



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4KBL / pdb_00004kbl
Title : Structure of HHARI, a RING-IBR-RING ubiquitin ligase: autoinhibition of an Ariadne-family E3 and insights into ligation mechanism
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Deposited on : 2013-04-23
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

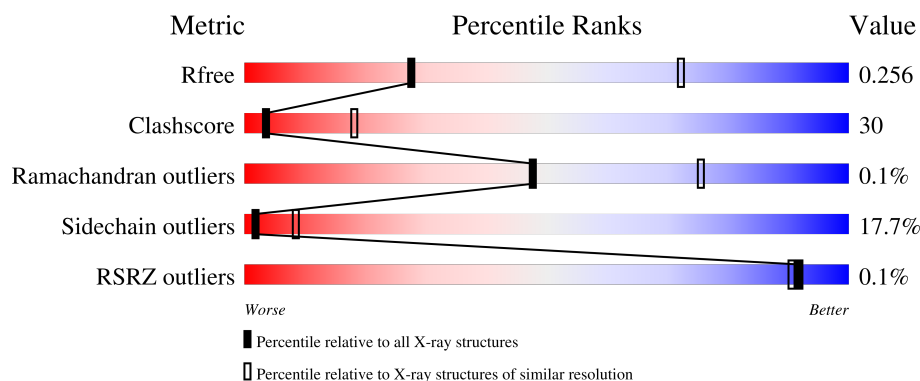
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

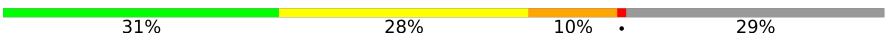
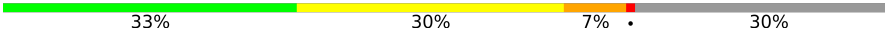
The reported resolution of this entry is 3.30 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of 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 $\leq 5\%$. 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	
1	B	559	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6581 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	395	Total	C	N	O	S	0	0	0
			3286	2084	579	582	41			
1	B	394	Total	C	N	O	S	0	0	0
			3283	2082	577	584	40			

There are 4 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
B	-1	GLY	-	expression tag	UNP Q9Y4X5
B	0	SER	-	expression tag	UNP Q9Y4X5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

L498	E499	F503	F504	L505	Y508	L509	E510	R511	D512	S513	S514	Q515	D516	I521	Q526	Y529	R530	E533	S534	R535	R536	R537	V538	L539	V543	H544	E545	E548	Y549	D550	L551	W552	E553	TYR	ILE	GLU	ASP																			
S407	L411	Q412	R413	Y414	L415	F416	R420	Y421	M425	Q426	S427	L428	R429	F430	E431	V438	M442	GLU	E443	NET	GLN	GLN	HIS	ASN	MET	SER	W452	I453	E454	K460	A461	Y462	D463	V464	L465	R469	A470	A471	T471	M473	Y474	T475	Y476	V477	F478	A479	F480	Y481	L482	T490	F491					
SER	GLU	THR	SER	ASN	TRP	I337	A338	A339	N340	T341	P345	K346	C347	T350	K353	D354	G355	H359	M360	V361	C367	E370	F371	C372	C375	L376	W379	E380	P381	H382	Y387	N388	C389	Y392	N393	E394	ASP	ASP	ALA	LYS	ALA	ALA	ALA	ARG	ARG	ASP	ALA	GLN	GLU	R406						
Q258	Y259	H260	L261	I262	T263	E268	C269	N270	R271	W275	A278	C281	V284	V285	R286	V287	Q288	Y289	K293	P294	V295	R296	C297	K298	C299	G300	R301	Q302	F303	C304	F305	E309	N310	W311	R312	D313	P314	V315	K316	C317	K318	W319	K322	W323	I324	K325	K326	C327	D328	ASP	ASP					
L191	N192	Y197	F198	L201	E202	H205	K206	F207	C208	M209	Q210	C211	W212	S213	E214	Y215	L216	T217	T218	K219	I220	M221	E222	GLU	GLY	M225	T228	I229	S230	C231	P232	A233	R234	G235	C236	S237	I238	L239	V240	D241	T244	V245	M246	R247	L248	I249	T250	D251	V254	K255	I256	K257				
I124	A128	T129	I130	I133	L134	L135	S136	H137	F138	K142	L145	M146	E147	R148	Y149	D151	G152	ASN	LEU	GLU	LYS	LEU	PHE	GLU	ALA	GLU	CYS	HIS	VAL	ILE	ASN	PRO	SER	LYS	LYS	SER	ARG	THR	THR	ARG	GLN	MET	ASN	THR	ARG	SER	SER	ALA	GLN	ASP	ASP	P185	C186	Q187	I188	C189

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	147.40Å 147.40Å 86.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 3.30 46.61 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (46.61-3.30) 97.8 (46.61-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.231 , 0.283 (Not available) , 0.256	Depositor DCC
R_{free} test set	2162 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	125.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 131.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6581	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.44	0/3366	1.08	33/4538 (0.7%)
1	B	0.43	0/3362	1.02	19/4531 (0.4%)
All	All	0.43	0/6728	1.05	52/9069 (0.6%)

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 outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	CYS	CA-C-N	11.43	132.35	119.32
1	B	231	CYS	C-N-CA	11.43	132.35	119.32
1	A	312	HIS	N-CA-C	9.99	124.11	112.72
1	A	276	CYS	CA-C-N	9.64	130.31	119.32
1	A	276	CYS	C-N-CA	9.64	130.31	119.32

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	312	HIS	Peptide
1	A	378	PRO	Peptide
1	A	456	GLN	Peptide
1	B	312	HIS	Peptide

5.2 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 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	3286	0	3180	203	0
1	B	3283	0	3172	192	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	6581	0	6352	382	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 30.

The worst 5 of 382 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:B:220:ILE:HD11	1:B:254:VAL:HG13	1.30	1.05
1:A:441:LYS:NZ	1:A:514:SER:OG	1.91	1.03
1:A:116:CYS:SG	1:A:142:LYS:NZ	2.36	0.98
1:B:213:SER:O	1:B:217:THR:OG1	1.83	0.96
1:B:100:ARG:HE	1:B:288:GLN:HG3	1.27	0.95

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	385/559 (69%)	363 (94%)	21 (6%)	1 (0%)	36	65
1	B	382/559 (68%)	361 (94%)	21 (6%)	0	100	100
All	All	767/1118 (69%)	724 (94%)	42 (6%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	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	364/489 (74%)	299 (82%)	65 (18%)	2	8
1	B	364/489 (74%)	300 (82%)	64 (18%)	2	9
All	All	728/978 (74%)	599 (82%)	129 (18%)	2	8

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	VAL
1	B	499	GLU
1	A	421	TYR
1	A	420	ARG
1	B	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	526	GLN
1	B	227	GLN
1	A	423	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	395/559 (70%)	-0.82	1 (0%) 90 82	84, 129, 186, 249	0
1	B	394/559 (70%)	-0.84	0 100 100	83, 127, 181, 265	0
All	All	789/1118 (70%)	-0.83	1 (0%) 92 90	83, 128, 183, 265	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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	0.99	0.03	159,159,159,159	0
2	ZN	B	606	1/1	0.99	0.03	163,163,163,163	0
2	ZN	A	603	1/1	1.00	0.01	136,136,136,136	0
2	ZN	A	604	1/1	1.00	0.01	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	605	1/1	1.00	0.01	136,136,136,136	0
2	ZN	A	601	1/1	1.00	0.02	157,157,157,157	0
2	ZN	B	601	1/1	1.00	0.02	163,163,163,163	0
2	ZN	B	602	1/1	1.00	0.01	109,109,109,109	0
2	ZN	B	603	1/1	1.00	0.02	138,138,138,138	0
2	ZN	B	604	1/1	1.00	0.02	120,120,120,120	0
2	ZN	B	605	1/1	1.00	0.01	139,139,139,139	0
2	ZN	A	602	1/1	1.00	0.02	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.