



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:02 PM UTC

PDB ID : 5LP8 / pdb\_00005lp8  
Title : Crystal structure of an asymmetric dimer of the ubiquitin ligase HUWE1  
Authors : Sander, B.; Lorenz, S.G.  
Deposited on : 2016-08-12  
Resolution : 2.70 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

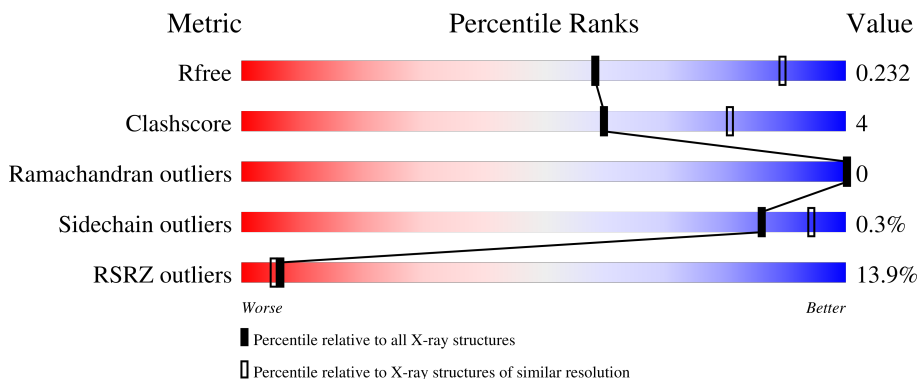
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

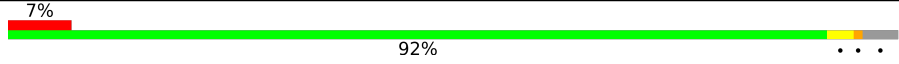
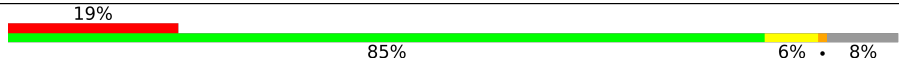
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	450	
1	B	450	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13785 atoms, of which 6770 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 HUWE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	416	6693	2170	3285	593	629	16	0	0	0
1	A	432	7060	2280	3485	616	663	16	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3925	MET	-	initiating methionine	UNP Q7Z6Z7
B	3926	LYS	-	expression tag	UNP Q7Z6Z7
B	3927	HIS	-	expression tag	UNP Q7Z6Z7
B	3928	HIS	-	expression tag	UNP Q7Z6Z7
B	3929	HIS	-	expression tag	UNP Q7Z6Z7
B	3930	HIS	-	expression tag	UNP Q7Z6Z7
B	3931	HIS	-	expression tag	UNP Q7Z6Z7
B	3932	HIS	-	expression tag	UNP Q7Z6Z7
B	3933	PRO	-	expression tag	UNP Q7Z6Z7
B	3934	MET	-	expression tag	UNP Q7Z6Z7
B	3935	SER	-	expression tag	UNP Q7Z6Z7
B	3936	ASP	-	expression tag	UNP Q7Z6Z7
B	3937	TYR	-	expression tag	UNP Q7Z6Z7
B	3938	ASP	-	expression tag	UNP Q7Z6Z7
B	3939	ILE	-	expression tag	UNP Q7Z6Z7
B	3940	PRO	-	expression tag	UNP Q7Z6Z7
B	3941	THR	-	expression tag	UNP Q7Z6Z7
B	3942	THR	-	expression tag	UNP Q7Z6Z7
B	3943	GLU	-	expression tag	UNP Q7Z6Z7
B	3944	ASN	-	expression tag	UNP Q7Z6Z7
B	3945	LEU	-	expression tag	UNP Q7Z6Z7
B	3946	TYR	-	expression tag	UNP Q7Z6Z7
B	3947	PHE	-	expression tag	UNP Q7Z6Z7
B	3948	GLN	-	expression tag	UNP Q7Z6Z7
B	3949	GLY	-	expression tag	UNP Q7Z6Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3950	ALA	-	expression tag	UNP Q7Z6Z7
A	3925	MET	-	initiating methionine	UNP Q7Z6Z7
A	3926	LYS	-	expression tag	UNP Q7Z6Z7
A	3927	HIS	-	expression tag	UNP Q7Z6Z7
A	3928	HIS	-	expression tag	UNP Q7Z6Z7
A	3929	HIS	-	expression tag	UNP Q7Z6Z7
A	3930	HIS	-	expression tag	UNP Q7Z6Z7
A	3931	HIS	-	expression tag	UNP Q7Z6Z7
A	3932	HIS	-	expression tag	UNP Q7Z6Z7
A	3933	PRO	-	expression tag	UNP Q7Z6Z7
A	3934	MET	-	expression tag	UNP Q7Z6Z7
A	3935	SER	-	expression tag	UNP Q7Z6Z7
A	3936	ASP	-	expression tag	UNP Q7Z6Z7
A	3937	TYR	-	expression tag	UNP Q7Z6Z7
A	3938	ASP	-	expression tag	UNP Q7Z6Z7
A	3939	ILE	-	expression tag	UNP Q7Z6Z7
A	3940	PRO	-	expression tag	UNP Q7Z6Z7
A	3941	THR	-	expression tag	UNP Q7Z6Z7
A	3942	THR	-	expression tag	UNP Q7Z6Z7
A	3943	GLU	-	expression tag	UNP Q7Z6Z7
A	3944	ASN	-	expression tag	UNP Q7Z6Z7
A	3945	LEU	-	expression tag	UNP Q7Z6Z7
A	3946	TYR	-	expression tag	UNP Q7Z6Z7
A	3947	PHE	-	expression tag	UNP Q7Z6Z7
A	3948	GLN	-	expression tag	UNP Q7Z6Z7
A	3949	GLY	-	expression tag	UNP Q7Z6Z7
A	3950	ALA	-	expression tag	UNP Q7Z6Z7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total O 2 2	0	0
2	A	30	Total O 30 30	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.46Å 177.46Å 106.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.70 46.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.15-2.70) 99.3 (46.15-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.194 , 0.225 0.206 , 0.232	Depositor DCC
$R_{free}$ test set	2551 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.47	5/3657 (0.1%)	0.69	1/4933 (0.0%)
1	B	0.64	8/3483 (0.2%)	0.75	1/4695 (0.0%)
All	All	0.56	13/7140 (0.2%)	0.72	2/9628 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3990	ARG	CZ-NH2	6.83	1.42	1.33
1	B	4063	ARG	CZ-NH2	6.74	1.42	1.33
1	B	3990	ARG	CZ-NH1	6.67	1.42	1.32
1	B	4071	ARG	CZ-NH2	6.67	1.42	1.33
1	B	4071	ARG	CZ-NH1	6.57	1.42	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4198	VAL	N-CA-C	6.22	116.20	107.37
1	B	3991	VAL	N-CA-C	5.22	119.34	112.04

There are no chirality outliers.

There are no planarity outliers.

### 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	3575	3485	3484	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3408	3285	3296	46	0
2	A	30	0	0	0	0
2	B	2	0	0	0	0
All	All	7015	6770	6780	59	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 4.

The worst 5 of 59 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:4073:MET:HE3	1:B:4110:VAL:CG2	1.32	1.54
1:B:4027:PHE:HD1	1:B:4069:ILE:CD1	1.45	1.29
1:B:4027:PHE:CD1	1:B:4069:ILE:HD11	1.77	1.17
1:A:3939:ILE:HD11	1:A:3966:LEU:HD23	1.28	1.14
1:B:4073:MET:CE	1:B:4110:VAL:CG2	2.26	1.13

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	428/450 (95%)	421 (98%)	7 (2%)	0	100	100
1	B	410/450 (91%)	398 (97%)	12 (3%)	0	100	100
All	All	838/900 (93%)	819 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	388/405 (96%)	387 (100%)	1 (0%)	86	94
1	B	362/405 (89%)	361 (100%)	1 (0%)	86	94
All	All	750/810 (93%)	748 (100%)	2 (0%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4061	LEU
1	A	4244	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4279	GLN
1	A	4208	HIS
1	A	4135	HIS
1	B	4339	HIS
1	A	4192	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](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/450 (96%)	0.14	33 (7%) 20 17	29, 56, 109, 176	0
1	B	416/450 (92%)	0.94	85 (20%) 3 2	30, 81, 144, 186	0
All	All	848/900 (94%)	0.54	118 (13%) 6 5	29, 68, 134, 186	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4190	LYS	8.7
1	B	3950	ALA	7.5
1	B	4173	THR	7.1
1	B	4198	VAL	6.7
1	B	4174	PHE	5.9

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.