



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 PM GMT

PDB ID : 3UPO
Title : Structure of penicillin-binding protein A from *M. tuberculosis*: penicillin G acyl-enzyme complex
Authors : Davies, C.; Fedorovich, A.
Deposited on : 2011-11-18
Resolution : 2.30 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

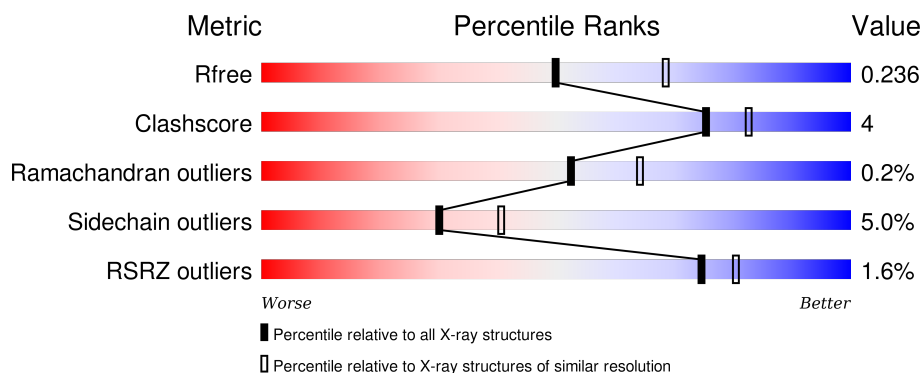
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	462	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 9% • • </div> </div>
1	B	462	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 9%, green 83%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 83% 9% • 6% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6558 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.

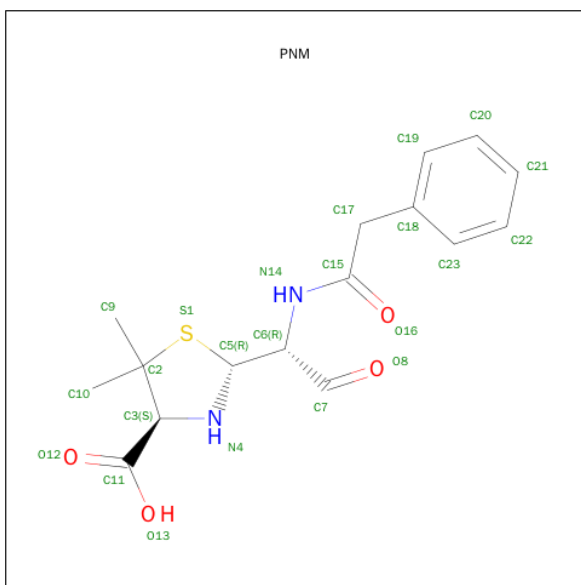
- Molecule 1 is a protein called Penicillin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3260	2040	585	626	9			
1	B	435	Total	C	N	O	S	0	0	0
			3204	2004	576	615	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP P71586
A	31	ALA	-	EXPRESSION TAG	UNP P71586
A	32	MET	-	EXPRESSION TAG	UNP P71586
A	33	GLY	-	EXPRESSION TAG	UNP P71586
A	34	SER	-	EXPRESSION TAG	UNP P71586
A	384	ARG	GLY	SEE REMARK 999	UNP P71586
B	30	GLY	-	EXPRESSION TAG	UNP P71586
B	31	ALA	-	EXPRESSION TAG	UNP P71586
B	32	MET	-	EXPRESSION TAG	UNP P71586
B	33	GLY	-	EXPRESSION TAG	UNP P71586
B	34	SER	-	EXPRESSION TAG	UNP P71586
B	384	ARG	GLY	SEE REMARK 999	UNP P71586

- Molecule 2 is OPEN FORM - PENICILLIN G (three-letter code: PNM) (formula: C₁₆H₂₀N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	16	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			23	16	2	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	19	Total	O	0	0
			19	19		

- Molecule 1: Penicillin-binding protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	123.21 Å 123.21 Å 97.32 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.28 – 2.30 44.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.28-2.30) 98.0 (44.27-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.243 0.193 , 0.236	Depositor DCC
R_{free} test set	1882 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 36562 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PNM

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	0/3330	0.62	0/4549
1	B	0.52	0/3272	0.64	2/4469 (0.0%)
All	All	0.52	0/6602	0.63	2/9018 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	TYR	N-CA-C	6.77	129.28	111.00
1	B	459	LEU	CA-CB-CG	-5.17	103.42	115.30

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	3260	0	3250	29	0
1	B	3204	0	3195	22	0
2	A	23	0	18	1	0
2	B	23	0	18	0	0
3	A	29	0	0	0	0
3	B	19	0	0	0	0
All	All	6558	0	6481	51	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 4.

All (51) 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:292:ARG:HG3	1:A:292:ARG:HH11	1.31	0.94
1:A:135:ASP:OD2	1:A:372:LYS:HE2	1.72	0.89
1:B:241:GLU:HG2	1:B:292:ARG:HH12	1.48	0.77
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.54	0.70
1:B:92:SER:HB2	1:B:186:LEU:O	1.97	0.63
1:A:190:ASN:HD22	1:A:193:VAL:H	1.47	0.62
1:A:251:LEU:HD21	1:A:258:LEU:HD22	1.82	0.62
1:A:438:PRO:HG2	1:A:462:ASN:HD22	1.68	0.59
1:A:427:THR:HG23	2:A:800:PNM:HC3	1.85	0.58
1:A:190:ASN:HD21	1:A:192:GLU:HG2	1.69	0.58
1:B:241:GLU:CG	1:B:292:ARG:HH12	2.17	0.57
1:B:485:ALA:HA	1:B:488:GLN:HE21	1.67	0.57
1:A:275:ARG:CG	1:A:275:ARG:HH11	2.18	0.56
1:A:199:GLN:NE2	1:A:203:ASP:OD2	2.41	0.53
1:B:361:ILE:HD11	1:B:389:ARG:NH1	2.24	0.52
1:A:292:ARG:CG	1:A:292:ARG:HH11	2.11	0.52
1:B:84:TYR:CE2	1:B:143:GLN:HG2	2.46	0.51
1:B:218:TYR:CE2	1:B:459:LEU:HD22	2.46	0.50
1:B:251:LEU:HD11	1:B:258:LEU:HD22	1.93	0.50
1:B:122:ASP:HA	1:B:125:THR:HG22	1.93	0.50
1:A:276:GLU:HG2	1:A:280:LYS:HE2	1.94	0.49
1:B:425:THR:HG22	1:B:443:TYR:HD1	1.78	0.49
1:A:53:GLY:HA3	1:A:132:GLY:O	2.13	0.48
1:A:312:ARG:HH11	1:A:312:ARG:HA	1.78	0.48
1:A:121:ALA:O	1:A:125:THR:HB	2.14	0.48
1:B:290:GLY:HA3	1:B:336:SER:OG	2.13	0.47
1:A:290:GLY:HA3	1:A:336:SER:OG	2.15	0.47
1:A:190:ASN:ND2	1:A:192:GLU:HG2	2.30	0.47
1:B:476:ALA:HB3	1:B:477:PRO:HD3	1.97	0.47
1:A:84:TYR:CE2	1:A:143:GLN:HG2	2.50	0.46
1:B:435:ARG:HE	1:B:435:ARG:HA	1.80	0.46
1:A:128:ASP:HA	1:A:129:PRO:HD3	1.86	0.45
1:A:441:ALA:HB1	1:A:471:GLY:HA2	1.99	0.44
1:B:50:ARG:HG3	1:B:129:PRO:HB2	2.00	0.44
1:A:308:ASP:OD2	1:A:323:VAL:HG12	2.19	0.43
1:A:115:LEU:HD21	1:A:379:ILE:HD11	2.00	0.43
1:A:292:ARG:NH1	1:A:292:ARG:HG3	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:HB2	1:A:399:LEU:HD11	2.00	0.42
1:B:152:GLN:HB2	1:B:152:GLN:HE21	1.57	0.42
1:A:108:LEU:O	1:A:131:GLY:HA3	2.19	0.42
1:B:219:PRO:HB2	1:B:428:ALA:HB1	2.01	0.42
1:B:304:ALA:HB1	1:B:390:ALA:HA	2.00	0.42
1:B:425:THR:HB	1:B:472:GLY:CA	2.49	0.42
1:A:192:GLU:O	1:A:196:GLN:HB2	2.20	0.42
1:A:82:GLU:HB3	1:A:180:SER:HB3	2.02	0.41
1:B:364:ARG:HD3	1:B:385:TYR:CE1	2.55	0.41
1:B:465:ASP:HB3	1:B:468:SER:O	2.21	0.41
1:A:269:GLU:CD	1:A:269:GLU:N	2.73	0.41
1:B:430:HIS:CE1	1:B:462:ASN:HD21	2.39	0.41
1:A:275:ARG:CG	1:A:275:ARG:NH1	2.82	0.41
1:B:364:ARG:HA	1:B:365:PRO:HD3	1.95	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	440/462 (95%)	429 (98%)	10 (2%)	1 (0%)	52	64
1	B	431/462 (93%)	416 (96%)	14 (3%)	1 (0%)	52	64
All	All	871/924 (94%)	845 (97%)	24 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	B	81	PRO

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	335/350 (96%)	318 (95%)	17 (5%)	29	39
1	B	330/350 (94%)	314 (95%)	16 (5%)	31	42
All	All	665/700 (95%)	632 (95%)	33 (5%)	30	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	66	VAL
1	A	125	THR
1	A	128	ASP
1	A	159	LYS
1	A	192	GLU
1	A	240	THR
1	A	258	LEU
1	A	275	ARG
1	A	292	ARG
1	A	309	SER
1	A	312	ARG
1	A	388	ARG
1	A	427	THR
1	A	432	THR
1	A	467	LEU
1	A	474	LEU
1	B	71	ARG
1	B	92	SER
1	B	109	ASN
1	B	118	ARG
1	B	123	PHE
1	B	152	GLN
1	B	186	LEU
1	B	199	GLN
1	B	241	GLU
1	B	248	THR

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Mol	Chain	Res	Type
1	B	254	SER
1	B	258	LEU
1	B	272	VAL
1	B	275	ARG
1	B	435	ARG
1	B	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	189	HIS
1	A	190	ASN
1	A	242	GLN
1	A	462	ASN
1	B	152	GLN
1	B	199	GLN
1	B	462	ASN
1	B	488	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PNM	A	800	1	17,24,24	2.88	3 (17%)	21,34,34	2.19	4 (19%)
2	PNM	B	800	1	17,24,24	2.96	3 (17%)	21,34,34	2.16	3 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNM	A	800	1	-	0/8/33/33	0/2/2/2
2	PNM	B	800	1	-	0/8/33/33	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	PNM	C2-S1	-4.13	1.77	1.85
2	A	800	PNM	C2-S1	-3.95	1.77	1.85
2	A	800	PNM	C15-N14	5.88	1.45	1.34
2	B	800	PNM	C15-N14	6.13	1.46	1.34
2	A	800	PNM	O16-C15	8.84	1.41	1.23
2	B	800	PNM	O16-C15	8.95	1.42	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	PNM	O16-C15-N14	-8.31	108.90	123.01
2	A	800	PNM	O16-C15-N14	-7.99	109.45	123.01
2	B	800	PNM	O16-C15-C17	-3.98	110.76	121.88
2	A	800	PNM	O16-C15-C17	-3.18	113.01	121.88
2	A	800	PNM	C17-C15-N14	-3.03	111.10	115.96
2	B	800	PNM	C5-C6-N14	2.22	114.75	109.57
2	A	800	PNM	C5-C6-N14	2.56	115.56	109.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	PNM	1	0

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	442/462 (95%)	-0.15	5 (1%) 82 86	33, 44, 64, 85	0
1	B	435/462 (94%)	-0.05	9 (2%) 67 74	36, 48, 73, 101	0
All	All	877/924 (94%)	-0.10	14 (1%) 74 80	33, 46, 70, 101	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	PHE	6.8
1	B	120	LEU	6.0
1	B	128	ASP	4.8
1	B	124	PHE	4.8
1	A	124	PHE	4.8
1	A	123	PHE	4.5
1	B	129	PRO	4.3
1	B	155	TYR	3.4
1	A	47	GLU	2.8
1	A	48	TYR	2.6
1	B	116	PHE	2.6
1	B	127	ARG	2.4
1	B	383	VAL	2.4
1	A	411	GLN	2.4

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PNM	B	800	23/23	0.90	0.19	1.57	47,50,69,69	0
2	PNM	A	800	23/23	0.91	0.14	0.39	42,47,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.