



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:21 pm GMT

PDB ID : 2P2M  
Title : Acetyl-CoA Synthetase, R194A mutation  
Authors : Reger, A.S.; Gulick, A.M.  
Deposited on : 2007-03-07  
Resolution : 2.11 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

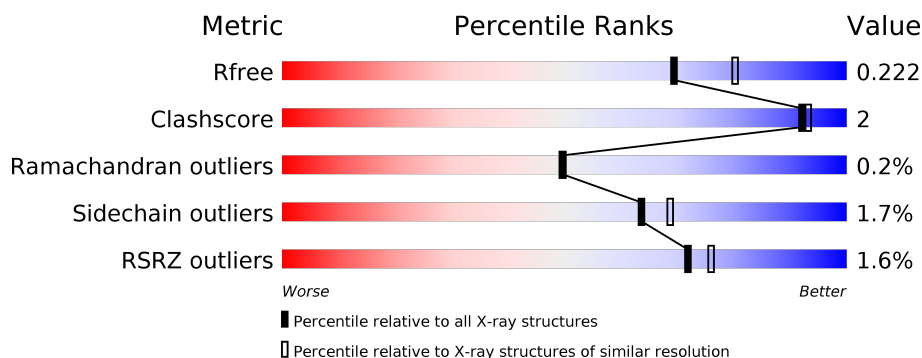
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	111664	5449 (2.14-2.10)
Clashscore	122126	5972 (2.14-2.10)
Ramachandran outliers	120053	5914 (2.14-2.10)
Sidechain outliers	120020	5915 (2.14-2.10)
RSRZ outliers	108989	5321 (2.14-2.10)

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. 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	652	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div></div> </div> <div></div> </div>
1	B	652	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10521 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.

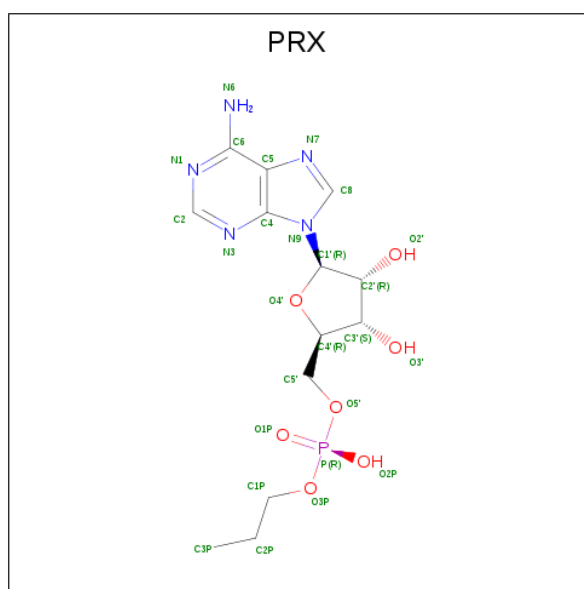
- Molecule 1 is a protein called Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4937	3141	842	936	18			
1	B	633	Total	C	N	O	S	0	0	0
			4906	3122	845	922	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	ARG	ENGINEERED	UNP Q8ZKF6
B	194	ALA	ARG	ENGINEERED	UNP Q8ZKF6

- Molecule 2 is ADENOSINE-5'-MONOPHOSPHATE-PROPYL ESTER (three-letter code: PRX) (formula:  $C_{13}H_{20}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

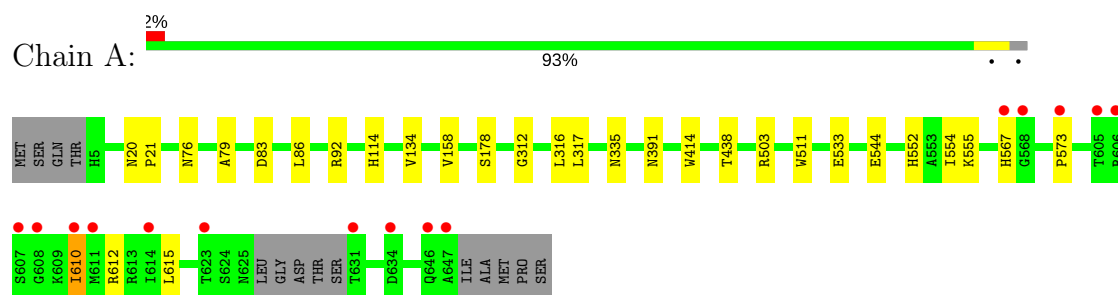
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	298	Total	O	0	0
			298	298		
3	B	328	Total	O	0	0
			328	328		

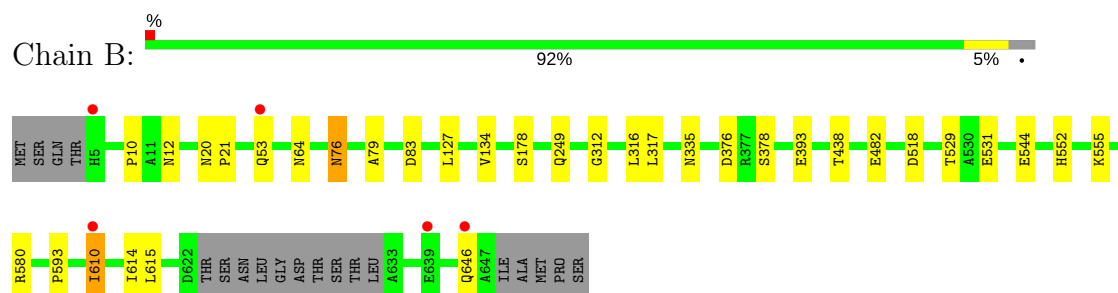
### 3 Residue-property plots [i](#)

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: Acetyl-coenzyme A synthetase



#### • Molecule 1: Acetyl-coenzyme A synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.72Å 95.50Å 163.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 2.11 47.35 – 2.11	Depositor EDS
% Data completeness (in resolution range)	92.6 (47.35-2.11) 91.9 (47.35-2.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.221 0.179 , 0.222	Depositor DCC
$R_{free}$ test set	3858 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

### 5.1 Standard geometry

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

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	0.49	0/5068	0.56	0/6916
1	B	0.47	0/5038	0.55	0/6873
All	All	0.48	0/10106	0.56	0/13789

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	4937	0	4754	18	0
1	B	4906	0	4740	15	1
2	A	26	0	19	1	0
2	B	26	0	19	0	0
3	A	298	0	0	2	2
3	B	328	0	0	1	3
All	All	10521	0	9532	32	3

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 2.

All (32) 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:B:552:HIS:HD2	1:B:555:LYS:H	1.28	0.79
1:A:610:ILE:HD11	1:A:615:LEU:HD12	1.68	0.74
1:B:610:ILE:HD11	1:B:615:LEU:CD1	2.18	0.73
1:B:552:HIS:CD2	1:B:555:LYS:H	2.12	0.66
1:A:610:ILE:HD11	1:A:615:LEU:CD1	2.25	0.66
1:B:610:ILE:HD11	1:B:615:LEU:HD12	1.76	0.65
1:A:533:GLU:OE2	1:A:612:ARG:NH2	2.30	0.64
1:A:552:HIS:CD2	1:A:555:LYS:H	2.15	0.64
1:A:552:HIS:HD2	1:A:555:LYS:H	1.47	0.61
1:A:316:LEU:HD12	1:A:317:LEU:HG	1.83	0.61
1:B:610:ILE:HD11	1:B:615:LEU:HD11	1.84	0.59
1:B:544:GLU:HG3	3:B:1104:HOH:O	2.05	0.54
1:B:20:ASN:HB2	1:B:21:PRO:CD	2.38	0.54
1:B:134:VAL:HG11	1:B:178:SER:HB2	1.90	0.53
1:B:376:ASP:OD1	1:B:378:SER:HB2	2.11	0.51
1:A:92:ARG:NE	3:A:1281:HOH:O	2.44	0.49
1:B:312:GLY:O	1:B:316:LEU:HB3	2.13	0.48
1:B:518:ASP:O	1:B:529:THR:HG23	2.15	0.47
1:A:76:ASN:HD22	1:A:79:ALA:H	1.62	0.45
1:A:312:GLY:O	1:A:316:LEU:HB3	2.16	0.45
1:A:20:ASN:HB2	1:A:21:PRO:CD	2.47	0.45
1:A:134:VAL:HA	1:A:158:VAL:O	2.17	0.44
1:A:503:ARG:HG2	1:A:511:TRP:HB2	2.00	0.43
1:B:76:ASN:HD22	1:B:79:ALA:H	1.66	0.42
1:B:580:ARG:HD2	1:B:593:PRO:O	2.20	0.42
1:A:134:VAL:HG11	1:A:178:SER:HB2	2.02	0.42
1:A:552:HIS:CD2	1:A:554:ILE:H	2.38	0.42
1:B:10:PRO:HB2	1:B:12:ASN:OD1	2.20	0.41
1:A:86:LEU:HD11	1:A:114:HIS:CG	2.56	0.41
1:A:414:TRP:CE2	2:A:998:PRX:H3P1	2.56	0.41
1:A:567:HIS:HB3	3:A:1199:HOH:O	2.20	0.40
1:A:573:PRO:HG2	1:B:393:GLU:HB3	2.03	0.40

All (3) 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)
1:B:482:GLU:OE2	3:B:1045:HOH:O[4_465]	1.72	0.48
3:A:1013:HOH:O	3:B:1020:HOH:O[4_555]	2.05	0.15
3:A:1013:HOH:O	3:B:1103:HOH:O[4_555]	2.18	0.02



## 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	634/652 (97%)	620 (98%)	13 (2%)	1 (0%)	49	50
1	B	629/652 (96%)	612 (97%)	16 (2%)	1 (0%)	49	50
All	All	1263/1304 (97%)	1232 (98%)	29 (2%)	2 (0%)	49	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	438	THR
1	A	438	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	512/537 (95%)	507 (99%)	5 (1%)	78	83
1	B	509/537 (95%)	497 (98%)	12 (2%)	52	55
All	All	1021/1074 (95%)	1004 (98%)	17 (2%)	63	69

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	335	ASN
1	A	391	ASN
1	A	544	GLU

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Mol	Chain	Res	Type
1	A	610	ILE
1	B	53	GLN
1	B	64	ASN
1	B	76	ASN
1	B	83	ASP
1	B	127	LEU
1	B	249	GLN
1	B	317	LEU
1	B	335	ASN
1	B	531	GLU
1	B	610	ILE
1	B	614	ILE
1	B	646	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	89	ASN
1	A	335	ASN
1	A	344	GLN
1	A	456	GLN
1	A	552	HIS
1	B	42	GLN
1	B	53	GLN
1	B	64	ASN
1	B	76	ASN
1	B	89	ASN
1	B	249	GLN
1	B	335	ASN
1	B	344	GLN
1	B	552	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
2	PRX	A	998	-	25,28,28	0.96	2 (8%)	25,41,41	1.99	2 (8%)
2	PRX	B	999	-	25,28,28	0.90	1 (4%)	25,41,41	1.98	1 (4%)

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	PRX	A	998	-	-	0/11/31/31	0/3/3/3
2	PRX	B	999	-	-	0/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	PRX	C8-N9	-2.79	1.33	1.36
2	A	998	PRX	O4'-C1'	2.36	1.44	1.41
2	B	999	PRX	O4'-C1'	2.67	1.45	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	PRX	N3-C2-N1	-9.46	120.76	128.86
2	A	998	PRX	N3-C2-N1	-9.18	121.00	128.86
2	A	998	PRX	C4-C5-N7	-2.44	107.06	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	PRX	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

### 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	638/652 (97%)	-0.17	15 (2%) 59 64	15, 21, 34, 45	0
1	B	633/652 (97%)	-0.22	5 (0%) 86 88	16, 23, 31, 50	0
All	All	1271/1304 (97%)	-0.19	20 (1%) 72 76	15, 23, 33, 50	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	HIS	5.1
1	A	567	HIS	5.0
1	A	610	ILE	4.4
1	A	607	SER	4.4
1	A	608	GLY	4.0
1	B	646	GLN	4.0
1	A	606	ARG	3.4
1	A	611	MET	3.2
1	A	605	THR	3.1
1	A	568	GLY	3.0
1	A	646	GLN	2.7
1	B	53	GLN	2.5
1	B	610	ILE	2.5
1	A	631	THR	2.4
1	A	573	PRO	2.4
1	A	647	ALA	2.3
1	A	614	ILE	2.2
1	A	623	THR	2.1
1	B	639	GLU	2.1
1	A	634	ASP	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, 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( $\text{\AA}^2$ )	Q<0.9
2	PRX	A	998	26/26	0.98	0.08	12,14,16,17	0
2	PRX	B	999	26/26	0.98	0.08	14,16,19,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.