



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3M8P
Title : HIV-1 RT with NNRTI TMC-125
Authors : Harris, S.F.; Villasenor, A.
Deposited on : 2010-03-18
Resolution : 2.67 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
<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

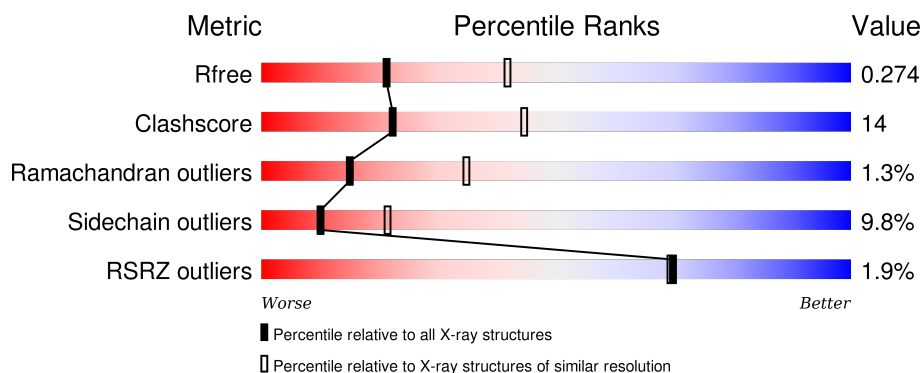
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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))
R_{free}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	561	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 65%, yellow 28%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 65% 28% 5% </div> </div>
2	B	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 61%, yellow 25%, orange 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 61% 25% 5% 9% </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8138 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.

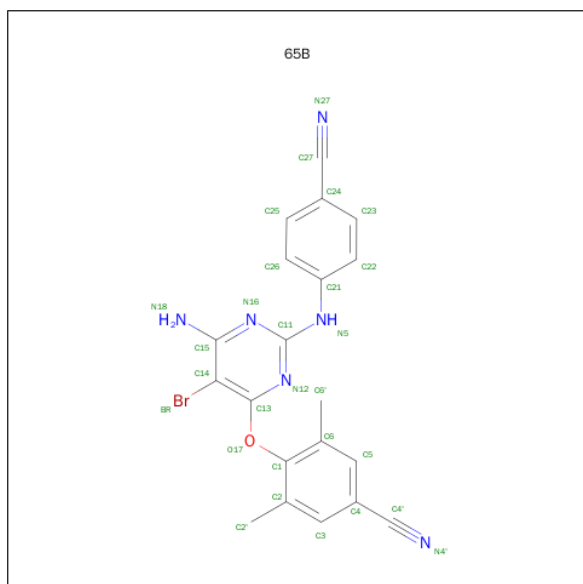
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4485	2900	748	829	8			

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3320	2166	545	602	7			

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (three-letter code: 65B) (formula: C₂₀H₁₅BrN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	20	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total 169	O 169	0	0
4	B	136	Total 136	O 136	0	0

L422	Y423	Y424	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.44Å 153.53Å 154.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 2.67 47.01 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.01-2.67) 99.7 (47.01-2.67)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.283 0.208 , 0.274	Depositor DCC
R_{free} test set	2042 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40211 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 65B

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	1.32	15/4601 (0.3%)	1.06	8/6252 (0.1%)
2	B	1.32	12/3414 (0.4%)	1.04	6/4640 (0.1%)
All	All	1.32	27/8015 (0.3%)	1.05	14/10892 (0.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	THR	CA-CB	7.82	1.73	1.53
1	A	402	TRP	CB-CG	7.63	1.64	1.50
2	B	36	GLU	CG-CD	7.32	1.62	1.51
1	A	478	GLU	CB-CG	7.21	1.65	1.52
2	B	399	GLU	CG-CD	6.60	1.61	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	B	123	ASP	CB-CG-OD2	-6.85	112.14	118.30
2	B	199	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	187	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	A	345	PRO	C-N-CA	5.84	136.31	121.70

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	4485	0	4530	132	0
2	B	3320	0	3341	90	0
3	A	28	0	15	4	0
4	A	169	0	0	19	0
4	B	136	0	0	9	0
All	All	8138	0	7886	217	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 14.

The worst 5 of 217 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)
1:A:80:LEU:O	1:A:84:THR:HG22	1.39	1.18
1:A:409:THR:HG21	4:A:695:HOH:O	1.63	0.98
1:A:27:THR:HG21	4:A:722:HOH:O	1.64	0.96
1:A:428:GLN:HE22	1:A:431:LYS:HZ3	0.97	0.96
1:A:428:GLN:NE2	1:A:431:LYS:HZ3	1.63	0.94

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	547/561 (98%)	509 (93%)	34 (6%)	4 (1%)	26	53
2	B	393/440 (89%)	364 (93%)	21 (5%)	8 (2%)	9	22
All	All	940/1001 (94%)	873 (93%)	55 (6%)	12 (1%)	15	35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
2	B	13	LYS
1	A	471	ASP
2	B	14	PRO
2	B	22	LYS

5.3.2 Protein sidechains ⓘ

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	491/501 (98%)	440 (90%)	51 (10%)	9	18
2	B	365/400 (91%)	332 (91%)	33 (9%)	12	25
All	All	856/901 (95%)	772 (90%)	84 (10%)	10	21

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	ILE
1	A	529	GLU
2	B	385	LYS
1	A	451	LYS
1	A	464	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
1	A	539	HIS
2	B	278	GLN
1	A	474	ASN
2	B	255	ASN

5.3.3 RNA ⓘ

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](#)

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	65B	A	562	-	30,30,30	1.47	4 (13%)	38,42,42	2.60	18 (47%)

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	65B	A	562	-	-	0/12/12/12	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	562	65B	C13-C14	-3.86	1.33	1.38
3	A	562	65B	C3-C2	-2.56	1.35	1.39
3	A	562	65B	C15-N16	-2.52	1.31	1.35
3	A	562	65B	C11-N5	2.62	1.40	1.36

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	562	65B	C14-C13-N12	-5.06	118.60	124.00
3	A	562	65B	C14-C15-N18	-4.84	118.71	122.87
3	A	562	65B	N16-C11-N12	-4.52	119.26	126.22
3	A	562	65B	BR-C14-C13	-4.00	114.74	121.48
3	A	562	65B	C5-C4-C4'	-3.59	114.97	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	562	65B	4	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](#)

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	551/561 (98%)	0.01	7 (1%) 79 79	25, 49, 75, 103	0
2	B	401/440 (91%)	0.02	11 (2%) 58 57	26, 46, 82, 95	0
All	All	952/1001 (95%)	0.02	18 (1%) 70 69	25, 48, 79, 103	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	5.9
1	A	219	LYS	5.2
1	A	221	HIS	4.9
2	B	13	LYS	4.5
1	A	220	LYS	4.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	65B	A	562	28/28	0.98	0.17	-0.13	24,33,40,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.