Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 04:57 PM EDT

PDB ID	:	2KIZ
Title	:	Solution structure of Arkadia RING-H2 finger domain
Authors	:	Kandias, N.G.; Chasapis, C.T.; Bentrop, D.; Episkopou, V.; Spyroulias, G.A.
Deposited on	:	2009-05-13

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

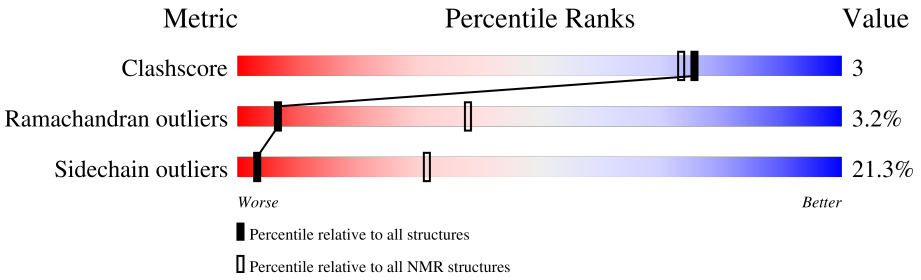
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	69	43% 20% 36%

2 Ensemble composition and analysis (i)

This entry contains 31 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:14-A:24, A:29-A:61 (44)	0.36	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 13, 15, 16, 17, 20, 21, 22, 23, 24, 25, 27, 30, 31
2	5, 18, 26, 29
3	19, 28
Single-model clusters	12; 14

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1079 atoms, of which 527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase Arkadia.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1077	336	527	92	114	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q6ZNA4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

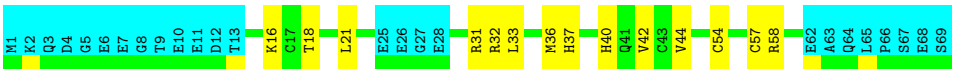
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: E3 ubiquitin-protein ligase Arkadia

Chain A: 43% 20% 36%



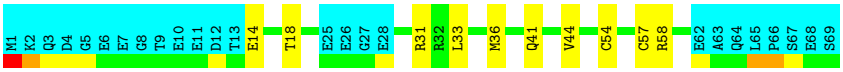
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: E3 ubiquitin-protein ligase Arkadia

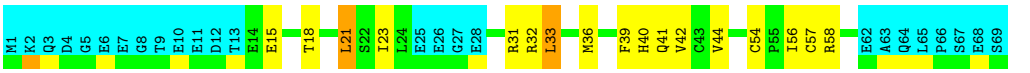
Chain A: 49% 14% 36%



4.2.2 Score per residue for model 2

• Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 39% 22% • 36%



4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 46% 16% • 36%

M1 K2 Q3 D4 G5 E6 E7 G8 T9 E10 E11 D12 T13 T18 L21 E25 E26 G27 E28 R31 R32 L33 M36 H37 V42 C43 V44 C54 C57 R58 E62 A63 Q64 L65 P66 S67 E68 S69

4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 45% 17% • 36%

M1 K2 Q3 D4 G5 E6 E7 G8 T9 E10 E11 D12 T13 L21 S22 I23 L24 E25 E26 G27 E28 D29 V30 R31 R32 L33 M36 H37 V42 C43 V44 C54 C57 R58 E62 A63 Q64 L65 P66 S67 E68 S69

4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 39% 20% • 36%

M1 K2 Q3 D4 G5 E6 E7 G8 T9 E10 E11 D12 T13 E14 E15 K16 C17 T18 E25 E26 G27 E28 D29 V30 R31 R32 L33 M36 H37 H40 Q41 V42 C43 V44 N51 K52 K53 C54 C57 R58 E62 A63 Q64 L65 P66 S67 E68 S69

4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 42% 20% • 36%

M1 K2 Q3 D4 G5 E6 E7 G8 T9 E10 E11 D12 T13 T18 I23 L24 E25 E26 G27 E28 R31 R32 L33 M36 H37 L38 F39 V42 C43 V44 C54 P55 I56 C57 R58 V59 D60 I61 E62 A63 Q64 L65 P66 S67 E68 S69

4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 43% 19% • 36%

M1 K2 Q3 D4 G5 E6 E7 G8 T9 E10 E11 D12 T13 T18 L21 E25 E26 G27 E28 D29 V30 R31 R32 L33 M36 H37 V42 C43 V44 T50 K53 C54 C57 R58 E62 A63 Q64 L65 P66 S67 E68 S69

4.2.8 Score per residue for model 8

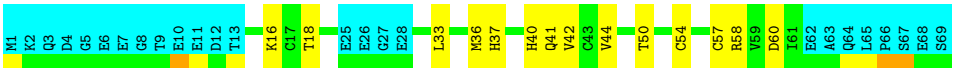
- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 49% 14% 36%

4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

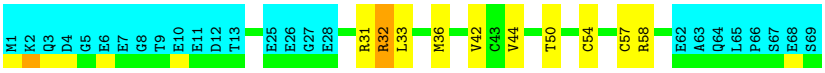
Chain A: 43% 20% 36%



4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

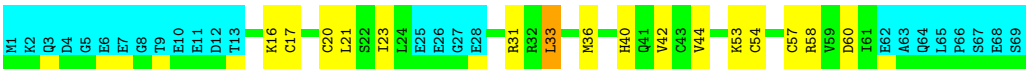
Chain A: 49% 13% • 36%



4.2.11 Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

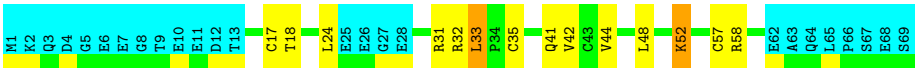
Chain A: 41% 22% • 36%



4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

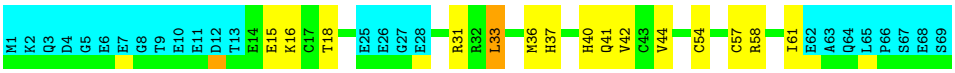
Chain A: 43% 17% • 36%



4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

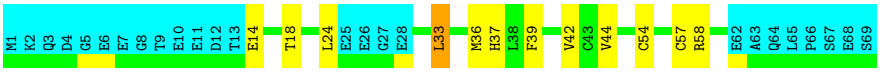
Chain A: 42% 20% • 36%



4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

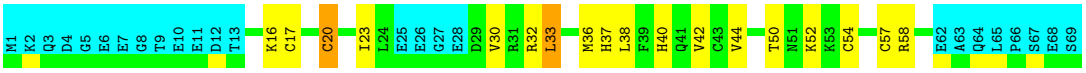
Chain A: 46% 16% • 36%



4.2.15 Score per residue for model 15

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

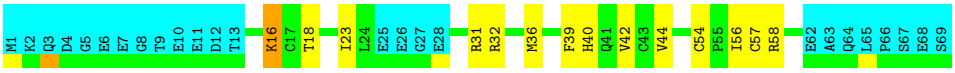
Chain A: 38% 23% • 36%



4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

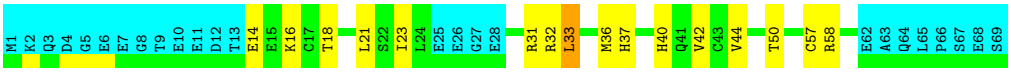
Chain A: 43% 19% • 36%



4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 41% 22% • 36%



4.2.18 Score per residue for model 18

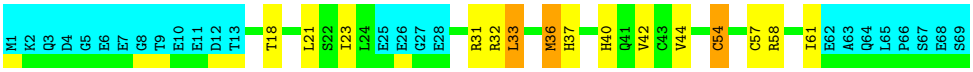
- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 36% 26% • 36%

4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

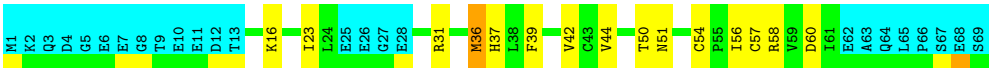
Chain A: 42% 17% • 36%



4.2.20 Score per residue for model 20

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

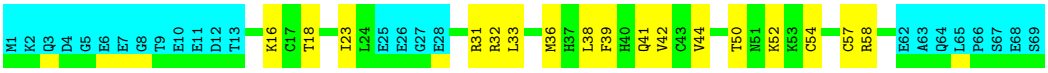
Chain A: 42% 20% • 36%



4.2.21 Score per residue for model 21

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 39% 25% 36%



4.2.22 Score per residue for model 22

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 49% 13% • 36%

4.2.23 Score per residue for model 23

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 46% 16% • 36%

4.2.24 Score per residue for model 24

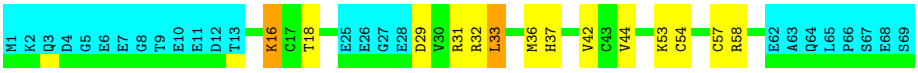
- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 38% 25% • 36%

4.2.25 Score per residue for model 25

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

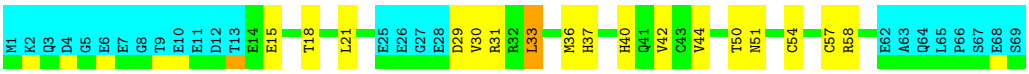
Chain A: 43% 17% • 36%



4.2.26 Score per residue for model 26

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 39% 23% • 36%



4.2.27 Score per residue for model 27

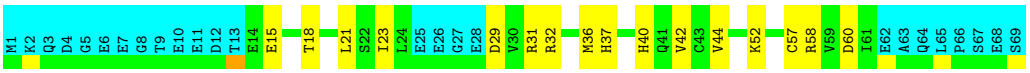
- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 48% 14% • 36%

4.2.28 Score per residue for model 28

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

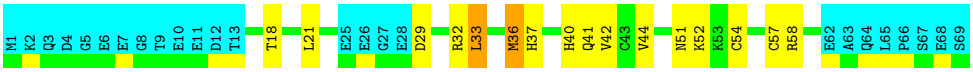
Chain A: 41% 23% 36%



4.2.29 Score per residue for model 29

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 41% 20% • 36%



4.2.30 Score per residue for model 30

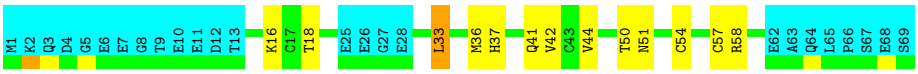
- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 41% 23% 36%

4.2.31 Score per residue for model 31

- Molecule 1: E3 ubiquitin-protein ligase Arkadia

Chain A: 45% 17% • 36%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 31 calculated structures, 31 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
AMBER 4.1	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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 (average) 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	0.51±0.01	0±0/366 (0.0± 0.0%)	0.94±0.04	0±0/496 (0.0± 0.1%)
All	All	0.51	0/11346 (0.0%)	0.94	5/15376 (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	Planarity
1	A	0.0±0.0	0.4±0.5
All	All	0	13

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	57	CYS	CA-CB-SG	7.80	128.04	114.00	28	4
1	A	32	ARG	CD-NE-CZ	5.39	131.15	123.60	10	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	40	HIS	Sidechain	12
1	A	31	ARG	Sidechain	1

6.2 Too-close contacts (i)

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	359	369	369	2±1
All	All	11191	11439	11439	70

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD12	1:A:33:LEU:H	0.67	1.48	12	3
1:A:54:CYS:CB	1:A:57:CYS:SG	0.63	2.87	25	26
1:A:33:LEU:HD12	1:A:37:HIS:O	0.59	1.97	23	15
1:A:33:LEU:HD22	1:A:37:HIS:O	0.50	2.07	13	2
1:A:33:LEU:HD22	1:A:33:LEU:H	0.48	1.68	13	2
1:A:17:CYS:CB	1:A:20:CYS:SG	0.48	3.00	11	2
1:A:38:LEU:HD13	1:A:39:PHE:N	0.47	2.25	21	1
1:A:30:VAL:HG12	1:A:40:HIS:HA	0.47	1.87	26	2
1:A:54:CYS:SG	1:A:55:PRO:HD2	0.45	2.52	18	1
1:A:61:ILE:HD12	1:A:61:ILE:H	0.45	1.70	19	3
1:A:33:LEU:HD11	1:A:39:PHE:CD2	0.44	2.47	14	1
1:A:48:LEU:O	1:A:52:LYS:CE	0.44	2.66	12	1
1:A:39:PHE:CZ	1:A:56:ILE:HD11	0.43	2.48	2	4
1:A:56:ILE:HD12	1:A:56:ILE:H	0.43	1.74	16	3
1:A:38:LEU:HD23	1:A:39:PHE:N	0.42	2.29	6	1
1:A:15:GLU:OE2	1:A:16:LYS:HE2	0.42	2.14	13	1
1:A:14:GLU:CD	1:A:24:LEU:HD12	0.42	2.35	14	1
1:A:14:GLU:CB	1:A:38:LEU:HD22	0.42	2.45	18	1

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	44/69 (64%)	36±2 (81±4%)	7±2 (16±4%)	1±1 (3±1%)	7 38
All	All	1364/2139 (64%)	1102 (81%)	219 (16%)	43 (3%)	7 38

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	MET	30
1	A	16	LYS	8
1	A	21	LEU	2
1	A	35	CYS	1
1	A	50	THR	1
1	A	52	LYS	1

6.3.2 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 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	44/65 (68%)	35±2 (79±5%)	9±2 (21±5%)	3 31
All	All	1364/2015 (68%)	1074 (79%)	290 (21%)	3 31

All 27 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	44	VAL	31
1	A	58	ARG	31
1	A	42	VAL	30
1	A	18	THR	24
1	A	33	LEU	24
1	A	31	ARG	22
1	A	32	ARG	16
1	A	21	LEU	14
1	A	23	ILE	14
1	A	41	GLN	11
1	A	29	ASP	11
1	A	50	THR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	16	LYS	8
1	A	52	LYS	7
1	A	51	ASN	6
1	A	60	ASP	6
1	A	15	GLU	5
1	A	36	MET	5
1	A	53	LYS	3
1	A	54	CYS	2
1	A	14	GLU	2
1	A	40	HIS	2
1	A	55	PRO	1
1	A	17	CYS	1
1	A	24	LEU	1
1	A	20	CYS	1
1	A	22	SER	1

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

No chemical shift data were provided