



# wwPDB X-ray Structure Validation Summary Report

Dec 3, 2023 – 02:03 pm GMT

PDB ID : 1UVI  
Title : The structural basis for RNA specificity and Ca<sup>2+</sup> inhibition of an RNA-dependent RNA polymerase phi6p2 with 6nt RNA  
Authors : Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.  
Deposited on : 2004-01-21  
Resolution : 2.15 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](mailto: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>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : **FAILED**  
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

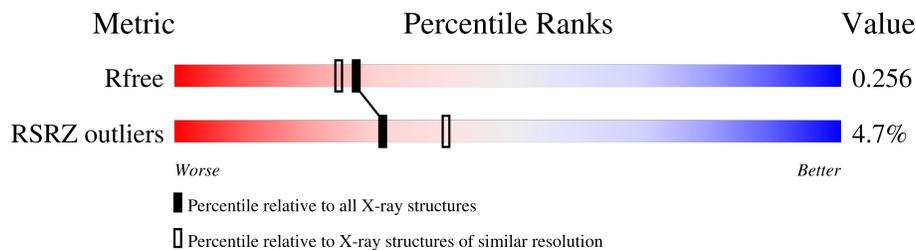
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16447 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5265	3342	914	977	32	0	0	0
1	B	664	5265	3342	914	977	32	0	0	0
1	C	664	5265	3342	914	977	32	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124

- Molecule 2 is a RNA chain called 5'-R(\*UP\*UP\*UP\*UP\*CP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	4	77	36	10	28	3	0	0	0
2	E	4	77	36	10	28	3	0	0	0
2	F	4	77	36	10	28	3	0	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	0	0
4	B	192	Total 192	O 192	0	0
4	C	109	Total 109	O 109	0	0
4	D	1	Total 1	O 1	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.13Å 93.71Å 140.74Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	19.93 – 2.15 19.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.93-2.15) 97.9 (19.93-2.15)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.15Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.256 0.230 , 0.256	Depositor DCC
$R_{free}$ test set	7208 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.631	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

#### 4.7 Other polymers

There are no such residues in this entry.

#### 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	664/664 (100%)	0.15	28 (4%) 36 45	17, 30, 52, 102	0
1	B	664/664 (100%)	0.16	19 (2%) 51 61	17, 28, 51, 102	0
1	C	664/664 (100%)	0.40	41 (6%) 20 27	18, 31, 53, 103	0
2	D	4/6 (66%)	1.91	1 (25%) 0 0	115, 116, 122, 128	0
2	E	4/6 (66%)	2.84	3 (75%) 0 0	115, 116, 123, 129	0
2	F	4/6 (66%)	2.39	2 (50%) 0 0	115, 116, 123, 129	0
All	All	2004/2010 (99%)	0.25	94 (4%) 31 41	17, 30, 53, 129	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	607	ARG	11.1
1	C	603	ALA	10.8
1	B	606	ALA	9.5
1	C	606	ALA	9.1
1	B	609	ALA	8.6

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.4 Ligands

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<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	MN	B	1665	1/1	0.98	0.06	26,26,26,26	0
3	MN	A	1665	1/1	0.99	0.08	29,29,29,29	0
3	MN	C	1665	1/1	0.99	0.05	30,30,30,30	0

## 5.5 Other polymers

There are no such residues in this entry.