



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NND  
Title : Arginine 116 is Essential for Nucleic Acid Recognition by the Fingers Domain of Moloney Murine Leukemia Virus Reverse Transcriptase  
Authors : Crowther, R.L.; Remeta, D.P.; Minetti, C.A.; Das, D.; Montano, S.P.; Georgiadis, M.M.  
Deposited on : 2003-01-13  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

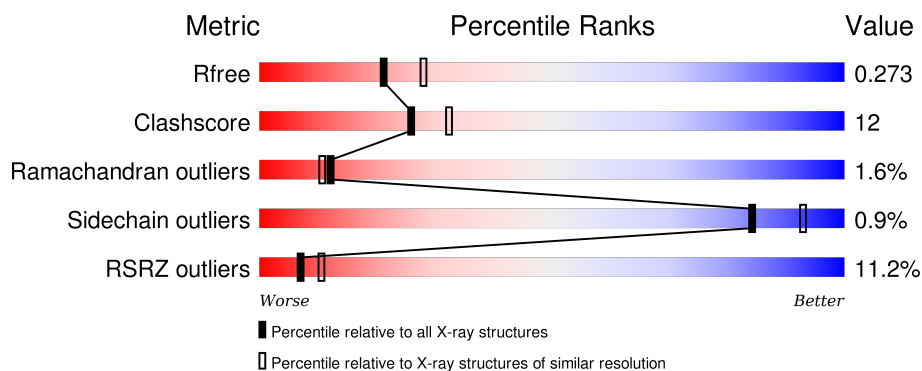
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	255	<div> <div>11%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2136 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 Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2001	1290	345	359	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	ARG	ENGINEERED	UNP P03355

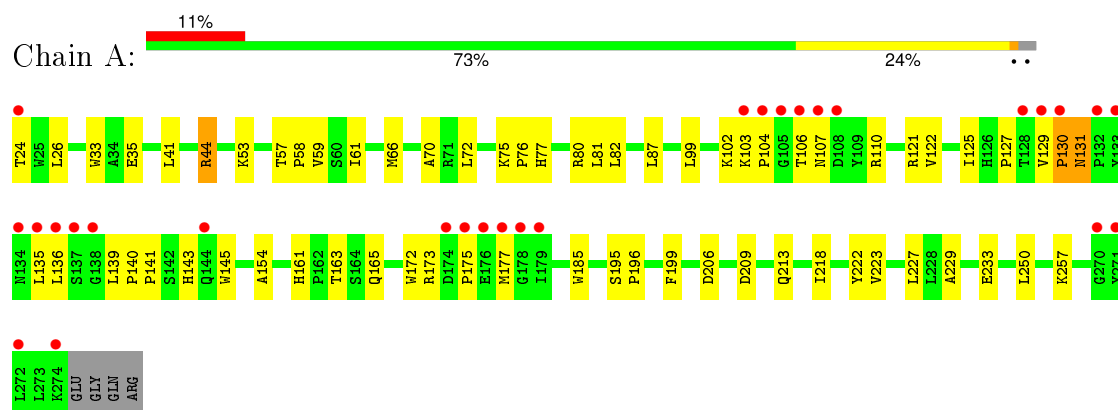
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total	O	0	0
			135	135		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Reverse Transcriptase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.80Å 116.65Å 61.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.84 – 2.30 32.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (32.84-2.30) 95.8 (32.84-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.63 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.274 0.204 , 0.273	Depositor DCC
$R_{free}$ test set	1219 reflections (9.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12449 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	0/2057	0.59	0/2808

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	2001	0	2018	50	1
2	A	135	0	0	2	0
All	All	2136	0	2018	50	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 12.

All (50) 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:A:103:LYS:HD2	1:A:104:PRO:HD2	1.55	0.87
1:A:102:LYS:NZ	1:A:107:ASN:HA	1.95	0.81
1:A:102:LYS:HZ2	1:A:107:ASN:HA	1.52	0.73
1:A:59:VAL:HG11	1:A:121:ARG:CZ	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HB3	1:A:44:ARG:HH11	1.56	0.69
1:A:209:ASP:O	1:A:213:GLN:HG2	1.96	0.65
1:A:57:THR:HG23	1:A:58:PRO:HD2	1.81	0.63
1:A:161:HIS:HD2	1:A:163:THR:H	1.46	0.63
1:A:59:VAL:CG1	1:A:121:ARG:CZ	2.76	0.63
1:A:75:LYS:HB3	1:A:76:PRO:HD3	1.81	0.61
1:A:206:ASP:HB3	1:A:250:LEU:HD13	1.83	0.60
1:A:139:LEU:HD23	1:A:218:ILE:HG21	1.86	0.57
1:A:125:ILE:O	1:A:127:PRO:HD3	2.05	0.57
1:A:102:LYS:HZ1	1:A:107:ASN:HA	1.70	0.56
1:A:106:THR:HG22	1:A:107:ASN:N	2.19	0.56
1:A:77:HIS:CD2	1:A:80:ARG:HH12	2.24	0.56
1:A:172:TRP:HE1	1:A:177:MET:CE	2.19	0.55
1:A:35:GLU:OE2	1:A:257:LYS:HG3	2.09	0.53
1:A:103:LYS:CD	1:A:104:PRO:HD2	2.35	0.53
1:A:44:ARG:CB	1:A:44:ARG:HH11	2.20	0.52
1:A:130:PRO:O	1:A:131:ASN:HB2	2.11	0.49
1:A:154:ALA:HB1	1:A:199:PHE:CZ	2.48	0.49
1:A:77:HIS:HD2	1:A:80:ARG:HH12	1.61	0.49
1:A:66:MET:HG2	1:A:70:ALA:HB3	1.94	0.48
1:A:227:LEU:C	1:A:227:LEU:HD23	2.35	0.47
1:A:195:SER:HB2	1:A:196:PRO:HD3	1.97	0.46
1:A:59:VAL:HG13	1:A:121:ARG:NE	2.30	0.46
1:A:57:THR:HG23	1:A:58:PRO:CD	2.46	0.46
1:A:131:ASN:O	1:A:135:LEU:HB2	2.16	0.45
1:A:24:THR:HG21	2:A:386:HOH:O	2.16	0.45
1:A:26:LEU:HD12	1:A:26:LEU:N	2.32	0.45
1:A:106:THR:CG2	1:A:107:ASN:N	2.81	0.44
1:A:173:ARG:NH1	1:A:173:ARG:HB2	2.31	0.44
1:A:110:ARG:HG3	1:A:110:ARG:O	2.17	0.44
1:A:161:HIS:CD2	1:A:163:THR:HG23	2.53	0.44
1:A:154:ALA:HB1	1:A:199:PHE:CE1	2.51	0.44
1:A:61:ILE:HD12	1:A:61:ILE:N	2.33	0.44
1:A:41:LEU:C	1:A:41:LEU:HD23	2.37	0.44
1:A:165:GLN:HG2	1:A:185:TRP:O	2.17	0.44
1:A:139:LEU:CD2	1:A:218:ILE:HG21	2.47	0.43
1:A:143:HIS:HB3	1:A:229:ALA:HB1	1.99	0.43
1:A:53:LYS:HE3	1:A:122:VAL:O	2.19	0.43
1:A:136:LEU:HD12	1:A:136:LEU:H	1.84	0.42
1:A:140:PRO:HA	1:A:141:PRO:HD3	1.90	0.42
1:A:222:TYR:HD1	2:A:279:HOH:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TRP:CH2	1:A:233:GLU:HB2	2.55	0.41
1:A:82:LEU:HD23	1:A:87:LEU:O	2.20	0.41
1:A:99:LEU:HD12	1:A:99:LEU:N	2.36	0.41
1:A:26:LEU:HA	1:A:33:TRP:NE1	2.35	0.41
1:A:129:VAL:HG11	1:A:222:TYR:CE2	2.55	0.41

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:CD1	1:A:72:LEU:CD1[2_655]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	249/255 (98%)	230 (92%)	15 (6%)	4 (2%)	12 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	130	PRO
1	A	223	VAL
1	A	131	ASN

### 5.3.2 Protein sidechains ⓘ

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	220/223 (99%)	218 (99%)	2 (1%)	84	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	81	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	HIS
1	A	84	GLN
1	A	161	HIS
1	A	190	GLN
1	A	249	ASN
1	A	265	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	251/255 (98%)	0.35	28 (11%) 7 10	10, 25, 84, 101	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	12.0
1	A	130	PRO	9.9
1	A	129	VAL	9.4
1	A	104	PRO	9.2
1	A	178	GLY	8.7
1	A	128	THR	7.9
1	A	179	ILE	6.7
1	A	132	PRO	5.7
1	A	272	LEU	4.7
1	A	103	LYS	4.6
1	A	271	TYR	4.5
1	A	106	THR	4.5
1	A	134	ASN	4.3
1	A	175	PRO	4.2
1	A	133	TYR	4.0
1	A	177	MET	3.1
1	A	176	GLU	2.8
1	A	24	THR	2.8
1	A	108	ASP	2.6
1	A	107	ASN	2.6
1	A	135	LEU	2.6
1	A	174	ASP	2.5
1	A	274	LYS	2.5
1	A	138	GLY	2.5
1	A	144	GLN	2.4
1	A	270	GLY	2.4
1	A	136	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	137	SER	2.3

## 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 carbohydrates 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.