wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:09 PM GMT

PDB ID	:	4KP3
Title	:	Crystal Structure of MyoVa-GTD in Complex with Two Cargos
Authors	:	Wei, Z.; Liu, X.; Yu, C.; Zhang, M.
Deposited on	:	2013-05-13
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

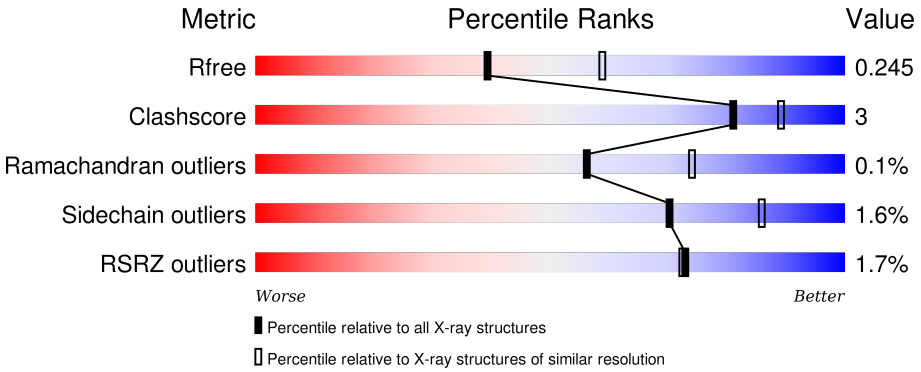
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 >=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 <=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	404	% 80% 9% 11%
1	B	404	% 80% 7% 12%
2	C	103	% 68% 11% 21%
2	D	103	73% 7% 20%
3	E	43	5% 33% 67%

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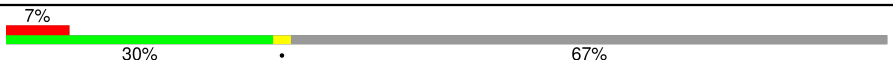
Mol	Chain	Length	Quality of chain
3	F	43	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7359 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 Unconventional myosin-Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2908	1850	501	536	21			
1	B	355	Total	C	N	O	S	0	0	0
			2847	1810	491	525	21			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1450	HIS	-	EXPRESSION TAG	UNP Q99104
A	1451	HIS	-	EXPRESSION TAG	UNP Q99104
A	1452	HIS	-	EXPRESSION TAG	UNP Q99104
A	1453	HIS	-	EXPRESSION TAG	UNP Q99104
A	1454	HIS	-	EXPRESSION TAG	UNP Q99104
A	1455	HIS	-	EXPRESSION TAG	UNP Q99104
A	1456	SER	-	EXPRESSION TAG	UNP Q99104
A	1457	SER	-	EXPRESSION TAG	UNP Q99104
A	1458	GLY	-	EXPRESSION TAG	UNP Q99104
A	1459	LEU	-	EXPRESSION TAG	UNP Q99104
A	1460	GLY	-	EXPRESSION TAG	UNP Q99104
A	1461	VAL	-	EXPRESSION TAG	UNP Q99104
A	1462	LEU	-	EXPRESSION TAG	UNP Q99104
A	1463	PHE	-	EXPRESSION TAG	UNP Q99104
A	1464	GLN	-	EXPRESSION TAG	UNP Q99104
A	1465	GLY	-	EXPRESSION TAG	UNP Q99104
A	1466	PRO	-	EXPRESSION TAG	UNP Q99104
A	1467	GLY	-	EXPRESSION TAG	UNP Q99104
A	1468	SER	-	EXPRESSION TAG	UNP Q99104
A	1674	SER	CYS	ENGINEERED MUTATION	UNP Q99104
B	1450	HIS	-	EXPRESSION TAG	UNP Q99104
B	1451	HIS	-	EXPRESSION TAG	UNP Q99104
B	1452	HIS	-	EXPRESSION TAG	UNP Q99104
B	1453	HIS	-	EXPRESSION TAG	UNP Q99104
B	1454	HIS	-	EXPRESSION TAG	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1455	HIS	-	EXPRESSION TAG	UNP Q99104
B	1456	SER	-	EXPRESSION TAG	UNP Q99104
B	1457	SER	-	EXPRESSION TAG	UNP Q99104
B	1458	GLY	-	EXPRESSION TAG	UNP Q99104
B	1459	LEU	-	EXPRESSION TAG	UNP Q99104
B	1460	GLY	-	EXPRESSION TAG	UNP Q99104
B	1461	VAL	-	EXPRESSION TAG	UNP Q99104
B	1462	LEU	-	EXPRESSION TAG	UNP Q99104
B	1463	PHE	-	EXPRESSION TAG	UNP Q99104
B	1464	GLN	-	EXPRESSION TAG	UNP Q99104
B	1465	GLY	-	EXPRESSION TAG	UNP Q99104
B	1466	PRO	-	EXPRESSION TAG	UNP Q99104
B	1467	GLY	-	EXPRESSION TAG	UNP Q99104
B	1468	SER	-	EXPRESSION TAG	UNP Q99104
B	1674	SER	CYS	ENGINEERED MUTATION	UNP Q99104

- Molecule 2 is a protein called RILP-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	81	Total	C	N	O	S	0	0	0
			642	398	110	130	4			
2	D	82	Total	C	N	O	S	0	1	0
			659	409	115	131	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	EXPRESSION TAG	UNP Q99LE1
C	-4	PRO	-	EXPRESSION TAG	UNP Q99LE1
C	-3	GLY	-	EXPRESSION TAG	UNP Q99LE1
C	-2	SER	-	EXPRESSION TAG	UNP Q99LE1
C	-1	GLU	-	EXPRESSION TAG	UNP Q99LE1
C	0	PHE	-	EXPRESSION TAG	UNP Q99LE1
D	-5	GLY	-	EXPRESSION TAG	UNP Q99LE1
D	-4	PRO	-	EXPRESSION TAG	UNP Q99LE1
D	-3	GLY	-	EXPRESSION TAG	UNP Q99LE1
D	-2	SER	-	EXPRESSION TAG	UNP Q99LE1
D	-1	GLU	-	EXPRESSION TAG	UNP Q99LE1
D	0	PHE	-	EXPRESSION TAG	UNP Q99LE1

- Molecule 3 is a protein called Melanophilin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	14	Total 121	C 78	N 22	O 21	0	0	0
3	F	14	Total 125	C 81	N 23	O 21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	166	GLY	-	EXPRESSION TAG	UNP Q91V27
E	167	PRO	-	EXPRESSION TAG	UNP Q91V27
E	168	GLY	-	EXPRESSION TAG	UNP Q91V27
E	169	SER	-	EXPRESSION TAG	UNP Q91V27
F	166	GLY	-	EXPRESSION TAG	UNP Q91V27
F	167	PRO	-	EXPRESSION TAG	UNP Q91V27
F	168	GLY	-	EXPRESSION TAG	UNP Q91V27
F	169	SER	-	EXPRESSION TAG	UNP Q91V27

- Molecule 4 is water.

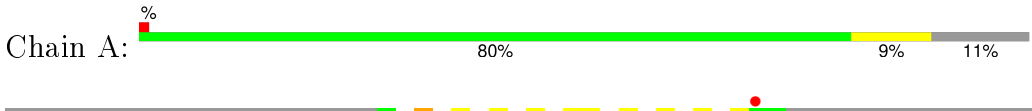
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	C	6	Total 6	O 6	0	0
4	E	1	Total 1	O 1	0	0
4	B	13	Total 13	O 13	0	0
4	D	3	Total 3	O 3	0	0
4	F	1	Total 1	O 1	0	0

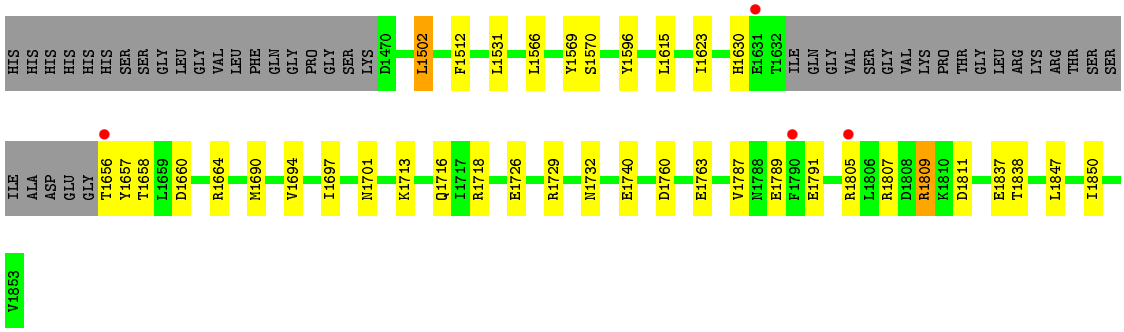
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (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: Unconventional myosin-Va

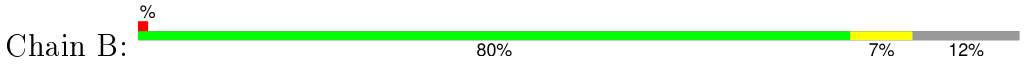
Chain A:

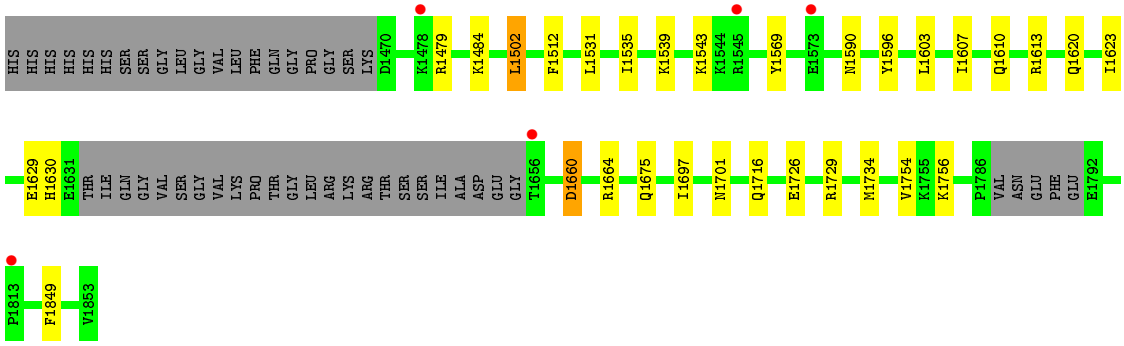




- Molecule 1: Unconventional myosin-Va

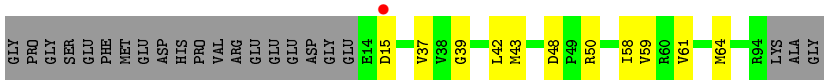
Chain B:





- Molecule 2: RILP-like protein 2

Chain C:

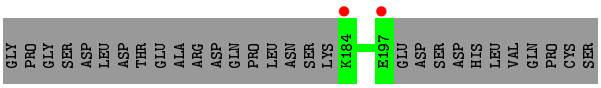


- Molecule 2: RILP-like protein 2

Chain D:

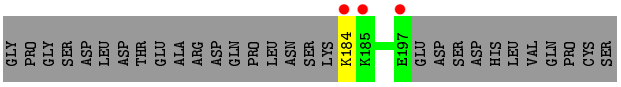
- Molecule 3: Melanophilin

Chain E:



- Molecule 3: Melanophilin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.85Å 107.93Å 83.51Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	38.69 – 2.40 38.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.69-2.40) 97.9 (38.69-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.192 , 0.241 0.201 , 0.245	Depositor DCC
R_{free} test set	2798 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.3	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 54945 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.26	0/2960	0.44	0/3995
1	B	0.24	0/2894	0.42	0/3906
2	C	0.25	0/646	0.44	0/869
2	D	0.25	0/666	0.41	0/894
3	E	0.24	0/122	0.36	0/160
3	F	0.24	0/126	0.34	0/164
All	All	0.25	0/7414	0.42	0/9988

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	2908	0	2960	24	0
1	B	2847	0	2890	16	0
2	C	642	0	650	7	0
2	D	659	0	676	6	0
3	E	121	0	121	0	0
3	F	125	0	132	1	0
4	A	33	0	0	0	0
4	B	13	0	0	0	0
4	C	6	0	0	0	0
4	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	7359	0	7429	48	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 3.

The worst 5 of 48 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:1726:GLU:OE2	1:A:1729:ARG:NH1	2.28	0.66
1:B:1630:HIS:O	1:B:1716:GLN:NE2	2.30	0.64
1:B:1539:LYS:HE3	1:B:1603:LEU:HD13	1.82	0.62
1:A:1623:ILE:HD12	1:A:1697:ILE:HD12	1.85	0.59
1:A:1763:GLU:OE1	1:A:1805:ARG:NH2	2.36	0.59

There are no symmetry-related clashes.

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	358/404 (89%)	351 (98%)	7 (2%)	0	100 100
1	B	349/404 (86%)	341 (98%)	7 (2%)	1 (0%)	46 63
2	C	79/103 (77%)	79 (100%)	0	0	100 100
2	D	81/103 (79%)	81 (100%)	0	0	100 100
3	E	12/43 (28%)	12 (100%)	0	0	100 100
3	F	12/43 (28%)	11 (92%)	1 (8%)	0	100 100
All	All	891/1100 (81%)	875 (98%)	15 (2%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1629	GLU

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	329/365 (90%)	323 (98%)	6 (2%)	66	84
1	B	321/365 (88%)	315 (98%)	6 (2%)	65	83
2	C	72/89 (81%)	71 (99%)	1 (1%)	74	88
2	D	74/89 (83%)	74 (100%)	0	100	100
3	E	13/40 (32%)	13 (100%)	0	100	100
3	F	14/40 (35%)	14 (100%)	0	100	100
All	All	823/988 (83%)	810 (98%)	13 (2%)	70	86

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1809	ARG
2	C	43	MET
1	B	1660	ASP
1	A	1760	ASP
1	B	1543	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1753	GLN
2	C	88	GLN
1	B	1586	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 carbohydrates 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

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^{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	361/404 (89%)	-0.24	4 (1%) 82 82	23, 44, 83, 118	0
1	B	355/404 (87%)	-0.08	5 (1%) 78 77	27, 55, 85, 119	1 (0%)
2	C	81/103 (78%)	-0.42	1 (1%) 81 81	28, 44, 73, 95	2 (2%)
2	D	82/103 (79%)	-0.26	0 100 100	27, 43, 71, 96	0
3	E	14/43 (32%)	-0.07	2 (14%) 4 3	41, 57, 84, 104	0
3	F	14/43 (32%)	0.97	3 (21%) 1 1	66, 86, 114, 124	0
All	All	907/1100 (82%)	-0.17	15 (1%) 73 72	23, 50, 87, 124	3 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	185	LYS	4.2
3	F	184	LYS	4.2
1	B	1656	THR	4.1
2	C	15	ASP	2.9
1	A	1656	THR	2.7

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.