



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:52 pm BST

PDB ID : 3UR5  
Title : Crystal Structure of PTE mutant K185R/I274N  
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Deposited on : 2011-11-21  
Resolution : 1.60 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)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

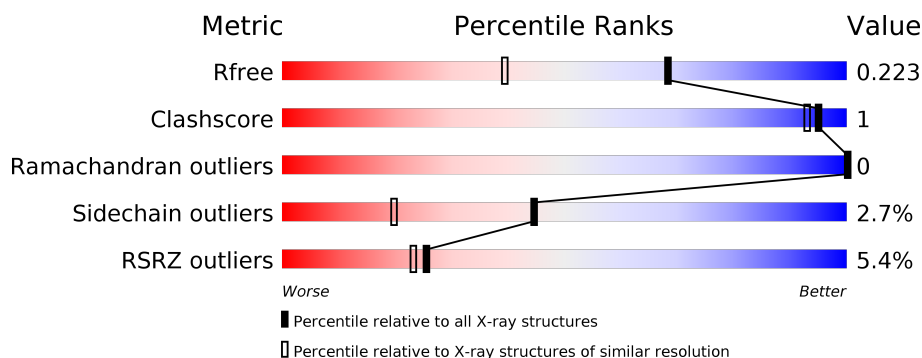
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	327	<div> <div>5%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	327	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5606 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.

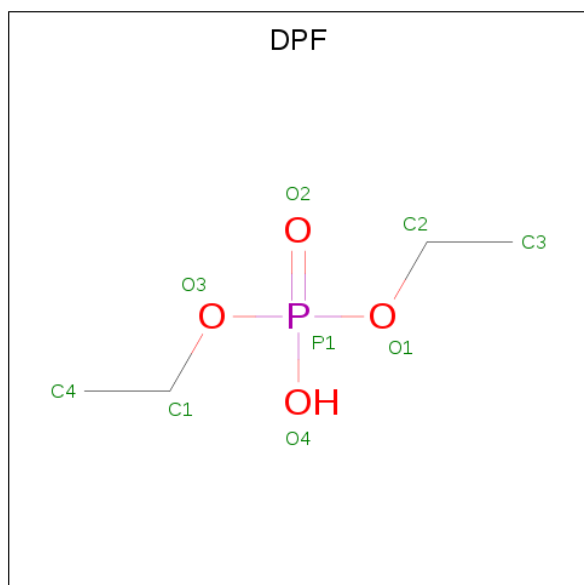
- Molecule 1 is a protein called Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2504	1580	447	470	7			
1	B	323	Total	C	N	O	S	0	0	0
			2471	1561	442	461	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ARG	LYS	engineered mutation	UNP P0A434
A	274	ASN	ILE	engineered mutation	UNP P0A434
B	185	ARG	LYS	engineered mutation	UNP P0A434
B	274	ASN	ILE	engineered mutation	UNP P0A434

- Molecule 2 is DIETHYL HYDROGEN PHOSPHATE (three-letter code: DPF) (formula:  $C_4H_{11}O_4P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	4	4	1		
2	B	1	Total	C	O	P	0	0
			9	4	4	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Co	0	0
			3	3		
3	A	2	Total	Co	0	0
			2	2		

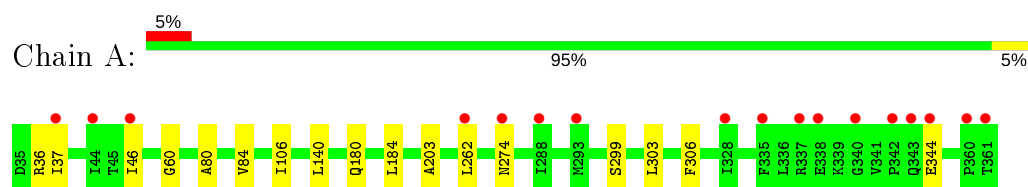
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	303	Total	O	0	0
			303	303		
4	B	305	Total	O	0	0
			305	305		

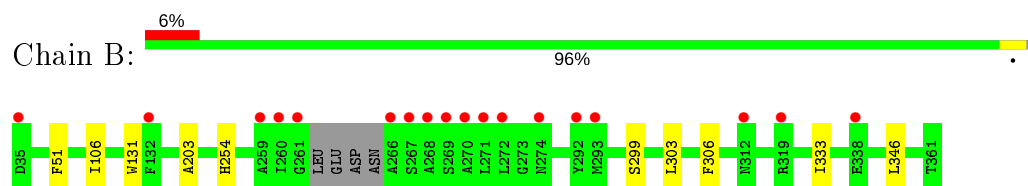
### 3 Residue-property plots [i](#)

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: Parathion hydrolase



- Molecule 1: Parathion hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.48Å 85.98Å 88.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 39.17 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.60) 99.9 (39.17-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.85 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.228 0.207 , 0.223	Depositor DCC
$R_{free}$ test set	4329 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.012 for -l,-k,-h 0.013 for k,h,-l 0.001 for k,l,h 0.001 for l,h,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: DPF, CO, KCX

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	0.59	0/2539	0.75	1/3447 (0.0%)
1	B	0.59	0/2505	0.74	1/3399 (0.0%)
All	All	0.59	0/5044	0.74	2/6846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ALA	N-CA-C	-6.14	94.41	111.00
1	A	203	ALA	N-CA-C	-6.04	94.69	111.00

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	2504	0	2511	4	0
1	B	2471	0	2483	4	0
2	A	9	0	10	3	0
2	B	9	0	10	4	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	303	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	305	0	0	2	0
All	All	5606	0	5014	12	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 1.

All (12) 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)
2:B:901:DPF:H21	4:B:1445:HOH:O	1.81	0.79
2:B:901:DPF:H31	4:B:1593:HOH:O	1.89	0.72
1:A:60:GLY:HA3	2:A:902:DPF:H41	1.96	0.47
2:A:902:DPF:H43	4:A:1007:HOH:O	2.14	0.47
2:A:902:DPF:H32	4:A:1313:HOH:O	2.15	0.45
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.98	0.45
1:B:254:HIS:NE2	2:B:901:DPF:H32	2.33	0.43
1:A:80:ALA:O	1:A:84:VAL:HG23	2.20	0.42
1:B:106:ILE:O	1:B:106:ILE:HG22	2.20	0.42
1:A:180:GLN:O	1:A:184:LEU:HD13	2.20	0.41
1:A:106:ILE:O	1:A:106:ILE:HG22	2.21	0.41
1:B:131:TRP:CZ2	2:B:901:DPF:H12	2.56	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	324/327 (99%)	314 (97%)	10 (3%)	0	100	100
1	B	318/327 (97%)	306 (96%)	12 (4%)	0	100	100
All	All	642/654 (98%)	620 (97%)	22 (3%)	0	100	100



There are no Ramachandran outliers to report.

### 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	262/262 (100%)	252 (96%)	10 (4%)	33	10
1	B	258/262 (98%)	254 (98%)	4 (2%)	62	41
All	All	520/524 (99%)	506 (97%)	14 (3%)	44	20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	37	ILE
1	A	46	ILE
1	A	140	LEU
1	A	262	LEU
1	A	274	ASN
1	A	299	SER
1	A	303	LEU
1	A	306	PHE
1	A	344	GLU
1	B	51	PHE
1	B	299	SER
1	B	303	LEU
1	B	306	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	B	169	1,3	7,11,12	0.53	0	4,12,14	0.51	0
1	KCX	A	169	1,3	7,11,12	0.53	0	4,12,14	0.45	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
1	KCX	B	169	1,3	-	0/7/10/12	-
1	KCX	A	169	1,3	-	0/7/10/12	-

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.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 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	$\# Z  > 2$
2	DPF	B	901	3	8,8,8	0.76	0	9,10,10	0.46	0
2	DPF	A	902	3	8,8,8	0.76	0	9,10,10	0.50	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
2	DPF	B	901	3	-	3/8/8/8	-
2	DPF	A	902	3	-	3/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	DPF	C1-O3-P1-O4
2	B	901	DPF	C2-O1-P1-O3
2	A	902	DPF	C1-O3-P1-O1
2	B	901	DPF	C2-O1-P1-O2
2	A	902	DPF	C1-O3-P1-O2
2	B	901	DPF	C3-C2-O1-P1

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	DPF	4	0
2	A	902	DPF	3	0

## 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	326/327 (99%)	0.41	17 (5%) 27 24	15, 26, 44, 56	0
1	B	322/327 (98%)	0.25	18 (5%) 24 22	13, 21, 43, 62	1 (0%)
All	All	648/654 (99%)	0.33	35 (5%) 25 23	13, 24, 43, 62	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	GLY	11.2
1	B	266	ALA	8.3
1	B	260	ILE	7.2
1	B	267	SER	6.4
1	B	269	SER	5.0
1	A	361	THR	5.0
1	A	293	MET	4.7
1	B	274	ASN	4.2
1	B	35	ASP	4.1
1	B	270	ALA	3.9
1	B	338	GLU	3.5
1	B	268	ALA	3.2
1	A	342	PRO	3.2
1	A	360	PRO	3.1
1	B	319	ARG	3.0
1	A	44	ILE	3.0
1	A	328	ILE	2.9
1	B	271	LEU	2.9
1	A	262	LEU	2.8
1	A	340	GLY	2.8
1	A	338	GLU	2.8
1	A	274	ASN	2.8
1	A	37	ILE	2.7
1	B	292	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	344	GLU	2.6
1	A	46	ILE	2.5
1	B	312	ASN	2.5
1	A	288	ILE	2.5
1	A	337	ARG	2.4
1	B	272	LEU	2.3
1	B	259	ALA	2.2
1	B	293	MET	2.2
1	A	343	GLN	2.1
1	A	335	PHE	2.1
1	B	132	PHE	2.0

## 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
1	KCX	A	169	12/13	0.92	0.12	17,19,20,20	0
1	KCX	B	169	12/13	0.96	0.09	13,14,16,17	0

## 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. 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	DPF	A	902	9/9	0.60	0.28	40,44,46,46	0
2	DPF	B	901	9/9	0.81	0.21	21,31,37,37	0
3	CO	B	805	1/1	0.97	0.12	50,50,50,50	0
3	CO	A	802	1/1	0.99	0.05	20,20,20,20	0
3	CO	A	801	1/1	0.99	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CO	B	804	1/1	1.00	0.05	17,17,17,17	0
3	CO	B	803	1/1	1.00	0.07	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.