



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:21 PM UTC

PDB ID : 2II1 / pdb_00002ii1
Title : Crystal structure of Acetamidase (10172637) from Bacillus Halodurans at 1.95 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2006-09-27
Resolution : 1.95 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

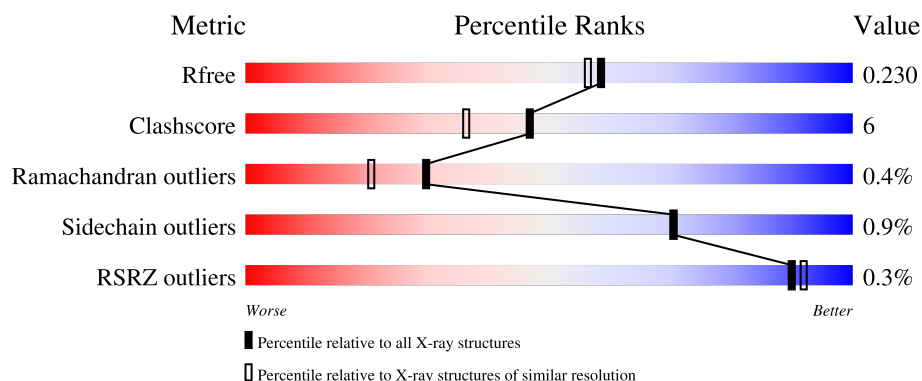
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	301	 86% 12% ..
1	B	301	 85% 13% .
1	C	301	 82% 15% ..
1	D	301	 88% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9233 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 Acetamidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	2	0
			2198	1395	363	428	3	9			
1	B	296	Total	C	N	O	S	Se	0	3	1
			2192	1393	358	429	3	9			
1	C	296	Total	C	N	O	S	Se	0	1	0
			2196	1392	360	432	3	9			
1	D	297	Total	C	N	O	S	Se	0	0	0
			2189	1388	357	431	3	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9KGN3
A	1	MSE	MET	modified residue	UNP Q9KGN3
A	13	MSE	MET	modified residue	UNP Q9KGN3
A	73	MSE	MET	modified residue	UNP Q9KGN3
A	89	MSE	MET	modified residue	UNP Q9KGN3
A	130	MSE	MET	modified residue	UNP Q9KGN3
A	186	MSE	MET	modified residue	UNP Q9KGN3
A	213	MSE	MET	modified residue	UNP Q9KGN3
A	226	MSE	MET	modified residue	UNP Q9KGN3
A	245	MSE	MET	modified residue	UNP Q9KGN3
A	262	MSE	MET	modified residue	UNP Q9KGN3
B	0	GLY	-	expression tag	UNP Q9KGN3
B	1	MSE	MET	modified residue	UNP Q9KGN3
B	13	MSE	MET	modified residue	UNP Q9KGN3
B	73	MSE	MET	modified residue	UNP Q9KGN3
B	89	MSE	MET	modified residue	UNP Q9KGN3
B	130	MSE	MET	modified residue	UNP Q9KGN3
B	186	MSE	MET	modified residue	UNP Q9KGN3
B	213	MSE	MET	modified residue	UNP Q9KGN3
B	226	MSE	MET	modified residue	UNP Q9KGN3
B	245	MSE	MET	modified residue	UNP Q9KGN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	262	MSE	MET	modified residue	UNP Q9KGN3
C	0	GLY	-	expression tag	UNP Q9KGN3
C	1	MSE	MET	modified residue	UNP Q9KGN3
C	13	MSE	MET	modified residue	UNP Q9KGN3
C	73	MSE	MET	modified residue	UNP Q9KGN3
C	89	MSE	MET	modified residue	UNP Q9KGN3
C	130	MSE	MET	modified residue	UNP Q9KGN3
C	186	MSE	MET	modified residue	UNP Q9KGN3
C	213	MSE	MET	modified residue	UNP Q9KGN3
C	226	MSE	MET	modified residue	UNP Q9KGN3
C	245	MSE	MET	modified residue	UNP Q9KGN3
C	262	MSE	MET	modified residue	UNP Q9KGN3
D	0	GLY	-	expression tag	UNP Q9KGN3
D	1	MSE	MET	modified residue	UNP Q9KGN3
D	13	MSE	MET	modified residue	UNP Q9KGN3
D	73	MSE	MET	modified residue	UNP Q9KGN3
D	89	MSE	MET	modified residue	UNP Q9KGN3
D	130	MSE	MET	modified residue	UNP Q9KGN3
D	186	MSE	MET	modified residue	UNP Q9KGN3
D	213	MSE	MET	modified residue	UNP Q9KGN3
D	226	MSE	MET	modified residue	UNP Q9KGN3
D	245	MSE	MET	modified residue	UNP Q9KGN3
D	262	MSE	MET	modified residue	UNP Q9KGN3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	5	Total Ca 5 5	0	0
2	C	5	Total Ca 5 5	0	0
2	D	3	Total Ca 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	115	Total O 115 115	0	0

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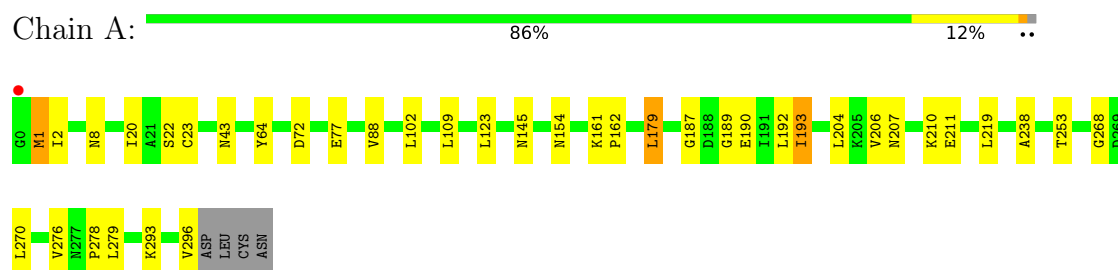
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	104	Total 104	O 104	0	0
3	C	106	Total 106	O 106	0	0
3	D	118	Total 118	O 118	0	0

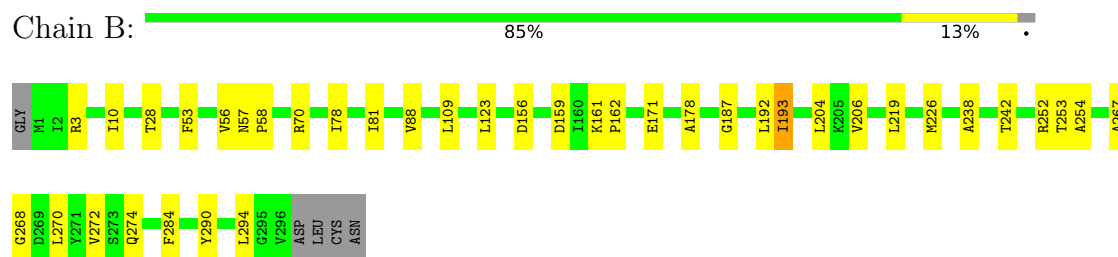
3 Residue-property plots [i](#)

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.

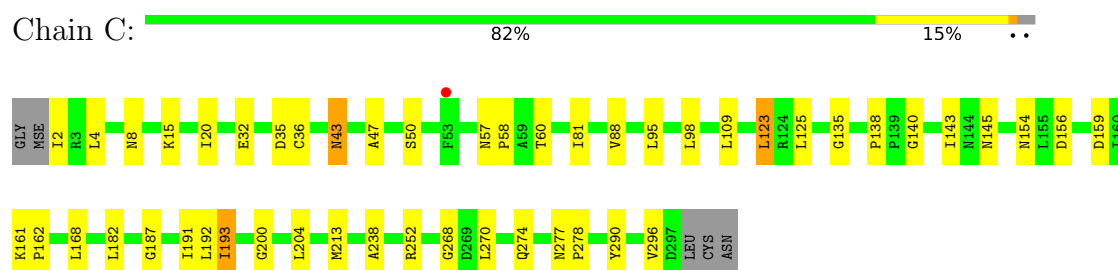
• Molecule 1: Acetamidase



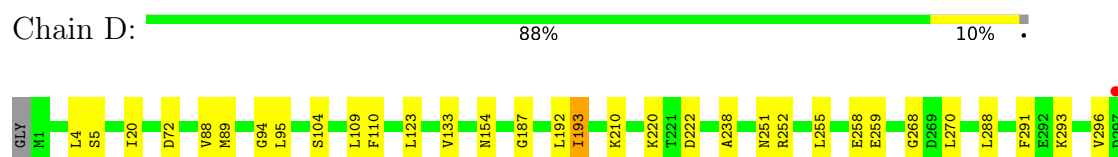
• Molecule 1: Acetamidase



• Molecule 1: Acetamidase



• Molecule 1: Acetamidase



LEU
CYS
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.76Å 69.61Å 94.98Å 73.95° 88.91° 86.63°	Depositor
Resolution (Å)	28.89 – 1.95 28.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.2 (28.89-1.95) 90.3 (28.89-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.228 0.178 , 0.230	Depositor DCC
R_{free} test set	3594 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9233	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.87	0/2231	0.91	1/3019 (0.0%)
1	B	0.85	0/2229	0.89	0/3018
1	C	0.83	0/2227	0.89	2/3016 (0.1%)
1	D	0.85	0/2217	0.90	1/3002 (0.0%)
All	All	0.85	0/8904	0.90	4/12055 (0.0%)

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	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	VAL	N-CA-C	8.61	119.46	111.45
1	A	1	MSE	N-CA-C	5.40	122.30	110.80
1	C	191	ILE	N-CA-C	5.01	117.35	111.09
1	D	251	ASN	N-CA-C	5.01	117.12	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	MSE	CA

There are no planarity outliers.

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	2198	0	2224	31	0
1	B	2192	0	2214	29	0
1	C	2196	0	2205	34	0
1	D	2189	0	2198	21	0
2	A	2	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0
3	A	115	0	0	0	0
3	B	104	0	0	1	0
3	C	106	0	0	2	0
3	D	118	0	0	1	0
All	All	9233	0	8841	101	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 6.

The worst 5 of 101 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:88:VAL:HG22	1:A:109:LEU:CD2	1.91	1.00
1:A:88:VAL:HG22	1:A:109:LEU:HD23	1.44	0.96
1:D:88:VAL:HG22	1:D:109:LEU:HD23	1.60	0.82
1:C:4:LEU:HD23	1:C:20:ILE:HD11	1.65	0.77
1:A:123:LEU:HD23	1:D:293:LYS:HD3	1.65	0.77

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	297/301 (99%)	287 (97%)	8 (3%)	2 (1%)	18	10
1	B	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	36	28
1	C	295/301 (98%)	285 (97%)	9 (3%)	1 (0%)	36	28
1	D	295/301 (98%)	285 (97%)	9 (3%)	1 (0%)	36	28
All	All	1184/1204 (98%)	1142 (96%)	37 (3%)	5 (0%)	30	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ILE
1	B	193	ILE
1	C	193	ILE
1	D	193	ILE
1	A	1	MSE

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	237/234 (101%)	234 (99%)	3 (1%)	61	58
1	B	237/234 (101%)	236 (100%)	1 (0%)	84	85
1	C	237/234 (101%)	235 (99%)	2 (1%)	73	74
1	D	236/234 (101%)	234 (99%)	2 (1%)	73	74
All	All	947/936 (101%)	939 (99%)	8 (1%)	70	74

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	222	ASP
1	D	5	SER
1	C	43	ASN

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Mol	Chain	Res	Type
1	B	28	THR
1	C	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	ASN
1	D	145	ASN
1	D	240	GLN
1	A	240	GLN
1	B	103	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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	287/301 (95%)	-0.30	1 (0%) 90 92	6, 14, 25, 35	2 (0%)
1	B	286/301 (95%)	-0.18	0 100 100	6, 16, 25, 33	3 (1%)
1	C	287/301 (95%)	0.01	1 (0%) 90 92	5, 16, 29, 39	1 (0%)
1	D	287/301 (95%)	-0.37	1 (0%) 90 92	6, 13, 25, 41	0
All	All	1147/1204 (95%)	-0.21	3 (0%) 90 92	5, 15, 26, 41	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	PHE	3.2
1	A	0	GLY	3.1
1	D	297	ASP	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 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, 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($\text{\AA}^2$)	Q<0.9
2	CA	C	403	1/1	0.90	0.11	31,31,31,31	0
2	CA	B	403	1/1	0.97	0.04	19,19,19,19	0
2	CA	C	401	1/1	0.98	0.04	18,18,18,18	0
2	CA	B	402	1/1	0.98	0.09	30,30,30,30	0
2	CA	D	401	1/1	0.98	0.02	13,13,13,13	0
2	CA	D	402	1/1	0.98	0.03	19,19,19,19	0
2	CA	B	404	1/1	0.99	0.03	19,19,19,19	0
2	CA	C	400	1/1	0.99	0.02	21,21,21,21	0
2	CA	B	400	1/1	0.99	0.02	17,17,17,17	0
2	CA	C	402	1/1	0.99	0.03	16,16,16,16	0
2	CA	B	401	1/1	0.99	0.02	15,15,15,15	0
2	CA	C	404	1/1	0.99	0.03	28,28,28,28	0
2	CA	D	400	1/1	0.99	0.02	16,16,16,16	0
2	CA	A	400	1/1	0.99	0.05	15,15,15,15	0
2	CA	A	401	1/1	0.99	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.