



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2025 – 12:32 am GMT

PDB ID : 9S1S / pdb\_00009s1s  
Title : Crystal structure of C278S mutant of mouse CDC14A in complex with a model phosphopeptide  
Authors : Shabbir, K.; Jackisch, G.; Sele, C.; Murina, V.; Knecht, W.; Wilson, E.; Dong, L.; Friedman, T.B.; Imtiaz, A.; Logan, D.T.  
Deposited on : 2025-07-21  
Resolution : 1.62 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](mailto: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>.

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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  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

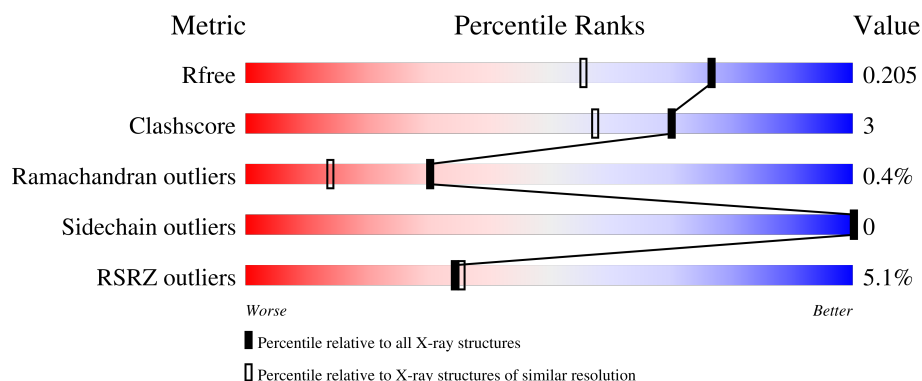
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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))
$R_{free}$	164625	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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	344	<div> <div>5%</div> <div>90%</div> <div>8%</div> </div>
1	B	344	<div> <div>5%</div> <div>91%</div> <div>8%</div> </div>
2	E	6	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11875 atoms, of which 5572 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 Dual specificity protein phosphatase CDC14A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	339	Total	C	H	N	O	S	0	8	0
			5581	1821	2769	485	493	13			
1	B	339	Total	C	H	N	O	S	0	5	0
			5565	1815	2763	484	491	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	SER	CYS	engineered mutation	UNP Q6GQT0
B	278	SER	CYS	engineered mutation	UNP Q6GQT0

- Molecule 2 is a protein called Model phosphohexapeptide.

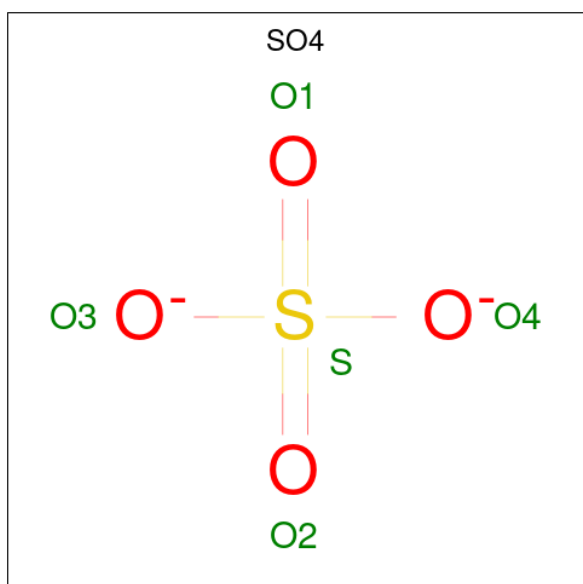
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			27	14	4	8	1			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

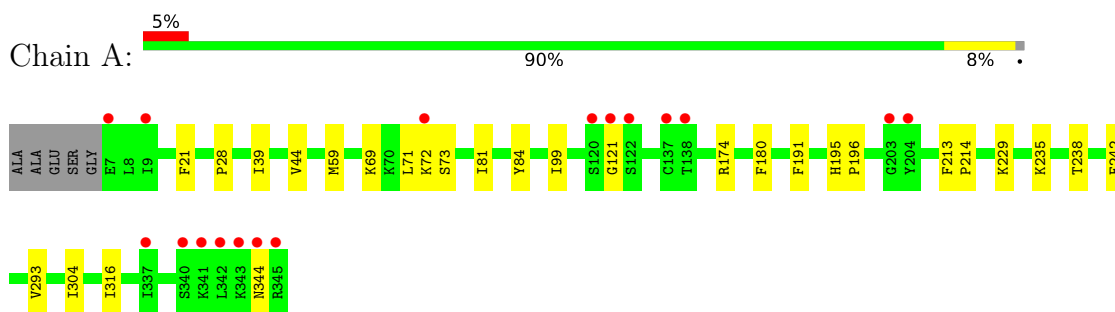
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	322	Total	O	0	0
			322	322		
5	B	291	Total	O	0	0
			291	291		
5	E	4	Total	O	0	0
			4	4		

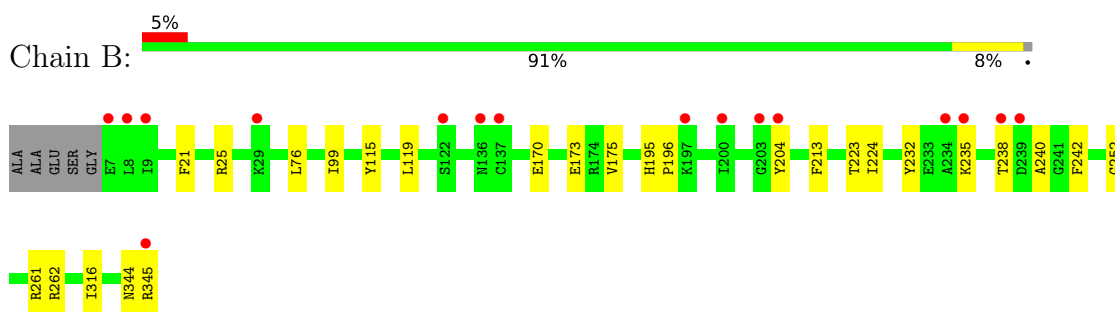
### 3 Residue-property plots [i](#)

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.

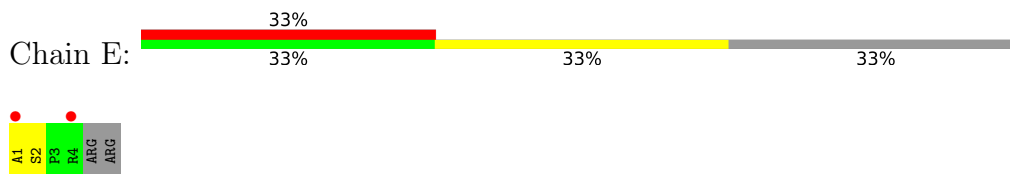
- Molecule 1: Dual specificity protein phosphatase CDC14A



- Molecule 1: Dual specificity protein phosphatase CDC14A



- Molecule 2: Model phosphohexapeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.34Å 158.09Å 69.27Å 90.00° 124.59° 90.00°	Depositor
Resolution (Å)	28.82 – 1.62 28.82 – 1.62	Depositor EDS
% Data completeness (in resolution range)	69.2 (28.82-1.62) 69.2 (28.82-1.62)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, $R_{free}$	0.168 , 0.207 0.168 , 0.205	Depositor DCC
$R_{free}$ test set	3978 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SEP, SO4, GOL

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	0.40	0/2929	0.51	0/3952
1	B	0.37	0/2904	0.50	0/3918
2	E	0.65	0/16	0.58	0/19
All	All	0.39	0/5849	0.51	0/7889

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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### 5.2 Torsion angles [i](#)

#### 5.2.1 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	345/344 (100%)	330 (96%)	13 (4%)	2 (1%)	22	7
1	B	342/344 (99%)	328 (96%)	13 (4%)	1 (0%)	37	20
2	E	1/6 (17%)	1 (100%)	0	0	100	100
All	All	688/694 (99%)	659 (96%)	26 (4%)	3 (0%)	30	14



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ILE
1	B	316	ILE
1	A	121	GLY

### 5.2.2 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	300/295 (102%)	300 (100%)	0	100	100
1	B	297/295 (101%)	297 (100%)	0	100	100
2	E	1/4 (25%)	1 (100%)	0	100	100
All	All	598/594 (101%)	598 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	B	177	ASN
1	B	344	ASN
1	B	334	GLN
1	A	177	ASN

### 5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
2	SEP	E	2	2	8,9,10	1.39	1 (12%)	8,12,14	1.42	2 (25%)

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
2	SEP	E	2	2	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	SEP	P-O1P	2.75	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	SEP	O3P-P-OG	-2.37	100.43	106.73
2	E	2	SEP	OG-P-O1P	2.11	112.39	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.4 Carbohydrates

There are no oligosaccharides in this entry.

## 5.5 Ligand geometry

8 ligands are modelled in this entry.

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	$\# Z  > 2$
4	SO4	A	403	-	4,4,4	0.52	0	6,6,6	0.56	0
3	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.46	0
3	GOL	B	403	-	5,5,5	0.32	0	5,5,5	0.44	0
4	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.38	0
3	GOL	B	401	-	5,5,5	0.26	0	5,5,5	0.27	0
4	SO4	B	404	-	4,4,4	0.64	0	6,6,6	0.40	0
3	GOL	A	401	-	5,5,5	0.22	0	5,5,5	0.42	0
3	GOL	A	402	-	5,5,5	0.18	0	5,5,5	0.56	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	GOL	B	402	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	401	-	-	4/4/4/4	-
3	GOL	A	401	-	-	1/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	C1-C2-C3-O3
3	B	401	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	403	GOL	O1-C1-C2-C3
3	B	401	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	SO4	1	0
3	B	401	GOL	1	0

## 5.6 Other polymers [i](#)

There are no such residues in this entry.

## 5.7 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, 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	339/344 (98%)	-0.22	17 (5%) 35 36	6, 23, 59, 95	4 (1%)
1	B	339/344 (98%)	-0.15	16 (4%) 37 39	7, 26, 63, 88	3 (0%)
2	E	3/6 (50%)	2.66	2 (66%) 0 0	34, 34, 43, 63	0
All	All	681/694 (98%)	-0.17	35 (5%) 34 35	6, 24, 63, 95	7 (1%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	ARG	4.4
1	A	344	ASN	4.1
1	A	345	ARG	3.8
1	A	137	CYS	3.5
1	A	342	LEU	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	E	2	10/11	0.96	0.11	21,33,43,45	0

### 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
3	GOL	A	401	6/6	0.82	0.16	42,60,75,75	0
3	GOL	B	403	6/6	0.85	0.14	29,52,65,65	0
3	GOL	A	402	6/6	0.87	0.14	33,55,72,72	0
3	GOL	B	402	6/6	0.92	0.10	22,36,51,53	0
3	GOL	B	401	6/6	0.93	0.11	24,37,67,67	0
4	SO4	B	404	5/5	0.95	0.08	30,34,40,43	0
4	SO4	A	403	5/5	0.98	0.07	12,16,29,30	0
4	SO4	A	404	5/5	0.99	0.04	16,18,20,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.