



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

PDB ID : 2FFF
Title : Open Form of a Class A Transpeptidase Domain
Authors : Lovering, A.L.; Strynadka, N.C.J.
Deposited on : 2005-12-19
Resolution : 2.23 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

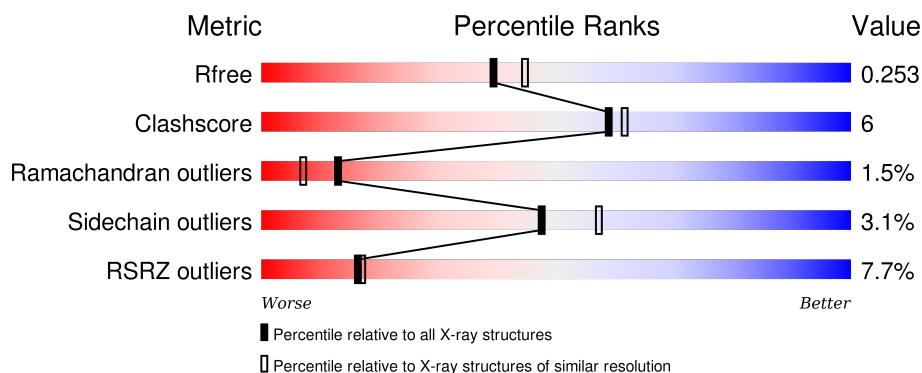
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	15	<div> <div>13%</div> <div>87%</div> <div>13%</div> </div>
2	B	453	<div> <div>8%</div> <div>88%</div> <div>10%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3849 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 1B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	0	0	0
			109	69	15	25			

- Molecule 2 is a protein called penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	453	Total	C	N	O	S	0	0	0
			3507	2193	601	698	15			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		

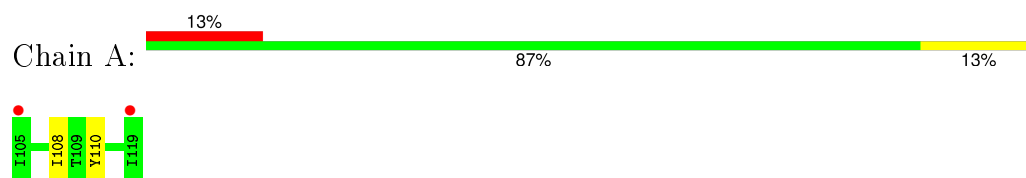
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	232	Total	O	0	0
			232	232		

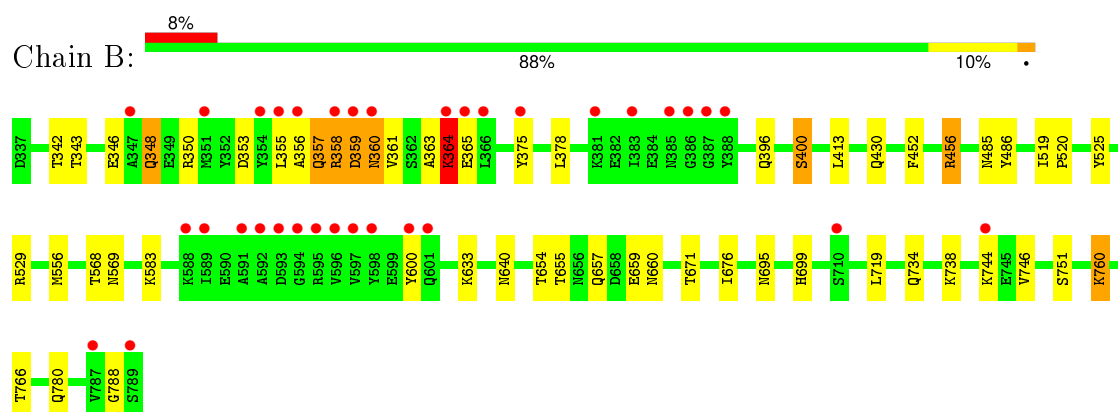
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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 1B



- Molecule 2: penicillin-binding protein 1B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.66Å 78.04Å 60.31Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	39.00 – 2.23 39.02 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.00-2.23) 99.5 (39.02-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.246 0.193 , 0.253	Depositor DCC
R_{free} test set	1405 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27505 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3849	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% 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: NI

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	0.46	0/109	0.59	0/148
2	B	0.61	0/3580	0.67	2/4857 (0.0%)
All	All	0.60	0/3689	0.67	2/5005 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	456	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	B	456	ARG	NE-CZ-NH2	5.32	122.96	120.30

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	109	0	108	3	0
2	B	3507	0	3383	41	0
3	B	1	0	0	0	0
4	B	232	0	0	6	0
All	All	3849	0	3491	41	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 (41) 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)
2:B:356:ALA:C	2:B:357:GLN:OE1	2.06	0.93
1:A:108:ILE:HG21	2:B:343:THR:HG21	1.57	0.86
2:B:353:ASP:O	2:B:357:GLN:NE2	2.09	0.85
2:B:357:GLN:OE1	2:B:357:GLN:N	2.12	0.81
2:B:485:ASN:HD22	2:B:520:PRO:HD3	1.50	0.76
1:A:108:ILE:CG2	2:B:343:THR:HG21	2.16	0.74
2:B:348:GLN:NE2	4:B:115:HOH:O	2.30	0.64
2:B:430:GLN:NE2	4:B:132:HOH:O	2.32	0.62
2:B:760:LYS:HD3	2:B:760:LYS:N	2.19	0.57
2:B:360:ASN:HB2	2:B:375:TYR:OH	2.05	0.57
2:B:355:LEU:HD13	2:B:378:LEU:HG	1.86	0.56
2:B:569:ASN:HD21	2:B:583:LYS:H	1.53	0.55
2:B:456:ARG:HD2	2:B:660:ASN:OD1	2.07	0.54
2:B:655:THR:HG22	2:B:659:GLU:OE2	2.07	0.54
2:B:734:GLN:HE21	2:B:766:THR:HA	1.73	0.53
2:B:760:LYS:HD3	2:B:760:LYS:H	1.74	0.52
2:B:734:GLN:NE2	2:B:766:THR:HA	2.26	0.51
2:B:525:TYR:CE2	2:B:529:ARG:HD2	2.47	0.50
2:B:600:TYR:HE1	4:B:116:HOH:O	1.96	0.49
2:B:485:ASN:ND2	2:B:520:PRO:HD3	2.25	0.49
2:B:357:GLN:N	2:B:357:GLN:CD	2.66	0.48
2:B:569:ASN:ND2	2:B:583:LYS:H	2.11	0.48
2:B:359:ASP:O	2:B:360:ASN:CB	2.62	0.47
2:B:760:LYS:CD	2:B:760:LYS:H	2.27	0.46
2:B:695:ASN:O	2:B:699:HIS:HD2	1.99	0.46
2:B:633:LYS:HD2	4:B:171:HOH:O	2.15	0.45
2:B:355:LEU:C	2:B:357:GLN:N	2.71	0.44
2:B:358:ARG:NE	2:B:359:ASP:OD1	2.51	0.44
2:B:342:THR:HG21	2:B:452:PHE:CE2	2.53	0.44
2:B:348:GLN:HG3	4:B:26:HOH:O	2.18	0.43
2:B:358:ARG:HG2	2:B:359:ASP:N	2.34	0.43
2:B:396:GLN:O	2:B:400:SER:HB3	2.19	0.42
2:B:363:ALA:HB1	2:B:364:LYS:HD2	2.00	0.42
2:B:356:ALA:O	2:B:357:GLN:OE1	2.34	0.41
2:B:486:TYR:O	2:B:519:ILE:HD13	2.20	0.41
2:B:738:LYS:HA	2:B:746:VAL:O	2.20	0.41
2:B:413:LEU:HD22	2:B:676:ILE:HG21	2.01	0.41
2:B:780:GLN:NE2	4:B:185:HOH:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:TYR:CZ	2:B:396:GLN:HG2	2.55	0.40
2:B:346:GLU:O	2:B:350:ARG:HG2	2.20	0.40
2:B:568:THR:HG23	2:B:671:THR:HG22	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	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
2	B	451/453 (100%)	428 (95%)	16 (4%)	7 (2%)	12	6
All	All	464/468 (99%)	440 (95%)	17 (4%)	7 (2%)	13	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	358	ARG
2	B	360	ASN
2	B	364	LYS
2	B	365	GLU
2	B	744	LYS
2	B	359	ASP
2	B	788	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	A	13/13 (100%)	13 (100%)	0	100	100
2	B	372/372 (100%)	360 (97%)	12 (3%)	46	56
All	All	385/385 (100%)	373 (97%)	12 (3%)	47	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	348	GLN
2	B	357	GLN
2	B	361	VAL
2	B	364	LYS
2	B	400	SER
2	B	556	MET
2	B	640	ASN
2	B	654	THR
2	B	657	GLN
2	B	719	LEU
2	B	751	SER
2	B	760	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	360	ASN
2	B	372	GLN
2	B	399	HIS
2	B	424	ASN
2	B	442	ASN
2	B	444	GLN
2	B	448	ASN
2	B	485	ASN
2	B	494	ASN
2	B	514	ASN
2	B	531	ASN
2	B	569	ASN
2	B	606	GLN
2	B	635	ASN
2	B	640	ASN
2	B	699	HIS

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Mol	Chain	Res	Type
2	B	734	GLN
2	B	780	GLN

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 ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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(Å ²)	Q<0.9
1	A	15/15 (100%)	1.20	2 (13%) 4 4	50, 54, 59, 59	0
2	B	453/453 (100%)	0.34	34 (7%) 17 18	25, 33, 55, 63	0
All	All	468/468 (100%)	0.36	36 (7%) 16 17	25, 33, 57, 63	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	ASN	6.1
2	B	594	GLY	5.6
2	B	595	ARG	4.8
2	B	593	ASP	4.8
2	B	385	ASN	4.4
2	B	355	LEU	4.3
2	B	592	ALA	4.2
2	B	591	ALA	4.0
2	B	386	GLY	4.0
1	A	119	ILE	3.8
2	B	358	ARG	3.6
2	B	381	LYS	3.6
2	B	383	ILE	3.5
1	A	105	ILE	3.3
2	B	596	VAL	3.3
2	B	366	LEU	3.2
2	B	787	VAL	3.2
2	B	744	LYS	3.0
2	B	354	TYR	3.0
2	B	351	MET	2.9
2	B	375	TYR	2.9
2	B	589	ILE	2.8
2	B	789	SER	2.8
2	B	597	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	359	ASP	2.8
2	B	347	ALA	2.8
2	B	356	ALA	2.7
2	B	387	GLY	2.7
2	B	600	TYR	2.6
2	B	365	GLU	2.3
2	B	388	TYR	2.3
2	B	598	TYR	2.3
2	B	710	SER	2.1
2	B	601	GLN	2.1
2	B	588	LYS	2.1
2	B	364	LYS	2.0

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(Å ²)	Q<0.9
3	NI	B	901	1/1	0.98	0.12	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.