



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 08:31 AM EDT

PDB ID : 4AXB  
Title : Crystal structure of soman-aged human butyrylcholinesterase in complex with 2-PAM  
Authors : Wandhammer, M.; de Koning, M.; Noort, D.; Goeldner, M.; Nachon, F.  
Deposited on : 2012-06-12  
Resolution : 2.40 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.

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

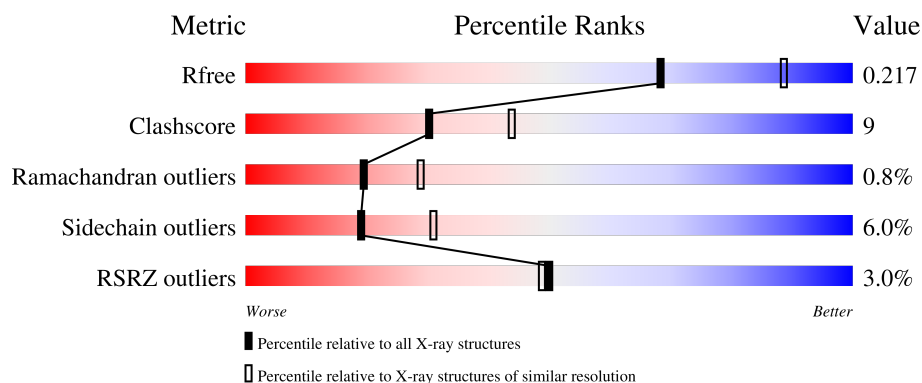
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	527	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div> </div>
2	B	3	<div> <div>100%</div> </div>
2	C	3	<div> <div>100%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	1	X	-	-	-
2	NAG	C	2	-	-	-	X
4	SO4	A	1531	-	-	X	-

## 2 Entry composition

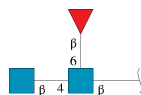
There are 9 unique types of molecules in this entry. The entry contains 4792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	P	S	0	10	0
			4261	2751	713	780	1	16			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total	0	0
			2 K		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

*Continued on next page...*

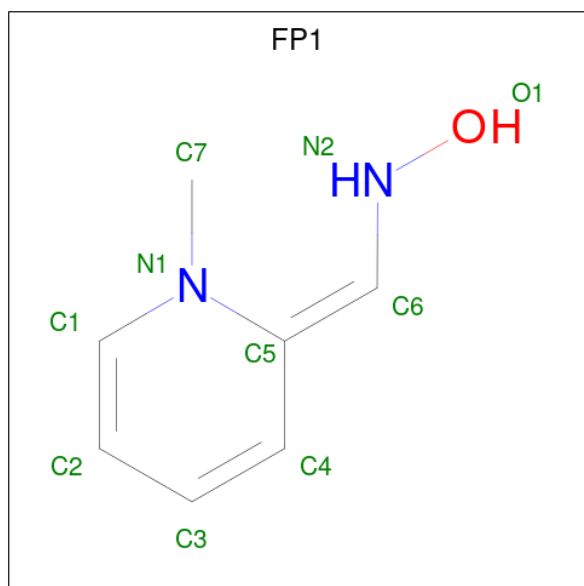
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is N-hydroxy-1-(1-methylpyridin-2(1H)-ylidene)methanamine (three-letter code: FP1) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

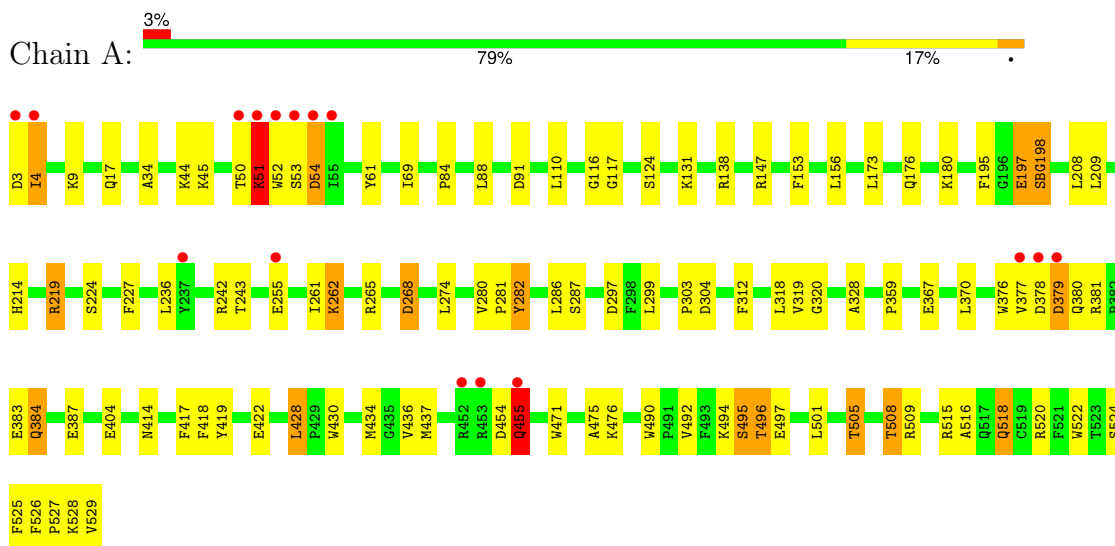
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	356	Total	O	0	0
			356	356		

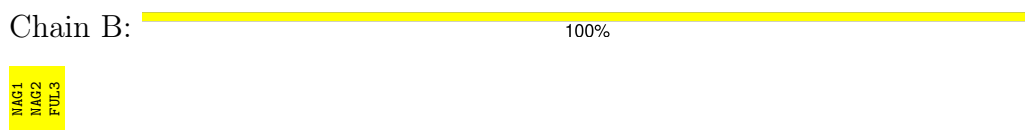
### 3 Residue-property plots

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.

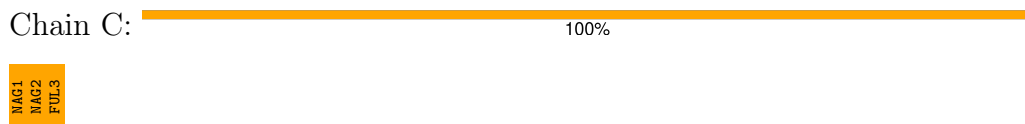
#### • Molecule 1: CHOLINESTERASE



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.95Å 155.95Å 127.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.27 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (110.27-2.40) 99.6 (49.32-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.168 , 0.221 0.165 , 0.217	Depositor DCC
$R_{free}$ test set	1563 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: NAG, GOL, SO4, CL, FP1, FUL, SBG, K

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	3.50	7/4406 (0.2%)	1.07	10/5978 (0.2%)

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	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	155.49	5.21	1.32
1	A	455[B]	GLN	CD-NE2	155.49	5.21	1.32
1	A	436	VAL	CB-CG2	6.42	1.66	1.52
1	A	153	PHE	CE1-CZ	5.99	1.48	1.37
1	A	404	GLU	CG-CD	5.88	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455[A]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[B]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[A]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	455[B]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	219	ARG	NE-CZ-NH2	-6.27	117.17	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455[A]	GLN	Sidechain
1	A	455[B]	GLN	Sidechain

## 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	4261	0	4165	77	0
2	B	38	0	34	0	0
2	C	38	0	34	3	0
3	A	2	0	0	0	1
4	A	10	0	0	2	0
5	A	18	0	24	3	0
6	A	3	0	0	1	0
7	A	10	0	10	2	0
8	A	56	0	52	1	0
9	A	356	0	0	12	0
All	All	4792	0	4319	81	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 9.

The worst 5 of 81 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:4:ILE:HD12	1:A:4:ILE:N	1.79	0.96
6:A:1536:CL:CL	9:A:2230:HOH:O	2.20	0.95
1:A:381:ARG:HH11	1:A:384:GLN:HE22	1.18	0.92
4:A:1531:SO4:O2	9:A:2269:HOH:O	1.93	0.87
1:A:518:GLN:HE21	1:A:518:GLN:H	1.28	0.81

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)
3:A:1538:K:K	3:A:1538:K:K[5_555]	1.93	0.27

## 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	534/527 (101%)	508 (95%)	22 (4%)	4 (1%)	22	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	379	ASP
1	A	496	THR
1	A	54	ASP

### 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	461/451 (102%)	432 (94%)	29 (6%)	18	28

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	SER
1	A	508	THR
1	A	367[B]	GLU
1	A	471	TRP
1	A	367[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	275	ASN
1	A	380	GLN
1	A	384	GLN
1	A	518	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	SBG	A	198	1	8,9,10	2.60	3 (37%)	3,12,14	2.74	1 (33%)

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
1	SBG	A	198	1	-	2/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SBG	P1-OG	6.33	1.67	1.57
1	A	198	SBG	P1-O2	2.30	1.54	1.50
1	A	198	SBG	P1-C1	-2.04	1.72	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SBG	OG-CB-CA	4.45	112.48	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SBG	N-CA-CB-OG
1	A	198	SBG	CB-OG-P1-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SBG	2	0

## 5.5 Carbohydrates [i](#)

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	NAG	B	1	1,2	14,14,15	0.97	1 (7%)	17,19,21	2.33	7 (41%)
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	2.08	5 (29%)
2	FUL	B	3	2	10,10,11	1.20	0	14,14,16	2.39	5 (35%)
2	NAG	C	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	2.06	6 (35%)
2	NAG	C	2	2	14,14,15	1.03	1 (7%)	17,19,21	1.98	3 (17%)
2	FUL	C	3	2	10,10,11	0.93	0	14,14,16	1.92	4 (28%)

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	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
2	NAG	C	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	FUL	C	3	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.29	1.39	1.43
2	C	2	NAG	C1-C2	2.24	1.55	1.52
2	C	1	NAG	C1-C2	2.22	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	5.11	129.75	122.90
2	C	2	NAG	C1-O5-C5	4.90	118.75	112.19
2	B	1	NAG	C2-N2-C7	4.87	129.43	122.90
2	B	1	NAG	C8-C7-N2	4.51	123.59	116.12
2	B	2	NAG	C4-C3-C2	4.28	117.30	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1

5 of 11 torsion outliers are listed below:

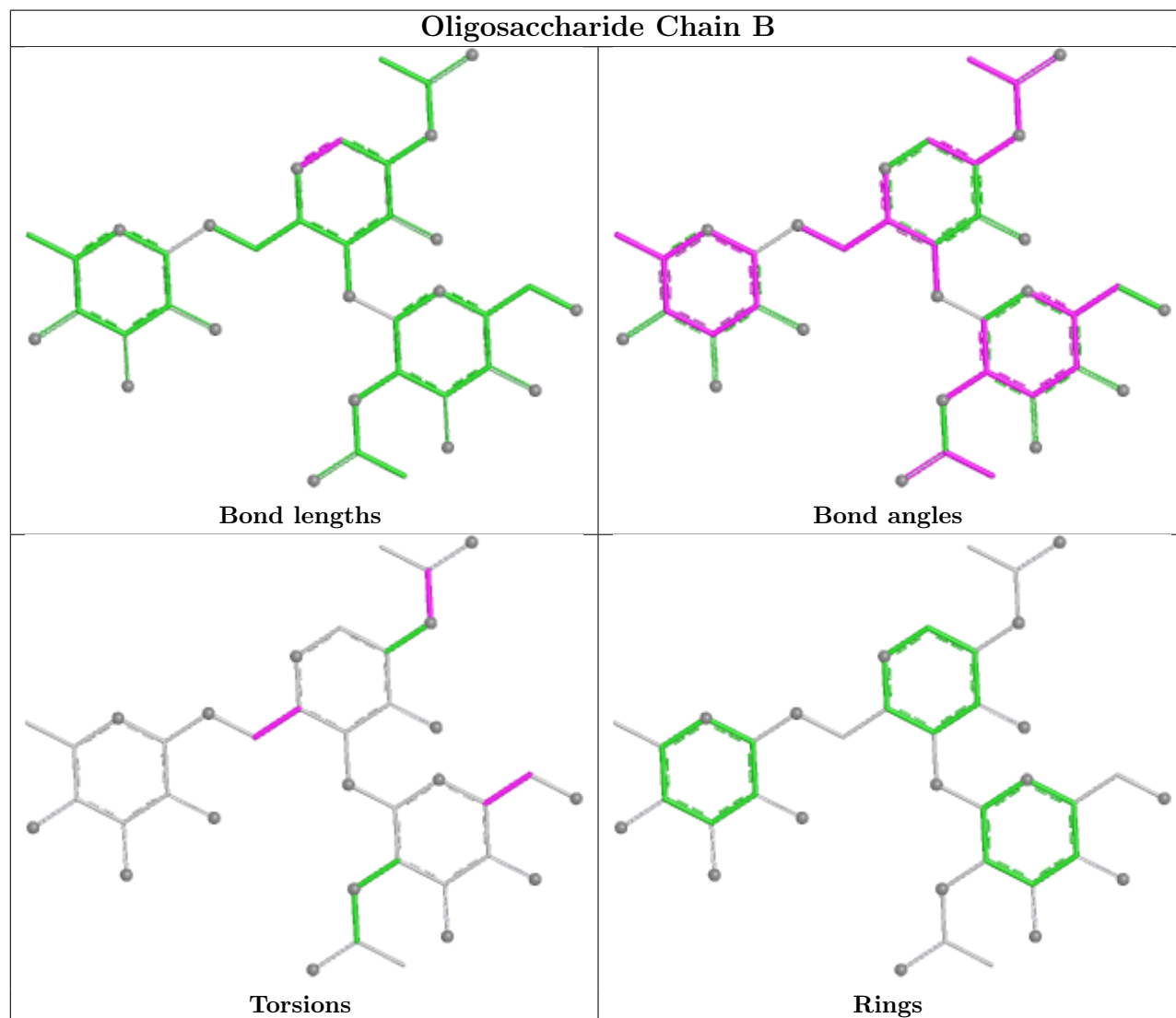
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2

There are no ring outliers.

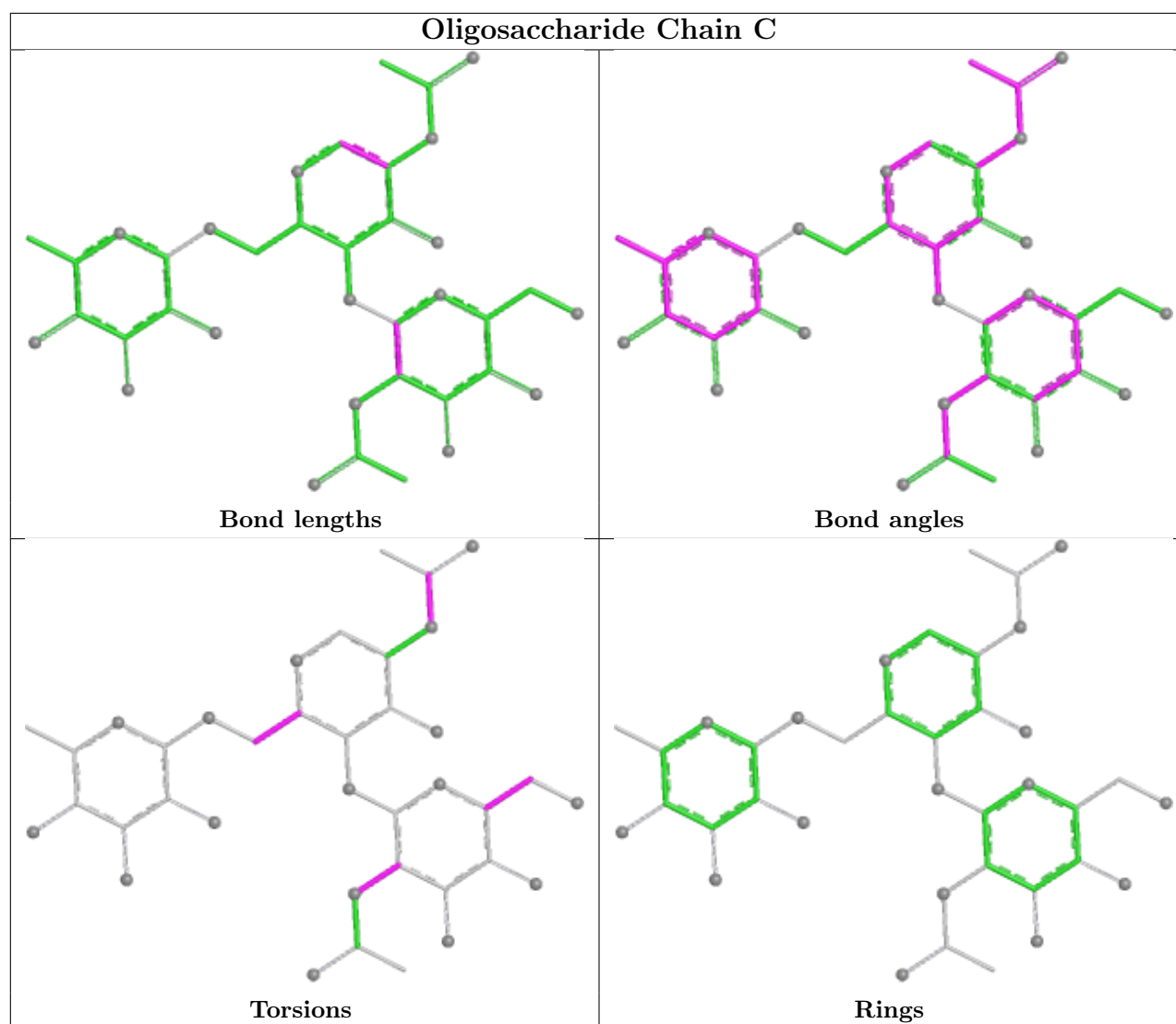
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	1	NAG	2	0
2	C	3	FUL	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](#)

Of 15 ligands modelled in this entry, 5 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	SO4	A	1531	-	4,4,4	0.47	0	6,6,6	0.45	0
8	NAG	A	1545	1	14,14,15	0.77	0	17,19,21	2.57	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	A	1546	1	14,14,15	0.74	0	17,19,21	2.77	6 (35%)
5	GOL	A	1533	-	5,5,5	0.32	0	5,5,5	1.63	1 (20%)
8	NAG	A	1547	1	14,14,15	0.82	0	17,19,21	1.39	1 (5%)
7	FP1	A	1535	-	9,10,10	2.44	3 (33%)	8,12,12	2.79	2 (25%)
5	GOL	A	1540	-	5,5,5	0.59	0	5,5,5	0.37	0
8	NAG	A	1544	1	14,14,15	1.16	1 (7%)	17,19,21	2.06	4 (23%)
4	SO4	A	1539	-	4,4,4	0.28	0	6,6,6	0.37	0
5	GOL	A	1532	-	5,5,5	0.43	0	5,5,5	0.82	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
8	NAG	A	1545	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1546	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1547	1	-	0/6/23/26	0/1/1/1
7	FP1	A	1535	-	-	0/0/3/3	0/1/1/1
5	GOL	A	1540	-	-	3/4/4/4	-
8	NAG	A	1544	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1533	-	-	2/4/4/4	-
5	GOL	A	1532	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1535	FP1	C7-N1	5.22	1.57	1.46
8	A	1544	NAG	C1-C2	3.27	1.56	1.52
7	A	1535	FP1	C6-N2	3.04	1.34	1.30
7	A	1535	FP1	C4-C5	-2.28	1.38	1.42

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1546	NAG	C1-O5-C5	9.05	124.31	112.19
7	A	1535	FP1	C5-C6-N2	-7.11	112.48	126.83
8	A	1545	NAG	C1-O5-C5	6.17	120.45	112.19
8	A	1544	NAG	C2-N2-C7	4.51	128.94	122.90
8	A	1547	NAG	O5-C5-C6	3.84	115.14	107.66

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1540	GOL	C1-C2-C3-O3
5	A	1540	GOL	O2-C2-C3-O3
8	A	1544	NAG	C8-C7-N2-C2
8	A	1544	NAG	O7-C7-N2-C2
8	A	1545	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1531	SO4	2	0
8	A	1545	NAG	1	0
5	A	1533	GOL	1	0
7	A	1535	FP1	2	0
5	A	1540	GOL	1	0
5	A	1532	GOL	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	526/527 (99%)	-0.36	16 (3%)	50 49	18, 33, 62, 80	1 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.2
1	A	378	ASP	3.6
1	A	55	ILE	3.4
1	A	54	ASP	3.3
1	A	453	ARG	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SBG	A	198	10/11	0.99	0.14	11,18,22,22	0

### 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.

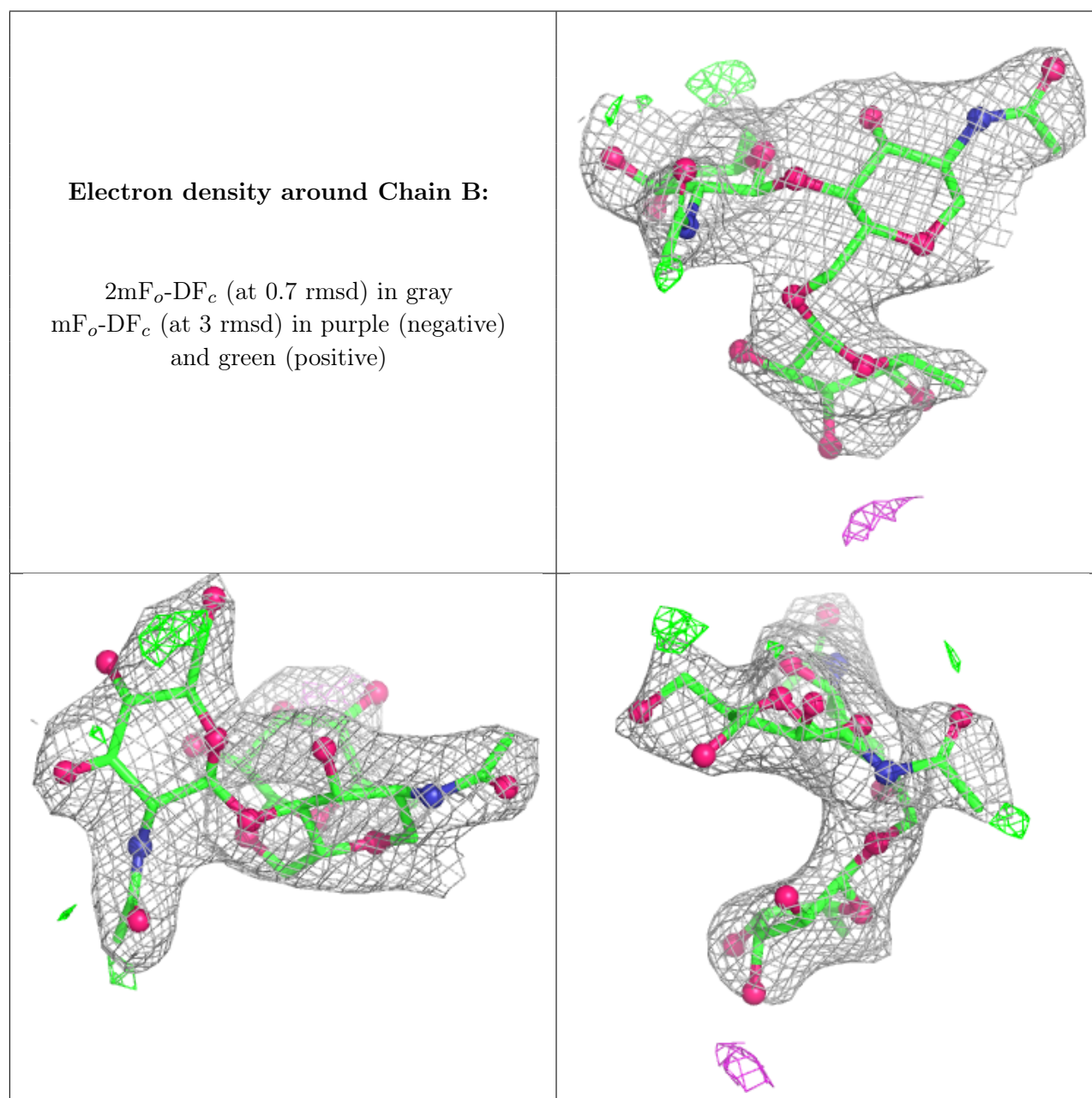
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	NAG	C	2	14/15	0.44	0.50	98,104,107,108	0

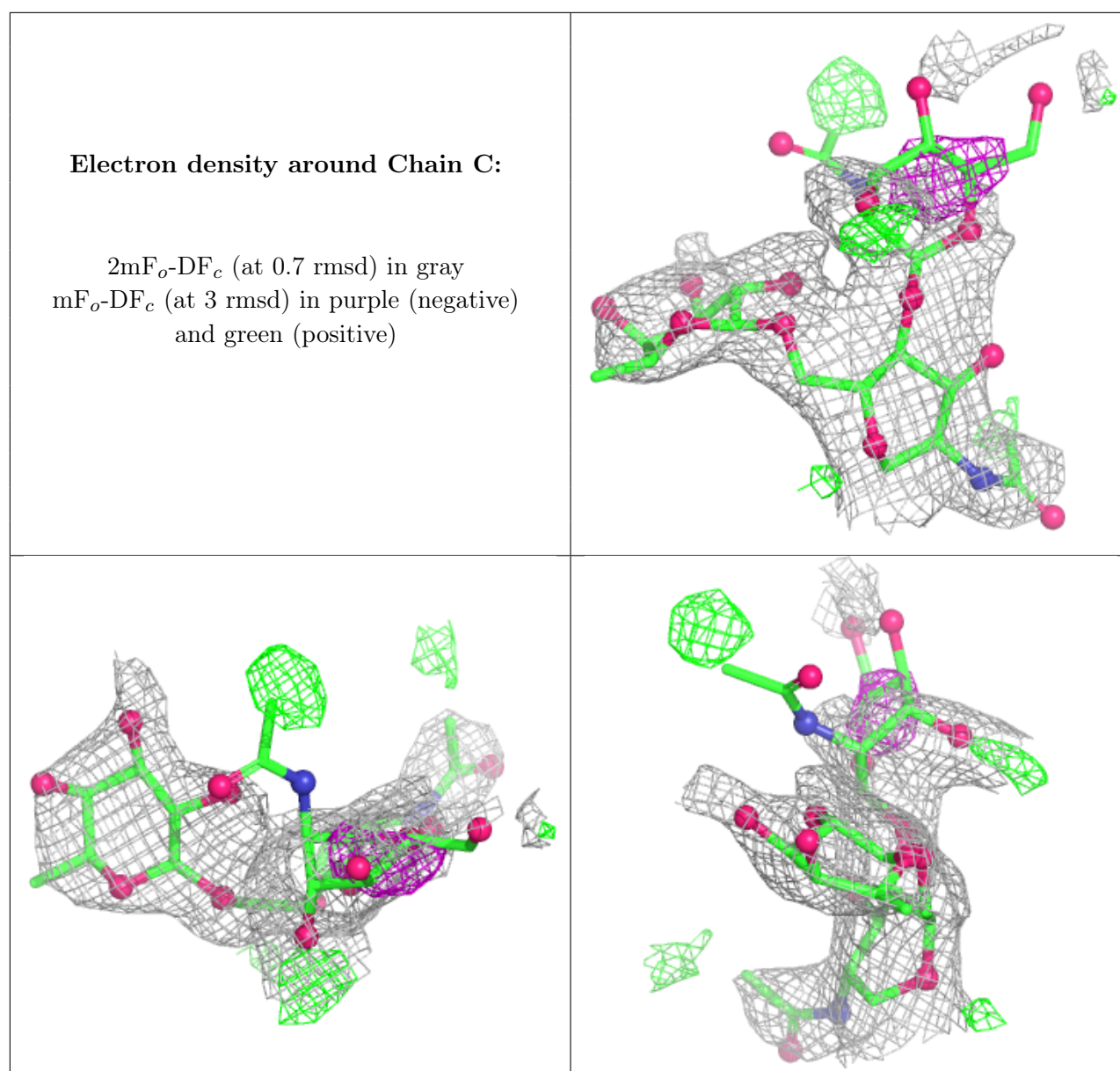
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1	14/15	0.86	0.24	70,80,85,90	0
2	NAG	B	2	14/15	0.87	0.16	69,73,77,79	0
2	FUL	B	3	10/11	0.89	0.26	71,76,77,77	0
2	FUL	C	3	10/11	0.94	0.30	77,79,80,80	0
2	NAG	B	1	14/15	0.96	0.14	42,53,63,68	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
5	GOL	A	1532	6/6	0.75	0.17	74,75,76,76	0
8	NAG	A	1546	14/15	0.76	0.23	60,73,80,81	0
8	NAG	A	1544	14/15	0.79	0.21	59,65,68,69	0
8	NAG	A	1545	14/15	0.81	0.29	66,72,77,79	0
8	NAG	A	1547	14/15	0.83	0.37	77,84,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	FP1	A	1535	10/10	0.84	0.27	50,56,57,59	0
4	SO4	A	1531	5/5	0.86	0.23	76,77,79,80	0
6	CL	A	1537	1/1	0.89	0.15	73,73,73,73	0
5	GOL	A	1533	6/6	0.89	0.21	47,54,55,56	0
5	GOL	A	1540	6/6	0.92	0.25	44,52,56,58	0
4	SO4	A	1539	5/5	0.95	0.15	94,94,94,95	0
3	K	A	1538	1/1	0.95	0.25	112,112,112,112	0
6	CL	A	1534	1/1	0.96	0.22	52,52,52,52	0
3	K	A	1530	1/1	0.98	0.14	63,63,63,63	0
6	CL	A	1536	1/1	0.98	0.05	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.