



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:08 PM UTC

PDB ID : 5Y28 / pdb_00005y28
Title : Crystal structure of H. pylori HtrA with PDZ2 deletion
Authors : Zhang, Z.; Huang, Q.; Tao, X.
Deposited on : 2017-07-24
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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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

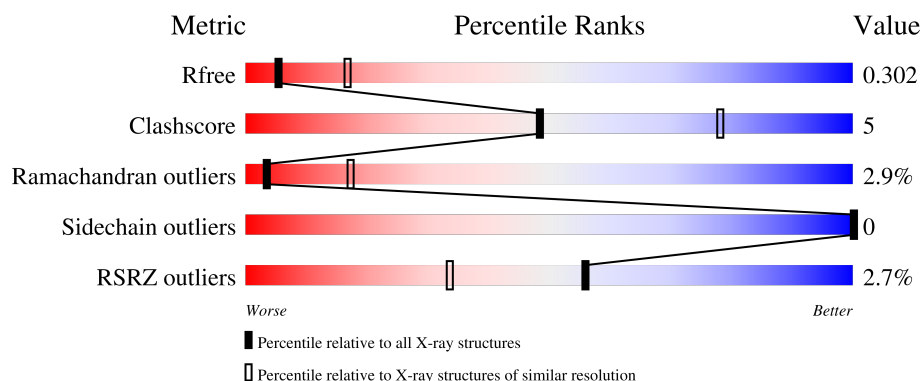
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	357	 3% 64% 11% 22%
1	B	357	 0% 50% 6% 43%
1	C	357	 2% 66% 12% 22%
2	G	4	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5193 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 Periplasmic serine endoprotease DegP-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1872	1166	323	380	3			
1	B	202	Total	C	N	O	S	0	0	0
			1393	871	238	281	3			
1	C	278	Total	C	N	O	S	0	0	0
			1899	1187	321	388	3			

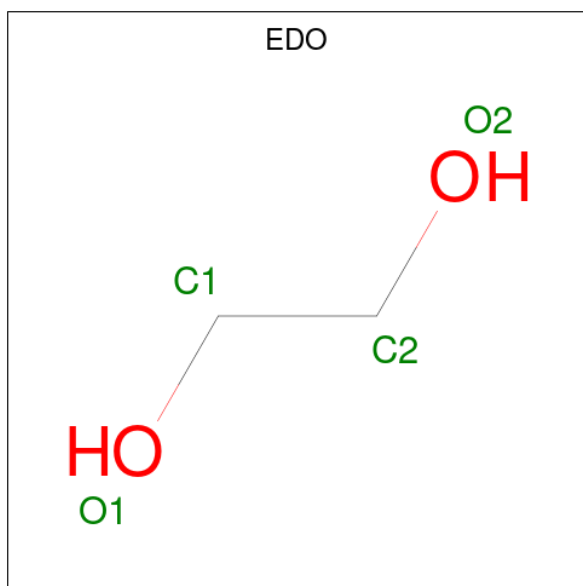
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP G2J5T2
A	12	PRO	-	expression tag	UNP G2J5T2
A	13	GLY	-	expression tag	UNP G2J5T2
A	14	TYR	-	expression tag	UNP G2J5T2
A	15	GLN	-	expression tag	UNP G2J5T2
A	16	ASP	-	expression tag	UNP G2J5T2
A	17	PRO	-	expression tag	UNP G2J5T2
B	11	GLY	-	expression tag	UNP G2J5T2
B	12	PRO	-	expression tag	UNP G2J5T2
B	13	GLY	-	expression tag	UNP G2J5T2
B	14	TYR	-	expression tag	UNP G2J5T2
B	15	GLN	-	expression tag	UNP G2J5T2
B	16	ASP	-	expression tag	UNP G2J5T2
B	17	PRO	-	expression tag	UNP G2J5T2
C	11	GLY	-	expression tag	UNP G2J5T2
C	12	PRO	-	expression tag	UNP G2J5T2
C	13	GLY	-	expression tag	UNP G2J5T2
C	14	TYR	-	expression tag	UNP G2J5T2
C	15	GLN	-	expression tag	UNP G2J5T2
C	16	ASP	-	expression tag	UNP G2J5T2
C	17	PRO	-	expression tag	UNP G2J5T2

- Molecule 2 is a protein called UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			20	12	4	4			

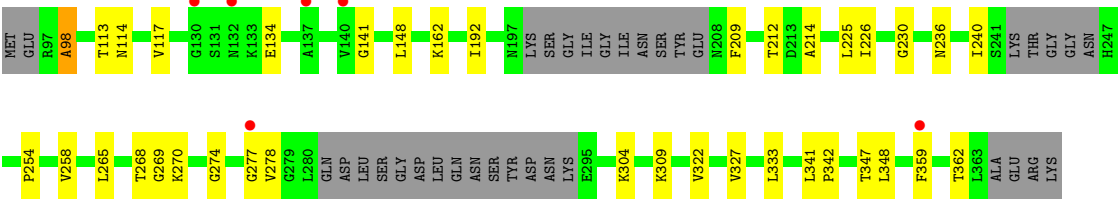
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		



● Molecule 2: UNK-UNK-UNK-UNK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.91Å 91.50Å 120.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.88 – 3.09 43.88 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.88-3.09) 99.5 (43.88-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.257 , 0.298 0.262 , 0.302	Depositor DCC
R_{free} test set	959 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5193	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: EDO

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	0.11	0/1888	0.35	0/2564
1	B	0.11	0/1405	0.30	0/1907
1	C	0.11	0/1914	0.33	0/2602
2	G	0.08	0/19	0.22	0/25
All	All	0.11	0/5226	0.33	0/7098

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	1872	0	1774	25	0
1	B	1393	0	1289	17	0
1	C	1899	0	1748	23	0
2	G	20	0	22	4	0
3	A	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
All	All	5193	0	4839	55	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 (55) 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:23:GLN:OE1	1:B:23:GLN:N	2.15	0.73
1:C:141:GLY:HA3	1:C:265:LEU:HD22	1.72	0.69
1:C:212:THR:HG22	1:C:214:ALA:H	1.56	0.69
1:C:268:THR:HG22	1:C:269:GLY:H	1.61	0.66
1:C:226:ILE:HD12	1:C:230:GLY:HA2	1.78	0.64
1:A:211:GLN:HB3	1:A:249:ILE:HD11	1.79	0.63
1:A:130:GLY:O	1:A:132:ASN:N	2.34	0.60
1:A:319:ILE:HG22	1:A:320:THR:HG23	1.84	0.60
1:A:341:LEU:HD23	2:G:4:ALA:HB3	1.84	0.59
1:A:35:PRO:HG2	1:C:32:VAL:HG21	1.85	0.58
1:A:41:ILE:HG22	1:B:229:ARG:HD3	1.84	0.58
1:A:114:ASN:HB2	1:A:117:VAL:HG23	1.86	0.57
1:B:114:ASN:ND2	1:B:221:SER:OG	2.38	0.56
1:B:178:ILE:HG23	1:B:188:VAL:HG12	1.88	0.56
1:A:161:ILE:O	1:B:23:GLN:NE2	2.38	0.56
1:B:46:ASP:HA	1:B:49:LYS:HD3	1.88	0.55
1:C:114:ASN:HB2	1:C:117:VAL:HG23	1.89	0.54
1:A:189:THR:HG21	1:A:215:SER:HB3	1.91	0.52
1:B:114:ASN:HB2	1:B:117:VAL:HG23	1.90	0.52
1:B:174:LEU:HD11	1:B:190:GLN:HE21	1.74	0.52
1:B:173:ASP:OD1	1:C:31:ARG:NH2	2.44	0.51
1:C:274:GLY:HA3	1:C:362:THR:HB	1.94	0.49
1:C:327:VAL:HG11	1:C:333:LEU:HB2	1.94	0.49
1:C:304:LYS:HA	1:C:309:LYS:HD3	1.94	0.49
1:A:340:MET:HA	2:G:3:ALA:HB1	1.96	0.47
1:A:226:ILE:HD12	1:A:230:GLY:HA2	1.95	0.47
1:A:259:LYS:HG3	1:B:22:ILE:HG21	1.96	0.47
1:C:113:THR:HG22	1:C:114:ASN:H	1.81	0.46
1:B:31:ARG:HG2	1:C:43:SER:HB3	1.98	0.46
1:A:99:LEU:HD12	1:A:117:VAL:O	2.15	0.46
1:C:347:THR:HG22	1:C:359:PHE:HD1	1.80	0.46
1:B:25:MET:HG2	1:B:26:PRO:HD2	1.98	0.45
1:A:274:GLY:HA2	2:G:3:ALA:HB3	1.98	0.45
1:A:352:ARG:NE	1:A:352:ARG:HA	2.32	0.45
1:C:322:VAL:HG22	1:C:348:LEU:HD22	1.98	0.44
1:A:275:TYR:HB3	2:G:3:ALA:H	1.83	0.44
1:A:124:ILE:HG22	1:A:137:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:MET:HE2	1:C:162:LYS:HB2	2.01	0.43
1:C:44:TYR:O	1:C:48:ILE:HG12	2.18	0.43
1:C:148:LEU:HD11	1:C:258:VAL:HG22	2.00	0.43
1:B:58:ILE:HG23	1:B:124:ILE:HG23	2.01	0.43
1:B:190:GLN:HB2	1:C:192:ILE:HD13	2.01	0.42
1:A:32:VAL:HG23	1:B:40:THR:HG21	2.02	0.42
1:C:225:LEU:HB2	1:C:236:ASN:OD1	2.19	0.42
1:A:216:ILE:HG23	1:A:236:ASN:HB3	2.01	0.42
1:A:353:ASP:OD1	1:A:354:LYS:N	2.52	0.42
1:C:48:ILE:HD12	1:C:226:ILE:HD11	2.02	0.42
1:B:114:ASN:ND2	1:B:221:SER:HG	2.17	0.42
1:B:164:SER:O	1:B:255:SER:OG	2.34	0.41
1:A:246:ASN:C	1:A:248:GLY:H	2.28	0.41
1:A:352:ARG:HB3	1:A:353:ASP:H	1.69	0.41
1:A:48:ILE:HG22	1:A:226:ILE:HD11	2.02	0.41
1:C:209:PHE:HA	1:C:254:PRO:HD3	2.03	0.41
1:A:41:ILE:HD11	1:C:31:ARG:CZ	2.51	0.40
1:C:59:SER:HA	1:C:98:ALA:HA	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	258/357 (72%)	228 (88%)	21 (8%)	9 (4%)	3	14
1	B	192/357 (54%)	174 (91%)	15 (8%)	3 (2%)	7	28
1	C	266/357 (74%)	235 (88%)	22 (8%)	9 (3%)	3	14
2	G	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
All	All	718/1075 (67%)	638 (89%)	59 (8%)	21 (3%)	3	17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	SER
1	A	340	MET
1	C	134	GLU
1	C	278	VAL
1	C	341	LEU
1	C	342	PRO
1	A	342	PRO
1	A	350	VAL
1	C	240	ILE
1	A	317	ASP
1	A	349	LYS
1	B	124	ILE
1	B	272	GLU
1	C	270	LYS
1	C	277	GLY
1	A	360	THR
1	B	134	GLU
1	A	327	VAL
1	C	35	PRO
1	C	98	ALA
1	A	319	ILE

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	191/300 (64%)	191 (100%)	0	100	100
1	B	140/300 (47%)	140 (100%)	0	100	100
1	C	184/300 (61%)	184 (100%)	0	100	100
All	All	515/900 (57%)	515 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	ASN
1	B	115	ASN
1	C	45	HIS
1	C	57	ASN
1	C	190	GLN
1	C	208	ASN
1	C	211	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](#)

1 ligand is 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	$\# Z > 2$
3	EDO	A	401	-	3,3,3	0.43	0	2,2,2	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	401	-	-	0/1/1/1	-

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	268/357 (75%)	0.23	9 (3%)	48	27	44, 77, 127, 143	0
1	B	202/357 (56%)	0.20	4 (1%)	65	42	48, 76, 112, 132	0
1	C	278/357 (77%)	0.28	7 (2%)	58	36	48, 90, 114, 131	0
2	G	4/4 (100%)	0.37	0	100	100	99, 99, 103, 104	0
All	All	752/1075 (69%)	0.24	20 (2%)	56	33	44, 82, 118, 143	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLY	4.0
1	C	140	VAL	3.9
1	C	130	GLY	3.2
1	B	132	ASN	3.2
1	A	135	TYR	2.8
1	B	220	ASN	2.7
1	C	359	PHE	2.6
1	A	281	GLN	2.5
1	C	36	SER	2.5
1	A	348	LEU	2.5
1	A	100	GLY	2.3
1	C	137	ALA	2.3
1	B	181	PRO	2.3
1	C	277	GLY	2.2
1	A	350	VAL	2.1
1	A	276	LEU	2.1
1	A	347	THR	2.1
1	A	340	MET	2.0
1	C	132	ASN	2.0
1	B	23	GLN	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($\text{\AA}^2$)	Q<0.9
3	EDO	A	401	4/4	0.73	0.22	78,82,83,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.