

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 10:58 PM BST

PDB ID	:	1Q9H
Title	:	3-Dimensional structure of native Cel7A from Talaromyces emersonii
Authors	:	Grassick, A.; Thompson, R.; Murray, P.G.; Collins, C.M.; Byrnes, L.; Tuohy,
		M.G.; Birrane, G.; Higgins, T.M.
Deposited on	:	2003-08-25
Resolution	:	2.35 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 following versions of software and data (see references (1)) were used in the production of this report:

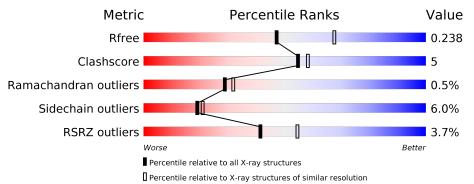
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.35 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	$1164 \ (2.36-2.36)$
Clashscore	141614	1232(2.36-2.36)
Ramachandran outliers	138981	1211(2.36-2.36)
Sidechain outliers	138945	1212(2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	А	437	83%	13%	•••
2	В	2	100%		



$1\mathrm{Q9H}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3504 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 cellobiohydrolase I catalytic domain.

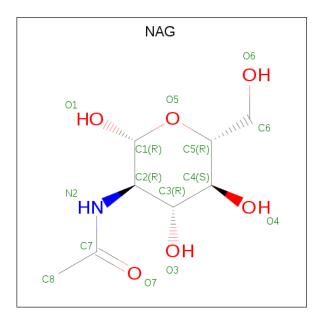
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	430	Total	С	Ν	Ο	\mathbf{S}	0	0	0
-		100	3208	1978	529	674	27		0	

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





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

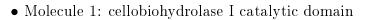
• Molecule 4 is water.

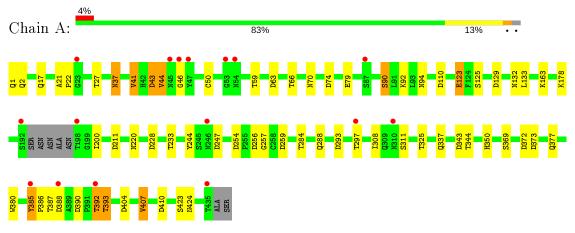
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	254	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 254 & 254 \end{array}$	1 0	0



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 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain B:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	74.39Å 74.39Å 177.05Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.65 - 2.35	Depositor
	19.63 - 2.35	EDS
% Data completeness	97.7(19.65-2.35)	Depositor
(in resolution range)	97.7(19.63-2.35)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.14 (at 2.35 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.1.24$	Depositor
R, R_{free}	0.161 , 0.229	Depositor
II, II, <i>free</i>	0.169 , 0.238	DCC
R_{free} test set	1083 reflections (5.16%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 36.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PCA, 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).

Mol	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.61	0/3279	0.90	16/4482~(0.4%)	

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	129	ASP	CB-CG-OD2	7.18	124.77	118.30
1	А	373	ASP	CB-CG-OD2	6.75	124.37	118.30
1	А	63	ASP	CB-CG-OD2	6.50	124.15	118.30
1	А	247	ASP	CB-CG-OD2	6.37	124.03	118.30
1	А	110	ASP	CB-CG-OD2	6.21	123.89	118.30
1	А	372	ASP	CB-CG-OD2	5.95	123.65	118.30
1	А	343	ASP	CB-CG-OD2	5.82	123.54	118.30
1	А	259	ASP	CB-CG-OD2	5.75	123.48	118.30
1	А	293	ASP	CB-CG-OD2	5.67	123.41	118.30
1	А	211	ASP	CB-CG-OD2	5.50	123.25	118.30
1	А	74	ASP	CB-CG-OD2	5.41	123.17	118.30
1	А	43	ASP	CB-CG-OD2	5.33	123.10	118.30
1	А	256	ASP	CB-CG-OD2	5.23	123.01	118.30
1	А	404	ASP	CB-CG-OD2	5.19	122.97	118.30
1	А	410	ASP	CB-CG-OD2	5.09	122.88	118.30
1	А	388	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.



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)	H(added)	Clashes	Symm-Clashes
1	А	3208	0	2899	31	0
2	В	28	0	25	0	0
3	А	14	0	13	1	0
4	А	254	0	0	11	0
All	All	3504	0	2937	32	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 5.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:79:GLU:CG	4:A:673:HOH:O	2.03	1.05
1:A:377:GLN:HG3	4:A:667:HOH:O	1.83	0.77
1:A:92:LYS:HE3	1:A:94:ASN:HD21	1.52	0.75
1:A:90:SER:HB2	1:A:423:SER:HB3	1.74	0.70
1:A:163:LYS:HD2	4:A:588:HOH:O	2.00	0.60
1:A:380:TRP:HA	1:A:385:TYR:HB2	1.85	0.57
1:A:385:TYR:O	1:A:387:THR:N	2.38	0.56
1:A:424:ASN:HB2	4:A:678:HOH:O	2.04	0.56
1:A:254:ASP:OD1	1:A:257:GLY:HA2	2.07	0.55
1:A:385:TYR:O	1:A:386:PRO:C	2.46	0.54
1:A:407:VAL:HG13	4:A:448:HOH:O	2.07	0.53
1:A:385:TYR:HB3	1:A:386:PRO:HD3	1.93	0.50
1:A:385:TYR:C	1:A:385:TYR:CD1	2.82	0.49
1:A:46:GLY:HA3	4:A:555:HOH:O	2.12	0.49
1:A:228:ASP:OD1	1:A:350:HIS:HD2	1.96	0.49
1:A:90:SER:HB2	1:A:423:SER:CB	2.43	0.49
1:A:17:GLN:HE21	1:A:27:THR:HG22	1.79	0.47
1:A:21:ALA:HB1	1:A:22:PRO:HD2	1.96	0.47
1:A:284:THR:HB	1:A:308:ILE:HB	1.97	0.47
1:A:424:ASN:CB	4:A:678:HOH:O	2.64	0.46
1:A:41:VAL:HG22	1:A:50:CYS:HB2	1.98	0.45
1:A:27:THR:HG23	4:A:607:HOH:O	2.17	0.44
1:A:244:TYR:CB	4:A:558:HOH:O	2.66	0.43

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Atom-1	Atom-2	${f Interatomic} \ {f distance} \ ({ m \AA})$	Clash overlap (Å)	
1:A:123:GLU:HB2	1:A:288:GLN:HG2	2.01	0.43	
1:A:390:ASP:OD2	1:A:392:THR:OG1	2.35	0.43	
1:A:390:ASP:HB3	1:A:393:THR:CG2	2.49	0.42	
1:A:37:ASN:O	1:A:178:LYS:NZ	2.53	0.42	
1:A:66:THR:HG22	1:A:70:ASN:ND2	2.35	0.42	
3:A:440:NAG:H5	4:A:612:HOH:O	2.19	0.41	
1:A:2:GLN:HG3	1:A:44:VAL:HG21	2.03	0.41	
1:A:92:LYS:HE3	1:A:94:ASN:ND2	2.28	0.41	
1:A:350:HIS:HE1	4:A:496:HOH:O	2.03	0.41	

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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 A		Allowed	Outliers	Percentiles
1	А	426/437~(98%)	410 (96%)	14 (3%)	2~(0%)	29 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	311	SER
1	А	385	TYR

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	А	351/361~(97%)	330 (94%)	21~(6%)	19 21	

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

Mol	Chain	Res	Type
1	А	37	ASN
1	А	41	VAL
1	А	43	ASP
1	А	44	VAL
1	А	59	THR
1	А	90	SER
1	А	123	GLU
1	А	125	SER
1	А	132	ASN
1	А	133	LEU
1	А	200	ILE
1	А	220	ASN
1	А	233	THR
1	А	297	THR
1	А	325	THR
1	А	337	GLN
1	А	344	THR
1	А	369	SER
1	А	392	THR
1	А	393	THR
1	А	407	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	17	GLN
1	А	45	ASN
1	А	69	GLN
1	А	94	ASN
1	А	109	GLN
1	А	115	GLN
1	А	121	ASN
1	А	220	ASN
1	А	350	HIS
1	А	417	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)

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).

ſ	Mal	Tune	Chain	Dog	Tink	B	ond leng	gths	B	ond ang	gles
		туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
	1	PCA	А	1	1	7,8,9	1.99	2 (28%)	$9,\!10,\!12$	2.17	4 (44%)

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	PCA	А	1	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	1	PCA	CD-N	4.22	1.45	1.34
1	А	1	PCA	CA-N	2.72	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1	PCA	CA-N-CD	-3.33	102.16	113.58
1	А	1	PCA	CB-CA-C	-3.20	108.31	112.70
1	А	1	PCA	OE-CD-CG	-2.95	121.61	126.76
1	А	1	PCA	CG-CD-N	2.40	114.61	108.39

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

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	Type	Chain	Res	Link	Bo	Bond lengths			ond ang	les
WIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	14, 14, 15	0.70	0	17,19,21	0.83	0
2	NAG	В	2	2	14,14,15	0.61	0	17,19,21	0.92	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	\mathbf{Link}	Chirals	Torsions	Rings
2	NAG	В	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

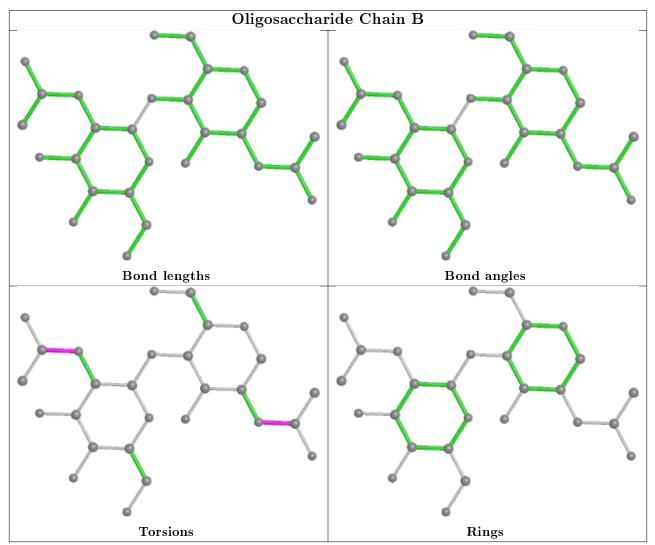
All (4) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	1	NAG	C8-C7-N2-C2
2	В	2	NAG	O7-C7-N2-C2
2	В	1	NAG	O7-C7-N2-C2

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)

1 ligand 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
	3	NAG	А	440	1	$14,\!14,\!15$	0.67	0	$17,\!19,\!21$	1.06	2 (11%)



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	\mathbf{Res}	Link	Chirals	Torsions	Rings
3	NAG	А	440	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	440	NAG	O5-C1-C2	-2.20	107.81	111.29
3	А	440	NAG	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	440	NAG	C8-C7-N2-C2
3	А	440	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mo	Chain	Res	Type	Clashes	Symm-Clashes
3	A	440	NAG	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	ain Analysed <rsrz< th=""><th>#RSRZ>2</th><th>$OWAB(Å^2)$</th><th>Q<0.9</th></rsrz<>		#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	429/437~(98%)	-0.29	16 (3%) 41 54	7, 18, 41, 50	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	47	TYR	4.4
1	А	192	SER	4.3
1	А	46	GLY	3.6
1	А	45	ASN	3.4
1	А	435	THR	3.3
1	А	392	THR	2.9
1	А	198	THR	2.8
1	А	297	THR	2.7
1	А	385	TYR	2.7
1	А	246	ASN	2.6
1	А	87	SER	2.5
1	А	388	ASP	2.4
1	А	23	GLY	2.2
1	А	54	ASN	2.2
1	А	310	ASN	2.0
1	А	53	GLY	2.0

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^{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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
1	PCA	А	1	8/9	0.95	0.13	$20,\!20,\!21,\!21$	0

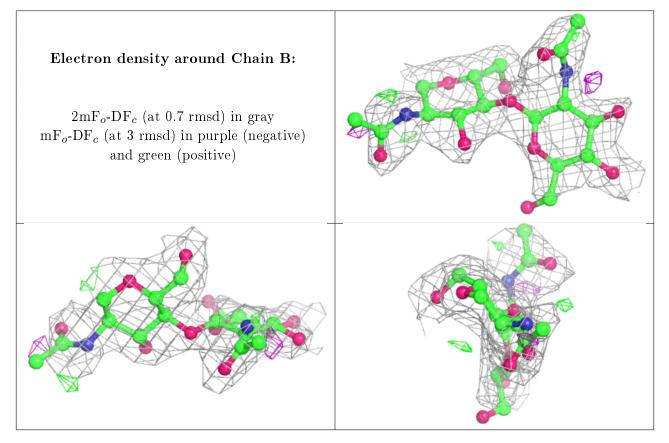


6.3 Carbohydrates (i)

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^{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	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
2	NAG	В	2	14/15	0.82	0.29	$50,\!53,\!55,\!56$	0
2	NAG	В	1	14/15	0.88	0.18	$32,\!41,\!47,\!48$	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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
3	NAG	А	440	14/15	0.87	0.29	$44,\!47,\!50,\!50$	0



6.5 Other polymers (i)

There are no such residues in this entry.

