



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:24 AM UTC

PDB ID : 7LY3 / pdb_00007ly3
Title : Crystal structure of SARS-CoV-2 S NTD bound to S2M28 Fab
Authors : McCallum, M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-03-05
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

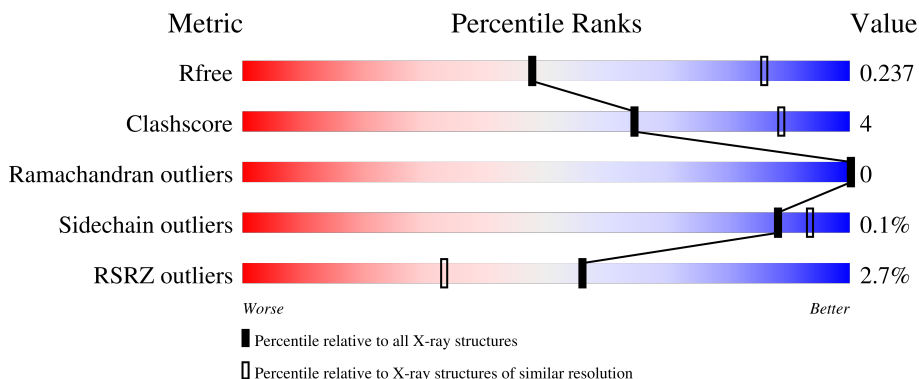
1 Overall quality at a glance

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.



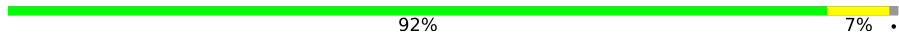



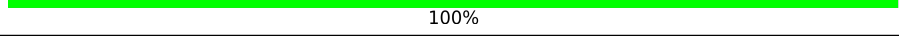


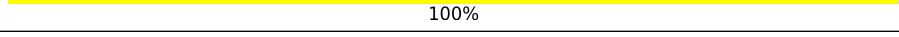
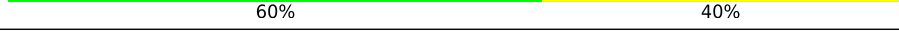

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	335	 4% 77% 7% 15%
1	B	335	 4% 75% 9% 16%
2	D	221	 % 89% 11%
2	F	221	 % 88% 12%
3	C	212	 % 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	212	 92% 7%
4	G	4	 75% 25%
4	I	4	 75% 25%
4	M	4	 75% 25%
5	H	2	 100%
5	J	2	 50% 50%
5	N	2	 50% 50%
5	O	2	 100%
6	K	5	 60% 40%
6	L	5	 40% 60%

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
8	UNX	A	1703	-	-	-	X
8	UNX	B	404	-	-	-	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 11292 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2209	1430	362	409	8	0	0	0
1	B	282	2212	1432	361	411	8	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P0DTC2
A	-17	GLY	-	expression tag	UNP P0DTC2
A	-16	ILE	-	expression tag	UNP P0DTC2
A	-15	LEU	-	expression tag	UNP P0DTC2
A	-14	PRO	-	expression tag	UNP P0DTC2
A	-13	SER	-	expression tag	UNP P0DTC2
A	-12	PRO	-	expression tag	UNP P0DTC2
A	-11	GLY	-	expression tag	UNP P0DTC2
A	-10	MET	-	expression tag	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	ALA	-	expression tag	UNP P0DTC2
A	-7	LEU	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	SER	-	expression tag	UNP P0DTC2
A	-4	LEU	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	MET	-	expression tag	UNP P0DTC2
A	6	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	CYS	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	303	ALA	LEU	conflict	UNP P0DTC2
A	308	ALA	-	expression tag	UNP P0DTC2
A	309	HIS	-	expression tag	UNP P0DTC2
A	310	HIS	-	expression tag	UNP P0DTC2
A	311	HIS	-	expression tag	UNP P0DTC2
A	312	HIS	-	expression tag	UNP P0DTC2
A	313	HIS	-	expression tag	UNP P0DTC2
A	314	HIS	-	expression tag	UNP P0DTC2
A	315	HIS	-	expression tag	UNP P0DTC2
A	316	HIS	-	expression tag	UNP P0DTC2
B	-18	MET	-	initiating methionine	UNP P0DTC2
B	-17	GLY	-	expression tag	UNP P0DTC2
B	-16	ILE	-	expression tag	UNP P0DTC2
B	-15	LEU	-	expression tag	UNP P0DTC2
B	-14	PRO	-	expression tag	UNP P0DTC2
B	-13	SER	-	expression tag	UNP P0DTC2
B	-12	PRO	-	expression tag	UNP P0DTC2
B	-11	GLY	-	expression tag	UNP P0DTC2
B	-10	MET	-	expression tag	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	ALA	-	expression tag	UNP P0DTC2
B	-7	LEU	-	expression tag	UNP P0DTC2
B	-6	LEU	-	expression tag	UNP P0DTC2
B	-5	SER	-	expression tag	UNP P0DTC2
B	-4	LEU	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	SER	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	MET	-	expression tag	UNP P0DTC2
B	6	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	CYS	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	303	ALA	LEU	conflict	UNP P0DTC2
B	308	ALA	-	expression tag	UNP P0DTC2
B	309	HIS	-	expression tag	UNP P0DTC2
B	310	HIS	-	expression tag	UNP P0DTC2
B	311	HIS	-	expression tag	UNP P0DTC2
B	312	HIS	-	expression tag	UNP P0DTC2
B	313	HIS	-	expression tag	UNP P0DTC2
B	314	HIS	-	expression tag	UNP P0DTC2
B	315	HIS	-	expression tag	UNP P0DTC2
B	316	HIS	-	expression tag	UNP P0DTC2

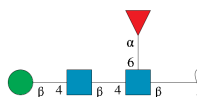
- Molecule 2 is a protein called S2M28 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	221	Total 1654	C 1048	N 278	O 322	S 6	0	0	0
2	F	221	Total 1651	C 1046	N 278	O 321	S 6	0	0	0

- Molecule 3 is a protein called S2M28 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	211	Total 1547	C 971	N 256	O 316	S 4	0	0	0
3	E	210	Total 1554	C 975	N 259	O 316	S 4	0	0	0

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



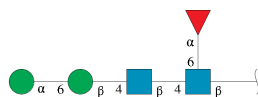
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



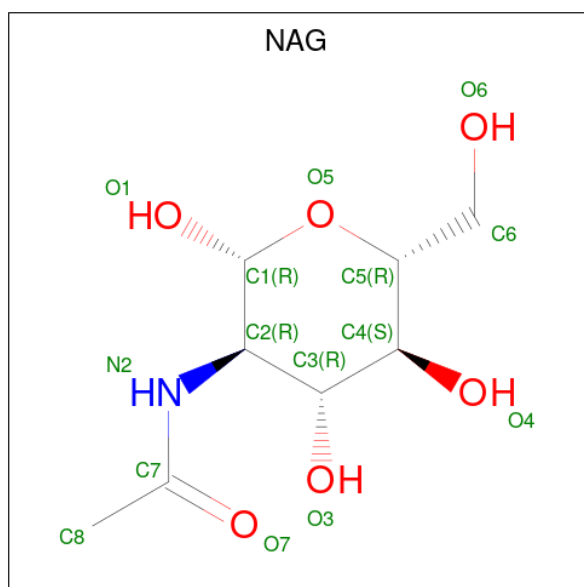
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	J	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	N	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	O	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	5	Total	C	N	O	0	0	0
			60	34	2	24			
6	L	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

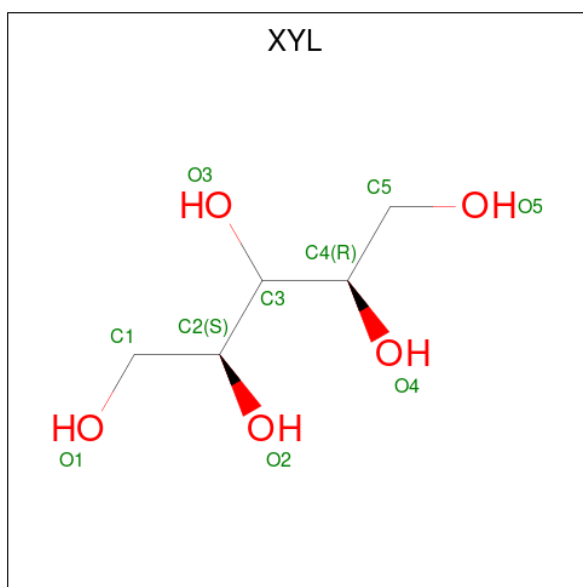


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
7	A	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0

- Molecule 8 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

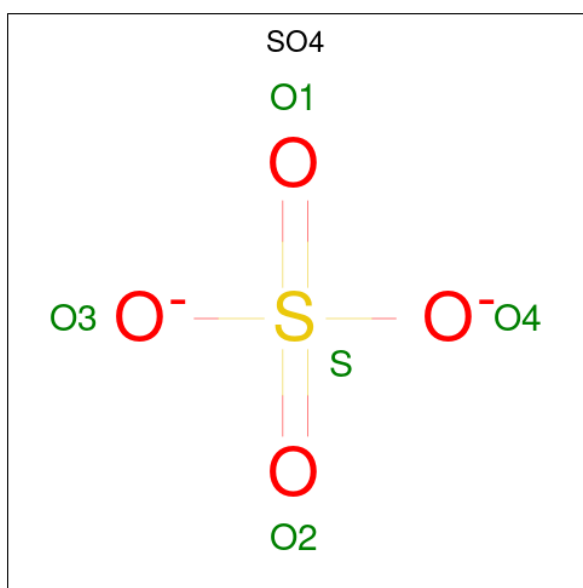
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total X 1 1	0	0
8	B	1	Total X 1 1	0	0

- Molecule 9 is Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	5	5		
9	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

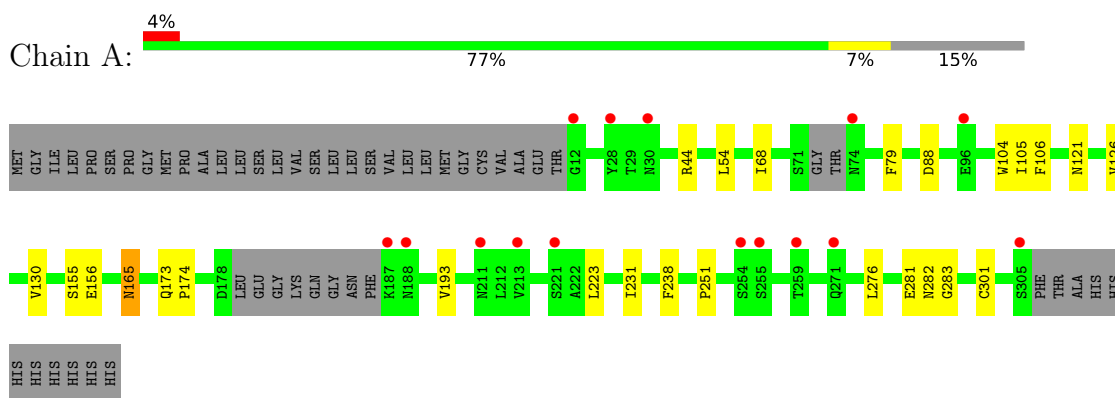


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		

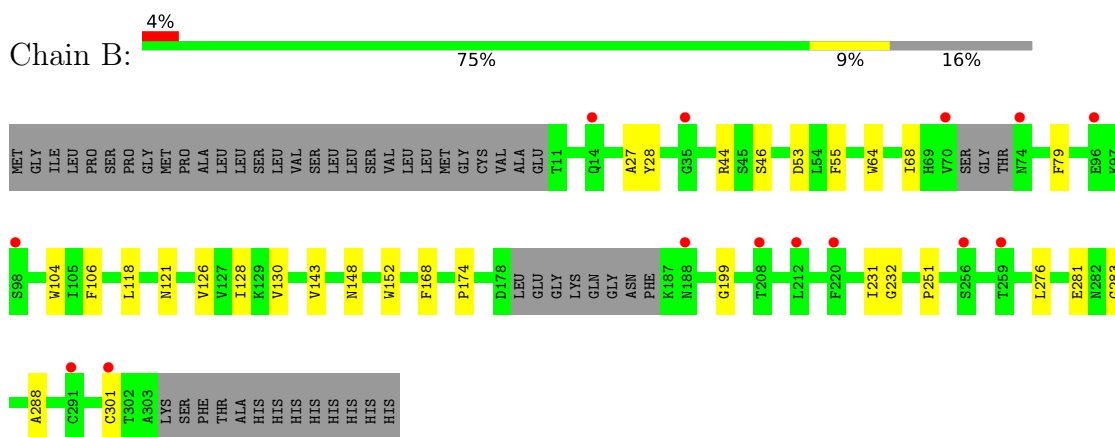
3 Residue-property plots [i](#)

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.

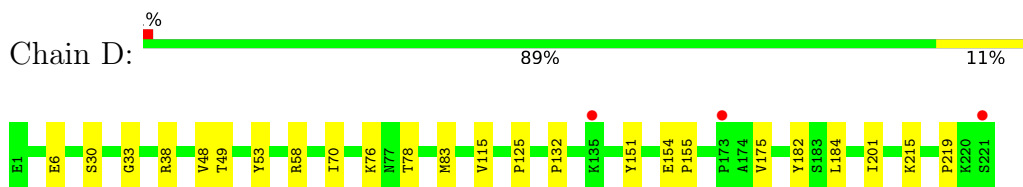
- Molecule 1: Spike protein S1



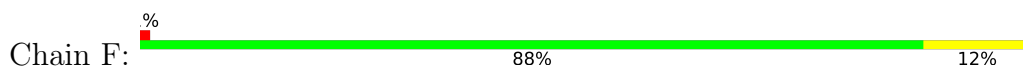
- Molecule 1: Spike protein S1



- Molecule 2: S2M28 Fab Heavy Chain



- Molecule 2: S2M28 Fab Heavy Chain

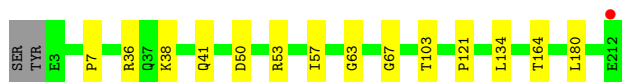




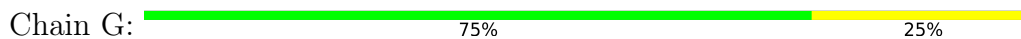
- Molecule 3: S2M28 Fab Light Chain



- Molecule 3: S2M28 Fab Light Chain



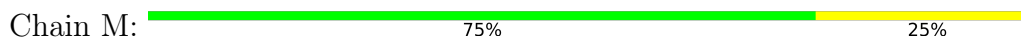
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
FUC2

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

Chain K:  60% 40%

MAG1
MAG2
BMA3
MAM4
FUC5

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

Chain L:  40% 60%

MAG1
MAG2
BMA3
MAM4
FUC5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.44Å 125.46Å 365.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.00 49.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.42-3.00) 91.9 (49.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.208 , 0.234 0.212 , 0.237	Depositor DCC
R_{free} test set	623 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11292	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: SO4, XYL, FUC, UNX, NAG, BMA, 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	0.25	0/2271	0.50	0/3104
1	B	0.24	0/2275	0.50	0/3107
2	D	0.28	0/1698	0.62	0/2320
2	F	0.30	0/1695	0.66	0/2316
3	C	0.27	0/1587	0.66	0/2177
3	E	0.27	0/1594	0.71	1/2183 (0.0%)
All	All	0.27	0/11120	0.60	1/15207 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	36	ARG	CB-CG-CD	-5.09	99.59	111.30

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	2209	0	2055	18	0
1	B	2212	0	2070	19	0
2	D	1654	0	1580	18	0
2	F	1651	0	1579	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1547	0	1454	13	1
3	E	1554	0	1488	10	0
4	G	49	0	43	3	0
4	I	49	0	43	0	0
4	M	49	0	43	0	0
5	H	24	0	22	0	0
5	J	24	0	22	1	0
5	N	24	0	22	0	0
5	O	24	0	22	1	0
6	K	60	0	52	0	0
6	L	60	0	52	0	0
7	A	28	0	26	0	0
7	B	42	0	39	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	10	0	12	0	0
9	B	10	0	12	0	0
10	D	5	0	0	0	0
10	F	5	0	0	0	0
All	All	11292	0	10636	86	1

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 4.

The worst 5 of 86 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:B:121:ASN:OD1	1:B:126:VAL:HG22	1.89	0.71
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.78	0.65
2:D:132:PRO:HD2	2:D:219:PRO:HA	1.83	0.61
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.82	0.60
1:A:121:ASN:OD1	1:A:126:VAL:HG22	2.01	0.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:GLN:O	3:C:173:LYS:NZ[4_445]	2.16	0.04

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	278/335 (83%)	264 (95%)	14 (5%)	0	100	100
1	B	276/335 (82%)	267 (97%)	9 (3%)	0	100	100
2	D	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
2	F	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
3	C	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
3	E	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
All	All	1409/1536 (92%)	1370 (97%)	39 (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	233/297 (78%)	232 (100%)	1 (0%)	84	90
1	B	237/297 (80%)	237 (100%)	0	100	100
2	D	179/185 (97%)	179 (100%)	0	100	100
2	F	179/185 (97%)	179 (100%)	0	100	100
3	C	166/178 (93%)	166 (100%)	0	100	100
3	E	171/178 (96%)	171 (100%)	0	100	100
All	All	1165/1320 (88%)	1164 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
3	E	172	ASN
1	A	271	GLN
1	B	30	ASN
1	B	49	HIS

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](#)

30 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	$\# Z > 2$
4	NAG	G	1	4,1	14,14,15	0.25	0	17,19,21	0.64	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.60	0
4	BMA	G	3	4	11,11,12	0.90	0	15,15,17	0.76	0
4	FUC	G	4	4	10,10,11	0.68	0	14,14,16	0.68	0
5	NAG	H	1	1,5	14,14,15	0.23	0	17,19,21	0.43	0
5	FUC	H	2	5	10,10,11	1.00	0	14,14,16	0.68	0
4	NAG	I	1	4,1	14,14,15	0.26	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.53	0
4	BMA	I	3	4	11,11,12	1.13	0	15,15,17	0.93	2 (13%)
4	FUC	I	4	4	10,10,11	0.77	0	14,14,16	0.67	0
5	NAG	J	1	1,5	14,14,15	0.43	0	17,19,21	0.66	1 (5%)
5	FUC	J	2	5	10,10,11	0.95	0	14,14,16	0.72	0
6	NAG	K	1	1,6	14,14,15	0.29	0	17,19,21	0.57	0
6	NAG	K	2	6	14,14,15	0.47	0	17,19,21	0.70	1 (5%)
6	BMA	K	3	6	11,11,12	0.79	0	15,15,17	0.77	0
6	MAN	K	4	6	11,11,12	0.77	0	15,15,17	1.04	2 (13%)
6	FUC	K	5	6	10,10,11	0.75	0	14,14,16	0.69	0
6	NAG	L	1	1,6	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
6	NAG	L	2	6	14,14,15	0.28	0	17,19,21	0.59	0
6	BMA	L	3	6	11,11,12	1.16	1 (9%)	15,15,17	1.08	2 (13%)
6	MAN	L	4	6	11,11,12	0.76	1 (9%)	15,15,17	1.10	2 (13%)
6	FUC	L	5	6	10,10,11	0.75	0	14,14,16	0.70	0
4	NAG	M	1	4,1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.51	0
4	BMA	M	3	4	11,11,12	0.97	1 (9%)	15,15,17	0.84	1 (6%)
4	FUC	M	4	4	10,10,11	0.76	0	14,14,16	0.89	0
5	NAG	N	1	1,5	14,14,15	0.75	1 (7%)	17,19,21	0.86	1 (5%)
5	FUC	N	2	5	10,10,11	0.85	0	14,14,16	0.74	0
5	NAG	O	1	1,5	14,14,15	0.45	0	17,19,21	0.53	0
5	FUC	O	2	5	10,10,11	1.63	4 (40%)	14,14,16	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	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	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	H	2	5	-	-	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	FUC	I	4	4	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
6	FUC	K	5	6	-	-	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	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
6	FUC	L	5	6	-	-	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	FUC	M	4	4	-	-	0/1/1/1
5	NAG	N	1	1,5	-	3/6/23/26	0/1/1/1
5	FUC	N	2	5	-	-	0/1/1/1
5	NAG	O	1	1,5	-	3/6/23/26	0/1/1/1
5	FUC	O	2	5	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2	FUC	C4-C5	2.56	1.58	1.52
5	N	1	NAG	C1-C2	2.55	1.55	1.52
5	O	2	FUC	C4-C3	2.44	1.58	1.52
6	L	3	BMA	C1-C2	2.44	1.58	1.52
5	O	2	FUC	C2-C3	2.22	1.55	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	4	MAN	C1-O5-C5	3.06	116.28	112.19
6	L	1	NAG	C4-C3-C2	2.72	115.00	111.02
6	L	3	BMA	C1-O5-C5	2.62	115.70	112.19
6	K	4	MAN	C1-O5-C5	2.60	115.67	112.19
6	K	2	NAG	C1-O5-C5	2.40	115.40	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

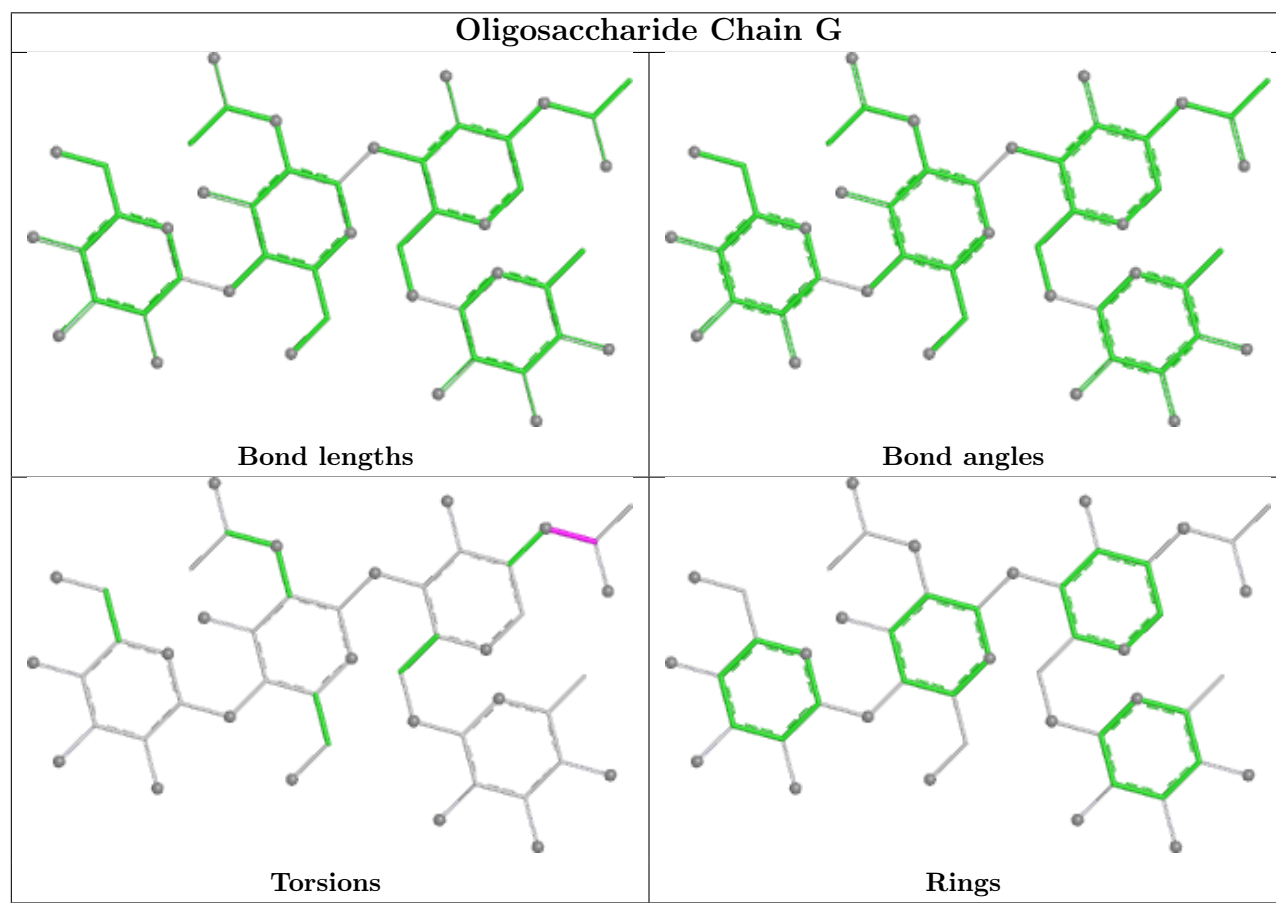
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
6	L	3	BMA	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6

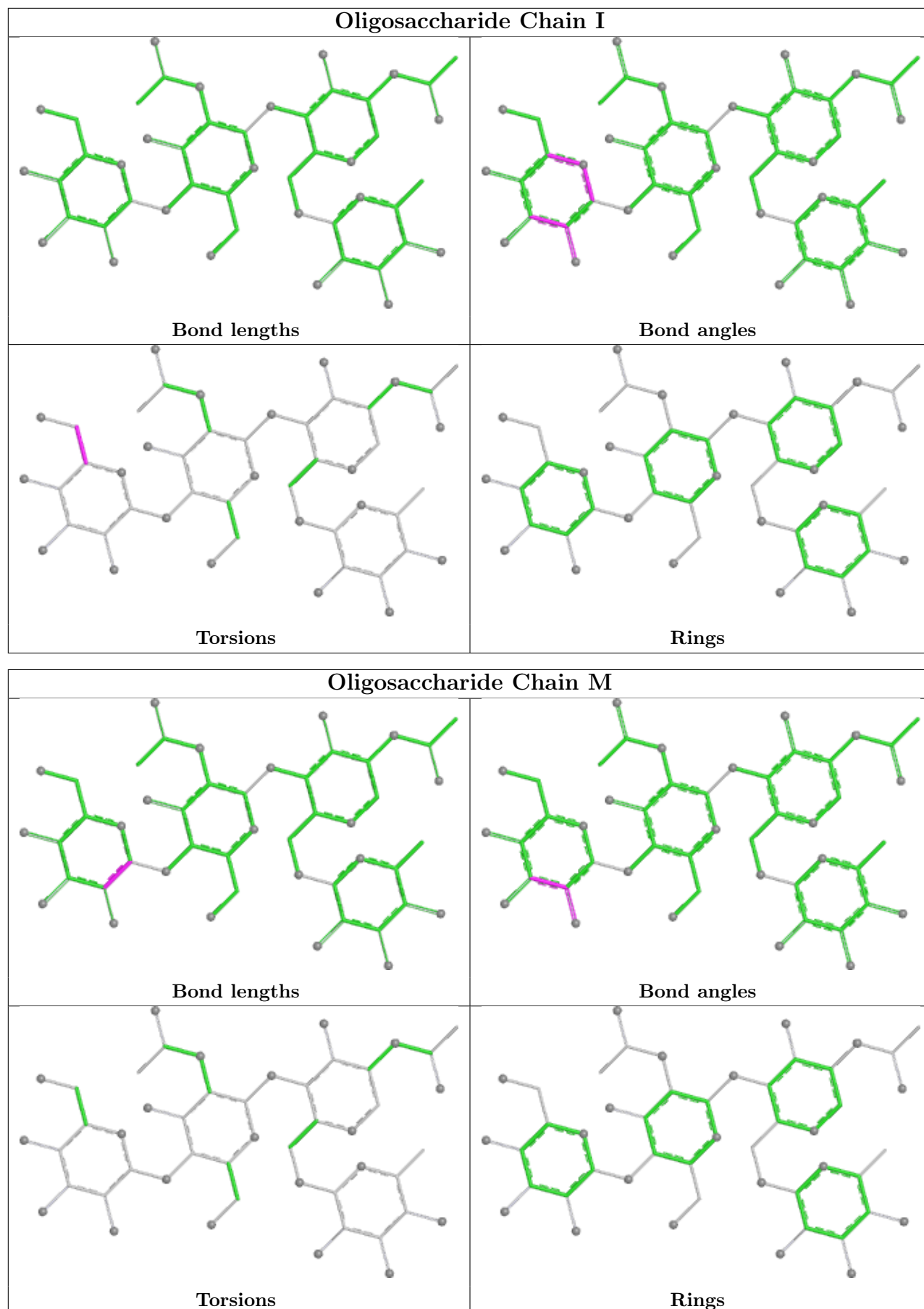
There are no ring outliers.

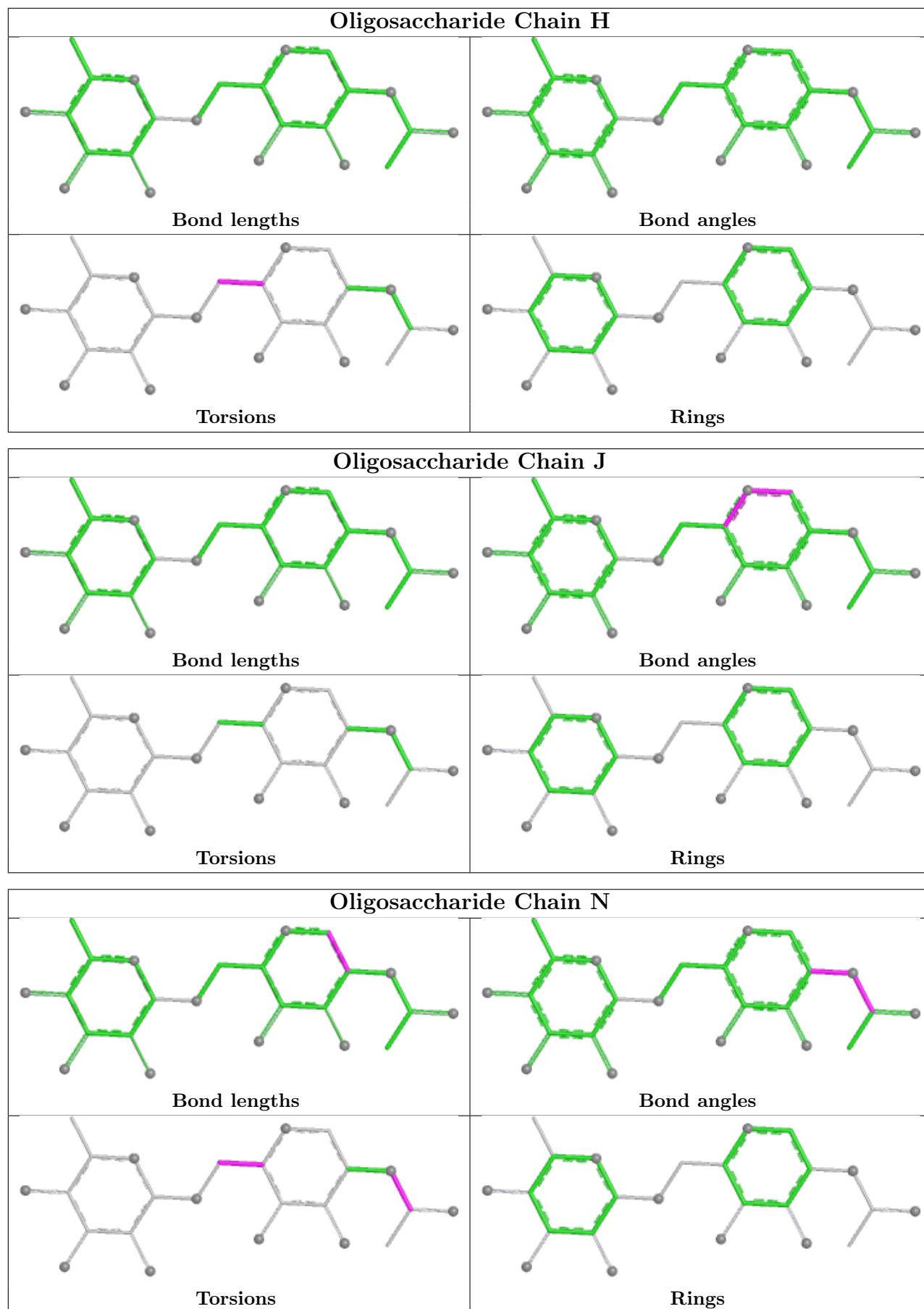
3 monomers are involved in 5 short contacts:

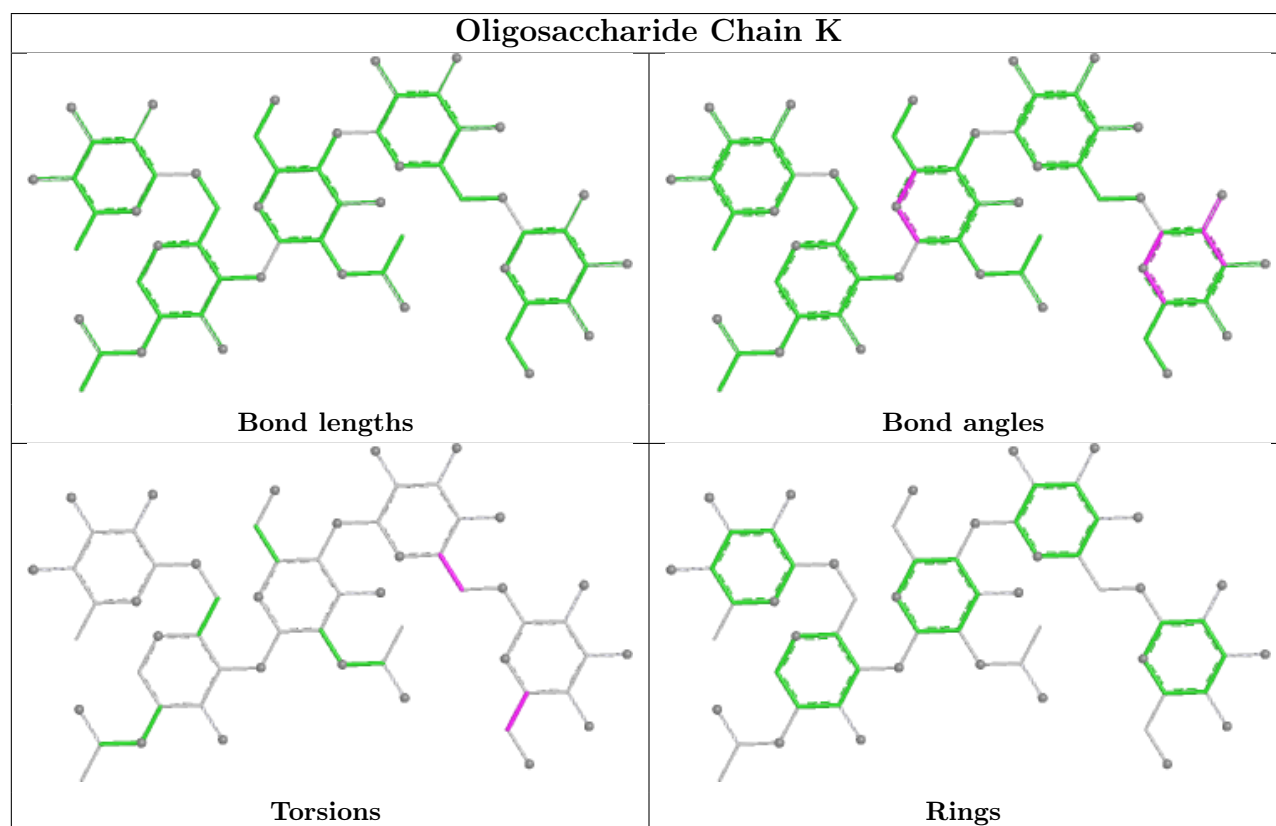
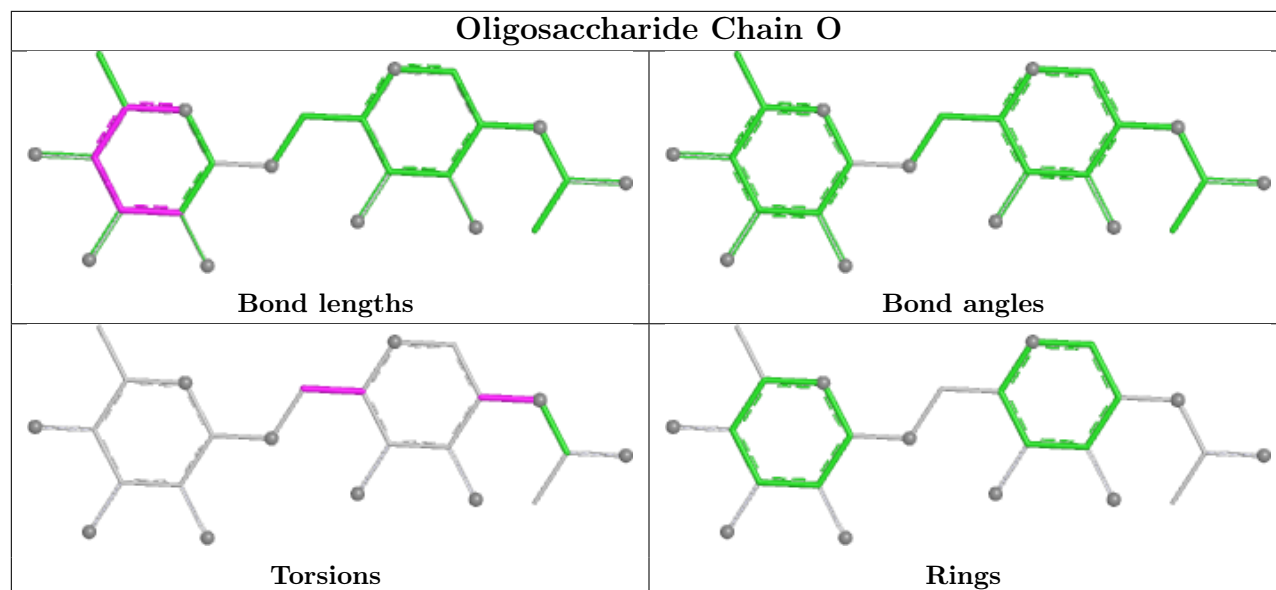
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
5	J	1	NAG	1	0
4	G	1	NAG	3	0

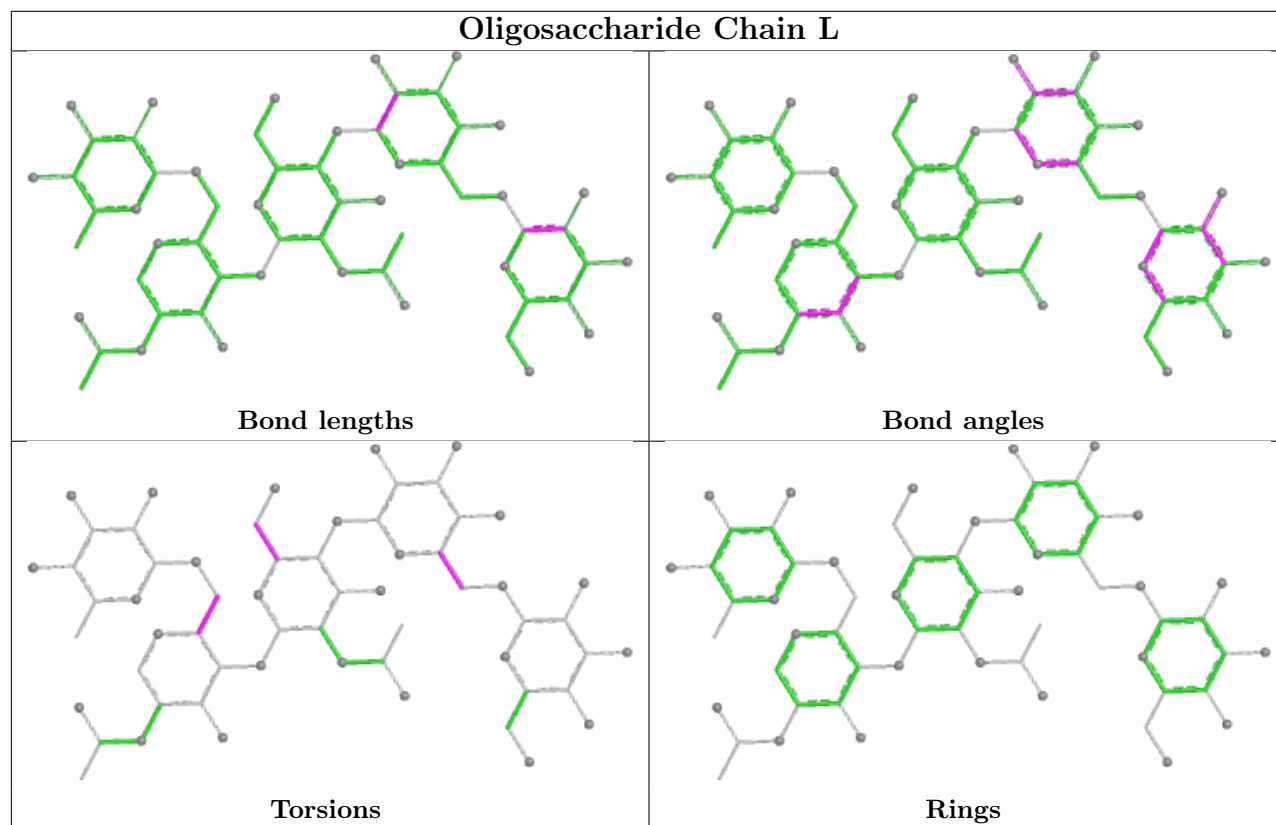
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are unknown - leaving 9 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$
10	SO4	D	301	-	4,4,4	0.26	0	6,6,6	0.28	0
7	NAG	B	402	1	14,14,15	0.38	0	17,19,21	0.57	0
7	NAG	A	1701	1	14,14,15	0.27	0	17,19,21	0.53	0
10	SO4	F	301	-	4,4,4	0.22	0	6,6,6	0.16	0
7	NAG	A	1702	1	14,14,15	0.48	0	17,19,21	0.62	0
9	XYL	B	405	-	9,9,9	0.75	0	11,11,11	0.65	0
7	NAG	B	401	1	14,14,15	0.70	1 (7%)	17,19,21	0.60	1 (5%)
7	NAG	B	403	1	14,14,15	0.39	0	17,19,21	0.52	0
9	XYL	A	1704	-	9,9,9	0.70	0	11,11,11	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	402	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1701	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1702	1	-	0/6/23/26	0/1/1/1
9	XYL	B	405	-	-	2/12/12/12	-
7	NAG	B	401	1	-	0/6/23/26	0/1/1/1
7	NAG	B	403	1	-	0/6/23/26	0/1/1/1
9	XYL	A	1704	-	-	0/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	NAG	O5-C1	2.52	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	401	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	405	XYL	O2-C2-C3-O3
9	B	405	XYL	O3-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	284/335 (84%)	0.38	15 (5%) 32 16	61, 88, 129, 151	0
1	B	282/335 (84%)	0.32	14 (4%) 34 18	61, 90, 122, 142	0
2	D	221/221 (100%)	0.01	3 (1%) 73 51	67, 88, 116, 126	0
2	F	221/221 (100%)	0.03	3 (1%) 73 51	68, 91, 120, 145	0
3	C	211/212 (99%)	0.11	2 (0%) 81 61	70, 93, 126, 141	0
3	E	210/212 (99%)	0.06	1 (0%) 87 72	67, 86, 117, 132	0
All	All	1429/1536 (93%)	0.17	38 (2%) 56 33	61, 90, 123, 151	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	3.8
1	A	255	SER	3.3
1	A	74	ASN	3.3
1	B	70	VAL	3.2
1	A	211	ASN	3.1

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](#)

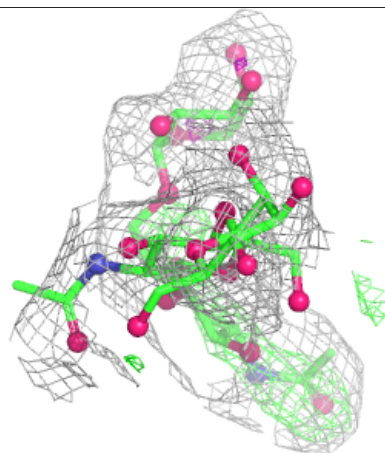
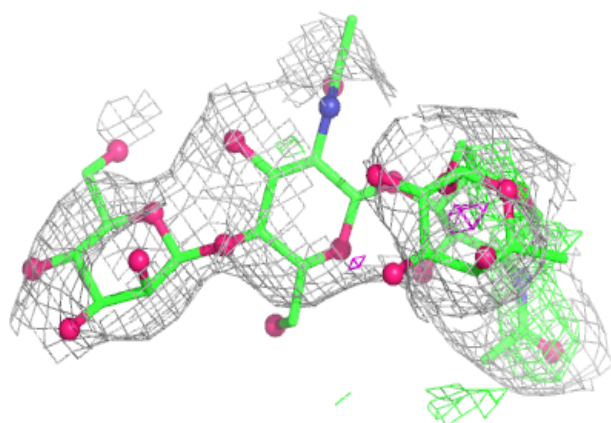
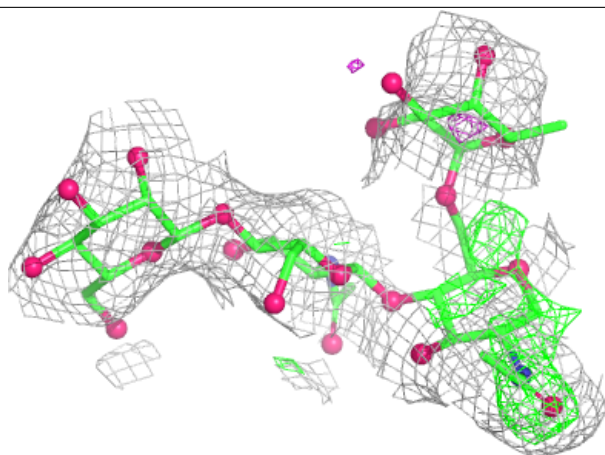
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	K	4	11/12	0.07	0.13	176,180,187,188	0
6	NAG	K	2	14/15	0.12	0.16	164,179,186,195	0
6	FUC	K	5	10/11	0.25	0.19	162,183,190,192	0
4	BMA	M	3	11/12	0.26	0.14	123,138,147,155	0
5	FUC	N	2	10/11	0.32	0.17	153,162,165,168	0
6	MAN	L	4	11/12	0.35	0.15	150,165,174,179	0
4	BMA	I	3	11/12	0.38	0.14	122,130,144,145	0
5	FUC	J	2	10/11	0.44	0.21	140,160,166,167	0
6	NAG	L	2	14/15	0.44	0.17	144,162,174,176	0
5	NAG	O	1	14/15	0.44	0.19	135,156,165,169	0
5	FUC	O	2	10/11	0.45	0.24	140,152,171,172	0
5	FUC	H	2	10/11	0.48	0.18	153,162,176,179	0
6	BMA	K	3	11/12	0.48	0.10	171,181,197,203	0
6	NAG	K	1	14/15	0.49	0.14	151,177,186,187	0
4	BMA	G	3	11/12	0.52	0.14	149,161,168,172	0
4	FUC	G	4	10/11	0.60	0.23	140,157,164,167	0
6	BMA	L	3	11/12	0.65	0.11	144,161,171,180	0
5	NAG	H	1	14/15	0.67	0.20	144,157,169,170	0
5	NAG	N	1	14/15	0.73	0.11	136,155,164,170	0
5	NAG	J	1	14/15	0.76	0.12	133,149,158,165	0
6	FUC	L	5	10/11	0.79	0.16	149,161,164,167	0
4	NAG	G	2	14/15	0.80	0.16	141,152,171,175	0
6	NAG	L	1	14/15	0.83	0.18	131,146,154,163	0
4	NAG	G	1	14/15	0.90	0.14	115,122,145,146	0
4	NAG	I	2	14/15	0.90	0.13	113,129,139,147	0
4	NAG	M	2	14/15	0.92	0.11	107,124,145,146	0
4	NAG	M	1	14/15	0.92	0.10	104,108,125,127	0
4	NAG	I	1	14/15	0.94	0.12	111,116,134,138	0
4	FUC	M	4	10/11	0.94	0.13	105,114,131,147	0
4	FUC	I	4	10/11	0.95	0.14	114,121,131,133	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.

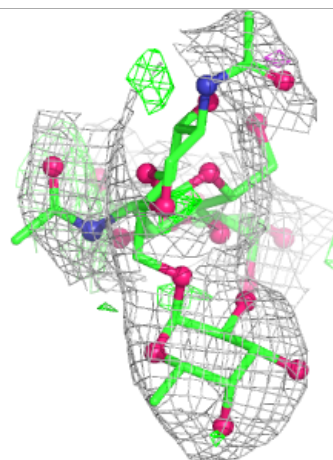
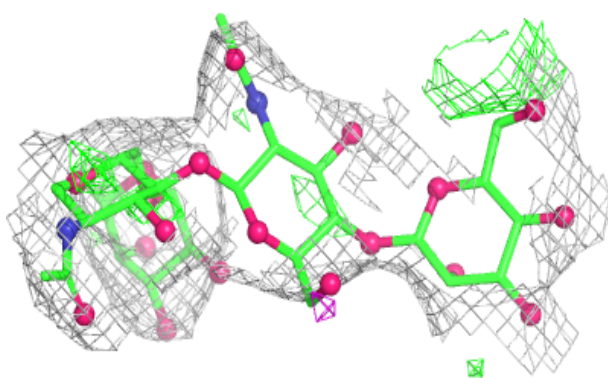
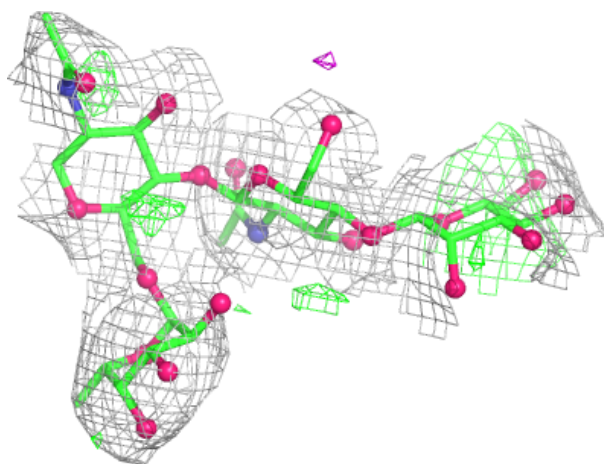
Electron density around Chain G:

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



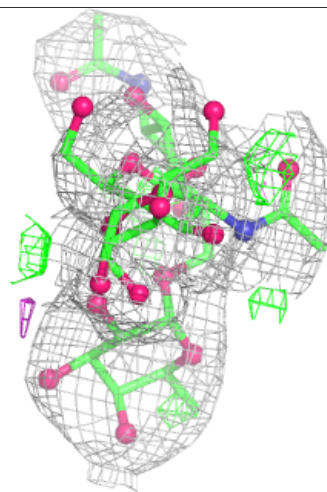
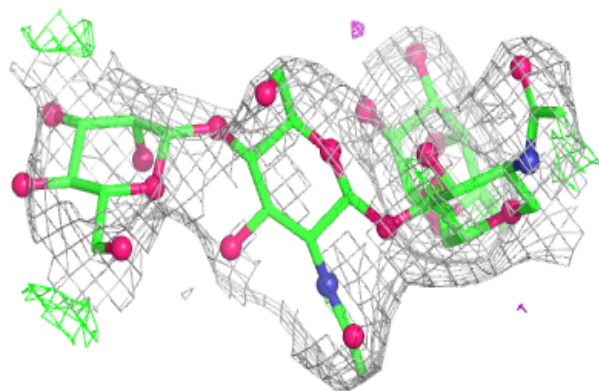
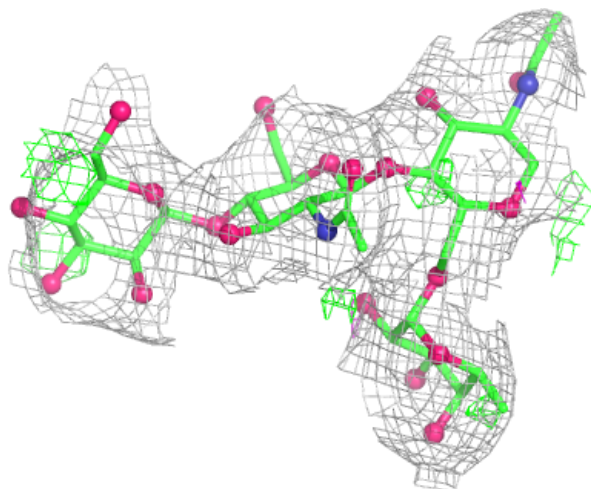
Electron density around Chain I:

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



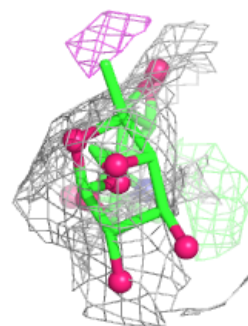
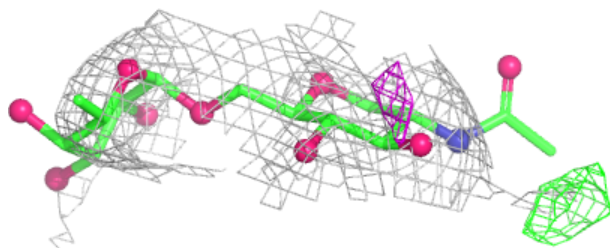
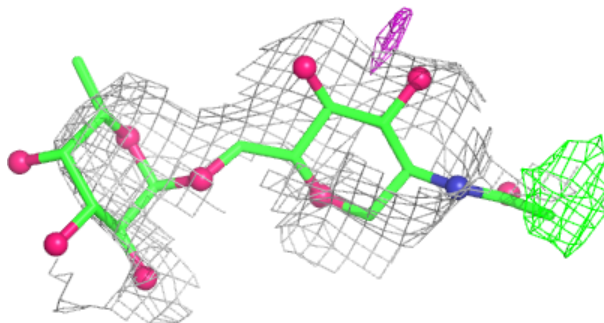
Electron density around Chain M:

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

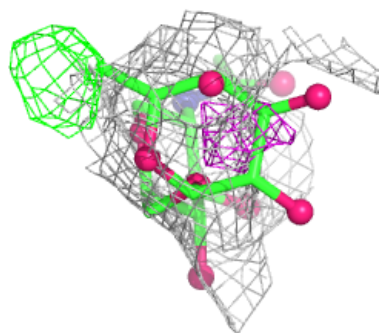
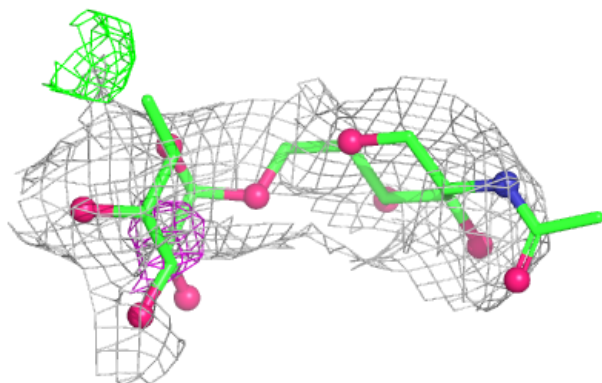
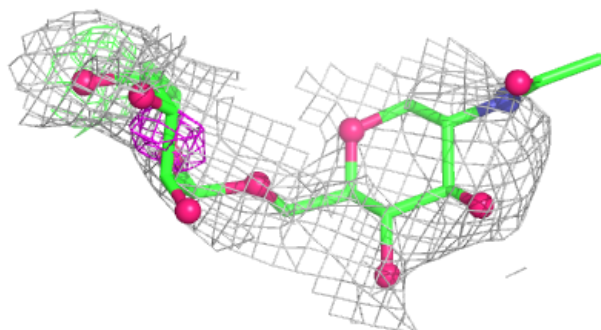


Electron density around Chain H:

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

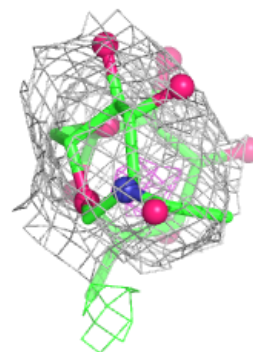
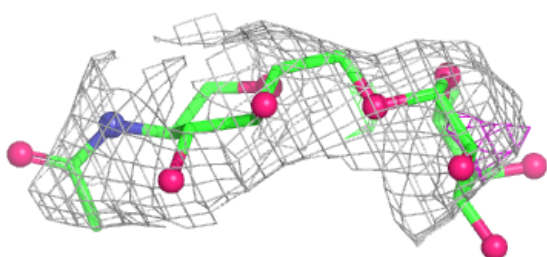
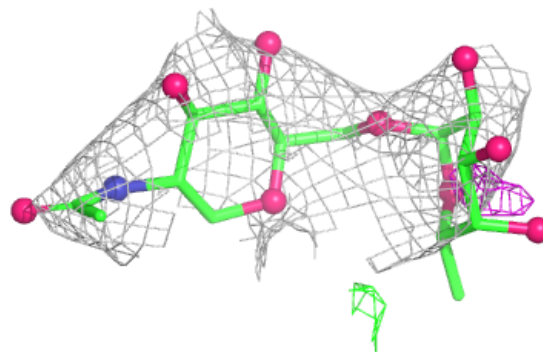
**Electron density around Chain J:**

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

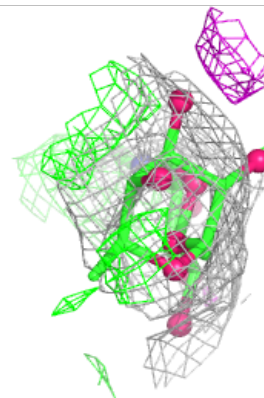
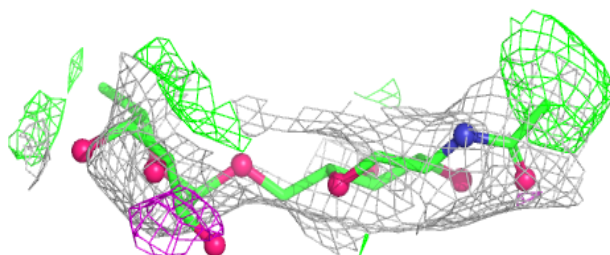
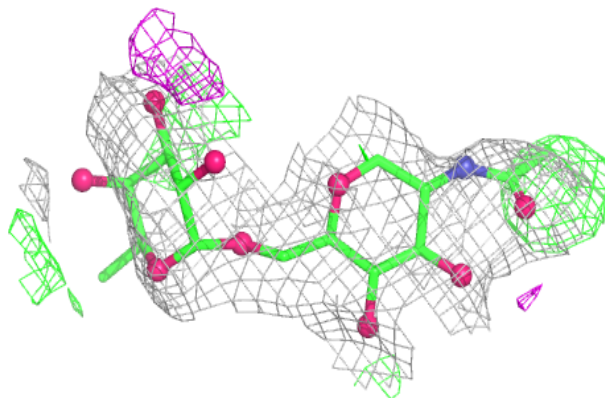


Electron density around Chain N:

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

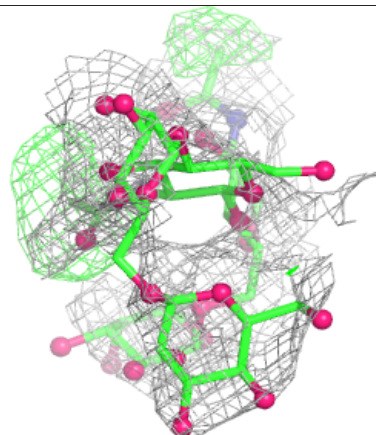
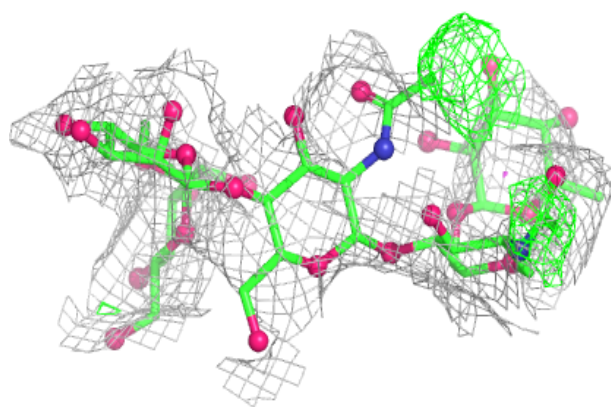
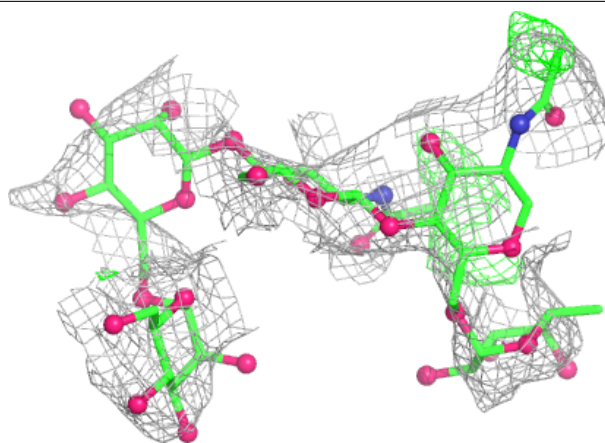
**Electron density around Chain O:**

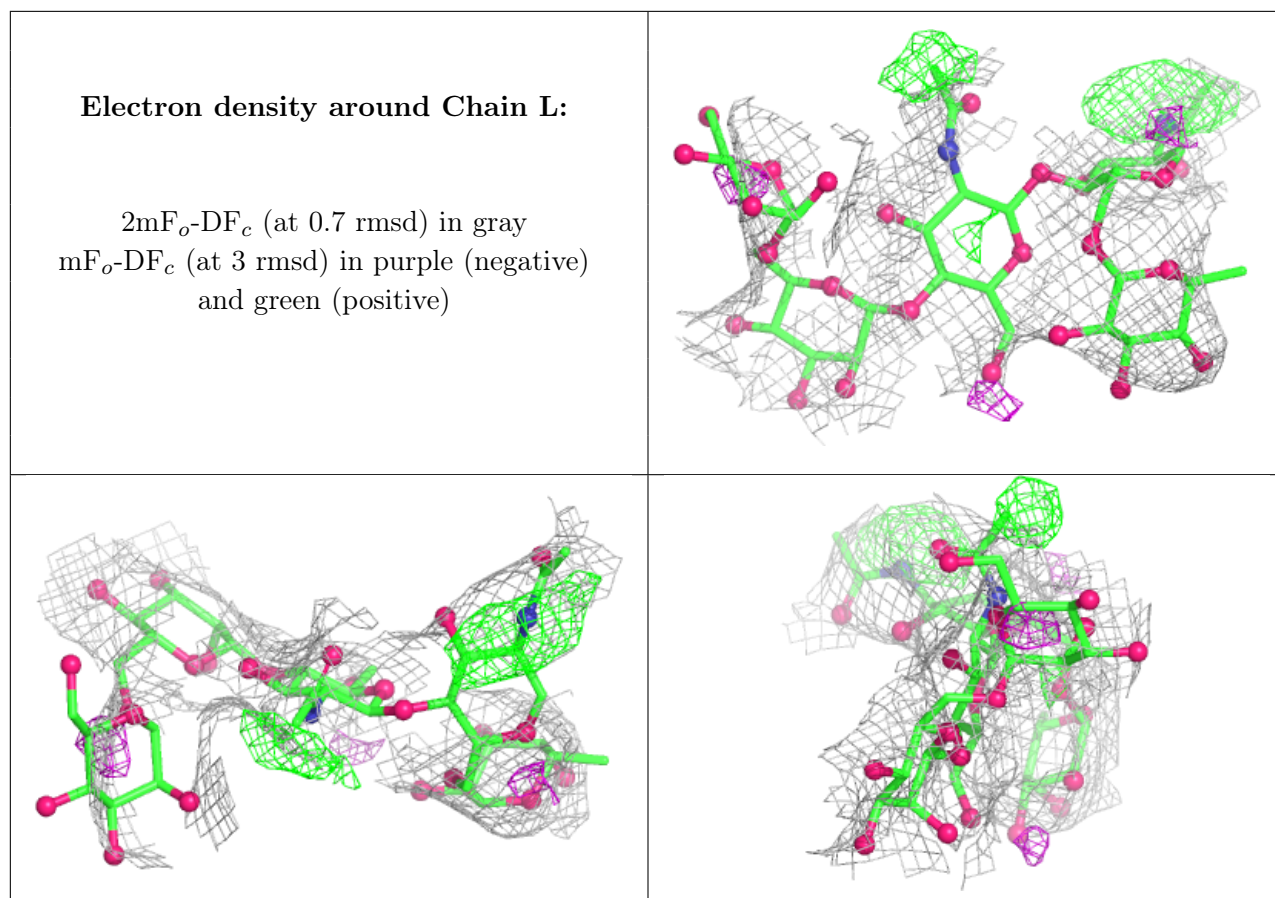
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
8	UNX	A	1703	1/1	0.33	0.50	90,90,90,90	0
8	UNX	B	404	1/1	0.33	0.73	78,78,78,78	0
7	NAG	B	401	14/15	0.37	0.15	138,150,163,164	0
10	SO4	D	301	5/5	0.39	0.11	155,160,170,215	0
7	NAG	B	403	14/15	0.54	0.13	132,166,175,179	0
10	SO4	F	301	5/5	0.58	0.11	147,161,178,195	0
7	NAG	A	1701	14/15	0.66	0.13	137,149,156,157	0
7	NAG	A	1702	14/15	0.74	0.15	124,142,161,174	0
7	NAG	B	402	14/15	0.76	0.14	135,147,157,161	0
9	XYL	B	405	10/10	0.80	0.17	107,118,138,141	0
9	XYL	A	1704	10/10	0.83	0.15	105,114,140,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.