Full wwPDB NMR Structure Validation Report (i)

Mar 12, 2026 – 07:23 AM UTC

PDB ID	:	1TER / pdb_00001ter
Title	:	SOLUTION STRUCTURE OF TERTIAPIN DETERMINED USING NUCLEAR MAGNETIC RESONANCE AND DISTANCE GEOMETRY
Authors	:	Xu, X.; Nelson, J.W.
Deposited on	:	1994-04-08

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 (i) 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 (i)) were used in the production of this report:

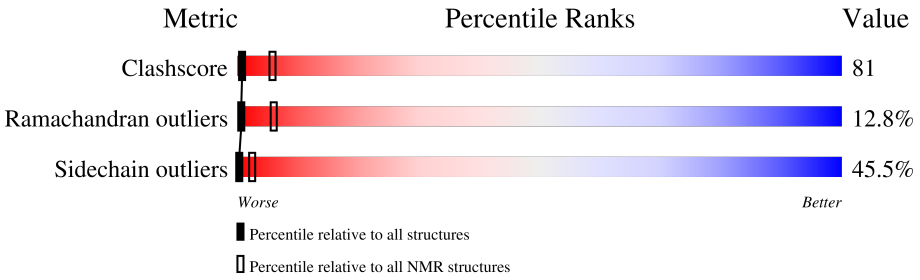
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

Mol	Chain	Length	Quality of chain
1	A	22	18% 41% 27% 14%

2 Ensemble composition and analysis

This entry contains 21 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:3-A:21 (19)	0.54	7

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 15
2	17, 20, 21
3	16, 18, 19
4	11, 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 351 atoms, of which 183 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TERTIAPIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	22	351	106	183	34	23	5	1

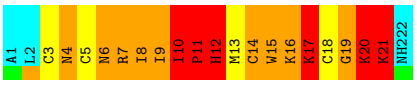
4 Residue-property plots

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: TERTIAPIN

Chain A:



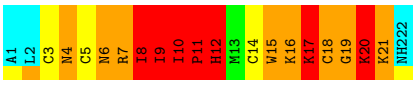
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TERTIAPIN

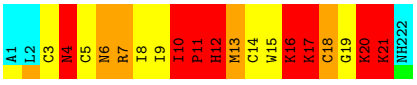
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: TERTIAPIN

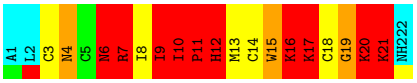
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: TERTIAPIN

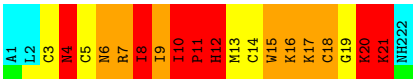
Chain A: 5% 23% 14% 45% 14%



4.2.4 Score per residue for model 4

• Molecule 1: TERTIAPIN

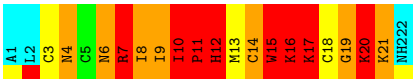
Chain A: 23% 32% 32% 14%



4.2.5 Score per residue for model 5

• Molecule 1: TERTIAPIN

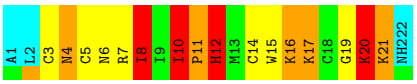
Chain A: 5% 14% 32% 36% 14%



4.2.6 Score per residue for model 6

• Molecule 1: TERTIAPIN

Chain A: 14% 32% 23% 18% 14%



4.2.7 Score per residue for model 7 (medoid)

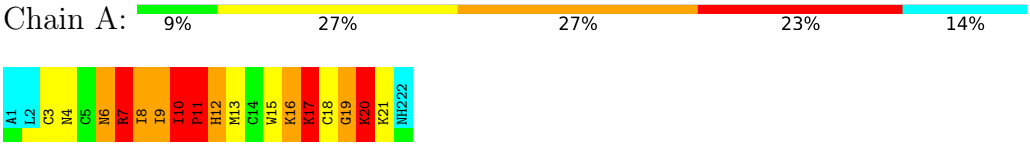
• Molecule 1: TERTIAPIN

Chain A: 5% 27% 23% 32% 14%

4.2.8 Score per residue for model 8

• Molecule 1: TERTIAPIN

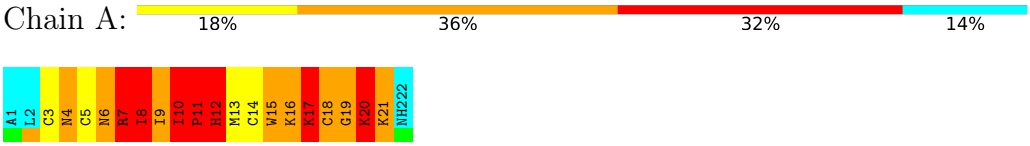
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: TERTIAPIN

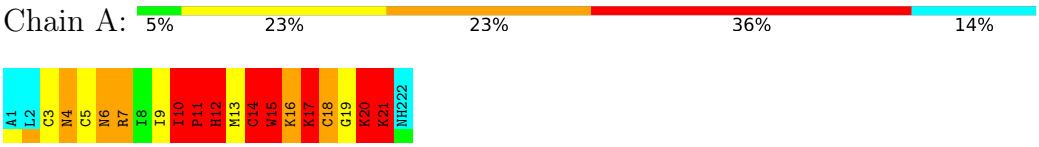
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: TERTIAPIN

Chain A:



4.2.11 Score per residue for model 11

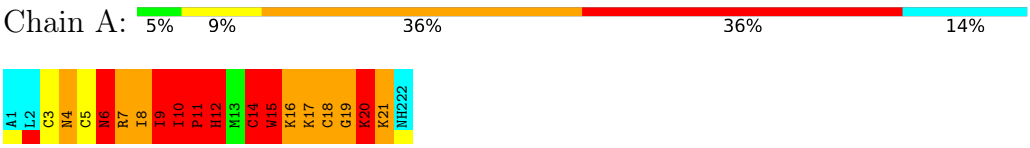
• Molecule 1: TERTIAPIN

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: TERTIAPIN

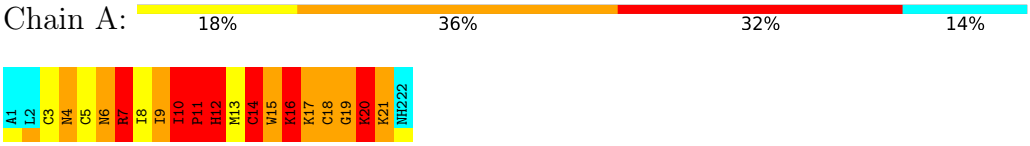
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: TERTIAPIN

Chain A:



4.2.14 Score per residue for model 14

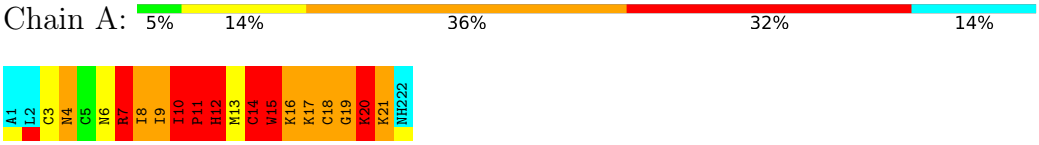
• Molecule 1: TERTIAPIN

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: TERTIAPIN

Chain A:



4.2.16 Score per residue for model 16

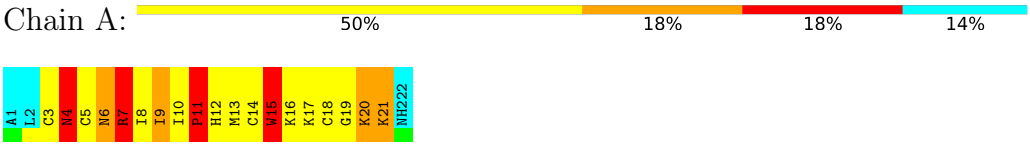
• Molecule 1: TERTIAPIN

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: TERTIAPIN

Chain A:



4.2.18 Score per residue for model 18

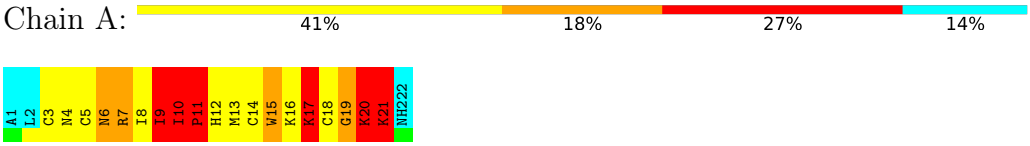
• Molecule 1: TERTIAPIN

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: TERTIAPIN

Chain A:



4.2.20 Score per residue for model 20

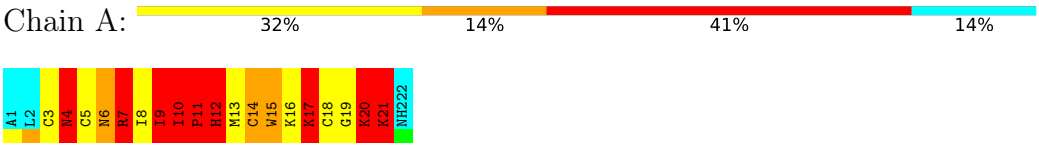
• Molecule 1: TERTIAPIN

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: TERTIAPIN

Chain A:



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 21 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	1.65±0.33	3±2/157 (1.6± 1.1%)	2.70±0.67	11±6/207 (5.4± 2.9%)
All	All	1.68	53/3297 (1.6%)	2.78	234/4347 (5.4%)

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	3.1±0.3	19.1±3.3
All	All	65	401

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	16	LYS	C-O	10.26	1.37	1.24	8	14
1	A	19	GLY	CA-C	9.44	1.65	1.51	14	7
1	A	15	TRP	CA-C	7.64	1.62	1.52	7	8
1	A	12	HIS	N-CA	6.80	1.54	1.46	5	7
1	A	16	LYS	C-N	5.93	1.42	1.33	12	8
1	A	12	HIS	C-O	5.69	1.32	1.24	14	4
1	A	10	ILE	N-CA	5.55	1.50	1.46	13	1
1	A	17	LYS	C-O	5.21	1.30	1.23	14	1
1	A	20	LYS	C-N	5.14	1.40	1.33	8	2
1	A	10	ILE	CA-CB	-5.02	1.47	1.54	14	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	20	LYS	N-CA-C	22.00	142.54	110.42	5	4
1	A	10	ILE	CB-CA-C	19.87	131.97	110.71	13	16
1	A	10	ILE	CA-CB-CG1	16.47	138.39	110.40	14	15
1	A	11	PRO	CB-CA-C	16.15	132.11	110.95	6	17
1	A	16	LYS	O-C-N	-13.21	104.86	122.43	13	15
1	A	11	PRO	N-CA-CB	-11.19	93.20	103.27	9	15
1	A	16	LYS	CA-C-O	-10.67	107.02	119.61	3	15
1	A	10	ILE	O-C-N	-9.92	113.72	121.46	7	7
1	A	15	TRP	CA-CB-CG	9.33	131.32	113.60	11	6
1	A	12	HIS	CB-CA-C	8.86	124.27	109.38	11	10
1	A	16	LYS	CA-C-N	-8.77	108.31	121.99	2	12
1	A	16	LYS	C-N-CA	-8.77	108.31	121.99	2	12
1	A	12	HIS	O-C-N	-7.80	112.97	122.34	5	9
1	A	17	LYS	N-CA-C	7.64	123.65	113.72	5	3
1	A	15	TRP	N-CA-CB	7.05	120.20	109.91	18	8
1	A	20	LYS	O-C-N	-7.05	115.21	123.11	5	13
1	A	14	CYS	O-C-N	-6.39	115.34	122.12	15	3
1	A	11	PRO	O-C-N	-6.30	115.32	123.00	6	6
1	A	10	ILE	CA-C-N	-6.29	113.81	120.03	14	5
1	A	10	ILE	C-N-CA	-6.29	113.81	120.03	14	5
1	A	17	LYS	O-C-N	-6.27	115.28	121.93	14	2
1	A	15	TRP	N-CA-C	-6.17	104.18	111.03	7	1
1	A	3	CYS	CA-CB-SG	6.14	128.53	114.40	11	1
1	A	12	HIS	CA-CB-CG	6.00	119.80	113.80	6	8
1	A	10	ILE	CA-C-O	5.81	124.87	119.76	1	3
1	A	15	TRP	CB-CA-C	-5.79	101.98	110.95	4	4
1	A	21	LYS	N-CA-CB	5.74	120.25	110.50	10	2
1	A	17	LYS	CA-C-N	5.74	128.24	120.38	10	1
1	A	17	LYS	C-N-CA	5.74	128.24	120.38	10	1
1	A	17	LYS	CA-CB-CG	5.52	125.14	114.10	2	1
1	A	11	PRO	N-CD-CG	-5.48	94.98	103.20	11	3
1	A	15	TRP	O-C-N	5.43	127.89	122.03	11	2
1	A	11	PRO	CA-C-O	-5.31	115.55	121.23	9	3
1	A	14	CYS	CA-C-O	-5.29	114.94	120.55	14	1
1	A	7	ARG	O-C-N	-5.27	117.16	123.06	8	1
1	A	20	LYS	CA-C-N	5.14	130.96	121.70	2	1
1	A	20	LYS	C-N-CA	5.14	130.96	121.70	2	1
1	A	17	LYS	N-CA-CB	-5.12	103.81	110.88	3	2

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	8	ILE	CB	21
1	A	9	ILE	CB	21
1	A	10	ILE	CB	21
1	A	20	LYS	CA	2

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	11	PRO	Mainchain,Peptide	21
1	A	16	LYS	Mainchain	21
1	A	20	LYS	Mainchain,Peptide	21
1	A	17	LYS	Mainchain,Peptide	20
1	A	3	CYS	Mainchain,Peptide	19
1	A	18	CYS	Mainchain,Peptide	19
1	A	7	ARG	Mainchain,Peptide,Sidechain	18
1	A	19	GLY	Peptide,Mainchain	18
1	A	9	ILE	Mainchain,Peptide	17
1	A	13	MET	Mainchain	17
1	A	10	ILE	Mainchain,Peptide	16
1	A	5	CYS	Mainchain	15
1	A	12	HIS	Peptide,Sidechain,Mainchain	15
1	A	14	CYS	Mainchain,Peptide	14
1	A	8	ILE	Mainchain,Peptide	13
1	A	4	ASN	Sidechain,Mainchain,Peptide	12
1	A	6	ASN	Mainchain,Peptide	12
1	A	15	TRP	Mainchain	8

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	154	163	162	24±13
All	All	3234	3423	3078	513

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 81.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ILE:HG22	1:A:14:CYS:HB3	0.93	1.39	7	8
1:A:10:ILE:HG13	1:A:15:TRP:HA	0.93	1.38	7	11
1:A:8:ILE:HD12	1:A:10:ILE:HD13	0.90	1.43	13	1
1:A:18:CYS:HB3	1:A:20:LYS:HB2	0.82	1.48	13	7
1:A:18:CYS:HB3	1:A:20:LYS:HB3	0.82	1.51	15	3
1:A:10:ILE:CG1	1:A:15:TRP:HA	0.81	2.06	1	13
1:A:10:ILE:HG22	1:A:11:PRO:HD2	0.80	1.54	14	13
1:A:18:CYS:HB3	1:A:20:LYS:CB	0.72	2.15	10	10
1:A:10:ILE:HG22	1:A:11:PRO:O	0.67	1.89	16	1
1:A:8:ILE:CD1	1:A:10:ILE:HD13	0.65	2.21	13	2
1:A:10:ILE:CG2	1:A:14:CYS:HB3	0.65	2.22	13	6
1:A:12:HIS:HA	1:A:15:TRP:HB2	0.64	1.70	2	4
1:A:10:ILE:HG12	1:A:21:LYS:HA	0.64	1.70	1	12
1:A:10:ILE:HG12	1:A:15:TRP:HA	0.63	1.71	15	7
1:A:8:ILE:HD11	1:A:20:LYS:HD3	0.62	1.71	13	2
1:A:10:ILE:HG22	1:A:14:CYS:CB	0.62	2.22	13	7
1:A:4:ASN:HB3	1:A:7:ARG:H	0.62	1.54	11	1
1:A:11:PRO:HD2	1:A:14:CYS:HB2	0.62	1.71	9	4
1:A:10:ILE:HD11	1:A:20:LYS:CG	0.62	2.24	14	1
1:A:9:ILE:HD13	1:A:9:ILE:N	0.61	2.11	19	3
1:A:10:ILE:HG13	1:A:15:TRP:N	0.60	2.11	5	8
1:A:18:CYS:HB3	1:A:20:LYS:HG2	0.60	1.74	12	3
1:A:10:ILE:HG13	1:A:15:TRP:CA	0.59	2.28	2	9
1:A:15:TRP:CD2	1:A:21:LYS:HG2	0.59	2.32	10	1
1:A:15:TRP:CG	1:A:21:LYS:HA	0.58	2.32	2	1
1:A:16:LYS:HA	1:A:20:LYS:HB3	0.58	1.75	5	2
1:A:9:ILE:N	1:A:9:ILE:HD13	0.58	2.13	3	1
1:A:9:ILE:HD12	1:A:9:ILE:N	0.58	2.13	21	2
1:A:20:LYS:HG3	1:A:21:LYS:N	0.57	2.14	14	4
1:A:12:HIS:HA	1:A:15:TRP:CG	0.57	2.34	12	12
1:A:18:CYS:HB3	1:A:20:LYS:CG	0.57	2.30	15	3
1:A:8:ILE:HD12	1:A:10:ILE:CD1	0.57	2.26	13	1
1:A:18:CYS:CB	1:A:20:LYS:HB2	0.56	2.29	1	7
1:A:10:ILE:HG12	1:A:15:TRP:CD1	0.55	2.37	12	12
1:A:10:ILE:HG22	1:A:11:PRO:CD	0.55	2.32	9	6
1:A:8:ILE:HD12	1:A:9:ILE:N	0.55	2.16	2	1
1:A:15:TRP:HB2	1:A:21:LYS:N	0.55	2.17	16	6
1:A:10:ILE:HG13	1:A:15:TRP:HB3	0.55	1.79	18	4
1:A:15:TRP:CE2	1:A:21:LYS:HG3	0.54	2.37	7	6
1:A:12:HIS:HB3	1:A:15:TRP:CD2	0.54	2.37	10	6
1:A:12:HIS:O	1:A:15:TRP:HB2	0.54	2.02	5	7
1:A:10:ILE:CG1	1:A:15:TRP:HB3	0.54	2.33	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:HB2	1:A:15:TRP:CD2	0.53	2.38	12	6
1:A:10:ILE:CD1	1:A:15:TRP:HA	0.53	2.34	19	3
1:A:10:ILE:HD13	1:A:21:LYS:O	0.53	2.03	5	2
1:A:15:TRP:NE1	1:A:21:LYS:HD3	0.52	2.19	5	2
1:A:15:TRP:HB3	1:A:21:LYS:N	0.52	2.20	11	2
1:A:15:TRP:CD2	1:A:21:LYS:HB2	0.52	2.40	2	5
1:A:9:ILE:H	1:A:9:ILE:HD13	0.52	1.65	12	1
1:A:4:ASN:HB3	1:A:7:ARG:HB2	0.52	1.81	7	4
1:A:8:ILE:C	1:A:9:ILE:HD13	0.52	2.29	11	1
1:A:10:ILE:HG22	1:A:15:TRP:N	0.52	2.18	21	1
1:A:10:ILE:HG23	1:A:11:PRO:HD2	0.52	1.82	16	2
1:A:8:ILE:N	1:A:8:ILE:HD13	0.52	2.20	11	2
1:A:7:ARG:NE	1:A:7:ARG:HA	0.51	2.20	14	3
1:A:15:TRP:CG	1:A:21:LYS:HB2	0.51	2.41	1	5
1:A:9:ILE:HD12	1:A:9:ILE:O	0.51	2.05	1	1
1:A:12:HIS:CD2	1:A:15:TRP:CE3	0.50	2.99	2	3
1:A:8:ILE:HD13	1:A:8:ILE:H	0.50	1.66	11	1
1:A:7:ARG:NE	1:A:7:ARG:N	0.50	2.60	13	1
1:A:10:ILE:HG22	1:A:14:CYS:HB2	0.50	1.81	9	1
1:A:4:ASN:C	1:A:6:ASN:H	0.50	2.15	4	13
1:A:12:HIS:CD2	1:A:15:TRP:CZ3	0.50	3.00	1	6
1:A:12:HIS:CG	1:A:15:TRP:CE3	0.50	3.00	5	2
1:A:10:ILE:HD11	1:A:18:CYS:CB	0.50	2.37	12	5
1:A:12:HIS:HB3	1:A:15:TRP:CE2	0.49	2.43	7	6
1:A:12:HIS:CD2	1:A:13:MET:N	0.49	2.81	16	1
1:A:10:ILE:HG21	1:A:18:CYS:SG	0.49	2.47	14	1
1:A:15:TRP:CE2	1:A:21:LYS:HG2	0.49	2.42	5	2
1:A:10:ILE:CG2	1:A:11:PRO:CD	0.49	2.91	4	7
1:A:10:ILE:HD11	1:A:20:LYS:HB3	0.48	1.85	7	1
1:A:4:ASN:ND2	1:A:7:ARG:NH2	0.48	2.60	15	1
1:A:15:TRP:CG	1:A:21:LYS:CB	0.48	2.97	4	5
1:A:8:ILE:HA	1:A:10:ILE:HD13	0.48	1.84	18	1
1:A:12:HIS:CB	1:A:15:TRP:CD2	0.48	2.96	10	6
1:A:10:ILE:CG2	1:A:11:PRO:HD2	0.47	2.37	5	7
1:A:15:TRP:C	1:A:20:LYS:HB3	0.47	2.33	5	2
1:A:12:HIS:CD2	1:A:13:MET:HG3	0.47	2.45	16	1
1:A:15:TRP:CZ3	1:A:16:LYS:HG3	0.47	2.44	16	1
1:A:15:TRP:C	1:A:17:LYS:N	0.47	2.72	3	13
1:A:15:TRP:CD2	1:A:21:LYS:HG3	0.47	2.43	15	1
1:A:12:HIS:CD2	1:A:15:TRP:CH2	0.47	3.03	11	1
1:A:19:GLY:N	1:A:20:LYS:CB	0.47	2.78	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:TRP:CE2	1:A:21:LYS:CG	0.46	2.98	15	4
1:A:12:HIS:CA	1:A:15:TRP:HB2	0.46	2.40	2	2
1:A:15:TRP:CG	1:A:21:LYS:HB3	0.46	2.45	9	3
1:A:6:ASN:HB3	1:A:7:ARG:NH2	0.46	2.26	12	2
1:A:15:TRP:CE3	1:A:20:LYS:CE	0.46	2.99	3	2
1:A:15:TRP:NE1	1:A:21:LYS:CD	0.46	2.79	3	2
1:A:12:HIS:HB2	1:A:15:TRP:CZ2	0.46	2.46	20	4
1:A:10:ILE:HD11	1:A:15:TRP:HA	0.45	1.87	19	1
1:A:7:ARG:NE	1:A:7:ARG:CA	0.45	2.79	3	2
1:A:15:TRP:CD2	1:A:21:LYS:CB	0.45	2.99	12	2
1:A:15:TRP:CD2	1:A:21:LYS:CG	0.45	3.00	10	2
1:A:12:HIS:NE2	1:A:13:MET:HG3	0.45	2.26	16	1
1:A:15:TRP:CE3	1:A:21:LYS:HB2	0.45	2.47	2	1
1:A:20:LYS:CG	1:A:21:LYS:N	0.45	2.78	12	3
1:A:12:HIS:HA	1:A:15:TRP:CB	0.45	2.42	2	3
1:A:12:HIS:HB2	1:A:15:TRP:CE2	0.45	2.47	11	2
1:A:12:HIS:CB	1:A:15:TRP:CG	0.45	2.99	10	1
1:A:9:ILE:HG23	1:A:9:ILE:O	0.45	2.12	13	1
1:A:15:TRP:CE3	1:A:20:LYS:HE3	0.45	2.47	5	1
1:A:15:TRP:CZ3	1:A:16:LYS:CG	0.45	3.00	16	1
1:A:15:TRP:CE2	1:A:21:LYS:CD	0.45	3.00	17	1
1:A:15:TRP:CE2	1:A:21:LYS:HD2	0.44	2.47	17	2
1:A:10:ILE:HD11	1:A:21:LYS:H	0.44	1.72	2	2
1:A:10:ILE:HD11	1:A:20:LYS:HG3	0.44	1.90	14	1
1:A:9:ILE:N	1:A:9:ILE:CD1	0.44	2.80	21	4
1:A:7:ARG:HA	1:A:7:ARG:HE	0.44	1.71	5	1
1:A:15:TRP:NE1	1:A:21:LYS:HG2	0.44	2.27	7	1
1:A:15:TRP:CH2	1:A:21:LYS:NZ	0.44	2.80	12	1
1:A:15:TRP:CE3	1:A:16:LYS:HG3	0.44	2.47	16	1
1:A:10:ILE:CG1	1:A:15:TRP:CA	0.44	2.94	12	2
1:A:15:TRP:CH2	1:A:21:LYS:CE	0.44	3.00	2	1
1:A:18:CYS:CB	1:A:20:LYS:HB3	0.44	2.35	12	2
1:A:12:HIS:HA	1:A:15:TRP:CE2	0.44	2.48	17	6
1:A:8:ILE:HG22	1:A:8:ILE:O	0.44	2.12	11	2
1:A:4:ASN:O	1:A:10:ILE:HG23	0.44	2.13	4	1
1:A:14:CYS:O	1:A:18:CYS:HB2	0.44	2.12	13	2
1:A:15:TRP:CZ2	1:A:21:LYS:HD2	0.43	2.48	13	2
1:A:10:ILE:C	1:A:15:TRP:CD1	0.43	2.96	10	9
1:A:15:TRP:CE3	1:A:20:LYS:HE2	0.43	2.48	3	1
1:A:15:TRP:HB3	1:A:21:LYS:HA	0.43	1.90	17	2
1:A:10:ILE:HG13	1:A:15:TRP:CB	0.43	2.42	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ILE:HD11	1:A:18:CYS:HB3	0.43	1.89	11	4
1:A:11:PRO:O	1:A:14:CYS:HB2	0.43	2.13	11	2
1:A:15:TRP:CZ2	1:A:21:LYS:HE3	0.43	2.49	2	3
1:A:12:HIS:HA	1:A:15:TRP:CD1	0.43	2.48	2	3
1:A:10:ILE:HA	1:A:11:PRO:HD3	0.43	1.68	9	1
1:A:10:ILE:HD12	1:A:15:TRP:HA	0.43	1.89	21	1
1:A:12:HIS:CE1	1:A:16:LYS:NZ	0.43	2.87	13	1
1:A:7:ARG:N	1:A:7:ARG:HD2	0.43	2.29	18	1
1:A:10:ILE:HG13	1:A:15:TRP:CD1	0.43	2.48	17	1
1:A:16:LYS:CA	1:A:20:LYS:HB3	0.43	2.43	5	1
1:A:4:ASN:C	1:A:6:ASN:N	0.42	2.76	2	12
1:A:10:ILE:CG1	1:A:21:LYS:HA	0.42	2.43	7	1
1:A:10:ILE:HD11	1:A:15:TRP:HB3	0.42	1.91	17	1
1:A:10:ILE:CD1	1:A:18:CYS:CB	0.42	2.97	7	3
1:A:11:PRO:C	1:A:14:CYS:HB2	0.42	2.39	11	1
1:A:15:TRP:CE3	1:A:21:LYS:HE2	0.42	2.49	14	1
1:A:9:ILE:O	1:A:9:ILE:HG23	0.42	2.13	17	1
1:A:15:TRP:NE1	1:A:21:LYS:HG3	0.42	2.30	13	2
1:A:19:GLY:O	1:A:20:LYS:HG2	0.42	2.13	1	3
1:A:8:ILE:HD11	1:A:20:LYS:CD	0.42	2.44	12	1
1:A:15:TRP:CH2	1:A:21:LYS:HD2	0.42	2.50	13	1
1:A:12:HIS:HA	1:A:15:TRP:CD2	0.42	2.50	17	1
1:A:15:TRP:CA	1:A:21:LYS:H	0.42	2.28	7	1
1:A:15:TRP:O	1:A:17:LYS:N	0.41	2.52	3	2
1:A:6:ASN:C	1:A:7:ARG:HE	0.41	2.23	21	1
1:A:20:LYS:HB3	1:A:21:LYS:O	0.41	2.15	7	1
1:A:15:TRP:CD2	1:A:21:LYS:HB3	0.41	2.50	9	3
1:A:17:LYS:C	1:A:19:GLY:N	0.41	2.77	14	1
1:A:10:ILE:HD12	1:A:10:ILE:HG21	0.41	1.81	2	1
1:A:12:HIS:C	1:A:15:TRP:HB2	0.41	2.41	5	1
1:A:4:ASN:CB	1:A:7:ARG:H	0.41	2.25	11	1
1:A:14:CYS:C	1:A:17:LYS:H	0.41	2.24	10	1
1:A:4:ASN:HB3	1:A:7:ARG:HD2	0.41	1.92	13	1
1:A:15:TRP:C	1:A:20:LYS:CB	0.41	2.93	3	1
1:A:20:LYS:HD3	1:A:21:LYS:CB	0.41	2.46	3	1
1:A:10:ILE:CD1	1:A:20:LYS:CG	0.41	2.96	14	1
1:A:15:TRP:HB2	1:A:20:LYS:HA	0.41	1.92	19	1
1:A:10:ILE:HD11	1:A:20:LYS:HG2	0.41	1.92	9	1
1:A:11:PRO:HD2	1:A:14:CYS:CB	0.41	2.41	9	1
1:A:8:ILE:O	1:A:8:ILE:HD13	0.40	2.16	1	1
1:A:8:ILE:HG12	1:A:10:ILE:HD13	0.40	1.92	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:TRP:CH2	1:A:21:LYS:HE3	0.40	2.51	2	1
1:A:12:HIS:HB2	1:A:15:TRP:CE3	0.40	2.51	3	1
1:A:7:ARG:CA	1:A:7:ARG:NE	0.40	2.85	7	1
1:A:15:TRP:CB	1:A:21:LYS:N	0.40	2.84	20	1
1:A:10:ILE:CG2	1:A:15:TRP:N	0.40	2.84	21	1
1:A:10:ILE:HG13	1:A:14:CYS:C	0.40	2.42	12	1
1:A:12:HIS:HB3	1:A:15:TRP:CG	0.40	2.51	14	1
1:A:15:TRP:CD1	1:A:21:LYS:HG3	0.40	2.52	16	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	19/22 (86%)	13±2 (68±9%)	4±2 (19±8%)	2±1 (13±3%)	0	6
All	All	398/462 (86%)	270 (68%)	77 (19%)	51 (13%)	0	6

All 8 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	21	LYS	21
1	A	20	LYS	17
1	A	19	GLY	5
1	A	15	TRP	3
1	A	8	ILE	2
1	A	3	CYS	1
1	A	9	ILE	1
1	A	18	CYS	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	18/19 (95%)	10±2 (54±9%)	8±2 (46±9%)	0 2
All	All	378/399 (95%)	206 (54%)	172 (46%)	0 2

All 16 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	20	LYS	20
1	A	7	ARG	19
1	A	10	ILE	17
1	A	9	ILE	16
1	A	12	HIS	16
1	A	17	LYS	14
1	A	4	ASN	14
1	A	8	ILE	12
1	A	6	ASN	12
1	A	21	LYS	11
1	A	11	PRO	5
1	A	15	TRP	5
1	A	16	LYS	4
1	A	14	CYS	4
1	A	13	MET	2
1	A	3	CYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided