WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2021 – 02:12 PM JST

PDB ID	:	5XLL
Title	:	Dimer form of M. tuberculosis PknI sensor domain
Authors	:	Rao, Z.; Yan, Q.
Deposited on	:	2017-05-10
Resolution	:	2.20 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:

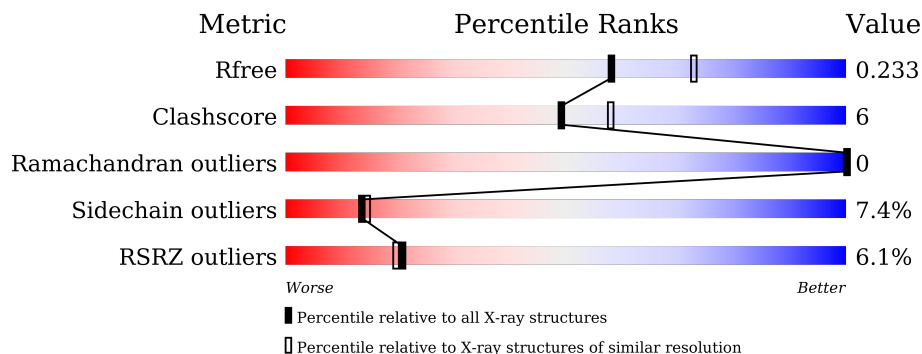|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.20 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		7.4%
RSRZ outliers		6.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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	184	4% 71% 14% · 14%
1	B	184	6% 70% 15% · 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2467 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 Serine/threonine-protein kinase PknI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	Se	0	0	0
			1201	751	209	234	4	3			
1	B	159	Total	C	N	O	S	Se	0	0	0
			1207	756	209	235	4	3			

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	28	Total	O	0	0
			28	28		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Serine/threonine-protein kinase PknI

Chain A:

• Molecule 1: Serine/threonine-protein kinase PknI

Chain B:
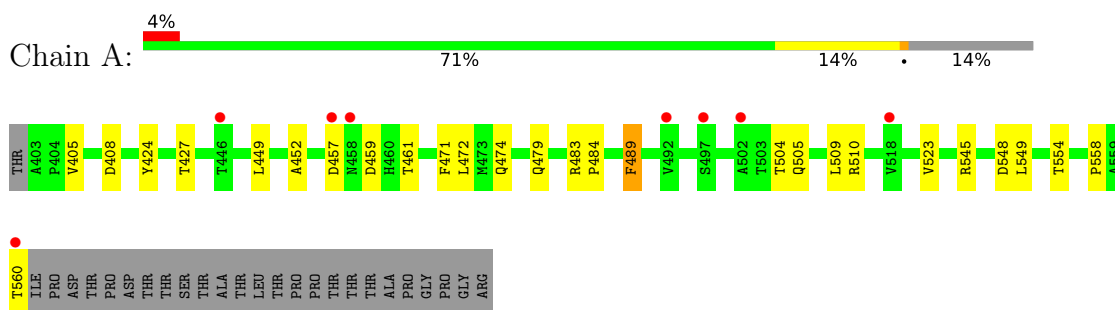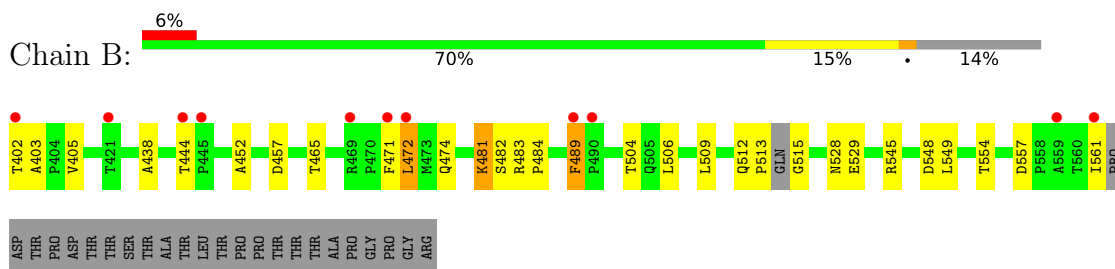
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	136.01Å 136.01Å 136.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.09 – 2.20 48.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.09-2.20) 100.0 (48.09-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.224 , 0.257 0.226 , 0.233	Depositor DCC
R_{free} test set	1087 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.486 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2467	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.48	0/1233	0.60	0/1693
1	B	0.48	0/1238	0.61	0/1699
All	All	0.48	0/2471	0.61	0/3392

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	1201	0	1160	11	1
1	B	1207	0	1169	17	1
2	A	31	0	0	2	0
2	B	28	0	0	4	0
All	All	2467	0	2329	28	1

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 6.

All (28) 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:465:THR:OG1	2:B:601:HOH:O	1.99	0.79

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLN:OE1	1:B:483:ARG:NH2	2.24	0.70
1:A:424:TYR:O	2:A:601:HOH:O	2.11	0.69
1:A:474:GLN:OE1	1:A:483:ARG:NH2	2.26	0.69
1:A:505:GLN:HG2	1:A:523:VAL:HG22	1.75	0.69
1:B:482:SER:OG	2:B:602:HOH:O	2.13	0.67
1:B:484:PRO:HB3	1:B:504:THR:HG23	1.85	0.58
1:A:452:ALA:HB3	1:A:471:PHE:HB3	1.86	0.57
1:B:557:ASP:OD2	2:B:603:HOH:O	2.17	0.57
1:B:452:ALA:HB3	1:B:471:PHE:HB3	1.87	0.57
1:B:529:GLU:OE1	1:B:529:GLU:N	2.21	0.56
1:A:545:ARG:NH2	1:A:548:ASP:OD2	2.40	0.54
1:B:528:ASN:HA	2:B:606:HOH:O	2.07	0.54
1:A:484:PRO:HB3	1:A:504:THR:HG23	1.90	0.53
1:B:545:ARG:NH2	1:B:548:ASP:OD2	2.44	0.51
1:B:402:THR:OG1	1:B:403:ALA:N	2.44	0.50
1:A:510:ARG:NH1	2:A:602:HOH:O	2.14	0.48
1:A:459:ASP:OD1	1:A:461:THR:OG1	2.31	0.46
1:A:449:LEU:HB2	1:A:558:PRO:HB2	1.98	0.45
1:B:481:LYS:HD2	1:B:506:LEU:HD22	1.98	0.45
1:A:479:GLN:OE1	1:A:510:ARG:NH1	2.49	0.45
1:B:472:LEU:HD22	1:B:472:LEU:HA	1.86	0.43
1:B:489:PHE:HD1	1:B:489:PHE:HA	1.71	0.42
1:B:513:PRO:O	1:B:515:GLY:N	2.53	0.42
1:B:484:PRO:HG3	1:B:506:LEU:HD23	2.02	0.41
1:B:484:PRO:HB3	1:B:504:THR:CG2	2.50	0.41
1:A:489:PHE:HD1	1:A:489:PHE:HA	1.76	0.40
1:B:438:ALA:O	1:B:452:ALA:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASP:O	1:B:545:ARG:NH1[23_555]	2.15	0.05

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

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	156/184 (85%)	151 (97%)	5 (3%)	0	100	100
1	B	155/184 (84%)	153 (99%)	2 (1%)	0	100	100
All	All	311/368 (84%)	304 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	135/154 (88%)	126 (93%)	9 (7%)	16	18
1	B	136/154 (88%)	125 (92%)	11 (8%)	11	12
All	All	271/308 (88%)	251 (93%)	20 (7%)	13	14

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	VAL
1	A	427	THR
1	A	457	ASP
1	A	472	LEU
1	A	489	PHE
1	A	509	LEU
1	A	549	LEU
1	A	554	THR
1	A	560	THR
1	B	405	VAL
1	B	444	THR
1	B	457	ASP
1	B	472	LEU
1	B	481	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	489	PHE
1	B	509	LEU
1	B	512	GLN
1	B	549	LEU
1	B	554	THR
1	B	561	ILE

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

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 monosaccharides 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, 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(Å²)	Q<0.9
1	A	155/184 (84%)	0.41	8 (5%)	27	26	34, 55, 98, 129	0
1	B	156/184 (84%)	0.51	11 (7%)	16	14	34, 54, 93, 120	0
All	All	311/368 (84%)	0.46	19 (6%)	21	20	34, 54, 96, 129	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	PHE	4.9
1	B	445	PRO	3.9
1	B	559	ALA	3.7
1	B	471	PHE	3.3
1	A	497	SER	2.7
1	A	560	THR	2.7
1	B	402	THR	2.7
1	A	457	ASP	2.6
1	A	502	ALA	2.5
1	B	469	ARG	2.3
1	B	421	THR	2.2
1	B	444	THR	2.2
1	A	518	VAL	2.1
1	B	561	ILE	2.1
1	A	492	VAL	2.1
1	A	446	THR	2.1
1	A	458	ASN	2.1
1	B	472	LEU	2.0
1	B	490	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.