



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2018 – 12:37 am GMT

PDB ID : 1K5K  
Title : Homonuclear <sup>1</sup>H Nuclear Magnetic Resonance Assignment and Structural Characterization of HIV-1 Tat Mal Protein  
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Deposited on : 2001-10-11

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

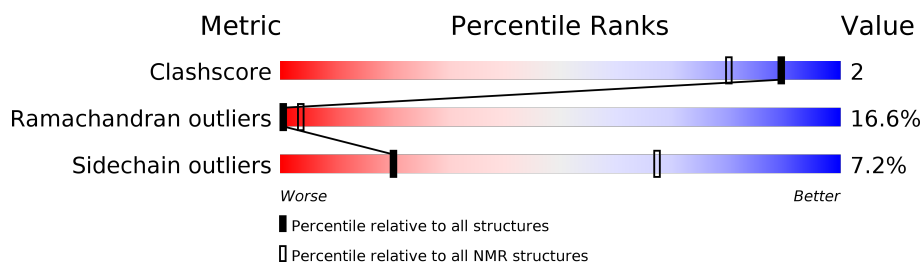
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	87	 63% 28% 7% •

## 2 Ensemble composition and analysis

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:87 (87)	0.16	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1379 atoms, of which 679 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TAT protein.

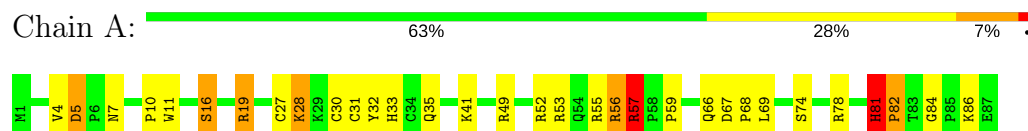
Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1379	426	679	141	124	9	

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: TAT protein

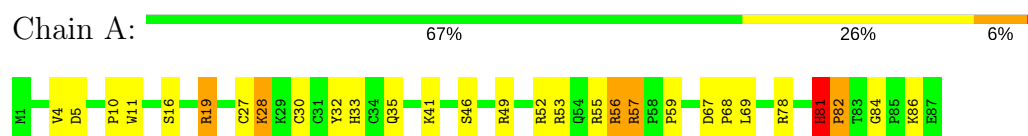


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

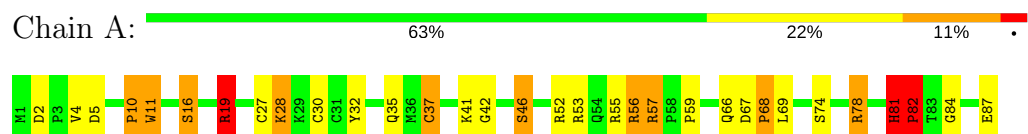
#### 4.2.1 Score per residue for model 1

- Molecule 1: TAT protein



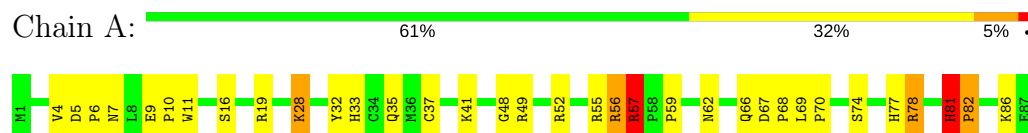
#### 4.2.2 Score per residue for model 2

- Molecule 1: TAT protein



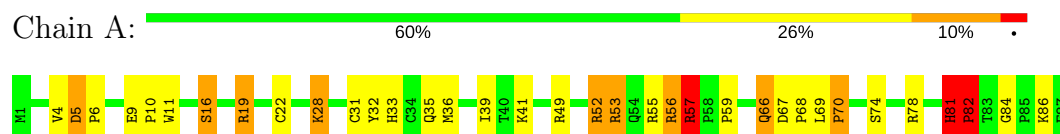
### 4.2.3 Score per residue for model 3

- Molecule 1: TAT protein



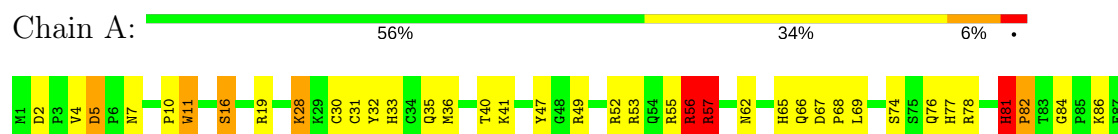
### 4.2.4 Score per residue for model 4

- Molecule 1: TAT protein



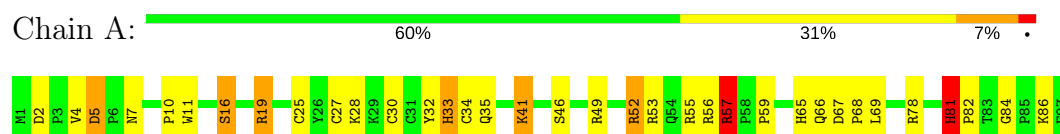
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: TAT protein



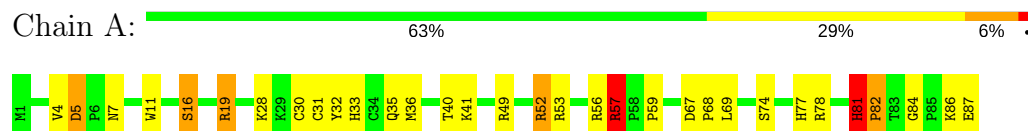
### 4.2.6 Score per residue for model 6

- Molecule 1: TAT protein



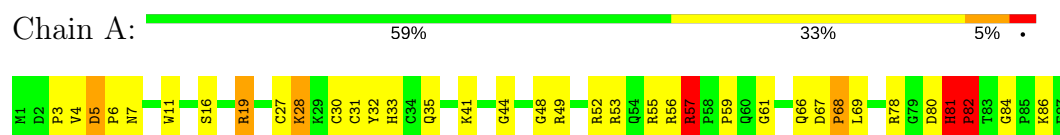
### 4.2.7 Score per residue for model 7

- Molecule 1: TAT protein



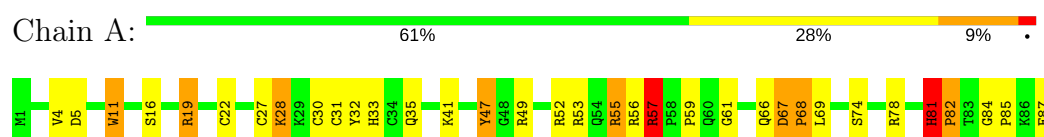
### 4.2.8 Score per residue for model 8

- Molecule 1: TAT protein



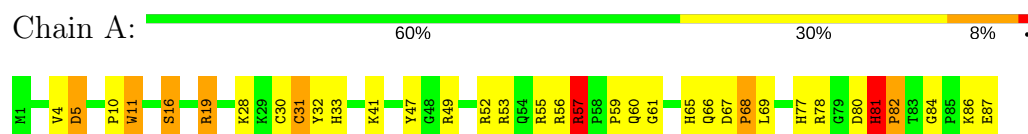
### 4.2.9 Score per residue for model 9

- Molecule 1: TAT protein



### 4.2.10 Score per residue for model 10

- Molecule 1: TAT protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DISCOVER	structure solution	2000
DISCOVER	refinement	2000

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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 (average) 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	1.51±0.07	1±1/723 (0.1±0.1%)	1.94±0.09	20±4/975 (2.1±0.5%)
All	All	1.51	8/7230 (0.1%)	1.95	203/9750 (2.1%)

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	Planarity
1	A	3.0±0.0	6.8±1.2
All	All	30	68

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	77	HIS	CG-CD2	6.20	1.46	1.35	5	1
1	A	16	SER	CA-CB	5.73	1.61	1.52	2	2
1	A	48	GLY	N-CA	5.43	1.54	1.46	3	2
1	A	53	ARG	CZ-NH2	-5.29	1.26	1.33	7	1
1	A	3	PRO	CA-C	5.17	1.63	1.52	8	1
1	A	61	GLY	N-CA	5.10	1.53	1.46	9	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	78	ARG	NE-CZ-NH1	13.23	126.92	120.30	2	8
1	A	56	ARG	NE-CZ-NH1	12.61	126.60	120.30	2	10
1	A	52	ARG	NE-CZ-NH2	-11.58	114.51	120.30	3	4
1	A	55	ARG	NE-CZ-NH1	10.62	125.61	120.30	5	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	ARG	NE-CZ-NH1	10.54	125.57	120.30	7	9
1	A	57	ARG	NE-CZ-NH1	10.54	125.57	120.30	5	9
1	A	57	ARG	NE-CZ-NH2	-10.32	115.14	120.30	7	8
1	A	49	ARG	NE-CZ-NH1	10.13	125.36	120.30	8	9
1	A	56	ARG	NE-CZ-NH2	-9.40	115.60	120.30	9	5
1	A	19	ARG	NE-CZ-NH1	8.63	124.61	120.30	7	8
1	A	53	ARG	NE-CZ-NH1	8.43	124.51	120.30	2	9
1	A	55	ARG	NE-CZ-NH2	-8.28	116.16	120.30	5	3
1	A	59	PRO	O-C-N	-8.13	109.69	122.70	3	9
1	A	49	ARG	NE-CZ-NH2	-8.11	116.24	120.30	3	3
1	A	59	PRO	CA-C-N	7.76	134.27	117.20	3	9
1	A	68	PRO	N-CA-CB	-7.43	94.38	103.30	2	4
1	A	30	CYS	O-C-N	-7.22	111.15	122.70	2	7
1	A	78	ARG	NE-CZ-NH2	-7.13	116.73	120.30	2	6
1	A	5	ASP	CB-CA-C	7.11	124.63	110.40	6	3
1	A	40	THR	CA-CB-CG2	7.10	122.34	112.40	7	2
1	A	87	GLU	N-CA-CB	6.85	122.92	110.60	2	2
1	A	53	ARG	NE-CZ-NH2	-6.78	116.91	120.30	4	2
1	A	66	GLN	N-CA-CB	-6.70	98.53	110.60	5	6
1	A	74	SER	N-CA-CB	-6.69	100.46	110.50	7	1
1	A	16	SER	N-CA-CB	6.68	120.53	110.50	4	4
1	A	5	ASP	CB-CG-OD1	6.41	124.07	118.30	4	4
1	A	2	ASP	CB-CG-OD2	6.41	124.06	118.30	5	2
1	A	80	ASP	CB-CG-OD2	6.32	123.98	118.30	10	1
1	A	53	ARG	CB-CA-C	6.14	122.68	110.40	7	3
1	A	77	HIS	CG-ND1-CE1	-6.08	97.80	105.70	10	1
1	A	59	PRO	N-CA-C	5.95	127.57	112.10	2	1
1	A	57	ARG	CB-CA-C	5.88	122.17	110.40	8	3
1	A	11	TRP	CD1-NE1-CE2	-5.76	103.81	109.00	9	10
1	A	82	PRO	N-CA-CB	-5.75	96.28	102.60	4	1
1	A	30	CYS	CA-C-N	5.72	129.79	117.20	2	6
1	A	87	GLU	CB-CG-CD	5.71	129.63	114.20	7	1
1	A	76	GLN	CB-CA-C	5.71	121.82	110.40	5	1
1	A	9	GLU	N-CA-CB	-5.68	100.37	110.60	4	2
1	A	19	ARG	NE-CZ-NH2	-5.64	117.48	120.30	8	4
1	A	41	LYS	CA-CB-CG	5.61	125.73	113.40	6	1
1	A	74	SER	CB-CA-C	5.61	120.75	110.10	9	1
1	A	22	CYS	N-CA-CB	-5.60	100.51	110.60	4	2
1	A	19	ARG	N-CA-CB	-5.48	100.73	110.60	2	1
1	A	31	CYS	CB-CA-C	5.40	121.20	110.40	10	1
1	A	77	HIS	ND1-CE1-NE2	5.39	121.76	109.90	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	80	ASP	N-CA-C	5.33	125.39	111.00	8	1
1	A	37	CYS	CA-CB-SG	-5.31	104.44	114.00	2	1
1	A	70	PRO	N-CA-CB	-5.28	96.79	102.60	4	1
1	A	49	ARG	CB-CA-C	5.16	120.72	110.40	7	1
1	A	39	ILE	CA-CB-CG1	5.14	120.77	111.00	4	1
1	A	5	ASP	CB-CG-OD2	-5.06	113.75	118.30	8	1
1	A	2	ASP	CA-C-N	5.00	131.11	117.10	2	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	31	CYS	CA	10
1	A	36	MET	CA	10
1	A	80	ASP	CA	10

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	TYR	Sidechain,Peptide	10
1	A	82	PRO	Peptide	10
1	A	33	HIS	Sidechain	9
1	A	86	LYS	Peptide	8
1	A	10	PRO	Peptide	7
1	A	78	ARG	Sidechain	3
1	A	46	SER	Peptide,Mainchain	3
1	A	66	GLN	Peptide	2
1	A	19	ARG	Sidechain	2
1	A	81	HIS	Sidechain	2
1	A	65	HIS	Peptide	2
1	A	16	SER	Peptide	1
1	A	60	GLN	Peptide	1
1	A	52	ARG	Sidechain	1
1	A	53	ARG	Peptide	1
1	A	57	ARG	Sidechain	1
1	A	55	ARG	Sidechain	1
1	A	56	ARG	Sidechain	1
1	A	47	TYR	Sidechain	1

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	700	679	675	3±1
All	All	7000	6785	6750	26

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 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:HIS:ND1	1:A:82:PRO:HD3	0.76	1.96	4	9
1:A:70:PRO:HD3	1:A:77:HIS:NE2	0.64	2.08	3	1
1:A:81:HIS:ND1	1:A:82:PRO:CD	0.61	2.63	4	6
1:A:33:HIS:CE1	1:A:34:CYS:O	0.58	2.56	6	1
1:A:77:HIS:O	1:A:77:HIS:CD2	0.58	2.56	7	1
1:A:11:TRP:HZ3	1:A:46:SER:OG	0.56	1.82	2	1
1:A:11:TRP:CZ2	1:A:47:TYR:CZ	0.54	2.95	9	3
1:A:65:HIS:O	1:A:81:HIS:HE1	0.41	1.98	10	1
1:A:19:ARG:HH21	1:A:87:GLU:CD	0.41	2.19	10	1
1:A:70:PRO:CD	1:A:77:HIS:NE2	0.41	2.83	3	1
1:A:81:HIS:ND1	1:A:82:PRO:HG3	0.40	2.31	9	1

## 6.3 Torsion angles [i](#)

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	85/87 (98%)	40±1 (47±2%)	31±3 (36±3%)	14±2 (17±2%)	0	4
All	All	850/870 (98%)	402 (47%)	307 (36%)	141 (17%)	0	4

All 26 unique Ramachandran outliers are listed below. They are sorted by the frequency of

occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	69	LEU	10
1	A	16	SER	10
1	A	68	PRO	10
1	A	5	ASP	10
1	A	57	ARG	10
1	A	81	HIS	10
1	A	4	VAL	10
1	A	35	GLN	9
1	A	84	GLY	9
1	A	28	LYS	7
1	A	19	ARG	6
1	A	31	CYS	6
1	A	27	CYS	5
1	A	7	ASN	5
1	A	74	SER	4
1	A	52	ARG	3
1	A	36	MET	3
1	A	6	PRO	3
1	A	37	CYS	2
1	A	82	PRO	2
1	A	61	GLY	2
1	A	85	PRO	1
1	A	42	GLY	1
1	A	67	ASP	1
1	A	44	GLY	1
1	A	25	CYS	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	79/79 (100%)	73±1 (93±1%)	6±1 (7±1%)	20	67
All	All	790/790 (100%)	733 (93%)	57 (7%)	20	67

All 10 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	41	LYS	10
1	A	28	LYS	10
1	A	67	ASP	10
1	A	81	HIS	10
1	A	57	ARG	7
1	A	56	ARG	5
1	A	62	ASN	2
1	A	10	PRO	1
1	A	70	PRO	1
1	A	66	GLN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided