



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2024 – 03:27 PM EDT

PDB ID : 1RTJ
Title : MECHANISM OF INHIBITION OF HIV-1 REVERSE TRANSCRIPTASE
BY NON-NUCLEOSIDE INHIBITORS
Authors : Ren, J.; Esnouf, R.; Ross, C.; Jones, Y.; Stammers, D.; Stuart, D.
Deposited on : 1995-05-03
Resolution : 2.35 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

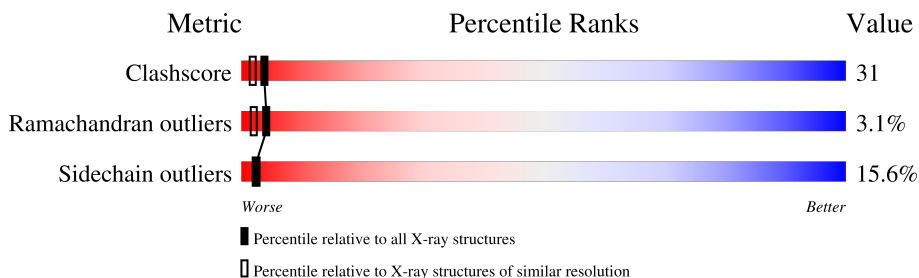
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	 41% 44% 11% ..
2	B	440	 38% 50% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8210 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4435	2869	739	819	8	0	0	0

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3508	2282	580	639	7	0	0	0

- Molecule 3 is water.

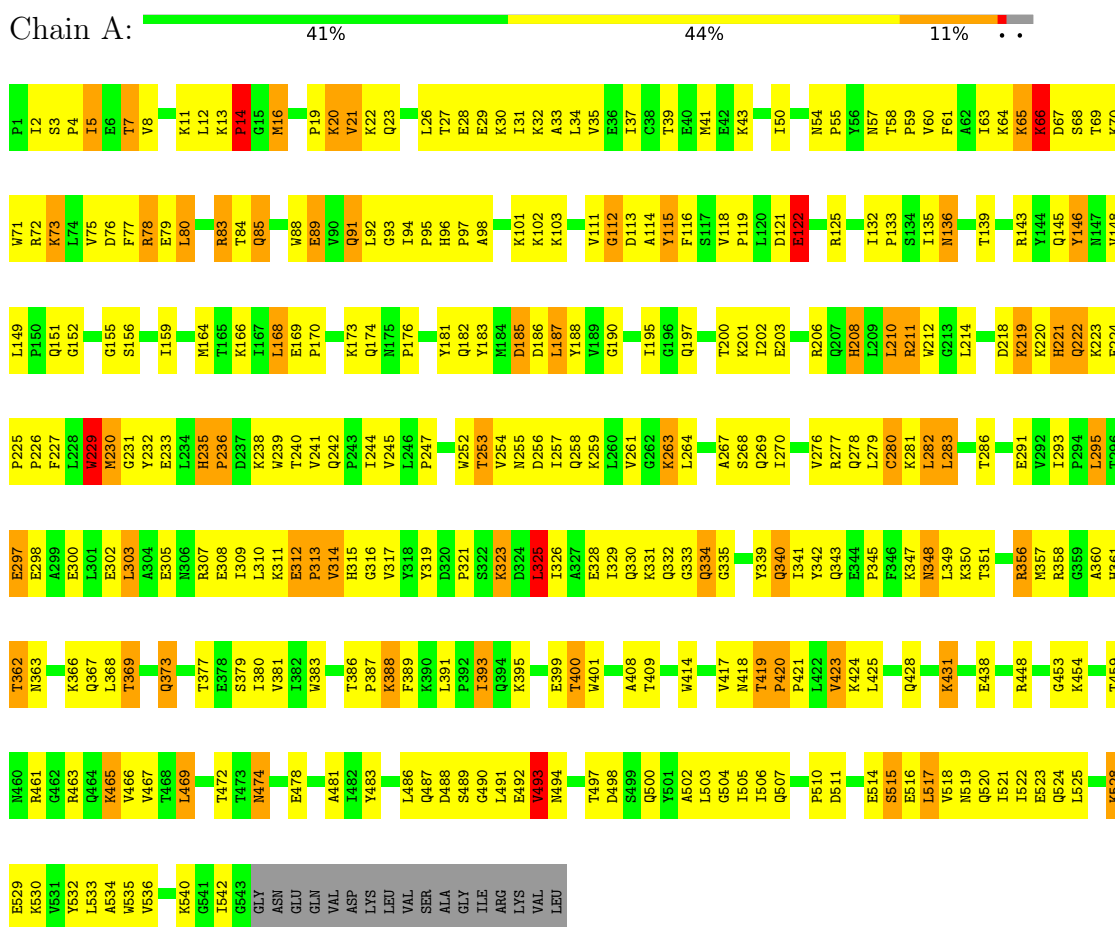
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	103	Total	O	0	0
			103	103		

3 Residue-property plots

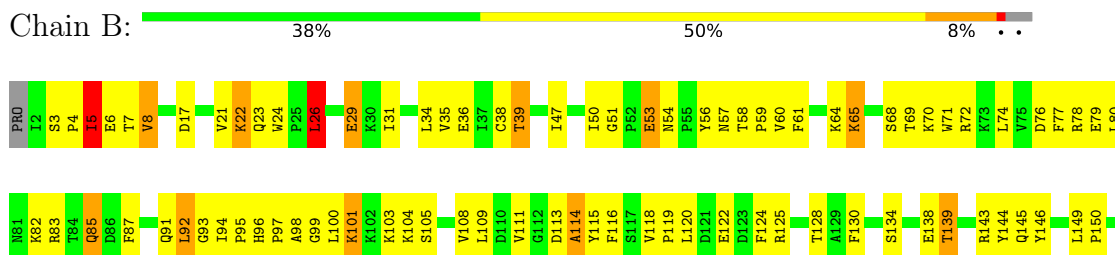
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



W153	W154	W155	W156	W157	W158	W159	W160	W161	W162	W163	W164	W165	W166	W167	W168	W169	W170	W171	W172	W173	W174	W175	W176	W177	W178	W179	W180	W181	W182	W183	W184	W185	W186	W187	W188	W189	W190	W191	W192	W193	W194	W195	W196	W197	W198	W199	W200	W201	W202	W203	W204	W205	W206	W207	W208	W209	W210	W211	W212	W213	W214	W215	W216
P217	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	G231	Y232	E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	P243	I244	V245	L246	P247	E248	K249	W252	T253	V254	W255	D256	I257	Q258	K259	L260	V261	W266	A267	Q268	I270	Y271	P272	G273	I274	K275	V276	R277	Q278	K281								
L282	L283	R284	A288	E291	V292	I293	P294	L295	E298	A299	E300	E302	L303	A304	R307	E308	I309	L310	K311	E312	F313	V314	V317	Y318	D320	P321	L325	I326	A327	E328	I329	Q332	G333	Q334	T338	Y339	I341	Y342	Q343	E344	P345	F346	K347	N348	L349	K350	T351	G352															
K353	Y354	A355	R356	G359	A360	H361	T362	N363	K366	Q367	L368	T369	E370	Q373	T376	I377	E378	S379	I380	V381	I382	W383	G384	K385	T386	P387	K388	F389	K390	L391	P392	I393	Q394	W398	E399	T400	W401	W402	T403	E404	Y405	W406	T409	W410	I411	P412	P421	L422	W423	K424	L425	W426											
L429	E430	K431	E432	I434	V435	G436	A437	E438	T439	F440																																																					

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.50Å 109.40Å 72.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35	Depositor
% Data completeness (in resolution range)	89.5 (25.00-2.35)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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: CSD

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	0.75	0/4544	0.94	7/6175 (0.1%)
2	B	0.75	0/3607	0.92	3/4903 (0.1%)
All	All	0.75	0/8151	0.94	10/11078 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LEU	CA-CB-CG	-7.04	99.12	115.30
1	A	139	THR	N-CA-C	-5.91	95.05	111.00
1	A	494	ASN	N-CA-C	-5.76	95.45	111.00
1	A	388	LYS	N-CA-C	-5.72	95.56	111.00
2	B	93	GLY	N-CA-C	-5.52	99.31	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	319	TYR	Sidechain
2	B	56	TYR	Sidechain

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	4435	0	4483	277	0
2	B	3508	0	3541	225	0
3	A	164	0	0	7	0
3	B	103	0	0	5	0
All	All	8210	0	8024	495	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 31.

The worst 5 of 495 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:178:ILE:HG12	2:B:191:SER:HB3	1.40	1.00
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.47	0.97
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.47	0.96
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.52	0.92
1:A:14:PRO:HG2	3:A:1024:HOH:O	1.73	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	540/560 (96%)	458 (85%)	65 (12%)	17 (3%)	4	2
2	B	422/440 (96%)	365 (86%)	44 (10%)	13 (3%)	4	2
All	All	962/1000 (96%)	823 (86%)	109 (11%)	30 (3%)	4	2

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	85	GLN
2	B	98	ALA
1	A	14	PRO
1	A	268	SER

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	485/499 (97%)	402 (83%)	83 (17%)	2	1
2	B	386/400 (96%)	333 (86%)	53 (14%)	3	3
All	All	871/899 (97%)	735 (84%)	136 (16%)	2	2

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	283	LEU
2	B	392	PRO
1	A	297	GLU
1	A	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	GLN
2	B	418	ASN
2	B	137	ASN
2	B	269	GLN
2	B	85	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	CSD	A	280	1	3,7,8	1.45	1 (33%)	1,8,10	10.61	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CB-SG	2.02	1.90	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	10.61	125.73	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.