Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:19 am BST

PDB ID	:	4KC9
Title	:	Structure of HHARI, a RING-IBR-RING ubiquitin ligase: autoinhibition of an Ariadne-family E3 and insights into ligation mechanism
Authors	:	Duda, D.M.; Olszewski, J.L.; Schulman, B.A.
Deposited on	:	2013-04-24
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

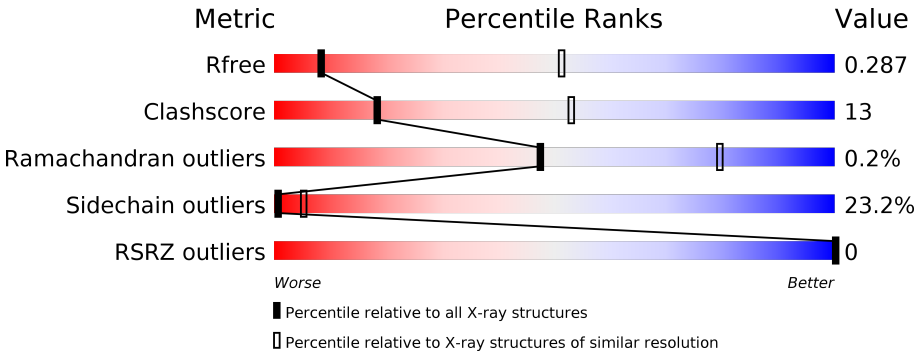
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 respectively. 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	559	47% 21% 6% 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3139 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 E3 ubiquitin-protein ligase ARIH1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	Se	0	0	0
			3133	1962	548	582	29	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Y4X5
A	0	SER	-	EXPRESSION TAG	UNP Q9Y4X5

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

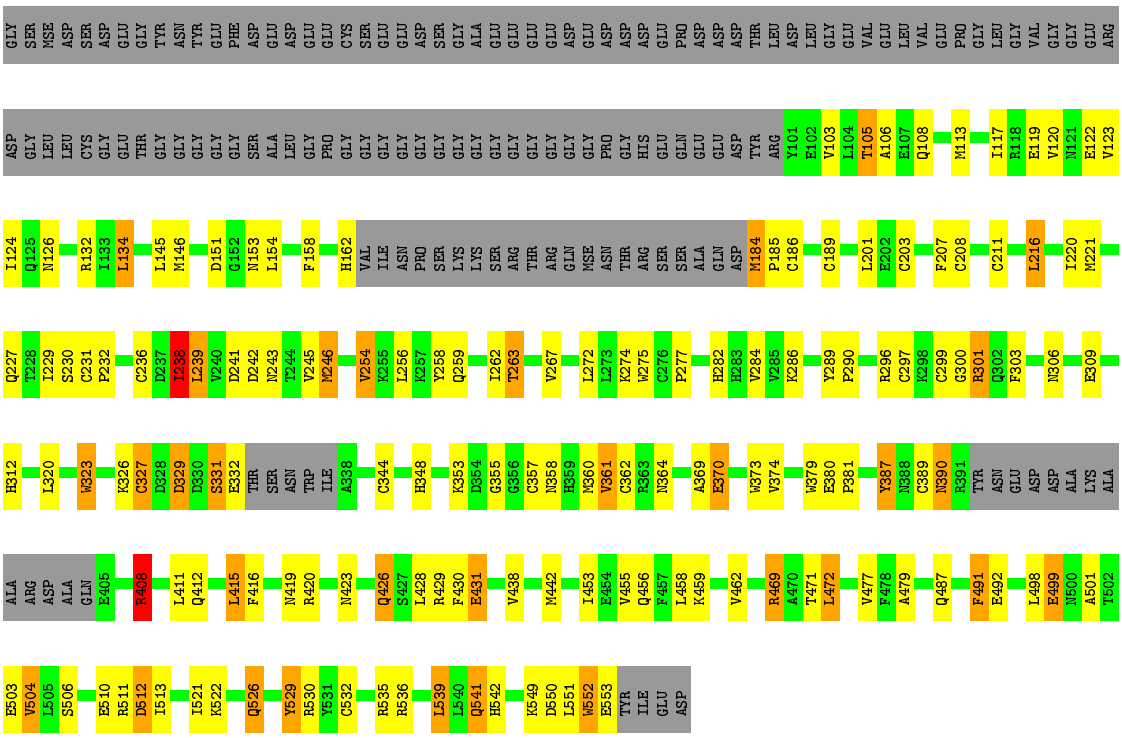
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Zn	0	0
			6	6		

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 the various outlier classes 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: E3 ubiquitin-protein ligase ARIH1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	96.13Å 96.13Å 151.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.47 – 3.60 36.47 – 3.60	Depositor EDS
% Data completeness (in resolution range)	90.6 (36.47-3.60) 90.4 (36.47-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	14.60 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.270 , 0.302 0.256 , 0.287	Depositor DCC
R_{free} test set	850 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	3139	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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 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	0.28	0/3191	0.56	2/4323 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	238	ILE	N-CA-C	-5.20	96.97	111.00

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	3133	0	2737	78	0
2	A	6	0	0	0	0
All	All	3139	0	2737	78	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 13.

All (78) 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:203:CYS:HB2	1:A:236:CYS:SG	2.00	1.01
1:A:231:CYS:SG	1:A:236:CYS:HB3	2.19	0.83
1:A:207:PHE:HE2	1:A:232:PRO:HB2	1.57	0.69
1:A:299:CYS:HB3	1:A:301:ARG:H	1.63	0.64
1:A:134:LEU:HD23	1:A:145:LEU:HD11	1.81	0.63
1:A:442:MSE:HE1	1:A:459:LYS:HB2	1.81	0.62
1:A:299:CYS:N	1:A:300:GLY:HA2	2.15	0.61
1:A:512:ASP:OD1	1:A:512:ASP:N	2.33	0.61
1:A:312:HIS:O	1:A:312:HIS:ND1	2.27	0.61
1:A:158:PHE:O	1:A:162:HIS:N	2.34	0.60
1:A:296:ARG:NH1	1:A:300:GLY:O	2.35	0.60
1:A:184:MSE:HB3	1:A:185:PRO:HD3	1.84	0.60
1:A:381:PRO:HB2	1:A:387:TYR:HD1	1.68	0.59
1:A:431:GLU:OE2	1:A:506:SER:OG	2.18	0.58
1:A:122:GLU:OE1	1:A:122:GLU:N	2.37	0.57
1:A:105:THR:OG1	1:A:106:ALA:N	2.38	0.56
1:A:230:SER:HA	1:A:239:LEU:HA	1.87	0.56
1:A:487:GLN:HG3	1:A:551:LEU:HD13	1.87	0.56
1:A:408:ARG:HH21	1:A:408:ARG:CG	2.19	0.56
1:A:510:GLU:HB3	1:A:511:ARG:HG3	1.88	0.55
1:A:472:LEU:HD13	1:A:498:LEU:HD23	1.89	0.55
1:A:361:VAL:HA	1:A:370:GLU:H	1.71	0.54
1:A:299:CYS:HB3	1:A:301:ARG:N	2.22	0.54
1:A:105:THR:HG23	1:A:108:GLN:HB2	1.90	0.53
1:A:344:CYS:O	1:A:348:HIS:HA	2.08	0.53
1:A:259:GLN:O	1:A:263:THR:HB	2.08	0.52
1:A:355:GLY:H	1:A:430:PHE:HD1	1.58	0.52
1:A:369:ALA:HA	1:A:370:GLU:HB3	1.93	0.51
1:A:390:ASN:N	1:A:390:ASN:OD1	2.44	0.51
1:A:522:LYS:O	1:A:526:GLN:NE2	2.43	0.51
1:A:256:LEU:HB3	1:A:282:HIS:ND1	2.26	0.50
1:A:236:CYS:O	1:A:238:ILE:HG22	2.12	0.50
1:A:113:MSE:HE2	1:A:117:ILE:HD11	1.93	0.50
1:A:241:ASP:N	1:A:241:ASP:OD2	2.38	0.49
1:A:415:LEU:O	1:A:419:ASN:HB2	2.13	0.49
1:A:220:ILE:HD13	1:A:254:VAL:HG23	1.95	0.48
1:A:256:LEU:HB3	1:A:282:HIS:CE1	2.48	0.48
1:A:323:TRP:O	1:A:327:CYS:N	2.28	0.48
1:A:208:CYS:HB2	1:A:211:CYS:SG	2.53	0.48
1:A:498:LEU:HD22	1:A:539:LEU:HD12	1.96	0.47
1:A:122:GLU:HA	1:A:123:VAL:HA	1.56	0.47
1:A:379:TRP:HA	1:A:380:GLU:HA	1.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:CYS:O	1:A:420:ARG:NH2	2.48	0.47
1:A:529:TYR:HA	1:A:532:CYS:HB2	1.97	0.47
1:A:499:GLU:O	1:A:503:GLU:HG2	2.14	0.46
1:A:320:LEU:HA	1:A:477:VAL:HG11	1.97	0.46
1:A:124:ILE:C	1:A:126:ASN:H	2.19	0.46
1:A:331:SER:O	1:A:332:GLU:HG2	2.15	0.46
1:A:323:TRP:CE3	1:A:477:VAL:HG22	2.50	0.46
1:A:221:MSE:HE2	1:A:254:VAL:HB	1.98	0.45
1:A:301:ARG:HH11	1:A:301:ARG:HB2	1.82	0.45
1:A:472:LEU:HD21	1:A:499:GLU:HG2	1.98	0.44
1:A:358:ASN:ND2	1:A:503:GLU:OE1	2.38	0.44
1:A:132:ARG:HH12	1:A:227:GLN:HB3	1.82	0.44
1:A:526:GLN:HA	1:A:529:TYR:CE2	2.52	0.44
1:A:487:GLN:HG3	1:A:551:LEU:HB3	1.99	0.44
1:A:353:LYS:HB2	1:A:373:TRP:CH2	2.52	0.44
1:A:258:TYR:CE1	1:A:262:ILE:HD13	2.53	0.44
1:A:243:ASN:HA	1:A:246:MSE:HG3	1.99	0.43
1:A:272:LEU:O	1:A:286:LYS:HA	2.19	0.43
1:A:369:ALA:HA	1:A:370:GLU:CB	2.46	0.43
1:A:479:ALA:HB2	1:A:491:PHE:CZ	2.54	0.43
1:A:479:ALA:HB2	1:A:491:PHE:HZ	1.83	0.43
1:A:289:TYR:HA	1:A:290:PRO:HD3	1.80	0.42
1:A:358:ASN:HB3	1:A:373:TRP:HB3	2.01	0.42
1:A:541:GLN:HB2	1:A:541:GLN:HE21	1.52	0.42
1:A:426:GLN:HA	1:A:429:ARG:HD2	2.01	0.42
1:A:501:ALA:O	1:A:504:VAL:HG12	2.19	0.42
1:A:186:CYS:HB3	1:A:189:CYS:O	2.19	0.41
1:A:552:TRP:O	1:A:553:GLU:HB2	2.20	0.41
1:A:277:PRO:HG3	1:A:303:PHE:CG	2.55	0.41
1:A:263:THR:HG22	1:A:275:TRP:CZ2	2.56	0.41
1:A:132:ARG:NH1	1:A:227:GLN:HB3	2.36	0.41
1:A:274:LYS:NZ	1:A:306:ASN:O	2.34	0.41
1:A:326:LYS:O	1:A:329:ASP:HB3	2.21	0.41
1:A:428:LEU:HD23	1:A:469:ARG:HB3	2.03	0.40
1:A:472:LEU:HD21	1:A:499:GLU:HA	2.03	0.40
1:A:216:LEU:O	1:A:220:ILE:HG22	2.21	0.40

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	406/559 (73%)	376 (93%)	29 (7%)	1 (0%)	47 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ILE

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	310/473 (66%)	238 (77%)	72 (23%)	1 5

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	105	THR
1	A	119	GLU
1	A	120	VAL
1	A	134	LEU
1	A	146	MSE
1	A	151	ASP
1	A	153	ASN
1	A	154	LEU
1	A	184	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	LEU
1	A	216	LEU
1	A	238	ILE
1	A	239	LEU
1	A	242	ASP
1	A	245	VAL
1	A	246	MSE
1	A	254	VAL
1	A	263	THR
1	A	267	VAL
1	A	284	VAL
1	A	297	CYS
1	A	301	ARG
1	A	309	GLU
1	A	323	TRP
1	A	327	CYS
1	A	329	ASP
1	A	331	SER
1	A	357	CYS
1	A	360	MSE
1	A	361	VAL
1	A	362	CYS
1	A	364	ASN
1	A	370	GLU
1	A	374	VAL
1	A	387	TYR
1	A	390	ASN
1	A	408	ARG
1	A	411	LEU
1	A	412	GLN
1	A	415	LEU
1	A	416	PHE
1	A	423	ASN
1	A	426	GLN
1	A	431	GLU
1	A	438	VAL
1	A	453	ILE
1	A	455	VAL
1	A	456	GLN
1	A	458	LEU
1	A	462	VAL
1	A	469	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	471	THR
1	A	472	LEU
1	A	491	PHE
1	A	492	GLU
1	A	499	GLU
1	A	504	VAL
1	A	512	ASP
1	A	513	ILE
1	A	521	ILE
1	A	526	GLN
1	A	529	TYR
1	A	530	ARG
1	A	535	ARG
1	A	536	ARG
1	A	539	LEU
1	A	541	GLN
1	A	542	HIS
1	A	549	LYS
1	A	550	ASP
1	A	552	TRP

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	111	GLN
1	A	448	HIS
1	A	541	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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.

No monomer is involved in short contacts.

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	400/559 (71%)	-0.49	0 100 100	28, 86, 136, 165	0

There are no RSRZ outliers to report.

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	606	1/1	0.97	0.08	113,113,113,113	0
2	ZN	A	604	1/1	0.97	0.07	124,124,124,124	0
2	ZN	A	605	1/1	0.98	0.14	90,90,90,90	0
2	ZN	A	601	1/1	0.99	0.08	99,99,99,99	0
2	ZN	A	602	1/1	0.99	0.15	81,81,81,81	0
2	ZN	A	603	1/1	1.00	0.10	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.