wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 10:39 am GMT

PDB ID	:	1E70
Title	:	2-F-glucosylated MYROSINASE FROM SINAPIS ALBA
Authors	:	Burmeister, W.P.
Deposited on	:	2000-08-23
Resolution	:	1.65 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 (i) 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 (1)) were used in the production of this report:

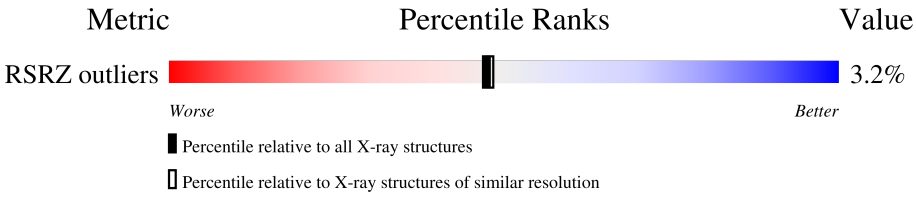
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
RSRZ outliers	127900	1791 (1.66-1.66)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	C	3	X	-	-	-
4	XYP	C	4	-	-	-	X
4	MAN	C	5	-	-	-	X
5	NAG	M	961	X	-	-	X
5	NAG	M	971	-	-	-	X
5	NAG	M	991	X	-	-	X
8	SO4	M	1507	-	-	-	X
9	GOL	M	1513	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5196 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.

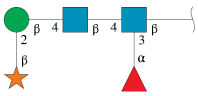
- Molecule 1 is a protein called MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	499	4086	2622	660	788	16	0	22	0

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

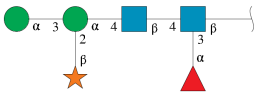
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0

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



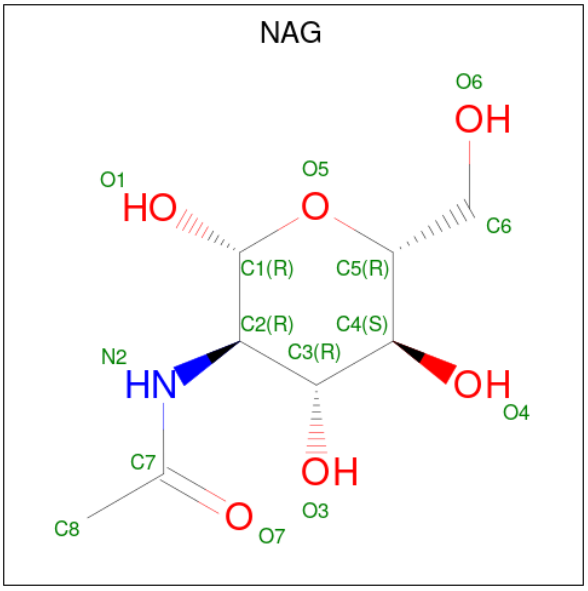
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	5	58	33	2	23	0	0	0

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



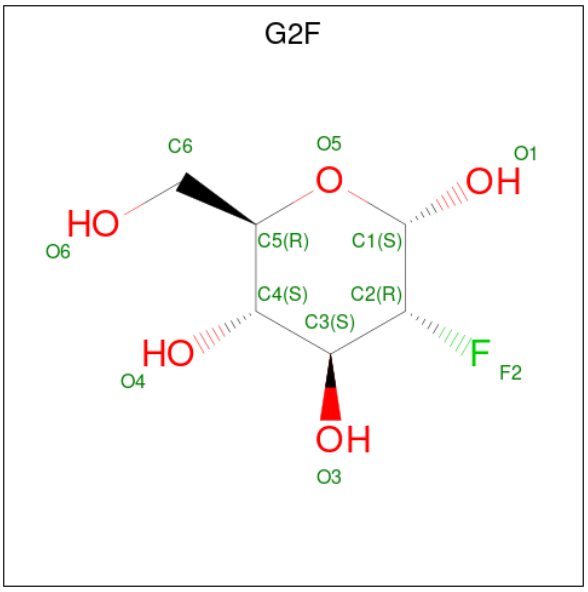
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	C	6	Total C N O 69 39 2 28	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 2-deoxy-2-fluoro-alpha-D-glucopyranose (three-letter code: G2F) (formula: $C_6H_{11}FO_5$).

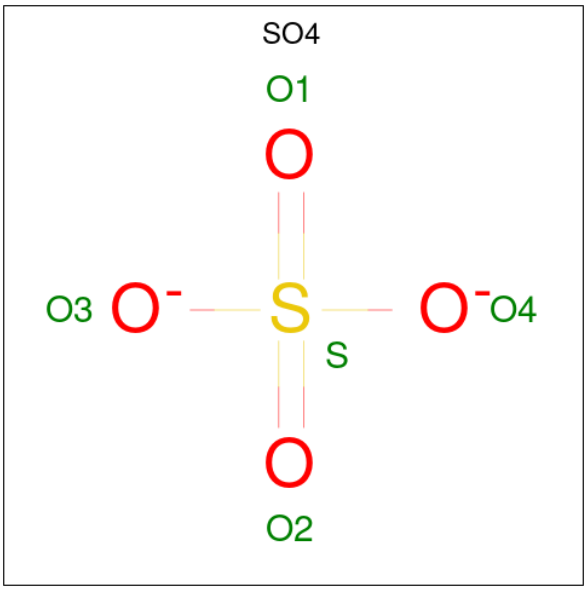


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total C F O 11 6 1 4	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

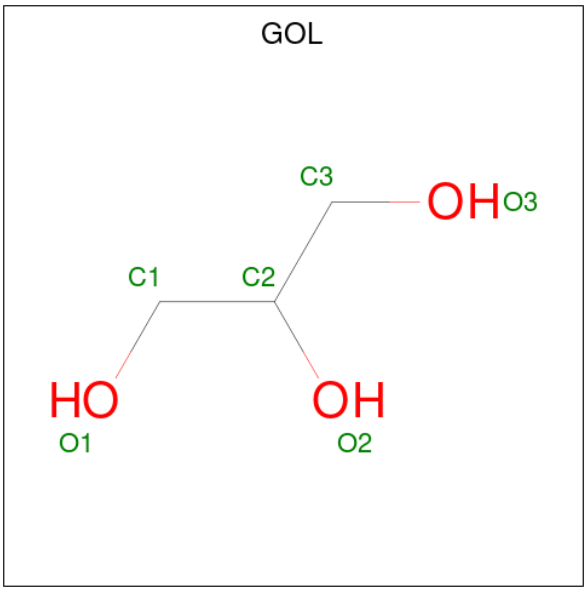
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total Zn 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 7 3 4	0	1
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	794	Total O 794 794	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65 9.99 – 1.65	Depositor EDS
% Data completeness (in resolution range)	82.3 (10.00-1.65) 82.3 (9.99-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.195 (Not available) , (Not available)	Depositor DCC
R_{free} test set	3755 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.49 , 72.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1	1,2	14,14,15	1.55	4 (28%)	17,19,21	3.30	9 (52%)
2	NAG	A	2	2	14,14,15	1.01	0	17,19,21	2.52	8 (47%)
3	NAG	B	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	4.07	11 (64%)
3	NAG	B	2	3	14,14,15	1.22	2 (14%)	17,19,21	1.53	4 (23%)
3	BMA	B	3	3	11,11,12	1.88	2 (18%)	15,15,17	1.44	3 (20%)
3	XYP	B	4	3	9,9,10	0.81	0	10,12,14	3.03	3 (30%)
3	FUC	B	5	3	10,10,11	1.50	2 (20%)	14,14,16	1.92	6 (42%)
4	NAG	C	1	1,4	14,14,15	1.21	1 (7%)	17,19,21	2.87	5 (29%)
4	NAG	C	2	4	14,14,15	1.43	2 (14%)	17,19,21	2.41	7 (41%)
4	MAN	C	3	4	11,11,12	2.03	3 (27%)	15,15,17	6.46	10 (66%)
4	XYP	C	4	4	9,9,10	1.36	1 (11%)	10,12,14	3.76	5 (50%)
4	MAN	C	5	4	11,11,12	1.22	2 (18%)	15,15,17	1.96	6 (40%)
4	FUC	C	6	4	10,10,11	1.75	3 (30%)	14,14,16	2.46	7 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	MAN	C	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	FUC	C	6	4	-	-	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	MAN	C2-C3	-4.66	1.45	1.52
3	B	3	BMA	C2-C3	-4.31	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	FUC	C2-C3	3.72	1.58	1.52
4	C	3	MAN	O5-C1	3.65	1.49	1.43
3	B	3	BMA	C4-C5	3.27	1.59	1.53

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3	MAN	C6-C5-C4	13.10	143.68	113.00
4	C	3	MAN	O4-C4-C5	9.97	134.06	109.30
4	C	3	MAN	C1-O5-C5	-9.59	99.20	112.19
4	C	3	MAN	O5-C5-C6	-8.94	93.19	107.20
2	A	1	NAG	C1-O5-C5	-8.44	100.75	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	3	MAN	C1

All (3) torsion outliers are listed below:

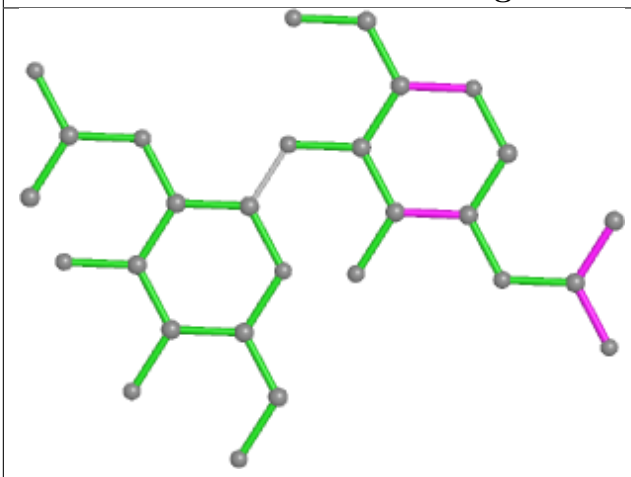
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

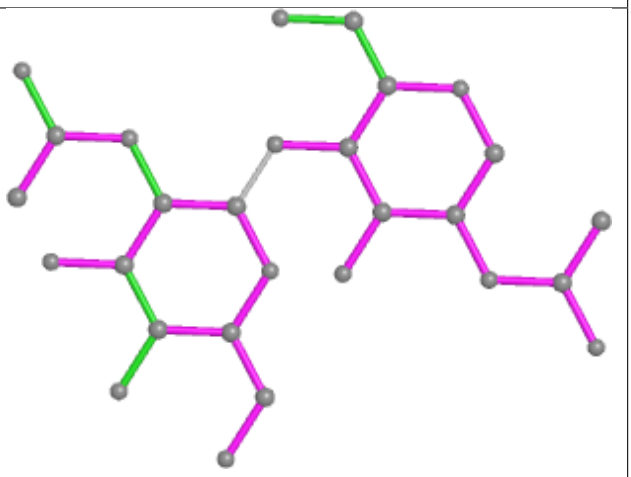
No monomer is involved in short contacts.

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

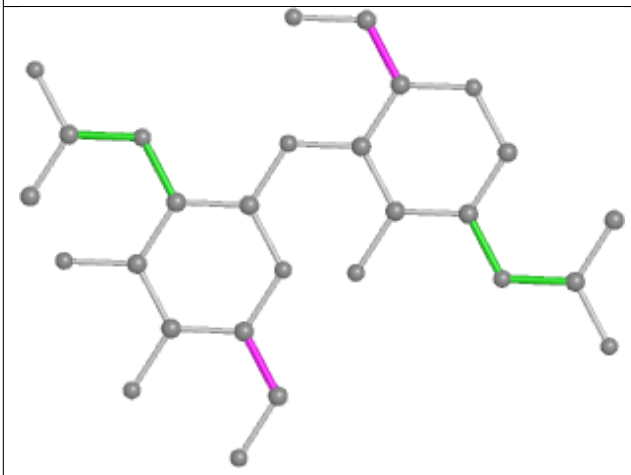
Oligosaccharide Chain A



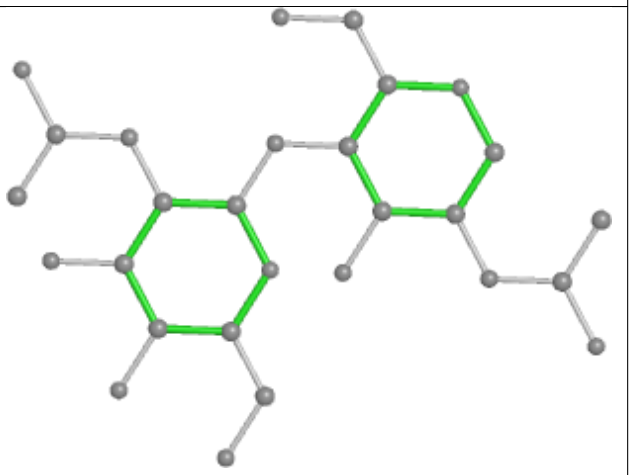
Bond lengths



Bond angles

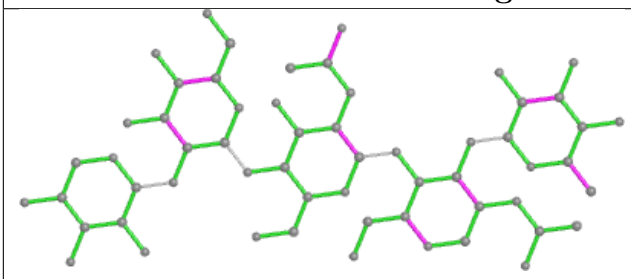


Torsions

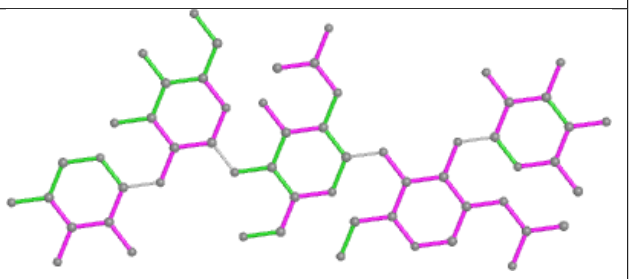


Rings

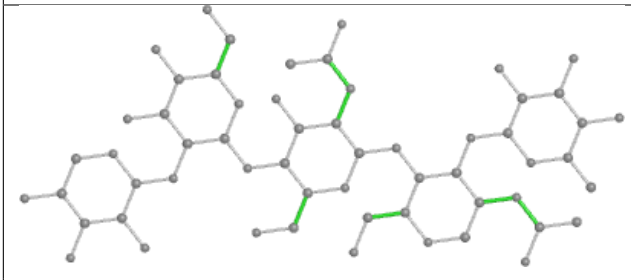
Oligosaccharide Chain B



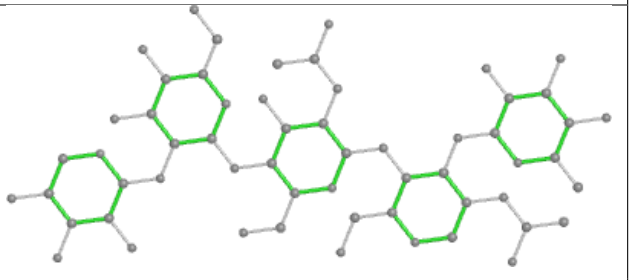
Bond lengths



Bond angles

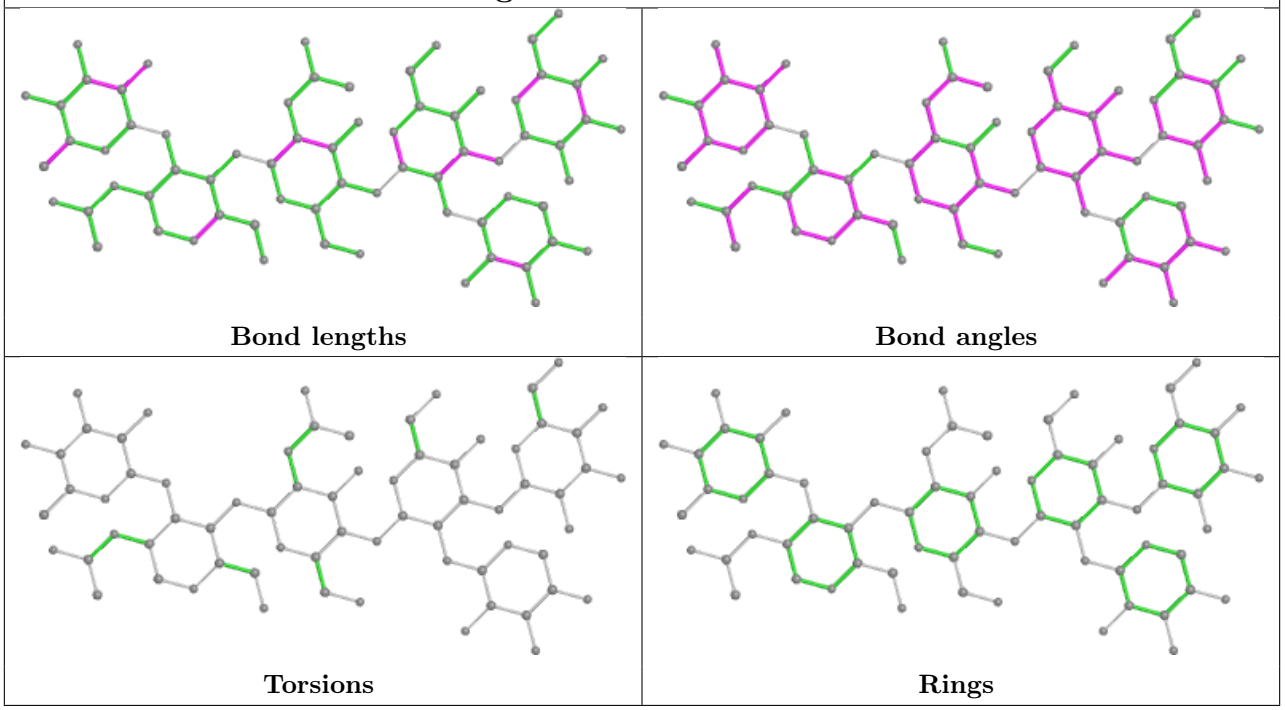


Torsions



Rings

Oligosaccharide Chain C



4.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	GOL	M	1513	-	5,5,5	3.95	4 (80%)	5,5,5	2.47	3 (60%)
5	NAG	M	991	1	14,14,15	1.29	1 (7%)	17,19,21	1.93	6 (35%)
8	SO4	M	1507	-	4,4,4	0.78	0	6,6,6	1.41	1 (16%)
8	SO4	M	1510	-	4,4,4	0.53	0	6,6,6	0.43	0
8	SO4	M	1509	-	4,4,4	0.63	0	6,6,6	0.23	0
8	SO4	M	1506	-	4,4,4	0.49	0	6,6,6	1.65	1 (16%)
8	SO4	M	1505	-	4,4,4	0.61	0	6,6,6	0.30	0
9	GOL	M	1512[A]	-	5,5,5	0.75	0	5,5,5	1.79	1 (20%)
8	SO4	M	1503	-	4,4,4	0.47	0	6,6,6	0.37	0
5	NAG	M	931	1	14,14,15	1.71	2 (14%)	17,19,21	7.71	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GOL	M	1514	-	5,5,5	0.25	0	5,5,5	0.79	0
5	NAG	M	911	1	14,14,15	1.19	1 (7%)	17,19,21	1.97	4 (23%)
6	G2F	M	999	-	11,11,12	1.86	2 (18%)	10,15,17	2.71	4 (40%)
9	GOL	M	1512[B]	-	5,5,5	0.73	0	5,5,5	2.11	2 (40%)
5	NAG	M	971	1	14,14,15	1.34	1 (7%)	17,19,21	1.36	2 (11%)
5	NAG	M	901	1	14,14,15	1.08	1 (7%)	17,19,21	1.64	5 (29%)
8	SO4	M	1504	-	4,4,4	0.60	0	6,6,6	0.28	0
5	NAG	M	961	1	14,14,15	1.47	2 (14%)	17,19,21	2.46	5 (29%)
8	SO4	M	1508	-	4,4,4	0.75	0	6,6,6	0.68	0
9	GOL	M	1511	-	5,5,5	0.32	0	5,5,5	0.55	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
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
6	G2F	M	999	-	-	0/2/19/22	0/1/1/1
9	GOL	M	1513	-	-	3/4/4/4	-
5	NAG	M	991	1	1/1/5/7	2/6/23/26	0/1/1/1
9	GOL	M	1512[A]	-	-	0/4/4/4	-
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1
9	GOL	M	1512[B]	-	-	2/4/4/4	-
5	NAG	M	901	1	-	2/6/23/26	0/1/1/1
5	NAG	M	931	1	-	3/6/23/26	0/1/1/1
9	GOL	M	1511	-	-	1/4/4/4	-
9	GOL	M	1514	-	-	1/4/4/4	-
5	NAG	M	961	1	1/1/5/7	0/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1513	GOL	O2-C2	6.33	1.62	1.43
5	M	931	NAG	O7-C7	-4.38	1.13	1.23
9	M	1513	GOL	O1-C1	4.22	1.60	1.42
6	M	999	G2F	C2-C3	4.06	1.57	1.51
5	M	971	NAG	O7-C7	-4.01	1.14	1.23

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	931	NAG	C2-N2-C7	28.95	164.12	122.90
5	M	931	NAG	O5-C1-C2	8.55	124.78	111.29
5	M	961	NAG	C1-O5-C5	7.90	122.89	112.19
5	M	931	NAG	O7-C7-N2	-6.27	110.43	121.95
6	M	999	G2F	C1-O5-C5	-5.11	105.27	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	961	NAG	C1
5	M	991	NAG	C1

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	1512[B]	GOL	O1-C1-C2-C3
5	M	971	NAG	O5-C5-C6-O6
5	M	971	NAG	C4-C5-C6-O6
5	M	931	NAG	O5-C5-C6-O6
5	M	901	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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, 95^{th} 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	M	499/501 (99%)	-0.13	16 (3%) 47 48	20, 25, 39, 66	1 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	9.0
1	M	380	ASP	5.6
1	M	375	LYS	4.7
1	M	374	ASP	4.3
1	M	417	ASP	3.9

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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^{th} 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
4	MAN	C	5	11/12	0.24	0.50	42,55,57,57	0
4	XYP	C	4	9/10	0.44	0.43	56,59,60,62	0
2	NAG	A	2	14/15	0.53	0.38	49,52,56,58	0
3	BMA	B	3	11/12	0.71	0.36	53,57,59,59	0
4	MAN	C	3	11/12	0.72	0.16	44,48,52,54	0
3	XYP	B	4	9/10	0.74	0.39	59,60,62,62	0
3	FUC	B	5	10/11	0.83	0.21	41,43,47,49	0

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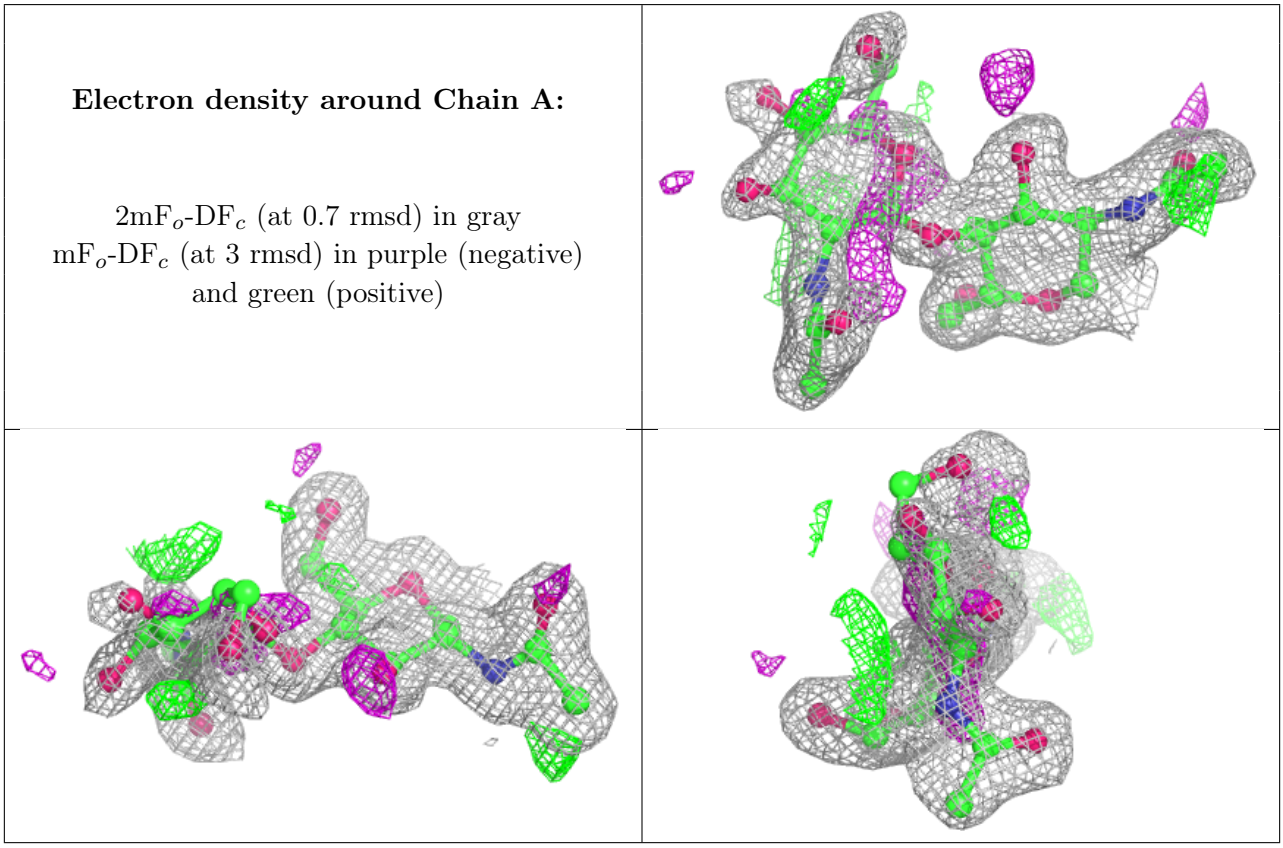
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	2	14/15	0.87	0.14	39,43,48,49	0
4	FUC	C	6	10/11	0.87	0.15	38,39,43,43	0
2	NAG	A	1	14/15	0.90	0.10	29,34,38,42	0
4	NAG	C	2	14/15	0.90	0.12	34,37,40,42	0
3	NAG	B	1	14/15	0.91	0.08	30,33,36,36	0
4	NAG	C	1	14/15	0.92	0.09	30,32,35,36	0

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.

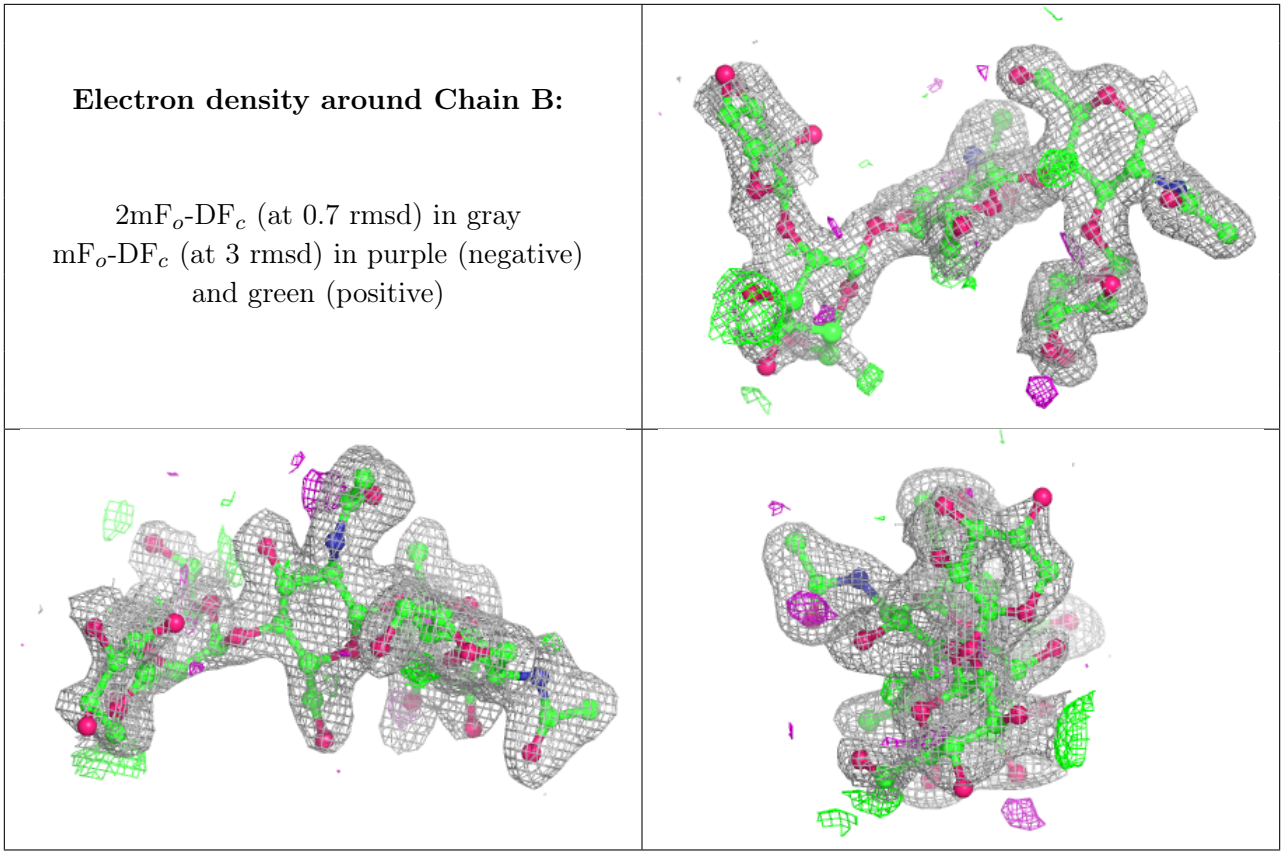
Electron density around Chain A:

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



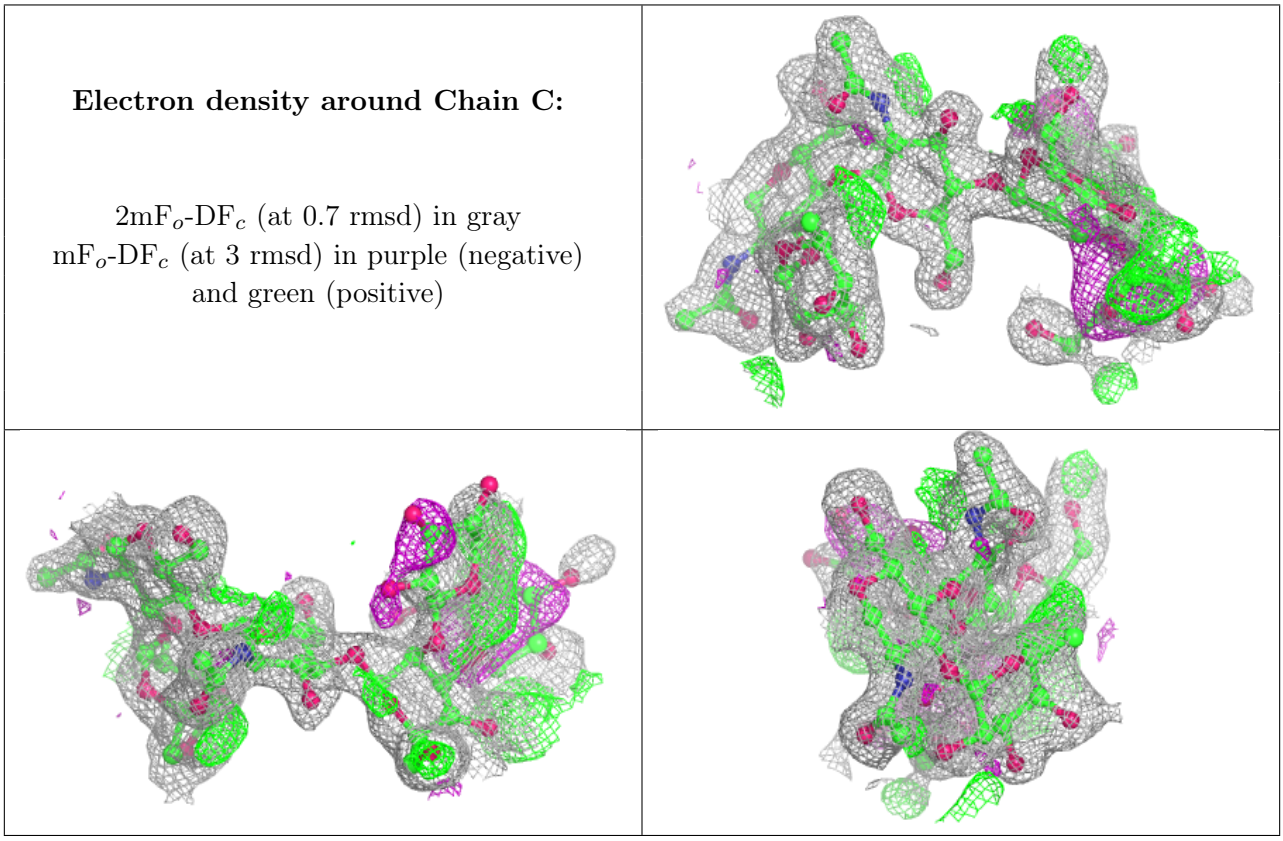
Electron density around Chain B:

$2mF_o$-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 C:

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



5.4 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, 95^{th} 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
5	NAG	M	961	14/15	0.36	0.56	59,63,66,67	0
5	NAG	M	991	14/15	0.43	0.62	57,58,63,64	0
8	SO4	M	1507	5/5	0.46	0.47	50,52,53,54	5
5	NAG	M	971	14/15	0.54	0.50	69,75,76,76	0
9	GOL	M	1511	6/6	0.60	0.34	55,56,56,56	6
5	NAG	M	931	14/15	0.64	0.34	53,58,60,60	0
8	SO4	M	1508	5/5	0.68	0.29	42,46,47,47	5
9	GOL	M	1514	6/6	0.68	0.29	57,59,59,60	6
5	NAG	M	901	14/15	0.71	0.20	42,45,50,52	0
8	SO4	M	1505	5/5	0.74	0.34	54,56,56,58	5
9	GOL	M	1513	6/6	0.76	0.29	20,26,29,36	0
8	SO4	M	1509	5/5	0.77	0.30	54,55,55,55	5
5	NAG	M	911	14/15	0.83	0.21	36,40,41,45	0
8	SO4	M	1510	5/5	0.87	0.37	62,62,63,64	1
9	GOL	M	1512[B]	6/6	0.91	0.14	23,26,28,29	2
6	G2F	M	999	11/12	0.91	0.10	27,32,35,37	0
9	GOL	M	1512[A]	6/6	0.91	0.14	16,23,28,28	2
8	SO4	M	1506	5/5	0.94	0.12	35,36,37,40	0
8	SO4	M	1504	5/5	0.96	0.15	36,39,41,41	5
8	SO4	M	1503	5/5	0.98	0.14	37,40,41,43	5
7	ZN	M	1502	1/1	0.99	0.02	21,21,21,21	1

5.5 Other polymers (i)

There are no such residues in this entry.