



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2025 – 12:46 PM JST

PDB ID : 8K6W
Title : dUTPase of helicobacter pylori 26695
Authors : Kumari, K.; Gourinath, S.
Deposited on : 2023-07-25
Resolution : 2.50 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 ⓘ 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

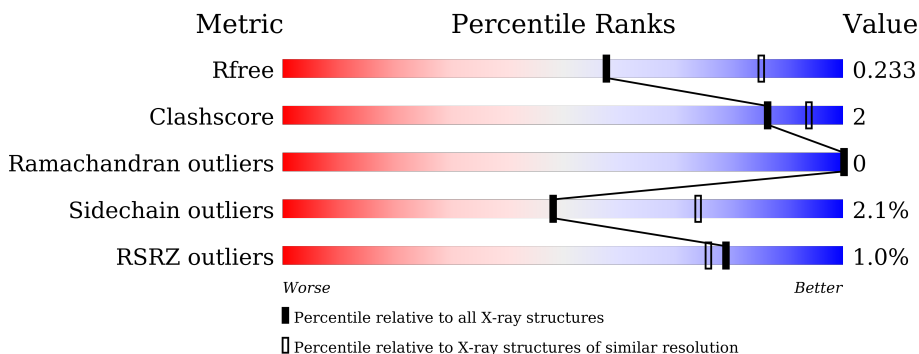
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	152	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% • • 16% </div> </div>
1	B	152	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% 9% 13% </div> </div>
1	C	152	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 81% • 15% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3004 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 Deoxyuridine 5'-triphosphate nucleotidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			977	620	167	185	5			
1	B	132	Total	C	N	O	S	0	0	0
			1010	639	172	194	5			
1	C	129	Total	C	N	O	S	0	0	0
			994	631	171	187	5			

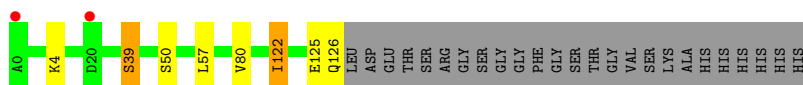
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP O25536
A	146	HIS	-	expression tag	UNP O25536
A	147	HIS	-	expression tag	UNP O25536
A	148	HIS	-	expression tag	UNP O25536
A	149	HIS	-	expression tag	UNP O25536
A	150	HIS	-	expression tag	UNP O25536
A	151	HIS	-	expression tag	UNP O25536
B	0	ALA	-	expression tag	UNP O25536
B	146	HIS	-	expression tag	UNP O25536
B	147	HIS	-	expression tag	UNP O25536
B	148	HIS	-	expression tag	UNP O25536
B	149	HIS	-	expression tag	UNP O25536
B	150	HIS	-	expression tag	UNP O25536
B	151	HIS	-	expression tag	UNP O25536
C	0	ALA	-	expression tag	UNP O25536
C	146	HIS	-	expression tag	UNP O25536
C	147	HIS	-	expression tag	UNP O25536
C	148	HIS	-	expression tag	UNP O25536
C	149	HIS	-	expression tag	UNP O25536
C	150	HIS	-	expression tag	UNP O25536
C	151	HIS	-	expression tag	UNP O25536

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	11	Total 11	O 11	0	0
2	C	1	Total 1	O 1	0	0

- Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase



	AQ	D20	F29	V23	I46	L57	QS8	T61	V70	V74	M72	V80	I108	Q114	C124	E129 T130 S131	ARG GLY SER GLY GLY PHE GLY GLY SER THR GLY VAL SER LYS ALA HIS HIS HIS HIS HIS
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AG	Q18	L57	Q58	P77	V50	K118	D128	GLU	THR	SER	ARG	GLY	SER	SER	GLY	GLY	PHE	GLY	SER	THR	GLY	VAL	SER	LYS	ALA	HTS	HTS	HTS	HTS	HTS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	102.36Å 102.36Å 78.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.70 – 2.50 58.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.70-2.50) 100.0 (58.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.175 , 0.238 0.182 , 0.233	Depositor DCC
R_{free} test set	1092 reflections (6.71%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3004	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	0.42	0/991	0.76	0/1338
1	B	0.39	0/1024	0.71	0/1385
1	C	0.38	0/1008	0.71	0/1361
All	All	0.40	0/3023	0.73	0/4084

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	977	0	990	5	0
1	B	1010	0	1014	6	0
1	C	994	0	1014	2	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	1	0	0	0	0
All	All	3004	0	3018	12	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 2.

The worst 5 of 12 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:45:ILE:HD11	1:B:108:ILE:HD11	1.89	0.55
1:A:57:LEU:HB3	1:A:80:VAL:HB	1.91	0.52
1:A:4:LYS:HB2	1:A:50:SER:HB3	1.93	0.51
1:B:57:LEU:HB3	1:B:80:VAL:HB	1.96	0.48
1:C:58:GLN:HB3	1:C:77:PRO:HB2	1.95	0.48

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	125/152 (82%)	123 (98%)	2 (2%)	0	100	100
1	B	130/152 (86%)	126 (97%)	4 (3%)	0	100	100
1	C	127/152 (84%)	125 (98%)	2 (2%)	0	100	100
All	All	382/456 (84%)	374 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	107/129 (83%)	105 (98%)	2 (2%)	52	77
1	B	110/129 (85%)	107 (97%)	3 (3%)	40	67
1	C	109/129 (84%)	107 (98%)	2 (2%)	54	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	326/387 (84%)	319 (98%)	7 (2%)	48 74

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	33	VAL
1	B	124	CYS
1	C	118	LYS
1	C	18	GLN
1	B	20	ASP

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	70	GLN
1	B	38	HIS
1	B	70	GLN
1	B	126	GLN
1	C	68	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	127/152 (83%)	-0.51	2 (1%) 70 67	28, 42, 68, 100	0
1	B	132/152 (86%)	-0.43	2 (1%) 71 68	29, 46, 70, 96	0
1	C	129/152 (84%)	-0.29	0 100 100	31, 49, 79, 103	0
All	All	388/456 (85%)	-0.41	4 (1%) 79 76	28, 46, 76, 103	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	3.7
1	B	129	GLU	2.3
1	A	20	ASP	2.2
1	B	130	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.