



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:04 am GMT

PDB ID : 1ZGK
Title : 1.35 angstrom structure of the Kelch domain of Keap1
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Deposited on : 2005-04-21
Resolution : 1.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

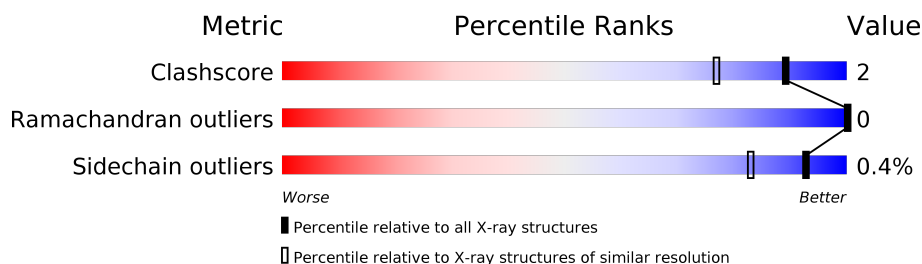
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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))
Clashscore	112137	1063 (1.38-1.34)
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	 90% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2651 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	288	Total	C	N	O	S	Se	0	25	0
			2274	1425	405	425	10	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	GLY	-	CLONING ARTIFACT	UNP Q14145
A	303	SER	-	CLONING ARTIFACT	UNP Q14145
A	304	SER	-	CLONING ARTIFACT	UNP Q14145
A	305	HIS	-	EXPRESSION TAG	UNP Q14145
A	306	HIS	-	EXPRESSION TAG	UNP Q14145
A	307	HIS	-	EXPRESSION TAG	UNP Q14145
A	308	HIS	-	EXPRESSION TAG	UNP Q14145
A	309	HIS	-	EXPRESSION TAG	UNP Q14145
A	310	HIS	-	EXPRESSION TAG	UNP Q14145
A	311	SER	-	CLONING ARTIFACT	UNP Q14145
A	312	SER	-	CLONING ARTIFACT	UNP Q14145
A	313	GLY	-	CLONING ARTIFACT	UNP Q14145
A	314	LEU	-	CLONING ARTIFACT	UNP Q14145
A	315	VAL	-	CLONING ARTIFACT	UNP Q14145
A	316	PRO	-	CLONING ARTIFACT	UNP Q14145
A	317	ARG	-	CLONING ARTIFACT	UNP Q14145
A	318	GLY	-	CLONING ARTIFACT	UNP Q14145
A	319	SER	-	CLONING ARTIFACT	UNP Q14145
A	320	HIS	-	CLONING ARTIFACT	UNP Q14145
A	399	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	409	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	456	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	499	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	503	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	550	MSE	MET	MODIFIED RESIDUE	UNP Q14145
A	597	MSE	MET	MODIFIED RESIDUE	UNP Q14145

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	377	Total 377	O 377	0	0

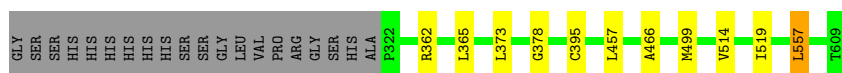
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

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

Chain A:  90% • 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.75Å 85.75Å 147.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.06 – 1.35	Depositor
% Data completeness (in resolution range)	100.0 (28.06-1.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.111 , 0.133	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2651	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

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	0.53	0/2414	0.73	0/3279

There are no bond length outliers.

There are no bond angle outliers.

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	2274	0	2172	10	0
2	A	377	0	0	0	0
All	All	2651	0	2172	10	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 2.

All (10) 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:514[B]:VAL:HG22	1:A:519:ILE:HD13	1.51	0.91
1:A:514[B]:VAL:HG22	1:A:519:ILE:CD1	2.11	0.80
1:A:466:ALA:HB1	1:A:514[B]:VAL:HG23	1.65	0.77
1:A:457:LEU:HD12	1:A:499[A]:MSE:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ALA:CB	1:A:514[B]:VAL:HG23	2.36	0.56
1:A:557:LEU:H	1:A:557:LEU:HD23	1.72	0.55
1:A:514[B]:VAL:CG2	1:A:519:ILE:CD1	2.88	0.50
1:A:365:LEU:H	1:A:365:LEU:HD23	1.81	0.44
1:A:373:LEU:HD13	1:A:395[A]:CYS:SG	2.61	0.41
1:A:362[B]:ARG:HD2	1:A:378:GLY:O	2.21	0.41

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	311/308 (101%)	304 (98%)	7 (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	247/243 (102%)	246 (100%)	1 (0%)	93	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	A	530	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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.