



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 07:22 PM EDT

PDB ID : 8F3Q
Title : Crystal structure of Penicillin Binding Protein 5 (PBP5) Y460A variant apo form from *Enterococcus faecium*
Authors : D'Andrea, E.D.; Schoenle, M.V.; Choy, M.S.; Page, R.; Peti, W.
Deposited on : 2022-11-10
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

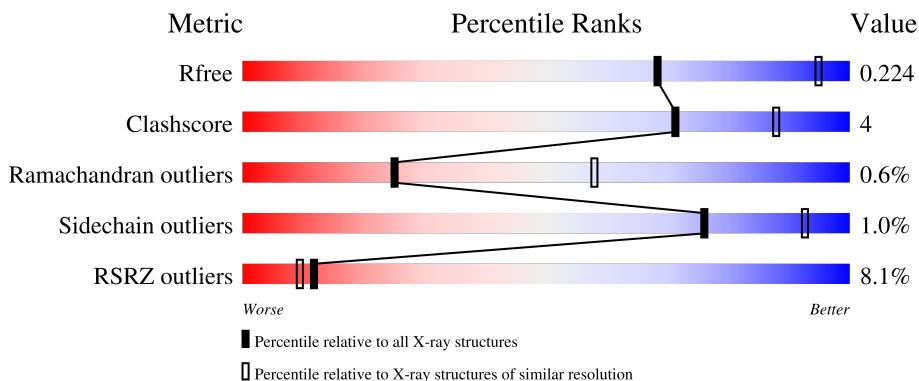
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	645	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	721	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4996 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
			Total	C	N	O	S			
1	A	640	4756	2982	781	981	12	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP G5CKR9
A	35	HIS	-	expression tag	UNP G5CKR9
A	36	MET	-	expression tag	UNP G5CKR9
A	460	ALA	TYR	engineered mutation	UNP G5CKR9
A	586	VAL	LEU	conflict	UNP G5CKR9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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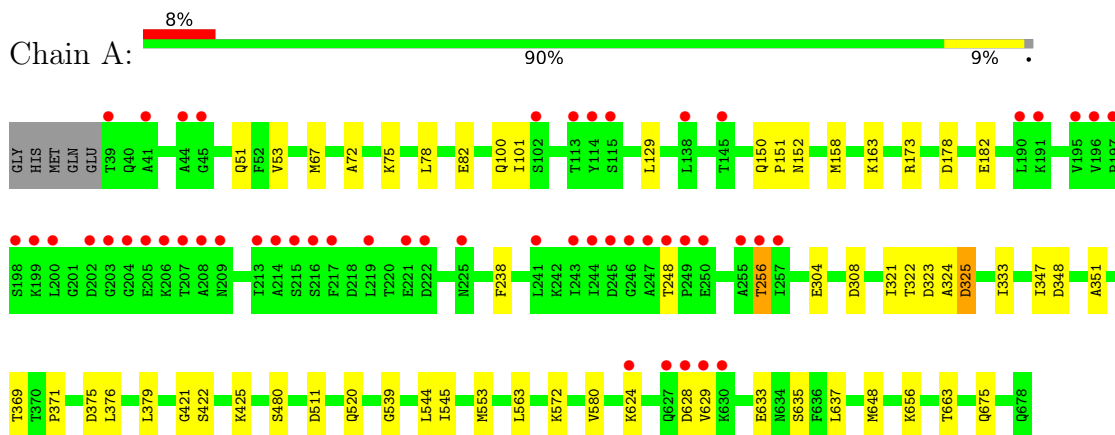
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	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 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.44Å 192.44Å 156.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.78 – 2.90 39.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.78-2.90) 99.3 (39.78-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.19.1-4122	Depositor
R, R_{free}	0.202 , 0.222 0.204 , 0.224	Depositor DCC
R_{free} test set	1863 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.24	0/4829	0.44	0/6557

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 [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	4756	0	4571	33	0
2	A	110	0	0	0	0
3	A	130	0	0	1	0
All	All	4996	0	4571	33	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 (33) 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:173:ARG:NH2	1:A:308:ASP:OD1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NH1	1:A:304:GLU:OE1	2.33	0.62
1:A:78:LEU:HD23	1:A:82:GLU:HB3	1.84	0.60
1:A:129:LEU:HB2	1:A:333:ILE:HD11	1.84	0.59
1:A:637:LEU:HD22	1:A:663:THR:HA	1.84	0.59
1:A:323:ASP:O	1:A:325:ASP:N	2.40	0.55
1:A:369:THR:HG22	1:A:376:LEU:HD23	1.90	0.53
1:A:150:GLN:HG3	1:A:151:PRO:HD2	1.92	0.52
1:A:376:LEU:HD13	1:A:379:LEU:HD11	1.92	0.51
1:A:323:ASP:O	3:A:801:HOH:O	2.19	0.51
1:A:53:VAL:HG21	1:A:101:ILE:HD13	1.93	0.51
1:A:51:GLN:HB2	1:A:67:MET:HE1	1.93	0.50
1:A:422:SER:HB2	1:A:425:LYS:HZ1	1.77	0.49
1:A:563:LEU:HB2	1:A:580:VAL:HG21	1.96	0.47
1:A:178:ASP:OD1	1:A:182:GLU:N	2.47	0.47
1:A:72:ALA:HB3	1:A:75:LYS:HB2	1.98	0.46
1:A:150:GLN:HB3	1:A:152:ASN:OD1	2.17	0.45
1:A:425:LYS:NZ	1:A:480:SER:OG	2.50	0.44
1:A:520:GLN:HG2	1:A:544:LEU:HB2	1.99	0.44
1:A:511:ASP:OD2	1:A:572:LYS:NZ	2.46	0.44
1:A:53:VAL:HG11	1:A:101:ILE:HG23	2.00	0.44
1:A:348:ASP:HB3	1:A:351:ALA:HB3	2.00	0.44
1:A:376:LEU:HD22	1:A:379:LEU:HD21	1.99	0.44
1:A:635:SER:HB2	1:A:656:LYS:HD2	2.00	0.43
1:A:633:GLU:O	1:A:656:LYS:HG2	2.19	0.42
1:A:163:LYS:HB2	1:A:322:THR:OG1	2.20	0.42
1:A:158:MET:HG2	1:A:321:ILE:HD13	2.01	0.42
1:A:371:PRO:HB3	1:A:648:MET:HE2	2.02	0.41
1:A:178:ASP:HB2	1:A:347:ILE:O	2.19	0.41
1:A:421:GLY:O	1:A:539:GLY:HA3	2.21	0.41
1:A:545:ILE:HD13	1:A:553:MET:HE1	2.03	0.40
1:A:238:PHE:HE1	1:A:256:THR:HG23	1.86	0.40
1:A:624:LYS:HA	1:A:624:LYS:HD2	1.84	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	638/645 (99%)	599 (94%)	35 (6%)	4 (1%)	25 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ALA
1	A	629	VAL
1	A	628	ASP
1	A	325	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	491/533 (92%)	486 (99%)	5 (1%)	76 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	248	THR
1	A	256	THR
1	A	375	ASP
1	A	675	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

22 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	SO4	A	717	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	712	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	715	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	721	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	705	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	704	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	703	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	722	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	719	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	708	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	710	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	702	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	714	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	720	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	709	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	A	711	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	716	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	707	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	713	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	718	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.05	0

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 [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

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	640/645 (99%)	0.17	52 (8%) 12 9	39, 63, 138, 166	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	GLN	9.7
1	A	247	ALA	5.4
1	A	628	ASP	5.3
1	A	257	ILE	4.8
1	A	217	PHE	4.4
1	A	195	VAL	4.4
1	A	256	THR	4.1
1	A	197	PRO	4.0
1	A	248	THR	3.9
1	A	114	TYR	3.9
1	A	41	ALA	3.8
1	A	198	SER	3.8
1	A	196	VAL	3.8
1	A	244	ILE	3.5
1	A	205	GLU	3.5
1	A	39	THR	3.4
1	A	204	GLY	3.4
1	A	145	THR	3.4
1	A	250	GLU	3.3
1	A	249	PRO	3.3
1	A	222	ASP	3.3
1	A	219	LEU	3.3
1	A	203	GLY	3.3
1	A	202	ASP	3.3
1	A	215	SER	3.3
1	A	245	ASP	3.2
1	A	213	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	3.1
1	A	190	LEU	3.0
1	A	241	LEU	3.0
1	A	199	LYS	2.9
1	A	207	THR	2.8
1	A	44	ALA	2.7
1	A	208	ALA	2.7
1	A	206	LYS	2.6
1	A	624	LYS	2.6
1	A	246	GLY	2.6
1	A	221	GLU	2.5
1	A	255	ALA	2.5
1	A	225	ASN	2.5
1	A	102	SER	2.4
1	A	216	SER	2.4
1	A	629	VAL	2.3
1	A	200	LEU	2.3
1	A	630	LYS	2.2
1	A	209	ASN	2.2
1	A	113	THR	2.1
1	A	45	GLY	2.1
1	A	115	SER	2.1
1	A	191	LYS	2.1
1	A	243	ILE	2.1
1	A	138	LEU	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](#)

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, 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	B-factors(\AA^2)	Q<0.9
2	SO4	A	721	5/5	0.76	0.42	107,107,134,135	5
2	SO4	A	716	5/5	0.84	0.23	93,96,106,110	5
2	SO4	A	718	5/5	0.86	0.32	72,78,106,109	5
2	SO4	A	710	5/5	0.88	0.25	68,84,104,113	5
2	SO4	A	722	5/5	0.90	0.19	95,100,104,124	5
2	SO4	A	712	5/5	0.91	0.15	49,84,103,107	5
2	SO4	A	720	5/5	0.91	0.40	97,120,142,142	5
2	SO4	A	719	5/5	0.92	0.30	49,55,64,70	5
2	SO4	A	717	5/5	0.92	0.20	73,74,75,98	5
2	SO4	A	708	5/5	0.93	0.21	67,70,89,115	5
2	SO4	A	713	5/5	0.93	0.24	62,87,101,105	5
2	SO4	A	715	5/5	0.93	0.39	106,107,145,160	0
2	SO4	A	706	5/5	0.93	0.14	54,61,95,108	5
2	SO4	A	711	5/5	0.93	0.15	81,95,110,117	5
2	SO4	A	707	5/5	0.94	0.24	71,76,95,110	5
2	SO4	A	705	5/5	0.95	0.16	64,77,89,99	5
2	SO4	A	709	5/5	0.95	0.21	53,58,75,76	5
2	SO4	A	704	5/5	0.96	0.15	47,54,77,78	5
2	SO4	A	714	5/5	0.96	0.23	67,84,92,94	5
2	SO4	A	703	5/5	0.97	0.08	65,68,85,90	5
2	SO4	A	701	5/5	0.97	0.11	49,67,83,96	5
2	SO4	A	702	5/5	0.98	0.10	45,67,71,77	5

6.5 Other polymers [i](#)

There are no such residues in this entry.