Full wwPDB X-ray Structure Validation Report (i)

May 1, 2017 – 04:32 PM EDT

PDB ID	:	5NI0
Title	:	VIM-2_10c. Metallo-beta-Lactamase Inhibitors by Bioisosteric Replacement: Preparation, Activity and Binding
Authors	:	Skagseth, S.; Akhter, S.; Paulsen, M.H.; Samuelsen, O.; Muhammad, Z.; Leiros, H.-K.S.; Bayer, A.
Deposited on	:	2017-03-22
Resolution	:	1.67 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

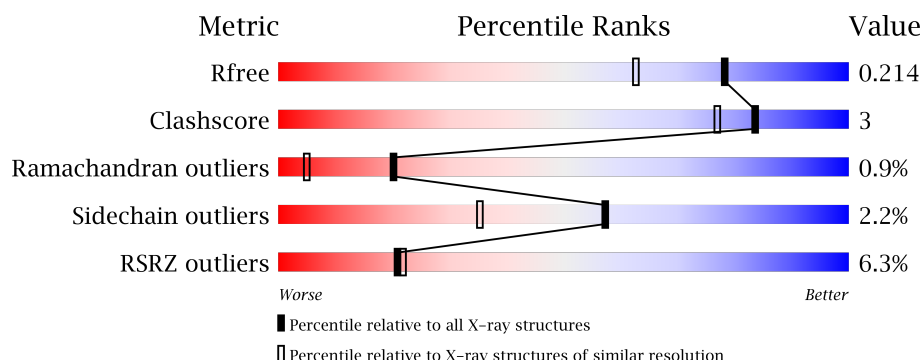|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

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 1.67 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	Percentile Ranks	Value
Rfree		0.214
Clashscore		3
Ramachandran outliers		0.9%
Sidechain outliers		2.2%
RSRZ outliers		6.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

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 >=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 <=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	266	5% / 81% / 6% / 14%
1	E	266	6% / 81% / 5% / 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7403 atoms, of which 3410 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 Beta-lactamase class B VIM-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	3	0
			3440	1105	1692	300	342	1			
1	E	229	Total	C	H	N	O	S	4	2	0
			3423	1099	1680	301	342	1			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		

- Molecule 3 is [(2 {R})-1-ethanoylsulfanyl-6-phenyl-hexan-2-yl]phosphonic acid (three-letter code: 8XW) (formula: $C_{14}H_{21}O_4PS$).
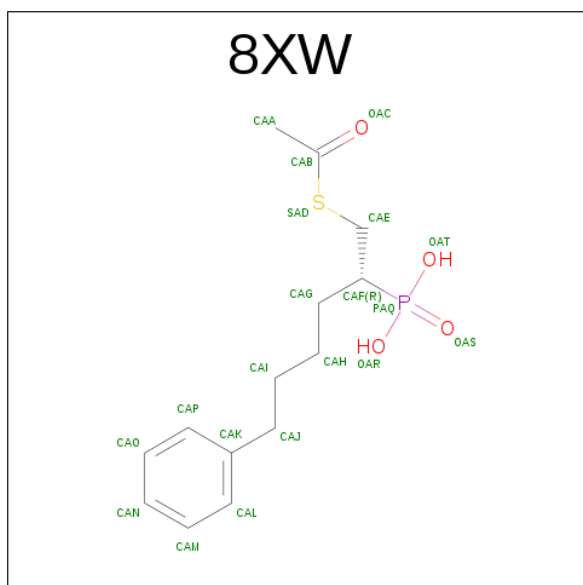
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	S	0	0
			39	14	19	4	1	1		
3	E	1	Total	C	H	O	P	S	0	0
			39	14	19	4	1	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	E	228	Total	O	0	0
			228	228		

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: Beta-lactamase class B VIM-2
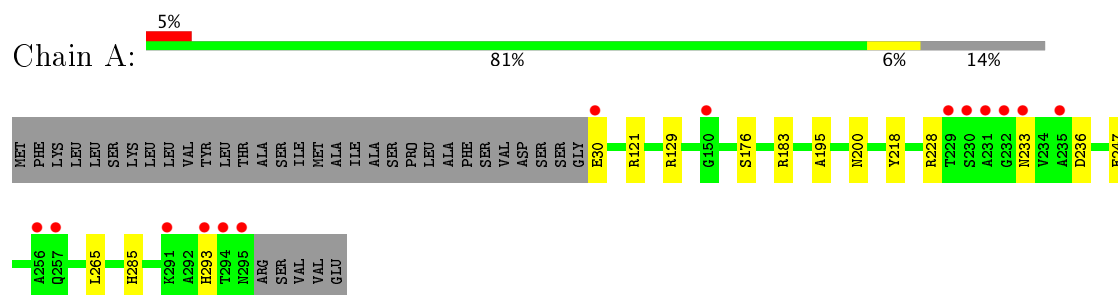
- Molecule 1: Beta-lactamase class B VIM-2
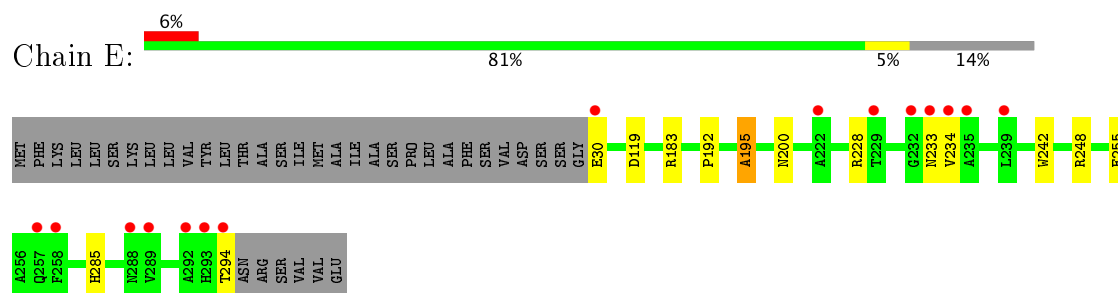
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.72Å 91.07Å 122.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.77 – 1.67	Depositor
	24.77 – 1.67	EDS
% Data completeness	94.1 (24.77-1.67)	Depositor
(in resolution range)	94.1 (24.77-1.67)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.67 (at 1.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.178 , 0.214	Depositor
	0.178 , 0.214	DCC
R_{free} test set	2781 reflections (4.92%)	DCC
Wilson B-factor (Å²)	20.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.40 , 50.4	EDS
L-test for twinning [2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7403	wwPDB-VP
Average B, all atoms (Å²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.14 % 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 5.8510e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 8XW

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	0.49	0/1795	0.64	0/2457
1	E	0.52	0/1784	0.64	0/2441
All	All	0.50	0/3579	0.64	0/4898

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	1748	1692	1694	10	0
1	E	1743	1680	1687	5	0
2	A	2	0	0	0	0
2	E	2	0	0	0	0
3	A	20	19	0	2	0
3	E	20	19	0	2	0
4	A	230	0	0	8	3
4	E	228	0	0	3	2
All	All	3993	3410	3381	19	3

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 3.

All (19) 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)
3:E:403:8XW:SAD	4:E:507:HOH:O	2.23	0.96
1:E:30:GLU:N	4:E:501:HOH:O	2.06	0.88
1:A:247:GLU:OE2	4:A:501:HOH:O	2.00	0.77
1:E:248[A]:ARG:NH1	4:E:502:HOH:O	2.16	0.77
1:A:236:ASP:OD2	4:A:502:HOH:O	2.10	0.69
1:A:176:SER:OG	4:A:503:HOH:O	2.16	0.61
1:A:129:ARG:NH1	4:A:510:HOH:O	2.34	0.58
1:A:129:ARG:NH2	4:A:510:HOH:O	2.42	0.53
1:E:228:ARG:O	1:E:285:HIS:NE2	2.41	0.52
1:A:30:GLU:OE2	4:A:504:HOH:O	2.19	0.51
1:E:192:PRO:O	1:E:248[A]:ARG:NH1	2.45	0.50
1:A:293:HIS:ND1	1:A:293:HIS:O	2.46	0.49
3:A:403:8XW:CAE	4:A:527:HOH:O	2.61	0.48
3:E:403:8XW:CAH	3:E:403:8XW:CAL	2.91	0.48
1:A:233:ASN:ND2	4:A:513:HOH:O	2.51	0.44
1:E:195:ALA:HB1	1:E:242:TRP:CD1	2.53	0.43
3:A:403:8XW:SAD	3:A:403:8XW:CAH	3.08	0.42
1:A:228:ARG:O	1:A:285:HIS:NE2	2.50	0.41
1:A:121:ARG:NH1	1:A:218:TYR:OH	2.53	0.40

All (3) 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:A:706:HOH:O	4:E:682:HOH:O[3_454]	2.07	0.13
4:A:706:HOH:O	4:E:548:HOH:O[3_454]	2.11	0.09
4:A:575:HOH:O	4:A:609:HOH:O[4_455]	2.18	0.02

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	231/266 (87%)	226 (98%)	4 (2%)	1 (0%)	38	18
1	E	229/266 (86%)	223 (97%)	3 (1%)	3 (1%)	14	2
All	All	460/532 (86%)	449 (98%)	7 (2%)	4 (1%)	20	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	233	ASN
1	A	195	ALA
1	E	195	ALA
1	E	234	VAL

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	186/214 (87%)	183 (98%)	3 (2%)	68	50
1	E	184/214 (86%)	178 (97%)	6 (3%)	43	19
All	All	370/428 (86%)	361 (98%)	9 (2%)	57	32

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	A	200	ASN
1	A	265	LEU
1	E	119[A]	ASP
1	E	119[B]	ASP
1	E	183	ARG
1	E	200	ASN
1	E	255	GLU
1	E	294	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	252	HIS

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 6 ligands modelled in this entry, 4 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	8XW	A	403	-	18,20,20	2.32	5 (27%)	17,26,26	1.30	2 (11%)
3	8XW	E	403	2	18,20,20	2.43	5 (27%)	17,26,26	1.21	2 (11%)

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	8XW	A	403	-	-	2/15/18/18	0/1/1/1
3	8XW	E	403	2	-	2/15/18/18	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	8XW	CAJ-CAK	-4.38	1.38	1.51
3	E	403	8XW	PAQ-OAR	-4.18	1.47	1.54
3	A	403	8XW	PAQ-OAR	-3.85	1.48	1.54
3	E	403	8XW	CAJ-CAK	-3.84	1.40	1.51
3	E	403	8XW	CAG-CAF	-2.39	1.52	1.54
3	A	403	8XW	CAE-SAD	-2.07	1.79	1.81
3	A	403	8XW	PAQ-OAT	4.43	1.62	1.54
3	E	403	8XW	PAQ-OAT	4.49	1.62	1.54
3	A	403	8XW	PAQ-OAS	5.75	1.60	1.49
3	E	403	8XW	PAQ-OAS	6.53	1.61	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	403	8XW	OAT-PAQ-OAS	-3.78	103.81	113.41
3	A	403	8XW	OAT-PAQ-OAS	-3.22	105.23	113.41
3	A	403	8XW	CAH-CAI-CAJ	-2.42	104.07	113.70
3	E	403	8XW	OAR-PAQ-OAT	2.86	115.79	107.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	8XW	CAA-CAB-SAD-CAE
3	A	403	8XW	OAC-CAB-SAD-CAE
3	E	403	8XW	CAA-CAB-SAD-CAE
3	E	403	8XW	OAC-CAB-SAD-CAE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	8XW	2	0
3	E	403	8XW	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 (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, 95th 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	A	230/266 (86%)	0.25	14 (6%)	22	23	13, 23, 42, 64	7 (3%)
1	E	229/266 (86%)	0.30	15 (6%)	19	20	12, 23, 46, 61	10 (4%)
All	All	459/532 (86%)	0.28	29 (6%)	21	22	12, 23, 45, 64	17 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	THR	6.7
1	A	231	ALA	5.9
1	A	295	ASN	5.8
1	E	234	VAL	4.9
1	E	294	THR	4.4
1	E	239	LEU	4.2
1	E	229	THR	4.1
1	A	229	THR	3.6
1	E	292	ALA	3.6
1	A	293	HIS	3.5
1	E	289	VAL	3.3
1	E	233	ASN	3.2
1	A	233	ASN	3.1
1	A	230	SER	2.7
1	E	232	GLY	2.7
1	E	235	ALA	2.7
1	E	257	GLN	2.5
1	E	222	ALA	2.4
1	A	235	ALA	2.3
1	E	288	ASN	2.3
1	A	232	GLY	2.3
1	E	30	GLU	2.2
1	A	257	GLN	2.2
1	A	291	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	293	HIS	2.2
1	E	258	PHE	2.2
1	A	150	GLY	2.1
1	A	256	ALA	2.1
1	A	30	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

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. 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, 95th 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(Å^2)	Q<0.9
3	8XW	A	403	20/20	0.84	0.23	1.93	46,62,77,86	14
3	8XW	E	403	20/20	0.86	0.24	1.81	36,64,79,80	15
2	ZN	A	401	1/1	1.00	0.06	-0.94	22,22,22,22	0
2	ZN	E	401	1/1	1.00	0.05	-0.95	25,25,25,25	0
2	ZN	E	402	1/1	0.97	0.08	-1.75	27,27,27,27	1
2	ZN	A	402	1/1	0.98	0.07	-1.92	29,29,29,29	1

6.5 Other polymers (i)

There are no such residues in this entry.