



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 12:00 am BST

PDB ID : 3WDZ  
Title : Crystal Structure of Keap1 in Complex with phosphorylated p62  
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Deposited on : 2013-06-26  
Resolution : 2.60 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](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.

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The following versions of software and data (see [references ⓘ](#)) 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

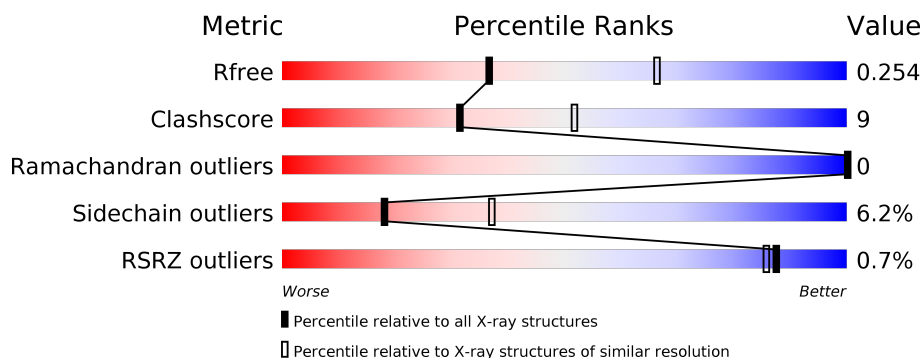
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	311	
2	B	14	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2281 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2189	1360	396	418	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	MET	-	EXPRESSION TAG	UNP Q9Z2X8
A	300	GLY	-	EXPRESSION TAG	UNP Q9Z2X8
A	301	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	302	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	303	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	304	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	305	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	306	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	307	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
A	308	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
A	309	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
A	310	ILE	-	EXPRESSION TAG	UNP Q9Z2X8
A	311	PRO	-	EXPRESSION TAG	UNP Q9Z2X8
A	312	THR	-	EXPRESSION TAG	UNP Q9Z2X8
A	313	THR	-	EXPRESSION TAG	UNP Q9Z2X8
A	314	GLU	-	EXPRESSION TAG	UNP Q9Z2X8
A	315	ASN	-	EXPRESSION TAG	UNP Q9Z2X8
A	316	LEU	-	EXPRESSION TAG	UNP Q9Z2X8
A	317	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
A	318	PHE	-	EXPRESSION TAG	UNP Q9Z2X8
A	319	GLN	-	EXPRESSION TAG	UNP Q9Z2X8
A	320	GLY	-	EXPRESSION TAG	UNP Q9Z2X8

- Molecule 2 is a protein called Peptide from Sequestosome-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			87	50	13	23	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		



- Molecule 1: Kelch-like ECH-associated protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.15Å 75.15Å 113.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.67 – 2.60 32.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.67-2.60) 99.0 (32.60-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.30 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.191 , 0.255 0.189 , 0.254	Depositor DCC
$R_{free}$ test set	551 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 14.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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](#)

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

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	0.80	3/2243 (0.1%)	0.92	2/3053 (0.1%)
2	B	0.68	0/76	1.05	0/100
All	All	0.80	3/2319 (0.1%)	0.92	2/3153 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	TRP	CD2-CE2	6.01	1.48	1.41
1	A	544	TRP	CD2-CE2	5.84	1.48	1.41
1	A	450	TRP	CD2-CE2	5.68	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	362	ARG	NE-CZ-NH1	5.53	123.06	120.30

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	2189	0	2075	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	87	0	77	2	0
3	A	5	0	0	0	0
All	All	2281	0	2152	40	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 9.

All (40) 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:479:ASP:HB3	1:A:484:LEU:HD11	1.70	0.73
1:A:382:ASN:HA	1:A:387:ASN:HB3	1.74	0.69
1:A:557:LEU:H	1:A:557:LEU:HD23	1.58	0.68
1:A:454:ALA:H	1:A:495:ASN:HD21	1.39	0.68
1:A:453:VAL:HG22	1:A:495:ASN:ND2	2.11	0.65
1:A:528:GLN:HG3	1:A:529:ASP:OD1	2.00	0.62
1:A:447:ARG:O	1:A:449:GLU:HG3	2.01	0.60
1:A:365:LEU:H	1:A:365:LEU:HD23	1.67	0.59
1:A:383:SER:HB2	1:A:384:PRO:HD2	1.87	0.56
1:A:570:GLY:HA3	1:A:597:MET:HE1	1.88	0.55
1:A:466:ALA:HB2	1:A:512:VAL:HG12	1.89	0.54
1:A:554:ARG:HD3	1:A:570:GLY:O	2.09	0.53
1:A:538:ASP:HB3	1:A:541:THR:OG1	2.08	0.53
1:A:446:GLU:CD	1:A:446:GLU:H	2.13	0.52
1:A:329:TYR:CE1	1:A:609:THR:HG22	2.46	0.51
1:A:415:ARG:NH1	2:B:351:SEP:O3P	2.43	0.50
1:A:365:LEU:HD12	1:A:376:ALA:HB1	1.92	0.50
1:A:485:ASN:HB3	1:A:506:ILE:HA	1.94	0.50
1:A:453:VAL:HG22	1:A:495:ASN:HD21	1.77	0.49
1:A:411:VAL:HG11	1:A:437:HIS:CE1	2.47	0.49
1:A:526:ASP:C	1:A:526:ASP:OD1	2.51	0.49
1:A:440:VAL:HG21	1:A:497:TRP:CZ2	2.48	0.48
1:A:483:ARG:HH11	1:A:527:GLY:HA2	1.79	0.47
1:A:515:LEU:HD21	1:A:586:PRO:HG3	1.95	0.47
1:A:369:VAL:HG21	1:A:609:THR:HB	1.97	0.47
1:A:418:VAL:HA	1:A:426:TYR:O	2.15	0.46
1:A:541:THR:HB	1:A:543:THR:HG23	1.97	0.46
1:A:553:HIS:H	1:A:553:HIS:CD2	2.35	0.45
1:A:569:LEU:N	1:A:569:LEU:HD12	2.32	0.45
1:A:561:VAL:HA	1:A:565:LYS:O	2.17	0.45
1:A:334:TYR:CE2	2:B:354:GLU:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:CYS:HB3	1:A:537:TYR:O	2.19	0.43
1:A:566:ILE:HB	1:A:584:TYR:HB3	2.01	0.43
1:A:440:VAL:HG21	1:A:497:TRP:HZ2	1.83	0.43
1:A:425:ILE:HB	1:A:443:TYR:HB3	2.01	0.43
1:A:444:GLU:HA	1:A:445:PRO:HD2	1.91	0.43
1:A:483:ARG:NH1	1:A:527:GLY:HA2	2.34	0.42
1:A:485:ASN:CB	1:A:506:ILE:HA	2.50	0.41
1:A:584:TYR:HB2	1:A:591:TRP:CZ3	2.55	0.41
1:A:345:TYR:CE1	1:A:350:GLY:HA2	2.56	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	283/311 (91%)	267 (94%)	16 (6%)	0	100	100
2	B	8/14 (57%)	8 (100%)	0	0	100	100
All	All	291/325 (90%)	275 (94%)	16 (6%)	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	232/255 (91%)	218 (94%)	14 (6%)	19	39
2	B	9/12 (75%)	8 (89%)	1 (11%)	6	11
All	All	241/267 (90%)	226 (94%)	15 (6%)	18	37

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	411	VAL
1	A	447	ARG
1	A	459	ARG
1	A	472	LEU
1	A	529	ASP
1	A	543	THR
1	A	545	THR
1	A	551	ARG
1	A	557	LEU
1	A	565	LYS
1	A	580	SER
1	A	593	GLU
1	A	596	ARG
2	B	356	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	ASN
1	A	495	ASN
1	A	553	HIS
1	A	563	GLN
2	B	356	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SEP	B	351	2	8,9,10	0.68	0	8,12,14	1.43	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	351	2	-	0/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	SEP	OG-P-O1P	-2.27	100.10	106.47
2	B	351	SEP	OG-CB-CA	-2.18	106.02	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	351	SEP	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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 [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	285/311 (91%)	-0.47	1 (0%) 92 91	33, 46, 65, 81	0
2	B	10/14 (71%)	-0.09	1 (10%) 7 4	47, 55, 75, 85	0
All	All	295/325 (90%)	-0.46	2 (0%) 87 86	33, 46, 67, 85	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	347	GLU	2.2
1	A	512	VAL	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SEP	B	351	10/11	0.97	0.10	48,51,56,60	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.