



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:38 pm BST

PDB ID : 6DJ6
Title : The X-ray crystal structure of the Streptococcus pneumoniae Fatty Acid Kinase (Fak) B2 protein loaded with cis-oleic acid to 1.9 Angstrom resolution
Authors : Cuypers, M.G.; Subramanian, C.; White, S.W.; Rock, C.O.
Deposited on : 2018-05-24
Resolution : 1.90 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

A user guide is available at

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

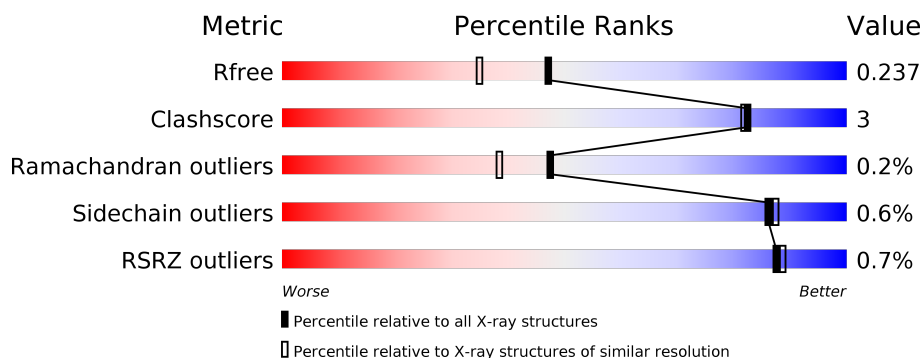
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	313	<div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
1	B	313	<div> <div>%</div> <div>84%</div> <div>.</div> <div>12%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5028 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 Fatty Acid Kinase (Fak) B2 protein (SPR1019).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	3	11	0
			2237	1414	371	440	12			
1	B	277	Total	C	N	O	S	3	4	0
			2169	1373	362	425	9			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP A0A0I9AIE4
A	-32	GLY	-	expression tag	UNP A0A0I9AIE4
A	-31	SER	-	expression tag	UNP A0A0I9AIE4
A	-30	SER	-	expression tag	UNP A0A0I9AIE4
A	-29	HIS	-	expression tag	UNP A0A0I9AIE4
A	-28	HIS	-	expression tag	UNP A0A0I9AIE4
A	-27	HIS	-	expression tag	UNP A0A0I9AIE4
A	-26	HIS	-	expression tag	UNP A0A0I9AIE4
A	-25	HIS	-	expression tag	UNP A0A0I9AIE4
A	-24	HIS	-	expression tag	UNP A0A0I9AIE4
A	-23	SER	-	expression tag	UNP A0A0I9AIE4
A	-22	SER	-	expression tag	UNP A0A0I9AIE4
A	-21	GLY	-	expression tag	UNP A0A0I9AIE4
A	-20	LEU	-	expression tag	UNP A0A0I9AIE4
A	-19	VAL	-	expression tag	UNP A0A0I9AIE4
A	-18	PRO	-	expression tag	UNP A0A0I9AIE4
A	-17	ARG	-	expression tag	UNP A0A0I9AIE4
A	-16	GLY	-	expression tag	UNP A0A0I9AIE4
A	-15	SER	-	expression tag	UNP A0A0I9AIE4
A	-14	HIS	-	expression tag	UNP A0A0I9AIE4
A	-13	MET	-	expression tag	UNP A0A0I9AIE4
A	-12	ALA	-	expression tag	UNP A0A0I9AIE4
A	-11	SER	-	expression tag	UNP A0A0I9AIE4
A	-10	MET	-	expression tag	UNP A0A0I9AIE4
A	-9	THR	-	expression tag	UNP A0A0I9AIE4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP A0A0I9AIE4
A	-7	GLY	-	expression tag	UNP A0A0I9AIE4
A	-6	GLN	-	expression tag	UNP A0A0I9AIE4
A	-5	GLN	-	expression tag	UNP A0A0I9AIE4
A	-4	MET	-	expression tag	UNP A0A0I9AIE4
A	-3	GLY	-	expression tag	UNP A0A0I9AIE4
A	-2	ARG	-	expression tag	UNP A0A0I9AIE4
A	-1	ASP	-	expression tag	UNP A0A0I9AIE4
A	0	PRO	-	expression tag	UNP A0A0I9AIE4
B	-33	MET	-	expression tag	UNP A0A0I9AIE4
B	-32	GLY	-	expression tag	UNP A0A0I9AIE4
B	-31	SER	-	expression tag	UNP A0A0I9AIE4
B	-30	SER	-	expression tag	UNP A0A0I9AIE4
B	-29	HIS	-	expression tag	UNP A0A0I9AIE4
B	-28	HIS	-	expression tag	UNP A0A0I9AIE4
B	-27	HIS	-	expression tag	UNP A0A0I9AIE4
B	-26	HIS	-	expression tag	UNP A0A0I9AIE4
B	-25	HIS	-	expression tag	UNP A0A0I9AIE4
B	-24	HIS	-	expression tag	UNP A0A0I9AIE4
B	-23	SER	-	expression tag	UNP A0A0I9AIE4
B	-22	SER	-	expression tag	UNP A0A0I9AIE4
B	-21	GLY	-	expression tag	UNP A0A0I9AIE4
B	-20	LEU	-	expression tag	UNP A0A0I9AIE4
B	-19	VAL	-	expression tag	UNP A0A0I9AIE4
B	-18	PRO	-	expression tag	UNP A0A0I9AIE4
B	-17	ARG	-	expression tag	UNP A0A0I9AIE4
B	-16	GLY	-	expression tag	UNP A0A0I9AIE4
B	-15	SER	-	expression tag	UNP A0A0I9AIE4
B	-14	HIS	-	expression tag	UNP A0A0I9AIE4
B	-13	MET	-	expression tag	UNP A0A0I9AIE4
B	-12	ALA	-	expression tag	UNP A0A0I9AIE4
B	-11	SER	-	expression tag	UNP A0A0I9AIE4
B	-10	MET	-	expression tag	UNP A0A0I9AIE4
B	-9	THR	-	expression tag	UNP A0A0I9AIE4
B	-8	GLY	-	expression tag	UNP A0A0I9AIE4
B	-7	GLY	-	expression tag	UNP A0A0I9AIE4
B	-6	GLN	-	expression tag	UNP A0A0I9AIE4
B	-5	GLN	-	expression tag	UNP A0A0I9AIE4
B	-4	MET	-	expression tag	UNP A0A0I9AIE4
B	-3	GLY	-	expression tag	UNP A0A0I9AIE4
B	-2	ARG	-	expression tag	UNP A0A0I9AIE4
B	-1	ASP	-	expression tag	UNP A0A0I9AIE4

Continued on next page...

Continued from previous page...

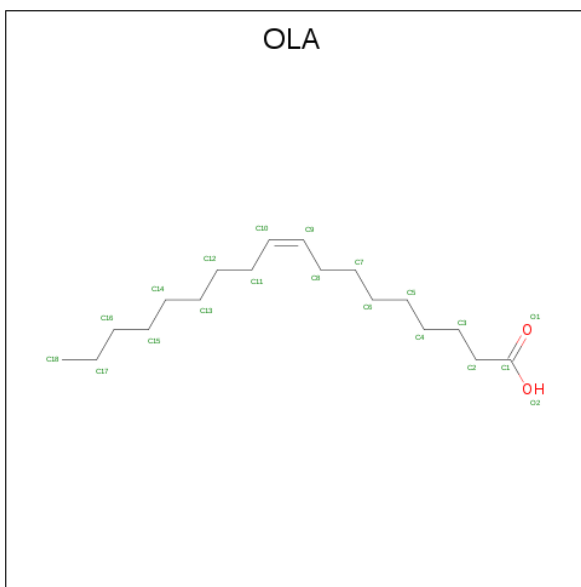
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PRO	-	expression tag	UNP A0A0I9AIE4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		

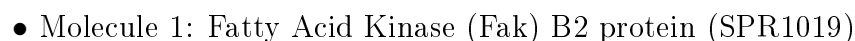
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		
5	B	257	Total	O	0	0
			257	257		

- Molecule 1: Fatty Acid Kinase (Fak) B2 protein (SPR1019)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.72Å 103.85Å 108.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.15 – 1.90 54.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (54.15-1.90) 97.8 (54.09-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.171 , 0.227 0.182 , 0.237	Depositor DCC
R_{free} test set	2659 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5028	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.51 % 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 3.1299e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, OLA, NA

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	0.60	0/2268	0.68	0/3062
1	B	0.55	0/2199	0.66	0/2969
All	All	0.57	0/4467	0.67	0/6031

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	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	2237	0	2276	11	0
1	B	2169	0	2223	12	0
2	A	24	0	31	1	0
2	B	6	0	8	0	0
3	A	20	0	33	0	0
3	B	20	0	33	0	0
4	A	1	0	0	0	0
5	A	294	0	0	7	0
5	B	257	0	0	5	0
All	All	5028	0	4604	23	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 3.

The worst 5 of 23 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:149:GLU:OE1	5:A:501:HOH:O	2.12	0.66
1:A:146[B]:HIS:CD2	5:A:583:HOH:O	2.49	0.65
1:A:129[A]:GLU:HG2	5:A:655:HOH:O	2.03	0.57
1:B:135:GLN:OE1	5:B:501:HOH:O	2.18	0.56
1:A:82:GLY:HA3	5:A:545:HOH:O	2.07	0.54

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	287/313 (92%)	281 (98%)	5 (2%)	1 (0%)	41	31
1	B	279/313 (89%)	276 (99%)	3 (1%)	0	100	100
All	All	566/626 (90%)	557 (98%)	8 (1%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR

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	252/269 (94%)	251 (100%)	1 (0%)	91	91
1	B	244/269 (91%)	242 (99%)	2 (1%)	81	82
All	All	496/538 (92%)	493 (99%)	3 (1%)	86	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	B	2	THR
1	B	234	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	B	35	ASN
1	B	165	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	GOL	A	404	-	5,5,5	0.22	0	5,5,5	0.33	0
2	GOL	A	403	-	5,5,5	0.44	0	5,5,5	0.14	0
3	OLA	B	402	-	16,19,19	0.29	0	15,19,19	0.39	0
3	OLA	A	405	-	16,19,19	0.33	0	15,19,19	0.55	0
2	GOL	B	401	-	5,5,5	0.23	0	5,5,5	0.20	0
2	GOL	A	401	4	5,5,5	0.50	0	5,5,5	0.72	0
2	GOL	A	402	-	5,5,5	0.72	0	5,5,5	0.74	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	GOL	A	404	-	-	2/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
3	OLA	B	402	-	-	0/15/17/17	-
3	OLA	A	405	-	-	0/15/17/17	-
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	A	401	4	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	GOL	C1-C2-C3-O3
2	A	403	GOL	C1-C2-C3-O3
2	A	403	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	GOL	1	0

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	278/313 (88%)	-0.36	1 (0%) 92 93	12, 18, 36, 60	3 (1%)
1	B	277/313 (88%)	-0.27	3 (1%) 80 82	15, 24, 45, 63	3 (1%)
All	All	555/626 (88%)	-0.31	4 (0%) 87 88	12, 21, 42, 63	6 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.4
1	B	179	LEU	3.1
1	B	214	GLU	2.5
1	B	178	LEU	2.1

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. 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(Å ²)	Q<0.9
2	GOL	A	404	6/6	0.83	0.17	51,53,55,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	402	6/6	0.83	0.16	43,45,47,47	0
2	GOL	A	403	6/6	0.87	0.14	34,54,57,58	0
2	GOL	A	401	6/6	0.89	0.16	36,37,37,39	0
2	GOL	B	401	6/6	0.89	0.14	47,48,52,54	0
4	NA	A	406	1/1	0.95	0.24	39,39,39,39	0
3	OLA	A	405	20/20	0.96	0.09	13,16,19,20	0
3	OLA	B	402	20/20	0.97	0.08	16,19,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.