Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 06:32 PM EDT

PDB ID	:	4U3T
Title	:	Crystal structure of the transpeptidase domain of Neisseria gonorrhoeae penicillin-binding protein 2 derived from the penicillin-resistant strain 6140
Authors	:	Fedarovich, A.; Davies, C.
Deposited on	:	2014-07-22
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 (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:

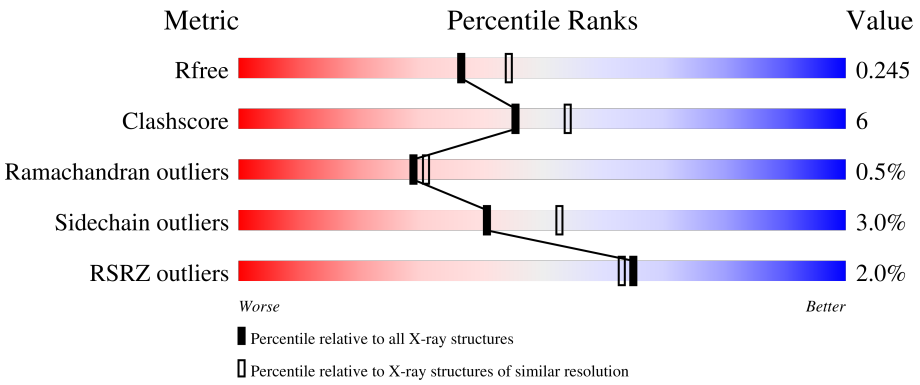
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	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	330	2% 82% 15% • •
1	B	330	2% 79% 15% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4911 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2443	1543	438	455	7	0	1	0
1	B	314	2376	1501	426	442	7	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP P08149
A	233	SER	-	expression tag	UNP P08149
A	234	GLY	-	expression tag	UNP P08149
A	235	GLY	-	expression tag	UNP P08149
A	236	ALA	-	expression tag	UNP P08149
A	?	-	ALA	deletion	UNP P08149
A	?	-	TYR	deletion	UNP P08149
A	?	-	ASP	deletion	UNP P08149
A	?	-	PRO	deletion	UNP P08149
A	?	-	ASN	deletion	UNP P08149
A	?	-	ARG	deletion	UNP P08149
A	?	-	PRO	deletion	UNP P08149
A	?	-	GLY	deletion	UNP P08149
A	?	-	ARG	deletion	UNP P08149
A	?	-	ALA	deletion	UNP P08149
A	?	-	ASP	deletion	UNP P08149
A	?	-	SER	deletion	UNP P08149
A	?	-	GLU	deletion	UNP P08149
A	?	-	GLN	deletion	UNP P08149
A	297	GLY	ARG	conflict	UNP P08149
A	346	ASP	-	insertion	UNP P08149
A	504	LEU	PHE	engineered mutation	UNP P08149
A	510	VAL	ALA	engineered mutation	UNP P08149
A	516	GLY	ALA	engineered mutation	UNP P08149
A	551	SER	PRO	engineered mutation	UNP P08149

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Chain	Residue	Modelled	Actual	Comment	Reference
B	232	GLY	-	expression tag	UNP P08149
B	233	SER	-	expression tag	UNP P08149
B	234	GLY	-	expression tag	UNP P08149
B	235	GLY	-	expression tag	UNP P08149
B	236	ALA	-	expression tag	UNP P08149
B	?	-	ALA	deletion	UNP P08149
B	?	-	TYR	deletion	UNP P08149
B	?	-	ASP	deletion	UNP P08149
B	?	-	PRO	deletion	UNP P08149
B	?	-	ASN	deletion	UNP P08149
B	?	-	ARG	deletion	UNP P08149
B	?	-	PRO	deletion	UNP P08149
B	?	-	GLY	deletion	UNP P08149
B	?	-	ARG	deletion	UNP P08149
B	?	-	ALA	deletion	UNP P08149
B	?	-	ASP	deletion	UNP P08149
B	?	-	SER	deletion	UNP P08149
B	?	-	GLU	deletion	UNP P08149
B	?	-	GLN	deletion	UNP P08149
B	297	GLY	ARG	conflict	UNP P08149
B	346	ASP	-	insertion	UNP P08149
B	504	LEU	PHE	engineered mutation	UNP P08149
B	510	VAL	ALA	engineered mutation	UNP P08149
B	516	GLY	ALA	engineered mutation	UNP P08149
B	551	SER	PRO	engineered mutation	UNP P08149

- Molecule 2 is water.

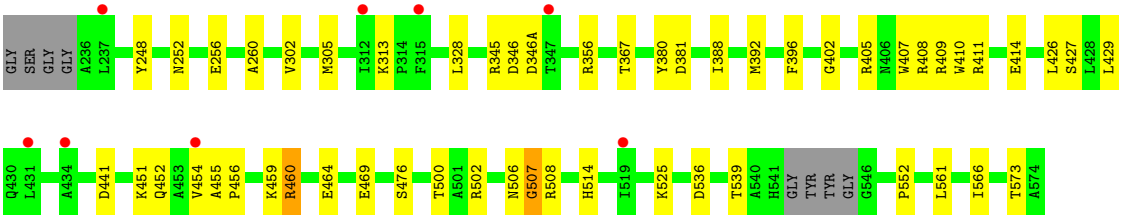
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	42	Total O 42 42	0	0

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.

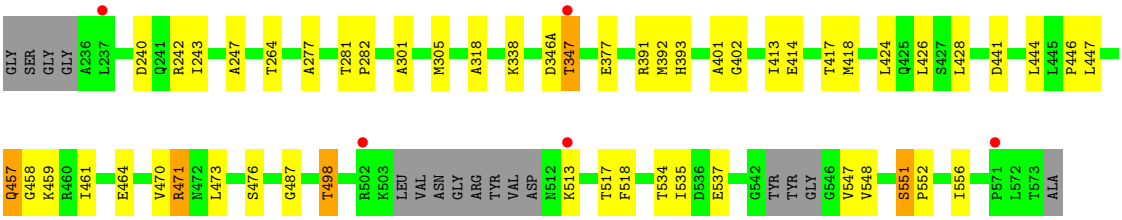
• Molecule 1: Penicillin-binding protein 2

Chain A:



• Molecule 1: Penicillin-binding protein 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.50Å 77.40Å 88.00Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	35.45 – 2.20 29.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.45-2.20) 96.6 (29.31-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.243 0.192 , 0.245	Depositor DCC
R_{free} test set	1496 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4911	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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)

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	0.52	0/2495	0.73	3/3381 (0.1%)
1	B	0.49	0/2421	0.68	1/3277 (0.0%)
All	All	0.50	0/4916	0.71	4/6658 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	471	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	460	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	460	ARG	CG-CD-NE	-5.02	101.26	111.80

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	2443	0	2481	34	0
1	B	2376	0	2413	32	0
2	A	50	0	0	2	0
2	B	42	0	0	1	0
All	All	4911	0	4894	62	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 6.

All (62) 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:441:ASP:OD1	1:B:471:ARG:NH1	2.02	0.93
1:B:281:THR:HB	1:B:282:PRO:HD2	1.66	0.76
1:B:305:MET:SD	1:B:402:GLY:HA2	2.29	0.73
1:B:457:GLN:OE1	1:B:458:GLY:N	2.26	0.68
1:A:305:MET:SD	1:A:402:GLY:HA2	2.35	0.67
1:B:457:GLN:OE1	1:B:457:GLN:HA	1.95	0.66
1:A:328:LEU:HD11	1:A:469:GLU:HG2	1.82	0.61
1:B:391:ARG:HG2	1:B:401:ALA:HA	1.81	0.61
1:A:459:LYS:HD3	1:B:377:GLU:HG2	1.81	0.60
1:B:414:GLU:O	1:B:418:MET:HG3	2.03	0.58
1:A:561:LEU:HD23	1:A:566:ILE:HD13	1.86	0.57
1:B:535:ILE:HG13	1:B:548:VAL:HG12	1.87	0.57
1:A:402:GLY:HA3	2:A:619:HOH:O	2.04	0.57
1:A:405:ARG:NH2	1:A:414:GLU:OE1	2.37	0.56
1:A:392:MET:HE1	1:A:429:LEU:HB3	1.88	0.56
1:A:345:ARG:HG2	1:A:346:ASP:O	2.07	0.55
1:A:506:ASN:HB3	1:A:507:GLY:HA2	1.89	0.54
1:B:444:LEU:HB2	1:B:461:ILE:HD12	1.90	0.53
1:A:454:VAL:HG13	1:A:455:ALA:C	2.30	0.52
1:B:428:LEU:HD13	1:B:534:THR:HG23	1.91	0.52
1:A:454:VAL:HG13	1:A:455:ALA:HA	1.92	0.52
1:A:455:ALA:HB1	1:A:456:PRO:CD	2.40	0.51
1:B:402:GLY:HA3	2:B:610:HOH:O	2.09	0.51
1:B:240:ASP:OD2	1:B:242:ARG:NH2	2.33	0.51
1:A:506:ASN:HB3	1:A:507:GLY:CA	2.42	0.50
1:B:517:THR:OG1	1:B:534:THR:HG22	2.12	0.50
1:B:391:ARG:CG	1:B:401:ALA:HA	2.41	0.50
1:B:247:ALA:HA	1:B:556:ILE:HG12	1.95	0.49
1:B:457:GLN:OE1	1:B:457:GLN:CA	2.61	0.49
1:A:408:ARG:HD3	1:B:392:MET:O	2.13	0.48
1:A:411:ARG:HG2	1:A:411:ARG:HH11	1.78	0.47
1:A:454:VAL:HG13	1:A:455:ALA:CA	2.44	0.47
1:A:525:LYS:HD3	2:A:644:HOH:O	2.14	0.47
1:B:498:THR:HB	1:B:518:PHE:CD2	2.50	0.47
1:B:473:LEU:O	1:B:476:SER:HB2	2.15	0.47
1:A:507:GLY:O	1:A:508:ARG:C	2.52	0.46
1:A:441:ASP:HB3	1:A:464:GLU:HG2	1.98	0.45
1:B:264:THR:HG21	1:B:301:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG11	1:A:396:PHE:HB2	1.99	0.44
1:A:381:ASP:OD1	1:B:459:LYS:HD2	2.18	0.43
1:B:551:SER:N	1:B:552:PRO:HD2	2.33	0.43
1:A:356:ARG:NH1	1:A:476:SER:HB3	2.32	0.43
1:B:243:ILE:HG22	1:B:277:ALA:HB2	2.01	0.42
1:A:305:MET:HE1	1:A:427:SER:HB3	2.01	0.42
1:A:248:TYR:CZ	1:A:252:ASN:ND2	2.88	0.41
1:B:487:GLY:HA3	1:B:518:PHE:CZ	2.55	0.41
1:B:513:LYS:HB3	1:B:537:GLU:HG2	2.02	0.41
1:A:313:LYS:HG2	1:A:367:THR:HG21	2.01	0.41
1:B:318:ALA:HB2	1:B:470:VAL:HG21	2.02	0.41
1:B:338:LYS:HB2	1:B:338:LYS:HE3	1.89	0.41
1:A:455:ALA:HB1	1:A:456:PRO:HD3	2.02	0.41
1:A:380:TYR:HB2	1:A:407:TRP:HB3	2.02	0.41
1:A:561:LEU:HA	1:A:566:ILE:HD12	2.03	0.41
1:B:413:ILE:HG13	1:B:417:THR:HG23	2.03	0.41
1:A:388:ILE:HG12	1:A:426:LEU:HD13	2.02	0.41
1:A:407:TRP:HA	1:A:410:TRP:CD1	2.56	0.41
1:A:409:ARG:HD2	1:B:393:HIS:CE1	2.54	0.41
1:A:260:ALA:HB1	1:A:536:ASP:O	2.21	0.40
1:B:446:PRO:O	1:B:447:LEU:HB2	2.21	0.40
1:A:502:ARG:HD3	1:A:514:HIS:CE1	2.56	0.40
1:B:441:ASP:HB3	1:B:464:GLU:HG3	2.03	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	319/330 (97%)	311 (98%)	7 (2%)	1 (0%)	41 46
1	B	308/330 (93%)	300 (97%)	6 (2%)	2 (1%)	25 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	627/660 (95%)	611 (97%)	13 (2%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	347	THR
1	A	507	GLY
1	B	346(A)	ASP

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	257/259 (99%)	249 (97%)	8 (3%)	40	51
1	B	249/259 (96%)	242 (97%)	7 (3%)	43	56
All	All	506/518 (98%)	491 (97%)	15 (3%)	41	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	A	346(A)	ASP
1	A	451	LYS
1	A	452	GLN
1	A	460	ARG
1	A	500	THR
1	A	539	THR
1	A	573	THR
1	B	347	THR
1	B	424	LEU
1	B	426	LEU
1	B	457	GLN
1	B	498	THR
1	B	547	VAL
1	B	551	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	HIS
1	A	393	HIS
1	A	514	HIS
1	B	393	HIS

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)

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	322/330 (97%)	-0.16	8 (2%)	57	55	26, 38, 63, 87	0
1	B	314/330 (95%)	-0.14	5 (1%)	72	70	27, 41, 63, 80	0
All	All	636/660 (96%)	-0.15	13 (2%)	65	63	26, 39, 63, 87	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	THR	4.8
1	A	454	VAL	4.5
1	B	347	THR	3.6
1	A	237	LEU	3.3
1	B	237	LEU	3.2
1	B	571	PRO	2.5
1	A	312	ILE	2.5
1	B	513	LYS	2.4
1	A	431	LEU	2.3
1	A	519	ILE	2.3
1	A	315	PHE	2.2
1	B	502	ARG	2.2
1	A	434	ALA	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.