wwPDB X-ray Structure Validation Summary Report (i)

Jan 21, 2025 – 06:52 pm GMT

PDB ID	:	9G7P
Title	:	Crystal structure of Shewanella putrefaciens PE-like toxin, Spx
Authors	:	Masuyer, G.
Deposited on	:	2024-07-22
Resolution	:	1.86 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

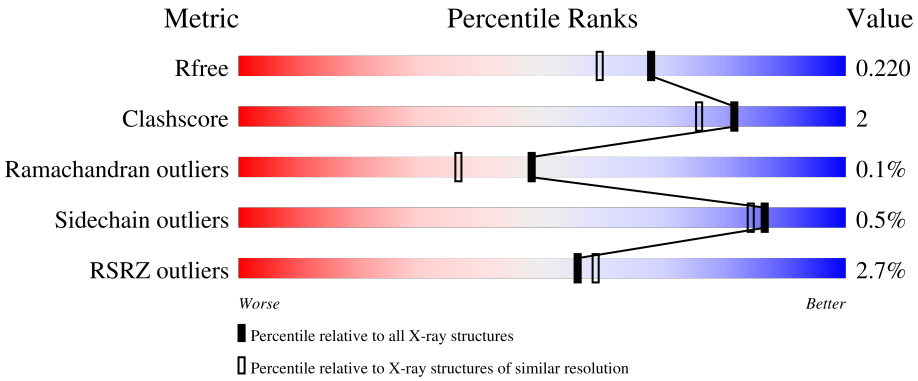
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.86 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 >=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	AAA	613	2% 94% 5% ·
1	BBB	613	3% 91% 8% ·
1	CCC	613	3% 92% 6% ·

2 Entry composition (i)

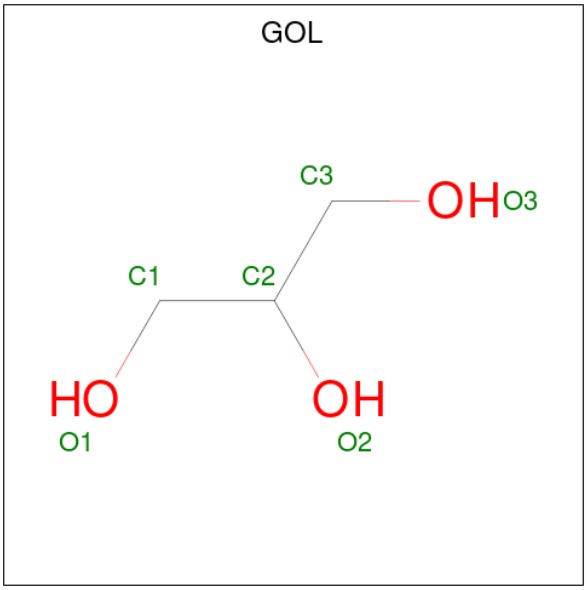
There are 4 unique types of molecules in this entry. The entry contains 28572 atoms, of which 13386 are hydrogens and 0 are deuteriums.

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 Shewanella putrefaciens PE-like toxin catalytically inactive mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	603	Total	C	H	N	O	S	156	0	0
			9081	2897	4446	819	908	11			
1	BBB	603	Total	C	H	N	O	S	156	0	0
			9081	2897	4446	819	908	11			
1	CCC	603	Total	C	H	N	O	S	156	0	0
			9081	2897	4446	819	908	11			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
2	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
2	BBB	1	Total	C	H	O	2	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total C H O 14 3 8 3	2	0
2	CCC	1	Total C H O 14 3 8 3	2	0
2	CCC	1	Total C H O 14 3 8 3	2	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Mg 1 1	0	0
3	BBB	2	Total Mg 2 2	0	0
3	CCC	1	Total Mg 1 1	0	0

- Molecule 4 is water.

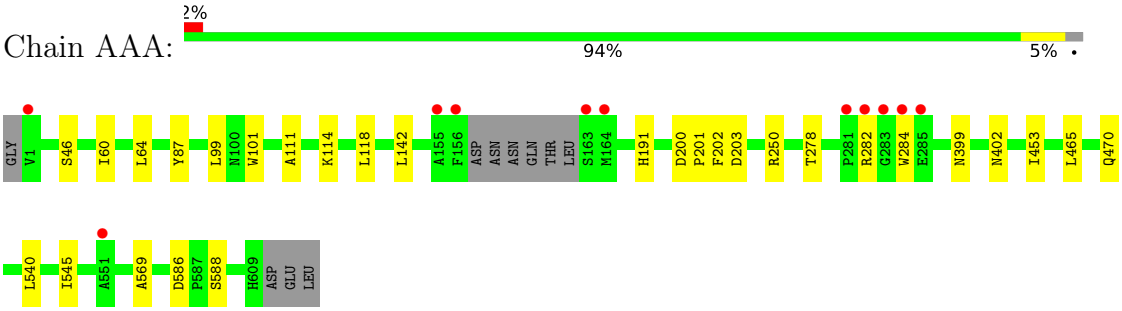
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	400	Total O 400 400	0	0
4	BBB	380	Total O 380 380	0	0
4	CCC	461	Total O 461 461	0	0

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.

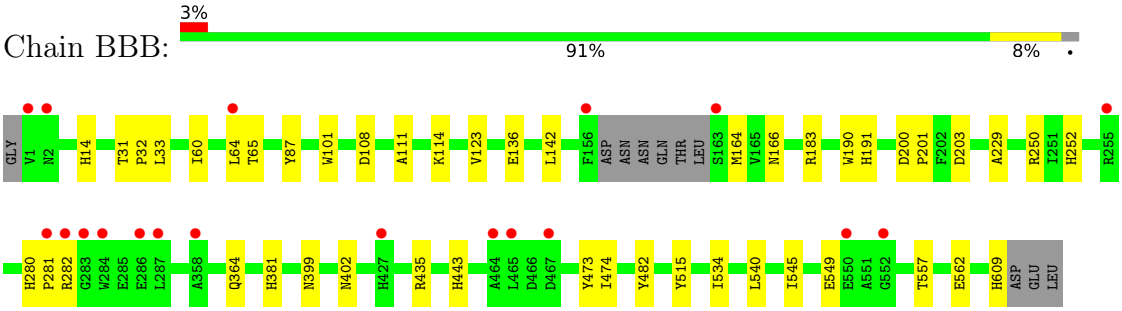
• Molecule 1: Shewanella putrefaciens PE-like toxin catalytically inactive mutant

Chain AAA:



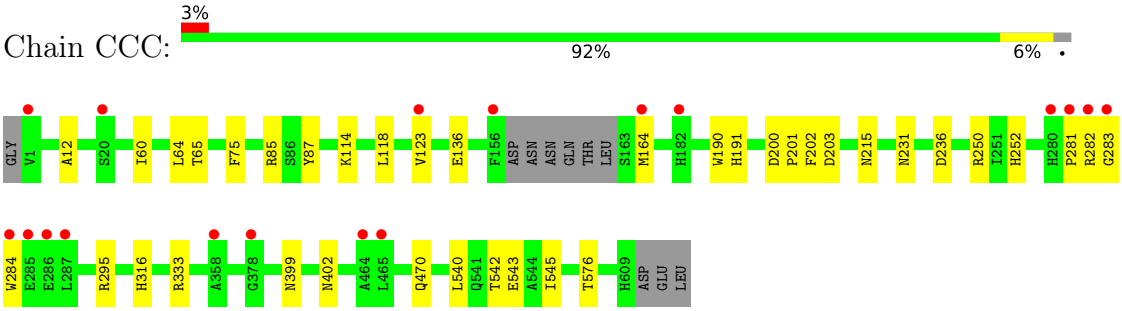
• Molecule 1: Shewanella putrefaciens PE-like toxin catalytically inactive mutant

Chain BBB:



• Molecule 1: Shewanella putrefaciens PE-like toxin catalytically inactive mutant

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	121.20Å 121.20Å 125.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	104.83 – 1.86 104.83 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (104.83-1.86) 99.5 (104.83-1.86)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.220 0.184 , 0.220	Depositor DCC
R_{free} test set	8476 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.059 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28572	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, GOL

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	AAA	0.63	0/4750	0.72	0/6495
1	BBB	0.63	0/4750	0.73	0/6495
1	CCC	0.63	0/4750	0.73	1/6495 (0.0%)
All	All	0.63	0/14250	0.73	1/19485 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	333	ARG	CG-CD-NE	-5.18	100.91	111.80

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	AAA	4635	4446	4424	15	0
1	BBB	4635	4446	4424	26	1
1	CCC	4635	4446	4424	22	1
2	AAA	12	16	16	0	0
2	BBB	12	16	16	1	0
2	CCC	12	16	16	2	0
3	AAA	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	2	0	0	0	1
3	CCC	1	0	0	0	0
4	AAA	400	0	0	1	0
4	BBB	380	0	0	3	0
4	CCC	461	0	0	6	0
All	All	15186	13386	13320	64	2

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.

The worst 5 of 64 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:CCC:470:GLN:NE2	4:CCC:804:HOH:O	2.29	0.62
1:CCC:215:ASN:HB2	4:CCC:1183:HOH:O	1.98	0.62
1:BBB:399:ASN:H	1:BBB:402:ASN:HD22	1.47	0.62
1:CCC:399:ASN:H	1:CCC:402:ASN:HD22	1.50	0.59
1:AAA:470:GLN:NE2	4:AAA:801:HOH:O	2.22	0.56

All (2) 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)
1:BBB:65:THR:HG23	1:BBB:609:HIS:HD1[3_644]	1.31	0.29
1:CCC:316:HIS:HE2	3:BBB:704:MG:MG[1_665]	1.58	0.02

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	AAA	599/613 (98%)	584 (98%)	15 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BBB	599/613 (98%)	582 (97%)	16 (3%)	1 (0%)	44 32
1	CCC	599/613 (98%)	581 (97%)	17 (3%)	1 (0%)	44 32
All	All	1797/1839 (98%)	1747 (97%)	48 (3%)	2 (0%)	48 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	281	PRO
1	CCC	281	PRO

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	AAA	496/505 (98%)	494 (100%)	2 (0%)	89 88
1	BBB	496/505 (98%)	494 (100%)	2 (0%)	89 88
1	CCC	496/505 (98%)	493 (99%)	3 (1%)	84 81
All	All	1488/1515 (98%)	1481 (100%)	7 (0%)	86 84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	203	ASP
1	CCC	164	MET
1	CCC	284	TRP
1	CCC	203	ASP
1	BBB	164	MET

Sometimes 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 molecules 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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	GOL	CCC	701	-	5,5,5	0.08	0	5,5,5	0.31	0
2	GOL	BBB	701	-	5,5,5	0.10	0	5,5,5	0.30	0
2	GOL	AAA	701	-	5,5,5	0.08	0	5,5,5	0.27	0
2	GOL	BBB	702	-	5,5,5	0.09	0	5,5,5	0.26	0
2	GOL	CCC	702	-	5,5,5	0.07	0	5,5,5	0.33	0
2	GOL	AAA	702	-	5,5,5	0.10	0	5,5,5	0.30	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	GOL	CCC	701	-	-	2/4/4/4	-
2	GOL	BBB	701	-	-	2/4/4/4	-
2	GOL	AAA	701	-	-	0/4/4/4	-
2	GOL	BBB	702	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	CCC	702	-	-	2/4/4/4	-
2	GOL	AAA	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	701	GOL	O1-C1-C2-C3
2	CCC	701	GOL	O1-C1-C2-C3
2	CCC	702	GOL	O1-C1-C2-O2
2	CCC	702	GOL	O1-C1-C2-C3
2	BBB	701	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	701	GOL	1	0
2	CCC	702	GOL	2	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^{th} 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^2)	Q<0.9
1	AAA	603/613 (98%)	-0.11	11 (1%)	67	70	21, 33, 54, 119	0
1	BBB	603/613 (98%)	-0.11	19 (3%)	50	53	23, 34, 55, 119	0
1	CCC	603/613 (98%)	-0.16	18 (2%)	52	56	20, 33, 52, 112	0
All	All	1809/1839 (98%)	-0.13	48 (2%)	56	59	20, 33, 54, 119	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	284	TRP	9.2
1	BBB	284	TRP	7.6
1	CCC	284	TRP	7.5
1	AAA	156	PHE	6.7
1	BBB	281	PRO	5.5

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	GOL	AAA	701	6/6	0.82	0.21	41,52,61,61	2
2	GOL	BBB	702	6/6	0.86	0.15	38,51,57,58	2
2	GOL	BBB	701	6/6	0.87	0.14	50,57,64,64	2
2	GOL	CCC	701	6/6	0.90	0.12	36,42,46,47	2
2	GOL	AAA	702	6/6	0.91	0.12	41,48,53,54	2
2	GOL	CCC	702	6/6	0.91	0.12	44,46,52,53	2
3	MG	AAA	703	1/1	0.98	0.04	29,29,29,29	0
3	MG	BBB	704	1/1	0.98	0.06	35,35,35,35	0
3	MG	CCC	703	1/1	0.99	0.02	27,27,27,27	0
3	MG	BBB	703	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.