



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 10:29 AM BST

PDB ID : 6VG1  
Title : xenopus protocadherin 8.1 EC1-6  
Authors : Harrison, O.J.; Brasch, B.; Shapiro, L.S.  
Deposited on : 2020-01-07  
Resolution : 2.00 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

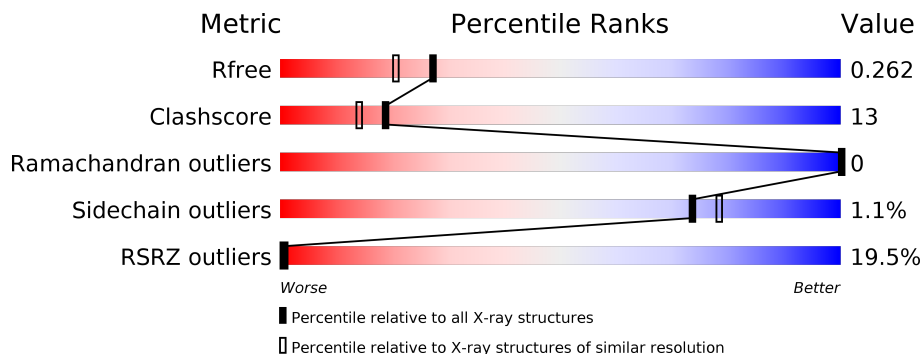
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	647	
1	B	647	
2	C	4	
2	D	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	MAN	B	722	-	-	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 19847 atoms, of which 9678 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.

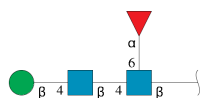
- Molecule 1 is a protein called protocadherin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	642	9697	3078	4771	838	997	13	0	0	0
1	B	641	9691	3075	4770	837	996	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	HIS	-	expression tag	UNP Q6GLU2
A	643	HIS	-	expression tag	UNP Q6GLU2
A	644	HIS	-	expression tag	UNP Q6GLU2
A	645	HIS	-	expression tag	UNP Q6GLU2
A	646	HIS	-	expression tag	UNP Q6GLU2
A	647	HIS	-	expression tag	UNP Q6GLU2
B	642	HIS	-	expression tag	UNP Q6GLU2
B	643	HIS	-	expression tag	UNP Q6GLU2
B	644	HIS	-	expression tag	UNP Q6GLU2
B	645	HIS	-	expression tag	UNP Q6GLU2
B	646	HIS	-	expression tag	UNP Q6GLU2
B	647	HIS	-	expression tag	UNP Q6GLU2

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



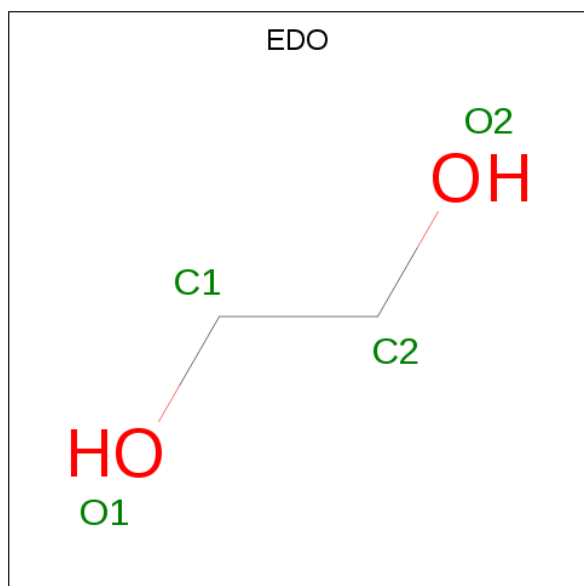
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	4	92	28	43	2	19	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
2	D	4	92	28	43	2	19	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	10	2	6	2	0	0
3	B	1	10	2	6	2	0	0

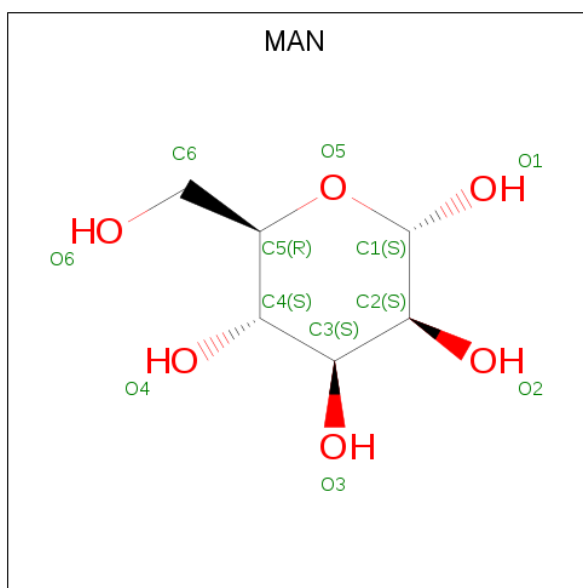
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	15	15	15	0	0
4	A	15	15	15	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	B	1	Total	C	H	O	0	0
			20	6	9	5		
6	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		

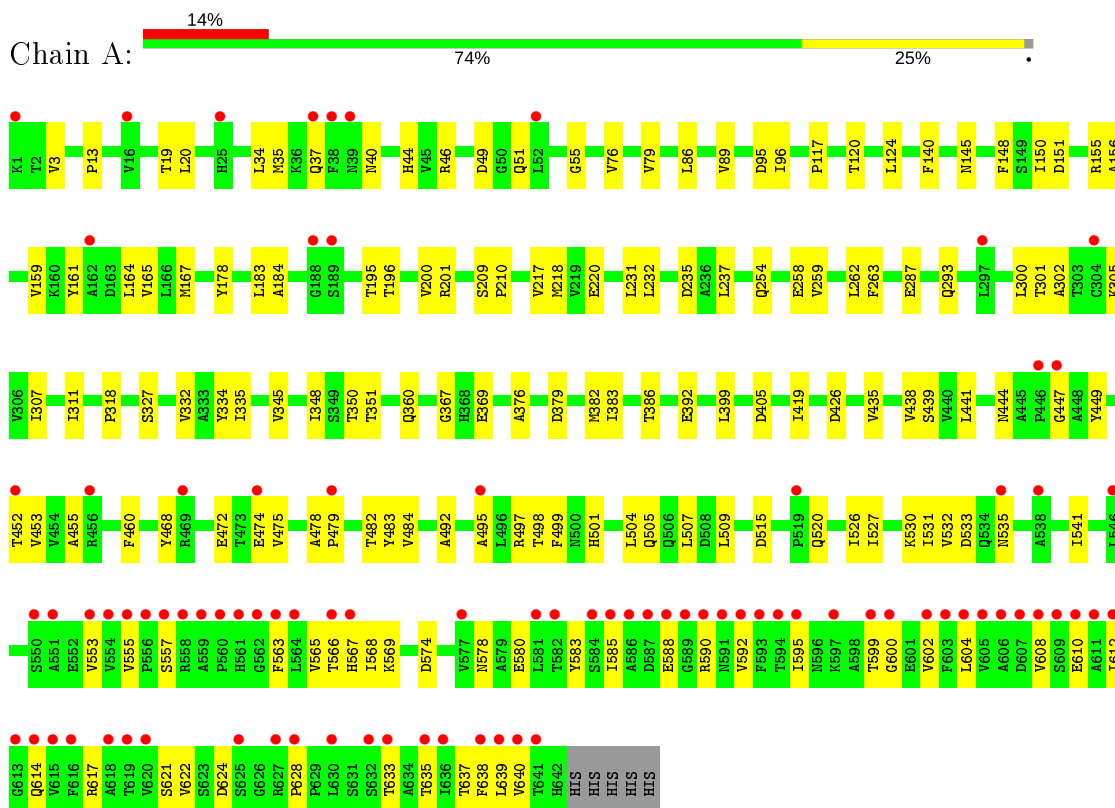
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total	O	0	0
			81	81		
8	B	57	Total	O	0	0
			57	57		

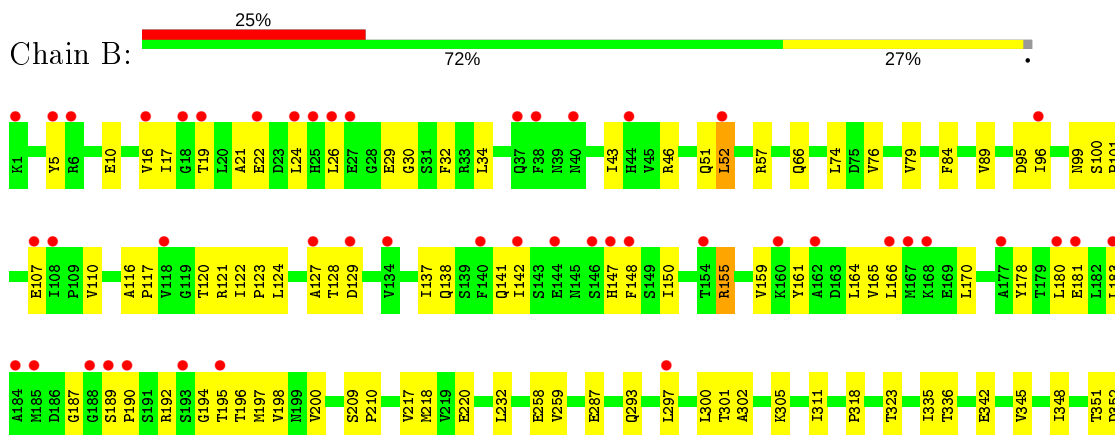
### 3 Residue-property plots

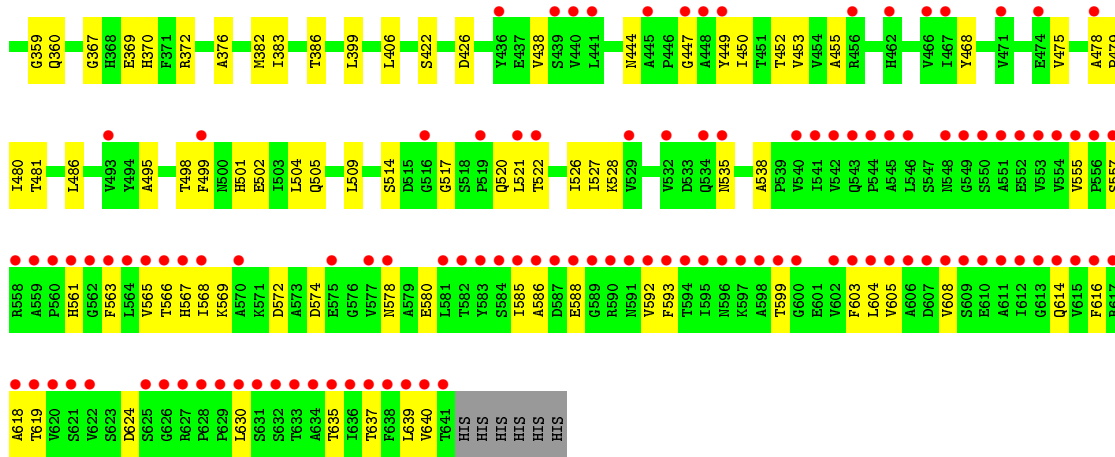
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: protocadherin protein

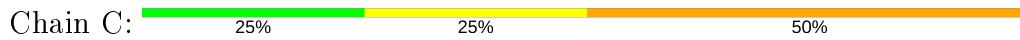


- Molecule 1: protocadherin protein





- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.65Å 42.39Å 167.47Å 90.00° 110.60° 90.00°	Depositor
Resolution (Å)	38.27 – 2.00 38.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	45.0 (38.27-2.00) 41.9 (38.27-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.253 , 0.297 0.255 , 0.262	Depositor DCC
$R_{free}$ test set	1775 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.26 % 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 9.6680e-04. 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, NA, CA, EDO, FUC, MAN

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	0.34	0/5010	0.55	0/6823
1	B	0.32	0/5005	0.53	0/6816
All	All	0.33	0/10015	0.54	0/13639

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 [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	4926	4771	4831	119	0
1	B	4921	4770	4828	141	0
2	C	49	43	43	1	0
2	D	49	43	43	2	0
3	A	4	6	6	1	0
3	B	4	6	6	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	20	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	19	19	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	81	0	0	0	0
8	B	57	0	0	1	0
All	All	10169	9678	9796	260	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 13.

The worst 5 of 260 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:572:ASP:OD2	1:B:578:ASN:O	1.73	1.06
1:B:574:ASP:OD2	1:B:578:ASN:OD1	1.84	0.94
1:A:567:HIS:HE1	1:A:599:THR:HG22	1.32	0.92
1:B:220:GLU:HB3	1:B:311:ILE:HD11	1.56	0.86
1:B:557:SER:O	1:B:608:VAL:HG21	1.76	0.84

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	640/647 (99%)	612 (96%)	28 (4%)	0	100	100
1	B	639/647 (99%)	615 (96%)	24 (4%)	0	100	100
All	All	1279/1294 (99%)	1227 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	549/555 (99%)	543 (99%)	6 (1%)	73	78
1	B	549/555 (99%)	543 (99%)	6 (1%)	73	78
All	All	1098/1110 (99%)	1086 (99%)	12 (1%)	73	78

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	PHE
1	B	52	LEU
1	B	297	LEU
1	A	262	LEU
1	B	218	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	B	229	HIS
1	B	368	HIS
1	A	147	HIS
1	B	277	GLN

### 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

8 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	NAG	C	1	1,2	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.51	0
2	BMA	C	3	2	11,11,12	1.00	0	15,15,17	0.84	1 (6%)
2	FUC	C	4	2	10,10,11	2.32	2 (20%)	14,14,16	2.07	2 (14%)
2	NAG	D	1	1,2	14,14,15	0.37	0	17,19,21	0.58	0
2	NAG	D	2	2	14,14,15	0.48	0	17,19,21	0.51	0
2	BMA	D	3	2	11,11,12	0.88	1 (9%)	15,15,17	1.04	1 (6%)
2	FUC	D	4	2	10,10,11	1.36	2 (20%)	14,14,16	2.26	2 (14%)

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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	FUC	C2-C3	5.20	1.60	1.52
2	C	4	FUC	C1-C2	4.10	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	O3-C3	2.78	1.49	1.43
2	D	4	FUC	O2-C2	2.31	1.48	1.43
2	D	3	BMA	C1-C2	2.15	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	FUC	C1-C2-C3	6.76	117.98	109.67
2	C	4	FUC	O2-C2-C1	6.48	122.41	109.15
2	D	4	FUC	C2-C3-C4	3.48	116.91	110.89
2	C	4	FUC	O2-C2-C3	-2.78	104.58	110.14
2	D	3	BMA	C1-C2-C3	2.15	112.30	109.67

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

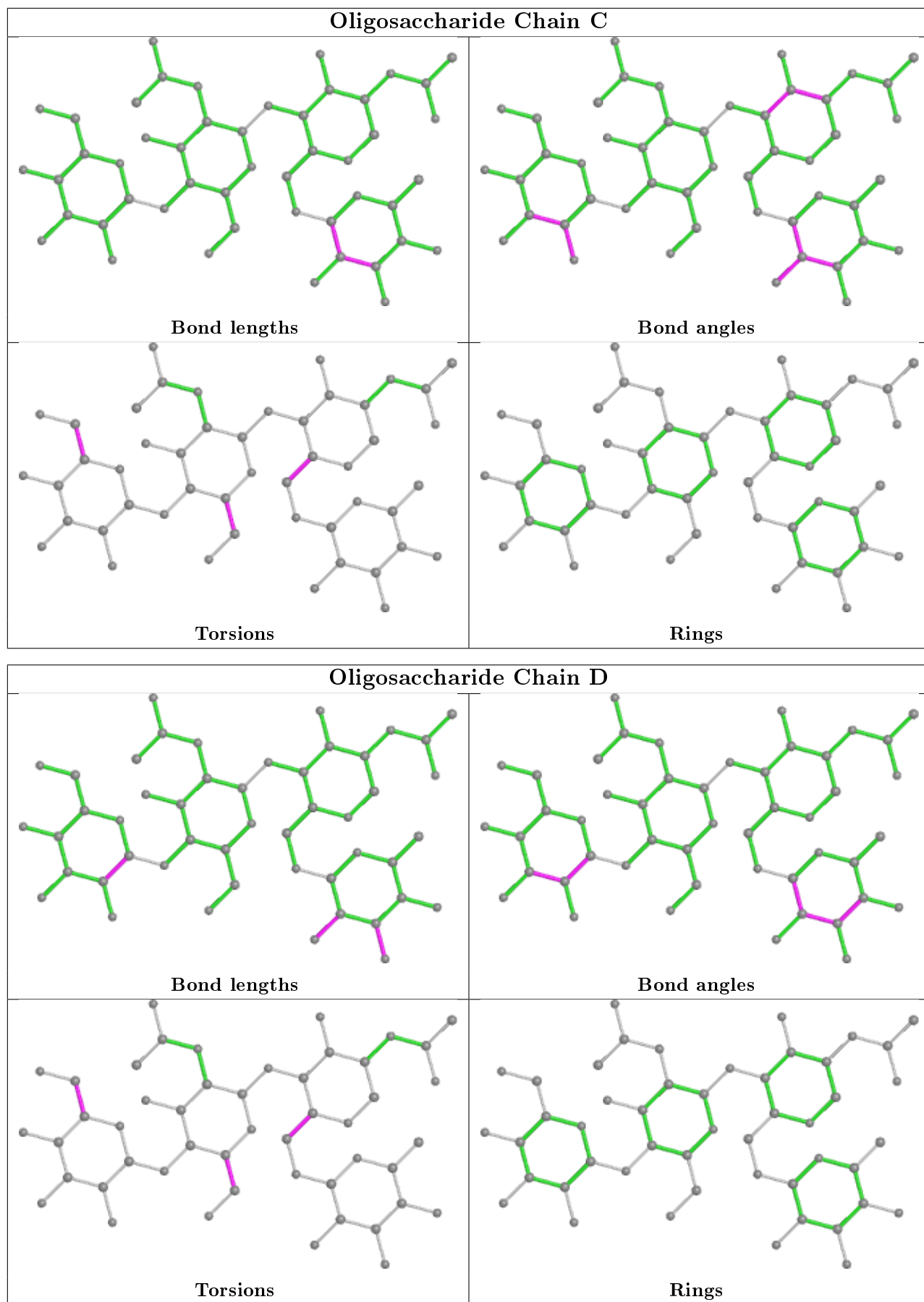
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	C	4	FUC	1	0
2	D	4	FUC	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

Of 40 ligands modelled in this entry, 34 are monoatomic - leaving 6 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
6	MAN	B	721	1	11,11,12	1.66	2 (18%)	15,15,17	1.37	4 (26%)
3	EDO	A	705	-	3,3,3	0.49	0	2,2,2	0.57	0
6	MAN	B	722	1	11,11,12	1.30	2 (18%)	15,15,17	1.14	1 (6%)
6	MAN	A	723	1	11,11,12	1.02	0	15,15,17	1.39	3 (20%)
3	EDO	B	724	-	3,3,3	0.49	0	2,2,2	0.46	0
6	MAN	A	722	1	11,11,12	0.93	0	15,15,17	1.19	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	B	721	1	-	2/2/19/22	0/1/1/1
3	EDO	A	705	-	-	0/1/1/1	-
6	MAN	B	722	1	-	0/2/19/22	0/1/1/1
6	MAN	A	723	1	-	2/2/19/22	0/1/1/1
3	EDO	B	724	-	-	1/1/1/1	-
6	MAN	A	722	1	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	721	MAN	O4-C4	3.28	1.50	1.43
6	B	721	MAN	O5-C1	-3.12	1.38	1.43
6	B	722	MAN	C2-C3	2.25	1.55	1.52
6	B	722	MAN	C1-C2	2.10	1.57	1.52

The worst 5 of 9 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	A	723	MAN	C1-O5-C5	3.44	116.85	112.19
6	A	722	MAN	C1-O5-C5	2.48	115.55	112.19
6	B	721	MAN	O2-C2-C3	-2.26	105.62	110.14
6	A	723	MAN	C2-C3-C4	2.20	114.71	110.89
6	A	723	MAN	O5-C5-C4	-2.14	105.63	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	723	MAN	O5-C5-C6-O6
6	A	723	MAN	C4-C5-C6-O6
6	B	721	MAN	O5-C5-C6-O6
6	B	721	MAN	C4-C5-C6-O6
3	B	724	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	EDO	1	0
6	B	722	MAN	2	0
6	A	723	MAN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	642/647 (99%)	0.81	88 (13%) 3 2	14, 60, 120, 182	0
1	B	641/647 (99%)	1.59	162 (25%) 0 0	21, 75, 143, 217	0
All	All	1283/1294 (99%)	1.20	250 (19%) 1 0	14, 66, 132, 217	0

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	PRO	21.4
1	B	616	PHE	20.8
1	B	555	VAL	14.0
1	B	618	ALA	13.0
1	B	554	VAL	12.7

### 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.

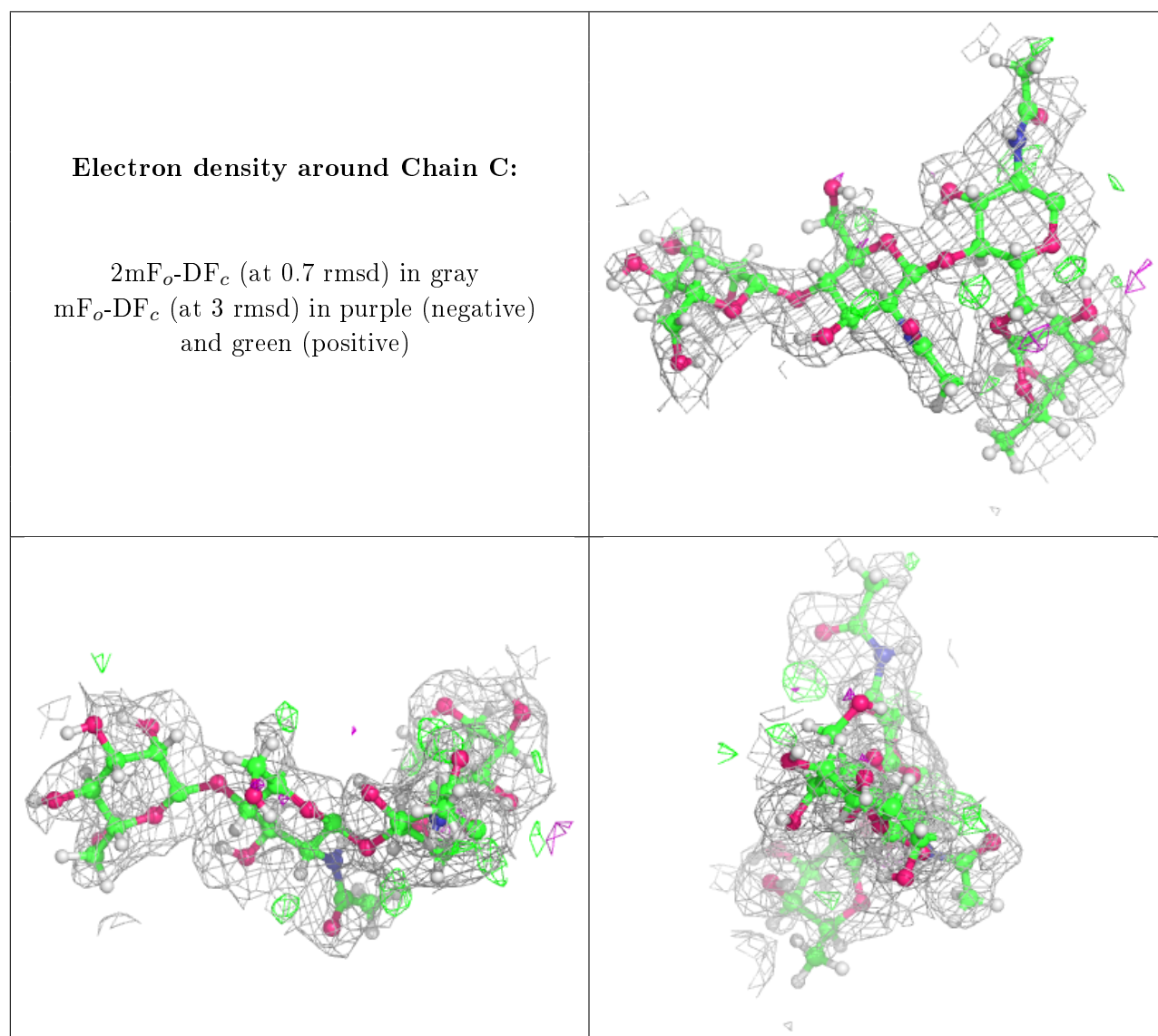
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	BMA	C	3	11/12	0.59	0.28	75,105,115,135	0
2	NAG	D	2	14/15	0.69	0.24	57,83,113,141	0
2	BMA	D	3	11/12	0.73	0.27	58,83,100,104	0
2	FUC	D	4	10/11	0.78	0.17	43,76,96,115	0
2	FUC	C	4	10/11	0.80	0.22	45,72,105,127	0

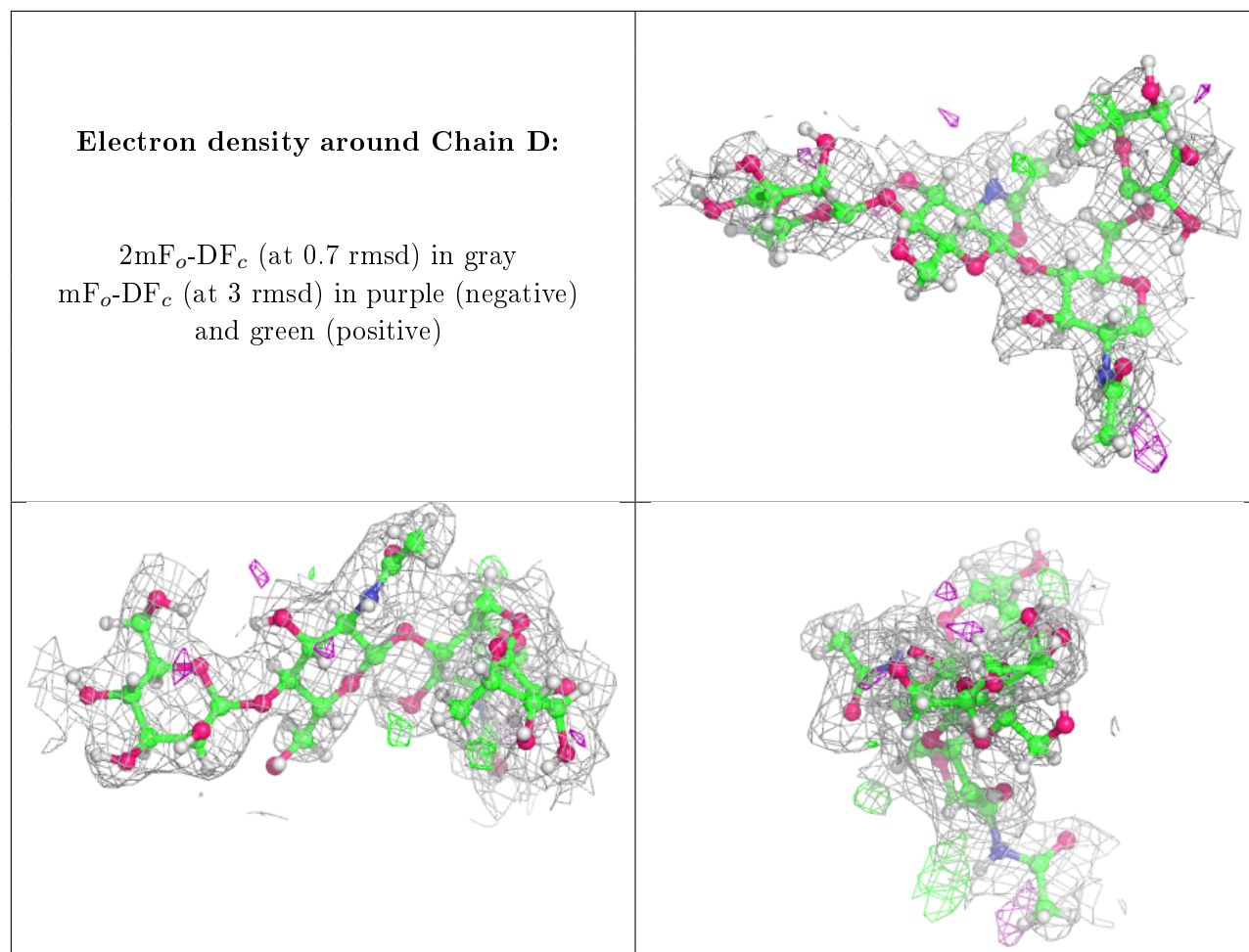
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	1	14/15	0.85	0.12	36,72,104,114	0
2	NAG	C	2	14/15	0.86	0.20	42,73,106,128	0
2	NAG	C	1	14/15	0.92	0.13	31,56,88,95	0

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(Å <sup>2</sup> )	Q<0.9
4	CA	B	719	1/1	0.54	0.15	154,154,154,154	0
4	CA	B	707	1/1	0.55	0.11	122,122,122,122	0
6	MAN	B	722	11/12	0.59	0.54	64,110,135,158	0
4	CA	B	706	1/1	0.67	0.07	92,92,92,92	0
6	MAN	A	723	11/12	0.69	0.23	56,81,104,132	0
4	CA	B	705	1/1	0.78	0.09	75,75,75,75	0
6	MAN	A	722	11/12	0.85	0.24	49,82,99,109	0
4	CA	A	719	1/1	0.85	0.07	91,91,91,91	0
6	MAN	B	721	11/12	0.86	0.29	66,94,131,142	0
4	CA	B	718	1/1	0.87	0.09	88,88,88,88	0
3	EDO	B	724	4/4	0.90	0.15	42,65,79,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	708	1/1	0.93	0.12	74,74,74,74	0
5	CL	B	720	1/1	0.94	0.26	69,69,69,69	0
4	CA	B	714	1/1	0.94	0.10	62,62,62,62	0
3	EDO	A	705	4/4	0.94	0.17	25,57,69,72	0
4	CA	A	718	1/1	0.96	0.12	69,69,69,69	0
4	CA	B	712	1/1	0.96	0.31	52,52,52,52	0
4	CA	B	717	1/1	0.97	0.09	83,83,83,83	0
5	CL	A	721	1/1	0.97	0.24	43,43,43,43	0
4	CA	B	716	1/1	0.97	0.07	59,59,59,59	0
4	CA	A	716	1/1	0.98	0.10	52,52,52,52	0
4	CA	A	707	1/1	0.98	0.14	58,58,58,58	0
4	CA	A	708	1/1	0.98	0.05	56,56,56,56	0
4	CA	A	717	1/1	0.98	0.12	62,62,62,62	0
4	CA	A	706	1/1	0.98	0.15	56,56,56,56	0
7	NA	B	723	1/1	0.98	0.16	46,46,46,46	0
4	CA	B	709	1/1	0.98	0.13	47,47,47,47	0
4	CA	A	711	1/1	0.99	0.14	34,34,34,34	0
4	CA	A	715	1/1	0.99	0.10	44,44,44,44	0
4	CA	A	712	1/1	0.99	0.19	33,33,33,33	0
4	CA	B	713	1/1	0.99	0.20	38,38,38,38	0
4	CA	B	715	1/1	0.99	0.11	44,44,44,44	0
4	CA	B	710	1/1	0.99	0.12	32,32,32,32	0
4	CA	A	720	1/1	0.99	0.08	48,48,48,48	0
4	CA	A	714	1/1	0.99	0.21	29,29,29,29	0
7	NA	A	724	1/1	0.99	0.15	14,14,14,14	0
4	CA	A	713	1/1	1.00	0.16	18,18,18,18	0
4	CA	A	709	1/1	1.00	0.12	21,21,21,21	0
4	CA	B	711	1/1	1.00	0.16	28,28,28,28	0
4	CA	A	710	1/1	1.00	0.13	23,23,23,23	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.