



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 7VBG / pdb_00007vbg
BMRB ID : 51070
Title : N Terminal Domain of PRC1
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Deposited on : 2021-08-31

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

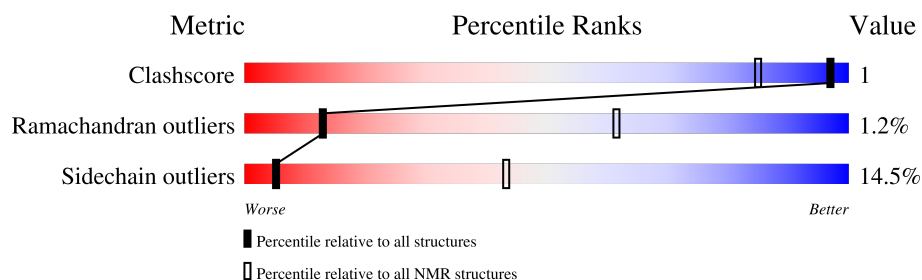
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	67	72% 22% 6%
1	B	67	73% 19% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:63, B:68-B:129 (125)	0.34	8

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 5 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2294 atoms, of which 1172 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein regulator of cytokinesis 1.

Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1147	350	586	101	106	4	
1	B	67	Total	C	H	N	O	S	0
			1147	350	586	101	106	4	

There are 4 discrepancies between the modelled and reference sequences:

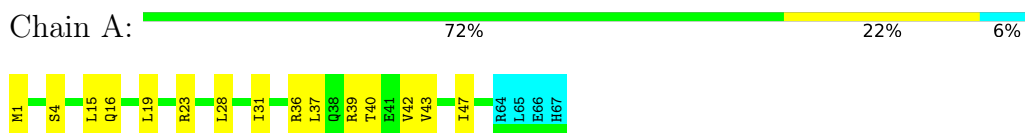
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	-	expression tag	UNP O43663
A	67	HIS	-	expression tag	UNP O43663
B	133	GLU	-	expression tag	UNP O43663
B	134	HIS	-	expression tag	UNP O43663

4 Residue-property plots

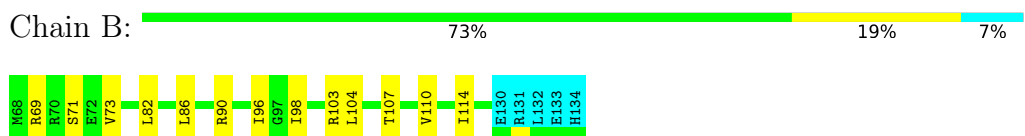
4.1 Average score per residue in the NMR ensemble

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: Protein regulator of cytokinesis 1



- Molecule 1: Protein regulator of cytokinesis 1

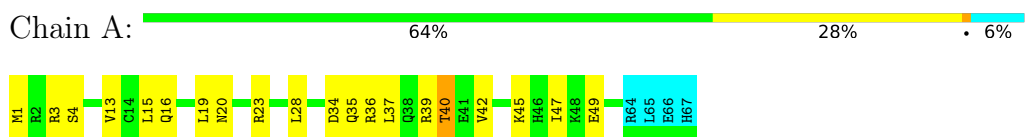


4.2 Scores per residue for each member of the ensemble

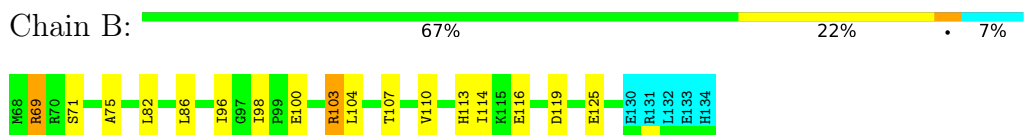
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein regulator of cytokinesis 1



- Molecule 1: Protein regulator of cytokinesis 1



4.2.2 Score per residue for model 2

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  75% 18% 6%



- Molecule 1: Protein regulator of cytokinesis 1

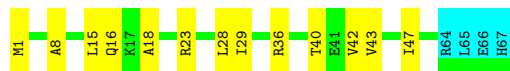
Chain B:  67% 22% 7%



4.2.3 Score per residue for model 3

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  75% 19% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  69% 22% 7%



4.2.4 Score per residue for model 4

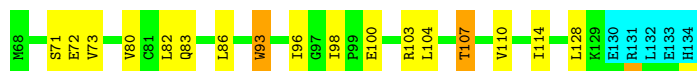
- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  73% 18% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  67% 22% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  75% 16% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  73% 16% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  75% 16% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  79% 12% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  69% 24% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  72% 21% 7%



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  67% 22% • • 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  73% 18% • 7%



4.2.9 Score per residue for model 9

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  75% 15% • 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  67% 24% • 7%



4.2.10 Score per residue for model 10

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  66% 25% • 6%



- Molecule 1: Protein regulator of cytokinesis 1

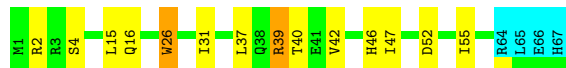
Chain B:  72% 21% 7%



4.2.11 Score per residue for model 11

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  73% 18% 6%



- Molecule 1: Protein regulator of cytokinesis 1

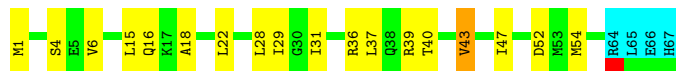
Chain B:  70% 21% 7%



4.2.12 Score per residue for model 12

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  67% 25% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  63% 25% 7%



4.2.13 Score per residue for model 13

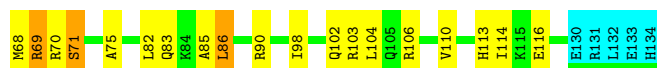
- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  70% 22% 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  64% 24% 7%



4.2.14 Score per residue for model 14

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  73% 19% • 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  75% 16% • 7%



4.2.15 Score per residue for model 15

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  66% 27% • 6%



- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  72% 18% • 7%



4.2.16 Score per residue for model 16

- Molecule 1: Protein regulator of cytokinesis 1

Chain A:  69% 24% • 6%



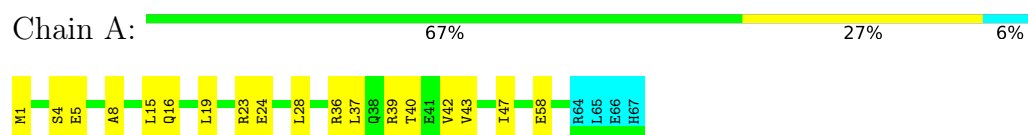
- Molecule 1: Protein regulator of cytokinesis 1

Chain B:  75% 18% 7%

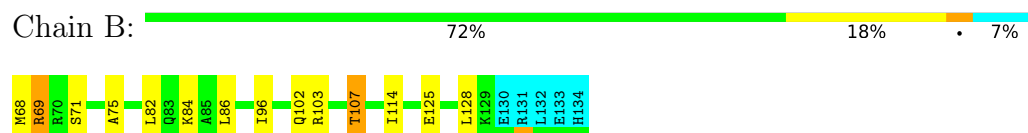


4.2.17 Score per residue for model 17

- Molecule 1: Protein regulator of cytokinesis 1

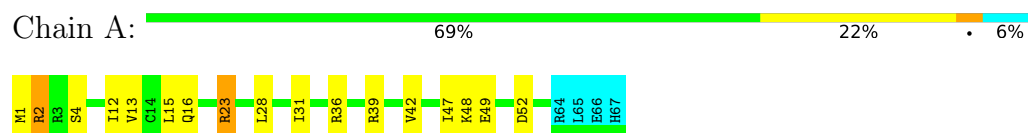


- Molecule 1: Protein regulator of cytokinesis 1

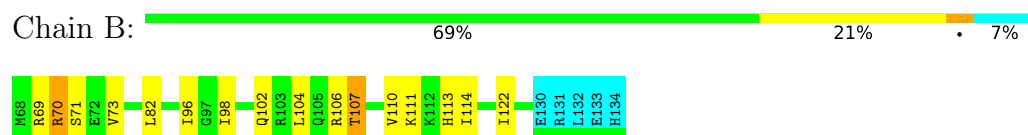


4.2.18 Score per residue for model 18

- Molecule 1: Protein regulator of cytokinesis 1

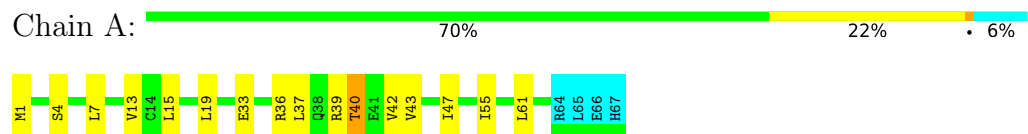


- Molecule 1: Protein regulator of cytokinesis 1

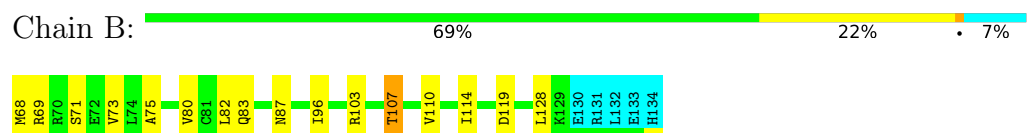


4.2.19 Score per residue for model 19

- Molecule 1: Protein regulator of cytokinesis 1

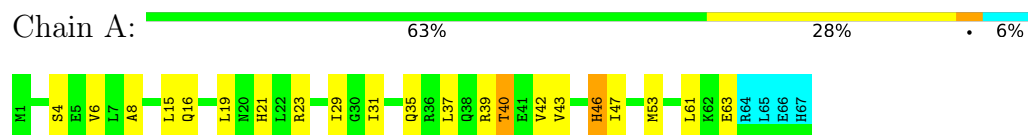


- Molecule 1: Protein regulator of cytokinesis 1

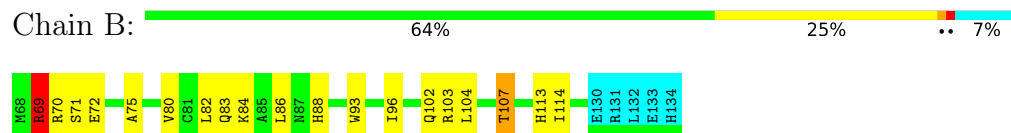


4.2.20 Score per residue for model 20

- Molecule 1: Protein regulator of cytokinesis 1



- Molecule 1: Protein regulator of cytokinesis 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	901
Number of shifts mapped to atoms	901
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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	1.11±0.03	0±0/527 (0.0± 0.0%)	1.78±0.05	8±3/706 (1.1± 0.4%)
1	B	1.11±0.04	0±0/518 (0.0± 0.0%)	1.77±0.05	7±3/694 (1.0± 0.5%)
All	All	1.11	0/20900 (0.0%)	1.78	291/28000 (1.0%)

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	0.0±0.0	1.4±0.9
1	B	0.0±0.0	1.4±0.8
All	All	0	54

There are no bond-length outliers.

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	39	ARG	NE-CZ-NH2	7.68	126.11	119.20	5	6
1	A	39	ARG	CD-NE-CZ	7.63	135.08	124.40	9	8
1	A	13	VAL	N-CA-C	-7.62	103.10	110.42	2	4
1	A	6	VAL	N-CA-C	7.41	119.06	110.62	10	3
1	A	16	GLN	CA-C-N	7.34	129.98	120.44	15	12
1	A	16	GLN	C-N-CA	7.34	129.98	120.44	15	12
1	B	106	ARG	NE-CZ-NH2	7.33	125.79	119.20	9	3
1	A	16	GLN	OE1-CD-NE2	-7.11	115.49	122.60	18	5
1	B	103	ARG	NE-CZ-NH2	6.97	125.48	119.20	12	5
1	A	52	ASP	N-CA-C	6.91	118.81	111.28	12	7
1	A	2	ARG	NE-CZ-NH2	6.77	125.29	119.20	18	1
1	B	109	VAL	N-CA-C	6.69	117.48	110.72	2	1
1	A	4	SER	CA-C-N	6.60	130.02	120.38	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	SER	C-N-CA	6.60	130.02	120.38	14	3
1	B	83	GLN	CA-C-N	6.48	128.87	120.44	19	9
1	B	83	GLN	C-N-CA	6.48	128.87	120.44	19	9
1	A	18	ALA	CA-C-N	6.47	128.95	120.28	9	4
1	A	18	ALA	C-N-CA	6.47	128.95	120.28	9	4
1	A	63	GLU	N-CA-C	6.46	119.31	111.82	20	1
1	A	36	ARG	NE-CZ-NH2	6.43	124.99	119.20	1	6
1	B	88	HIS	CA-CB-CG	6.39	120.19	113.80	5	2
1	B	93	TRP	N-CA-C	6.37	118.22	111.28	2	1
1	B	80	VAL	N-CA-C	-6.35	104.33	110.42	4	4
1	B	90	ARG	NE-CZ-NH2	6.32	124.89	119.20	15	3
1	B	107	THR	N-CA-C	6.32	117.83	111.07	20	6
1	B	72	GLU	CA-C-N	6.32	129.44	120.53	20	7
1	B	72	GLU	C-N-CA	6.32	129.44	120.53	20	7
1	B	106	ARG	CD-NE-CZ	6.22	133.11	124.40	13	4
1	A	17	LYS	N-CA-CB	-6.20	101.03	110.01	6	2
1	B	83	GLN	OE1-CD-NE2	-6.11	116.49	122.60	11	4
1	A	35	GLN	OE1-CD-NE2	-6.11	116.49	122.60	1	4
1	B	73	VAL	N-CA-C	6.10	117.58	110.62	3	3
1	A	36	ARG	CA-CB-CG	-6.04	102.01	114.10	17	2
1	B	103	ARG	CA-CB-CG	-6.04	102.02	114.10	8	4
1	B	70	ARG	NE-CZ-NH2	5.99	124.59	119.20	18	2
1	B	101	ASP	N-CA-C	5.91	118.68	111.82	12	1
1	B	113	HIS	CB-CG-CD2	-5.89	123.54	131.20	13	8
1	B	102	GLN	OE1-CD-NE2	-5.84	116.76	122.60	13	4
1	A	5	GLU	CA-C-N	5.78	128.68	120.53	4	4
1	A	5	GLU	C-N-CA	5.78	128.68	120.53	4	4
1	A	32	PRO	CA-C-N	5.76	128.58	120.28	16	1
1	A	32	PRO	C-N-CA	5.76	128.58	120.28	16	1
1	A	20	ASN	OD1-CG-ND2	-5.72	116.88	122.60	13	2
1	A	3	ARG	NE-CZ-NH2	5.72	124.35	119.20	7	2
1	A	36	ARG	CD-NE-CZ	5.72	132.41	124.40	6	1
1	A	32	PRO	N-CA-CB	5.72	108.33	103.19	13	2
1	B	119	ASP	N-CA-C	5.69	117.57	111.36	19	3
1	B	103	ARG	NH1-CZ-NH2	-5.68	111.92	119.30	1	2
1	A	21	HIS	CB-CG-CD2	-5.67	123.83	131.20	20	1
1	A	28	LEU	CB-CA-C	5.62	120.14	110.86	7	1
1	B	86	LEU	N-CA-CB	-5.62	101.85	110.12	13	1
1	B	111	LYS	O-C-N	-5.60	116.30	122.07	18	1
1	B	71	SER	CA-C-N	5.58	128.53	120.38	12	3
1	B	71	SER	C-N-CA	5.58	128.53	120.38	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	96	ILE	N-CA-C	5.58	116.36	110.72	5	2
1	B	106	ARG	NE-CZ-NH1	-5.58	115.92	121.50	9	1
1	A	46	HIS	CB-CG-CD2	-5.58	123.95	131.20	11	2
1	A	43	VAL	CA-CB-CG1	5.56	119.86	110.40	12	1
1	A	36	ARG	N-CA-C	5.56	117.02	111.07	15	2
1	A	26	TRP	CA-CB-CG	5.54	124.12	113.60	11	1
1	B	87	ASN	OD1-CG-ND2	-5.52	117.08	122.60	19	2
1	B	85	ALA	CA-C-N	5.51	127.97	120.54	10	2
1	B	85	ALA	C-N-CA	5.51	127.97	120.54	10	2
1	A	58	GLU	N-CA-CB	5.49	117.92	109.91	9	1
1	A	36	ARG	CA-C-O	-5.46	115.08	120.70	13	1
1	B	115	LYS	CA-C-N	5.46	127.59	120.28	7	1
1	B	115	LYS	C-N-CA	5.46	127.59	120.28	7	1
1	A	20	ASN	CA-CB-CG	5.45	118.05	112.60	1	2
1	B	128	LEU	CB-CA-C	5.45	120.62	109.67	19	2
1	B	95	LEU	N-CA-CB	-5.44	101.76	110.19	9	1
1	B	84	LYS	CA-C-N	5.42	127.81	120.44	20	1
1	B	84	LYS	C-N-CA	5.42	127.81	120.44	20	1
1	A	39	ARG	NE-CZ-NH1	-5.40	116.10	121.50	20	2
1	A	40	THR	N-CA-C	5.39	117.16	111.28	1	3
1	A	23	ARG	CD-NE-CZ	5.37	131.92	124.40	1	2
1	A	7	LEU	CA-C-N	5.36	127.72	120.44	19	1
1	A	7	LEU	C-N-CA	5.36	127.72	120.44	19	1
1	B	105	GLN	OE1-CD-NE2	-5.34	117.26	122.60	6	2
1	A	61	LEU	CB-CA-C	5.34	120.40	109.67	16	3
1	A	21	HIS	CA-CB-CG	5.31	119.11	113.80	6	1
1	B	103	ARG	N-CA-C	5.30	117.14	111.36	17	1
1	A	34	ASP	CA-CB-CG	5.29	117.89	112.60	1	1
1	B	87	ASN	CA-CB-CG	5.26	117.86	112.60	15	1
1	A	42	VAL	N-CA-C	5.26	117.67	111.09	11	1
1	B	87	ASN	CA-C-N	5.26	127.28	120.44	12	1
1	B	87	ASN	C-N-CA	5.26	127.28	120.44	12	1
1	A	13	VAL	CB-CA-C	-5.26	105.15	111.88	19	2
1	A	48	LYS	CA-C-N	5.25	127.32	120.28	15	2
1	A	48	LYS	C-N-CA	5.25	127.32	120.28	15	2
1	A	42	VAL	CA-C-N	5.24	127.16	120.56	17	2
1	A	42	VAL	C-N-CA	5.24	127.16	120.56	17	2
1	B	127	SER	CA-C-O	-5.23	113.49	119.60	15	1
1	A	29	ILE	CA-CB-CG1	5.20	119.25	110.40	3	1
1	A	19	LEU	N-CA-CB	-5.19	102.50	110.12	9	1
1	B	80	VAL	CB-CA-C	-5.17	105.35	111.97	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	GLU	CA-C-N	5.15	129.23	120.88	16	1
1	A	27	GLU	C-N-CA	5.15	129.23	120.88	16	1
1	A	19	LEU	CB-CA-C	5.14	119.59	110.85	8	1
1	B	125	GLU	N-CA-CB	5.14	117.42	109.91	9	1
1	A	24	GLU	N-CA-CB	5.14	117.46	110.01	17	1
1	B	69	ARG	NE-CZ-NH2	5.13	123.82	119.20	20	1
1	B	93	TRP	N-CA-CB	5.13	117.62	109.82	4	1
1	B	90	ARG	NE-CZ-NH1	5.12	126.62	121.50	6	1
1	A	45	LYS	CA-CB-CG	-5.12	103.86	114.10	1	1
1	B	99	PRO	N-CA-CB	5.11	107.78	103.19	3	1
1	A	31	ILE	CA-C-N	5.10	125.39	119.93	8	1
1	A	31	ILE	C-N-CA	5.10	125.39	119.93	8	1
1	A	23	ARG	NE-CZ-NH2	5.09	123.78	119.20	2	1
1	B	103	ARG	CD-NE-CZ	5.09	131.52	124.40	8	1
1	B	110	VAL	CA-CB-CG1	5.05	118.99	110.40	9	1
1	B	84	LYS	N-CA-CB	-5.05	102.69	110.01	17	1
1	A	12	ILE	CA-CB-CG1	5.04	118.97	110.40	18	1
1	A	8	ALA	CA-C-N	5.04	126.99	120.44	15	1
1	A	8	ALA	C-N-CA	5.04	126.99	120.44	15	1
1	B	96	ILE	CA-CB-CG1	5.04	118.96	110.40	2	1
1	A	36	ARG	NH1-CZ-NH2	-5.02	112.77	119.30	3	1
1	A	2	ARG	CA-C-N	5.02	127.71	120.38	10	1
1	A	2	ARG	C-N-CA	5.02	127.71	120.38	10	1
1	A	21	HIS	N-CA-C	5.02	116.75	111.28	9	1

There are no chirality outliers.

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	1	MET	Peptide	12
1	B	68	MET	Peptide	9
1	B	69	ARG	Sidechain	6
1	A	36	ARG	Sidechain	6
1	B	103	ARG	Sidechain	5
1	B	90	ARG	Sidechain	3
1	A	23	ARG	Sidechain	3
1	A	3	ARG	Peptide,Sidechain	2
1	A	39	ARG	Sidechain	2
1	B	106	ARG	Sidechain	2
1	B	70	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	2	ARG	Sidechain	1
1	A	46	HIS	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	522	548	546	1±1
1	B	513	542	537	1±1
All	All	20700	21800	21660	28

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:MET:HE1	1:B:85:ALA:HB1	0.66	1.68	5	2
1:A:54:MET:CE	1:B:85:ALA:HB1	0.59	2.27	5	1
1:A:8:ALA:HB1	1:B:86:LEU:HD22	0.55	1.77	5	4
1:A:19:LEU:HD22	1:B:75:ALA:HB1	0.53	1.81	7	8
1:A:40:THR:HG23	1:B:75:ALA:HB2	0.47	1.86	13	3
1:B:81:CYS:HA	1:B:84:LYS:HE2	0.45	1.87	10	1
1:B:93:TRP:CE2	1:B:103:ARG:CZ	0.44	3.00	4	1
1:A:8:ALA:HB2	1:B:107:THR:HG23	0.44	1.90	17	4
1:B:93:TRP:HB2	1:B:103:ARG:CD	0.43	2.44	20	1
1:A:26:TRP:CD1	1:A:36:ARG:HD2	0.41	2.50	5	1
1:A:54:MET:HE1	1:B:85:ALA:CB	0.41	2.46	12	2

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	62/67 (93%)	58±1 (94±1%)	3±1 (5±2%)	1±0 (1±1%)	14	63
1	B	61/67 (91%)	58±1 (95±2%)	2±1 (4±2%)	1±0 (1±1%)	12	60
All	All	2460/2680 (92%)	2328 (95%)	102 (4%)	30 (1%)	13	61

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	71	SER	16
1	A	4	SER	13
1	A	58	GLU	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	59/63 (94%)	50±2 (85±3%)	9±2 (15±3%)	5	43
1	B	58/63 (92%)	50±2 (86±4%)	8±2 (14±4%)	5	44
All	All	2340/2520 (93%)	2000 (85%)	340 (15%)	5	43

All 47 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	47	ILE	20
1	B	114	ILE	20
1	A	15	LEU	19
1	B	82	LEU	18
1	A	40	THR	17
1	B	107	THR	17
1	B	96	ILE	15
1	A	42	VAL	13
1	B	110	VAL	12
1	A	31	ILE	12
1	A	43	VAL	12
1	A	28	LEU	11
1	A	37	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	B	98	ILE	11
1	B	104	LEU	11
1	B	69	ARG	8
1	B	116	GLU	8
1	B	73	VAL	8
1	B	86	LEU	7
1	A	23	ARG	7
1	B	90	ARG	7
1	A	49	GLU	6
1	B	125	GLU	6
1	A	55	ILE	6
1	A	6	VAL	6
1	A	29	ILE	5
1	B	93	TRP	5
1	A	26	TRP	5
1	B	109	VAL	4
1	A	33	GLU	4
1	A	58	GLU	4
1	B	100	GLU	3
1	A	36	ARG	3
1	A	19	LEU	3
1	A	2	ARG	3
1	A	39	ARG	2
1	A	3	ARG	1
1	A	7	LEU	1
1	B	120	MET	1
1	B	72	GLU	1
1	A	22	LEU	1
1	B	80	VAL	1
1	A	10	GLU	1
1	B	128	LEU	1
1	B	70	ARG	1
1	B	122	ILE	1
1	A	53	MET	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 [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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	901
Number of shifts mapped to atoms	901
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	67	-0.54 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	66	0.17 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	64	-0.63 ± 0.15	Should be applied
^{15}N	62	-0.20 ± 0.27	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 46%, i.e. 852 atoms were assigned a chemical shift out of a possible 1866. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	305/623 (49%)	124/250 (50%)	123/250 (49%)	58/123 (47%)
Sidechain	529/1187 (45%)	357/768 (46%)	166/371 (45%)	6/48 (12%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	18/56 (32%)	9/28 (32%)	9/18 (50%)	0/10 (0%)
Overall	852/1866 (46%)	490/1046 (47%)	298/639 (47%)	64/181 (35%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 901 atoms were assigned a chemical shift out of a possible 2016. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	325/668 (49%)	132/268 (49%)	131/268 (49%)	62/132 (47%)
Sidechain	558/1276 (44%)	376/824 (46%)	176/398 (44%)	6/54 (11%)
Aromatic	18/72 (25%)	9/36 (25%)	9/22 (41%)	0/14 (0%)
Overall	901/2016 (45%)	517/1128 (46%)	316/688 (46%)	68/200 (34%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

