



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 11:03 AM UTC

PDB ID : 1K5K / pdb_00001k5k
Title : Homonuclear ¹H Nuclear Magnetic Resonance Assignment and Structural Characterization of HIV-1 Tat Mal Protein
Authors : Gregoire, C.; Peloponese, J.M.; Esquieu, D.; Opi, S.; Campbell, G.; Solomiac, M.; Lebrun, E.; Lebreton, J.; Loret, E.P.
Deposited on : 2001-10-11

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

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	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

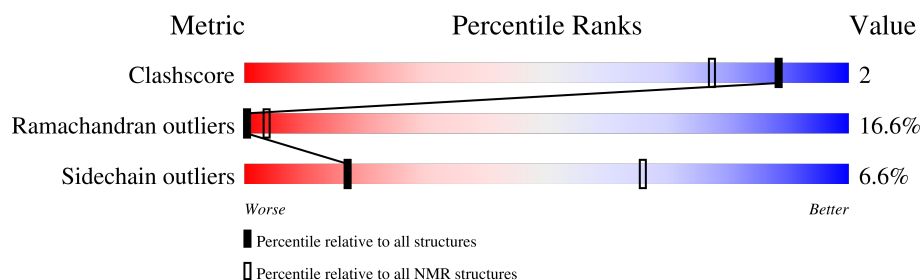
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 ≥ 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	39% 47% 13% .

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)	0.28	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	

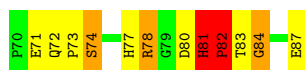
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

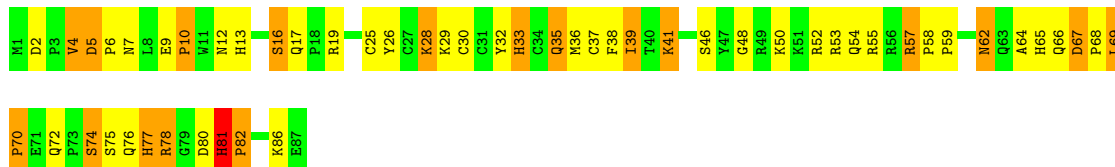
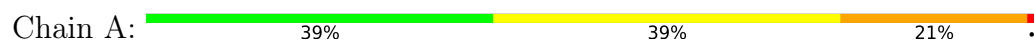
- Molecule 1: TAT protein





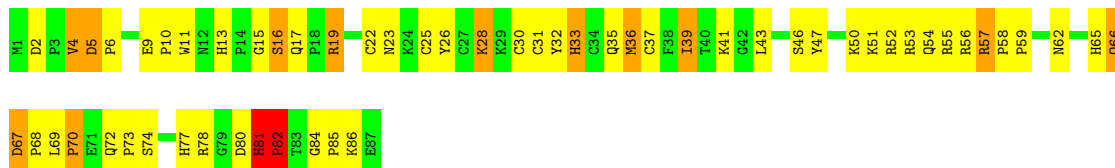
4.2.3 Score per residue for model 3

- Molecule 1: TAT protein



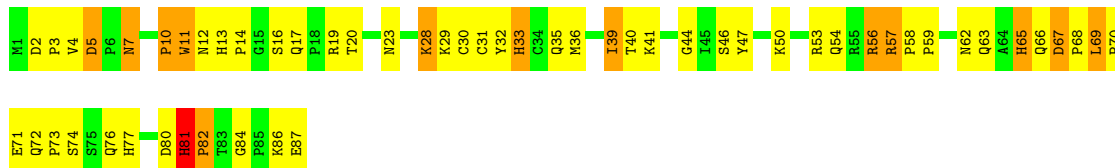
4.2.4 Score per residue for model 4

- Molecule 1: TAT protein



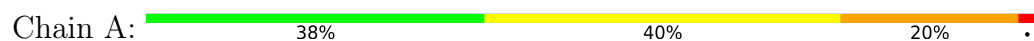
4.2.5 Score per residue for model 5 (medoid)

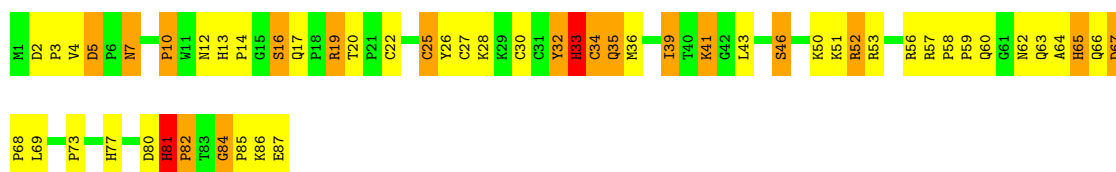
- Molecule 1: TAT protein



4.2.6 Score per residue for model 6

- Molecule 1: TAT protein

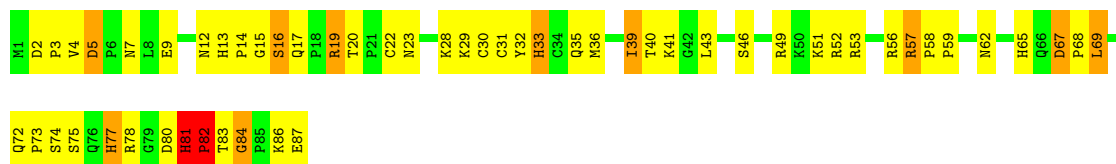




4.2.7 Score per residue for model 7

- Molecule 1: TAT protein

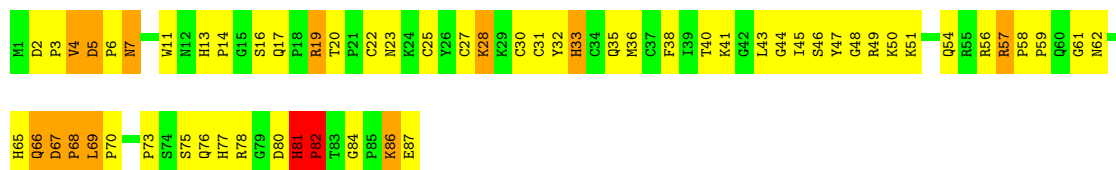
Chain A: 37% 49% 11% .



4.2.8 Score per residue for model 8

- Molecule 1: TAT protein

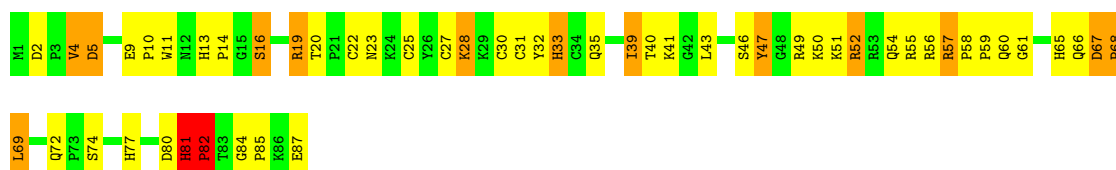
Chain A: 31% 53% 14% .



4.2.9 Score per residue for model 9

- Molecule 1: TAT protein

Chain A: 39% 44% 15% .



4.2.10 Score per residue for model 10

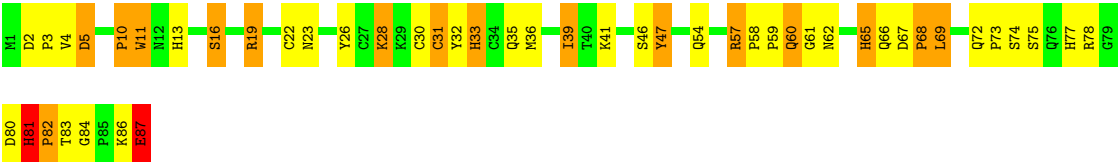
- Molecule 1: TAT protein

Chain A:

45%

34%

18%



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.

6 Model quality i

6.1 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 (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	2.28±0.10	27±9/723 (3.8± 1.2%)	2.43±0.09	50±5/975 (5.1± 0.5%)
All	All	2.28	274/7230 (3.8%)	2.43	499/9750 (5.1%)

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	58	PRO	CA-C	9.89	1.61	1.52	3	10
1	A	53	ARG	CA-C	9.61	1.62	1.53	5	2
1	A	77	HIS	CG-CD2	9.49	1.46	1.35	5	2
1	A	73	PRO	CA-C	9.32	1.61	1.52	4	6
1	A	33	HIS	CA-C	9.11	1.62	1.52	4	1
1	A	77	HIS	CE1-NE2	8.85	1.41	1.32	4	5
1	A	51	LYS	CA-C	8.50	1.64	1.52	7	5
1	A	43	LEU	CA-C	8.25	1.61	1.53	9	6
1	A	17	GLN	CA-C	8.24	1.63	1.52	7	4
1	A	13	HIS	CA-C	8.08	1.62	1.52	4	8
1	A	19	ARG	CA-C	8.00	1.63	1.52	9	4
1	A	30	CYS	CA-C	7.96	1.59	1.52	3	3
1	A	65	HIS	CA-C	7.85	1.62	1.52	9	5
1	A	69	LEU	CA-C	7.75	1.62	1.52	8	4
1	A	83	THR	CA-C	7.73	1.63	1.52	10	3
1	A	2	ASP	CA-C	7.46	1.62	1.52	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	TRP	CA-C	7.31	1.60	1.52	4	4
1	A	25	CYS	CA-C	7.30	1.62	1.52	9	4
1	A	40	THR	CA-C	7.30	1.61	1.53	9	2
1	A	77	HIS	ND1-CE1	7.30	1.39	1.32	4	4
1	A	4	VAL	CA-C	7.25	1.61	1.52	3	4
1	A	5	ASP	CA-C	7.12	1.61	1.52	3	4
1	A	75	SER	CA-C	7.09	1.61	1.52	10	4
1	A	39	ILE	N-CA	7.06	1.54	1.46	4	1
1	A	23	ASN	CA-C	7.03	1.62	1.52	4	3
1	A	62	ASN	CA-C	7.02	1.61	1.52	3	4
1	A	3	PRO	CA-C	7.01	1.63	1.52	8	1
1	A	38	PHE	CA-C	6.96	1.60	1.53	2	1
1	A	69	LEU	C-N	6.94	1.42	1.33	5	3
1	A	67	ASP	CA-C	6.89	1.61	1.52	3	3
1	A	36	MET	CA-C	6.83	1.61	1.52	4	4
1	A	81	HIS	CA-C	6.80	1.61	1.52	9	4
1	A	39	ILE	CA-CB	6.70	1.62	1.54	9	1
1	A	68	PRO	CA-C	6.67	1.61	1.52	8	1
1	A	50	LYS	CA-C	6.63	1.60	1.53	8	6
1	A	71	GLU	CA-C	6.60	1.61	1.52	5	2
1	A	26	TYR	CA-C	6.57	1.61	1.52	3	3
1	A	70	PRO	CA-C	6.55	1.60	1.52	5	3
1	A	52	ARG	CA-C	6.53	1.61	1.52	9	1
1	A	39	ILE	CA-C	6.52	1.60	1.52	5	1
1	A	19	ARG	N-CA	6.34	1.54	1.46	7	4
1	A	32	TYR	CA-C	6.27	1.61	1.52	6	1
1	A	14	PRO	CA-C	6.22	1.60	1.52	7	3
1	A	54	GLN	CA-C	6.19	1.61	1.52	2	4
1	A	45	ILE	CA-C	6.18	1.60	1.52	8	1
1	A	29	LYS	CA-C	6.16	1.60	1.52	7	3
1	A	20	THR	CA-C	6.16	1.60	1.52	6	3
1	A	57	ARG	C-N	6.15	1.40	1.33	7	2
1	A	4	VAL	N-CA	6.15	1.54	1.46	8	2
1	A	77	HIS	CA-C	6.14	1.60	1.53	9	3
1	A	85	PRO	CA-C	6.12	1.61	1.52	4	2
1	A	48	GLY	N-CA	6.08	1.54	1.45	3	2
1	A	49	ARG	CA-C	6.07	1.60	1.52	9	2
1	A	26	TYR	N-CA	6.06	1.53	1.46	6	1
1	A	12	ASN	CA-C	6.06	1.59	1.53	5	2
1	A	78	ARG	CA-C	6.02	1.60	1.52	3	1
1	A	72	GLN	CA-C	5.99	1.59	1.52	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	56	ARG	CA-C	5.98	1.60	1.52	9	6
1	A	46	SER	CA-C	5.97	1.60	1.52	10	2
1	A	65	HIS	N-CA	5.92	1.53	1.46	6	4
1	A	55	ARG	CA-C	5.92	1.59	1.52	3	2
1	A	16	SER	CA-C	5.92	1.60	1.52	3	1
1	A	84	GLY	N-CA	5.90	1.52	1.44	6	2
1	A	10	PRO	CA-C	5.89	1.60	1.52	3	1
1	A	56	ARG	N-CA	5.85	1.53	1.46	5	1
1	A	64	ALA	CA-C	5.84	1.60	1.52	2	3
1	A	66	GLN	CA-C	5.83	1.60	1.52	6	1
1	A	34	CYS	CA-C	5.82	1.59	1.52	6	1
1	A	43	LEU	CA-CB	5.79	1.59	1.52	2	1
1	A	13	HIS	CA-CB	5.78	1.60	1.53	7	2
1	A	61	GLY	N-CA	5.74	1.53	1.45	9	1
1	A	83	THR	CA-CB	5.70	1.60	1.52	10	1
1	A	57	ARG	CA-C	5.69	1.60	1.52	2	3
1	A	35	GLN	CA-C	5.67	1.60	1.52	3	1
1	A	47	TYR	CA-C	5.67	1.60	1.52	8	3
1	A	78	ARG	CD-NE	5.65	1.54	1.46	4	3
1	A	27	CYS	CA-C	5.61	1.60	1.52	2	1
1	A	74	SER	N-CA	5.61	1.53	1.46	9	2
1	A	72	GLN	CA-CB	5.60	1.59	1.53	4	1
1	A	53	ARG	CZ-NH2	-5.59	1.26	1.33	7	1
1	A	76	GLN	CA-C	5.58	1.60	1.52	3	1
1	A	65	HIS	CA-CB	5.57	1.60	1.53	2	4
1	A	74	SER	CA-C	5.56	1.59	1.53	10	2
1	A	29	LYS	N-CA	5.52	1.52	1.46	2	1
1	A	47	TYR	N-CA	5.52	1.53	1.46	4	1
1	A	77	HIS	CB-CG	5.50	1.57	1.50	10	1
1	A	82	PRO	CA-C	5.48	1.60	1.52	7	2
1	A	2	ASP	C-N	5.47	1.39	1.34	4	2
1	A	9	GLU	CA-C	5.46	1.60	1.52	7	2
1	A	28	LYS	CA-C	5.44	1.60	1.52	10	1
1	A	22	CYS	CA-C	5.44	1.59	1.52	10	1
1	A	2	ASP	N-CA	5.39	1.51	1.46	8	2
1	A	41	LYS	CA-C	5.38	1.60	1.53	3	2
1	A	15	GLY	CA-C	5.28	1.59	1.51	4	2
1	A	25	CYS	N-CA	5.26	1.52	1.46	6	2
1	A	63	GLN	N-CA	5.23	1.53	1.46	6	2
1	A	63	GLN	CA-C	5.20	1.60	1.52	6	2
1	A	7	ASN	CA-C	5.17	1.59	1.52	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	53	ARG	CD-NE	5.17	1.53	1.46	5	2
1	A	19	ARG	CA-CB	5.17	1.62	1.53	3	1
1	A	52	ARG	N-CA	5.17	1.52	1.46	9	1
1	A	55	ARG	CD-NE	5.13	1.53	1.46	4	1
1	A	51	LYS	N-CA	5.12	1.52	1.46	8	1
1	A	76	GLN	N-CA	5.07	1.52	1.46	8	1
1	A	16	SER	N-CA	5.07	1.52	1.46	9	1
1	A	57	ARG	CZ-NH2	-5.05	1.26	1.33	4	1
1	A	59	PRO	CA-C	5.05	1.59	1.52	4	1
1	A	56	ARG	CZ-NH2	-5.03	1.26	1.33	2	1
1	A	44	GLY	CA-C	5.01	1.58	1.51	5	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	77	HIS	ND1-CE1-NE2	13.36	121.76	108.40	10	10
1	A	77	HIS	CE1-NE2-CD2	-11.80	97.20	109.00	8	10
1	A	5	ASP	CA-CB-CG	11.21	123.81	112.60	5	10
1	A	33	HIS	CB-CG-CD2	-11.21	116.63	131.20	9	10
1	A	72	GLN	O-C-N	-10.84	113.64	121.23	10	1
1	A	23	ASN	CA-CB-CG	10.29	122.89	112.60	10	4
1	A	87	GLU	CB-CG-CD	10.02	129.63	112.60	7	5
1	A	80	ASP	N-CA-C	9.93	124.49	112.38	2	10
1	A	33	HIS	ND1-CE1-NE2	9.78	118.18	108.40	5	10
1	A	81	HIS	ND1-CE1-NE2	9.77	118.17	108.40	5	10
1	A	13	HIS	ND1-CE1-NE2	9.71	118.11	108.40	1	10
1	A	65	HIS	ND1-CE1-NE2	9.71	118.11	108.40	1	10
1	A	59	PRO	O-C-N	-9.59	109.69	122.64	3	10
1	A	81	HIS	CB-CG-CD2	-9.18	119.27	131.20	6	10
1	A	62	ASN	CA-CB-CG	9.16	121.76	112.60	7	7
1	A	22	CYS	N-CA-C	8.97	121.14	111.36	4	7
1	A	30	CYS	O-C-N	-8.84	113.13	121.79	7	10
1	A	67	ASP	CA-CB-CG	8.69	121.29	112.60	3	8
1	A	46	SER	N-CA-C	8.66	121.50	111.11	5	8
1	A	68	PRO	N-CA-CB	-8.45	94.38	103.25	2	4
1	A	35	GLN	OE1-CD-NE2	-8.45	114.15	122.60	6	3
1	A	2	ASP	CA-CB-CG	8.42	121.02	112.60	7	2
1	A	58	PRO	N-CA-C	8.21	120.71	110.70	8	7
1	A	66	GLN	N-CA-CB	-8.04	98.86	110.36	4	8
1	A	65	HIS	CB-CG-CD2	-8.02	120.78	131.20	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	GLN	N-CA-C	7.92	121.41	110.24	2	4
1	A	54	GLN	OE1-CD-NE2	-7.68	114.92	122.60	9	5
1	A	13	HIS	CB-CG-CD2	-7.51	121.44	131.20	1	10
1	A	9	GLU	N-CA-CB	-7.50	100.96	110.03	3	3
1	A	12	ASN	CA-CB-CG	7.44	120.04	112.60	3	2
1	A	5	ASP	CB-CA-C	7.34	124.63	110.17	6	3
1	A	59	PRO	N-CA-C	7.33	127.57	112.47	2	4
1	A	87	GLU	N-CA-CB	7.31	122.92	110.50	2	2
1	A	66	GLN	OE1-CD-NE2	-7.27	115.33	122.60	2	4
1	A	2	ASP	N-CA-C	7.23	122.65	113.25	9	3
1	A	62	ASN	N-CA-C	7.22	119.83	111.02	5	1
1	A	72	GLN	OE1-CD-NE2	-7.16	115.44	122.60	2	3
1	A	65	HIS	CA-C-N	7.01	130.78	120.90	2	2
1	A	65	HIS	C-N-CA	7.01	130.78	120.90	2	2
1	A	40	THR	CA-CB-CG2	6.96	122.34	110.50	7	2
1	A	77	HIS	CB-CG-CD2	-6.96	122.15	131.20	9	6
1	A	38	PHE	CA-CB-CG	6.92	120.72	113.80	8	3
1	A	77	HIS	CG-ND1-CE1	-6.77	97.80	109.30	10	7
1	A	60	GLN	OE1-CD-NE2	-6.72	115.88	122.60	9	2
1	A	2	ASP	CA-C-O	-6.65	112.21	118.33	7	3
1	A	82	PRO	N-CA-CB	-6.64	96.28	103.25	4	3
1	A	14	PRO	N-CA-C	6.63	122.95	113.47	5	3
1	A	3	PRO	N-CA-C	6.56	122.07	114.20	2	7
1	A	22	CYS	N-CA-CB	-6.52	100.51	110.16	4	2
1	A	81	HIS	CE1-NE2-CD2	-6.51	102.48	109.00	4	10
1	A	33	HIS	CE1-NE2-CD2	-6.49	102.51	109.00	5	10
1	A	65	HIS	N-CA-C	6.45	119.56	111.24	4	1
1	A	13	HIS	CE1-NE2-CD2	-6.44	102.56	109.00	1	10
1	A	65	HIS	CE1-NE2-CD2	-6.42	102.58	109.00	1	10
1	A	2	ASP	O-C-N	-6.42	114.63	120.92	4	2
1	A	17	GLN	OE1-CD-NE2	-6.41	116.19	122.60	6	3
1	A	20	THR	O-C-N	-6.16	114.23	121.32	8	3
1	A	39	ILE	CA-CB-CG1	6.10	120.77	110.40	4	7
1	A	77	HIS	N-CA-C	6.09	119.65	111.24	10	2
1	A	57	ARG	CB-CA-C	6.09	122.17	110.17	8	3
1	A	81	HIS	N-CA-C	6.04	123.15	109.81	4	3
1	A	7	ASN	CA-CB-CG	6.02	118.62	112.60	5	3
1	A	62	ASN	CB-CG-ND2	6.02	125.42	116.40	6	1
1	A	67	ASP	O-C-N	-5.95	114.48	121.32	5	1
1	A	16	SER	N-CA-CB	5.94	120.53	110.49	4	3
1	A	74	SER	N-CA-CB	-5.93	100.46	110.49	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	ASP	CA-C-O	-5.85	112.14	120.16	2	1
1	A	65	HIS	CA-C-O	5.85	126.94	120.80	9	1
1	A	58	PRO	CB-CA-C	5.85	118.05	110.92	6	1
1	A	12	ASN	CB-CA-C	5.84	118.42	110.94	7	1
1	A	31	CYS	CB-CA-C	5.84	121.20	110.10	10	1
1	A	41	LYS	CA-CB-CG	5.82	125.73	114.10	6	1
1	A	36	MET	CB-CA-C	5.78	119.46	110.67	3	1
1	A	5	ASP	O-C-N	-5.78	114.67	121.32	10	3
1	A	19	ARG	N-CA-CB	-5.77	100.73	110.49	2	1
1	A	12	ASN	OD1-CG-ND2	-5.75	116.85	122.60	3	2
1	A	39	ILE	CB-CA-C	5.75	118.56	111.25	2	1
1	A	76	GLN	CB-CA-C	5.73	121.82	110.42	5	1
1	A	13	HIS	CA-C-N	5.72	125.19	119.24	2	2
1	A	13	HIS	C-N-CA	5.72	125.19	119.24	2	2
1	A	53	ARG	CB-CA-C	5.67	122.68	111.22	7	1
1	A	56	ARG	CA-C-O	-5.61	114.66	121.28	9	1
1	A	81	HIS	CG-ND1-CE1	-5.60	99.79	109.30	3	10
1	A	33	HIS	CG-ND1-CE1	-5.59	99.79	109.30	8	10
1	A	65	HIS	CG-ND1-CE1	-5.59	99.80	109.30	1	10
1	A	13	HIS	CG-ND1-CE1	-5.59	99.80	109.30	1	10
1	A	17	GLN	O-C-N	-5.58	116.18	121.20	2	1
1	A	63	GLN	N-CA-C	5.58	119.56	112.87	2	1
1	A	10	PRO	N-CA-C	5.52	123.84	112.47	10	4
1	A	80	ASP	CA-CB-CG	5.51	118.11	112.60	6	1
1	A	77	HIS	ND1-CG-CD2	5.51	111.61	106.10	4	5
1	A	5	ASP	CA-C-O	-5.50	112.63	120.16	3	1
1	A	19	ARG	N-CA-C	5.47	122.46	110.80	8	2
1	A	68	PRO	CB-CA-C	5.46	120.56	111.56	2	2
1	A	13	HIS	ND1-CG-CD2	5.43	111.53	106.10	1	10
1	A	78	ARG	NE-CZ-NH1	5.42	126.92	121.50	2	1
1	A	65	HIS	ND1-CG-CD2	5.41	111.51	106.10	1	10
1	A	81	HIS	ND1-CG-CD2	5.41	111.51	106.10	8	10
1	A	33	HIS	ND1-CG-CD2	5.41	111.51	106.10	7	10
1	A	25	CYS	O-C-N	-5.40	117.84	123.56	3	1
1	A	9	GLU	N-CA-C	5.39	117.72	110.29	3	1
1	A	73	PRO	N-CA-CB	-5.38	98.99	102.65	7	1
1	A	69	LEU	O-C-N	-5.36	115.16	121.32	10	1
1	A	60	GLN	CB-CG-CD	5.35	121.70	112.60	10	1
1	A	69	LEU	CA-C-N	5.32	125.22	119.85	9	1
1	A	69	LEU	C-N-CA	5.32	125.22	119.85	9	1
1	A	87	GLU	CB-CA-C	5.32	120.20	110.10	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	GLY	O-C-N	-5.29	116.48	121.77	2	1
1	A	50	LYS	CB-CA-C	5.29	118.22	111.40	6	1
1	A	52	ARG	NE-CZ-NH2	-5.21	114.51	119.20	3	1
1	A	52	ARG	N-CA-C	5.20	121.87	110.80	6	1
1	A	74	SER	CB-CA-C	5.19	120.75	110.42	9	1
1	A	5	ASP	N-CA-C	5.18	121.25	109.81	9	2
1	A	49	ARG	CB-CA-C	5.18	120.72	110.42	7	1
1	A	86	LYS	CB-CA-C	5.17	119.63	111.77	8	1
1	A	70	PRO	CB-CA-C	5.17	117.74	110.60	3	1
1	A	77	HIS	CB-CA-C	5.13	118.73	111.86	5	1
1	A	77	HIS	CG-CD2-NE2	5.13	112.33	107.20	8	1
1	A	23	ASN	OD1-CG-ND2	-5.12	117.48	122.60	9	1
1	A	70	PRO	N-CA-CB	-5.11	96.79	102.72	4	1
1	A	56	ARG	NE-CZ-NH1	5.10	126.60	121.50	2	1
1	A	11	TRP	CA-C-O	-5.07	114.87	120.24	2	1
1	A	58	PRO	O-C-N	-5.05	115.50	121.46	4	1
1	A	37	CYS	N-CA-CB	-5.01	102.02	110.49	4	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	Peptide,Sidechain	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	46	SER	Peptide,Mainchain	3
1	A	78	ARG	Sidechain	3
1	A	19	ARG	Sidechain	2
1	A	66	GLN	Peptide	2
1	A	65	HIS	Peptide	2
1	A	81	HIS	Sidechain	2
1	A	52	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	53	ARG	Peptide	1
1	A	56	ARG	Sidechain	1
1	A	16	SER	Peptide	1
1	A	47	TYR	Sidechain	1
1	A	55	ARG	Sidechain	1
1	A	57	ARG	Sidechain	1
1	A	60	GLN	Peptide	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:11:TRP:HZ3	1:A:46:SER:HG	0.91	0.99	2	1
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:CZ2	1:A:47:TYR:CZ	0.54	2.95	9	3
1:A:19:ARG:HH21	1:A:87:GLU:CD	0.44	2.19	10	1
1:A:65:HIS:O	1:A:81:HIS:HE1	0.41	1.98	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

6.3.1 Protein backbone

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	4	VAL	10
1	A	5	ASP	10
1	A	16	SER	10
1	A	57	ARG	10
1	A	68	PRO	10
1	A	69	LEU	10
1	A	81	HIS	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	6	PRO	3
1	A	36	MET	3
1	A	52	ARG	3
1	A	37	CYS	2
1	A	82	PRO	2
1	A	61	GLY	2
1	A	42	GLY	1
1	A	25	CYS	1
1	A	44	GLY	1
1	A	67	ASP	1
1	A	85	PRO	1

6.3.2 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 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%)	74±1 (93±1%)	5±1 (7±1%)	17 66
All	All	790/790 (100%)	738 (93%)	52 (7%)	17 66

All 9 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	28	LYS	10
1	A	41	LYS	10
1	A	81	HIS	10
1	A	39	ILE	9
1	A	67	ASP	9
1	A	10	PRO	1
1	A	62	ASN	1
1	A	70	PRO	1
1	A	87	GLU	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 oligosaccharides 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