



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:18 PM BST

PDB ID : 4FLS  
Title : Crystal structure of Amylosucrase inactive double mutant F290K-E328Q from *Neisseria polysaccharea* in complex with sucrose.  
Authors : Guerin, F.; Champion, E.; Moulis, C.; Barbe, S.; Tran, T.H.; Morel, S.; Descroix, K.; Monsan, P.; Mulard, L.A.; Remaud-Simeon, M.; Andre, I.; Mourey, L.; Tranier, S.  
Deposited on : 2012-06-15  
Resolution : 2.30 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.

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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 : 2.13.1  
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) : 2.13.1

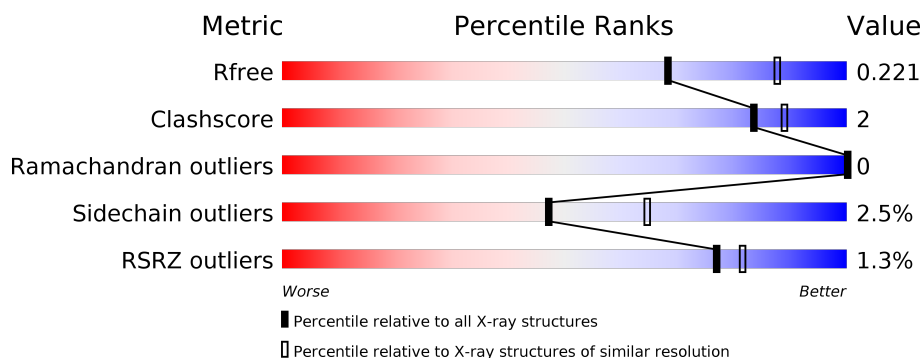
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	628	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>92%</span> <span>8%</span> </div> </div>
2	B	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>50%</span> <span>50%</span> </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 100%);"></div> <div style="text-align: center; margin-top: 5px;">100%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5370 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.

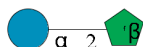
- Molecule 1 is a protein called Amylosucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	628	5037	3206	876	934	21	0	5	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9ZEU2
A	2	PRO	-	expression tag	UNP Q9ZEU2
A	3	ASN	-	expression tag	UNP Q9ZEU2
A	4	SER	-	expression tag	UNP Q9ZEU2
A	290	LYS	PHE	engineered mutation	UNP Q9ZEU2
A	328	GLN	GLU	engineered mutation	UNP Q9ZEU2
A	537	ASP	GLY	cloning artifact	UNP Q9ZEU2

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



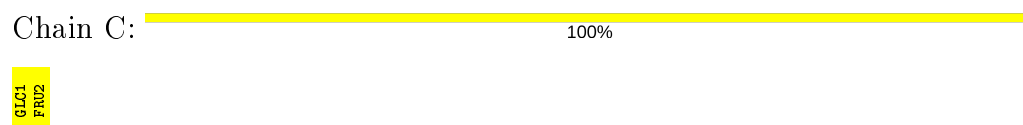
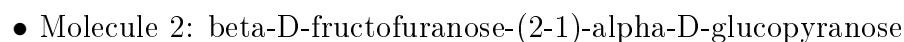
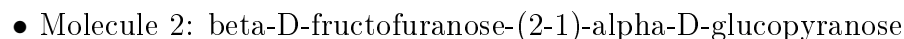
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total	O	0	0
			280	280		



- Molecule 1: Amylosucrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.11Å 114.70Å 54.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 2.30 11.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (11.98-2.30) 98.8 (11.98-2.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.176 , 0.220 0.176 , 0.221	Depositor DCC
$R_{free}$ test set	1340 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GLC, FRU, CL

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	0.53	5/5181 (0.1%)	0.56	0/7051

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	TRP	CD2-CE2	5.28	1.47	1.41
1	A	245	TRP	CD2-CE2	5.18	1.47	1.41
1	A	624	TRP	CD2-CE2	5.15	1.47	1.41
1	A	397	TRP	CD2-CE2	5.11	1.47	1.41
1	A	498	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5037	0	4786	24	0
2	B	23	0	21	0	0
2	C	23	0	21	0	0
3	A	1	0	0	0	0
4	A	6	0	8	0	0
5	A	280	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5370	0	4836	24	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 2.

All (24) 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:618:GLN:HG2	5:A:1067:HOH:O	1.84	0.76
1:A:63:MET:HG2	1:A:67[A]:GLN:HE21	1.59	0.67
1:A:357:LEU:HB3	1:A:471:LEU:HD22	1.79	0.63
1:A:290:LYS:HE2	5:A:938:HOH:O	2.01	0.60
1:A:67[A]:GLN:HE22	1:A:266:ARG:HD3	1.67	0.59
1:A:580:ASN:O	1:A:620:TYR:HA	2.05	0.55
1:A:210:TYR:HB2	1:A:247:TRP:HB2	1.89	0.54
1:A:20:ARG:NH2	1:A:24:GLU:OE2	2.41	0.54
1:A:423:VAL:O	1:A:423:VAL:HG12	2.07	0.53
1:A:7:LEU:HD13	1:A:65:LEU:HD13	1.91	0.52
1:A:15:TYR:HB3	1:A:19:GLN:HG3	1.92	0.50
1:A:180:VAL:HG22	1:A:282:ILE:HB	1.93	0.50
1:A:423:VAL:O	1:A:423:VAL:CG1	2.59	0.50
1:A:249:THR:HG21	1:A:290:LYS:HD3	1.97	0.46
1:A:116:LYS:HB2	1:A:168:VAL:HG22	1.97	0.46
1:A:36:MET:SD	1:A:65:LEU:HD22	2.56	0.46
1:A:289:ALA:HA	1:A:339:TYR:OH	2.17	0.45
1:A:585:PRO:HG3	5:A:1015:HOH:O	2.17	0.45
1:A:287:ALA:HB1	1:A:290:LYS:HG3	2.00	0.43
1:A:67[A]:GLN:NE2	1:A:266:ARG:HD3	2.32	0.43
1:A:195:ALA:HA	1:A:209:TYR:CE1	2.55	0.41
1:A:325:PHE:HB2	1:A:345:CYS:HA	2.03	0.41
1:A:313:ASN:O	1:A:317:ARG:HG2	2.20	0.40
1:A:129:TYR:CZ	1:A:180:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	631/628 (100%)	616 (98%)	15 (2%)	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	527/533 (99%)	514 (98%)	13 (2%)	47	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	14	ILE
1	A	20	ARG
1	A	61	LEU
1	A	135	LEU
1	A	185	PHE
1	A	256	ASP
1	A	290	LYS
1	A	434	VAL
1	A	446	ARG
1	A	560	ASN
1	A	599	LYS
1	A	622	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	123	GLN
1	A	186	ASN
1	A	196	GLN
1	A	207	ASN
1	A	338	GLN
1	A	419	ASN
1	A	560	ASN
1	A	573	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 ⓘ

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	GLC	B	1	2	11,11,12	0.32	0	15,15,17	2.00	1 (6%)
2	FRU	B	2	2	11,12,12	0.70	0	10,18,18	0.90	0
2	GLC	C	1	2	11,11,12	0.35	0	15,15,17	1.09	2 (13%)
2	FRU	C	2	2	11,12,12	0.70	1 (9%)	10,18,18	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	FRU	B	2	2	-	0/5/24/24	0/1/1/1
2	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	FRU	C	2	2	-	3/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FRU	O2-C2	2.02	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C1-O5-C5	6.80	121.41	112.19
2	C	1	GLC	O5-C5-C6	2.95	111.82	107.20
2	C	1	GLC	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

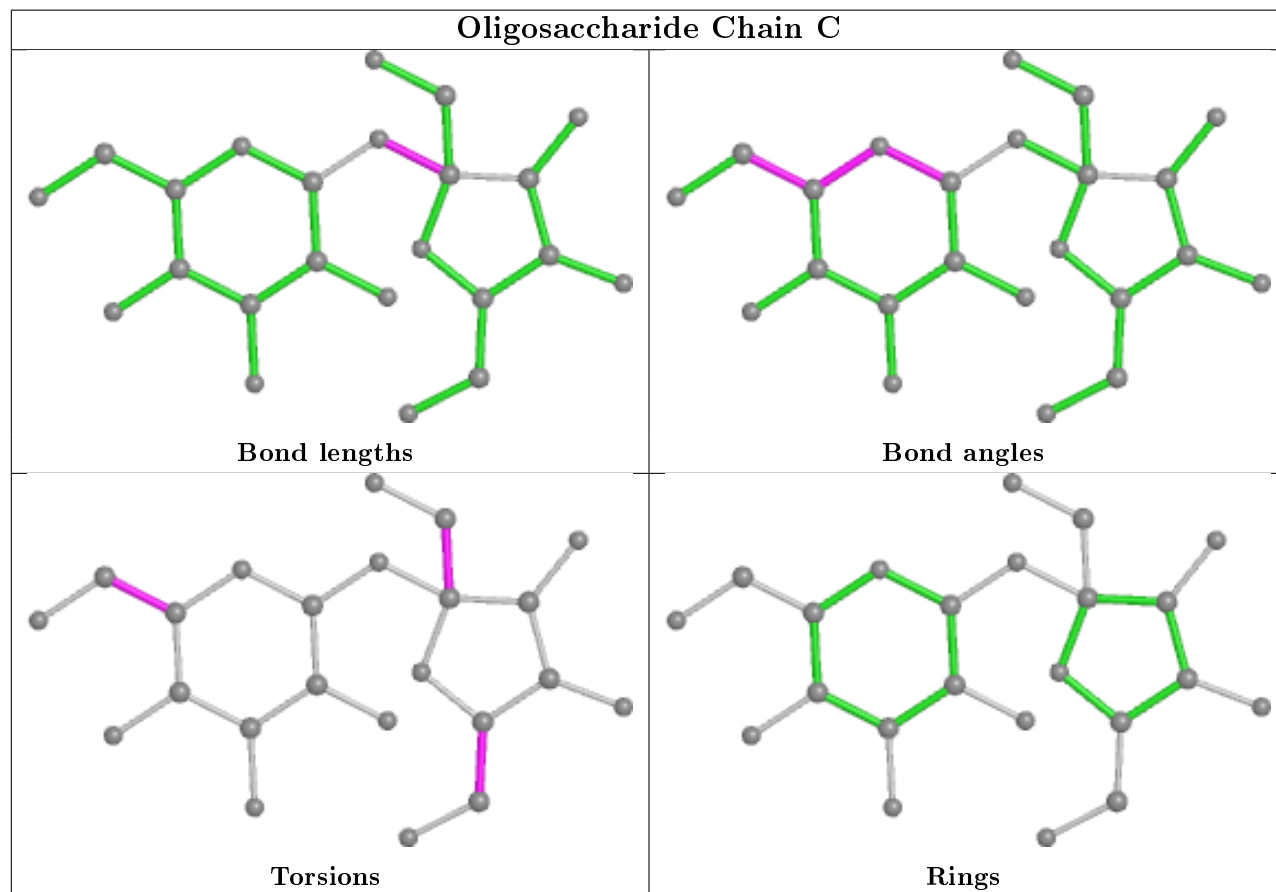
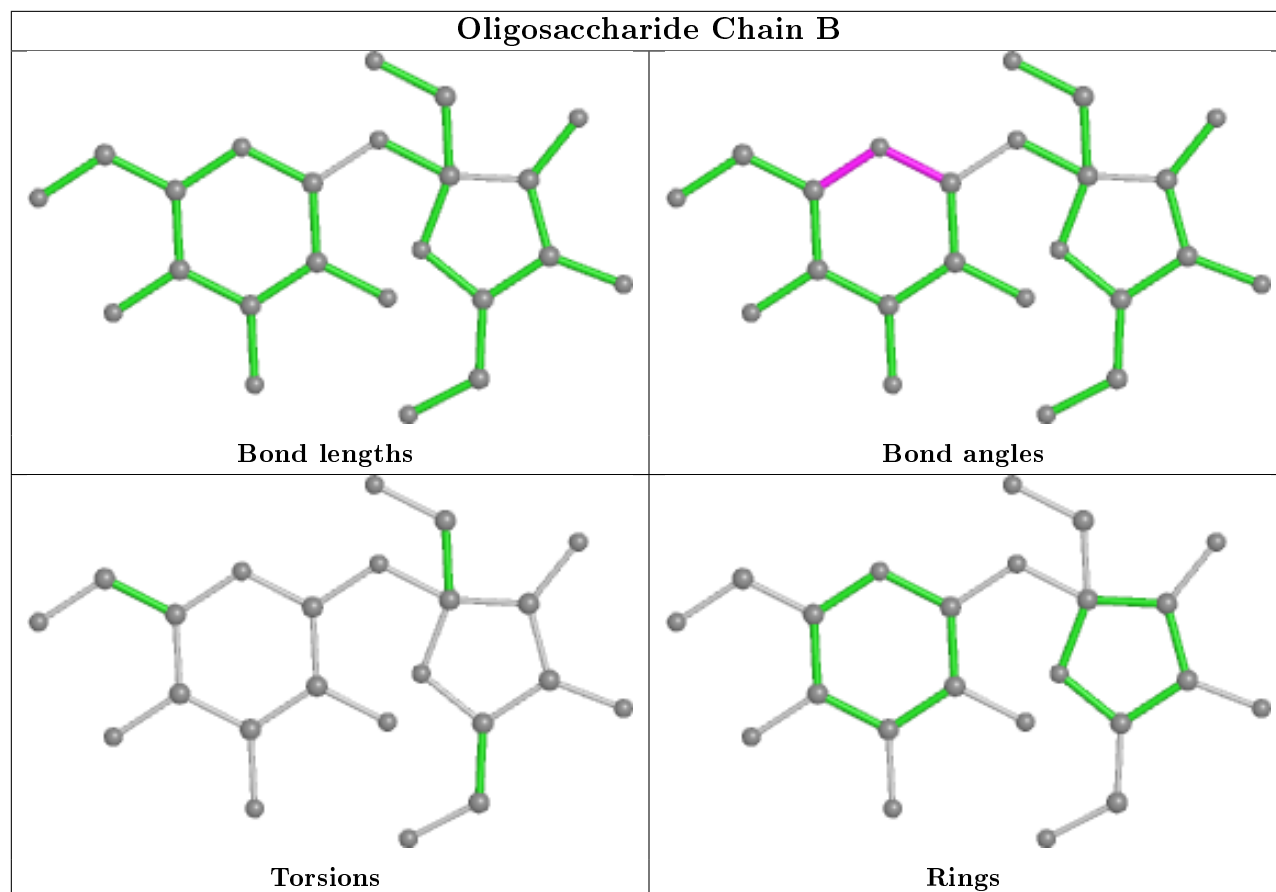
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	FRU	O1-C1-C2-O5
2	C	2	FRU	O5-C5-C6-O6
2	C	2	FRU	O1-C1-C2-C3

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.



## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GOL	A	703	-	5,5,5	0.25	0	5,5,5	0.18	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
4	GOL	A	703	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	GOL	O1-C1-C2-C3
4	A	703	GOL	O1-C1-C2-O2

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	628/628 (100%)	-0.33	8 (1%) 77 81	11, 16, 26, 41	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	4.2
1	A	496	ASP	2.6
1	A	425	ARG	2.5
1	A	408	GLY	2.5
1	A	427	ASP	2.3
1	A	207	ASN	2.3
1	A	14	ILE	2.1
1	A	426	PHE	2.1

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

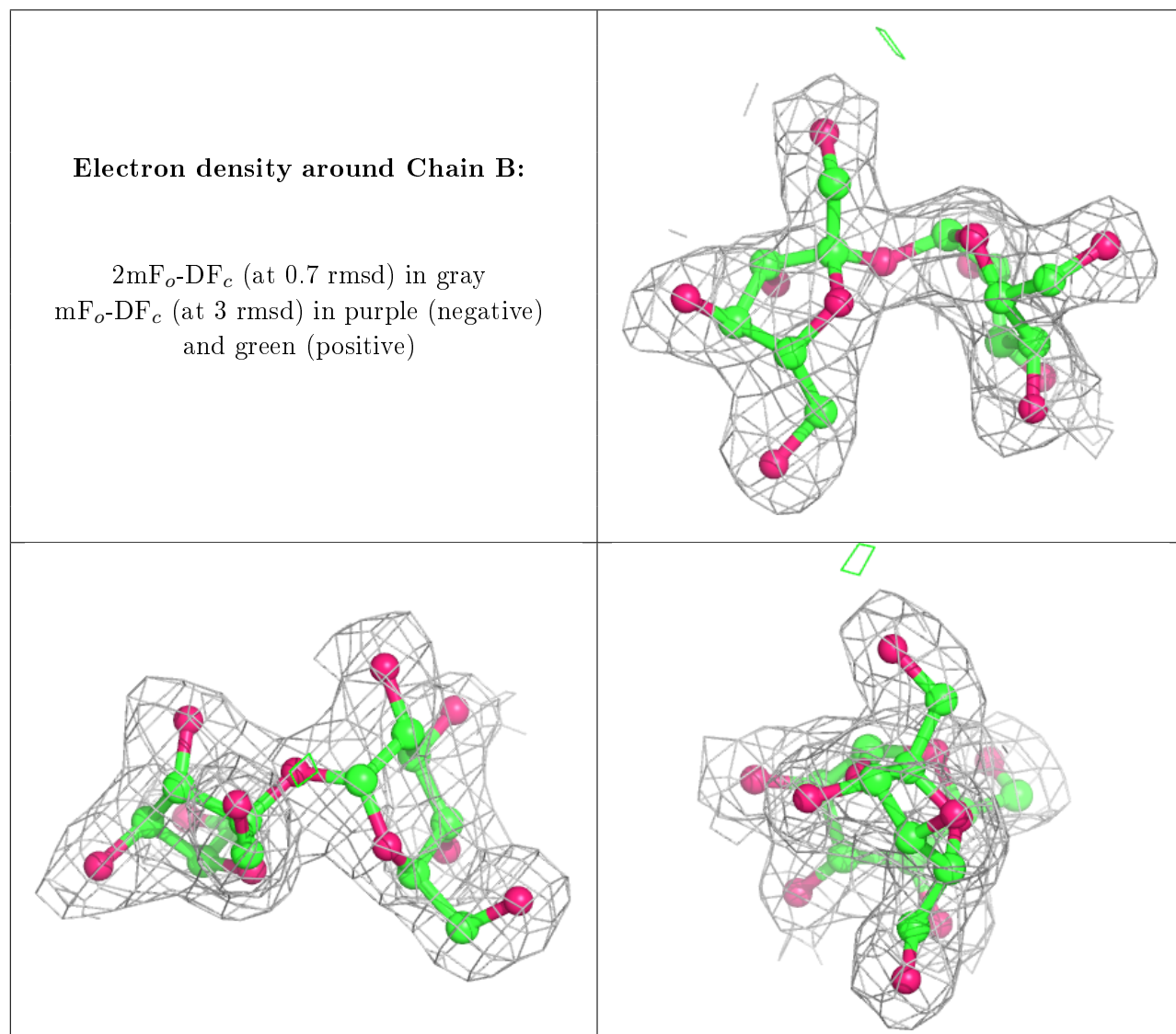
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

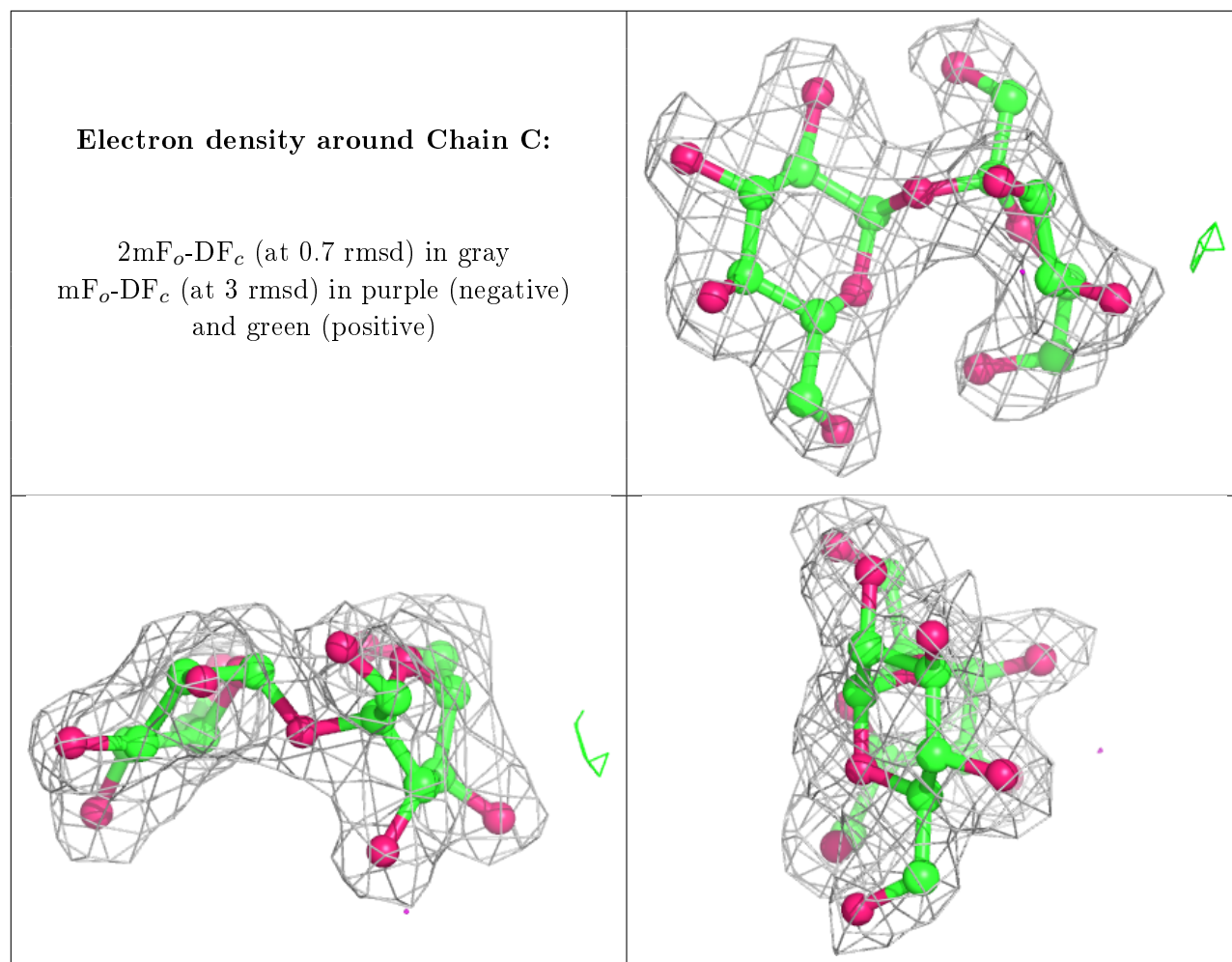
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	GLC	C	1	11/12	0.90	0.14	21,21,22,22	0
2	FRU	C	2	12/12	0.92	0.19	21,22,23,24	0
2	FRU	B	2	12/12	0.97	0.07	13,13,14,14	0
2	GLC	B	1	11/12	0.98	0.08	13,13,13,14	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.







## 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
4	GOL	A	703	6/6	0.91	0.14	23,25,25,26	0
3	CL	A	702	1/1	0.99	0.03	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.