



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2021 – 10:43 AM EDT

PDB ID : 7LY3  
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](mailto: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.

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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	:	2.18
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)	:	2.18

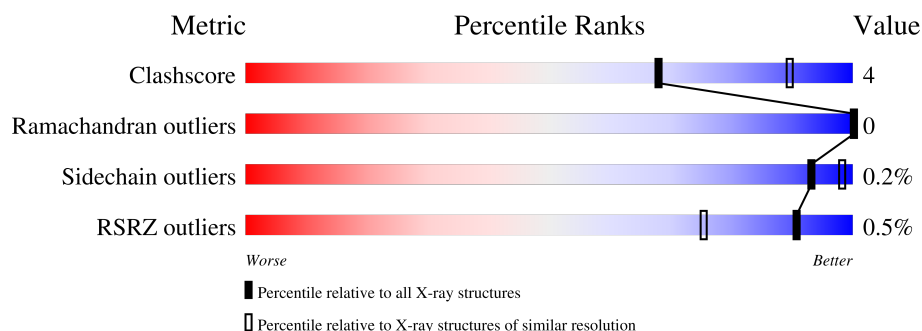
# 1 Overall quality at a glance ⓘ

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.






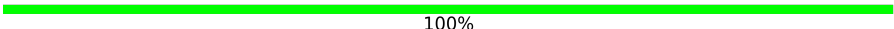


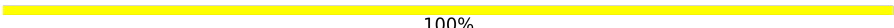

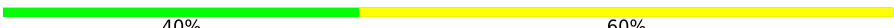
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	
1	B	335	
2	D	221	
2	F	221	
3	C	212	
3	E	212	

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Mol	Chain	Length	Quality of chain
4	G	4	 50% 50%
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
10	SO4	D	301	-	-	-	X
10	SO4	F	301	-	-	-	X
5	FUC	H	2	-	-	-	X
5	NAG	J	1	-	-	-	X
5	FUC	J	2	-	-	-	X
6	NAG	K	1	-	-	-	X
6	NAG	K	2	-	-	-	X
6	BMA	K	3	-	-	-	X
6	FUC	K	5	-	-	-	X
6	MAN	L	4	-	-	-	X
9	XYL	B	405	-	-	-	X

## 2 Entry composition

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
1	A	284	Total	C	N	O	S	0	0	0
			2209	1430	362	409	8			
1	B	282	Total	C	N	O	S	0	0	0
			2212	1432	361	411	8			

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

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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

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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

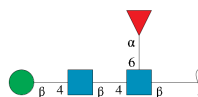
- Molecule 2 is a protein called S2M28 Fab Heavy Chain.

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

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

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

- 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.



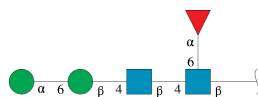
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

- 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 (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



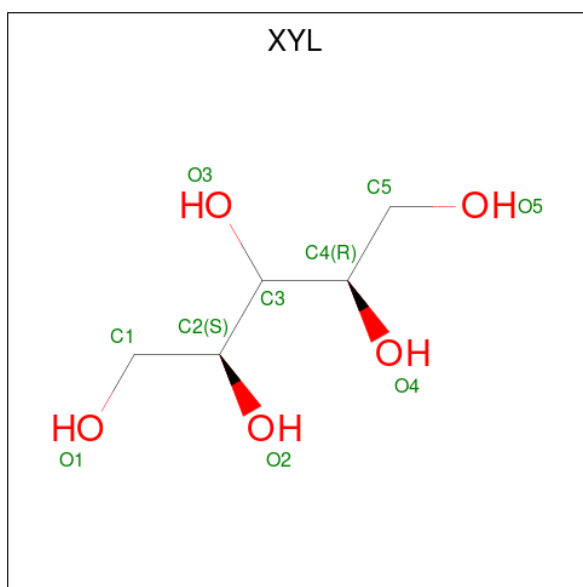
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

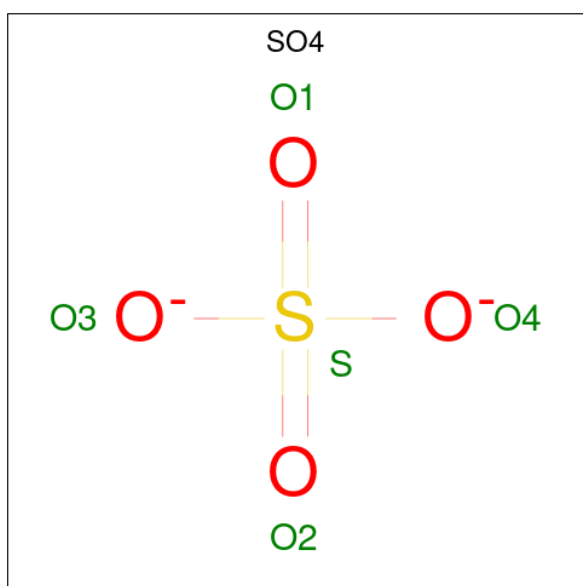
- Molecule 9 is Xylitol (three-letter code: XYL) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).





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 (three-letter code: SO4) (formula: O<sub>4</sub>S).

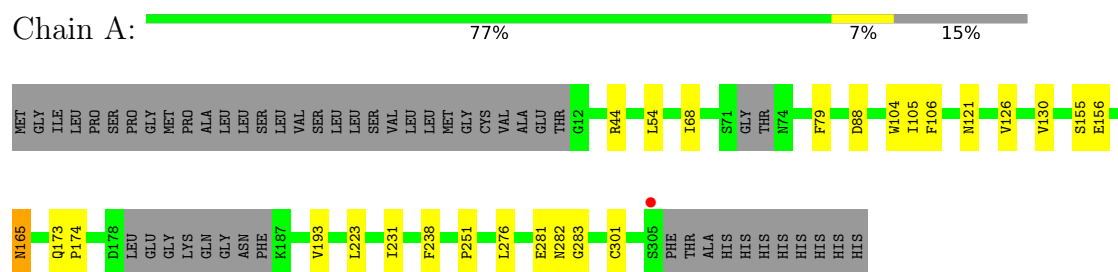


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		

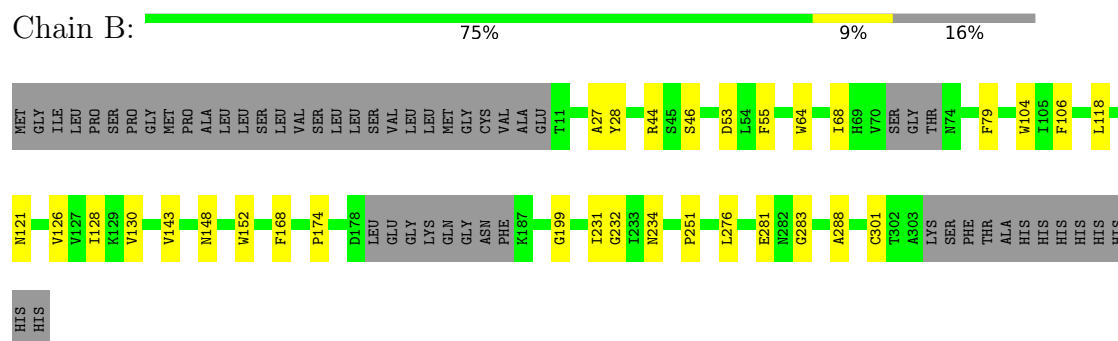
### 3 Residue-property plots [i](#)

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.

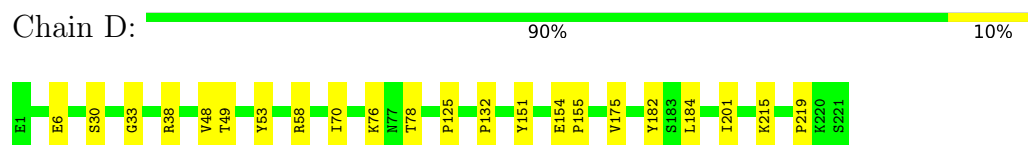
- Molecule 1: Spike protein S1



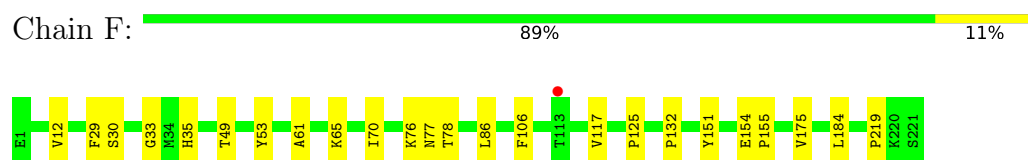
- Molecule 1: Spike protein S1



- Molecule 2: S2M28 Fab Heavy Chain



- Molecule 2: S2M28 Fab Heavy Chain



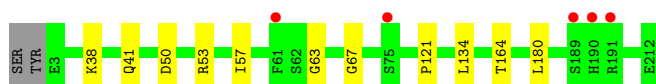
- Molecule 3: S2M28 Fab Light Chain

Chain C:  93% 7%



- Molecule 3: S2M28 Fab Light Chain

Chain E:  2% 94% 5%



- 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

Chain G:  50% 50%



- 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

Chain I:  75% 25%



- 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

Chain M:  75% 25%



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

Chain H:  100%



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

Chain J:  50% 50%



- 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  
MAN4  
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  
MAN4  
FUC5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, $R_{free}$	0.208 , 0.234 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	623 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XYL, FUC, UNX, BMA, NAG, MAN, SO4

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	0.34	0/2271	0.56	0/3104
1	B	0.34	0/2275	0.55	0/3107
2	D	0.37	0/1698	0.65	0/2320
2	F	0.38	0/1695	0.65	0/2316
3	C	0.35	0/1587	0.65	0/2177
3	E	0.35	0/1594	0.66	0/2183
All	All	0.36	0/11120	0.62	0/15207

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	2209	0	2055	18	0
1	B	2212	0	2070	19	0
2	D	1654	0	1580	17	0
2	F	1651	0	1579	16	0
3	C	1547	0	1454	13	1
3	E	1554	0	1488	9	0
4	G	49	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	83	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 83 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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	91	97
1	B	237/297 (80%)	236 (100%)	1 (0%)	91	97
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%)	1163 (100%)	2 (0%)	93	98



All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	B	234	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	ASN

### 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 ⓘ

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	1,4	14,14,15	0.24	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.58	0
4	BMA	G	3	4	11,11,12	0.91	1 (9%)	15,15,17	0.80	0
4	FUC	G	4	4	10,10,11	0.70	0	14,14,16	0.75	0
5	NAG	H	1	1,5	14,14,15	0.22	0	17,19,21	0.42	0
5	FUC	H	2	5	10,10,11	1.02	0	14,14,16	0.75	0
4	NAG	I	1	1,4	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.51	0
4	BMA	I	3	4	11,11,12	1.14	1 (9%)	15,15,17	0.96	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUC	I	4	4	10,10,11	0.81	0	14,14,16	0.72	0
5	NAG	J	1	1,5	14,14,15	0.41	0	17,19,21	0.64	1 (5%)
5	FUC	J	2	5	10,10,11	0.96	0	14,14,16	0.79	0
6	NAG	K	1	1,6	14,14,15	0.28	0	17,19,21	0.55	0
6	NAG	K	2	6	14,14,15	0.47	0	17,19,21	0.68	1 (5%)
6	BMA	K	3	6	11,11,12	0.81	0	15,15,17	0.81	0
6	MAN	K	4	6	11,11,12	0.78	0	15,15,17	1.08	2 (13%)
6	FUC	K	5	6	10,10,11	0.77	0	14,14,16	0.74	0
6	NAG	L	1	1,6	14,14,15	0.42	0	17,19,21	1.09	1 (5%)
6	NAG	L	2	6	14,14,15	0.28	0	17,19,21	0.58	0
6	BMA	L	3	6	11,11,12	1.19	1 (9%)	15,15,17	1.11	2 (13%)
6	MAN	L	4	6	11,11,12	0.78	1 (9%)	15,15,17	1.12	2 (13%)
6	FUC	L	5	6	10,10,11	0.75	0	14,14,16	0.77	0
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.49	0
4	BMA	M	3	4	11,11,12	0.98	1 (9%)	15,15,17	0.91	1 (6%)
4	FUC	M	4	4	10,10,11	0.80	0	14,14,16	0.95	0
5	NAG	N	1	1,5	14,14,15	0.69	1 (7%)	17,19,21	0.84	1 (5%)
5	FUC	N	2	5	10,10,11	0.85	0	14,14,16	0.81	0
5	NAG	O	1	1,5	14,14,15	0.42	0	17,19,21	0.52	0
5	FUC	O	2	5	10,10,11	1.63	4 (40%)	14,14,16	1.00	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	1,4	-	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	1,4	-	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
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	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	-	4/6/23/26	0/1/1/1
5	FUC	O	2	5	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	3	BMA	C1-C2	2.55	1.58	1.52
5	O	2	FUC	C4-C5	2.53	1.58	1.52
5	O	2	FUC	C4-C3	2.49	1.58	1.52
5	N	1	NAG	C1-C2	2.33	1.55	1.52
5	O	2	FUC	C2-C3	2.29	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	3.02	116.28	112.19
6	L	1	NAG	C4-C3-C2	2.72	115.00	111.02
6	L	3	BMA	C1-O5-C5	2.59	115.70	112.19
6	K	4	MAN	C1-O5-C5	2.57	115.67	112.19
6	K	2	NAG	C1-O5-C5	2.36	115.40	112.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

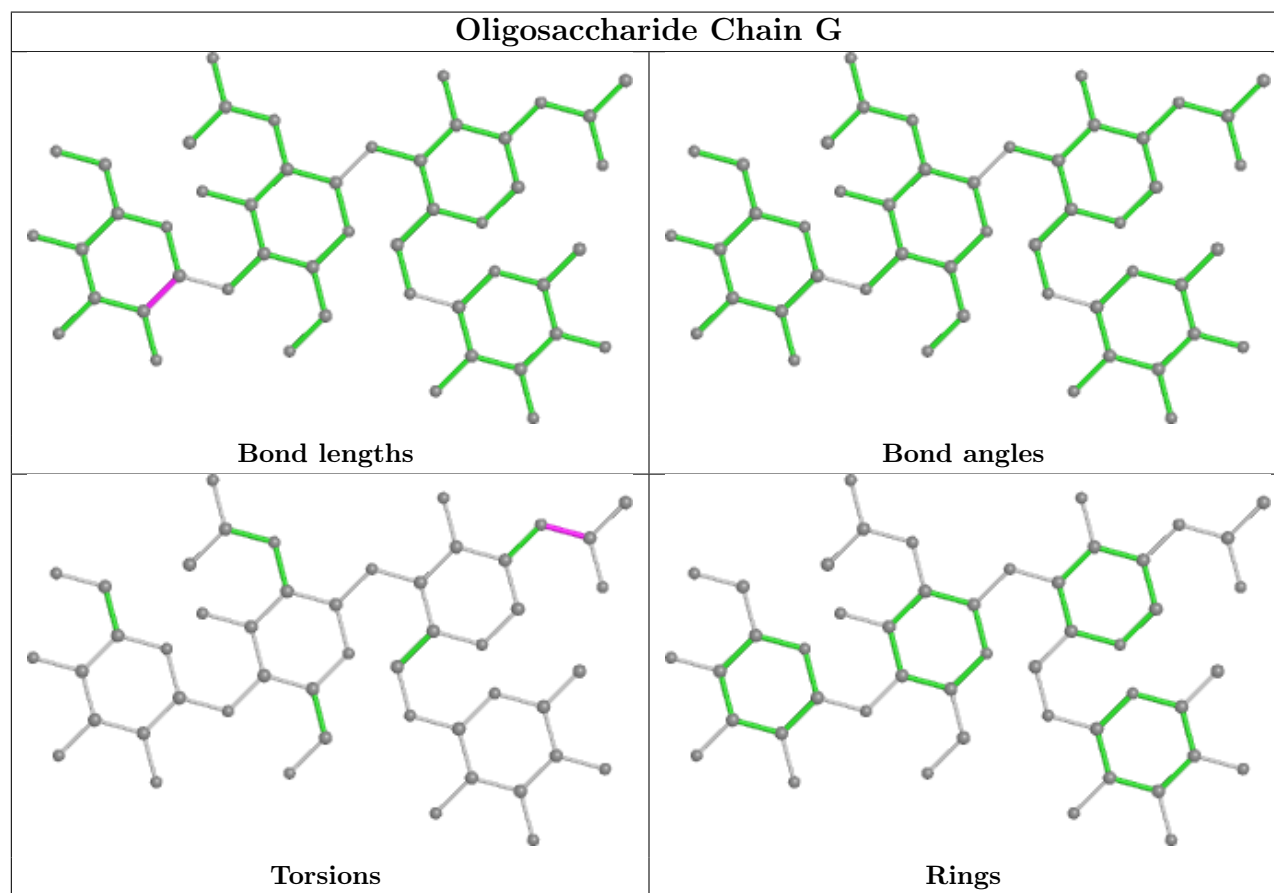
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
6	L	2	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6

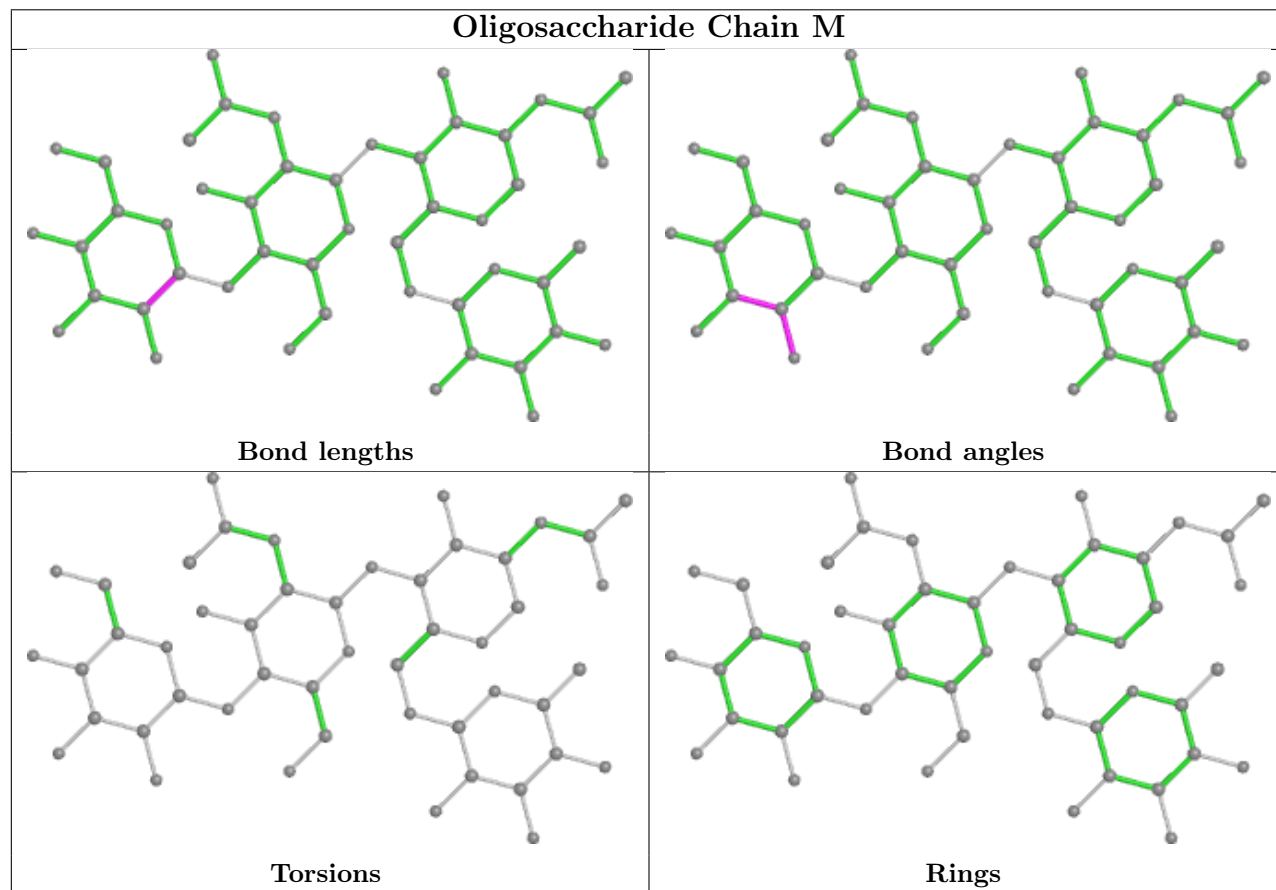
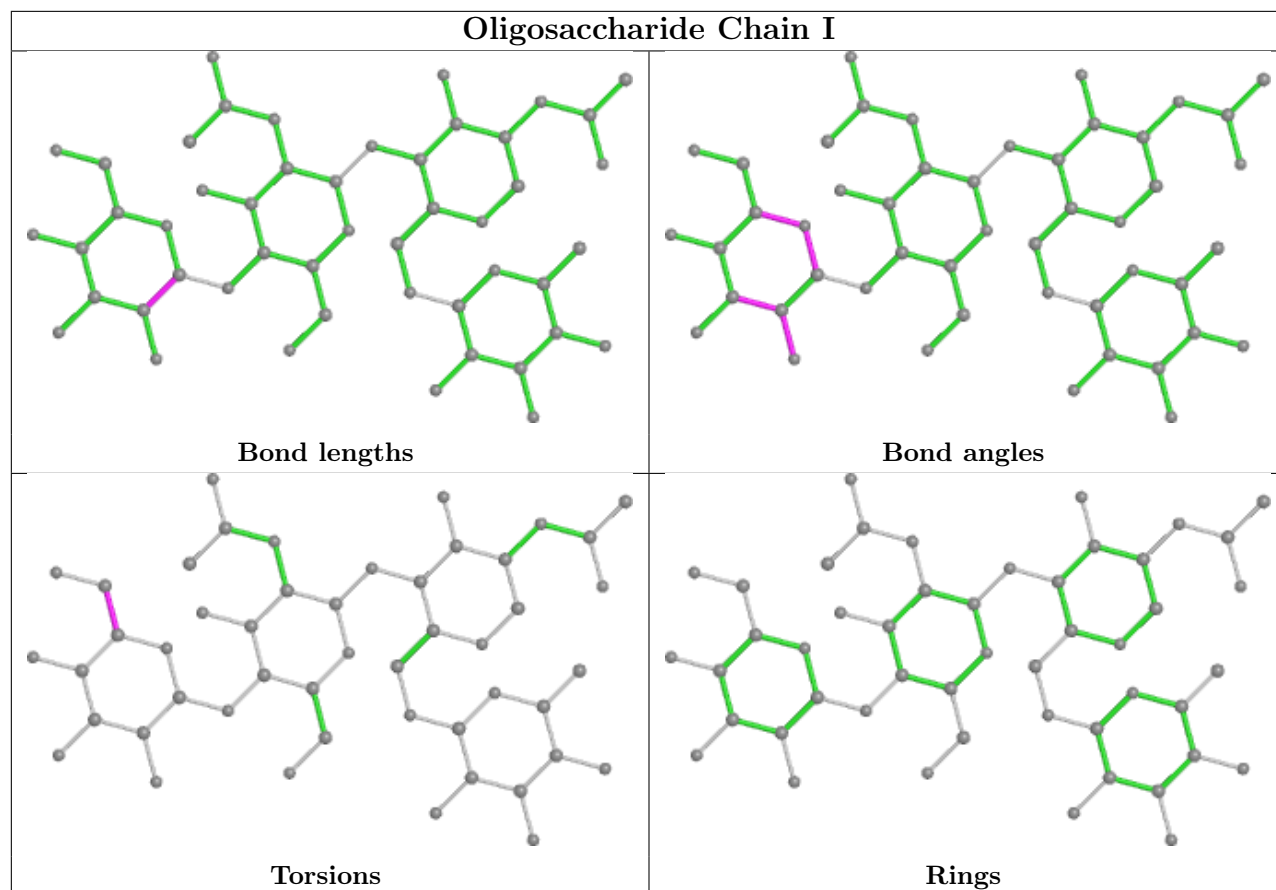
There are no ring outliers.

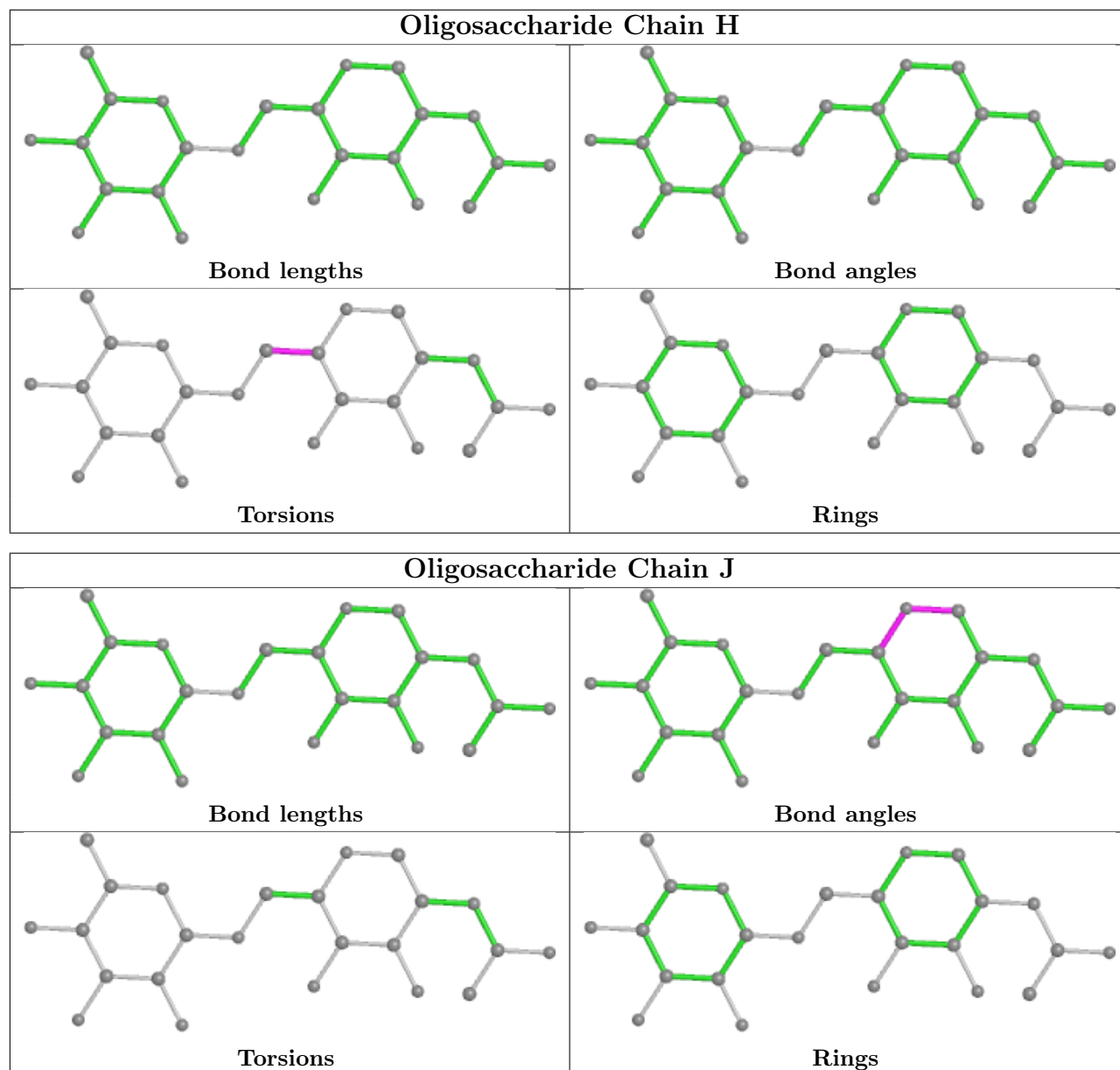
3 monomers are involved in 5 short contacts:

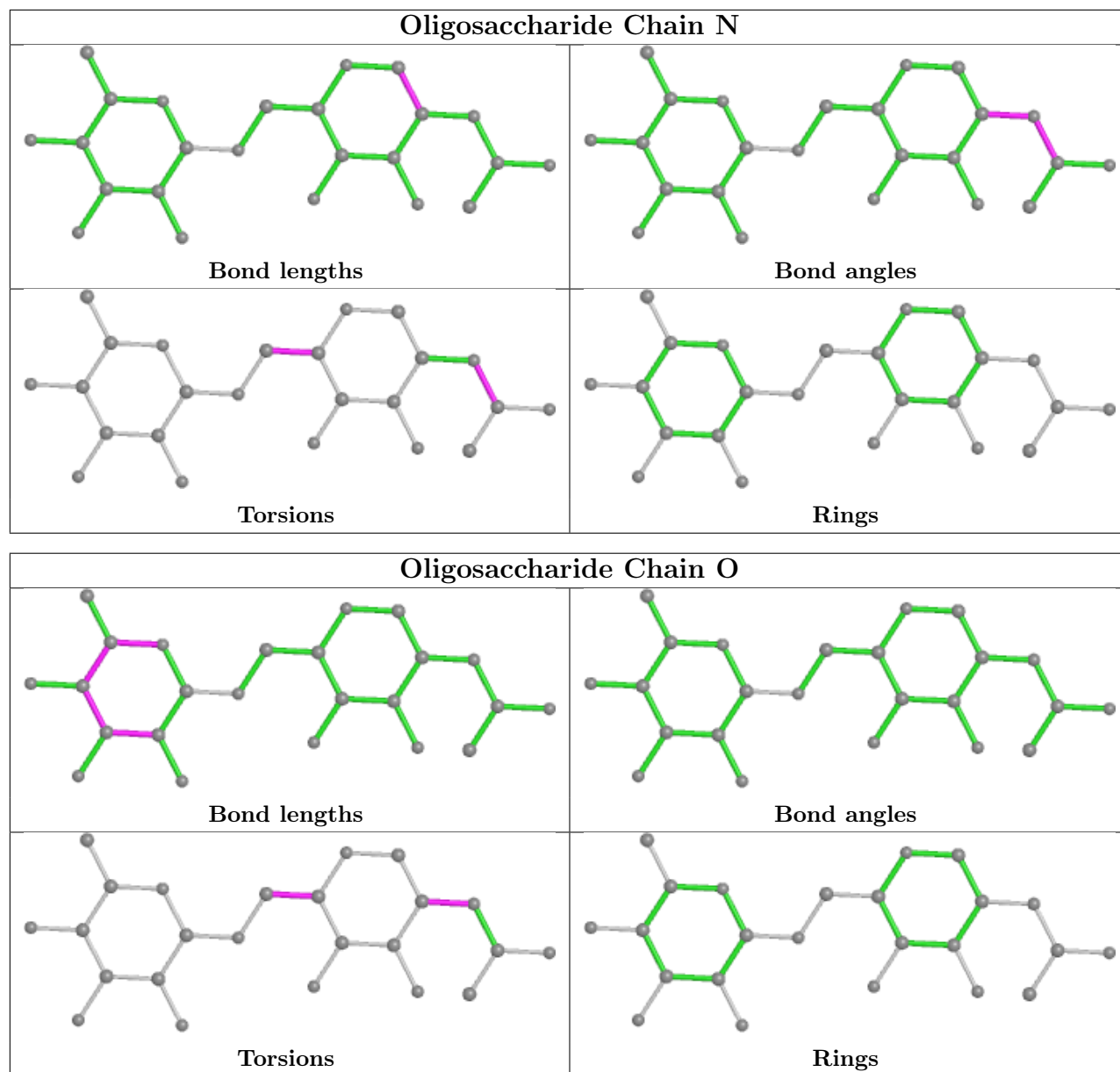
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
4	G	1	NAG	3	0
5	J	1	NAG	1	0

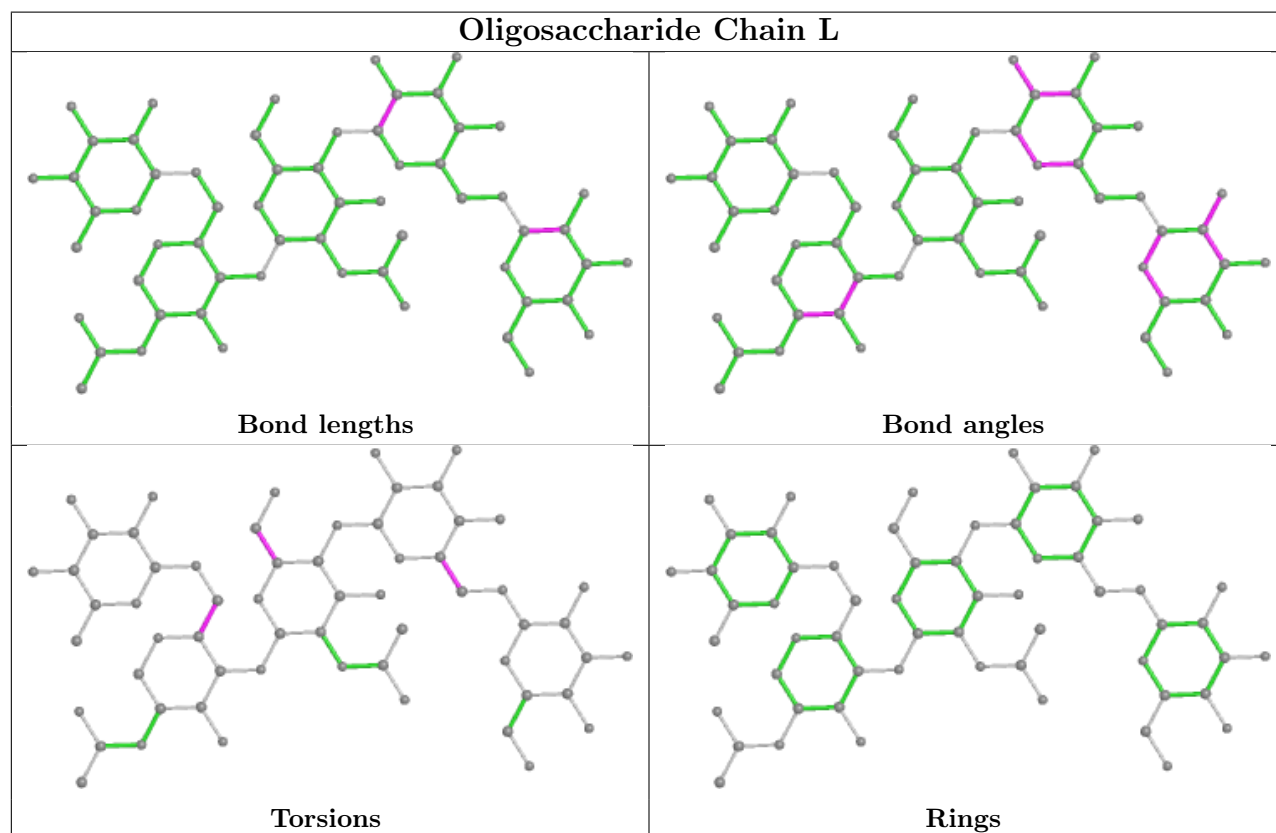
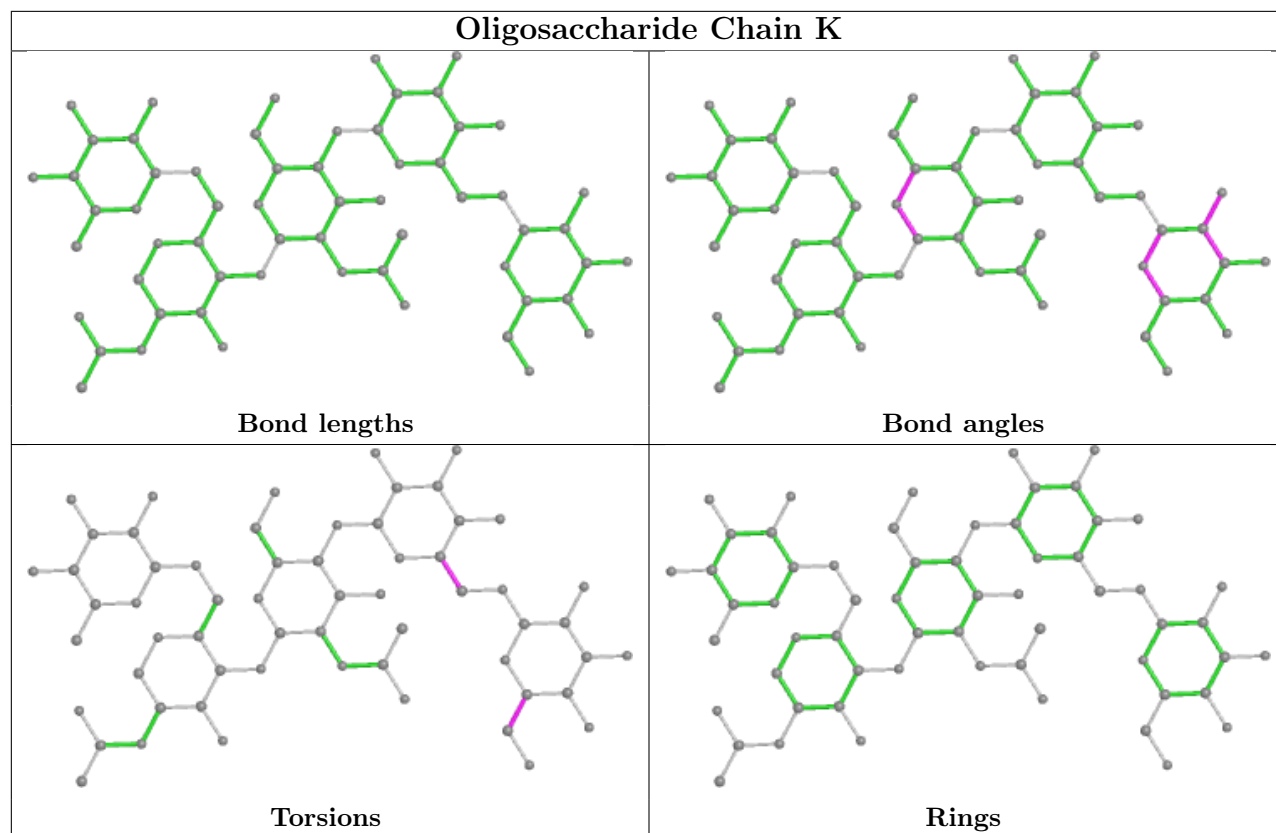
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.













## 5.6 Ligand geometry

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
7	NAG	B	402	1	14,14,15	0.36	0	17,19,21	0.56	0
7	NAG	B	401	1	14,14,15	0.73	1 (7%)	17,19,21	0.59	0
7	NAG	A	1701	1	14,14,15	0.26	0	17,19,21	0.51	0
9	XYL	B	405	-	9,9,9	0.75	0	11,11,11	0.59	0
10	SO4	F	301	-	4,4,4	0.15	0	6,6,6	0.14	0
9	XYL	A	1704	-	9,9,9	0.69	0	11,11,11	0.52	0
7	NAG	B	403	1	14,14,15	0.39	0	17,19,21	0.50	0
7	NAG	A	1702	1	14,14,15	0.48	0	17,19,21	0.61	0
10	SO4	D	301	-	4,4,4	0.30	0	6,6,6	0.28	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	B	401	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1701	1	-	0/6/23/26	0/1/1/1
9	XYL	B	405	-	-	1/12/12/12	-
9	XYL	A	1704	-	-	0/12/12/12	-
7	NAG	B	403	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1702	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	NAG	O5-C1	2.63	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	284/335 (84%)	-0.19	1 (0%) 92 79	61, 88, 129, 151	0
1	B	282/335 (84%)	-0.20	0 100 100	61, 90, 122, 142	0
2	D	221/221 (100%)	-0.09	0 100 100	67, 88, 116, 126	0
2	F	221/221 (100%)	-0.07	1 (0%) 91 75	68, 91, 120, 145	0
3	C	211/212 (99%)	-0.21	0 100 100	70, 93, 126, 141	0
3	E	210/212 (99%)	-0.08	5 (2%) 59 30	67, 86, 117, 132	0
All	All	1429/1536 (93%)	-0.15	7 (0%) 91 75	61, 90, 123, 151	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	3.3
3	E	189	SER	2.5
3	E	75	SER	2.4
3	E	191	ARG	2.1
3	E	61	PHE	2.1

### 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](#)

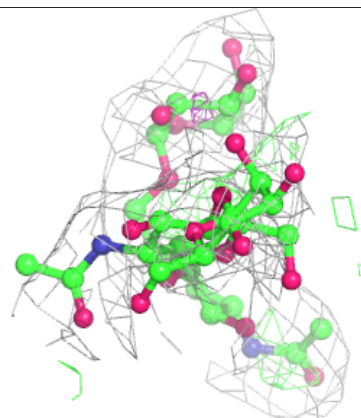
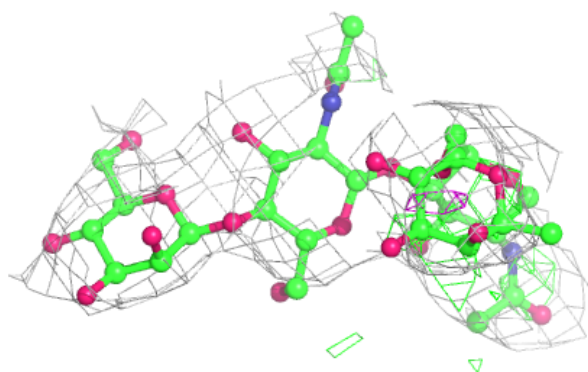
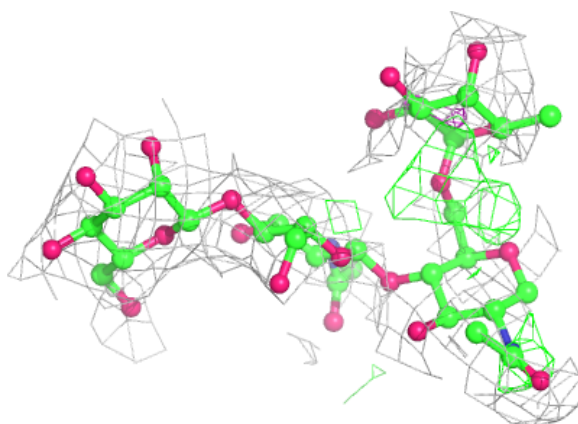
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	L	3	11/12	0.42	0.31	144,161,171,180	0
5	FUC	J	2	10/11	0.49	0.42	140,160,166,167	0
6	NAG	K	1	14/15	0.58	0.44	151,177,186,187	0
6	MAN	L	4	11/12	0.58	0.46	150,165,174,179	0
6	NAG	K	2	14/15	0.61	0.60	164,179,186,195	0
5	NAG	O	1	14/15	0.62	0.23	135,156,165,169	0
6	NAG	L	2	14/15	0.65	0.27	144,162,174,176	0
4	BMA	G	3	11/12	0.65	0.31	149,161,168,172	0
5	FUC	H	2	10/11	0.65	0.48	153,162,176,179	0
5	FUC	O	2	10/11	0.67	0.40	140,152,171,172	0
6	FUC	K	5	10/11	0.69	0.67	162,183,190,192	0
6	BMA	K	3	11/12	0.70	0.60	171,181,197,203	0
5	NAG	H	1	14/15	0.72	0.36	144,157,169,170	0
4	BMA	I	3	11/12	0.72	0.20	122,130,144,145	0
4	BMA	M	3	11/12	0.72	0.25	123,138,147,155	0
4	FUC	G	4	10/11	0.79	0.33	140,157,164,167	0
5	NAG	J	1	14/15	0.79	0.43	133,149,158,165	0
4	NAG	I	2	14/15	0.81	0.21	113,129,139,147	0
4	NAG	G	2	14/15	0.81	0.22	141,152,171,175	0
5	FUC	N	2	10/11	0.82	0.71	153,162,165,168	0
6	NAG	L	1	14/15	0.84	0.21	131,146,154,163	0
6	MAN	K	4	11/12	0.84	0.65	176,180,187,188	0
4	NAG	M	2	14/15	0.85	0.19	107,124,145,146	0
5	NAG	N	1	14/15	0.86	0.40	136,155,164,170	0
6	FUC	L	5	10/11	0.87	0.35	149,161,164,167	0
4	NAG	G	1	14/15	0.89	0.16	115,122,145,146	0
4	NAG	I	1	14/15	0.93	0.20	111,116,134,138	0
4	NAG	M	1	14/15	0.93	0.14	104,108,125,127	0
4	FUC	I	4	10/11	0.94	0.21	114,121,131,133	0
4	FUC	M	4	10/11	0.94	0.23	105,114,131,147	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.

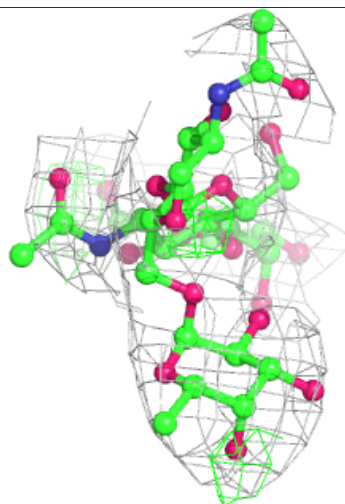
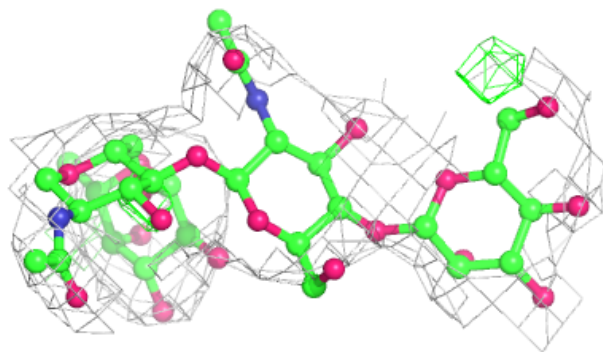
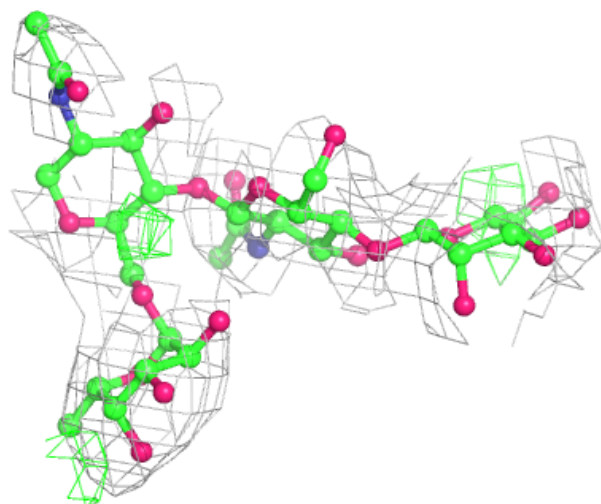
**Electron density around Chain G:**

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



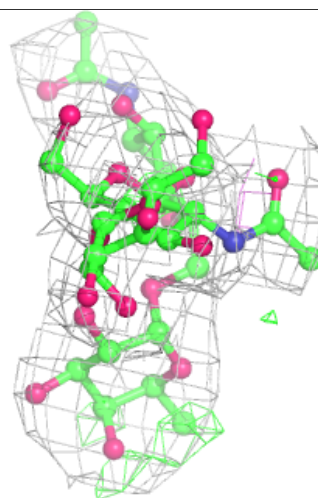
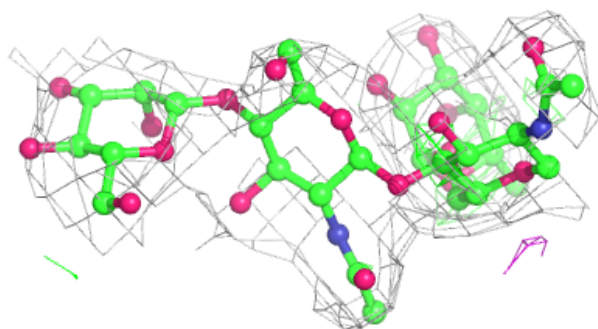
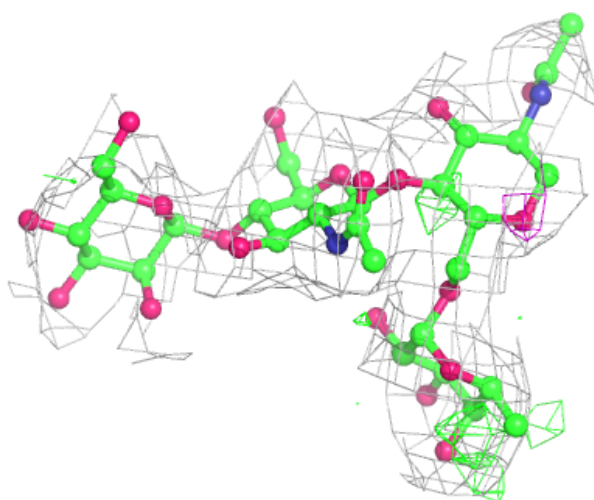
**Electron density around Chain I:**

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



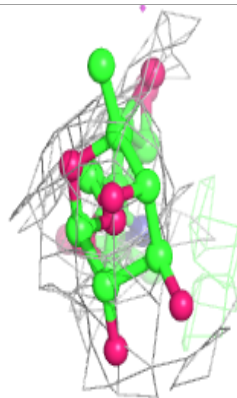
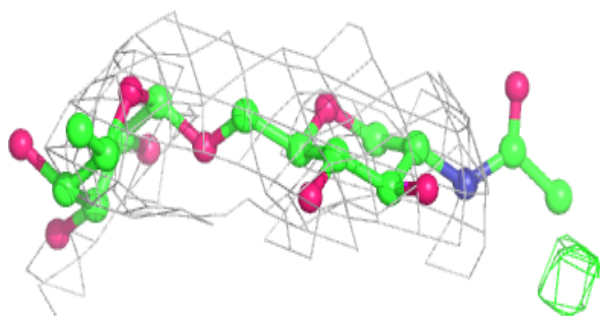
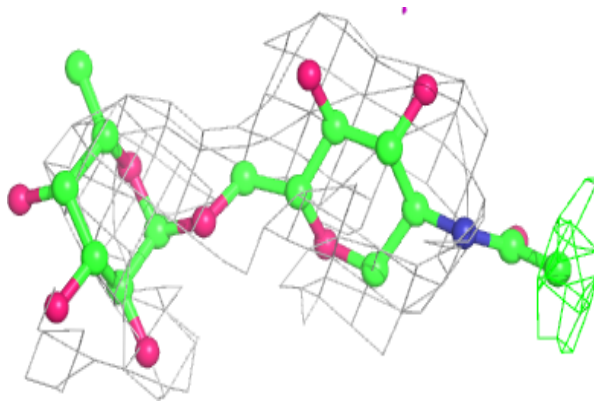
**Electron density around Chain M:**

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

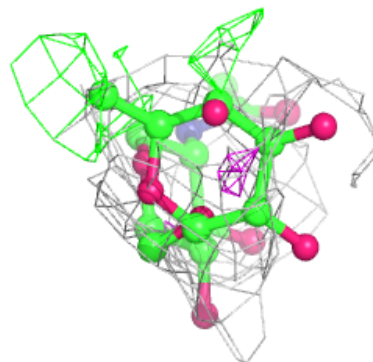
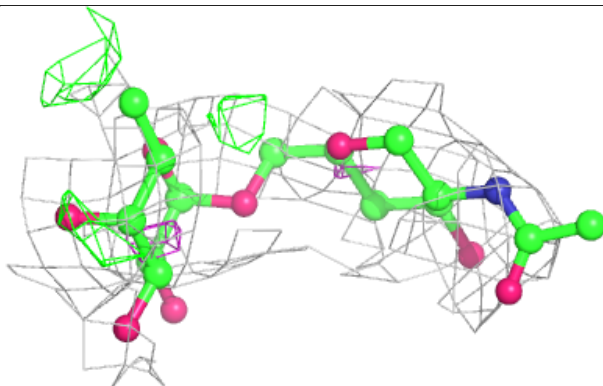
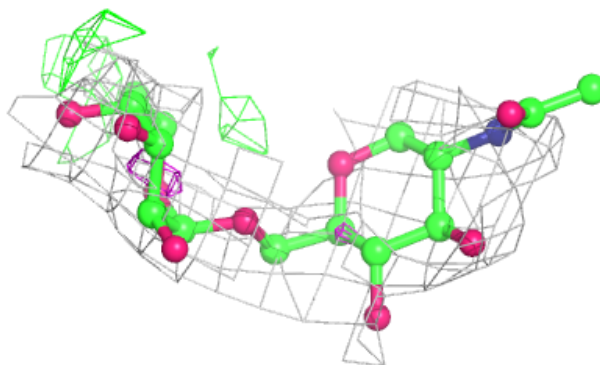


**Electron density around Chain H:**

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

**Electron density around Chain J:**

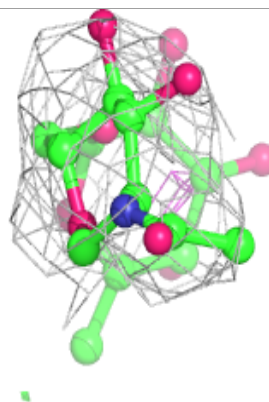
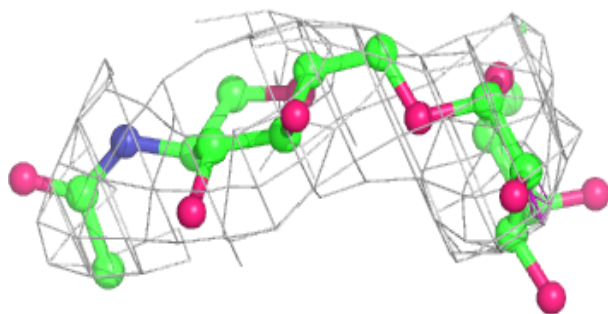
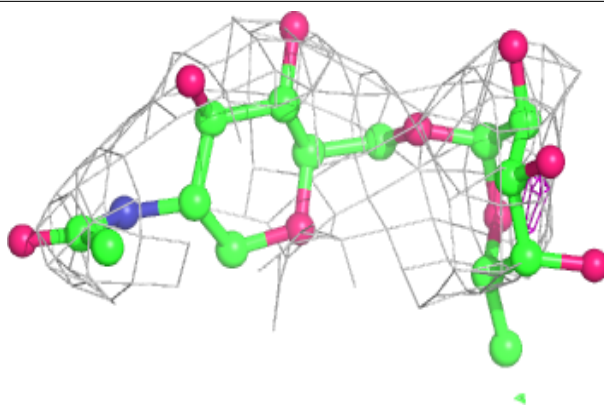
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



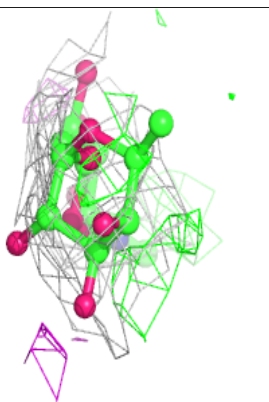
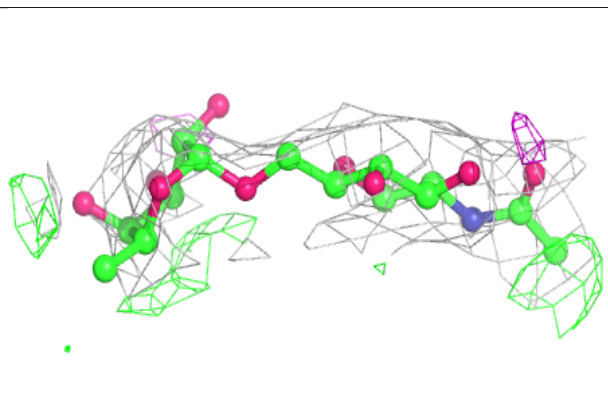
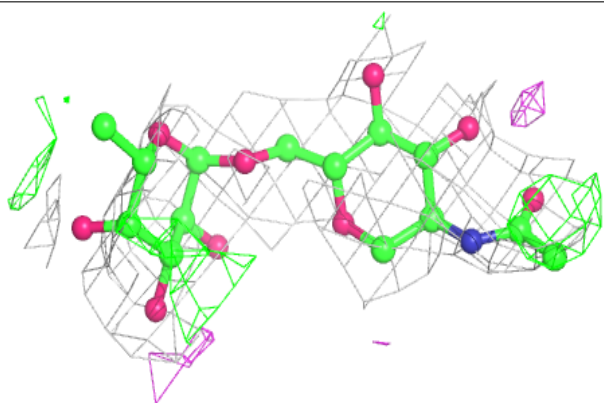


**Electron density around Chain N:**

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

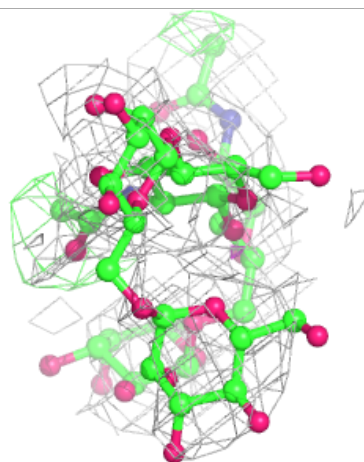
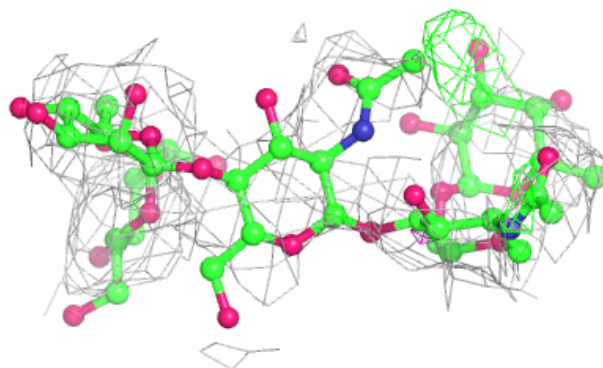
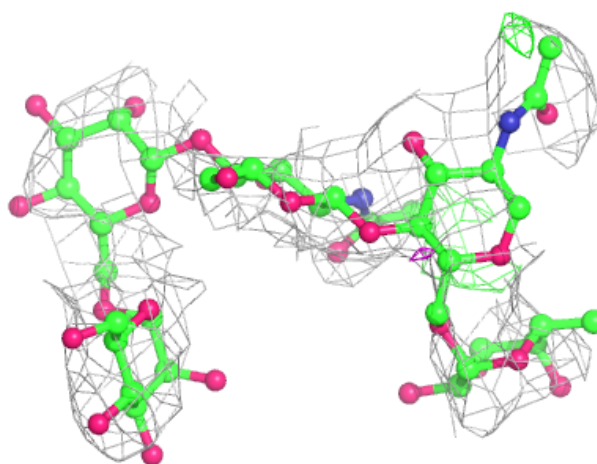
**Electron density around Chain O:**

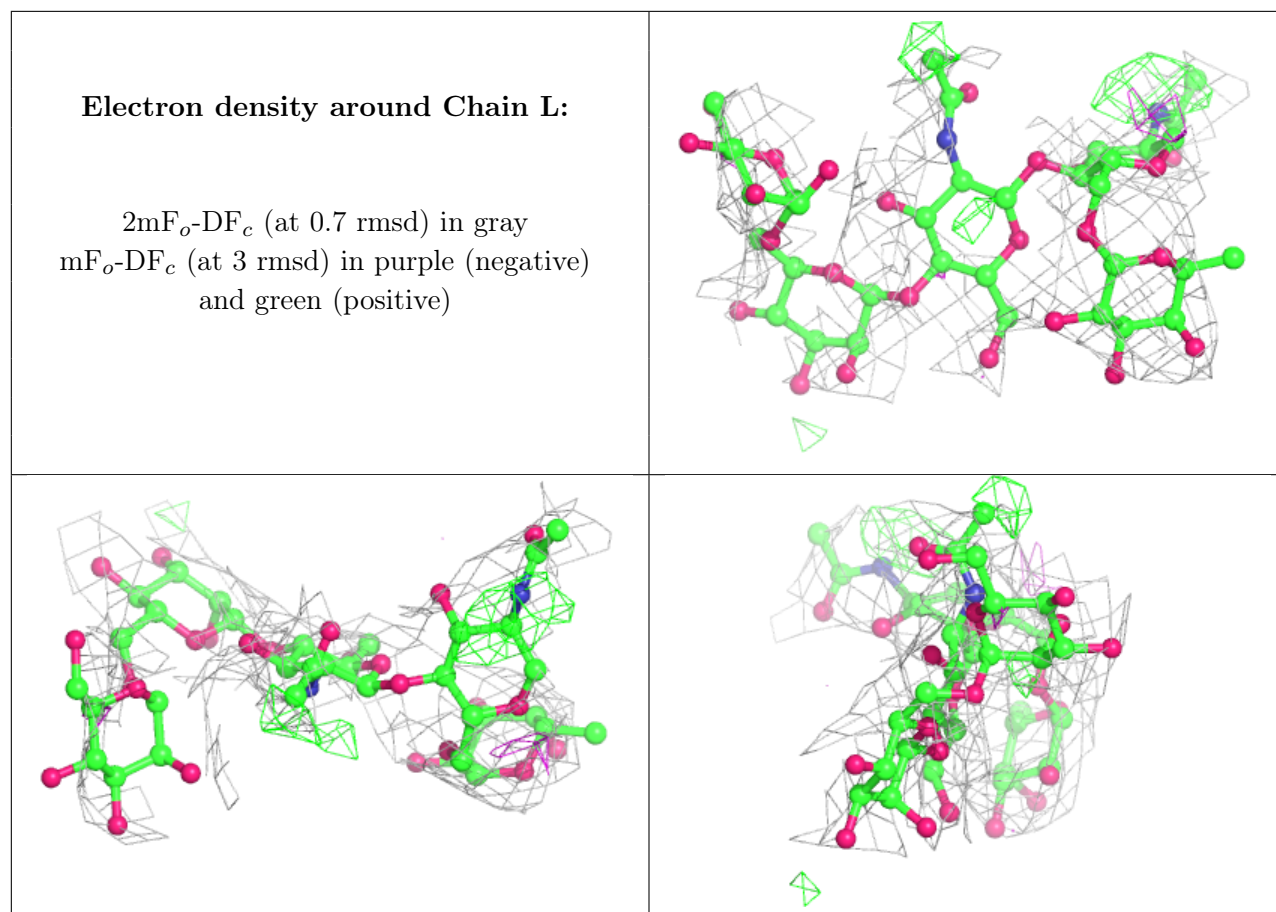
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	SO4	D	301	5/5	0.48	0.55	155,160,170,215	0
10	SO4	F	301	5/5	0.75	0.48	147,161,178,195	0
7	NAG	A	1702	14/15	0.77	0.32	124,142,161,174	0
7	NAG	B	401	14/15	0.80	0.47	138,150,163,164	0
9	XYL	B	405	10/10	0.80	0.47	107,118,138,141	0
9	XYL	A	1704	10/10	0.81	0.35	105,114,140,142	0
7	NAG	B	403	14/15	0.81	0.38	132,166,175,179	0
8	UNX	B	404	1/1	0.83	1.28	78,78,78,78	0
8	UNX	A	1703	1/1	0.87	1.21	90,90,90,90	0
7	NAG	B	402	14/15	0.89	0.17	135,147,157,161	0
7	NAG	A	1701	14/15	0.89	0.33	137,149,156,157	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.