



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:43 AM UTC

PDB ID : 2PS0 / pdb\_00002ps0  
Title : Structure and metal binding properties of ZnuA, a periplasmic zinc transporter from Escherichia coli  
Authors : Yatsunyk, L.A.; Kim, L.R.; Vorontsov, I.I.; Rosenzweig, A.C.  
Deposited on : 2007-05-04  
Resolution : 2.00 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)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

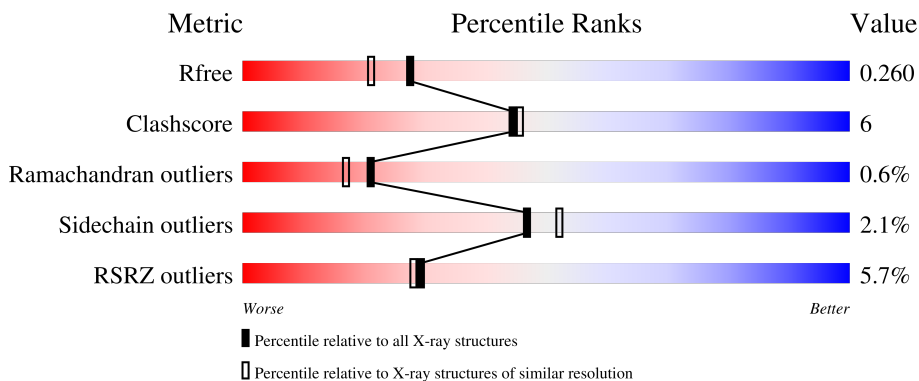
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	284	
1	B	284	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	503	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4488 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 High-affinity zinc uptake system protein znuA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	Total 2049	C 1305	N 348	O 388	S 8	4	3	0
1	B	263	Total 2041	C 1304	N 345	O 384	S 8	5	3	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

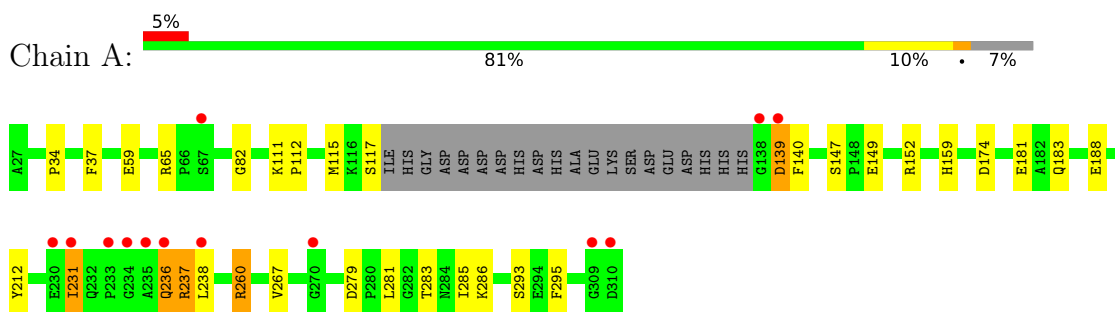
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total 191	O 191	0	0
3	B	203	Total 203	O 203	0	0

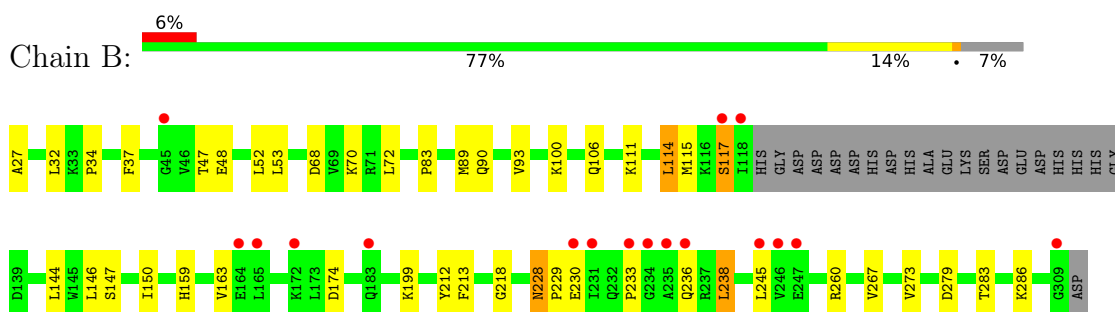
### 3 Residue-property plots [i](#)

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: High-affinity zinc uptake system protein znuA



- Molecule 1: High-affinity zinc uptake system protein znuA



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.44Å 86.27Å 88.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.20 – 2.00 37.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.20-2.00) 99.7 (37.20-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.250 (Not available) , 0.260	Depositor DCC
$R_{free}$ test set	1925 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.97 % 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 3.9545e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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:  
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	0.88	1/2094 (0.0%)	0.88	5/2840 (0.2%)
1	B	0.57	0/2089	0.91	4/2832 (0.1%)
All	All	0.74	1/4183 (0.0%)	0.89	9/5672 (0.2%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ARG	CD-NE	30.76	1.89	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	GLN	CA-C-N	7.21	134.69	121.70
1	A	236	GLN	C-N-CA	7.21	134.69	121.70
1	B	260	ARG	CB-CG-CD	6.37	125.94	111.30
1	B	117	SER	N-CA-C	5.99	123.55	110.80
1	A	236	GLN	N-CA-C	5.79	120.86	111.37
1	B	228	ASN	CA-C-N	5.68	125.30	119.56
1	B	228	ASN	C-N-CA	5.68	125.30	119.56
1	A	82	GLY	CA-C-N	5.10	124.76	119.56
1	A	82	GLY	C-N-CA	5.10	124.76	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	ARG	Sidechain

## 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	2049	0	2052	24	0
1	B	2041	0	2058	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	191	0	0	4	0
3	B	203	0	0	5	0
All	All	4488	0	4110	49	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 6.

All (49) 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:236:GLN:HB3	1:A:237:ARG:HB2	1.35	1.07
1:A:231:ILE:HG13	1:A:231:ILE:O	1.75	0.85
1:A:152:ARG:HD3	1:A:181:GLU:OE1	1.83	0.78
1:B:199:LYS:HG2	1:B:218:GLY:O	1.95	0.67
1:B:68:ASP:OD2	3:B:521:HOH:O	2.14	0.64
1:A:236:GLN:HB3	1:A:237:ARG:CB	2.22	0.64
1:A:183:GLN:HG3	1:A:293:SER:OG	2.02	0.60
1:A:147:SER:HB2	1:A:212:TYR:HB3	1.85	0.59
1:B:111:LYS:HA	1:B:114:LEU:HD22	1.83	0.59
1:B:286:LYS:HA	1:B:286:LYS:HE2	1.84	0.58
1:B:83:PRO:HB3	1:B:90[B]:GLN:HG3	1.85	0.58
1:B:147:SER:HB2	1:B:212:TYR:HB3	1.87	0.56
1:A:65:ARG:HD3	3:A:614:HOH:O	2.04	0.56
1:B:115:MET:HG2	1:B:212:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:CB	1:B:47:THR:OG1	2.55	0.54
1:B:34:PRO:HA	1:B:37:PHE:CD2	2.43	0.54
1:A:159:HIS:HE1	1:A:174:ASP:OD1	1.91	0.53
1:A:115:MET:HG3	1:A:117:SER:HB2	1.92	0.52
1:A:152:ARG:HH22	1:A:188:GLU:CD	2.18	0.51
1:A:236:GLN:CB	1:A:237:ARG:HB2	2.25	0.51
1:B:233:PRO:HB2	1:B:238:LEU:HD13	1.93	0.50
1:A:34:PRO:HA	1:A:37:PHE:CD2	2.48	0.49
1:A:279:ASP:OD2	1:A:283:THR:HG23	2.12	0.48
1:A:286:LYS:NZ	3:A:606:HOH:O	2.47	0.48
1:B:48:GLU:H	1:B:48:GLU:CD	2.22	0.47
1:A:159:HIS:HD2	3:A:516:HOH:O	1.97	0.47
1:A:139:ASP:HB3	1:A:140:PHE:H	1.50	0.47
1:A:285:ILE:HD13	1:A:295:PHE:HA	1.97	0.46
1:B:115:MET:HG2	1:B:212:TYR:CE1	2.49	0.46
1:B:144:LEU:HB3	1:B:150:ILE:HG21	1.96	0.46
1:A:237:ARG:HA	1:A:237:ARG:HD2	1.70	0.46
1:B:32:LEU:HD22	1:B:53:LEU:HD22	1.96	0.46
1:B:106:GLN:NE2	3:B:634:HOH:O	2.46	0.45
1:B:245:LEU:HG	1:B:273:VAL:HG21	1.98	0.45
1:B:70:LYS:HG3	3:B:597:HOH:O	2.17	0.44
1:B:89:MET:HE2	1:B:93:VAL:HG21	1.99	0.44
1:A:149:GLU:OE2	1:A:152:ARG:NH2	2.50	0.44
1:B:279:ASP:OD2	1:B:283:THR:HG23	2.17	0.44
1:A:111:LYS:N	1:A:112:PRO:HD2	2.33	0.44
1:B:159:HIS:HD2	3:B:553:HOH:O	1.99	0.43
1:B:52:LEU:HD11	1:B:72:LEU:HD21	2.00	0.43
1:B:100:LYS:HE2	3:B:698:HOH:O	2.18	0.42
1:B:228:ASN:HA	1:B:229:PRO:HD2	1.94	0.42
1:B:159:HIS:HE1	1:B:174:ASP:OD1	2.03	0.42
1:A:115:MET:HG2	1:A:212:TYR:CZ	2.55	0.41
1:A:117:SER:HB3	3:A:594:HOH:O	2.21	0.41
1:A:285:ILE:CD1	1:A:295:PHE:HA	2.50	0.41
1:A:59:GLU:OE2	1:A:281:LEU:HD11	2.20	0.41
1:B:146:LEU:HB3	1:B:213:PHE:HB2	2.03	0.41

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	263/284 (93%)	255 (97%)	6 (2%)	2 (1%)	16	11
1	B	262/284 (92%)	257 (98%)	4 (2%)	1 (0%)	30	27
All	All	525/568 (92%)	512 (98%)	10 (2%)	3 (1%)	21	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	B	117	SER
1	A	139	ASP

### 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	221/236 (94%)	218 (99%)	3 (1%)	59	66
1	B	221/236 (94%)	215 (97%)	6 (3%)	39	42
All	All	442/472 (94%)	433 (98%)	9 (2%)	47	54

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

Mol	Chain	Res	Type
1	A	231	ILE
1	A	238	LEU
1	A	267	VAL

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Mol	Chain	Res	Type
1	B	114	LEU
1	B	163	VAL
1	B	230	GLU
1	B	236	GLN
1	B	238	LEU
1	B	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	159	HIS
1	B	74	ASN
1	B	101	GLN
1	B	106	GLN
1	B	159	HIS
1	B	168	GLN
1	B	190	GLN
1	B	193	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 oligosaccharides 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, 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	264/284 (92%)	0.19	13 (4%) 35 34	14, 25, 44, 55	4 (1%)
1	B	263/284 (92%)	0.33	17 (6%) 25 23	13, 26, 45, 50	4 (1%)
All	All	527/568 (92%)	0.26	30 (5%) 29 28	13, 26, 45, 55	8 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	4.8
1	B	118	ILE	3.9
1	B	233	PRO	3.9
1	A	310	ASP	3.8
1	A	138	GLY	3.8
1	B	235	ALA	3.5
1	B	117	SER	3.4
1	B	246	VAL	3.4
1	A	238	LEU	3.2
1	A	231	ILE	3.1
1	A	309	GLY	3.1
1	B	165	LEU	2.8
1	A	139	ASP	2.7
1	A	270	GLY	2.7
1	B	183	GLN	2.6
1	A	230	GLU	2.6
1	A	67	SER	2.6
1	B	245	LEU	2.6
1	B	236	GLN	2.5
1	B	172	LYS	2.5
1	A	235	ALA	2.4
1	A	234	GLY	2.4
1	B	230	GLU	2.4
1	B	45	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	GLU	2.2
1	B	164	GLU	2.2
1	B	231	ILE	2.1
1	B	309	GLY	2.1
1	A	236	GLN	2.0
1	A	233	PRO	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	ZN	B	503	1/1	0.78	0.42	42,42,42,42	1
2	ZN	A	504	1/1	0.80	0.33	40,40,40,40	1
2	ZN	B	501	1/1	0.99	0.08	28,28,28,28	0
2	ZN	A	502	1/1	0.99	0.09	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.