

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 2, 2024 - 10:12 pm GMT

PDB ID	:	4UHQ
Title	:	Crystal structure of the pyocin AP41 DNase
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Deposited on		
Resolution	:	1.50  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 (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:

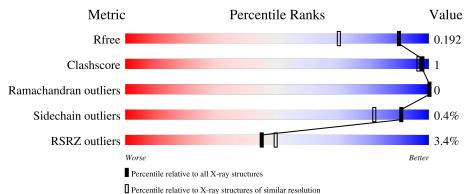
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	А	136	2% 95% •	•				
1	В	136	98%					



#### $4 \mathrm{UHQ}$

## 2 Entry composition (i)

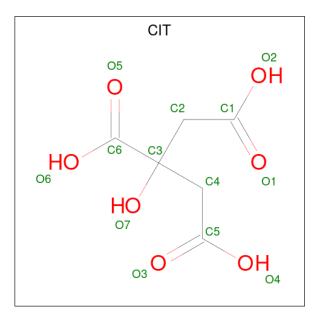
There are 4 unique types of molecules in this entry. The entry contains 2313 atoms, of which 20 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	133	Total	С	Ν	0	S	0	2	0
	1 A	155	1051	667	187	196	1	0	2	0
1	В	134	Total	С	Ν	0	S	0	1	0
I D	154	1053	667	187	198	1	0		0	

• Molecule 1 is a protein called LARGE COMPONENT OF PYOCIN AP41.

• Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 18 & 6 & 5 & 7 \end{array}$	0	0
2	А	1	Total         C         H         O           36         12         10         14	0	1
2	В	1	Total C H O 18 6 5 7	0	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ni 1 1	0	0
3	В	1	Total Ni 1 1	0	0

• Molecule 4 is water.

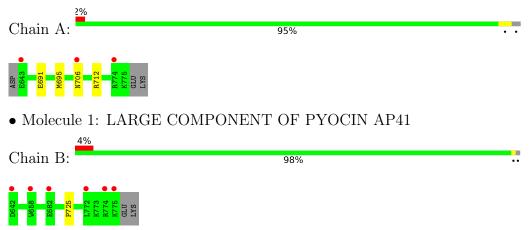
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	86	Total         O           86         86	0	0
4	В	49	Total         O           49         49	0	0



# 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: LARGE COMPONENT OF PYOCIN AP41





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	100.58Å 100.58Å 71.53Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.98 - 1.50	Depositor
Resolution (A)	44.98 - 1.50	EDS
% Data completeness	100.0 (44.98 - 1.50)	Depositor
(in resolution range)	$100.0 \ (44.98 - 1.50)$	EDS
R <sub>merge</sub>	0.06	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.53 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D	0.174 , $0.191$	Depositor
$R, R_{free}$	0.176 , $0.192$	DCC
$R_{free}$ test set	2960 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35 , $42.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2313	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: CIT, NI

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).

Mal	Mol Chain		lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.67	0/1085	0.74	1/1471~(0.1%)	
1	В	0.60	0/1084	0.66	0/1470	
All	All	0.63	0/2169	0.70	1/2941~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	rpe Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	A	712	ARG	NE-CZ-NH2	-5.28	117.66	120.30

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	А	1051	0	1030	2	0
1	В	1053	0	1026	0	0
2	А	39	15	14	1	0
2	В	13	5	4	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	86	0	0	1	0
4	В	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2293	20	2074	3	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 1.

All (3) 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)
2:A:1777[B]:CIT:O4	4:A:2039:HOH:O	1.78	0.98
1:A:691:GLU:O	1:A:695:MET:HG3	2.19	0.43
1:A:706[B]:ASN:ND2	1:A:706[B]:ASN:H	2.17	0.42

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	Perce	ntiles
1	А	133/136~(98%)	133 (100%)	0	0	100	100
1	В	133/136~(98%)	133 (100%)	0	0	100	100
All	All	266/272~(98%)	266 (100%)	0	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	А	113/115~(98%)	113 (100%)	0	100 100		
1	В	113/115~(98%)	112 (99%)	1 (1%)	78 61		
All	All	226/230~(98%)	225~(100%)	1 (0%)	91 82		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	В	725	PRO	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	True	Chain	Dec Lin		Res Link G Bond lengths				Bond angles		
IVIOI	Type	Chain	nes 1	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
2	CIT	А	1776	3	12,12,12	1.33	2 (16%)	$17,\!17,\!17$	2.07	5 (29%)	
2	CIT	А	1777[B]	-	12,12,12	1.04	0	17,17,17	1.77	5 (29%)	



Mol	Mal Truna Chain Dag		Tinle	Bo	Bond lengths			Bond angles		
10101	Type	Chain	$\operatorname{Res}$	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	CIT	В	1776	3	12,12,12	1.01	1 (8%)	17,17,17	1.54	3 (17%)
2	CIT	А	1777[A]	-	12,12,12	1.07	0	17,17,17	2.46	7 (41%)

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
2	CIT	А	1776	3	-	3/16/16/16	-
2	CIT	А	1777[B]	-	-	8/16/16/16	-
2	CIT	В	1776	3	-	4/16/16/16	-
2	CIT	А	1777[A]	-	-	6/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1776	CIT	O2-C1	-2.25	1.23	1.30
2	В	1776	CIT	O2-C1	-2.14	1.23	1.30
2	А	1776	CIT	01-C1	2.01	1.28	1.22

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	1777[A]	CIT	O6-C6-C3	5.77	123.06	113.05
2	А	1776	CIT	O5-C6-C3	-4.88	115.35	122.25
2	А	1777[A]	CIT	O5-C6-C3	-4.85	115.39	122.25
2	А	1776	CIT	O6-C6-C3	4.74	121.27	113.05
2	А	1777[B]	CIT	O6-C6-C3	4.68	121.17	113.05
2	В	1776	CIT	O6-C6-C3	3.75	119.56	113.05
2	А	1777[A]	CIT	O2-C1-C2	3.52	125.64	114.35
2	А	1776	CIT	O2-C1-C2	2.66	122.89	114.35
2	А	1777[A]	CIT	O1-C1-C2	-2.65	115.20	122.94
2	А	1777[A]	CIT	O7-C3-C6	2.60	112.51	108.86
2	А	1777[A]	CIT	O4-C5-C4	2.58	122.65	114.35
2	А	1777[B]	CIT	O4-C5-C4	2.41	122.08	114.35
2	А	1776	CIT	C2-C3-C6	2.40	115.27	110.11
2	В	1776	CIT	C2-C3-C6	2.33	115.12	110.11
2	А	1777[B]	CIT	O2-C1-C2	2.21	121.45	114.35
2	А	1776	CIT	O2-C1-O1	-2.20	117.82	123.30
2	А	1777[B]	CIT	O4-C5-O3	-2.16	117.91	123.30

All (20) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	1777[A]	CIT	O4-C5-O3	-2.11	118.04	123.30
2	В	1776	CIT	C4-C3-C6	-2.10	105.58	110.11
2	А	1777[B]	CIT	O6-C6-O5	-2.02	117.38	123.82

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There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1777[B]	CIT	O7-C3-C6-O5
2	А	1777[B]	CIT	O7-C3-C6-O6
2	А	1777[B]	CIT	C4-C3-C6-O5
2	А	1777[B]	CIT	C4-C3-C6-O6
2	А	1777[A]	CIT	C3-C4-C5-O3
2	А	1777[A]	CIT	C3-C4-C5-O4
2	А	1777[A]	CIT	C4-C3-C6-O6
2	А	1776	CIT	C4-C3-C6-O5
2	В	1776	CIT	C2-C3-C6-O6
2	А	1777[A]	CIT	O2-C1-C2-C3
2	В	1776	CIT	C2-C3-C6-O5
2	А	1777[A]	CIT	O1-C1-C2-C3
2	А	1777[B]	CIT	O2-C1-C2-C3
2	А	1776	CIT	O2-C1-C2-C3
2	А	1777[B]	CIT	O1-C1-C2-C3
2	А	1777[B]	CIT	C3-C4-C5-O3
2	В	1776	CIT	O2-C1-C2-C3
2	А	1776	CIT	O1-C1-C2-C3
2	А	1777[B]	CIT	C3-C4-C5-O4
2	А	1777[A]	CIT	C2-C3-C6-O6
2	В	1776	CIT	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1777[B]	CIT	1	0

## 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 $>$	$\#RSRZ{>}2$		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	133/136~(97%)	0.12	3 (2%)	60 65	17, 25, 42, 62	0
1	В	134/136~(98%)	0.24	6 (4%)	33 36	17, 30, 56, 89	0
All	All	267/272 (98%)	0.18	9 (3%)	45 49	17, 27, 49, 89	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	774	ARG	4.3
1	В	772	LEU	4.0
1	А	774	ARG	3.3
1	В	775	LYS	2.7
1	В	658	TRP	2.5
1	А	706[A]	ASN	2.5
1	В	642	ASP	2.3
1	В	682	GLU	2.2
1	A	643	GLU	2.2

## 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,



Mol	Type	Chain	$\mathbf{Res}$	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	$\mathbf{Q}{<}0.9$
2	CIT	А	1777[A]	13/13	0.86	0.20	22,26,36,40	18
2	CIT	А	1777[B]	13/13	0.86	0.20	21,26,31,32	18
2	CIT	А	1776	13/13	0.94	0.09	18,21,27,33	0
2	CIT	В	1776	13/13	0.95	0.08	19,25,31,33	0
3	NI	В	1777	1/1	0.99	0.10	21,21,21,21	0
3	NI	А	1778	1/1	1.00	0.11	18,18,18,18	0

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.

## 6.5 Other polymers (i)

There are no such residues in this entry.

