



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 11:08 am GMT

PDB ID : 6YHN  
Title : Crystal structure of domains 4-5 of CNFy from Yersinia pseudotuberculosis  
Authors : Lukat, P.; Gazdag, E.M.; Heidler, T.V.; Blankenfeldt, W.  
Deposited on : 2020-03-30  
Resolution : 1.80 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 : 2.16  
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) : 2.16

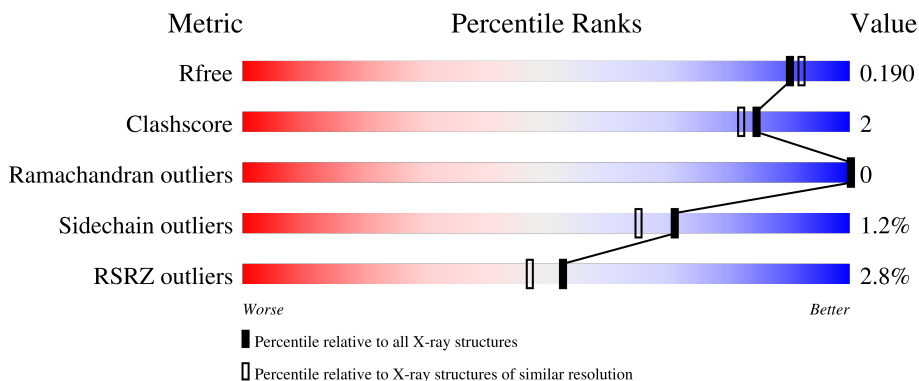
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	A	519	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7667 atoms, of which 3598 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 Cytotoxic necrotizing factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	460	7272	2331	3588	603	742	8	1	24	0

There are 30 discrepancies between the modelled and reference sequences:

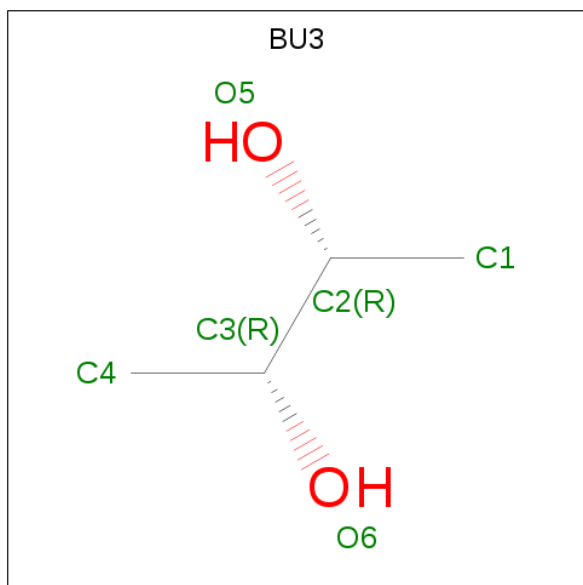
Chain	Residue	Modelled	Actual	Comment	Reference
A	522	GLY	-	expression tag	UNP A0A0N9JNY6
A	523	GLY	-	expression tag	UNP A0A0N9JNY6
A	524	GLY	-	expression tag	UNP A0A0N9JNY6
A	525	ARG	-	expression tag	UNP A0A0N9JNY6
A	1015	SER	-	expression tag	UNP A0A0N9JNY6
A	1016	ALA	-	expression tag	UNP A0A0N9JNY6
A	1017	GLY	-	expression tag	UNP A0A0N9JNY6
A	1018	GLY	-	expression tag	UNP A0A0N9JNY6
A	1019	ASP	-	expression tag	UNP A0A0N9JNY6
A	1020	TYR	-	expression tag	UNP A0A0N9JNY6
A	1021	LYS	-	expression tag	UNP A0A0N9JNY6
A	1022	ASP	-	expression tag	UNP A0A0N9JNY6
A	1023	HIS	-	expression tag	UNP A0A0N9JNY6
A	1024	ASP	-	expression tag	UNP A0A0N9JNY6
A	1025	GLY	-	expression tag	UNP A0A0N9JNY6
A	1026	ASP	-	expression tag	UNP A0A0N9JNY6
A	1027	TYR	-	expression tag	UNP A0A0N9JNY6
A	1028	LYS	-	expression tag	UNP A0A0N9JNY6
A	1029	ASP	-	expression tag	UNP A0A0N9JNY6
A	1030	HIS	-	expression tag	UNP A0A0N9JNY6
A	1031	ASP	-	expression tag	UNP A0A0N9JNY6
A	1032	ILE	-	expression tag	UNP A0A0N9JNY6
A	1033	ASP	-	expression tag	UNP A0A0N9JNY6
A	1034	TYR	-	expression tag	UNP A0A0N9JNY6
A	1035	LYS	-	expression tag	UNP A0A0N9JNY6
A	1036	ASP	-	expression tag	UNP A0A0N9JNY6
A	1037	ASP	-	expression tag	UNP A0A0N9JNY6

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1038	ASP	-	expression tag	UNP A0A0N9JNY6
A	1039	ASP	-	expression tag	UNP A0A0N9JNY6
A	1040	LYS	-	expression tag	UNP A0A0N9JNY6

- Molecule 2 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	16	4	10	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	4	4	4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0

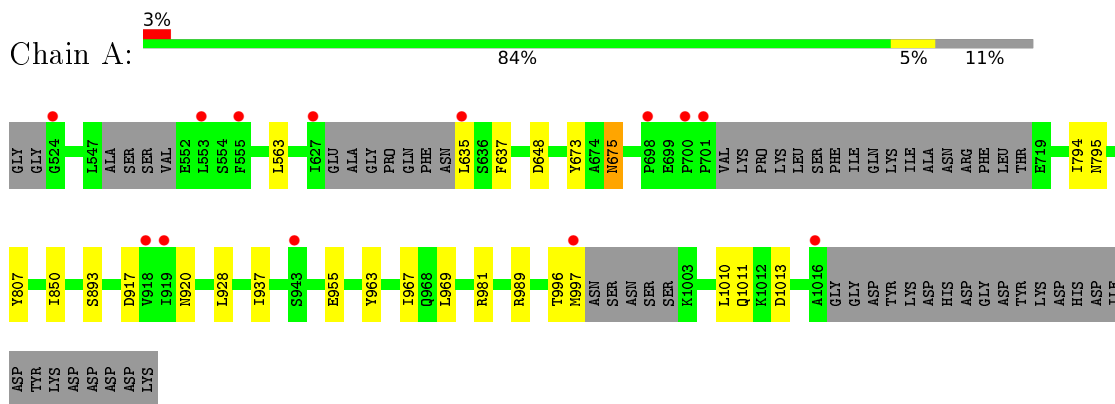
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	367	Total O 367 367	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: Cytotoxic necrotizing factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.27Å 90.53Å 120.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.27 – 1.80 45.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.27-1.80) 100.0 (45.27-1.80)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.14rc1_3177	Depositor
R, $R_{free}$	0.158 , 0.191 0.158 , 0.190	Depositor DCC
$R_{free}$ test set	2412 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.868	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, BU3, CSO, SO4, NA

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	0.30	0/3849	0.50	0/5225

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 [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	3684	3588	3490	17	0
2	A	6	10	10	1	0
3	A	4	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	367	0	0	2	1
All	All	4069	3598	3500	17	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 2.

All (17) 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:989[B]:ARG:NH2	1:A:1013[B]:ASP:OD2	2.27	0.67
1:A:981:ARG:NH1	7:A:1303:HOH:O	2.37	0.58
1:A:807:TYR:OH	7:A:1301:HOH:O	2.17	0.56
1:A:850:ILE:O	1:A:981:ARG:HG3	2.06	0.56
1:A:563:LEU:HD12	1:A:648:ASP:HA	1.89	0.55
1:A:955:GLU:OE1	1:A:955:GLU:N	2.36	0.52
1:A:893:SER:O	1:A:920:ASN:HA	2.11	0.51
1:A:850:ILE:O	1:A:981:ARG:CG	2.64	0.46
1:A:963:TYR:HA	1:A:967:ILE:HD12	1.97	0.46
1:A:794:ILE:HD12	1:A:794:ILE:N	2.31	0.45
1:A:635:LEU:HB3	1:A:637:PHE:CE2	2.54	0.42
1:A:996:THR:O	1:A:997:MET:HB2	2.19	0.42
1:A:673:TYR:CE1	2:A:1201:BU3:H42	2.56	0.41
1:A:675:ASN:N	1:A:675:ASN:HD22	2.19	0.41
1:A:928:LEU:HD12	1:A:937:ILE:HD11	2.03	0.41
1:A:1010:LEU:C	1:A:1010:LEU:HD23	2.42	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)
7:A:1312:HOH:O	7:A:1314:HOH:O[1_455]	2.08	0.12

## 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	473/519 (91%)	462 (98%)	11 (2%)	0	<b>100</b> <b>100</b>

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	A	427/459 (93%)	421 (99%)	6 (1%)	67 59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	ASN
1	A	795	ASN
1	A	917	ASP
1	A	969	LEU
1	A	1011[A]	GLN
1	A	1011[B]	GLN

Sometimes 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](#)

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSO	A	866	1	3,6,7	0.69	0	0,6,8	0.00	-

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	CSO	A	866	1	-	0/1/5/7	-

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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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	$\# Z  > 2$
6	SO4	A	1209	-	4,4,4	0.15	0	6,6,6	0.05	0
2	BU3	A	1201	-	4,5,5	0.74	0	6,6,6	0.38	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
2	BU3	A	1201	-	-	0/4/4/4	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	BU3	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	A	459/519 (88%)	-0.27	13 (2%) 53 47	16, 29, 65, 117	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	701	PRO	3.6
1	A	943	SER	3.5
1	A	555	PHE	3.3
1	A	524	GLY	3.1
1	A	700	PRO	3.1
1	A	627	ILE	2.9
1	A	635	LEU	2.9
1	A	698	PRO	2.9
1	A	1016	ALA	2.4
1	A	919	ILE	2.3
1	A	997	MET	2.3
1	A	918	VAL	2.2
1	A	553	LEU	2.1

### 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
1	CSO	A	866	7/8	0.92	0.10	17,25,60,72	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	1209	5/5	0.74	0.20	119,120,131,134	0
4	NA	A	1207	1/1	0.83	0.10	64,64,64,64	0
3	MG	A	1205	1/1	0.94	0.12	32,32,32,32	0
2	BU3	A	1201	6/6	0.95	0.12	37,72,77,86	0
3	MG	A	1203	1/1	0.98	0.10	31,31,31,31	0
4	NA	A	1206	1/1	0.98	0.21	65,65,65,65	0
3	MG	A	1204	1/1	0.99	0.09	25,25,25,25	0
3	MG	A	1202	1/1	0.99	0.22	19,19,19,19	0
5	CL	A	1208	1/1	0.99	0.06	29,29,29,29	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.