



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1R4K
Title : Solution Structure of the Drosophila Argonaute 1 PAZ Domain
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Deposited on : 2003-10-07

This is a Full wwPDB NMR Structure 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/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

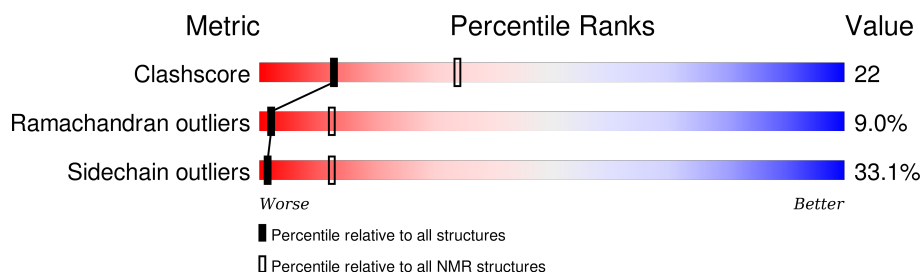
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	169	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2794 atoms, of which 1417 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Argonaute 1.

Mol	Chain	Residues	Atoms						Trace
1	A	168	Total	C	H	N	O	S	0
			2794	863	1417	255	246	13	

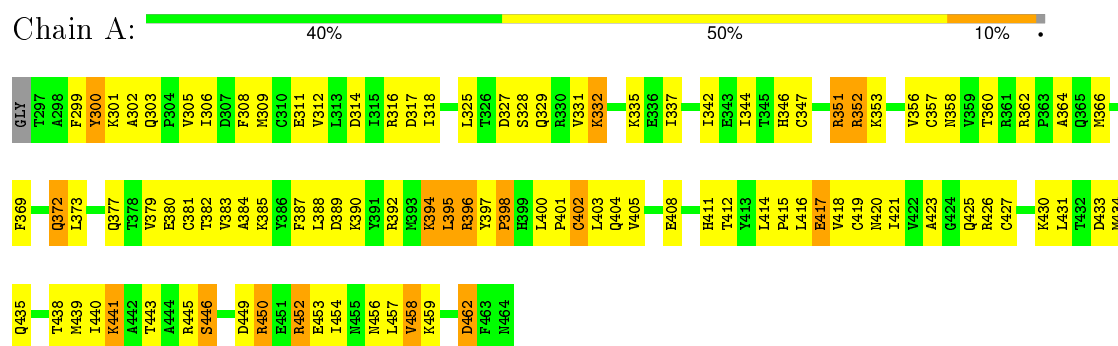
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLY	-	CLONING ARTIFACT	UNP Q9V6V6

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Argonaute 1



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.1
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1377	1417	1416	61
All	All	1377	1417	1416	61

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 22.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:342:ILE:HD11	1:A:405:VAL:HG11	0.84	1.49
1:A:412:THR:HG22	1:A:414:LEU:HD21	0.80	1.52
1:A:342:ILE:HD13	1:A:419:CYS:SG	0.77	2.19
1:A:306:ILE:HG23	1:A:318:ILE:HG12	0.77	1.57
1:A:342:ILE:CD1	1:A:405:VAL:HG11	0.72	2.12
1:A:346:HIS:HB3	1:A:418:VAL:HG22	0.72	1.60
1:A:344:ILE:HD11	1:A:352:ARG:HB2	0.67	1.67
1:A:369:PHE:CD1	1:A:383:VAL:HG23	0.67	2.24
1:A:346:HIS:CB	1:A:418:VAL:HG22	0.66	2.19
1:A:346:HIS:ND1	1:A:418:VAL:HG13	0.64	2.08
1:A:414:LEU:N	1:A:414:LEU:HD22	0.61	2.10
1:A:327:ASP:O	1:A:331:VAL:HG23	0.61	1.96
1:A:412:THR:CG2	1:A:414:LEU:HD21	0.60	2.25
1:A:458:VAL:O	1:A:458:VAL:HG22	0.60	1.96
1:A:412:THR:HG22	1:A:414:LEU:CD2	0.59	2.24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:383:VAL:O	1:A:384:ALA:HB3	0.58	1.99
1:A:364:ALA:O	1:A:384:ALA:HB3	0.57	2.00
1:A:397:TYR:N	1:A:398:PRO:CD	0.55	2.71
1:A:356:VAL:HA	1:A:405:VAL:HG12	0.53	1.80
1:A:416:LEU:HD22	1:A:416:LEU:N	0.53	2.18
1:A:364:ALA:HB3	1:A:398:PRO:HA	0.52	1.81
1:A:342:ILE:HG23	1:A:356:VAL:CG2	0.51	2.35
1:A:308:PHE:O	1:A:312:VAL:HG23	0.50	2.06
1:A:346:HIS:CD2	1:A:347:CYS:N	0.48	2.81
1:A:440:ILE:O	1:A:440:ILE:HG23	0.48	2.08
1:A:299:PHE:N	1:A:299:PHE:CD1	0.48	2.79
1:A:373:LEU:HD23	1:A:379:VAL:HB	0.48	1.86
1:A:342:ILE:CG2	1:A:356:VAL:CG2	0.48	2.92
1:A:414:LEU:CD2	1:A:414:LEU:N	0.48	2.76
1:A:373:LEU:CD2	1:A:373:LEU:N	0.47	2.77
1:A:416:LEU:N	1:A:416:LEU:CD2	0.47	2.78
1:A:372:GLN:C	1:A:373:LEU:HD22	0.47	2.30
1:A:299:PHE:O	1:A:299:PHE:CD2	0.46	2.69
1:A:394:LYS:O	1:A:396:ARG:N	0.46	2.47
1:A:325:LEU:HD12	1:A:401:PRO:CG	0.45	2.42
1:A:346:HIS:CG	1:A:347:CYS:N	0.45	2.84
1:A:344:ILE:HD11	1:A:352:ARG:CB	0.45	2.39
1:A:342:ILE:HG22	1:A:421:ILE:HD13	0.44	1.89
1:A:417:GLU:C	1:A:418:VAL:HG23	0.44	2.32
1:A:373:LEU:HD22	1:A:373:LEU:N	0.44	2.26
1:A:417:GLU:O	1:A:419:CYS:N	0.44	2.50
1:A:397:TYR:N	1:A:398:PRO:HD3	0.44	2.27
1:A:379:VAL:HG12	1:A:380:GLU:N	0.44	2.28
1:A:383:VAL:O	1:A:384:ALA:CB	0.43	2.66
1:A:360:THR:OG1	1:A:402:CYS:CB	0.43	2.67
1:A:417:GLU:O	1:A:418:VAL:CB	0.43	2.67
1:A:299:PHE:CB	1:A:426:ARG:NE	0.43	2.82
1:A:309:MET:CE	1:A:318:ILE:CD1	0.43	2.96
1:A:379:VAL:CG1	1:A:380:GLU:N	0.42	2.82
1:A:387:PHE:O	1:A:392:ARG:N	0.42	2.52
1:A:449:ASP:OD1	1:A:450:ARG:N	0.42	2.53
1:A:395:LEU:O	1:A:396:ARG:CB	0.41	2.67
1:A:405:VAL:HG23	1:A:412:THR:HB	0.41	1.93
1:A:344:ILE:CD1	1:A:352:ARG:CB	0.41	2.98
1:A:452:ARG:O	1:A:454:ILE:N	0.41	2.53
1:A:369:PHE:N	1:A:369:PHE:CD1	0.41	2.89
1:A:305:VAL:CG2	1:A:419:CYS:O	0.41	2.69

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:312:VAL:CG1	1:A:332:LYS:CD	0.41	2.98
1:A:300:TYR:HB3	1:A:425:GLN:CB	0.41	2.46
1:A:364:ALA:C	1:A:384:ALA:CB	0.41	2.89
1:A:458:VAL:O	1:A:458:VAL:CG2	0.40	2.68

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	166/169 (98%)	109 (66%)	42 (25%)	15 (9%)	2	12
All	All	166/169 (98%)	109 (66%)	42 (25%)	15 (9%)	2	12

All 15 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	456	ASN
1	A	417	GLU
1	A	423	ALA
1	A	351	ARG
1	A	398	PRO
1	A	459	LYS
1	A	337	ILE
1	A	415	PRO
1	A	458	VAL
1	A	441	LYS
1	A	314	ASP
1	A	457	LEU
1	A	446	SER
1	A	462	ASP
1	A	302	ALA

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	154/154 (100%)	103 (67%)	51 (33%)	1	12
All	All	154/154 (100%)	103 (67%)	51 (33%)	1	12

All 51 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	395	LEU
1	A	301	LYS
1	A	441	LYS
1	A	402	CYS
1	A	381	CYS
1	A	439	MET
1	A	450	ARG
1	A	452	ARG
1	A	362	ARG
1	A	316	ARG
1	A	443	THR
1	A	332	LYS
1	A	434	MET
1	A	427	CYS
1	A	404	GLN
1	A	435	GLN
1	A	431	LEU
1	A	403	LEU
1	A	390	LYS
1	A	358	ASN
1	A	388	LEU
1	A	382	THR
1	A	389	ASP
1	A	446	SER
1	A	411	HIS
1	A	372	GLN
1	A	385	LYS
1	A	400	LEU
1	A	300	TYR

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Mol	Chain	Res	Type
1	A	328	SER
1	A	357	CYS
1	A	445	ARG
1	A	353	LYS
1	A	352	ARG
1	A	394	LYS
1	A	433	ASP
1	A	408	GLU
1	A	438	THR
1	A	420	ASN
1	A	311	GLU
1	A	396	ARG
1	A	335	LYS
1	A	366	MET
1	A	303	GLN
1	A	351	ARG
1	A	462	ASP
1	A	377	GLN
1	A	430	LYS
1	A	317	ASP
1	A	453	GLU
1	A	329	GLN

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided