



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 10:58 AM EDT

PDB ID : 4QLL  
Title : Crystal structure of rice BGlu1 E176Q/Y341A/Q187A mutant complexed with cellotetraose  
Authors : Pengthaisong, S.; Ketudat Cairns, J.R.  
Deposited on : 2014-06-12  
Resolution : 1.85 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

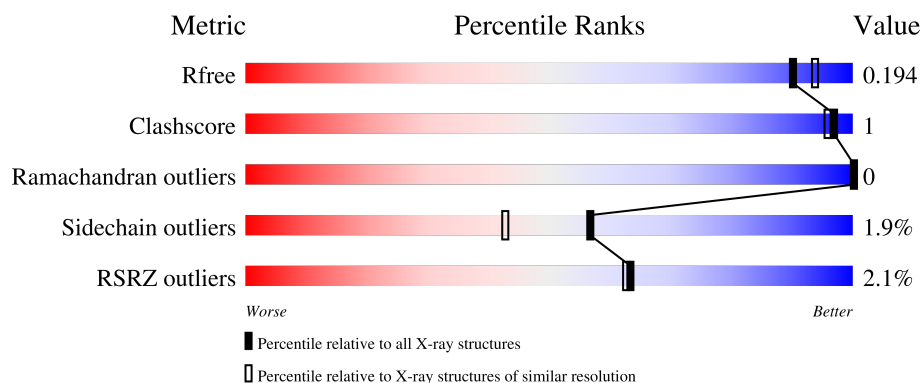
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	481	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	B	481	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
2	D	4	<div> <div>50%</div> <div>25%</div> <div>25%</div> </div>
2	E	4	<div> <div>100%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8605 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 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3798	2442	655	688	13			
1	B	472	Total	C	N	O	S	0	0	0
			3798	2442	655	688	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	expression tag	UNP Q75I93
A	-3	MET	-	expression tag	UNP Q75I93
A	-2	ALA	-	expression tag	UNP Q75I93
A	-1	ASP	-	expression tag	UNP Q75I93
A	0	VAL	-	expression tag	UNP Q75I93
A	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
A	176	GLN	GLU	engineered mutation	UNP Q75I93
A	187	ALA	GLN	engineered mutation	UNP Q75I93
A	341	ALA	TYR	expression tag	UNP Q75I93
B	-4	ALA	-	expression tag	UNP Q75I93
B	-3	MET	-	expression tag	UNP Q75I93
B	-2	ALA	-	expression tag	UNP Q75I93
B	-1	ASP	-	expression tag	UNP Q75I93
B	0	VAL	-	expression tag	UNP Q75I93
B	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
B	176	GLN	GLU	engineered mutation	UNP Q75I93
B	187	ALA	GLN	engineered mutation	UNP Q75I93
B	341	ALA	TYR	engineered mutation	UNP Q75I93

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

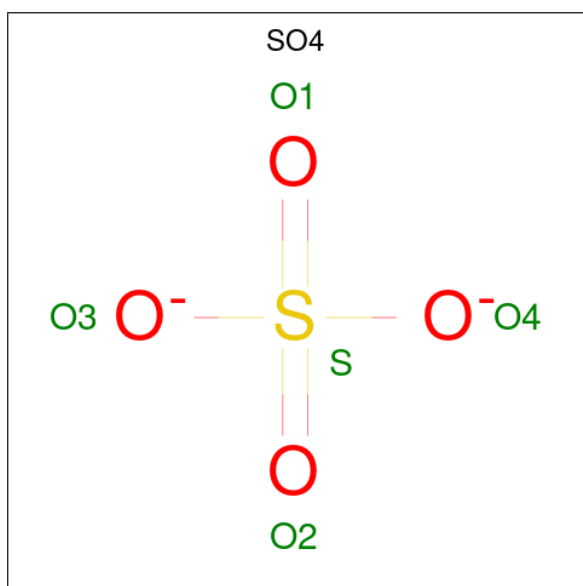


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	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	411	Total	O	0	0
			411	411		
6	B	428	Total	O	0	0
			428	428		

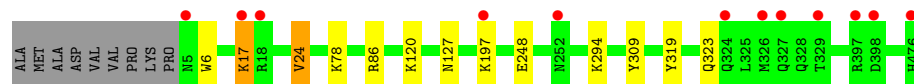
### 3 Residue-property plots [i](#)

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 7



- Molecule 1: Beta-glucosidase 7



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.58Å 101.26Å 127.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.93 – 1.85 27.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (27.93-1.85) 96.9 (27.93-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.161 , 0.185 0.172 , 0.194	Depositor DCC
$R_{free}$ test set	4250 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9849e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SO4, BGC, MES, ZN

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	0/3913	0.58	0/5319
1	B	0.42	0/3913	0.58	0/5319
All	All	0.42	0/7826	0.58	0/10638

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	3798	0	3639	10	0
1	B	3798	0	3639	4	0
2	C	45	0	39	0	0
2	D	45	0	39	3	0
2	E	45	0	39	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	12	0	12	0	0
5	B	12	0	12	0	0
6	A	411	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	428	0	0	0	0
All	All	8605	0	7419	14	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 (14) 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:5:ASN:ND2	2:D:1:BGC:H3	1.45	1.30
1:A:5:ASN:HD22	2:D:1:BGC:H3	1.13	0.90
1:A:235:GLN:HG2	6:A:1146:HOH:O	1.75	0.86
1:A:5:ASN:HD22	2:D:1:BGC:C3	1.94	0.80
1:A:255:GLU:HG2	6:A:1119:HOH:O	2.07	0.54
1:B:24:VAL:HB	1:B:86:ARG:HB3	1.95	0.49
1:A:24:VAL:HB	1:A:86:ARG:HB3	1.96	0.48
1:A:17:LYS:H	1:A:17:LYS:NZ	2.15	0.44
1:A:29:GLN:O	1:A:438:ASN:HB2	2.18	0.44
1:A:119:GLN:NE2	6:A:1234:HOH:O	2.50	0.43
1:A:78:LYS:HD2	1:A:120:LYS:HE3	2.00	0.43
1:B:17:LYS:H	1:B:17:LYS:NZ	2.16	0.43
1:B:78:LYS:HD2	1:B:120:LYS:HE3	2.01	0.42
1:B:248:GLU:O	1:B:319:TYR:HA	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	470/481 (98%)	458 (97%)	12 (3%)	0	100	100
1	B	470/481 (98%)	458 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	940/962 (98%)	916 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	388/395 (98%)	381 (98%)	7 (2%)	59	45
1	B	388/395 (98%)	380 (98%)	8 (2%)	53	38
All	All	776/790 (98%)	761 (98%)	15 (2%)	57	43

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

Mol	Chain	Res	Type
1	A	6	TRP
1	A	17	LYS
1	A	24	VAL
1	A	197	LYS
1	A	294	LYS
1	A	309	TYR
1	A	323	GLN
1	B	6	TRP
1	B	17	LYS
1	B	24	VAL
1	B	127	ASN
1	B	197	LYS
1	B	294	LYS
1	B	309	TYR
1	B	323	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	B	119	GLN
1	B	353	GLN

### 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 ⓘ

12 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	C	1	2	12,12,12	0.55	0	17,17,17	0.84	0
2	BGC	C	2	2	11,11,12	0.43	0	15,15,17	1.41	2 (13%)
2	BGC	C	3	2	11,11,12	0.45	0	15,15,17	1.61	4 (26%)
2	BGC	C	4	2	11,11,12	0.94	1 (9%)	15,15,17	2.68	7 (46%)
2	BGC	D	1	2	12,12,12	0.56	0	17,17,17	1.48	4 (23%)
2	BGC	D	2	2	11,11,12	0.28	0	15,15,17	0.98	1 (6%)
2	BGC	D	3	2	11,11,12	0.20	0	15,15,17	0.84	0
2	BGC	D	4	2	11,11,12	0.46	0	15,15,17	0.68	0
2	BGC	E	1	2	12,12,12	0.55	0	17,17,17	0.87	1 (5%)
2	BGC	E	2	2	11,11,12	0.41	0	15,15,17	1.59	2 (13%)
2	BGC	E	3	2	11,11,12	0.53	0	15,15,17	1.50	3 (20%)
2	BGC	E	4	2	11,11,12	0.93	1 (9%)	15,15,17	2.61	7 (46%)

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	C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
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	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	2/2/19/22	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
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	BGC	C1-C2	2.59	1.58	1.52
2	E	4	BGC	C1-C2	2.54	1.58	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	BGC	C1-O5-C5	6.55	121.07	112.19
2	E	4	BGC	C1-O5-C5	6.07	120.42	112.19
2	E	4	BGC	C1-C2-C3	4.84	115.62	109.67
2	C	4	BGC	C1-C2-C3	4.80	115.56	109.67
2	E	2	BGC	C1-C2-C3	4.29	114.94	109.67
2	C	2	BGC	C1-C2-C3	3.68	114.19	109.67
2	E	4	BGC	O5-C1-C2	3.52	116.20	110.77
2	C	3	BGC	O5-C1-C2	-3.43	105.47	110.77
2	E	3	BGC	O5-C1-C2	-3.43	105.48	110.77
2	E	2	BGC	C1-O5-C5	3.28	116.64	112.19
2	C	4	BGC	O2-C2-C3	-3.26	103.61	110.14
2	C	2	BGC	C1-O5-C5	2.92	116.16	112.19
2	E	4	BGC	O2-C2-C1	2.86	114.99	109.15
2	C	4	BGC	O5-C1-C2	2.79	115.08	110.77
2	C	4	BGC	C2-C3-C4	-2.72	106.19	110.89
2	C	4	BGC	O2-C2-C1	2.72	114.71	109.15
2	D	1	BGC	C3-C4-C5	2.66	114.98	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	BGC	C2-C3-C4	-2.58	106.43	110.89
2	C	3	BGC	C2-C3-C4	2.57	115.35	110.89
2	C	4	BGC	C3-C4-C5	-2.51	105.76	110.24
2	D	1	BGC	O5-C5-C4	2.50	114.24	109.69
2	E	3	BGC	C2-C3-C4	2.47	115.17	110.89
2	E	4	BGC	C3-C4-C5	-2.46	105.84	110.24
2	E	4	BGC	O2-C2-C3	-2.38	105.36	110.14
2	C	3	BGC	C1-C2-C3	2.30	112.49	109.67
2	D	2	BGC	O5-C5-C6	2.24	110.71	107.20
2	E	3	BGC	C1-C2-C3	2.20	112.37	109.67
2	D	1	BGC	C4-C3-C2	2.09	114.47	110.82
2	E	1	BGC	C4-C3-C2	-2.09	107.18	110.82
2	D	1	BGC	O4-C4-C3	-2.03	105.65	110.35
2	C	3	BGC	O4-C4-C5	2.01	114.28	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

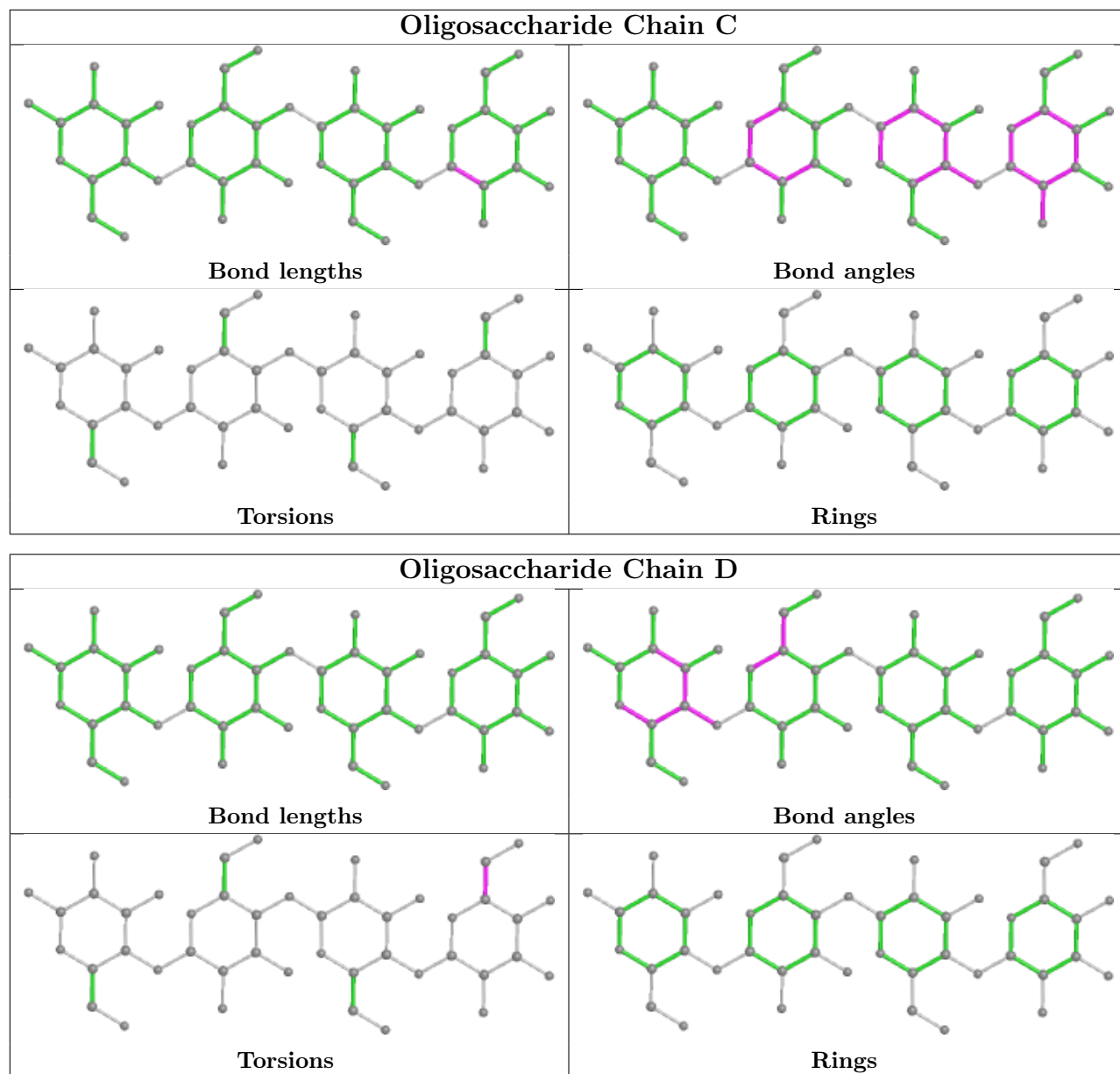
Mol	Chain	Res	Type	Atoms
2	D	4	BGC	C4-C5-C6-O6
2	D	4	BGC	O5-C5-C6-O6

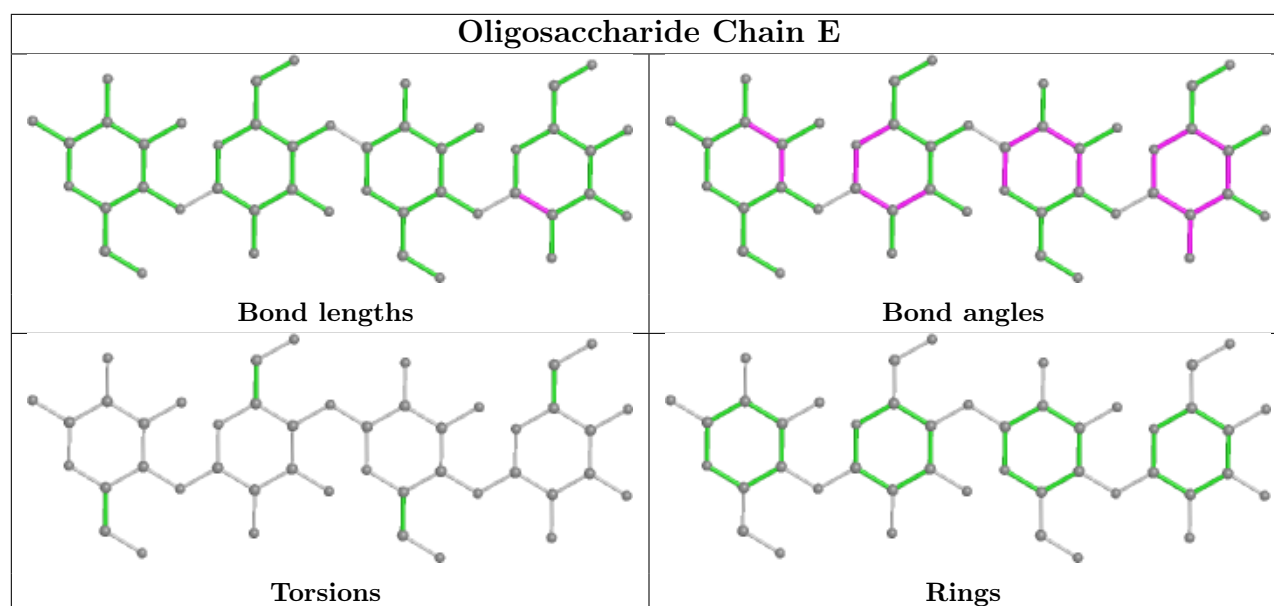
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	3	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.





## 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	SO4	A	1004	-	4,4,4	0.23	0	6,6,6	0.20	0
5	MES	B	503	-	12,12,12	2.12	1 (8%)	14,16,16	3.05	8 (57%)
4	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.15	0
5	MES	A	1005	-	12,12,12	2.14	1 (8%)	14,16,16	3.31	6 (42%)

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	B	503	-	-	2/6/14/14	0/1/1/1
5	MES	A	1005	-	-	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)
5	A	1005	MES	C8-S	-6.59	1.68	1.77
5	B	503	MES	C8-S	-6.44	1.68	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1005	MES	C5-N4-C3	7.08	124.76	108.83
5	B	503	MES	C5-N4-C3	6.69	123.89	108.83
5	B	503	MES	O1S-S-C8	-6.40	99.20	106.92
5	A	1005	MES	O1S-S-C8	-5.22	100.63	106.92
5	A	1005	MES	O2S-S-C8	-4.89	101.03	106.92
5	A	1005	MES	O3S-S-C8	-4.76	98.07	105.77
5	A	1005	MES	C7-N4-C3	3.42	119.99	111.23
5	B	503	MES	O3S-S-C8	-3.05	100.83	105.77
5	B	503	MES	C7-N4-C5	3.02	118.97	111.23
5	B	503	MES	C2-C3-N4	2.61	114.06	110.10
5	A	1005	MES	O3S-S-O2S	2.41	117.17	111.27
5	B	503	MES	C7-N4-C3	2.15	116.73	111.23
5	B	503	MES	O2S-S-C8	-2.12	104.36	106.92
5	B	503	MES	O2S-S-O1S	2.08	121.16	113.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1005	MES	C8-C7-N4-C5
5	B	503	MES	C8-C7-N4-C5
5	A	1005	MES	C8-C7-N4-C3
5	B	503	MES	C8-C7-N4-C3

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	472/481 (98%)	-0.24	8 (1%) 70 70	10, 15, 25, 44	0
1	B	472/481 (98%)	-0.20	12 (2%) 57 56	11, 15, 26, 46	0
All	All	944/962 (98%)	-0.22	20 (2%) 63 63	10, 15, 26, 46	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	HIS	5.7
1	A	324	GLN	4.4
1	B	327	GLN	4.4
1	A	5	ASN	3.8
1	B	5	ASN	3.7
1	A	476	HIS	3.7
1	B	324	GLN	3.4
1	A	327	GLN	3.4
1	A	252	ASN	3.2
1	B	197	LYS	3.2
1	B	326	MET	3.0
1	B	252	ASN	3.0
1	A	197	LYS	2.9
1	A	326	MET	2.8
1	A	18	ARG	2.6
1	B	18	ARG	2.6
1	B	329	THR	2.6
1	B	17	LYS	2.5
1	B	398	ASP	2.2
1	B	397	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

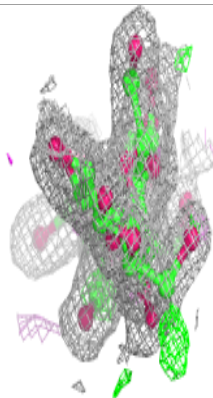
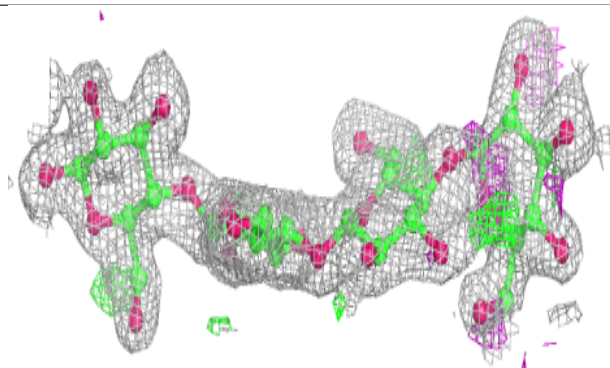
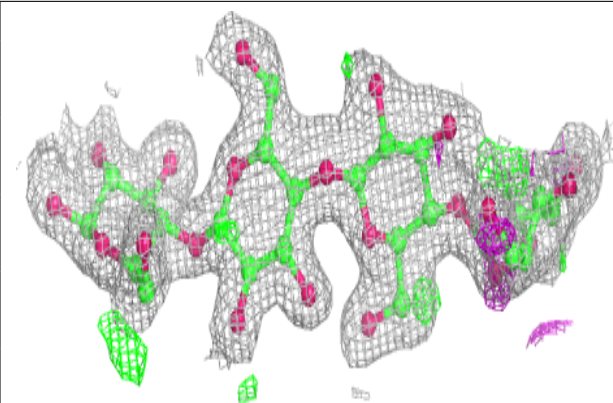
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	D	1	12/12	0.65	0.40	44,51,53,55	0
2	BGC	C	4	11/12	0.81	0.19	19,24,28,29	0
2	BGC	E	4	11/12	0.83	0.17	19,24,27,27	0
2	BGC	E	1	12/12	0.86	0.17	26,32,34,34	0
2	BGC	C	3	11/12	0.86	0.13	27,29,31,33	0
2	BGC	D	2	11/12	0.87	0.13	35,37,39,40	0
2	BGC	D	4	11/12	0.87	0.18	34,35,37,39	0
2	BGC	C	1	12/12	0.88	0.13	26,31,32,32	0
2	BGC	E	3	11/12	0.89	0.11	28,30,32,35	0
2	BGC	D	3	11/12	0.89	0.11	33,34,35,35	0
2	BGC	C	2	11/12	0.91	0.10	27,29,30,31	0
2	BGC	E	2	11/12	0.93	0.10	27,29,31,31	0

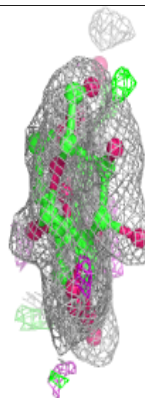
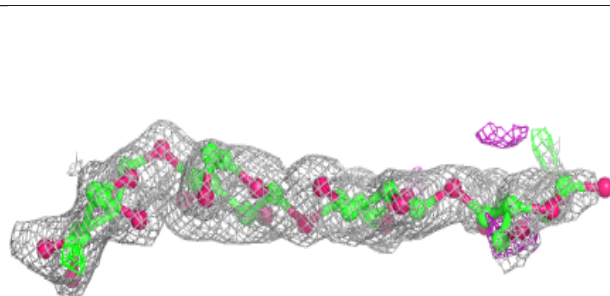
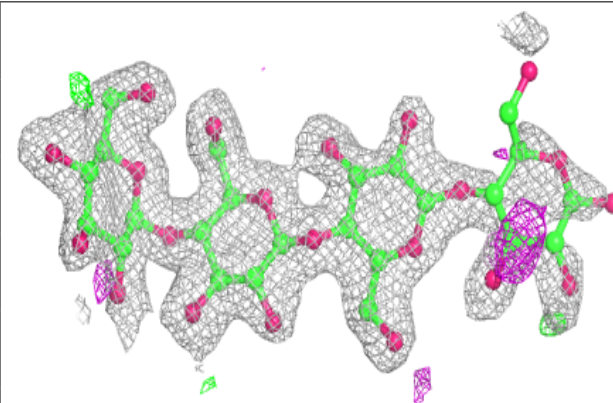
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

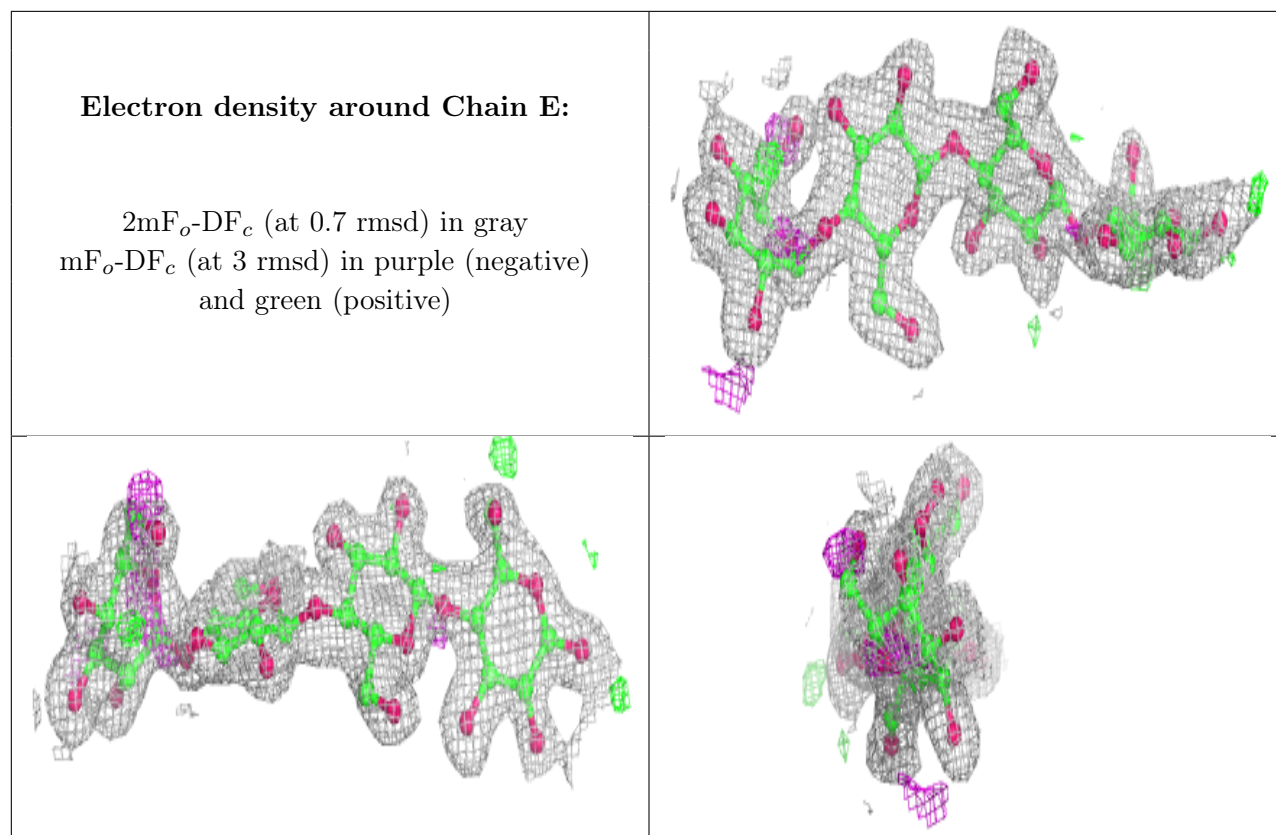
**Electron density around Chain C:**

$2mF_o-DF_c$  (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)





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	MES	A	1005	12/12	0.94	0.13	25,30,34,35	0
5	MES	B	503	12/12	0.95	0.13	26,30,34,34	0
4	SO4	A	1004	5/5	0.98	0.15	30,31,32,34	0
4	SO4	B	502	5/5	0.98	0.12	32,34,35,35	0
3	ZN	A	1003	1/1	1.00	0.05	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.