



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:35 AM GMT

PDB ID : 3QW9  
Title : Crystal structure of betaglycan ZP-C domain  
Authors : Lin, S.J.; Jardetzky, T.S.  
Deposited on : 2011-02-27  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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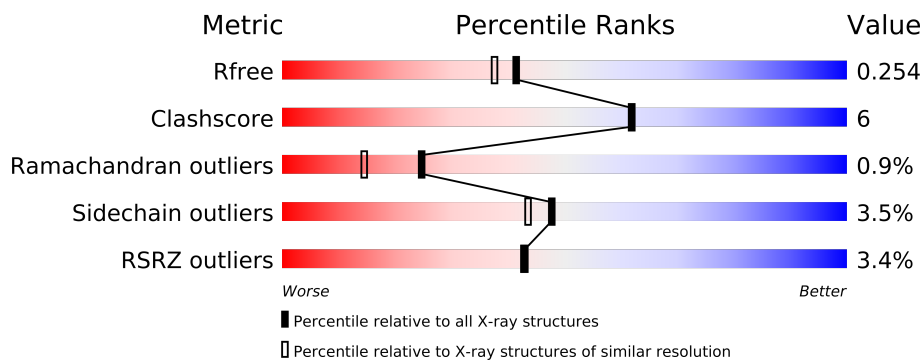
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	176	
1	B	176	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2982 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transforming growth factor beta receptor type 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1347	867	218	251	11			
1	B	166	Total	C	N	O	S	0	1	0
			1322	851	214	246	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PRO	-	EXPRESSION TAG	UNP P26342
A	12	ASN	-	EXPRESSION TAG	UNP P26342
A	13	SER	-	EXPRESSION TAG	UNP P26342
B	11	PRO	-	EXPRESSION TAG	UNP P26342
B	12	ASN	-	EXPRESSION TAG	UNP P26342
B	13	SER	-	EXPRESSION TAG	UNP P26342

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			59	34	2	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PRO	-	EXPRESSION TAG	UNP P26342
A	12	ASN	-	EXPRESSION TAG	UNP P26342
A	13	SER	-	EXPRESSION TAG	UNP P26342

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			81	46	2	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PRO	-	EXPRESSION TAG	UNP P26342
A	12	ASN	-	EXPRESSION TAG	UNP P26342
A	13	SER	-	EXPRESSION TAG	UNP P26342

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	87	Total	O	0	0
			87	87		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

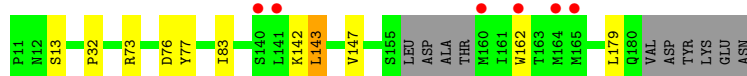
- Molecule 1: Transforming growth factor beta receptor type 3

Chain A: 



- Molecule 1: Transforming growth factor beta receptor type 3

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.53Å 63.57Å 107.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 47.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.00) 98.7 (47.89-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.186 , 0.245 0.201 , 0.254	Depositor DCC
$R_{free}$ test set	1278 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25073 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, NAG, MAN

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	0.88	0/1381	0.88	1/1874 (0.1%)
1	B	0.89	0/1358	0.85	1/1842 (0.1%)
All	All	0.88	0/2739	0.86	2/3716 (0.1%)

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	B	0	1
3	A	3	0
All	All	3	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	163	THR	CB-CA-C	-5.01	98.07	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	205	MAN	C1
3	A	190	FUC	C1
3	A	206	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	32	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1347	0	14	8	0
1	B	1322	0	19	3	0
2	A	59	0	52	3	0
3	A	81	0	69	6	0
4	A	86	0	0	4	0
4	B	87	0	0	1	0
All	All	2982	0	154	17	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:188:NAG:H5	3:A:190:FUC:H61	1.49	0.94
3:A:188:NAG:H83	3:A:206:MAN:H5	1.55	0.89
1:A:136:ARG:NH2	4:A:280:HOH:O	2.23	0.70
2:A:200:NAG:H61	2:A:202:FUC:H5	1.74	0.68
1:A:42:HIS:CD2	1:A:115:LEU:CD2	2.80	0.65
1:A:165:MET:CE	4:A:265:HOH:O	2.49	0.59
1:A:42:HIS:NE2	1:A:115:LEU:CD2	2.68	0.57
1:A:121:ASN:N	3:A:206:MAN:HO4	2.04	0.55
3:A:188:NAG:HN2	3:A:206:MAN:H61	1.76	0.51
1:B:142:LYS:O	1:B:143:LEU:CD1	2.64	0.45
3:A:188:NAG:H83	3:A:206:MAN:C5	2.38	0.45
1:A:13:SER:OG	2:A:200:NAG:H81	2.18	0.44
1:B:76:ASP:N	4:B:213:HOH:O	2.51	0.43
2:A:200:NAG:H61	2:A:202:FUC:C5	2.47	0.42
1:A:142:LYS:CA	4:A:223:HOH:O	2.67	0.42
1:A:108:ASP:OD2	4:A:279:HOH:O	2.22	0.41
3:A:187:NAG:H81	1:B:13:SER:OG	2.21	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	168/176 (96%)	164 (98%)	2 (1%)	2 (1%)	19	9
1	B	163/176 (93%)	156 (96%)	6 (4%)	1 (1%)	33	24
All	All	331/352 (94%)	320 (97%)	8 (2%)	3 (1%)	25	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ILE
1	B	83	ILE
1	A	25	ASP

### 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	157/165 (95%)	151 (96%)	6 (4%)	44	39
1	B	154/165 (93%)	149 (97%)	5 (3%)	51	47
All	All	311/330 (94%)	300 (96%)	11 (4%)	48	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	45	VAL
1	A	75	SER

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Mol	Chain	Res	Type
1	A	77	TYR
1	A	163	THR
1	A	164	MET
1	B	77	TYR
1	B	143	LEU
1	B	147	VAL
1	B	162	TRP
1	B	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 carbohydrates 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	$\# Z  > 2$
3	NAG	A	187	1,3	12,14,15	1.17	1 (8%)	15,19,21	1.66	3 (20%)
3	NAG	A	188	3	12,14,15	0.71	0	15,19,21	1.75	4 (26%)
3	BMA	A	189	3	10,11,12	0.84	0	11,15,17	2.16	4 (36%)
3	FUC	A	190	3	9,10,11	0.89	0	10,14,16	2.12	3 (30%)
3	FUC	A	191	3	9,10,11	0.73	0	10,14,16	1.33	2 (20%)
2	NAG	A	200	1,2	12,14,15	1.04	0	15,19,21	2.90	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	201	2	12,14,15	0.93	0	15,19,21	1.88	3 (20%)
2	FUC	A	202	2	9,10,11	0.84	0	10,14,16	1.53	1 (10%)
2	FUC	A	203	2	9,10,11	0.91	0	10,14,16	1.08	0
2	BMA	A	204	2	10,11,12	0.63	0	11,15,17	3.10	3 (27%)
3	MAN	A	205	3	10,11,12	0.72	0	11,15,17	1.04	1 (9%)
3	MAN	A	206	1,3	10,11,12	1.49	2 (20%)	11,15,17	2.67	5 (45%)

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
3	NAG	A	187	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	188	3	-	0/6/23/26	0/1/1/1
3	BMA	A	189	3	-	0/2/19/22	0/1/1/1
3	FUC	A	190	3	1/1/4/5	0/0/17/20	1/1/1/1
3	FUC	A	191	3	-	0/0/17/20	0/1/1/1
2	NAG	A	200	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	201	2	-	0/6/23/26	0/1/1/1
2	FUC	A	202	2	-	0/0/17/20	0/1/1/1
2	FUC	A	203	2	-	0/0/17/20	0/1/1/1
2	BMA	A	204	2	-	0/2/19/22	0/1/1/1
3	MAN	A	205	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	206	1,3	1/1/4/5	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	NAG	C2-N2	-3.05	1.42	1.46
3	A	206	MAN	C4-C5	2.91	1.59	1.53
3	A	206	MAN	O4-C4	2.65	1.49	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	204	BMA	O5-C5-C6	7.15	114.48	106.98
2	A	200	NAG	O3-C3-C2	-5.95	96.60	109.09
2	A	200	NAG	O5-C5-C6	-5.74	100.96	106.98
3	A	206	MAN	O4-C4-C5	5.50	123.77	109.28
2	A	204	BMA	C4-C3-C2	5.07	117.31	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	204	BMA	O5-C5-C4	-4.90	104.44	110.65
3	A	190	FUC	O5-C5-C6	4.80	115.75	108.03
3	A	188	NAG	O5-C5-C6	4.61	111.82	106.98
3	A	189	BMA	O5-C5-C4	-4.52	104.91	110.65
2	A	200	NAG	O5-C5-C4	4.39	116.22	110.65
3	A	206	MAN	O5-C5-C6	-4.00	102.78	106.98
2	A	201	NAG	O4-C4-C3	-3.99	101.40	110.35
3	A	206	MAN	C6-C5-C4	3.64	121.80	113.00
3	A	187	NAG	O3-C3-C2	-3.45	101.84	109.09
3	A	190	FUC	C3-C4-C5	-3.38	104.20	109.84
2	A	202	FUC	C6-C5-C4	-3.35	107.63	113.06
2	A	201	NAG	O5-C5-C6	3.22	110.36	106.98
2	A	200	NAG	C6-C5-C4	-3.16	105.37	113.00
3	A	189	BMA	O5-C5-C6	3.06	110.19	106.98
2	A	201	NAG	C3-C2-N2	-2.96	107.25	111.76
2	A	200	NAG	C3-C4-C5	2.95	115.47	110.20
3	A	205	MAN	O5-C5-C6	2.85	109.97	106.98
3	A	189	BMA	O3-C3-C2	2.84	115.13	109.94
3	A	187	NAG	O5-C5-C6	-2.64	104.21	106.98
3	A	206	MAN	O5-C5-C4	2.59	113.94	110.65
3	A	189	BMA	C4-C3-C2	2.55	113.93	110.50
3	A	187	NAG	C3-C2-N2	-2.48	107.98	111.76
3	A	191	FUC	O5-C5-C6	2.46	111.98	108.03
3	A	206	MAN	C3-C4-C5	-2.42	105.88	110.20
3	A	191	FUC	C6-C5-C4	-2.29	109.34	113.06
3	A	190	FUC	O3-C3-C2	2.23	114.02	109.94
3	A	188	NAG	O4-C4-C5	-2.15	103.62	109.28
3	A	188	NAG	C6-C5-C4	-2.15	107.81	113.00
2	A	200	NAG	O6-C6-C5	-2.13	104.04	111.36
3	A	188	NAG	O3-C3-C2	-2.07	104.75	109.09
2	A	200	NAG	O3-C3-C4	2.04	114.92	110.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	205	MAN	C1
3	A	190	FUC	C1
3	A	206	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	190	FUC	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	170/176 (96%)	0.08	6 (3%)	42	41	22, 36, 64, 88	0
1	B	166/176 (94%)	0.18	6 (3%)	41	40	21, 35, 75, 100	0
All	All	336/352 (95%)	0.13	12 (3%)	43	40	21, 36, 71, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	6.0
1	A	167	ASN	5.1
1	B	162	TRP	4.5
1	A	140	SER	3.9
1	B	164	MET	3.1
1	B	160	MET	3.1
1	A	139	GLY	3.0
1	B	140	SER	2.9
1	A	166	GLN	2.9
1	B	165	MET	2.9
1	A	74	MET	2.2
1	A	179	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	A	190	10/11	0.14	2.32	36,42,58,58	0
3	MAN	A	206	11/12	0.28	1.54	36,86,91,95	0
2	FUC	A	202	10/11	0.12	0.81	26,42,47,52	0
2	NAG	A	201	14/15	0.13	0.05	30,36,48,58	0
3	NAG	A	187	14/15	0.09	-0.55	22,27,33,41	0
2	NAG	A	200	14/15	0.09	-0.68	22,28,36,39	0
3	NAG	A	188	14/15	0.10	-0.84	27,38,62,64	0
3	FUC	A	191	10/11	0.10	-1.42	33,44,50,51	0
2	FUC	A	203	10/11	0.11	-2.15	26,32,43,53	0
3	MAN	A	205	11/12	0.25	-3.10	76,83,89,93	0
3	BMA	A	189	11/12	0.22	-5.57	56,82,93,94	0
2	BMA	A	204	11/12	0.32	-	61,72,82,82	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.