Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2023 – 01:34 pm BST

PDB ID	:	8BBH
Title	:	The crystal structure of a mouse Fab fragment TL1 in complex with a human Glucose-6-phosphate isomerase peptide 293-307
Authors	:	Ge, C.; Holmdahl, R.; Li, T.
Deposited on	:	2022-10-13
Resolution	:	1.62 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:

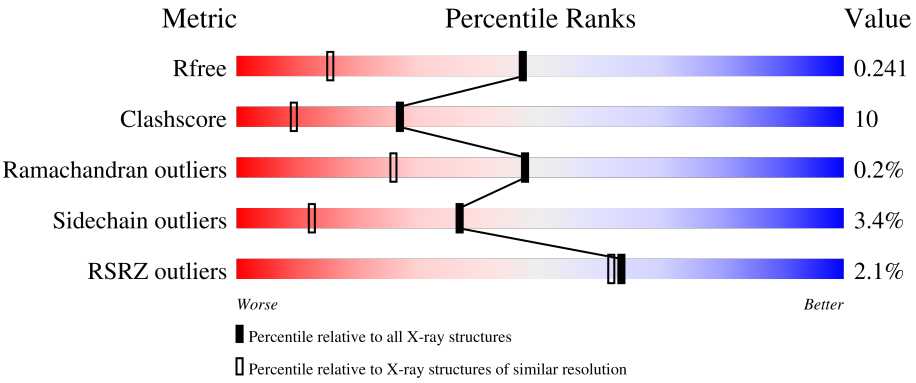
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (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 >=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 <=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	19	32% 11% 58%
2	H	213	% 92% 6%
3	L	218	3% 83% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6947 atoms, of which 3266 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	8	Total	C	H	N	O	S	6	0	0
			136	49	61	14	11	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ACA	-	expression tag	UNP P06744
A	292	CYS	-	expression tag	UNP P06744
A	308	CYS	-	expression tag	UNP P06744
A	309	ALA	-	expression tag	UNP P06744

- Molecule 2 is a protein called Heavy Chain of TL1 Fab fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	213	Total	C	H	N	O	S	104	0	0
			3159	1018	1563	256	314	8			

- Molecule 3 is a protein called Light Chain of TL1 Fab fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	218	Total	C	H	N	O	S	115	0	0
			3316	1051	1642	281	337	5			

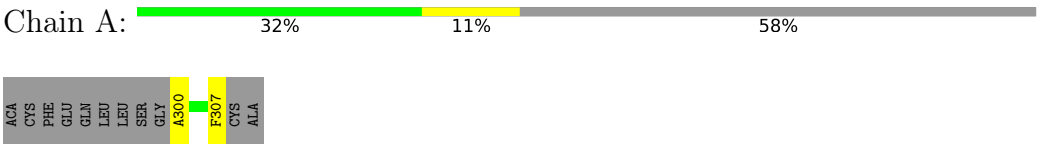
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	H	164	Total	O	0	0
			164	164		
4	L	162	Total	O	0	0
			162	162		

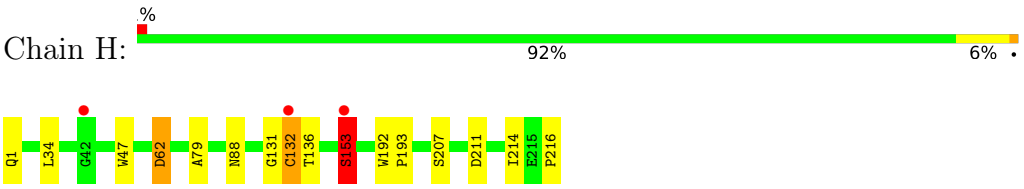
3 Residue-property plots (i)

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.

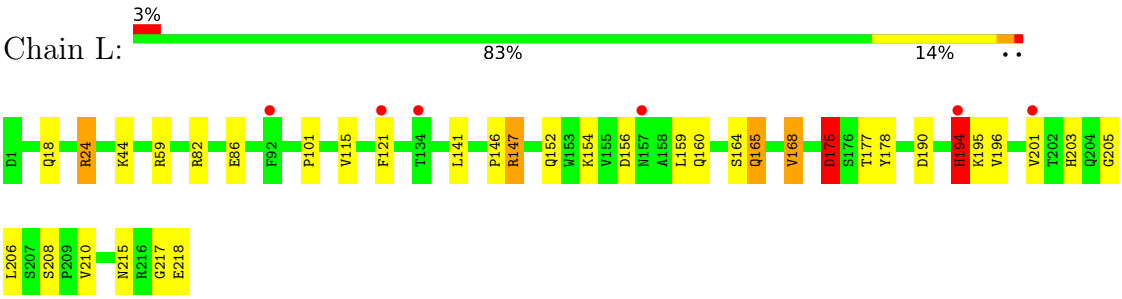
• Molecule 1: Glucose-6-phosphate isomerase



• Molecule 2: Heavy Chain of TL1 Fab fragment



• Molecule 3: Light Chain of TL1 Fab fragment



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.66Å 75.55Å 96.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.41 – 1.62 55.35 – 1.62	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.41-1.62) 100.0 (55.35-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.198 , 0.229 0.207 , 0.241	Depositor DCC
R_{free} test set	3038 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6947	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.50	0/79	0.72	0/106
2	H	0.44	0/1640	0.77	0/2241
3	L	0.73	1/1710 (0.1%)	0.89	6/2321 (0.3%)
All	All	0.60	1/3429 (0.0%)	0.83	6/4668 (0.1%)

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
2	H	0	1
3	L	0	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	194	HIS	CE1-NE2	-22.28	0.81	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	194	HIS	ND1-CG-CD2	-8.73	93.78	106.00
3	L	165	GLN	CB-CG-CD	6.58	128.70	111.60
3	L	194	HIS	CA-CB-CG	-6.31	102.87	113.60
3	L	194	HIS	CB-CG-CD2	5.28	147.16	130.80
3	L	175	ASP	CB-CA-C	-5.19	100.01	110.40
3	L	194	HIS	CE1-NE2-CD2	5.11	119.36	106.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	153	SER	Peptide
3	L	147	ARG	Sidechain
3	L	194	HIS	Sidechain
3	L	24	ARG	Sidechain
3	L	59	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	75	61	58	3	0
2	H	1596	1563	1560	10	3
3	L	1674	1642	1639	55	2
4	A	10	0	0	3	0
4	H	164	0	0	5	1
4	L	162	0	0	27	1
All	All	3681	3266	3257	67	4

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 10.

All (67) 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)
3:L:115:VAL:HG11	4:L:445:HOH:O	1.17	1.27
3:L:164:SER:HB3	4:L:357:HOH:O	1.11	1.24
1:A:307:PHE:C	4:A:406:HOH:O	1.77	1.21
3:L:218:GLU:C	4:L:304:HOH:O	1.81	1.15
3:L:194:HIS:CE1	4:L:305:HOH:O	1.99	1.13
3:L:168:VAL:HG12	4:L:404:HOH:O	1.47	1.11
2:H:153:SER:HA	4:H:301:HOH:O	1.62	0.98
3:L:205:GLY:HA3	4:L:362:HOH:O	1.62	0.97
3:L:194:HIS:CE1	3:L:194:HIS:NE2	0.81	0.97
3:L:206:LEU:HD12	3:L:206:LEU:O	1.66	0.95
3:L:196:VAL:HG12	3:L:215:ASN:OD1	1.67	0.95
3:L:194:HIS:NE2	3:L:194:HIS:HE1	1.54	0.92
3:L:205:GLY:HA3	4:L:403:HOH:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:HIS:CD2	4:L:422:HOH:O	2.26	0.89
3:L:194:HIS:HD2	4:L:422:HOH:O	1.58	0.85
3:L:206:LEU:HD13	3:L:208:SER:O	1.75	0.85
3:L:115:VAL:HG21	4:L:445:HOH:O	1.78	0.84
3:L:115:VAL:CG1	4:L:445:HOH:O	1.92	0.82
3:L:206:LEU:CD2	3:L:210:VAL:HG23	2.10	0.81
3:L:115:VAL:CG2	4:L:445:HOH:O	2.34	0.75
3:L:175:ASP:OD1	4:L:301:HOH:O	2.05	0.75
3:L:194:HIS:CE1	3:L:194:HIS:HE2	1.45	0.74
3:L:156:ASP:HA	3:L:196:VAL:HG22	1.70	0.73
3:L:152:GLN:HE21	3:L:154:LYS:HE3	1.53	0.72
3:L:141:LEU:HD21	3:L:201:VAL:HG22	1.70	0.72
3:L:194:HIS:NE2	4:L:305:HOH:O	2.23	0.70
3:L:121:PHE:CD2	4:L:360:HOH:O	2.44	0.70
3:L:206:LEU:HD23	3:L:210:VAL:HG23	1.72	0.70
2:H:153:SER:CA	4:H:301:HOH:O	2.30	0.69
3:L:152:GLN:HG3	3:L:159:LEU:HD13	1.74	0.68
1:A:300:ALA:N	4:A:401:HOH:O	2.27	0.67
3:L:156:ASP:HA	3:L:196:VAL:CG2	2.27	0.65
2:H:153:SER:N	4:H:301:HOH:O	2.29	0.64
3:L:190:ASP:OD2	4:L:302:HOH:O	2.15	0.64
3:L:115:VAL:CB	4:L:445:HOH:O	2.36	0.63
2:H:153:SER:HB2	4:H:369:HOH:O	2.01	0.61
3:L:203:HIS:HD2	4:L:362:HOH:O	1.82	0.60
3:L:206:LEU:HD23	4:L:453:HOH:O	2.02	0.58
3:L:121:PHE:HD2	4:L:360:HOH:O	1.83	0.55
3:L:205:GLY:CA	4:L:403:HOH:O	2.41	0.50
1:A:300:ALA:N	4:A:402:HOH:O	2.44	0.50
3:L:196:VAL:HG23	4:L:433:HOH:O	2.12	0.49
3:L:190:ASP:CG	4:L:302:HOH:O	2.49	0.49
3:L:206:LEU:O	3:L:206:LEU:CD1	2.51	0.49
3:L:146:PRO:O	3:L:203:HIS:HE1	1.95	0.49
2:H:131:GLY:O	2:H:132:CYS:C	2.51	0.48
3:L:196:VAL:HG11	4:L:427:HOH:O	2.13	0.47
3:L:205:GLY:CA	4:L:362:HOH:O	2.40	0.47
3:L:24:ARG:NH2	4:L:313:HOH:O	2.48	0.47
3:L:44:LYS:NZ	3:L:86:GLU:O	2.48	0.45
3:L:152:GLN:NE2	3:L:154:LYS:HE3	2.28	0.45
3:L:175:ASP:HB3	3:L:177:THR:H	1.82	0.45
3:L:141:LEU:HD23	3:L:201:VAL:CG1	2.46	0.45
3:L:178:TYR:HB3	4:L:404:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:ASN:ND2	4:H:306:HOH:O	2.50	0.44
2:H:192:TRP:CG	2:H:193:PRO:HA	2.53	0.44
3:L:141:LEU:CD2	3:L:201:VAL:HG22	2.43	0.43
3:L:206:LEU:HD13	3:L:208:SER:C	2.36	0.43
2:H:34:LEU:HD13	2:H:79:ALA:HB2	2.00	0.43
2:H:214:ILE:O	2:H:214:ILE:HG22	2.17	0.43
3:L:44:LYS:CE	3:L:86:GLU:O	2.67	0.42
3:L:195:LYS:HZ3	3:L:217:GLY:HA3	1.84	0.42
3:L:156:ASP:OD1	3:L:196:VAL:HG22	2.20	0.41
3:L:159:LEU:HD12	3:L:160:GLN:N	2.36	0.41
3:L:115:VAL:HG12	3:L:146:PRO:HD3	2.01	0.40
3:L:152:GLN:CG	3:L:159:LEU:HD13	2.45	0.40
2:H:47:TRP:CE3	3:L:101:PRO:HD2	2.56	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:211:ASP:OD2	3:L:194:HIS:NE2[3_355]	1.88	0.32
2:H:211:ASP:OD2	3:L:194:HIS:HE2[3_355]	1.43	0.17
2:H:62:ASP:OD2	2:H:62:ASP:OD2[2_545]	2.14	0.06
4:H:436:HOH:O	4:L:457:HOH:O[3_455]	2.18	0.02

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	6/19 (32%)	6 (100%)	0	0	100 100
2	H	209/213 (98%)	205 (98%)	3 (1%)	1 (0%)	29 11
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
All	All	431/450 (96%)	422 (98%)	8 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	153	SER

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	7/15 (47%)	7 (100%)	0	100	100
2	H	180/180 (100%)	174 (97%)	6 (3%)	38	13
3	L	194/194 (100%)	187 (96%)	7 (4%)	35	11
All	All	381/389 (98%)	368 (97%)	13 (3%)	37	12

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1	GLN
2	H	62	ASP
2	H	132	CYS
2	H	136	THR
2	H	207	SER
2	H	216	PRO
3	L	18	GLN
3	L	82	ARG
3	L	147	ARG
3	L	165	GLN
3	L	168	VAL
3	L	175	ASP
3	L	194	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	82	GLN
2	H	84	ASN
3	L	43	GLN
3	L	152	GLN
3	L	163	ASN
3	L	203	HIS

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	132:CYS	C	136:THR	N	10.82

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^{th} 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	8/19 (42%)	-0.09	0	100	100	22, 26, 33, 43	0
2	H	213/213 (100%)	-0.17	3 (1%)	75	74	18, 26, 46, 65	0
3	L	218/218 (100%)	-0.07	6 (2%)	53	50	20, 27, 41, 53	0
All	All	439/450 (97%)	-0.12	9 (2%)	63	62	18, 27, 44, 65	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	132	CYS	4.5
3	L	121	PHE	4.2
3	L	157	ASN	3.4
3	L	134	THR	3.1
3	L	201	VAL	3.0
2	H	42	GLY	2.8
2	H	153	SER	2.5
3	L	92	PHE	2.4
3	L	194	HIS	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.