



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 5AVA / pdb_00005ava
Title : Crystal structure of PHA-E lectin in complex with bisected glycan
Authors : Nagae, M.; Yamaguchi, Y.
Deposited on : 2015-06-12
Resolution : 3.00 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

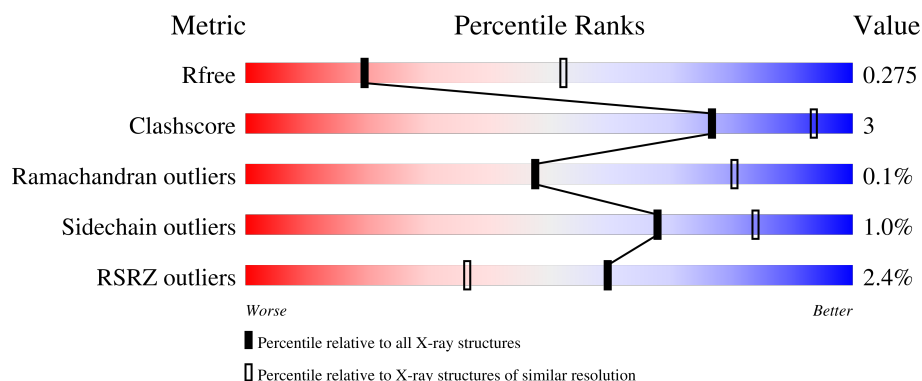
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



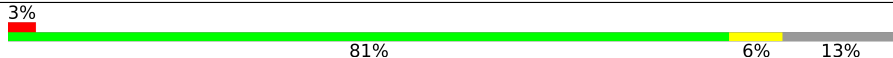
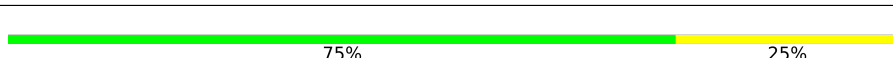
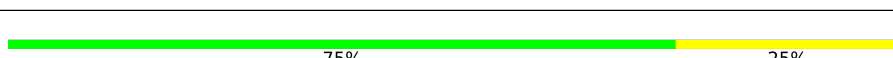
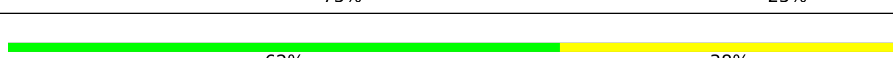
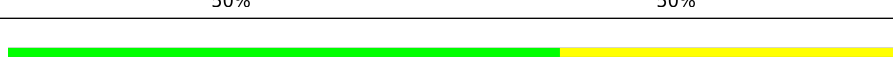
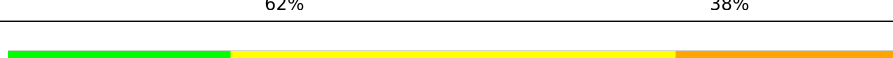
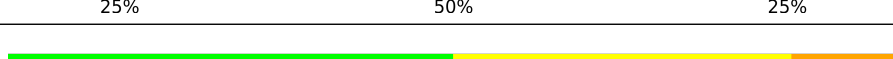
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	275	2% 78% 8% 13%
1	B	275	% 77% 9% 13%
1	C	275	2% 80% 6% 13%
1	D	275	2% 80% 7% 13%
1	E	275	% 81% 5% 13%

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Mol	Chain	Length	Quality of chain
1	F	275	 % 77% 9% 13%
1	G	275	 4% 77% 9% 13%
1	H	275	 3% 81% 6% 13%
2	I	8	 75% 25%
2	J	8	 50% 38% 12%
2	K	8	 75% 25%
2	L	8	 62% 38%
2	M	8	 50% 50%
2	N	8	 62% 38%
2	O	8	 25% 50% 25%
2	P	8	 50% 38% 12%

2 Entry composition [i](#)

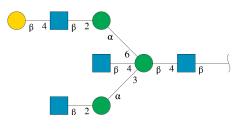
There are 5 unique types of molecules in this entry. The entry contains 15504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Erythroagglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	B	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	C	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	D	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	E	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	F	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	G	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	H	238	Total	C	N	O	0	0	0
			1832	1169	300	363			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	J	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	K	8	Total	C	N	O	0	0	0
			100	56	4	40			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	M	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	N	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	O	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	P	8	Total	C	N	O	0	0	0
			100	56	4	40			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

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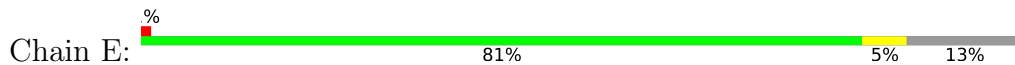
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0
4	G	1	Total 1	Ca 1	0	0
4	H	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	4	Total 4	O 4	0	0
5	C	4	Total 4	O 4	0	0
5	D	4	Total 4	O 4	0	0
5	E	4	Total 4	O 4	0	0
5	F	4	Total 4	O 4	0	0
5	G	4	Total 4	O 4	0	0
5	H	4	Total 4	O 4	0	0

THR
SER
GLU
ALA
LEU
ASN
LEU
ALA
PHE
ASN
LEU
GLN
LEU

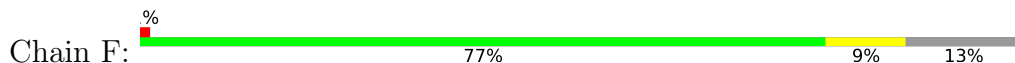
• Molecule 1: Erythroagglutinin



MET ALA SER SER ASN LEU LEU SER LEU ALA ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 L53 G68 Y72 S73 A74 I78 N102 A106 A143 L149 D164 S170 T173 E185 L196 V202 D257 G258 T259 THR SER GLU ALA

LEU ASN LEU LEU ALA ALA PHE LEU LEU ASN LEU ASN GLN ILE LEU

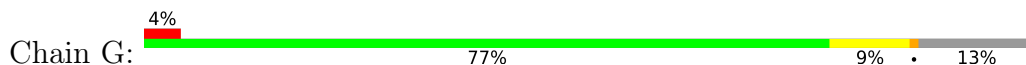
• Molecule 1: Erythroagglutinin



MET ALA SER SER ASN LEU LEU SER LEU ALA ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 T25 Q30 L51 R52 L53 G68 I78 W79 P105 A106 D107 V112 Q119 D122 L126 L129 A143 T148 L149 Y150 N151 D155 P156 K157

L196 V226 I246 S256 D257 G258 T259 THR SER GLU ALA LEU LEU THR HIS ALA ASN PHE LEU ALA ASN SER A22 S23 Q24 L51 R52 L53 T54 G68 Y72 S73 A74 I78 F95 N101 N102 P105 A106 D107 V112 L113 L126 L129 F130 T148 L149 H153

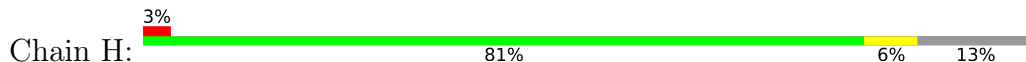
• Molecule 1: Erythroagglutinin



MET ALA SER SER ASN LEU LEU SER LEU ALA ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 S23 Q24 L51 R52 L53 T54 G68 Y72 S73 A74 I78 F95 N101 N102 P105 A106 D107 V112 L113 L126 L129 F130 T148 L149 H153

P204 V228 A232 T236 T237 N240 N244 D245 I246 K254 L255 S256 D257 G258 T259 THR SER GLU ALA LEU LEU ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 S23 Q24 L51 R52 L53 T54 G68 Y72 S73 A74 I78 F95 N101 N102 P105 A106 D107 V112 L113 L126 L129 F130 T148 L149 H153

• Molecule 1: Erythroagglutinin



MET ALA SER SER ASN LEU LEU SER LEU ALA ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 L51 F62 Y72 S73 A74 P105 V112 L126 L129 F130 T148 L149 N150 N151 V152 H153 V202 Y203 P204 S209 T233 T237 T243 T246

G258 T259 THR SER GLU ALA LEU LEU ASN PHE LEU VAL LEU LEU THR HIS ALA ASN SER A22 S23 Q24 L51 R52 L53 T54 G68 Y72 S73 A74 I78 F95 N101 N102 P105 A106 D107 V112 L113 L126 L129 F130 T148 L149 H153

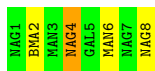
• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  75% 25%



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

Chain J:  50% 38% 12%



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

Chain K:  75% 25%



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

Chain L:  62% 38%



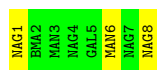
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

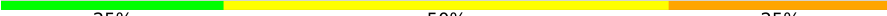


- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  62% 38%



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

Chain O:  25% 50% 25%



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

Chain P:  50% 38% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.21Å 122.84Å 97.66Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 97.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-3.00) 99.8 (97.66-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.24 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.229 , 0.274 0.229 , 0.275	Depositor DCC
R_{free} test set	2268 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 7.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.019 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15504	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: NAG, CA, GAL, MAN, BMA, MN

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	0.41	0/1874	0.72	0/2559
1	B	0.43	0/1874	0.72	1/2559 (0.0%)
1	C	0.41	0/1874	0.71	0/2559
1	D	0.41	0/1874	0.72	0/2559
1	E	0.43	0/1874	0.72	0/2559
1	F	0.42	0/1874	0.71	0/2559
1	G	0.41	0/1874	0.70	1/2559 (0.0%)
1	H	0.44	0/1874	0.72	0/2559
All	All	0.42	0/14992	0.72	2/20472 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	112	VAL	N-CA-C	5.09	116.05	108.46
1	B	160	HIS	N-CA-C	5.01	116.60	109.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1832	0	1796	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1832	0	1796	13	0
1	C	1832	0	1796	9	0
1	D	1832	0	1796	10	0
1	E	1832	0	1796	9	0
1	F	1832	0	1796	16	0
1	G	1832	0	1796	15	0
1	H	1832	0	1796	8	0
2	I	100	0	85	0	0
2	J	100	0	85	1	0
2	K	100	0	85	0	0
2	L	100	0	85	1	0
2	M	100	0	85	0	0
2	N	100	0	85	0	0
2	O	100	0	85	3	0
2	P	100	0	85	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
All	All	15504	0	15048	89	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 3.

The worst 5 of 89 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:202:VAL:HG12	1:A:209:SER:HB3	1.70	0.72
1:A:58:ASP:HB3	1:F:119:GLN:HG3	1.78	0.65
1:F:196:LEU:HD22	1:H:204:PRO:HA	1.83	0.61
1:B:78:ILE:HG22	1:B:79:TRP:HD1	1.67	0.59
1:F:22:ALA:HB3	1:F:256:SER:HA	1.85	0.58

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	236/275 (86%)	227 (96%)	8 (3%)	1 (0%)	30	65
1	B	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
1	C	236/275 (86%)	226 (96%)	10 (4%)	0	100	100
1	D	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
1	E	236/275 (86%)	222 (94%)	14 (6%)	0	100	100
1	F	236/275 (86%)	223 (94%)	13 (6%)	0	100	100
1	G	236/275 (86%)	227 (96%)	9 (4%)	0	100	100
1	H	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
All	All	1888/2200 (86%)	1800 (95%)	87 (5%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA

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	207/238 (87%)	207 (100%)	0	100	100
1	B	207/238 (87%)	203 (98%)	4 (2%)	50	76
1	C	207/238 (87%)	203 (98%)	4 (2%)	50	76
1	D	207/238 (87%)	205 (99%)	2 (1%)	68	84
1	E	207/238 (87%)	207 (100%)	0	100	100
1	F	207/238 (87%)	205 (99%)	2 (1%)	68	84
1	G	207/238 (87%)	205 (99%)	2 (1%)	68	84
1	H	207/238 (87%)	205 (99%)	2 (1%)	68	84
All	All	1656/1904 (87%)	1640 (99%)	16 (1%)	68	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	237	THR
1	G	107	ASP
1	D	103	SER
1	G	78	ILE
1	C	205	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	240	ASN
1	H	240	ASN
1	G	30	GLN
1	G	153	HIS
1	C	153	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

56 non-standard protein/DNA/RNA residues 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	N	4	2	14,14,15	0.48	0	17,19,21	0.80	0
2	MAN	N	3	2	11,11,12	0.60	0	15,15,17	0.62	0
2	NAG	I	1	2	14,14,15	0.54	0	17,19,21	0.94	0
2	NAG	P	8	2	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
2	NAG	I	7	2	14,14,15	0.47	0	17,19,21	0.85	0
2	MAN	L	6	2	11,11,12	0.49	0	15,15,17	1.18	1 (6%)
2	NAG	I	4	2	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
2	NAG	J	4	2	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
2	GAL	L	5	2	11,11,12	0.58	0	15,15,17	0.58	0
2	NAG	L	1	2	14,14,15	0.51	0	17,19,21	0.88	0
2	NAG	K	7	2	14,14,15	0.51	0	17,19,21	0.70	0
2	GAL	M	5	2	11,11,12	0.65	0	15,15,17	0.76	0
2	NAG	J	7	2	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	L	8	2	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
2	NAG	N	7	2	14,14,15	0.48	0	17,19,21	1.03	0
2	NAG	P	7	2	14,14,15	0.52	0	17,19,21	0.59	0
2	NAG	K	1	2	14,14,15	0.50	0	17,19,21	0.98	0
2	NAG	N	8	2	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
2	MAN	N	6	2	11,11,12	0.53	0	15,15,17	0.85	1 (6%)
2	MAN	M	3	2	11,11,12	0.59	0	15,15,17	0.98	1 (6%)
2	MAN	I	6	2	11,11,12	0.48	0	15,15,17	1.07	1 (6%)
2	NAG	P	1	2	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
2	NAG	I	8	2	14,14,15	0.46	0	17,19,21	0.73	0
2	NAG	K	8	2	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	GAL	J	5	2	11,11,12	0.61	0	15,15,17	0.64	0
2	NAG	K	4	2	14,14,15	0.52	0	17,19,21	0.84	0
2	NAG	L	7	2	14,14,15	0.53	0	17,19,21	0.79	0
2	NAG	N	1	2	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
2	NAG	M	7	2	14,14,15	0.50	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	M	6	2	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
2	MAN	J	3	2	11,11,12	0.61	0	15,15,17	0.76	0
2	NAG	P	4	2	14,14,15	0.55	0	17,19,21	1.14	3 (17%)
2	MAN	K	3	2	11,11,12	0.62	0	15,15,17	0.62	0
2	NAG	O	4	2	14,14,15	0.49	0	17,19,21	0.93	0
2	MAN	I	3	2	11,11,12	0.68	0	15,15,17	0.88	0
2	NAG	O	7	2	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
2	MAN	P	3	2	11,11,12	0.63	0	15,15,17	0.85	0
2	MAN	O	3	2	11,11,12	0.65	0	15,15,17	0.61	0
2	GAL	N	5	2	11,11,12	0.59	0	15,15,17	0.59	0
2	NAG	M	1	2	14,14,15	0.53	0	17,19,21	0.87	0
2	NAG	L	4	2	14,14,15	0.50	0	17,19,21	0.88	0
2	MAN	O	6	2	11,11,12	0.51	0	15,15,17	1.06	1 (6%)
2	NAG	M	4	2	14,14,15	0.45	0	17,19,21	0.80	0
2	NAG	M	8	2	14,14,15	0.39	0	17,19,21	1.37	1 (5%)
2	MAN	J	6	2	11,11,12	0.51	0	15,15,17	1.68	1 (6%)
2	GAL	O	5	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	K	6	2	11,11,12	0.51	0	15,15,17	0.88	1 (6%)
2	NAG	O	1	2	14,14,15	0.53	0	17,19,21	1.12	1 (5%)
2	MAN	P	6	2	11,11,12	0.56	0	15,15,17	0.71	0
2	GAL	I	5	2	11,11,12	0.60	0	15,15,17	0.57	0
2	GAL	K	5	2	11,11,12	0.59	0	15,15,17	0.63	0
2	NAG	O	8	2	14,14,15	0.37	0	17,19,21	1.31	1 (5%)
2	NAG	J	1	2	14,14,15	0.54	0	17,19,21	0.88	0
2	MAN	L	3	2	11,11,12	0.62	0	15,15,17	0.59	0
2	GAL	P	5	2	11,11,12	0.60	0	15,15,17	0.77	1 (6%)
2	NAG	J	8	2	14,14,15	0.49	0	17,19,21	1.30	2 (11%)

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	N	4	2	-	0/6/23/26	0/1/1/1
2	MAN	N	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	NAG	P	8	2	-	0/6/23/26	0/1/1/1
2	NAG	I	7	2	-	2/6/23/26	0/1/1/1
2	MAN	L	6	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	4	2	-	0/6/23/26	0/1/1/1
2	NAG	J	4	2	-	2/6/23/26	0/1/1/1
2	GAL	L	5	2	-	2/2/19/22	0/1/1/1
2	NAG	L	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	7	2	-	2/6/23/26	0/1/1/1
2	GAL	M	5	2	-	2/2/19/22	0/1/1/1
2	NAG	J	7	2	-	2/6/23/26	0/1/1/1
2	NAG	L	8	2	-	0/6/23/26	0/1/1/1
2	NAG	N	7	2	-	2/6/23/26	0/1/1/1
2	NAG	P	7	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2	-	2/6/23/26	0/1/1/1
2	NAG	N	8	2	-	0/6/23/26	0/1/1/1
2	MAN	N	6	2	-	0/2/19/22	0/1/1/1
2	MAN	M	3	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	1/2/19/22	0/1/1/1
2	NAG	P	1	2	-	0/6/23/26	0/1/1/1
2	NAG	I	8	2	-	0/6/23/26	0/1/1/1
2	NAG	K	8	2	-	0/6/23/26	0/1/1/1
2	GAL	J	5	2	-	2/2/19/22	0/1/1/1
2	NAG	K	4	2	-	0/6/23/26	0/1/1/1
2	NAG	L	7	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2	-	2/6/23/26	0/1/1/1
2	NAG	M	7	2	-	2/6/23/26	0/1/1/1
2	MAN	M	6	2	-	2/2/19/22	0/1/1/1
2	MAN	J	3	2	-	0/2/19/22	0/1/1/1
2	NAG	P	4	2	-	0/6/23/26	0/1/1/1
2	MAN	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	O	4	2	-	0/6/23/26	0/1/1/1
2	MAN	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	O	7	2	-	2/6/23/26	0/1/1/1
2	MAN	P	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	3	2	-	0/2/19/22	0/1/1/1
2	GAL	N	5	2	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2	-	0/6/23/26	0/1/1/1
2	NAG	L	4	2	-	0/6/23/26	0/1/1/1
2	MAN	O	6	2	-	1/2/19/22	0/1/1/1
2	NAG	M	4	2	-	0/6/23/26	0/1/1/1
2	NAG	M	8	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	J	6	2	-	2/2/19/22	0/1/1/1
2	GAL	O	5	2	-	2/2/19/22	0/1/1/1
2	MAN	K	6	2	-	2/2/19/22	0/1/1/1
2	NAG	O	1	2	-	1/6/23/26	0/1/1/1
2	MAN	P	6	2	-	1/2/19/22	0/1/1/1
2	GAL	I	5	2	-	2/2/19/22	0/1/1/1
2	GAL	K	5	2	-	2/2/19/22	0/1/1/1
2	NAG	O	8	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2	-	0/6/23/26	0/1/1/1
2	MAN	L	3	2	-	0/2/19/22	0/1/1/1
2	GAL	P	5	2	-	2/2/19/22	0/1/1/1
2	NAG	J	8	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	6	MAN	C1-O5-C5	5.53	119.60	112.19
2	M	8	NAG	C1-O5-C5	4.63	118.40	112.19
2	O	8	NAG	C1-O5-C5	4.57	118.31	112.19
2	K	8	NAG	C1-O5-C5	3.97	117.51	112.19
2	J	8	NAG	C1-O5-C5	3.46	116.83	112.19

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	L	7	NAG	O5-C5-C6-O6
2	O	8	NAG	O5-C5-C6-O6
2	J	7	NAG	C4-C5-C6-O6
2	O	8	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	4	NAG	1	0
2	P	4	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	4	NAG	1	0
2	L	4	NAG	1	0
2	O	6	MAN	1	0
2	O	5	GAL	1	0
2	O	8	NAG	1	0

5.5 Carbohydrates [i](#)

64 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	I	1	2	14,14,15	0.54	0	17,19,21	0.94	0
2	BMA	I	2	2	11,11,12	0.63	0	15,15,17	0.66	0
2	MAN	I	3	2	11,11,12	0.68	0	15,15,17	0.88	0
2	NAG	I	4	2	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
2	GAL	I	5	2	11,11,12	0.60	0	15,15,17	0.57	0
2	MAN	I	6	2	11,11,12	0.48	0	15,15,17	1.07	1 (6%)
2	NAG	I	7	2	14,14,15	0.47	0	17,19,21	0.85	0
2	NAG	I	8	2	14,14,15	0.46	0	17,19,21	0.73	0
2	NAG	J	1	2	14,14,15	0.54	0	17,19,21	0.88	0
2	BMA	J	2	2	11,11,12	0.57	0	15,15,17	0.80	1 (6%)
2	MAN	J	3	2	11,11,12	0.61	0	15,15,17	0.76	0
2	NAG	J	4	2	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
2	GAL	J	5	2	11,11,12	0.61	0	15,15,17	0.64	0
2	MAN	J	6	2	11,11,12	0.51	0	15,15,17	1.68	1 (6%)
2	NAG	J	7	2	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	J	8	2	14,14,15	0.49	0	17,19,21	1.30	2 (11%)
2	NAG	K	1	2	14,14,15	0.50	0	17,19,21	0.98	0
2	BMA	K	2	2	11,11,12	0.59	0	15,15,17	0.71	0
2	MAN	K	3	2	11,11,12	0.62	0	15,15,17	0.62	0
2	NAG	K	4	2	14,14,15	0.52	0	17,19,21	0.84	0
2	GAL	K	5	2	11,11,12	0.59	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	6	2	11,11,12	0.51	0	15,15,17	0.88	1 (6%)
2	NAG	K	7	2	14,14,15	0.51	0	17,19,21	0.70	0
2	NAG	K	8	2	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	NAG	L	1	2	14,14,15	0.51	0	17,19,21	0.88	0
2	BMA	L	2	2	11,11,12	0.53	0	15,15,17	0.59	0
2	MAN	L	3	2	11,11,12	0.62	0	15,15,17	0.59	0
2	NAG	L	4	2	14,14,15	0.50	0	17,19,21	0.88	0
2	GAL	L	5	2	11,11,12	0.58	0	15,15,17	0.58	0
2	MAN	L	6	2	11,11,12	0.49	0	15,15,17	1.18	1 (6%)
2	NAG	L	7	2	14,14,15	0.53	0	17,19,21	0.79	0
2	NAG	L	8	2	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
2	NAG	M	1	2	14,14,15	0.53	0	17,19,21	0.87	0
2	BMA	M	2	2	11,11,12	0.54	0	15,15,17	0.74	0
2	MAN	M	3	2	11,11,12	0.59	0	15,15,17	0.98	1 (6%)
2	NAG	M	4	2	14,14,15	0.45	0	17,19,21	0.80	0
2	GAL	M	5	2	11,11,12	0.65	0	15,15,17	0.76	0
2	MAN	M	6	2	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
2	NAG	M	7	2	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
2	NAG	M	8	2	14,14,15	0.39	0	17,19,21	1.37	1 (5%)
2	NAG	N	1	2	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
2	BMA	N	2	2	11,11,12	0.54	0	15,15,17	0.63	0
2	MAN	N	3	2	11,11,12	0.60	0	15,15,17	0.62	0
2	NAG	N	4	2	14,14,15	0.48	0	17,19,21	0.80	0
2	GAL	N	5	2	11,11,12	0.59	0	15,15,17	0.59	0
2	MAN	N	6	2	11,11,12	0.53	0	15,15,17	0.85	1 (6%)
2	NAG	N	7	2	14,14,15	0.48	0	17,19,21	1.03	0
2	NAG	N	8	2	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
2	NAG	O	1	2	14,14,15	0.53	0	17,19,21	1.12	1 (5%)
2	BMA	O	2	2	11,11,12	0.56	0	15,15,17	0.71	0
2	MAN	O	3	2	11,11,12	0.65	0	15,15,17	0.61	0
2	NAG	O	4	2	14,14,15	0.49	0	17,19,21	0.93	0
2	GAL	O	5	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	O	6	2	11,11,12	0.51	0	15,15,17	1.06	1 (6%)
2	NAG	O	7	2	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
2	NAG	O	8	2	14,14,15	0.37	0	17,19,21	1.31	1 (5%)
2	NAG	P	1	2	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
2	BMA	P	2	2	11,11,12	0.51	0	15,15,17	0.47	0
2	MAN	P	3	2	11,11,12	0.63	0	15,15,17	0.85	0
2	NAG	P	4	2	14,14,15	0.55	0	17,19,21	1.14	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	P	5	2	11,11,12	0.60	0	15,15,17	0.77	1 (6%)
2	MAN	P	6	2	11,11,12	0.56	0	15,15,17	0.71	0
2	NAG	P	7	2	14,14,15	0.52	0	17,19,21	0.59	0
2	NAG	P	8	2	14,14,15	0.47	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	BMA	I	2	2	-	0/2/19/22	0/1/1/1
2	MAN	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	I	4	2	-	0/6/23/26	0/1/1/1
2	GAL	I	5	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	1/2/19/22	0/1/1/1
2	NAG	I	7	2	-	2/6/23/26	0/1/1/1
2	NAG	I	8	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2	-	0/6/23/26	0/1/1/1
2	BMA	J	2	2	-	0/2/19/22	0/1/1/1
2	MAN	J	3	2	-	0/2/19/22	0/1/1/1
2	NAG	J	4	2	-	2/6/23/26	0/1/1/1
2	GAL	J	5	2	-	2/2/19/22	0/1/1/1
2	MAN	J	6	2	-	2/2/19/22	0/1/1/1
2	NAG	J	7	2	-	2/6/23/26	0/1/1/1
2	NAG	J	8	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	2	-	2/6/23/26	0/1/1/1
2	BMA	K	2	2	-	0/2/19/22	0/1/1/1
2	MAN	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	K	4	2	-	0/6/23/26	0/1/1/1
2	GAL	K	5	2	-	2/2/19/22	0/1/1/1
2	MAN	K	6	2	-	2/2/19/22	0/1/1/1
2	NAG	K	7	2	-	2/6/23/26	0/1/1/1
2	NAG	K	8	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2	-	0/6/23/26	0/1/1/1
2	BMA	L	2	2	-	0/2/19/22	0/1/1/1
2	MAN	L	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	4	2	-	0/6/23/26	0/1/1/1
2	GAL	L	5	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	L	6	2	-	0/2/19/22	0/1/1/1
2	NAG	L	7	2	-	2/6/23/26	0/1/1/1
2	NAG	L	8	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2	-	0/6/23/26	0/1/1/1
2	BMA	M	2	2	-	0/2/19/22	0/1/1/1
2	MAN	M	3	2	-	2/2/19/22	0/1/1/1
2	NAG	M	4	2	-	0/6/23/26	0/1/1/1
2	GAL	M	5	2	-	2/2/19/22	0/1/1/1
2	MAN	M	6	2	-	2/2/19/22	0/1/1/1
2	NAG	M	7	2	-	2/6/23/26	0/1/1/1
2	NAG	M	8	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2	-	2/6/23/26	0/1/1/1
2	BMA	N	2	2	-	0/2/19/22	0/1/1/1
2	MAN	N	3	2	-	0/2/19/22	0/1/1/1
2	NAG	N	4	2	-	0/6/23/26	0/1/1/1
2	GAL	N	5	2	-	2/2/19/22	0/1/1/1
2	MAN	N	6	2	-	0/2/19/22	0/1/1/1
2	NAG	N	7	2	-	2/6/23/26	0/1/1/1
2	NAG	N	8	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2	-	1/6/23/26	0/1/1/1
2	BMA	O	2	2	-	0/2/19/22	0/1/1/1
2	MAN	O	3	2	-	0/2/19/22	0/1/1/1
2	NAG	O	4	2	-	0/6/23/26	0/1/1/1
2	GAL	O	5	2	-	2/2/19/22	0/1/1/1
2	MAN	O	6	2	-	1/2/19/22	0/1/1/1
2	NAG	O	7	2	-	2/6/23/26	0/1/1/1
2	NAG	O	8	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	2	-	0/6/23/26	0/1/1/1
2	BMA	P	2	2	-	0/2/19/22	0/1/1/1
2	MAN	P	3	2	-	2/2/19/22	0/1/1/1
2	NAG	P	4	2	-	0/6/23/26	0/1/1/1
2	GAL	P	5	2	-	2/2/19/22	0/1/1/1
2	MAN	P	6	2	-	1/2/19/22	0/1/1/1
2	NAG	P	7	2	-	0/6/23/26	0/1/1/1
2	NAG	P	8	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	J	6	MAN	C1-O5-C5	5.53	119.60	112.19
2	M	8	NAG	C1-O5-C5	4.63	118.40	112.19
2	O	8	NAG	C1-O5-C5	4.57	118.31	112.19
2	K	8	NAG	C1-O5-C5	3.97	117.51	112.19
2	J	8	NAG	C1-O5-C5	3.46	116.83	112.19

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

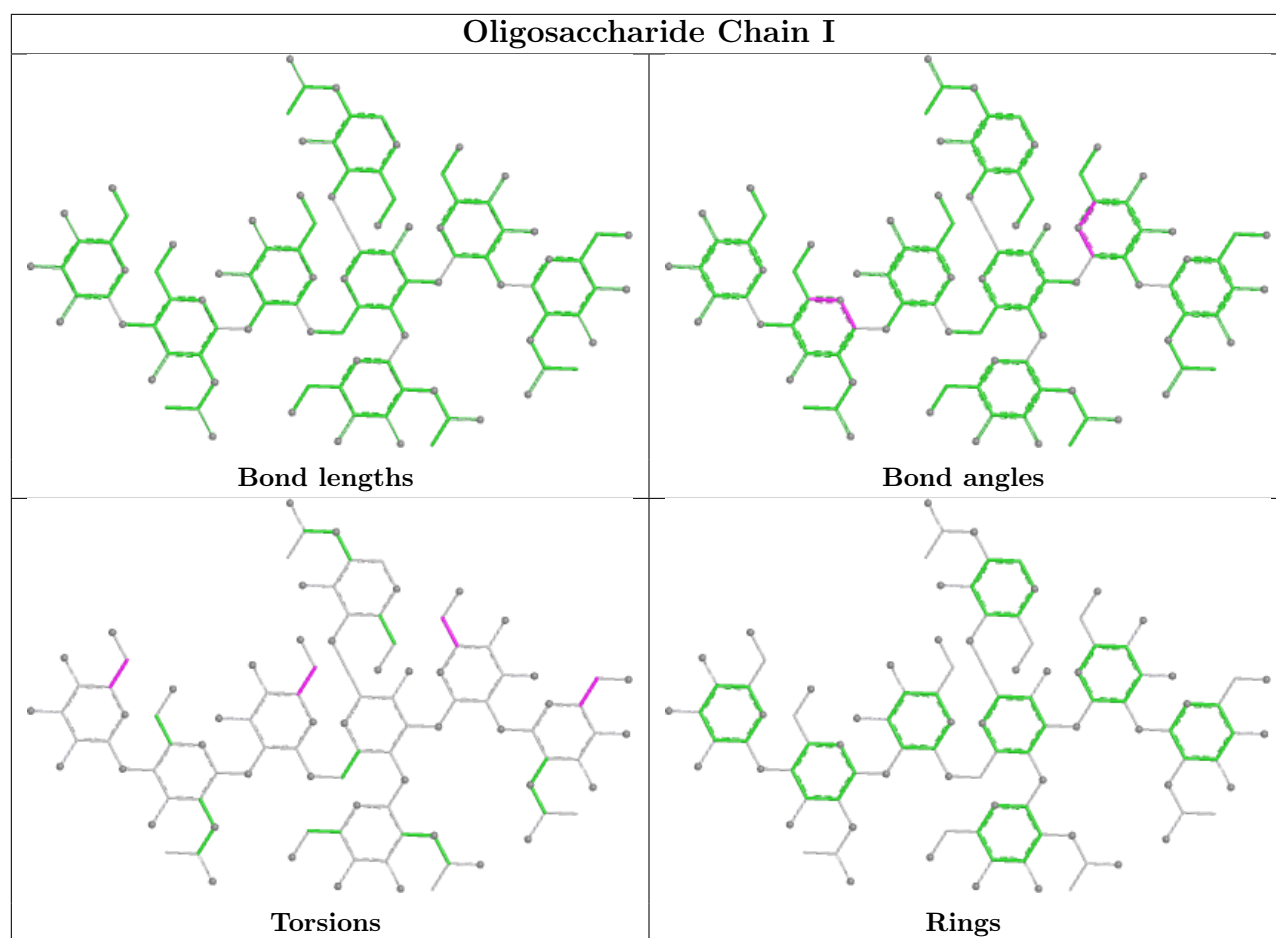
Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	L	7	NAG	O5-C5-C6-O6
2	O	8	NAG	O5-C5-C6-O6
2	J	7	NAG	C4-C5-C6-O6
2	O	8	NAG	C4-C5-C6-O6

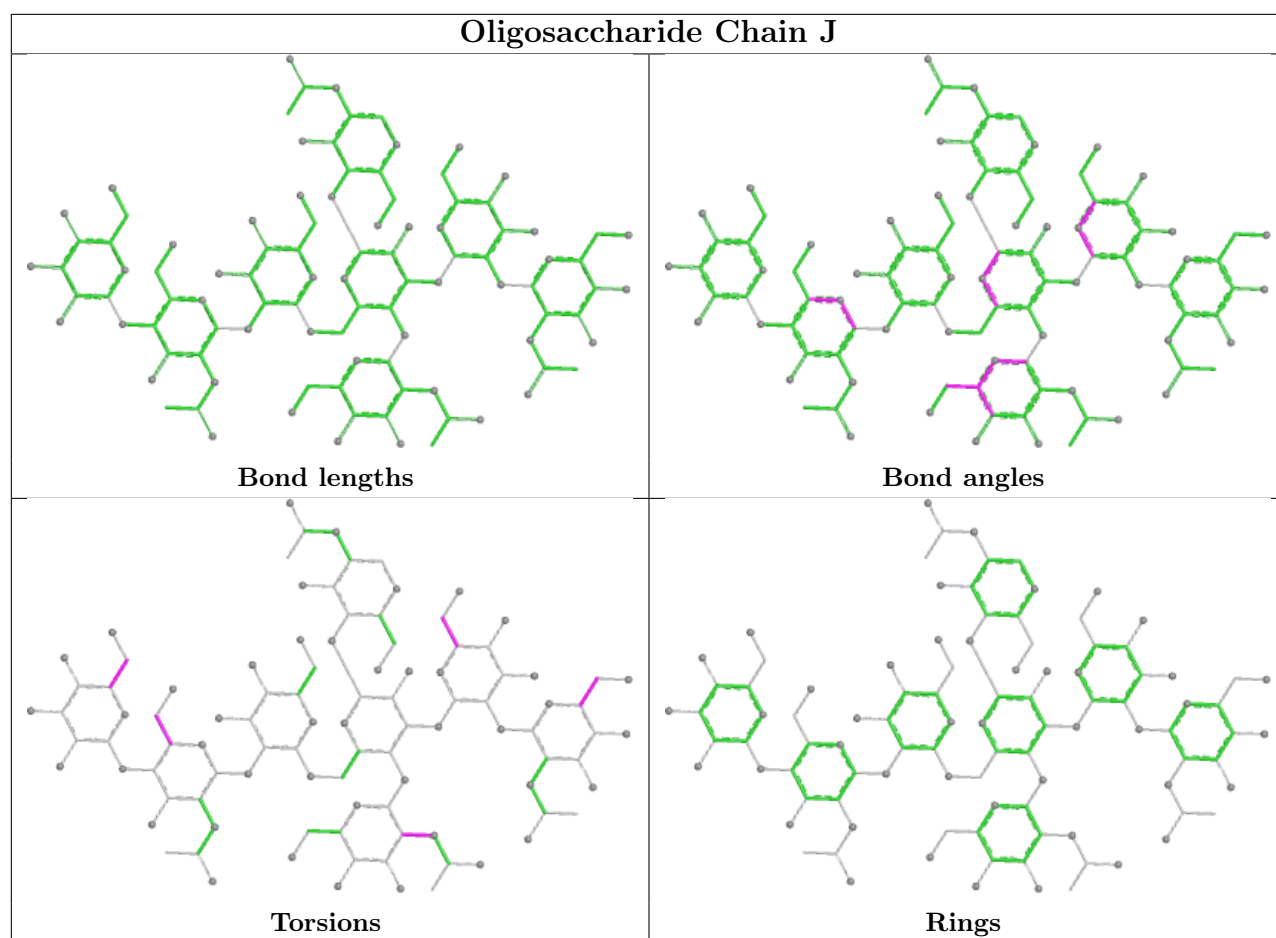
There are no ring outliers.

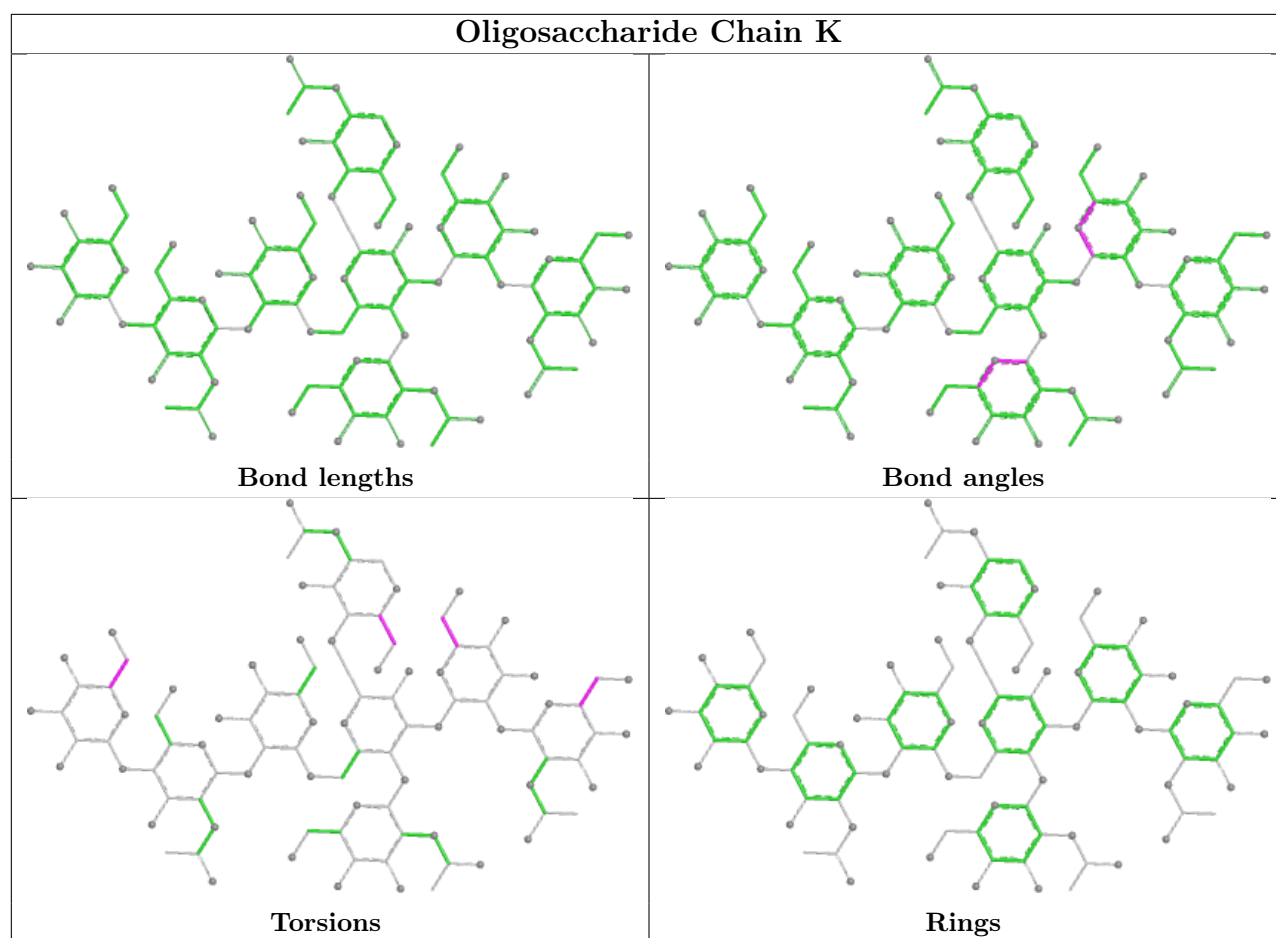
7 monomers are involved in 6 short contacts:

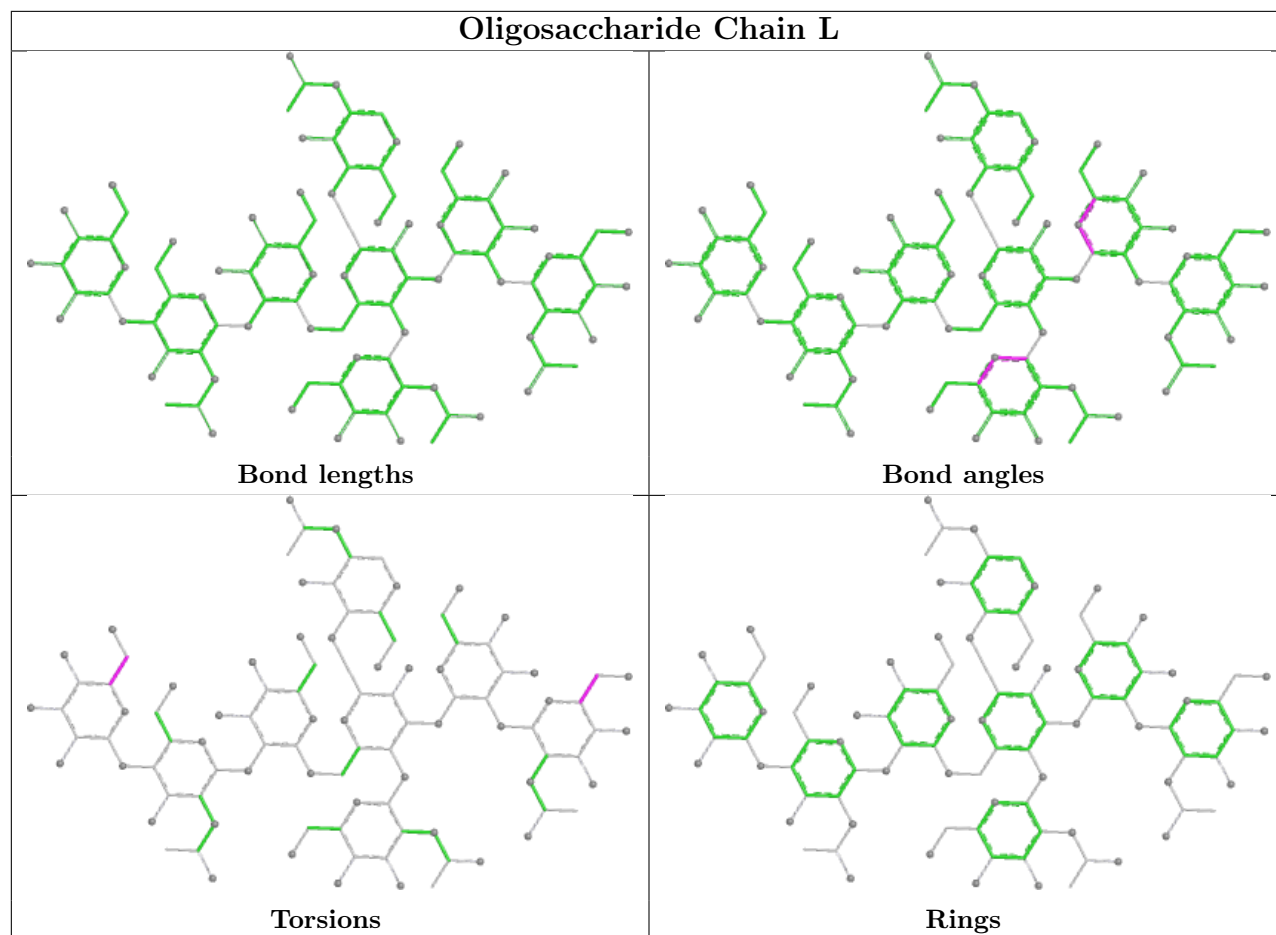
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	4	NAG	1	0
2	O	8	NAG	1	0
2	P	4	NAG	1	0
2	O	4	NAG	1	0
2	L	4	NAG	1	0
2	O	6	MAN	1	0
2	O	5	GAL	1	0

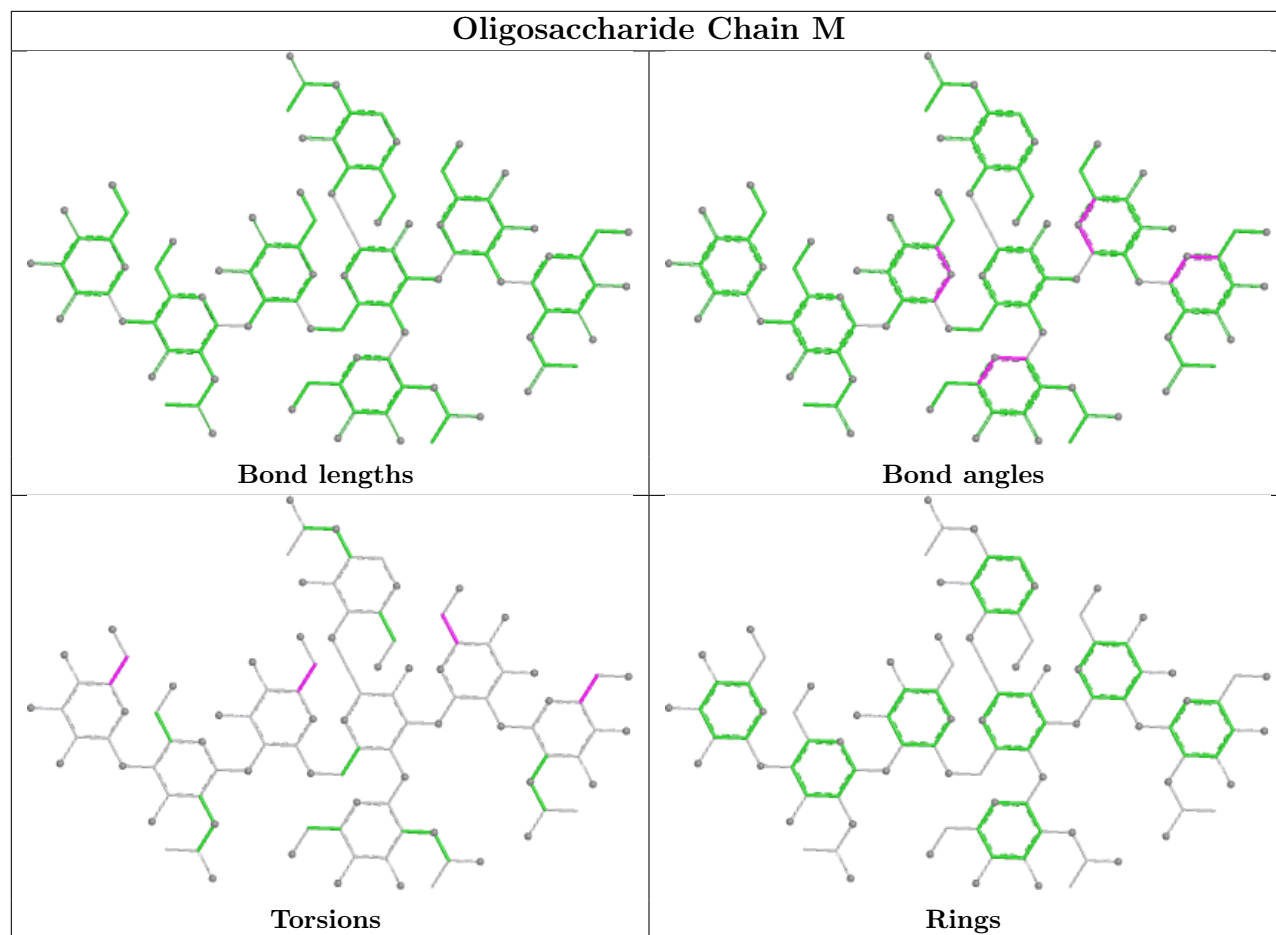
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

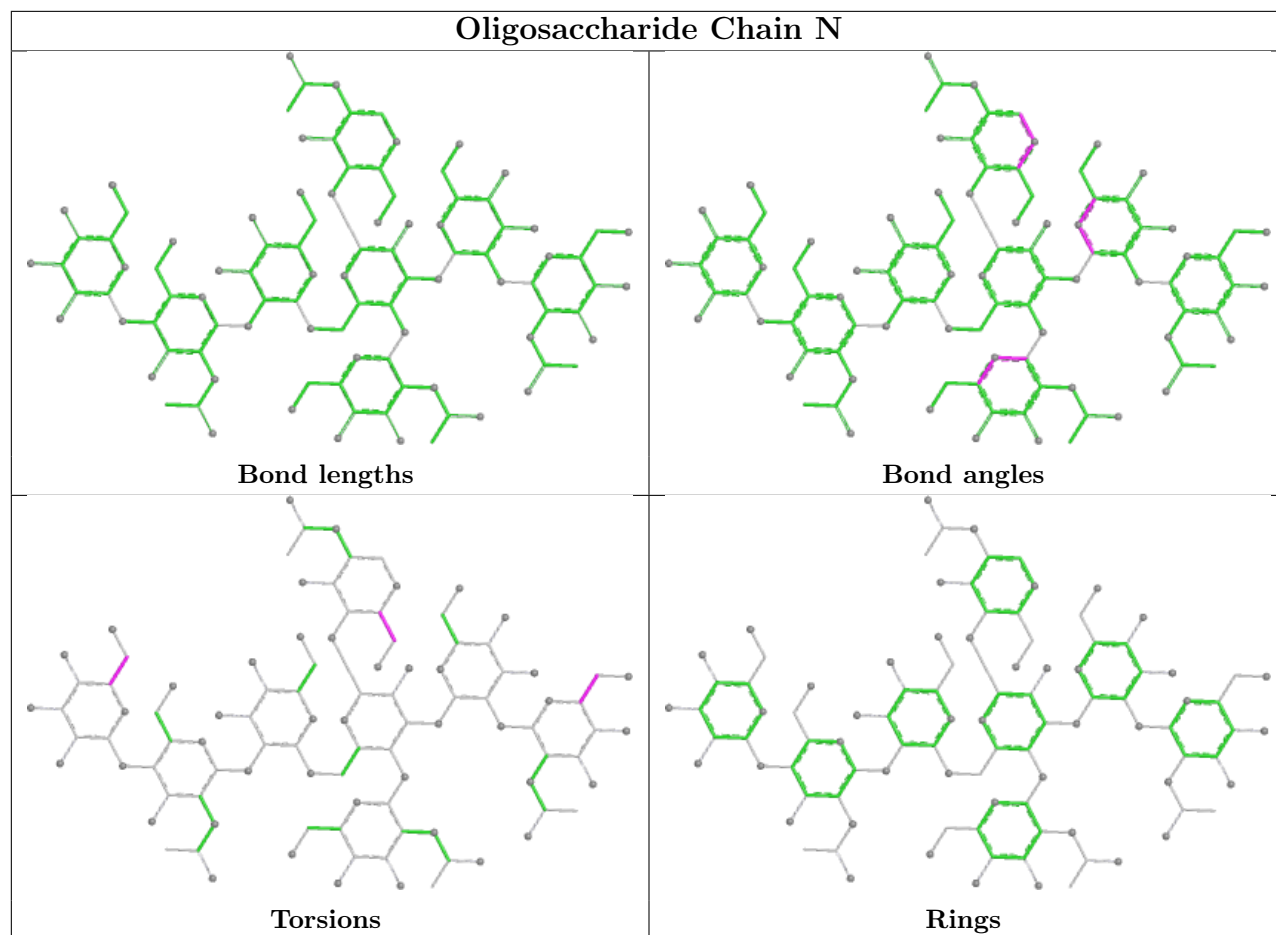


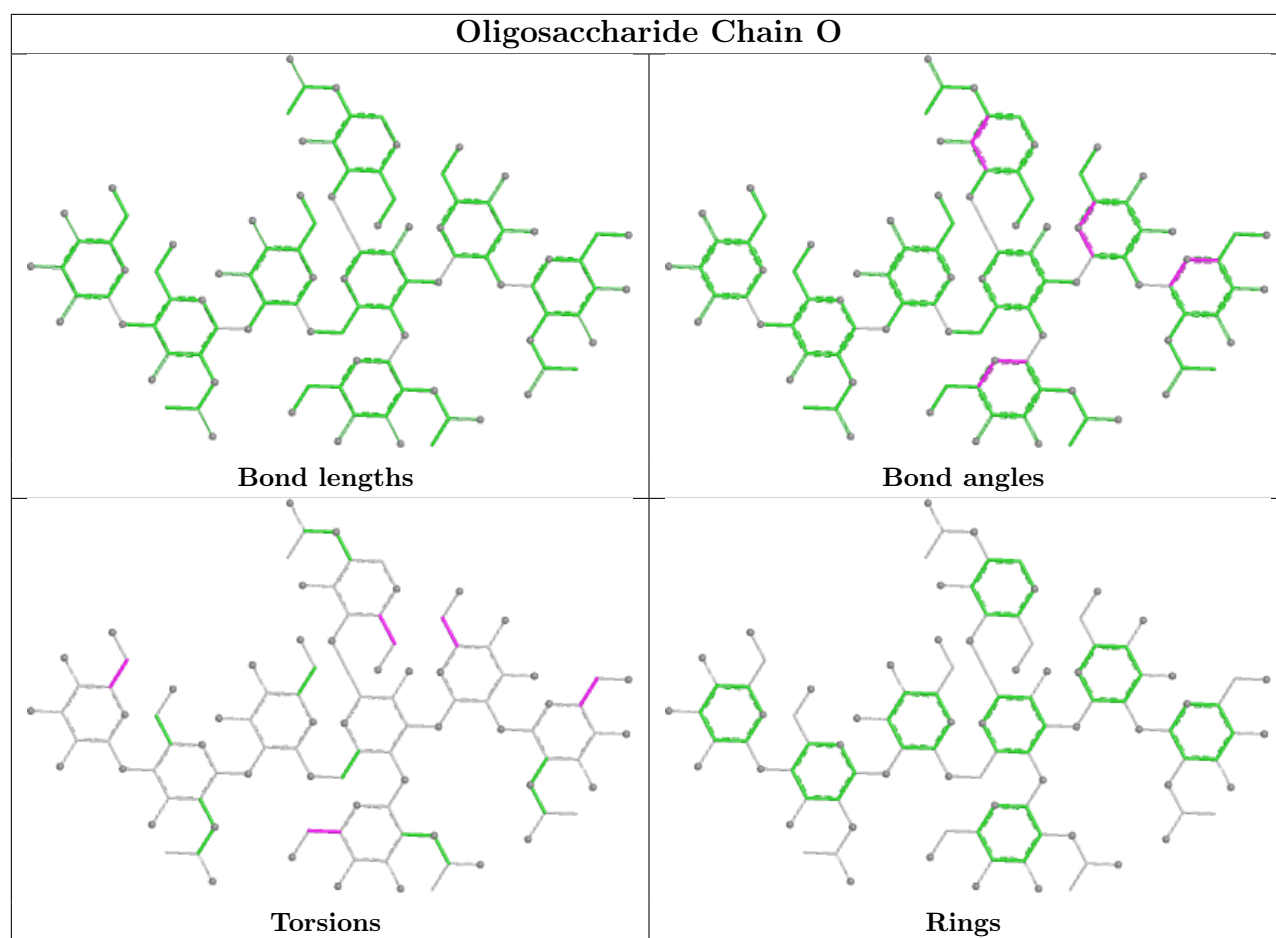


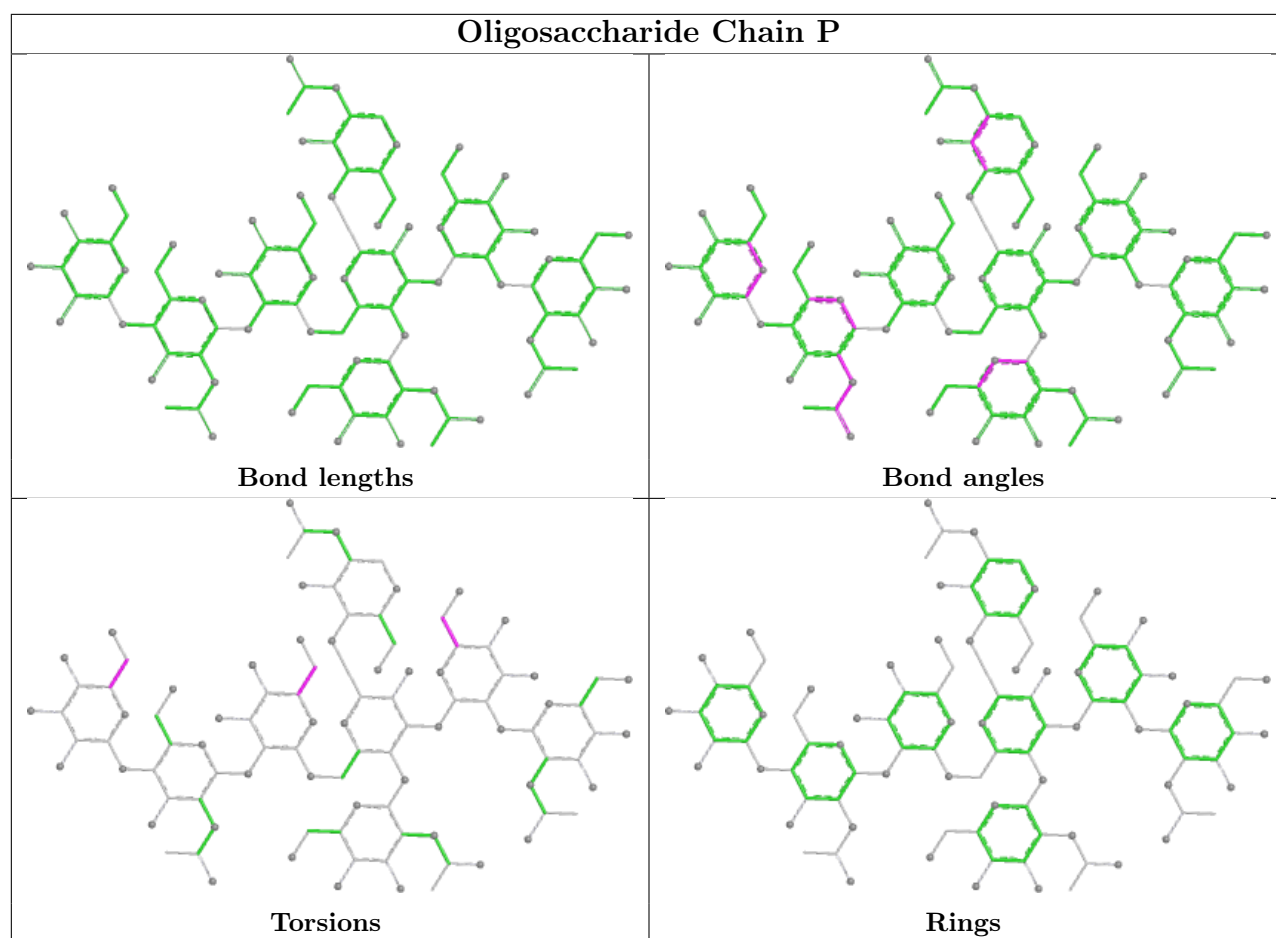












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	238/275 (86%)	-0.26	5 (2%) 63 40	20, 32, 50, 139	0
1	B	238/275 (86%)	-0.17	4 (1%) 69 45	22, 33, 50, 97	0
1	C	238/275 (86%)	-0.00	5 (2%) 63 40	23, 38, 68, 115	0
1	D	238/275 (86%)	-0.03	6 (2%) 58 35	24, 36, 61, 116	0
1	E	238/275 (86%)	-0.26	4 (1%) 69 45	19, 32, 51, 116	0
1	F	238/275 (86%)	-0.12	3 (1%) 75 53	20, 35, 62, 119	0
1	G	238/275 (86%)	0.43	10 (4%) 40 22	25, 50, 82, 131	0
1	H	238/275 (86%)	0.62	8 (3%) 48 27	30, 54, 83, 120	0
All	All	1904/2200 (86%)	0.03	45 (2%) 59 36	19, 37, 73, 139	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	259	THR	5.5
1	F	259	THR	5.1
1	G	258	GLY	4.9
1	C	22	ALA	4.9
1	D	259	THR	4.8

6.2 Non-standard residues in protein, DNA, RNA chains [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	O	7	14/15	0.47	0.15	75,80,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	P	1	14/15	0.53	0.20	84,89,96,97	0
2	NAG	J	1	14/15	0.61	0.17	45,48,49,51	0
2	NAG	O	1	14/15	0.64	0.16	55,60,66,66	0
2	NAG	N	7	14/15	0.66	0.15	83,86,87,90	0
2	NAG	K	1	14/15	0.66	0.16	57,59,61,61	0
2	NAG	L	7	14/15	0.67	0.14	69,72,74,76	0
2	NAG	I	7	14/15	0.69	0.14	66,68,72,73	0
2	NAG	M	7	14/15	0.71	0.13	71,71,72,74	0
2	NAG	N	1	14/15	0.71	0.16	63,66,70,71	0
2	MAN	M	6	11/12	0.71	0.14	66,70,74,76	0
2	MAN	O	6	11/12	0.73	0.14	79,82,86,86	0
2	MAN	K	6	11/12	0.74	0.17	67,69,72,73	0
2	NAG	P	8	14/15	0.75	0.13	69,73,80,81	0
2	MAN	P	6	11/12	0.75	0.14	77,80,82,82	0
2	NAG	P	4	14/15	0.76	0.19	67,71,79,82	0
2	MAN	P	3	11/12	0.77	0.16	78,83,84,85	0
2	MAN	O	3	11/12	0.77	0.16	65,68,69,72	0
2	MAN	I	6	11/12	0.78	0.11	55,56,57,62	0
2	NAG	K	7	14/15	0.79	0.14	62,67,71,72	0
2	MAN	L	6	11/12	0.79	0.10	66,68,70,71	0
2	NAG	M	1	14/15	0.80	0.13	48,54,57,58	0
2	NAG	O	8	14/15	0.80	0.14	57,58,60,60	0
2	MAN	N	6	11/12	0.80	0.12	74,76,77,82	0
2	NAG	J	7	14/15	0.81	0.13	59,61,63,64	0
2	NAG	L	1	14/15	0.81	0.14	53,58,59,60	0
2	NAG	N	8	14/15	0.81	0.14	55,59,61,62	0
2	NAG	P	7	14/15	0.81	0.13	82,84,84,84	0
2	GAL	O	5	11/12	0.82	0.14	64,65,66,66	0
2	NAG	I	1	14/15	0.82	0.11	40,42,43,43	0
2	GAL	P	5	11/12	0.83	0.11	64,66,69,69	0
2	GAL	N	5	11/12	0.83	0.12	54,57,58,59	0
2	MAN	J	6	11/12	0.84	0.11	50,51,52,56	0
2	GAL	K	5	11/12	0.85	0.11	47,49,50,50	0
2	NAG	K	8	14/15	0.86	0.12	48,49,51,53	0
2	GAL	M	5	11/12	0.86	0.12	40,41,41,41	0
2	MAN	N	3	11/12	0.87	0.11	53,55,57,58	0
2	MAN	M	3	11/12	0.88	0.12	47,49,50,50	0
2	NAG	N	4	14/15	0.89	0.11	55,58,62,63	0
2	NAG	M	8	14/15	0.89	0.10	43,44,45,46	0
2	NAG	I	8	14/15	0.89	0.10	39,40,43,45	0
2	MAN	I	3	11/12	0.89	0.11	37,38,38,39	0
2	GAL	L	5	11/12	0.89	0.10	40,41,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	J	8	14/15	0.89	0.11	35,38,40,40	0
2	NAG	O	4	14/15	0.90	0.13	58,61,62,64	0
2	NAG	K	4	14/15	0.90	0.12	45,47,48,49	0
2	MAN	K	3	11/12	0.90	0.11	49,52,53,54	0
2	NAG	L	4	14/15	0.90	0.10	45,47,51,51	0
2	NAG	L	8	14/15	0.91	0.12	51,53,61,63	0
2	GAL	I	5	11/12	0.92	0.10	31,32,33,34	0
2	GAL	J	5	11/12	0.93	0.07	40,42,43,44	0
2	NAG	M	4	14/15	0.93	0.09	42,44,45,46	0
2	MAN	J	3	11/12	0.93	0.10	35,37,38,38	0
2	MAN	L	3	11/12	0.94	0.08	48,50,52,53	0
2	NAG	I	4	14/15	0.94	0.10	34,36,40,41	0
2	NAG	J	4	14/15	0.95	0.10	33,34,35,38	0

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($\text{\AA}^2$)	Q<0.9
2	NAG	O	7	14/15	0.47	0.15	75,80,81,81	0
2	NAG	P	1	14/15	0.53	0.20	84,89,96,97	0
2	NAG	J	1	14/15	0.61	0.17	45,48,49,51	0
2	NAG	O	1	14/15	0.64	0.16	55,60,66,66	0
2	NAG	N	7	14/15	0.66	0.15	83,86,87,90	0
2	NAG	K	1	14/15	0.66	0.16	57,59,61,61	0
2	NAG	L	7	14/15	0.67	0.14	69,72,74,76	0
2	NAG	I	7	14/15	0.69	0.14	66,68,72,73	0
2	NAG	M	7	14/15	0.71	0.13	71,71,72,74	0
2	NAG	N	1	14/15	0.71	0.16	63,66,70,71	0
2	MAN	M	6	11/12	0.71	0.14	66,70,74,76	0
2	MAN	O	6	11/12	0.73	0.14	79,82,86,86	0
2	MAN	K	6	11/12	0.74	0.17	67,69,72,73	0
2	MAN	P	6	11/12	0.75	0.14	77,80,82,82	0
2	NAG	P	8	14/15	0.75	0.13	69,73,80,81	0
2	NAG	P	4	14/15	0.76	0.19	67,71,79,82	0
2	MAN	O	3	11/12	0.77	0.16	65,68,69,72	0
2	BMA	P	2	11/12	0.77	0.12	76,79,83,84	0
2	MAN	P	3	11/12	0.77	0.16	78,83,84,85	0
2	MAN	I	6	11/12	0.78	0.11	55,56,57,62	0

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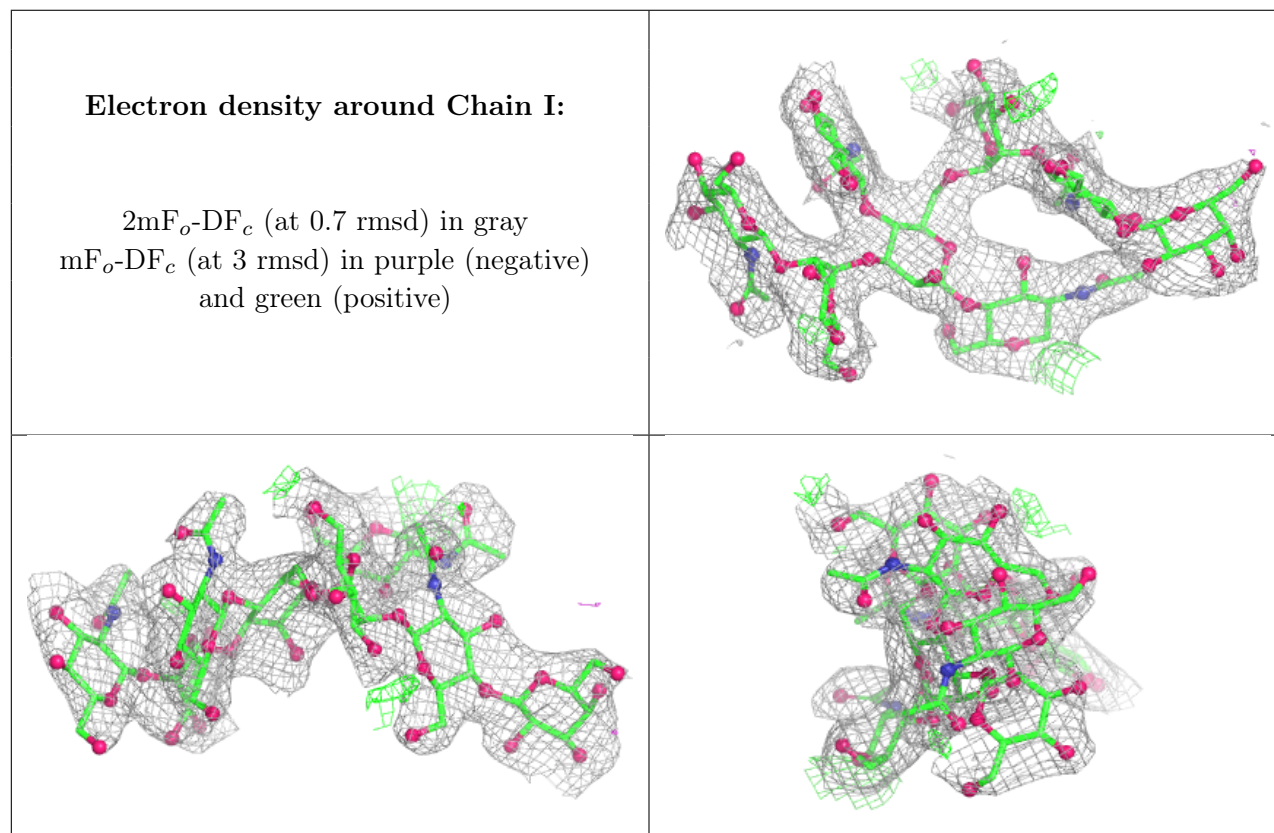
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	L	6	11/12	0.79	0.10	66,68,70,71	0
2	NAG	K	7	14/15	0.79	0.14	62,67,71,72	0
2	MAN	N	6	11/12	0.80	0.12	74,76,77,82	0
2	NAG	M	1	14/15	0.80	0.13	48,54,57,58	0
2	NAG	O	8	14/15	0.80	0.14	57,58,60,60	0
2	NAG	N	8	14/15	0.81	0.14	55,59,61,62	0
2	NAG	J	7	14/15	0.81	0.13	59,61,63,64	0
2	NAG	P	7	14/15	0.81	0.13	82,84,84,84	0
2	NAG	L	1	14/15	0.81	0.14	53,58,59,60	0
2	NAG	I	1	14/15	0.82	0.11	40,42,43,43	0
2	GAL	O	5	11/12	0.82	0.14	64,65,66,66	0
2	GAL	P	5	11/12	0.83	0.11	64,66,69,69	0
2	GAL	N	5	11/12	0.83	0.12	54,57,58,59	0
2	MAN	J	6	11/12	0.84	0.11	50,51,52,56	0
2	BMA	L	2	11/12	0.84	0.10	52,57,59,63	0
2	BMA	K	2	11/12	0.85	0.11	53,55,58,63	0
2	GAL	K	5	11/12	0.85	0.11	47,49,50,50	0
2	GAL	M	5	11/12	0.86	0.12	40,41,41,41	0
2	BMA	O	2	11/12	0.86	0.11	62,64,69,73	0
2	NAG	K	8	14/15	0.86	0.12	48,49,51,53	0
2	MAN	N	3	11/12	0.87	0.11	53,55,57,58	0
2	BMA	J	2	11/12	0.88	0.10	39,43,44,47	0
2	MAN	M	3	11/12	0.88	0.12	47,49,50,50	0
2	NAG	J	8	14/15	0.89	0.11	35,38,40,40	0
2	NAG	N	4	14/15	0.89	0.11	55,58,62,63	0
2	MAN	I	3	11/12	0.89	0.11	37,38,38,39	0
2	NAG	I	8	14/15	0.89	0.10	39,40,43,45	0
2	NAG	M	8	14/15	0.89	0.10	43,44,45,46	0
2	GAL	L	5	11/12	0.89	0.10	40,41,43,43	0
2	BMA	N	2	11/12	0.89	0.09	58,63,66,69	0
2	MAN	K	3	11/12	0.90	0.11	49,52,53,54	0
2	NAG	K	4	14/15	0.90	0.12	45,47,48,49	0
2	NAG	L	4	14/15	0.90	0.10	45,47,51,51	0
2	BMA	M	2	11/12	0.90	0.09	50,53,55,60	0
2	BMA	I	2	11/12	0.90	0.09	39,42,45,50	0
2	NAG	O	4	14/15	0.90	0.13	58,61,62,64	0
2	NAG	L	8	14/15	0.91	0.12	51,53,61,63	0
2	GAL	I	5	11/12	0.92	0.10	31,32,33,34	0
2	MAN	J	3	11/12	0.93	0.10	35,37,38,38	0
2	NAG	M	4	14/15	0.93	0.09	42,44,45,46	0
2	GAL	J	5	11/12	0.93	0.07	40,42,43,44	0
2	MAN	L	3	11/12	0.94	0.08	48,50,52,53	0

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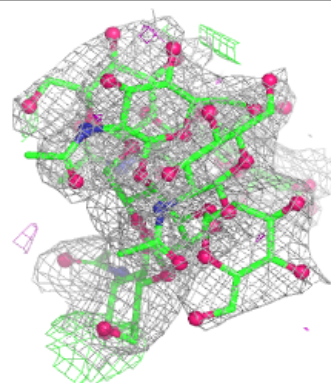
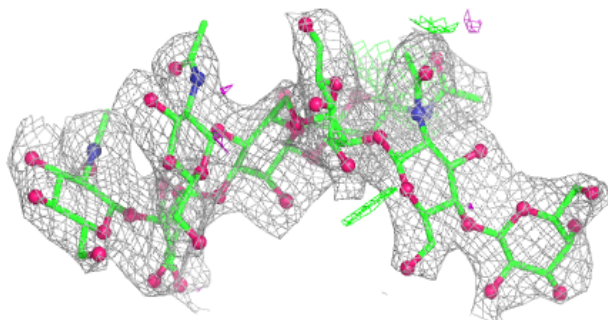
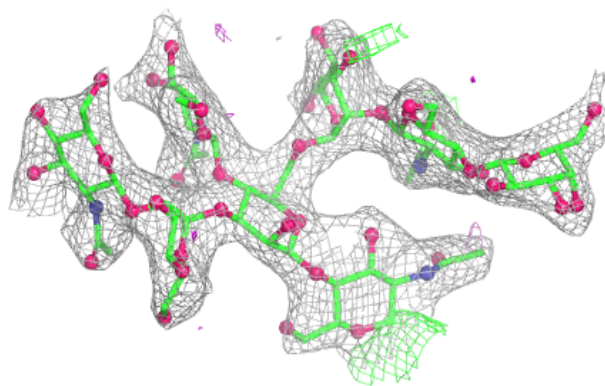
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	4	14/15	0.94	0.10	34,36,40,41	0
2	NAG	J	4	14/15	0.95	0.10	33,34,35,38	0

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.

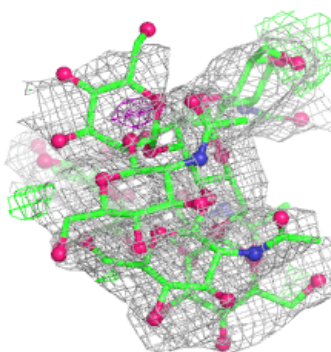
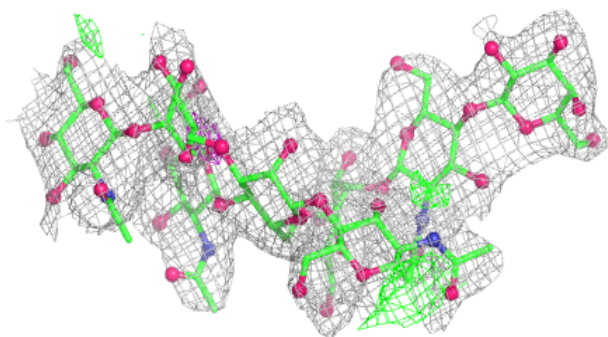
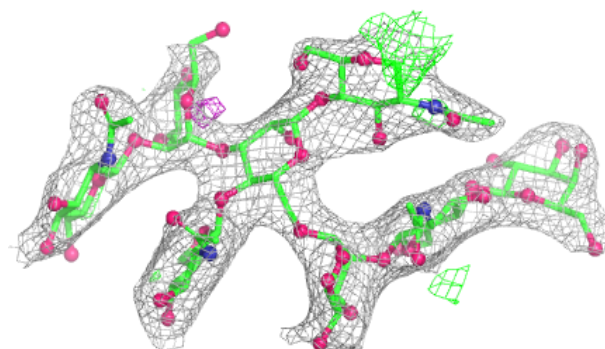


Electron density around Chain J:

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

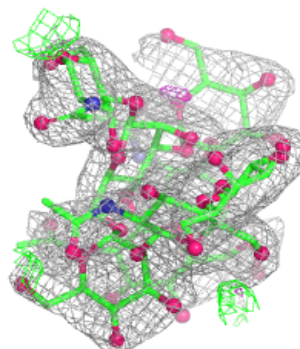
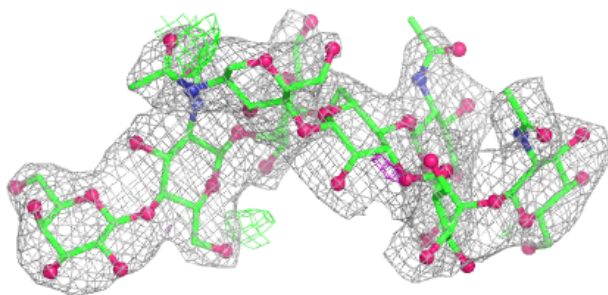
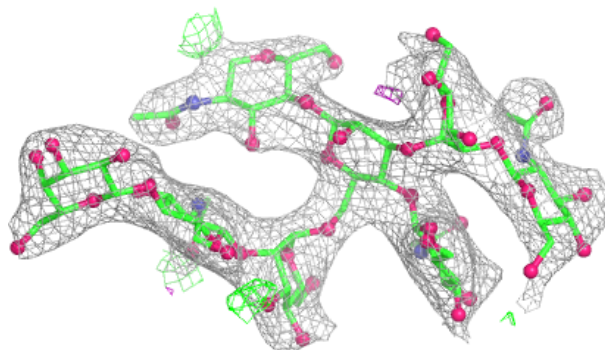
**Electron density around Chain K:**

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

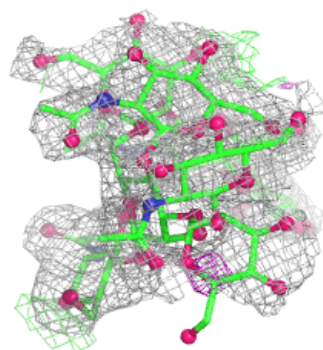
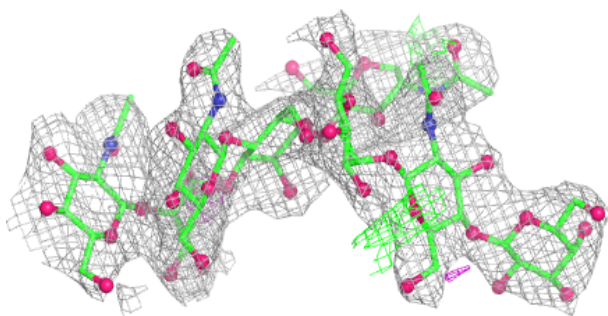
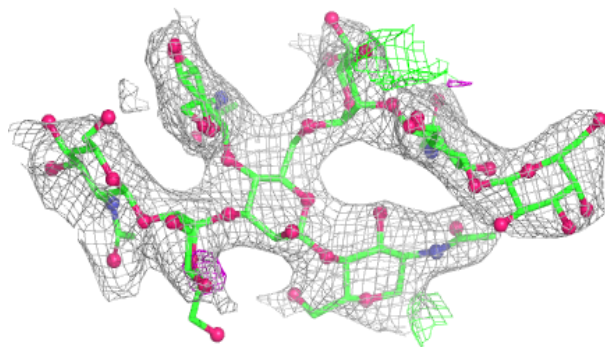


Electron density around Chain L:

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

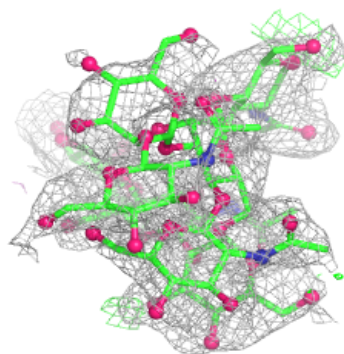
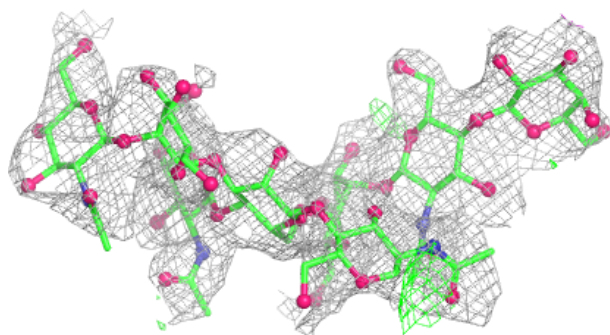
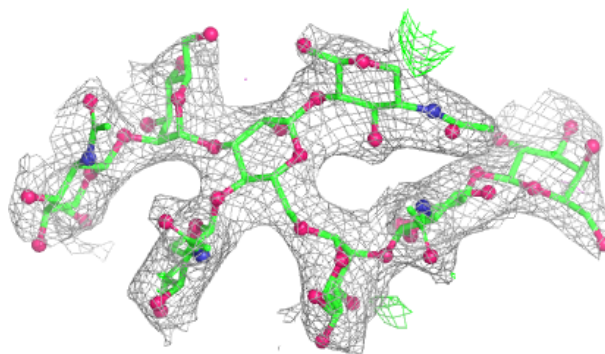
**Electron density around Chain M:**

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

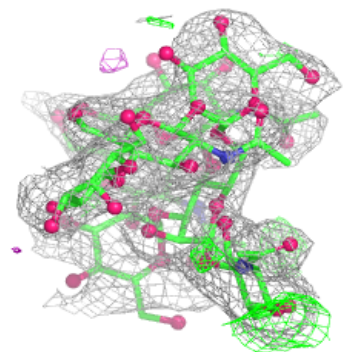
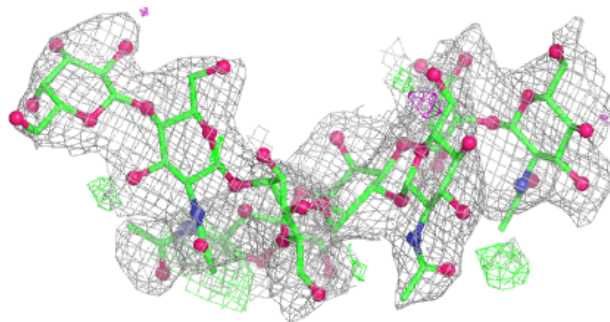
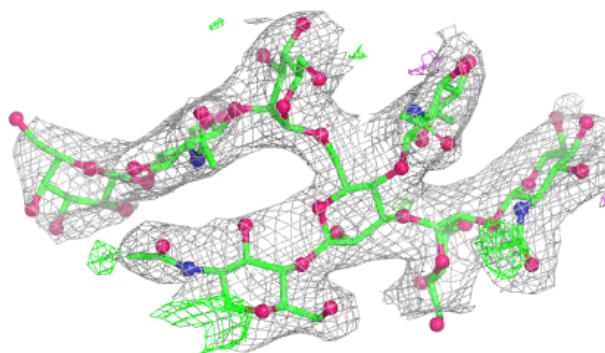


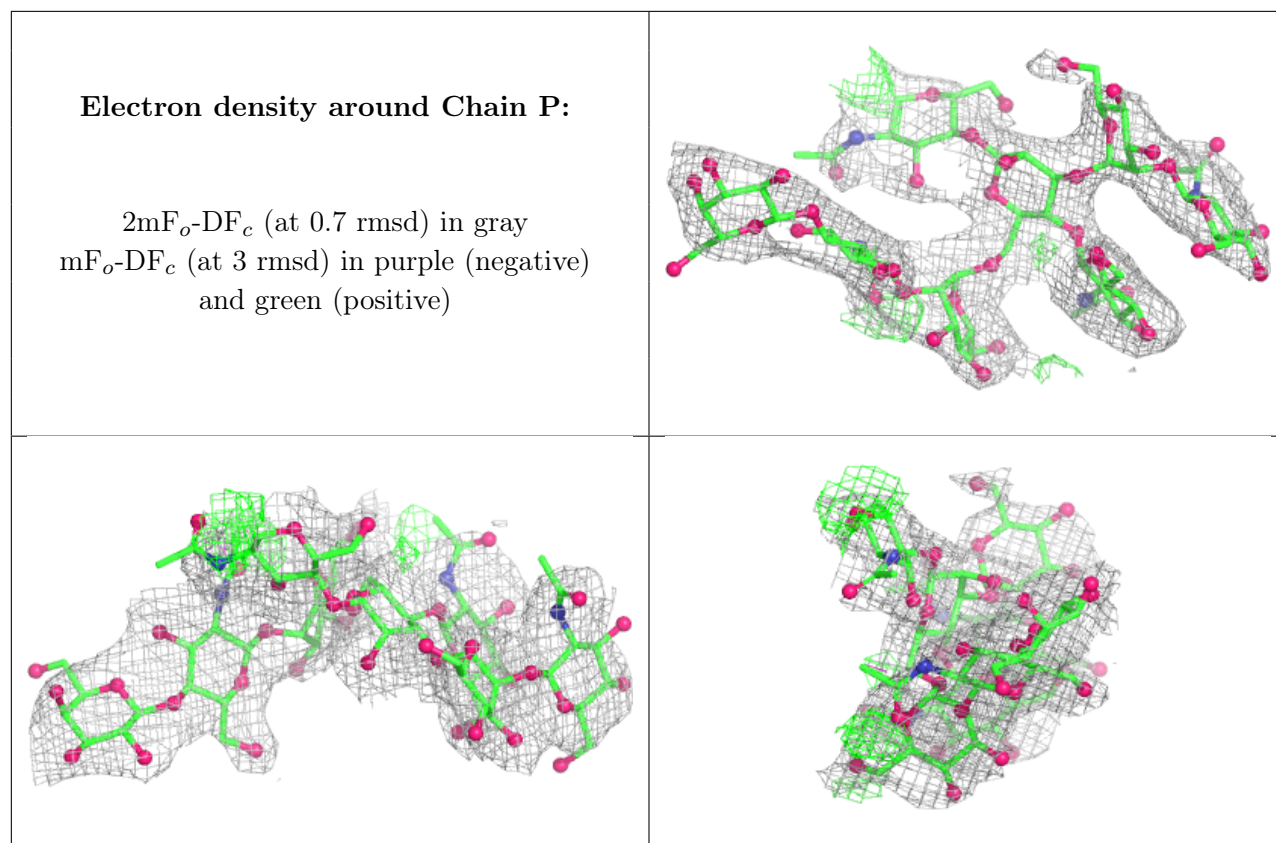
Electron density around Chain N:

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

**Electron density around Chain O:**

$2mF_o-DF_c$ (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
4	CA	H	2002	1/1	0.93	0.07	72,72,72,72	0
4	CA	G	2002	1/1	0.94	0.06	61,61,61,61	0
4	CA	D	2002	1/1	0.96	0.05	44,44,44,44	0
4	CA	C	2002	1/1	0.97	0.07	42,42,42,42	0
4	CA	A	2002	1/1	0.98	0.04	34,34,34,34	0
4	CA	B	2002	1/1	0.98	0.11	35,35,35,35	0
3	MN	B	2001	1/1	0.98	0.07	34,34,34,34	0
3	MN	C	2001	1/1	0.98	0.04	41,41,41,41	0
3	MN	G	2001	1/1	0.98	0.03	54,54,54,54	0
3	MN	H	2001	1/1	0.98	0.07	63,63,63,63	0
3	MN	E	2001	1/1	0.99	0.04	40,40,40,40	0
4	CA	E	2002	1/1	0.99	0.03	40,40,40,40	0
4	CA	F	2002	1/1	0.99	0.06	44,44,44,44	0
3	MN	A	2001	1/1	0.99	0.04	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	D	2001	1/1	0.99	0.06	40,40,40,40	0
3	MN	F	2001	1/1	1.00	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.