



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8U55 / pdb_00008u55
Title : Crystal structure of Enterococcus faecium EnGen25 Penicillin-binding protein 5 (PBP5)
Authors : Pemberton, O.A.; Shamoo, Y.
Deposited on : 2023-09-12
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

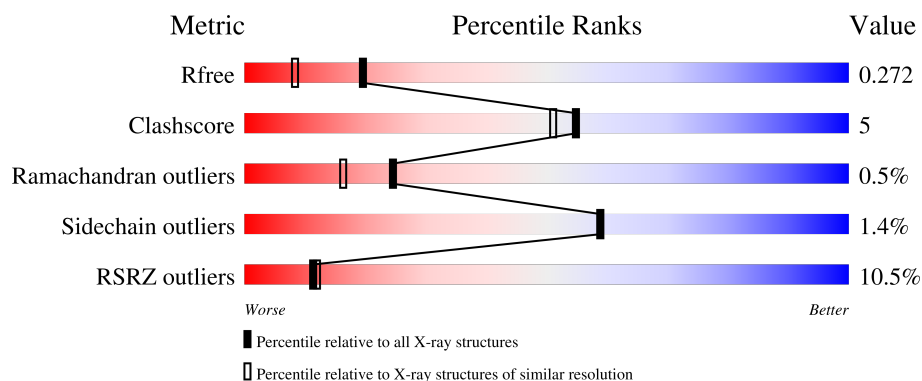
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	664	10% 81% 12% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5033 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	1	0
			4766	2988	786	980	12			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP M1RM73
A	16	ALA	-	expression tag	UNP M1RM73
A	17	HIS	-	expression tag	UNP M1RM73
A	18	HIS	-	expression tag	UNP M1RM73
A	19	HIS	-	expression tag	UNP M1RM73
A	20	HIS	-	expression tag	UNP M1RM73
A	21	HIS	-	expression tag	UNP M1RM73
A	22	HIS	-	expression tag	UNP M1RM73
A	23	ASP	-	expression tag	UNP M1RM73
A	24	TYR	-	expression tag	UNP M1RM73
A	25	ASP	-	expression tag	UNP M1RM73
A	26	ILE	-	expression tag	UNP M1RM73
A	27	PRO	-	expression tag	UNP M1RM73
A	28	THR	-	expression tag	UNP M1RM73
A	29	THR	-	expression tag	UNP M1RM73
A	30	GLU	-	expression tag	UNP M1RM73
A	31	ASN	-	expression tag	UNP M1RM73
A	32	LEU	-	expression tag	UNP M1RM73
A	33	TYR	-	expression tag	UNP M1RM73
A	34	PHE	-	expression tag	UNP M1RM73
A	35	GLN	-	expression tag	UNP M1RM73
A	36	GLY	-	expression tag	UNP M1RM73
A	497	PHE	LEU	conflict	UNP M1RM73

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	267	Total 267	O 267	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.23Å 62.23Å 372.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 1.90 44.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.00-1.90) 91.1 (44.00-1.90)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.226 , 0.274 0.226 , 0.272	Depositor DCC
R_{free} test set	3042 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5033	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.333 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	0.38	0/4837	0.62	4/6535 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	VAL	N-CA-C	-11.82	90.85	108.46
1	A	466	SER	N-CA-C	7.63	120.02	109.18
1	A	467	ASP	N-CA-C	6.07	119.68	107.41
1	A	540	GLN	CB-CA-C	-5.02	109.84	117.07

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	4766	0	4712	45	0
2	A	267	0	0	2	0
All	All	5033	0	4712	45	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.

All (45) 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:560:ASN:ND2	1:A:583:GLU:OE1	2.27	0.66
1:A:452:GLN:HG3	1:A:457:TRP:HB2	1.83	0.60
1:A:369:THR:HG22	1:A:376:LEU:HD23	1.85	0.58
1:A:423:THR:O	1:A:426:MET:HG2	2.05	0.57
1:A:649:MET:HE2	1:A:669:LEU:HD23	1.88	0.55
1:A:283:ALA:HA	1:A:286:ILE:HD12	1.89	0.55
1:A:584:THR:HG23	1:A:585:ALA:H	1.73	0.53
1:A:635:SER:HB2	1:A:656:LYS:HD3	1.90	0.53
1:A:178:ASP:HB2	1:A:347:ILE:O	2.09	0.53
1:A:200:LEU:HD12	1:A:254:GLY:HA3	1.90	0.52
1:A:53:VAL:HG21	1:A:101:ILE:HG21	1.92	0.52
1:A:389:LYS:N	1:A:389:LYS:HD3	2.25	0.51
1:A:536:THR:HG23	1:A:543:LEU:HG	1.93	0.51
1:A:269:GLU:HB2	1:A:384:SER:HB3	1.94	0.49
1:A:222:ASP:O	1:A:226:GLN:HG3	2.13	0.48
1:A:300:ARG:C	1:A:305:MET:HE3	2.39	0.48
1:A:426:MET:HE1	1:A:638:PHE:CD2	2.49	0.48
1:A:99:LEU:HD13	1:A:122:MET:HE2	1.96	0.47
1:A:193:LEU:HB2	1:A:244:ILE:HD13	1.96	0.47
1:A:572:LYS:HB3	1:A:572:LYS:HE2	1.50	0.47
1:A:353:LYS:NZ	1:A:357:ASP:OD1	2.43	0.47
1:A:297:LYS:HE2	2:A:792:HOH:O	2.14	0.47
1:A:129:LEU:HG	1:A:333:ILE:HD11	1.98	0.46
1:A:167:THR:O	1:A:317:GLY:HA3	2.16	0.46
1:A:234:GLN:HB2	1:A:237:TYR:CE2	2.51	0.45
1:A:460:TYR:OH	1:A:535:ASP:OD1	2.27	0.45
1:A:65:ALA:HB1	1:A:80:GLU:HG3	1.99	0.45
1:A:425:LYS:HB2	1:A:425:LYS:HE2	1.73	0.45
1:A:244:ILE:HD11	1:A:257:ILE:HD11	1.98	0.45
1:A:336:GLU:H	1:A:336:GLU:HG2	1.56	0.44
1:A:575:LYS:HB2	1:A:575:LYS:HE2	1.72	0.44
1:A:390:MET:HE1	1:A:399:TYR:CD2	2.54	0.43
1:A:466:SER:OG	1:A:467:ASP:N	2.51	0.43
1:A:53:VAL:HG11	1:A:101:ILE:HG23	2.00	0.43
1:A:652:MET:HE2	1:A:652:MET:HB3	1.90	0.43
1:A:457:TRP:HA	1:A:531:ILE:HD11	2.01	0.42
1:A:106:VAL:HA	1:A:115:SER:O	2.19	0.42
1:A:191:LYS:HB2	1:A:244:ILE:O	2.20	0.42
1:A:108:LYS:HE3	1:A:114:TYR:CZ	2.55	0.42
1:A:212:ALA:O	1:A:216:SER:HB3	2.19	0.42
1:A:468:VAL:HG11	1:A:479[B]:TYR:CD2	2.55	0.41
1:A:591:PRO:HG3	2:A:916:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASP:OD1	1:A:297:LYS:HE3	2.20	0.41
1:A:79:SER:N	1:A:82:GLU:OE1	2.39	0.41
1:A:121:LYS:HB3	1:A:121:LYS:HE2	1.78	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	615/664 (93%)	590 (96%)	22 (4%)	3 (0%)	24 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	SER
1	A	231	SER
1	A	230	GLN

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	516/551 (94%)	509 (99%)	7 (1%)	59 59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	A	110	ASP
1	A	125	SER
1	A	465	VAL
1	A	468	VAL
1	A	480	SER
1	A	572	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	335	HIS
1	A	338	GLN
1	A	396	GLN
1	A	520	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 oligosaccharides 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 ⓘ

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	622/664 (93%)	0.84	65 (10%)	11 12	17, 44, 74, 96	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	THR	4.2
1	A	145	THR	4.2
1	A	230	GLN	4.1
1	A	245	ASP	4.1
1	A	394	ILE	4.0
1	A	106	VAL	3.8
1	A	286	ILE	3.8
1	A	217	PHE	3.7
1	A	114	TYR	3.6
1	A	222	ASP	3.6
1	A	244	ILE	3.5
1	A	288	LYS	3.4
1	A	289	ASN	3.1
1	A	255	ALA	3.1
1	A	233	VAL	3.0
1	A	44	ALA	3.0
1	A	401	ALA	3.0
1	A	200	LEU	3.0
1	A	237	TYR	3.0
1	A	571	ASP	3.0
1	A	290	PRO	3.0
1	A	283	ALA	3.0
1	A	251	LEU	2.9
1	A	528	ASN	2.9
1	A	232	TRP	2.9
1	A	231	SER	2.9
1	A	337	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	2.8
1	A	256	THR	2.8
1	A	257	ILE	2.8
1	A	195	VAL	2.7
1	A	291	GLU	2.6
1	A	223	ALA	2.6
1	A	193	LEU	2.5
1	A	140	ARG	2.5
1	A	250	GLU	2.4
1	A	623	ILE	2.4
1	A	584	THR	2.4
1	A	468	VAL	2.4
1	A	216	SER	2.4
1	A	219	LEU	2.4
1	A	236	ASP	2.4
1	A	658	ASP	2.4
1	A	227	ALA	2.4
1	A	43	GLU	2.4
1	A	389	LYS	2.3
1	A	287	ASP	2.3
1	A	138	LEU	2.2
1	A	533	LEU	2.2
1	A	622	GLU	2.2
1	A	467	ASP	2.2
1	A	336	GLU	2.2
1	A	235	PRO	2.2
1	A	402	TYR	2.2
1	A	104	LEU	2.2
1	A	123	ASN	2.1
1	A	465	VAL	2.1
1	A	224	ILE	2.1
1	A	399	TYR	2.1
1	A	161	ASN	2.1
1	A	95	ASP	2.1
1	A	190	LEU	2.1
1	A	439	ASP	2.1
1	A	198	SER	2.0
1	A	260	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.