WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:21 AM GMT

PDB ID : 3HG0
Title : Crystal structure of a DARPin in complex with ORF49 from Lactococcal phage TP901-1
Authors : Veesler, D.; Dreier, B.; Blangy, S.; Lichiere, J.; Tremblay, D.; Moineau, S.; Spinelli, S.; Tegoni, M.; Pluckthun, A.; Campanacci, V.; Cambillau, C.
Deposited on : 2009-05-13
Resolution : 2.10 Å(reported)

This is a full wwPDB validation 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/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 2.10 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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.4%
Sidechain outliers		7.5%
RSRZ outliers		2.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
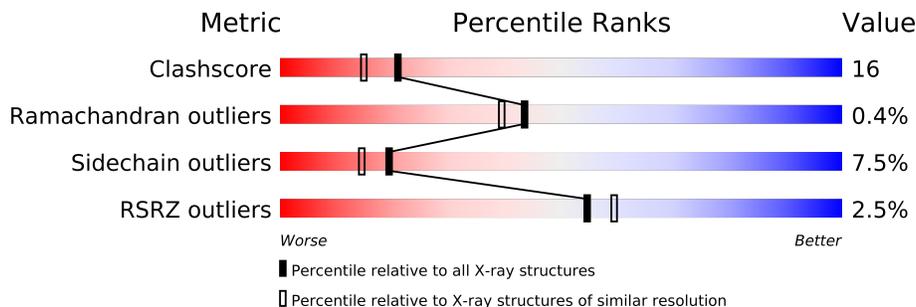
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 >=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	169	
1	B	169	
1	C	169	
2	D	136	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4379 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 Baseplate protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	3	0
			1035	646	189	196	4			
1	B	130	Total	C	N	O	S	0	3	0
			977	610	172	191	4			
1	C	132	Total	C	N	O	S	0	3	0
			989	618	177	190	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	EXPRESSION TAG	UNP Q9G096
A	165	HIS	-	EXPRESSION TAG	UNP Q9G096
A	166	HIS	-	EXPRESSION TAG	UNP Q9G096
A	167	HIS	-	EXPRESSION TAG	UNP Q9G096
A	168	HIS	-	EXPRESSION TAG	UNP Q9G096
A	169	HIS	-	EXPRESSION TAG	UNP Q9G096
B	164	HIS	-	EXPRESSION TAG	UNP Q9G096
B	165	HIS	-	EXPRESSION TAG	UNP Q9G096
B	166	HIS	-	EXPRESSION TAG	UNP Q9G096
B	167	HIS	-	EXPRESSION TAG	UNP Q9G096
B	168	HIS	-	EXPRESSION TAG	UNP Q9G096
B	169	HIS	-	EXPRESSION TAG	UNP Q9G096
C	164	HIS	-	EXPRESSION TAG	UNP Q9G096
C	165	HIS	-	EXPRESSION TAG	UNP Q9G096
C	166	HIS	-	EXPRESSION TAG	UNP Q9G096
C	167	HIS	-	EXPRESSION TAG	UNP Q9G096
C	168	HIS	-	EXPRESSION TAG	UNP Q9G096
C	169	HIS	-	EXPRESSION TAG	UNP Q9G096

- Molecule 2 is a protein called Designed Ankyrin Repeat Protein (DARPin) 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	124	932	583	159	187	3	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total 158	O 158	0	0
3	B	93	Total 93	O 93	0	0
3	C	107	Total 107	O 107	0	0
3	D	88	Total 88	O 88	0	0

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 (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: Baseplate protein

Chain A:
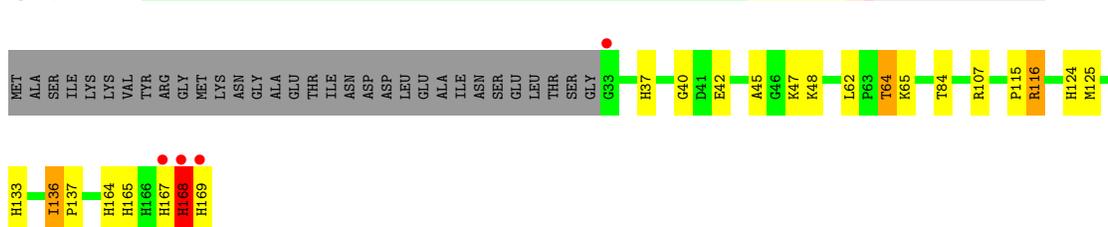
- Molecule 1: Baseplate protein

Chain B:
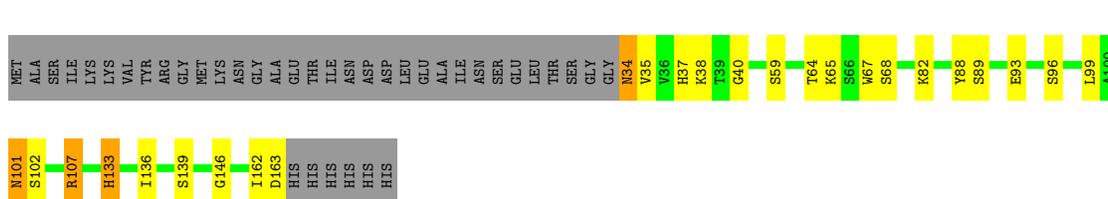
- Molecule 1: Baseplate protein

Chain C:
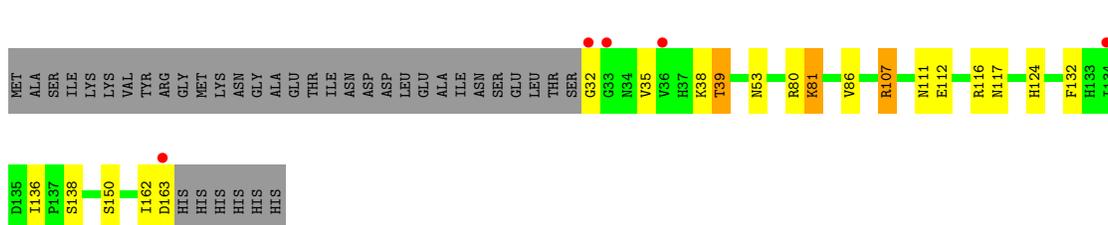
- Molecule 2: Designed Ankyrin Repeat Protein (DARPin) 20

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.65Å 80.44Å 182.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.10 19.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.89-2.10) 97.0 (19.89-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.09Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.4_56)	Depositor
R, R_{free}	0.208 , 0.243 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, \ < L^2 > = 0.32$	Xtriage
Outliers	0 of 39881 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4379	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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	0.62	0/1071	0.82	2/1456 (0.1%)
1	B	0.61	0/1001	0.79	2/1361 (0.1%)
1	C	0.63	0/1016	0.85	2/1377 (0.1%)
2	D	0.56	0/941	0.73	0/1273
All	All	0.61	0/4029	0.80	6/5467 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	HIS	N-CA-CB	7.91	124.84	110.60
1	A	133	HIS	N-CA-CB	6.47	122.25	110.60
1	B	146	GLY	N-CA-C	-5.99	98.13	113.10
1	C	81[A]	LYS	CB-CA-C	-5.78	98.83	110.40
1	C	81[B]	LYS	CB-CA-C	-5.78	98.83	110.40
1	A	168	HIS	N-CA-C	5.72	126.44	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1035	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	977	0	0	21	0
1	C	989	0	0	19	0
2	D	932	0	0	12	0
3	A	158	0	0	4	0
3	B	93	0	0	8	0
3	C	107	0	0	5	0
3	D	88	0	0	3	0
All	All	4379	0	0	61	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 16.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:81[A]:LYS:NZ	1:C:112:GLU:CG	1.97	1.28
1:C:81[A]:LYS:NZ	1:C:112:GLU:O	2.03	0.91
1:A:169:HIS:CD2	3:A:429:HOH:O	2.33	0.81
1:B:162:ILE:CG2	3:B:405:HOH:O	2.35	0.75
1:A:167:HIS:O	1:A:168:HIS:CB	2.36	0.74
1:B:35:VAL:O	1:B:37:HIS:CE1	2.41	0.74
1:C:81[A]:LYS:NZ	1:C:112:GLU:CB	2.51	0.74
2:D:45:LYS:NZ	3:D:283:HOH:O	2.20	0.73
2:D:112:PHE:N	2:D:112:PHE:CD1	2.56	0.71
1:C:81[A]:LYS:NZ	1:C:112:GLU:C	2.44	0.71
1:B:139[B]:SER:OG	3:B:421:HOH:O	2.09	0.69
1:A:84:THR:OG1	1:B:82:LYS:NZ	2.26	0.68
1:B:35:VAL:O	1:B:37:HIS:ND1	2.27	0.67
1:C:116:ARG:NH1	1:C:117:ASN:OD1	2.28	0.67
1:B:107:ARG:CG	1:B:107:ARG:NH1	2.59	0.66
1:C:162:ILE:O	1:C:163:ASP:C	2.35	0.65
1:C:81[A]:LYS:CE	1:C:112:GLU:CG	2.75	0.64
1:B:40:GLY:N	3:B:199:HOH:O	2.32	0.62
2:D:117:PHE:CE1	2:D:133:GLN:OE1	2.52	0.62
1:B:64[A]:THR:CG2	3:B:441:HOH:O	2.48	0.61
2:D:45:LYS:N	2:D:45:LYS:CD	2.64	0.60
1:A:45:ALA:N	1:B:38:LYS:O	2.33	0.60
1:C:32:GLY:N	3:C:271:HOH:O	2.32	0.60
1:B:59:SER:OG	1:C:53:ASN:OD1	2.20	0.60
2:D:12:SER:N	3:D:251:HOH:O	2.35	0.59
1:C:80:ARG:CZ	3:C:407:HOH:O	2.51	0.59
1:A:115:PRO:CD	1:A:136[A]:ILE:CD1	2.82	0.57
1:C:162:ILE:CG2	1:C:163:ASP:N	2.66	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:LEU:N	3:B:194:HOH:O	2.39	0.55
1:A:124:HIS:CE1	1:A:125:MET:O	2.60	0.55
2:D:110:ASP:OD1	2:D:110:ASP:C	2.45	0.55
1:B:34:ASN:ND2	1:C:39:THR:OG1	2.41	0.54
1:A:40:GLY:N	3:A:252:HOH:O	2.41	0.53
1:B:133:HIS:ND1	1:C:124:HIS:CD2	2.77	0.52
2:D:134:LYS:CG	2:D:135:LEU:N	2.74	0.51
1:A:62:LEU:N	3:A:254:HOH:O	2.42	0.51
1:B:101:ASN:ND2	3:B:272:HOH:O	2.42	0.51
1:C:107[A]:ARG:CG	1:C:107[A]:ARG:NH2	2.76	0.49
1:A:64[A]:THR:CG2	1:A:65:LYS:N	2.75	0.48
2:D:123:ASN:ND2	2:D:123:ASN:C	2.67	0.48
1:A:168:HIS:C	1:A:168:HIS:ND1	2.68	0.46
1:B:64[A]:THR:CG2	1:B:65:LYS:N	2.78	0.46
1:A:37:HIS:CD2	1:A:42:GLU:OE2	2.70	0.45
1:B:68:SER:N	3:B:203:HOH:O	2.49	0.45
1:B:38:LYS:NZ	3:B:323:HOH:O	2.50	0.44
1:A:45:ALA:O	1:A:48:LYS:NZ	2.51	0.43
1:C:107[A]:ARG:NH1	3:C:174:HOH:O	2.50	0.43
1:C:111:ASN:N	3:C:188:HOH:O	2.52	0.43
2:D:77:ASP:OD2	2:D:81:GLU:OE1	2.37	0.42
1:B:136[B]:ILE:O	1:B:136[B]:ILE:CG2	2.67	0.42
1:B:67:TRP:CG	1:B:68:SER:N	2.87	0.42
1:C:86:VAL:CG2	1:C:162:ILE:CD1	2.98	0.42
1:B:162:ILE:O	1:B:163:ASP:CB	2.68	0.42
2:D:106:VAL:O	3:D:169:HOH:O	2.22	0.41
1:A:116:ARG:NH1	1:A:165:HIS:CE1	2.89	0.41
1:B:88:TYR:C	1:B:88:TYR:CD2	2.93	0.41
1:C:162:ILE:CG2	3:C:438:HOH:O	2.69	0.41
2:D:49:THR:OG1	2:D:52:HIS:ND1	2.54	0.40
1:A:164:HIS:N	3:A:185:HOH:O	2.54	0.40
2:D:129:ALA:O	2:D:130:GLU:C	2.59	0.40
1:C:132:PHE:C	1:C:132:PHE:CD1	2.94	0.40

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	138/169 (82%)	134 (97%)	2 (1%)	2 (1%)	16	9
1	B	131/169 (78%)	125 (95%)	6 (5%)	0	100	100
1	C	133/169 (79%)	126 (95%)	7 (5%)	0	100	100
2	D	122/136 (90%)	115 (94%)	7 (6%)	0	100	100
All	All	524/643 (82%)	500 (95%)	22 (4%)	2 (0%)	43	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	137	PRO

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	116/139 (84%)	109 (94%)	7 (6%)	27	22
1	B	110/139 (79%)	103 (94%)	7 (6%)	25	20
1	C	110/139 (79%)	102 (93%)	8 (7%)	20	15
2	D	98/108 (91%)	85 (87%)	13 (13%)	6	3
All	All	434/525 (83%)	399 (92%)	35 (8%)	19	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	64[A]	THR
1	A	64[B]	THR
1	A	107	ARG
1	A	116	ARG
1	A	136[A]	ILE
1	A	136[B]	ILE

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Mol	Chain	Res	Type
1	B	34	ASN
1	B	89	SER
1	B	93	GLU
1	B	96	SER
1	B	101	ASN
1	B	102	SER
1	B	107	ARG
1	C	35	VAL
1	C	38	LYS
1	C	39	THR
1	C	107[A]	ARG
1	C	107[B]	ARG
1	C	136	ILE
1	C	138	SER
1	C	150	SER
2	D	13	ASP
2	D	32	ILE
2	D	40	VAL
2	D	45	LYS
2	D	68	LYS
2	D	86	LEU
2	D	106	VAL
2	D	109	GLN
2	D	112	PHE
2	D	114	LYS
2	D	123	ASN
2	D	131	ILE
2	D	134	LYS

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 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 ⓘ

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, 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(Å²)	Q<0.9
1	A	137/169 (81%)	-0.34	4 (2%)	49	54	27, 37, 70, 114	0
1	B	130/169 (76%)	-0.15	0	100	100	32, 51, 75, 105	0
1	C	132/169 (78%)	-0.22	5 (3%)	38	43	32, 47, 75, 103	0
2	D	124/136 (91%)	-0.04	4 (3%)	45	50	23, 47, 81, 137	1 (0%)
All	All	523/643 (81%)	-0.19	13 (2%)	54	59	23, 46, 77, 137	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	135	LEU	4.9
1	C	32	GLY	4.9
2	D	134	LYS	4.4
1	A	169	HIS	4.3
2	D	12	SER	3.9
1	A	33	GLY	2.7
1	A	168	HIS	2.7
1	C	33	GLY	2.6
1	C	163	ASP	2.5
1	A	167	HIS	2.4
1	C	36	VAL	2.2
1	C	134	ILE	2.1
2	D	112	PHE	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.