



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 10:45 PM EST

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 : unknown
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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

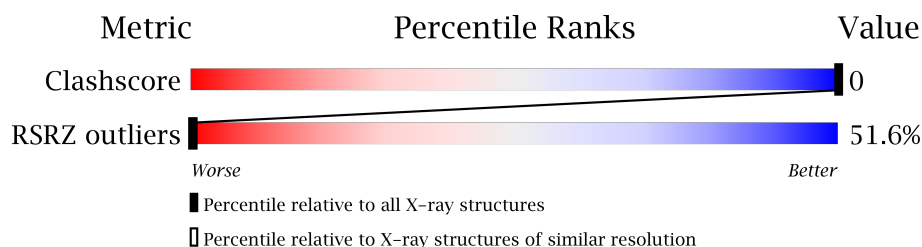
1 Overall quality at a glance

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	112137	3033 (2.80-2.80)
RSRZ outliers	101464	2610 (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.

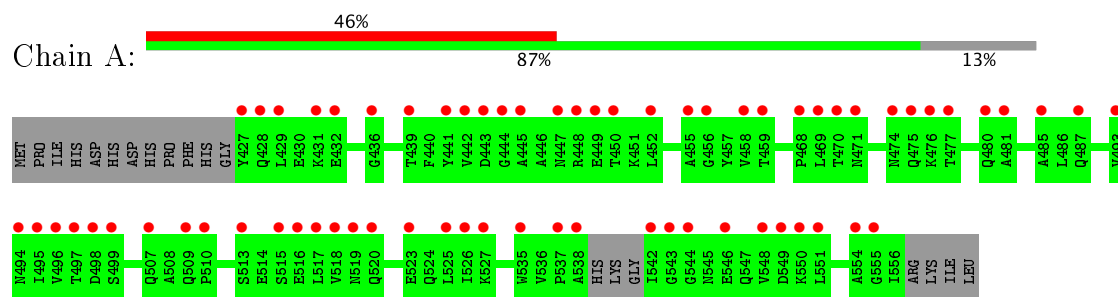
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (RIBONUCLEASE H DOMAIN).

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

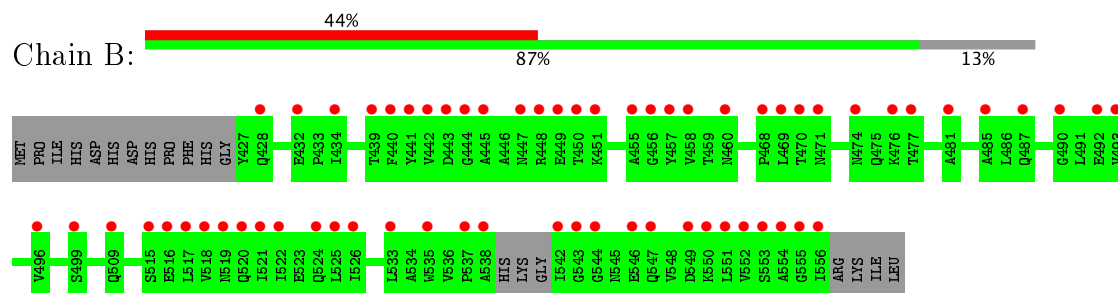
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.058 for h,-h-k,-l 0.036 for -k,-h,-l	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, 0.333 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).

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%)	3.44	67 (52%)  	12, 27, 46, 53	0
1	B	127/146 (86%)	3.29	64 (50%)  	11, 25, 45, 50	0
All	All	254/292 (86%)	3.36	131 (51%)  	11, 26, 46, 53	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	GLY	23.2
1	B	556	ILE	21.1
1	A	549	ASP	17.7
1	A	555	GLY	17.4
1	B	554	ALA	16.9
1	B	432	GLU	16.7
1	A	450	THR	16.2
1	A	487	GLN	15.5
1	A	480	GLN	14.7
1	A	449	GLU	13.6
1	A	523	GLU	13.5
1	A	519	ASN	13.4
1	B	450	THR	13.3
1	B	538	ALA	12.8
1	A	470	THR	12.7
1	B	550	LYS	12.1
1	A	476	LYS	12.0
1	A	471	ASN	11.8
1	B	551	LEU	10.9
1	A	544	GLY	10.8
1	B	509	GLN	10.5
1	B	542	ILE	10.5
1	A	507	GLN	10.3
1	B	470	THR	9.7

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Mol	Chain	Res	Type	RSRZ
1	B	520	GLN	9.7
1	A	537	PRO	9.6
1	A	436	GLY	9.4
1	B	476	LYS	9.4
1	A	550	LYS	9.2
1	A	475	GLN	9.2
1	A	520	GLN	8.5
1	B	519	ASN	8.4
1	A	546	GLU	8.3
1	A	554	ALA	8.2
1	A	515	SER	7.9
1	B	546	GLU	7.8
1	B	447	ASN	7.4
1	B	460	ASN	7.4
1	A	474	ASN	7.2
1	B	449	GLU	7.2
1	B	518	VAL	7.1
1	B	525	LEU	6.7
1	B	490	GLY	6.7
1	A	429	LEU	6.6
1	B	515	SER	6.1
1	A	447	ASN	6.0
1	B	471	ASN	5.9
1	A	516	GLU	5.9
1	B	547	GLN	5.3
1	A	535	TRP	5.1
1	B	517	LEU	5.0
1	A	525	LEU	5.0
1	A	468	PRO	4.9
1	B	443	ASP	4.6
1	B	543	GLY	4.6
1	A	542	ILE	4.6
1	B	524	GLN	4.6
1	A	538	ALA	4.6
1	A	432	GLU	4.6
1	B	535	TRP	4.6
1	A	452	LEU	4.4
1	B	487	GLN	4.4
1	A	551	LEU	4.1
1	A	509	GLN	4.1
1	B	555	GLY	3.9
1	A	497	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	549	ASP	3.6
1	B	537	PRO	3.5
1	B	521	ILE	3.5
1	A	455	ALA	3.5
1	B	441	TYR	3.4
1	A	498	ASP	3.4
1	A	517	LEU	3.3
1	B	493	VAL	3.3
1	A	428	GLN	3.3
1	A	499	SER	3.2
1	B	456	GLY	3.1
1	A	548	VAL	3.1
1	A	442	VAL	3.1
1	B	455	ALA	3.1
1	A	495	ILE	3.1
1	B	492	GLU	3.1
1	A	527	LYS	3.1
1	B	445	ALA	3.0
1	B	474	ASN	3.0
1	B	434	ILE	3.0
1	A	494	ASN	2.9
1	A	526	ILE	2.9
1	A	448	ARG	2.9
1	B	442	VAL	2.9
1	B	457	TYR	2.9
1	B	553	SER	2.9
1	A	485	ALA	2.8
1	A	431	LYS	2.8
1	B	469	LEU	2.8
1	A	496	VAL	2.7
1	A	427	TYR	2.6
1	A	543	GLY	2.6
1	B	428	GLN	2.6
1	B	477	THR	2.6
1	A	518	VAL	2.6
1	A	445	ALA	2.6
1	B	448	ARG	2.5
1	B	444	GLY	2.5
1	B	451	LYS	2.5
1	B	516	GLU	2.5
1	B	481	ALA	2.5
1	A	477	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	2.4
1	B	496	VAL	2.4
1	B	468	PRO	2.4
1	B	439	THR	2.4
1	B	485	ALA	2.4
1	A	493	VAL	2.4
1	B	458	VAL	2.4
1	B	552	VAL	2.3
1	A	439	THR	2.3
1	A	456	GLY	2.3
1	A	443	ASP	2.2
1	A	481	ALA	2.2
1	A	513	SER	2.2
1	B	440	PHE	2.2
1	A	441	TYR	2.2
1	B	499	SER	2.2
1	B	533	LEU	2.2
1	A	459	THR	2.2
1	A	469	LEU	2.1
1	A	510	PRO	2.1
1	B	526	ILE	2.1
1	A	458	VAL	2.1
1	B	522	ILE	2.0

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.