wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 11:22 AM EDT

PDB ID	:	6TII
Title	:	Crystal structure of penicillin-binding protein 2 from Yersinia pestis
Authors	:	Pankov, G.; Hunter, W.N.; Dawson, A.
Deposited on	:	2019-11-22
Resolution	:	2.26 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

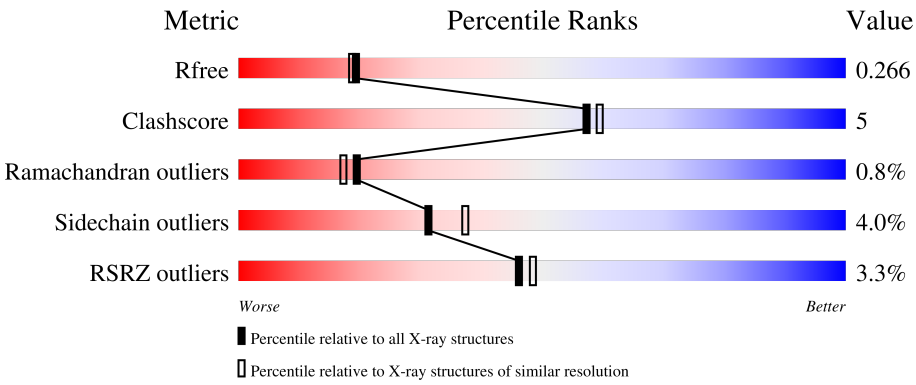
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	AAA	583	4% 77% 14% • 8%
1	BBB	583	2% 80% 11% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8753 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 Peptidoglycan D,D-transpeptidase MrdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	534	4216	2686	735	786	9	0	1	0
1	BBB	534	4230	2692	739	790	9	0	3	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	31	HIS	-	expression tag	UNP A0A384KFW3
AAA	32	HIS	-	expression tag	UNP A0A384KFW3
AAA	33	HIS	-	expression tag	UNP A0A384KFW3
AAA	34	HIS	-	expression tag	UNP A0A384KFW3
AAA	35	HIS	-	expression tag	UNP A0A384KFW3
AAA	36	HIS	-	expression tag	UNP A0A384KFW3
AAA	37	SER	-	expression tag	UNP A0A384KFW3
AAA	38	SER	-	expression tag	UNP A0A384KFW3
AAA	39	GLY	-	expression tag	UNP A0A384KFW3
AAA	40	GLU	-	expression tag	UNP A0A384KFW3
AAA	41	ASN	-	expression tag	UNP A0A384KFW3
AAA	42	LEU	-	expression tag	UNP A0A384KFW3
AAA	43	TYR	-	expression tag	UNP A0A384KFW3
AAA	44	PHE	-	expression tag	UNP A0A384KFW3
AAA	45	GLN	-	expression tag	UNP A0A384KFW3
AAA	46	GLY	-	expression tag	UNP A0A384KFW3
AAA	47	HIS	-	expression tag	UNP A0A384KFW3
AAA	48	MET	-	expression tag	UNP A0A384KFW3
BBB	31	HIS	-	expression tag	UNP A0A384KFW3
BBB	32	HIS	-	expression tag	UNP A0A384KFW3
BBB	33	HIS	-	expression tag	UNP A0A384KFW3
BBB	34	HIS	-	expression tag	UNP A0A384KFW3
BBB	35	HIS	-	expression tag	UNP A0A384KFW3
BBB	36	HIS	-	expression tag	UNP A0A384KFW3
BBB	37	SER	-	expression tag	UNP A0A384KFW3

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	38	SER	-	expression tag	UNP A0A384KFW3
BBB	39	GLY	-	expression tag	UNP A0A384KFW3
BBB	40	GLU	-	expression tag	UNP A0A384KFW3
BBB	41	ASN	-	expression tag	UNP A0A384KFW3
BBB	42	LEU	-	expression tag	UNP A0A384KFW3
BBB	43	TYR	-	expression tag	UNP A0A384KFW3
BBB	44	PHE	-	expression tag	UNP A0A384KFW3
BBB	45	GLN	-	expression tag	UNP A0A384KFW3
BBB	46	GLY	-	expression tag	UNP A0A384KFW3
BBB	47	HIS	-	expression tag	UNP A0A384KFW3
BBB	48	MET	-	expression tag	UNP A0A384KFW3

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
2	AAA	1	1	1	0	0
			Total	Br		
2	BBB	1	1	1	0	0

- Molecule 3 is water.

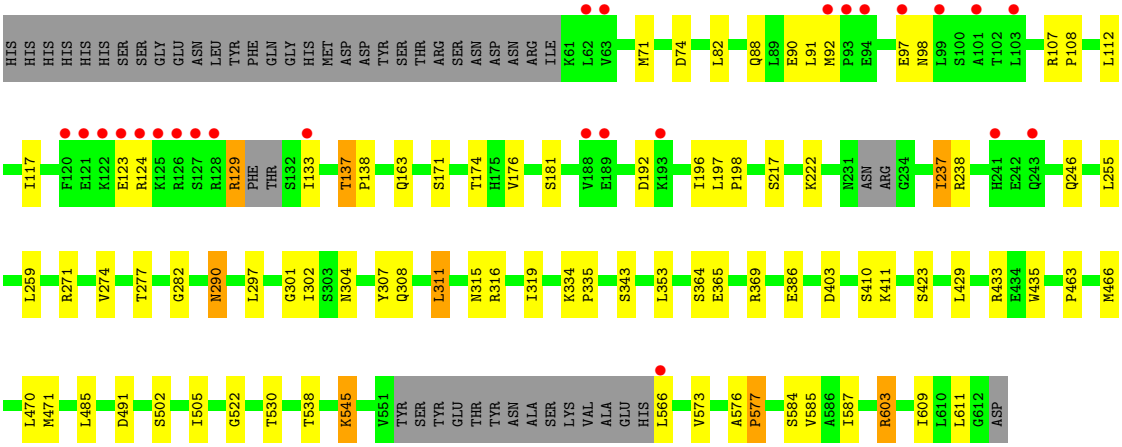
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	AAA	160	160	160	0	0
			Total	O		
3	BBB	145	145	145	0	0

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.

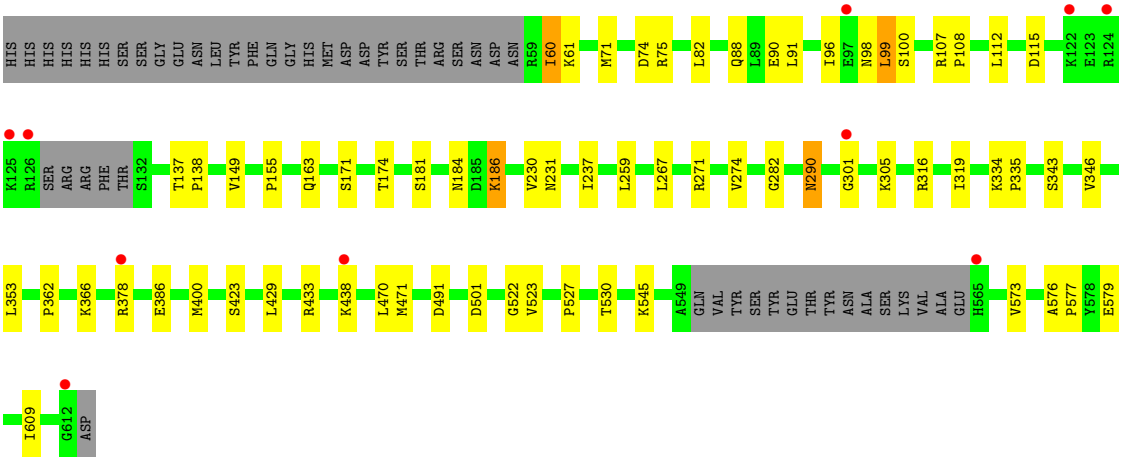
• Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain AAA:



• Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.66Å 84.77Å 88.36Å 113.47° 94.97° 103.72°	Depositor
Resolution (Å)	50.01 – 2.26 46.28 – 2.26	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.01-2.26) 90.4 (46.28-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.191 , 0.253 0.204 , 0.266	Depositor DCC
R_{free} test set	2616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 (i)

5.1 Standard geometry (i)

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

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	AAA	0.69	0/4311	0.85	0/5847
1	BBB	0.69	0/4327	0.85	1/5870 (0.0%)
All	All	0.69	0/8638	0.85	1/11717 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	4
1	BBB	0	4
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	75	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	THR	Peptide
1	AAA	290	ASN	Peptide,Mainchain
1	AAA	576	ALA	Peptide
1	BBB	137	THR	Peptide
1	BBB	290	ASN	Mainchain

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	AAA	4216	0	4222	54	0
1	BBB	4230	0	4227	31	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	160	0	0	4	0
3	BBB	145	0	0	3	0
All	All	8753	0	8449	83	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 5.

The worst 5 of 83 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:AAA:271:ARG:HD3	1:AAA:315:ASN:HD22	1.41	0.83
1:BBB:231:ASN:HD22	1:BBB:237:ILE:HD11	1.47	0.79
1:AAA:112:LEU:HD21	1:AAA:117:ILE:HG13	1.71	0.72
1:AAA:163:GLN:NE2	1:BBB:491:ASP:O	2.26	0.67
1:AAA:176:VAL:HG11	1:AAA:255:LEU:HD11	1.79	0.63

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	AAA	527/583 (90%)	503 (95%)	20 (4%)	4 (1%)	19 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	531/583 (91%)	512 (96%)	15 (3%)	4 (1%)	19	17
All	All	1058/1166 (91%)	1015 (96%)	35 (3%)	8 (1%)	19	17

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	138	PRO
1	AAA	364	SER
1	AAA	577	PRO
1	BBB	577	PRO
1	AAA	301	GLY

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	AAA	450/494 (91%)	432 (96%)	18 (4%)	31	37
1	BBB	452/494 (92%)	434 (96%)	18 (4%)	31	37
All	All	902/988 (91%)	866 (96%)	36 (4%)	31	37

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	378	ARG
1	BBB	579	GLU
1	BBB	423	SER
1	BBB	438	LYS
1	AAA	423	SER

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	534/583 (91%)	0.06	25 (4%)	31	34	26, 49, 96, 115	0
1	BBB	534/583 (91%)	-0.09	10 (1%)	66	69	26, 48, 90, 127	0
All	All	1068/1166 (91%)	-0.02	35 (3%)	46	48	26, 48, 95, 127	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	99	LEU	4.5
1	BBB	126	ARG	4.3
1	AAA	128	ARG	4.1
1	BBB	122	LYS	4.0
1	BBB	438	LYS	3.9

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 monosaccharides in this entry.

6.4 Ligands (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, 95th 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^2)	Q<0.9
2	BR	AAA	701	1/1	0.84	0.08	103,103,103,103	0
2	BR	BBB	701	1/1	0.95	0.08	93,93,93,93	0

6.5 Other polymers (i)

There are no such residues in this entry.