wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 03:29 pm BST

PDB ID	:	5YZV
Title	:	Biophysical and structural characterization of the thermostable WD40 domain of a prokaryotic protein, Thermomonospora curvata PkwA
Authors	:	Li, D.Y.; Shen, C.; Du, Y.; Qiao, F.F.; Kong, T.; Yuan, L.R.; Zhang, D.L.; Wu, X.H.; Wu, Y.D.
Deposited on	:	2017-12-15
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

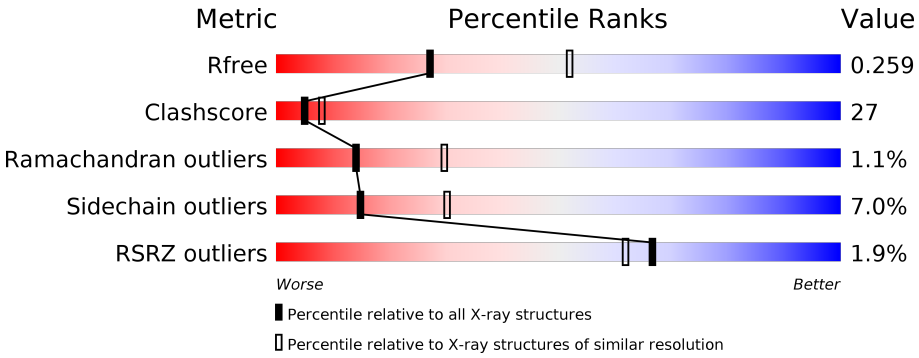
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 >=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 <=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	302	2% 58% 30% 6% 5%
1	B	302	79% 15% • 5%
1	C	302	4% 56% 31% 9% •
1	D	302	4% 51% 32% 9% • 6%
1	E	302	71% 22% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10922 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 Probable serine/threonine-protein kinase PkwA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2124	1325	369	427	3			
1	B	288	Total	C	N	O	S	0	0	0
			2154	1341	377	433	3			
1	C	290	Total	C	N	O	S	0	0	0
			2152	1341	373	435	3			
1	D	284	Total	C	N	O	S	0	0	0
			2111	1319	364	425	3			
1	E	288	Total	C	N	O	S	0	0	0
			2151	1340	376	432	3			

- Molecule 2 is water.

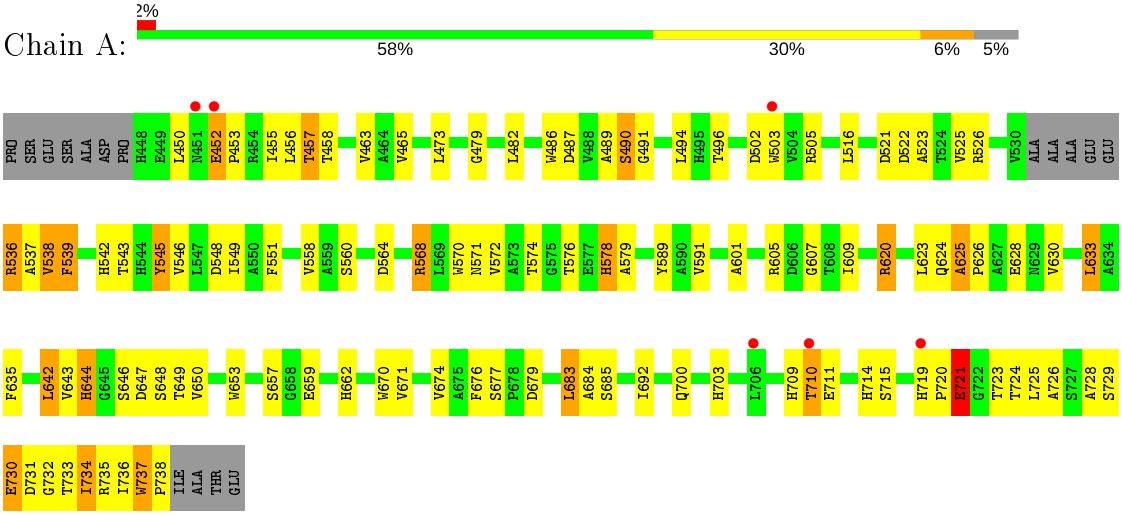
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total	O	0	0
			57	57		
2	B	44	Total	O	0	0
			44	44		
2	C	44	Total	O	0	0
			44	44		
2	D	42	Total	O	0	0
			42	42		
2	E	43	Total	O	0	0
			43	43		

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.

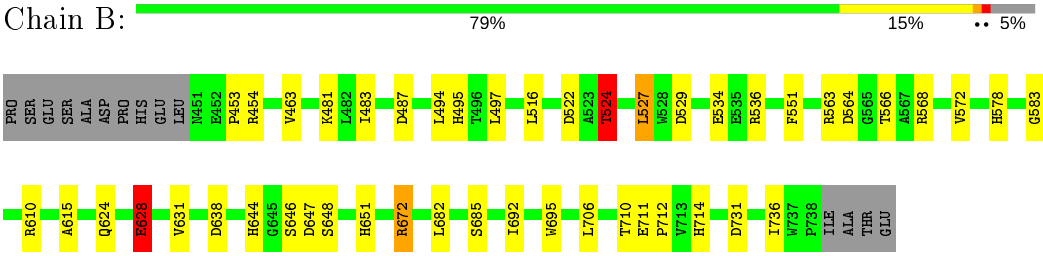
- Molecule 1: Probable serine/threonine-protein kinase PkwA

Chain A:



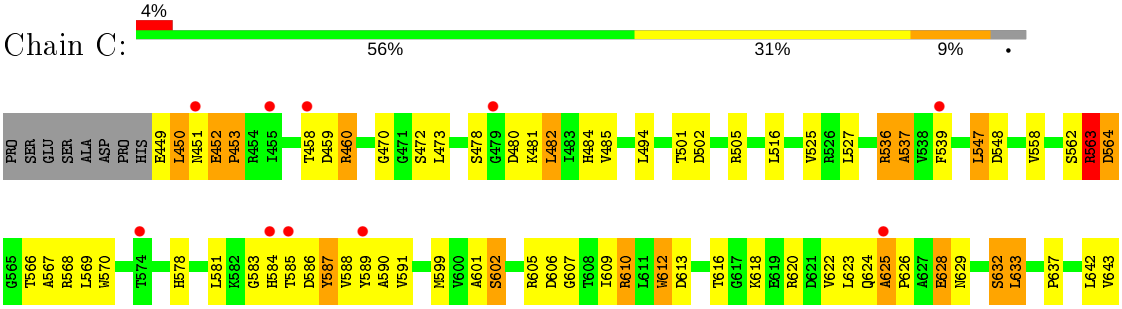
- Molecule 1: Probable serine/threonine-protein kinase PkwA

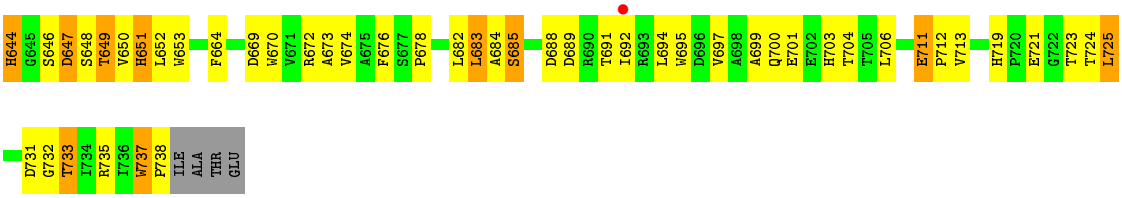
Chain B:



- Molecule 1: Probable serine/threonine-protein kinase PkwA

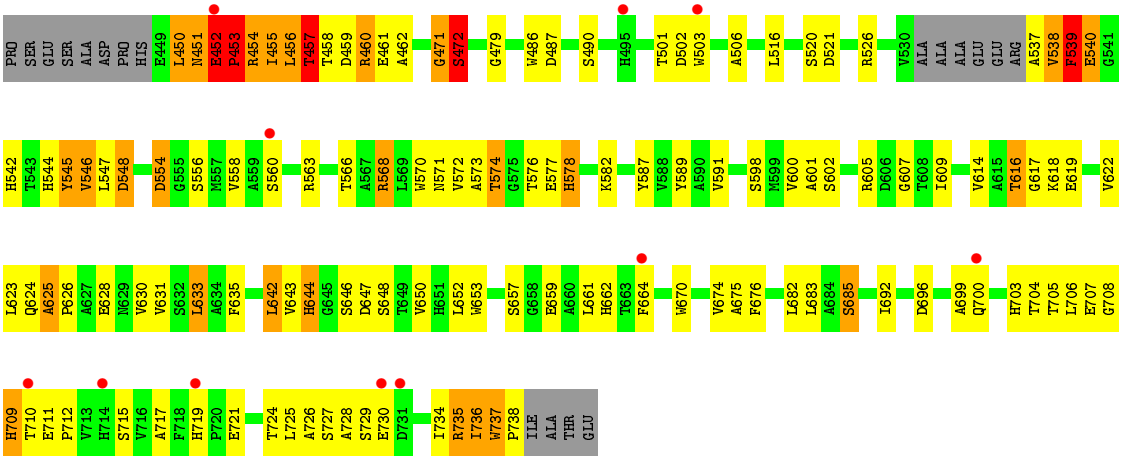
Chain C:





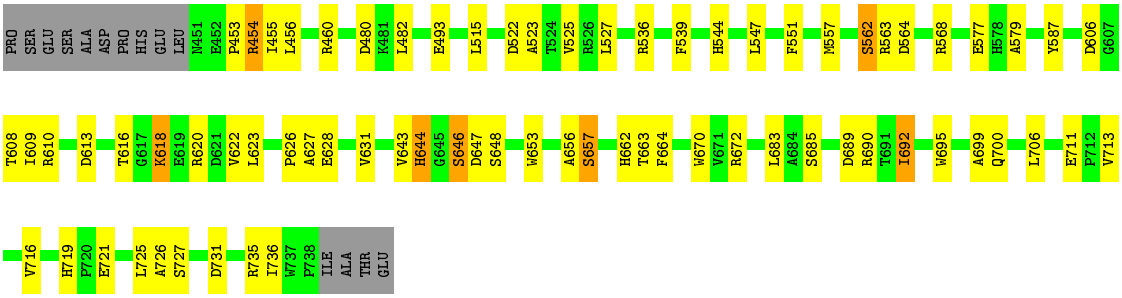
• Molecule 1: Probable serine/threonine-protein kinase PkwA

Chain D:



• Molecule 1: Probable serine/threonine-protein kinase PkwA

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.69Å 107.26Å 110.27Å 78.77° 89.33° 88.91°	Depositor
Resolution (Å)	50.01 – 2.60 44.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.01-2.60) 87.3 (44.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.225 , 0.259 0.230 , 0.259	Depositor DCC
R_{free} test set	2895 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l 0.013 for -h,l,k 0.118 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.14	7/2178 (0.3%)	1.12	5/2981 (0.2%)
1	B	1.03	2/2209 (0.1%)	1.04	6/3022 (0.2%)
1	C	1.12	9/2207 (0.4%)	1.15	16/3022 (0.5%)
1	D	1.21	10/2165 (0.5%)	1.16	11/2964 (0.4%)
1	E	1.01	2/2206 (0.1%)	1.01	7/3018 (0.2%)
All	All	1.10	30/10965 (0.3%)	1.10	45/15007 (0.3%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	453	PRO	N-CA	12.93	1.69	1.47
1	D	539	PHE	CB-CG	-8.56	1.36	1.51
1	C	649	THR	CB-CG2	-8.28	1.25	1.52
1	D	540	GLU	CG-CD	-7.67	1.40	1.51
1	D	727	SER	CB-OG	7.21	1.51	1.42

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	610	ARG	NE-CZ-NH1	-13.24	113.68	120.30
1	C	453	PRO	CA-N-CD	-10.29	97.10	111.50
1	D	460	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	C	610	ARG	NE-CZ-NH2	8.77	124.69	120.30
1	E	454	ARG	NE-CZ-NH2	-8.37	116.11	120.30

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	2124	0	1969	151	0
1	B	2154	0	2013	29	0
1	C	2152	0	1995	167	0
1	D	2111	0	1963	172	0
1	E	2151	0	2009	46	0
2	A	57	0	0	3	0
2	B	44	0	0	0	0
2	C	44	0	0	4	0
2	D	42	0	0	0	0
2	E	43	0	0	0	0
All	All	10922	0	9949	559	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 27.

The worst 5 of 559 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:452:GLU:HG2	1:A:453:PRO:CD	1.31	1.57
1:C:453:PRO:CA	1:C:453:PRO:N	1.69	1.34
1:A:452:GLU:CG	1:A:453:PRO:CD	2.13	1.27
1:A:452:GLU:CG	1:A:453:PRO:HD3	1.64	1.24
1:C:605:ARG:HG3	1:C:629:ASN:ND2	1.60	1.16

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	282/302 (93%)	268 (95%)	10 (4%)	4 (1%)	11 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	286/302 (95%)	273 (96%)	12 (4%)	1 (0%)	41 64
1	C	288/302 (95%)	270 (94%)	15 (5%)	3 (1%)	15 32
1	D	280/302 (93%)	258 (92%)	15 (5%)	7 (2%)	5 9
1	E	286/302 (95%)	273 (96%)	12 (4%)	1 (0%)	41 64
All	All	1422/1510 (94%)	1342 (94%)	64 (4%)	16 (1%)	14 30

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	452	GLU
1	A	625	ALA
1	C	625	ALA
1	D	453	PRO
1	D	457	THR

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	219/235 (93%)	204 (93%)	15 (7%)	16 32
1	B	223/235 (95%)	212 (95%)	11 (5%)	25 48
1	C	221/235 (94%)	202 (91%)	19 (9%)	10 20
1	D	219/235 (93%)	195 (89%)	24 (11%)	6 11
1	E	222/235 (94%)	214 (96%)	8 (4%)	35 61
All	All	1104/1175 (94%)	1027 (93%)	77 (7%)	15 30

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	632	SER
1	C	725	LEU
1	E	551	PHE
1	C	633	LEU

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Mol	Chain	Res	Type
1	C	676	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	629	ASN
1	C	651	HIS
1	D	700	GLN
1	C	495	HIS
1	D	651	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

6.1 Protein, DNA and RNA chains

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^{th} 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	286/302 (94%)	0.03	6 (2%) 63 58	19, 37, 68, 101	0
1	B	288/302 (95%)	-0.30	0 100 100	20, 36, 60, 79	0
1	C	290/302 (96%)	0.07	11 (3%) 40 33	19, 38, 69, 93	0
1	D	284/302 (94%)	0.06	11 (3%) 39 32	22, 40, 69, 92	0
1	E	288/302 (95%)	-0.30	0 100 100	23, 40, 61, 85	0
All	All	1436/1510 (95%)	-0.09	28 (1%) 66 62	19, 38, 67, 101	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	585	THR	4.2
1	A	710	THR	3.9
1	D	700	GLN	3.5
1	A	452	GLU	3.3
1	A	451	ASN	3.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.