Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 04:28 PM JST

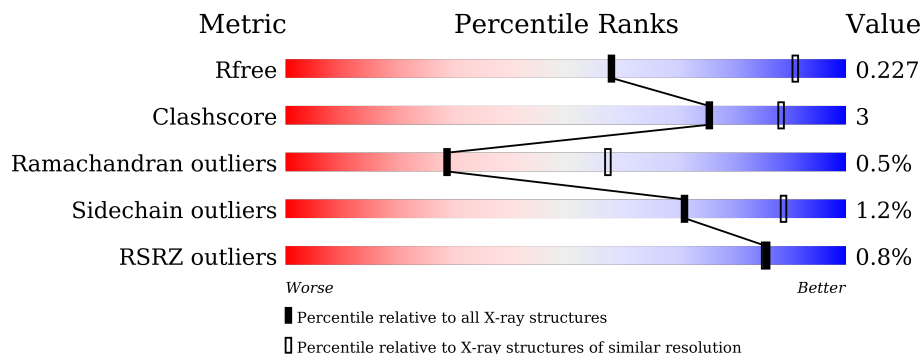|		
PDB ID	:	6JPN
Title	:	Crystal structure of the catalytic domain of a multi-domain alginate lyase Dp0100 from thermophilic bacterium Defluviitalea phaphyphila
Authors	:	Ji, S.Q.; Dix, S.R.; Aziz, A.; Sedelnikova, S.E.; Li, F.L.; Rice, D.W.
Deposited on	:	2019-03-27
Resolution	:	2.85 Å(reported)

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 2.85 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		1.2%
RSRZ outliers		0.8%

Worse → Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	772	.% 91% 9%
2	B	5	20% 80%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6337 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 Alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total 6235	C 3958	N 1015	O 1246	S 16	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-beta-D-manno pyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic aci d-(1-4)-beta-D-mannopyranuronic acid.

◆ β 4 ◇ β 4 ◆ β 4 ◆ β 4 ◆ β 4 ◇ β
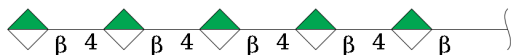
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	5	Total 61	C 30	O 31	0	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total 37	O 37	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: Alginate lyase
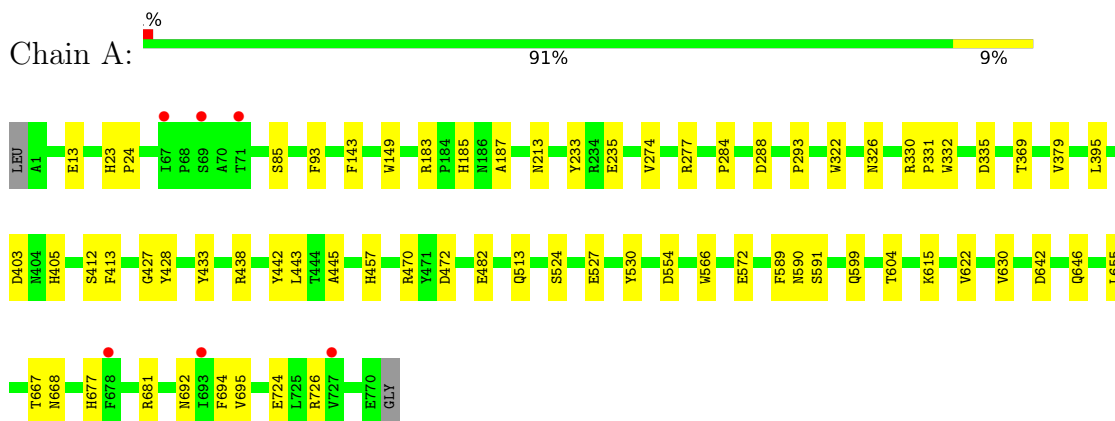
• Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.38Å 261.38Å 58.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.86 – 2.85 62.78 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.86-2.85) 100.0 (62.78-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.207 , 0.223 0.215 , 0.227	Depositor DCC
R_{free} test set	2701 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6337	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: MN, MG, CA, BEM

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	0/6407	0.76	0/8719

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 ⓘ

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	6235	0	5796	34	0
2	B	61	0	33	4	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	37	0	0	1	0
All	All	6337	0	5829	37	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.

All (37) 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:183:ARG:HH21	2:B:1:BEM:H5	1.45	0.82
2:B:3:BEM:O3	2:B:4:BEM:O5	2.03	0.71
1:A:293:PRO:HD3	1:A:332:TRP:CZ2	2.31	0.65
1:A:668:ASN:HD22	1:A:677:HIS:HD2	1.43	0.65
1:A:724:GLU:OE2	1:A:726:ARG:NH2	2.37	0.58
1:A:668:ASN:ND2	1:A:677:HIS:HD2	2.04	0.55
1:A:274:VAL:O	1:A:277:ARG:HG2	2.09	0.53
1:A:445:ALA:HB2	1:A:457:HIS:HB3	1.92	0.52
1:A:322:TRP:CD1	1:A:326:ASN:ND2	2.80	0.50
1:A:185:HIS:CE1	1:A:187:ALA:HB3	2.46	0.50
1:A:646:GLN:HE21	1:A:681:ARG:HH22	1.60	0.49
1:A:524:SER:HB2	1:A:530:TYR:OH	2.14	0.47
1:A:85:SER:HA	1:A:143:PHE:CE1	2.50	0.47
1:A:642:ASP:HA	1:A:667:THR:O	2.15	0.47
1:A:13:GLU:O	1:A:213:ASN:ND2	2.45	0.46
1:A:470:ARG:NH2	1:A:482:GLU:OE2	2.46	0.46
1:A:330:ARG:N	1:A:331:PRO:CD	2.78	0.46
1:A:630:VAL:HG12	1:A:655:LEU:HD12	1.98	0.45
1:A:668:ASN:HD22	1:A:677:HIS:CD2	2.29	0.45
1:A:288:ASP:HB2	1:A:405:HIS:HB3	1.99	0.45
1:A:395:LEU:O	1:A:413:PHE:HA	2.17	0.45
2:B:2:BEM:O3	2:B:3:BEM:O5	2.25	0.45
2:B:2:BEM:C3	2:B:3:BEM:O5	2.66	0.44
1:A:566:TRP:CE3	1:A:622:VAL:HG21	2.53	0.43
1:A:566:TRP:CD2	1:A:622:VAL:HG21	2.54	0.43
1:A:599:GLN:NE2	1:A:604:THR:OG1	2.51	0.42
1:A:438:ARG:HA	1:A:442:TYR:HB2	2.01	0.42
1:A:23:HIS:HA	1:A:24:PRO:HA	1.87	0.42
1:A:233:TYR:CE2	1:A:235:GLU:HB2	2.56	0.41
1:A:433:TYR:CE1	1:A:438:ARG:NH1	2.88	0.41
1:A:284:PRO:HG3	1:A:395:LEU:HD22	2.02	0.41
1:A:589:PHE:O	1:A:590:ASN:ND2	2.53	0.41
1:A:692:ASN:HD21	1:A:695:VAL:HG13	1.85	0.41
1:A:93:PHE:HB2	1:A:149:TRP:CZ3	2.55	0.41
1:A:427:GLY:N	6:A:901:HOH:O	2.53	0.41
1:A:369:THR:HA	1:A:379:VAL:O	2.21	0.40
1:A:443:LEU:C	1:A:443:LEU:HD12	2.42	0.40

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	768/772 (100%)	721 (94%)	43 (6%)	4 (0%)	29	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	ASP
1	A	335	ASP
1	A	615	LYS
1	A	513	GLN

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	670/671 (100%)	662 (99%)	8 (1%)	71	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ASP
1	A	412	SER
1	A	428	TYR
1	A	472	ASP
1	A	527	GLU
1	A	572	GLU
1	A	591	SER

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Mol	Chain	Res	Type
1	A	694	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	232	HIS
1	A	361	GLN
1	A	419	ASN
1	A	464	ASN
1	A	529	GLN
1	A	559	GLN
1	A	590	ASN
1	A	599	GLN
1	A	646	GLN
1	A	650	ASN
1	A	668	ASN
1	A	677	HIS
1	A	692	ASN
1	A	711	GLN
1	A	744	ASN
1	A	767	ASN

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)

5 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	BEM	B	1	2	13,13,13	0.92	1 (7%)	18,19,19	1.66	4 (22%)
2	BEM	B	2	2	12,12,13	0.92	1 (8%)	14,17,19	1.48	2 (14%)
2	BEM	B	3	2	12,12,13	1.08	1 (8%)	14,17,19	0.80	0
2	BEM	B	4	2	12,12,13	0.90	1 (8%)	14,17,19	1.12	1 (7%)
2	BEM	B	5	2	12,12,13	0.92	1 (8%)	14,17,19	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEM	B	1	2	-	2/4/24/24	0/1/1/1
2	BEM	B	2	2	-	0/4/21/24	0/1/1/1
2	BEM	B	3	2	-	1/4/21/24	0/1/1/1
2	BEM	B	4	2	-	0/4/21/24	0/1/1/1
2	BEM	B	5	2	-	1/4/21/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	BEM	O6B-C6	-3.13	1.20	1.30
2	B	4	BEM	O6B-C6	-2.93	1.21	1.30
2	B	5	BEM	O6B-C6	-2.90	1.21	1.30
2	B	3	BEM	O6B-C6	-2.84	1.21	1.30
2	B	2	BEM	O6B-C6	-2.72	1.21	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	BEM	C3-C4-C5	3.29	114.87	109.25
2	B	2	BEM	O4-C4-C5	-3.22	102.53	109.74
2	B	1	BEM	O4-C4-C5	-3.01	102.98	109.74
2	B	2	BEM	O4-C4-C3	2.63	116.43	110.35
2	B	1	BEM	O5-C5-C6	2.41	112.36	105.88
2	B	4	BEM	O5-C5-C6	2.25	113.71	106.31
2	B	1	BEM	C1-O5-C5	-2.23	108.95	112.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	BEM	C4-C5-C6-O6A
2	B	1	BEM	O5-C5-C6-O6B
2	B	1	BEM	O5-C5-C6-O6A
2	B	5	BEM	O5-C5-C6-O6B

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BEM	1	0
2	B	3	BEM	3	0
2	B	1	BEM	1	0
2	B	2	BEM	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.

Oligosaccharide Chain B

Bond lengths   Bond angles

Torsions   Rings
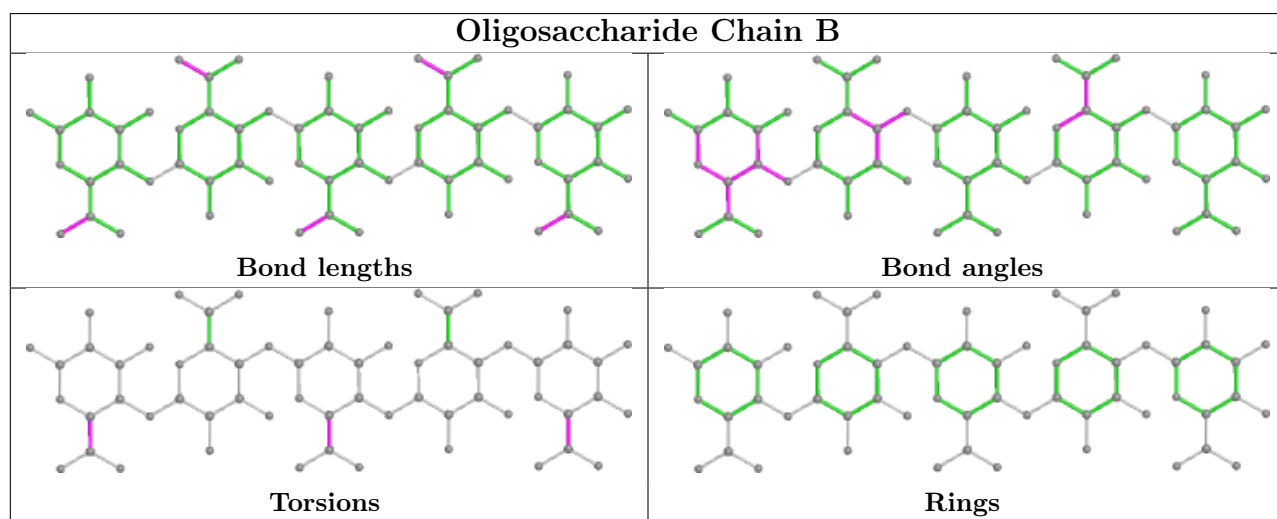
5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

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	770/772 (99%)	0.21	6 (0%)	86	85	53, 72, 97, 125	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	2.5
1	A	678	PHE	2.3
1	A	69	SER	2.2
1	A	71	THR	2.2
1	A	727	VAL	2.1
1	A	693	ILE	2.0

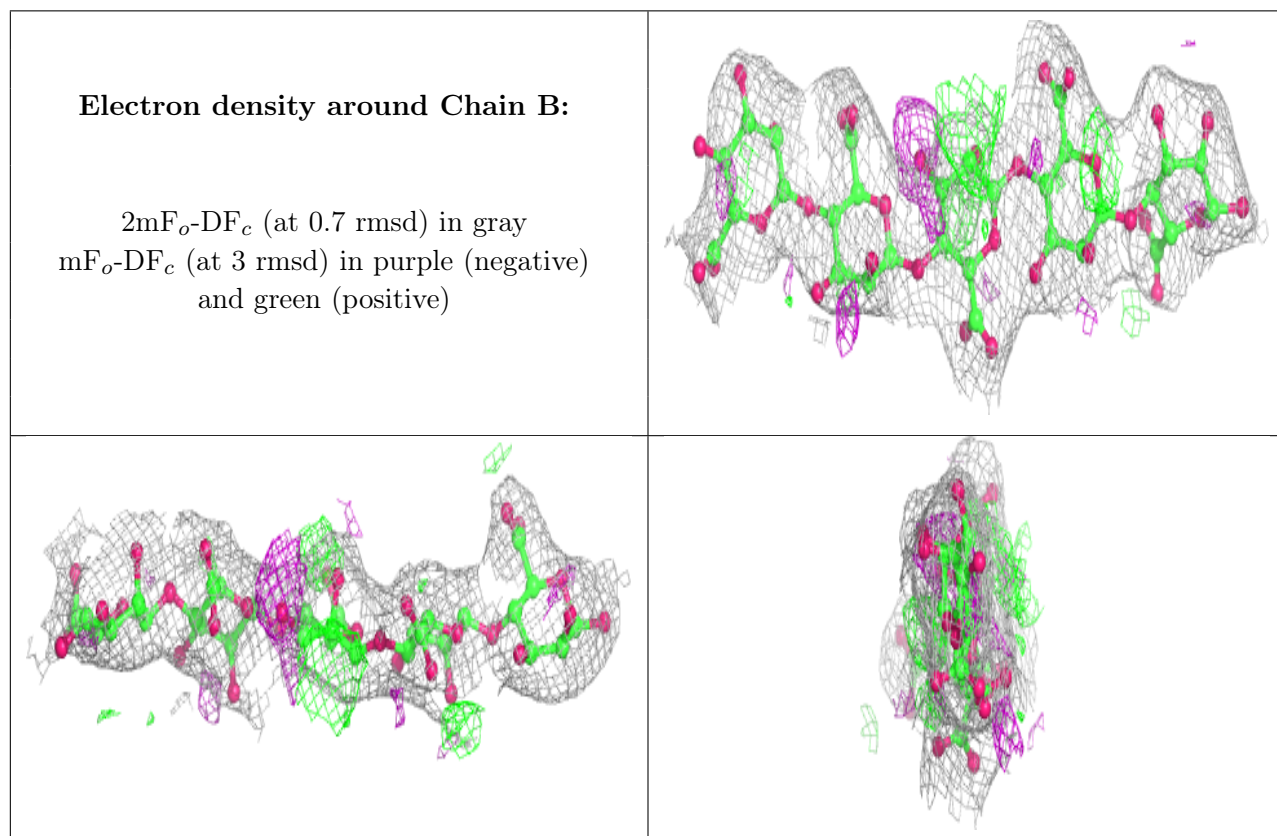## 6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

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	BEM	B	5	12/13	0.87	0.18	102,107,111,115	0
2	BEM	B	3	12/13	0.90	0.19	72,78,85,95	0
2	BEM	B	1	13/13	0.92	0.15	83,84,89,90	0
2	BEM	B	4	12/13	0.93	0.17	84,88,95,101	0
2	BEM	B	2	12/13	0.94	0.17	71,78,84,88	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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
3	MN	A	801	1/1	0.95	0.19	61,61,61,61	0
5	MG	A	804	1/1	0.97	0.08	45,45,45,45	0
4	CA	A	802	1/1	0.98	0.16	69,69,69,69	0
4	CA	A	803	1/1	0.99	0.12	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.