



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:07 AM UTC

PDB ID : 1ZCZ / pdb_00001zcz
Title : Crystal structure of Phosphoribosylaminoimidazolecarboxamide formyltransferase / IMP cyclohydrolase (TM1249) from THERMOTOGA MARITIMA at 1.88 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-04-13
Resolution : 1.88 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

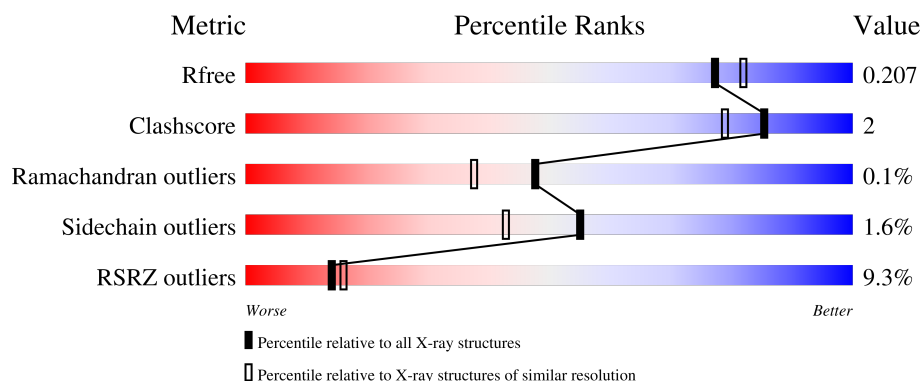
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	464	4% 91% 7% .
1	B	464	14% 92% 6% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7676 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 Bifunctional purine biosynthesis protein purH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	6	0
			3503	2259	581	655	8			
1	B	454	Total	C	N	O	S	0	11	0
			3509	2261	582	656	10			

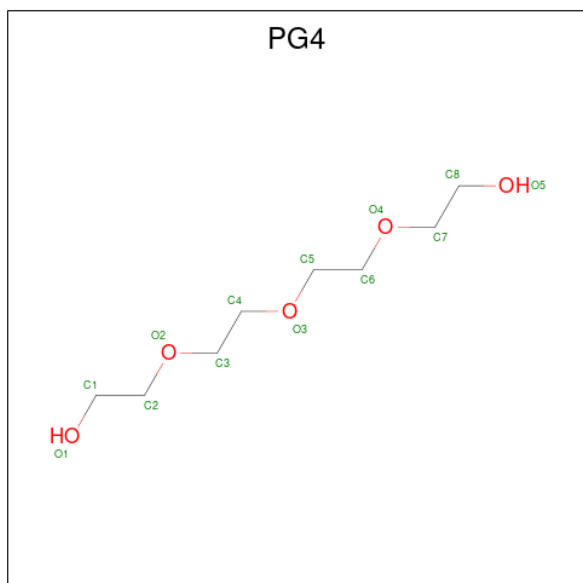
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X0X6
A	-10	GLY	-	expression tag	UNP Q9X0X6
A	-9	SER	-	expression tag	UNP Q9X0X6
A	-8	ASP	-	expression tag	UNP Q9X0X6
A	-7	LYS	-	expression tag	UNP Q9X0X6
A	-6	ILE	-	expression tag	UNP Q9X0X6
A	-5	HIS	-	expression tag	UNP Q9X0X6
A	-4	HIS	-	expression tag	UNP Q9X0X6
A	-3	HIS	-	expression tag	UNP Q9X0X6
A	-2	HIS	-	expression tag	UNP Q9X0X6
A	-1	HIS	-	expression tag	UNP Q9X0X6
A	0	HIS	-	expression tag	UNP Q9X0X6
B	-11	MET	-	expression tag	UNP Q9X0X6
B	-10	GLY	-	expression tag	UNP Q9X0X6
B	-9	SER	-	expression tag	UNP Q9X0X6
B	-8	ASP	-	expression tag	UNP Q9X0X6
B	-7	LYS	-	expression tag	UNP Q9X0X6
B	-6	ILE	-	expression tag	UNP Q9X0X6
B	-5	HIS	-	expression tag	UNP Q9X0X6
B	-4	HIS	-	expression tag	UNP Q9X0X6
B	-3	HIS	-	expression tag	UNP Q9X0X6
B	-2	HIS	-	expression tag	UNP Q9X0X6
B	-1	HIS	-	expression tag	UNP Q9X0X6
B	0	HIS	-	expression tag	UNP Q9X0X6

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	333	Total O 333 333	0	0
4	B	303	Total O 303 303	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.08Å 58.63Å 72.75Å 99.26° 96.89° 106.13°	Depositor
Resolution (Å)	50.00 – 1.88 50.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.88) 94.6 (50.00-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.156 , 0.197 0.166 , 0.207	Depositor DCC
R_{free} test set	3700 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7676	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: PG4, K

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	0.82	0/3604	0.87	1/4874 (0.0%)
1	B	0.79	0/3638	0.86	0/4926
All	All	0.81	0/7242	0.86	1/9800 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASN	CA-CB-CG	5.55	118.15	112.60

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	3503	0	3502	17	0
1	B	3509	0	3451	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	18	0	0
3	B	13	0	18	0	0
4	A	333	0	0	4	0
4	B	303	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7676	0	6989	31	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 2.

All (31) 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:B:408:LEU:HG	1:B:440:ILE:HD11	1.70	0.73
1:A:195:THR:HG23	4:A:533:HOH:O	1.90	0.72
1:B:248:ASP:O	1:B:272:LYS:NZ	2.29	0.66
1:B:251:SER:OG	1:B:272:LYS:NZ	2.32	0.61
1:A:108:TRP:CZ3	1:A:133:LYS:HG3	2.40	0.56
1:A:50[B]:THR:HG23	1:A:51:ILE:HG23	1.89	0.54
1:A:126:ILE:HD13	1:A:131:THR:HB	1.91	0.52
1:A:195:THR:CG2	4:A:533:HOH:O	2.55	0.51
1:B:213:ASN:O	1:B:348:ARG:HD3	2.13	0.49
1:B:48:VAL:O	1:B:51:ILE:HG22	2.12	0.49
1:A:408:LEU:HD21	1:A:435:ALA:HB2	1.95	0.49
1:A:133:LYS:NZ	4:A:573:HOH:O	2.47	0.47
1:B:163:LYS:HD2	1:B:164:ARG:O	2.14	0.47
1:B:121:LYS:O	1:B:125:GLU:HG2	2.15	0.47
1:A:213:ASN:ND2	4:A:579:HOH:O	2.44	0.47
1:A:227:PRO:HD2	1:A:353:ALA:HA	1.96	0.47
1:B:235:ASP:OD1	1:B:235:ASP:C	2.58	0.46
1:A:62:VAL:HG22	1:A:62:VAL:O	2.15	0.46
1:A:401:PHE:CD1	1:A:425:SER:HB2	2.51	0.46
1:A:196:ILE:HG13	1:A:200:ASN:CB	2.46	0.45
1:A:240:VAL:HG11	1:A:270:LEU:HD21	1.99	0.43
1:B:6:VAL:HG12	1:B:8:LEU:HG	2.00	0.43
1:B:37:PHE:O	1:B:40:SER:OG	2.23	0.43
1:A:217:MET:HG3	1:A:260:PHE:CD2	2.54	0.43
1:B:51:ILE:HG12	1:B:79:ARG:CZ	2.49	0.43
1:A:354:LYS:HA	1:A:451:ARG:O	2.20	0.42
1:B:210[B]:MET:HE1	1:B:227:PRO:HD3	2.02	0.42
1:B:126:ILE:HG22	1:B:127:ASP:N	2.36	0.41
1:A:381:TRP:CE3	1:A:382:ILE:HG13	2.55	0.41
1:B:212:LYS:NZ	4:B:547:HOH:O	2.54	0.41
1:A:422:PRO:HG3	1:A:448:ARG:HA	2.03	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	456/464 (98%)	448 (98%)	7 (2%)	1 (0%)	43	34
1	B	463/464 (100%)	453 (98%)	10 (2%)	0	100	100
All	All	919/928 (99%)	901 (98%)	17 (2%)	1 (0%)	48	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	HIS

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	362/378 (96%)	358 (99%)	4 (1%)	65	56
1	B	360/378 (95%)	353 (98%)	7 (2%)	50	36
All	All	722/756 (96%)	711 (98%)	11 (2%)	55	46

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	350	VAL
1	A	359	LEU
1	A	376	ARG
1	B	9	TYR

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Mol	Chain	Res	Type
1	B	61	LEU
1	B	63	LYS
1	B	126	ILE
1	B	127	ASP
1	B	350	VAL
1	B	376	ARG

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

Mol	Chain	Res	Type
1	A	284	GLN
1	B	56	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, 2 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	PG4	B	454	-	12,12,12	0.32	0	11,11,11	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PG4	A	454	-	12,12,12	0.38	0	11,11,11	0.57	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
3	PG4	B	454	-	-	4/10/10/10	-
3	PG4	A	454	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	454	PG4	O3-C5-C6-O4
3	A	454	PG4	O2-C3-C4-O3
3	A	454	PG4	C4-C3-O2-C2
3	A	454	PG4	O1-C1-C2-O2
3	B	454	PG4	C5-C6-O4-C7
3	A	454	PG4	C1-C2-O2-C3
3	A	454	PG4	C6-C5-O3-C4
3	B	454	PG4	O3-C5-C6-O4
3	B	454	PG4	C8-C7-O4-C6
3	B	454	PG4	C1-C2-O2-C3

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

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	452/464 (97%)	0.73	17 (3%)	44 48	23, 39, 49, 60	6 (1%)
1	B	454/464 (97%)	1.03	67 (14%)	5 6	24, 39, 49, 60	11 (2%)
All	All	906/928 (97%)	0.88	84 (9%)	14 16	23, 39, 49, 60	17 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	VAL	6.5
1	B	160	LEU	6.4
1	B	158	ILE	6.3
1	B	161	ALA	5.6
1	B	10	GLU	5.4
1	B	154	PHE	5.1
1	B	162	PHE	4.6
1	B	149	ILE	4.6
1	B	151	ALA	4.4
1	B	148[A]	SER	4.3
1	B	144	SER	4.2
1	B	38	LEU	4.2
1	B	9	TYR	4.1
1	B	143	THR	4.1
1	B	157	GLY	4.1
1	B	141	ALA	4.0
1	B	159[A]	SER	4.0
1	B	37	PHE	3.9
1	B	40	SER	3.8
1	A	54	PHE	3.7
1	B	88	TYR	3.7
1	B	145	VAL	3.6
1	B	152	ASN	3.5
1	B	14	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	PHE	3.5
1	B	150	ARG	3.5
1	B	93	ILE	3.4
1	B	43	ILE	3.3
1	B	45	ALA	3.3
1	B	46	ASN	3.2
1	A	1	MET	3.2
1	B	153	GLN	3.2
1	B	147	ASP	3.2
1	B	163	LYS	3.1
1	A	191	HIS	3.0
1	B	139	THR	2.9
1	B	146	TYR	2.9
1	B	142	PHE	2.9
1	B	31	SER	2.8
1	A	440	ILE	2.8
1	B	91	PRO	2.8
1	B	156	GLU	2.7
1	B	25	GLY	2.6
1	B	-1	HIS	2.6
1	B	44	GLU	2.6
1	B	102	ARG	2.5
1	A	57	LEU	2.5
1	B	17	ILE	2.5
1	B	99	ALA	2.5
1	B	90	PRO	2.5
1	A	195	THR	2.5
1	B	41	ASN	2.4
1	B	105	ALA	2.4
1	A	59	GLY	2.4
1	B	108	TRP	2.4
1	B	61	LEU	2.3
1	B	0	HIS	2.3
1	B	213	ASN	2.3
1	A	381	TRP	2.3
1	A	234	GLU	2.3
1	A	61	LEU	2.3
1	A	167	LEU	2.3
1	B	58	LEU	2.3
1	B	51	ILE	2.3
1	B	133	LYS	2.2
1	B	166	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	158	ILE	2.1
1	B	29	TRP	2.1
1	B	137	GLY	2.1
1	A	101	LEU	2.1
1	B	324	GLU	2.1
1	B	95	ILE	2.1
1	A	438	LEU	2.1
1	B	92	ASP	2.1
1	A	52	THR	2.1
1	B	111	VAL	2.1
1	B	101	LEU	2.1
1	B	35	ALA	2.1
1	B	136	ALA	2.1
1	A	126	ILE	2.0
1	A	450	PHE	2.0
1	B	11	LYS	2.0
1	B	106	LYS	2.0
1	B	273	TYR	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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	PG4	A	454	13/13	0.90	0.12	34,47,52,52	0
3	PG4	B	454	13/13	0.93	0.10	34,40,47,49	0
2	K	A	453	1/1	0.99	0.19	33,33,33,33	0
2	K	B	453	1/1	0.99	0.21	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.