

Full wwPDB X-ray Structure Validation Report (i)

Feb 8, 2023 – 02:01 PM EST

PDB ID : 1AY2

Title : STRUCTURE OF THE FIBER-FORMING PROTEIN PILIN AT 2.6

ANGSTROMS RESOLUTION

Authors: Forest, K.T.; Parge, H.E.; Tainer, J.A.

Deposited on : 1997-11-13

Resolution : 2.60 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.32.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

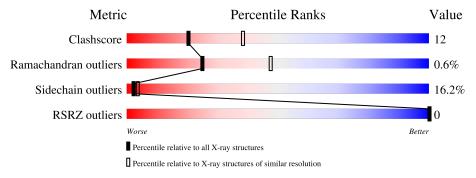
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.60 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	158	57%	34% 9%				
2	В	2	100%					



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1373 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 TYPE 4 PILIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	158	Total	С	N	О	S	0	0	0
_	11	100	1208	761	206	237	4			

• Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



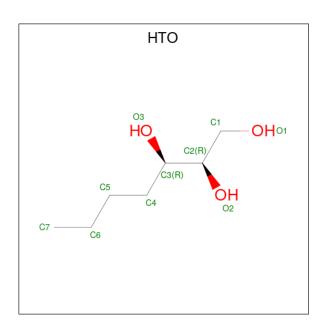
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	2	Total 25	C 14	N 1	O 10	0	0	0

• Molecule 3 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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

• Molecule 4 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 7	O 3	0	0

• Molecule 5 is water.

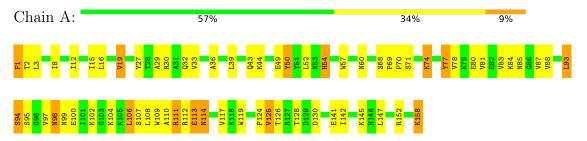
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 129 129	0	0



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: TYPE 4 PILIN



• Molecule 2: alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1 GLA2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants	127.58Å 121.08Å 26.86Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 2.60	Depositor
Resolution (A)	9.97 - 2.60	EDS
% Data completeness	95.0 (10.00-2.60)	Depositor
(in resolution range)	96.2 (9.97-2.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
P. P.	0.194 , (Not available)	Depositor
R, R_{free}	0.191 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.09, 61.4	EDS
L-test for twinning ¹	$< L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1373	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, HTO, PT, NAG

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).

Mal	Chain	Bond	lengths	Bond angles		
MOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	1 A 0.95		0/1229	1.79	$34/1666 \ (2.0\%)$	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	106	LEU	CA-CB-CG	9.36	136.82	115.30
1	A	2	THR	N-CA-C	8.94	135.12	111.00
1	A	77	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	A	109	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	119	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	57	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	A	152	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	57	TRP	CE2-CD2-CG	-7.52	101.29	107.30
1	A	119	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	109	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	27	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	57	TRP	CG-CD2-CE3	7.04	140.24	133.90
1	A	19	VAL	CA-CB-CG2	-6.82	100.67	110.90
1	A	119	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	30	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	1	PHE	N-CA-CB	-6.48	98.94	110.60

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	57	TRP	CB-CG-CD1	-6.35	118.75	127.00
1	A	68	SER	CA-CB-OG	6.28	128.15	111.20
1	A	152	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	125	VAL	N-CA-CB	-6.08	98.12	111.50
1	A	104	LYS	CA-CB-CG	5.93	126.44	113.40
1	A	32	GLN	O-C-N	-5.89	113.28	122.70
1	A	1	PHE	C-N-CA	5.70	135.94	121.70
1	A	19	VAL	CA-CB-CG1	5.63	119.34	110.90
1	A	119	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	A	2	THR	OG1-CB-CG2	5.57	122.80	110.00
1	A	2	THR	CB-CA-C	-5.50	96.76	111.60
1	A	109	TRP	CG-CD1-NE1	-5.45	104.66	110.10
1	A	32	GLN	CA-C-N	5.44	129.17	117.20
1	A	142	ILE	CB-CA-C	-5.34	100.91	111.60
1	A	113	GLU	N-CA-C	-5.32	96.63	111.00
1	A	113	GLU	CA-C-N	-5.24	105.67	117.20
1	A	119	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	87	VAL	CG1-CB-CG2	-5.12	102.72	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	TYR	Sidechain

5.2 Too-close contacts (i)

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1208	0	1212	31	0
2	В	25	0	22	0	0
3	A	1	0	0	0	0
4	A	10	0	16	2	0
5	A	129	0	0	0	0
All	All	1373	0	1250	31	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 12.

All (31) 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:1:PHE:HE2	4:A:162:HTO:H41	1.53	0.72
1:A:111:ARG:NH2	1:A:158:LYS:HG2	2.08	0.68
1:A:70:PRO:HB2	1:A:80:GLU:HB2	1.81	0.62
1:A:39:LEU:HB3	1:A:81:VAL:HG21	1.83	0.59
1:A:8:ILE:O	1:A:12:ILE:HG23	2.04	0.57
1:A:93:LEU:HD12	1:A:94:SER:H	1.69	0.56
1:A:112:ARG:HH11	1:A:114:ASN:HA	1.71	0.55
1:A:124:PRO:HD2	1:A:141:GLU:HB3	1.88	0.55
1:A:98:ASN:OD1	1:A:100:GLU:HG2	2.07	0.54
1:A:36:ALA:HA	1:A:78:VAL:HG21	1.88	0.53
1:A:60:ASN:HA	1:A:83:VAL:O	2.09	0.53
1:A:112:ARG:NH1	1:A:114:ASN:HA	2.23	0.53
1:A:1:PHE:CE2	4:A:162:HTO:H41	2.38	0.52
1:A:107:SER:OG	1:A:124:PRO:HA	2.09	0.52
1:A:44:LYS:HD3	1:A:108:LEU:HD23	1.92	0.51
1:A:71:SER:O	1:A:74:LYS:HE3	2.11	0.51
1:A:77:TYR:HB3	1:A:97:VAL:HG22	1.92	0.50
1:A:111:ARG:HH21	1:A:158:LYS:HG2	1.78	0.48
1:A:94:SER:HA	1:A:102:LYS:HB2	1.95	0.47
1:A:15:ILE:HG13	1:A:16:LEU:N	2.30	0.46
1:A:110:ALA:HB1	1:A:117:VAL:HB	1.98	0.45
1:A:69:PRO:HA	1:A:70:PRO:HD2	1.62	0.43
1:A:29:ALA:HB2	1:A:98:ASN:ND2	2.34	0.43
1:A:84:LYS:HB3	1:A:84:LYS:HE2	1.91	0.43
1:A:99:ASN:HA	1:A:102:LYS:HE3	2.01	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.78	0.42
1:A:43:GLN:HE21	1:A:81:VAL:HG11	1.85	0.42
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.92	0.42
1:A:113:GLU:O	1:A:113:GLU:HG3	2.20	0.41
1:A:112:ARG:HD3	1:A:114:ASN:ND2	2.36	0.41
1:A:50:TYR:O	1:A:54:HIS:ND1	2.54	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	156/158 (99%)	145 (93%)	10 (6%)	1 (1%)	25 47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ASN

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	Analysed Rotameric Outliers		Percentiles	
1	A	130/130 (100%)	109 (84%)	21 (16%)	2 4	

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	33	VAL
1	A	49	GLU
1	A	52	LEU
1	A	54	HIS
1	A	74	LYS
1	A	85	ASN
1	A	88	VAL
1	A	93	LEU
1	A	94	SER

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Mol	Chain	Res	Type
1	A	95	SER
1	A	98	ASN
1	A	106	LEU
1	A	111	ARG
1	A	125	VAL
1	A	126	THR
1	A	128	THR
1	A	130	ASP
1	A	145	LYS
1	A	147	LEU
1	A	158	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	53	ASN
1	A	114	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)

2 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	Trees	Type Chain Res Link				Bond lengths			Bond angles		
IVIOI	туре	Chain Res		Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	NAG	В	1	1,2	14,14,15	0.50	0	17,19,21	0.98	2 (11%)	
2	GLA	В	2	2	11,11,12	0.28	0	15,15,17	0.68	1 (6%)	

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.

N	Лol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	NAG	В	1	1,2	-	1/6/23/26	0/1/1/1
	2	GLA	В	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	В	1	NAG	C4-C3-C2	-2.54	107.30	111.02
2	В	1	NAG	C2-N2-C7	-2.24	119.71	122.90
2	В	2	GLA	C1-O5-C5	2.16	115.11	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

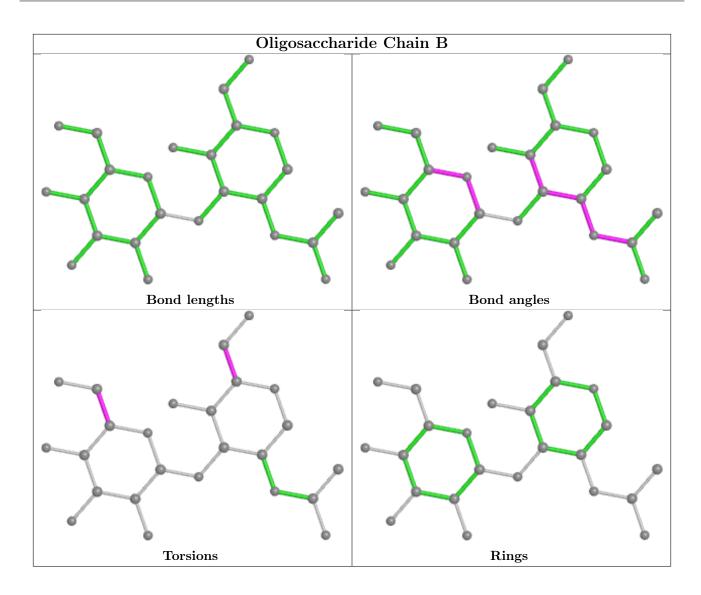
Mol	Chain	Res	Type	Atoms
2	В	2	GLA	O5-C5-C6-O6
2	В	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 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	В	ond leng	${ m gths}$	В	ond ang	les
	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	НТО	A	162	-	9,9,9	0.90	1 (11%)	10,10,10	1.37	1 (10%)

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	НТО	A	162	-	-	3/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	A	162	НТО	C3-C2	2.26	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	162	НТО	O2-C2-C3	-2.53	104.52	109.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	162	НТО	O1-C1-C2-O2
4	A	162	НТО	O1-C1-C2-C3
4	A	162	НТО	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	162	НТО	2	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^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2			$OWAB(Å^2)$	Q<0.9
1	A	158/158 (100%)	-0.93	0 10	00	100	5, 29, 47, 61	0

There are no RSRZ outliers to report.

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

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

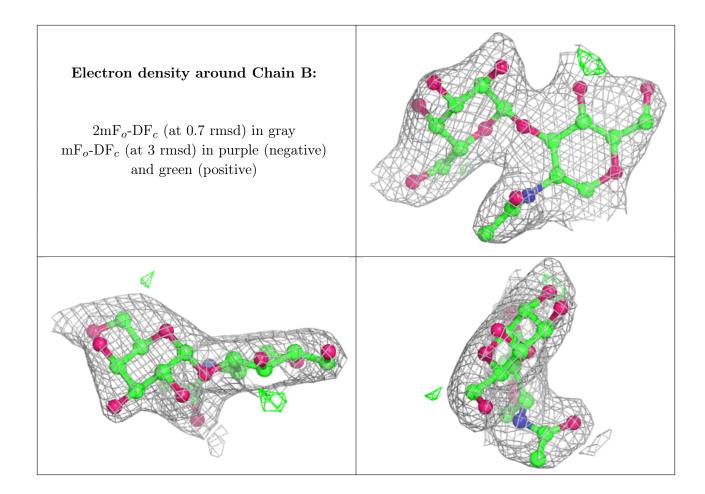
6.3 Carbohydrates (i)

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GLA	В	2	11/12	0.95	0.11	31,38,47,50	0
2	NAG	В	1	14/15	0.96	0.11	24,28,36,43	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	НТО	A	162	10/10	0.86	0.16	88,94,98,101	0
3	PT	A	200	1/1	0.99	0.07	73,73,73,73	1

6.5 Other polymers (i)

There are no such residues in this entry.

