



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:55 am GMT

PDB ID : 3FAK
Title : Structural and Functional Analysis of a Hormone-Sensitive Lipase like EstE5
from a Metagenome Library
Authors : Hwang, K.Y.; Nam, K.H.
Deposited on : 2008-11-17
Resolution : 1.90 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 : 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

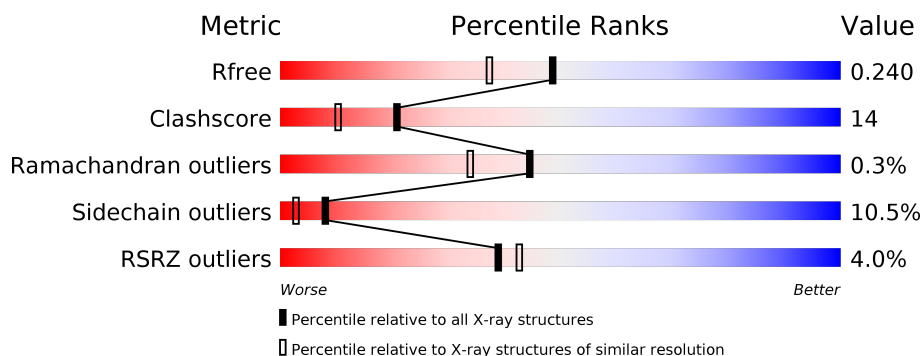
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	322	<div> <div>4%</div> <div>69%</div> <div>17%</div> <div>5%</div> <div>8%</div> </div>

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	CL	A	310	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2438 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 Esterase/lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2241	1426	393	407	15			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	INITIATING METHIONINE	UNP Q0GMU2
A	-11	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	-10	SER	-	EXPRESSION TAG	UNP Q0GMU2
A	-9	MET	-	EXPRESSION TAG	UNP Q0GMU2
A	-8	THR	-	EXPRESSION TAG	UNP Q0GMU2
A	-7	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-6	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-5	GLN	-	EXPRESSION TAG	UNP Q0GMU2
A	-4	GLN	-	EXPRESSION TAG	UNP Q0GMU2
A	-3	MET	-	EXPRESSION TAG	UNP Q0GMU2
A	-2	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-1	ARG	-	EXPRESSION TAG	UNP Q0GMU2
A	0	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	298	LEU	-	EXPRESSION TAG	UNP Q0GMU2
A	299	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	300	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	301	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	302	LEU	-	EXPRESSION TAG	UNP Q0GMU2
A	303	GLU	-	EXPRESSION TAG	UNP Q0GMU2
A	304	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	305	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	306	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	307	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	308	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	309	HIS	-	EXPRESSION TAG	UNP Q0GMU2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

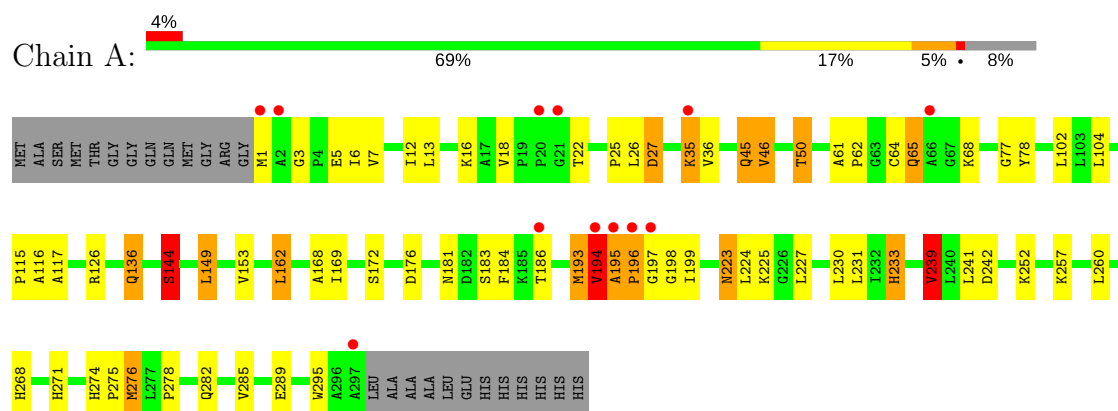
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		

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: Esterase/lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 61.00Å 149.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 1.90 19.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.79-1.90) 97.1 (19.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.243 0.210 , 0.240	Depositor DCC
R_{free} test set	2206 reflections (9.90%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2438	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: NA, CL

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	1/2295 (0.0%)	0.91	12/3116 (0.4%)

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	1	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	THR	CA-CB	5.80	1.68	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ALA	N-CA-C	20.57	166.53	111.00
1	A	197	GLY	N-CA-C	-12.87	80.92	113.10
1	A	195	ALA	N-CA-CB	-12.46	92.65	110.10
1	A	194	VAL	CA-C-N	-10.89	93.24	117.20
1	A	46	VAL	CG1-CB-CG2	6.42	121.16	110.90
1	A	195	ALA	CB-CA-C	-6.24	100.73	110.10
1	A	239	VAL	CG1-CB-CG2	5.55	119.78	110.90
1	A	239	VAL	N-CA-CB	-5.50	99.39	111.50
1	A	144	SER	CA-CB-OG	-5.41	96.60	111.20
1	A	46	VAL	N-CA-CB	-5.26	99.92	111.50
1	A	195	ALA	C-N-CD	-5.16	109.24	120.60
1	A	239	VAL	CB-CA-C	5.11	121.11	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	195	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	VAL	Mainchain,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	2241	0	2254	62	0
2	A	1	0	0	2	0
3	A	1	0	0	0	0
4	A	195	0	0	7	0
All	All	2438	0	2254	62	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 14.

All (62) 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:194:VAL:HA	1:A:195:ALA:CB	1.69	1.19
1:A:194:VAL:CA	1:A:195:ALA:HB2	1.87	1.04
1:A:196:PRO:HB2	1:A:199:ILE:H	1.27	0.97
1:A:194:VAL:HA	1:A:195:ALA:HB2	0.92	0.88
1:A:25:PRO:HB2	4:A:550:HOH:O	1.79	0.81
1:A:276:MET:HE2	1:A:276:MET:H	1.46	0.80
1:A:183:SER:HA	1:A:186:THR:CG2	2.12	0.79
1:A:136:GLN:H	1:A:136:GLN:HE21	1.38	0.72
1:A:136:GLN:H	1:A:136:GLN:NE2	1.88	0.72
1:A:183:SER:HA	1:A:186:THR:HG23	1.72	0.70
1:A:196:PRO:HB2	1:A:199:ILE:HG22	1.75	0.67
1:A:196:PRO:HB2	1:A:199:ILE:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:CA	1:A:195:ALA:CB	2.53	0.66
1:A:13:LEU:HD13	1:A:193:MET:CE	2.27	0.64
1:A:18:VAL:HG12	1:A:22:THR:OG1	1.96	0.64
1:A:196:PRO:CB	1:A:199:ILE:H	2.08	0.64
1:A:285:VAL:O	1:A:289:GLU:HG3	1.99	0.63
1:A:5:GLU:HG2	1:A:278:PRO:HD3	1.80	0.63
1:A:13:LEU:HD13	1:A:193:MET:HE1	1.82	0.60
1:A:276:MET:HE2	1:A:276:MET:N	2.16	0.59
1:A:233:HIS:HD2	1:A:271:HIS:NE2	2.00	0.59
1:A:183:SER:HA	1:A:186:THR:HG22	1.84	0.59
1:A:169:ILE:HD12	1:A:169:ILE:N	2.19	0.57
1:A:116:ALA:HB3	2:A:310:CL:CL	2.42	0.56
1:A:184:PHE:HA	1:A:239:VAL:HG22	1.90	0.53
1:A:274:HIS:CG	1:A:275:PRO:HD3	2.44	0.52
1:A:271:HIS:HD1	1:A:271:HIS:H	1.58	0.52
1:A:136:GLN:HE21	1:A:136:GLN:N	2.04	0.52
1:A:168:ALA:C	1:A:169:ILE:HD12	2.30	0.52
1:A:35:LYS:HG3	1:A:36:VAL:HG13	1.92	0.51
1:A:224:LEU:O	1:A:227:LEU:HG	2.11	0.51
1:A:64:CYS:HB2	4:A:456:HOH:O	2.10	0.50
1:A:117:ALA:N	2:A:310:CL:CL	2.82	0.50
1:A:144:SER:OG	1:A:268:HIS:CE1	2.65	0.50
1:A:149:LEU:HD22	1:A:153:VAL:HG23	1.95	0.48
1:A:27:ASP:N	4:A:550:HOH:O	2.46	0.48
1:A:144:SER:HA	1:A:172:SER:O	2.14	0.48
1:A:13:LEU:HD13	1:A:193:MET:HE2	1.95	0.47
1:A:176:ASP:HB3	4:A:416:HOH:O	2.15	0.46
1:A:278:PRO:O	1:A:282:GLN:HG3	2.16	0.46
1:A:181:ASN:HB3	1:A:242:ASP:HB2	1.97	0.45
1:A:252:LYS:HG2	4:A:432:HOH:O	2.17	0.45
1:A:61:ALA:HB1	1:A:62:PRO:HD2	1.99	0.45
1:A:193:MET:O	1:A:195:ALA:HB2	2.16	0.45
1:A:45:GLN:HG2	4:A:582:HOH:O	2.16	0.45
1:A:25:PRO:C	4:A:550:HOH:O	2.55	0.44
1:A:12:ILE:HG23	1:A:16:LYS:HE3	2.00	0.44
1:A:196:PRO:O	1:A:196:PRO:HD2	2.18	0.44
1:A:68:LYS:HD3	1:A:295:TRP:CD2	2.53	0.43
1:A:126:ARG:HG3	1:A:162:LEU:HD21	2.00	0.43
1:A:77:GLY:O	1:A:78:TYR:HB2	2.19	0.43
1:A:144:SER:HG	1:A:268:HIS:CE1	2.37	0.42
1:A:196:PRO:HB2	1:A:199:ILE:CG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:HA	1:A:65:GLN:OE1	2.19	0.42
1:A:6:ILE:HG23	1:A:7:VAL:N	2.35	0.41
1:A:196:PRO:HA	1:A:198:GLY:H	1.85	0.41
1:A:196:PRO:HG2	1:A:199:ILE:CG2	2.50	0.41
1:A:3:GLY:O	1:A:6:ILE:HG22	2.21	0.41
1:A:274:HIS:N	1:A:275:PRO:CD	2.84	0.41
1:A:196:PRO:CB	1:A:199:ILE:HG22	2.47	0.40
1:A:223:ASN:ND2	1:A:225:LYS:H	2.19	0.40
1:A:168:ALA:HB3	1:A:230:LEU:HD12	2.04	0.40

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	295/322 (92%)	288 (98%)	6 (2%)	1 (0%)	44 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	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	229/246 (93%)	205 (90%)	24 (10%)	8 3

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	LEU
1	A	27	ASP
1	A	35	LYS
1	A	45	GLN
1	A	46	VAL
1	A	50	THR
1	A	65	GLN
1	A	102	LEU
1	A	104	LEU
1	A	115	PRO
1	A	136	GLN
1	A	144	SER
1	A	149	LEU
1	A	162	LEU
1	A	193	MET
1	A	223	ASN
1	A	231	LEU
1	A	233	HIS
1	A	239	VAL
1	A	241	LEU
1	A	257	LYS
1	A	260	LEU
1	A	276	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	98	GLN
1	A	136	GLN
1	A	181	ASN
1	A	223	ASN
1	A	233	HIS
1	A	282	GLN

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 2 ligands modelled in this entry, 2 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	297/322 (92%)	0.40	12 (4%) 39 43	13, 24, 56, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	11.5
1	A	194	VAL	9.5
1	A	196	PRO	6.7
1	A	1	MET	6.3
1	A	66	ALA	5.3
1	A	197	GLY	4.0
1	A	186	THR	3.6
1	A	35	LYS	2.7
1	A	2	ALA	2.7
1	A	21	GLY	2.5
1	A	297	ALA	2.4
1	A	20	PRO	2.3

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	CL	A	310	1/1	0.98	0.38	26.04	19,19,19,19	0
3	NA	A	311	1/1	0.55	1.21	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.