



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:06 PM JST

PDB ID : 5GOP  
Title : Crystal structure of alkaline invertase InvA from *Anabaena* sp. PCC 7120 complexed with sucrose  
Authors : Xie, J.; Cai, K.; Hu, H.X.; Jiang, Y.L.; Yang, F.; Hu, P.F.; Chen, Y.; Zhou, C.Z.  
Deposited on : 2016-07-28  
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](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 : 2.36  
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

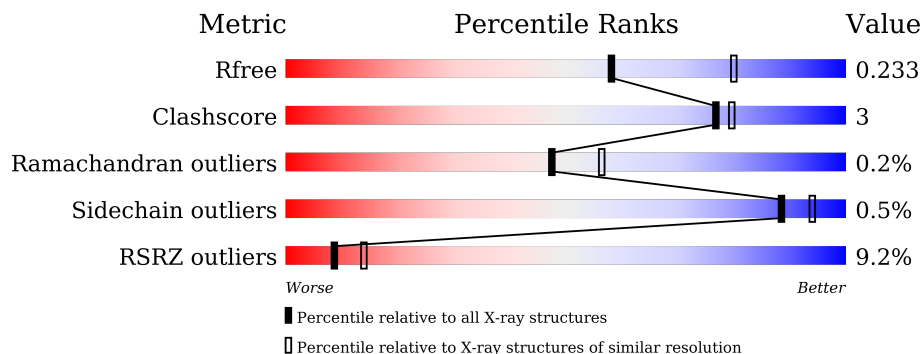
# 1 Overall quality at a glance

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  $\geq 3$ , 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	461	 10% 89% 8%
1	B	461	 7% 88% 7% 5%
1	C	461	 9% 85% 9% 6%
2	D	2	 50% 50%
2	E	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11010 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 Alkaline Invertase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	447	Total 3597	C 2336	N 600	O 643	S 6	Se 12	0	0	0
1	B	437	Total 3514	C 2284	N 584	O 628	S 6	Se 12	0	0	0
1	C	434	Total 3506	C 2282	N 584	O 622	S 6	Se 12	0	1	0

There are 27 discrepancies between the modelled and reference sequences:

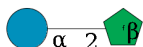
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP Q8YWS9
A	1	GLY	-	expression tag	UNP Q8YWS9
A	2	HIS	-	expression tag	UNP Q8YWS9
A	3	HIS	-	expression tag	UNP Q8YWS9
A	4	HIS	-	expression tag	UNP Q8YWS9
A	5	HIS	-	expression tag	UNP Q8YWS9
A	6	HIS	-	expression tag	UNP Q8YWS9
A	7	HIS	-	expression tag	UNP Q8YWS9
A	8	MSE	-	expression tag	UNP Q8YWS9
B	0	MSE	-	expression tag	UNP Q8YWS9
B	1	GLY	-	expression tag	UNP Q8YWS9
B	2	HIS	-	expression tag	UNP Q8YWS9
B	3	HIS	-	expression tag	UNP Q8YWS9
B	4	HIS	-	expression tag	UNP Q8YWS9
B	5	HIS	-	expression tag	UNP Q8YWS9
B	6	HIS	-	expression tag	UNP Q8YWS9
B	7	HIS	-	expression tag	UNP Q8YWS9
B	8	MSE	-	expression tag	UNP Q8YWS9
C	0	MSE	-	expression tag	UNP Q8YWS9
C	1	GLY	-	expression tag	UNP Q8YWS9
C	2	HIS	-	expression tag	UNP Q8YWS9
C	3	HIS	-	expression tag	UNP Q8YWS9
C	4	HIS	-	expression tag	UNP Q8YWS9

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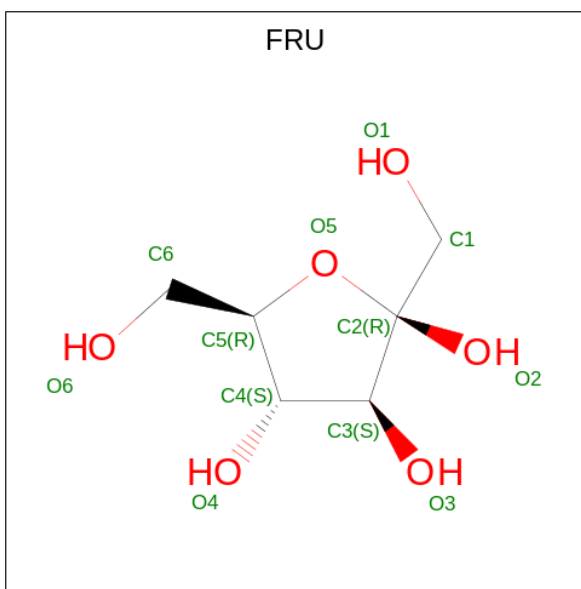
Chain	Residue	Modelled	Actual	Comment	Reference
C	5	HIS	-	expression tag	UNP Q8YWS9
C	6	HIS	-	expression tag	UNP Q8YWS9
C	7	HIS	-	expression tag	UNP Q8YWS9
C	8	MSE	-	expression tag	UNP Q8YWS9

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



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

- Molecule 3 is beta-D-fructofuranose (three-letter code: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		

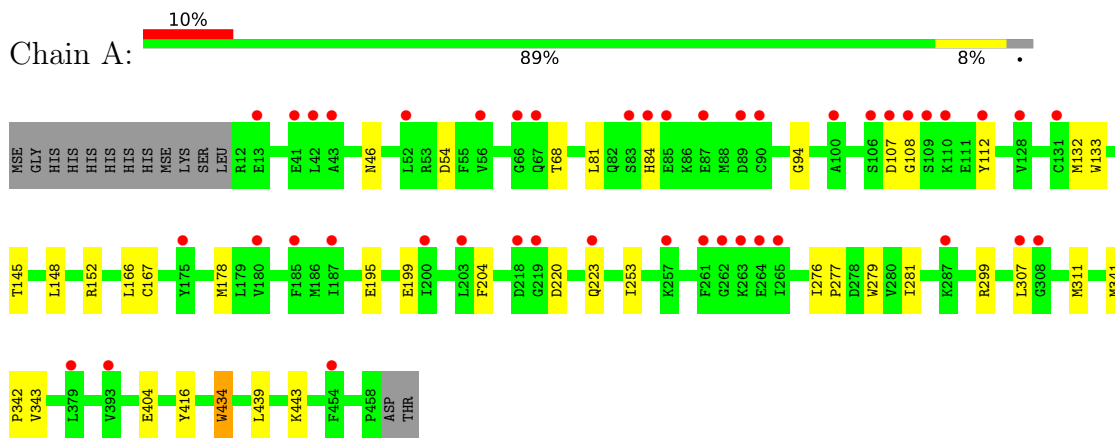
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	119	Total 119	O 119	0	0
4	B	109	Total 109	O 109	0	0
4	C	107	Total 107	O 107	0	0

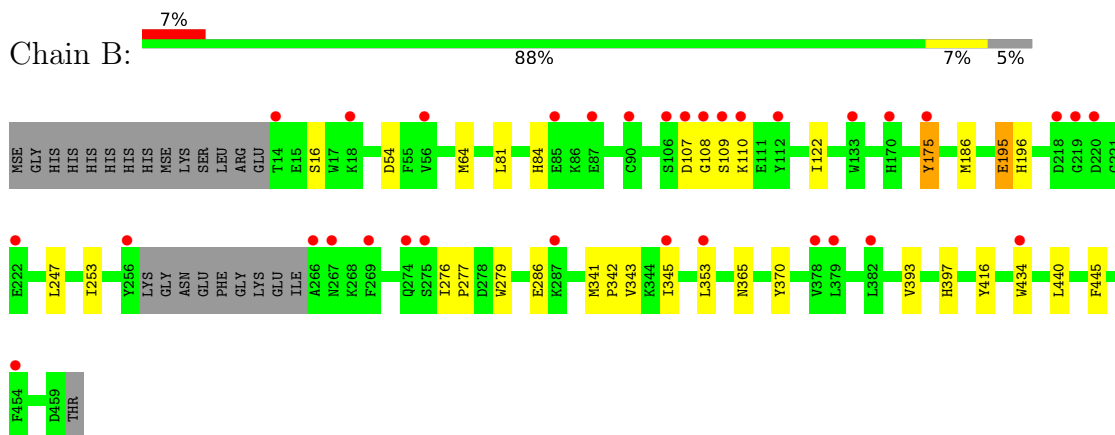
### 3 Residue-property plots [i](#)

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.

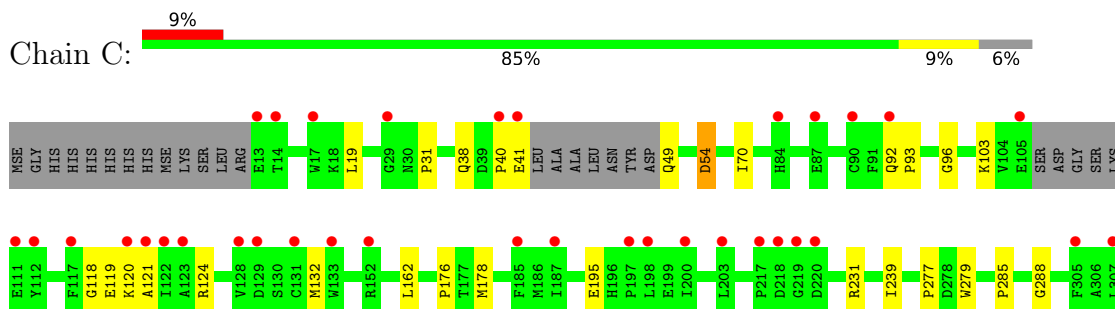
- Molecule 1: Alkaline Invertase

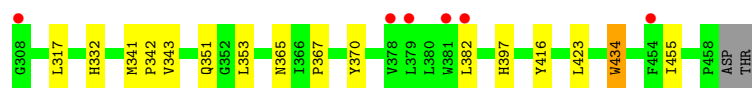


- Molecule 1: Alkaline Invertase



- Molecule 1: Alkaline Invertase





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

Chain D:  50%

  
GLC1  
FRU2

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

Chain E:  100%

  
GLC1  
FRU2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.87Å 178.92Å 181.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.94 – 2.35 33.94 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.5 (33.94-2.35) 98.2 (33.94-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.207 , 0.235 0.206 , 0.233	Depositor DCC
$R_{free}$ test set	3415 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: GLC, FRU

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	0.26	0/3685	0.51	1/4979 (0.0%)
1	B	0.25	0/3600	0.46	0/4867
1	C	0.26	0/3595	0.48	1/4855 (0.0%)
All	All	0.26	0/10880	0.49	2/14701 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	GLY	N-CA-C	-7.28	94.91	113.10
1	C	382	LEU	CA-CB-CG	5.39	127.69	115.30

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	3597	0	3537	22	0
1	B	3514	0	3451	17	0
1	C	3506	0	3448	27	0
2	D	23	0	21	1	0
2	E	23	0	21	0	0
3	B	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	119	0	0	1	0
4	B	109	0	0	0	0
4	C	107	0	0	2	1
All	All	11010	0	10490	64	1

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 3.

All (64) 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:C:397[B]:HIS:NE2	4:C:601:HOH:O	2.23	0.70
1:C:119:GLU:HG3	1:C:120:LYS:HG3	1.74	0.69
1:C:118:GLY:HA2	1:C:121:ALA:HB3	1.75	0.69
1:A:94:GLY:HA3	1:A:166:LEU:HD21	1.76	0.68
1:C:119:GLU:O	1:C:124:ARG:CZ	2.42	0.67
1:A:148:LEU:O	1:A:152:ARG:HG2	1.96	0.65
1:B:64:MSE:HE1	1:B:445:PHE:CE1	2.32	0.65
1:A:132:MSE:HE1	1:A:178:MSE:SE	2.48	0.64
1:C:231:ARG:NH2	4:C:603:HOH:O	2.31	0.62
1:A:281:ILE:HG12	1:C:423:LEU:HD11	1.83	0.60
1:A:133:TRP:HH2	1:A:311:MSE:HE3	1.67	0.59
1:A:107:ASP:HB2	1:A:112:TYR:HE1	1.68	0.58
1:A:81:LEU:HA	1:A:84:HIS:CD2	2.39	0.58
1:C:285:PRO:HG2	1:C:288:GLY:HA3	1.86	0.57
1:B:122:ILE:HD12	3:B:501:FRU:H5	1.87	0.56
1:A:68:THR:HG21	1:A:145:THR:HG22	1.89	0.55
1:C:351:GLN:HG2	1:C:367:PRO:HB3	1.90	0.54
1:C:132:MSE:HE1	1:C:178:MSE:SE	2.59	0.53
1:A:133:TRP:CH2	1:A:311:MSE:HE3	2.43	0.52
1:C:19:LEU:O	1:C:38:GLN:NE2	2.43	0.52
1:A:439:LEU:O	1:A:443:LYS:HG3	2.10	0.52
1:C:341:MSE:HG2	1:C:416:TYR:CD1	2.46	0.50
1:B:277:PRO:HB2	1:B:279:TRP:CD1	2.46	0.50
1:B:81:LEU:O	1:B:84:HIS:HB2	2.12	0.50
1:B:341:MSE:HG2	1:B:416:TYR:CD1	2.47	0.50
1:C:285:PRO:HB3	1:C:332:HIS:CG	2.47	0.49
1:C:49:GLN:HB3	1:C:103:LYS:HB3	1.92	0.49
1:A:253:ILE:HG22	1:A:276:ILE:HD11	1.94	0.49
1:C:118:GLY:HA2	1:C:121:ALA:CB	2.43	0.49
1:B:16:SER:HB3	1:B:440:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:NH2	4:A:604:HOH:O	2.34	0.48
1:A:277:PRO:HB2	1:A:279:TRP:CD1	2.48	0.48
1:C:54:ASP:HA	1:C:434:TRP:CE3	2.48	0.48
1:C:176:PRO:O	1:C:231:ARG:NH1	2.46	0.47
1:C:239:ILE:HD13	1:C:317:LEU:HD21	1.95	0.47
1:B:186:MSE:HE2	1:B:345:ILE:HD12	1.96	0.47
1:B:247:LEU:HD12	1:B:286:GLU:HA	1.95	0.47
1:C:31:PRO:HB2	1:C:70:ILE:HD12	1.98	0.46
1:A:46:ASN:OD1	2:D:2:FRU:O1	2.30	0.46
1:A:404:GLU:OE2	1:A:443:LYS:NZ	2.36	0.46
1:B:342:PRO:HA	1:B:343:VAL:HA	1.73	0.46
1:C:96:GLY:HA2	1:C:162:LEU:HB3	1.98	0.46
1:A:342:PRO:HA	1:A:343:VAL:HA	1.74	0.44
1:A:54:ASP:HA	1:A:434:TRP:CE3	2.53	0.44
1:A:199:GLU:HG3	1:A:307:LEU:HD22	1.99	0.44
1:C:365:ASN:OD1	1:C:370:TYR:HB3	2.17	0.44
1:B:353:LEU:HB3	1:C:353:LEU:HD23	2.00	0.44
1:C:40:PRO:O	1:C:41:GLU:HB2	2.19	0.43
1:A:167:CYS:HB3	1:A:204:PHE:CE1	2.54	0.43
1:B:107:ASP:N	1:B:110:LYS:O	2.38	0.43
1:C:277:PRO:HB2	1:C:279:TRP:CD1	2.53	0.43
1:C:342:PRO:HA	1:C:343:VAL:HA	1.70	0.43
1:B:175:TYR:HE2	1:B:196:HIS:CE1	2.36	0.42
1:A:341:MSE:HG2	1:A:416:TYR:CD1	2.54	0.42
1:B:393:VAL:HG12	1:B:397:HIS:CD2	2.55	0.42
1:B:253:ILE:HG22	1:B:276:ILE:HD11	2.02	0.42
1:C:455:ILE:HG13	1:C:455:ILE:O	2.19	0.42
1:B:195:GLU:HB3	1:B:196:HIS:H	1.65	0.42
1:B:108:GLY:O	1:B:109:SER:HB3	2.19	0.41
1:A:220:ASP:O	1:A:223:GLN:HG2	2.20	0.41
1:C:92:GLN:HA	1:C:93:PRO:HD3	1.92	0.41
1:A:281:ILE:H	1:A:281:ILE:HD12	1.85	0.41
1:B:365:ASN:OD1	1:B:370:TYR:HB3	2.21	0.41
1:C:118:GLY:O	1:C:124:ARG:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:601:HOH:O	4:C:687:HOH:O[3_555]	2.10	0.10

## 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	445/461 (96%)	438 (98%)	6 (1%)	1 (0%)	47	56
1	B	433/461 (94%)	423 (98%)	9 (2%)	1 (0%)	47	56
1	C	429/461 (93%)	419 (98%)	9 (2%)	1 (0%)	47	56
All	All	1307/1383 (94%)	1280 (98%)	24 (2%)	3 (0%)	47	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	GLU
1	A	195	GLU
1	C	195	GLU

### 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	372/371 (100%)	371 (100%)	1 (0%)	92	96
1	B	364/371 (98%)	361 (99%)	3 (1%)	81	89
1	C	363/371 (98%)	361 (99%)	2 (1%)	86	93
All	All	1099/1113 (99%)	1093 (100%)	6 (0%)	88	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	TRP
1	B	54	ASP
1	B	175	TYR
1	B	434	TRP
1	C	54	ASP
1	C	434	TRP

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

### 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	GLC	D	1	2	11,11,12	0.27	0	15,15,17	0.98	1 (6%)
2	FRU	D	2	2	11,12,12	0.70	1 (9%)	10,18,18	0.96	0
2	GLC	E	1	2	11,11,12	0.27	0	15,15,17	0.94	0
2	FRU	E	2	2	11,12,12	0.52	0	10,18,18	0.67	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	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	5/5/24/24	0/1/1/1
2	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	FRU	E	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	D	2	FRU	O2-C2	2.17	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-O5-C5	2.48	115.56	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

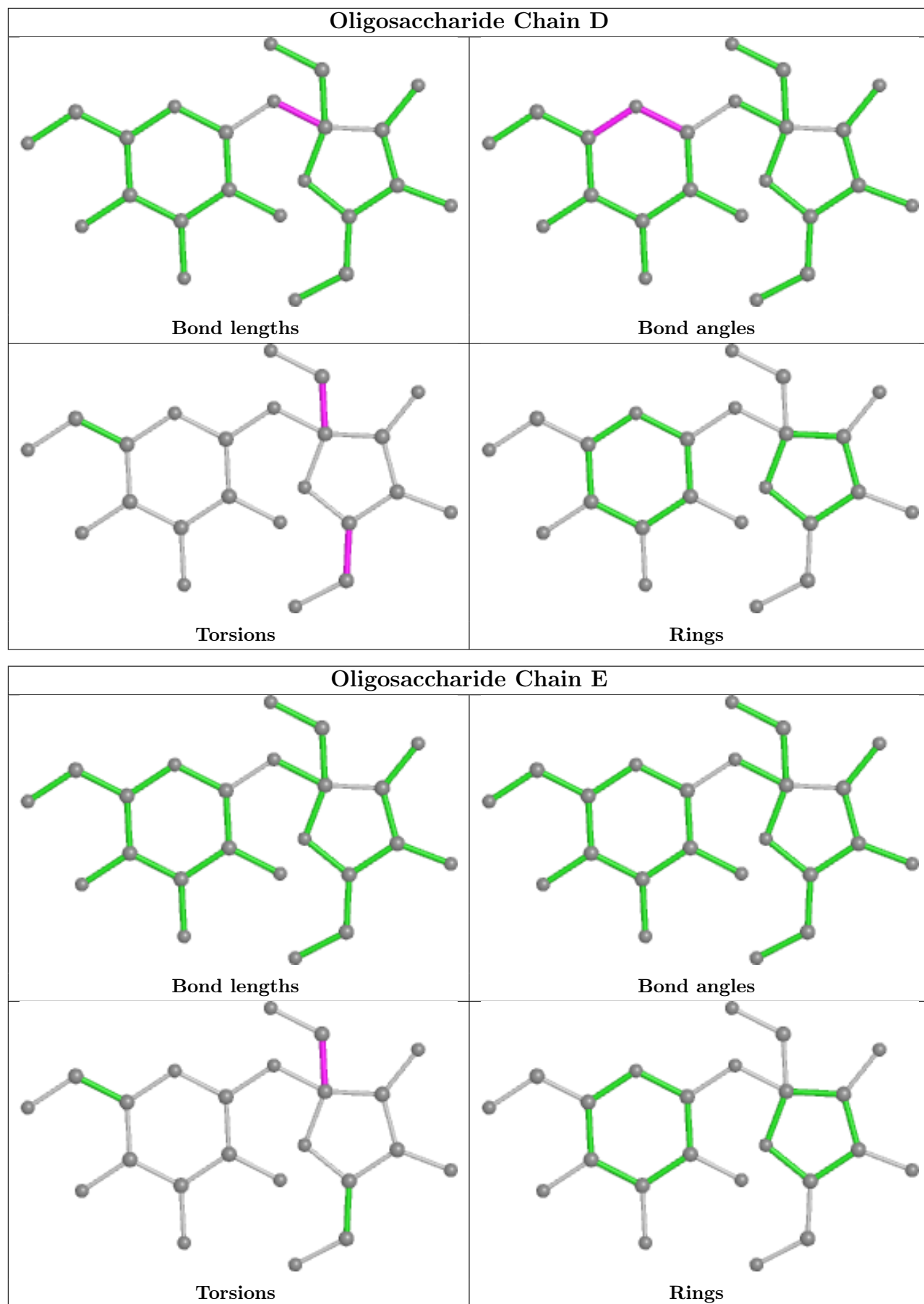
Mol	Chain	Res	Type	Atoms
2	D	2	FRU	O1-C1-C2-O2
2	D	2	FRU	O5-C5-C6-O6
2	E	2	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-O2
2	E	2	FRU	O1-C1-C2-O5
2	D	2	FRU	C4-C5-C6-O6
2	D	2	FRU	O1-C1-C2-O5
2	D	2	FRU	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	FRU	1	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](#)

1 ligand is 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
3	FRU	B	501	-	11,12,12	0.71	0	10,18,18	0.61	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
3	FRU	B	501	-	-	1/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	FRU	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	FRU	1	0

## 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

### 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	435/461 (94%)	0.53	44 (10%) <b>7</b> <b>11</b>	19, 30, 46, 79	1 (0%)
1	B	425/461 (92%)	0.35	33 (7%) <b>13</b> <b>19</b>	18, 28, 41, 57	1 (0%)
1	C	422/461 (91%)	0.52	41 (9%) <b>7</b> <b>12</b>	19, 30, 50, 66	1 (0%)
All	All	1282/1383 (92%)	0.47	118 (9%) <b>9</b> <b>14</b>	18, 29, 46, 79	3 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	ALA	8.9
1	A	109	SER	8.0
1	A	107	ASP	8.0
1	A	42	LEU	7.2
1	C	122	ILE	7.2
1	A	43	ALA	6.9
1	A	110	LYS	6.5
1	A	265	ILE	6.1
1	A	108	GLY	5.9
1	C	120	LYS	5.9
1	A	106	SER	5.7
1	C	117	PHE	5.6
1	B	274	GLN	5.4
1	A	175	TYR	5.2
1	A	264	GLU	5.2
1	C	112	TYR	5.1
1	C	121	ALA	5.0
1	A	41	GLU	4.8
1	A	85	GLU	4.7
1	A	454	PHE	4.4
1	A	13	GLU	4.4
1	C	84	HIS	4.2
1	B	109	SER	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	110	LYS	4.1
1	A	223	GLN	3.9
1	B	106	SER	3.9
1	B	175	TYR	3.9
1	A	307	LEU	3.8
1	B	275	SER	3.8
1	C	40	PRO	3.8
1	C	87	GLU	3.8
1	C	105	GLU	3.6
1	B	256	TYR	3.6
1	A	90	CYS	3.5
1	C	14	THR	3.5
1	B	218	ASP	3.5
1	A	112	TYR	3.5
1	C	307	LEU	3.4
1	C	128	VAL	3.4
1	C	217	PRO	3.3
1	B	107	ASP	3.3
1	C	219	GLY	3.2
1	C	218	ASP	3.2
1	C	203	LEU	3.1
1	B	14	THR	3.1
1	C	152	ARG	3.1
1	A	131	CYS	3.0
1	B	133	TRP	3.0
1	A	185	PHE	3.0
1	C	220	ASP	3.0
1	C	381	TRP	3.0
1	B	108	GLY	2.9
1	C	111	GLU	2.9
1	C	200	ILE	2.9
1	C	378	VAL	2.9
1	C	90	CYS	2.8
1	C	131	CYS	2.8
1	B	353	LEU	2.8
1	A	218	ASP	2.8
1	A	56	VAL	2.8
1	A	87	GLU	2.7
1	C	13	GLU	2.7
1	C	29	GLY	2.7
1	C	379	LEU	2.7
1	C	17	TRP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	41	GLU	2.6
1	B	287	LYS	2.5
1	C	198	LEU	2.5
1	C	133	TRP	2.5
1	C	92	GLN	2.5
1	B	220	ASP	2.4
1	A	52	LEU	2.4
1	A	100	ALA	2.4
1	B	219	GLY	2.4
1	B	378	VAL	2.4
1	B	85	GLU	2.4
1	C	382	LEU	2.4
1	B	90	CYS	2.4
1	A	67	GLN	2.4
1	B	112	TYR	2.4
1	C	129	ASP	2.4
1	C	185	PHE	2.4
1	A	393	VAL	2.3
1	A	84	HIS	2.3
1	A	257	LYS	2.3
1	A	89	ASP	2.3
1	B	56	VAL	2.3
1	A	200	ILE	2.3
1	B	267	ASN	2.3
1	A	66	GLY	2.3
1	C	454	PHE	2.3
1	A	261	PHE	2.2
1	B	434	TRP	2.2
1	A	308	GLY	2.2
1	B	87	GLU	2.2
1	C	187	ILE	2.2
1	B	266	ALA	2.2
1	A	203	LEU	2.2
1	B	382	LEU	2.2
1	A	262	GLY	2.2
1	A	263	LYS	2.2
1	A	187	ILE	2.2
1	B	222	GLU	2.2
1	C	197	PRO	2.2
1	C	308	GLY	2.1
1	B	269	PHE	2.1
1	C	305	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	83	SER	2.1
1	B	345	ILE	2.1
1	A	128	VAL	2.1
1	A	219	GLY	2.1
1	B	18	LYS	2.1
1	A	379	LEU	2.1
1	B	170	HIS	2.1
1	A	287	LYS	2.1
1	A	180	VAL	2.1
1	B	454	PHE	2.1
1	B	379	LEU	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](#)

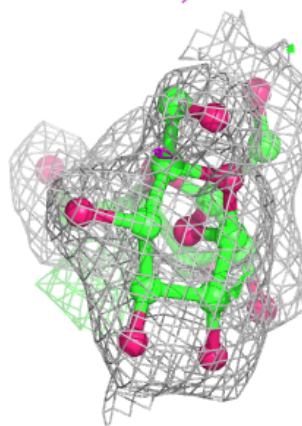
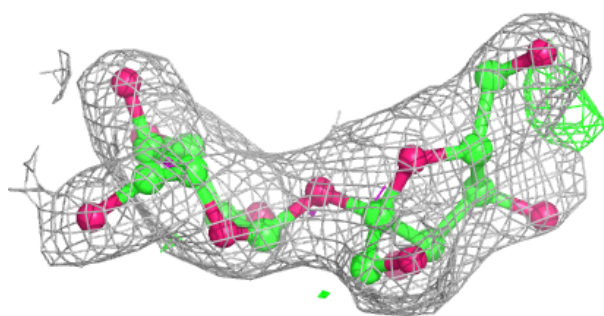
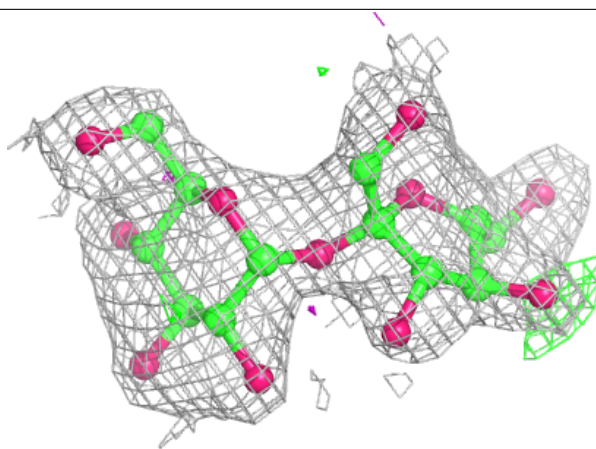
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

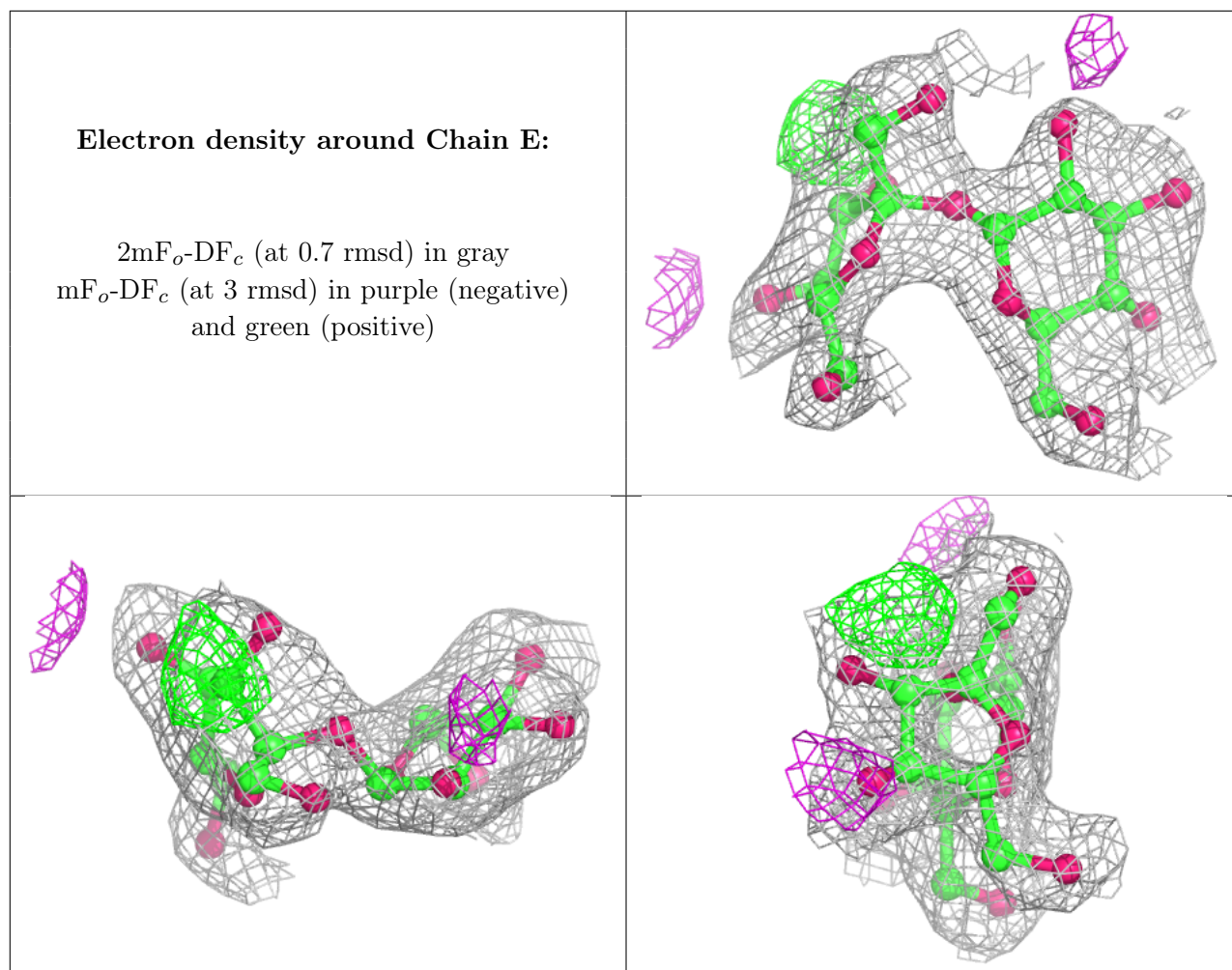
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	E	2	12/12	0.84	0.19	31,34,36,37	12
2	GLC	E	1	11/12	0.88	0.28	27,29,32,32	11
2	GLC	D	1	11/12	0.89	0.22	25,27,28,29	0
2	FRU	D	2	12/12	0.89	0.21	27,30,33,35	0

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)





## 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
3	FRU	B	501	12/12	0.96	0.13	18,20,22,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.