



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:17 am GMT

PDB ID : 4CYW
Title : Structure of the A_mallard_Sweden_51_2002 H10 Avian Haemmagglutinin in complex with human receptor analog 6-SLN
Authors : Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Martin, S.R.; Haire, L.F.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-04-15
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

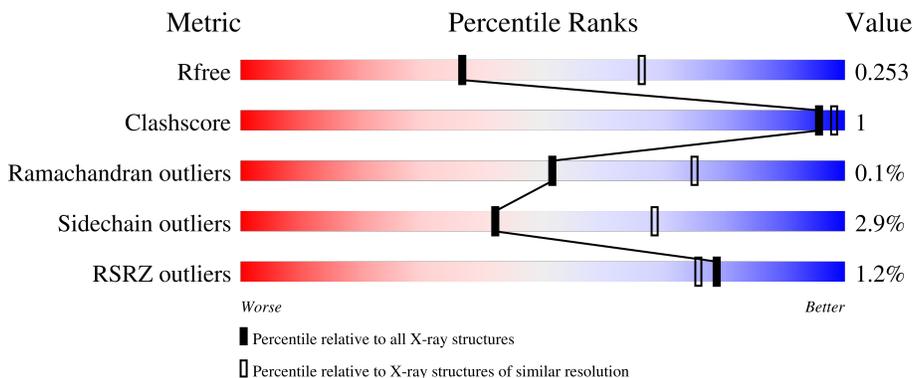
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

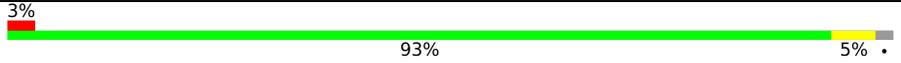
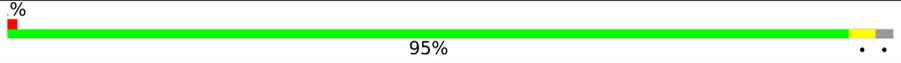
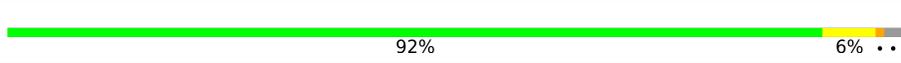
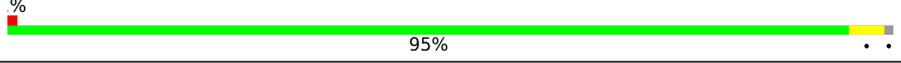
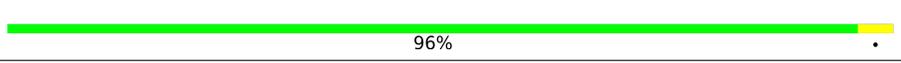
The reported resolution of this entry is 2.60 Å.

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.



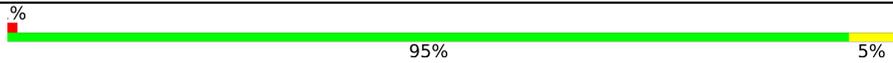
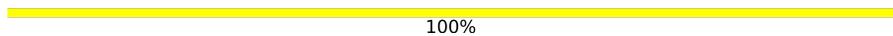
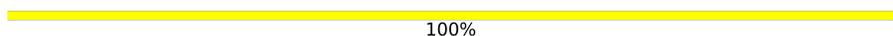
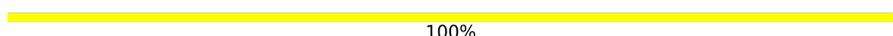
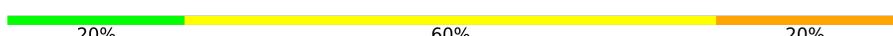
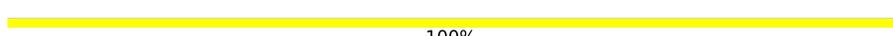
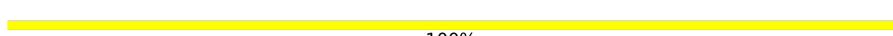
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	324	 3% 93% 5%
1	C	324	 % 95% ..
1	E	324	 92% 6% ..
2	B	173	 % 95% ..
2	D	173	 96% .

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Mol	Chain	Length	Quality of chain
2	F	173	 % 95% 5%
3	G	3	 100%
3	I	3	 100%
3	K	3	 100%
4	H	5	 20% 60% 20%
5	J	5	 100%
6	L	4	 100%

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
4	MAN	H	4	-	-	-	X
4	MAN	H	5	-	-	-	X
5	MAN	J	5	X	-	-	-
6	MAN	L	4	-	-	-	X
7	NAG	A	420	X	-	-	-
7	NAG	C	420	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12105 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.

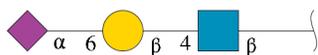
- Molecule 1 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	Total 2411	C 1490	N 434	O 471	S 16	0	0	0
1	C	319	Total 2430	C 1504	N 437	O 473	S 16	0	0	0
1	E	319	Total 2430	C 1504	N 437	O 473	S 16	0	0	0

- Molecule 2 is a protein called HEMAGGLUTININ.

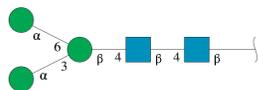
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	Total 1381	C 853	N 238	O 282	S 8	0	0	0
2	D	173	Total 1384	C 856	N 239	O 281	S 8	0	0	0
2	F	173	Total 1391	C 860	N 240	O 283	S 8	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



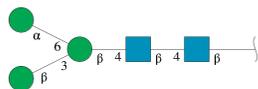
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	3	Total 46	C 25	N 2	O 19	0	0	0
3	I	3	Total 46	C 25	N 2	O 19	0	0	0
3	K	3	Total 45	C 25	N 2	O 18	0	0	0

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



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

- Molecule 5 is an oligosaccharide called beta-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.



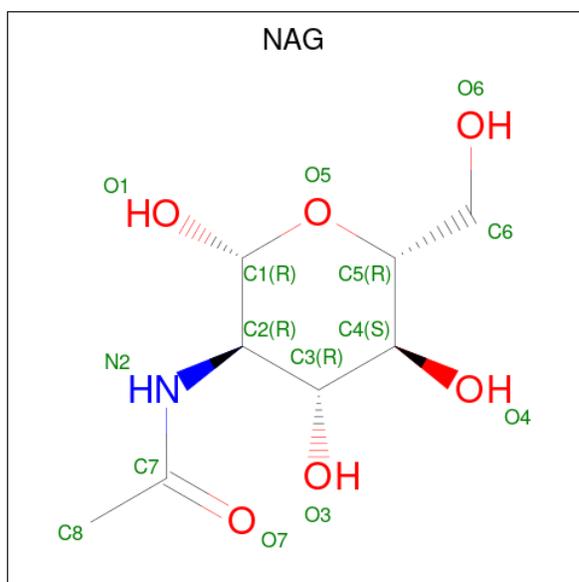
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	5	61	34	2	25	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	L	4	50	28	2	20	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

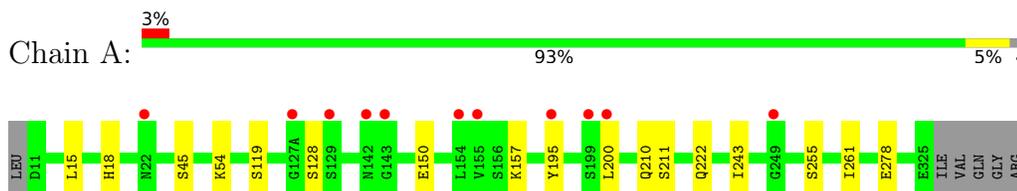
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	48	48	48	0	0
8	B	47	47	47	0	0
8	C	52	52	52	0	0
8	D	42	42	42	0	0
8	E	73	73	73	0	0
8	F	23	23	23	0	0

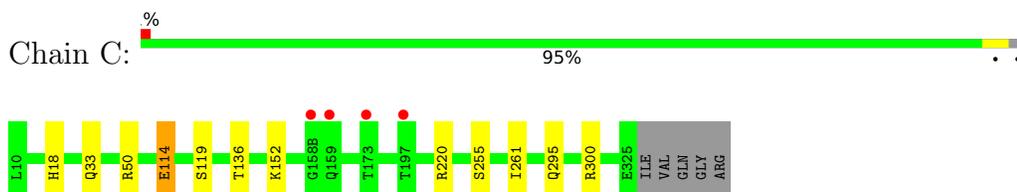
3 Residue-property plots [i](#)

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.

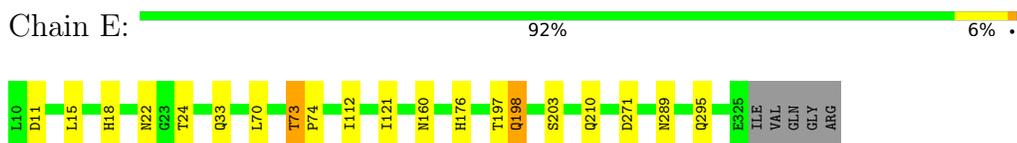
- Molecule 1: HEMAGGLUTININ



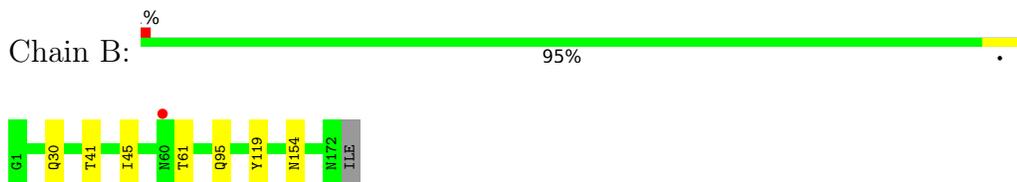
- Molecule 1: HEMAGGLUTININ



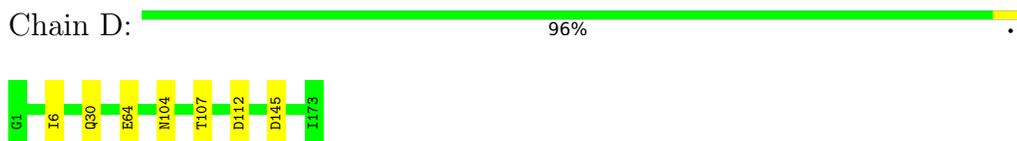
- Molecule 1: HEMAGGLUTININ



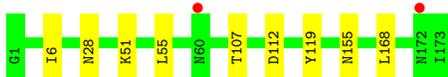
- Molecule 2: HEMAGGLUTININ



- Molecule 2: HEMAGGLUTININ



- Molecule 2: HEMAGGLUTININ



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



- Molecule 5: beta-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



- Molecule 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



MAG1
MAG2
BMA3
MAY4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.97Å 215.45Å 79.36Å 90.00° 104.91° 90.00°	Depositor
Resolution (Å)	107.72 – 2.60 48.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (107.72-2.60) 99.1 (48.85-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.208 , 0.254 0.211 , 0.253	Depositor DCC
R_{free} test set	3428 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtrriage
Anisotropy	0.689	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12105	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: SIA, BMA, GAL, MAN, NAG

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	0.28	0/2460	0.50	0/3337
1	C	0.28	0/2479	0.50	0/3361
1	E	0.30	0/2479	0.53	0/3361
2	B	0.31	0/1406	0.50	0/1899
2	D	0.31	0/1409	0.49	0/1904
2	F	0.30	0/1416	0.49	0/1912
All	All	0.30	0/11649	0.50	0/15774

There are no bond length outliers.

There are no bond angle outliers.

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	2411	0	2330	6	0
1	C	2430	0	2367	3	0
1	E	2430	0	2367	7	0
2	B	1381	0	1268	2	0
2	D	1384	0	1273	5	0
2	F	1391	0	1286	4	0
3	G	46	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	46	0	40	0	0
3	K	45	0	38	0	0
4	H	61	0	52	1	0
5	J	61	0	52	0	0
6	L	50	0	43	0	0
7	A	28	0	26	0	0
7	C	28	0	26	3	0
7	E	28	0	26	0	0
8	A	48	0	0	0	0
8	B	47	0	0	0	0
8	C	52	0	0	0	0
8	D	42	0	0	0	0
8	E	73	0	0	0	0
8	F	23	0	0	0	0
All	All	12105	0	11234	26	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 1.

All (26) 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)
7:C:401:NAG:H83	7:C:401:NAG:H3	1.87	0.57
1:A:128:SER:O	1:A:157:LYS:NZ	2.40	0.55
2:D:104:ASN:HA	2:D:107:THR:HG22	1.89	0.54
1:E:121:ILE:HD13	1:E:176:HIS:CE1	2.42	0.54
1:E:70:LEU:HD11	1:E:112:ILE:HD11	1.92	0.52
1:C:114:GLU:OE2	4:H:1:NAG:H81	2.09	0.52
1:C:114:GLU:OE2	2:D:64:GLU:OE1	2.29	0.50
7:C:401:NAG:H3	7:C:401:NAG:C8	2.44	0.48
1:A:119:SER:OG	1:A:261:ILE:HD11	2.15	0.47
1:A:54:LYS:HB3	1:A:278:GLU:HB3	1.97	0.45
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.98	0.45
1:A:243:ILE:HG23	1:A:243:ILE:O	2.17	0.44
2:D:30:GLN:HE22	2:D:145:ASP:HA	1.82	0.44
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.98	0.44
1:E:15:LEU:HD13	2:F:119:TYR:HA	1.99	0.44
1:E:73:THR:HG22	1:E:74:PRO:HD2	1.99	0.44
1:A:222:GLN:NE2	3:G:2:GAL:O3	2.51	0.43
1:C:119:SER:OG	1:C:261:ILE:HD11	2.19	0.43
2:F:6:ILE:HD12	2:F:112:ASP:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:THR:HG22	2:B:45:ILE:HD12	2.02	0.42
1:E:160:ASN:CB	1:E:198:GLN:HE21	2.32	0.42
2:F:51:LYS:NZ	2:F:107:THR:HG23	2.34	0.42
1:E:11:ASP:HB3	2:F:28:ASN:HA	2.02	0.42
1:E:160:ASN:HB3	1:E:198:GLN:HE21	1.85	0.41
7:C:401:NAG:H83	7:C:401:NAG:C3	2.51	0.41
2:D:104:ASN:HA	2:D:107:THR:CG2	2.51	0.41

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	316/324 (98%)	306 (97%)	10 (3%)	0	100	100
1	C	317/324 (98%)	304 (96%)	13 (4%)	0	100	100
1	E	317/324 (98%)	310 (98%)	6 (2%)	1 (0%)	41	64
2	B	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
2	D	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
2	F	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
All	All	1462/1491 (98%)	1415 (97%)	46 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	198	GLN

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	266/275 (97%)	258 (97%)	8 (3%)	41	67
1	C	270/275 (98%)	260 (96%)	10 (4%)	34	60
1	E	270/275 (98%)	259 (96%)	11 (4%)	30	56
2	B	144/147 (98%)	140 (97%)	4 (3%)	43	69
2	D	144/147 (98%)	144 (100%)	0	100	100
2	F	146/147 (99%)	143 (98%)	3 (2%)	53	77
All	All	1240/1266 (98%)	1204 (97%)	36 (3%)	42	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	45	SER
1	A	150	GLU
1	A	195	TYR
1	A	200	LEU
1	A	210	GLN
1	A	211	SER
1	A	255	SER
2	B	30	GLN
2	B	61	THR
2	B	95	GLN
2	B	154	ASN
1	C	18	HIS
1	C	33	GLN
1	C	50	ARG
1	C	114	GLU
1	C	136	THR
1	C	152	LYS
1	C	220	ARG
1	C	255	SER
1	C	295	GLN
1	C	300	ARG

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Mol	Chain	Res	Type
1	E	18	HIS
1	E	22	ASN
1	E	24	THR
1	E	33	GLN
1	E	73	THR
1	E	197	THR
1	E	203	SER
1	E	210	GLN
1	E	271	ASP
1	E	289	ASN
1	E	295	GLN
2	F	55	LEU
2	F	155	ASN
2	F	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	104	ASN
1	A	166	ASN
1	A	222	GLN
2	B	172	ASN
1	C	22	ASN
2	D	30	GLN
2	D	161	GLN
1	E	276	ASN
2	F	30	GLN
2	F	155	ASN

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

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	3	15,15,15	0.44	0	21,21,21	1.18	2 (9%)
3	GAL	G	2	3	11,11,12	0.67	0	15,15,17	0.73	0
3	SIA	G	3	3	20,20,21	0.60	0	24,28,31	1.68	4 (16%)
4	NAG	H	1	2,4	14,14,15	0.51	0	17,19,21	1.60	4 (23%)
4	NAG	H	2	4	14,14,15	0.57	0	17,19,21	0.97	1 (5%)
4	BMA	H	3	4	11,11,12	0.39	0	15,15,17	0.76	0
4	MAN	H	4	4	11,11,12	0.61	0	15,15,17	1.05	2 (13%)
4	MAN	H	5	4	11,11,12	0.54	0	15,15,17	1.14	2 (13%)
3	NAG	I	1	3	15,15,15	0.47	0	21,21,21	1.36	3 (14%)
3	GAL	I	2	3	11,11,12	0.62	0	15,15,17	1.07	1 (6%)
3	SIA	I	3	3	20,20,21	0.57	0	24,28,31	1.52	4 (16%)
5	NAG	J	1	2,5	14,14,15	0.60	0	17,19,21	0.83	1 (5%)
5	NAG	J	2	5	14,14,15	0.43	0	17,19,21	1.77	3 (17%)
5	BMA	J	3	5	11,11,12	0.47	0	15,15,17	1.08	1 (6%)
5	BMA	J	4	5	11,11,12	0.92	1 (9%)	15,15,17	2.15	3 (20%)
5	MAN	J	5	5	11,11,12	0.69	0	15,15,17	1.68	3 (20%)
3	NAG	K	1	3	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
3	GAL	K	2	3	11,11,12	0.65	0	15,15,17	1.44	2 (13%)
3	SIA	K	3	3	20,20,21	0.48	0	24,28,31	1.05	2 (8%)
6	NAG	L	1	2,6	14,14,15	0.63	0	17,19,21	1.12	1 (5%)
6	NAG	L	2	6	14,14,15	0.40	0	17,19,21	1.44	2 (11%)
6	BMA	L	3	6	11,11,12	0.62	0	15,15,17	2.28	6 (40%)
6	MAN	L	4	6	11,11,12	0.57	0	15,15,17	1.20	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3	-	1/6/26/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	SIA	G	3	3	-	1/18/34/38	0/1/1/1
4	NAG	H	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
4	MAN	H	5	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3	-	4/6/26/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	SIA	I	3	3	-	2/18/34/38	0/1/1/1
5	NAG	J	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	BMA	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	K	1	3	-	4/6/23/26	0/1/1/1
3	GAL	K	2	3	-	0/2/19/22	0/1/1/1
3	SIA	K	3	3	-	0/18/34/38	0/1/1/1
6	NAG	L	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	BMA	C2-C3	2.12	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4	BMA	C1-C2-C3	6.64	117.83	109.67
5	J	2	NAG	C1-O5-C5	5.92	120.22	112.19
3	G	3	SIA	C6-C5-N5	5.55	120.12	110.91
6	L	3	BMA	C1-O5-C5	5.16	119.18	112.19
3	K	1	NAG	C4-C3-C2	4.32	117.35	111.02
6	L	2	NAG	C1-O5-C5	4.31	118.03	112.19
4	H	1	NAG	C1-O5-C5	4.14	117.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	GAL	C1-O5-C5	3.93	117.52	112.19
3	I	3	SIA	C4-C5-N5	3.91	118.11	110.38
6	L	3	BMA	C1-C2-C3	3.91	114.47	109.67
5	J	5	MAN	C1-O5-C5	3.77	117.31	112.19
5	J	5	MAN	O5-C1-C2	3.68	116.46	110.77
6	L	3	BMA	O5-C5-C6	3.60	112.85	107.20
3	K	1	NAG	C3-C4-C5	3.51	116.51	110.24
4	H	5	MAN	C1-O5-C5	3.49	116.91	112.19
6	L	4	MAN	C1-O5-C5	3.45	116.87	112.19
3	I	1	NAG	C1-C2-N2	3.43	114.70	110.73
3	G	3	SIA	C6-O6-C2	3.13	118.04	111.34
5	J	4	BMA	C2-C3-C4	3.11	116.28	110.89
5	J	5	MAN	C1-C2-C3	2.94	113.27	109.67
6	L	3	BMA	C2-C3-C4	2.93	115.97	110.89
5	J	3	BMA	O5-C5-C6	2.80	111.59	107.20
3	K	3	SIA	C6-O6-C2	2.77	117.27	111.34
4	H	4	MAN	C1-C2-C3	2.75	113.04	109.67
4	H	1	NAG	C8-C7-N2	2.71	120.69	116.10
4	H	1	NAG	O5-C1-C2	-2.70	107.02	111.29
3	I	1	NAG	O5-C1-C2	-2.67	106.83	109.52
3	K	2	GAL	C1-C2-C3	2.64	112.91	109.67
3	G	1	NAG	C4-C3-C2	2.63	114.20	110.34
6	L	2	NAG	C4-C3-C2	-2.63	107.17	111.02
3	I	3	SIA	C6-O6-C2	2.62	116.94	111.34
6	L	3	BMA	O5-C1-C2	2.52	114.67	110.77
3	I	3	SIA	O6-C2-C1	2.46	112.53	107.70
5	J	2	NAG	O5-C5-C6	2.45	111.05	107.20
5	J	4	BMA	C1-O5-C5	2.40	115.45	112.19
6	L	1	NAG	C1-O5-C5	2.38	115.42	112.19
3	I	1	NAG	C3-C4-C5	2.38	114.48	110.24
4	H	1	NAG	C4-C3-C2	-2.37	107.55	111.02
3	I	3	SIA	O1B-C1-C2	2.32	119.66	113.03
3	G	1	NAG	C3-C4-C5	2.23	114.22	110.24
3	G	3	SIA	C5-N5-C10	2.21	128.56	123.18
5	J	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	H	2	NAG	C1-O5-C5	2.16	115.12	112.19
6	L	3	BMA	C3-C4-C5	2.15	114.08	110.24
3	G	3	SIA	O1B-C1-C2	2.11	119.04	113.03
4	H	5	MAN	C1-C2-C3	2.09	112.24	109.67
3	I	2	GAL	O5-C5-C6	2.09	110.48	107.20
4	H	4	MAN	C1-O5-C5	2.06	114.98	112.19
3	K	3	SIA	O1B-C1-C2	2.05	118.90	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	O5-C1-C2	-2.03	108.08	111.29
5	J	2	NAG	C3-C4-C5	2.02	113.84	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	J	5	MAN	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	SIA	C6-C5-N5-C10
3	I	3	SIA	C4-C5-N5-C10
3	K	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
5	J	5	MAN	C4-C5-C6-O6
5	J	4	BMA	C4-C5-C6-O6
5	J	4	BMA	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	3	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
3	K	1	NAG	C1-C2-N2-C7
4	H	2	NAG	O5-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
4	H	4	MAN	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C3-C2-N2-C7

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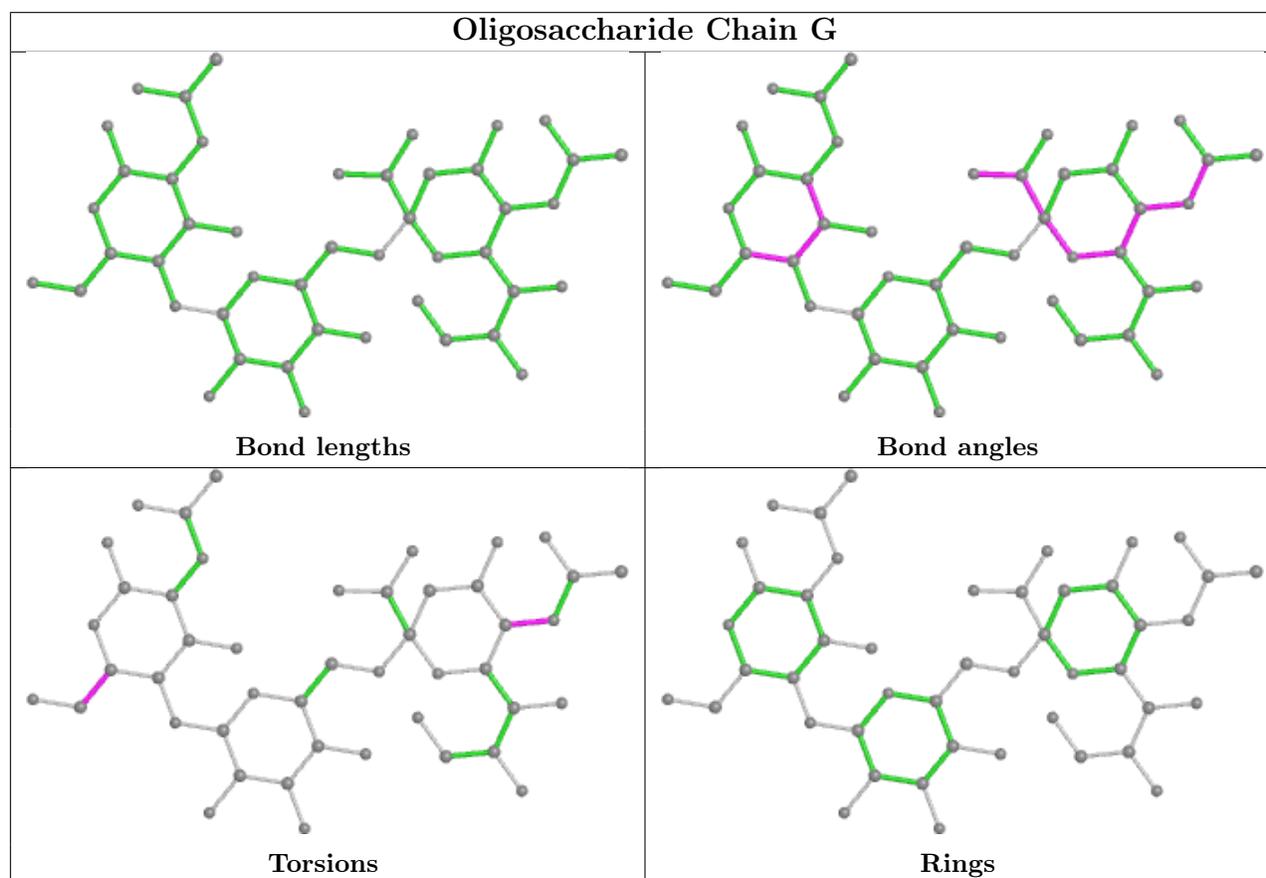
Mol	Chain	Res	Type	Atoms
3	I	3	SIA	O1A-C1-C2-C3

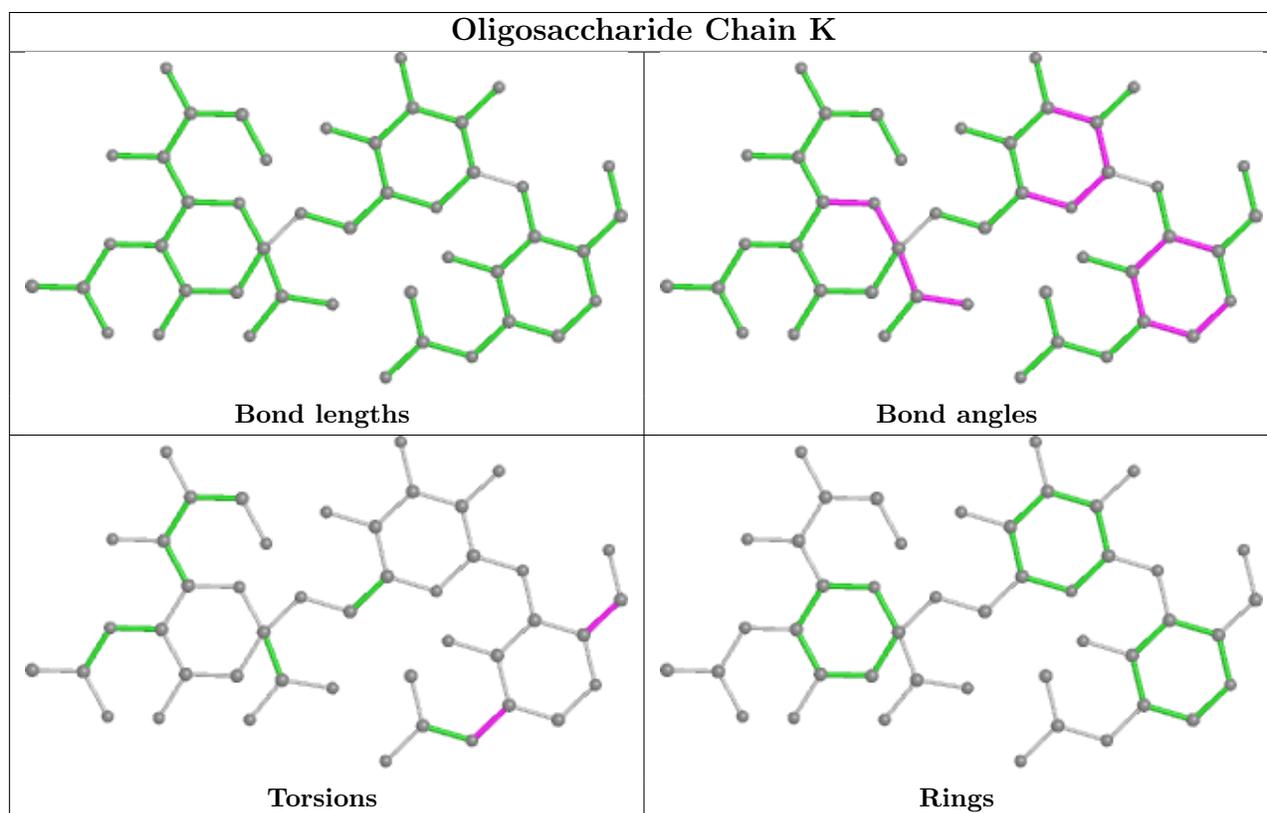
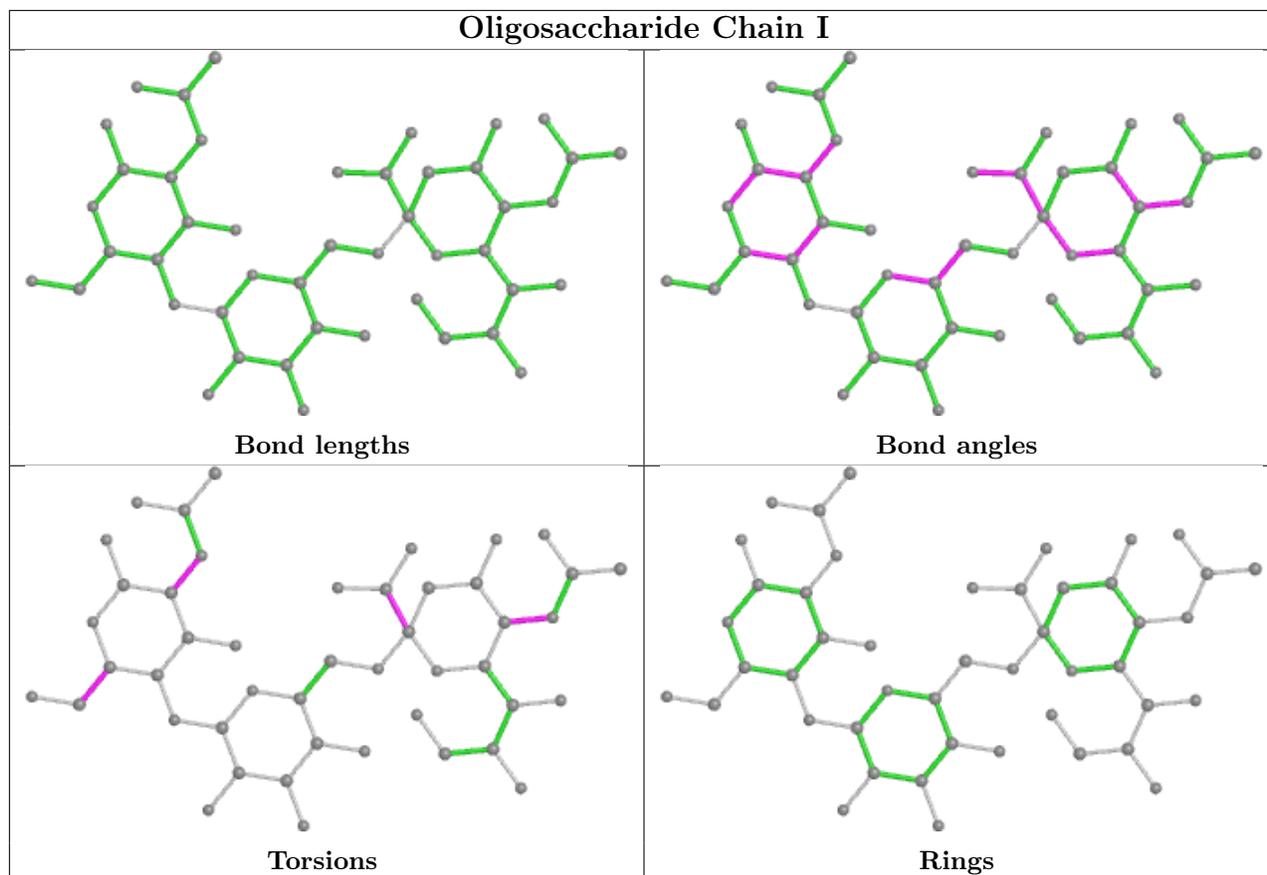
There are no ring outliers.

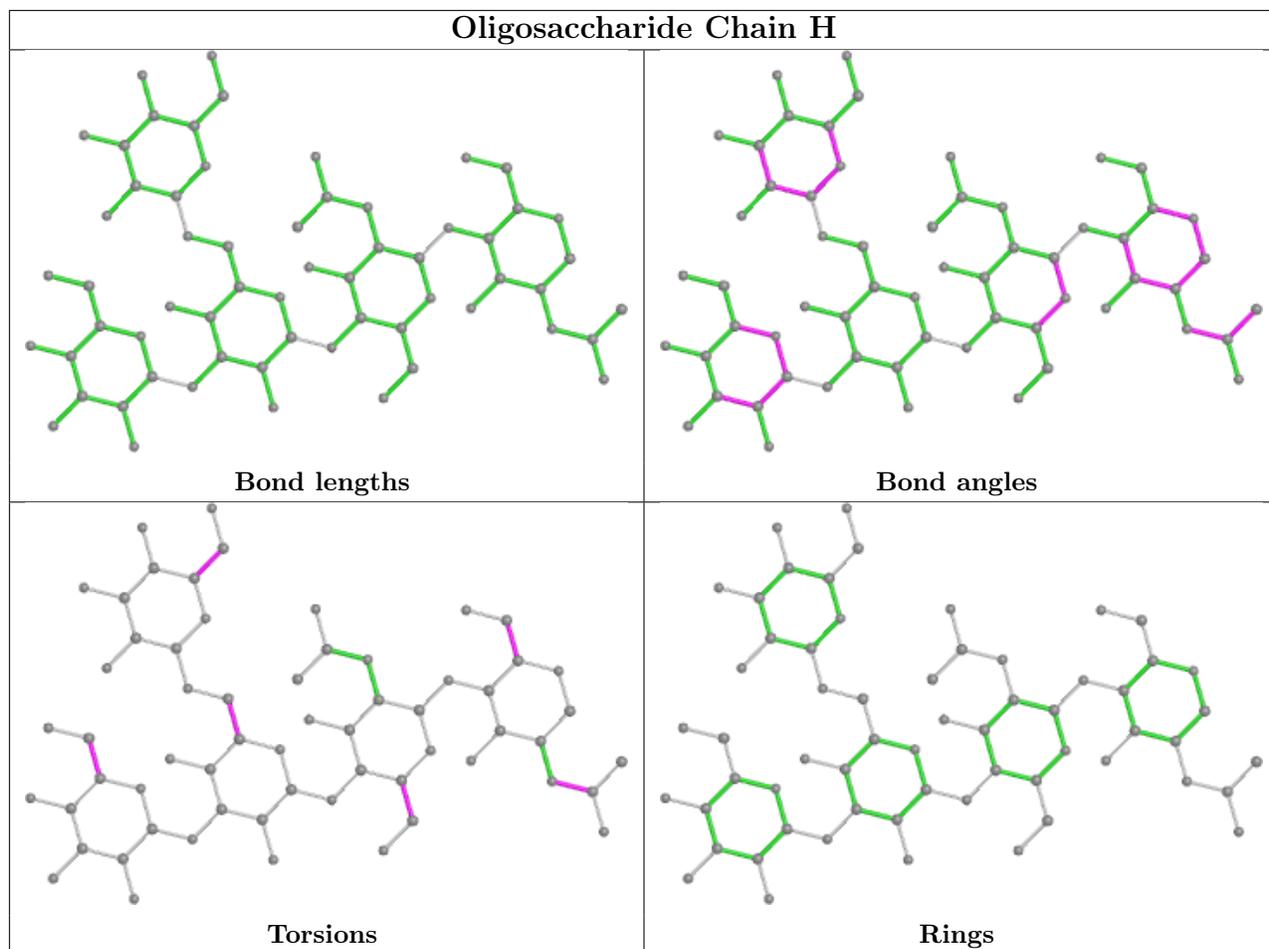
2 monomers are involved in 2 short contacts:

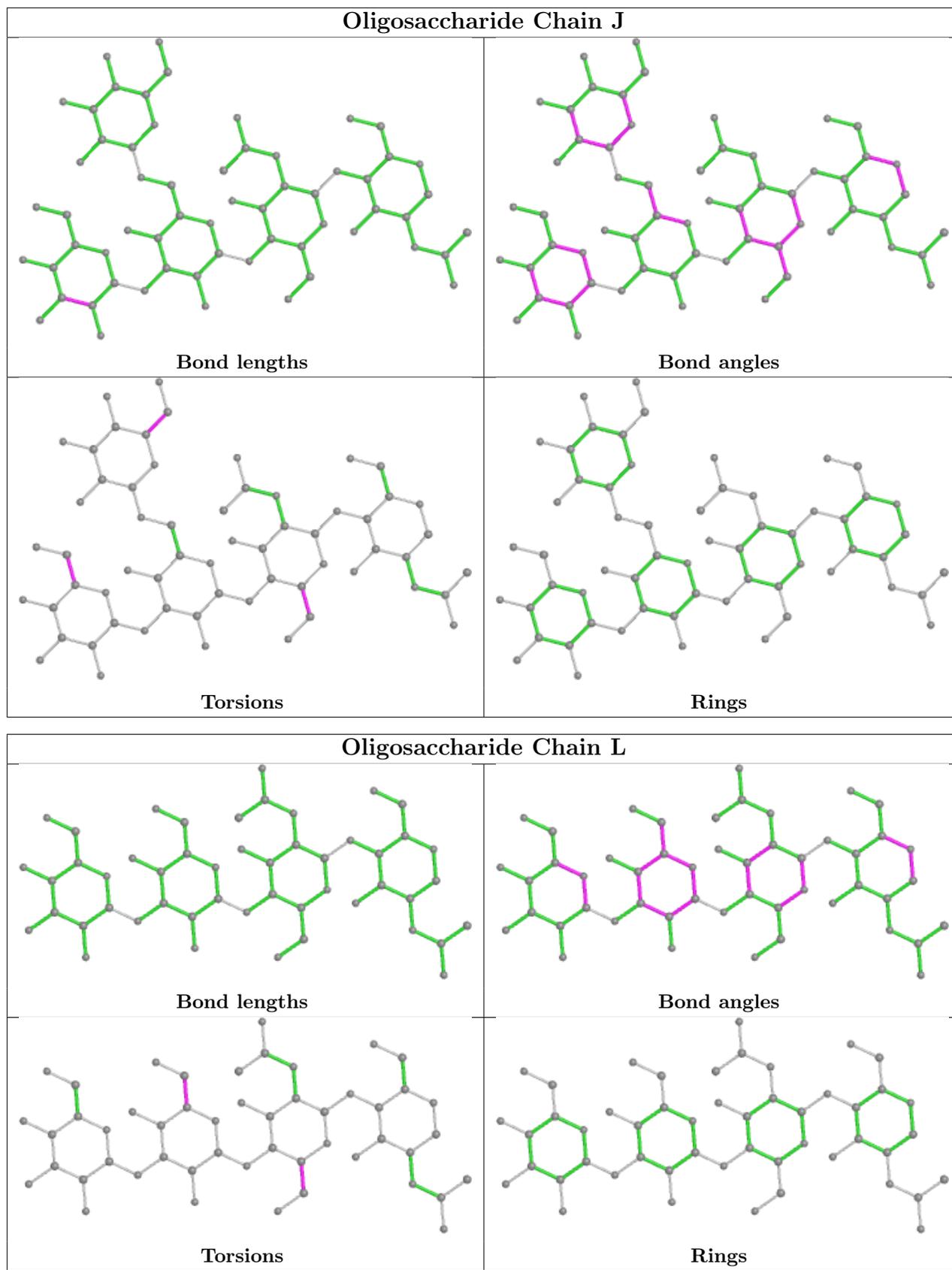
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
3	G	2	GAL	1	0

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

6 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
7	NAG	C	420	1	14,14,15	0.63	0	17,19,21	0.92	1 (5%)
7	NAG	C	401	1	14,14,15	0.43	0	17,19,21	1.81	4 (23%)
7	NAG	A	401	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
7	NAG	E	420	1	14,14,15	0.37	0	17,19,21	1.57	3 (17%)
7	NAG	E	401	1	14,14,15	0.43	0	17,19,21	1.51	5 (29%)
7	NAG	A	420	1	14,14,15	0.48	0	17,19,21	1.61	3 (17%)

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
7	NAG	C	420	1	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	C	401	1	-	4/6/23/26	0/1/1/1
7	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	NAG	E	420	1	-	2/6/23/26	0/1/1/1
7	NAG	E	401	1	-	1/6/23/26	0/1/1/1
7	NAG	A	420	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	420	NAG	C1-O5-C5	4.33	118.05	112.19
7	C	401	NAG	C1-O5-C5	4.17	117.84	112.19
7	E	420	NAG	C1-O5-C5	3.52	116.96	112.19
7	C	401	NAG	C8-C7-N2	3.46	121.95	116.10
7	C	401	NAG	C2-N2-C7	3.40	127.75	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	NAG	C4-C3-C2	-3.09	106.49	111.02
7	C	420	NAG	O5-C1-C2	-2.89	106.72	111.29
7	A	401	NAG	O5-C1-C2	-2.75	106.94	111.29
7	A	420	NAG	C3-C4-C5	2.64	114.95	110.24
7	E	401	NAG	C1-O5-C5	2.54	115.63	112.19
7	E	420	NAG	C8-C7-N2	2.45	120.25	116.10
7	E	401	NAG	O5-C1-C2	-2.40	107.50	111.29
7	E	401	NAG	C2-N2-C7	2.38	126.29	122.90
7	C	401	NAG	O7-C7-C8	-2.21	117.95	122.06
7	E	401	NAG	C4-C3-C2	-2.16	107.86	111.02
7	A	420	NAG	O5-C5-C4	2.10	115.94	110.83
7	E	401	NAG	C1-C2-N2	2.08	114.03	110.49
7	E	420	NAG	C4-C3-C2	-2.07	107.98	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	420	NAG	C1
7	C	420	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	401	NAG	C3-C2-N2-C7
7	C	401	NAG	C8-C7-N2-C2
7	C	401	NAG	O7-C7-N2-C2
7	E	420	NAG	C8-C7-N2-C2
7	E	420	NAG	O7-C7-N2-C2
7	A	401	NAG	C4-C5-C6-O6
7	C	401	NAG	C3-C2-N2-C7
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C3-C2-N2-C7
7	C	420	NAG	C3-C2-N2-C7
7	C	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	NAG	3	0

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	318/324 (98%)	0.15	11 (3%) 44 36	45, 69, 110, 120	0
1	C	319/324 (98%)	-0.11	4 (1%) 77 73	38, 62, 87, 99	0
1	E	319/324 (98%)	-0.27	0 100 100	36, 52, 83, 94	0
2	B	172/173 (99%)	-0.11	1 (0%) 89 88	38, 55, 74, 94	0
2	D	173/173 (100%)	-0.12	0 100 100	35, 51, 70, 81	0
2	F	173/173 (100%)	-0.02	2 (1%) 79 76	36, 56, 80, 90	0
All	All	1474/1491 (98%)	-0.08	18 (1%) 79 76	35, 58, 94, 120	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	5.0
1	C	158(B)	GLY	4.7
1	A	249	GLY	4.7
1	A	127(A)	GLY	4.0
1	A	195	TYR	3.8
1	A	155	VAL	3.4
1	C	197	THR	3.2
1	A	143	GLY	3.0
2	F	60	ASN	2.9
2	B	60	ASN	2.7
1	C	159	GLN	2.5
1	A	142	ASN	2.5
2	F	172	ASN	2.4
1	A	199	SER	2.2
1	C	173	THR	2.2
1	A	154	LEU	2.1
1	A	22	ASN	2.0
1	A	129	SER	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](#)

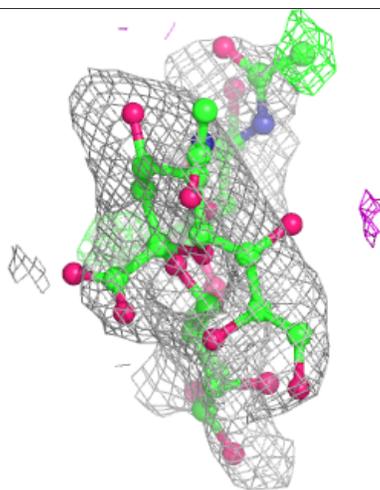
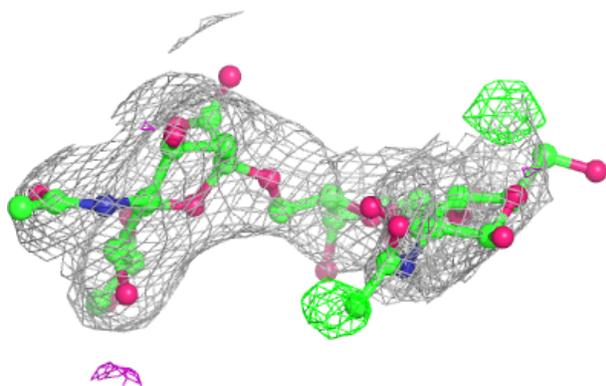
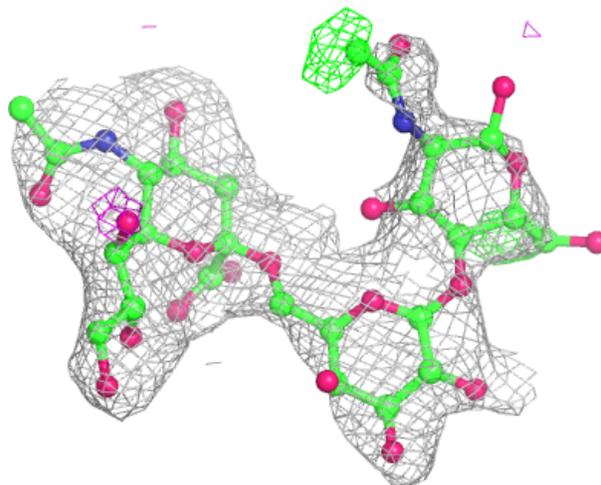
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	L	4	11/12	0.42	0.51	111,120,125,127	0
5	BMA	J	4	11/12	0.45	0.36	103,105,110,110	0
4	MAN	H	4	11/12	0.56	0.41	114,116,122,126	0
6	BMA	L	3	11/12	0.62	0.27	98,101,107,114	0
4	MAN	H	5	11/12	0.64	0.41	108,112,116,117	0
3	NAG	I	1	15/15	0.71	0.35	104,107,110,110	0
3	NAG	G	1	15/15	0.76	0.36	132,137,143,145	0
3	GAL	G	2	11/12	0.78	0.33	118,128,132,133	0
5	MAN	J	5	11/12	0.79	0.28	97,101,104,104	0
5	BMA	J	3	11/12	0.79	0.30	95,101,105,109	0
3	NAG	K	1	14/15	0.79	0.38	110,115,122,122	0
4	BMA	H	3	11/12	0.82	0.25	102,109,115,115	0
3	GAL	K	2	11/12	0.83	0.28	94,105,109,109	0
3	GAL	I	2	11/12	0.86	0.29	86,96,102,102	0
6	NAG	L	2	14/15	0.87	0.17	70,74,82,90	0
4	NAG	H	1	14/15	0.89	0.15	57,62,66,73	0
4	NAG	H	2	14/15	0.91	0.20	79,83,92,97	0
3	SIA	G	3	20/21	0.91	0.21	101,105,109,110	0
5	NAG	J	2	14/15	0.92	0.20	76,83,87,89	0
5	NAG	J	1	14/15	0.93	0.13	53,56,62,68	0
3	SIA	I	3	20/21	0.93	0.15	67,70,73,74	0
6	NAG	L	1	14/15	0.94	0.12	51,54,59,64	0
3	SIA	K	3	20/21	0.96	0.15	68,72,79,81	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.

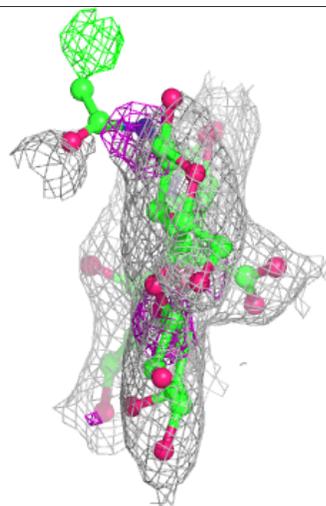
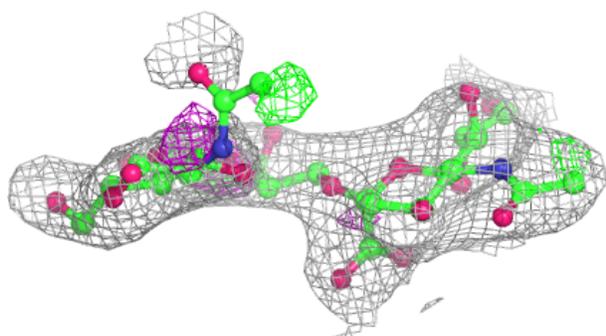
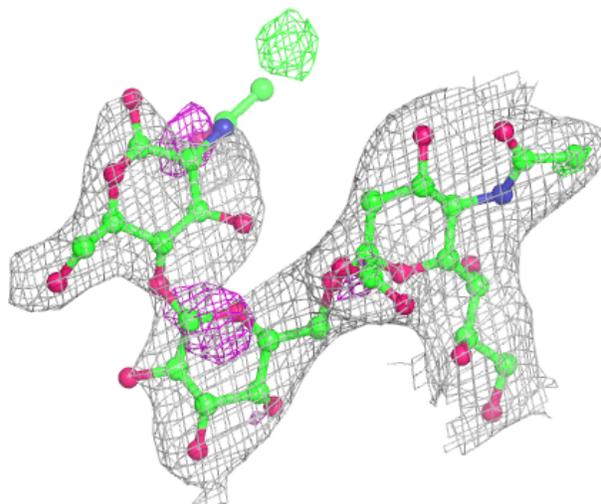
Electron density around Chain G:

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



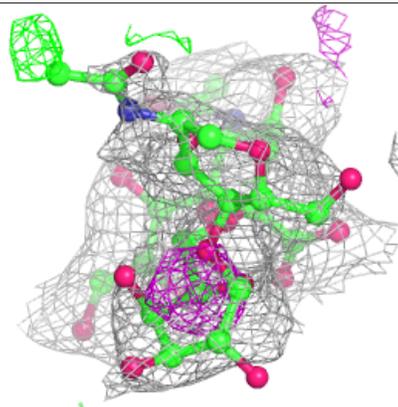
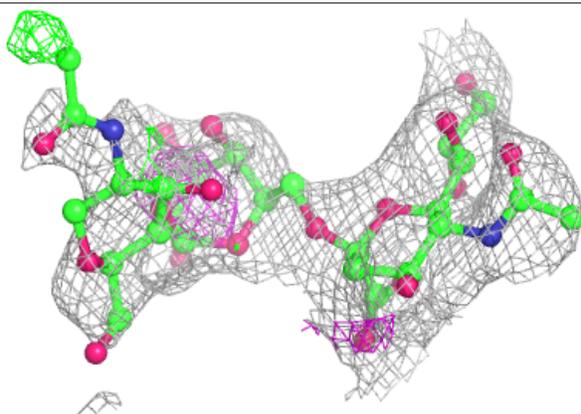
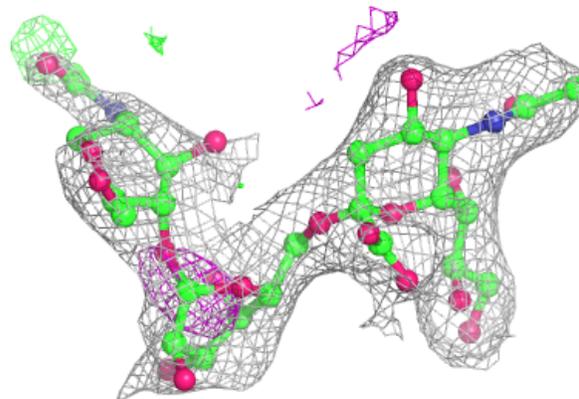
Electron density around Chain I:

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



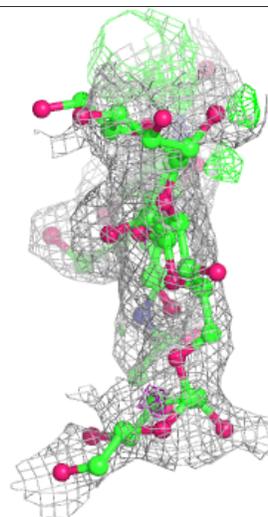
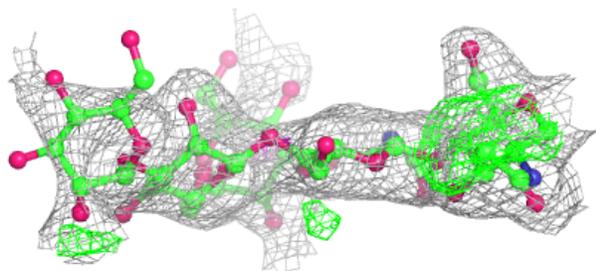
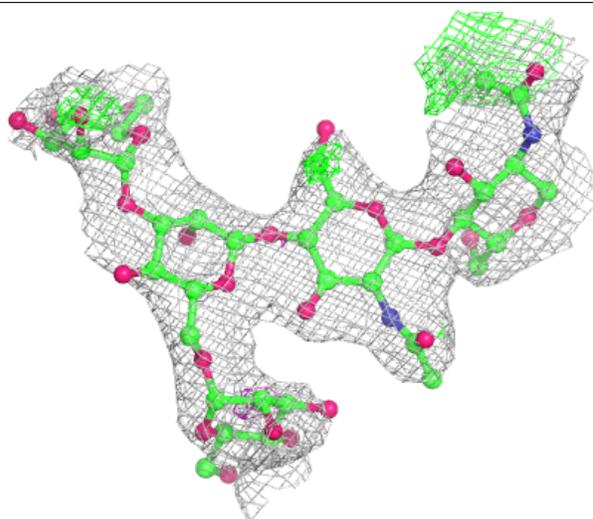
Electron density around Chain K:

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



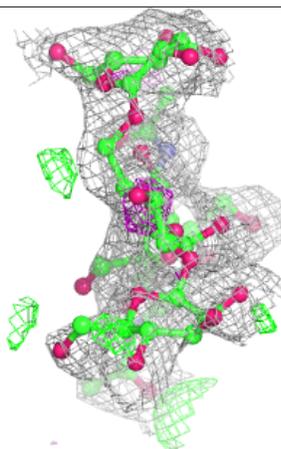
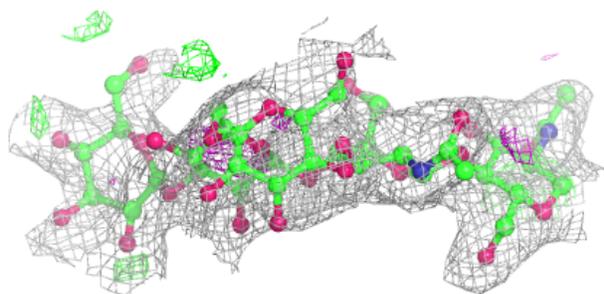
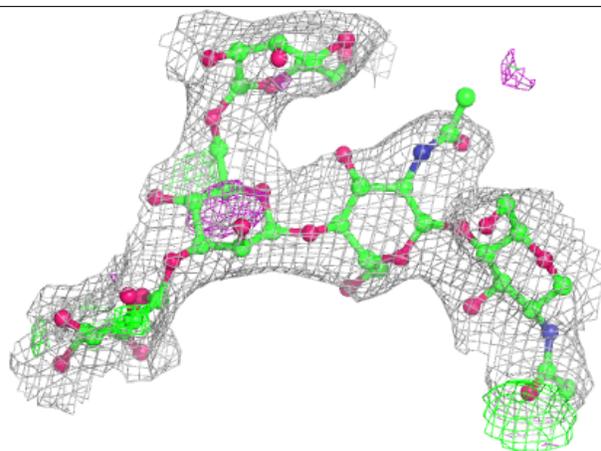
Electron density around Chain H:

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

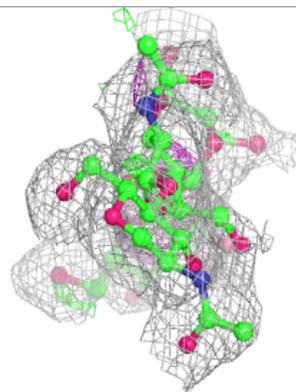
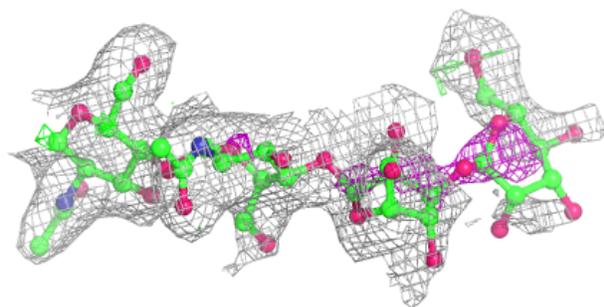
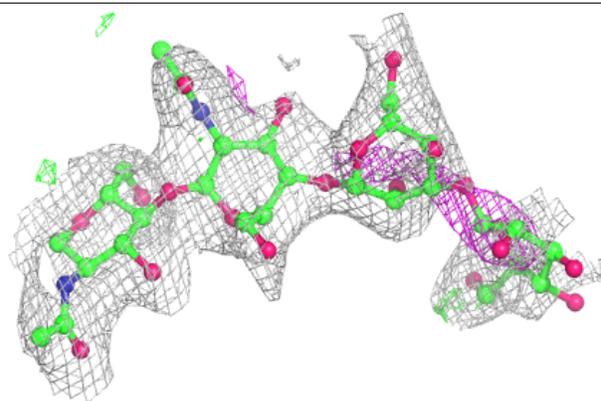


Electron density around Chain J:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	420	14/15	0.72	0.36	90,97,98,100	0
7	NAG	E	401	14/15	0.78	0.24	79,85,88,90	0
7	NAG	C	401	14/15	0.80	0.36	97,102,106,108	0
7	NAG	C	420	14/15	0.82	0.28	77,83,89,90	0
7	NAG	E	420	14/15	0.87	0.29	77,83,86,88	0
7	NAG	A	401	14/15	0.88	0.20	77,79,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.