W O R L D W I D E
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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 10:29 PM EDT

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PDB ID	:	1RWF
Title	:	Crystal structure of Arthrobacter aurescens chondroitin AC lyase in complex with chondroitin tetrasaccharide
Authors	:	Lunin, V.V.; Li, Y.; Miyazono, H.; Kyogashima, M.; Bell, A.W.; Cygler, M.
Deposited on	:	2003-12-16
Resolution	:	1.45 Å(reported)

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 1.45 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.
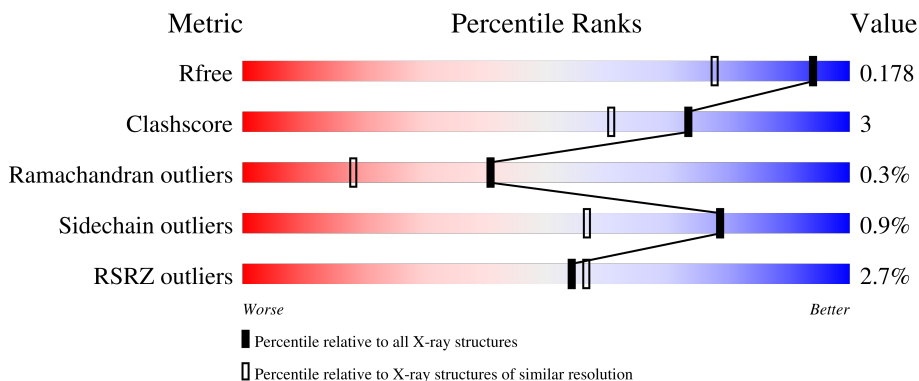
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 >=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 <=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	757	3% red; 93% green; 6%
2	B	4	25% yellow; 75% orange

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	GCT	B	2	-	-	X	-
4	PO4	A	850	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6732 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 chondroitin AC lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total 5617	C 3525	N 990	O 1084	S 18	0	4	0

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-2,6-anhydro-3-deoxy-L-xylo-hexonic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose.
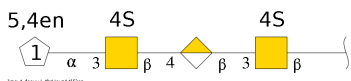
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total 60	C 28	N 2	O 28	S 2	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P = O O1

P

O⁻

O4

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1049	Total 1049	O 1049	0	0

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: chondroitin AC lyase
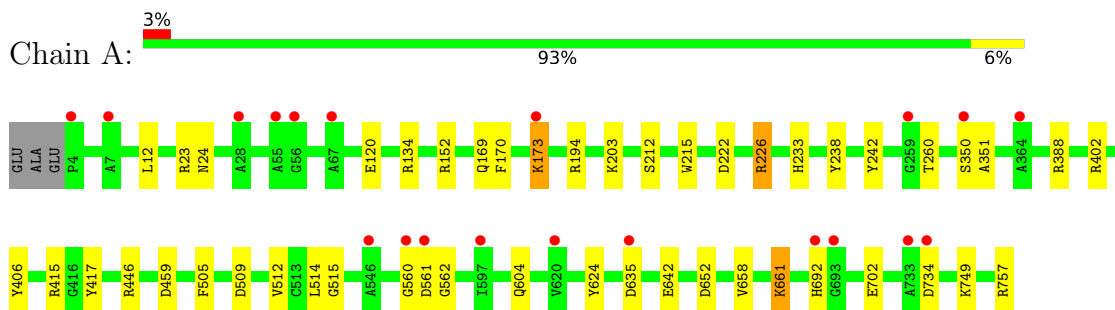
• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-2,6-anhydro-3-deoxy-L-xylo-hexonic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.89Å 86.91Å 81.50Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	27.12 – 1.45 27.16 – 1.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.12-1.45) 99.6 (27.16-1.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.138 , 0.177 0.140 , 0.178	Depositor DCC
R_{free} test set	1473 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6732	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, GAD, GCT, ASG

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	1.15	3/5759 (0.1%)	0.96	17/7845 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	LYS	CB-CG	-9.67	1.26	1.52
1	A	24	ASN	CB-CG	5.78	1.64	1.51
1	A	661	LYS	CE-NZ	5.16	1.61	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757[A]	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	757[B]	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	459	ASP	CB-CG-OD2	7.78	125.30	118.30
1	A	152	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	23	ARG	NE-CZ-NH2	-6.61	117.00	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5617	0	5508	28	0
2	B	60	0	28	11	0
3	A	1	0	0	0	0
4	A	5	0	0	3	0
5	A	1049	0	0	17	0
All	All	6732	0	5536	36	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 3.

The worst 5 of 36 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:509:ASP:HB3	5:A:1559:HOH:O	1.10	1.28
1:A:749:LYS:HG2	5:A:1529:HOH:O	1.45	1.12
1:A:604:GLN:NE2	5:A:1468:HOH:O	1.94	1.01
1:A:642[A]:GLU:OE1	5:A:1986:HOH:O	1.91	0.88
1:A:242:TYR:OH	2:B:2:GCT:HC5	1.81	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	755/757 (100%)	739 (98%)	14 (2%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	560	GLY
1	A	170	PHE

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	571/570 (100%)	566 (99%)	5 (1%)	78	57

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	238	TYR
1	A	406	TYR
1	A	417	TYR
1	A	702	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	19	GLN
1	A	418	HIS
1	A	582	HIS
1	A	598	ASN
1	A	604	GLN

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   ⓘ

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	ASG	B	1	2	19,19,19	1.30	2 (10%)	23,28,28	1.52	7 (30%)
2	GCT	B	2	2	11,11,11	1.05	0	12,15,15	2.77	5 (41%)
2	ASG	B	3	2	19,19,19	1.20	2 (10%)	23,28,28	1.52	4 (17%)
2	GAD	B	4	2	10,11,11	2.47	5 (50%)	13,15,15	3.19	5 (38%)

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	ASG	B	1	2	-	5/11/31/31	0/1/1/1
2	GCT	B	2	2	-	0/4/17/17	0/1/1/1
2	ASG	B	3	2	-	1/11/31/31	0/1/1/1
2	GAD	B	4	2	-	2/4/17/17	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ASG	OSC-S	4.02	1.62	1.45
2	B	4	GAD	O5-C5	3.94	1.42	1.37
2	B	4	GAD	C3-C4	3.90	1.55	1.50
2	B	3	ASG	OSC-S	3.59	1.60	1.45
2	B	4	GAD	O2-C2	3.54	1.50	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	GAD	O5-C5-C4	-8.81	117.37	124.81
2	B	4	GAD	O2-C2-C1	4.81	119.00	109.15
2	B	2	GCT	C1-O5-C5	4.71	121.11	113.92
2	B	2	GCT	O5-C1-C2	4.43	117.60	110.77
2	B	2	GCT	C3-C4-C5	4.25	117.42	109.81

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	ASG	C5-C4-O4-S
2	B	1	ASG	C4-O4-S-OSA
2	B	4	GAD	C4-C5-C6-O6A
2	B	1	ASG	C4-O4-S-OSB
2	B	4	GAD	O5-C5-C6-O6A

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	ASG	4	0
2	B	1	ASG	3	0
2	B	2	GCT	7	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.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
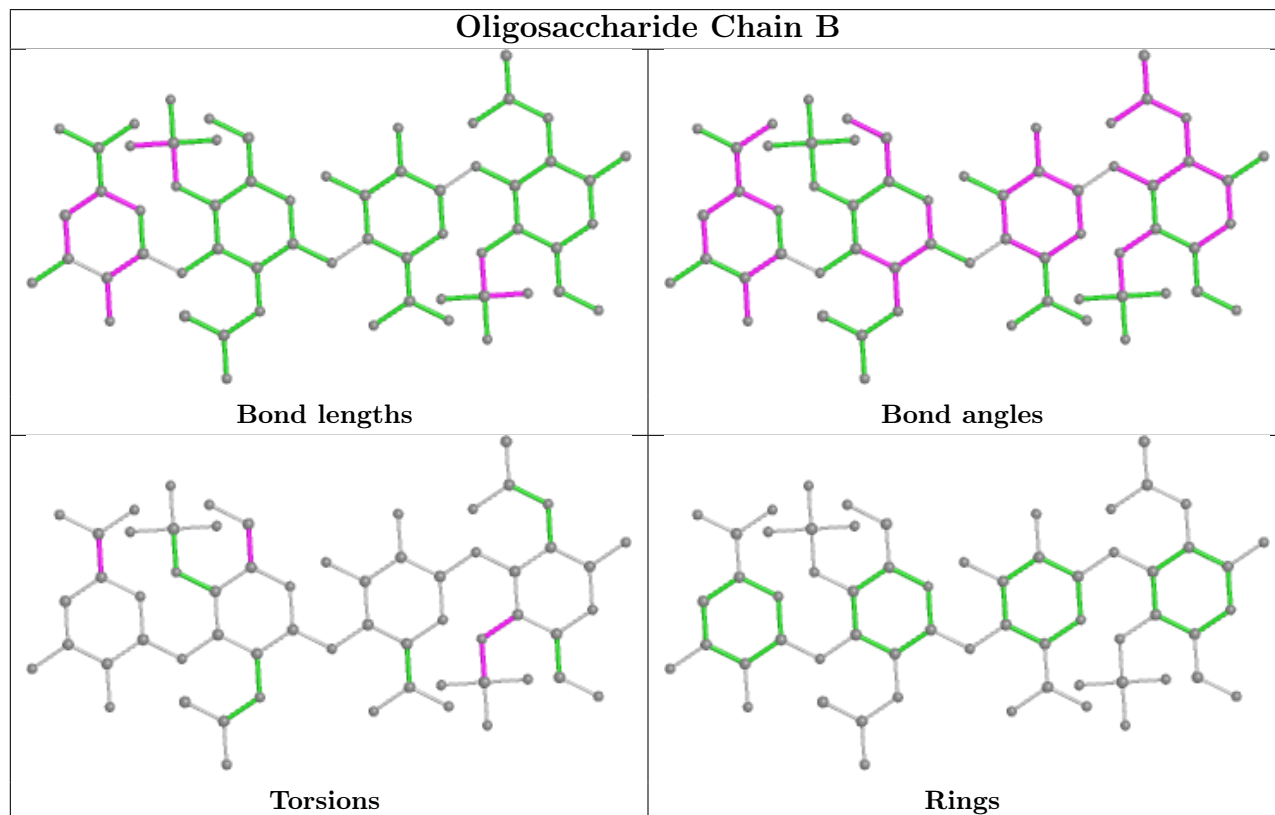
5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PO4	A	850	-	4,4,4	1.15	0	6,6,6	0.91	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	850	PO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

W O R L D W I D E
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PROTEIN DATA BANK

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, 95th 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^2)	Q<0.9
1	A	754/757 (99%)	-0.08	20 (2%)	54	56	8, 16, 30, 48	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	7.7
1	A	560	GLY	6.5
1	A	561	ASP	6.1
1	A	4	PRO	5.8
1	A	734	ASP	4.1

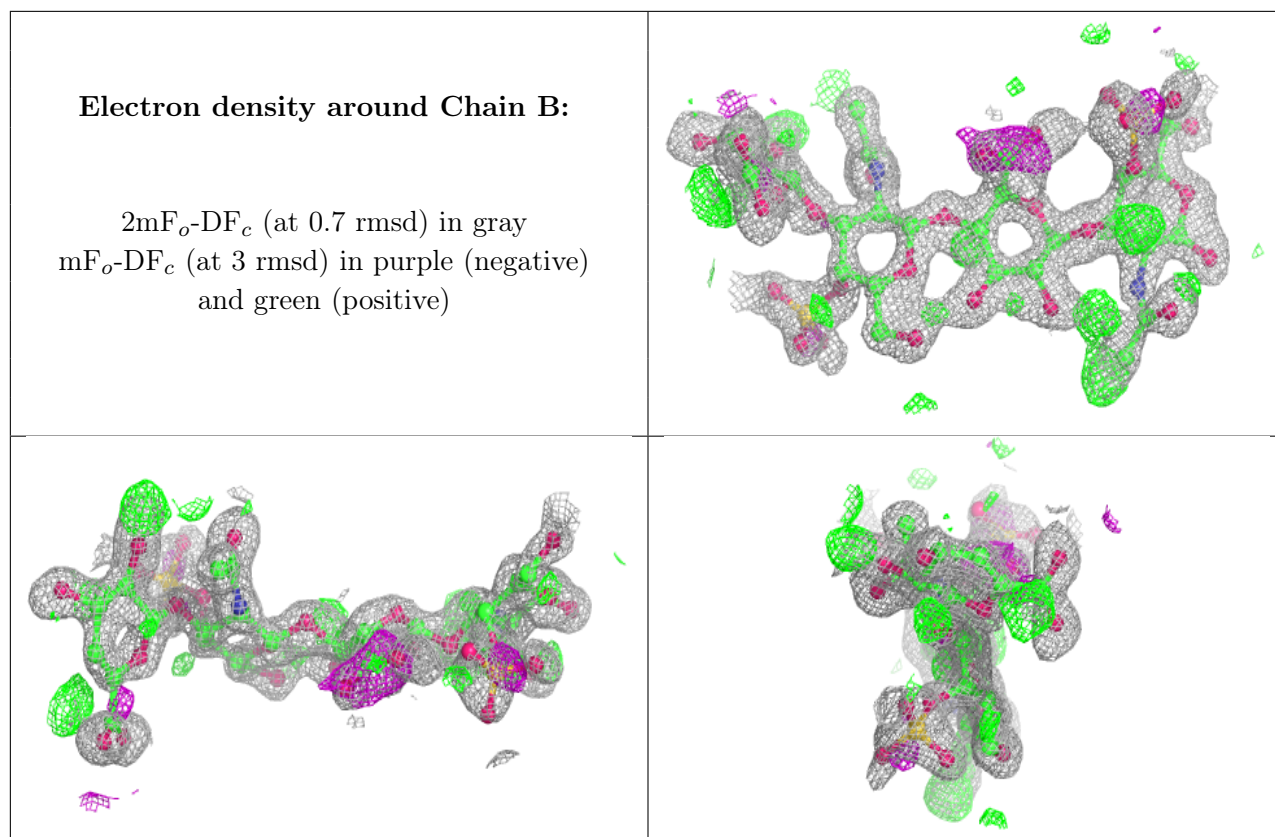## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 95th 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^2)	Q<0.9
2	ASG	B	1	19/19	0.84	0.18	21,26,38,39	19
2	GCT	B	2	11/11	0.84	0.20	21,24,35,35	11
2	GAD	B	4	11/11	0.86	0.15	17,19,20,21	11
2	ASG	B	3	19/19	0.88	0.16	11,22,33,33	19

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 B:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
4	PO4	A	850	5/5	0.95	0.13	10,13,15,15	5
3	NA	A	900	1/1	0.99	0.14	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.