

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

Dec 18, 2023 - 02:20 am GMT

PDB ID	:	4B3P
Title	:	Structures of HIV-1 RT and RNA-DNA Complex Reveal a Unique RT Con-
		formation and Substrate Interface
Authors	:	Lapkouski, M.; Tian, L.; Miller, J.T.; Le Grice, S.F.J.; Yang, W.
Deposited on	:	2012-07-25
Resolution	:	4.84  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
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 4.84 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
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1098 (5.82 - 3.80)
Clashscore	141614	1172(5.82-3.80)
Ramachandran outliers	138981	1107 (5.82 - 3.80)
Sidechain outliers	138945	1087 (5.82 - 3.80)
RNA backbone	3102	$1065 \ (6.46-3.00)$

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%

Mol	Chain	Length	Qualit	y of chain	
1	А	560	83%		9% • 7%
2	В	454	81%		8% 11%
3	D	29	48%	24%	28%
4	R	34	53%	9%	38%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8162 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	А	519	Total 4054	C 2612	N 669	O 766	${ m S} 7$	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	68	GLY	SER	engineered mutation	UNP P04585
А	83	LYS	ARG	engineered mutation	UNP P04585
А	411	VAL	ILE	engineered mutation	UNP P04585
A	447	SER	ASN	engineered mutation	UNP P04585
А	461	LYS	ARG	engineered mutation	UNP P04585
А	483	HIS	TYR	engineered mutation	UNP P04585
А	498	ALA	ASP	engineered mutation	UNP P04585
А	559	ILE	VAL	engineered mutation	UNP P04585

• Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	404	Total 3230	C 2102	N 524	O 597	${ m S} 7$	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-13	MET	-	expression tag	UNP P04585
В	-12	ARG	-	expression tag	UNP P04585
В	-11	GLY	-	expression tag	UNP P04585
В	-10	SER	-	expression tag	UNP P04585
В	-9	HIS	-	expression tag	UNP P04585
В	-8	HIS	-	expression tag	UNP P04585
В	-7	HIS	-	expression tag	UNP P04585
В	-6	HIS	-	expression tag	UNP P04585

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-5	HIS	-	expression tag	UNP P04585
В	-4	HIS	-	expression tag	UNP P04585
В	-3	GLY	-	expression tag	UNP P04585
В	-2	SER	-	expression tag	UNP P04585
В	-1	GLN	-	expression tag	UNP P04585
В	0	LEU	-	expression tag	UNP P04585
В	68	GLY	SER	engineered mutation	UNP P04585
В	83	LYS	ARG	engineered mutation	UNP P04585
В	411	VAL	ILE	engineered mutation	UNP P04585

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• Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total 433	C 207	N 75	O 130	Р 21	0	0	0

• Molecule 4 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	21	Total 445	C 200	N 81	0 143	Р 21	0	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. 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. 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



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	163.00Å 163.00Å 229.60Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{ascolution}}(\hat{\mathbf{A}})$	46.10 - 4.84	Depositor
Resolution (A)	48.38 - 4.84	EDS
% Data completeness	99.2 (46.10-4.84)	Depositor
(in resolution range)	99.4 (48.38-4.84)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.16	Depositor
$< I/\sigma(I) > 1$	$0.90 (at 4.85 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.364 , $0.404$	Depositor
II, II, <i>free</i>	0.583 , $0.406$	DCC
$R_{free}$ test set	433 reflections $(2.39%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	130.1	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.31, 139.3	EDS
L-test for $twinning^2$	$ < L >=0.28, < L^2>=0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.60	EDS
Total number of atoms	8162	wwPDB-VP
Average B, all atoms $(Å^2)$	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.73% 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)

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	Chain	Bo	Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.49	4/4146~(0.1%)	0.47	0/5648
2	В	0.53	4/3315~(0.1%)	0.47	0/4513
3	D	0.30	0/484	0.70	0/746
4	R	0.29	1/497~(0.2%)	0.65	0/771
All	All	0.49	9/8442~(0.1%)	0.50	0/11678

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	410	TRP	CD2-CE2	5.06	1.47	1.41
1	А	383	TRP	CD2-CE2	5.05	1.47	1.41
2	В	426	TRP	CD2-CE2	5.03	1.47	1.41
2	В	24	TRP	CD2-CE2	5.03	1.47	1.41
2	В	212	TRP	CD2-CE2	5.03	1.47	1.41
4	R	21	A	C3'-C2'	5.03	1.58	1.52
1	А	212	TRP	CD2-CE2	5.01	1.47	1.41
1	A	401	TRP	CD2-CE2	5.01	1.47	1.41
2	В	398	TRP	CD2-CE2	5.01	1.47	1.41

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	А	4054	0	3965	23	0
2	В	3230	0	3186	14	0
3	D	433	0	240	5	0
4	R	445	0	228	2	0
All	All	8162	0	7619	43	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.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1 Atom-2		distance (Å)	overlap (Å)
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.69	0.74
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.45	0.63
3:D:3:DG:H2'	3:D:4:DG:H8	1.69	0.58
1:A:482:ILE:HD13	1:A:506:ILE:HD11	1.85	0.57
3:D:16:DT:H2'	3:D:17:DA:C8	2.40	0.56
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.89	0.55
3:D:3:DG:H2'	3:D:4:DG:C8	2.42	0.54
1:A:482:ILE:HD11	1:A:502:ALA:HB1	1.90	0.53
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.90	0.52
2:B:185:ASP:HB2	2:B:409:THR:HG21	1.90	0.52
4:R:28:C:H2'	4:R:29:G:H8	1.75	0.51
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.94	0.50
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.93	0.50
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.92	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.48
1:A:363:ASN:HD22	1:A:509:GLN:HB2	1.79	0.48
1:A:295:LEU:H	1:A:295:LEU:HD13	1.79	0.47
1:A:479:LEU:HD21	1:A:518:VAL:HG23	1.97	0.46
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.98	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.46
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.99	0.45
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.85	0.45
4:R:28:C:H2'	4:R:29:G:C8	2.51	0.45
2:B:169:GLU:N	2:B:170:PRO:HD2	2.32	0.45
1:A:253:THR:HA	1:A:292:VAL:HA	1.99	0.44
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.99	0.44
1:A:449:GLU:C	1:A:451:LYS:H	2.21	0.43
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.00	0.43
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.87	0.43
1:A:515:SER:C	1:A:517:LEU:N	2.72	0.43

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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:325:LEU:HD23	2:B:387:PRO:HB3	2.02	0.42
2:B:295:LEU:HB3	2:B:300:GLU:HG2	2.02	0.42
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.85	0.41
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.01	0.41
2:B:264:LEU:HD12	2:B:274:ILE:HG12	2.01	0.41
3:D:11:DG:H2"	3:D:12:DC:H5'	2.03	0.41
1:A:376:THR:O	1:A:380:ILE:HG12	2.21	0.41
2:B:180:ILE:HG22	2:B:189:VAL:HG22	2.03	0.40
3:D:10:DT:H2'	3:D:11:DG:C8	2.56	0.40
2:B:125:ARG:HE	2:B:147:ASN:HA	1.86	0.40
1:A:515:SER:C	1:A:517:LEU:H	2.25	0.40
2:B:341:ILE:HD12	2:B:350:LYS:HB3	2.03	0.40
1:A:97:PRO:HA	1:A:100:LEU:HD12	2.03	0.40

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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	А	507/560~(90%)	473 (93%)	29 (6%)	5 (1%)	15 53
2	В	396/454~(87%)	383~(97%)	11 (3%)	2~(0%)	29 68
All	All	903/1014 (89%)	856 (95%)	40 (4%)	7 (1%)	19 59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	360	ALA
1	А	6	GLU
1	А	363	ASN
2	В	355	ALA
1	А	184	MET

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Mol	Chain	Res	Type
1	А	421	PRO
1	А	292	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	$\mathbf{ntiles}$
1	А	426/498~(86%)	415 (97%)	11 (3%)	46	67
2	В	344/411~(84%)	339~(98%)	5(2%)	65	80
All	All	770/909~(85%)	754 (98%)	16 (2%)	53	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	185	ASP
1	А	250	ASP
1	А	260	LEU
1	А	295	LEU
1	А	301	LEU
1	А	323	LYS
1	А	353	LYS
1	А	442	VAL
1	А	448	ARG
1	А	516	GLU
1	А	517	LEU
2	В	86	ASP
2	В	113	ASP
2	В	186	ASP
2	В	303	LEU
2	В	305	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:



Mol	Chain	Res	Type
1	А	222	GLN
1	А	367	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	20/34~(58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

#### 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)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

