Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2020 – 11:10 pm GMT

PDB ID	:	6HZN
Title	:	Crystal structure of human dermatan sulfate epimerase 1
Authors	:	Hasan, M.; Unge, J.; Westergren-Thorsson, G.; Ellervik, U.; Mueller, U.; Malmstrom, A.; Tykesson, E.
Deposited on	:	2018-10-23
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

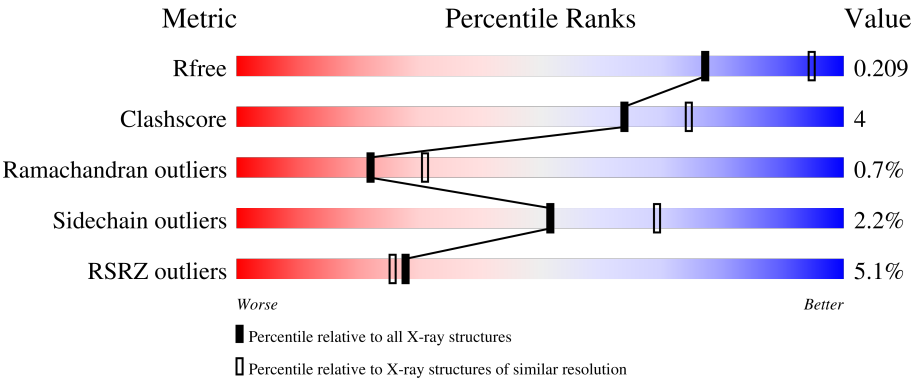
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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% 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	761	5% 86% 10%
2	B	2	100%
3	C	5	40% 20% 40%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6304 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 Dermatan-sulfate epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	1	0	0
			6009	3876	1018	1091	24			

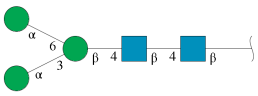
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	HIS	-	expression tag	UNP Q9UL01
A	777	HIS	-	expression tag	UNP Q9UL01
A	778	HIS	-	expression tag	UNP Q9UL01
A	779	HIS	-	expression tag	UNP Q9UL01
A	780	HIS	-	expression tag	UNP Q9UL01
A	781	HIS	-	expression tag	UNP Q9UL01
A	782	HIS	-	expression tag	UNP Q9UL01
A	783	HIS	-	expression tag	UNP Q9UL01

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

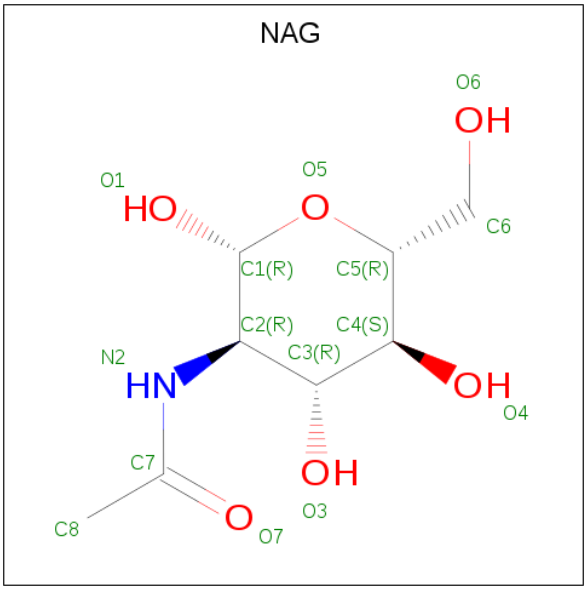
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

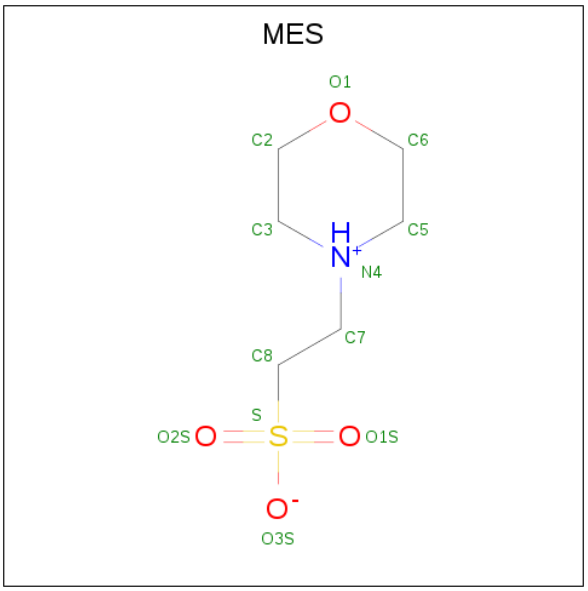


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is water.

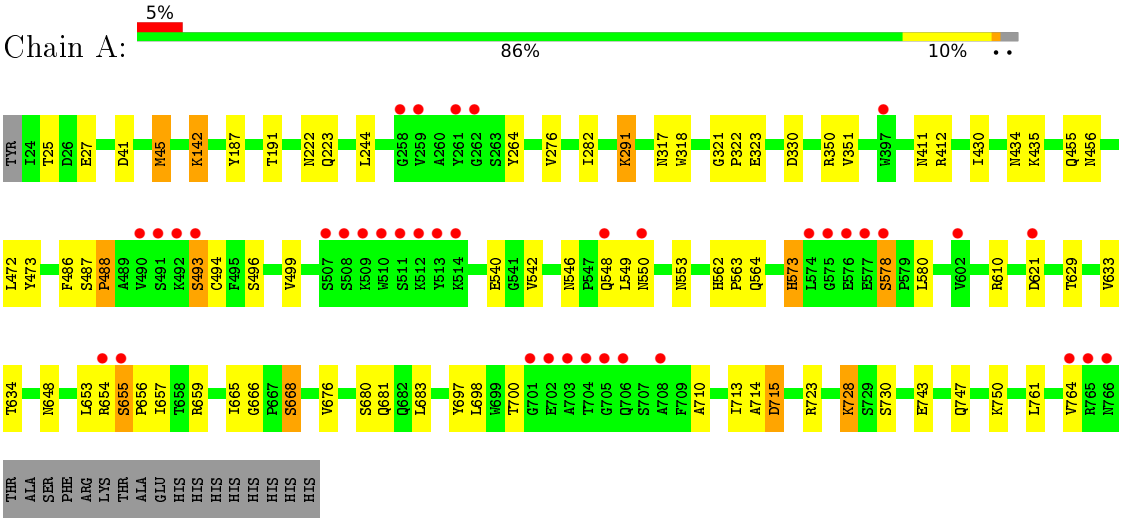
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	153	Total	O	0	0
			153	153		

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.

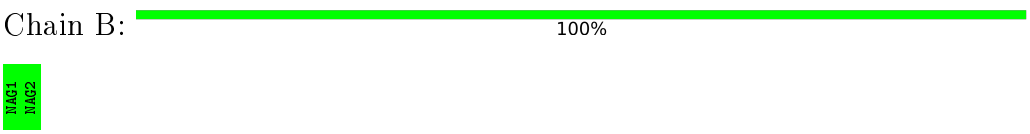
• Molecule 1: Dermatan-sulfate epimerase

Chain A:



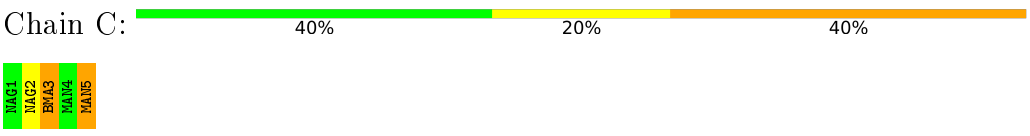
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



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

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	182.68Å 213.91Å 86.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 2.41 48.57 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.57-2.41) 100.0 (48.57-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.176 , 0.209 0.176 , 0.209	Depositor DCC
R_{free} test set	3272 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6304	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, MES, MN

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	0.29	0/6194	0.50	0/8428

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	486	PHE	Peptide

5.2 Too-close contacts

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	6009	0	5777	49	0
2	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	61	0	52	1	0
4	A	28	0	26	0	0
5	A	1	0	0	0	0
6	A	24	0	24	0	0
7	A	153	0	0	1	0
All	All	6304	0	5904	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (50) 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:A:728:LYS:NZ	1:A:730:SER:OG	2.16	0.77
1:A:25:THR:HG23	1:A:27:GLU:H	1.60	0.66
1:A:621:ASP:HA	1:A:676:VAL:HG23	1.81	0.63
1:A:434:ASN:ND2	1:A:434:ASN:O	2.32	0.62
1:A:747:GLN:OE1	1:A:750:LYS:NZ	2.30	0.62
1:A:493:SER:OG	1:A:494:CYS:N	2.34	0.61
1:A:681:GLN:HA	1:A:700:THR:HG22	1.87	0.57
1:A:317:ASN:OD1	1:A:318:TRP:N	2.35	0.56
1:A:276:VAL:CG1	1:A:282:ILE:HB	2.36	0.56
1:A:633:VAL:HG12	1:A:634:THR:O	2.06	0.56
1:A:276:VAL:HG12	1:A:282:ILE:HB	1.89	0.55
1:A:487:SER:OG	1:A:488:PRO:HD3	2.06	0.55
1:A:317:ASN:HB2	1:A:318:TRP:CE3	2.42	0.55
1:A:665:ILE:HG22	1:A:666:GLY:O	2.06	0.55
1:A:45:MET:SD	1:A:222:ASN:HB2	2.47	0.54
1:A:549:LEU:O	1:A:578:SER:HB2	2.09	0.53
1:A:549:LEU:HB3	1:A:580:LEU:HD21	1.92	0.52
1:A:761:LEU:HA	1:A:764:VAL:HG12	1.90	0.52
1:A:659:ARG:HE	1:A:683:LEU:HD12	1.75	0.51
3:C:3:BMA:H62	3:C:5:MAN:H5	1.91	0.51
1:A:656:PRO:HB2	1:A:657:ILE:HD12	1.92	0.51
1:A:41:ASP:OD1	1:A:223:GLN:NE2	2.44	0.50
1:A:291:LYS:O	1:A:291:LYS:HG3	2.12	0.49
1:A:323:GLU:OE2	1:A:350:ARG:NH1	2.46	0.49
1:A:540:GLU:OE1	1:A:542:VAL:HG23	2.14	0.48
1:A:546:ASN:OD1	1:A:548:GLN:HG3	2.14	0.47
1:A:698:LEU:HD23	1:A:710:ALA:HB2	1.97	0.47
1:A:621:ASP:OD1	1:A:654:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:SER:HB2	1:A:656:PRO:HD2	1.98	0.45
1:A:564:GLN:NE2	1:A:668:SER:HB2	2.31	0.45
1:A:142:LYS:NZ	7:A:908:HOH:O	2.49	0.45
1:A:564:GLN:HE22	1:A:668:SER:HB2	1.82	0.45
1:A:430:ILE:HA	1:A:435:LYS:HD3	1.99	0.44
1:A:697:TYR:HE2	1:A:713:ILE:CD1	2.29	0.44
1:A:629:THR:OG1	1:A:648:ASN:HB3	2.18	0.44
1:A:553:ASN:HB2	1:A:573:HIS:HB3	1.99	0.44
1:A:621:ASP:HA	1:A:676:VAL:CG2	2.45	0.43
1:A:411:ASN:O	1:A:412:ARG:HD3	2.19	0.43
1:A:743:GLU:O	1:A:747:GLN:HG2	2.19	0.43
1:A:550:ASN:HB3	1:A:578:SER:HB3	2.00	0.42
1:A:546:ASN:O	1:A:549:LEU:HD12	2.19	0.42
1:A:455:GLN:O	1:A:456:ASN:HB2	2.20	0.42
1:A:714:ALA:O	1:A:715:ASP:C	2.58	0.42
1:A:562:HIS:CG	1:A:563:PRO:HD2	2.55	0.41
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.92	0.41
1:A:321:GLY:HA3	1:A:322:PRO:HA	1.81	0.41
1:A:350:ARG:HG3	1:A:351:VAL:N	2.35	0.41
1:A:653:LEU:HA	1:A:653:LEU:HD23	1.91	0.40
1:A:499:VAL:HG11	1:A:549:LEU:HD21	2.03	0.40
1:A:187:TYR:O	1:A:191:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	741/761 (97%)	709 (96%)	27 (4%)	5 (1%)	22 31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	SER
1	A	472	LEU
1	A	655	SER
1	A	488	PRO
1	A	715	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	639/655 (98%)	625 (98%)	14 (2%)	52 69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	MET
1	A	142	LYS
1	A	264	TYR
1	A	291	LYS
1	A	330	ASP
1	A	473	TYR
1	A	493	SER
1	A	573	HIS
1	A	578	SER
1	A	610	ARG
1	A	668	SER
1	A	680	SER
1	A	723	ARG
1	A	728	LYS

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

Mol	Chain	Res	Type
1	A	434	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

7 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	B	1	1,2	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	B	2	2	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	C	1	1,3	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.22	0	17,19,21	0.85	1 (5%)
3	BMA	C	3	3	11,11,12	0.25	0	15,15,17	0.96	1 (6%)
3	MAN	C	4	3	11,11,12	0.21	0	15,15,17	0.44	0
3	MAN	C	5	3	11,11,12	0.75	1 (9%)	15,15,17	1.50	2 (13%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	MAN	C1-C2	2.10	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5	MAN	C1-C2-C3	5.05	115.87	109.67
3	C	3	BMA	C1-O5-C5	2.91	116.14	112.19
3	C	2	NAG	C1-O5-C5	2.43	115.48	112.19
3	C	5	MAN	C1-O5-C5	2.40	115.45	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

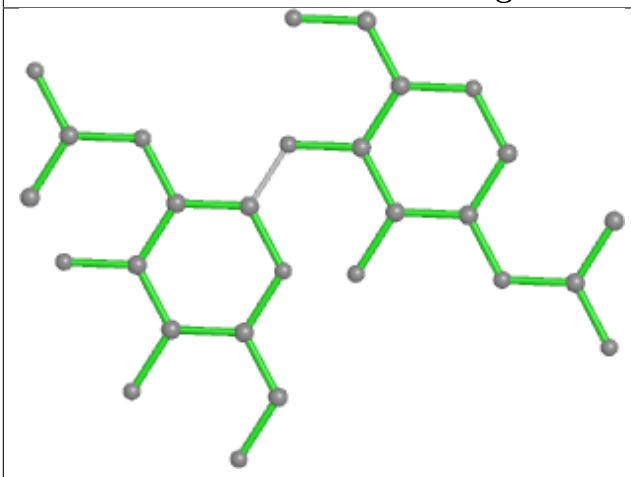
There are no ring outliers.

2 monomers are involved in 1 short contact:

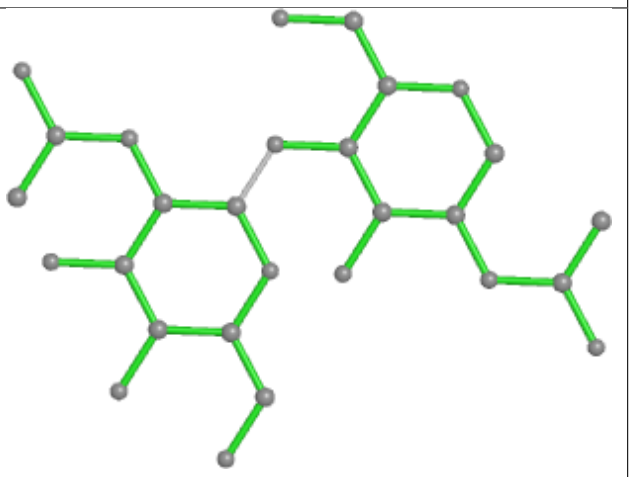
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BMA	1	0
3	C	5	MAN	1	0

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

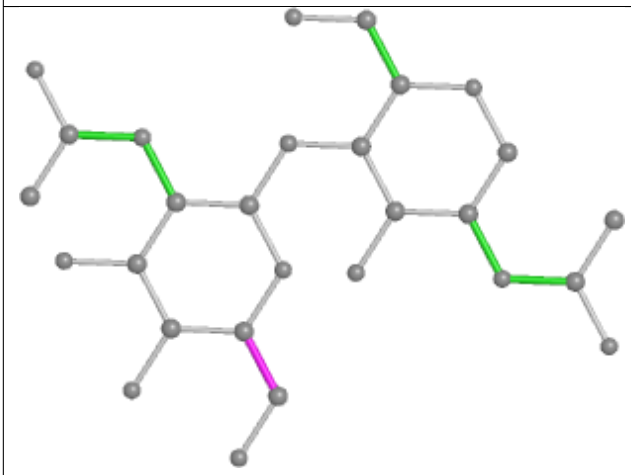
Oligosaccharide Chain B



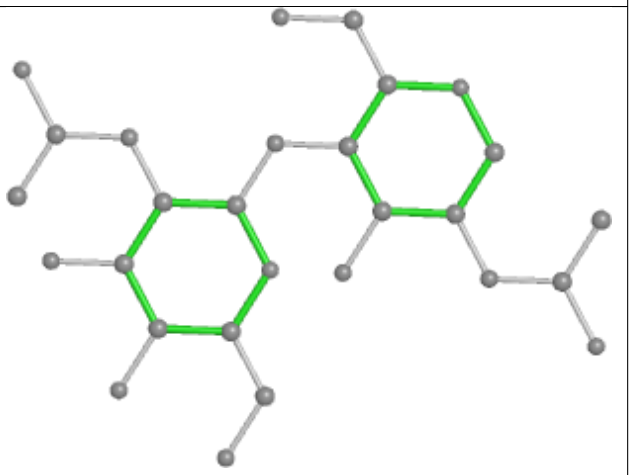
Bond lengths



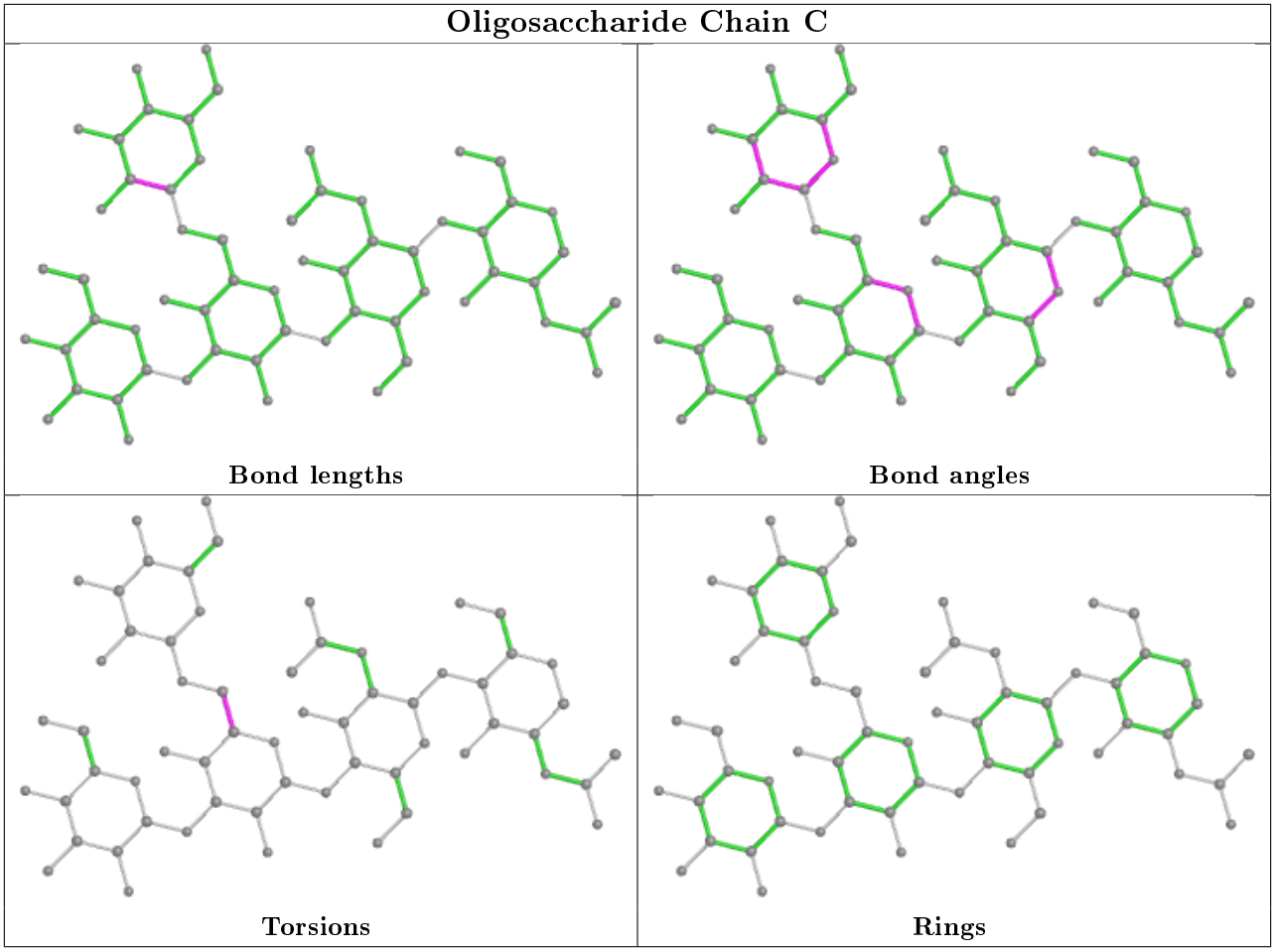
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	NAG	A	809	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	A	803	1	14,14,15	0.23	0	17,19,21	0.49	0
6	MES	A	812	-	12,12,12	2.05	1 (8%)	14,16,16	2.12	5 (35%)
6	MES	A	811	-	12,12,12	2.20	1 (8%)	14,16,16	1.91	5 (35%)

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	A	809	1	-	1/6/23/26	0/1/1/1
4	NAG	A	803	1	-	0/6/23/26	0/1/1/1
6	MES	A	812	-	-	2/6/14/14	0/1/1/1
6	MES	A	811	-	-	2/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	811	MES	C8-S	-7.36	1.67	1.77
6	A	812	MES	C8-S	-6.81	1.67	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	812	MES	O2S-S-C8	4.23	112.01	106.92
6	A	812	MES	C5-N4-C3	3.55	116.83	108.83
6	A	811	MES	C5-N4-C3	3.53	116.77	108.83
6	A	811	MES	O2S-S-C8	2.99	110.52	106.92
6	A	812	MES	C7-N4-C5	2.93	118.72	111.23
6	A	811	MES	C7-N4-C5	2.71	118.17	111.23
6	A	811	MES	C6-C5-N4	-2.53	106.27	110.10
6	A	812	MES	O3S-S-C8	2.47	109.76	105.77
6	A	811	MES	O1S-S-C8	2.33	109.72	106.92
6	A	812	MES	C6-C5-N4	-2.15	106.84	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	811	MES	C8-C7-N4-C5
6	A	812	MES	C8-C7-N4-C5
6	A	812	MES	C8-C7-N4-C3
4	A	809	NAG	C1-C2-N2-C7
6	A	811	MES	C7-C8-S-O2S

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	743/761 (97%)	0.23	38 (5%) 28 26	50, 74, 127, 190	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	704	THR	15.7
1	A	513	TYR	11.4
1	A	508	SER	9.7
1	A	509	LYS	9.0
1	A	511	SER	8.5
1	A	706	GLN	7.6
1	A	703	ALA	6.7
1	A	510	TRP	4.8
1	A	514	LYS	4.2
1	A	705	GLY	4.2
1	A	654	ARG	4.2
1	A	512	LYS	4.1
1	A	702	GLU	4.0
1	A	576	GLU	3.8
1	A	577	GLU	3.5
1	A	655	SER	3.1
1	A	490	VAL	2.9
1	A	507	SER	2.9
1	A	701	GLY	2.8
1	A	765	ARG	2.8
1	A	621	ASP	2.7
1	A	550	ASN	2.6
1	A	258	GLY	2.5
1	A	708	ALA	2.5
1	A	575	GLY	2.5
1	A	578	SER	2.4
1	A	764	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	493	SER	2.3
1	A	766	ASN	2.3
1	A	491	SER	2.3
1	A	574	LEU	2.2
1	A	259	VAL	2.2
1	A	602	VAL	2.2
1	A	397	TRP	2.1
1	A	261	TYR	2.1
1	A	492	LYS	2.1
1	A	262	GLY	2.0
1	A	548	GLN	2.0

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

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

6.3 Carbohydrates (i)

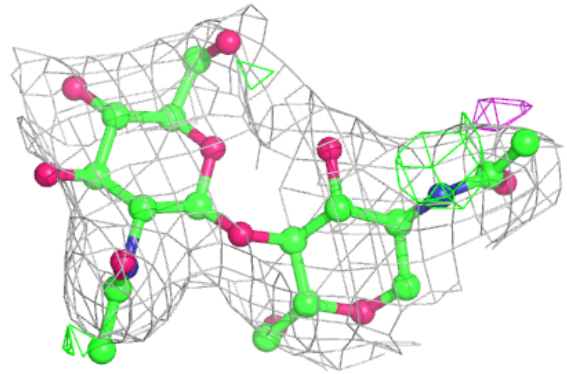
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

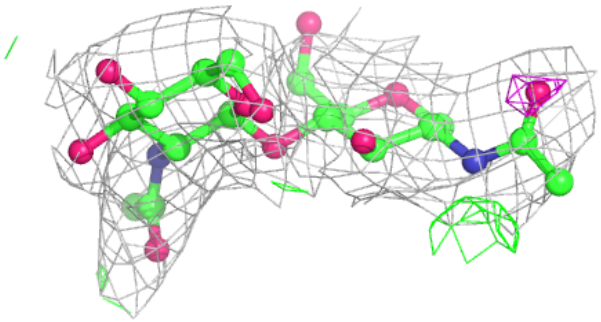
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	4	11/12	0.60	0.22	125,139,146,149	0
3	MAN	C	5	11/12	0.71	0.22	115,123,135,140	0
3	BMA	C	3	11/12	0.84	0.13	106,115,131,143	0
2	NAG	B	2	14/15	0.91	0.12	113,133,142,153	0
2	NAG	B	1	14/15	0.94	0.12	73,105,124,130	0
3	NAG	C	2	14/15	0.95	0.09	68,78,91,102	0
3	NAG	C	1	14/15	0.96	0.13	56,65,77,80	0

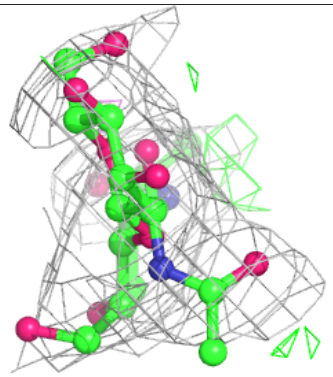
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

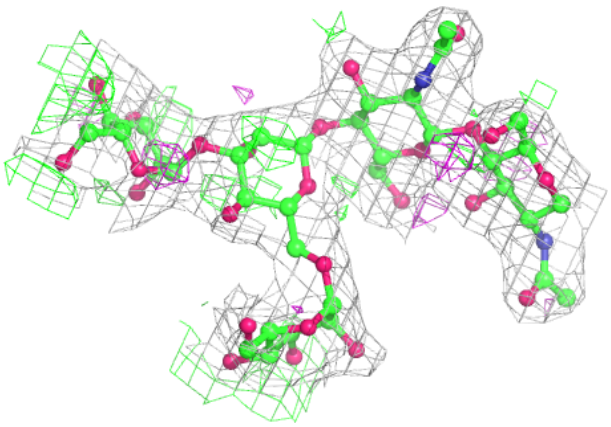


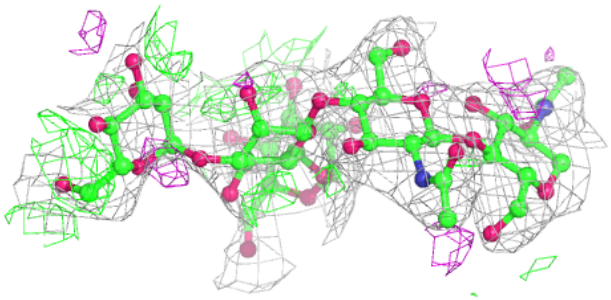


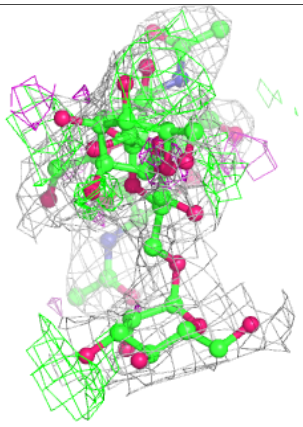


Electron density around Chain C:

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







6.4 Ligands

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	NAG	A	803	14/15	0.61	0.35	97,141,153,157	0
4	NAG	A	809	14/15	0.88	0.17	149,163,169,171	0
6	MES	A	812	12/12	0.93	0.30	79,88,103,112	0
6	MES	A	811	12/12	0.94	0.42	99,103,113,117	0
5	MN	A	810	1/1	0.99	0.16	72,72,72,72	0

6.5 Other polymers

There are no such residues in this entry.