wwPDB X-ray Structure Validation Summary Report (i)

Nov 28, 2023 – 07:29 pm GMT

PDB ID	:	1DWJ
Title	:	study on radiation damage on a cryocooled crystal. Refined part 6: structure after a radiation dose of 54*10e15 photons/mm2
Authors	:	Burmeister, W.P.
Deposited on	:	1999-12-05
Resolution	:	2.40 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 (i)) were used in the production of this report:

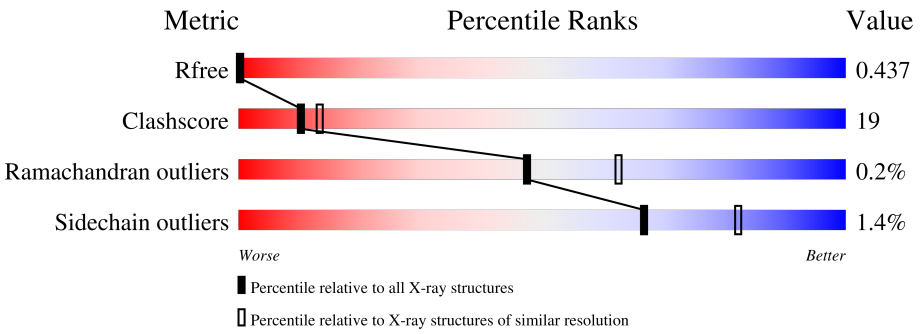
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Mol	Chain	Length	Quality of chain
1	M	499	72% 27% .
2	A	2	50% 50%
2	D	2	100%
3	B	5	20% 80%
4	C	7	29% 29% 43%

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	6	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5220 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	4083	2619	660	788	16	0	21	0

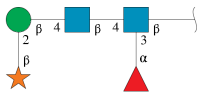
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

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

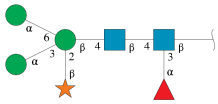
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- 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.



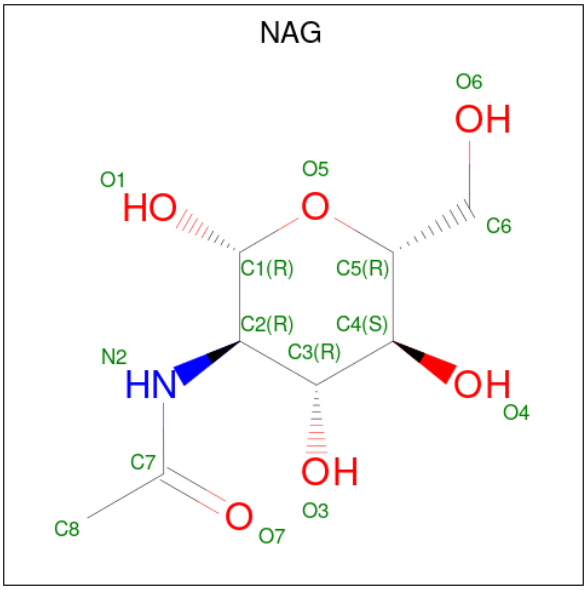
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	5	58	33	2	23	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]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			
4	C	7	80	45	2	33	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
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0

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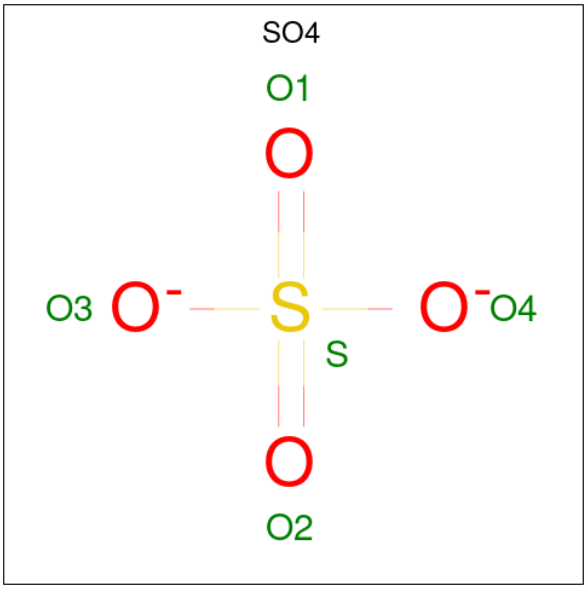
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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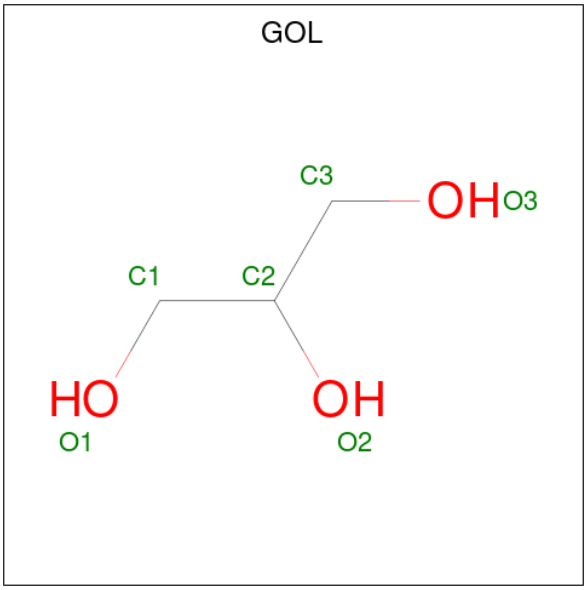
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

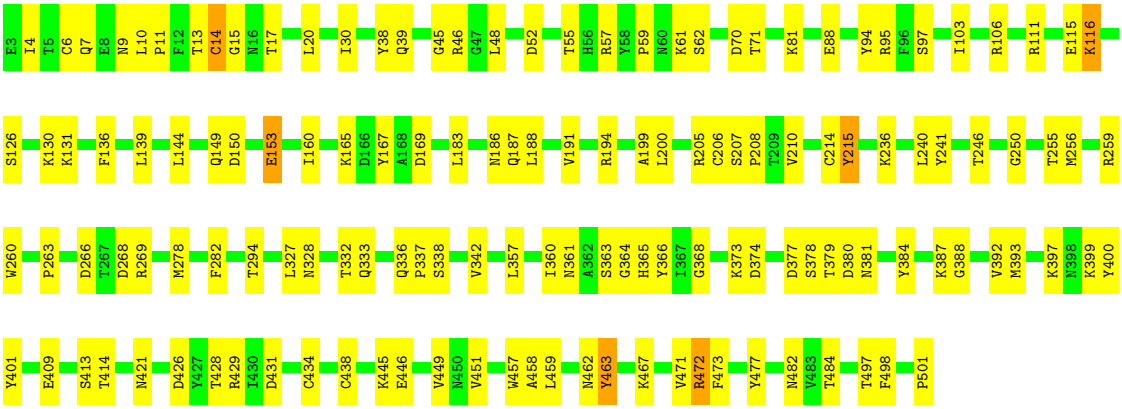
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	788	Total O 788 788	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: MYROSINASE MA1

Chain M: 72% 27%



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

Chain A: 50% 50%

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

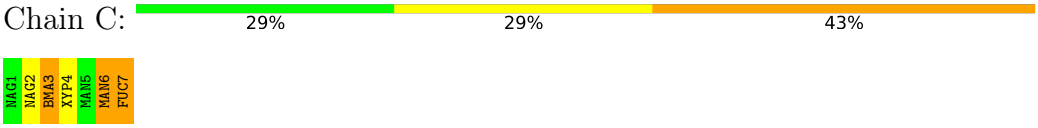
Chain D: 100%

• Molecule 3: 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

Chain B: 20% 80%

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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.40) 95.1 (9.94-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.93 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.186 , 0.245 0.407 , 0.437	Depositor DCC
R_{free} test set	2570 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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.

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: FUC, BMA, NAG, ZN, XYP, SO4, GOL, 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	M	0.82	2/4291 (0.0%)	0.79	1/5835 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	2	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	14	CYS	CB-SG	5.68	1.92	1.82
1	M	153	GLU	CG-CD	5.11	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	472	ARG	NE-CZ-NH1	5.32	122.96	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	M	360[A]	ILE	CB
1	M	360[B]	ILE	CB

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	215	TYR	Sidechain
1	M	401	TYR	Sidechain
1	M	446	GLU	Mainchain
1	M	94	TYR	Sidechain
1	M	97	SER	Mainchain

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	M	4083	0	3838	143	8
2	A	28	0	25	0	0
2	D	28	0	25	2	0
3	B	58	0	42	0	0
4	C	80	0	60	11	0
5	M	84	0	78	9	0
6	M	1	0	0	0	1
7	M	40	0	0	1	0
8	M	30	0	40	1	0
9	M	788	0	0	84	15
All	All	5220	0	4108	159	23

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 19.

The worst 5 of 159 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)
9:M:3053:HOH:O	4:C:6:MAN:O6	1.55	1.22
1:M:15:GLY:HA3	9:M:2027:HOH:O	1.06	1.20
9:M:3055:HOH:O	4:C:6:MAN:H61	1.01	1.19
9:M:3066:HOH:O	2:D:2:NAG:H83	1.44	1.17
1:M:428:THR:HG23	9:M:2608:HOH:O	1.44	1.17

The worst 5 of 23 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)
6:M:1001:ZN:ZN	6:M:1001:ZN:ZN[3_656]	1.10	1.10
9:M:2272:HOH:O	9:M:2272:HOH:O[3_656]	1.10	1.10
9:M:2010:HOH:O	9:M:2505:HOH:O[4_576]	1.43	0.77
9:M:2546:HOH:O	9:M:2546:HOH:O[4_576]	1.44	0.76
9:M:2017:HOH:O	9:M:2017:HOH:O[4_576]	1.63	0.57

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	M	518/499 (104%)	498 (96%)	19 (4%)	1 (0%)	47 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	456/435 (105%)	450 (99%)	6 (1%)	69 84

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	263	PRO

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Mol	Chain	Res	Type
1	M	266	ASP
1	M	268	ASP
1	M	183	LEU
1	M	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

16 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	2,1	14,14,15	0.51	0	17,19,21	0.81	0
2	NAG	A	2	2	14,14,15	1.03	1 (7%)	17,19,21	0.84	0
3	NAG	B	1	1,3	14,14,15	0.61	0	17,19,21	0.86	1 (5%)
3	NAG	B	2	3	14,14,15	0.77	0	17,19,21	0.62	0
3	BMA	B	3	3	11,11,12	1.25	1 (9%)	15,15,17	0.72	0
3	XYP	B	4	3	9,9,10	0.90	0	10,12,14	1.51	1 (10%)
3	FUC	B	5	3	10,10,11	1.18	1 (10%)	14,14,16	0.87	1 (7%)
4	NAG	C	1	1,4	14,14,15	0.65	0	17,19,21	0.82	0
4	NAG	C	2	4	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
4	BMA	C	3	4	11,11,12	1.05	1 (9%)	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	XYP	C	4	4	9,9,10	0.75	0	10,12,14	1.30	1 (10%)
4	MAN	C	5	4	11,11,12	0.84	0	15,15,17	0.55	0
4	MAN	C	6	4	11,11,12	1.02	1 (9%)	15,15,17	1.51	2 (13%)
4	FUC	C	7	4	10,10,11	0.94	0	14,14,16	1.42	2 (14%)
2	NAG	D	1	2,1	14,14,15	0.58	0	17,19,21	0.53	0
2	NAG	D	2	2	14,14,15	0.80	0	17,19,21	0.79	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
2	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	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	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	1/2/19/22	0/1/1/1
4	MAN	C	6	4	-	2/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	FUC	C2-C3	2.74	1.56	1.52
4	C	3	BMA	C2-C3	-2.68	1.48	1.52
2	A	2	NAG	C1-C2	2.61	1.56	1.52
3	B	3	BMA	C4-C5	2.50	1.58	1.53
4	C	6	MAN	C2-C3	2.47	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	6	MAN	C6-C5-C4	4.36	123.21	113.00
3	B	4	XYP	C1-C2-C3	4.13	114.74	109.67
4	C	4	XYP	C5-C4-C3	3.65	114.16	109.67
4	C	7	FUC	C1-C2-C3	-3.05	105.92	109.67
4	C	2	NAG	C3-C4-C5	2.68	115.03	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	6	MAN	C4-C5-C6-O6
4	C	6	MAN	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6

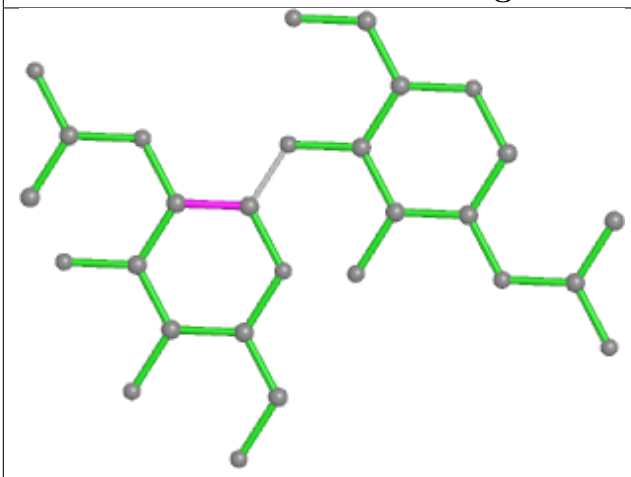
There are no ring outliers.

5 monomers are involved in 13 short contacts:

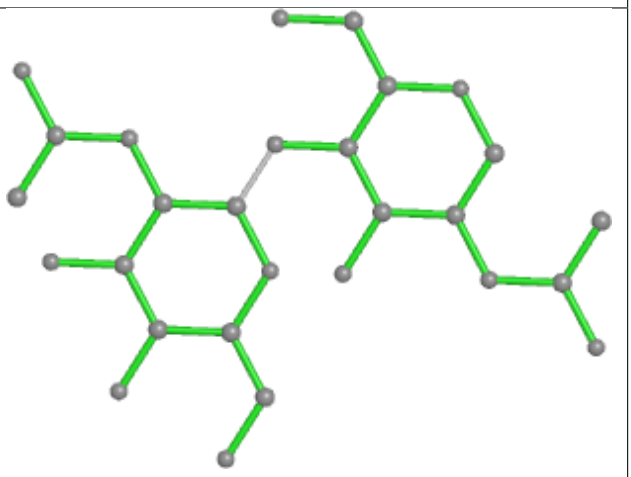
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	BMA	5	0
4	C	6	MAN	9	0
2	D	2	NAG	1	0
2	D	1	NAG	1	0
4	C	7	FUC	1	0

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

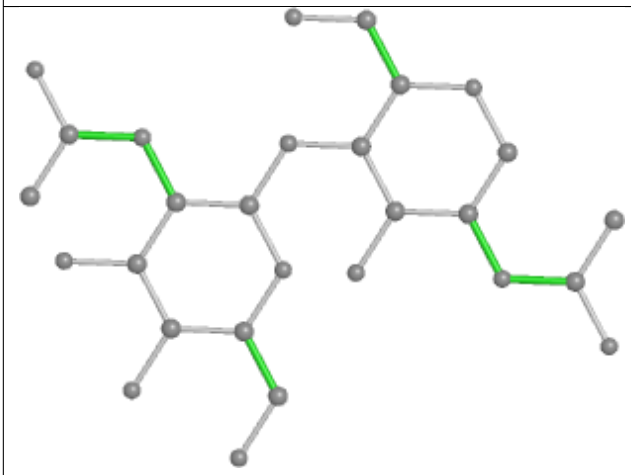
Oligosaccharide Chain A



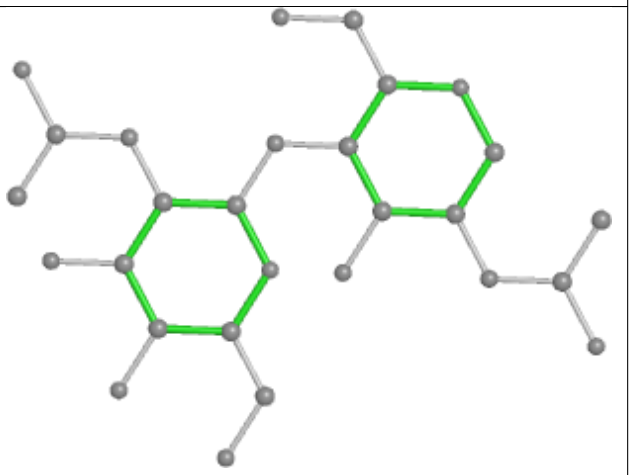
Bond lengths



Bond angles

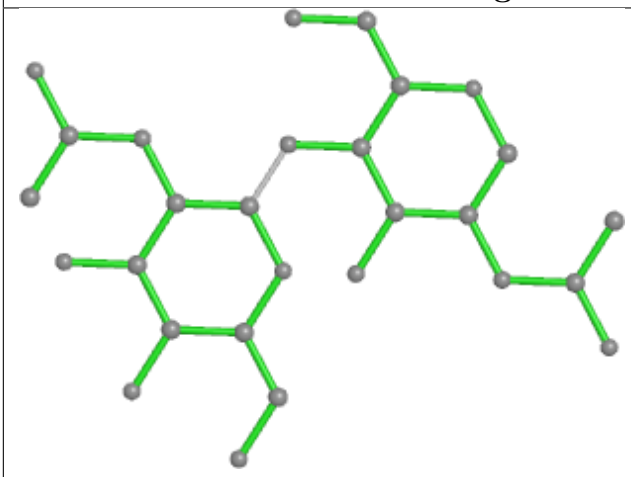


Torsions

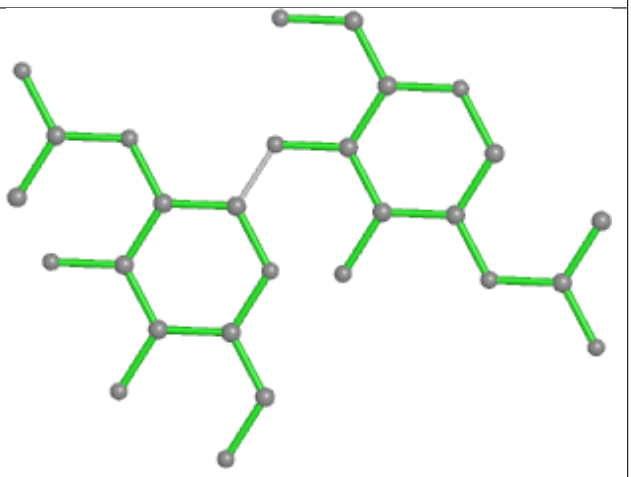


Rings

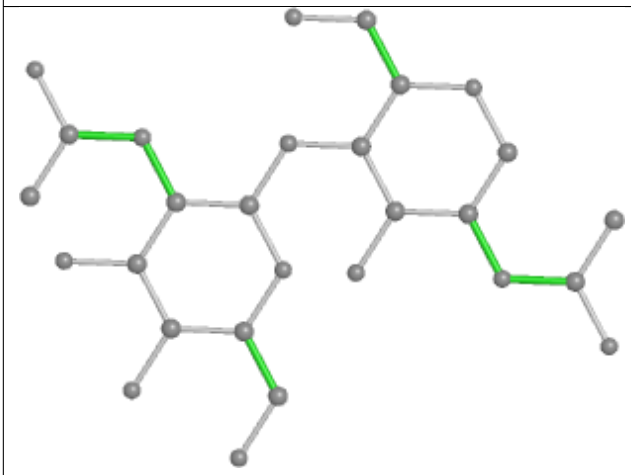
Oligosaccharide Chain D



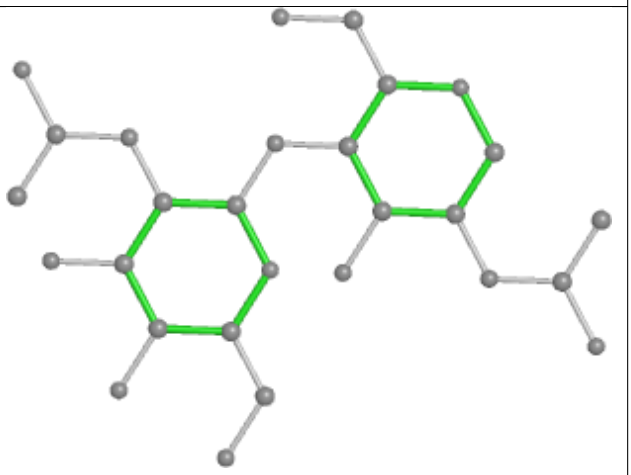
Bond lengths



Bond angles

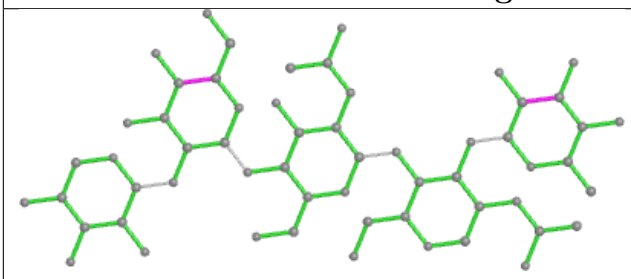


Torsions

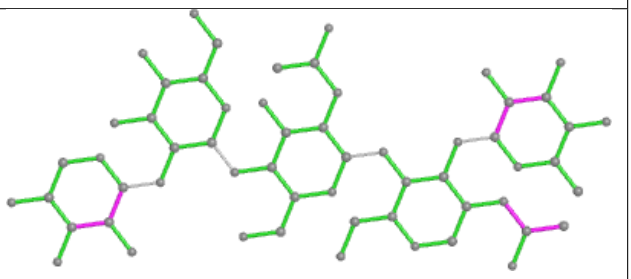


Rings

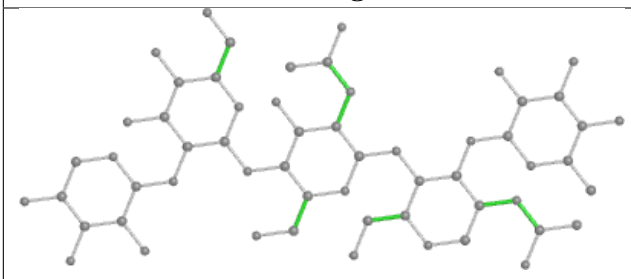
Oligosaccharide Chain B



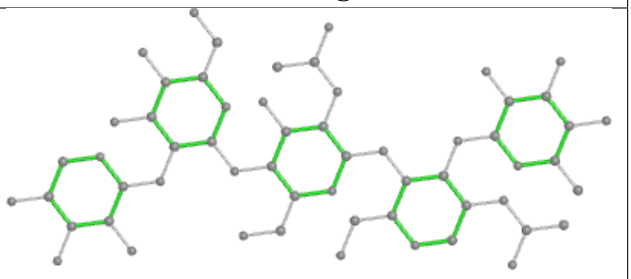
Bond lengths



Bond angles

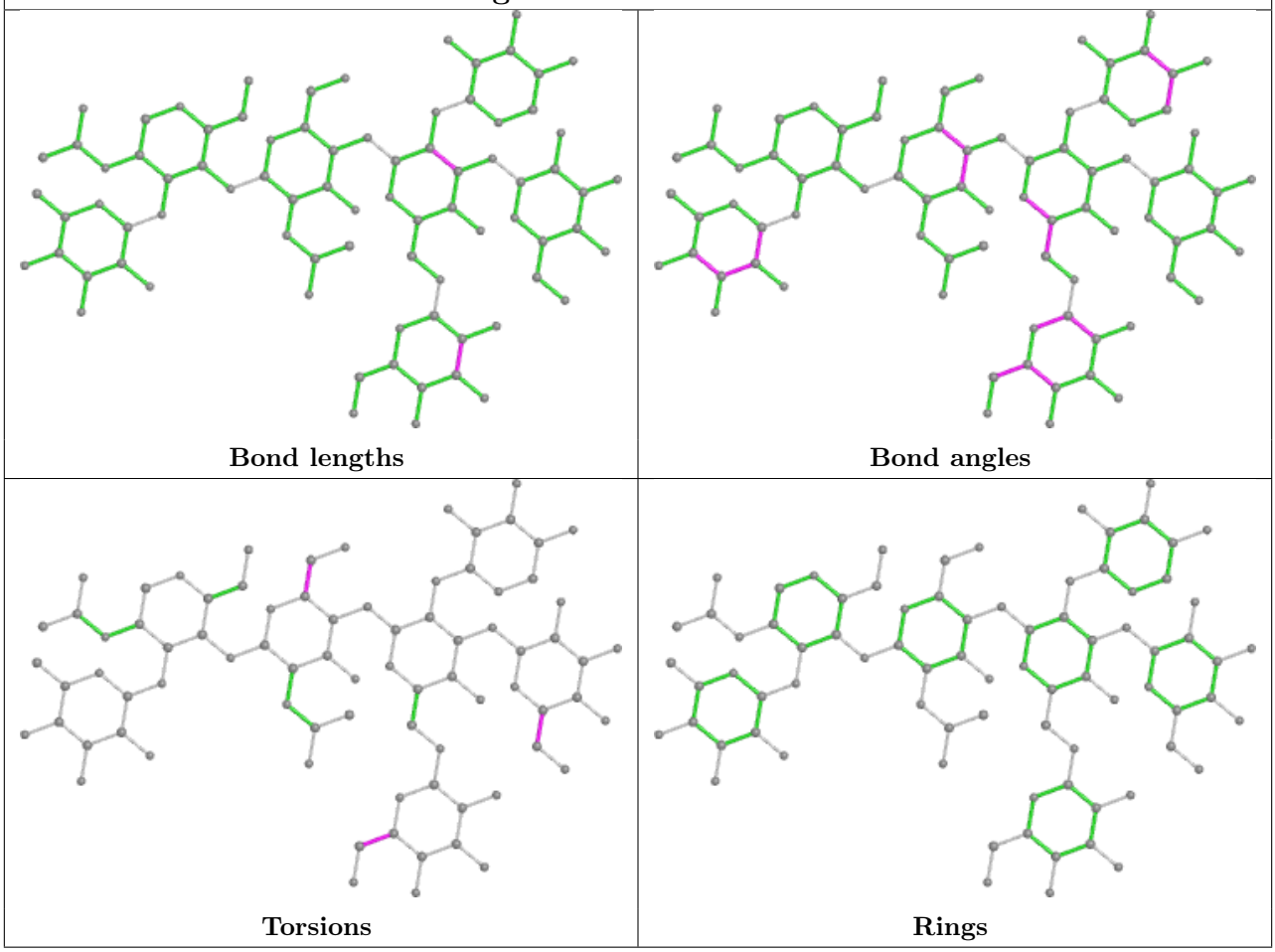


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
8	GOL	M	1010	-	5,5,5	0.15	0	5,5,5	0.50	0
5	NAG	M	911	1	14,14,15	0.81	0	17,19,21	0.69	0
8	GOL	M	1024	-	5,5,5	0.59	0	5,5,5	0.32	0
5	NAG	M	991	1	14,14,15	0.83	0	17,19,21	0.88	1 (5%)
8	GOL	M	1021	-	5,5,5	0.34	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	M	961	1	14,14,15	0.89	0	17,19,21	0.90	1 (5%)
5	NAG	M	931	1	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
7	SO4	M	1006	-	4,4,4	0.39	0	6,6,6	0.23	0
7	SO4	M	1002	-	4,4,4	0.43	0	6,6,6	0.17	0
7	SO4	M	1003	-	4,4,4	0.22	0	6,6,6	0.12	0
8	GOL	M	1020	-	5,5,5	0.43	0	5,5,5	0.69	0
7	SO4	M	1004	-	4,4,4	0.26	0	6,6,6	0.30	0
5	NAG	M	971	1	14,14,15	1.29	2 (14%)	17,19,21	0.59	0
5	NAG	M	901	1	14,14,15	0.65	0	17,19,21	0.85	0
7	SO4	M	1008	-	4,4,4	0.35	0	6,6,6	0.12	0
7	SO4	M	1007	-	4,4,4	0.16	0	6,6,6	0.18	0
7	SO4	M	1005	-	4,4,4	0.30	0	6,6,6	0.25	0
7	SO4	M	1009	-	4,4,4	0.42	0	6,6,6	0.20	0
8	GOL	M	1023	-	5,5,5	0.39	0	5,5,5	0.39	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
8	GOL	M	1010	-	-	4/4/4/4	-
8	GOL	M	1024	-	-	0/4/4/4	-
5	NAG	M	991	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1020	-	-	0/4/4/4	-
8	GOL	M	1021	-	-	0/4/4/4	-
5	NAG	M	961	1	-	2/6/23/26	0/1/1/1
5	NAG	M	931	1	-	2/6/23/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1023	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	971	NAG	C1-C2	2.88	1.56	1.52
5	M	971	NAG	C4-C5	2.63	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	931	NAG	C2-N2-C7	3.40	127.74	122.90
5	M	991	NAG	C4-C3-C2	-2.74	107.01	111.02
5	M	961	NAG	C8-C7-N2	-2.15	112.45	116.10

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1010	GOL	O1-C1-C2-C3
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
5	M	971	NAG	O5-C5-C6-O6
5	M	971	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1024	GOL	1	0
5	M	961	NAG	3	0
5	M	931	NAG	4	0
5	M	901	NAG	2	0
7	M	1009	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

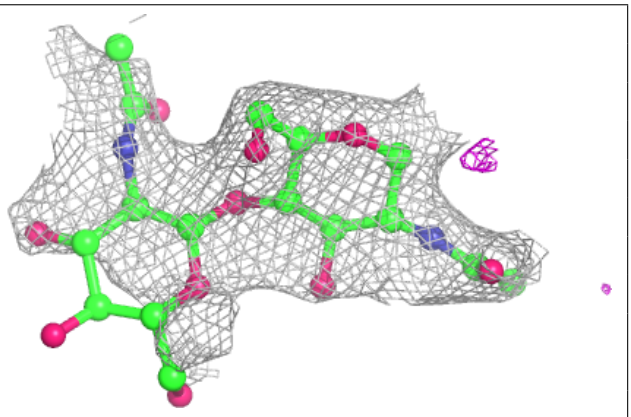
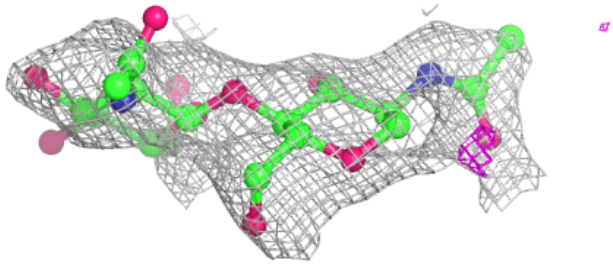
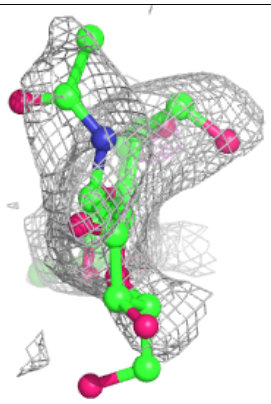
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

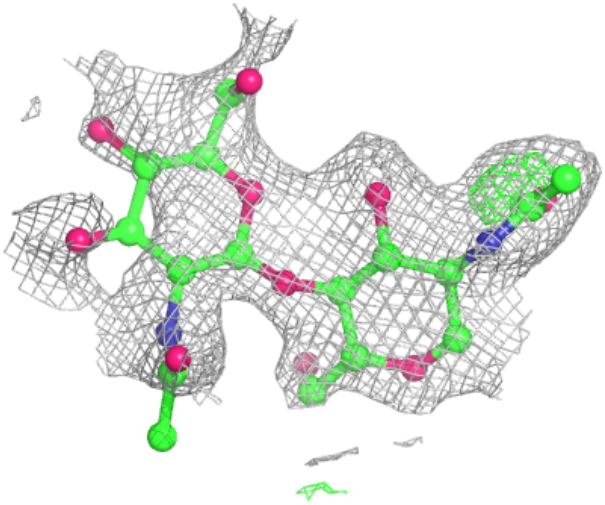
Unable to reproduce the depositors R factor - this section is therefore empty.

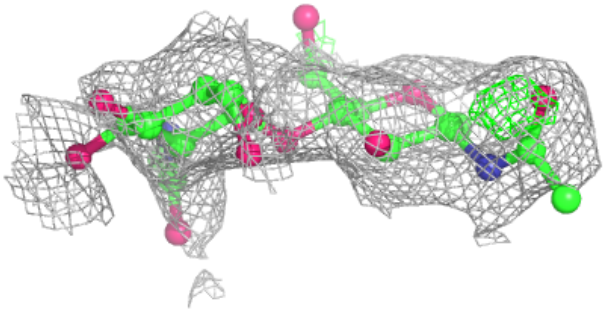
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

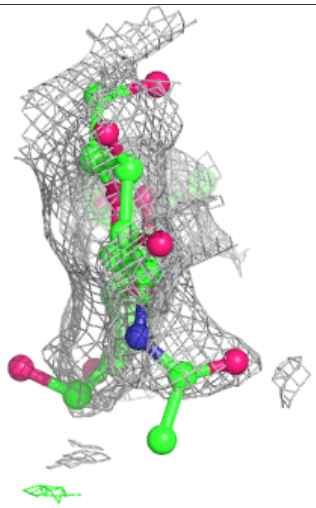
Electron density around Chain A: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around Chain D:

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

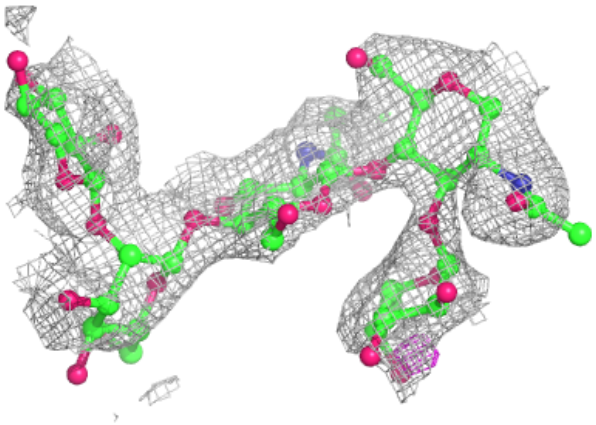


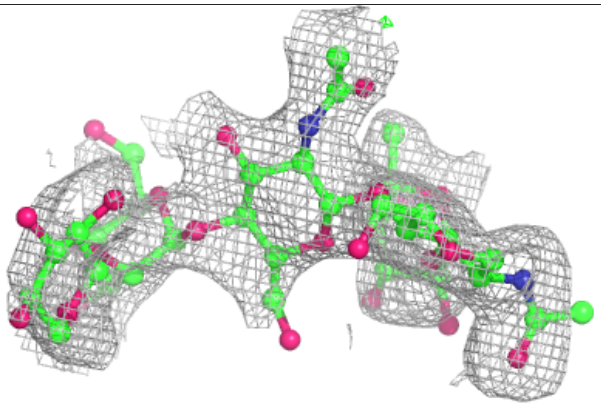


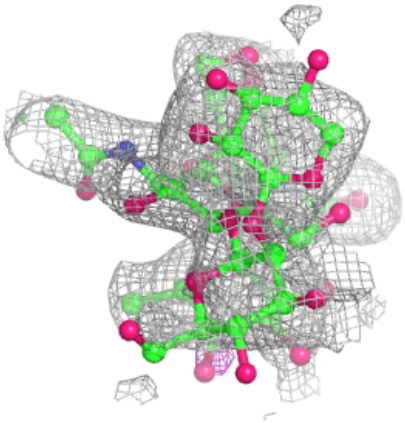


Electron density around Chain B:

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

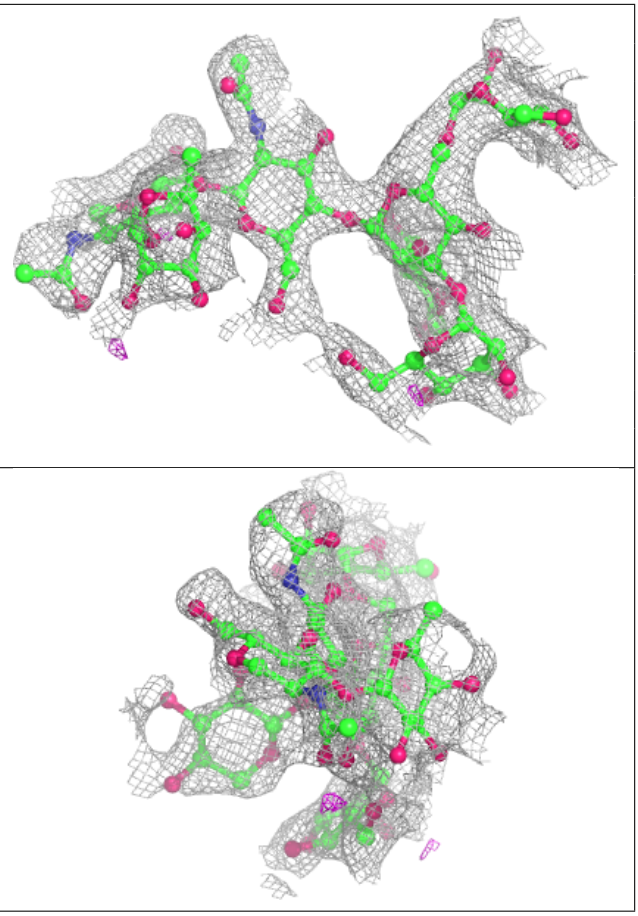






Electron density around Chain C:

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



6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.