

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2021 – 06:07 PM EST

PDB ID : 3IVD

Title: Putative 5'-Nucleotidase (c4898) from Escherichia Coli in complex with Uri-

dine

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Deposited on : 2009-08-31

Resolution : 1.90 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 following versions of software and data (see references (1)) 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 : 2.16

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) oteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

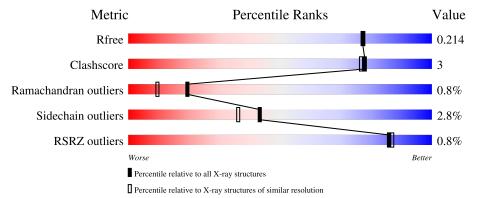
Validation Pipeline (wwPDB-VP) : 2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	509	89%	9%	.
1	В	509	90%	8%	



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8223 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 Nucleotidase.

\mathbf{Mol}	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	499	Total 3863	C 2462	N 651	O 741	Se 9	0	5	0
1	В	499	Total 3860	C 2455	N 654	O 743	Se 8	0	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MSE	-	expression tag	UNP Q8FBB1
A	20	SER	-	expression tag	UNP Q8FBB1
A	21	LEU	-	expression tag	UNP Q8FBB1
A	520	GLU	-	expression tag	UNP Q8FBB1
A	521	GLY	-	expression tag	UNP Q8FBB1
A	522	HIS	_	expression tag	UNP Q8FBB1
A	523	HIS	-	expression tag	UNP Q8FBB1
A	524	HIS	_	expression tag	UNP Q8FBB1
A	525	HIS	-	expression tag	UNP Q8FBB1
A	526	HIS	-	expression tag	UNP Q8FBB1
A	527	HIS	-	expression tag	UNP Q8FBB1
В	19	MSE	-	expression tag	UNP Q8FBB1
В	20	SER	-	expression tag	UNP Q8FBB1
В	21	LEU	-	expression tag	UNP Q8FBB1
В	520	GLU	-	expression tag	UNP Q8FBB1
В	521	GLY	-	expression tag	UNP Q8FBB1
В	522	HIS	-	expression tag	UNP Q8FBB1
В	523	HIS	-	expression tag	UNP Q8FBB1
В	524	HIS	-	expression tag	UNP Q8FBB1
В	525	HIS	-	expression tag	UNP Q8FBB1
В	526	HIS	-	expression tag	UNP Q8FBB1
В	527	HIS	-	expression tag	UNP Q8FBB1

• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

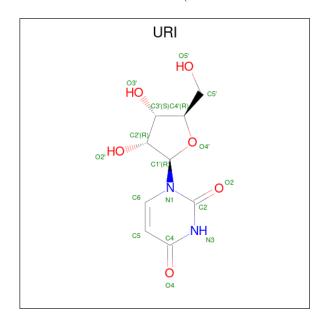


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

• Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0

 \bullet Molecule 4 is URIDINE (three-letter code: URI) (formula: $\mathrm{C_9H_{12}N_2O_6}).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 17				0	0
4	В	1	Total 17		N 2	O 6	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	230	Total O 230 230	0	0
6	В	230	Total O 230 230	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: Nucleotidase

Chain A:

89%

9%

• Molecule 1: Nucleotidase

Chain B:

90%

88%

• Molecule 1: Nucleotidase

Chain B:

90%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	47.60Å 67.28Å 86.42Å	Donositor
a, b, c, α , β , γ	74.04° 77.55° 83.76°	Depositor
Resolution (Å)	50.00 - 1.90	Depositor
Resolution (A)	45.24 - 1.90	EDS
% Data completeness	95.9 (50.00-1.90)	Depositor
(in resolution range)	95.9 (45.24-1.90)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.10 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.167 , 0.210	Depositor
R, R_{free}	0.172 , 0.214	DCC
R_{free} test set	3828 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 42.0	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	0.96	EDS
Total number of atoms	8223	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.57% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN, FE, URI

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.58	0/3948	0.65	0/5341	
1	В	0.61	0/3936	0.65	0/5324	
All	All	0.60	0/7884	0.65	0/10665	

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	3863	0	3861	26	0
1	В	3860	0	3846	19	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	17	0	12	0	0
4	В	17	0	12	0	0
5	A	1	0	0	0	0
5	В	1	0	0	0	0
6	A	230	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	230	0	0	1	0
All	All	8223	0	7731	45	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.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:490:TYR:H	1:B:493:HIS:HD2	1.10	0.92
1:A:490:TYR:H	1:A:493:HIS:HD2	1.18	0.86
1:B:490:TYR:H	1:B:493:HIS:CD2	2.01	0.70
1:A:311:GLN:HG2	6:A:685:HOH:O	1.91	0.70
1:A:412:MSE:CE	1:A:423:LEU:HD12	2.26	0.65

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	Favoured Allowed		Percentiles		
1	A	502/509 (99%)	488 (97%)	10 (2%)	4 (1%)	19 9		
1	В	499/509 (98%)	487 (98%)	8 (2%)	4 (1%)	19 9		
All	All	1001/1018 (98%)	975 (97%)	18 (2%)	8 (1%)	19 9		

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASP
1	A	251	HIS
1	В	188	ASP

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Mol	Chain	Res	Type
1	В	251	HIS
1	A	227	VAL

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	413/411 (100%)	401 (97%)	12 (3%)	42 35		
1	В	412/411 (100%)	400 (97%)	12 (3%)	42 35		
All	All	825/822 (100%)	801 (97%)	24 (3%)	43 35		

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	GLN
1	В	181	ARG
1	В	464	GLN
1	A	500	LYS
1	В	80	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	36	HIS
1	В	493	HIS
1	В	295	ASN
1	A	320	ASN
1	В	290	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)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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 Ty	Trme	Type Chain		Chain	Chain	Dag	Res Link	Bo	Bond lengths			Bond angles		
IVIOI	туре	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2				
4	URI	В	603	-	14,18,18	1.21	1 (7%)	14,26,26	1.45	2 (14%)				
4	URI	A	603	-	14,18,18	1.23	2 (14%)	14,26,26	1.21	1 (7%)				

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
4	URI	В	603	-	-	0/4/22/22	0/2/2/2
4	URI	A	603	-	-	0/4/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	В	603	URI	C4-N3	3.62	1.39	1.33
4	A	603	URI	C4-N3	3.28	1.38	1.33
4	A	603	URI	O3'-C3'	2.10	1.47	1.43

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	603	URI	C5-C4-N3	-3.62	115.35	123.31
4	A	603	URI	C5-C4-N3	-3.19	116.30	123.31
4	В	603	URI	C3'-C2'-C1'	2.23	104.33	100.98

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 (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	<RSRZ $>$	# RSRZ > 2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	491/509 (96%)	-0.38	3 (0%) 89	90	13, 20, 36, 50	0
1	В	491/509~(96%)	-0.37	5 (1%) 82	84	11, 20, 35, 52	1 (0%)
All	All	982/1018 (96%)	-0.38	8 (0%) 86	87	11, 20, 35, 52	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	362	LYS	3.8
1	В	22	ALA	3.4
1	A	21	LEU	3.3
1	В	286	GLU	3.2
1	A	22	ALA	2.4

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	URI	A	603	17/17	0.97	0.10	14,17,19,19	0
4	URI	В	603	17/17	0.98	0.07	14,17,19,19	0
5	CL	A	604	1/1	0.99	0.03	19,19,19,19	0
5	CL	В	604	1/1	0.99	0.08	16,16,16,16	0
2	FE	В	601	1/1	1.00	0.08	15,15,15,15	0
3	MN	В	602	1/1	1.00	0.07	19,19,19,19	0
2	FE	A	601	1/1	1.00	0.07	19,19,19,19	0
3	MN	A	602	1/1	1.00	0.04	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.

