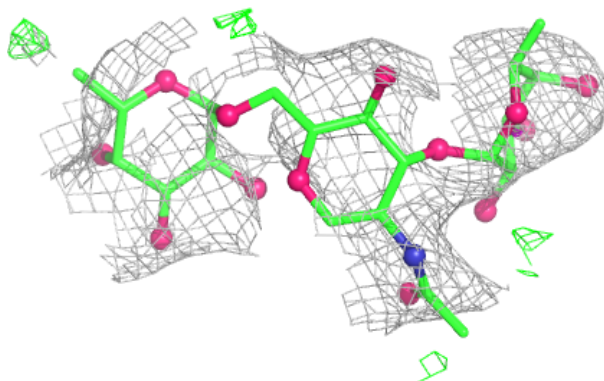


Electron density around Chain R:

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

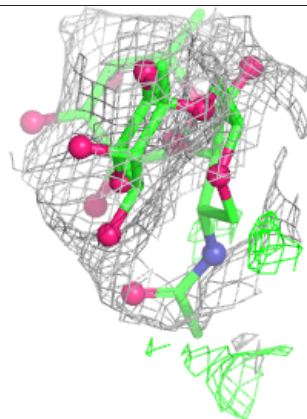
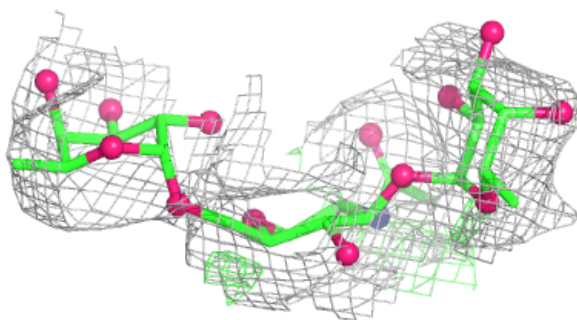
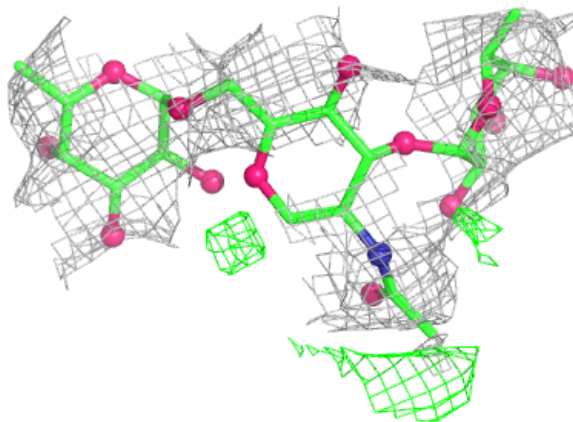
**Electron density around Chain K:**

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

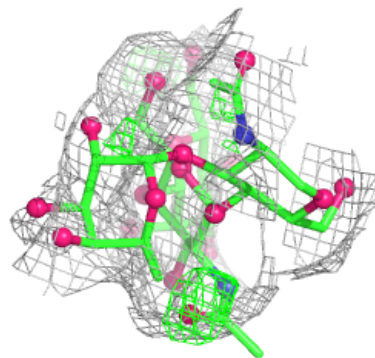
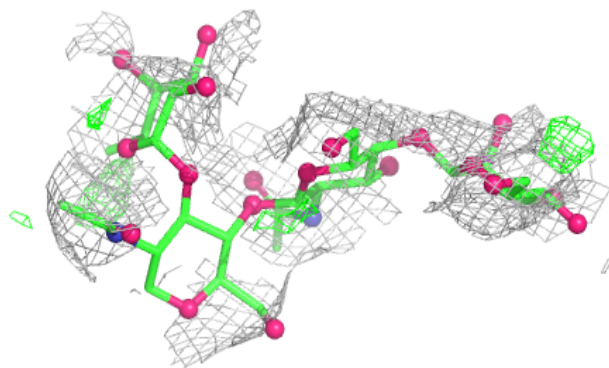
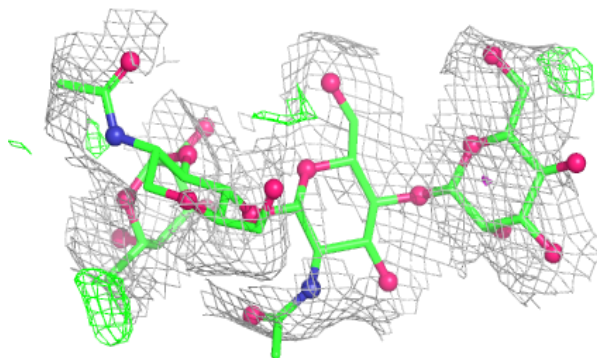


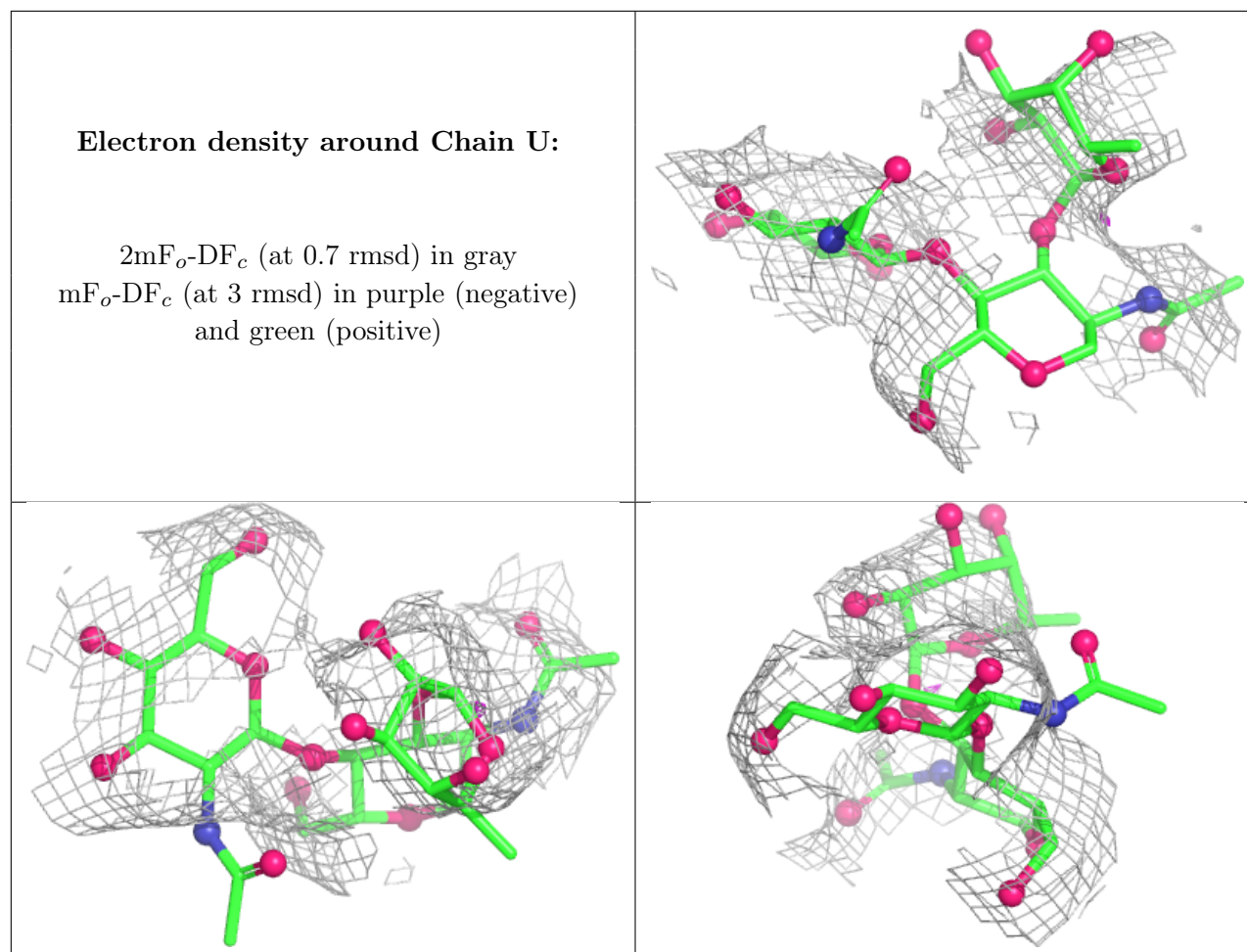
Electron density around Chain S:

$2mF_o-DF_c$ (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.