



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:26 PM UTC

PDB ID : 2H6O / pdb_00002h6o
Title : Epstein Barr Virus Major Envelope Glycoprotein
Authors : Chen, X.S.
Deposited on : 2006-05-31
Resolution : 3.50 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

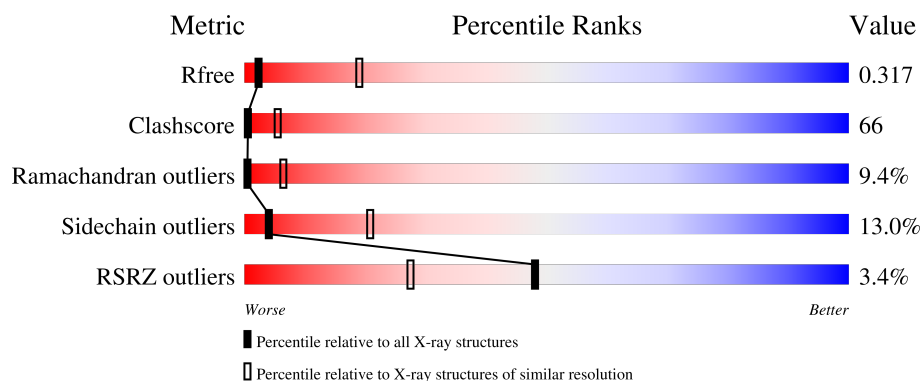
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	470	3% 27% 47% 16% 6%
2	B	7	100%
3	D	7	29% 71%
4	F	8	100%
5	J	9	22% 78%

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Mol	Chain	Length	Quality of chain
6	M	10	 50% 50%
7	Q	9	 11% 89%
8	U	11	 9% 91%
9	Y	3	 100%
10	Z	5	 20% 80%
11	b	8	 100%
12	d	9	 22% 78%
13	f	10	 10% 90%
14	i	3	 100%
15	j	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	b	1	-	-	X	-
11	MAN	b	6	-	-	X	-
14	NAG	i	2	-	-	X	-
2	MAN	B	3	-	-	X	-
2	MAN	B	4	-	-	X	-
3	MAN	D	3	-	-	X	-
5	NAG	J	1	-	-	X	-
7	MAN	Q	3	-	-	X	-
8	MAN	U	5	-	-	X	-

2 Entry composition [i](#)

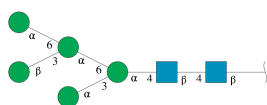
There are 15 unique types of molecules in this entry. The entry contains 4500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Major outer envelope glycoprotein gp350.

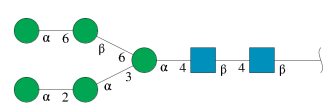
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3301	2082	542	660	17			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

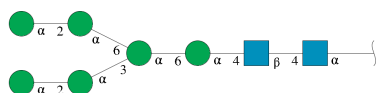
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			83	46	2	35			

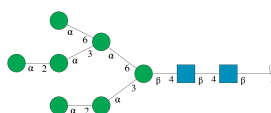
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-

2-acetamido-2-deoxy-alpha-D-glucopyranose.



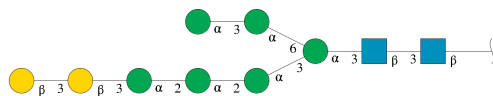
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



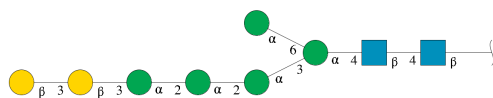
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



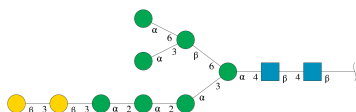
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



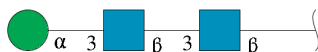
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 8 is an oligosaccharide called beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



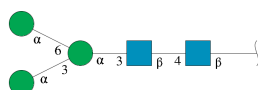
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	U	11	Total	C	N	O	0	0	0
			127	70	2	55			

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



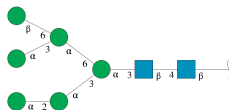
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



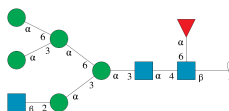
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Z	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



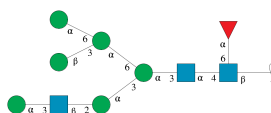
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	b	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



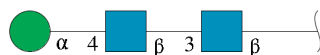
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	d	9	Total	C	N	O	0	0	0
			107	60	3	44			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



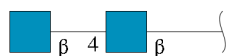
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	f	10	Total	C	N	O	0	0	0
			118	66	3	49			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	i	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 15 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	j	2	Total	C	N	O	0	0	0
			28	16	2	10			

MAG1
MAG2
MAN3
MAN4
BMA5
MAG6
MAN7

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

Chain D:  29% 71%

MAG1
MAG2
MAN3
MAN4
MAN5
BMA6
MAN7

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

Chain F:  100%

NDG1
MAG2
MAN3
MAN4
MAN5
MAG6
MAN7
MAN8

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

Chain J:  22% 78%

MAG1
MAG2
MAN3
BMA4
MAN5
MAG6
MAN7
MAN8
MAN9

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

Chain M:  50% 50%

MAG1
MAG2
MAN3
MAN4
MAN5
MAG6
GAL7
GAL8
MAN9
MAN10

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

Chain Q:  11% 89%

MAG1
MAG2
MAN3
MAN4
MAN5
MAG6
GAL7
GAL8
MAN9

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

Chain U:  9% 91%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
GAL7
GAL8
BMA9
MAN10
MAN11

- Molecule 9: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1
MAG2
MAN3

- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  20% 80%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7
BMA8

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  22% 78%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
FUC9

- Molecule 13: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  10% 90%

NAG1	NAG2	MAN3	MAN4	NAG5	MAN6	MAN7	MAN8	MAN9	FUC10
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- Molecule 14: α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%

NAG1	NAG2	MAN3
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- Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  50% 50%

NAG1	NAG2
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.01Å 110.01Å 146.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 91.9 (20.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.326 , 0.368 0.287 , 0.317	Depositor DCC
R_{free} test set	947 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4500	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: GAL, NAG, FUC, BMA, NDG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	4/3377 (0.1%)	1.42	75/4621 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	ASN	CA-C	8.85	1.71	1.52
1	A	352	TRP	NE1-CE2	-7.58	1.29	1.37
1	A	443	ASN	C-O	6.59	1.36	1.23
1	A	404	ILE	CA-CB	-5.04	1.47	1.53

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASN	N-CA-C	-11.39	98.96	112.86
1	A	23	PRO	N-CA-C	-9.58	101.20	114.80
1	A	101	GLU	N-CA-C	8.98	122.72	109.07
1	A	163	ASP	N-CA-C	8.67	129.26	110.80
1	A	399	ALA	CA-C-N	8.35	130.28	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PHE	Sidechain

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	3301	0	3132	363	0
2	B	83	0	72	21	0
3	D	83	0	71	11	0
4	F	94	0	81	10	0
5	J	105	0	89	18	0
6	M	116	0	96	6	0
7	Q	105	0	89	15	0
8	U	127	0	108	20	0
9	Y	39	0	34	5	0
10	Z	61	0	53	9	0
11	b	94	0	82	19	0
12	d	107	0	94	15	0
13	f	118	0	99	14	0
14	i	39	0	34	8	0
15	j	28	0	24	3	0
All	All	4500	0	4158	492	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 66.

The worst 5 of 492 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:HD21	5:J:1:NAG:C1	1.07	1.60
1:A:386:ASN:HD21	13:f:1:NAG:C1	1.06	1.59
1:A:345:ASN:HD21	11:b:1:NAG:C1	1.12	1.53
1:A:87:ASN:HD22	3:D:1:NAG:C1	1.31	1.41
1:A:318:ASN:ND2	9:Y:1:NAG:C1	1.92	1.31

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	438/470 (93%)	327 (75%)	70 (16%)	41 (9%)	0 6

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	32	GLU
1	A	85	SER
1	A	115	ILE
1	A	158	PRO

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	362/404 (90%)	315 (87%)	47 (13%)	4 21

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	MET
1	A	299	ILE
1	A	203	LEU
1	A	246	THR
1	A	304	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	328	ASN
1	A	435	ASN
1	A	318	ASN
1	A	342	ASN

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 ⓘ

101 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2	14,14,15	1.60	4 (28%)	17,19,21	1.43	3 (17%)
2	NAG	B	2	2	14,14,15	1.13	2 (14%)	17,19,21	1.83	5 (29%)
2	MAN	B	3	2	11,11,12	1.36	1 (9%)	15,15,17	0.93	0
2	MAN	B	4	2	11,11,12	1.54	2 (18%)	15,15,17	1.30	1 (6%)
2	BMA	B	5	2	11,11,12	1.20	2 (18%)	15,15,17	1.41	3 (20%)
2	MAN	B	6	2	11,11,12	1.17	1 (9%)	15,15,17	1.37	2 (13%)
2	MAN	B	7	2	11,11,12	1.26	1 (9%)	15,15,17	1.22	1 (6%)
3	NAG	D	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	0.83	1 (5%)
3	NAG	D	2	3	14,14,15	0.93	1 (7%)	17,19,21	0.91	2 (11%)
3	MAN	D	3	3	11,11,12	1.29	2 (18%)	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	4	3	11,11,12	1.48	3 (27%)	15,15,17	1.13	1 (6%)
3	MAN	D	5	3	11,11,12	1.19	1 (9%)	15,15,17	1.37	2 (13%)
3	BMA	D	6	3	11,11,12	1.63	3 (27%)	15,15,17	1.46	4 (26%)
3	MAN	D	7	3	11,11,12	0.94	1 (9%)	15,15,17	1.16	2 (13%)
4	NDG	F	1	4,1	14,14,15	1.54	2 (14%)	17,19,21	1.38	4 (23%)
4	NAG	F	2	4	14,14,15	0.88	0	17,19,21	1.25	2 (11%)
4	MAN	F	3	4	11,11,12	1.54	2 (18%)	15,15,17	1.09	0
4	MAN	F	4	4	11,11,12	1.22	3 (27%)	15,15,17	1.55	4 (26%)
4	MAN	F	5	4	11,11,12	1.38	2 (18%)	15,15,17	1.17	1 (6%)
4	MAN	F	6	4	11,11,12	1.27	1 (9%)	15,15,17	1.24	2 (13%)
4	MAN	F	7	4	11,11,12	1.32	2 (18%)	15,15,17	0.88	1 (6%)
4	MAN	F	8	4	11,11,12	1.00	0	15,15,17	1.00	1 (6%)
5	NAG	J	1	5,1	14,14,15	1.00	1 (7%)	17,19,21	0.77	0
5	NAG	J	2	5	14,14,15	1.03	1 (7%)	17,19,21	0.89	1 (5%)
5	BMA	J	3	5	11,11,12	1.77	3 (27%)	15,15,17	2.39	5 (33%)
5	MAN	J	4	5	11,11,12	1.97	4 (36%)	15,15,17	2.32	5 (33%)
5	MAN	J	5	5	11,11,12	1.16	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	J	6	5	11,11,12	1.25	1 (9%)	15,15,17	1.11	1 (6%)
5	MAN	J	7	5	11,11,12	1.07	1 (9%)	15,15,17	1.10	2 (13%)
5	MAN	J	8	5	11,11,12	1.63	3 (27%)	15,15,17	0.92	0
5	MAN	J	9	5	11,11,12	0.91	0	15,15,17	1.63	4 (26%)
6	NAG	M	1	6,1	14,14,15	2.58	4 (28%)	17,19,21	2.14	4 (23%)
6	MAN	M	10	6	11,11,12	1.06	1 (9%)	15,15,17	1.10	1 (6%)
6	NAG	M	2	6	14,14,15	1.05	0	17,19,21	1.64	5 (29%)
6	MAN	M	3	6	11,11,12	2.86	5 (45%)	15,15,17	1.96	4 (26%)
6	MAN	M	4	6	11,11,12	1.84	4 (36%)	15,15,17	1.04	1 (6%)
6	MAN	M	5	6	11,11,12	1.90	3 (27%)	15,15,17	1.80	3 (20%)
6	MAN	M	6	6	11,11,12	1.32	3 (27%)	15,15,17	0.82	0
6	GAL	M	7	6	11,11,12	1.14	2 (18%)	15,15,17	0.84	0
6	GAL	M	8	6	11,11,12	0.32	0	15,15,17	0.81	0
6	MAN	M	9	6	11,11,12	1.27	2 (18%)	15,15,17	1.16	2 (13%)
7	NAG	Q	1	1,7	14,14,15	1.05	1 (7%)	17,19,21	1.49	3 (17%)
7	NAG	Q	2	7	14,14,15	1.11	1 (7%)	17,19,21	1.75	5 (29%)
7	MAN	Q	3	7	11,11,12	1.47	1 (9%)	15,15,17	2.34	6 (40%)
7	MAN	Q	4	7	11,11,12	1.26	1 (9%)	15,15,17	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	Q	5	7	11,11,12	1.49	3 (27%)	15,15,17	0.96	1 (6%)
7	MAN	Q	6	7	11,11,12	1.16	1 (9%)	15,15,17	1.15	1 (6%)
7	GAL	Q	7	7	11,11,12	1.09	1 (9%)	15,15,17	1.00	2 (13%)
7	GAL	Q	8	7	11,11,12	0.36	0	15,15,17	0.81	0
7	MAN	Q	9	7	11,11,12	0.87	0	15,15,17	1.32	2 (13%)
8	NAG	U	1	8	14,14,15	1.00	1 (7%)	17,19,21	1.43	3 (17%)
8	MAN	U	10	8	11,11,12	1.09	1 (9%)	15,15,17	1.17	2 (13%)
8	MAN	U	11	8	11,11,12	1.15	2 (18%)	15,15,17	1.28	2 (13%)
8	NAG	U	2	8	14,14,15	0.94	1 (7%)	17,19,21	1.44	2 (11%)
8	MAN	U	3	8	11,11,12	1.36	2 (18%)	15,15,17	0.86	0
8	MAN	U	4	8	11,11,12	1.35	2 (18%)	15,15,17	1.16	2 (13%)
8	MAN	U	5	8	11,11,12	1.24	3 (27%)	15,15,17	1.14	1 (6%)
8	MAN	U	6	8	11,11,12	1.38	3 (27%)	15,15,17	1.33	2 (13%)
8	GAL	U	7	8	11,11,12	1.04	1 (9%)	15,15,17	1.15	2 (13%)
8	GAL	U	8	8	11,11,12	1.09	1 (9%)	15,15,17	0.76	0
8	BMA	U	9	8	11,11,12	1.43	1 (9%)	15,15,17	1.72	4 (26%)
9	NAG	Y	1	9	14,14,15	2.42	3 (21%)	17,19,21	1.66	3 (17%)
9	NAG	Y	2	9	14,14,15	1.69	3 (21%)	17,19,21	1.57	5 (29%)
9	MAN	Y	3	9	11,11,12	1.54	3 (27%)	15,15,17	1.60	2 (13%)
10	NAG	Z	1	1,10	14,14,15	1.27	2 (14%)	17,19,21	1.61	4 (23%)
10	NAG	Z	2	10	14,14,15	1.46	2 (14%)	17,19,21	2.20	5 (29%)
10	MAN	Z	3	10	11,11,12	1.81	3 (27%)	15,15,17	1.58	1 (6%)
10	MAN	Z	4	10	11,11,12	1.05	1 (9%)	15,15,17	1.17	1 (6%)
10	MAN	Z	5	10	11,11,12	0.99	0	15,15,17	0.69	0
11	NAG	b	1	11,1	14,14,15	1.49	3 (21%)	17,19,21	1.72	4 (23%)
11	NAG	b	2	11	14,14,15	2.03	1 (7%)	17,19,21	2.15	6 (35%)
11	MAN	b	3	11	11,11,12	1.61	2 (18%)	15,15,17	2.38	8 (53%)
11	MAN	b	4	11	11,11,12	1.06	1 (9%)	15,15,17	0.96	0
11	MAN	b	5	11	11,11,12	1.00	0	15,15,17	1.12	1 (6%)
11	MAN	b	6	11	11,11,12	1.53	2 (18%)	15,15,17	1.12	1 (6%)
11	MAN	b	7	11	11,11,12	2.15	3 (27%)	15,15,17	1.52	1 (6%)
11	BMA	b	8	11	11,11,12	2.28	3 (27%)	15,15,17	1.57	2 (13%)
12	NAG	d	1	1,12	14,14,15	1.25	2 (14%)	17,19,21	1.41	2 (11%)
12	NDG	d	2	12	14,14,15	1.58	4 (28%)	17,19,21	1.36	4 (23%)
12	MAN	d	3	12	11,11,12	1.06	1 (9%)	15,15,17	1.83	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	d	4	12	11,11,12	1.01	1 (9%)	15,15,17	1.30	2 (13%)
12	NAG	d	5	12	14,14,15	1.71	3 (21%)	17,19,21	1.37	2 (11%)
12	MAN	d	6	12	11,11,12	1.02	0	15,15,17	1.40	1 (6%)
12	MAN	d	7	12	11,11,12	1.05	1 (9%)	15,15,17	1.28	1 (6%)
12	MAN	d	8	12	11,11,12	0.65	0	15,15,17	1.32	1 (6%)
12	FUC	d	9	12	10,10,11	0.57	0	14,14,16	0.64	0
13	NAG	f	1	1,13	14,14,15	1.23	1 (7%)	17,19,21	1.94	5 (29%)
13	FUC	f	10	13	10,10,11	1.23	2 (20%)	14,14,16	0.29	0
13	NDG	f	2	13	14,14,15	1.02	1 (7%)	17,19,21	1.89	6 (35%)
13	MAN	f	3	13	11,11,12	1.34	1 (9%)	15,15,17	1.09	2 (13%)
13	MAN	f	4	13	11,11,12	1.85	3 (27%)	15,15,17	1.44	4 (26%)
13	NAG	f	5	13	14,14,15	1.48	2 (14%)	17,19,21	2.22	6 (35%)
13	MAN	f	6	13	11,11,12	1.14	1 (9%)	15,15,17	0.90	0
13	MAN	f	7	13	11,11,12	1.41	1 (9%)	15,15,17	1.51	3 (20%)
13	BMA	f	8	13	11,11,12	1.24	2 (18%)	15,15,17	1.15	1 (6%)
13	MAN	f	9	13	11,11,12	1.66	3 (27%)	15,15,17	2.17	7 (46%)
14	NAG	i	1	1,14	14,14,15	2.03	2 (14%)	17,19,21	2.01	4 (23%)
14	NAG	i	2	14	14,14,15	1.37	2 (14%)	17,19,21	1.97	5 (29%)
14	MAN	i	3	14	11,11,12	1.40	1 (9%)	15,15,17	0.86	0
15	NAG	j	1	15	14,14,15	1.36	2 (14%)	17,19,21	1.57	5 (29%)
15	NAG	j	2	15	14,14,15	0.99	0	17,19,21	1.78	4 (23%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	BMA	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
4	NDG	F	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	MAN	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	2/2/19/22	0/1/1/1
5	MAN	J	6	5	-	0/2/19/22	0/1/1/1
5	MAN	J	7	5	-	2/2/19/22	0/1/1/1
5	MAN	J	8	5	-	0/2/19/22	0/1/1/1
5	MAN	J	9	5	-	0/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	4/6/23/26	0/1/1/1
6	MAN	M	10	6	-	0/2/19/22	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	MAN	M	3	6	-	0/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	1/2/19/22	0/1/1/1
6	MAN	M	6	6	-	0/2/19/22	0/1/1/1
6	GAL	M	7	6	-	2/2/19/22	0/1/1/1
6	GAL	M	8	6	-	2/2/19/22	0/1/1/1
6	MAN	M	9	6	-	2/2/19/22	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	MAN	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GAL	Q	7	7	-	2/2/19/22	0/1/1/1
7	GAL	Q	8	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	9	7	-	2/2/19/22	0/1/1/1
8	NAG	U	1	8	-	4/6/23/26	0/1/1/1
8	MAN	U	10	8	-	0/2/19/22	0/1/1/1
8	MAN	U	11	8	-	2/2/19/22	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1
8	MAN	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	0/2/19/22	0/1/1/1
8	MAN	U	5	8	-	2/2/19/22	0/1/1/1
8	MAN	U	6	8	-	0/2/19/22	0/1/1/1
8	GAL	U	7	8	-	2/2/19/22	0/1/1/1
8	GAL	U	8	8	-	2/2/19/22	0/1/1/1
8	BMA	U	9	8	-	0/2/19/22	0/1/1/1
9	NAG	Y	1	9	-	4/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	MAN	Y	3	9	-	0/2/19/22	0/1/1/1
10	NAG	Z	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	MAN	Z	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
11	NAG	b	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	b	2	11	-	1/6/23/26	0/1/1/1
11	MAN	b	3	11	-	0/2/19/22	0/1/1/1
11	MAN	b	4	11	-	2/2/19/22	0/1/1/1
11	MAN	b	5	11	-	2/2/19/22	0/1/1/1
11	MAN	b	6	11	-	0/2/19/22	0/1/1/1
11	MAN	b	7	11	-	2/2/19/22	0/1/1/1
11	BMA	b	8	11	-	2/2/19/22	0/1/1/1
12	NAG	d	1	1,12	-	4/6/23/26	0/1/1/1
12	NDG	d	2	12	-	1/6/23/26	0/1/1/1
12	MAN	d	3	12	-	0/2/19/22	0/1/1/1
12	MAN	d	4	12	-	2/2/19/22	0/1/1/1
12	NAG	d	5	12	-	4/6/23/26	0/1/1/1
12	MAN	d	6	12	-	2/2/19/22	0/1/1/1
12	MAN	d	7	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	d	8	12	-	2/2/19/22	0/1/1/1
12	FUC	d	9	12	-	-	0/1/1/1
13	NAG	f	1	1,13	-	2/6/23/26	0/1/1/1
13	FUC	f	10	13	-	-	0/1/1/1
13	NDG	f	2	13	-	3/6/23/26	0/1/1/1
13	MAN	f	3	13	-	0/2/19/22	0/1/1/1
13	MAN	f	4	13	-	0/2/19/22	0/1/1/1
13	NAG	f	5	13	-	2/6/23/26	0/1/1/1
13	MAN	f	6	13	-	0/2/19/22	0/1/1/1
13	MAN	f	7	13	-	0/2/19/22	0/1/1/1
13	BMA	f	8	13	-	0/2/19/22	0/1/1/1
13	MAN	f	9	13	-	0/2/19/22	0/1/1/1
14	NAG	i	1	1,14	-	2/6/23/26	0/1/1/1
14	NAG	i	2	14	-	2/6/23/26	0/1/1/1
14	MAN	i	3	14	-	0/2/19/22	0/1/1/1
15	NAG	j	1	15	-	0/6/23/26	0/1/1/1
15	NAG	j	2	15	-	6/6/23/26	0/1/1/1

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1	NAG	C1-C2	-7.81	1.41	1.52
11	b	2	NAG	O5-C1	6.46	1.54	1.43
14	i	1	NAG	C1-C2	-6.25	1.43	1.52
9	Y	1	NAG	O3-C3	-6.23	1.27	1.43
6	M	3	MAN	O3-C3	-5.57	1.29	1.43

The worst 5 of 234 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	2	NAG	O5-C1-C2	6.67	121.60	111.29
6	M	1	NAG	C1-O5-C5	-6.51	103.47	112.19
14	i	1	NAG	O5-C1-C2	5.96	120.51	111.29
7	Q	3	MAN	O5-C1-C2	5.65	124.28	110.79
12	d	3	MAN	O5-C1-C2	5.54	124.01	110.79

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
11	b	1	NAG	O7-C7-N2-C2
15	j	2	NAG	C1-C2-N2-C7
12	d	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2

There are no ring outliers.

88 monomers are involved in 174 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Y	1	NAG	4	0
8	U	9	BMA	4	0
2	B	5	BMA	2	0
6	M	1	NAG	3	0
8	U	8	GAL	3	0
2	B	7	MAN	1	0
12	d	9	FUC	1	0
4	F	3	MAN	3	0
7	Q	1	NAG	2	0
12	d	4	MAN	4	0
13	f	4	MAN	1	0
14	i	2	NAG	7	0
5	J	8	MAN	5	0
11	b	2	NAG	2	0
6	M	7	GAL	1	0
13	f	7	MAN	4	0
3	D	4	MAN	3	0
5	J	3	BMA	4	0
7	Q	9	MAN	1	0
13	f	6	MAN	4	0
12	d	1	NAG	6	0
9	Y	3	MAN	1	0
4	F	1	NDG	2	0
12	d	6	MAN	3	0
4	F	2	NAG	4	0
5	J	2	NAG	3	0
5	J	4	MAN	1	0
14	i	1	NAG	6	0
4	F	5	MAN	1	0
7	Q	4	MAN	2	0
6	M	3	MAN	1	0
11	b	8	BMA	2	0
7	Q	8	GAL	1	0

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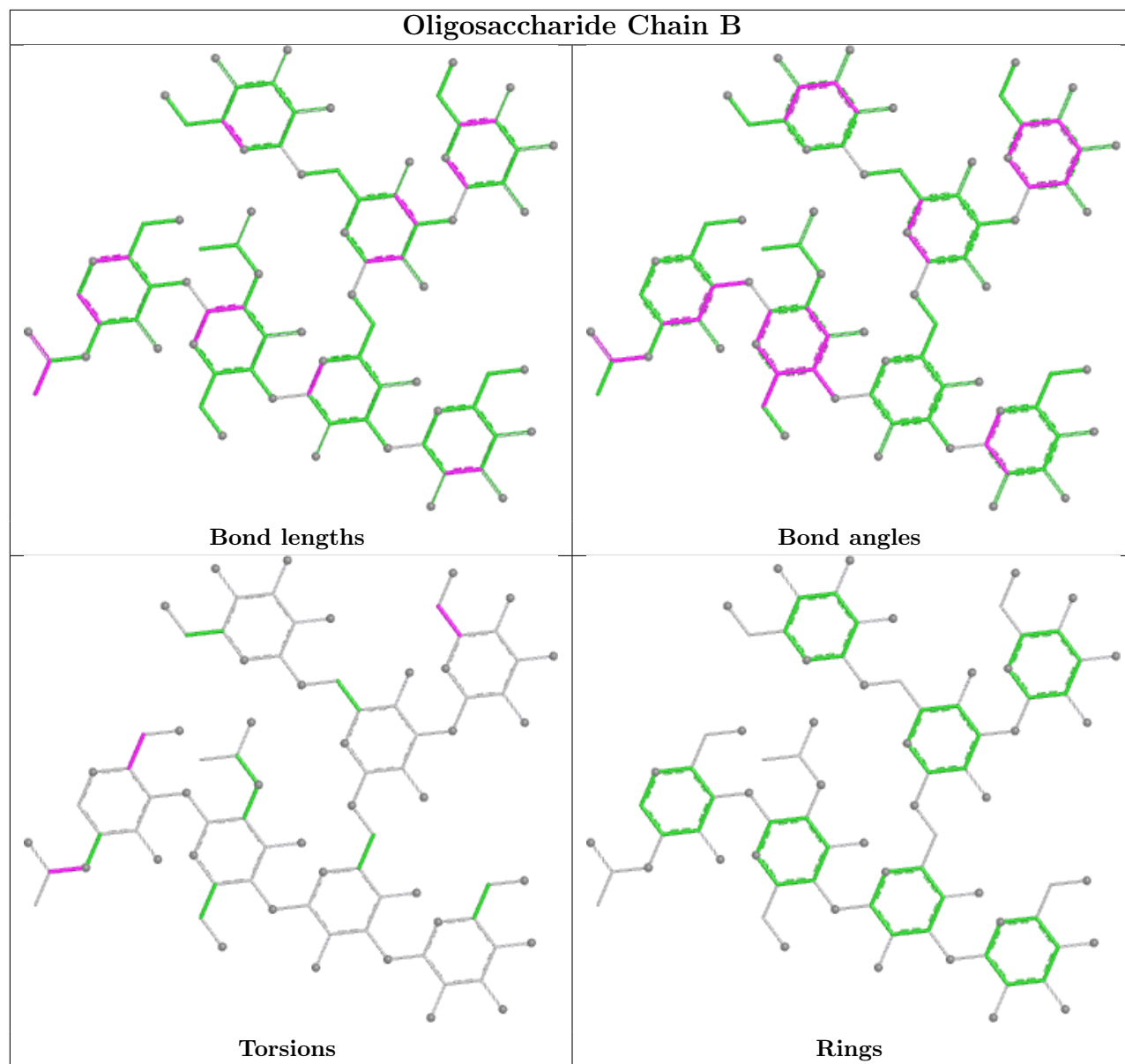
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	d	5	NAG	3	0
11	b	3	MAN	4	0
7	Q	7	GAL	4	0
4	F	4	MAN	3	0
2	B	1	NAG	6	0
11	b	6	MAN	6	0
3	D	2	NAG	1	0
8	U	10	MAN	2	0
10	Z	3	MAN	4	0
13	f	8	BMA	1	0
4	F	7	MAN	4	0
13	f	3	MAN	1	0
15	j	1	NAG	3	0
10	Z	1	NAG	5	0
5	J	1	NAG	8	0
12	d	7	MAN	3	0
8	U	2	NAG	1	0
11	b	1	NAG	9	0
9	Y	2	NAG	2	0
7	Q	5	MAN	3	0
12	d	3	MAN	3	0
3	D	3	MAN	9	0
13	f	9	MAN	3	0
7	Q	3	MAN	6	0
11	b	5	MAN	2	0
13	f	10	FUC	2	0
8	U	7	GAL	3	0
12	d	2	NDG	3	0
2	B	3	MAN	9	0
13	f	5	NAG	4	0
8	U	4	MAN	5	0
4	F	8	MAN	2	0
2	B	6	MAN	4	0
8	U	3	MAN	4	0
7	Q	6	MAN	5	0
14	i	3	MAN	2	0
10	Z	4	MAN	3	0
6	M	8	GAL	1	0
8	U	1	NAG	3	0
2	B	2	NAG	6	0
2	B	4	MAN	9	0
3	D	1	NAG	2	0

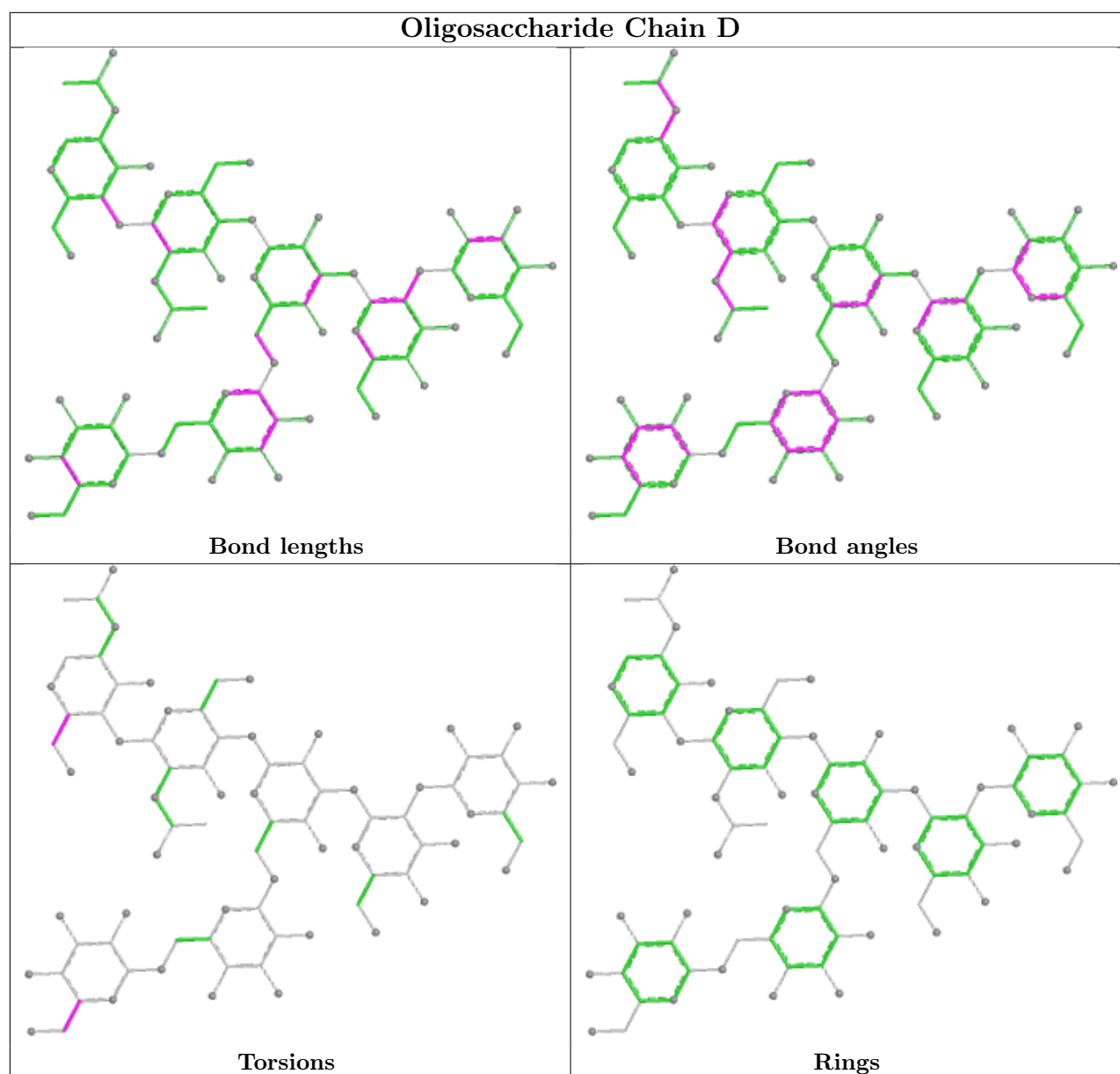
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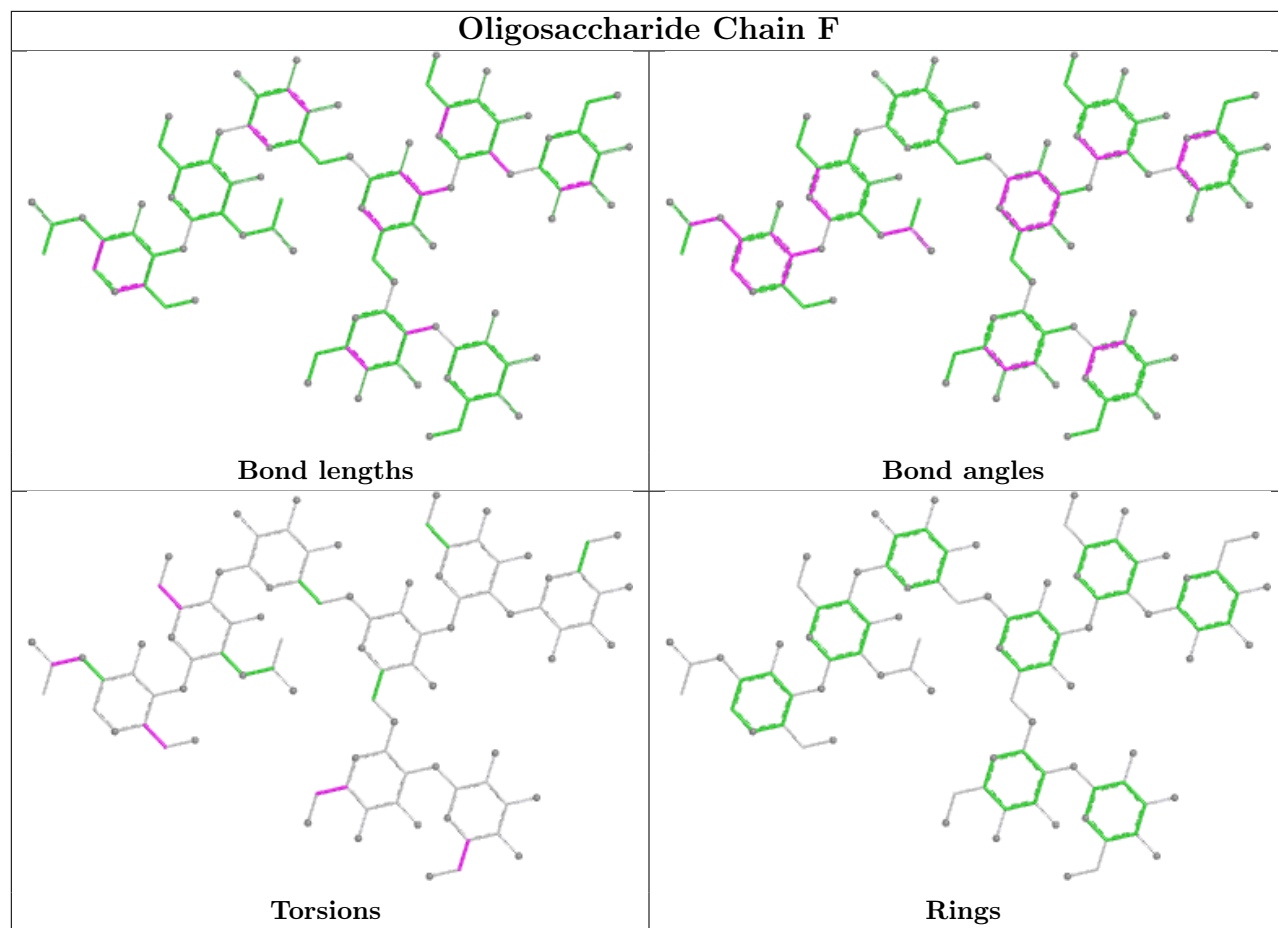
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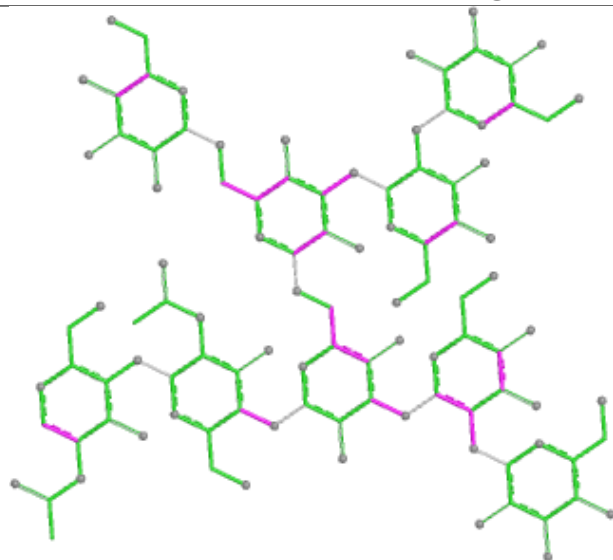
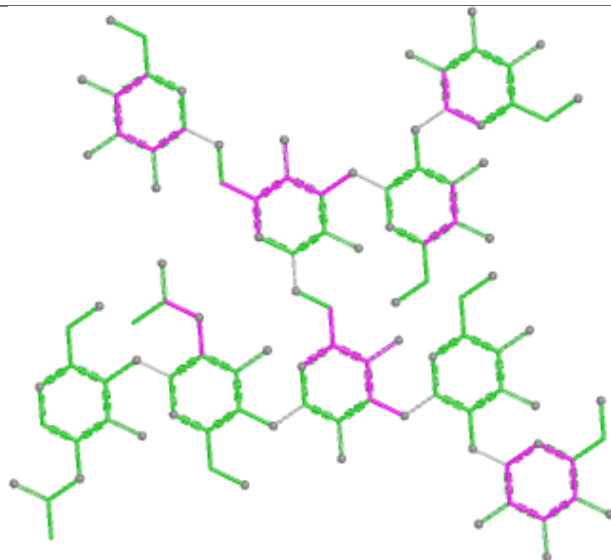
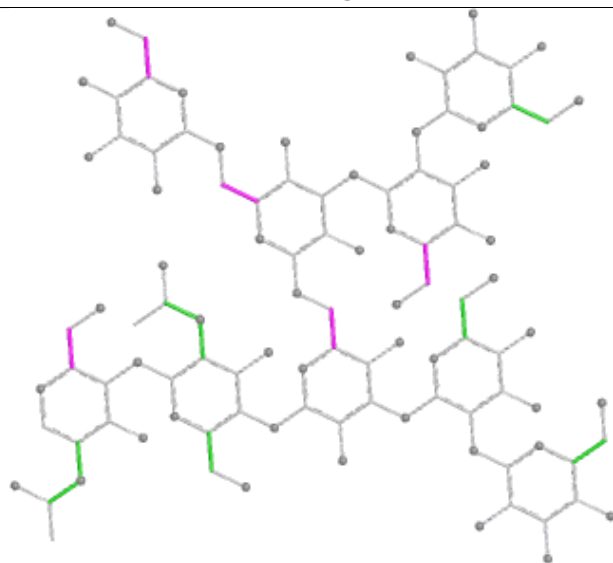
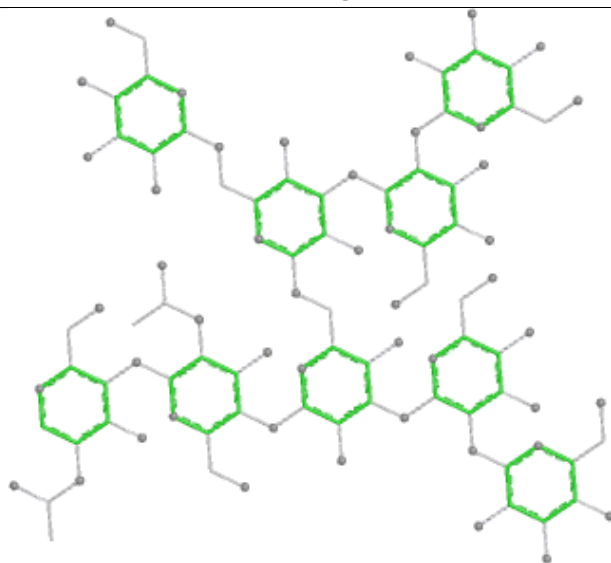
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	5	MAN	8	0
11	b	7	MAN	2	0
5	J	6	MAN	3	0
3	D	6	BMA	5	0
6	M	2	NAG	2	0
6	M	4	MAN	1	0
5	J	5	MAN	3	0
11	b	4	MAN	4	0
10	Z	2	NAG	4	0
4	F	6	MAN	1	0
13	f	1	NAG	5	0
7	Q	2	NAG	6	0
8	U	6	MAN	4	0

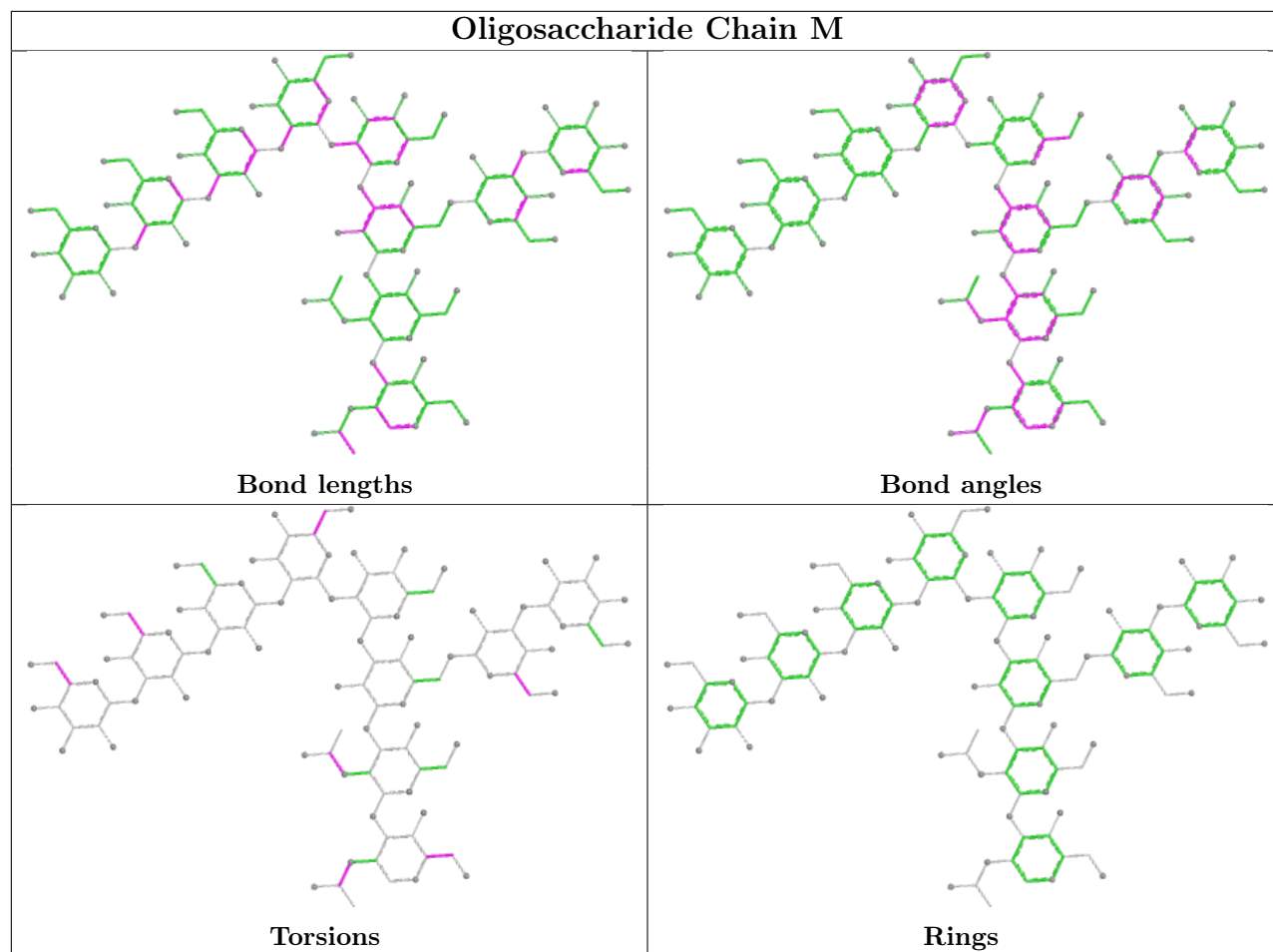
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



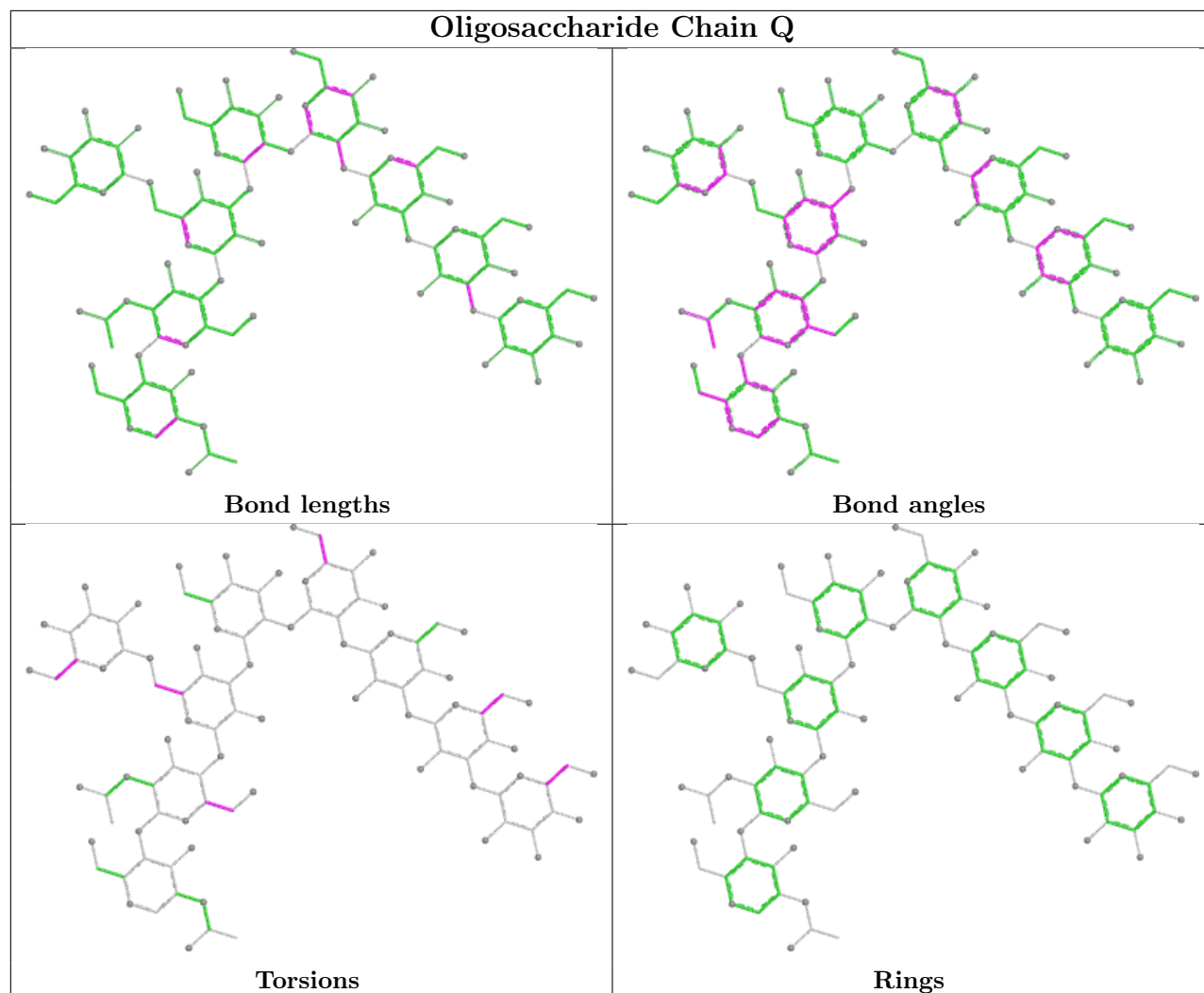


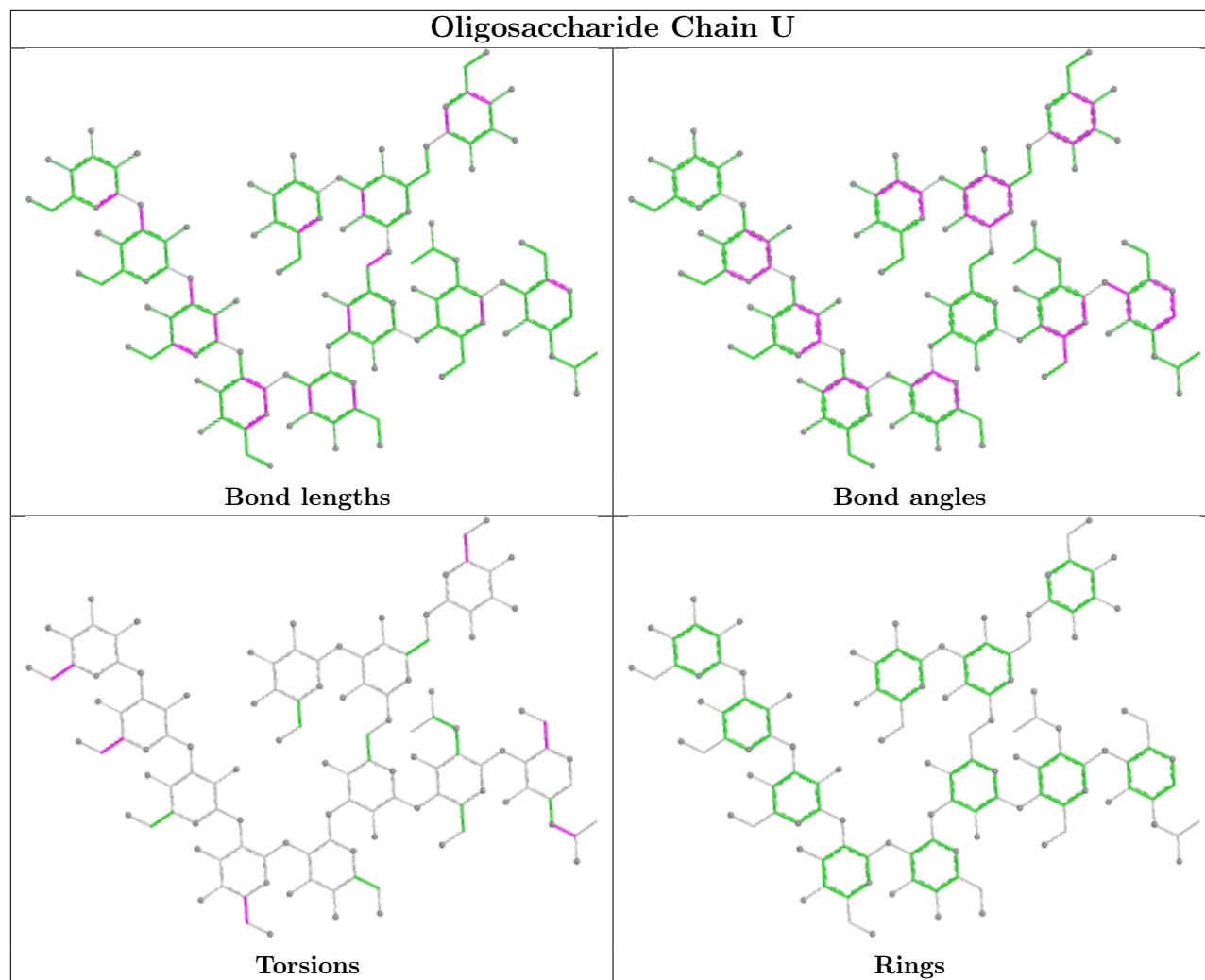


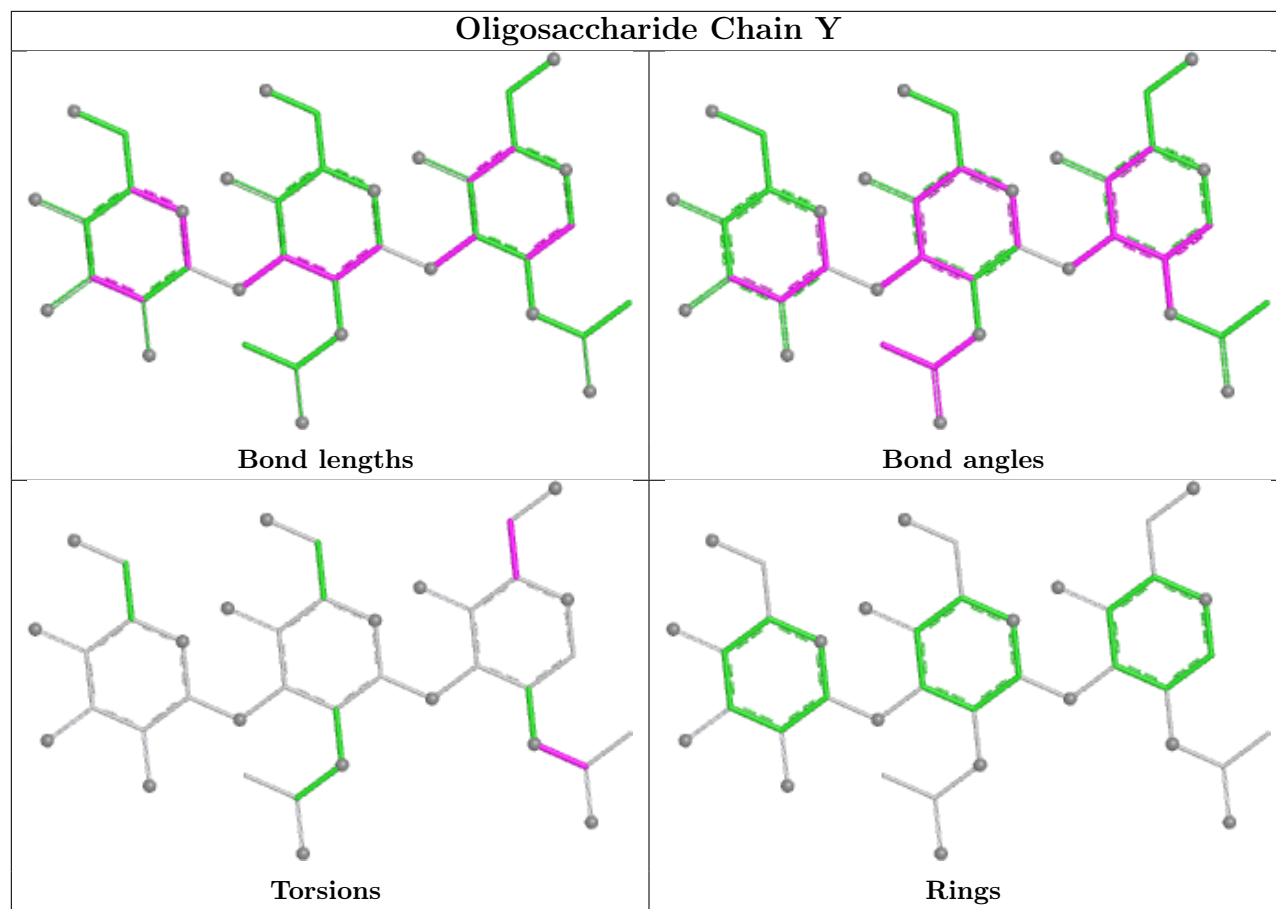
Oligosaccharide Chain J**Bond lengths****Bond angles****Torsions****Rings**

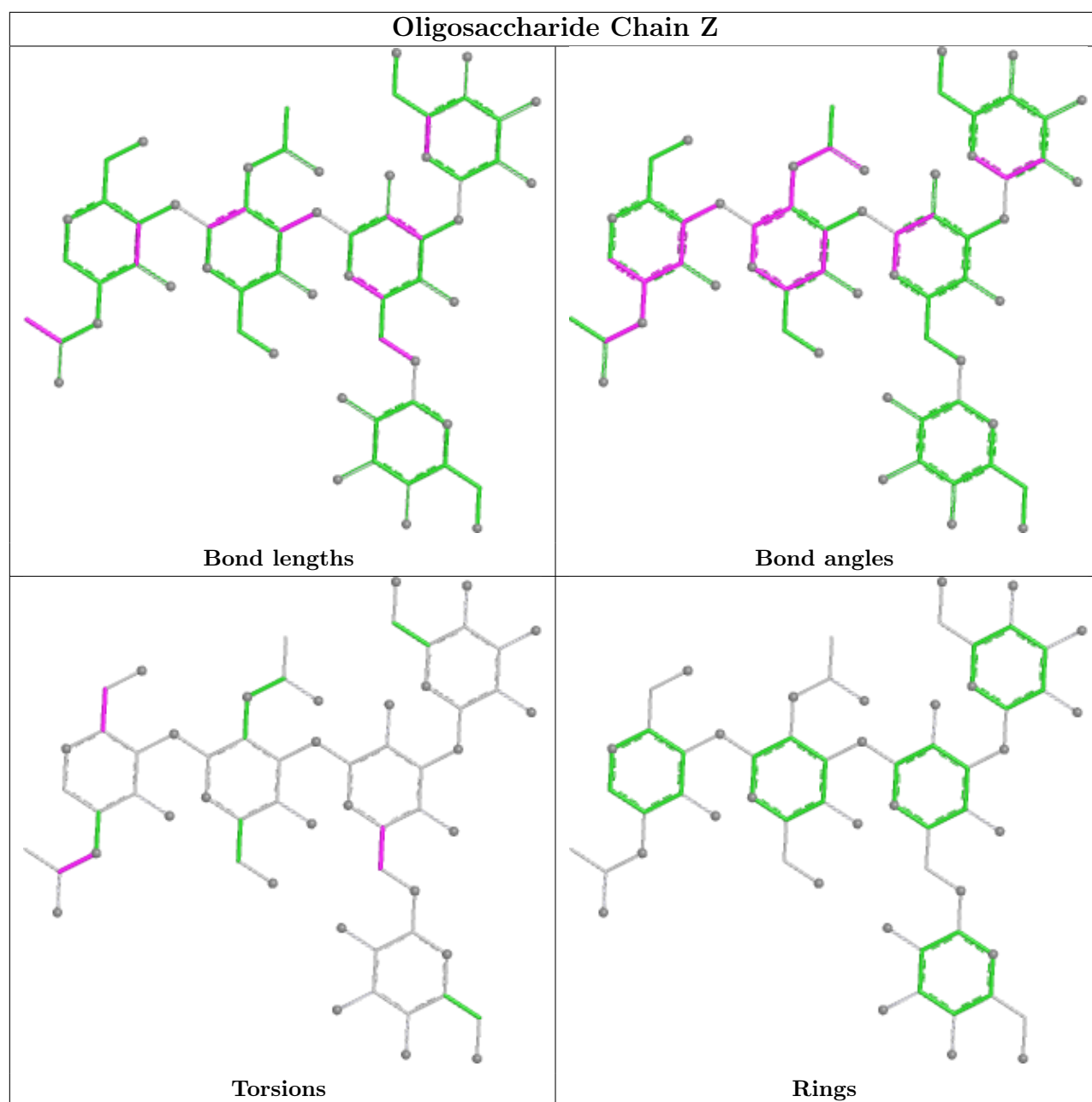


Oligosaccharide Chain Q

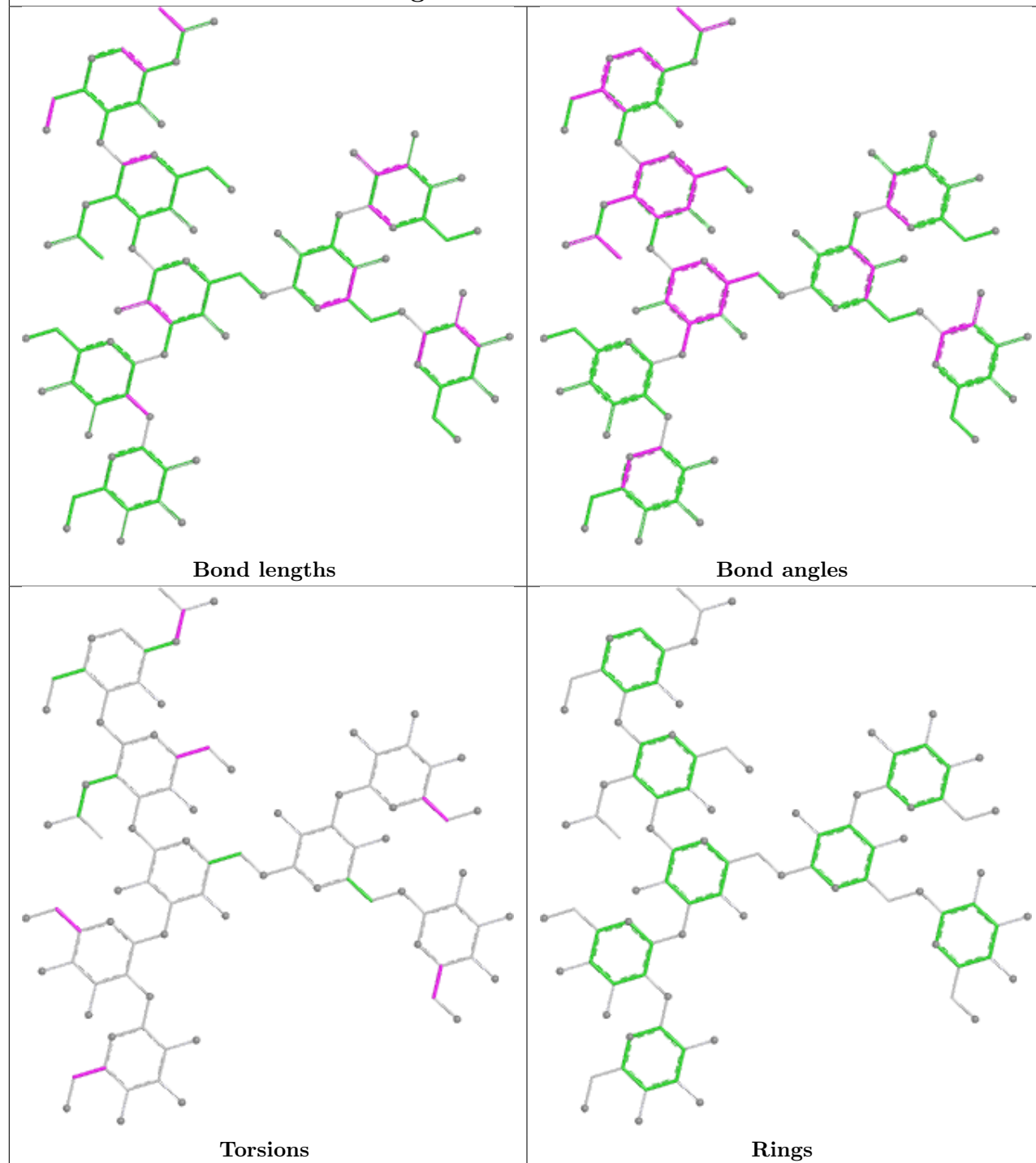


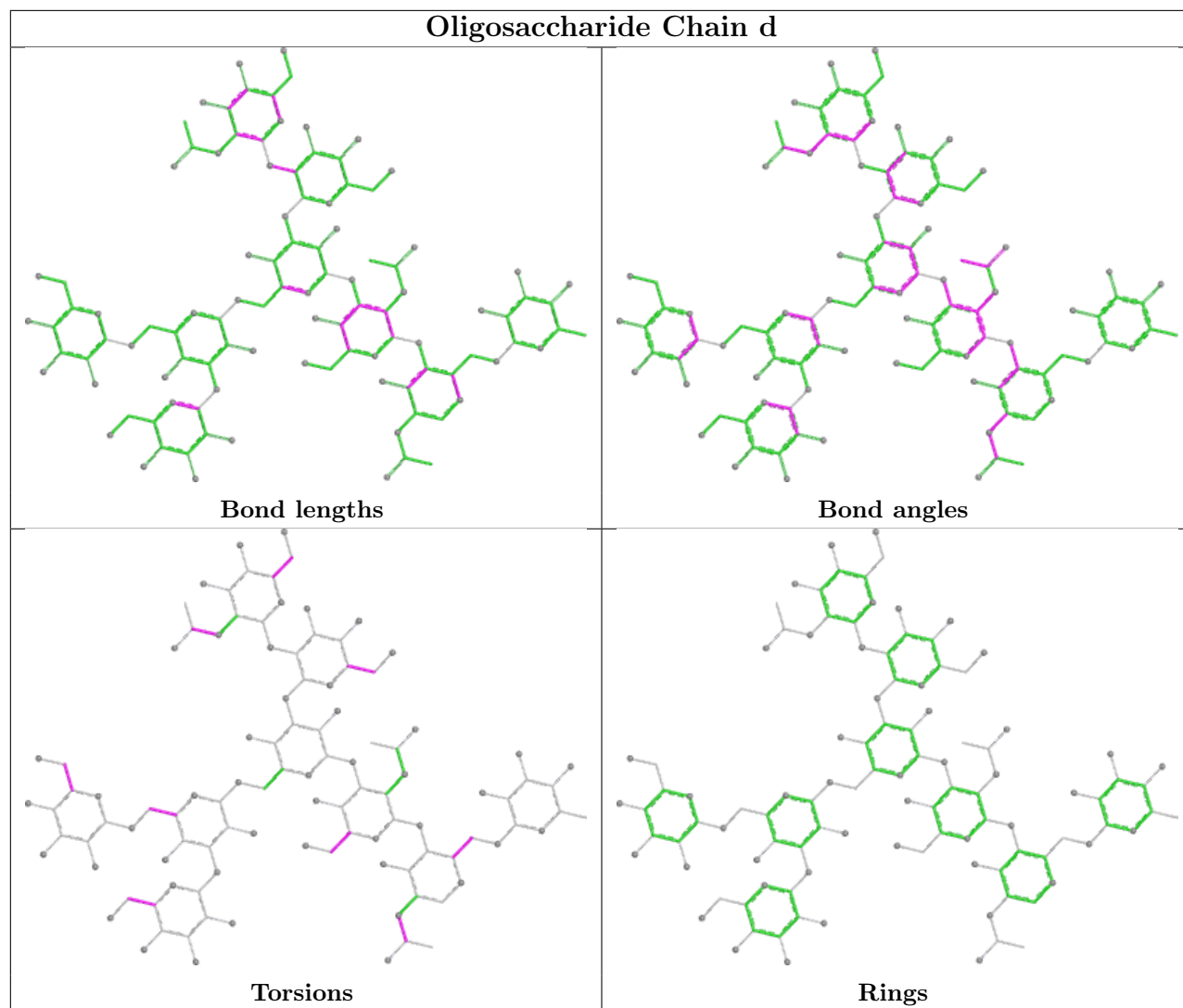


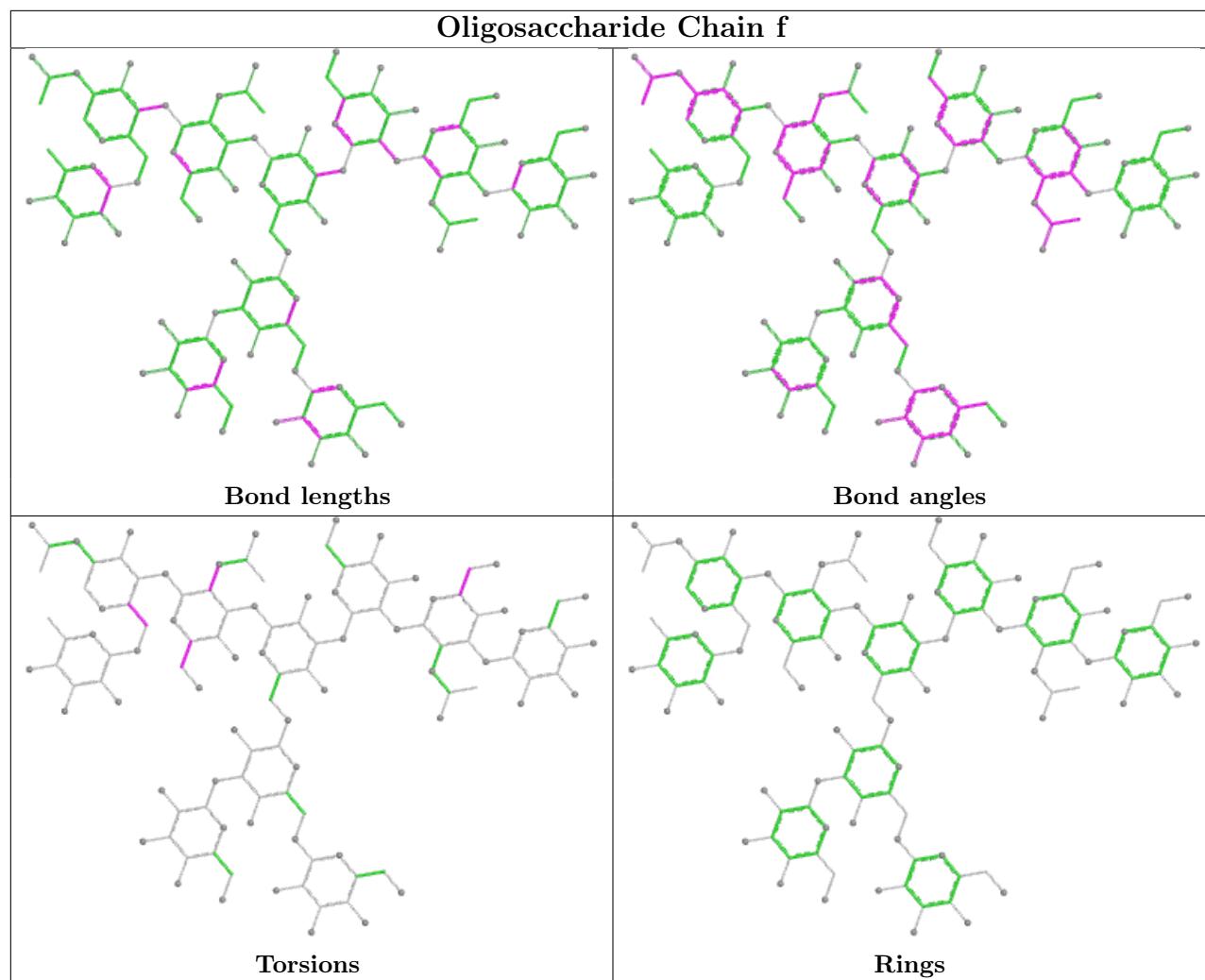


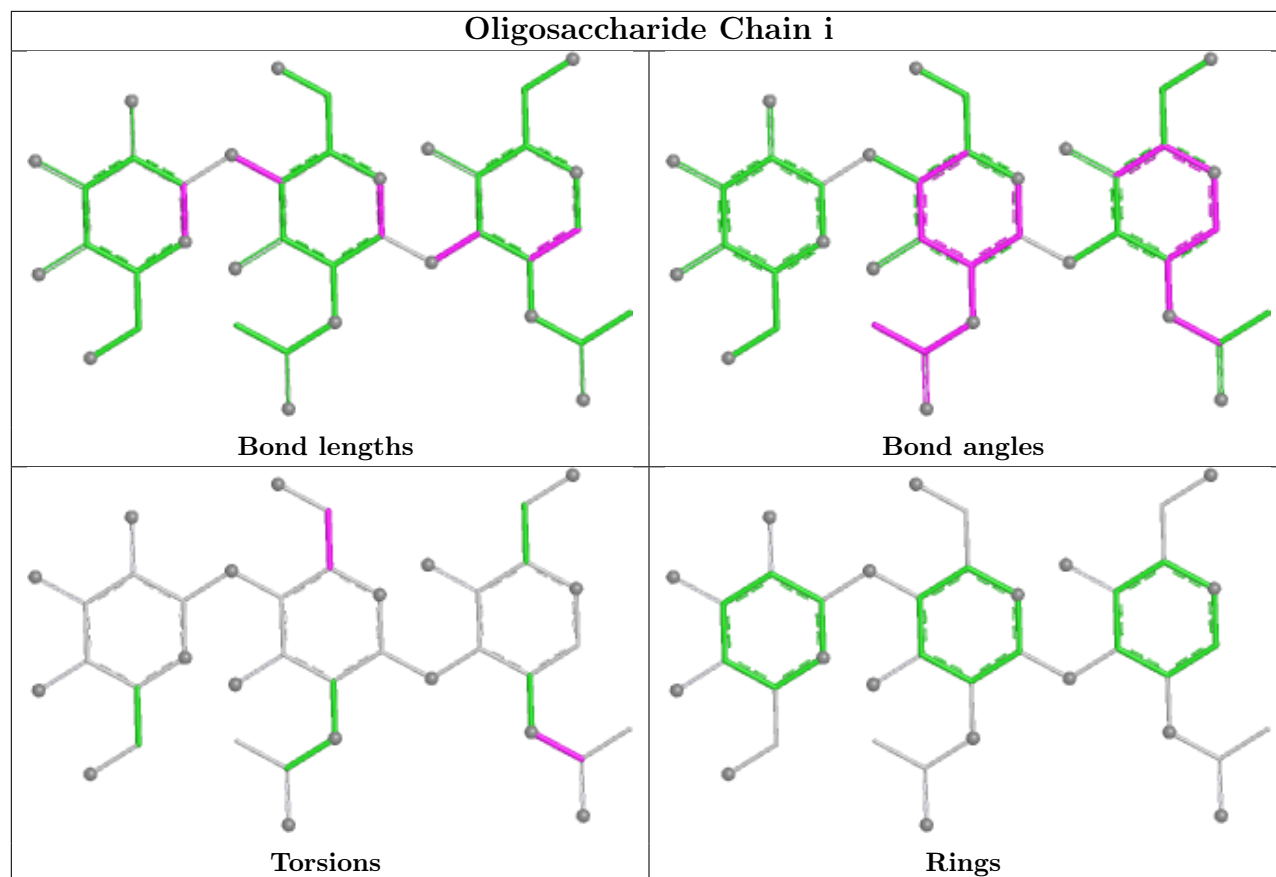


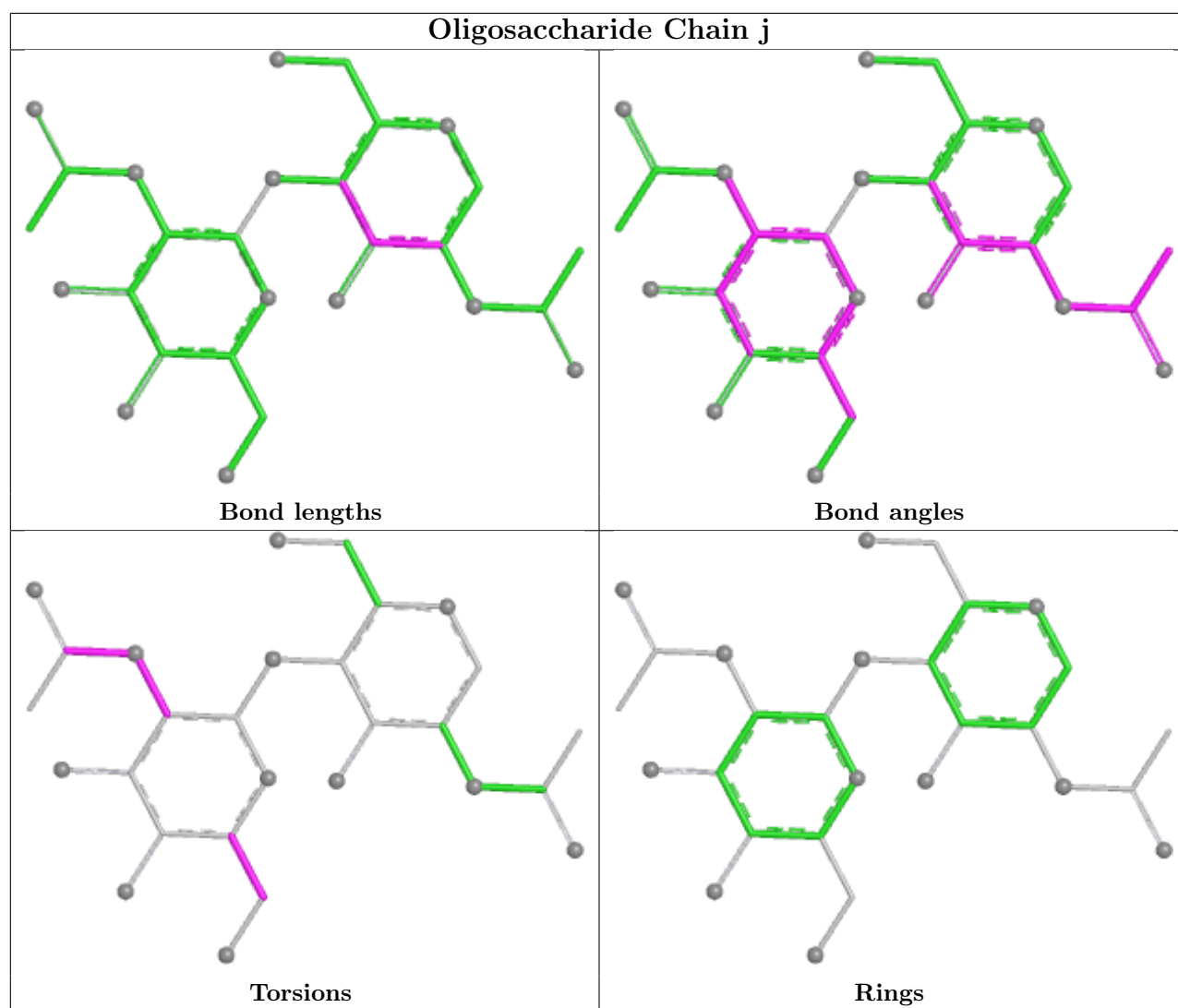
Oligosaccharide Chain b











5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	440/470 (93%)	0.18	15 (3%) 48 27	22, 46, 85, 97	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	ASN	4.8
1	A	292	ALA	3.4
1	A	258	THR	3.3
1	A	431	SER	3.0
1	A	433	THR	2.9

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
2	MAN	B	4	11/12	-0.29	0.17	129,129,129,129	0
2	BMA	B	5	11/12	-0.27	0.18	129,129,129,129	0
4	NAG	F	2	14/15	-0.22	0.20	129,129,129,129	0
6	MAN	M	3	11/12	-0.14	0.15	129,129,129,129	0
3	NAG	D	2	14/15	-0.05	0.16	129,129,129,129	0
3	MAN	D	3	11/12	-0.00	0.19	129,129,129,129	0
6	MAN	M	9	11/12	0.04	0.13	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	1	14/15	-	-	129,129,129,129	0
2	MAN	B	6	11/12	0.06	0.15	129,129,129,129	0
3	MAN	D	5	11/12	0.09	0.12	129,129,129,129	0
3	MAN	D	7	11/12	0.10	0.12	129,129,129,129	0
5	MAN	J	5	11/12	0.12	0.16	129,129,129,129	0
3	BMA	D	6	11/12	-	-	129,129,129,129	0
4	MAN	F	6	11/12	0.20	0.15	129,129,129,129	0
4	NDG	F	1	14/15	-	-	129,129,129,129	0
4	MAN	F	4	11/12	0.20	0.15	129,129,129,129	0
6	MAN	M	4	11/12	0.26	0.14	129,129,129,129	0
4	MAN	F	5	11/12	0.26	0.12	129,129,129,129	0
3	MAN	D	4	11/12	0.30	0.12	129,129,129,129	0
4	MAN	F	3	11/12	0.31	0.11	129,129,129,129	0
4	MAN	F	7	11/12	-	-	129,129,129,129	0
4	MAN	F	8	11/12	-	-	129,129,129,129	0
2	MAN	B	3	11/12	0.39	0.11	129,129,129,129	0
5	NAG	J	1	14/15	0.42	0.23	129,129,129,129	0
5	BMA	J	3	11/12	-	-	129,129,129,129	0
5	NAG	J	2	14/15	0.44	0.11	129,129,129,129	0
6	MAN	M	6	11/12	0.49	0.10	129,129,129,129	0
5	MAN	J	6	11/12	-	-	129,129,129,129	0
5	MAN	J	7	11/12	-	-	129,129,129,129	0
5	MAN	J	8	11/12	-	-	129,129,129,129	0
5	MAN	J	9	11/12	-	-	129,129,129,129	0
2	MAN	B	7	11/12	0.62	0.20	129,129,129,129	0
6	NAG	M	2	14/15	-	-	129,129,129,129	0
5	MAN	J	4	11/12	0.64	0.11	129,129,129,129	0
2	NAG	B	1	14/15	0.66	0.23	129,129,129,129	0
6	MAN	M	5	11/12	-	-	129,129,129,129	0
2	NAG	B	2	14/15	0.70	0.15	129,129,129,129	0
6	GAL	M	7	11/12	-	-	129,129,129,129	0
6	GAL	M	8	11/12	-	-	129,129,129,129	0
6	NAG	M	1	14/15	0.75	0.18	129,129,129,129	0
6	MAN	M	10	11/12	-	-	129,129,129,129	0
7	NAG	Q	1	14/15	-	-	129,129,129,129	0
7	NAG	Q	2	14/15	-	-	129,129,129,129	0
7	MAN	Q	3	11/12	-	-	129,129,129,129	0
7	MAN	Q	4	11/12	-	-	129,129,129,129	0
7	MAN	Q	5	11/12	-	-	129,129,129,129	0
7	MAN	Q	6	11/12	-	-	129,129,129,129	0
7	GAL	Q	7	11/12	-	-	129,129,129,129	0
7	GAL	Q	8	11/12	-	-	129,129,129,129	0

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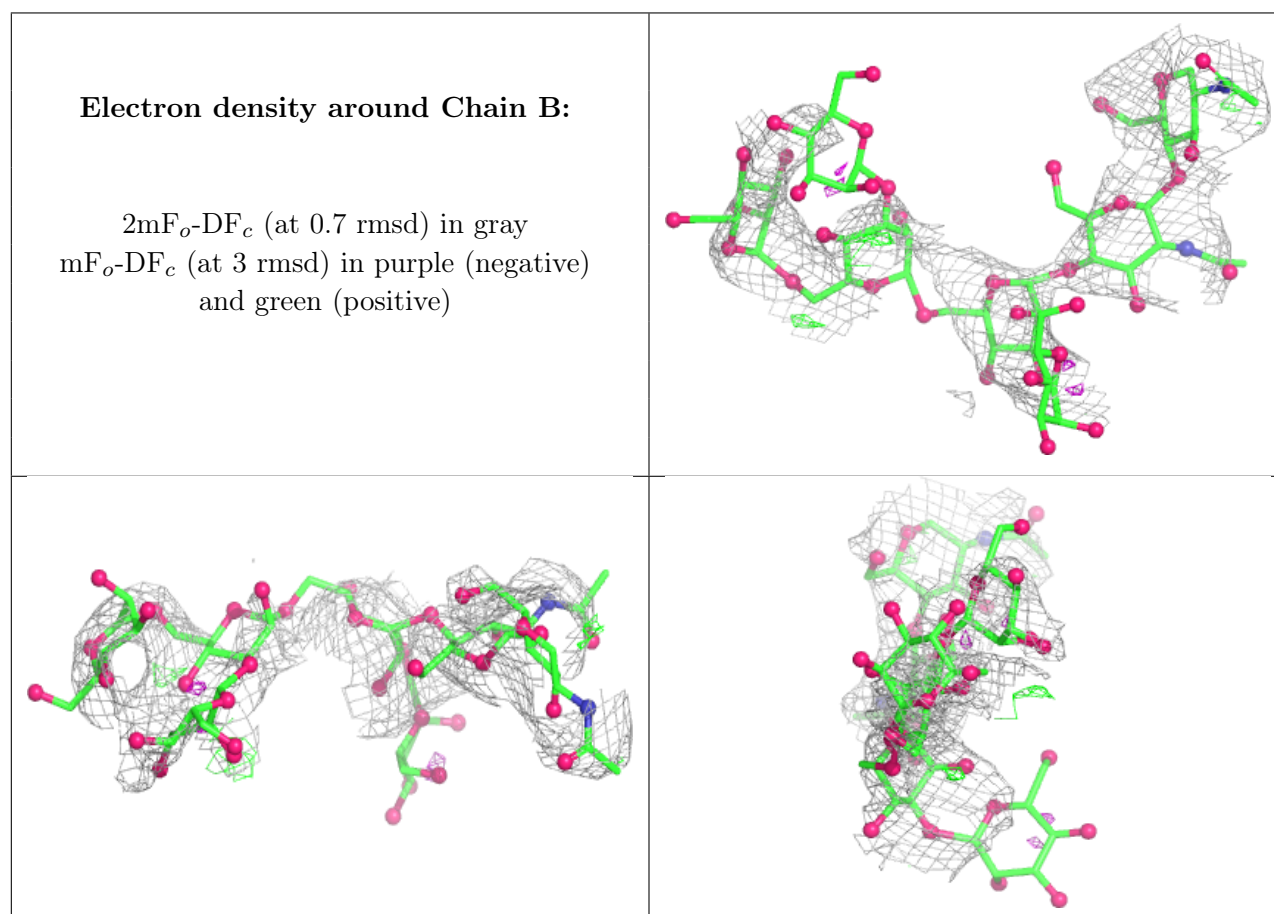
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	Q	9	11/12	-	-	129,129,129,129	0
8	NAG	U	1	14/15	-	-	129,129,129,129	0
8	NAG	U	2	14/15	-	-	129,129,129,129	0
8	MAN	U	3	11/12	-	-	129,129,129,129	0
8	MAN	U	4	11/12	-	-	129,129,129,129	0
8	MAN	U	5	11/12	-	-	129,129,129,129	0
8	MAN	U	6	11/12	-	-	129,129,129,129	0
8	GAL	U	7	11/12	-	-	129,129,129,129	0
8	GAL	U	8	11/12	-	-	129,129,129,129	0
8	BMA	U	9	11/12	-	-	129,129,129,129	0
8	MAN	U	10	11/12	-	-	129,129,129,129	0
8	MAN	U	11	11/12	-	-	129,129,129,129	0
9	NAG	Y	1	14/15	-	-	129,129,129,129	0
9	NAG	Y	2	14/15	-	-	129,129,129,129	0
9	MAN	Y	3	11/12	-	-	129,129,129,129	0
10	NAG	Z	1	14/15	-	-	129,129,129,129	0
10	NAG	Z	2	14/15	-	-	129,129,129,129	0
10	MAN	Z	3	11/12	-	-	129,129,129,129	0
10	MAN	Z	4	11/12	-	-	129,129,129,129	0
10	MAN	Z	5	11/12	-	-	129,129,129,129	0
11	NAG	b	1	14/15	-	-	129,129,129,129	0
11	NAG	b	2	14/15	-	-	129,129,129,129	0
11	MAN	b	3	11/12	-	-	129,129,129,129	0
11	MAN	b	4	11/12	-	-	129,129,129,129	0
11	MAN	b	5	11/12	-	-	129,129,129,129	0
11	MAN	b	6	11/12	-	-	129,129,129,129	0
11	MAN	b	7	11/12	-	-	129,129,129,129	0
11	BMA	b	8	11/12	-	-	129,129,129,129	0
12	NAG	d	1	14/15	-	-	129,129,129,129	0
12	NDG	d	2	14/15	-	-	129,129,129,129	0
12	MAN	d	3	11/12	-	-	129,129,129,129	0
12	MAN	d	4	11/12	-	-	129,129,129,129	0
12	NAG	d	5	14/15	-	-	129,129,129,129	0
12	MAN	d	6	11/12	-	-	129,129,129,129	0
12	MAN	d	7	11/12	-	-	129,129,129,129	0
12	MAN	d	8	11/12	-	-	129,129,129,129	0
12	FUC	d	9	10/11	-	-	129,129,129,129	0
13	NAG	f	1	14/15	-	-	129,129,129,129	0
13	NDG	f	2	14/15	-	-	129,129,129,129	0
13	MAN	f	3	11/12	-	-	129,129,129,129	0
13	MAN	f	4	11/12	-	-	129,129,129,129	0
13	NAG	f	5	14/15	-	-	129,129,129,129	0

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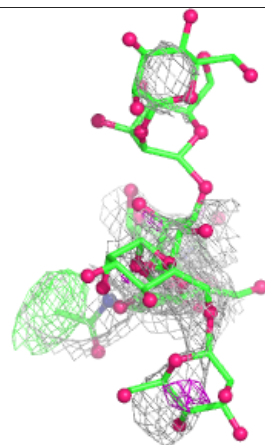
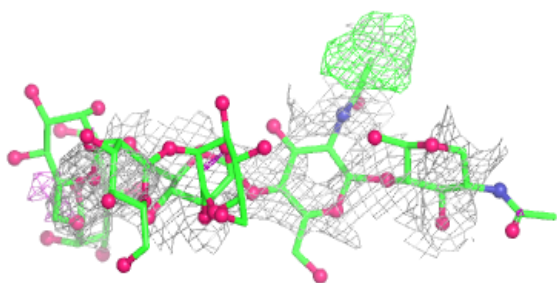
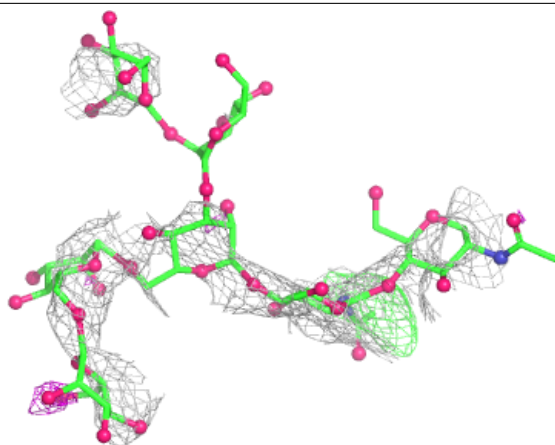
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	MAN	f	6	11/12	-	-	129,129,129,129	0
13	MAN	f	7	11/12	-	-	129,129,129,129	0
13	BMA	f	8	11/12	-	-	129,129,129,129	0
13	MAN	f	9	11/12	-	-	129,129,129,129	0
13	FUC	f	10	10/11	-	-	129,129,129,129	0
14	NAG	i	1	14/15	-	-	129,129,129,129	0
14	NAG	i	2	14/15	-	-	129,129,129,129	0
14	MAN	i	3	11/12	-	-	129,129,129,129	0
15	NAG	j	1	14/15	-	-	129,129,129,129	0
15	NAG	j	2	14/15	-	-	129,129,129,129	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.



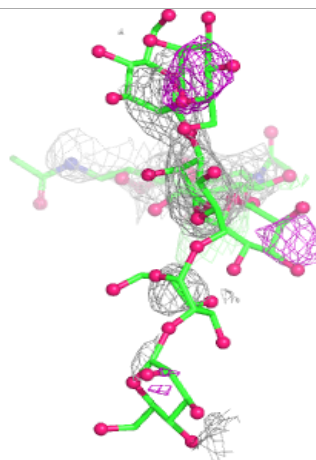
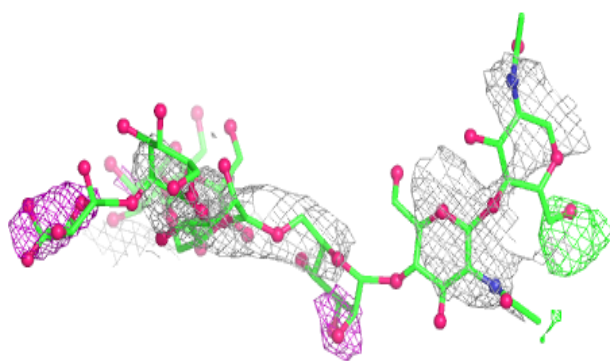
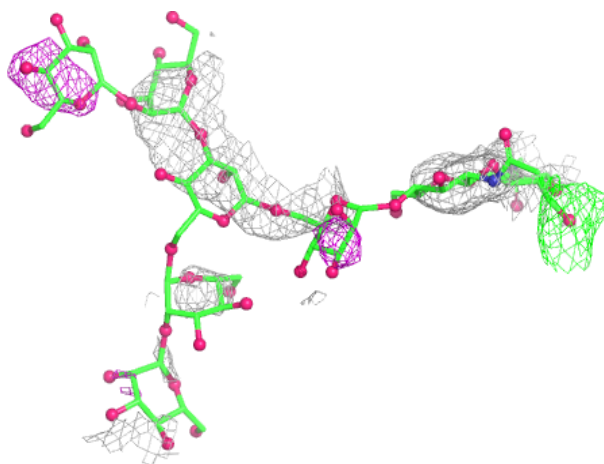
Electron density around Chain D:

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



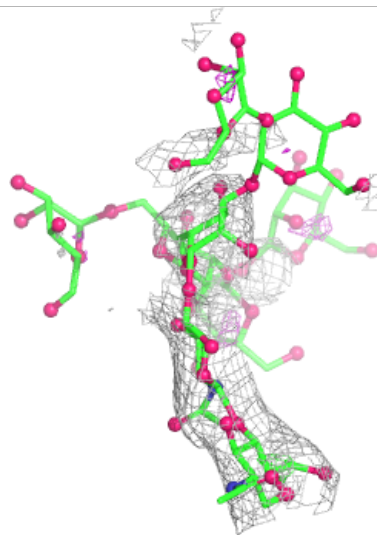
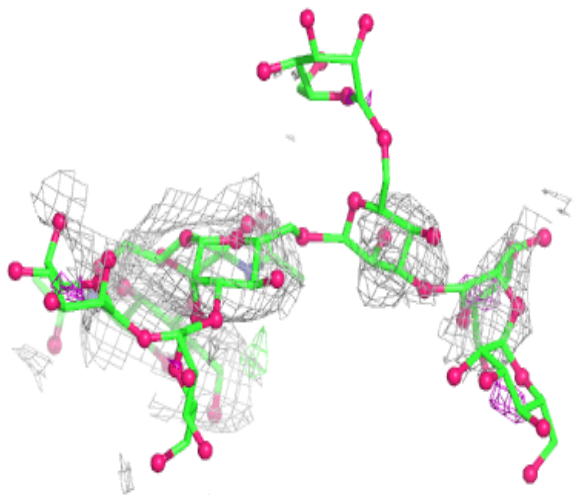
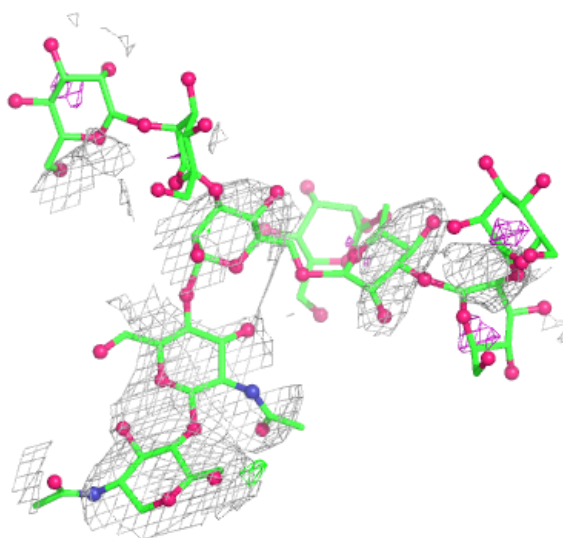
Electron density around Chain F:

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



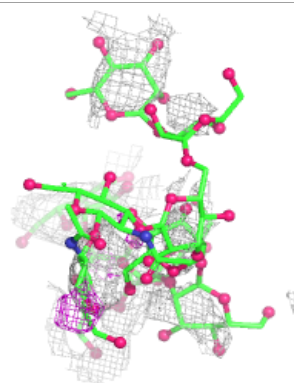
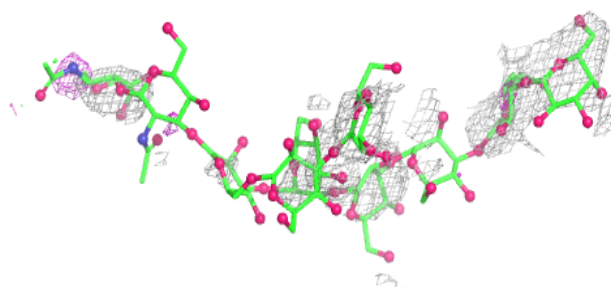
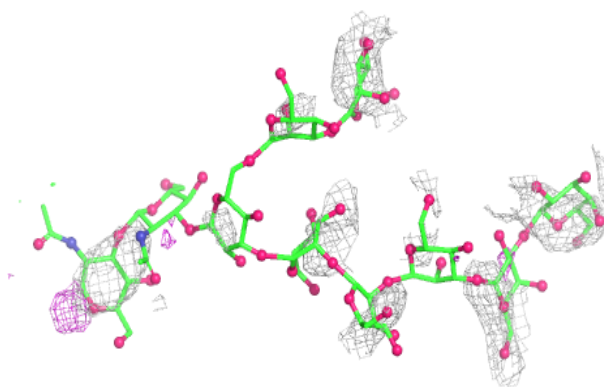
Electron density around Chain J:

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

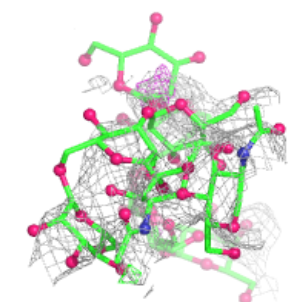
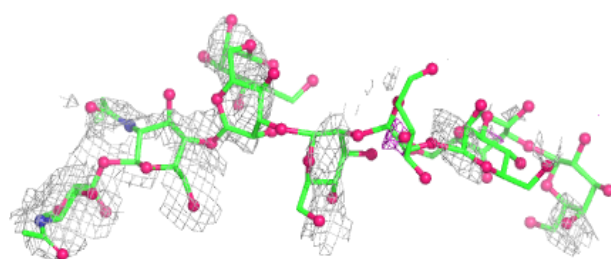
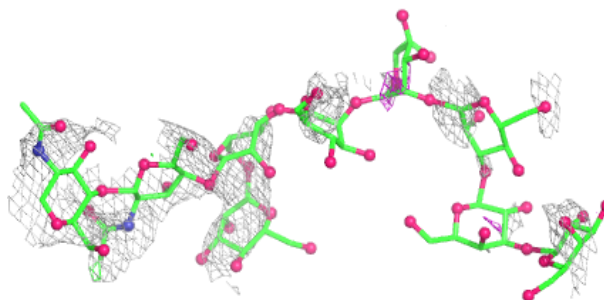


Electron density around Chain M:

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

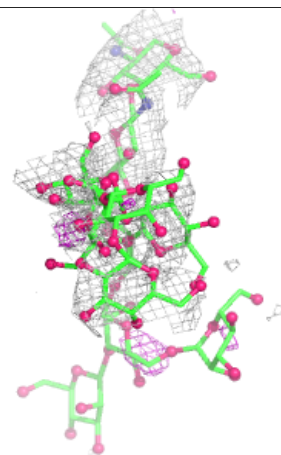
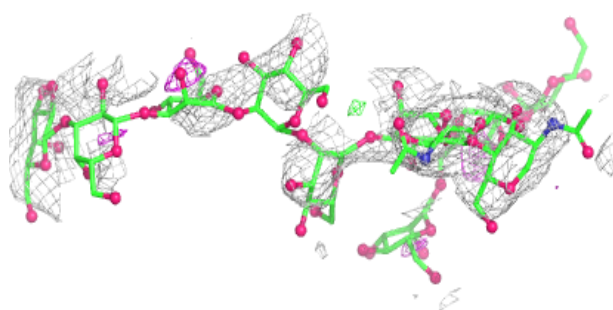
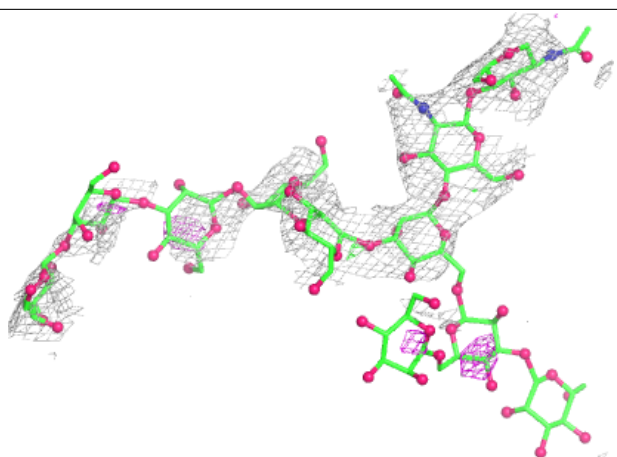
**Electron density around Chain Q:**

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

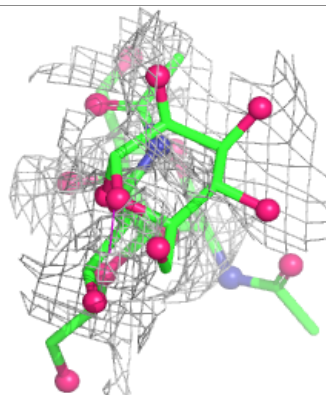
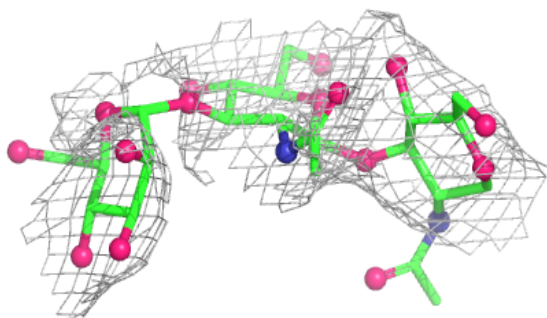
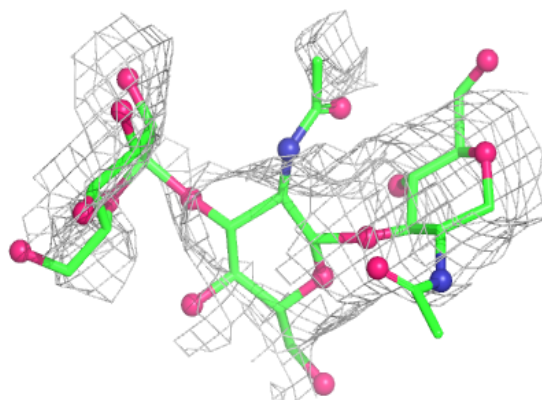


Electron density around Chain U:

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

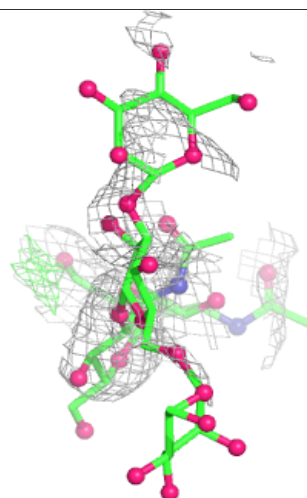
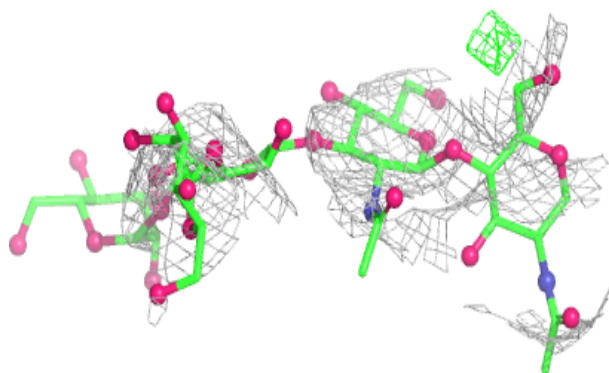
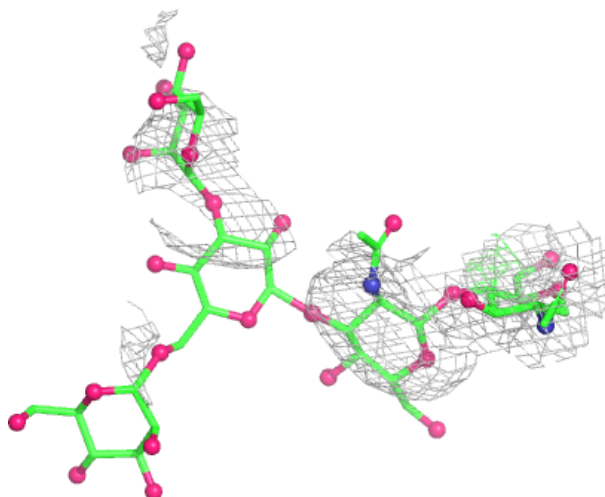
**Electron density around Chain Y:**

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



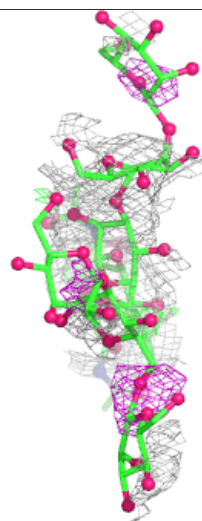
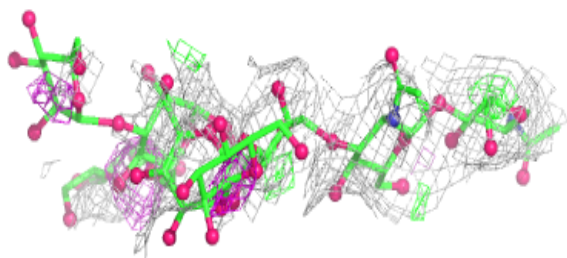
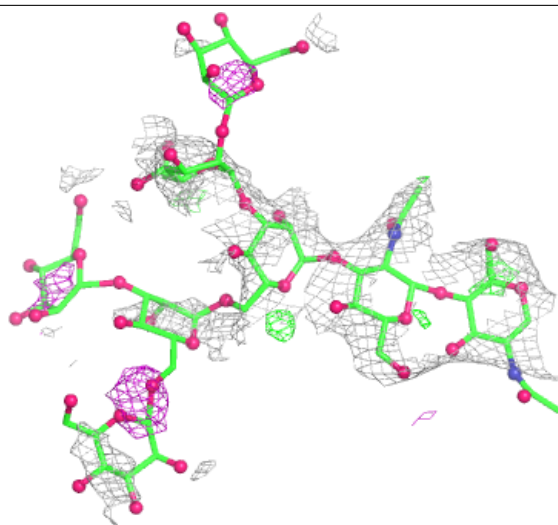
Electron density around Chain Z:

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



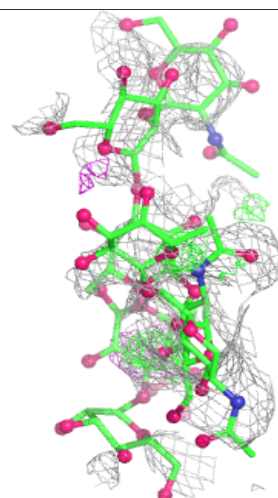
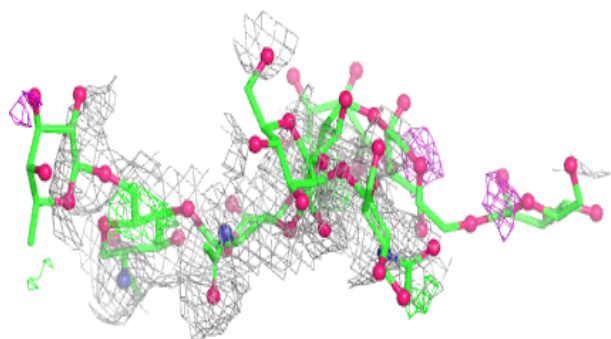
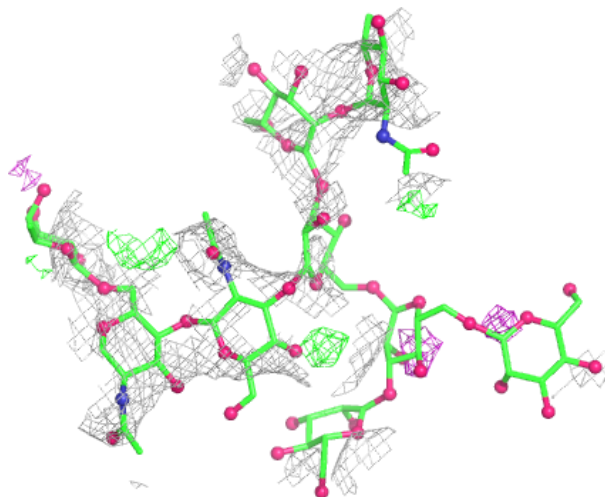
Electron density around Chain b:

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



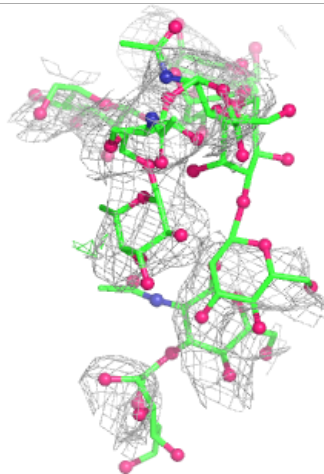
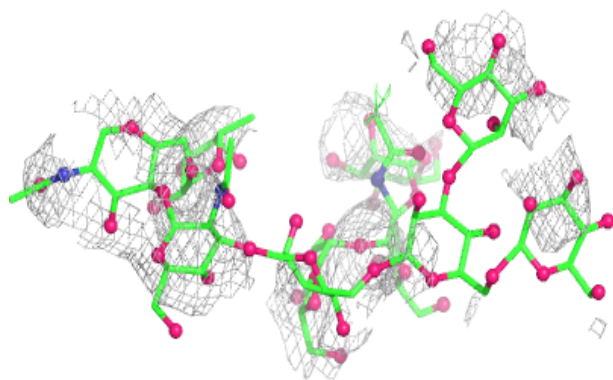
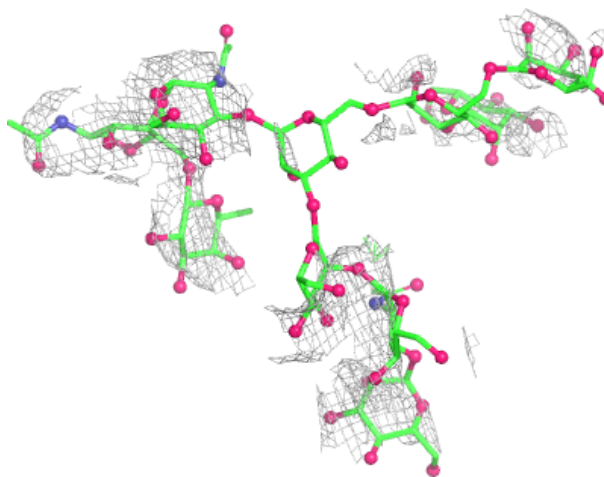
Electron density around Chain d:

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



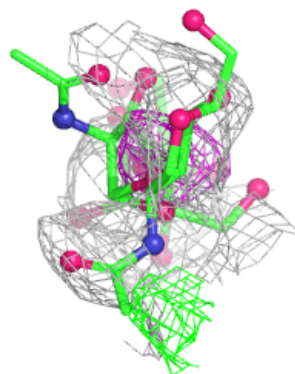
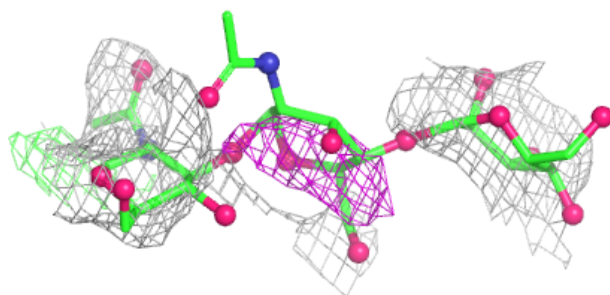
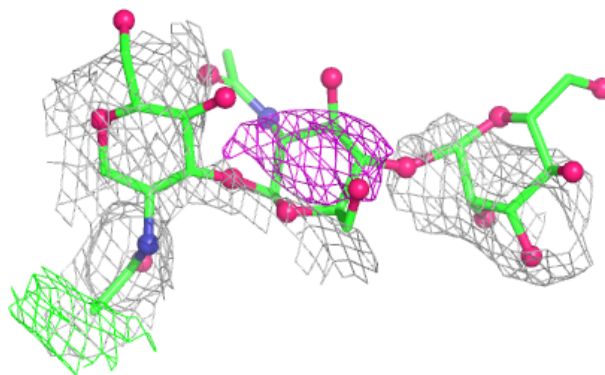
Electron density around Chain f:

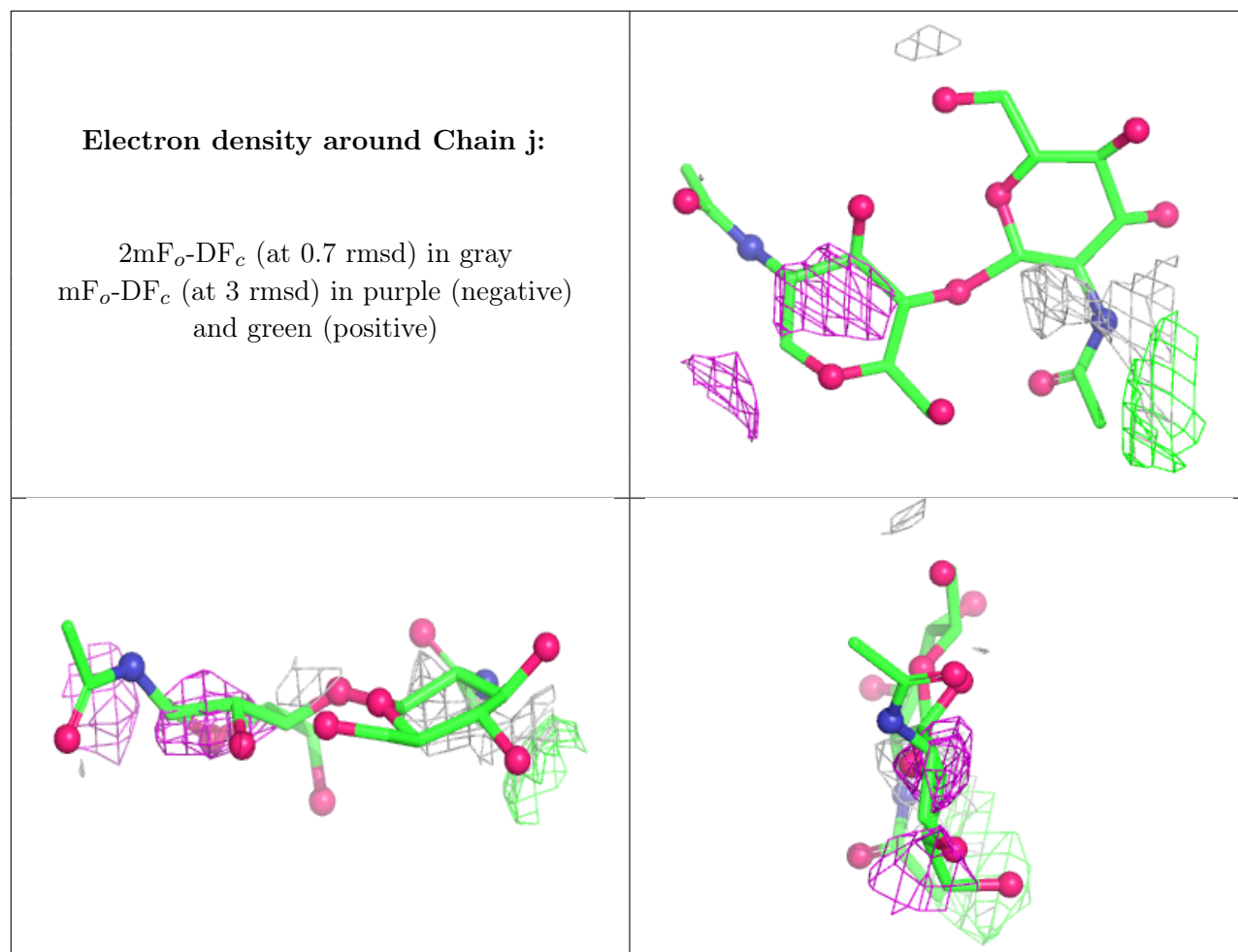
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain i:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.