



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:57 PM GMT

PDB ID : 2HT4  
Title : Structure of the Escherichia coli ClC chloride channel Y445W mutant and Fab complex  
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.  
Deposited on : 2006-07-25  
Resolution : 3.20 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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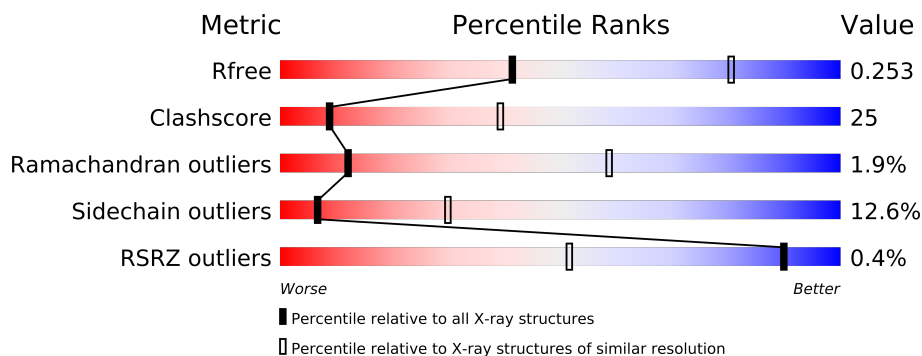
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	
2	C	221	
2	E	221	
3	D	211	
3	F	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	BR	A	475	-	X
4	BR	B	475	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13231 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3335	2192	561	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3306	2176	554	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	TRP	TYR	ENGINEERED	UNP P37019
B	445	TRP	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Br	0	0
			2	2		

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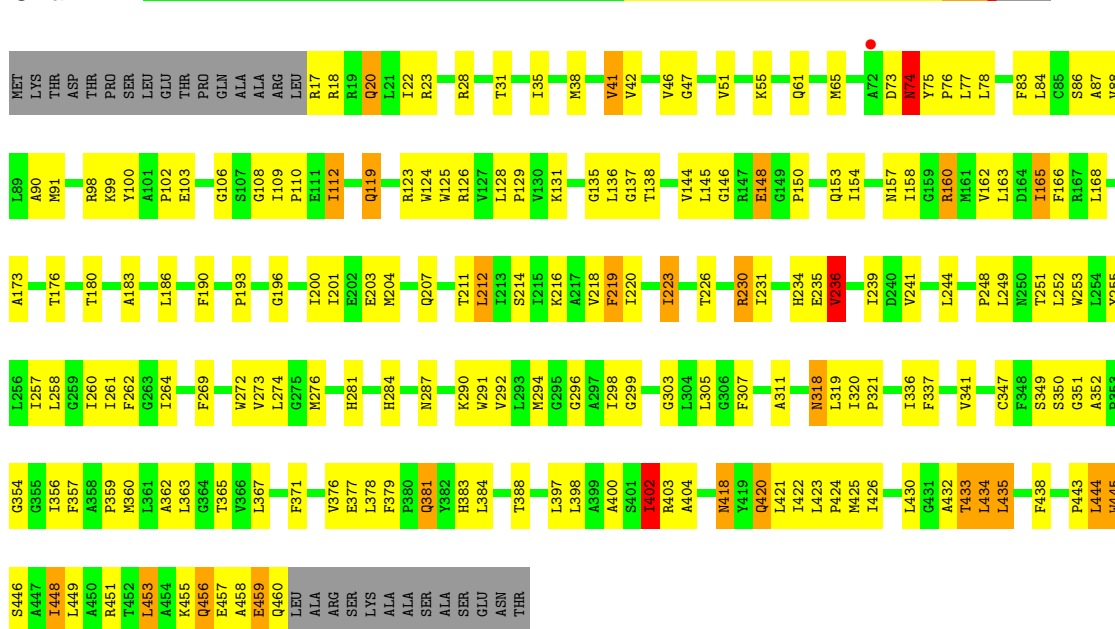
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Br	0	0
			2	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: H(+)/Cl(-) exchange transporter clcA

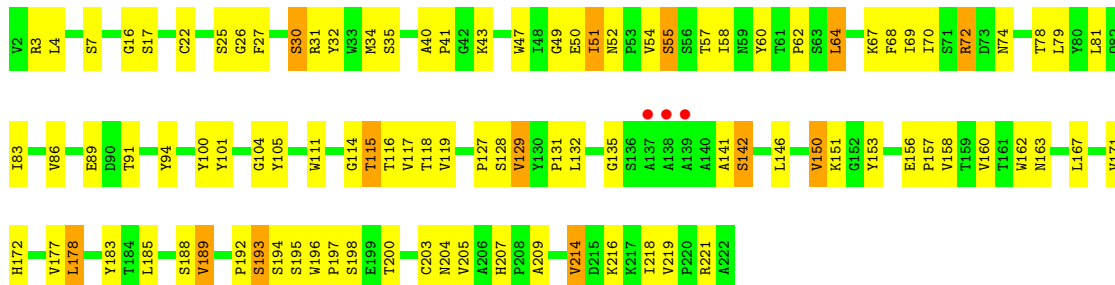
Chain A:





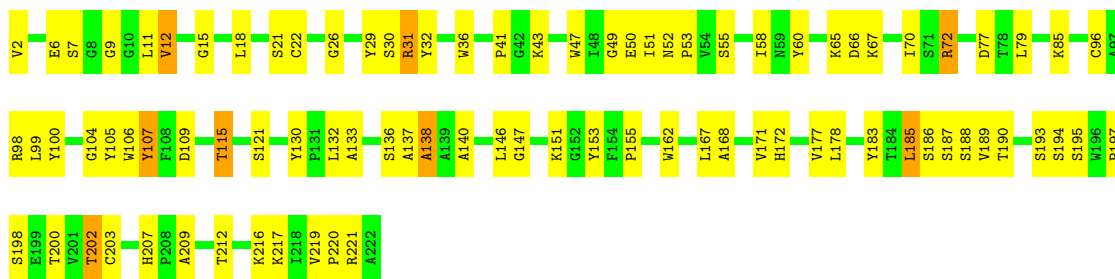
• Molecule 2: Fab fragment, Heavy chain

Chain C:



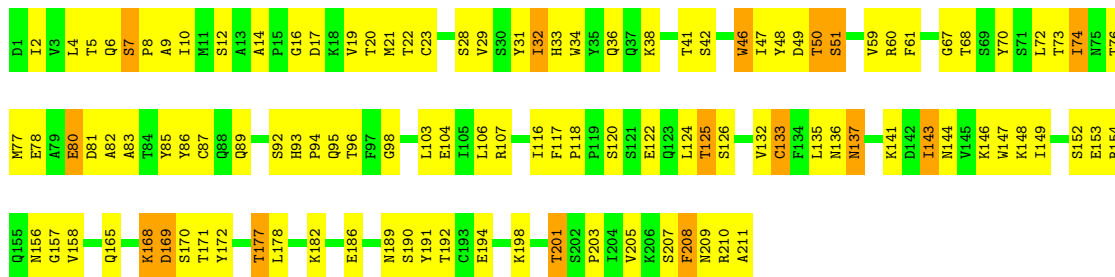
• Molecule 2: Fab fragment, Heavy chain

Chain E:



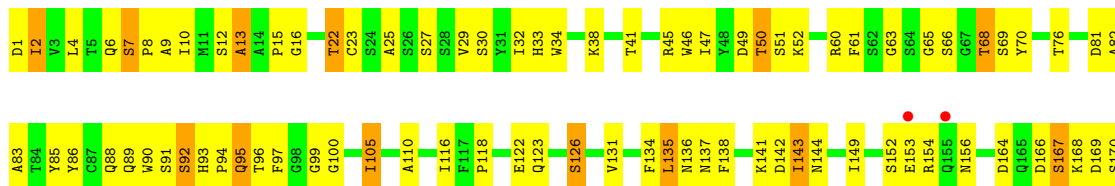
• Molecule 3: Fab fragment, Light chain

Chain D:



• Molecule 3: Fab fragment, Light chain

Chain F:



S173	M174	S175	L178	T181	K182	D183	E184	Y185	E186	R187	H188	N189	S190	Y191	T192	G193	E194	K198	T201	T204	V205	K206	S207	R210	A211
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.01Å 95.94Å 175.33Å 90.00° 133.20° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 19.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-3.20) 97.0 (19.87-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.239 , 0.261 0.232 , 0.253	Depositor DCC
$R_{free}$ test set	2228 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 100.0	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 46773 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.59	1/3408 (0.0%)	0.76	2/4626 (0.0%)
1	B	0.60	1/3379 (0.0%)	0.76	0/4588
2	C	0.68	0/1721	0.78	0/2355
2	E	0.62	0/1721	0.78	1/2355 (0.0%)
3	D	0.62	1/1660 (0.1%)	0.75	0/2257
3	F	0.58	0/1660	0.75	0/2257
All	All	0.61	3/13549 (0.0%)	0.76	3/18438 (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
2	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	LYS	CD-CE	7.41	1.69	1.51
1	B	85	CYS	CB-SG	-5.94	1.72	1.81
1	A	445	TRP	CG-CD1	-5.66	1.28	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ILE	CG1-CB-CG2	-10.39	88.55	111.40
2	E	185	LEU	CA-CB-CG	6.83	131.01	115.30
1	A	223	ILE	CG1-CB-CG2	-5.39	99.53	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	196	TRP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3335	0	3485	185	0
1	B	3306	0	3458	198	0
2	C	1672	0	1654	80	0
2	E	1672	0	1654	61	0
3	D	1621	0	1546	99	0
3	F	1621	0	1546	105	0
4	A	2	0	0	5	0
4	B	2	0	0	7	0
All	All	13231	0	13343	677	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 677 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:402:ILE:HD13	1:B:445:TRP:CD1	1.64	1.33
1:B:402:ILE:HD13	1:B:445:TRP:NE1	1.52	1.21
1:B:445:TRP:HH2	4:B:474:BR:BR	1.81	1.18
1:A:109:ILE:HG21	1:A:445:TRP:CZ3	1.77	1.18
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.16	1.15

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	442/473 (93%)	400 (90%)	37 (8%)	5 (1%)	21	72
1	B	439/473 (93%)	399 (91%)	38 (9%)	2 (0%)	38	85
2	C	219/221 (99%)	189 (86%)	25 (11%)	5 (2%)	10	52
2	E	219/221 (99%)	190 (87%)	23 (10%)	6 (3%)	8	46
3	D	209/211 (99%)	169 (81%)	32 (15%)	8 (4%)	5	34
3	F	209/211 (99%)	180 (86%)	22 (10%)	7 (3%)	6	38
All	All	1737/1810 (96%)	1527 (88%)	177 (10%)	33 (2%)	12	59

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
2	C	41	PRO
2	C	141	ALA
3	D	7	SER
3	D	50	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	335/358 (94%)	298 (89%)	37 (11%)	9	36
1	B	332/358 (93%)	290 (87%)	42 (13%)	6	29
2	C	181/181 (100%)	154 (85%)	27 (15%)	4	20
2	E	181/181 (100%)	158 (87%)	23 (13%)	6	29
3	D	185/185 (100%)	165 (89%)	20 (11%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	185/185 (100%)	158 (85%)	27 (15%)	5	21
All	All	1399/1448 (97%)	1223 (87%)	176 (13%)	7	30

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	30	SER
2	C	189	VAL
3	F	143	ILE
2	C	35	SER
2	C	118	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	GLN
1	B	327	ASN
3	F	137	ASN
1	B	270	ASN
1	B	277	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	444/473 (93%)	-0.06	1 (0%) 93 66	41, 79, 124, 162	0
1	B	441/473 (93%)	-0.06	1 (0%) 93 66	36, 79, 124, 173	0
2	C	221/221 (100%)	0.13	3 (1%) 72 22	37, 75, 127, 168	0
2	E	221/221 (100%)	0.02	0 100 100	29, 77, 122, 172	0
3	D	211/211 (100%)	0.09	0 100 100	50, 88, 118, 141	0
3	F	211/211 (100%)	0.05	2 (0%) 81 32	32, 73, 121, 155	0
All	All	1749/1810 (96%)	0.01	7 (0%) 90 51	29, 79, 124, 173	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	3.2
2	C	139	ALA	2.6
1	A	72	ALA	2.6
2	C	137	ALA	2.5
3	F	155	GLN	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BR	B	475	1/1	0.35	4.88	51,51,51,51	0
4	BR	A	475	1/1	0.41	3.91	51,51,51,51	0
4	BR	A	474	1/1	0.29	1.87	51,51,51,51	0
4	BR	B	474	1/1	0.27	1.15	51,51,51,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.