



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:05 AM UTC

PDB ID : 5LP4 / pdb_00005lp4
Title : Penicillin-Binding Protein (PBP2) from *Helicobacter pylori*
Authors : Contreras-Martel, C.; Martins, A.; Ecobichon, C.; Maragno, D.M.; Mattei, P.J.; El Ghachi, M.; Boneca, I.G.; Dessen, A.
Deposited on : 2016-08-11
Resolution : 3.03 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

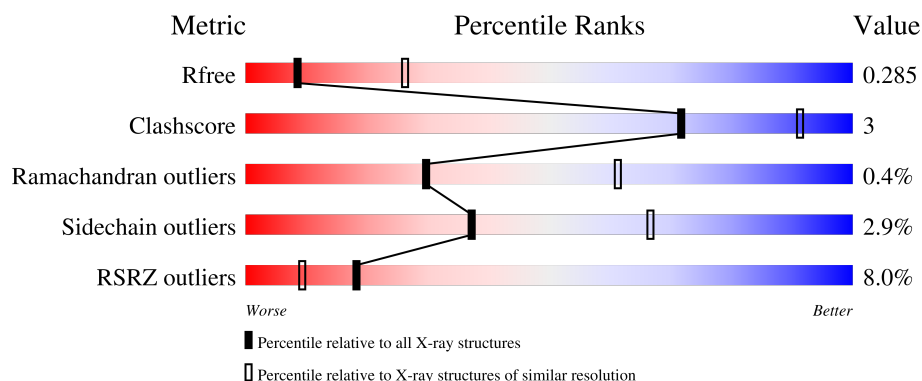
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	594	6% 78% 10% 12%
1	B	594	8% 78% 10% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8371 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 (Pbp2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4178	2697	705	768	8			
1	B	522	Total	C	N	O	S	0	0	0
			4154	2683	699	764	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	589	HIS	-	expression tag	UNP O26085
A	590	HIS	-	expression tag	UNP O26085
A	591	HIS	-	expression tag	UNP O26085
A	592	HIS	-	expression tag	UNP O26085
A	593	HIS	-	expression tag	UNP O26085
A	594	HIS	-	expression tag	UNP O26085
B	589	HIS	-	expression tag	UNP O26085
B	590	HIS	-	expression tag	UNP O26085
B	591	HIS	-	expression tag	UNP O26085
B	592	HIS	-	expression tag	UNP O26085
B	593	HIS	-	expression tag	UNP O26085
B	594	HIS	-	expression tag	UNP O26085

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.40Å 140.97Å 81.30Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	45.39 – 3.03 45.39 – 3.03	Depositor EDS
% Data completeness (in resolution range)	91.0 (45.39-3.03) 91.0 (45.39-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.251 , 0.288 0.252 , 0.285	Depositor DCC
R_{free} test set	2766 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8371	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.72	0/4268	0.88	4/5772 (0.1%)
1	B	0.73	0/4244	0.87	2/5740 (0.0%)
All	All	0.73	0/8512	0.88	6/11512 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	LYS	CA-C-N	7.43	127.88	119.93
1	A	553	LYS	C-N-CA	7.43	127.88	119.93
1	B	553	LYS	CA-C-N	6.96	127.37	119.93
1	B	553	LYS	C-N-CA	6.96	127.37	119.93
1	A	570	LYS	N-CA-C	-5.33	107.33	113.88
1	A	166	VAL	CB-CA-C	-5.08	106.01	111.59

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	4178	0	4243	31	0
1	B	4154	0	4216	29	0
2	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
3	A	13	0	0	1	0
3	B	11	0	0	0	0
All	All	8371	0	8459	56	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 3.

All (56) 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:399:ASP:N	1:B:399:ASP:OD1	2.31	0.61
1:B:56:ILE:HB	1:B:65:ALA:HB3	1.82	0.60
1:A:56:ILE:HB	1:A:65:ALA:HB3	1.82	0.60
1:A:399:ASP:N	1:A:399:ASP:OD1	2.33	0.60
1:B:465:ASN:HB3	1:B:467:GLN:HE21	1.71	0.56
1:A:465:ASN:HB3	1:A:467:GLN:HE21	1.72	0.55
1:A:210:VAL:HG22	1:A:220:LEU:HD23	1.90	0.54
1:A:504:ARG:HD2	3:A:809:HOH:O	2.08	0.53
1:B:135:ALA:O	1:B:139:GLN:HG2	2.09	0.53
1:B:171:LEU:HD23	1:B:171:LEU:O	2.09	0.53
1:B:210:VAL:HG22	1:B:220:LEU:HD23	1.89	0.53
1:A:364:ARG:HD3	1:A:494:HIS:ND1	2.23	0.53
1:B:364:ARG:HD3	1:B:494:HIS:ND1	2.23	0.52
1:A:171:LEU:O	1:A:171:LEU:HD23	2.10	0.52
1:A:379:SER:HB3	1:A:382:LYS:HE3	1.91	0.52
1:A:340:GLU:HB3	1:A:345:LYS:HG2	1.93	0.51
1:B:340:GLU:HB3	1:B:345:LYS:HG2	1.92	0.51
1:A:517:ALA:HB3	1:A:542:HIS:HB2	1.93	0.50
1:A:135:ALA:O	1:A:139:GLN:HG2	2.11	0.49
1:B:210:VAL:HG22	1:B:220:LEU:CD2	2.43	0.49
1:A:182:TYR:HB2	1:B:119:ILE:HD13	1.94	0.49
1:B:517:ALA:HB3	1:B:542:HIS:HB2	1.94	0.48
1:A:210:VAL:HG22	1:A:220:LEU:CD2	2.43	0.48
1:A:465:ASN:HB3	1:A:467:GLN:NE2	2.29	0.48
1:B:465:ASN:HB3	1:B:467:GLN:NE2	2.30	0.47
1:A:379:SER:HB3	1:A:382:LYS:CE	2.45	0.47
1:A:396:THR:HG21	1:A:442:LEU:HB3	1.95	0.47
1:B:396:THR:HG21	1:B:442:LEU:HB3	1.96	0.47
1:A:157:ALA:O	1:A:158:LEU:C	2.58	0.46
1:B:465:ASN:O	1:B:466:LYS:C	2.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HD13	1:B:182:TYR:HB2	1.96	0.46
1:A:315:MET:HE3	1:A:488:MET:SD	2.56	0.46
1:B:315:MET:HE3	1:B:488:MET:SD	2.56	0.46
1:B:157:ALA:O	1:B:158:LEU:C	2.59	0.45
1:A:251:ARG:HD3	1:A:295:TYR:CD1	2.52	0.45
1:A:162:VAL:HG11	1:A:235:LEU:HD11	2.00	0.44
1:B:50:VAL:HG21	1:B:208:MET:SD	2.58	0.44
1:A:50:VAL:HG21	1:A:208:MET:SD	2.58	0.44
1:A:465:ASN:O	1:A:466:LYS:C	2.58	0.44
1:A:54:GLY:O	1:A:151:ARG:NH1	2.46	0.43
1:A:308:PRO:HD2	1:A:517:ALA:HB1	1.99	0.43
1:A:224:LEU:HD22	1:B:224:LEU:HD22	2.00	0.43
1:A:317:VAL:HG21	1:A:431:ALA:O	2.18	0.43
1:B:54:GLY:O	1:B:151:ARG:NH1	2.45	0.42
1:A:242:GLU:O	1:A:246:LEU:HG	2.19	0.42
1:B:519:VAL:HG22	1:B:542:HIS:NE2	2.34	0.42
1:A:445:LEU:HA	1:A:559:THR:OG1	2.20	0.42
1:B:308:PRO:HD2	1:B:517:ALA:HB1	2.00	0.42
1:B:317:VAL:HG21	1:B:431:ALA:O	2.18	0.42
1:A:304:ASN:ND2	1:A:402:ASN:O	2.53	0.42
1:B:445:LEU:HA	1:B:559:THR:OG1	2.20	0.41
1:B:146:LEU:HA	1:B:147:PRO:HD3	1.97	0.41
1:B:420:GLN:HE22	1:B:436:SER:HB2	1.85	0.40
1:B:50:VAL:HG13	1:B:147:PRO:O	2.20	0.40
1:B:322:LEU:HD13	1:B:480:LYS:HD2	2.04	0.40
1:A:138:ILE:HD12	1:B:180:ASN:CG	2.46	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	521/594 (88%)	479 (92%)	40 (8%)	2 (0%)	30	61
1	B	518/594 (87%)	479 (92%)	37 (7%)	2 (0%)	30	61
All	All	1039/1188 (88%)	958 (92%)	77 (7%)	4 (0%)	30	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	B	97	ASN
1	B	342	GLY
1	A	342	GLY

5.3.2 Protein sidechains ⓘ

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	454/518 (88%)	441 (97%)	13 (3%)	37	67
1	B	451/518 (87%)	438 (97%)	13 (3%)	37	67
All	All	905/1036 (87%)	879 (97%)	26 (3%)	37	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	175	LYS
1	A	183	SER
1	A	219	THR
1	A	251	ARG
1	A	294	ILE
1	A	311	SER
1	A	350	LYS
1	A	399	ASP
1	A	475	SER
1	A	492	CYS
1	A	541	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	566	GLU
1	B	46	LYS
1	B	175	LYS
1	B	183	SER
1	B	188	LYS
1	B	219	THR
1	B	235	LEU
1	B	251	ARG
1	B	311	SER
1	B	399	ASP
1	B	463	ILE
1	B	475	SER
1	B	479	LYS
1	B	492	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	117	ASN
1	A	155	ASN
1	A	276	ASN
1	A	288	GLN
1	A	344	HIS
1	A	354	HIS
1	A	434	GLN
1	B	117	ASN
1	B	288	GLN
1	B	354	HIS
1	B	420	GLN
1	B	434	GLN
1	B	467	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	B	701	-	4,4,4	0.55	0	6,6,6	0.24	0
2	SO4	B	700	-	4,4,4	0.51	0	6,6,6	0.18	0
2	SO4	A	700	-	4,4,4	0.54	0	6,6,6	0.12	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	525/594 (88%)	0.65	36 (6%)	23 11	26, 47, 82, 139	0
1	B	522/594 (87%)	0.67	48 (9%)	14 7	26, 46, 90, 114	0
All	All	1047/1188 (88%)	0.66	84 (8%)	18 9	26, 46, 86, 139	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	LEU	5.1
1	B	569	SER	4.4
1	B	99	SER	4.1
1	B	213	LEU	4.0
1	A	420	GLN	3.9
1	A	466	LYS	3.9
1	B	215	GLN	3.9
1	A	569	SER	3.8
1	B	519	VAL	3.8
1	A	568	GLY	3.7
1	B	518	GLN	3.7
1	B	501	HIS	3.7
1	B	517	ALA	3.6
1	B	568	GLY	3.4
1	B	416	LYS	3.4
1	A	215	GLN	3.4
1	A	294	ILE	3.2
1	A	111	ASN	3.0
1	B	349	TRP	3.0
1	A	492	CYS	3.0
1	B	214	ASN	3.0
1	B	228	ASN	2.9
1	A	512	CYS	2.9
1	A	411	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	285	ASP	2.8
1	A	421	ASP	2.8
1	A	343	LYS	2.7
1	B	566	GLU	2.6
1	B	97	ASN	2.6
1	B	98	PHE	2.6
1	A	336	PRO	2.5
1	A	344	HIS	2.5
1	B	283	SER	2.5
1	B	344	HIS	2.5
1	A	567	GLY	2.5
1	B	423	ARG	2.5
1	B	80	LYS	2.4
1	A	520	VAL	2.4
1	B	230	HIS	2.4
1	A	212	ALA	2.4
1	A	100	LYS	2.4
1	A	417	ARG	2.4
1	B	284	GLN	2.4
1	B	343	LYS	2.3
1	B	110	GLU	2.3
1	A	93	LYS	2.3
1	B	345	LYS	2.3
1	B	351	LYS	2.3
1	A	565	GLY	2.3
1	A	211	ASN	2.3
1	A	110	GLU	2.3
1	B	347	ARG	2.3
1	B	381	GLU	2.3
1	B	352	THR	2.3
1	B	211	ASN	2.3
1	A	588	LEU	2.2
1	B	176	ASP	2.2
1	B	415	LEU	2.2
1	B	279	VAL	2.2
1	B	101	GLU	2.2
1	B	340	GLU	2.2
1	A	518	GLN	2.2
1	A	419	ASN	2.2
1	A	566	GLU	2.2
1	B	93	LYS	2.2
1	B	78	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	2.1
1	B	142	GLY	2.1
1	B	61	ASP	2.1
1	B	512	CYS	2.1
1	B	100	LYS	2.1
1	A	101	GLU	2.1
1	A	416	LYS	2.1
1	B	45	LYS	2.1
1	B	82	LYS	2.1
1	B	350	LYS	2.1
1	B	86	GLU	2.1
1	A	365	GLU	2.1
1	A	418	PHE	2.0
1	B	104	LEU	2.0
1	A	349	TRP	2.0
1	A	108	GLN	2.0
1	B	570	LYS	2.0
1	A	216	GLU	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 oligosaccharides 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(Å ²)	Q<0.9
2	SO4	B	700	5/5	0.76	0.17	85,85,92,93	0
2	SO4	A	700	5/5	0.89	0.14	72,75,77,77	0
2	SO4	B	701	5/5	0.90	0.13	64,66,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.