



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:06 AM UTC

PDB ID : 6FHW / pdb_00006fhw
Title : Structure of Hormoconis resinae Glucoamylase
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Deposited on : 2018-01-15
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

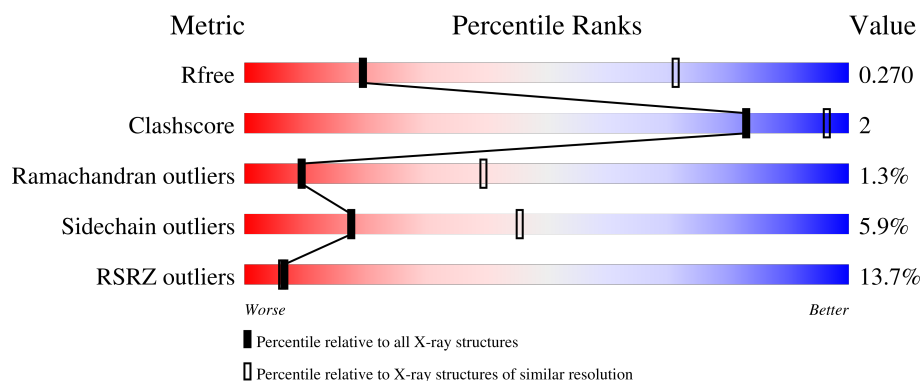
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



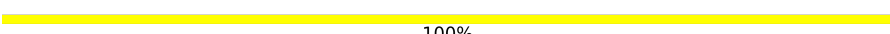
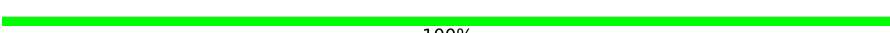
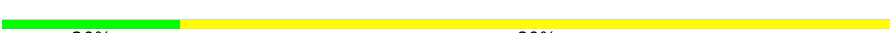
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	616	
1	B	616	
2	C	2	
2	D	2	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	G	2	 50% 50%
2	H	2	 100%
2	I	2	 50% 50%
2	J	2	 50% 50%
2	K	2	 100%
2	L	2	 100%
3	F	5	 20% 80%
4	M	3	 67% 33%
4	N	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9385 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 Glucoamylase P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4474	2838	740	879	17			
1	B	587	Total	C	N	O	S	0	0	0
			4482	2842	742	881	17			

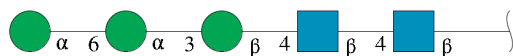
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

ose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

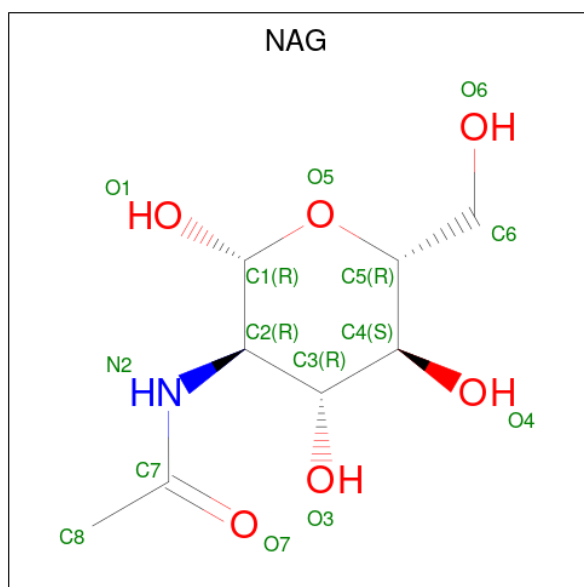


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			44	25	1	18			
4	N	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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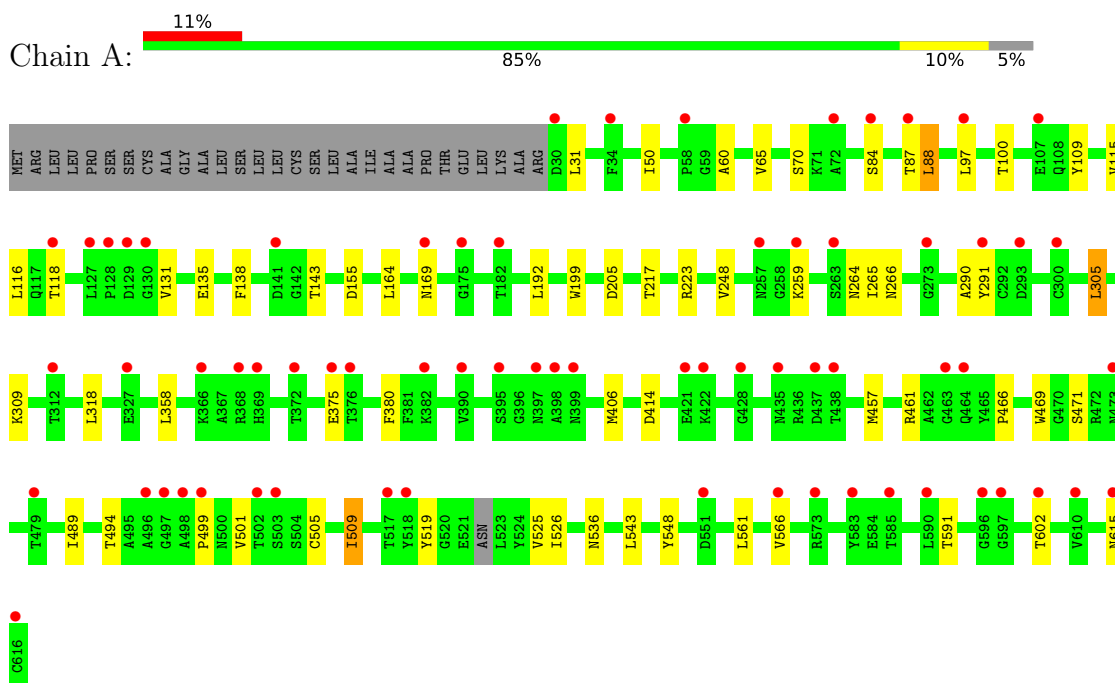
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

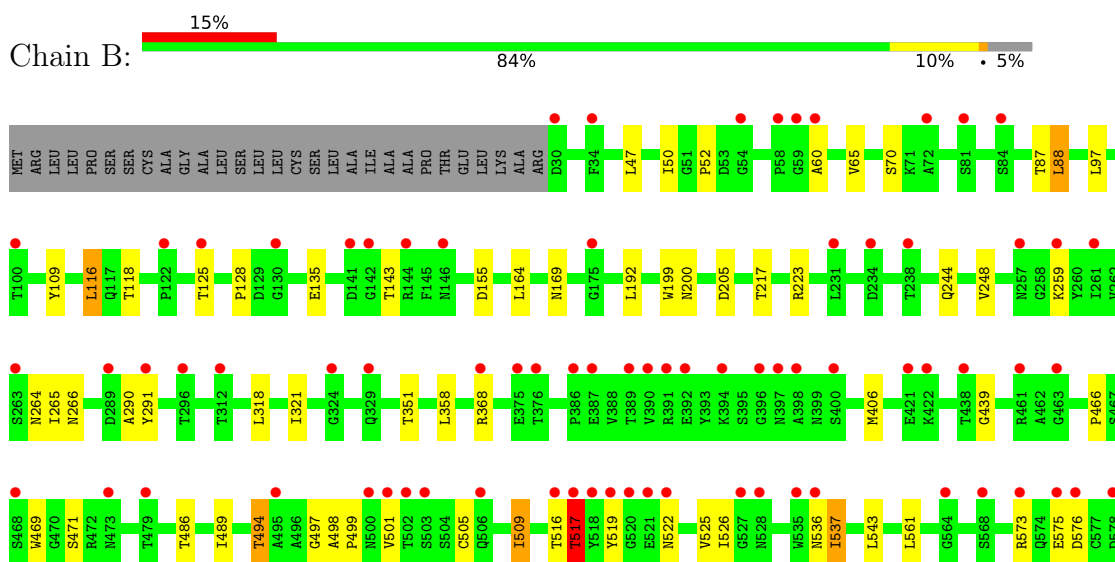
3 Residue-property plots [i](#)

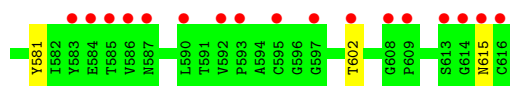
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glucoamylase P



• Molecule 1: Glucoamylase P





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

Chain C: 100%



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

Chain D: 50% 50%



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

Chain E: 100%



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

Chain G: 50% 50%



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

Chain H: 100%



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

Chain I: 50% 50%

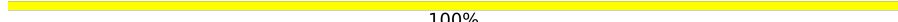


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

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

Chain K:  100%

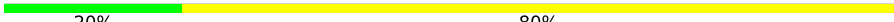
MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-6)-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 F:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 4: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  67% 33%

GLC1
GLC2
AC13

- Molecule 4: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:  67% 33%

GLC1
GLC2
AC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.97Å 149.83Å 192.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.58 – 3.60 59.58 – 3.60	Depositor EDS
% Data completeness (in resolution range)	79.1 (59.58-3.60) 79.1 (59.58-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.264 , 0.273 0.265 , 0.270	Depositor DCC
R_{free} test set	1887 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9385	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: MAN, GLC, NAG, BMA, AC1

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	0.56	0/4592	0.81	0/6284
1	B	0.57	0/4601	0.82	0/6298
All	All	0.57	0/9193	0.82	0/12582

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	575	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4241	18	0
1	B	4482	0	4250	24	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	F	61	0	52	0	0
4	M	44	0	30	0	0
4	N	44	0	30	0	0
5	A	28	0	26	0	0
All	All	9385	0	8854	44	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 2.

All (44) 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:115:VAL:O	1:A:118:THR:HG22	1.91	0.70
1:B:52:PRO:HA	1:B:60:ALA:HB1	1.79	0.65
1:A:65:VAL:HG11	1:A:87:THR:HG21	1.78	0.65
1:B:65:VAL:HG11	1:B:87:THR:HG21	1.78	0.64
1:B:88:LEU:HD22	1:B:109:TYR:CD1	2.35	0.61
1:A:88:LEU:HD22	1:A:109:TYR:CD1	2.35	0.61
1:B:517:THR:HG21	1:B:573:ARG:CZ	2.34	0.58
1:A:116:LEU:HD11	1:A:138:PHE:CD1	2.40	0.57
1:A:116:LEU:HD11	1:A:138:PHE:CG	2.39	0.57
1:B:118:THR:HG21	1:B:499:PRO:HD2	1.90	0.54
1:B:125:THR:HG23	1:B:128:PRO:HD2	1.94	0.50
1:B:537:ILE:HG21	1:B:581:TYR:CD2	2.47	0.50
1:B:498:ALA:HB1	1:B:499:PRO:HD2	1.93	0.49
1:A:414:ASP:OD1	1:A:461:ARG:NH2	2.46	0.49
2:J:1:NAG:H82	2:J:1:NAG:O3	2.13	0.49
1:B:116:LEU:C	1:B:116:LEU:HD12	2.37	0.48
1:B:88:LEU:HD22	1:B:109:TYR:CG	2.48	0.48
1:A:88:LEU:HD22	1:A:109:TYR:CG	2.48	0.48
1:A:305:LEU:HD12	1:A:380:PHE:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TRP:CD2	1:A:248:VAL:HG22	2.52	0.45
1:A:205:ASP:HB3	1:A:264:ASN:HD21	1.81	0.45
1:B:205:ASP:HB3	1:B:264:ASN:HD21	1.81	0.45
2:H:1:NAG:O3	2:H:2:NAG:O5	2.29	0.45
1:B:200:ASN:HD22	2:I:1:NAG:H83	1.82	0.45
1:B:516:THR:O	1:B:517:THR:HG23	2.17	0.45
1:B:199:TRP:CD2	1:B:248:VAL:HG22	2.52	0.44
1:B:498:ALA:HB1	1:B:499:PRO:CD	2.47	0.44
1:B:50:ILE:HG12	1:B:65:VAL:HG13	2.00	0.44
1:A:155:ASP:HB3	1:A:217:THR:HG23	2.00	0.43
1:B:244:GLN:NE2	1:B:486:THR:HG23	2.32	0.43
1:A:290:ALA:HB2	1:A:471:SER:OG	2.18	0.43
1:A:509:ILE:HG21	1:A:561:LEU:HD11	2.00	0.43
1:B:155:ASP:HB3	1:B:217:THR:HG23	2.00	0.43
1:A:566:VAL:HG12	1:A:591:THR:HB	2.01	0.43
1:B:290:ALA:HB2	1:B:471:SER:OG	2.18	0.43
1:A:50:ILE:HG12	1:A:65:VAL:HG13	2.00	0.43
1:B:509:ILE:HG21	1:B:561:LEU:HD11	2.00	0.43
1:A:525:VAL:HG12	1:A:543:LEU:HD11	2.01	0.42
1:A:519:TYR:HA	1:A:548:TYR:CD1	2.55	0.42
1:B:525:VAL:HG12	1:B:543:LEU:HD11	2.01	0.42
1:B:494:THR:H	1:B:498:ALA:HB3	1.84	0.41
1:A:223:ARG:HG3	1:A:469:TRP:CD2	2.56	0.41
1:B:321:ILE:HD11	1:B:439:GLY:HA2	2.03	0.41
1:B:223:ARG:HG3	1:B:469:TRP:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	582/616 (94%)	531 (91%)	45 (8%)	6 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	585/616 (95%)	531 (91%)	45 (8%)	9 (2%)	8	37
All	All	1167/1232 (95%)	1062 (91%)	90 (8%)	15 (1%)	9	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	519	TYR
1	A	60	ALA
1	A	70	SER
1	A	499	PRO
1	B	70	SER
1	A	466	PRO
1	B	466	PRO
1	B	522	ASN
1	B	497	GLY
1	B	517	THR
1	B	576	ASP
1	A	494	THR
1	B	494	THR
1	B	505	CYS
1	A	505	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	472/495 (95%)	443 (94%)	29 (6%)	17	45
1	B	473/495 (96%)	446 (94%)	27 (6%)	18	46
All	All	945/990 (96%)	889 (94%)	56 (6%)	18	45

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	84	SER
1	A	88	LEU
1	A	97	LEU
1	A	100	THR
1	A	131	VAL
1	A	135	GLU
1	A	143	THR
1	A	164	LEU
1	A	169	ASN
1	A	192	LEU
1	A	259	LYS
1	A	265	ILE
1	A	266	ASN
1	A	291	TYR
1	A	305	LEU
1	A	309	LYS
1	A	318	LEU
1	A	358	LEU
1	A	375	GLU
1	A	406	MET
1	A	457	MET
1	A	489	ILE
1	A	501	VAL
1	A	509	ILE
1	A	526	ILE
1	A	536	ASN
1	A	602	THR
1	A	615	ASN
1	B	47	LEU
1	B	88	LEU
1	B	97	LEU
1	B	116	LEU
1	B	135	GLU
1	B	143	THR
1	B	164	LEU
1	B	169	ASN
1	B	192	LEU
1	B	259	LYS
1	B	265	ILE
1	B	266	ASN
1	B	291	TYR
1	B	318	LEU

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Mol	Chain	Res	Type
1	B	351	THR
1	B	358	LEU
1	B	368	ARG
1	B	406	MET
1	B	489	ILE
1	B	501	VAL
1	B	509	ILE
1	B	517	THR
1	B	526	ILE
1	B	536	ASN
1	B	537	ILE
1	B	602	THR
1	B	615	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	49	ASN
1	A	103	GLN
1	A	108	GLN
1	A	111	HIS
1	A	174	ASN
1	A	190	ASN
1	A	220	ASN
1	A	253	GLN
1	A	257	ASN
1	A	264	ASN
1	A	303	GLN
1	A	307	ASN
1	A	317	ASN
1	A	329	GLN
1	A	364	GLN
1	A	433	GLN
1	A	506	GLN
1	A	536	ASN
1	A	574	GLN
1	A	579	GLN
1	B	48	ASN
1	B	49	ASN
1	B	73	ASN
1	B	103	GLN

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Mol	Chain	Res	Type
1	B	113	GLN
1	B	174	ASN
1	B	190	ASN
1	B	220	ASN
1	B	264	ASN
1	B	317	ASN
1	B	329	GLN
1	B	364	GLN
1	B	433	GLN
1	B	536	ASN
1	B	574	GLN
1	B	579	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

29 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	C	1	2,1	14,14,15	0.36	0	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.90	0
2	NAG	D	1	2,1	14,14,15	0.30	0	17,19,21	1.15	2 (11%)
2	NAG	D	2	2	14,14,15	0.31	0	17,19,21	0.65	0
2	NAG	E	1	2,1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.34	0	17,19,21	1.25	2 (11%)
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.63	0
3	BMA	F	3	3	11,11,12	0.43	0	15,15,17	1.02	2 (13%)
3	MAN	F	4	3	11,11,12	0.33	0	15,15,17	0.71	1 (6%)
3	MAN	F	5	3	11,11,12	0.51	0	15,15,17	1.97	2 (13%)
2	NAG	G	1	2,1	14,14,15	0.26	0	17,19,21	0.98	2 (11%)
2	NAG	G	2	2	14,14,15	0.28	0	17,19,21	0.61	0
2	NAG	H	1	2,1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
2	NAG	H	2	2	14,14,15	0.40	0	17,19,21	1.30	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.39	0	17,19,21	1.49	3 (17%)
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.71	0
2	NAG	J	1	2,1	14,14,15	0.48	0	17,19,21	1.80	3 (17%)
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.84	0
2	NAG	K	1	2,1	14,14,15	0.37	0	17,19,21	1.29	1 (5%)
2	NAG	K	2	2	14,14,15	0.33	0	17,19,21	1.76	2 (11%)
2	NAG	L	1	2,1	14,14,15	0.41	0	17,19,21	0.72	0
2	NAG	L	2	2	14,14,15	0.33	0	17,19,21	0.69	0
4	GLC	M	1	4	12,12,12	0.58	0	17,17,17	0.69	0
4	GLC	M	2	4	11,11,12	0.33	0	15,15,17	1.37	2 (13%)
4	AC1	M	3	4	21,22,23	0.48	0	22,32,34	0.73	0
4	GLC	N	1	4	12,12,12	0.52	0	17,17,17	0.59	0
4	GLC	N	2	4	11,11,12	0.32	0	15,15,17	1.06	2 (13%)
4	AC1	N	3	4	21,22,23	0.60	0	22,32,34	0.77	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
4	GLC	M	1	4	-	0/2/22/22	0/1/1/1
4	GLC	M	2	4	-	0/2/19/22	0/1/1/1
4	AC1	M	3	4	-	4/6/43/46	0/2/2/2
4	GLC	N	1	4	-	2/2/22/22	0/1/1/1
4	GLC	N	2	4	-	0/2/19/22	0/1/1/1
4	AC1	N	3	4	-	5/6/43/46	0/2/2/2

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	MAN	C1-O5-C5	5.73	119.87	112.19
2	K	2	NAG	C2-N2-C7	5.28	129.97	122.90
2	J	1	NAG	C2-N2-C7	4.64	129.12	122.90
2	J	1	NAG	C8-C7-N2	3.93	122.64	116.12
3	F	5	MAN	C1-C2-C3	3.93	115.37	109.64
2	I	1	NAG	C8-C7-N2	3.56	122.02	116.12
4	M	2	GLC	C1-C2-C3	3.53	114.79	109.64
2	K	1	NAG	C1-C2-N2	3.44	115.86	110.43
2	I	1	NAG	C2-N2-C7	3.34	127.38	122.90
2	K	2	NAG	C8-C7-N2	3.33	121.63	116.12
3	F	1	NAG	O5-C1-C2	-2.94	106.75	111.29
2	H	2	NAG	C1-O5-C5	2.84	116.00	112.19
2	E	1	NAG	O5-C1-C2	-2.67	107.17	111.29
2	D	1	NAG	C8-C7-N2	2.63	120.49	116.12
3	F	3	BMA	C1-C2-C3	2.61	113.44	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C1-C2-N2	2.56	114.47	110.43
3	F	1	NAG	C1-C2-N2	2.54	114.44	110.43
2	H	2	NAG	C2-N2-C7	2.47	126.21	122.90
2	D	1	NAG	C2-N2-C7	2.47	126.20	122.90
2	E	2	NAG	C2-N2-C7	2.42	126.14	122.90
3	F	4	MAN	C1-O5-C5	2.37	115.36	112.19
2	E	2	NAG	O5-C1-C2	-2.31	107.72	111.29
3	F	3	BMA	C1-O5-C5	2.28	115.24	112.19
4	N	2	GLC	C1-O5-C5	2.22	115.16	112.19
2	I	1	NAG	O7-C7-C8	-2.19	118.16	122.05
2	H	2	NAG	C1-C2-N2	2.15	113.82	110.43
2	G	1	NAG	O5-C1-C2	-2.15	107.97	111.29
2	G	1	NAG	C1-O5-C5	2.14	115.06	112.19
4	M	2	GLC	C2-C3-C4	2.11	114.57	110.86
2	J	1	NAG	O7-C7-C8	-2.02	118.45	122.05
4	N	2	GLC	C1-C2-C3	2.01	112.57	109.64

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	3	AC1	C3-C4-N4A-C1B
4	M	3	AC1	C5-C4-N4A-C1B
4	M	3	AC1	C4A-C5B-C6B-O6B
4	M	3	AC1	C7B-C5B-C6B-O6B
4	N	3	AC1	C5-C4-N4A-C1B
2	G	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
4	N	1	GLC	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

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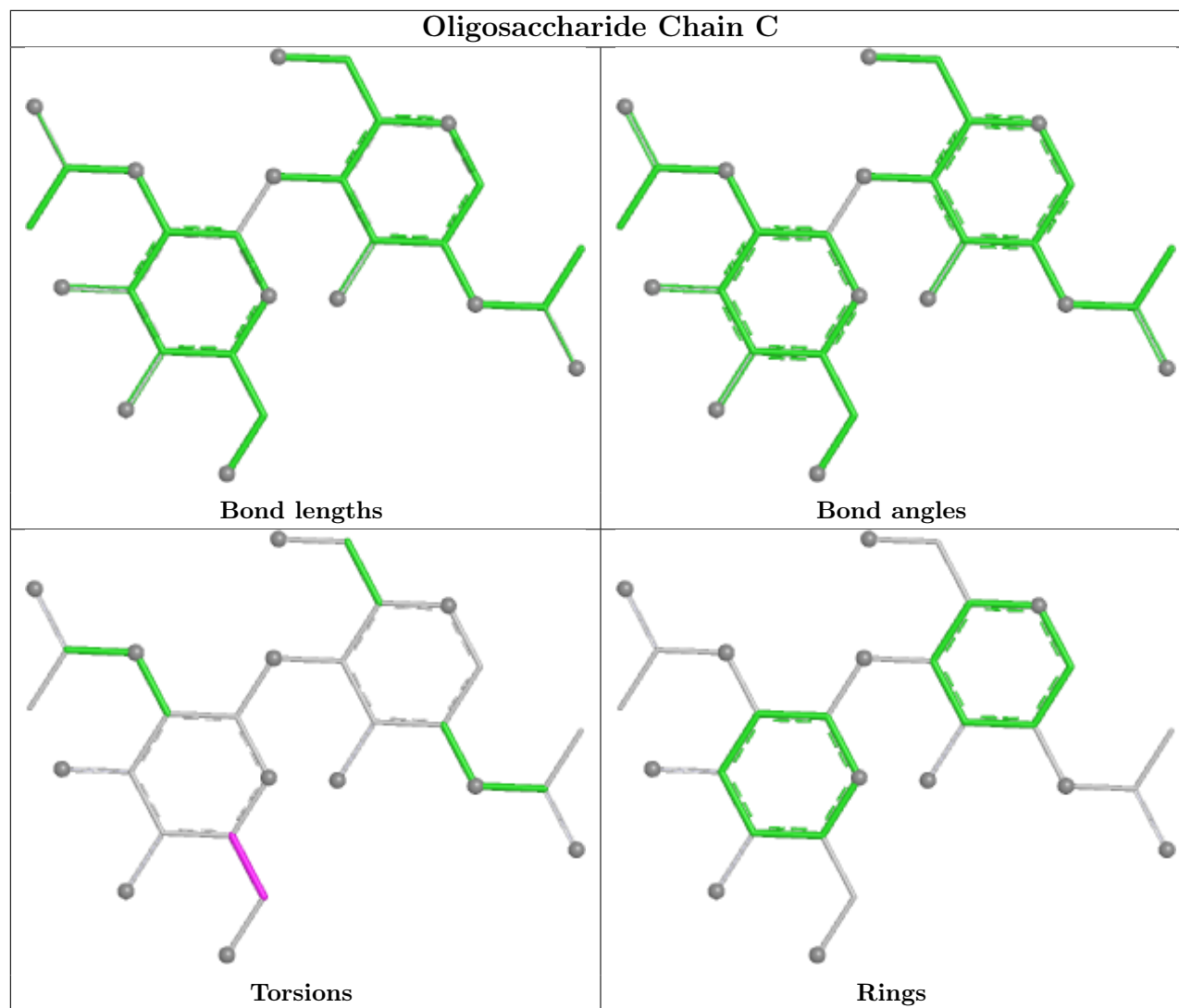
Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C4-C5-C6-O6
4	N	1	GLC	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	K	1	NAG	C1-C2-N2-C7
4	N	3	AC1	C7B-C5B-C6B-O6B
2	K	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
4	N	3	AC1	C2B-C1B-N4A-C4
4	N	3	AC1	C3-C4-N4A-C1B
2	G	2	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
2	H	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	K	1	NAG	O5-C5-C6-O6
4	N	3	AC1	C4A-C5B-C6B-O6B
3	F	1	NAG	C4-C5-C6-O6

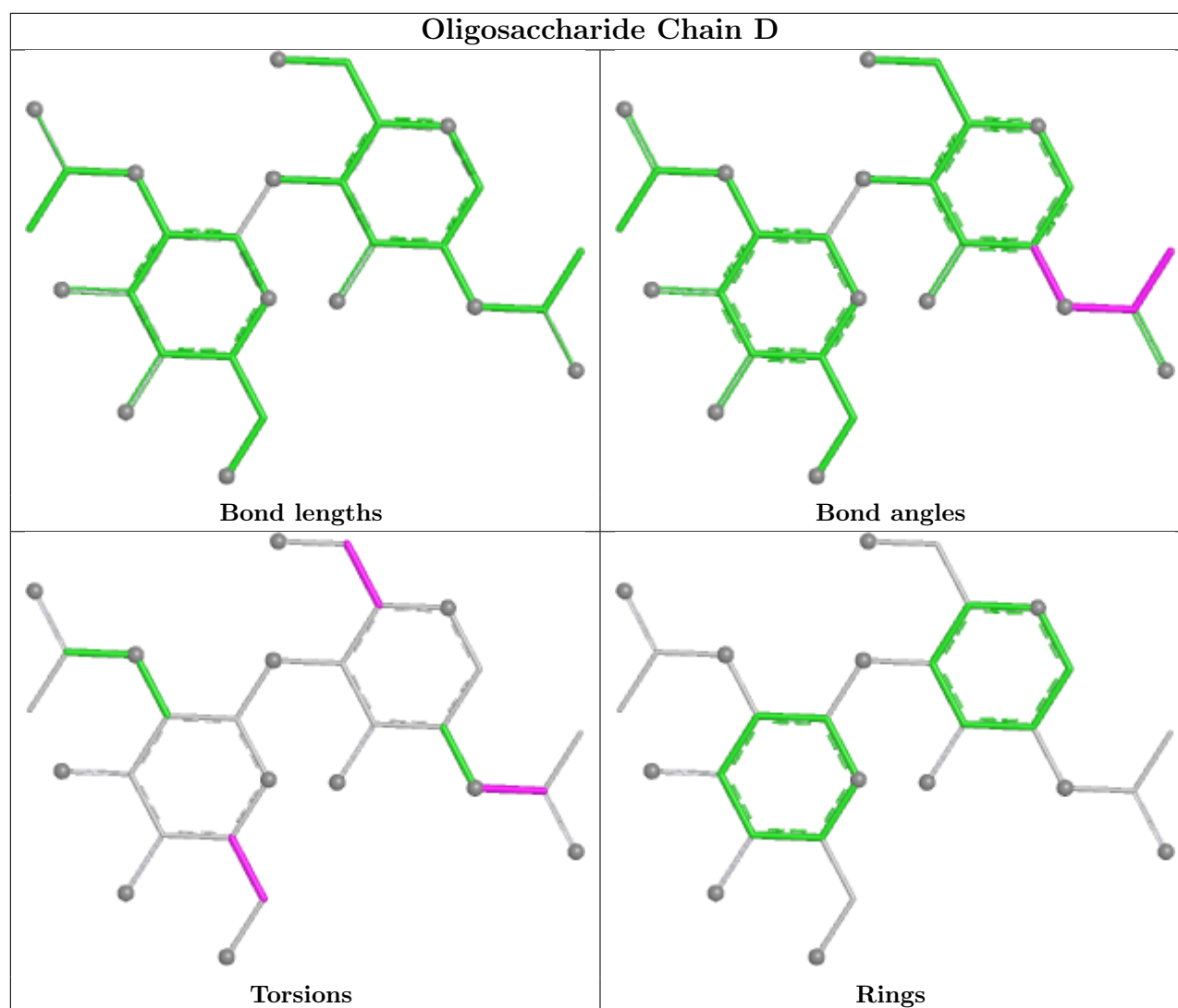
There are no ring outliers.

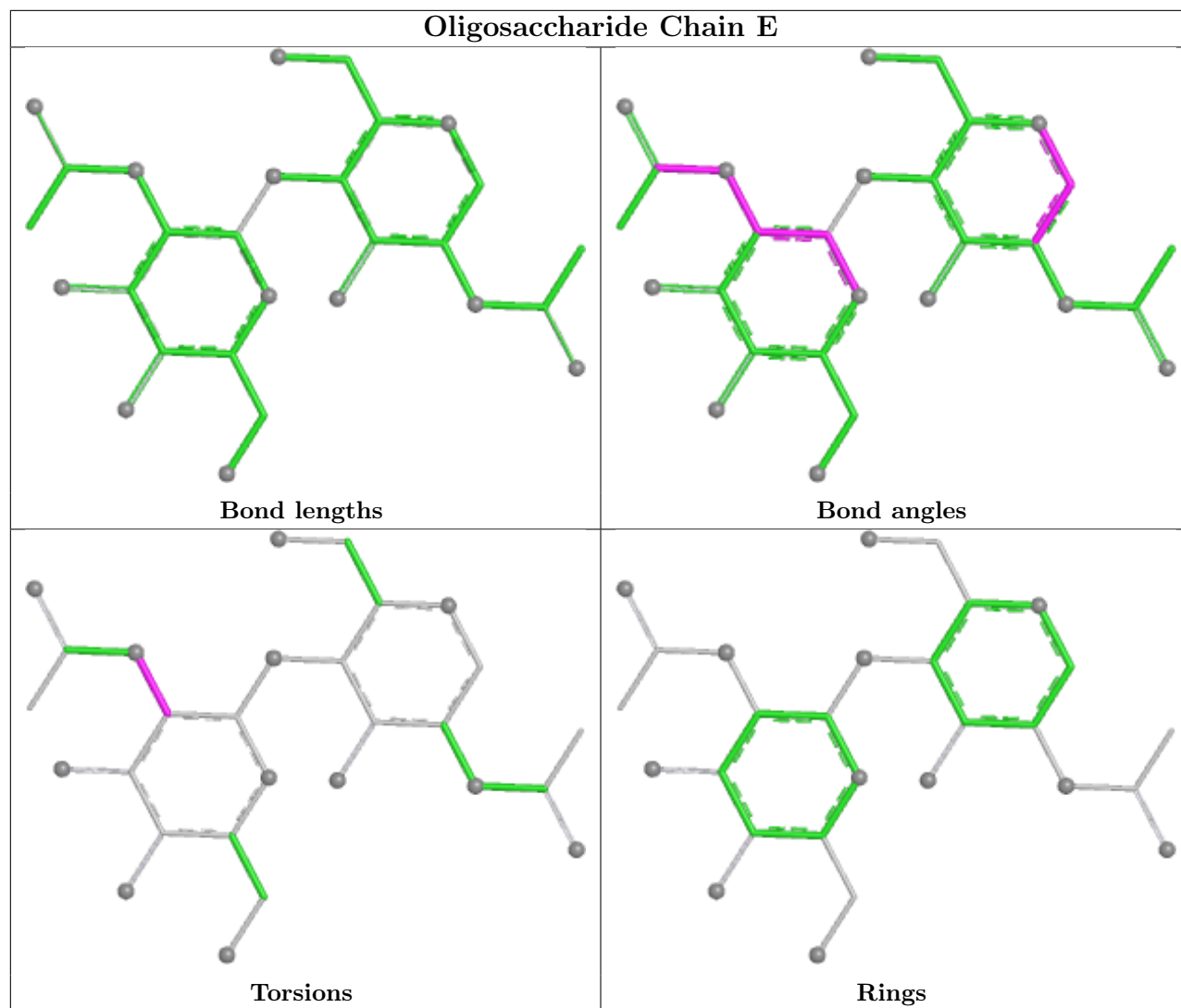
4 monomers are involved in 3 short contacts:

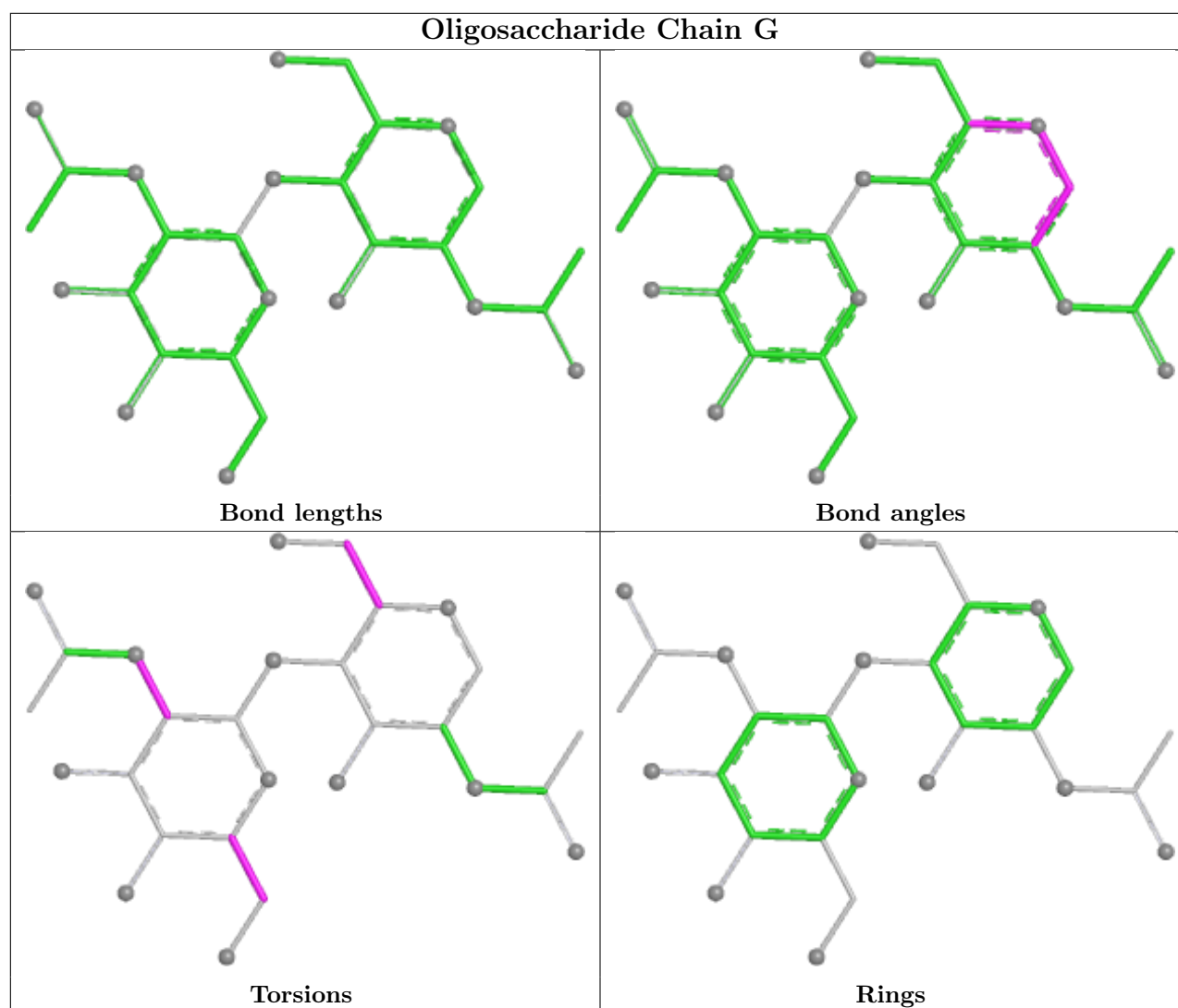
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	J	1	NAG	1	0
2	H	2	NAG	1	0
2	I	1	NAG	1	0

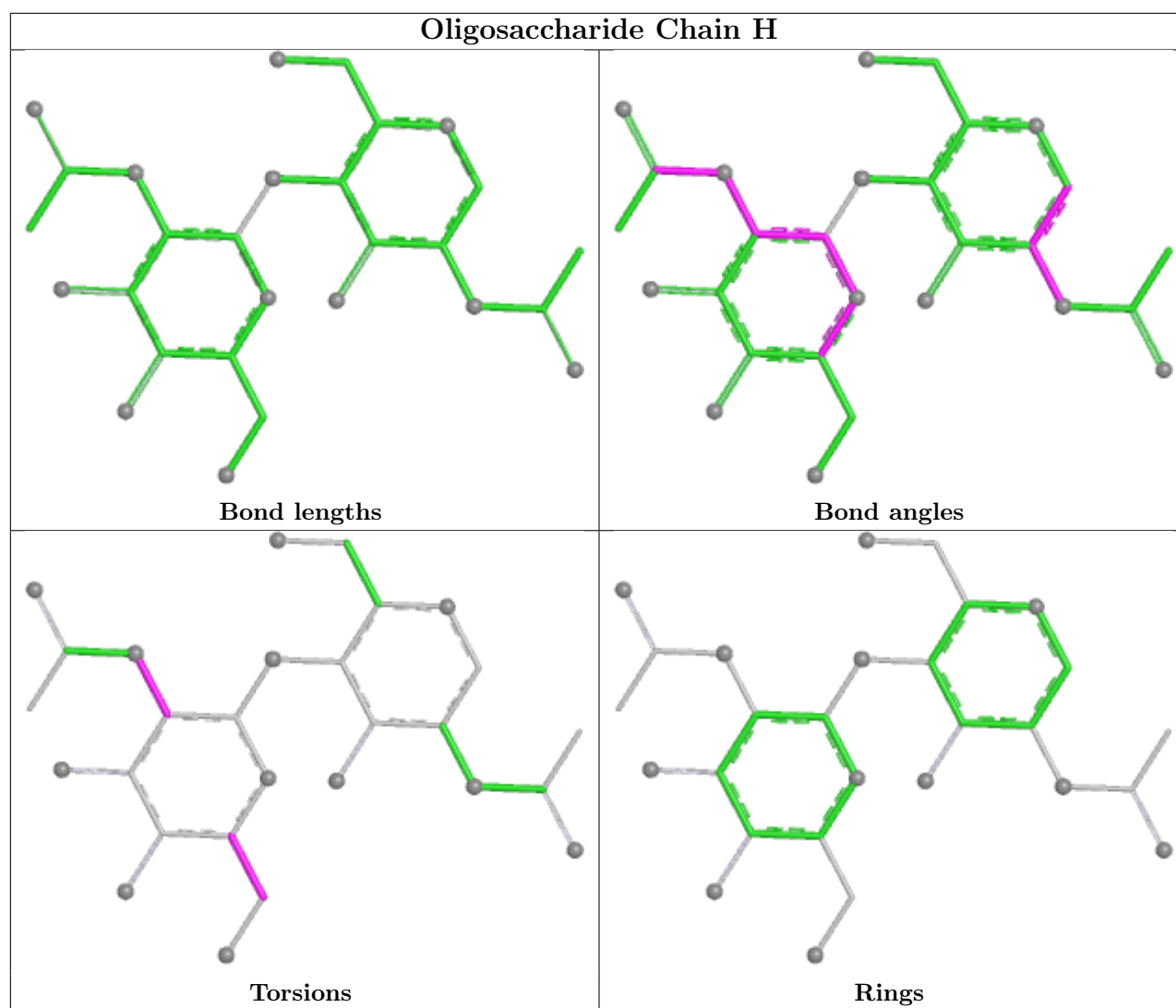
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

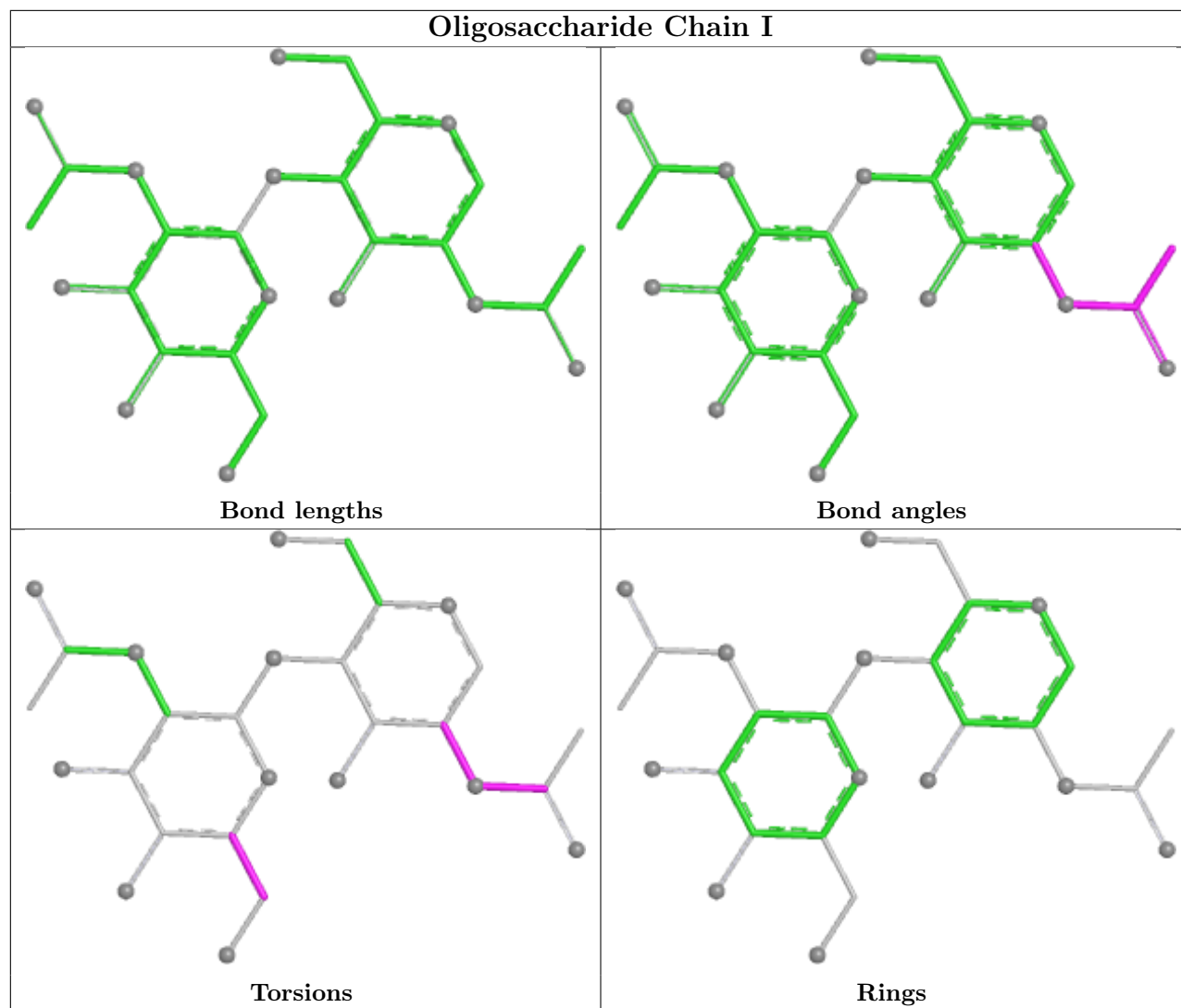


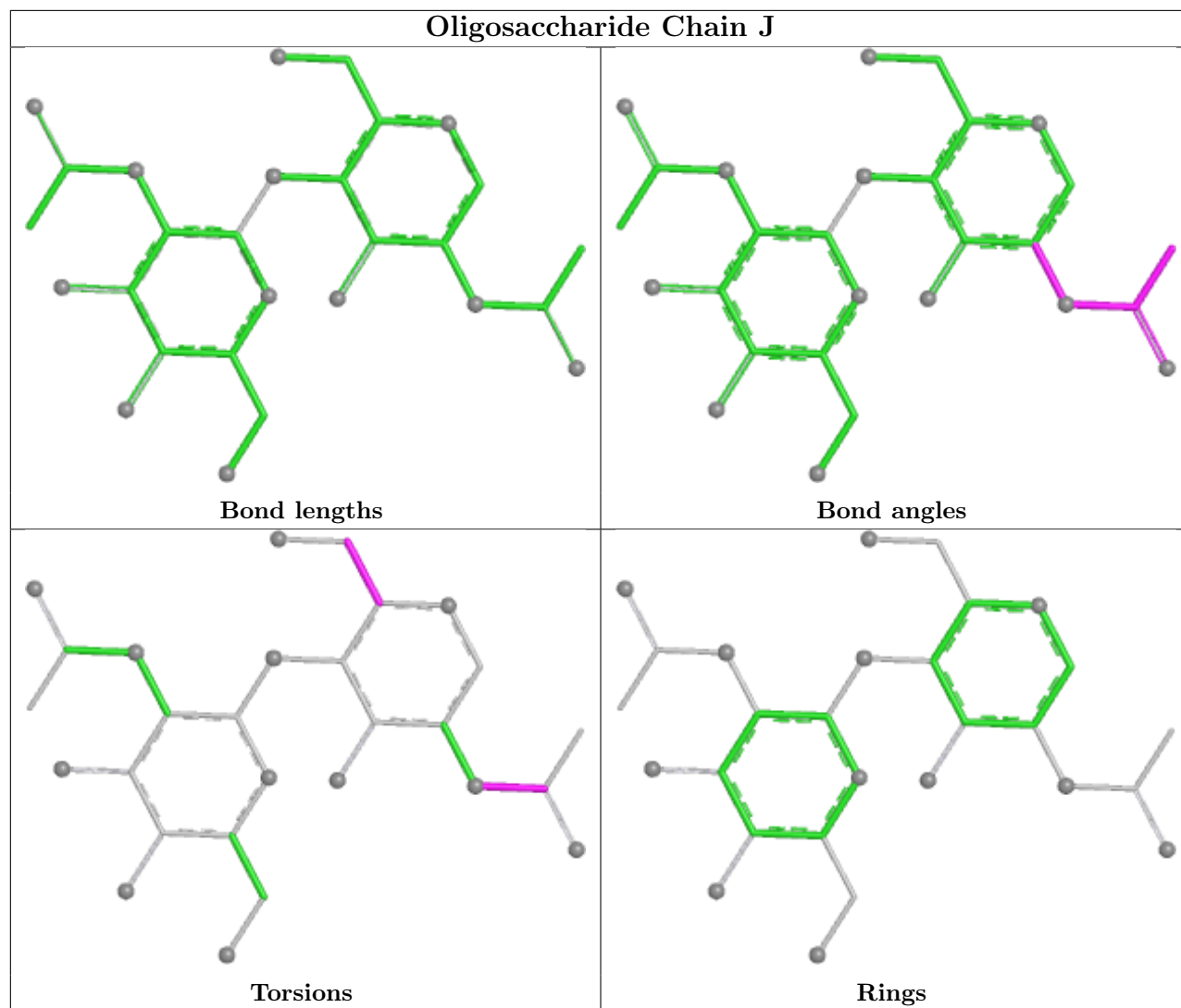


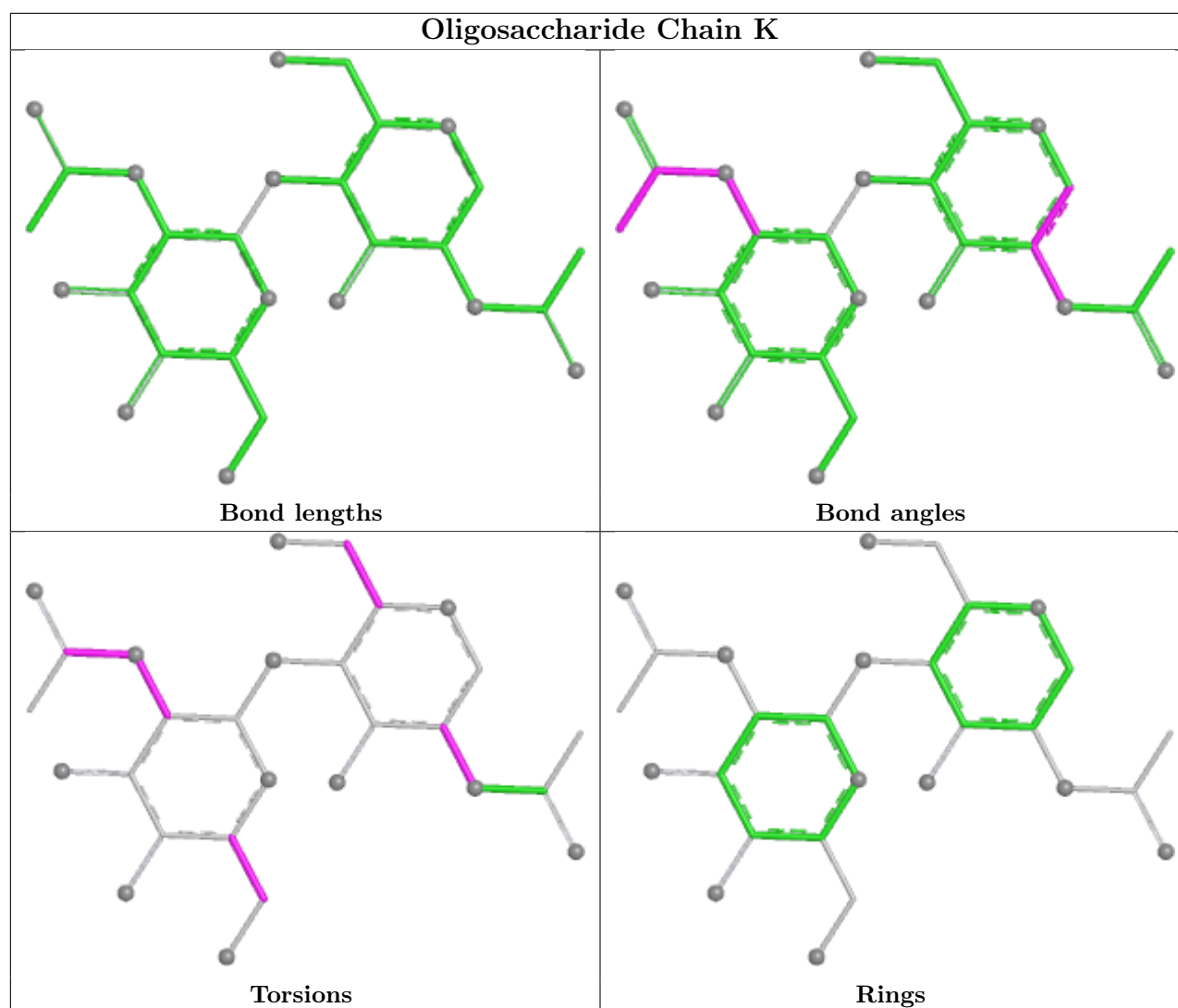


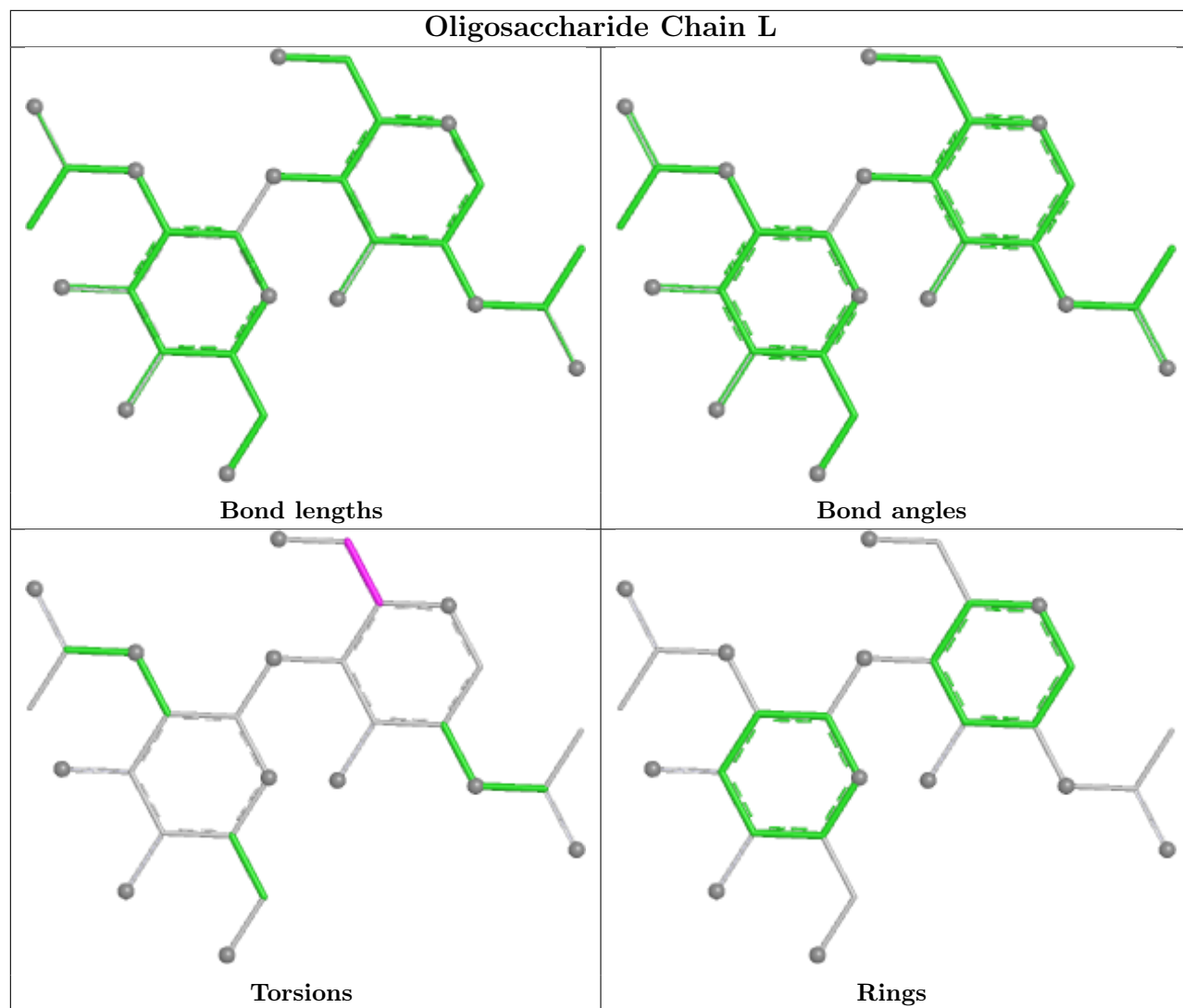


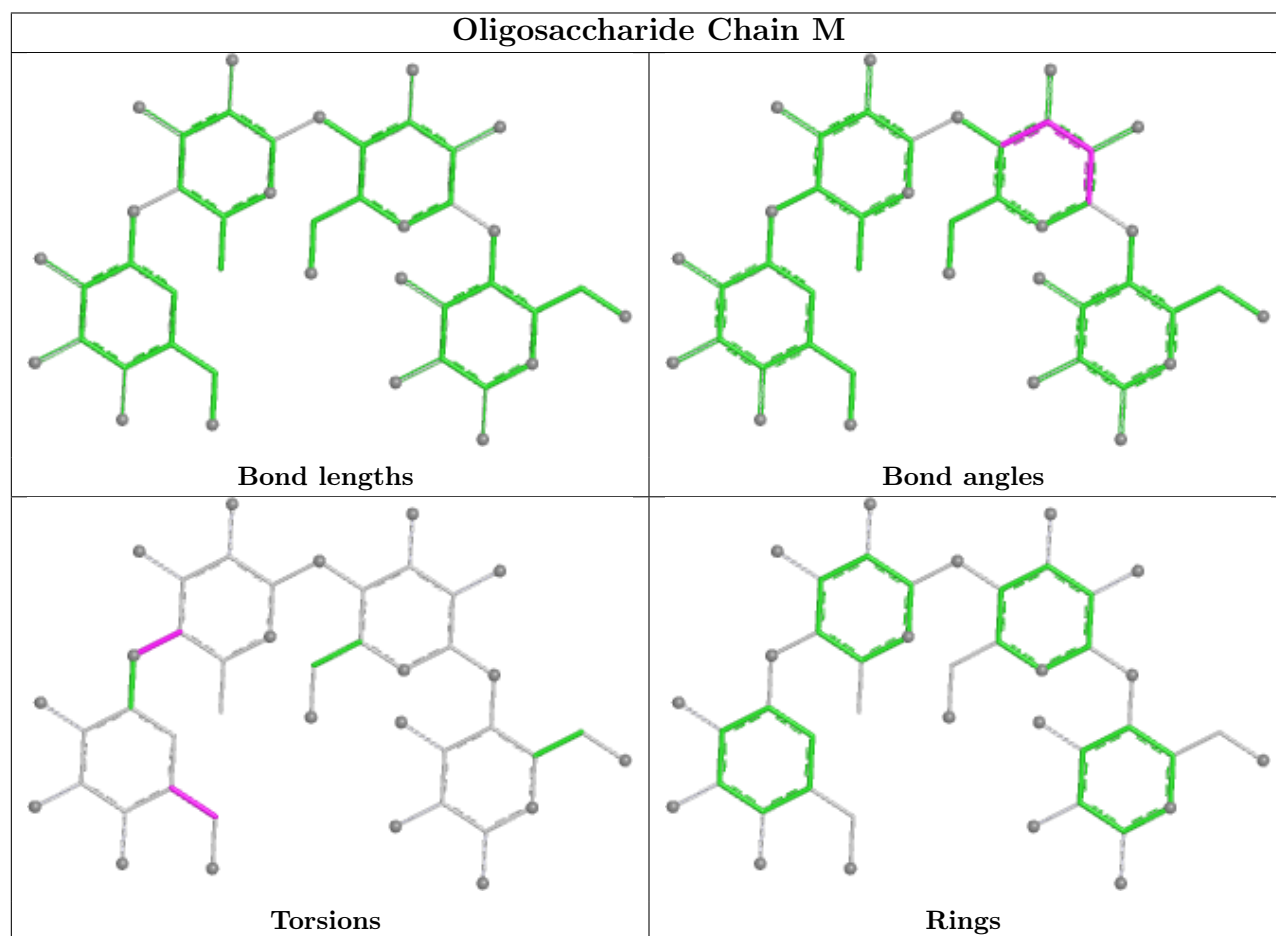
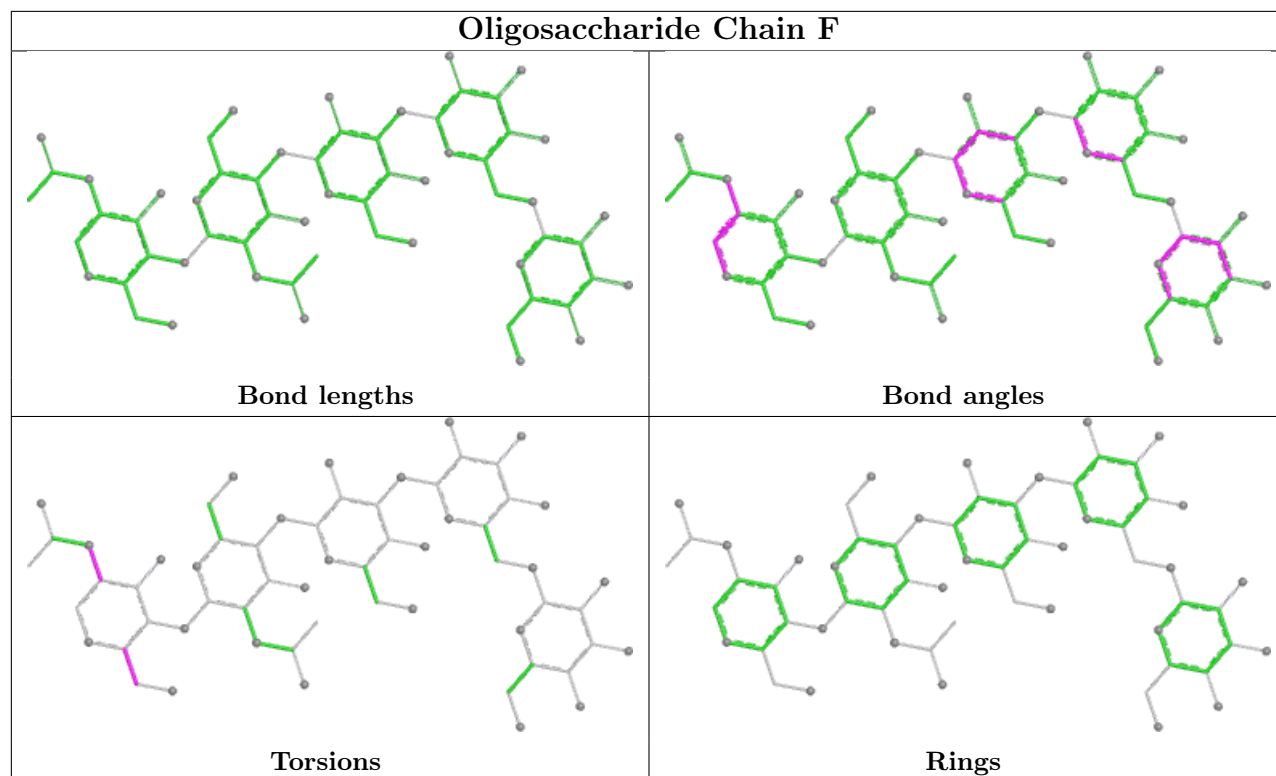


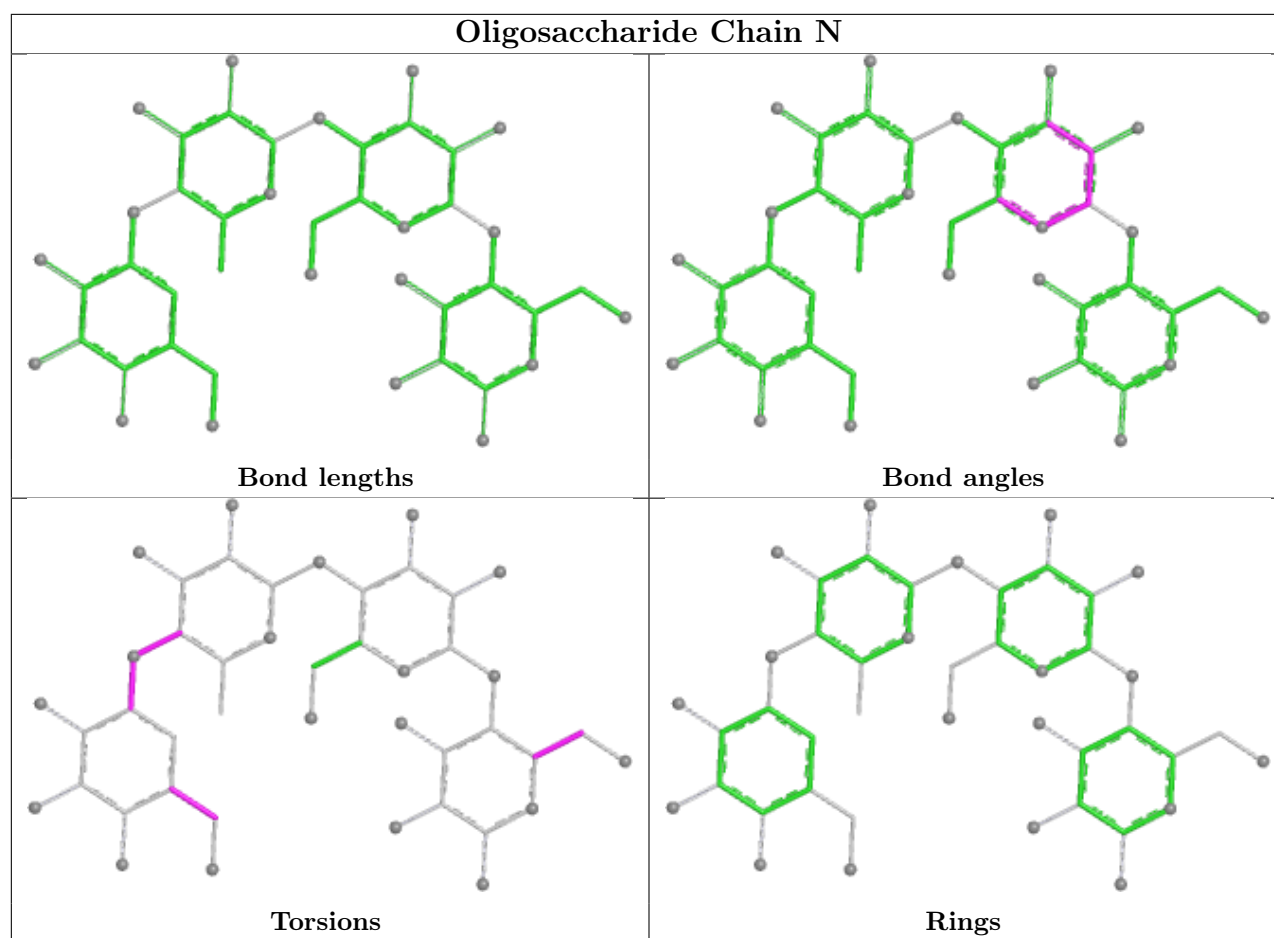












5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	814	1	14,14,15	0.32	0	17,19,21	1.42	4 (23%)
5	NAG	A	808	1	14,14,15	0.35	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	814	1	-	3/6/23/26	0/1/1/1
5	NAG	A	808	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	814	NAG	C8-C7-N2	2.73	120.65	116.12
5	A	814	NAG	C1-O5-C5	2.67	115.77	112.19
5	A	814	NAG	C2-N2-C7	2.62	126.41	122.90
5	A	814	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	814	NAG	C8-C7-N2-C2
5	A	814	NAG	O7-C7-N2-C2
5	A	814	NAG	O5-C5-C6-O6
5	A	808	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	586/616 (95%)	0.95	68 (11%) 9 8	32, 51, 84, 104	0
1	B	587/616 (95%)	1.03	93 (15%) 5 5	33, 55, 87, 104	0
All	All	1173/1232 (95%)	0.99	161 (13%) 6 6	32, 53, 86, 104	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ALA	6.8
1	B	257	ASN	6.0
1	B	519	TYR	5.5
1	A	616	CYS	5.2
1	B	234	ASP	5.2
1	B	473	ASN	5.2
1	B	613	SER	4.7
1	B	528	ASN	4.6
1	B	518	TYR	4.6
1	A	369	HIS	4.4
1	A	590	LEU	4.3
1	B	392	GLU	4.2
1	B	259	LYS	4.2
1	B	30	ASP	4.1
1	B	584	GLU	4.1
1	B	291	TYR	4.1
1	A	422	LYS	4.1
1	A	499	PRO	4.0
1	B	34	PHE	3.8
1	A	30	ASP	3.8
1	A	58	PRO	3.8
1	B	142	GLY	3.7
1	B	522	ASN	3.7
1	A	395	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	578	ASP	3.7
1	A	257	ASN	3.5
1	B	461	ARG	3.5
1	B	100	THR	3.4
1	B	590	LEU	3.4
1	B	130	GLY	3.4
1	A	517	THR	3.4
1	B	616	CYS	3.3
1	B	421	GLU	3.3
1	B	324	GLY	3.3
1	A	107	GLU	3.3
1	A	435	ASN	3.3
1	A	273	GLY	3.2
1	A	382	LYS	3.2
1	B	141	ASP	3.2
1	B	479	THR	3.1
1	B	386	PRO	3.1
1	A	372	THR	3.1
1	A	602	THR	3.1
1	B	368	ARG	3.1
1	A	130	GLY	3.1
1	A	397	ASN	3.0
1	B	520	GLY	3.0
1	B	564	GLY	3.0
1	B	502	THR	3.0
1	B	602	THR	3.0
1	B	81	SER	3.0
1	A	585	THR	3.0
1	B	521	GLU	2.9
1	B	398	ALA	2.9
1	B	58	PRO	2.9
1	A	518	TYR	2.9
1	A	34	PHE	2.9
1	A	84	SER	2.9
1	A	175	GLY	2.9
1	B	231	LEU	2.9
1	A	398	ALA	2.9
1	B	468	SER	2.8
1	A	263	SER	2.8
1	B	583	TYR	2.8
1	B	615	ASN	2.8
1	A	463	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	463	GLY	2.8
1	B	389	THR	2.8
1	B	60	ALA	2.7
1	A	291	TYR	2.7
1	A	583	TYR	2.7
1	A	566	VAL	2.7
1	A	399	ASN	2.7
1	A	473	ASN	2.7
1	A	141	ASP	2.7
1	B	614	GLY	2.7
1	A	375	GLU	2.7
1	B	597	GLY	2.6
1	A	259	LYS	2.6
1	B	394	LYS	2.6
1	A	293	ASP	2.6
1	A	503	SER	2.6
1	B	536	ASN	2.6
1	B	59	GLY	2.6
1	A	182	THR	2.5
1	B	585	THR	2.5
1	A	437	ASP	2.5
1	B	122	PRO	2.5
1	B	263	SER	2.5
1	B	72	ALA	2.5
1	A	502	THR	2.5
1	A	421	GLU	2.4
1	A	72	ALA	2.4
1	B	595	CYS	2.4
1	B	400	SER	2.4
1	B	375	GLU	2.4
1	B	391	ARG	2.4
1	A	97	LEU	2.4
1	A	438	THR	2.4
1	B	422	LYS	2.4
1	B	54	GLY	2.4
1	B	587	ASN	2.4
1	B	376	THR	2.4
1	B	503	SER	2.3
1	B	506	GLN	2.3
1	B	261	ILE	2.3
1	A	127	LEU	2.3
1	B	312	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	366	LYS	2.3
1	B	329	GLN	2.3
1	B	527	GLY	2.3
1	A	615	ASN	2.3
1	B	238	THR	2.3
1	A	597	GLY	2.3
1	A	376	THR	2.2
1	A	390	VAL	2.2
1	B	586	VAL	2.2
1	A	551	ASP	2.2
1	B	125	THR	2.2
1	B	175	GLY	2.2
1	B	608	GLY	2.2
1	A	464	GLN	2.2
1	B	593	PRO	2.2
1	A	129	ASP	2.2
1	B	576	ASP	2.2
1	B	84	SER	2.2
1	A	497	GLY	2.2
1	B	609	PRO	2.2
1	A	428	GLY	2.2
1	B	438	THR	2.2
1	B	387	GLU	2.1
1	A	573	ARG	2.1
1	A	596	GLY	2.1
1	B	575	GLU	2.1
1	A	610	VAL	2.1
1	B	390	VAL	2.1
1	B	592	VAL	2.1
1	B	396	GLY	2.1
1	B	517	THR	2.1
1	B	568	SER	2.1
1	B	289	ASP	2.1
1	B	535	TRP	2.1
1	B	144	ARG	2.1
1	B	495	ALA	2.1
1	A	169	ASN	2.1
1	B	397	ASN	2.1
1	B	296	THR	2.1
1	A	496	ALA	2.1
1	B	146	ASN	2.1
1	B	516	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	2.0
1	A	128	PRO	2.0
1	A	368	ARG	2.0
1	A	87	THR	2.0
1	A	118	THR	2.0
1	A	479	THR	2.0
1	A	327	GLU	2.0
1	A	300	CYS	2.0
1	B	500	ASN	2.0
1	B	573	ARG	2.0
1	A	312	THR	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
2	NAG	E	2	14/15	0.49	0.20	93,95,95,96	0
3	BMA	F	3	11/12	0.58	0.22	78,83,86,90	0
2	NAG	H	2	14/15	0.62	0.24	85,87,93,95	0
3	MAN	F	5	11/12	0.63	0.27	97,98,100,102	0
2	NAG	D	2	14/15	0.69	0.21	94,97,99,100	0
2	NAG	K	2	14/15	0.70	0.25	81,85,88,88	0
3	MAN	F	4	11/12	0.71	0.20	93,95,96,97	0
2	NAG	L	2	14/15	0.77	0.18	103,104,105,105	0
2	NAG	J	2	14/15	0.82	0.18	79,82,83,83	0
2	NAG	D	1	14/15	0.82	0.18	80,84,85,90	0
2	NAG	E	1	14/15	0.82	0.17	80,84,87,91	0
2	NAG	G	2	14/15	0.83	0.18	73,75,77,77	0
2	NAG	C	1	14/15	0.84	0.16	58,60,62,65	0
2	NAG	L	1	14/15	0.84	0.19	101,102,103,103	0
2	NAG	C	2	14/15	0.85	0.14	68,71,72,72	0
2	NAG	J	1	14/15	0.86	0.17	67,69,71,75	0
2	NAG	I	1	14/15	0.87	0.17	60,62,64,66	0

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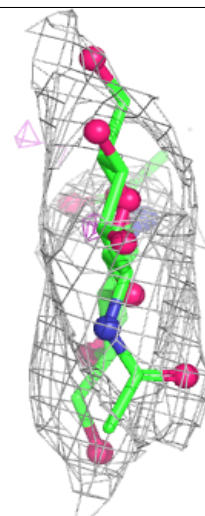
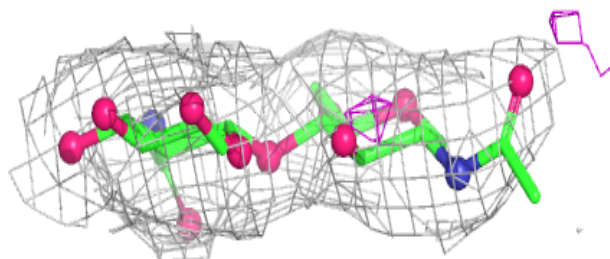
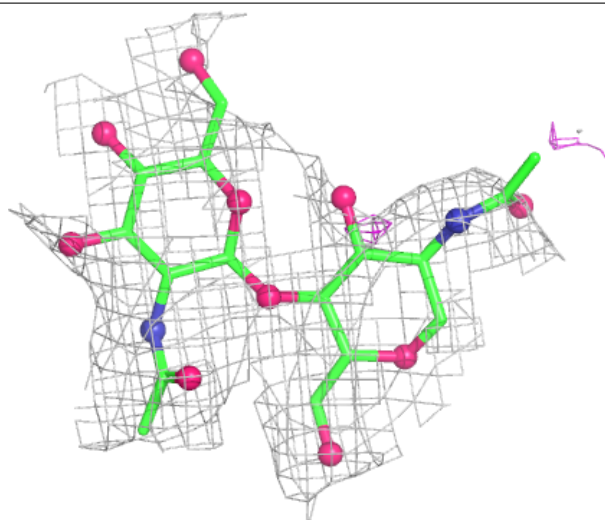
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	2	14/15	0.87	0.16	68,69,71,72	0
2	NAG	G	1	14/15	0.88	0.14	62,66,68,70	0
2	NAG	H	1	14/15	0.92	0.14	71,75,78,81	0
2	NAG	K	1	14/15	0.92	0.15	71,73,75,79	0
3	NAG	F	2	14/15	0.93	0.11	56,59,63,71	0
3	NAG	F	1	14/15	0.93	0.14	46,48,49,53	0
4	AC1	N	3	21/22	0.93	0.15	40,41,43,43	0
4	GLC	N	1	12/12	0.94	0.12	44,45,45,45	0
4	AC1	M	3	21/22	0.95	0.12	35,35,36,36	0
4	GLC	M	1	12/12	0.95	0.12	41,43,43,44	0
4	GLC	M	2	11/12	0.95	0.11	37,39,39,40	0
4	GLC	N	2	11/12	0.96	0.10	42,44,44,44	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.

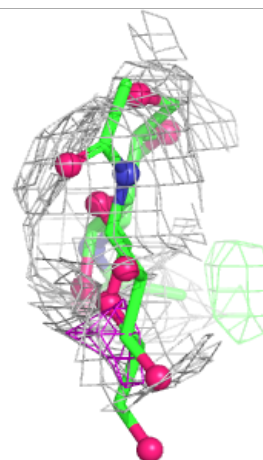
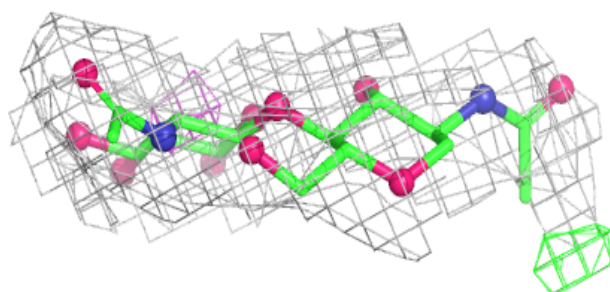
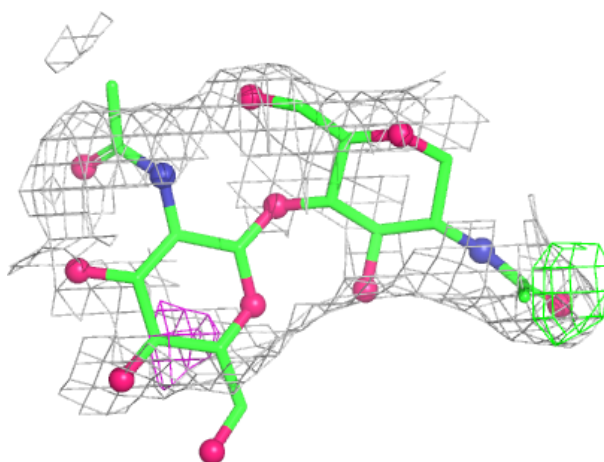
Electron density around Chain C:

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



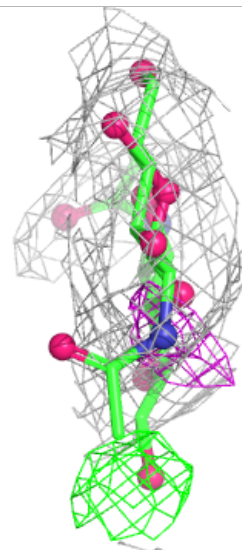
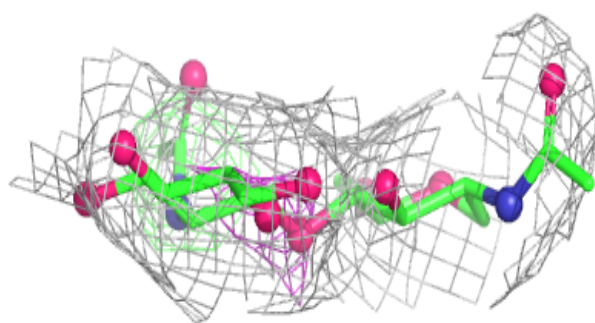
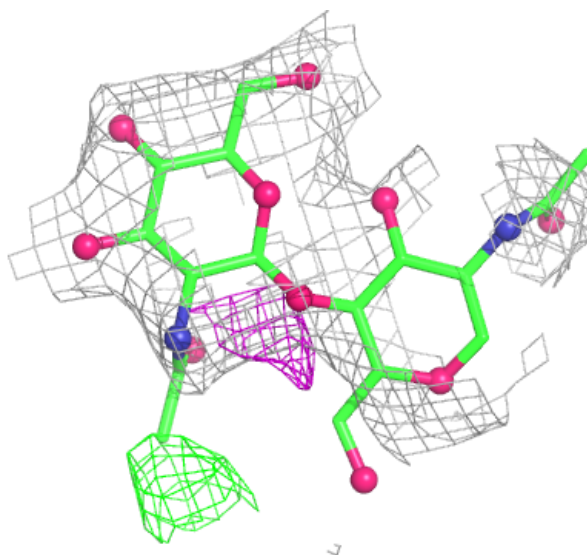
Electron density around Chain D:

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



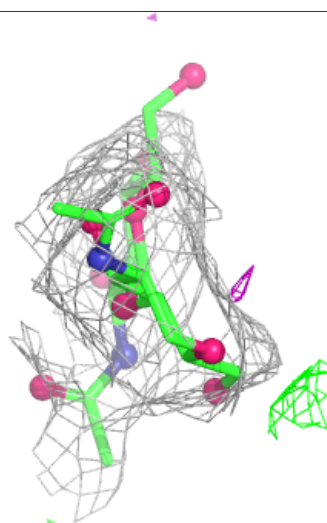
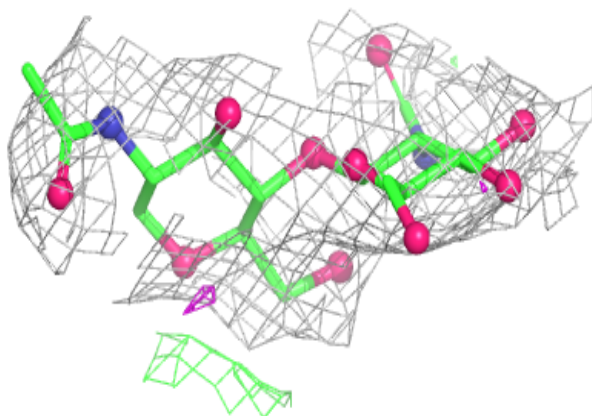
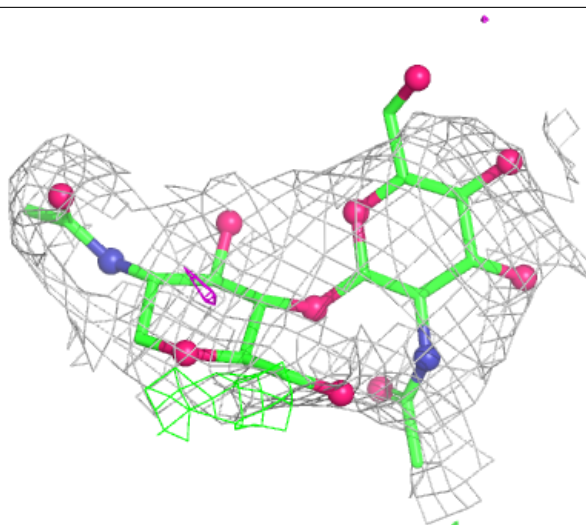
Electron density around Chain E:

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



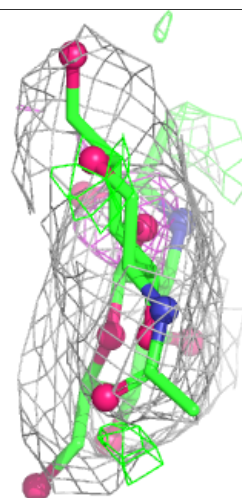
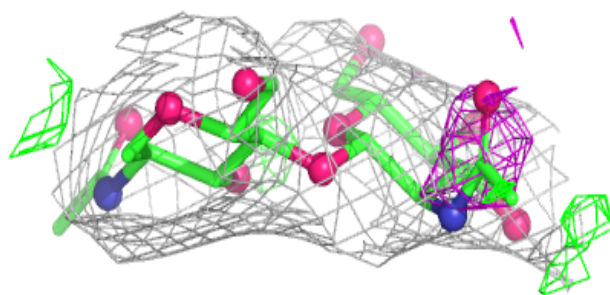
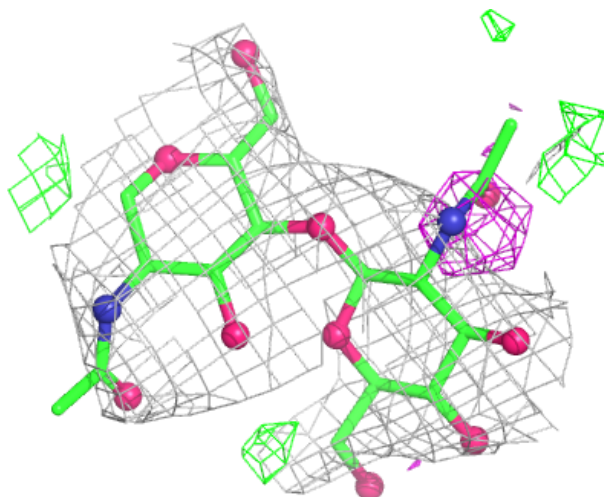
Electron density around Chain G:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



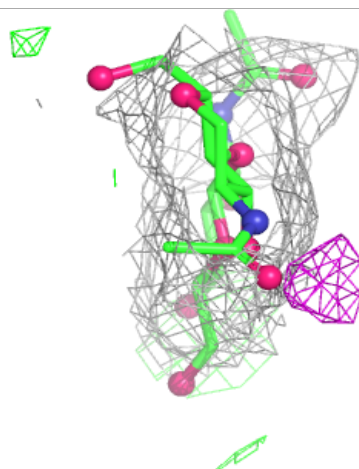
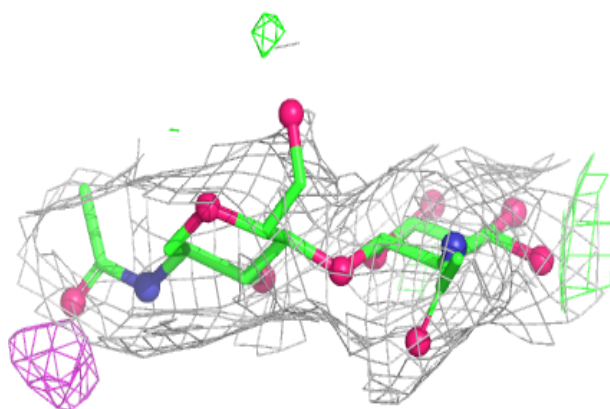
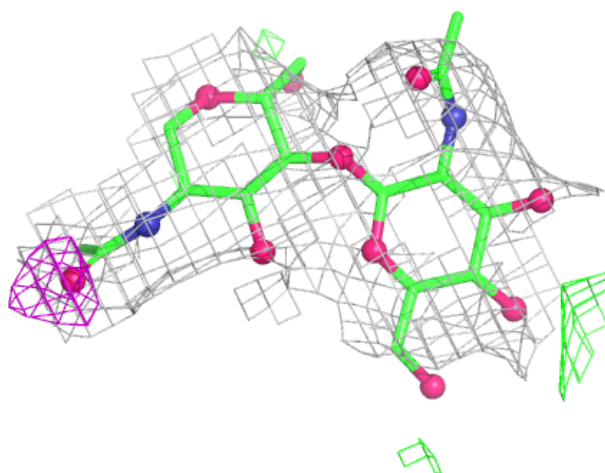
Electron density around Chain H:

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



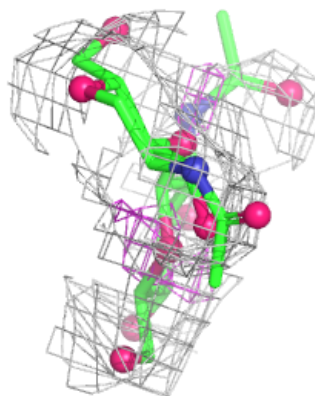
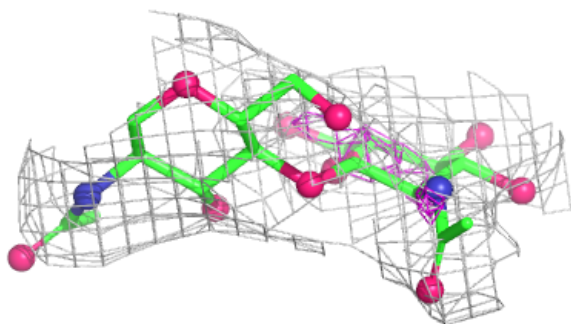
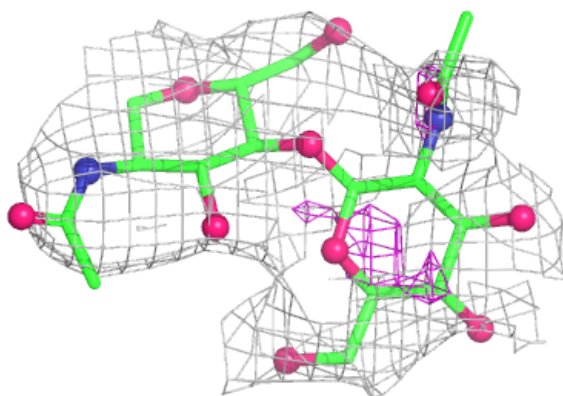
Electron density around Chain I:

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

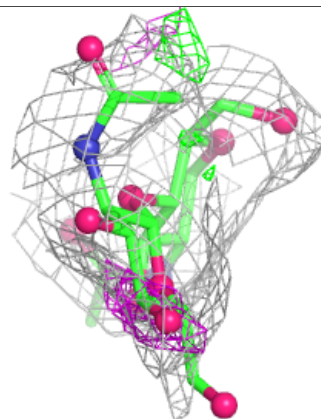
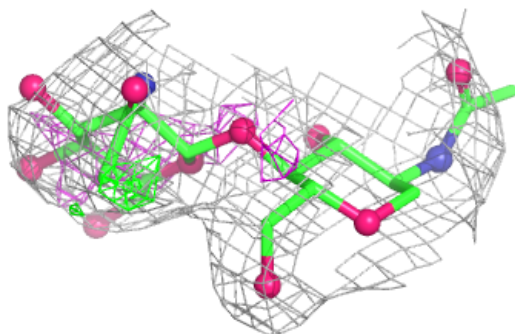
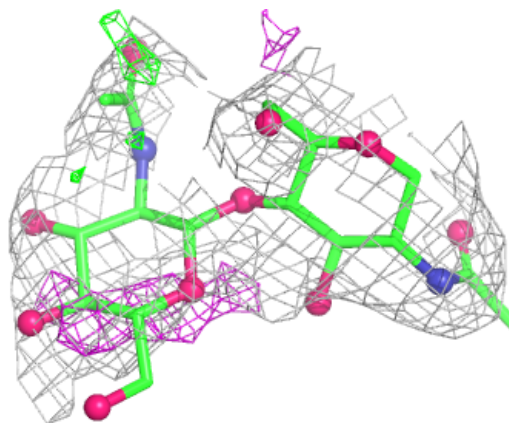


Electron density around Chain J:

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

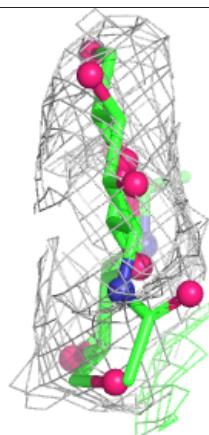
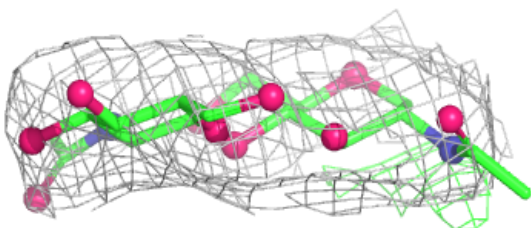
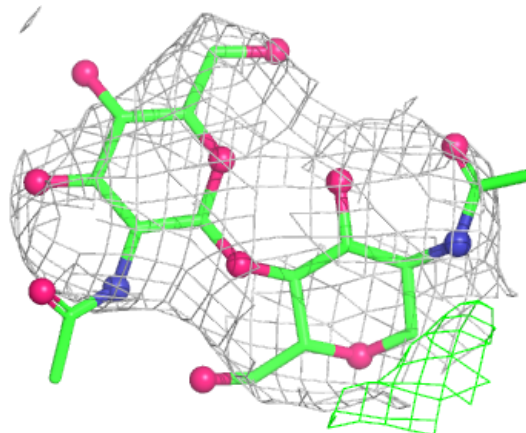
**Electron density around Chain K:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

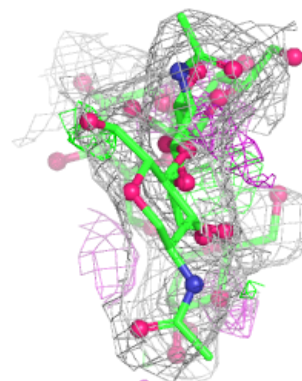
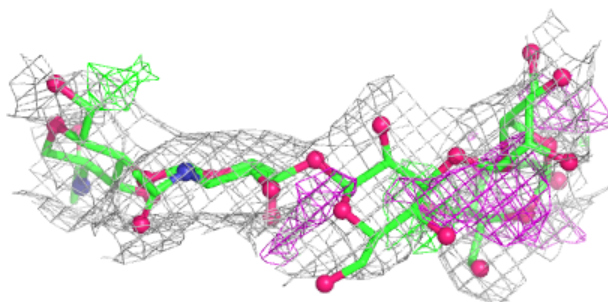
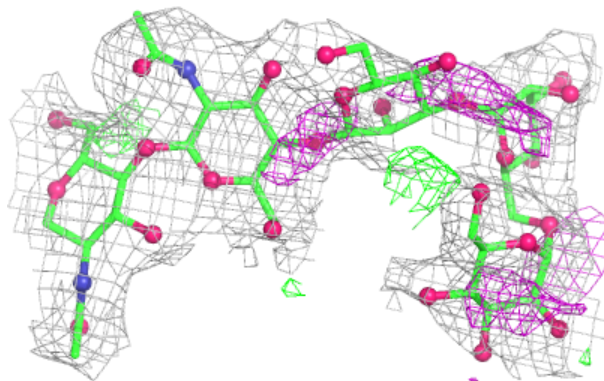


Electron density around Chain L:

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

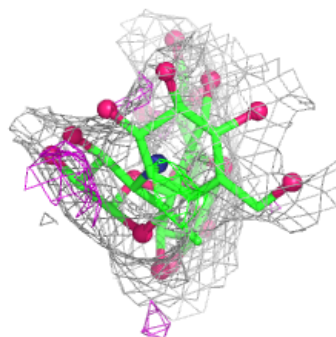
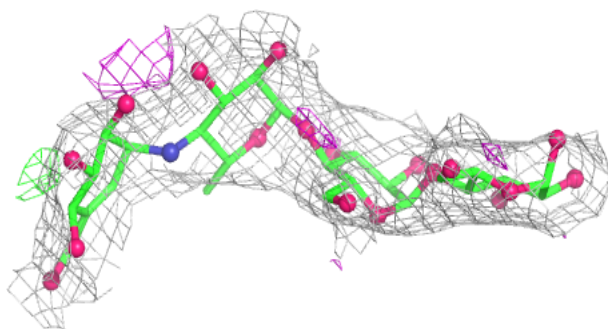
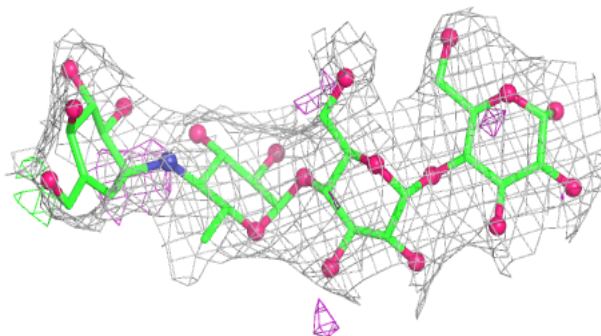
**Electron density around Chain F:**

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

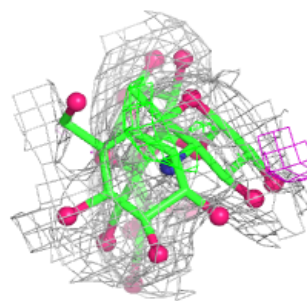
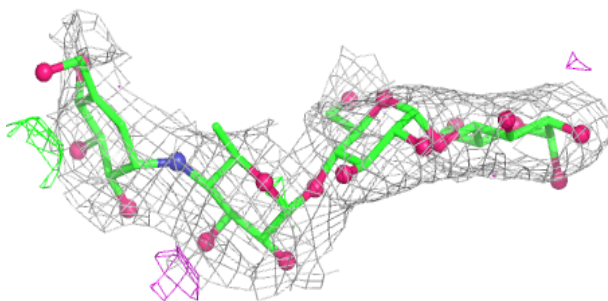
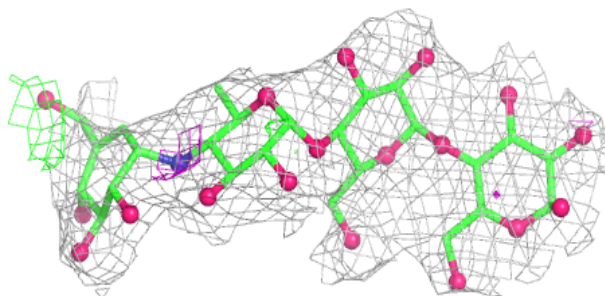


Electron density around Chain M:

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

**Electron density around Chain N:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	814	14/15	0.54	0.23	76,78,79,80	0
5	NAG	A	808	14/15	0.80	0.18	85,86,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.