



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1RDH
Title : CRYSTALLOGRAPHIC ANALYSES OF AN ACTIVE HIV-1 RIBONUCLEASE H DOMAIN SHOW STRUCTURAL FEATURES THAT DISTINGUISH IT FROM THE INACTIVE FORM
Authors : Finzel, B.C.; Chattopadhyay, D.; Einspahr, H.M.
Deposited on : 1993-03-05
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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
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

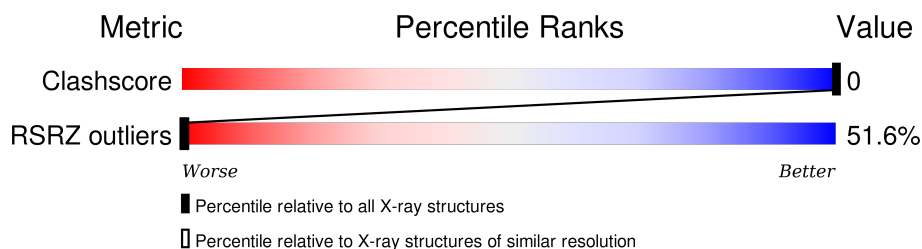
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


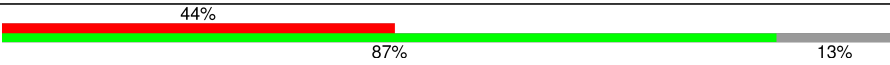
The reported resolution of this entry is 2.80 Å.

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	102246	2827 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	146	
1	B	146	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 254 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.

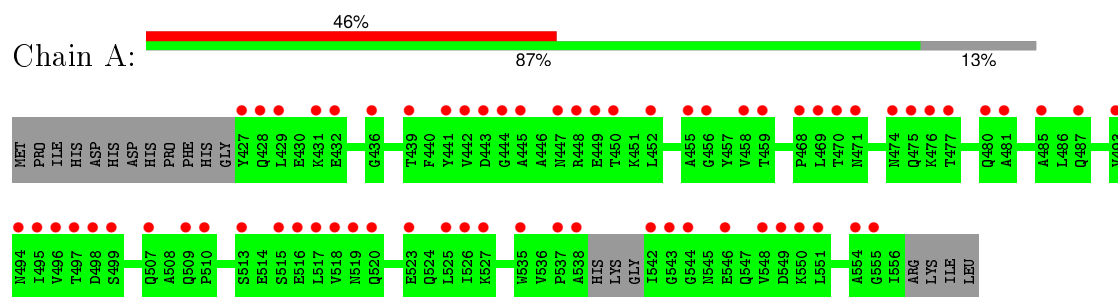
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (RIBONUCLEASE H DOMAIN).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	127	Total	C	0	0	127
			127	127			
1	B	127	Total	C	0	0	127
			127	127			

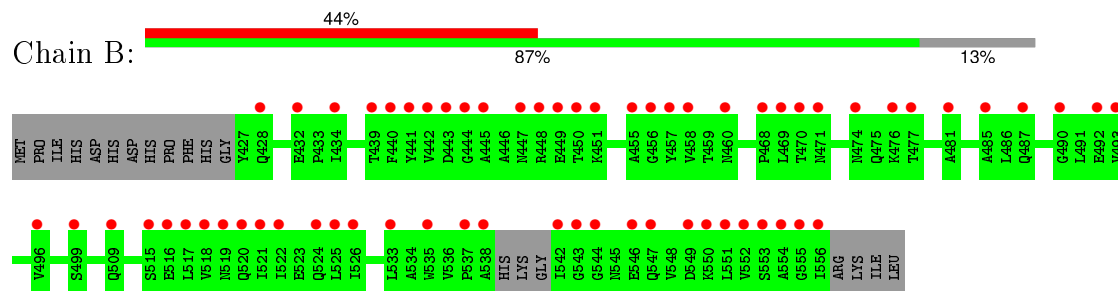
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: HIV-1 REVERSE TRANSCRIPTASE (RIBONUCLEASE H DOMAIN)



- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (RIBONUCLEASE H DOMAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	52.03Å 52.03Å 113.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 96.3 (19.38-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.79Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available) 0.398 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , -10.0	EDS
Estimated twinning fraction	0.009 for -h,-k,l 0.058 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 8148 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	254	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	127	0	0	0	0
1	B	127	0	0	0	0
All	All	254	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates 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

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, 95th 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 ²)	Q<0.9
1	A	127/146 (86%)	3.51	67 (52%)  	12, 27, 46, 53	0
1	B	127/146 (86%)	3.35	64 (50%)  	11, 25, 45, 50	0
All	All	254/292 (86%)	3.43	131 (51%)  	11, 26, 46, 53	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	GLY	23.4
1	B	556	ILE	21.5
1	A	549	ASP	18.2
1	A	555	GLY	17.6
1	B	432	GLU	17.0
1	B	554	ALA	16.8
1	A	450	THR	16.7
1	A	487	GLN	15.9
1	A	480	GLN	15.1
1	A	449	GLU	13.8
1	A	519	ASN	13.8
1	A	523	GLU	13.8
1	B	450	THR	13.6
1	A	470	THR	13.0
1	B	538	ALA	12.8
1	B	550	LYS	12.3
1	A	476	LYS	12.2
1	A	471	ASN	12.2
1	B	551	LEU	11.1
1	A	544	GLY	11.0
1	B	509	GLN	10.8
1	B	542	ILE	10.7
1	A	507	GLN	10.6
1	B	520	GLN	10.0

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Mol	Chain	Res	Type	RSRZ
1	B	470	THR	10.0
1	A	537	PRO	9.9
1	B	476	LYS	9.6
1	A	436	GLY	9.5
1	A	475	GLN	9.4
1	A	550	LYS	9.4
1	A	520	GLN	8.7
1	B	519	ASN	8.6
1	A	546	GLU	8.5
1	A	554	ALA	8.2
1	A	515	SER	8.1
1	B	546	GLU	8.0
1	B	447	ASN	7.7
1	B	460	ASN	7.6
1	A	474	ASN	7.5
1	B	449	GLU	7.3
1	B	518	VAL	7.2
1	B	525	LEU	6.8
1	B	490	GLY	6.7
1	A	429	LEU	6.7
1	B	515	SER	6.2
1	A	447	ASN	6.2
1	B	471	ASN	6.1
1	A	516	GLU	6.0
1	B	547	GLN	5.5
1	A	535	TRP	5.3
1	B	517	LEU	5.1
1	A	468	PRO	5.1
1	A	525	LEU	5.1
1	B	443	ASP	4.8
1	B	524	GLN	4.7
1	B	535	TRP	4.7
1	A	432	GLU	4.7
1	A	542	ILE	4.7
1	B	543	GLY	4.7
1	A	538	ALA	4.5
1	B	487	GLN	4.5
1	A	452	LEU	4.5
1	A	509	GLN	4.3
1	A	551	LEU	4.2
1	B	555	GLY	3.9
1	A	497	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	549	ASP	3.7
1	B	537	PRO	3.6
1	B	521	ILE	3.6
1	B	441	TYR	3.5
1	A	498	ASP	3.5
1	A	455	ALA	3.4
1	A	428	GLN	3.4
1	A	517	LEU	3.4
1	B	493	VAL	3.4
1	A	499	SER	3.3
1	B	456	GLY	3.2
1	B	492	GLU	3.2
1	A	548	VAL	3.1
1	A	442	VAL	3.1
1	B	474	ASN	3.1
1	A	495	ILE	3.1
1	A	527	LYS	3.1
1	B	455	ALA	3.1
1	A	494	ASN	3.1
1	B	445	ALA	3.0
1	B	434	ILE	3.0
1	A	526	ILE	3.0
1	B	457	TYR	2.9
1	B	553	SER	2.9
1	B	442	VAL	2.9
1	A	431	LYS	2.9
1	B	469	LEU	2.8
1	A	448	ARG	2.8
1	A	485	ALA	2.8
1	B	428	GLN	2.7
1	A	427	TYR	2.7
1	A	496	VAL	2.7
1	A	543	GLY	2.7
1	B	477	THR	2.6
1	A	518	VAL	2.6
1	B	444	GLY	2.6
1	B	451	LYS	2.6
1	B	516	GLU	2.6
1	A	477	THR	2.5
1	A	445	ALA	2.5
1	B	468	PRO	2.5
1	B	439	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	2.5
1	B	481	ALA	2.5
1	B	448	ARG	2.4
1	B	496	VAL	2.4
1	A	493	VAL	2.4
1	B	458	VAL	2.4
1	B	485	ALA	2.4
1	B	552	VAL	2.4
1	A	439	THR	2.4
1	A	443	ASP	2.3
1	A	456	GLY	2.3
1	A	513	SER	2.3
1	A	441	TYR	2.3
1	B	499	SER	2.3
1	B	440	PHE	2.2
1	A	459	THR	2.2
1	B	533	LEU	2.2
1	A	481	ALA	2.2
1	A	510	PRO	2.2
1	A	469	LEU	2.2
1	B	526	ILE	2.1
1	A	458	VAL	2.1
1	B	522	ILE	2.1

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.