



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:12 pm BST

PDB ID : 6Q41  
Title : Atomic resolution crystal structure of a BAA collagen heterotrimer  
Authors : Jalan, A.A.; Hartgerink, J.D.; Brear, P.; Leitinger, B.; Farndale, R.W.  
Deposited on : 2018-12-05  
Resolution : 1.03 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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) : 2.11

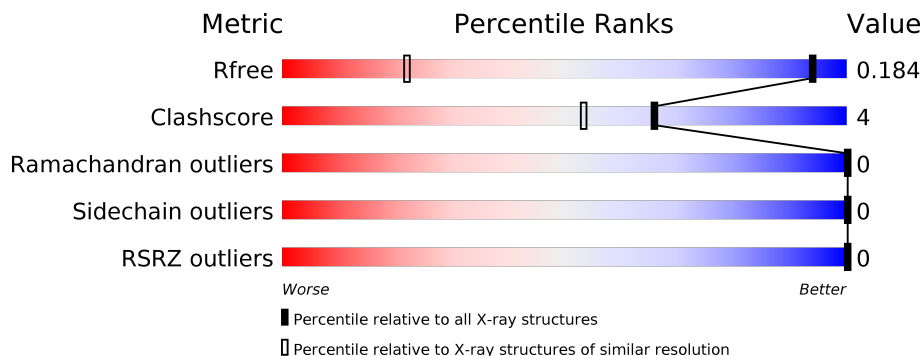
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.03 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))
$R_{free}$	130704	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)
RSRZ outliers	127900	1557 (1.10-0.98)

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 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	B	50	
1	C	50	
2	A	50	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2274 atoms, of which 969 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.

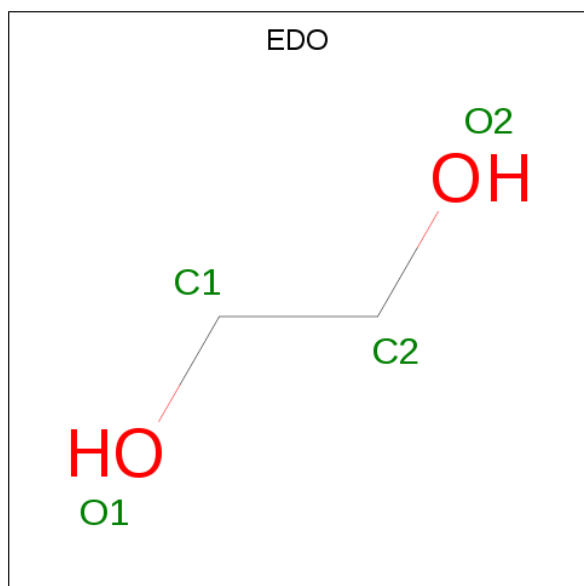
- Molecule 1 is a protein called Middle and Trailing Chains of the BAA collagen heterotrimer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	B	50	Total 633	C 203	H 310	N 59	O 61	4	1	1
1	C	50	Total 623	C 201	H 301	N 58	O 63	4	1	1

- Molecule 2 is a protein called Leading chain of the BAA collagen heterotrimer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	A	50	Total 651	C 211	H 312	N 61	O 67	3	4	1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



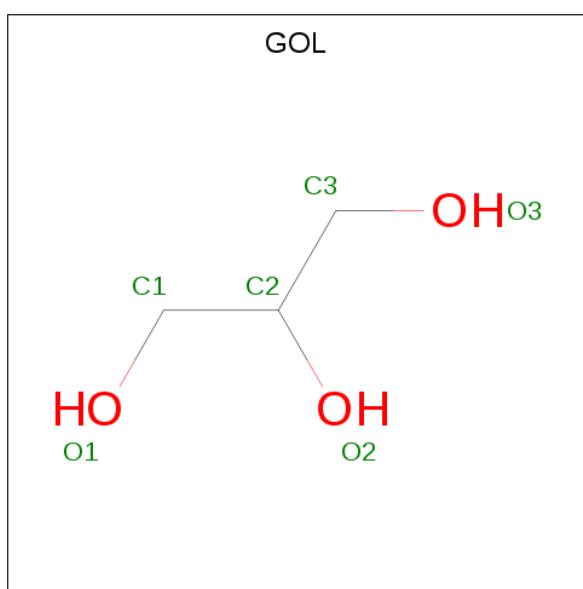
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	Total 10	C 2	H 6	O 2	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	1	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	C	1	Total 14	C 3	H 8	O 3	0	0
4	A	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 5 is water.

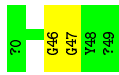
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	100	Total 100	O 100	0	0
5	C	97	Total 97	O 97	0	0
5	A	92	Total 92	O 92	0	0

### 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 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: Middle and Trailing Chains of the BAA collagen heterotrimer

Chain B:  96%



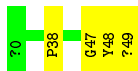
- Molecule 1: Middle and Trailing Chains of the BAA collagen heterotrimer

Chain C:  96%



- Molecule 2: Leading chain of the BAA collagen heterotrimer

Chain A:  92% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	18.78Å 38.66Å 45.33Å 69.04° 79.58° 77.44°	Depositor
Resolution (Å)	42.06 – 1.03 42.06 – 1.03	Depositor EDS
% Data completeness (in resolution range)	90.3 (42.06-1.03) 91.7 (42.06-1.03)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.03Å)	Xtrriage
Refinement program	PHENIX 1.13_2998, REFMAC 5.8.0158, CCP4	Depositor
R, $R_{free}$	0.143 , 0.177 0.151 , 0.184	Depositor DCC
$R_{free}$ test set	2631 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtrriage
Anisotropy	0.732	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.024 for h,h-k,h-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5961e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, ACE, EDO, HYP, NLE, NH2

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	B	0.57	0/317	0.73	0/429
1	C	0.62	0/316	0.83	0/429
2	A	0.70	0/332	0.84	0/448
All	All	0.63	0/965	0.80	0/1306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	B	323	310	307	2	0
1	C	322	301	298	2	0
2	A	339	312	308	5	0
3	B	16	24	24	1	0
3	C	4	6	6	3	0
4	A	6	8	8	0	0
4	C	6	8	8	1	1
5	A	92	0	0	1	1
5	B	100	0	0	1	0
5	C	97	0	0	0	0
All	All	1305	969	959	8	1

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 4.

All (8) 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:46:GLY:HA3	2:A:47[B]:GLY:O	2.05	0.57
2:A:49[B]:NH2:N	5:A:202:HOH:O	2.44	0.50
3:C:101:EDO:H22	2:A:38:PRO:HD3	1.96	0.47
3:C:101:EDO:C2	2:A:38:PRO:HD3	2.46	0.46
1:C:33:PRO:HB2	3:C:101:EDO:H11	1.98	0.46
1:C:0:ACE:O	4:C:102:GOL:H11	2.16	0.46
3:B:104:EDO:H11	5:B:260:HOH:O	2.15	0.45
1:B:47:GLY:HA2	2:A:48[A]:TYR:OH	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:102:GOL:O1	5:A:203:HOH:O[1_447]	2.17	0.03

## 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	B	47/50 (94%)	47 (100%)	0	0	100	100
1	C	47/50 (94%)	47 (100%)	0	0	100	100
2	A	49/50 (98%)	49 (100%)	0	0	100	100
All	All	143/150 (95%)	143 (100%)	0	0	100	100

There are no Ramachandran outliers to report.



### 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	B	28/27 (104%)	28 (100%)	0	100	100
1	C	28/27 (104%)	28 (100%)	0	100	100
2	A	29/28 (104%)	29 (100%)	0	100	100
All	All	85/82 (104%)	85 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	HYP	C	30	1	6,8,9	0.59	0	5,10,12	1.55	1 (20%)
2	HYP	A	24	2	6,8,9	0.69	0	5,10,12	2.10	1 (20%)
1	HYP	B	30	1	6,8,9	0.41	0	5,10,12	0.97	0
1	NLE	B	27	1	6,7,8	0.69	0	2,7,9	1.03	0
1	NLE	C	27	1	6,7,8	0.52	0	2,7,9	0.45	0
2	HYP	A	30	2	6,8,9	0.69	0	5,10,12	3.02	3 (60%)

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	HYP	C	30	1	-	0/0/11/13	0/1/1/1
2	HYP	A	24	2	-	0/0/11/13	0/1/1/1
1	HYP	B	30	1	-	0/0/11/13	0/1/1/1
1	NLE	B	27	1	-	1/5/6/8	-
1	NLE	C	27	1	-	0/5/6/8	-
2	HYP	A	30	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	30	HYP	CB-CG-CD	5.53	110.05	103.27
2	A	24	HYP	CB-CG-CD	-4.24	98.07	103.27
1	C	30	HYP	OD1-CG-CD	-2.22	105.49	110.35
2	A	30	HYP	CG-CB-CA	-2.22	101.16	103.96
2	A	30	HYP	OD1-CG-CB	-2.21	104.58	110.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	27	NLE	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands 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	EDO	B	102	-	3,3,3	0.41	0	2,2,2	0.48	0
4	GOL	C	102	-	5,5,5	0.28	0	5,5,5	0.23	0
3	EDO	C	101	-	3,3,3	0.77	0	2,2,2	0.45	0
3	EDO	B	103	-	3,3,3	0.67	0	2,2,2	0.16	0
4	GOL	A	101	-	5,5,5	0.58	0	5,5,5	0.45	0
3	EDO	B	104	-	3,3,3	0.50	0	2,2,2	0.26	0
3	EDO	B	101	-	3,3,3	0.56	0	2,2,2	0.21	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	EDO	B	102	-	-	0/1/1/1	-
4	GOL	C	102	-	-	2/4/4/4	-
3	EDO	C	101	-	-	0/1/1/1	-
3	EDO	B	103	-	-	0/1/1/1	-
4	GOL	A	101	-	-	0/4/4/4	-
3	EDO	B	104	-	-	0/1/1/1	-
3	EDO	B	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	102	GOL	O1-C1-C2-C3
4	C	102	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	102	GOL	1	1
3	C	101	EDO	3	0
3	B	104	EDO	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, 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	B	46/50 (92%)	-0.45	0 100 100	9, 14, 27, 27	0
1	C	46/50 (92%)	-0.52	0 100 100	10, 14, 23, 27	0
2	A	46/50 (92%)	-0.45	0 100 100	9, 14, 22, 25	0
All	All	138/150 (92%)	-0.48	0 100 100	9, 14, 25, 27	0

There are no RSRZ outliers to report.

### 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<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	B-factors(Å <sup>2</sup> )	Q < 0.9
2	HYP	A	24	8/9	0.96	0.10	17,20,24,25	1
1	HYP	C	30	8/9	0.98	0.04	16,19,24,25	1
1	NLE	C	27	8/9	0.98	0.05	14,19,27,27	0
2	HYP	A	30	8/9	0.98	0.06	12,18,24,26	0
1	HYP	B	30	8/9	0.99	0.04	12,16,20,20	1
1	NLE	B	27	8/9	0.99	0.06	13,20,30,30	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	102	6/6	0.69	0.21	55,66,68,69	0
3	EDO	B	102	4/4	0.74	0.16	50,60,63,63	1
3	EDO	C	101	4/4	0.78	0.14	41,49,49,49	1
3	EDO	B	103	4/4	0.80	0.14	30,37,43,44	1
3	EDO	B	104	4/4	0.80	0.18	52,62,67,68	0
4	GOL	A	101	6/6	0.97	0.12	15,19,23,23	0
3	EDO	B	101	4/4	0.97	0.15	17,29,33,37	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.