



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 10:35 pm GMT

PDB ID : 4PYQ  
Title : Humanized rat apo-COMT in complex with a ureido-benzamidine  
Authors : Ehler, A.; Benz, J.; Schlatter, D.; Rudolph, M.G.  
Deposited on : 2014-03-27  
Resolution : 1.39 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](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 : trunk30967  
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) : trunk30967

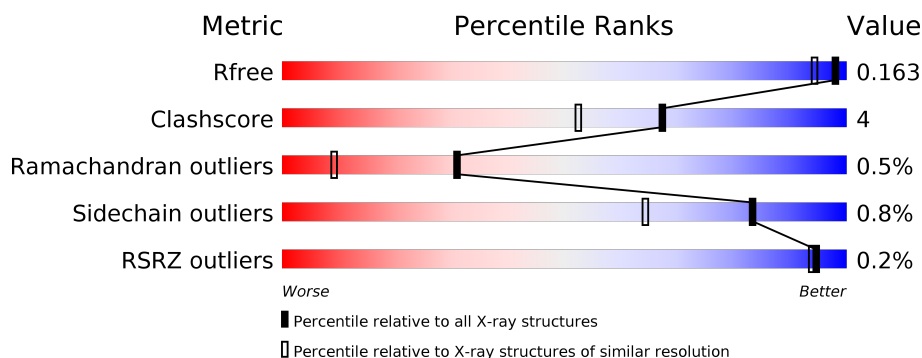
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.39 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	1450 (1.40-1.40)
Clashscore	122126	1541 (1.40-1.40)
Ramachandran outliers	120053	1500 (1.40-1.40)
Sidechain outliers	120020	1499 (1.40-1.40)
RSRZ outliers	108989	1412 (1.40-1.40)

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	221	<div> <div style="width: 90%;"></div> <div style="width: 6%;"></div> <div style="width: 4%;"></div> <div style="width: 0%;"></div> </div> <div>90% 6% .</div>
1	B	221	<div> <div style="width: 85%;"></div> <div style="width: 11%;"></div> <div style="width: 4%;"></div> <div style="width: 0%;"></div> </div> <div>85% 11% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	303	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7087 atoms, of which 3422 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.

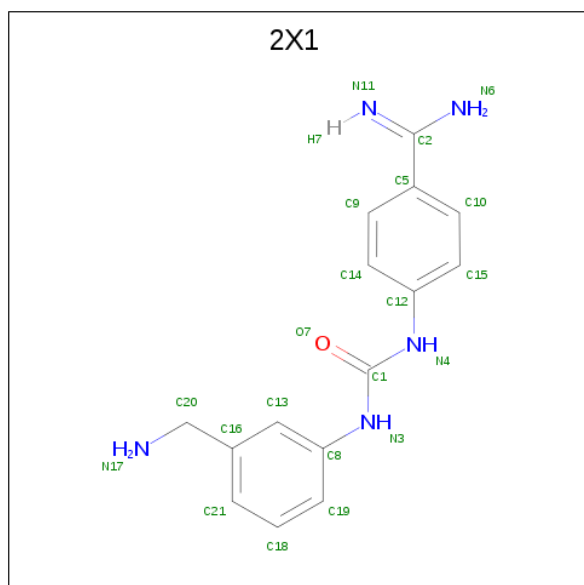
- Molecule 1 is a protein called Catechol O-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	3	0
			3392	1076	1704	278	321	13			
1	B	213	Total	C	H	N	O	S	0	4	0
			3415	1085	1718	278	320	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ILE	MET	ENGINEERED MUTATION	UNP P22734
A	138	CYS	TYR	ENGINEERED MUTATION	UNP P22734
B	134	ILE	MET	ENGINEERED MUTATION	UNP P22734
B	138	CYS	TYR	ENGINEERED MUTATION	UNP P22734

- Molecule 2 is 4-([3-(aminomethyl)phenyl]carbamoyl)amino)benzenecarboximidamide (three-letter code: 2X1) (formula: C<sub>15</sub>H<sub>17</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	15	5	1		
2	B	1	Total	C	N	O	0	0
			21	15	5	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		


- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	110	Total	O	0	0
			110	110		
7	B	97	Total	O	0	0
			97	97		

### 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.

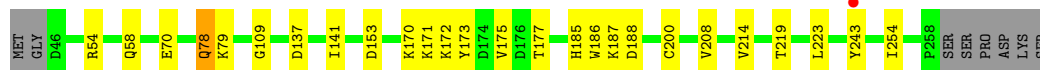
- Molecule 1: Catechol O-methyltransferase

Chain A:  90% 6% •



- Molecule 1: Catechol O-methyltransferase

Chain B:  85% 11% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.37Å 125.37Å 77.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.41 – 1.39 36.41 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.41-1.39) 96.3 (36.41-1.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1589)	Depositor
R, $R_{free}$	0.132 , 0.161 0.136 , 0.163	Depositor DCC
$R_{free}$ test set	4560 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 29.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.095 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.108 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.096 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.108 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.095 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.096 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.457 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for K,H,-L	Depositor
Outliers	0 of 91065 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: 2X1, NA, ACT, SO4, CL

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	0.66	0/1728	0.66	0/2342
1	B	0.70	0/1741	0.64	0/2359
All	All	0.68	0/3469	0.65	0/4701

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	1688	1704	1704	8	3
1	B	1697	1718	1718	19	4
2	A	21	0	16	3	0
2	B	21	0	17	2	0
3	A	4	0	3	0	0
3	B	4	0	3	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	110	0	0	0	0
7	B	97	0	0	2	0
All	All	3665	3422	3461	29	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 4.

The worst 5 of 29 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:B:303:ACT:H1	7:B:468:HOH:O	1.81	0.79
1:A:135:ASN:ND2	2:A:301:2X1:H15	2.13	0.62
1:B:188:ASP:OD1	2:B:302:2X1:N11	2.31	0.61
1:B:188:ASP:OD1	7:B:485:HOH:O	2.16	0.61
1:A:181:VAL:HB	1:A:209:LEU:HD22	1.93	0.51

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)
1:A:70:GLU:CD	1:B:70:GLU:OE2[3_555]	1.91	0.29
1:A:70:GLU:OE2	1:B:70:GLU:OE2[3_555]	1.96	0.24
1:A:70:GLU:OE1	1:B:70:GLU:OE2[3_555]	2.13	0.07
1:B:153:ASP:OD2	1:B:177:THR:OG1[2_555]	2.14	0.06

## 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	214/221 (97%)	204 (95%)	10 (5%)	0	100	100
1	B	215/221 (97%)	201 (94%)	12 (6%)	2 (1%)	19	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	429/442 (97%)	405 (94%)	22 (5%)	2 (0%)	31	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	LYS
1	B	185	HIS

### 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	186/190 (98%)	184 (99%)	2 (1%)	76	53
1	B	187/190 (98%)	186 (100%)	1 (0%)	90	77
All	All	373/380 (98%)	370 (99%)	3 (1%)	83	64

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

Mol	Chain	Res	Type
1	A	78	GLN
1	A	174	ASP
1	B	78	GLN

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 ⓘ

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	2X1	A	301	-	22,22,22	1.19	3 (13%)	27,29,29	1.02	2 (7%)
3	ACT	A	302	-	1,3,3	0.70	0	0,3,3	0.00	-
5	SO4	A	304	-	4,4,4	0.37	0	6,6,6	0.41	0
5	SO4	A	305	-	4,4,4	0.19	0	6,6,6	0.15	0
2	2X1	B	302	-	22,22,22	1.39	3 (13%)	27,29,29	1.31	3 (11%)
3	ACT	B	303	-	1,3,3	0.39	0	0,3,3	0.00	-
5	SO4	B	305	-	4,4,4	0.26	0	6,6,6	0.28	0
5	SO4	B	306	-	4,4,4	0.16	0	6,6,6	0.19	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	2X1	A	301	-	-	0/14/14/14	0/2/2/2
3	ACT	A	302	-	-	0/0/0/0	0/0/0/0
5	SO4	A	304	-	-	0/0/0/0	0/0/0/0
5	SO4	A	305	-	-	0/0/0/0	0/0/0/0
2	2X1	B	302	-	-	0/14/14/14	0/2/2/2
3	ACT	B	303	-	-	0/0/0/0	0/0/0/0
5	SO4	B	305	-	-	0/0/0/0	0/0/0/0
5	SO4	B	306	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	2X1	C1-N3	2.63	1.43	1.37
2	A	301	2X1	C1-N3	2.66	1.43	1.37
2	A	301	2X1	C1-N4	2.84	1.43	1.37
2	B	302	2X1	C1-N4	3.02	1.44	1.37
2	A	301	2X1	C2-N6	3.46	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	2X1	C9-C5-C2	-4.04	115.78	120.65
2	B	302	2X1	C5-C2-N6	-3.03	113.45	118.08
2	A	301	2X1	C9-C5-C2	-2.00	118.23	120.65
2	A	301	2X1	C9-C5-C10	2.26	121.77	118.58
2	B	302	2X1	C9-C5-C10	2.38	121.95	118.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	2X1	3	0
2	B	302	2X1	2	0
3	B	303	ACT	6	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, 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	213/221 (96%)	-0.39	0	100   100	12, 16, 31, 45	0
1	B	213/221 (96%)	-0.38	1 (0%)	90   90	12, 17, 32, 42	0
All	All	426/442 (96%)	-0.38	1 (0%)	94   94	12, 17, 31, 45	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243[A]	TYR	3.2

### 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(Å <sup>2</sup> )	Q < 0.9
5	SO4	A	305	5/5	0.93	0.13	75,76,77,78	0
6	CL	B	304	1/1	0.94	0.09	48,48,48,48	0
3	ACT	B	303	4/4	0.96	0.08	24,24,26,28	0
5	SO4	B	306	5/5	0.96	0.13	75,76,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2X1	B	302	21/21	0.97	0.11	24,30,42,45	0
3	ACT	A	302	4/4	0.98	0.06	18,21,21,22	0
2	2X1	A	301	21/21	0.98	0.08	20,25,36,40	0
4	NA	B	301	1/1	1.00	0.07	14,14,14,14	0
5	SO4	A	304	5/5	1.00	0.06	18,18,18,23	0
4	NA	A	303	1/1	1.00	0.06	13,13,13,13	0
5	SO4	B	305	5/5	1.00	0.05	19,21,22,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.