



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:27 pm BST

PDB ID : 6TYU
Title : Structure of Ku80 von Willebrand domain complexed with MRI Ku Binding Motif
Authors : Min, J.; Pedersen, L.C.
Deposited on : 2019-08-09
Resolution : 1.47 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

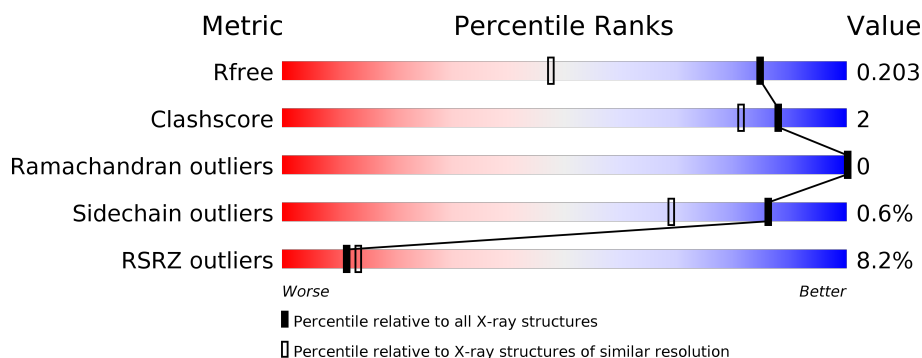
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 $\leq 5\%$. 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	231	<div> <div>7%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
2	B	16	<div> <div>6%</div> <div>69%</div> <div>31%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3679 atoms, of which 1723 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 X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	209	3312	1073	1635	264	328	12	0	13	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A1L8EVE5
A	-5	HIS	-	expression tag	UNP A0A1L8EVE5
A	-4	HIS	-	expression tag	UNP A0A1L8EVE5
A	-3	HIS	-	expression tag	UNP A0A1L8EVE5
A	-2	HIS	-	expression tag	UNP A0A1L8EVE5
A	-1	HIS	-	expression tag	UNP A0A1L8EVE5
A	0	HIS	-	expression tag	UNP A0A1L8EVE5
A	?	-	GLU	deletion	UNP A0A1L8EVE5
A	?	-	GLU	deletion	UNP A0A1L8EVE5
A	?	-	PHE	deletion	UNP A0A1L8EVE5
A	?	-	GLY	deletion	UNP A0A1L8EVE5
A	?	-	GLY	deletion	UNP A0A1L8EVE5
A	?	-	SER	deletion	UNP A0A1L8EVE5
A	?	-	SER	deletion	UNP A0A1L8EVE5
A	?	-	ASN	deletion	UNP A0A1L8EVE5
A	?	-	ASN	deletion	UNP A0A1L8EVE5
A	?	-	ARG	deletion	UNP A0A1L8EVE5
A	?	-	GLY	deletion	UNP A0A1L8EVE5
A	?	-	ASN	deletion	UNP A0A1L8EVE5
A	?	-	ALA	deletion	UNP A0A1L8EVE5
A	?	-	GLY	deletion	UNP A0A1L8EVE5
A	?	-	SER	deletion	UNP A0A1L8EVE5
A	?	-	SER	deletion	UNP A0A1L8EVE5
A	?	-	ASP	deletion	UNP A0A1L8EVE5
A	?	-	ARG	deletion	UNP A0A1L8EVE5
A	190	SER	CYS	engineered mutation	UNP A0A1L8EVE5

- Molecule 2 is a protein called LYS-THR-ARG-VAL-LEU-PRO-SER-TRP-LEU-THR-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	0	0	0
			174	57	88	15	14			


- Molecule 3 is water.

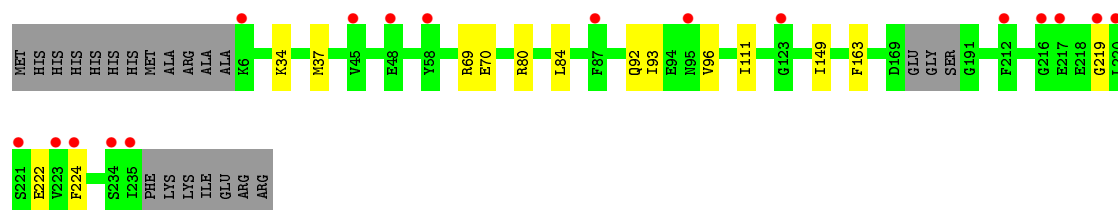
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	2
			178	178		
3	B	15	Total	O	0	0
			15	15		

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.

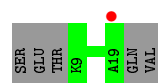
- Molecule 1: X-ray repair cross-complementing protein 5

Chain A: 



- Molecule 2: LYS-THR-ARG-VAL-LEU-PRO-SER-TRP-LEU-THR-ALA

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.57Å 71.35Å 79.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 1.47 37.80 – 1.47	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.80-1.47) 98.2 (37.80-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.178 , 0.201 0.179 , 0.203	Depositor DCC
R_{free} test set	2152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3679	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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

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	0.42	0/1712	0.60	0/2313
2	B	0.31	0/88	0.53	0/121
All	All	0.42	0/1800	0.60	0/2434

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

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	1677	1635	1621	7	0
2	B	86	88	88	0	0
3	A	178	0	0	0	0
3	B	15	0	0	0	0
All	All	1956	1723	1709	7	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 (7) 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:69:ARG:O	1:A:70:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80[B]:ARG:NH2	1:A:84:LEU:O	2.43	0.43
1:A:34:LYS:NZ	1:A:93:ILE:O	2.47	0.43
1:A:111:ILE:HD11	1:A:149:ILE:HD11	2.00	0.42
1:A:163:PHE:CD1	1:A:224:PHE:HB2	2.55	0.41
1:A:92:GLN:O	1:A:96:VAL:N	2.54	0.41
1:A:219:GLY:HA2	1:A:222:GLU:OE1	2.22	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	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	B	9/16 (56%)	9 (100%)	0	0	100	100
All	All	227/247 (92%)	223 (98%)	4 (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	182/204 (89%)	180 (99%)	2 (1%)	73	48
2	B	9/15 (60%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	191/219 (87%)	189 (99%)	2 (1%)	86	52

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

Mol	Chain	Res	Type
1	A	37[A]	MET
1	A	37[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [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	209/231 (90%)	0.49	17 (8%) 12 14	14, 26, 56, 84	0
2	B	11/16 (68%)	0.08	1 (9%) 9 11	19, 24, 38, 56	0
All	All	220/247 (89%)	0.47	18 (8%) 11 13	14, 26, 56, 84	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	7.8
1	A	216	GLY	4.3
1	A	87	PHE	4.1
2	B	19	ALA	3.8
1	A	212	PHE	3.7
1	A	221	SER	3.5
1	A	219	GLY	3.1
1	A	217	GLU	2.9
1	A	234	SER	2.9
1	A	224	PHE	2.8
1	A	95	ASN	2.5
1	A	45	VAL	2.5
1	A	123	GLY	2.4
1	A	223	VAL	2.4
1	A	6	LYS	2.3
1	A	235	ILE	2.2
1	A	58	TYR	2.2
1	A	48	GLU	2.2

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 carbohydrates 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.