



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 02:58 PM EDT

PDB ID : 3KLI  
Title : Crystal structure of unliganded AZT-resistant HIV-1 Reverse Transcriptase  
Authors : Tu, X.; Sarafianos, S.G.; Arnold, E.  
Deposited on : 2009-11-08  
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

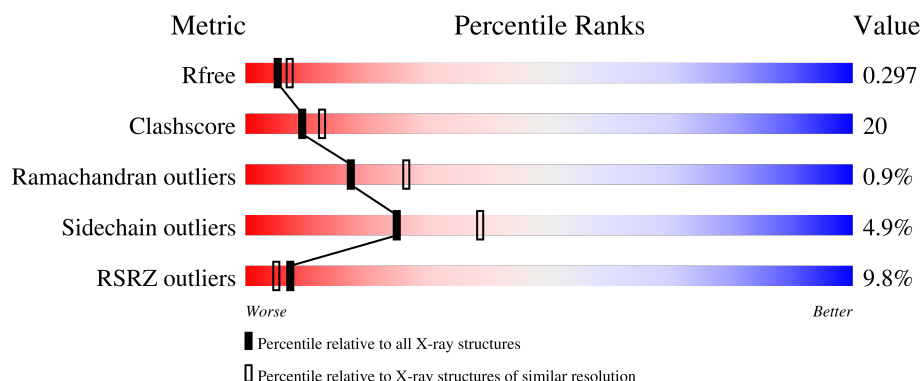
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	562	<div> <div>10%</div> <div>58%</div> <div>36%</div> <div>..</div> </div>
2	B	437	<div> <div>8%</div> <div>62%</div> <div>34%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8062 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4495	2911	749	828	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	41	LEU	MET	engineered mutation	UNP P03366
A	67	ASN	ASP	engineered mutation	UNP P03366
A	70	ARG	LYS	engineered mutation	UNP P03366
A	215	TYR	THR	engineered mutation	UNP P03366
A	219	GLN	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	559	VAL	ILE	SEE REMARK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3529	2300	584	638	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	429	GLY	-	expression tag	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	HIS	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

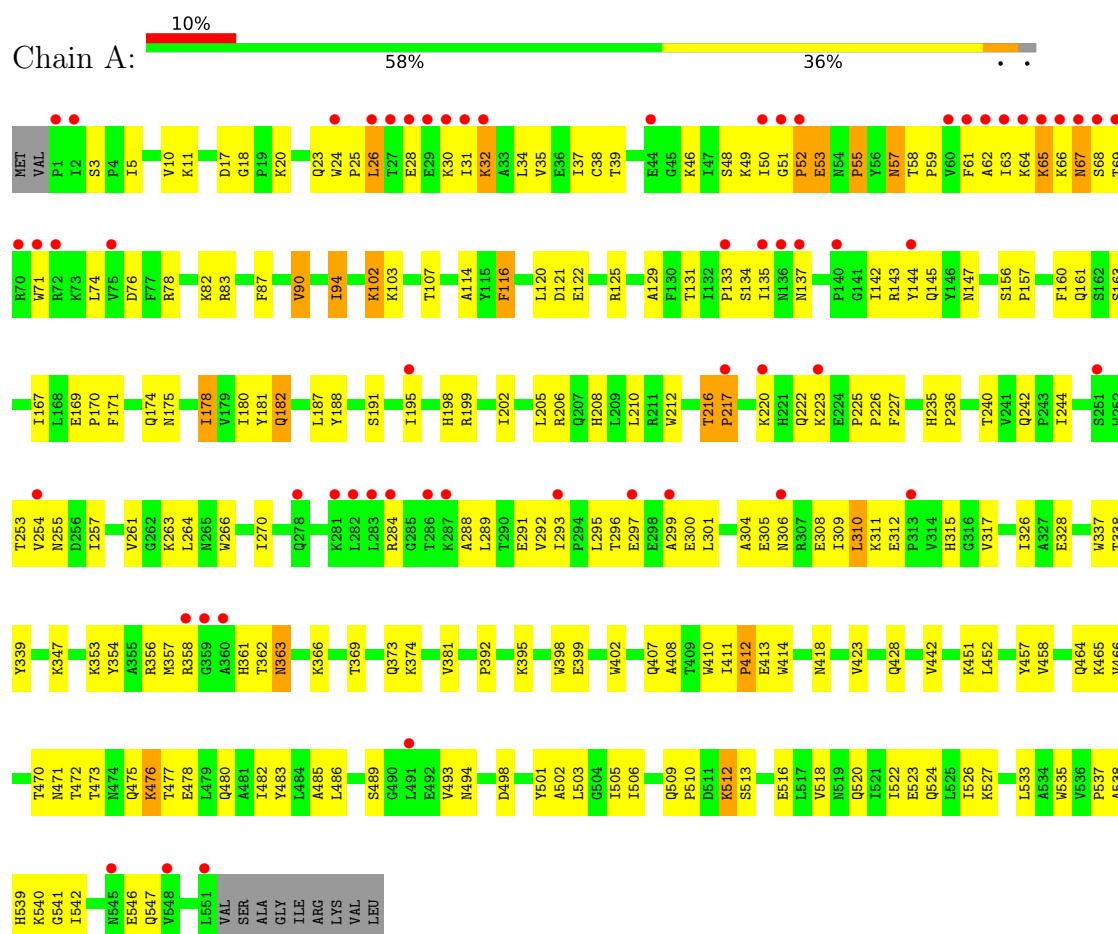
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	19	Total	O	0	0
			19	19		

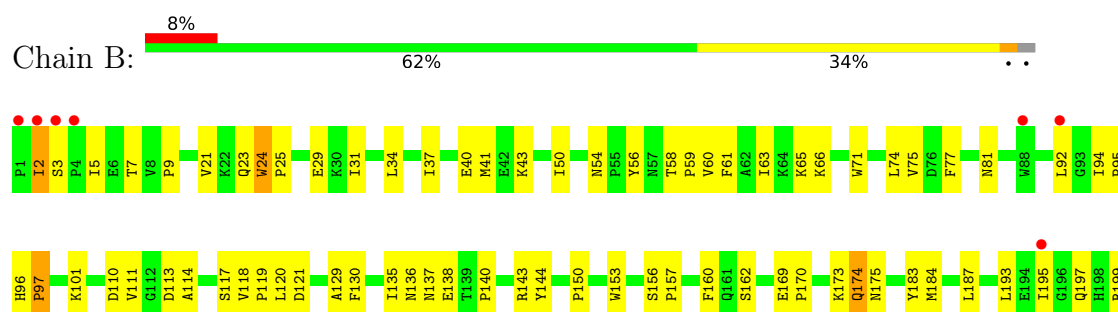
### 3 Residue-property plots [i](#)

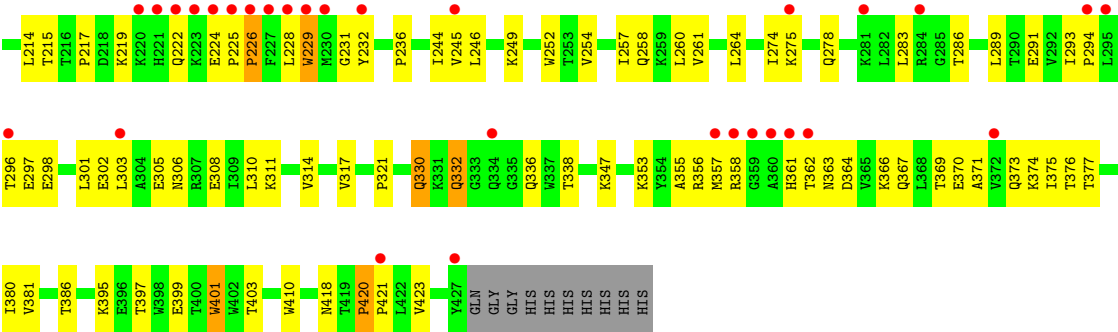
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase/ribonuclease H



#### • Molecule 2: p51 RT





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	237.07Å 71.22Å 94.63Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.65 28.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (28.64-2.65) 92.5 (28.64-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.260 , 0.294 0.260 , 0.297	Depositor DCC
$R_{free}$ test set	1334 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.3	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	0.93	EDS
Total number of atoms	8062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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.

## 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	0.43	0/4614	0.61	2/6270 (0.0%)
2	B	0.50	0/3634	0.67	1/4940 (0.0%)
All	All	0.46	0/8248	0.64	3/11210 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	SER	CB-CA-C	-5.45	99.74	110.10
1	A	57	ASN	CB-CA-C	5.33	121.06	110.40
1	A	58	THR	N-CA-CB	5.22	120.22	110.30

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	A	4495	0	4549	208	0
2	B	3529	0	3568	130	0
3	A	19	0	0	0	0
3	B	19	0	0	3	0
All	All	8062	0	8117	319	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 20.



The worst 5 of 319 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:494:ASN:HD22	2:B:289:LEU:HD12	1.19	1.06
1:A:51:GLY:N	1:A:52:PRO:HD3	1.76	0.95
1:A:222:GLN:O	1:A:222:GLN:HG3	1.67	0.93
1:A:63:ILE:HG12	1:A:64:LYS:H	1.34	0.90
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.54	0.89

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	549/562 (98%)	491 (89%)	53 (10%)	5 (1%)	17	26
2	B	425/437 (97%)	381 (90%)	40 (9%)	4 (1%)	17	26
All	All	974/999 (98%)	872 (90%)	93 (10%)	9 (1%)	17	26

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	217	PRO
1	A	412	PRO
1	A	55	PRO
1	A	90	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	493/502 (98%)	464 (94%)	29 (6%)	19	30
2	B	389/397 (98%)	375 (96%)	14 (4%)	35	51
All	All	882/899 (98%)	839 (95%)	43 (5%)	25	38

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	LEU
2	B	174	GLN
2	B	2	ILE
2	B	58	THR
2	B	229	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	207	GLN
2	B	278	GLN
2	B	332	GLN
1	A	363	ASN
1	A	336	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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, 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	551/562 (98%)	0.63	59 (10%) 6 4	53, 97, 138, 148	0
2	B	427/437 (97%)	0.55	37 (8%) 10 8	43, 86, 138, 152	0
All	All	978/999 (97%)	0.60	96 (9%) 7 5	43, 94, 138, 152	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PRO	9.9
2	B	360	ALA	9.8
2	B	230	MET	8.8
2	B	359	GLY	8.4
2	B	227	PHE	8.2

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.