Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 08:36 PM JST

PDB ID	:	8I5Q
Title	:	Crystal structure of TxGH116 D593A acid/base mutant from Thermoanaerobacterium xylanolyticum with laminaribiose
Authors	:	Pengthaisong, S.; Ketudat Cairns, J.R.
Deposited on	:	2023-01-26
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

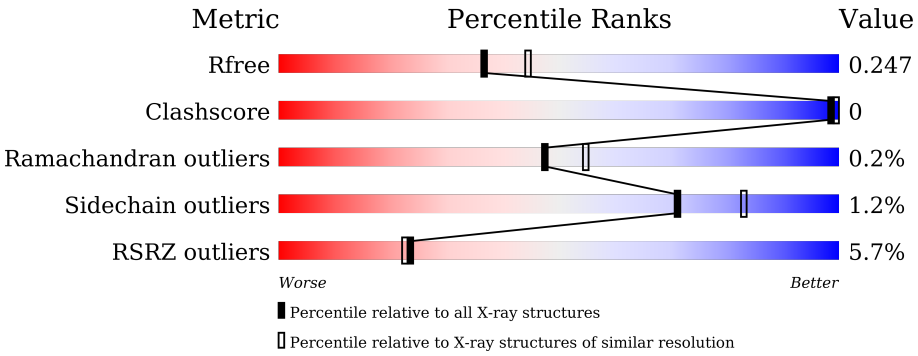
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	799	2% 94%
1	B	799	9% 93%
2	D	2	100%
2	E	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12843 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.

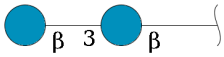
- Molecule 1 is a protein called beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	0	4	0
			6229	4021	1003	1177	28			
1	B	769	Total	C	N	O	S	0	2	0
			6112	3944	978	1163	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	expression tag	UNP F6BL85
A	17	MET	-	expression tag	UNP F6BL85
A	18	ALA	-	expression tag	UNP F6BL85
A	593	ALA	ASP	engineered mutation	UNP F6BL85
A	807	LEU	-	expression tag	UNP F6BL85
A	808	GLU	-	expression tag	UNP F6BL85
A	809	HIS	-	expression tag	UNP F6BL85
A	810	HIS	-	expression tag	UNP F6BL85
A	811	HIS	-	expression tag	UNP F6BL85
A	812	HIS	-	expression tag	UNP F6BL85
A	813	HIS	-	expression tag	UNP F6BL85
A	814	HIS	-	expression tag	UNP F6BL85
B	16	ALA	-	expression tag	UNP F6BL85
B	17	MET	-	expression tag	UNP F6BL85
B	18	ALA	-	expression tag	UNP F6BL85
B	593	ALA	ASP	engineered mutation	UNP F6BL85
B	807	LEU	-	expression tag	UNP F6BL85
B	808	GLU	-	expression tag	UNP F6BL85
B	809	HIS	-	expression tag	UNP F6BL85
B	810	HIS	-	expression tag	UNP F6BL85
B	811	HIS	-	expression tag	UNP F6BL85
B	812	HIS	-	expression tag	UNP F6BL85
B	813	HIS	-	expression tag	UNP F6BL85
B	814	HIS	-	expression tag	UNP F6BL85

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.

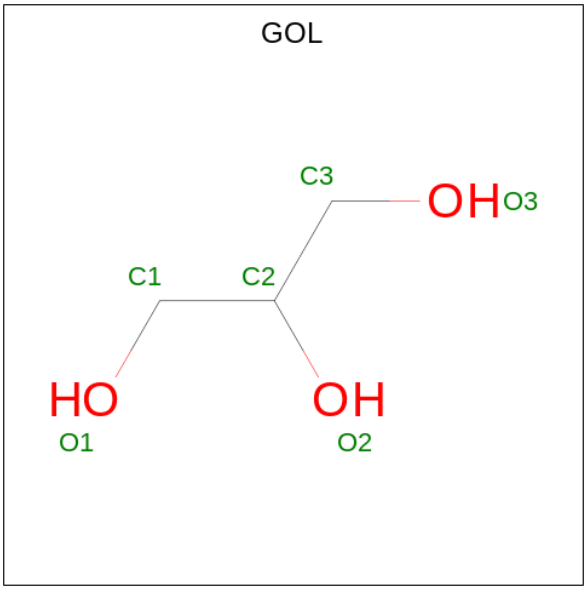


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	2	Total C O 23 12 11	0	0	0
2	E	2	Total C O 23 12 11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

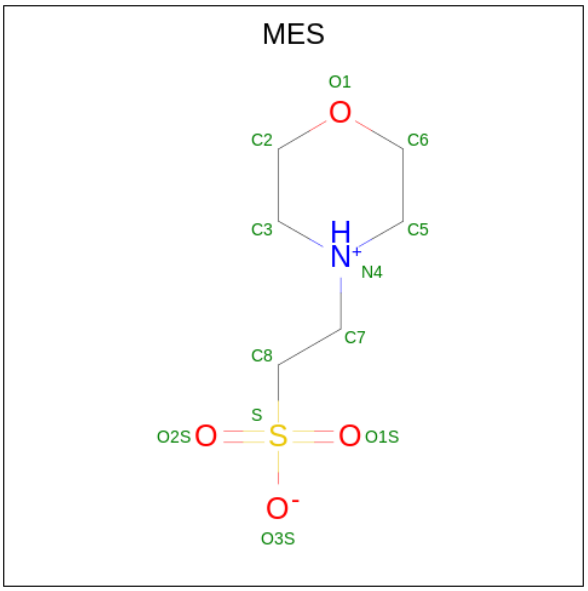
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 6 is water.

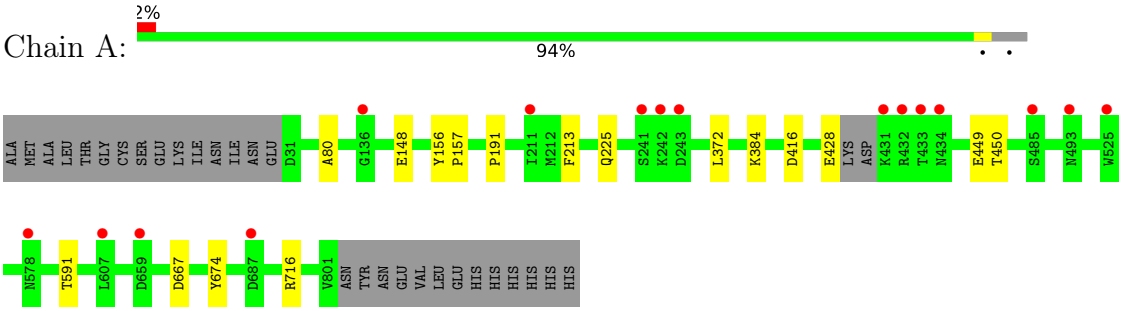
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	273	Total	O	0	0
			273	273		
6	B	163	Total	O	0	0
			163	163		

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.

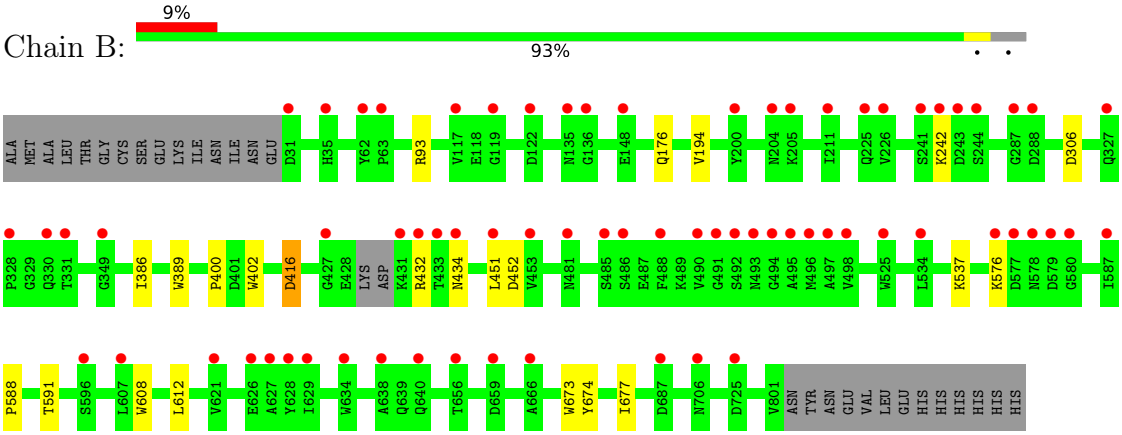
• Molecule 1: beta-glucosidase

Chain A:



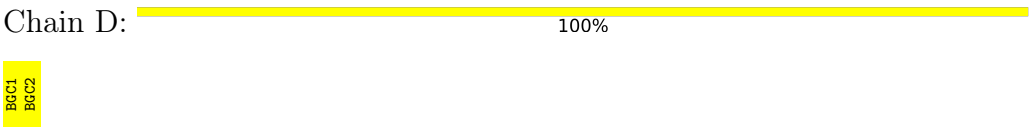
• Molecule 1: beta-glucosidase

Chain B:



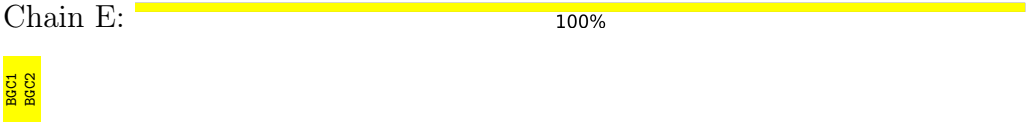
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain D:



• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.90Å 100.62Å 173.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 27.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.20) 99.8 (27.38-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.241 0.199 , 0.247	Depositor DCC
R_{free} test set	4292 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12843	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: MES, GOL, BGC, CA

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	0.48	0/6410	0.64	0/8695
1	B	0.49	0/6288	0.62	0/8548
All	All	0.49	0/12698	0.63	0/17243

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

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	6229	0	5930	4	0
1	B	6112	0	5722	8	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
5	A	12	0	13	0	0
6	A	273	0	0	1	0
6	B	163	0	0	0	0
All	All	12843	0	11715	12	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 0.

All (12) 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:93:ARG:NH2	1:B:416:ASP:OD2	2.32	0.60
1:B:432:ARG:NH1	1:B:434:ASN:O	2.46	0.48
1:A:80:ALA:HB1	1:A:191:PRO:HB3	1.97	0.46
1:B:608:TRP:CE2	1:B:612:LEU:HD11	2.52	0.45
1:B:537:LYS:NZ	1:B:591:THR:OG1	2.50	0.44
1:A:156:TYR:CD1	1:A:157:PRO:HA	2.54	0.43
1:B:400:PRO:HB2	1:B:402:TRP:CD1	2.56	0.41
1:B:386:ILE:HA	1:B:389[A]:TRP:CD1	2.55	0.41
1:B:673:TRP:NE1	1:B:677:ILE:HD11	2.36	0.41
1:A:449:GLU:O	1:A:450:THR:C	2.59	0.41
1:A:225:GLN:NE2	6:A:1103:HOH:O	2.54	0.40
1:B:176:GLN:HA	1:B:194:VAL:O	2.21	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	769/799 (96%)	738 (96%)	30 (4%)	1 (0%)	51 60
1	B	767/799 (96%)	730 (95%)	35 (5%)	2 (0%)	41 46
All	All	1536/1598 (96%)	1468 (96%)	65 (4%)	3 (0%)	47 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	THR
1	B	588	PRO

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Mol	Chain	Res	Type
1	B	242	LYS

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	651/684 (95%)	642 (99%)	9 (1%)	67 80
1	B	625/684 (91%)	619 (99%)	6 (1%)	76 86
All	All	1276/1368 (93%)	1261 (99%)	15 (1%)	71 83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLU
1	A	213	PHE
1	A	372	LEU
1	A	384	LYS
1	A	416	ASP
1	A	428	GLU
1	A	667	ASP
1	A	674	TYR
1	A	716	ARG
1	B	306	ASP
1	B	416	ASP
1	B	451	LEU
1	B	452	ASP
1	B	576	LYS
1	B	674	TYR

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	225	GLN

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)

4 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	BGC	D	1	2	12,12,12	0.76	0	17,17,17	1.88	5 (29%)
2	BGC	D	2	2	11,11,12	0.56	0	15,15,17	1.82	2 (13%)
2	BGC	E	1	2	12,12,12	0.56	0	17,17,17	1.29	3 (17%)
2	BGC	E	2	2	11,11,12	0.55	0	15,15,17	2.24	3 (20%)

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	BGC	D	1	2	-	1/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	BGC	C1-C2-C3	5.77	116.76	109.67
2	E	2	BGC	C1-O5-C5	5.23	119.28	112.19
2	D	2	BGC	C1-C2-C3	4.77	115.53	109.67
2	D	2	BGC	C1-O5-C5	4.48	118.26	112.19
2	D	1	BGC	C1-C2-C3	-3.49	103.08	110.31
2	D	1	BGC	O3-C3-C2	3.23	117.82	110.35
2	D	1	BGC	O3-C3-C4	3.02	117.33	110.35
2	E	2	BGC	O5-C1-C2	3.00	115.40	110.77
2	D	1	BGC	O2-C2-C1	2.97	116.05	109.16
2	D	1	BGC	C1-O5-C5	2.36	118.12	113.66
2	E	1	BGC	C3-C4-C5	-2.15	106.40	110.24
2	E	1	BGC	O3-C3-C2	2.10	115.20	110.35
2	E	1	BGC	C4-C3-C2	-2.06	107.23	110.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

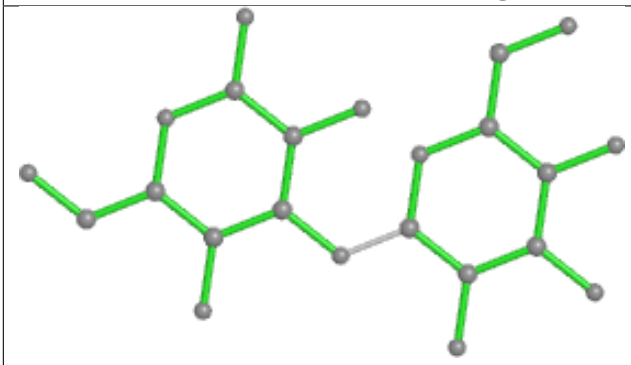
Mol	Chain	Res	Type	Atoms
2	D	1	BGC	O5-C5-C6-O6

There are no ring outliers.

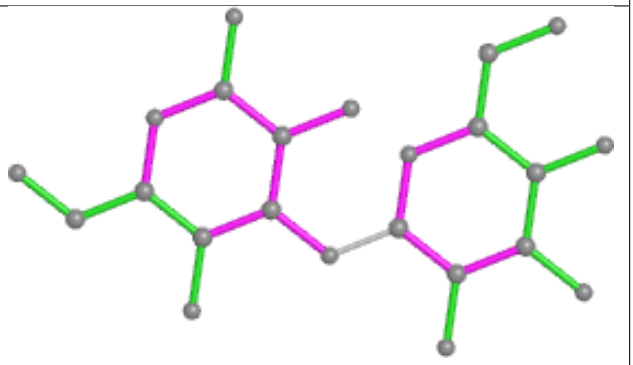
No monomer is involved in short contacts.

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

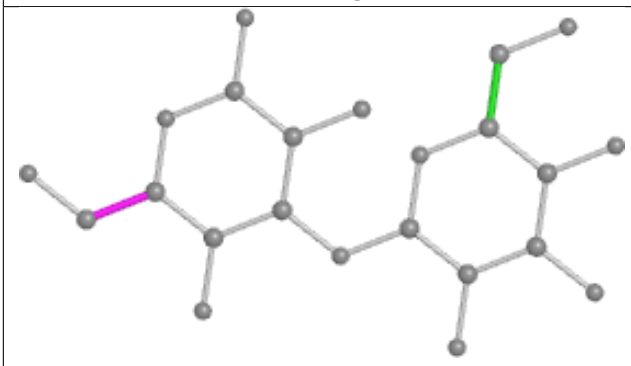
Oligosaccharide Chain D



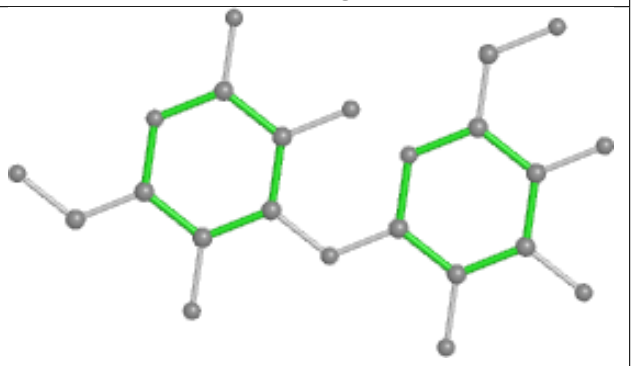
Bond lengths



Bond angles

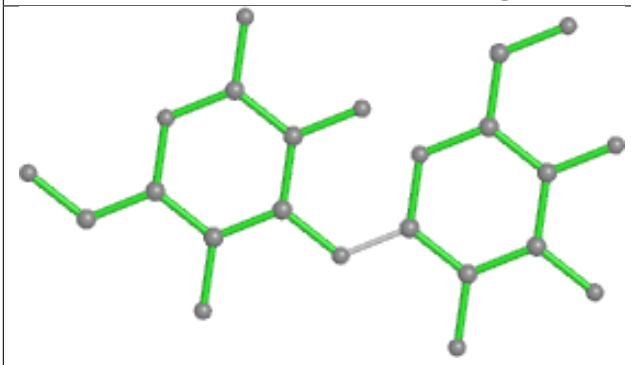


Torsions

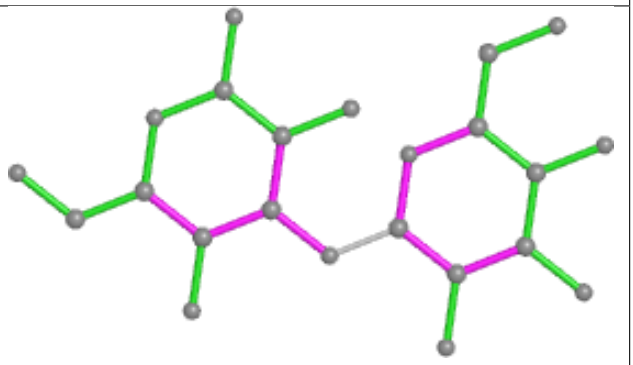


Rings

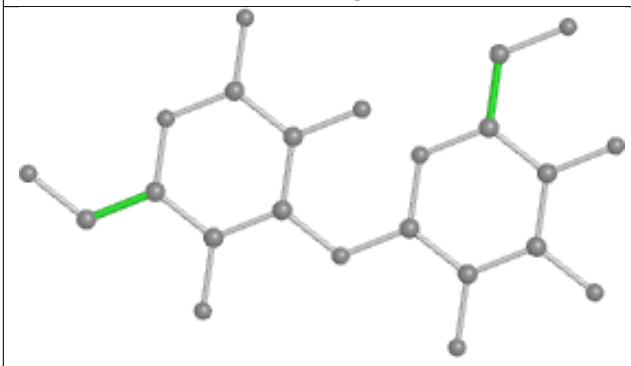
Oligosaccharide Chain E



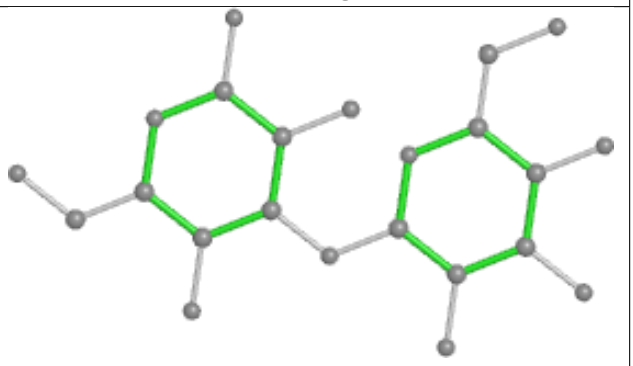
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	MES	A	1003	-	12,12,12	2.39	1 (8%)	14,16,16	1.31	1 (7%)
4	GOL	A	1002	-	5,5,5	0.42	0	5,5,5	0.66	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	MES	A	1003	-	-	1/6/14/14	0/1/1/1
4	GOL	A	1002	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MES	C8-S	-8.02	1.66	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	MES	O1S-S-C8	3.17	110.74	106.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MES	C7-C8-S-O2S

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

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	769/799 (96%)	-0.24	16 (2%) 63 61	15, 27, 48, 93	1 (0%)
1	B	769/799 (96%)	0.45	71 (9%) 9 7	19, 40, 76, 98	1 (0%)
All	All	1538/1598 (96%)	0.11	87 (5%) 23 22	15, 32, 68, 98	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	VAL	5.9
1	A	243	ASP	5.9
1	B	491	GLY	5.8
1	B	242	LYS	5.6
1	B	493	ASN	5.5
1	B	492	SER	5.4
1	B	433	THR	5.1
1	B	241	SER	5.0
1	B	119	GLY	4.8
1	B	225	GLN	4.7
1	B	204	ASN	4.6
1	B	495	ALA	4.5
1	B	496	MET	4.4
1	B	494	GLY	4.4
1	B	629	ILE	4.4
1	B	243	ASP	4.3
1	A	241	SER	4.2
1	A	242	LYS	4.0
1	B	525	TRP	4.0
1	A	433	THR	4.0
1	B	244	SER	3.9
1	B	628	TYR	3.7
1	B	485	SER	3.7
1	B	122	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	656	THR	3.6
1	B	226	VAL	3.6
1	B	659	ASP	3.6
1	A	485	SER	3.5
1	B	576	LYS	3.5
1	B	135	ASN	3.4
1	B	63	PRO	3.4
1	B	577	ASP	3.4
1	B	431	LYS	3.3
1	B	330	GLN	3.2
1	B	498	VAL	3.1
1	B	607	LEU	3.1
1	B	287	GLY	3.0
1	B	497	ALA	3.0
1	B	434	ASN	3.0
1	B	488	PHE	2.9
1	B	481	ASN	2.8
1	B	578	ASN	2.8
1	B	587	ILE	2.8
1	B	627	ALA	2.8
1	B	31	ASP	2.8
1	B	62	TYR	2.8
1	B	666	ALA	2.7
1	B	331	THR	2.7
1	B	621	VAL	2.7
1	B	327	GLN	2.6
1	A	659	ASP	2.6
1	B	432	ARG	2.6
1	B	687	ASP	2.6
1	B	200	TYR	2.6
1	B	706	ASN	2.6
1	B	136	GLY	2.6
1	B	486	SER	2.5
1	B	211	ILE	2.5
1	A	525	TRP	2.5
1	A	493	ASN	2.5
1	B	596	SER	2.5
1	B	534	LEU	2.4
1	B	427	GLY	2.4
1	B	117	VAL	2.4
1	B	328	PRO	2.4
1	B	35	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	580	GLY	2.3
1	B	634	TRP	2.3
1	A	434	ASN	2.3
1	B	148	GLU	2.3
1	A	687	ASP	2.2
1	B	349	GLY	2.2
1	B	640	GLN	2.2
1	A	432	ARG	2.2
1	B	451	LEU	2.2
1	B	638	ALA	2.2
1	A	431	LYS	2.1
1	A	607	LEU	2.1
1	A	136	GLY	2.1
1	B	288	ASP	2.1
1	B	579	ASP	2.0
1	B	626	GLU	2.0
1	A	578	ASN	2.0
1	B	725	ASP	2.0
1	B	205	LYS	2.0
1	B	453	VAL	2.0
1	A	211	ILE	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)

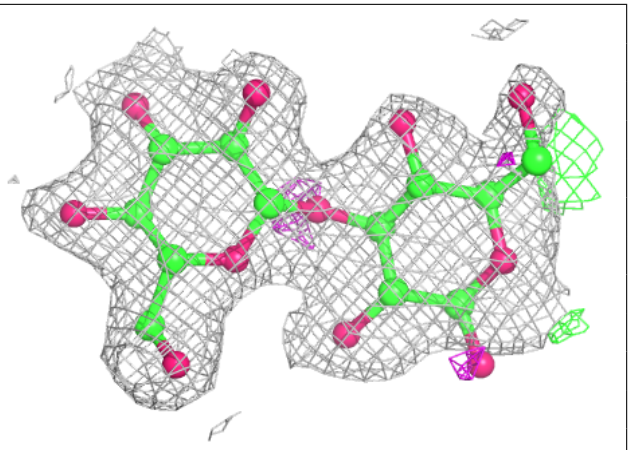
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

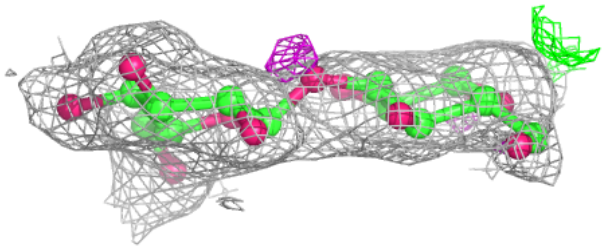
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	E	1	12/12	0.82	0.19	62,71,76,77	0
2	BGC	E	2	11/12	0.85	0.17	42,47,52,54	0
2	BGC	D	1	12/12	0.87	0.20	42,45,49,57	0
2	BGC	D	2	11/12	0.93	0.12	31,34,37,38	0

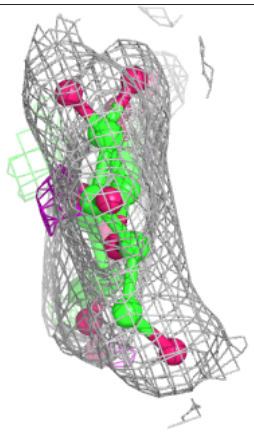
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

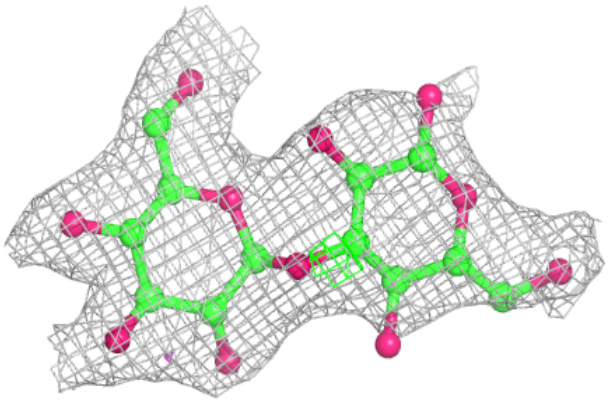


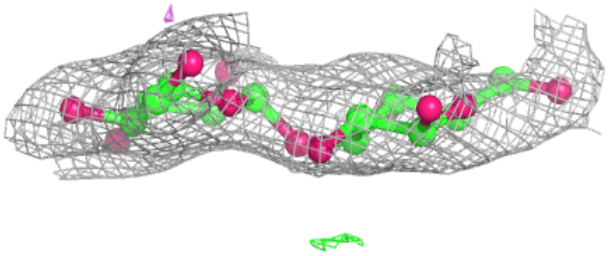


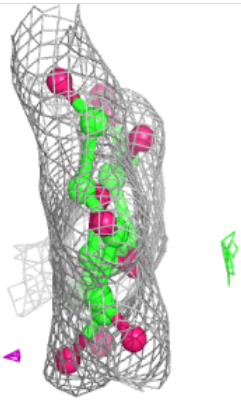


Electron density around Chain E:

$2mF_o$-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
3	CA	B	901	1/1	0.89	0.08	75,75,75,75	0
4	GOL	A	1002	6/6	0.90	0.12	37,41,44,47	0
3	CA	A	1001	1/1	0.96	0.08	43,43,43,43	0
5	MES	A	1003	12/12	0.98	0.09	27,29,32,32	0

6.5 Other polymers

There are no such residues in this entry.