Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2021 – 08:05 am GMT

PDB ID	:	6YN0
Title	:	Structure of E. coli PBP1b with a FtsN peptide activating transglycosylase activity
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Deposited on	:	2020-04-10
Resolution	:	2.40 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 ①) were used in the production of this report:

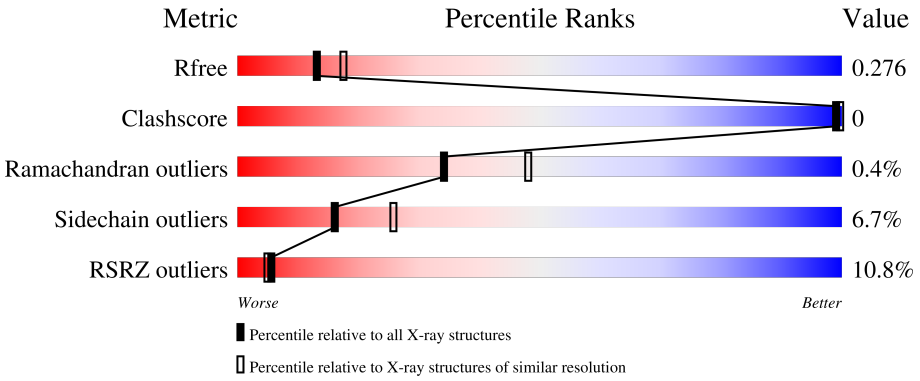
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	747	10% 86% 6% 8%
2	B	19	16% 63% 5% 32%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11288 atoms, of which 5631 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.

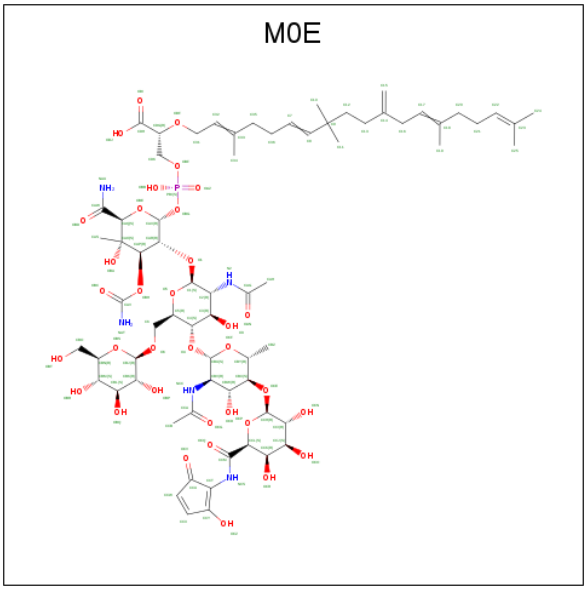
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	689	Total	C	H	N	O	S	7	0	0
			10857	3423	5454	953	1001	26			

- Molecule 2 is a protein called Cell division protein FtsN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	H	N	O	2	0	0
			239	78	117	21	23			

- Molecule 3 is MOENOMYCIN (three-letter code: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			137	39	60	5	32	1		

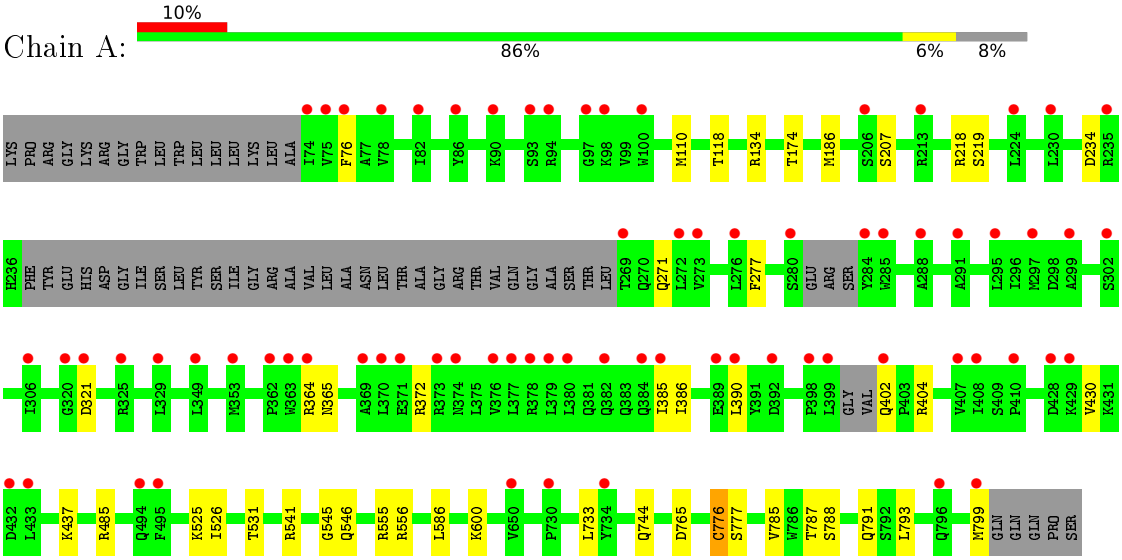
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0

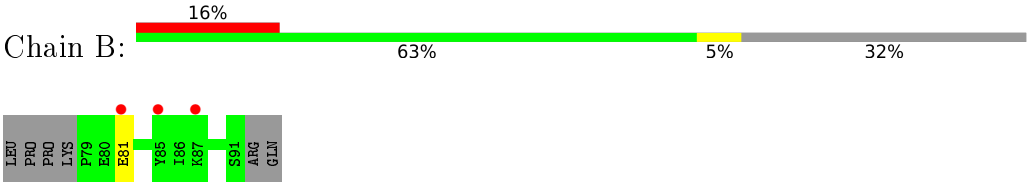
3 Residue-property plots (i)

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 1B



- Molecule 2: Cell division protein FtsN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.14Å 283.02Å 62.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.40 47.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	57.3 (47.17-2.40) 57.3 (47.11-2.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.225 , 0.256 0.242 , 0.276	Depositor DCC
R_{free} test set	1320 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.067 for l,-k,h	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11288	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

Bond lengths and bond angles in the following residue types are not validated in this section: M0E

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	0.38	0/5510	0.56	0/7475
2	B	0.39	0/125	0.47	0/166
All	All	0.38	0/5635	0.56	0/7641

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	5403	5454	5446	3	0
2	B	122	117	116	0	0
3	A	77	60	59	0	0
4	A	55	0	0	0	0
All	All	5657	5631	5621	3	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 0.

All (3) 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:776:CYS:HA	1:A:793:LEU:HD13	1.90	0.53
1:A:776:CYS:HB3	1:A:793:LEU:HD13	1.98	0.45
1:A:386:ILE:HG23	1:A:390:LEU:HD11	2.02	0.41

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	681/747 (91%)	641 (94%)	37 (5%)	3 (0%)	34 48
2	B	11/19 (58%)	11 (100%)	0	0	100 100
All	All	692/766 (90%)	652 (94%)	37 (5%)	3 (0%)	34 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ILE
1	A	545	GLY
1	A	430	VAL

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	581/627 (93%)	542 (93%)	39 (7%)	16 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	13/19 (68%)	12 (92%)	1 (8%)	13 20
All	All	594/646 (92%)	554 (93%)	40 (7%)	16 26

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	110	MET
1	A	118	THR
1	A	134	ARG
1	A	174	THR
1	A	186	MET
1	A	207	SER
1	A	218	ARG
1	A	219	SER
1	A	234	ASP
1	A	271	GLN
1	A	277	PHE
1	A	321	ASP
1	A	364	ARG
1	A	365	ASN
1	A	372	ARG
1	A	402	GLN
1	A	404	ARG
1	A	437	LYS
1	A	485	ARG
1	A	525	LYS
1	A	526	ILE
1	A	531	THR
1	A	541	ARG
1	A	546	GLN
1	A	555	ARG
1	A	556	ARG
1	A	586	LEU
1	A	600	LYS
1	A	733	LEU
1	A	744	GLN
1	A	765	ASP
1	A	776	CYS
1	A	777	SER
1	A	785	VAL
1	A	787	THR

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Mol	Chain	Res	Type
1	A	788	SER
1	A	791	GLN
1	A	799	MET
2	B	81	GLU

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

1 ligand is modelled in this entry.

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, 95^{th} 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	689/747 (92%)	0.44	73 (10%) 6 5	26, 60, 153, 169	0
2	B	13/19 (68%)	1.10	3 (23%) 0 0	107, 122, 140, 143	0
All	All	702/766 (91%)	0.45	76 (10%) 5 5	26, 61, 153, 169	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ALA	7.7
1	A	369	ALA	7.1
1	A	285	TRP	6.6
1	A	213	ARG	6.4
1	A	382	GLN	6.3
1	A	284	TYR	5.9
1	A	76	PHE	5.4
2	B	85	TYR	5.4
1	A	206	SER	5.1
1	A	74	ILE	5.0
1	A	329	LEU	4.8
1	A	734	TYR	4.8
1	A	320	GLY	4.6
1	A	392	ASP	4.6
1	A	380	LEU	4.6
1	A	98	LYS	4.6
1	A	432	ASP	4.5
1	A	363	TRP	4.5
1	A	306	ILE	4.5
1	A	321	ASP	4.5
1	A	93	SER	4.4
1	A	799	MET	4.4
1	A	370	LEU	4.1
1	A	276	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	4.0
1	A	399	LEU	4.0
1	A	495	PHE	3.9
1	A	100	TRP	3.9
1	A	371	GLU	3.8
1	A	97	GLY	3.7
1	A	433	LEU	3.7
1	A	295	LEU	3.7
1	A	378	ARG	3.5
1	A	407	VAL	3.5
1	A	408	ILE	3.5
1	A	90	LYS	3.5
1	A	273	VAL	3.4
1	A	390	LEU	3.4
1	A	796	GLN	3.3
1	A	384	GLN	3.3
1	A	235	ARG	3.2
1	A	291	ALA	3.2
1	A	650	VAL	3.2
1	A	94	ARG	3.1
1	A	373	ARG	3.1
1	A	224	LEU	3.1
2	B	87	LYS	3.0
1	A	385	ILE	2.9
1	A	349	LEU	2.9
1	A	86	TYR	2.8
1	A	428	ASP	2.7
1	A	429	LYS	2.7
1	A	376	VAL	2.7
1	A	82	ILE	2.7
1	A	269	THR	2.6
1	A	402	GLN	2.6
1	A	272	LEU	2.6
1	A	302	SER	2.6
1	A	230	LEU	2.5
1	A	280	SER	2.5
1	A	362	PRO	2.5
1	A	364	ARG	2.5
1	A	377	LEU	2.4
1	A	78	VAL	2.4
2	B	81	GLU	2.4
1	A	398	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	75	VAL	2.3
1	A	730	PRO	2.3
1	A	410	PRO	2.2
1	A	297	MET	2.2
1	A	299	ALA	2.2
1	A	389	GLU	2.2
1	A	374	ASN	2.1
1	A	353	MET	2.1
1	A	494	GLN	2.1
1	A	325	ARG	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 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, 95^{th} 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
3	M0E	A	901	77/109	0.77	0.19	142,152,156,156	0

6.5 Other polymers (i)

There are no such residues in this entry.