



wwPDB X-ray Structure Validation Summary Report

Feb 15, 2017 – 01:43 am GMT

PDB ID : 2DKF
Title : Crystal Structure of TTHA0252 from *Thermus thermophilus* HB8, a RNA Degradation Protein of the Metallo-beta-lactamase Superfamily
Authors : Ishikawa, I.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-04-10
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

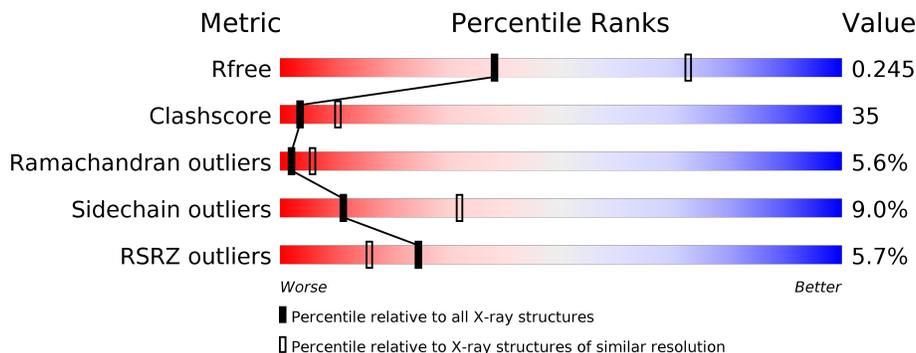
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 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 $\leq 5\%$. 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	431	
1	B	431	
1	C	431	
1	D	431	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	433	-	-	-	X
2	ZN	B	432	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13404 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 metallo-beta-lactamase superfamily protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	431	3326	2127	597	594	1	7	0	0	0
1	B	431	3326	2127	597	594	1	7	0	0	0
1	C	431	3326	2127	597	594	1	7	0	0	0
1	D	431	3326	2127	597	594	1	7	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	32	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	90	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	101	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	253	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	307	MSE	MET	MODIFIED RESIDUE	GB 55771634
A	315	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	1	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	32	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	90	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	101	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	253	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	307	MSE	MET	MODIFIED RESIDUE	GB 55771634
B	315	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	1	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	32	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	90	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	101	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	253	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	307	MSE	MET	MODIFIED RESIDUE	GB 55771634
C	315	MSE	MET	MODIFIED RESIDUE	GB 55771634

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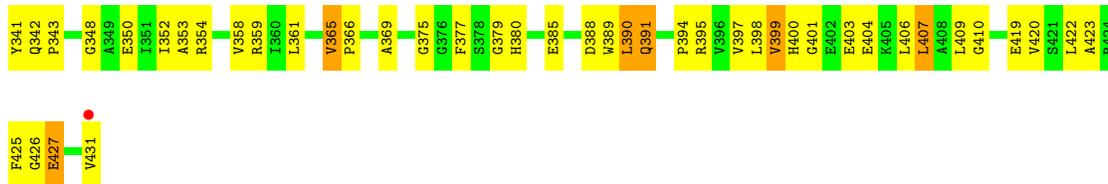
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	32	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	90	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	101	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	253	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	307	MSE	MET	MODIFIED RESIDUE	GB 55771634
D	315	MSE	MET	MODIFIED RESIDUE	GB 55771634

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

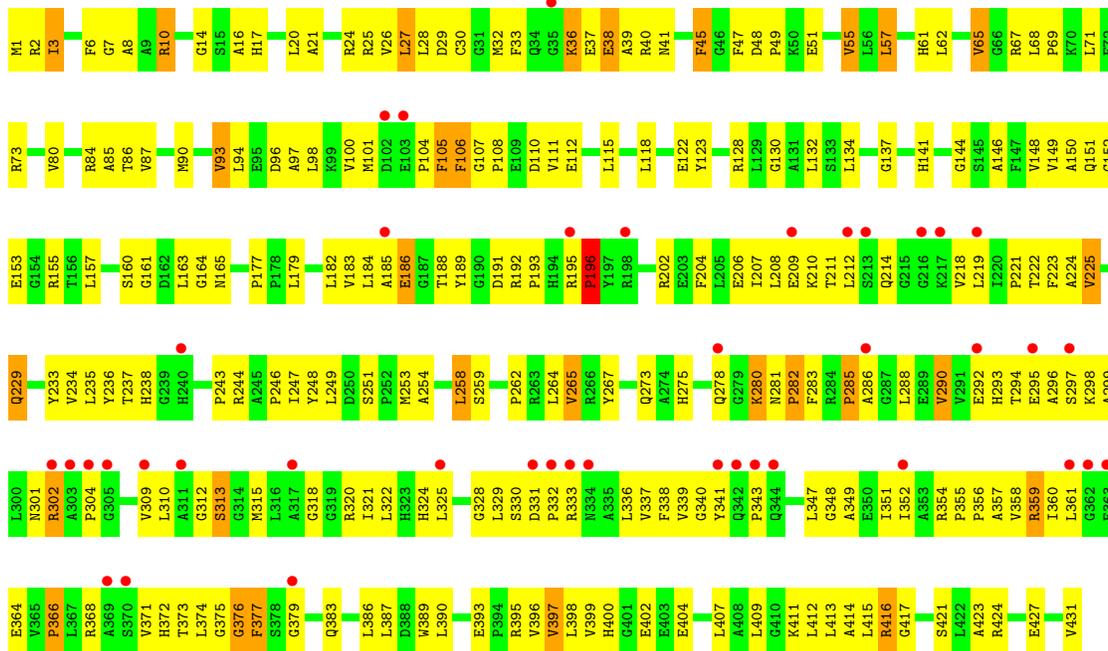
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

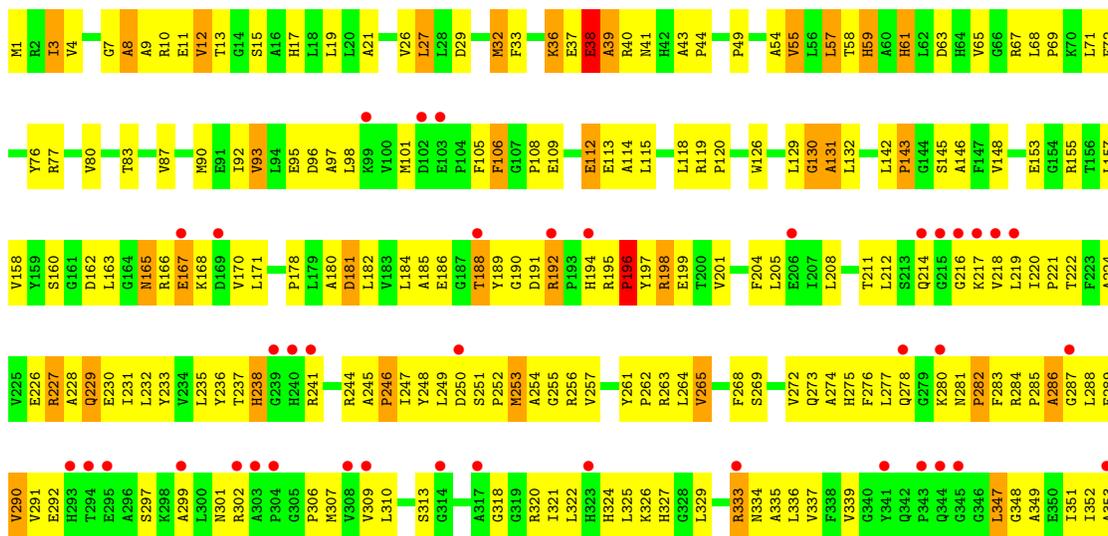
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	28	Total 28	O 28	0	0
3	C	16	Total 16	O 16	0	0
3	D	16	Total 16	O 16	0	0

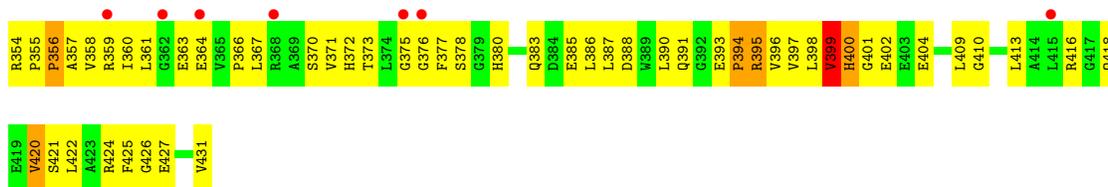


• Molecule 1: metallo-beta-lactamase superfamily protein



• Molecule 1: metallo-beta-lactamase superfamily protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.22Å 147.10Å 121.23Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.99-2.80) 96.1 (19.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	28.81 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.285 0.246 , 0.245	Depositor DCC
R_{free} test set	2847 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	59.7	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13404	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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:
ZN

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	0.59	4/3401 (0.1%)	0.84	5/4603 (0.1%)
1	B	0.59	1/3401 (0.0%)	0.80	2/4603 (0.0%)
1	C	0.47	0/3401	0.67	2/4603 (0.0%)
1	D	0.45	1/3401 (0.0%)	0.65	0/4603
All	All	0.53	6/13604 (0.0%)	0.75	9/18412 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	MSE	CG-SE	-6.77	1.72	1.95
1	A	90	MSE	SE-CE	-6.12	1.59	1.95
1	B	90	MSE	CG-SE	-6.07	1.74	1.95
1	A	90	MSE	CG-SE	-5.91	1.75	1.95
1	A	32	MSE	SE-CE	-5.21	1.64	1.95

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	GLY	N-CA-C	-8.06	92.94	113.10
1	B	375	GLY	N-CA-C	-6.94	95.75	113.10
1	C	161	GLY	N-CA-C	-5.78	98.66	113.10
1	A	161	GLY	N-CA-C	-5.76	98.69	113.10
1	C	105	PHE	N-CA-C	-5.18	97.00	111.00

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	3326	0	3351	206	0
1	B	3326	0	3351	224	0
1	C	3326	0	3351	242	0
1	D	3326	0	3351	272	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	32	0	0	3	0
3	B	28	0	0	0	0
3	C	16	0	0	1	0
3	D	16	0	0	0	0
All	All	13404	0	13404	933	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 35.

The worst 5 of 933 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:C:37:GLU:HB3	1:C:40:ARG:HH11	0.97	1.13
1:C:37:GLU:HB3	1:C:40:ARG:NH1	1.76	1.00
1:D:227:ARG:HB2	1:D:227:ARG:HH21	1.25	0.99
1:C:73:ARG:HE	1:C:106:PHE:HA	1.24	0.98
1:C:235:LEU:HD23	1:C:247:ILE:HD13	1.45	0.97

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	429/431 (100%)	361 (84%)	45 (10%)	23 (5%)	2	6
1	B	429/431 (100%)	364 (85%)	45 (10%)	20 (5%)	3	8
1	C	429/431 (100%)	340 (79%)	64 (15%)	25 (6%)	2	5
1	D	429/431 (100%)	333 (78%)	68 (16%)	28 (6%)	1	4
All	All	1716/1724 (100%)	1398 (82%)	222 (13%)	96 (6%)	2	6

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	59	HIS
1	A	106	PHE
1	A	286	ALA
1	A	304	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	A	342/335 (102%)	299 (87%)	43 (13%)	5	16
1	B	342/335 (102%)	313 (92%)	29 (8%)	12	35
1	C	342/335 (102%)	317 (93%)	25 (7%)	16	42
1	D	342/335 (102%)	316 (92%)	26 (8%)	15	40
All	All	1368/1340 (102%)	1245 (91%)	123 (9%)	11	32

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	B	390	LEU
1	D	188	THR

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Mol	Chain	Res	Type
1	B	184	LEU
1	B	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	324	HIS
1	C	117	HIS
1	D	278	GLN
1	B	383	GLN
1	C	41	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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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	424/431 (98%)	-0.31	1 (0%) 94 94	21, 44, 66, 81	0
1	B	424/431 (98%)	-0.19	7 (1%) 70 63	22, 45, 77, 93	0
1	C	424/431 (98%)	0.41	41 (9%) 8 4	33, 78, 134, 141	0
1	D	424/431 (98%)	0.56	47 (11%) 6 3	36, 90, 146, 160	0
All	All	1696/1724 (98%)	0.12	96 (5%) 24 16	21, 56, 136, 160	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ARG	8.2
1	D	215	GLY	6.9
1	D	216	GLY	6.4
1	C	341	TYR	4.6
1	D	341	TYR	4.6

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
2	ZN	B	432	1/1	0.91	0.22	3.64	28,28,28,28	1
2	ZN	A	433	1/1	0.86	0.21	2.06	37,37,37,37	1
2	ZN	B	433	1/1	0.84	0.18	0.81	42,42,42,42	1
2	ZN	D	432	1/1	0.81	0.23	0.68	59,59,59,59	1
2	ZN	C	432	1/1	0.91	0.20	0.23	48,48,48,48	1
2	ZN	C	433	1/1	0.96	0.19	-0.08	44,44,44,44	1
2	ZN	D	433	1/1	0.90	0.17	-0.36	73,73,73,73	1
2	ZN	A	432	1/1	0.97	0.12	-1.50	19,19,19,19	1

6.5 Other polymers [i](#)

There are no such residues in this entry.