



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2016 – 03:04 PM EDT

PDB ID : 2WQZ  
Title : Crystal structure of synaptic protein neuroligin-4 in complex with neurexin-beta 1: alternative refinement  
Authors : Fabrichny, I.P.; Leone, P.; Sulzenbacher, G.; Comoletti, D.; Miller, M.T.; Taylor, P.; Bourne, Y.; Marchot, P.  
Deposited on : 2009-08-28  
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

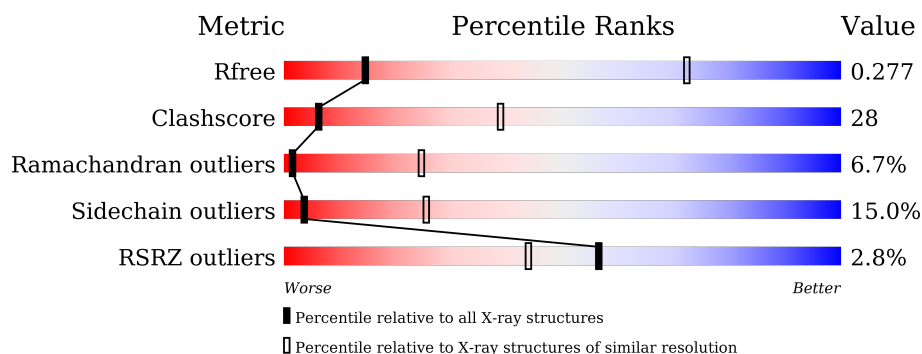
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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. 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	588	<div> <div>0% (Poor fit)</div> <div> <div>42% (Green)</div> <div>38% (Yellow)</div> <div>11% (Orange)</div> <div>7% (Red)</div> </div> </div>
1	B	588	<div> <div>3% (Poor fit)</div> <div> <div>47% (Green)</div> <div>36% (Yellow)</div> <div>8% (Orange)</div> <div>7% (Red)</div> </div> </div>
2	C	179	<div> <div>3% (Poor fit)</div> <div> <div>54% (Green)</div> <div>36% (Yellow)</div> <div>9% (Orange)</div> <div>2% (Red)</div> </div> </div>
2	D	179	<div> <div>9% (Poor fit)</div> <div> <div>54% (Green)</div> <div>36% (Yellow)</div> <div>8% (Orange)</div> <div>1% (Red)</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11360 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 NEUROLIGIN 4, X-LINKED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4310	2756	712	821	21			
1	B	544	Total	C	N	O	S	0	0	0
			4302	2749	713	819	21			

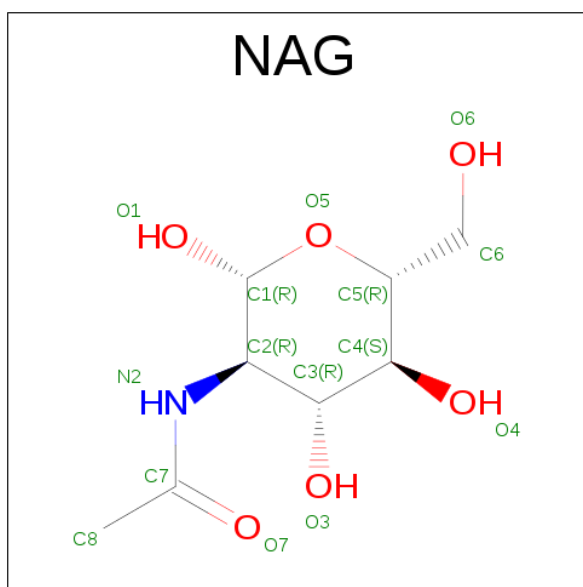
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ARG	LYS	CONFLICT	UNP Q8N0W4
B	561	ARG	LYS	CONFLICT	UNP Q8N0W4

- Molecule 2 is a protein called NEUREXIN-1-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	D	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

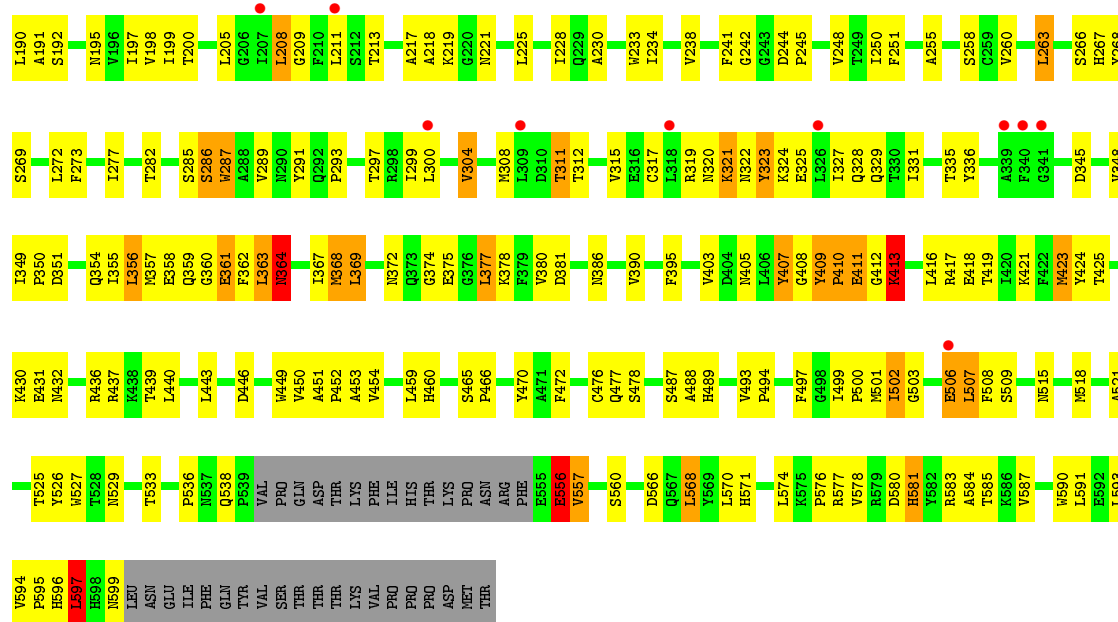


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

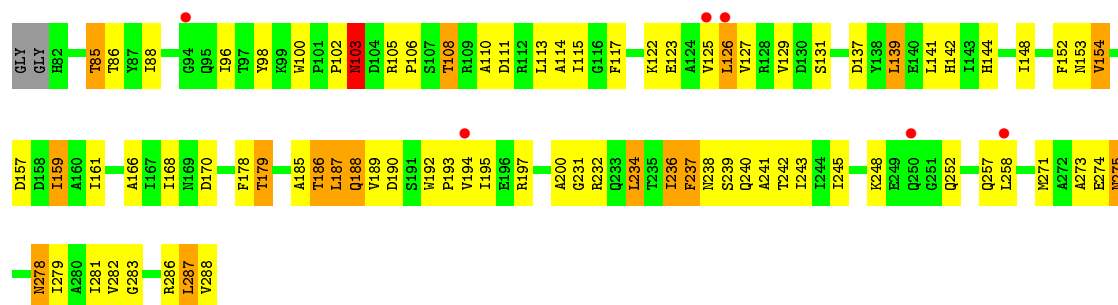
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

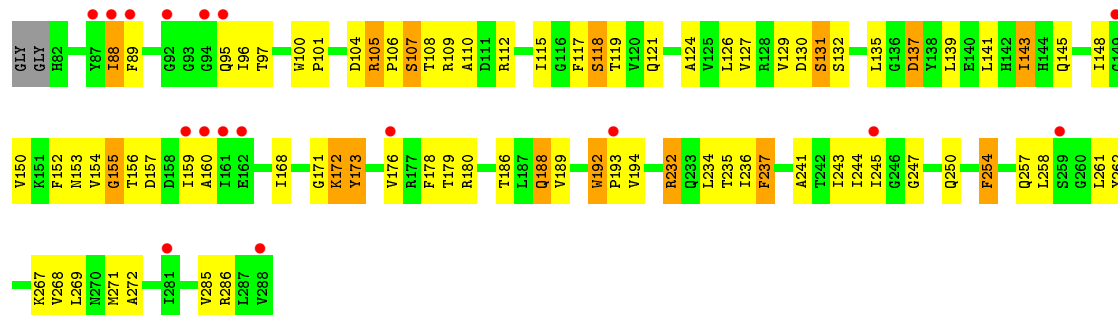




• Molecule 2: NEUREXIN-1-BETA



• Molecule 2: NEUREXIN-1-BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.52Å 198.67Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.90 47.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.90) 96.2 (47.40-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.205 , 0.276 0.208 , 0.277	Depositor DCC
$R_{free}$ test set	1261 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 93.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: CA, 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/4429	0.70	1/6040 (0.0%)
1	B	0.50	0/4422	0.66	0/6033
2	C	0.47	0/1384	0.67	0/1874
2	D	0.59	0/1384	0.68	0/1874
All	All	0.53	0/11619	0.68	1/15821 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	LEU	CA-CB-CG	5.89	128.85	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	410	PRO	Peptide
1	A	411	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	537	ASN	Peptide
1	A	597	LEU	Peptide

## 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	A	4310	0	4133	277	0
1	B	4302	0	4122	211	0
2	C	1359	0	1346	69	0
2	D	1359	0	1346	88	0
3	A	28	0	26	8	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	11360	0	10973	625	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 28.

The worst 5 of 625 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:B:119:LEU:O	1:B:120:LEU:HD22	1.53	1.08
1:A:189:ILE:HD11	1:A:502:ILE:HD12	1.28	1.08
1:A:139:VAL:HG13	1:A:140:GLN:H	1.24	0.98
1:A:149:LEU:CD1	1:A:151:ILE:HD11	1.96	0.95
2:D:141:LEU:HD11	2:D:148:ILE:HG23	1.47	0.94

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	539/588 (92%)	388 (72%)	105 (20%)	46 (8%)	1	17
1	B	540/588 (92%)	419 (78%)	81 (15%)	40 (7%)	1	21
2	C	173/179 (97%)	142 (82%)	28 (16%)	3 (2%)	11	55
2	D	173/179 (97%)	125 (72%)	41 (24%)	7 (4%)	4	37
All	All	1425/1534 (93%)	1074 (75%)	255 (18%)	96 (7%)	1	25

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLY
1	A	87	ARG
1	A	118	SER
1	A	121	HIS
1	A	126	ILE

### 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	467/510 (92%)	390 (84%)	77 (16%)	3	21
1	B	466/510 (91%)	400 (86%)	66 (14%)	4	28
2	C	143/143 (100%)	119 (83%)	24 (17%)	2	20
2	D	143/143 (100%)	127 (89%)	16 (11%)	7	37
All	All	1219/1306 (93%)	1036 (85%)	183 (15%)	3	25

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	ARG
1	B	166	LYS

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Mol	Chain	Res	Type
2	D	105	ARG
1	B	101	ARG
1	B	121	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	ASN
1	B	386	ASN
2	D	145	GLN
1	B	364	ASN
1	B	405	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	NAG	A	1599	-	14,14,15	0.38	0	15,19,21	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1600	-	14,14,15	0.32	0	15,19,21	0.84	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
3	NAG	A	1599	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1600	-	-	0/6/23/26	0/1/1/1

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.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1599	NAG	5	0
3	A	1600	NAG	3	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 ⓘ

### 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	545/588 (92%)	-0.26	3 (0%) 90 86	50, 72, 77, 86	0
1	B	544/588 (92%)	-0.05	15 (2%) 56 44	63, 73, 78, 84	0
2	C	177/179 (98%)	0.12	6 (3%) 49 37	59, 72, 81, 83	0
2	D	177/179 (98%)	0.51	17 (9%) 10 7	61, 76, 84, 86	0
All	All	1443/1534 (94%)	-0.04	41 (2%) 56 44	50, 73, 80, 86	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	94	GLY	10.8
2	D	162	GLU	6.5
2	C	94	GLY	5.7
2	D	89	PHE	4.9
2	D	160	ALA	4.0

### 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 ⓘ

There are no carbohydrates in this entry.

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	D	1289	1/1	0.97	0.14	-1.27	134,134,134,134	0
4	CA	C	1289	1/1	0.99	0.07	-1.84	109,109,109,109	0
3	NAG	A	1600	14/15	0.79	0.14	-	191,192,193,193	0
3	NAG	A	1599	14/15	0.80	0.17	-	221,222,224,225	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.