



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2017 – 08:27 AM EDT

PDB ID : 3CJP
Title : Crystal structure of an uncharacterized amidohydrolase CAC3332 from *Clostridium acetobutylicum*
Authors : Malashkevich, V.N.; Toro, R.; Ramagopal, U.A.; Bonanno, J.B.; Meyer, A.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 1.85 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 ⓘ 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	:	rb-20030345
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-20030345

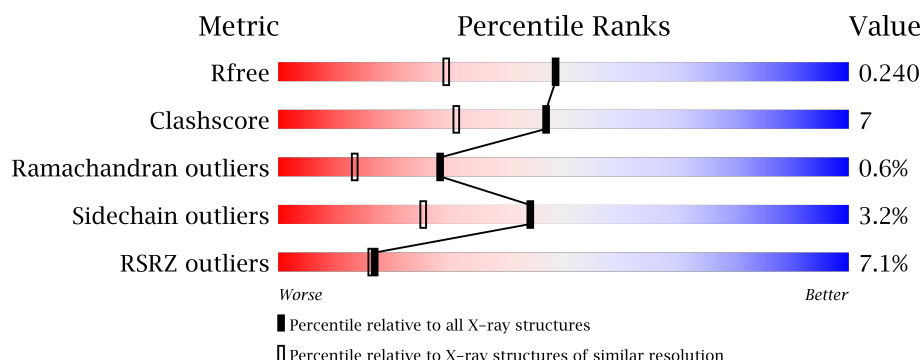
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (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 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	272	<div> <div>10%</div> <div>83%</div> <div>12%</div> <div>••</div> </div>
1	B	272	<div> <div>4%</div> <div>81%</div> <div>15%</div> <div>•</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4436 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 Predicted amidohydrolase, dihydroorotase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	2	0
			2046	1314	337	385	10			
1	B	262	Total	C	N	O	S	0	1	0
			2043	1312	337	384	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q97DY3
A	2	SER	-	EXPRESSION TAG	UNP Q97DY3
A	3	LEU	-	EXPRESSION TAG	UNP Q97DY3
A	265	GLU	-	EXPRESSION TAG	UNP Q97DY3
A	266	GLY	-	EXPRESSION TAG	UNP Q97DY3
A	267	HIS	-	EXPRESSION TAG	UNP Q97DY3
A	268	HIS	-	EXPRESSION TAG	UNP Q97DY3
A	269	HIS	-	EXPRESSION TAG	UNP Q97DY3
A	270	HIS	-	EXPRESSION TAG	UNP Q97DY3
A	271	HIS	-	EXPRESSION TAG	UNP Q97DY3
A	272	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	1	MET	-	EXPRESSION TAG	UNP Q97DY3
B	2	SER	-	EXPRESSION TAG	UNP Q97DY3
B	3	LEU	-	EXPRESSION TAG	UNP Q97DY3
B	265	GLU	-	EXPRESSION TAG	UNP Q97DY3
B	266	GLY	-	EXPRESSION TAG	UNP Q97DY3
B	267	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	268	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	269	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	270	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	271	HIS	-	EXPRESSION TAG	UNP Q97DY3
B	272	HIS	-	EXPRESSION TAG	UNP Q97DY3

- 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

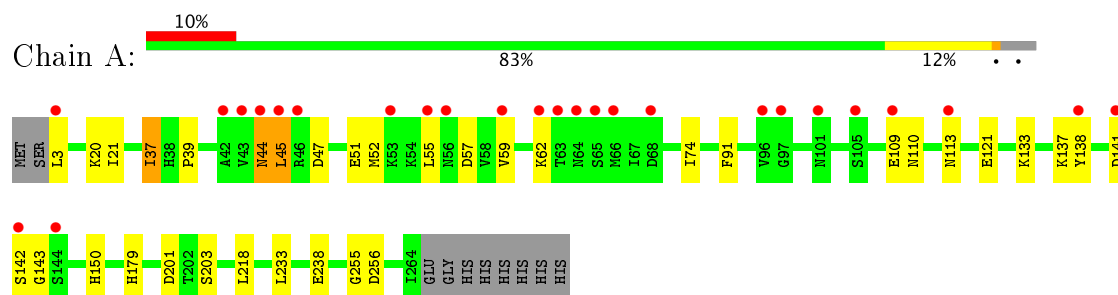
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total 160	O 160	0	0
3	B	183	Total 183	O 183	0	0

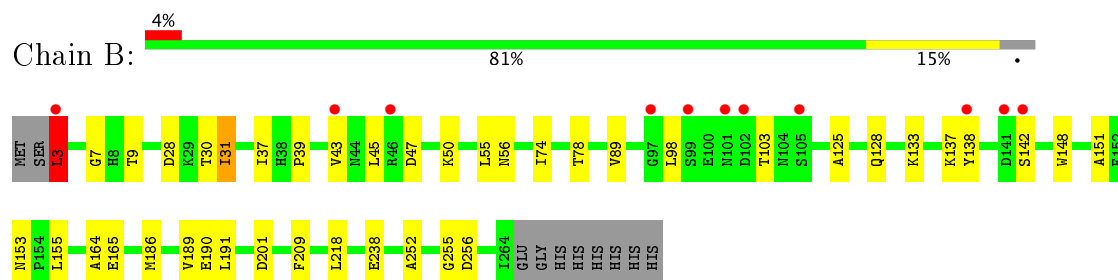
3 Residue-property plots [i](#)

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: Predicted amidohydrolase, dihydroorotase family



- Molecule 1: Predicted amidohydrolase, dihydroorotase family



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.63Å 77.27Å 72.66Å 90.00° 96.09° 90.00°	Depositor
Resolution (Å)	9.97 – 1.85 9.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (9.97-1.85) 99.7 (9.97-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	26.75 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.184 , 0.241 0.185 , 0.240	Depositor DCC
R_{free} test set	2247 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4436	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.17% 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

5.1 Standard geometry

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	0.72	0/2089	0.72	0/2831
1	B	0.73	0/2083	0.73	0/2823
All	All	0.72	0/4172	0.73	0/5654

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3	LEU	Peptide

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	A	2046	0	2109	31	0
1	B	2043	0	2104	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	160	0	0	4	0
3	B	183	0	0	6	0
All	All	4436	0	4213	59	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 7.

All (59) 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:52:MET:CE	1:B:209:PHE:CE2	2.40	1.04
1:A:52:MET:HE2	1:B:209:PHE:CE2	1.95	1.01
1:A:37:ILE:CD1	1:A:55:LEU:HB2	1.94	0.98
1:B:189:VAL:HG23	1:B:218:LEU:HD12	1.46	0.94
1:A:52:MET:HE2	1:B:209:PHE:HE2	1.28	0.92
1:A:37:ILE:HD12	1:A:55:LEU:HB2	1.49	0.91
1:A:52:MET:CE	1:B:209:PHE:CD2	2.54	0.89
1:B:28:ASP:OD1	3:B:611:HOH:O	1.96	0.82
1:A:52:MET:HE3	1:B:209:PHE:CD2	2.17	0.79
1:A:37:ILE:HD11	1:A:55:LEU:HB2	1.69	0.74
1:A:57:ASP:HB2	1:A:62:LYS:HD2	1.68	0.74
1:B:3:LEU:O	3:B:470:HOH:O	2.07	0.73
1:A:91:PHE:O	3:A:453:HOH:O	2.11	0.69
1:A:133:LYS:HG2	1:A:137:LYS:HE2	1.78	0.65
1:B:189:VAL:CG2	1:B:218:LEU:HD12	2.23	0.64
1:A:52:MET:HE1	1:B:209:PHE:CE2	2.30	0.63
1:A:52:MET:HE3	1:B:209:PHE:HD2	1.61	0.62
1:A:52:MET:CE	1:B:209:PHE:HE2	1.95	0.62
1:A:138:TYR:CD2	1:A:138:TYR:C	2.77	0.58
1:A:138:TYR:CE2	1:A:142:SER:HB2	2.39	0.57
1:B:186:MET:O	1:B:190:GLU:HG3	2.05	0.57
1:B:31:ILE:HD13	1:B:89:VAL:CG2	2.35	0.56
1:A:74:ILE:HD12	1:A:110:ASN:HB3	1.89	0.55
1:B:37:ILE:HG21	1:B:55:LEU:HG	1.88	0.55
1:B:37:ILE:HG22	1:B:39:PRO:HD3	1.87	0.55
1:A:45:LEU:H	1:A:45:LEU:HD22	1.72	0.55
1:B:133:LYS:HD3	1:B:137:LYS:NZ	2.22	0.54
1:B:43:VAL:HB	3:B:609:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:O	1:B:78:THR:HG23	2.08	0.53
1:B:138:TYR:C	1:B:138:TYR:CD2	2.81	0.53
1:A:109:GLU:O	1:A:113:ASN:HB2	2.09	0.52
1:B:125:ALA:HB3	1:B:128:GLN:HG3	1.91	0.52
1:A:21:ILE:HG22	1:A:233:LEU:HD23	1.93	0.51
1:A:3:LEU:N	3:A:369:HOH:O	2.44	0.51
1:A:47:ASP:O	1:A:51:GLU:HG2	2.11	0.51
1:A:142:SER:OG	1:A:143:GLY:N	2.43	0.50
1:A:52:MET:HE2	1:B:209:PHE:CD2	2.36	0.49
1:B:7:GLY:HA2	1:B:31:ILE:HG13	1.95	0.49
1:B:164:ALA:HB2	1:B:191:LEU:HD13	1.95	0.48
1:A:37:ILE:HG12	1:A:39:PRO:HD3	1.95	0.47
1:B:3:LEU:HD22	3:B:508:HOH:O	2.15	0.46
3:A:331:HOH:O	1:B:45:LEU:HD11	2.15	0.45
1:B:151:ALA:HA	1:B:155:LEU:HD12	1.97	0.45
1:B:153:ASN:H	1:B:153:ASN:HD22	1.64	0.45
1:A:218:LEU:HD12	3:A:457:HOH:O	2.16	0.45
1:B:189:VAL:HG23	1:B:218:LEU:CD1	2.32	0.45
1:A:238:GLU:OE1	1:B:238:GLU:OE1	2.36	0.44
1:A:138:TYR:CE2	1:A:142:SER:CB	3.01	0.43
1:B:9:THR:HB	1:B:30:THR:HG21	2.01	0.43
1:B:37:ILE:HG22	1:B:55:LEU:HD11	2.00	0.43
1:A:121:GLU:OE2	1:A:150:HIS:HB2	2.18	0.42
1:B:165:GLU:HG3	3:B:479:HOH:O	2.18	0.42
1:B:133:LYS:HD3	1:B:137:LYS:HZ2	1.85	0.41
1:A:133:LYS:CG	1:A:137:LYS:HE2	2.47	0.41
1:B:43:VAL:O	1:B:47:ASP:HB2	2.21	0.41
1:B:252:ALA:HA	1:B:256:ASP:HB2	2.02	0.41
1:B:3:LEU:HD11	3:B:545:HOH:O	2.21	0.40
1:B:98:LEU:HB2	1:B:103:THR:HG23	2.04	0.40
1:A:179:HIS:HA	1:A:203:SER:O	2.22	0.40

There are no symmetry-related clashes.

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	262/272 (96%)	251 (96%)	9 (3%)	2 (1%)	22	8
1	B	261/272 (96%)	254 (97%)	6 (2%)	1 (0%)	38	22
All	All	523/544 (96%)	505 (97%)	15 (3%)	3 (1%)	28	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	255	GLY
1	B	255	GLY

5.3.2 Protein sidechains ⓘ

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	235/242 (97%)	227 (97%)	8 (3%)	42	22
1	B	234/242 (97%)	227 (97%)	7 (3%)	46	28
All	All	469/484 (97%)	454 (97%)	15 (3%)	44	25

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	37	ILE
1	A	44	ASN
1	A	45	LEU
1	A	59	VAL
1	A	141	ASP
1	A	201	ASP
1	A	256	ASP
1	B	3	LEU
1	B	31	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	50	LYS
1	B	56	ASN
1	B	142	SER
1	B	148	TRP
1	B	201	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	153	ASN
1	A	196	GLN
1	B	56	ASN
1	B	82	GLN
1	B	153	ASN
1	B	184	ASN
1	B	196	GLN
1	B	234	GLN
1	B	263	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 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	262/272 (96%)	0.24	26 (9%) 8 8	14, 23, 48, 61	0
1	B	262/272 (96%)	0.09	11 (4%) 37 35	15, 22, 43, 60	0
All	All	524/544 (96%)	0.17	37 (7%) 17 16	14, 23, 47, 61	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	VAL	7.1
1	B	141	ASP	6.4
1	A	141	ASP	6.2
1	B	97	GLY	4.8
1	A	66	MET	4.4
1	A	97	GLY	4.3
1	A	43	VAL	4.0
1	A	105	SER	4.0
1	B	142	SER	3.8
1	B	46	ARG	3.7
1	A	46	ARG	3.6
1	A	65	SER	3.6
1	A	55	LEU	3.6
1	A	44	ASN	3.2
1	A	101	ASN	3.1
1	A	64	ASN	3.1
1	B	3	LEU	3.1
1	B	99	SER	2.9
1	A	113	ASN	2.8
1	A	56	ASN	2.7
1	A	144	SER	2.6
1	B	101	ASN	2.6
1	B	105	SER	2.5
1	A	63	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	TYR	2.5
1	A	53	LYS	2.4
1	A	62	LYS	2.4
1	A	45	LEU	2.3
1	B	138	TYR	2.3
1	A	42	ALA	2.2
1	A	59	VAL	2.2
1	B	102	ASP	2.1
1	A	3	LEU	2.1
1	A	68	ASP	2.1
1	A	96	VAL	2.0
1	A	109	GLU	2.0
1	A	142	SER	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(\AA^2)	Q<0.9
2	ZN	A	301	1/1	1.00	0.03	-1.84	22,22,22,22	0
2	ZN	B	302	1/1	0.99	0.03	-2.98	22,22,22,22	0
2	ZN	B	301	1/1	1.00	0.03	-3.28	20,20,20,20	0
2	ZN	A	302	1/1	0.99	0.03	-5.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.