



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:48 PM BST

PDB ID : 1V0Z
Title : Structure of Neuraminidase from English duck subtype N6
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on : 2004-03-12
Resolution : 1.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

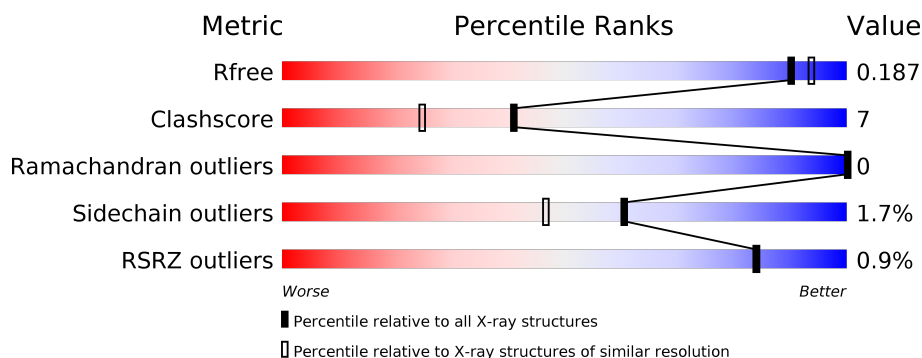
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



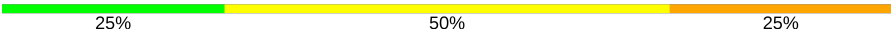
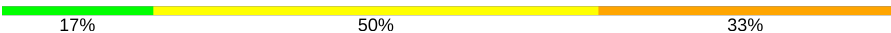


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 91%, green 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 91% 8% </div> </div>
1	B	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 92%, green 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 92% 7% </div> </div>
1	C	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 89%, green 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 89% 10% </div> </div>
1	D	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 89%, green 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 10% </div> </div>
2	E	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>
2	I	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	4	
4	G	6	
5	H	3	
6	J	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEG	C	503	-	X	X	-
2	NAG	E	2	-	-	-	X
3	MAN	F	3	-	-	-	X
6	MAN	J	2	-	-	-	X
9	NAG	A	506	-	-	X	-
9	NAG	A	513	-	-	-	X
9	NAG	B	503	-	-	-	X
9	NAG	C	501	-	-	-	X
9	NAG	D	506	-	-	-	X
9	NAG	D	508	-	-	X	-

2 Entry composition [i](#)

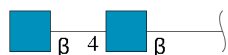
There are 12 unique types of molecules in this entry. The entry contains 14347 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE.

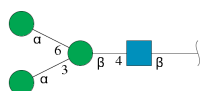
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	B	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	C	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

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



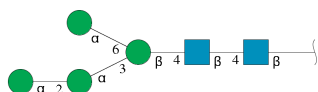
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



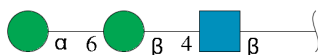
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			47	26	1	20			

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



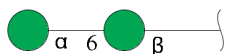
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			36	20	1	15			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	J	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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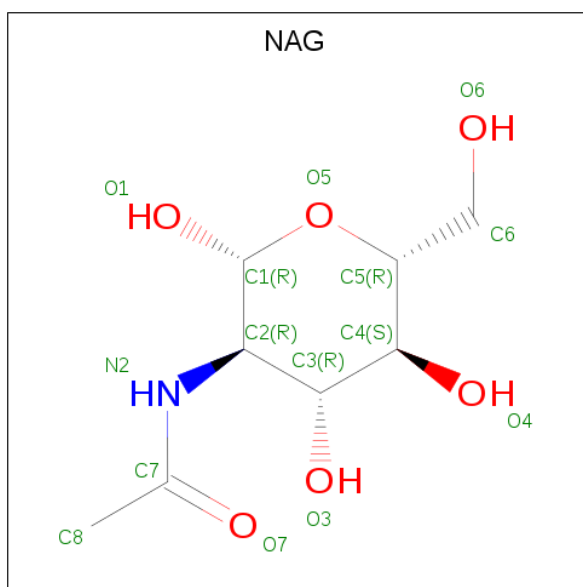
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



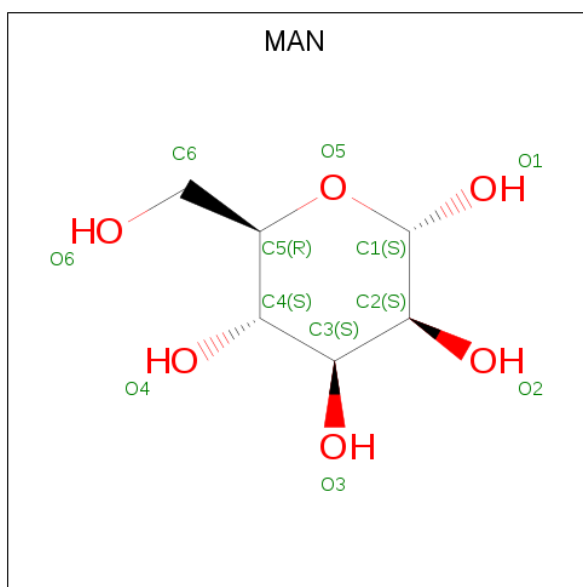
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



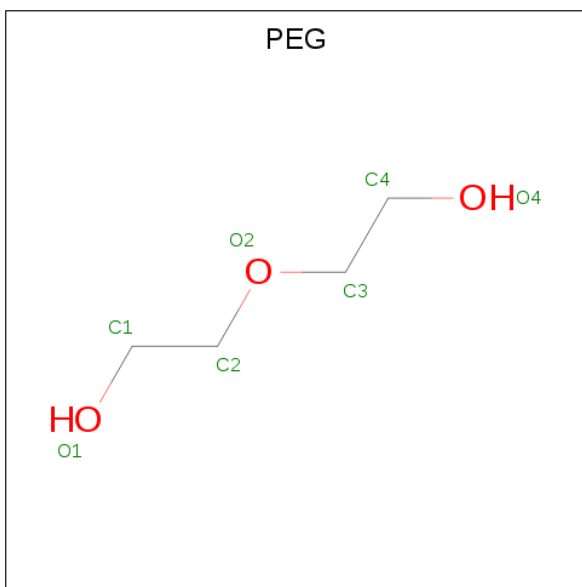
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1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

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	460	Total	O	0	0
			460	460		
12	B	442	Total	O	0	0
			442	442		
12	C	454	Total	O	0	0
			454	454		
12	D	442	Total	O	0	0
			442	442		



- Molecule 1: NEURAMINIDASE



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

Chain E:  50% 50%

UAG1
UAG2

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

Chain I:  50% 50%


UAG1
UAG2

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

Chain F:  25% 50% 25%

UAG1
UAG2
MAN3
MAN4

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

Chain G:  17% 50% 33%

UAG1
UAG2
MAN3
MAN4
MAN5
MAN6

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

Chain H:  33% 67%

UAG1
MAN2
MAN3

- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain J:  100%

MAN1
MAN2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.48Å 73.75Å 106.81Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.96 – 1.84 19.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.84) 93.2 (19.98-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.149 , 0.190 0.150 , 0.187	Depositor DCC
R_{free} test set	6696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14347	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, PEG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/3084	0.67	1/4185 (0.0%)
1	B	0.65	1/3084 (0.0%)	0.67	1/4185 (0.0%)
1	C	0.66	0/3084	0.66	1/4185 (0.0%)
1	D	0.65	0/3084	0.69	1/4185 (0.0%)
All	All	0.65	1/12336 (0.0%)	0.67	4/16740 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	TRP	CB-CG	-5.11	1.41	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	CA-CB-CG	7.07	131.57	115.30
1	D	128	LEU	CA-CB-CG	6.70	130.71	115.30
1	B	128	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	128	LEU	CA-CB-CG	6.12	129.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3009	0	2885	26	0
1	B	3009	0	2888	31	0
1	C	3009	0	2888	53	0
1	D	3009	0	2888	50	0
2	E	28	0	25	0	0
2	I	28	0	25	7	0
3	F	47	0	40	7	0
4	G	72	0	61	8	0
5	H	36	0	31	6	0
6	J	22	0	19	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	6	0	8	2	0
8	B	6	0	8	1	0
8	C	6	0	8	1	0
8	D	6	0	8	0	0
9	A	42	0	39	9	0
9	B	28	0	26	4	0
9	C	42	0	39	5	0
9	D	56	0	52	16	0
10	A	44	0	40	9	0
10	B	22	0	20	1	0
10	D	11	0	10	2	0
11	C	7	0	10	16	0
12	A	460	0	0	5	0
12	B	442	0	0	1	0
12	C	454	0	0	6	0
12	D	442	0	0	1	0
All	All	14347	0	12018	174	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 7.

The worst 5 of 174 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:D:207:ASN:HD21	9:D:508:NAG:C1	1.03	1.63
1:D:152:ASN:HD21	9:D:507:NAG:C1	1.01	1.55
1:B:152:ASN:HD21	9:B:504:NAG:C1	0.97	1.54
1:C:152:ASN:HD21	9:C:506:NAG:C1	0.92	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ASN:HD21	2:I:1:NAG:C1	0.94	1.52

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	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	B	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	C	387/389 (100%)	374 (97%)	13 (3%)	0	100	100
1	D	387/389 (100%)	373 (96%)	14 (4%)	0	100	100
All	All	1548/1556 (100%)	1497 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	327 (99%)	4 (1%)	71	61
1	B	331/331 (100%)	325 (98%)	6 (2%)	59	44
1	C	331/331 (100%)	327 (99%)	4 (1%)	71	61
1	D	331/331 (100%)	323 (98%)	8 (2%)	49	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	60 47

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	TRP
1	C	445	LEU
1	D	460	ARG
1	C	128	LEU
1	C	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	ASN
1	C	207	ASN
1	D	406	ASN
1	B	427	ASN
1	B	467	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 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	E	1	1,2	14,14,15	0.64	0	17,19,21	0.93	0
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.77	1 (5%)
3	NAG	F	1	3	14,14,15	0.59	0	17,19,21	0.65	0
3	BMA	F	2	3	11,11,12	0.26	0	15,15,17	1.20	2 (13%)
3	MAN	F	3	3	11,11,12	0.41	0	15,15,17	0.86	0
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	1.45	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.77	0	17,19,21	2.50	6 (35%)
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	1.41	2 (11%)
4	BMA	G	3	4	11,11,12	0.56	0	15,15,17	0.99	1 (6%)
4	MAN	G	4	4	11,11,12	0.51	0	15,15,17	0.86	0
4	MAN	G	5	4	11,11,12	0.43	0	15,15,17	0.94	1 (6%)
4	MAN	G	6	4	11,11,12	0.38	0	15,15,17	1.34	2 (13%)
5	NAG	H	1	5	14,14,15	0.68	0	17,19,21	2.54	6 (35%)
5	BMA	H	2	5	11,11,12	0.42	0	15,15,17	1.16	1 (6%)
5	MAN	H	3	5	11,11,12	0.41	0	15,15,17	1.07	1 (6%)
2	NAG	I	1	2	14,14,15	0.63	0	17,19,21	1.56	3 (17%)
2	NAG	I	2	2	14,14,15	0.61	0	17,19,21	0.63	0
6	BMA	J	1	6	11,11,12	0.45	0	15,15,17	1.13	2 (13%)
6	MAN	J	2	6	11,11,12	0.50	0	15,15,17	1.61	2 (13%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	H	2	5	-	0/2/19/22	0/1/1/1
5	MAN	H	3	5	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
6	BMA	J	1	6	-	0/2/19/22	0/1/1/1
6	MAN	J	2	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C3-C4-C5	-6.03	99.49	110.24
5	H	1	NAG	C4-C3-C2	-5.51	102.94	111.02
4	G	1	NAG	O5-C5-C6	5.18	115.32	107.20
5	H	1	NAG	C2-N2-C7	4.49	129.29	122.90
5	H	1	NAG	O5-C1-C2	-4.32	104.47	111.29

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

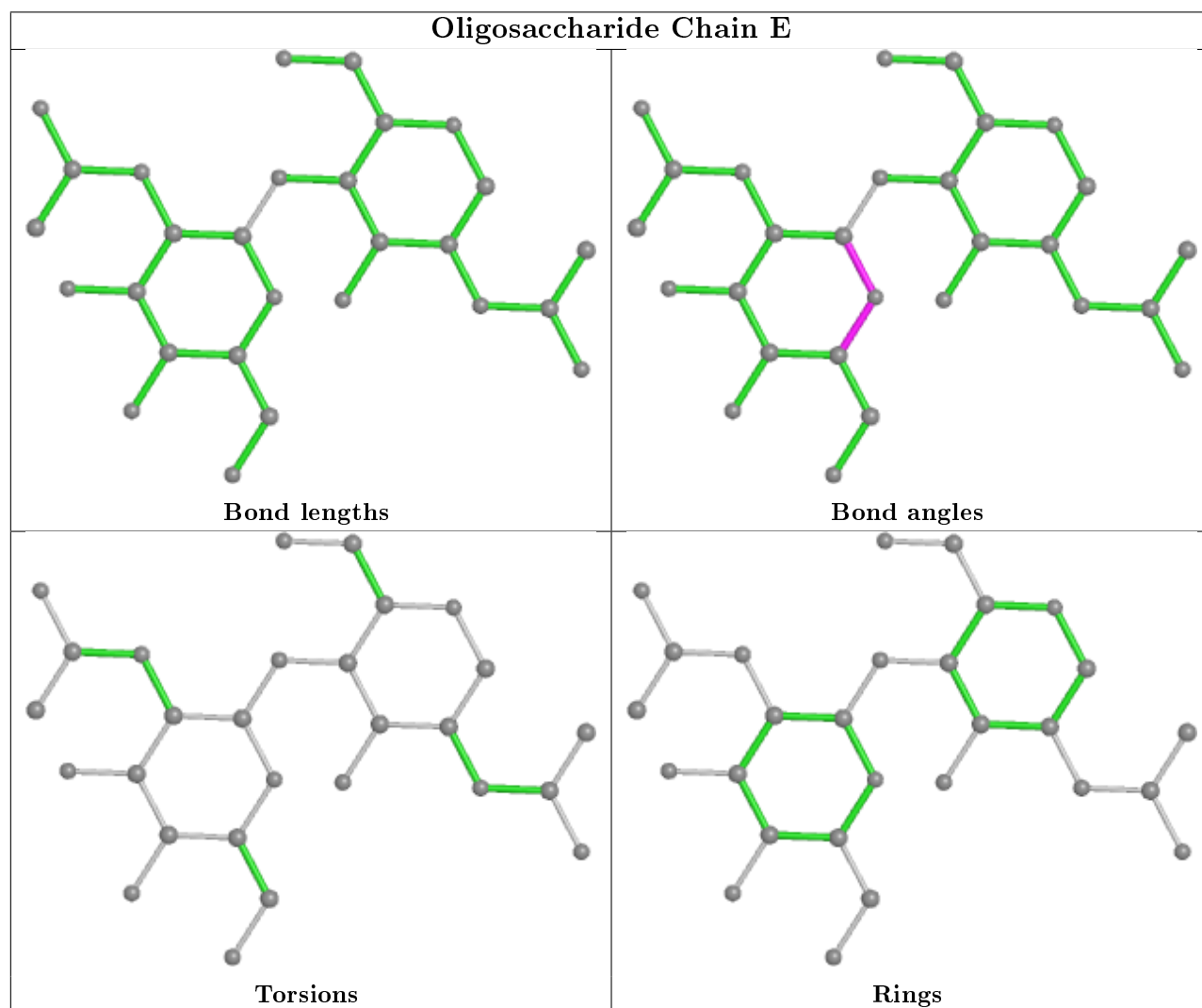
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
3	F	3	MAN	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

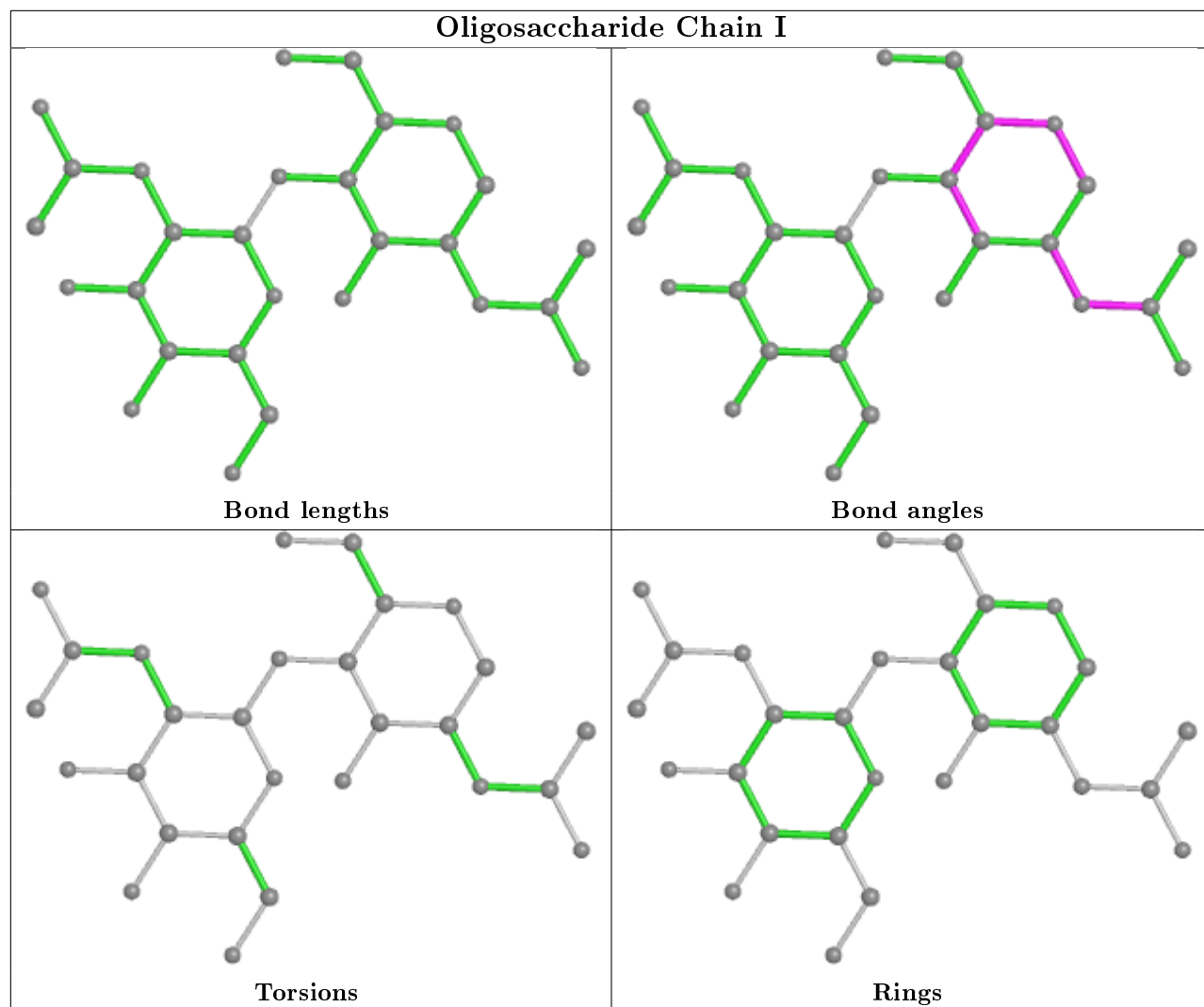
There are no ring outliers.

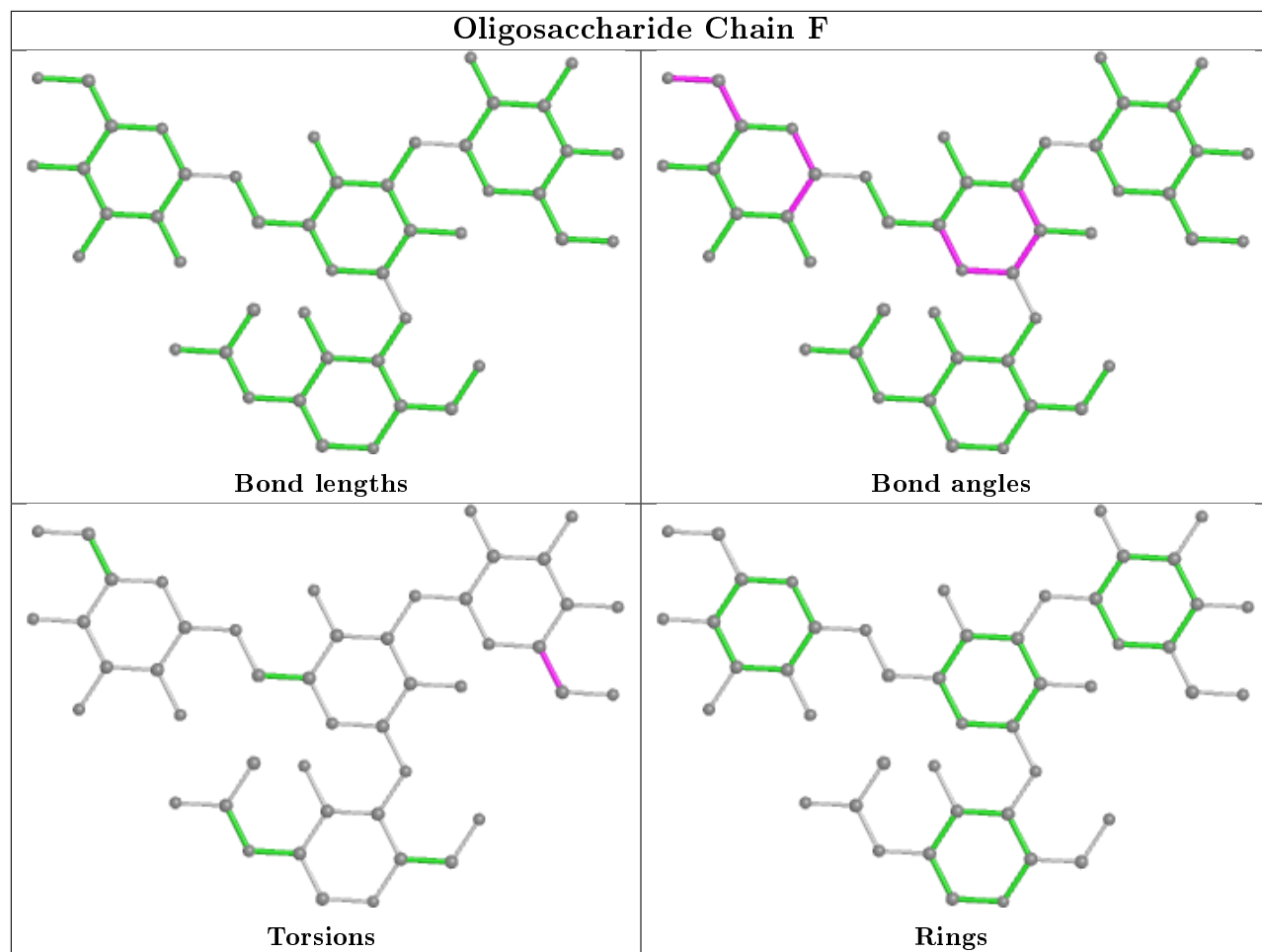
10 monomers are involved in 30 short contacts:

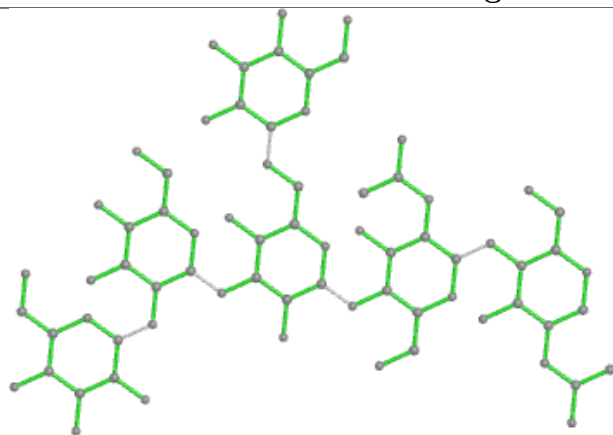
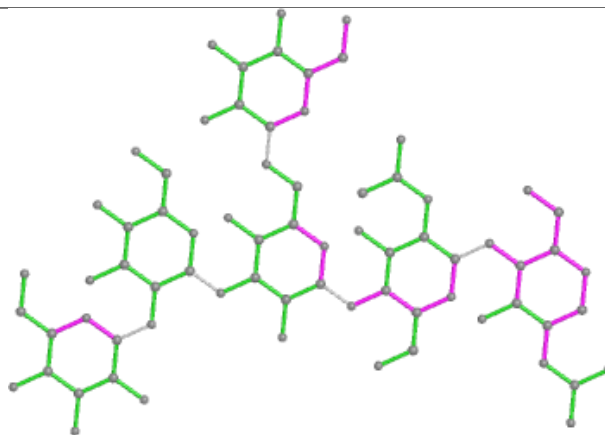
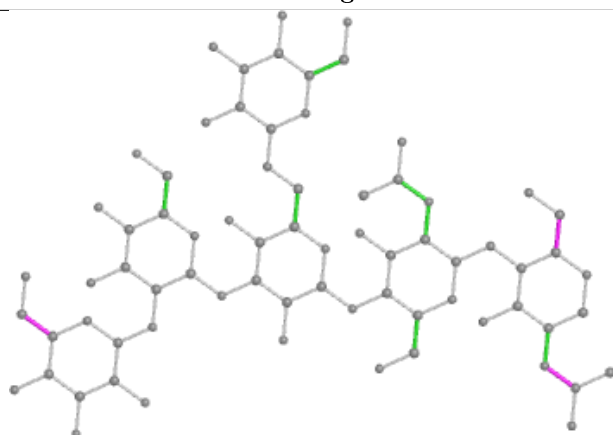
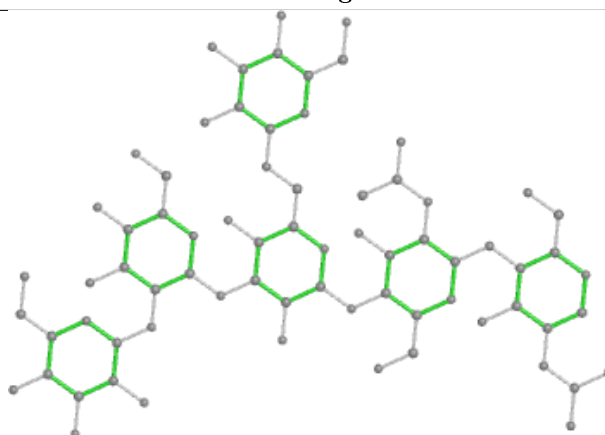
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	BMA	3	0
3	F	4	MAN	4	0
2	I	2	NAG	3	0
4	G	1	NAG	3	0
3	F	1	NAG	3	0
6	J	2	MAN	2	0
2	I	1	NAG	4	0
4	G	6	MAN	5	0
5	H	3	MAN	1	0
5	H	1	NAG	5	0

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

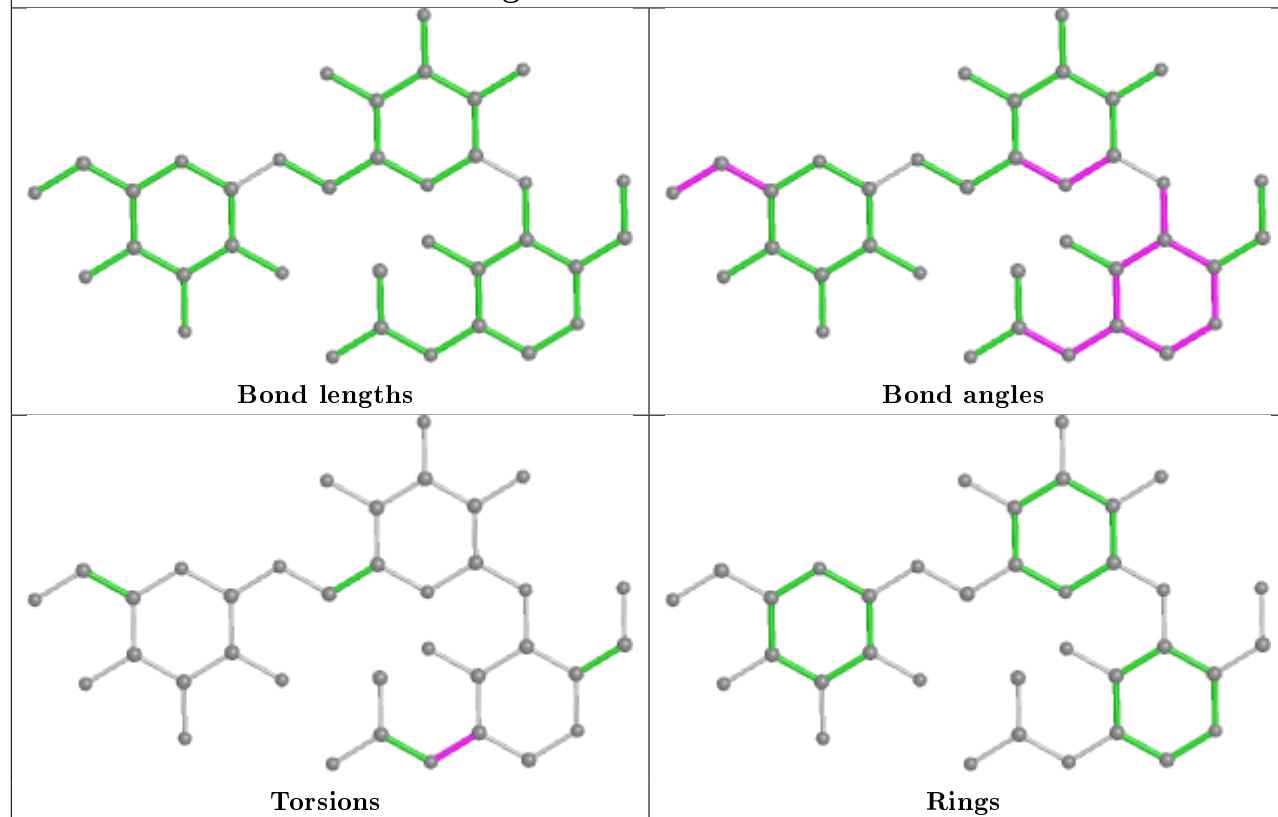




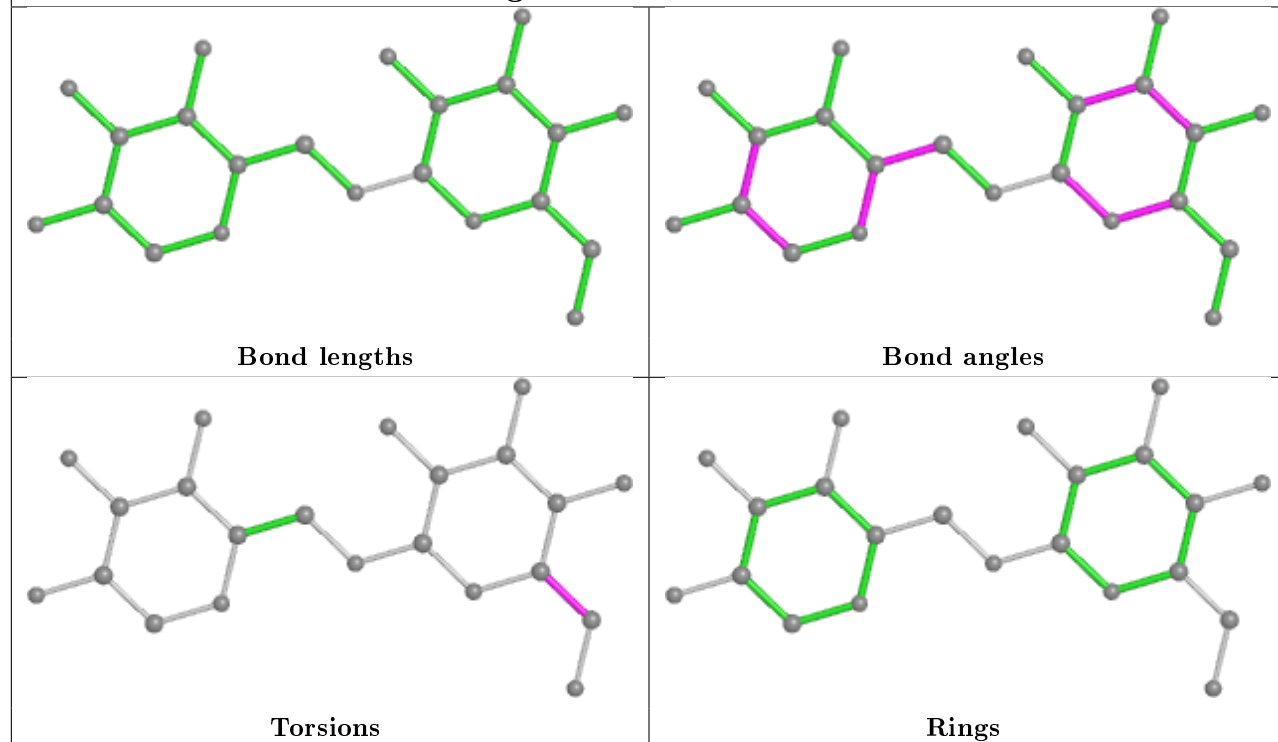


Oligosaccharide Chain G**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain H



Oligosaccharide Chain J



5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	C	505	-	14,14,15	0.56	0	17,19,21	1.49	5 (29%)
9	NAG	A	513	-	14,14,15	0.52	0	17,19,21	1.12	2 (11%)
8	GOL	D	505	-	5,5,5	1.38	0	5,5,5	1.88	1 (20%)
9	NAG	C	501	-	14,14,15	0.54	0	17,19,21	1.21	2 (11%)
10	MAN	B	509	-	11,11,12	0.50	0	15,15,17	1.87	3 (20%)
8	GOL	A	502	-	5,5,5	1.20	0	5,5,5	1.83	1 (20%)
11	PEG	C	503	-	6,6,6	0.27	0	5,5,5	6.29	5 (100%)
8	GOL	B	502	-	5,5,5	1.72	1 (20%)	5,5,5	2.12	2 (40%)
9	NAG	A	505	1	14,14,15	0.63	0	17,19,21	0.91	0
8	GOL	C	504	-	5,5,5	1.62	1 (20%)	5,5,5	2.10	2 (40%)
9	NAG	D	501	-	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
9	NAG	D	508	-	14,14,15	0.64	0	17,19,21	1.69	3 (17%)
9	NAG	A	506	-	14,14,15	0.58	0	17,19,21	1.66	3 (17%)
10	MAN	B	506	-	11,11,12	0.37	0	15,15,17	1.14	1 (6%)
10	MAN	A	521	-	11,11,12	0.59	0	15,15,17	1.78	4 (26%)
9	NAG	B	503	-	14,14,15	0.45	0	17,19,21	1.33	3 (17%)
9	NAG	B	504	-	14,14,15	0.71	0	17,19,21	1.06	2 (11%)
9	NAG	D	507	-	14,14,15	0.60	0	17,19,21	1.20	2 (11%)
9	NAG	D	506	-	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
10	MAN	A	514	-	11,11,12	0.43	0	15,15,17	1.55	2 (13%)
10	MAN	A	508	-	11,11,12	0.37	0	15,15,17	1.44	2 (13%)
10	MAN	D	509	-	11,11,12	0.59	0	15,15,17	1.22	2 (13%)
10	MAN	A	509	-	11,11,12	0.52	0	15,15,17	1.39	2 (13%)
9	NAG	C	506	-	14,14,15	0.67	0	17,19,21	1.11	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
9	NAG	C	505	-	-	2/6/23/26	0/1/1/1
9	NAG	A	513	-	-	4/6/23/26	0/1/1/1
8	GOL	D	505	-	-	1/4/4/4	-
9	NAG	C	501	-	-	1/6/23/26	0/1/1/1
10	MAN	B	509	-	-	0/2/19/22	0/1/1/1
8	GOL	A	502	-	-	1/4/4/4	-
11	PEG	C	503	-	-	2/4/4/4	-
8	GOL	B	502	-	-	0/4/4/4	-
9	NAG	A	505	1	-	0/6/23/26	0/1/1/1
8	GOL	C	504	-	-	1/4/4/4	-
9	NAG	D	501	-	-	4/6/23/26	0/1/1/1
9	NAG	D	508	-	-	0/6/23/26	0/1/1/1
9	NAG	A	506	-	-	4/6/23/26	0/1/1/1
10	MAN	B	506	-	-	0/2/19/22	0/1/1/1
10	MAN	A	521	-	-	0/2/19/22	0/1/1/1
9	NAG	B	503	-	-	3/6/23/26	0/1/1/1
9	NAG	B	504	-	-	0/6/23/26	0/1/1/1
9	NAG	D	507	-	-	0/6/23/26	0/1/1/1
9	NAG	D	506	-	-	2/6/23/26	0/1/1/1
10	MAN	A	514	-	-	2/2/19/22	0/1/1/1
10	MAN	A	508	-	-	1/2/19/22	0/1/1/1
10	MAN	D	509	-	-	2/2/19/22	0/1/1/1
10	MAN	A	509	-	-	0/2/19/22	0/1/1/1
9	NAG	C	506	-	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	GOL	O3-C3	2.69	1.53	1.42
8	C	504	GOL	O3-C3	2.33	1.52	1.42

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	503	PEG	O1-C1-C2	9.11	164.65	111.81
11	C	503	PEG	O2-C2-C1	7.83	144.49	110.07
11	C	503	PEG	C3-O2-C2	-6.14	86.66	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	509	MAN	C1-O5-C5	4.93	118.86	112.19
10	A	514	MAN	C1-O5-C5	4.73	118.59	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	501	NAG	C8-C7-N2-C2
9	D	501	NAG	O7-C7-N2-C2
9	A	506	NAG	C8-C7-N2-C2
9	A	506	NAG	O7-C7-N2-C2
9	B	503	NAG	C8-C7-N2-C2

There are no ring outliers.

17 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	502	GOL	2	0
11	C	503	PEG	16	0
8	B	502	GOL	1	0
8	C	504	GOL	1	0
9	D	501	NAG	1	0
9	D	508	NAG	8	0
9	A	506	NAG	9	0
10	B	506	MAN	1	0
10	A	521	MAN	3	0
9	B	504	NAG	4	0
9	D	507	NAG	4	0
9	D	506	NAG	3	0
10	A	514	MAN	2	0
10	A	508	MAN	2	0
10	D	509	MAN	2	0
10	A	509	MAN	2	0
9	C	506	NAG	5	0

5.7 Other polymers

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	389/389 (100%)	-0.48	3 (0%) 86 86	7, 12, 20, 31	0
1	B	389/389 (100%)	-0.49	2 (0%) 91 91	7, 12, 18, 37	0
1	C	389/389 (100%)	-0.52	6 (1%) 73 73	7, 11, 19, 33	0
1	D	389/389 (100%)	-0.47	3 (0%) 86 86	7, 12, 18, 33	0
All	All	1556/1556 (100%)	-0.49	14 (0%) 84 84	7, 12, 19, 37	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	4.3
1	C	350	GLY	3.5
1	C	349	GLY	3.2
1	A	88	ARG	3.2
1	C	88	ARG	2.9

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	J	2	11/12	0.60	0.42	45,49,51,51	0
2	NAG	E	2	14/15	0.68	0.45	39,43,45,45	0

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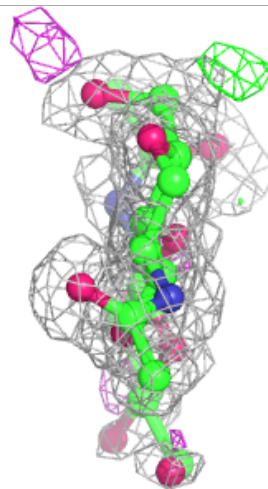
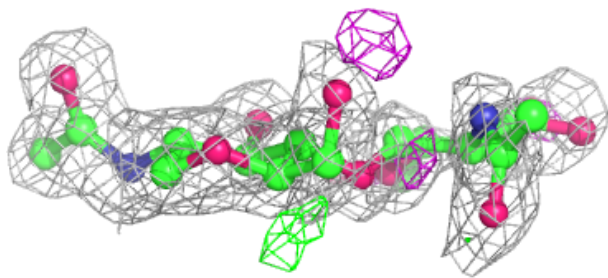
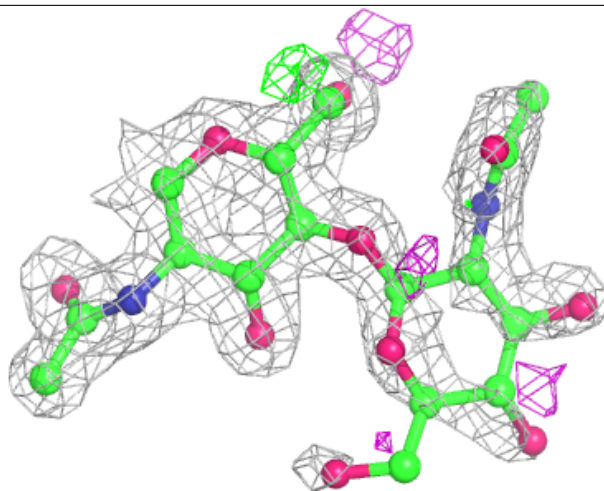
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	H	1	14/15	0.69	0.26	26,35,39,43	0
3	MAN	F	3	11/12	0.75	0.44	45,48,49,50	0
3	NAG	F	1	14/15	0.80	0.28	20,24,27,30	0
4	NAG	G	1	14/15	0.81	0.32	26,31,35,38	0
2	NAG	I	2	14/15	0.81	0.21	18,24,29,33	0
5	MAN	H	3	11/12	0.82	0.26	35,37,37,37	0
4	MAN	G	5	11/12	0.84	0.41	38,42,44,44	0
6	BMA	J	1	11/12	0.85	0.28	32,35,36,40	0
5	BMA	H	2	11/12	0.85	0.24	35,36,37,38	0
2	NAG	I	1	14/15	0.86	0.24	25,29,32,34	0
2	NAG	E	1	14/15	0.90	0.16	20,22,26,32	0
3	MAN	F	4	11/12	0.90	0.20	22,24,24,27	0
4	NAG	G	2	14/15	0.92	0.15	14,20,24,25	0
4	BMA	G	3	11/12	0.94	0.13	16,19,19,21	0
4	MAN	G	4	11/12	0.94	0.13	24,25,27,27	0
3	BMA	F	2	11/12	0.94	0.21	21,25,26,31	0
4	MAN	G	6	11/12	0.94	0.14	14,15,16,19	0

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

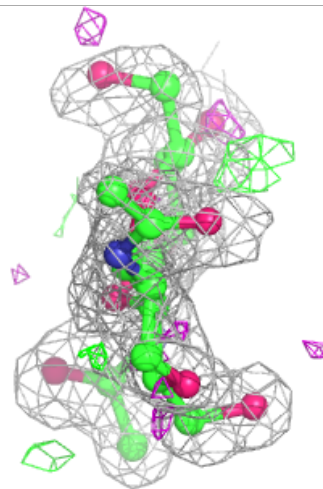
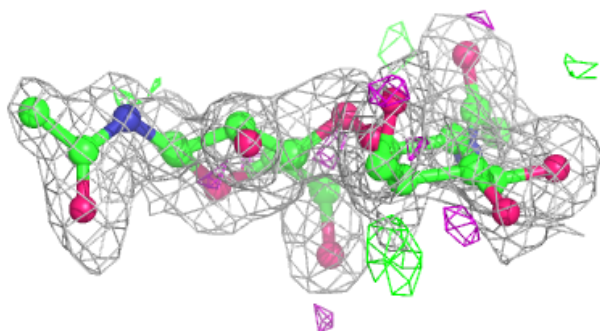
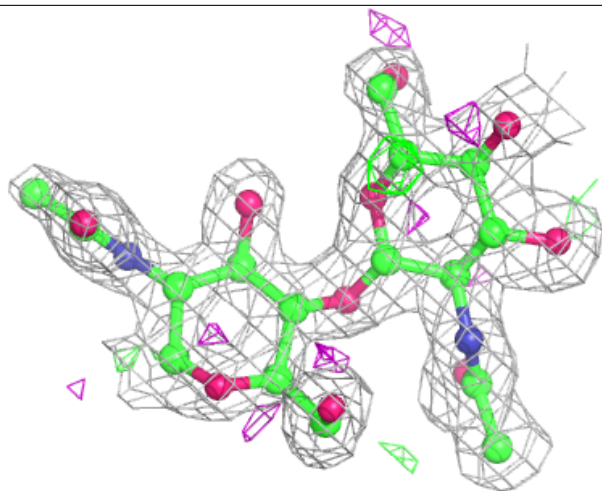
Electron density around Chain E:

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



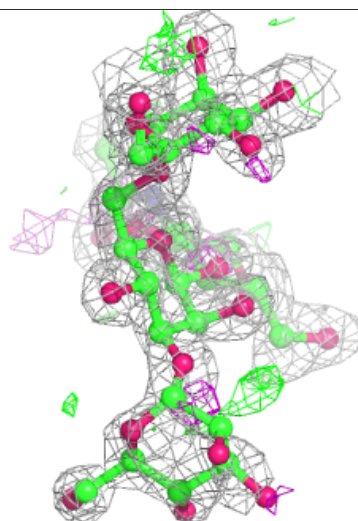
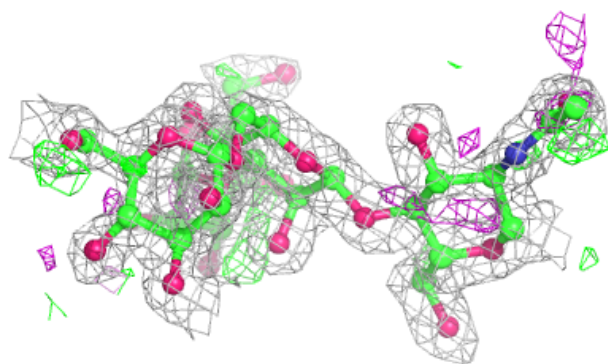
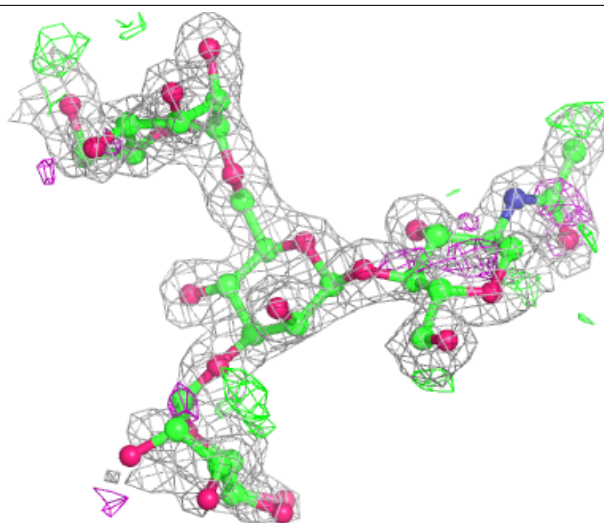
Electron density around Chain I:

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



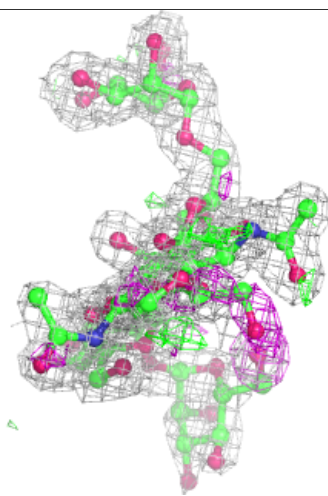
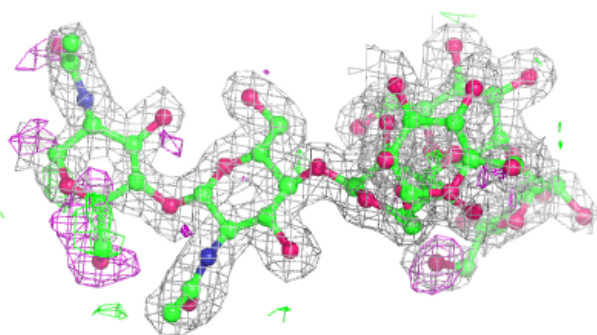
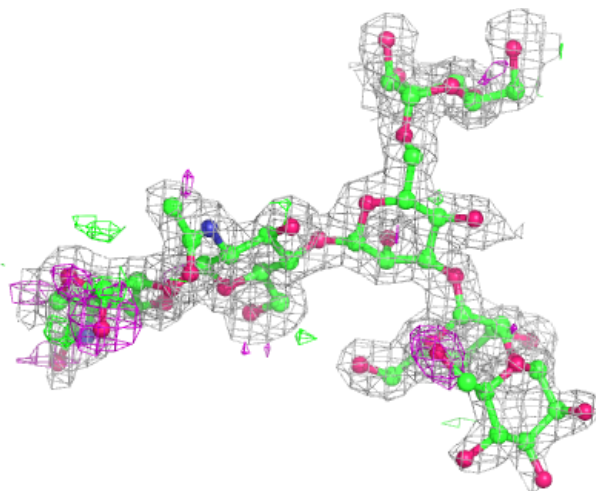
Electron density around Chain F:

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



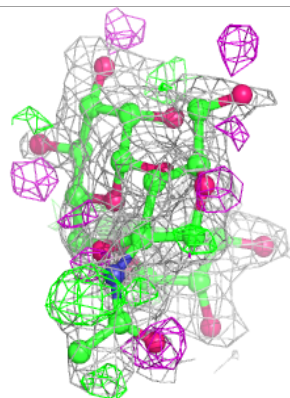
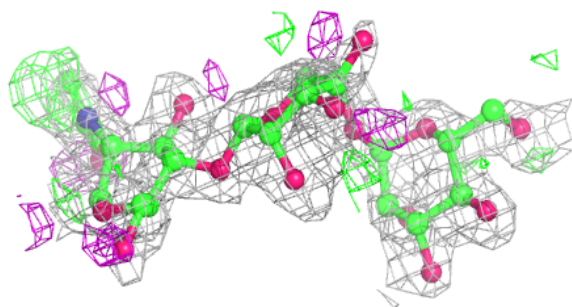
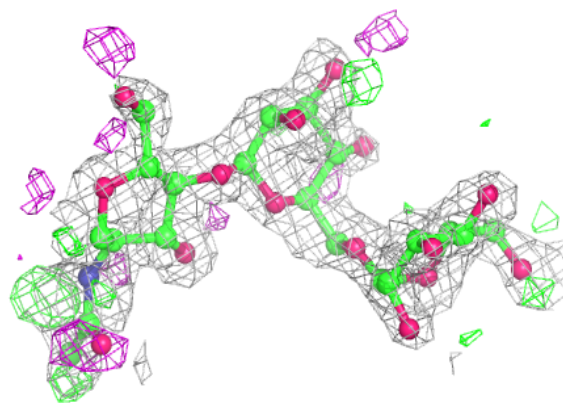
Electron density around Chain G:

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

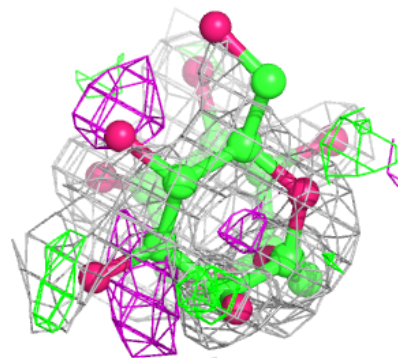
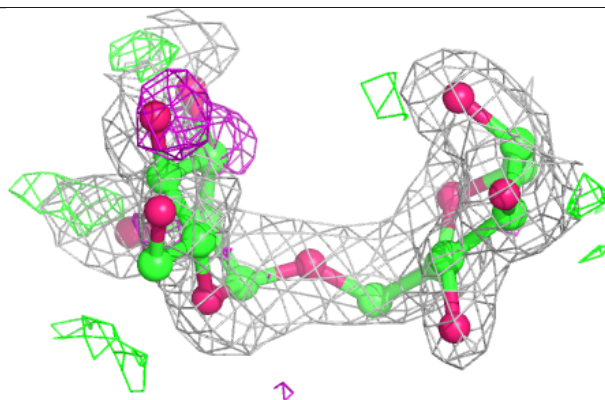
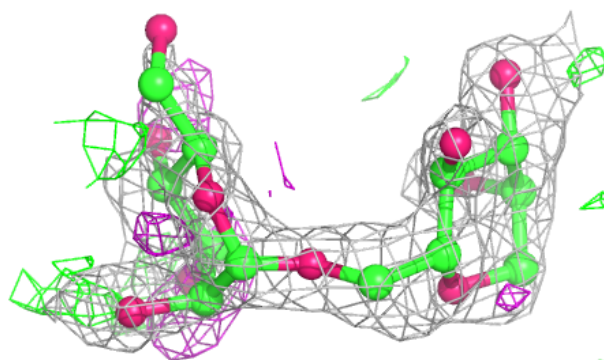


Electron density around Chain H:

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

**Electron density around Chain J:**

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



6.4 Ligands ⓘ

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
9	NAG	A	513	14/15	0.15	0.47	95,96,97,97	0
9	NAG	B	503	14/15	0.31	0.43	98,99,99,99	0
9	NAG	D	501	14/15	0.42	0.37	74,77,77,77	0
9	NAG	C	505	14/15	0.46	0.37	62,63,64,64	0
9	NAG	C	501	14/15	0.47	0.49	64,67,68,68	0
9	NAG	D	506	14/15	0.50	0.43	105,105,106,106	0
10	MAN	D	509	11/12	0.53	0.39	67,68,68,68	0
11	PEG	C	503	7/7	0.67	0.25	20,24,28,29	0
8	GOL	B	502	6/6	0.67	0.29	12,25,26,28	0
8	GOL	A	502	6/6	0.69	0.25	19,29,30,31	0
9	NAG	A	506	14/15	0.73	0.30	42,44,45,45	0
8	GOL	D	505	6/6	0.73	0.29	17,29,30,30	0
10	MAN	B	509	11/12	0.74	0.33	44,47,48,49	0
8	GOL	C	504	6/6	0.76	0.26	13,26,28,29	0
10	MAN	B	506	11/12	0.79	0.29	32,33,36,38	0
10	MAN	A	508	11/12	0.81	0.20	26,30,35,38	0
9	NAG	D	508	14/15	0.82	0.21	23,26,27,27	0
10	MAN	A	514	11/12	0.85	0.19	30,33,36,38	0
10	MAN	A	509	11/12	0.85	0.18	24,27,28,29	0
9	NAG	A	505	14/15	0.89	0.16	19,22,27,28	0
9	NAG	B	504	14/15	0.90	0.15	16,22,26,29	0
10	MAN	A	521	11/12	0.91	0.14	19,20,21,21	0
9	NAG	D	507	14/15	0.92	0.15	17,22,26,26	0
9	NAG	C	506	14/15	0.93	0.13	15,18,25,26	0
7	CA	C	502	1/1	0.98	0.17	19,19,19,19	0
7	CA	B	501	1/1	0.99	0.09	19,19,19,19	0
7	CA	D	504	1/1	0.99	0.14	19,19,19,19	0
7	CA	A	501	1/1	0.99	0.14	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.