



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2026 – 11:48 pm BST

PDB ID : 9SIN / pdb_00009sin
Title : Phage epsilon15 tailspike gp20 containing domains beta-helix, beta-sandwich and petal domains with three hexasaccharides of the Salmonella Anatum O-antigen
Authors : Seoane-Blanco, M.; van Raaij, M.J.
Deposited on : 2025-08-28
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

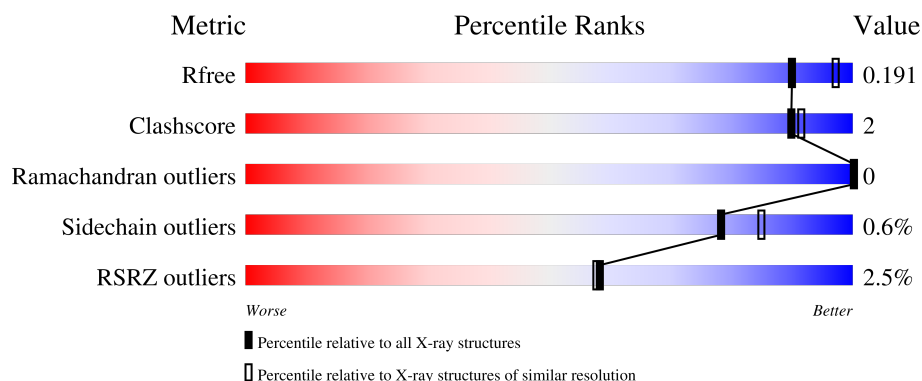
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	857	2% 93% 17%
2	B	6	83% 17%
3	D	6	83% 17%
3	E	6	83% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13624 atoms, of which 6359 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 Tail spike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	832	Total	C	H	N	O	S	241	15	0
			12516	3967	6139	1111	1271	28			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	initiating methionine	UNP Q858F5
A	215	GLY	-	expression tag	UNP Q858F5
A	216	SER	-	expression tag	UNP Q858F5
A	217	SER	-	expression tag	UNP Q858F5
A	218	HIS	-	expression tag	UNP Q858F5
A	219	HIS	-	expression tag	UNP Q858F5
A	220	HIS	-	expression tag	UNP Q858F5
A	221	HIS	-	expression tag	UNP Q858F5
A	222	HIS	-	expression tag	UNP Q858F5
A	223	HIS	-	expression tag	UNP Q858F5
A	224	SER	-	expression tag	UNP Q858F5
A	225	SER	-	expression tag	UNP Q858F5
A	226	GLY	-	expression tag	UNP Q858F5
A	227	LEU	-	expression tag	UNP Q858F5
A	228	VAL	-	expression tag	UNP Q858F5
A	229	PRO	-	expression tag	UNP Q858F5
A	230	ARG	-	expression tag	UNP Q858F5
A	231	GLY	-	expression tag	UNP Q858F5
A	232	SER	-	expression tag	UNP Q858F5
A	233	HIS	-	expression tag	UNP Q858F5
A	234	MET	-	expression tag	UNP Q858F5
A	235	ALA	-	expression tag	UNP Q858F5
A	236	SER	-	expression tag	UNP Q858F5
A	237	MET	-	expression tag	UNP Q858F5
A	238	THR	-	expression tag	UNP Q858F5
A	239	GLY	-	expression tag	UNP Q858F5
A	240	GLY	-	expression tag	UNP Q858F5

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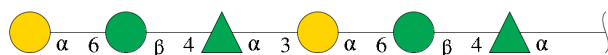
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Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLN	-	expression tag	UNP Q858F5
A	242	GLN	-	expression tag	UNP Q858F5
A	243	MET	-	expression tag	UNP Q858F5
A	244	GLY	-	expression tag	UNP Q858F5
A	245	ARG	-	expression tag	UNP Q858F5
A	246	ILE	-	expression tag	UNP Q858F5
A	247	LEU	-	expression tag	UNP Q858F5
A	308	ILE	CYS	conflict	UNP Q858F5

- Molecule 2 is an oligosaccharide called 6-O-acetyl-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-6-O-acetyl-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.

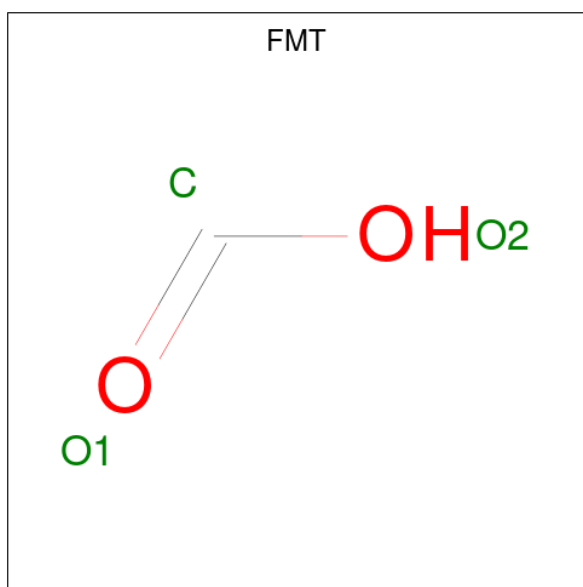
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	H	O	22	0	0
			137	40	66	31			

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	6	Total	C	H	O	18	0	0
			127	36	62	29			
3	E	6	Total	C	H	O	18	0	0
			127	36	62	29			

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		
4	A	1	Total	C	H	O	1	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

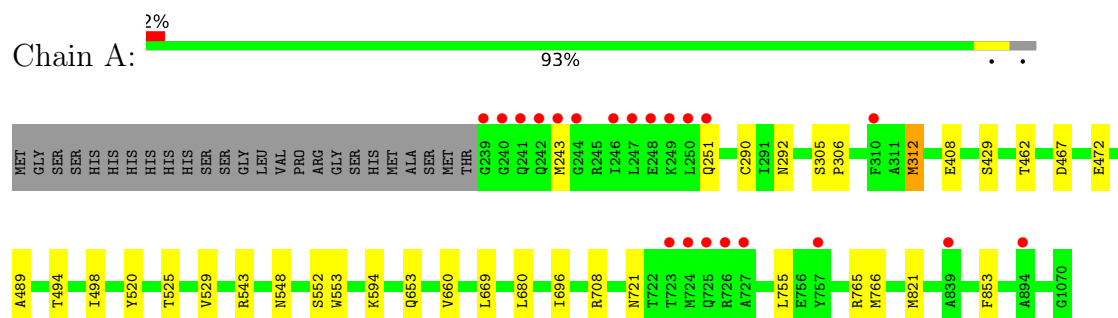
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	629	Total	O	0	11
			640	640		

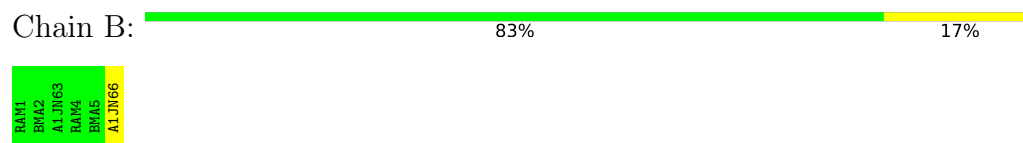
3 Residue-property plots [i](#)

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.

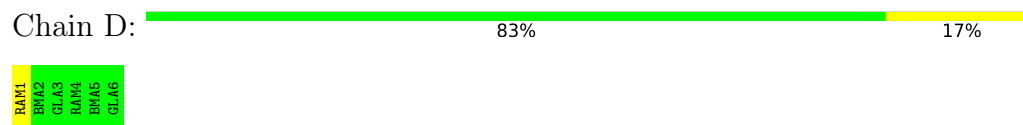
- Molecule 1: Tail spike protein



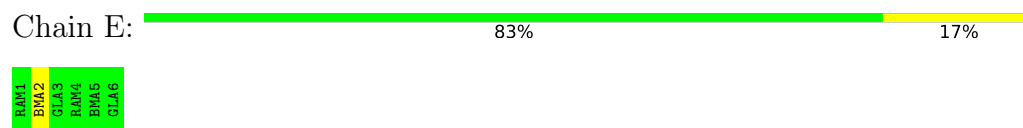
- Molecule 2: 6-O-acetyl-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-6-O-acetyl-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose



- Molecule 3: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose



- Molecule 3: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	117.52Å 117.52Å 250.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.07 – 2.00 48.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.07-2.00) 99.2 (48.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.166 , 0.191 0.167 , 0.191	Depositor DCC
R_{free} test set	4438 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13624	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, A1JN6, NA, GLA, RAM, BMA

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	0.46	0/6554	0.79	0/8912

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	653[A]	GLN	Mainchain
1	A	708	ARG	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	6377	6139	6111	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	71	66	38	1	0
3	D	65	62	57	1	0
3	E	65	62	57	0	0
4	A	45	30	15	1	0
5	A	2	0	0	0	0
6	A	640	0	0	0	0
All	All	7265	6359	6278	23	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 2.

All (23) 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:290[A]:CYS:SG	1:A:312[A]:MET:SD	2.68	0.91
1:A:821:MET:HE1	1:A:853:PHE:CZ	2.33	0.63
1:A:696:ILE:CD1	1:A:766:MET:HE1	2.33	0.59
1:A:696:ILE:HD12	1:A:766:MET:HE1	1.89	0.55
1:A:765[A]:ARG:HH22	4:A:1108:FMT:C	2.23	0.52
1:A:462:THR:HA	1:A:489:ALA:O	2.11	0.50
1:A:553:TRP:HA	1:A:594:LYS:O	2.11	0.49
1:A:292:ASN:HA	1:A:312[B]:MET:HG3	1.96	0.47
1:A:525:THR:HA	1:A:548:ASN:O	2.15	0.46
1:A:408:GLU:HA	1:A:429:SER:O	2.16	0.46
1:A:660:VAL:HG21	1:A:755:LEU:HD22	1.96	0.46
1:A:489:ALA:HA	1:A:520:TYR:O	2.16	0.45
2:B:6:A1JN6:O3	3:D:1:RAM:O1	2.28	0.45
1:A:494:THR:HA	1:A:525:THR:O	2.16	0.45
1:A:680:LEU:C	1:A:680:LEU:HD23	2.43	0.44
1:A:305:SER:HB2	1:A:306:PRO:CD	2.48	0.43
1:A:529:VAL:O	1:A:552:SER:HA	2.19	0.42
1:A:467:ASP:HA	1:A:494:THR:O	2.19	0.41
1:A:520:TYR:HA	1:A:543:ARG:O	2.21	0.41
1:A:669:LEU:HD13	1:A:669:LEU:C	2.45	0.41
1:A:305:SER:HB2	1:A:306:PRO:HD2	2.03	0.41
1:A:498:ILE:O	1:A:529:VAL:HA	2.21	0.41
1:A:243:MET:HA	1:A:243:MET:HE3	2.03	0.40

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	845/857 (99%)	813 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	697/703 (99%)	692 (99%)	5 (1%)	76	82

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

Mol	Chain	Res	Type
1	A	251	GLN
1	A	312[A]	MET
1	A	312[B]	MET
1	A	472	GLU
1	A	721	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	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 ⓘ

18 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	RAM	B	1	2	11,11,11	0.18	0	15,16,16	0.31	0
2	BMA	B	2	2	11,11,12	0.22	0	15,15,17	0.44	0
2	A1JN6	B	3	2	14,14,15	0.28	0	19,19,21	0.48	0
2	RAM	B	4	2	10,10,11	0.31	0	14,14,16	0.39	0
2	BMA	B	5	2	11,11,12	0.25	0	15,15,17	0.51	0
2	A1JN6	B	6	2	14,14,15	0.27	0	19,19,21	0.62	0
3	RAM	D	1	3	11,11,11	0.30	0	15,16,16	0.45	0
3	BMA	D	2	3	11,11,12	0.40	0	15,15,17	0.47	0
3	GLA	D	3	3	11,11,12	0.30	0	15,15,17	0.58	0
3	RAM	D	4	3	10,10,11	0.32	0	14,14,16	0.40	0
3	BMA	D	5	3	11,11,12	0.27	0	15,15,17	0.42	0
3	GLA	D	6	3	11,11,12	0.28	0	15,15,17	0.60	0
3	RAM	E	1	3	11,11,11	0.27	0	15,16,16	0.45	0
3	BMA	E	2	3	11,11,12	0.31	0	15,15,17	0.72	1 (6%)
3	GLA	E	3	3	11,11,12	0.36	0	15,15,17	0.73	0
3	RAM	E	4	3	10,10,11	0.30	0	14,14,16	0.42	0
3	BMA	E	5	3	11,11,12	0.25	0	15,15,17	0.48	0
3	GLA	E	6	3	11,11,12	0.34	0	15,15,17	0.61	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	RAM	B	1	2	-	-	0/1/1/1
2	BMA	B	2	2	-	0/2/19/22	0/1/1/1
2	A1JN6	B	3	2	-	0/5/22/25	0/1/1/1
2	RAM	B	4	2	-	-	0/1/1/1
2	BMA	B	5	2	-	0/2/19/22	0/1/1/1
2	A1JN6	B	6	2	-	1/5/22/25	0/1/1/1
3	RAM	D	1	3	-	-	0/1/1/1
3	BMA	D	2	3	-	0/2/19/22	0/1/1/1
3	GLA	D	3	3	-	0/2/19/22	0/1/1/1
3	RAM	D	4	3	-	-	0/1/1/1
3	BMA	D	5	3	-	0/2/19/22	0/1/1/1
3	GLA	D	6	3	-	0/2/19/22	0/1/1/1
3	RAM	E	1	3	-	-	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	GLA	E	3	3	-	2/2/19/22	0/1/1/1
3	RAM	E	4	3	-	-	0/1/1/1
3	BMA	E	5	3	-	0/2/19/22	0/1/1/1
3	GLA	E	6	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	BMA	C1-C2-C3	2.06	112.20	109.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

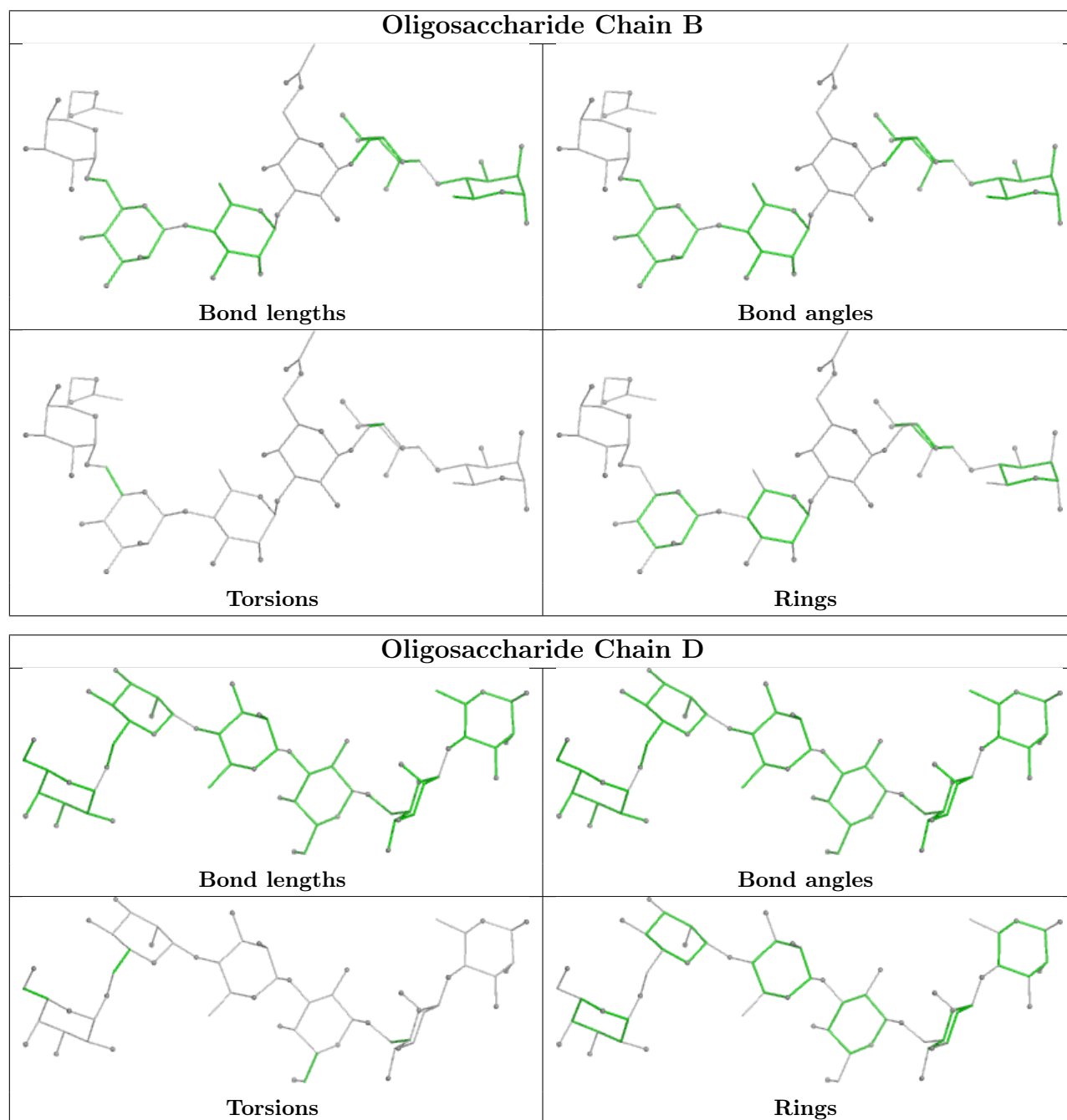
Mol	Chain	Res	Type	Atoms
3	E	3	GLA	C4-C5-C6-O6
3	E	3	GLA	O5-C5-C6-O6
2	B	6	A1JN6	O5-C5-C6-O6

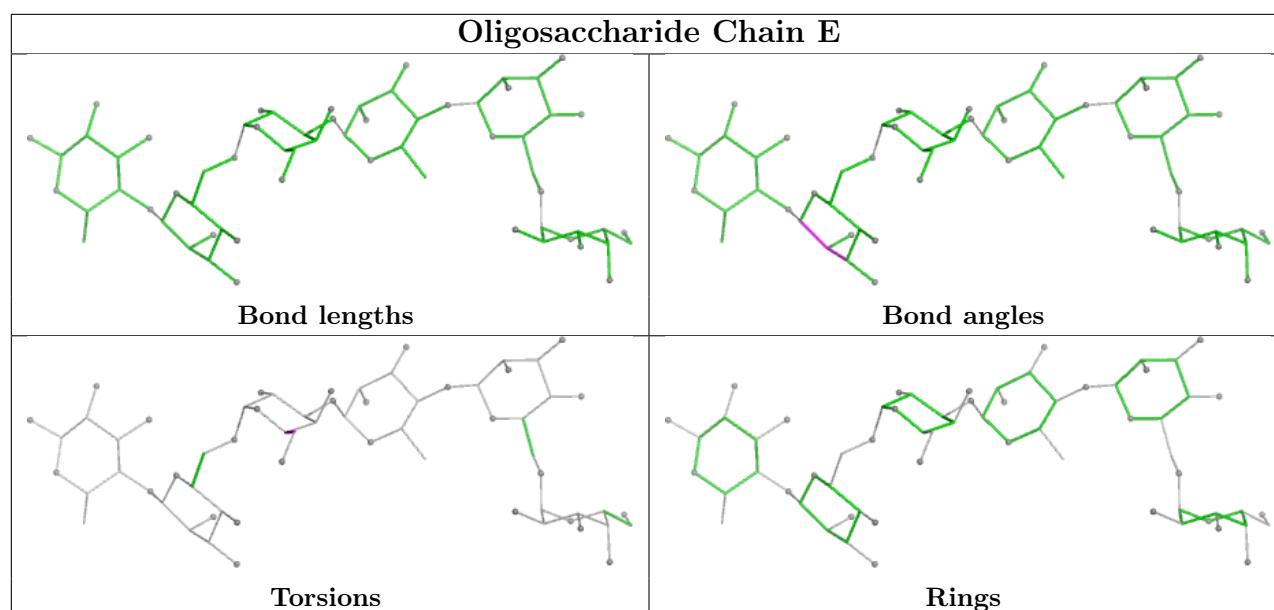
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	A1JN6	1	0
3	D	1	RAM	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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	FMT	A	1112	-	2,2,2	0.99	0	1,1,1	0.25	0
4	FMT	A	1114	-	2,2,2	1.00	0	1,1,1	0.24	0
4	FMT	A	1103	-	2,2,2	1.01	0	1,1,1	0.24	0
4	FMT	A	1108	-	2,2,2	1.00	0	1,1,1	0.23	0
4	FMT	A	1106	-	2,2,2	1.01	0	1,1,1	0.24	0
4	FMT	A	1111	-	2,2,2	0.99	0	1,1,1	0.25	0
4	FMT	A	1109	-	2,2,2	1.00	0	1,1,1	0.23	0
4	FMT	A	1113	-	2,2,2	1.01	0	1,1,1	0.23	0
4	FMT	A	1101	-	2,2,2	0.97	0	1,1,1	0.25	0
4	FMT	A	1102	-	2,2,2	1.03	0	1,1,1	0.23	0
4	FMT	A	1105	-	2,2,2	0.93	0	1,1,1	0.27	0
4	FMT	A	1115	-	2,2,2	1.00	0	1,1,1	0.23	0
4	FMT	A	1107	-	2,2,2	0.98	0	1,1,1	0.25	0
4	FMT	A	1110	-	2,2,2	1.01	0	1,1,1	0.24	0
4	FMT	A	1104	-	2,2,2	1.05	0	1,1,1	0.23	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1108	FMT	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, 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	831/857 (96%)	-0.14	21 (2%) 58 58	16, 33, 59, 108	13 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	727	ALA	5.6
1	A	248	GLU	4.6
1	A	724	MET	4.2
1	A	240	GLY	4.0
1	A	247	LEU	3.7
1	A	241	GLN	3.6
1	A	726	ARG	3.5
1	A	249	LYS	3.1
1	A	242	GLN	2.9
1	A	839	ALA	2.9
1	A	243	MET	2.8
1	A	239	GLY	2.7
1	A	246	ILE	2.7
1	A	250	LEU	2.6
1	A	723	THR	2.5
1	A	244	GLY	2.4
1	A	894	ALA	2.3
1	A	725	GLN	2.2
1	A	310	PHE	2.2
1	A	757	TYR	2.1
1	A	251	GLN	2.1

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

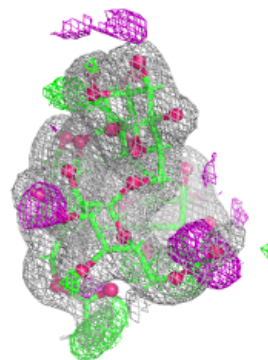
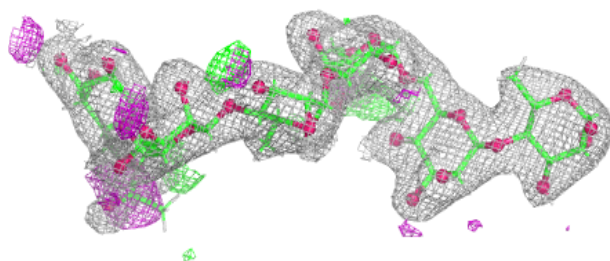
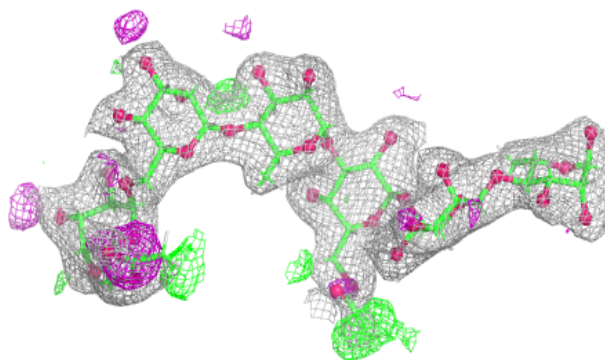
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RAM	D	1	11/11	0.77	0.14	39,43,44,65	3
3	GLA	D	3	11/12	0.83	0.14	38,42,47,61	3
3	BMA	D	2	11/12	0.87	0.12	33,38,40,41	3
3	GLA	D	6	11/12	0.87	0.10	69,73,82,92	4
2	RAM	B	1	11/11	0.93	0.08	46,52,59,66	3
2	A1JN6	B	6	14/15	0.93	0.11	30,35,63,63	6
2	A1JN6	B	3	14/15	0.94	0.09	28,33,34,35	8
3	RAM	D	4	10/11	0.95	0.08	40,44,46,49	2
2	BMA	B	5	11/12	0.95	0.06	33,37,38,40	3
3	BMA	D	5	11/12	0.96	0.07	49,55,60,64	3
2	RAM	B	4	10/11	0.96	0.06	36,37,40,42	2
2	BMA	B	2	11/12	0.97	0.06	34,39,42,44	3
3	RAM	E	1	11/11	-	-	87,94,105,114	3
3	BMA	E	2	11/12	-	-	73,79,81,83	3
3	GLA	E	3	11/12	-	-	55,68,77,85	3
3	RAM	E	4	10/11	-	-	39,44,48,49	2
3	BMA	E	5	11/12	-	-	37,41,46,50	3
3	GLA	E	6	11/12	-	-	53,57,63,71	4

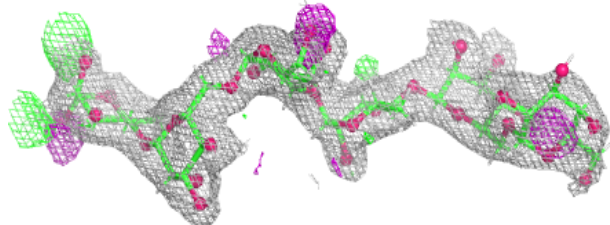
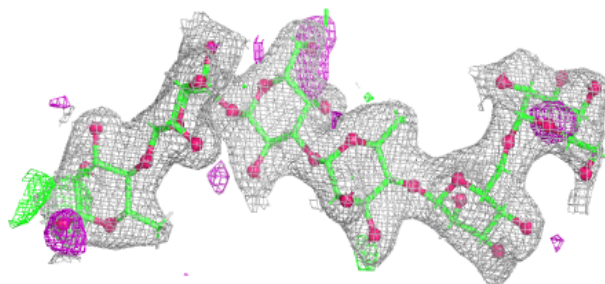
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

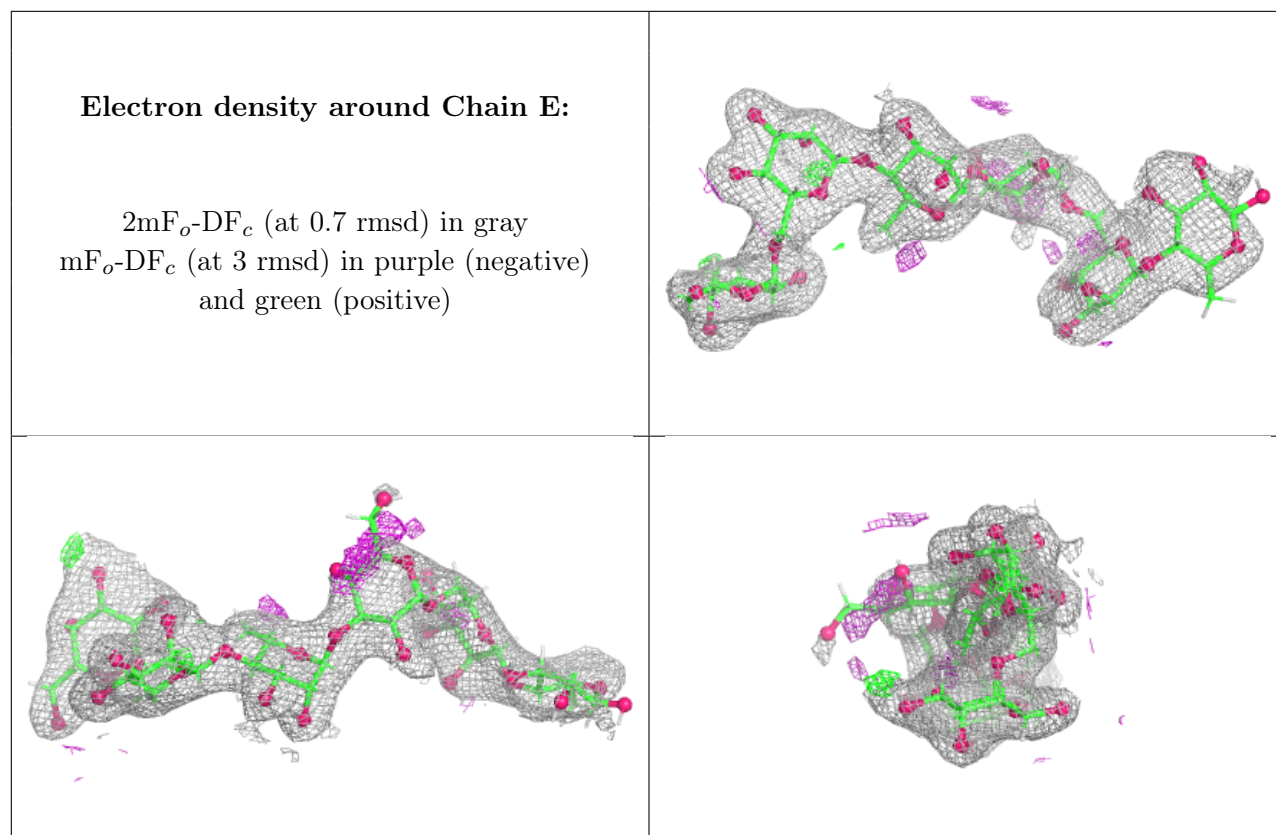
Electron density around Chain B:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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, 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($\text{\AA}^2$)	Q<0.9
4	FMT	A	1104	3/3	0.71	0.25	51,56,58,58	1
4	FMT	A	1112	3/3	0.74	0.21	72,72,72,73	1
4	FMT	A	1103	3/3	0.86	0.19	59,61,61,64	1
4	FMT	A	1106	3/3	0.87	0.23	66,66,67,67	1
4	FMT	A	1101	3/3	0.88	0.15	49,52,52,53	1
4	FMT	A	1115	3/3	0.88	0.18	65,65,66,68	1
4	FMT	A	1114	3/3	0.89	0.20	65,66,67,68	1
4	FMT	A	1110	3/3	0.89	0.17	54,60,63,63	1
4	FMT	A	1111	3/3	0.91	0.16	62,62,63,63	1
4	FMT	A	1113	3/3	0.91	0.17	68,68,69,71	1
4	FMT	A	1107	3/3	0.92	0.10	63,63,64,64	1
4	FMT	A	1109	3/3	0.92	0.15	48,50,51,54	1
5	NA	A	1117	1/1	0.92	0.09	58,58,58,58	0
4	FMT	A	1108	3/3	0.93	0.16	65,66,66,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	A	1105	3/3	0.95	0.09	39,39,41,42	1
4	FMT	A	1102	3/3	0.97	0.09	40,40,40,41	1
5	NA	A	1116	1/1	0.98	0.04	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.