

wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2024 – 08:43 AM EST

PDB ID : 2PVP

Title : Crystal structure of D-Alanine-D-Alanine Ligase from Helicobacter pylori

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Deposited on : 2007-05-10

Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$

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)

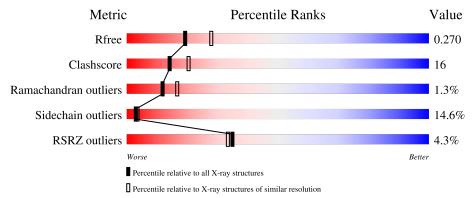
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
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	367	57%	24%	7% • 10%		
1	В	367	59%	20%	7% • 14%		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5286 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 D-alanine-D-alanine ligase.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	329	Total 2660	C 1741	N 422	O 490	S 7	0	0	0
1	В	315	Total 2531	C 1656	N 401	O 467	S 7	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q2N4T5
A	-18	GLY	_	expression tag	UNP Q2N4T5
A	-17	SER	-	expression tag	UNP Q2N4T5
A	-16	SER	-	expression tag	UNP Q2N4T5
A	-15	HIS	-	expression tag	UNP Q2N4T5
A	-14	HIS	-	expression tag	UNP Q2N4T5
A	-13	HIS	-	expression tag	UNP Q2N4T5
A	-12	HIS	-	expression tag	UNP Q2N4T5
A	-11	HIS	-	expression tag	UNP Q2N4T5
A	-10	HIS	-	expression tag	UNP Q2N4T5
A	-9	SER	-	expression tag	UNP Q2N4T5
A	-8	SER	-	expression tag	UNP Q2N4T5
A	-7	GLY	-	expression tag	UNP Q2N4T5
A	-6	LEU	-	expression tag	UNP Q2N4T5
A	-5	VAL	-	expression tag	UNP Q2N4T5
A	-4	PRO	-	expression tag	UNP Q2N4T5
A	-3	ARG	-	expression tag	UNP Q2N4T5
A	-2	GLY	-	expression tag	UNP Q2N4T5
A	-1	SER	-	expression tag	UNP Q2N4T5
A	0	HIS	-	expression tag	UNP Q2N4T5
В	-19	MET	-	expression tag	UNP Q2N4T5
В	-18	GLY	-	expression tag	UNP Q2N4T5
В	-17	SER	-	expression tag	UNP Q2N4T5
В	-16	SER	-	expression tag	UNP Q2N4T5
В	-15	HIS	-	expression tag	UNP Q2N4T5

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-14	HIS	-	expression tag	UNP Q2N4T5
В	-13	HIS	-	expression tag	UNP Q2N4T5
В	-12	HIS	-	expression tag	UNP Q2N4T5
В	-11	HIS	-	expression tag	UNP Q2N4T5
В	-10	HIS	-	expression tag	UNP Q2N4T5
В	-9	SER	-	expression tag	UNP Q2N4T5
В	-8	SER	-	expression tag	UNP Q2N4T5
В	-7	GLY	-	expression tag	UNP Q2N4T5
В	-6	LEU	-	expression tag	UNP Q2N4T5
В	-5	VAL	-	expression tag	UNP Q2N4T5
В	-4	PRO	-	expression tag	UNP Q2N4T5
В	-3	ARG	-	expression tag	UNP Q2N4T5
В	-2	GLY	-	expression tag	UNP Q2N4T5
В	-1	SER	-	expression tag	UNP Q2N4T5
В	0	HIS	-	expression tag	UNP Q2N4T5

• Molecule 2 is water.

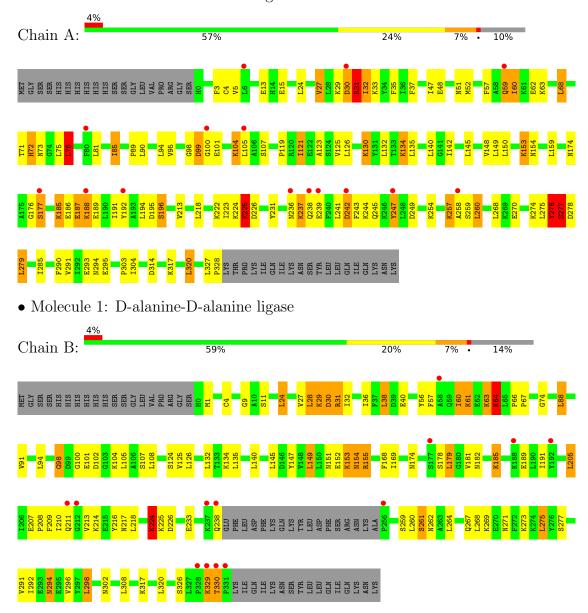
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	43	Total O 43 43	0	0
2	В	52	Total O 52 52	0	0



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: D-alanine-D-alanine ligase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.97Å 89.02Å 121.88Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 - 2.40	Depositor
rtesolution (A)	32.78 - 2.40	EDS
% Data completeness	97.5 (15.00-2.40)	Depositor
(in resolution range)	97.6 (32.78-2.40)	EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.229 , 0.283	Depositor
R, R_{free}	0.232 , 0.270	DCC
R_{free} test set	1521 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 44.3	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5286	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	Mol Chain		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	1.03	$10/2720 \ (0.4\%)$	1.33	20/3667~(0.5%)	
1	В	0.80	7/2587 (0.3%)	1.03	14/3489 (0.4%)	
All	All	0.92	$17/5307 \ (0.3\%)$	1.19	34/7156 (0.5%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	В	0	1
All	All	0	3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
1	A	277	SER	CB-OG	26.23	1.76	1.42
1	A	27	VAL	CB-CG2	-17.43	1.16	1.52
1	В	178	SER	CB-OG	15.21	1.62	1.42
1	A	27	VAL	CB-CG1	13.47	1.81	1.52
1	В	30	ASP	CB-CG	-13.24	1.24	1.51

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	276	TYR	CB-CG-CD1	-41.08	96.35	121.00
1	A	276	TYR	CB-CG-CD2	32.89	140.73	121.00
1	В	30	ASP	CB-CG-OD1	21.71	137.84	118.30
1	В	30	ASP	CB-CG-OD2	-20.40	99.94	118.30
1	A	278	ASP	CB-CG-OD1	16.42	133.08	118.30

There are no chirality outliers.



All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	TYR	Sidechain
1	A	30	ASP	Peptide
1	В	63	LYS	Peptide

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	2660	0	2678	107	1
1	В	2531	0	2558	59	1
2	A	43	0	0	3	0
2	В	52	0	0	4	0
All	All	5286	0	5236	163	1

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 16.

The worst 5 of 163 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \AA) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:31:ARG:CB	1:B:31:ARG:CG	1.83	1.56
1:A:225:LYS:CB	1:A:225:LYS:CG	1.80	1.54
1:A:27:VAL:CB	1:A:27:VAL:CG1	1.81	1.54
1:A:231:TYR:CE1	1:A:242:ASP:OD1	1.81	1.32
1:A:277:SER:CB	1:A:277:SER:OG	1.76	1.32

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$	
1:A:249:ASP:OD1	1:B:261:SER:OG[1_655]	1.93	0.27	



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	Perc	entiles
1	A	327/367 (89%)	307 (94%)	17 (5%)	3 (1%)	17	25
1	В	311/367 (85%)	293 (94%)	13 (4%)	5 (2%)	9	13
All	All	638/734 (87%)	600 (94%)	30 (5%)	8 (1%)	12	17

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	SER
1	A	154	ASN
1	В	64	LYS
1	В	98	GLY
1	В	153	LYS

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	Pe	erce	\mathbf{ent} i	iles
1	A	291/326 (89%)	249 (86%)	42 (14%)		3	3	
1	В	278/326 (85%)	237 (85%)	41 (15%)		3	3	
All	All	569/652 (87%)	486 (85%)	83 (15%)		3	3	

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	149	LEU

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Mol	Chain	Res	Type
1	В	261	SER
1	В	153	LYS
1	В	205	LEU
1	В	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	В	294	ASN
1	В	154	ASN
1	В	302	ASN
1	В	174	ASN

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)

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 (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle { m RSRZ} \rangle$	#RSI	$\mathbf{RZ}>$	2	$OWAB(A^2)$	Q<0.9
1	A	329/367 (89%)	0.21	15 (4%)	32	31	20, 51, 82, 102	0
1	В	315/367~(85%)	0.19	13 (4%)	37	36	20, 58, 86, 118	0
All	All	644/734 (87%)	0.20	28 (4%)	35	33	20, 54, 85, 118	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	ALA	9.4
1	В	331	PRO	7.0
1	В	328	PRO	5.5
1	В	330	THR	5.4
1	A	236	ASN	4.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

