



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 09:48 AM BST

PDB ID : 2I58  
Title : Crystal Structure of RafE from Streptococcus pneumoniae complexed with raffinose  
Authors : Paterson, N.G.; Riboldi-Tunncliffe, A.; Mitchell, T.J.; Isaacs, N.W.  
Deposited on : 2006-08-24  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

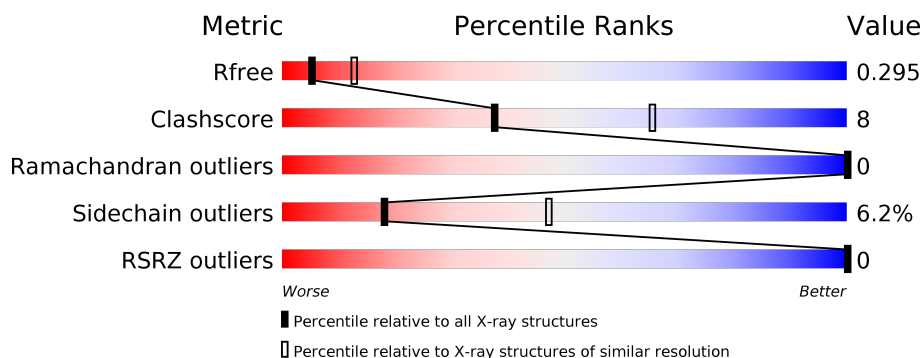
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	388	<div> <div>78%</div> <div>21%</div> <div>..</div> </div>
1	B	388	<div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6157 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 Sugar ABC transporter, sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	60	0	0
			3043	1945	499	587	12			
1	B	385	Total	C	N	O	S	56	0	0
			3043	1945	499	587	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q97NW2
A	2	PRO	-	cloning artifact	UNP Q97NW2
A	3	SER	-	cloning artifact	UNP Q97NW2
A	4	SER	-	cloning artifact	UNP Q97NW2
A	388	MET	-	cloning artifact	UNP Q97NW2
B	1	GLY	-	cloning artifact	UNP Q97NW2
B	2	PRO	-	cloning artifact	UNP Q97NW2
B	3	SER	-	cloning artifact	UNP Q97NW2
B	4	SER	-	cloning artifact	UNP Q97NW2
B	388	MET	-	cloning artifact	UNP Q97NW2

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

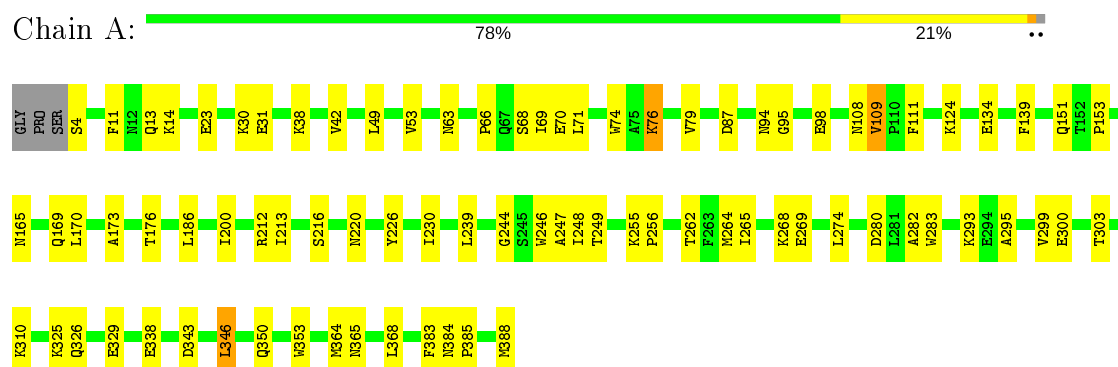
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Cl 2	0	0
3	A	1	Total 1	Cl 1	0	0

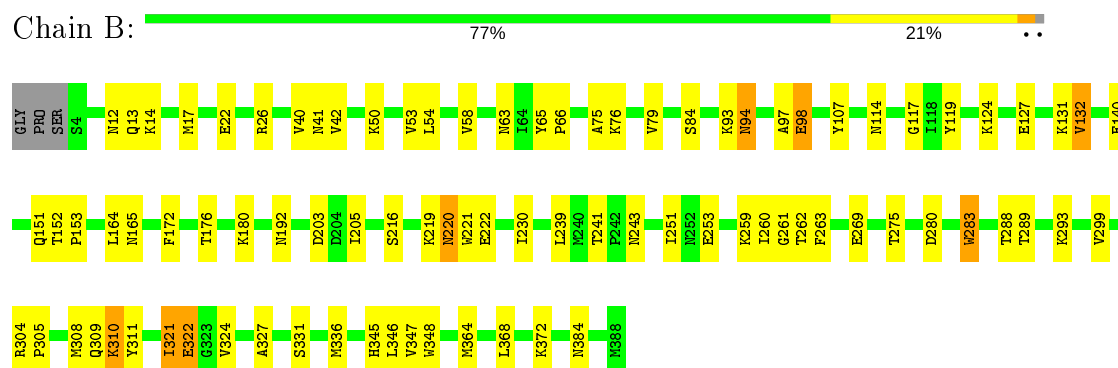
### 3 Residue-property plots [i](#)

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.

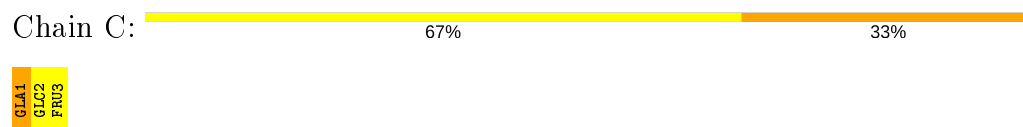
- Molecule 1: Sugar ABC transporter, sugar-binding protein



- Molecule 1: Sugar ABC transporter, sugar-binding protein



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranos e



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranos e



GLA1  
GLC2  
FRU3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.21Å 119.44Å 146.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.27 – 2.80 46.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (46.27-2.80) 91.5 (46.26-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.211 , 0.296 0.216 , 0.295	Depositor DCC
$R_{free}$ test set	971 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, 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	0.93	5/3113 (0.2%)	0.89	4/4219 (0.1%)
1	B	0.97	6/3113 (0.2%)	0.85	1/4219 (0.0%)
All	All	0.95	11/6226 (0.2%)	0.87	5/8438 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	PRO	N-CD	7.08	1.57	1.47
1	A	268	LYS	CA-CB	-6.70	1.39	1.53
1	B	140	GLU	CG-CD	5.82	1.60	1.51
1	B	259	LYS	CD-CE	-5.57	1.37	1.51
1	B	203	ASP	CB-CG	5.54	1.63	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	76	LYS	CG-CD-CE	6.80	132.32	111.90
1	A	212	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	26	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	30	LYS	CB-CG-CD	-5.05	98.48	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3043	0	2982	39	0
1	B	3043	0	2982	52	0
2	C	34	0	31	2	0
2	D	34	0	31	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
All	All	6157	0	6026	91	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 8.

The worst 5 of 91 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:13:GLN:H	1:B:63:ASN:HD22	1.10	0.98
1:B:321:ILE:HG22	1:B:324:VAL:HG23	1.57	0.83
1:B:164:LEU:HD12	1:B:364:MET:HE2	1.62	0.81
1:B:124:LYS:NZ	1:B:127:GLU:OE1	2.14	0.80
1:A:66:PRO:HA	1:A:71:LEU:HD22	1.65	0.78

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	383/388 (99%)	362 (94%)	21 (6%)	0	100	100
1	B	383/388 (99%)	352 (92%)	31 (8%)	0	100	100
All	All	766/776 (99%)	714 (93%)	52 (7%)	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	322/324 (99%)	300 (93%)	22 (7%)	16	42
1	B	322/324 (99%)	304 (94%)	18 (6%)	21	51
All	All	644/648 (99%)	604 (94%)	40 (6%)	18	47

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	GLU
1	B	22	GLU
1	B	310	LYS
1	A	346	LEU
1	B	76	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	B	380	ASN
1	B	151	GLN
1	A	151	GLN
1	B	63	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 ⓘ

6 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	GLA	C	1	2	11,11,12	0.74	0	15,15,17	1.26	3 (20%)
2	GLC	C	2	2	12,12,12	1.12	0	17,17,17	1.37	2 (11%)
2	FRU	C	3	2	11,11,12	0.69	0	15,15,18	1.79	3 (20%)
2	GLA	D	1	2	11,11,12	0.58	0	15,15,17	0.97	1 (6%)
2	GLC	D	2	2	12,12,12	0.85	0	17,17,17	1.46	4 (23%)
2	FRU	D	3	2	11,11,12	0.67	0	15,15,18	1.74	4 (26%)

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	GLA	C	1	2	-	1/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/22/22	0/1/1/1
2	FRU	C	3	2	-	4/4/20/24	0/1/1/1
2	GLA	D	1	2	-	2/2/19/22	0/1/1/1
2	GLC	D	2	2	-	0/2/22/22	0/1/1/1
2	FRU	D	3	2	-	2/4/20/24	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	FRU	C1-C2-C3	-4.68	103.81	115.09
2	D	3	FRU	C6-C5-C4	-3.79	105.96	115.09
2	D	3	FRU	O5-C5-C6	3.37	116.50	109.21
2	C	3	FRU	C6-C5-C4	-3.13	107.55	115.09
2	C	2	GLC	O3-C3-C2	-2.90	103.65	110.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

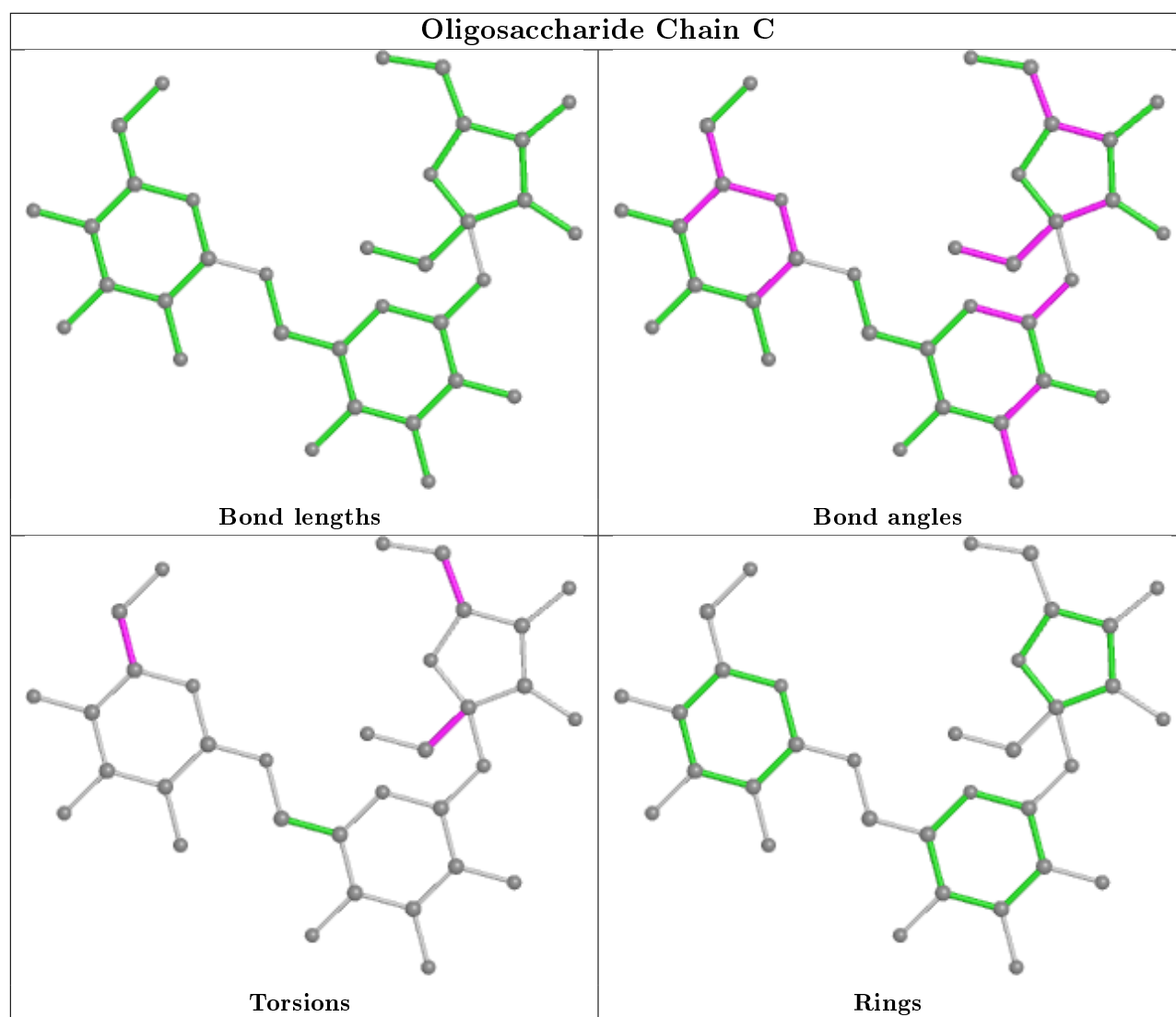
Mol	Chain	Res	Type	Atoms
2	D	3	FRU	O5-C5-C6-O6
2	D	3	FRU	C4-C5-C6-O6
2	C	3	FRU	O1-C1-C2-O5
2	D	1	GLA	O5-C5-C6-O6
2	C	1	GLA	O5-C5-C6-O6

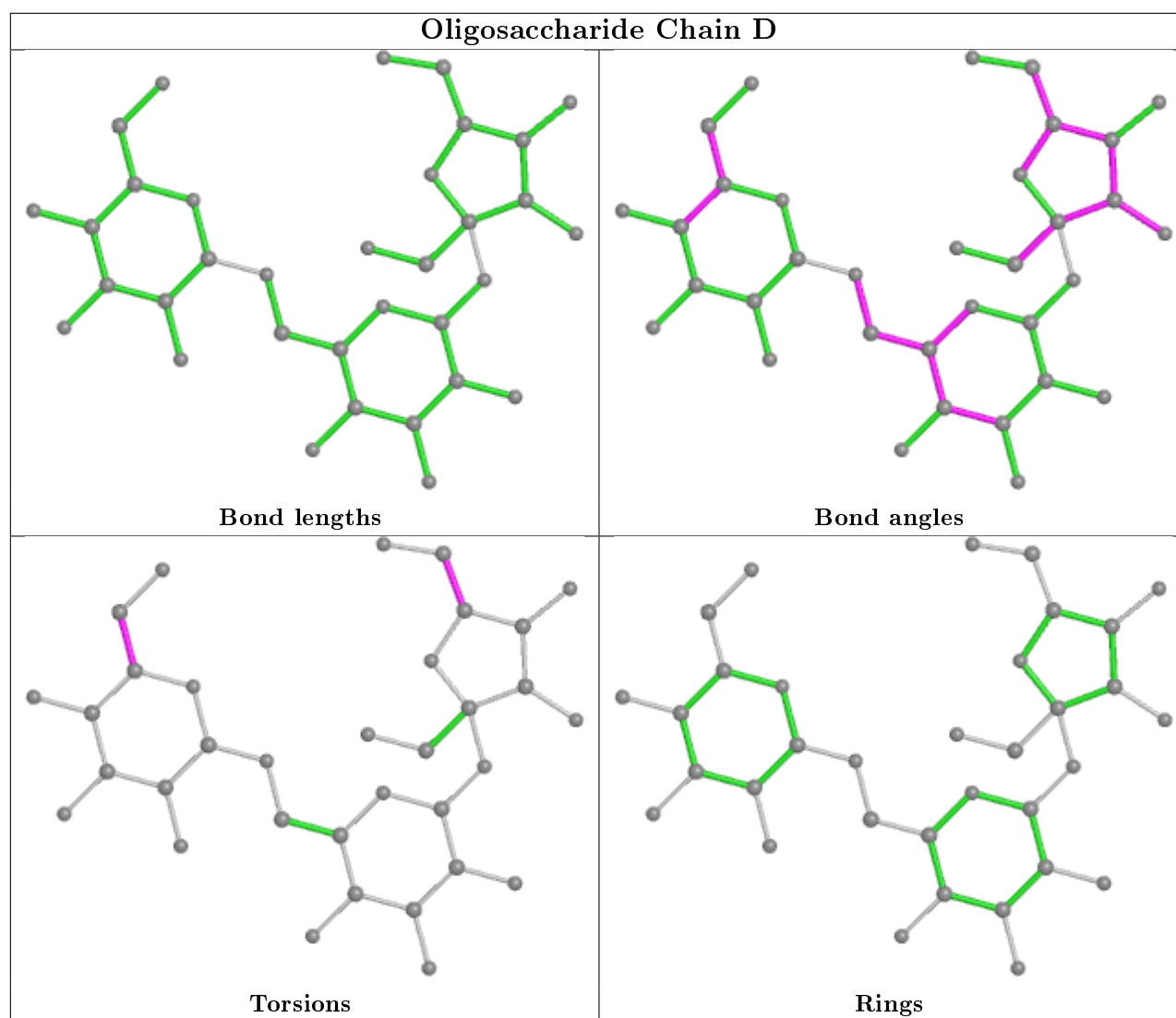
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLA	1	0
2	C	1	GLA	2	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	385/388 (99%)	-0.59	0 100 100	27, 55, 84, 131	19 (4%)
1	B	385/388 (99%)	-0.58	0 100 100	30, 58, 86, 106	18 (4%)
All	All	770/776 (99%)	-0.58	0 100 100	27, 57, 86, 131	37 (4%)

There are no RSRZ outliers to report.

### 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](#)

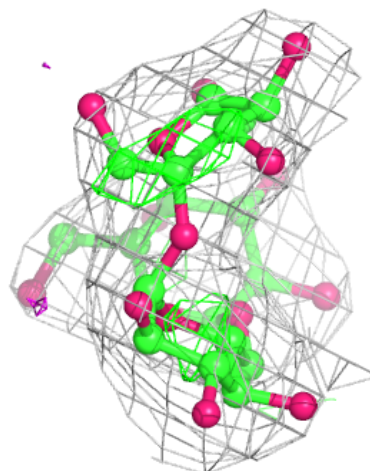
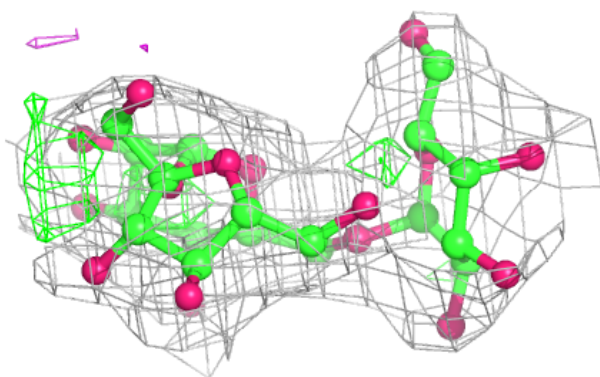
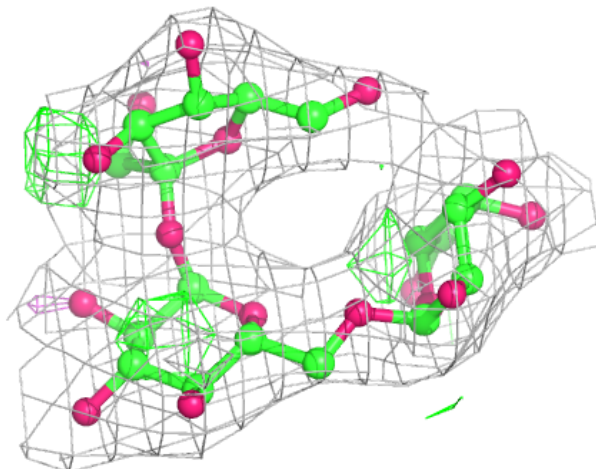
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

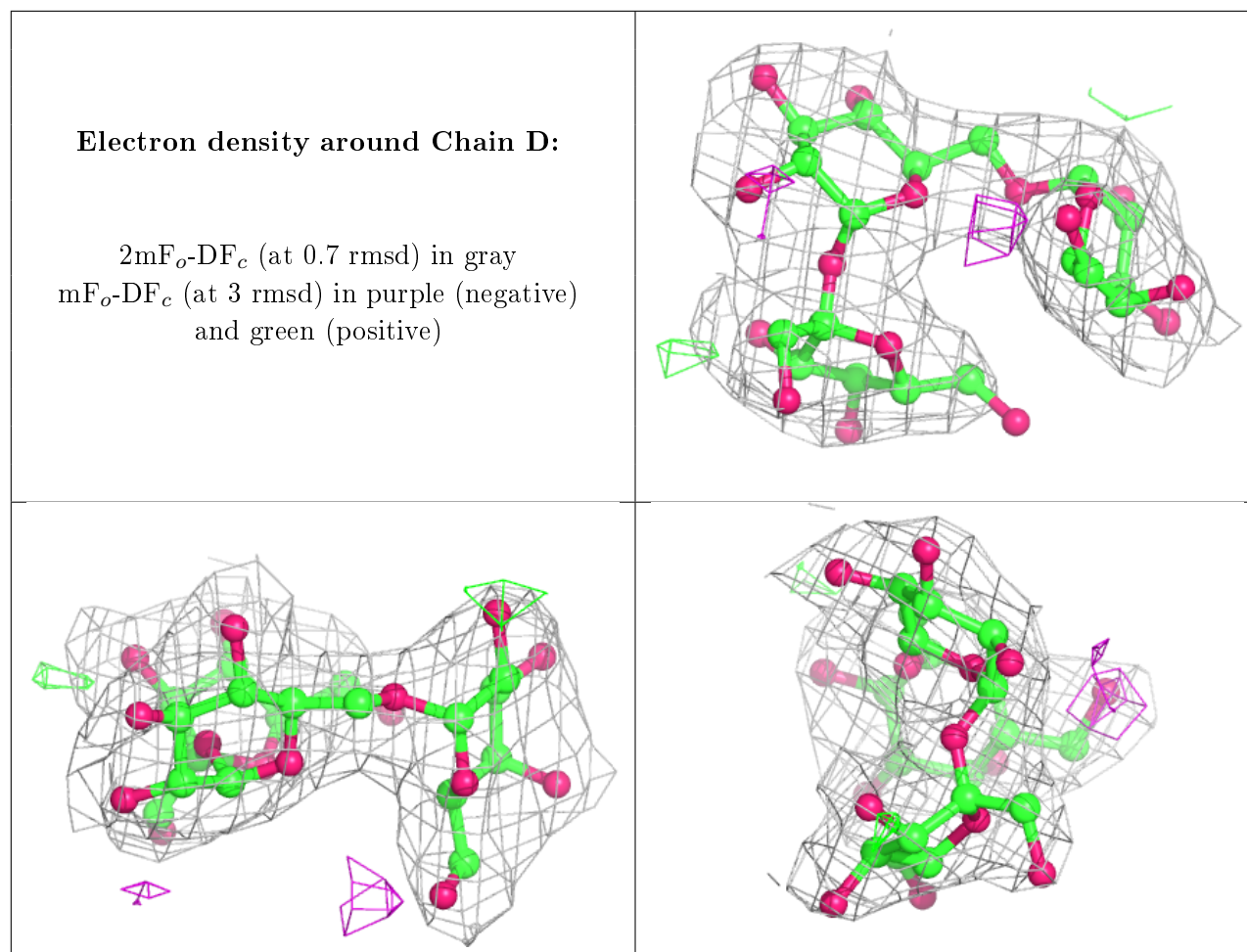
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	D	3	11/12	0.90	0.21	48,50,55,58	0
2	GLA	C	1	11/12	0.93	0.18	49,51,55,57	0
2	FRU	C	3	11/12	0.93	0.15	47,48,56,57	0
2	GLA	D	1	11/12	0.96	0.14	36,38,40,40	0
2	GLC	D	2	12/12	0.97	0.10	34,40,43,44	0
2	GLC	C	2	12/12	0.97	0.14	40,43,50,50	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)





## 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<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
3	CL	A	401	1/1	0.90	0.13	34,34,34,34	0
3	CL	B	401	1/1	0.90	0.15	33,33,33,33	0
3	CL	B	402	1/1	0.95	0.24	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.