



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:22 AM BST

PDB ID : 4BSW  
Title : Heterodimeric Fc Antibody Azymetric Variant 2  
Authors : Suits, M.D.L.; Spreter, T.; Cabrera, E.E.; Dixit, S.B.; Lario, P.I.; Poon, D.K.Y.; D'Angelo, I.E.P.; Boulanger, M.J.  
Deposited on : 2013-06-11  
Resolution : 2.15 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

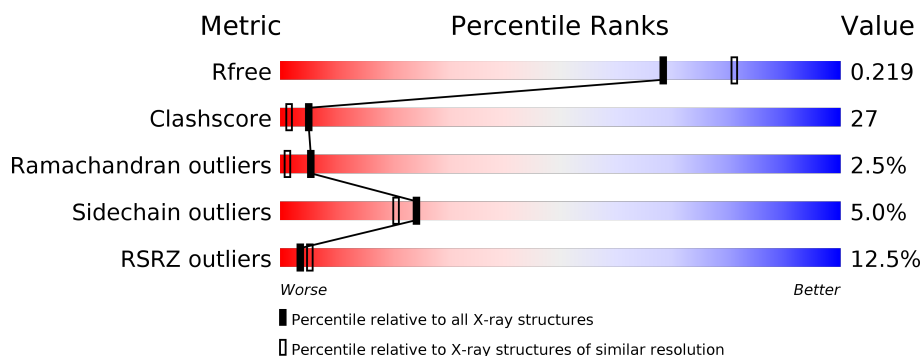
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	232	<div> <div>13%</div> <div>41%</div> <div>44%</div> <div>7%</div> <div>7%</div> </div>
2	B	232	<div> <div>10%</div> <div>38%</div> <div>47%</div> <div>7%</div> <div>7%</div> </div>
3	C	9	<div> <div>11%</div> <div>44%</div> <div>44%</div> </div>
3	D	9	<div> <div>11%</div> <div>89%</div> </div>

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2[B]	-	-	X	-
3	NAG	C	5[A]	-	-	X	-
3	GAL	C	6[A]	-	-	-	X
3	GAL	C	6[B]	-	-	-	X
3	NAG	D	1[B]	-	-	X	-
3	FUC	D	9[B]	-	-	X	-
4	EDO	A	1446[A]	-	-	-	X
4	EDO	A	1446[B]	-	-	-	X
4	EDO	A	1449[A]	-	-	X	-
4	EDO	B	1446[A]	-	-	X	-
4	EDO	B	1448[A]	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7555 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 HETERODIMERIC FC ANTIBODY AZYMETRIC VARIANT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	210	0
			3350	2136	564	638	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	GLY	-	expression tag	UNP P01857
A	350	VAL	THR	engineered mutation	UNP P01857
A	351	TYR	LEU	microheterogeneity	UNP P01857
A	366	LEU	THR	microheterogeneity	UNP P01857
A	392	LEU	LYS	microheterogeneity	UNP P01857
A	394	THR	TRP	microheterogeneity	UNP P01857
A	405	ALA	PHE	microheterogeneity	UNP P01857
A	407	VAL	TYR	microheterogeneity	UNP P01857

- Molecule 2 is a protein called HETERODIMERIC FC ANTIBODY AZYMETRIC VARIANT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	210	0
			3350	2136	564	638	12			

There are 8 discrepancies between the modelled and reference sequences:

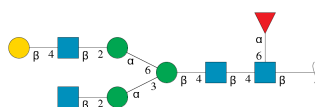
Chain	Residue	Modelled	Actual	Comment	Reference
B	222	GLY	-	expression tag	UNP P01857
B	350	VAL	THR	engineered mutation	UNP P01857
B	351	TYR	LEU	microheterogeneity	UNP P01857
B	366	LEU	THR	microheterogeneity	UNP P01857
B	392	LEU	LYS	microheterogeneity	UNP P01857
B	394	THR	TRP	microheterogeneity	UNP P01857

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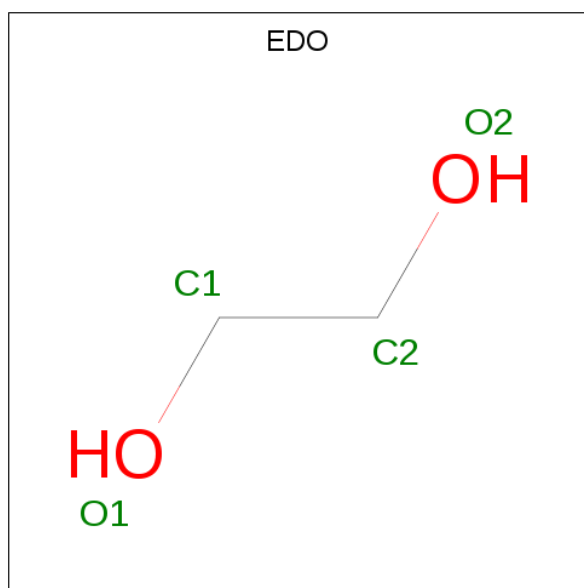
Chain	Residue	Modelled	Actual	Comment	Reference
B	405	ALA	PHE	microheterogeneity	UNP P01857
B	407	VAL	TYR	microheterogeneity	UNP P01857

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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
3	C	9	Total	C	N	O	0	9	0
			220	124	8	88			
3	D	9	Total	C	N	O	0	9	0
			220	124	8	88			

- Molecule 4 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
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	1
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			8	4	4		
4	B	1	Total	C	O	0	1
			8	4	4		
4	B	1	Total	C	O	0	1
			8	4	4		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

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

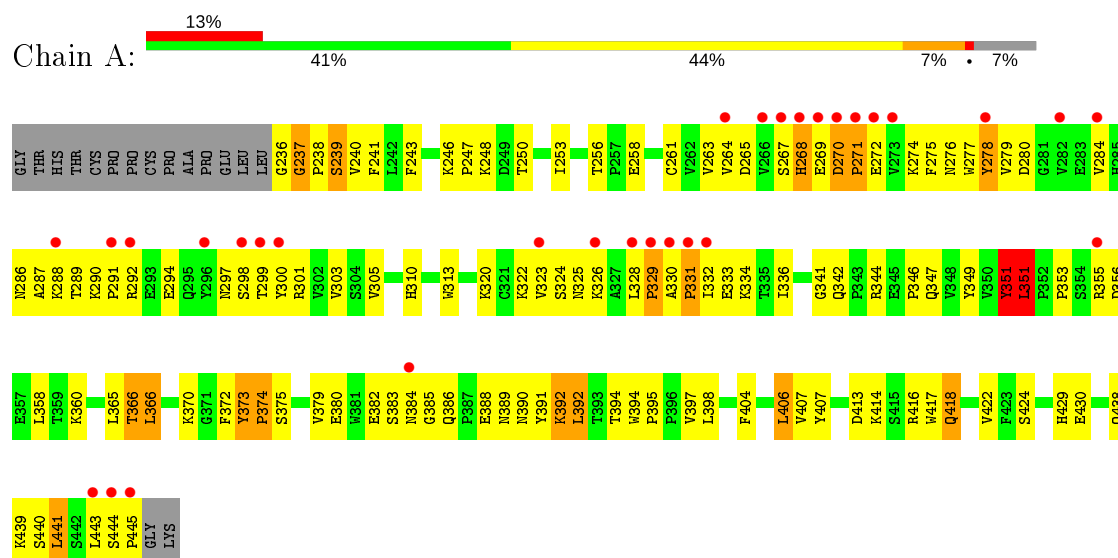
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	204	Total	O	0	0
			204	204		

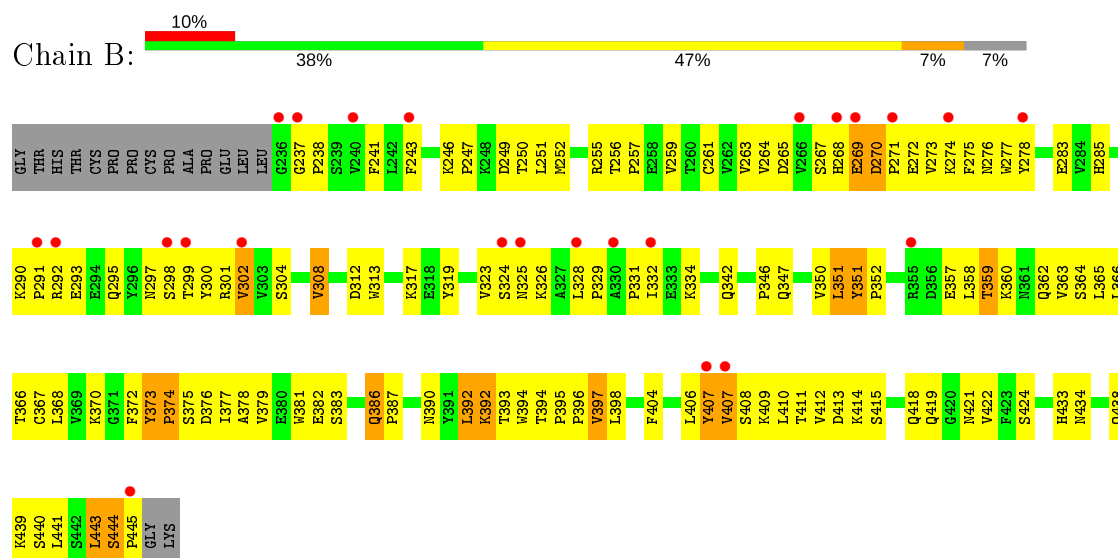
### 3 Residue-property plots

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: HETERODIMERIC FC ANTIBODY AZYMETRIC VARIANT 2



#### • Molecule 2: HETERODIMERIC FC ANTIBODY AZYMETRIC VARIANT 2



#### • Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr

anose-(1-3)]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

Chain C:  11% 44% 44%

NAG1	NAG2	BMA3	MAN4	NAG5	GAL6	MAN7	NAG8	FUC9
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● Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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

Chain D:  11% 89%

NAG1	NAG2	BMA3	MAN4	NAG5	GAL6	MAN7	NAG8	FUC9
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.68 Å 74.72 Å 148.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.26 – 2.15 47.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.26-2.15) 99.9 (47.12-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.200 , 0.259 0.207 , 0.219	Depositor DCC
$R_{free}$ test set	1679 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7555	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.25% 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: BMA, NAG, EDO, GAL, FUC, IOD, 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	0.64	7/3439 (0.2%)	0.66	0/4678
2	B	0.72	8/3439 (0.2%)	0.80	10/4678 (0.2%)
All	All	0.68	15/6878 (0.2%)	0.73	10/9356 (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	A	0	3
2	B	0	5
All	All	0	8

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392[B]	LEU	C-N	13.03	1.64	1.34
2	B	397[A]	VAL	C-N	-12.13	1.06	1.34
2	B	397[B]	VAL	C-N	-12.13	1.06	1.34
2	B	270[A]	ASP	C-N	10.67	1.54	1.34
2	B	270[B]	ASP	C-N	10.67	1.54	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	396[A]	PRO	O-C-N	-13.85	100.54	122.70
2	B	396[B]	PRO	O-C-N	-13.85	100.54	122.70
2	B	396[A]	PRO	CA-C-N	10.05	139.32	117.20
2	B	396[B]	PRO	CA-C-N	10.05	139.32	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	396[A]	PRO	C-N-CA	7.95	141.57	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373[A]	TYR	Mainchain,Peptide
1	A	373[B]	TYR	Peptide
2	B	373[A]	TYR	Mainchain,Peptide
2	B	373[B]	TYR	Mainchain,Peptide
2	B	397[A]	VAL	Mainchain

## 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	3350	0	3273	159	0
2	B	3350	0	3271	173	0
3	C	220	0	187	28	0
3	D	220	0	190	31	0
4	A	16	0	24	11	0
4	B	24	0	36	19	0
5	A	3	0	0	0	0
5	B	1	0	0	1	0
6	A	167	0	0	27	0
6	B	204	0	0	32	0
All	All	7555	0	6981	367	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 27.

The worst 5 of 367 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:322[B]:LYS:CE	1:A:333[B]:GLU:OE2	1.89	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386[A]:GLN:NE2	6:A:2121:HOH:O	1.74	1.20
1:A:322[B]:LYS:HE2	1:A:333[B]:GLU:OE2	1.00	1.16
2:B:238[A]:PRO:HG2	2:B:328[A]:LEU:HD21	1.22	1.15
4:B:1446[B]:EDO:H12	6:B:2204:HOH:O	1.48	1.13

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	404/232 (174%)	360 (89%)	28 (7%)	16 (4%)	3	0
2	B	404/232 (174%)	380 (94%)	20 (5%)	4 (1%)	15	9
All	All	808/464 (174%)	740 (92%)	48 (6%)	20 (2%)	5	1

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374[A]	PRO
1	A	374[B]	PRO
2	B	359[A]	THR
2	B	359[B]	THR
2	B	374[A]	PRO

### 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	389/213 (183%)	369 (95%)	20 (5%)	24	20
2	B	389/213 (183%)	373 (96%)	16 (4%)	30	29
All	All	778/426 (183%)	742 (95%)	36 (5%)	24	23

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418[A]	GLN
2	B	302[A]	VAL
2	B	443[B]	LEU
1	A	441[A]	LEU
2	B	302[B]	VAL

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

### 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 ⓘ

36 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	$\# Z  > 2$
3	NAG	C	1[A]	1,3	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
3	NAG	C	1[B]	1,3	14,14,15	0.35	0	17,19,21	0.67	0
3	NAG	C	2[A]	3	14,14,15	0.69	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	2[B]	3	14,14,15	0.68	0	17,19,21	1.43	3 (17%)
3	BMA	C	3[A]	3	11,11,12	0.40	0	15,15,17	1.30	3 (20%)
3	BMA	C	3[B]	3	11,11,12	0.36	0	15,15,17	0.92	1 (6%)
3	MAN	C	4[A]	3	11,11,12	0.79	1 (9%)	15,15,17	1.23	2 (13%)
3	MAN	C	4[B]	3	11,11,12	0.37	0	15,15,17	0.83	0
3	NAG	C	5[A]	3	14,14,15	0.38	0	17,19,21	0.81	0
3	NAG	C	5[B]	3	14,14,15	0.29	0	17,19,21	0.62	0
3	GAL	C	6[A]	1,3	11,11,12	0.38	0	15,15,17	1.18	1 (6%)
3	GAL	C	6[B]	3	11,11,12	0.26	0	15,15,17	0.63	0
3	MAN	C	7[A]	3	11,11,12	0.29	0	15,15,17	0.97	1 (6%)
3	MAN	C	7[B]	3	11,11,12	0.30	0	15,15,17	0.97	1 (6%)
3	NAG	C	8[A]	3	14,14,15	0.30	0	17,19,21	0.69	0
3	NAG	C	8[B]	3	14,14,15	0.31	0	17,19,21	0.68	0
3	FUC	C	9[A]	3	10,10,11	0.92	1 (10%)	14,14,16	1.11	1 (7%)
3	FUC	C	9[B]	3	10,10,11	0.31	0	14,14,16	0.72	0
3	NAG	D	1[A]	3,2	14,14,15	0.39	0	17,19,21	0.64	0
3	NAG	D	1[B]	3,2	14,14,15	0.38	0	17,19,21	2.27	3 (17%)
3	NAG	D	2[A]	3	14,14,15	0.54	0	17,19,21	1.21	3 (17%)
3	NAG	D	2[B]	3	14,14,15	0.53	0	17,19,21	1.23	2 (11%)
3	BMA	D	3[A]	3	11,11,12	0.38	0	15,15,17	0.72	0
3	BMA	D	3[B]	3	11,11,12	0.45	0	15,15,17	1.38	3 (20%)
3	MAN	D	4[A]	3	11,11,12	0.35	0	15,15,17	0.83	1 (6%)
3	MAN	D	4[B]	3	11,11,12	0.75	1 (9%)	15,15,17	0.72	0
3	NAG	D	5[A]	3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	D	5[B]	3	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
3	GAL	D	6[A]	3	11,11,12	0.26	0	15,15,17	0.64	0
3	GAL	D	6[B]	3	11,11,12	0.35	0	15,15,17	0.94	1 (6%)
3	MAN	D	7[A]	3	11,11,12	0.92	1 (9%)	15,15,17	0.77	0
3	MAN	D	7[B]	3	11,11,12	0.36	0	15,15,17	1.06	0
3	NAG	D	8[A]	3	14,14,15	0.52	0	17,19,21	1.11	1 (5%)
3	NAG	D	8[B]	3	14,14,15	0.39	0	17,19,21	0.60	0
3	FUC	D	9[A]	3	10,10,11	0.33	0	14,14,16	0.97	1 (7%)
3	FUC	D	9[B]	3	10,10,11	0.67	0	14,14,16	1.20	1 (7%)

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	NAG	C	1[A]	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1[B]	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2[A]	3	-	2/6/23/26	0/1/1/1
3	NAG	C	2[B]	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3[A]	3	-	0/2/19/22	0/1/1/1
3	BMA	C	3[B]	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4[A]	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4[B]	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5[A]	3	-	0/6/23/26	0/1/1/1
3	NAG	C	5[B]	3	-	2/6/23/26	0/1/1/1
3	GAL	C	6[A]	1,3	-	2/2/19/22	0/1/1/1
3	GAL	C	6[B]	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7[A]	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7[B]	3	-	2/2/19/22	0/1/1/1
3	NAG	C	8[A]	3	-	4/6/23/26	0/1/1/1
3	NAG	C	8[B]	3	-	4/6/23/26	0/1/1/1
3	FUC	C	9[A]	3	-	-	0/1/1/1
3	FUC	C	9[B]	3	-	-	0/1/1/1
3	NAG	D	1[A]	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	1[B]	3,2	-	1/6/23/26	0/1/1/1
3	NAG	D	2[A]	3	-	2/6/23/26	0/1/1/1
3	NAG	D	2[B]	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3[A]	3	-	1/2/19/22	0/1/1/1
3	BMA	D	3[B]	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4[A]	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4[B]	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5[A]	3	-	1/6/23/26	0/1/1/1
3	NAG	D	5[B]	3	-	0/6/23/26	0/1/1/1
3	GAL	D	6[A]	3	-	1/2/19/22	0/1/1/1
3	GAL	D	6[B]	3	-	1/2/19/22	0/1/1/1
3	MAN	D	7[A]	3	-	1/2/19/22	0/1/1/1
3	MAN	D	7[B]	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8[A]	3	-	4/6/23/26	0/1/1/1
3	NAG	D	8[B]	3	-	4/6/23/26	0/1/1/1
3	FUC	D	9[A]	3	-	-	0/1/1/1
3	FUC	D	9[B]	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7[A]	MAN	O6-C6	2.95	1.54	1.42
3	C	4[A]	MAN	O5-C1	-2.16	1.40	1.43
3	C	9[A]	FUC	O5-C1	-2.03	1.40	1.43
3	D	4[B]	MAN	O5-C1	-2.01	1.40	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1[B]	NAG	C1-O5-C5	7.82	122.79	112.19
3	D	3[B]	BMA	C1-C2-C3	3.37	113.81	109.67
3	C	2[B]	NAG	O5-C1-C2	-3.31	106.06	111.29
3	C	9[A]	FUC	O5-C1-C2	-2.87	106.34	110.77
3	C	6[A]	GAL	C1-C2-C3	2.84	113.16	109.67

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	8[A]	NAG	C8-C7-N2-C2
3	C	8[A]	NAG	O7-C7-N2-C2
3	C	8[B]	NAG	C8-C7-N2-C2
3	C	8[B]	NAG	O7-C7-N2-C2
3	D	8[B]	NAG	C8-C7-N2-C2

There are no ring outliers.

22 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	7[A]	MAN	4	0
3	D	7[B]	MAN	5	0
3	C	9[A]	FUC	1	0
3	D	9[B]	FUC	7	0
3	C	6[A]	GAL	2	0
3	C	6[B]	GAL	4	0
3	D	2[A]	NAG	2	0
3	D	5[A]	NAG	2	0
3	D	6[B]	GAL	1	0
3	D	6[A]	GAL	1	0
3	D	2[B]	NAG	5	0
3	D	3[B]	BMA	5	0
3	D	1[B]	NAG	7	0
3	D	8[B]	NAG	2	0

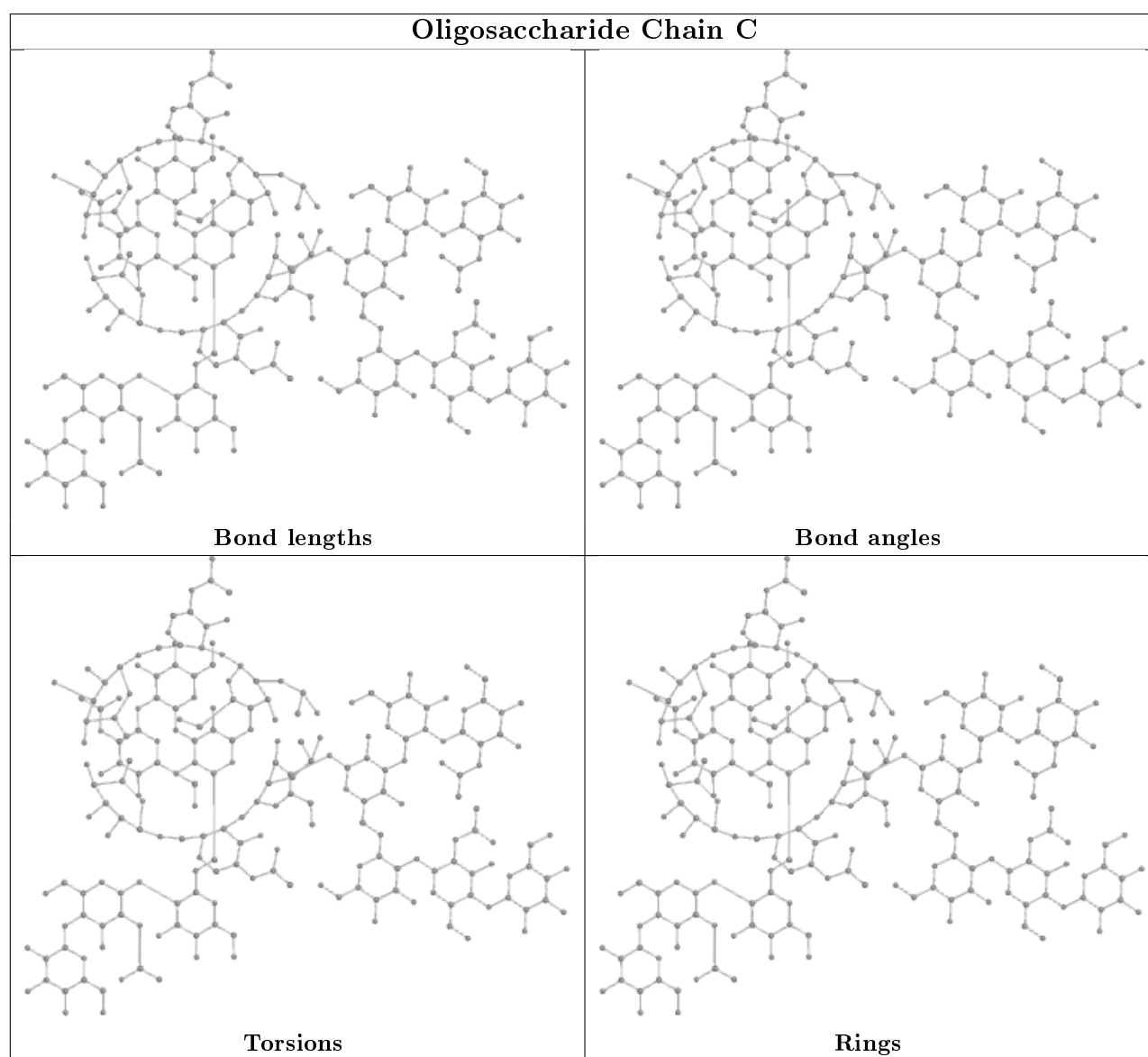
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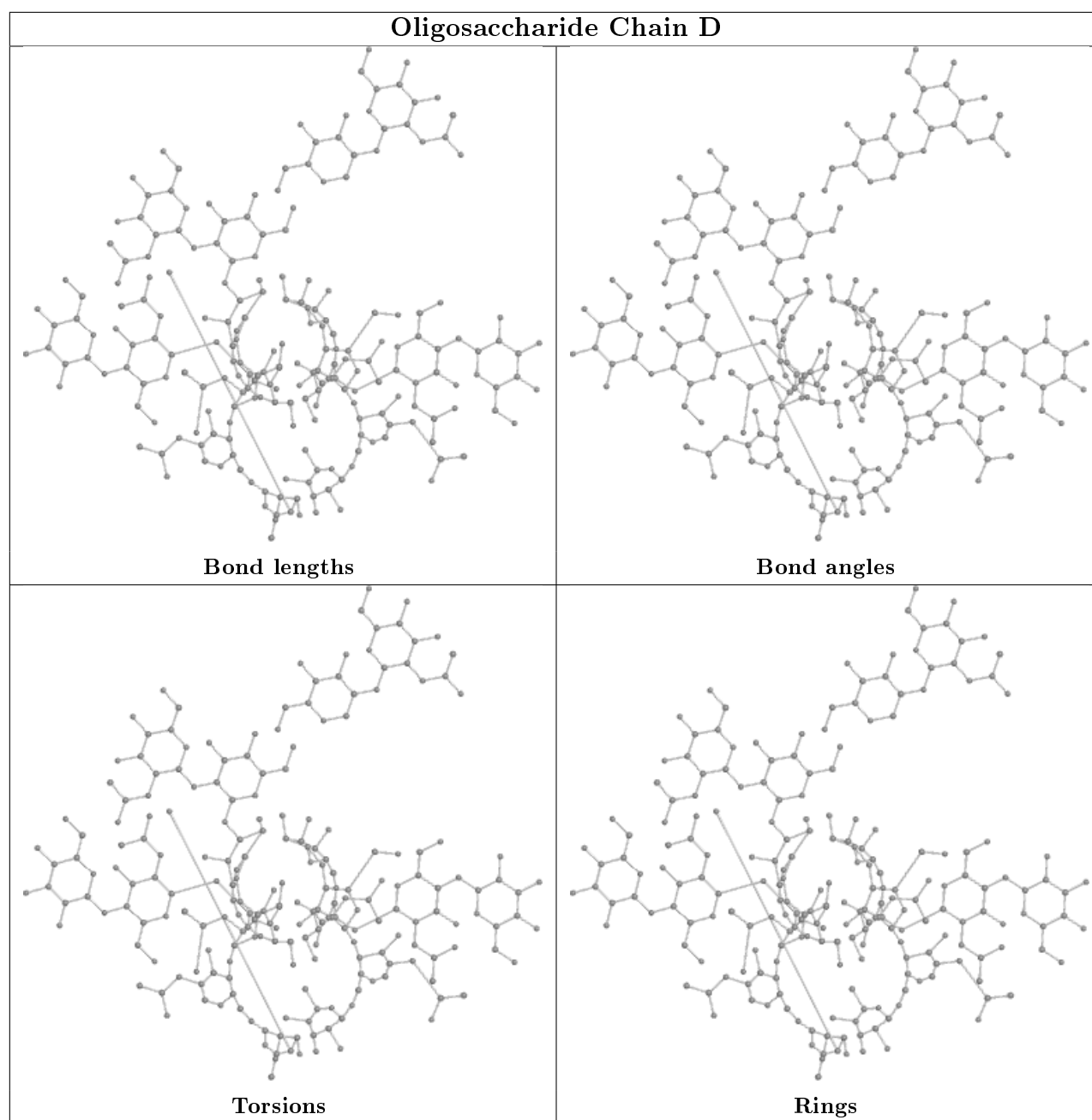


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3[A]	BMA	4	0
3	D	8[A]	NAG	2	0
3	C	1[A]	NAG	1	0
3	C	1[B]	NAG	1	0
3	C	2[B]	NAG	7	0
3	C	5[A]	NAG	7	0
3	C	2[A]	NAG	4	0
3	C	5[B]	NAG	4	0

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	EDO	B	1446[A]	-	3,3,3	0.44	0	2,2,2	0.72	0
4	EDO	B	1448[B]	-	3,3,3	0.56	0	2,2,2	0.33	0
4	EDO	B	1447[B]	-	3,3,3	0.69	0	2,2,2	0.28	0
4	EDO	B	1446[B]	-	3,3,3	0.52	0	2,2,2	0.07	0
4	EDO	B	1448[A]	-	3,3,3	0.55	0	2,2,2	0.30	0
4	EDO	A	1449[A]	-	3,3,3	0.55	0	2,2,2	0.34	0
4	EDO	B	1447[A]	-	3,3,3	0.45	0	2,2,2	0.16	0
4	EDO	A	1446[A]	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	A	1446[B]	-	3,3,3	0.54	0	2,2,2	0.42	0
4	EDO	A	1449[B]	-	3,3,3	0.56	0	2,2,2	0.30	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	EDO	B	1446[A]	-	-	1/1/1/1	-
4	EDO	B	1448[B]	-	-	0/1/1/1	-
4	EDO	B	1447[B]	-	-	1/1/1/1	-
4	EDO	B	1446[B]	-	-	1/1/1/1	-
4	EDO	B	1448[A]	-	-	0/1/1/1	-
4	EDO	A	1449[A]	-	-	1/1/1/1	-
4	EDO	B	1447[A]	-	-	0/1/1/1	-
4	EDO	A	1446[A]	-	-	0/1/1/1	-
4	EDO	A	1446[B]	-	-	1/1/1/1	-
4	EDO	A	1449[B]	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1449[B]	EDO	O1-C1-C2-O2
4	A	1449[A]	EDO	O1-C1-C2-O2
4	A	1446[B]	EDO	O1-C1-C2-O2
4	B	1446[A]	EDO	O1-C1-C2-O2
4	B	1447[B]	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1446[A]	EDO	7	0
4	B	1448[B]	EDO	3	0
4	B	1447[B]	EDO	1	0
4	B	1446[B]	EDO	3	0
4	B	1448[A]	EDO	5	0
4	A	1449[A]	EDO	6	0
4	A	1446[B]	EDO	3	0
4	A	1449[B]	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	396[A]:PRO	C	397[A]:VAL	N	1.15
1	B	269[B]:GLU	C	270[B]:ASP	N	1.07
1	B	397[A]:VAL	C	398[A]:LEU	N	1.06

## 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	216/232 (93%)	0.91	31 (14%) <b>2</b> <b>3</b>	26, 42, 71, 83	12 (5%)
2	B	216/232 (93%)	0.87	22 (10%) <b>6</b> <b>10</b>	24, 40, 66, 86	12 (5%)
All	All	432/464 (93%)	0.89	53 (12%) <b>3</b> <b>5</b>	24, 41, 69, 86	24 (5%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330[A]	ALA	5.4
1	A	296[A]	TYR	5.3
2	B	445[A]	PRO	4.8
2	B	266[A]	VAL	4.4
1	A	300[A]	TYR	4.2

### 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
3	NAG	C	8[A]	14/15	0.68	0.29	97,102,111,114	14
3	NAG	C	8[B]	14/15	0.68	0.29	94,99,115,130	14
3	GAL	C	6[A]	11/12	<b>0.71</b>	<b>0.46</b>	59,65,76,87	11
3	GAL	C	6[B]	11/12	<b>0.71</b>	<b>0.46</b>	40,50,57,65	11
3	GAL	D	6[B]	11/12	0.74	0.32	52,68,77,89	11

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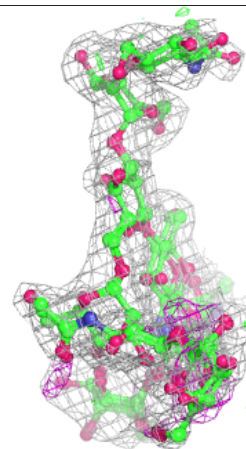
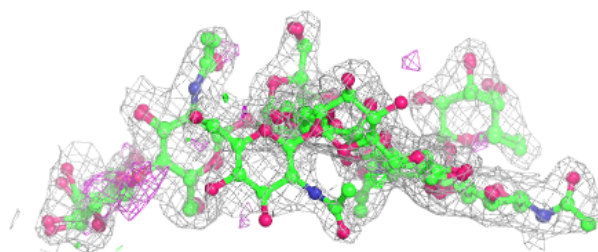
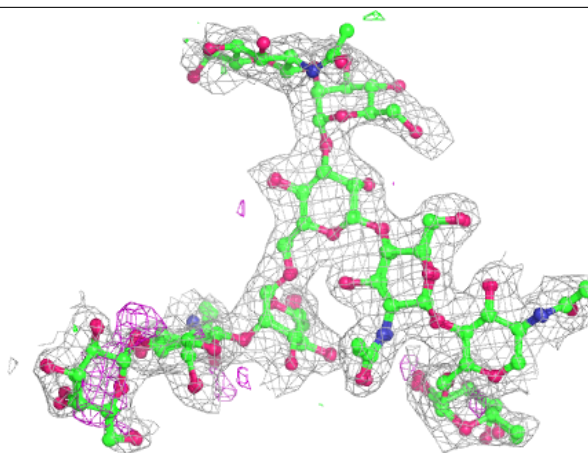
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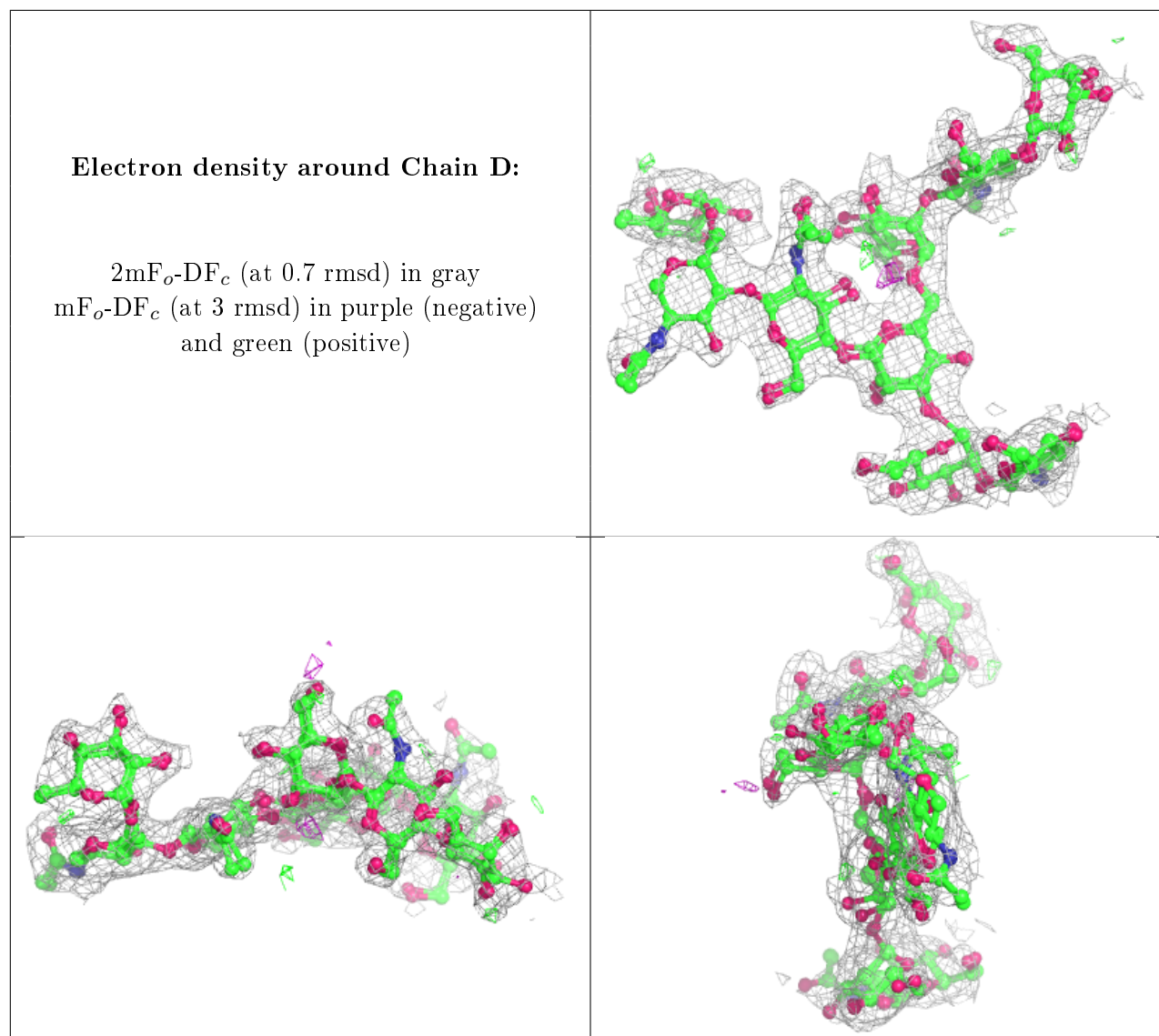
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	D	6[A]	11/12	0.74	0.32	81,86,96,104	11
3	NAG	D	8[B]	14/15	0.74	0.28	85,100,103,103	14
3	NAG	D	8[A]	14/15	0.74	0.28	101,116,123,124	14
3	MAN	D	7[B]	11/12	0.82	0.29	50,61,76,88	11
3	FUC	D	9[A]	10/11	0.82	0.24	57,67,78,79	10
3	FUC	C	9[A]	10/11	0.82	0.22	63,72,78,81	10
3	FUC	D	9[B]	10/11	0.82	0.24	67,72,76,78	10
3	MAN	C	7[A]	11/12	0.82	0.20	65,75,84,87	11
3	FUC	C	9[B]	10/11	0.82	0.22	64,73,83,85	10
3	MAN	D	7[A]	11/12	0.82	0.29	65,82,86,100	11
3	MAN	C	7[B]	11/12	0.82	0.20	64,75,78,80	11
3	NAG	C	5[A]	14/15	0.85	0.17	43,47,52,52	14
3	NAG	C	5[B]	14/15	0.85	0.17	41,45,50,53	14
3	MAN	D	4[B]	11/12	0.88	0.20	46,48,53,58	11
3	MAN	D	4[A]	11/12	0.88	0.20	51,58,65,66	11
3	NAG	D	5[B]	14/15	0.89	0.24	38,47,52,55	14
3	NAG	D	5[A]	14/15	0.89	0.24	76,84,95,96	14
3	BMA	D	3[A]	11/12	0.91	0.14	59,68,75,76	11
3	BMA	D	3[B]	11/12	0.91	0.14	42,49,53,53	11
3	NAG	D	2[B]	14/15	0.93	0.16	34,44,50,55	14
3	NAG	D	1[B]	14/15	0.93	0.18	44,52,61,72	14
3	NAG	D	2[A]	14/15	0.93	0.16	65,70,72,74	14
3	NAG	D	1[A]	14/15	0.93	0.18	69,71,76,80	14
3	NAG	C	1[B]	14/15	0.94	0.13	46,56,63,71	14
3	NAG	C	2[B]	14/15	0.94	0.15	41,44,56,57	14
3	NAG	C	1[A]	14/15	0.94	0.13	53,62,68,71	14
3	BMA	C	3[A]	11/12	0.94	0.11	42,48,54,55	11
3	NAG	C	2[A]	14/15	0.94	0.15	40,50,58,62	14
3	BMA	C	3[B]	11/12	0.94	0.11	40,46,53,54	11
3	MAN	C	4[B]	11/12	0.95	0.13	41,46,51,52	11
3	MAN	C	4[A]	11/12	0.95	0.13	43,49,56,59	11

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 [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	EDO	A	1446[B]	4/4	0.73	0.46	25,30,38,38	4
4	EDO	A	1446[A]	4/4	0.73	0.46	26,27,30,32	4
4	EDO	B	1447[A]	4/4	0.88	0.27	42,55,64,64	4
4	EDO	B	1447[B]	4/4	0.88	0.27	37,43,51,53	4
4	EDO	A	1449[A]	4/4	0.91	0.26	45,50,52,53	4
4	EDO	A	1449[B]	4/4	0.91	0.26	52,52,52,57	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	1448[B]	4/4	0.93	0.24	34,43,43,48	4
4	EDO	B	1446[A]	4/4	0.93	0.20	41,42,47,52	4
4	EDO	B	1446[B]	4/4	0.93	0.20	41,45,47,48	4
4	EDO	B	1448[A]	4/4	0.93	0.24	34,35,36,36	4
5	IOD	A	1447[A]	1/1	0.99	0.10	48,48,48,48	1
5	IOD	A	1447[B]	1/1	0.99	0.10	48,48,48,48	1
5	IOD	A	1451	1/1	1.00	0.18	37,37,37,37	1
5	IOD	B	1449[B]	1/1	1.00	0.18	31,31,31,31	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.