



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1BQM  
Title : HIV-1 RT/HBY 097  
Authors : Hsiou, Y.; Das, K.; Ding, J.; Arnold, E.  
Deposited on : 1998-08-17  
Resolution : 3.10 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

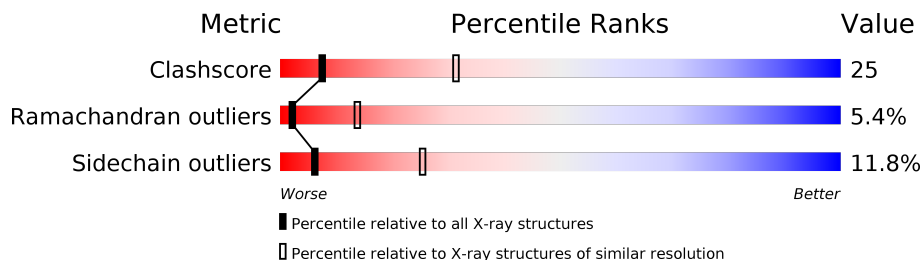
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>51%</div> <div>42%</div> <div>6%</div> </div>
2	B	430	<div> <div>47%</div> <div>46%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HBV	A	557	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7799 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	556	Total	C	N	O	S	0	0	0
			4338	2804	719	808	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

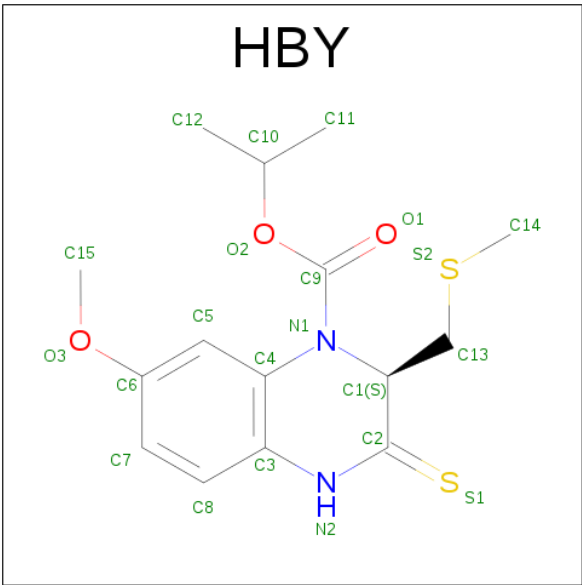
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3439	2240	567	627	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (three-letter code: HBY) (formula: C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).



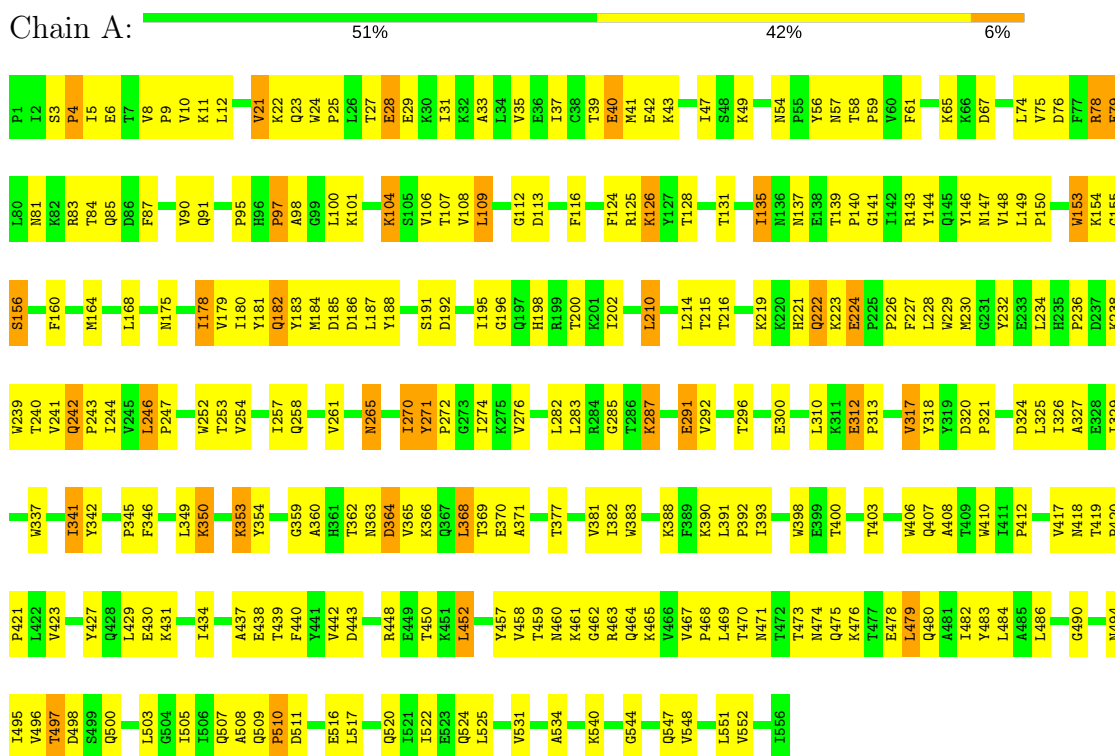
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	22	15	2	3	2	0	0

### 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 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.

Note EDS was not executed.

#### • Molecule 1: REVERSE TRANSCRIPTASE



#### • Molecule 2: REVERSE TRANSCRIPTASE



E404	I329	T244
Y405	K330	V245
W406	Q331	L246
Q407		P247
	Q336	
T409	W337	D250
F410	T338	S251
I411	Y339	W252
P412	Q340	V253
E413		
W414	Q343	V254
	E344	
	P345	T257
M418	F346	Q258
T419		K259
P420		L260
	L349	V261
L425	K350	
W426	T351	W266
Y427	G352	A267
Q428	K353	S268
L429	Y354	Q269
E430	A355	L270
	R356	Y271
		P272
	T362	G273
	N363	L274
	D364	
	V365	L279
	K366	
	Q367	L282
	L368	
	T369	L289
	E370	T290
	A371	E291
	V372	V292
	K373	T293
	Q374	P294
	L375	L295
	T376	
	T377	L303
		A304
	I380	E305
	V381	N306
	L382	R307
	W383	E308
		L309
	F389	L310
	K390	K311
	L391	
	P392	V314
	I393	H315
	Q394	G316
	K395	V317
		Y318
	W398	Y319
	E399	
	T400	D324
	W401	
	W402	A327
	T403	F328

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.20 Å   69.40 Å   104.60 Å 90.00°   106.40°   90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	99.1 (10.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, $R_{free}$	0.258 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

## 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: HBY

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	0.50	0/4451	0.77	0/6070
2	B	0.54	0/3538	0.84	1/4821 (0.0%)
All	All	0.52	0/7989	0.80	1/10891 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	TRP	N-CA-C	5.35	125.44	111.00

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	4338	0	4229	213	0
2	B	3439	0	3390	172	0
3	A	22	0	20	25	0
All	All	7799	0	7639	379	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 25.

The worst 5 of 379 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:B:26:LEU:HD12	2:B:133:PRO:HG3	1.41	1.03
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.46	0.97
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.50	0.92
1:A:234:LEU:HB3	3:A:557:HBY:H153	1.53	0.90
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.55	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	554/556 (100%)	453 (82%)	75 (14%)	26 (5%)	3	17
2	B	428/430 (100%)	342 (80%)	59 (14%)	27 (6%)	1	10
All	All	982/986 (100%)	795 (81%)	134 (14%)	53 (5%)	2	14

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	67	ASP
1	A	104	LYS
1	A	195	ILE
1	A	222	GLN

### 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	450/496 (91%)	390 (87%)	60 (13%)	4	20
2	B	363/392 (93%)	327 (90%)	36 (10%)	9	34
All	All	813/888 (92%)	717 (88%)	96 (12%)	6	25

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	LEU
1	A	484	LEU
2	B	362	THR
1	A	431	LYS
1	A	452	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	ASN
2	B	145	GLN
2	B	348	ASN
2	B	57	ASN
2	B	96	HIS

### 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 ⓘ

1 ligand is modelled in this entry.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HBY	A	557	-	21,23,23	6.35	17 (80%)	23,32,32	2.05	5 (21%)

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
3	HBY	A	557	-	-	0/13/29/29	0/1/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	HBY	C5-C4	2.19	1.43	1.39
3	A	557	HBY	C4-N1	2.20	1.45	1.42
3	A	557	HBY	O3-C15	3.04	1.51	1.42
3	A	557	HBY	C8-C3	3.38	1.45	1.39
3	A	557	HBY	C3-N2	3.88	1.46	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	HBY	C3-N2-C2	-4.43	120.51	124.70
3	A	557	HBY	C14-S2-C13	-2.73	96.81	101.19
3	A	557	HBY	O1-C9-N1	-2.64	119.29	124.12
3	A	557	HBY	O2-C10-C12	2.47	113.65	107.11
3	A	557	HBY	O2-C9-N1	6.23	118.10	110.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	HBV	25	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.