Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 08:37 PM JST

PDB ID	:	8I5P
Title	:	Crystal structure of TxGH116 D593A acid/base mutant from Thermoanaerobacterium xylanolyticum with cellobiose
Authors	:	Pengthaisong, S.; Ketudat Cairns, J.R.
Deposited on	:	2023-01-26
Resolution	:	2.35 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:

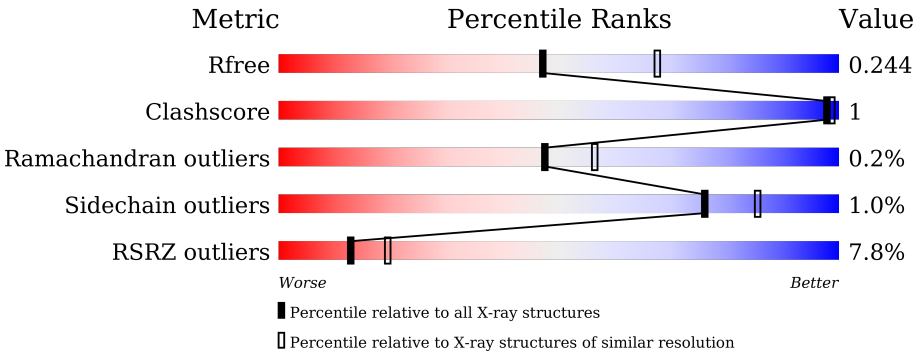
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	4% 93%
1	B	799	11% 93%
2	D	2	50% 50%
2	E	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12615 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
			6192	3997	993	1174	28			
1	B	769	Total	C	N	O	S	0	3	0
			6054	3915	965	1146	28			

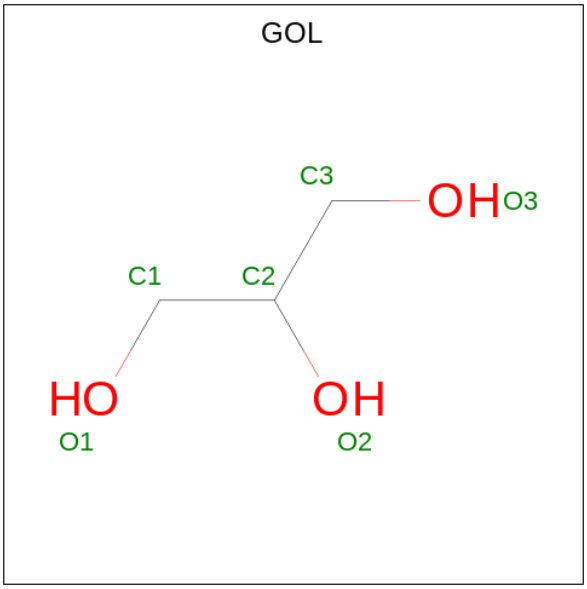
There are 24 discrepancies between the modelled and reference sequences:

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-(1-4)-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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

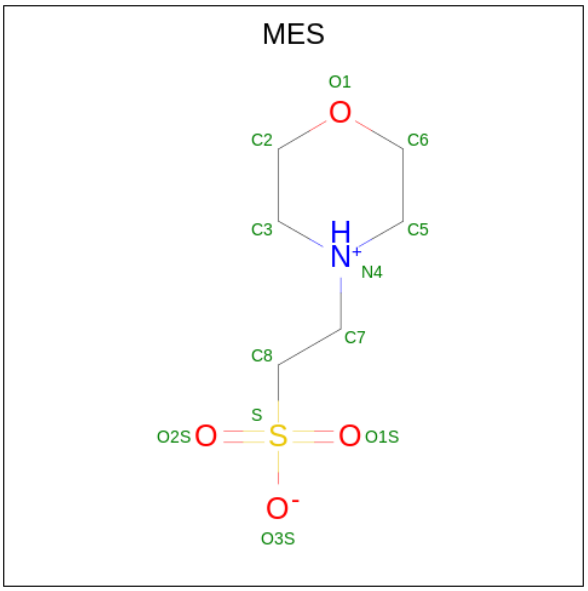


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

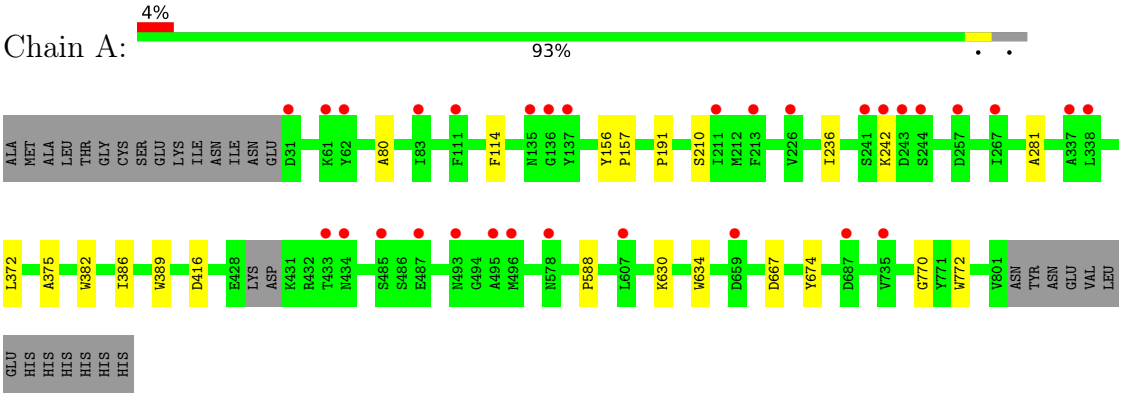
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	114	Total	O	0	0
			114	114		

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.

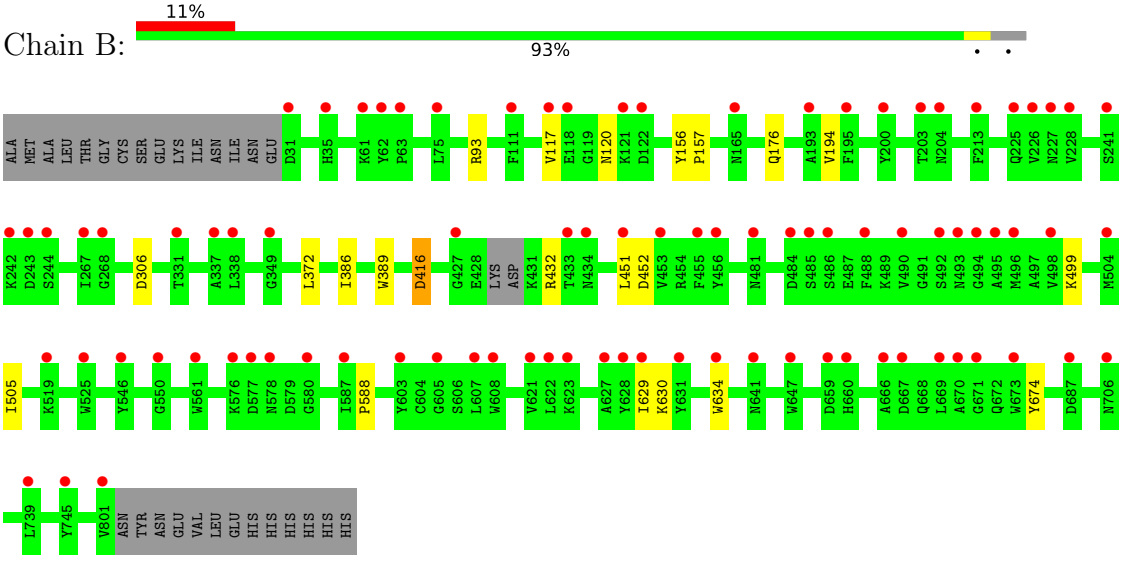
• Molecule 1: beta-glucosidase

Chain A:



• Molecule 1: beta-glucosidase

Chain B:



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

Chain D:

• Molecule 2: beta-D-glucopyranose-(1-4)-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	98.07Å 100.50Å 173.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 29.27 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.35) 100.0 (29.27-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.190 , 0.241 0.196 , 0.244	Depositor DCC
R_{free} test set	3529 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12615	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 2.85% 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: GOL, MES, CA, BGC

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	0.42	0/6373	0.62	0/8655
1	B	0.43	0/6233	0.60	0/8488
All	All	0.42	0/12606	0.61	0/17143

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	6192	0	5845	8	0
1	B	6054	0	5600	9	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
3	A	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	13	0	0
6	A	189	0	0	0	0
6	B	114	0	0	0	0
All	All	12615	0	11508	17	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 1.

All (17) 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:451:LEU:HD22	1:B:505:ILE:HG21	1.78	0.65
1:A:630:LYS:HE2	1:A:634:TRP:CZ2	2.35	0.61
1:B:93:ARG:NH2	1:B:416:ASP:OD2	2.38	0.56
1:B:386:ILE:HA	1:B:389[A]:TRP:CD1	2.49	0.48
1:B:630:LYS:HE2	1:B:634:TRP:CZ2	2.48	0.48
1:A:80:ALA:HB1	1:A:191:PRO:HB3	1.96	0.47
1:B:117:VAL:HB	1:B:120:ASN:OD1	2.16	0.45
1:A:156:TYR:CD1	1:A:157:PRO:HA	2.53	0.44
1:A:386:ILE:HA	1:A:389[A]:TRP:CD1	2.53	0.44
1:B:156:TYR:CD1	1:B:157:PRO:HA	2.53	0.43
1:A:236:ILE:HG12	1:A:281:ALA:HB2	2.00	0.43
1:B:389[B]:TRP:O	1:B:389[B]:TRP:CD1	2.71	0.43
1:A:114:PHE:HB3	1:A:210:SER:HB2	2.02	0.41
1:A:770:GLY:HA2	1:A:772:TRP:CZ3	2.56	0.41
1:B:389[B]:TRP:CD1	1:B:389[B]:TRP:C	2.95	0.40
1:B:176:GLN:HA	1:B:194:VAL:O	2.21	0.40
1:A:375:ALA:HA	1:A:382:TRP:CH2	2.56	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%)	741 (96%)	26 (3%)	2 (0%)	41	47
1	B	768/799 (96%)	739 (96%)	28 (4%)	1 (0%)	51	63
All	All	1537/1598 (96%)	1480 (96%)	54 (4%)	3 (0%)	47	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	588	PRO
1	A	242	LYS
1	A	588	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	642/684 (94%)	638 (99%)	4 (1%)	86 93
1	B	608/684 (89%)	600 (99%)	8 (1%)	69 80
All	All	1250/1368 (91%)	1238 (99%)	12 (1%)	76 85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LEU
1	A	416	ASP
1	A	667	ASP
1	A	674	TYR
1	B	306	ASP
1	B	372	LEU
1	B	416	ASP
1	B	432	ARG
1	B	452	ASP
1	B	499	LYS
1	B	629	ILE
1	B	674	TYR

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

5.3.3 RNA

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	0.48	0	17,17,17	0.85	0
2	BGC	D	2	2	11,11,12	0.35	0	15,15,17	1.23	1 (6%)
2	BGC	E	1	2	12,12,12	0.50	0	17,17,17	0.92	0
2	BGC	E	2	2	11,11,12	0.35	0	15,15,17	1.36	1 (6%)

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	-	0/2/22/22	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	BGC	C1-C2-C3	3.39	113.83	109.67
2	D	2	BGC	C1-C2-C3	3.37	113.81	109.67

There are no chirality outliers.

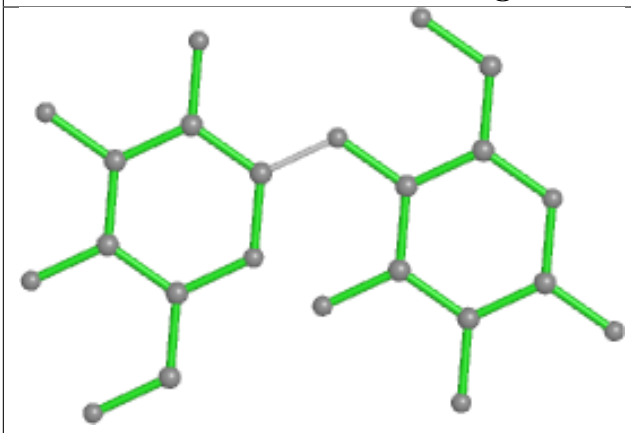
There are no torsion outliers.

There are no ring outliers.

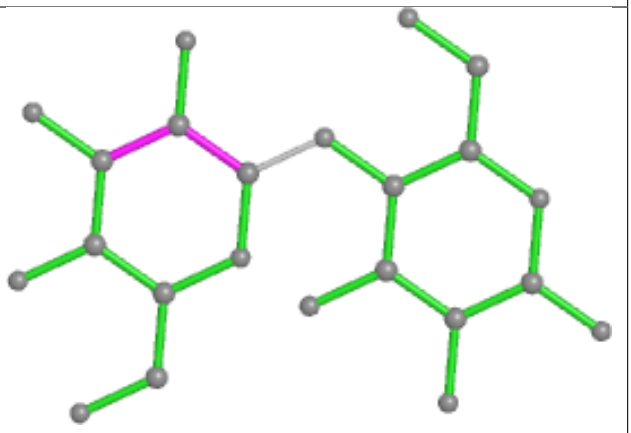
No monomer is involved in short contacts.

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

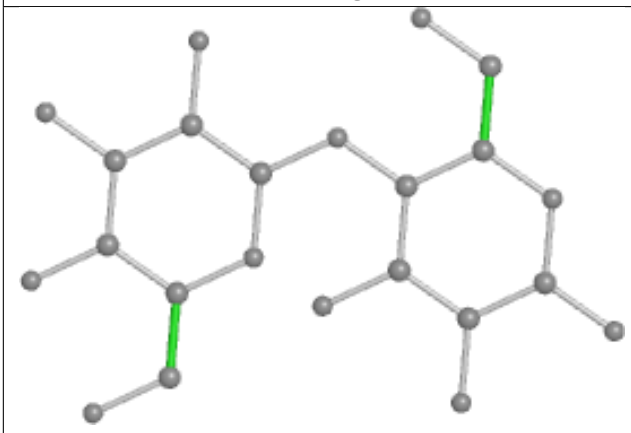
Oligosaccharide Chain D



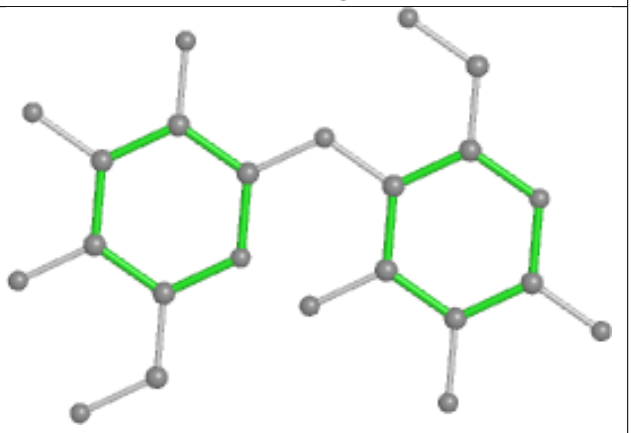
Bond lengths



Bond angles

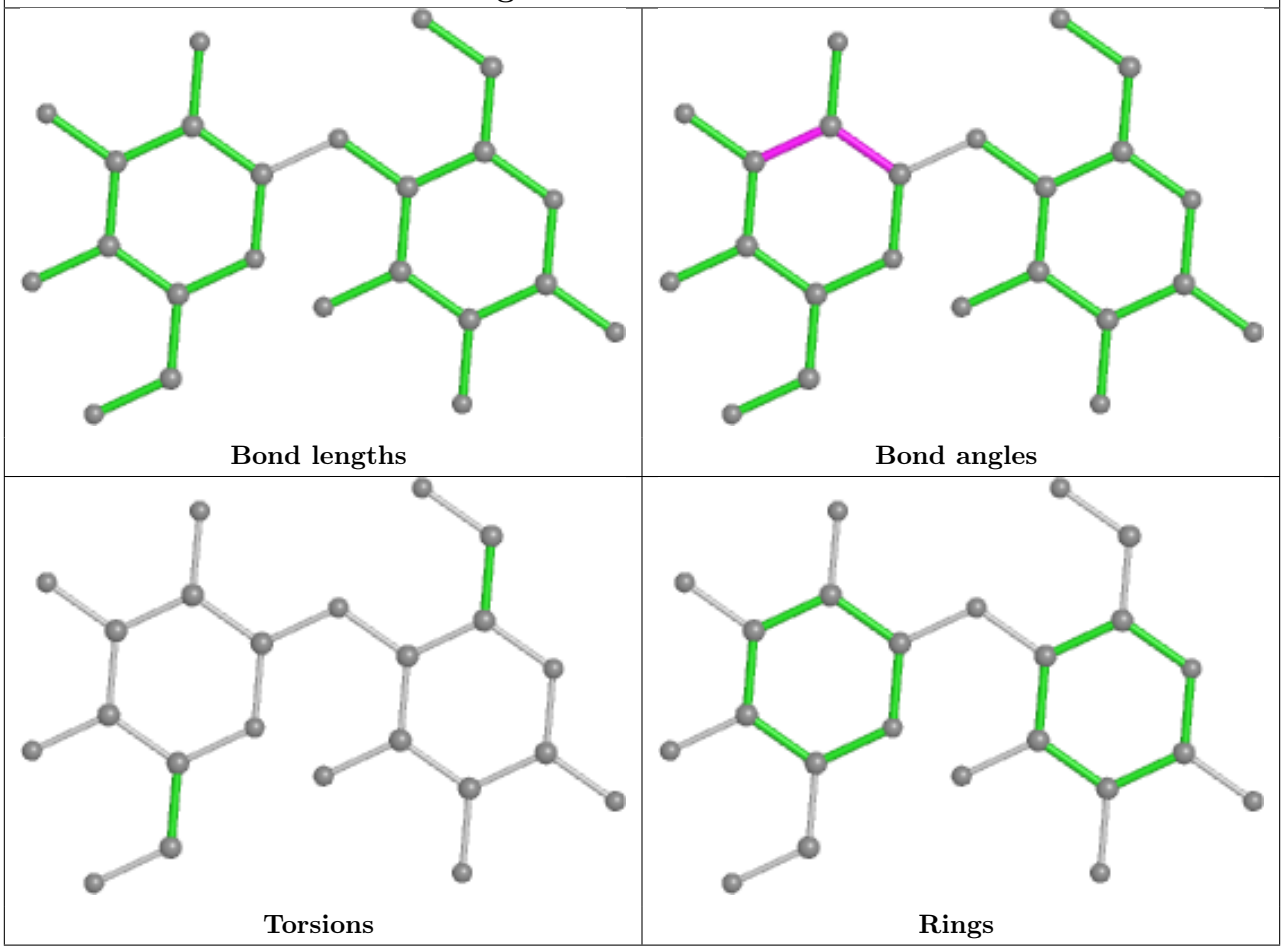


Torsions



Rings

Oligosaccharide Chain E



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	2.37	1 (8%)	14,16,16	1.73	2 (14%)
3	GOL	A	1001	-	5,5,5	0.36	0	5,5,5	0.44	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	-	-	5/6/14/14	0/1/1/1
3	GOL	A	1001	-	-	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	-7.83	1.66	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	MES	O1S-S-C8	5.05	113.00	106.92
5	A	1003	MES	O2S-S-C8	2.63	110.08	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MES	C7-C8-S-O3S
5	A	1003	MES	C8-C7-N4-C5
5	A	1003	MES	C7-C8-S-O1S
5	A	1003	MES	C7-C8-S-O2S
5	A	1003	MES	C8-C7-N4-C3

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%)	0.03	31 (4%) 38 51	22, 34, 55, 98	0
1	B	769/799 (96%)	0.59	89 (11%) 4 7	24, 47, 82, 105	0
All	All	1538/1598 (96%)	0.31	120 (7%) 13 19	22, 39, 74, 105	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	5.9
1	B	493	ASN	5.3
1	B	226	VAL	5.0
1	B	495	ALA	4.8
1	B	627	ALA	4.8
1	A	485	SER	4.7
1	B	242	LYS	4.7
1	B	122	ASP	4.6
1	B	494	GLY	4.4
1	B	492	SER	4.4
1	B	587	ILE	4.3
1	B	204	ASN	4.2
1	B	666	ALA	4.1
1	B	607	LEU	4.1
1	A	243	ASP	4.0
1	B	629	ILE	3.9
1	B	490	VAL	3.9
1	A	242	LYS	3.9
1	B	453	VAL	3.8
1	B	225	GLN	3.7
1	B	576	LYS	3.6
1	B	628	TYR	3.6
1	A	241	SER	3.5
1	B	117	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	241	SER	3.5
1	B	525	TRP	3.5
1	A	659	ASP	3.5
1	B	121	LYS	3.4
1	B	603	TYR	3.4
1	A	607	LEU	3.4
1	B	433	THR	3.3
1	B	669	LEU	3.3
1	B	427	GLY	3.2
1	B	62	TYR	3.2
1	B	621	VAL	3.2
1	A	135	ASN	3.2
1	B	488	PHE	3.1
1	A	137	TYR	3.1
1	B	228	VAL	3.1
1	A	136	GLY	3.1
1	B	496	MET	3.0
1	B	578	ASN	3.0
1	B	485	SER	3.0
1	A	433	THR	3.0
1	B	434	ASN	3.0
1	B	670	ALA	2.9
1	B	35	HIS	2.9
1	B	244[A]	SER	2.8
1	B	623	LYS	2.8
1	B	577	ASP	2.8
1	B	267	ILE	2.7
1	B	622	LEU	2.7
1	B	200	TYR	2.7
1	B	745	TYR	2.7
1	B	634	TRP	2.7
1	A	226	VAL	2.6
1	B	349	GLY	2.6
1	B	687	ASP	2.6
1	B	331	THR	2.6
1	B	195	PHE	2.6
1	B	118	GLU	2.6
1	B	647	TRP	2.5
1	B	63	PRO	2.5
1	A	267	ILE	2.5
1	B	213	PHE	2.5
1	B	504	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	546	TYR	2.5
1	A	61	LYS	2.5
1	A	111	PHE	2.5
1	B	227	ASN	2.5
1	B	31	ASP	2.5
1	B	706	ASN	2.4
1	A	735	VAL	2.4
1	B	561	TRP	2.4
1	B	605	GLY	2.4
1	A	578	ASN	2.4
1	A	434	ASN	2.4
1	B	673	TRP	2.4
1	B	193	ALA	2.3
1	B	451	LEU	2.3
1	B	111	PHE	2.3
1	B	455	PHE	2.3
1	A	62	TYR	2.3
1	B	498	VAL	2.3
1	B	75	LEU	2.3
1	B	481	ASN	2.3
1	A	244	SER	2.3
1	B	660	HIS	2.3
1	A	495	ALA	2.3
1	B	203	THR	2.3
1	B	338	LEU	2.3
1	B	801	VAL	2.2
1	B	456	TYR	2.2
1	B	667	ASP	2.2
1	A	213	PHE	2.2
1	A	257	ASP	2.2
1	A	687	ASP	2.2
1	A	338	LEU	2.2
1	A	337	ALA	2.2
1	B	671	GLY	2.2
1	A	83	ILE	2.1
1	B	739	LEU	2.1
1	B	165	ASN	2.1
1	B	659	ASP	2.1
1	A	211	ILE	2.1
1	A	493	ASN	2.1
1	B	268	GLY	2.1
1	B	580	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	519	LYS	2.1
1	B	608	TRP	2.1
1	B	631	TYR	2.1
1	A	31	ASP	2.1
1	B	484	ASP	2.1
1	A	496	MET	2.1
1	B	550	GLY	2.1
1	A	487	GLU	2.0
1	B	641	ASN	2.0
1	B	337	ALA	2.0
1	B	486	SER	2.0
1	B	61	LYS	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)

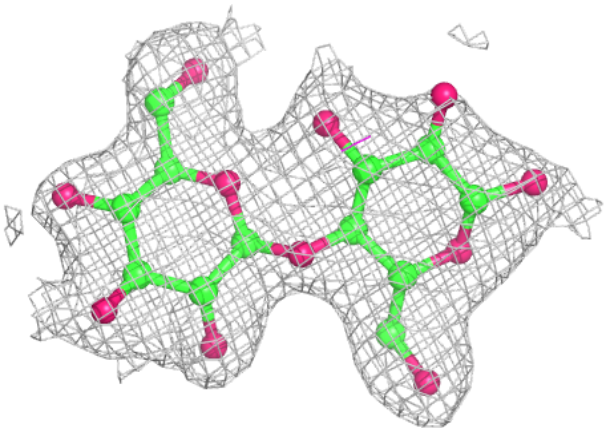
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

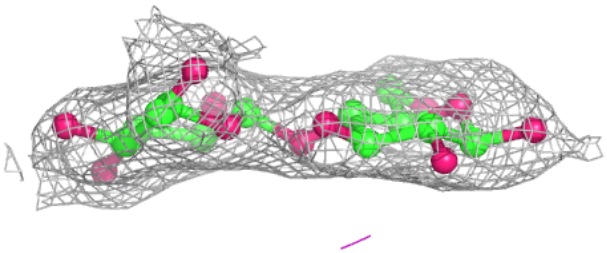
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	E	1	12/12	0.90	0.13	51,56,58,59	0
2	BGC	D	1	12/12	0.93	0.10	38,39,46,46	0
2	BGC	E	2	11/12	0.93	0.13	41,44,47,48	0
2	BGC	D	2	11/12	0.96	0.13	33,34,35,36	0

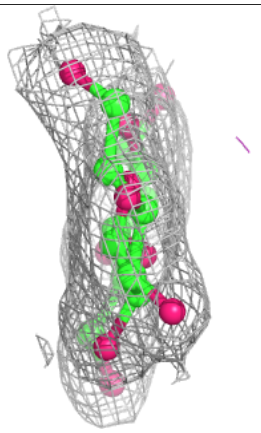
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

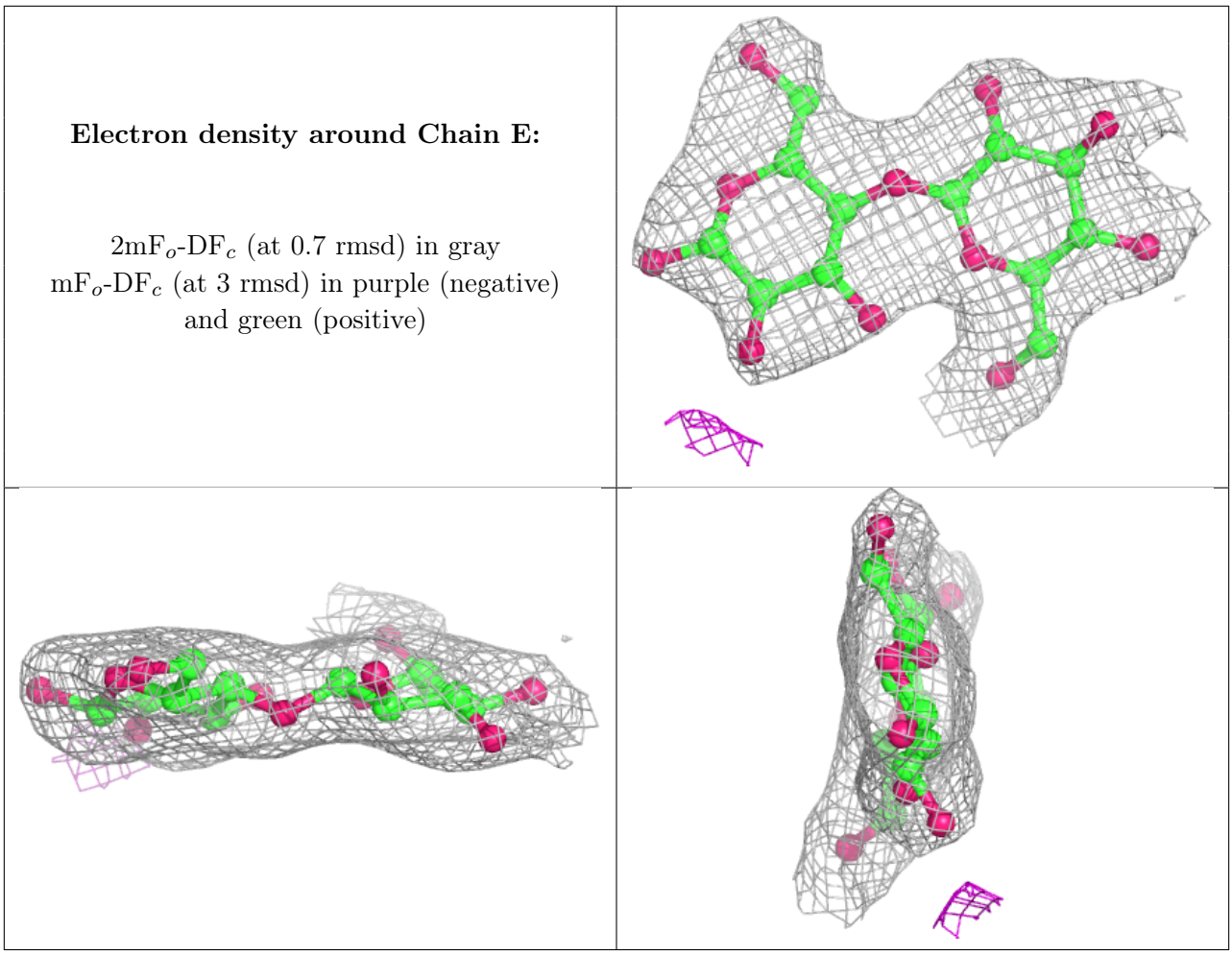






Electron density around Chain E:

$2mF_o$-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
4	CA	B	901	1/1	0.83	0.06	75,75,75,75	0
3	GOL	A	1001	6/6	0.88	0.16	44,48,51,56	0
4	CA	A	1002	1/1	0.97	0.08	50,50,50,50	0
5	MES	A	1003	12/12	0.97	0.14	35,37,38,39	0

6.5 Other polymers

There are no such residues in this entry.