wwPDB NMR Structure Validation Summary Report

Apr 26, 2016 – 03:06 PM BST

PDB ID	:	1K1Z
Title	:	Solution structure of N-terminal SH3 domain mutant(P33G) of murine Vav
Authors	:	Ogura, K.; Nagata, K.; Horiuchi, M.; Ebisui, E.; Hasuda, T.; Yuzawa, S.; Nishida, M.; Hatanaka, H.; Inagaki, F.
Deposited on	:	2001-09-26

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

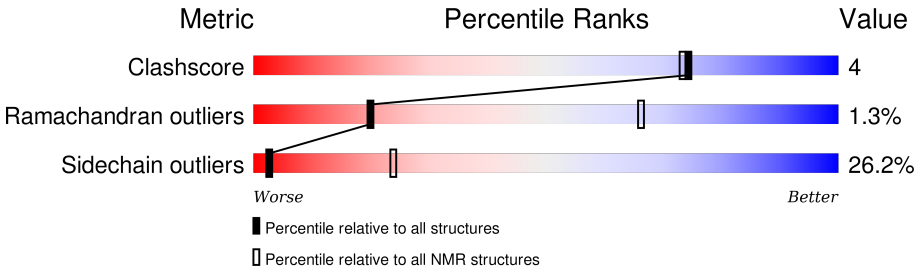
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 76%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	78	69% 27% .

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1243 atoms, of which 606 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called vav.

Mol	Chain	Residues	Atoms						Trace
1	A	78	Total	C	H	N	O	S	0
			1243	408	606	114	113	2	

There is a discrepancy between the modelled and reference sequences:

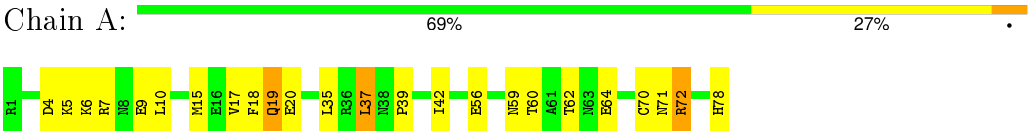
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	PRO	ENGINEERED	UNP P27870

4 Residue-property plots (i)

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: vav

Chain A:



5 Refinement protocol and experimental data overview

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

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
ARIA	structure solution	1.0
ARIA	refinement	1.0

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)	BMRB entry 5179
Number of chemical shift lists	1
Total number of shifts	845
Number of shifts mapped to atoms	844
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	637	606	603	5
All	All	637	606	603	5

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:15:MET:O	1:A:42:ILE:HA	0.51	2.05
1:A:17:VAL:HG11	1:A:37:LEU:HB3	0.50	1.83
1:A:42:ILE:O	1:A:60:THR:HG22	0.44	2.13
1:A:35:LEU:HD21	1:A:59:ASN:HB2	0.42	1.89
1:A:19:GLN:NE2	1:A:72:ARG:HB3	0.41	2.31

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	76/78 (97%)	70 (92%)	5 (7%)	1 (1%)	20 66
All	All	76/78 (97%)	70 (92%)	5 (7%)	1 (1%)	20 66

All 1 Ramachandran outliers are listed below.

Mol	Chain	Res	Type
1	A	39	PRO

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	65/65 (100%)	48 (74%)	17 (26%)	3 24
All	All	65/65 (100%)	48 (74%)	17 (26%)	3 24

5 of 17 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	72	ARG
1	A	19	GLN
1	A	20	GLU
1	A	71	ASN
1	A	18	PHE

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

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

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5179

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	845
Number of shifts mapped to atoms	844
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	200

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. The only occurence is reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	NH2	HN1	8.49	-1.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	77	0.30 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	69	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	67	0.12 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 761 atoms were assigned a chemical shift out of a possible 999. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	286/374 (76%)	142/148 (96%)	77/156 (49%)	67/70 (96%)
Sidechain	374/505 (74%)	229/301 (76%)	138/177 (78%)	7/27 (26%)
Aromatic	101/120 (84%)	53/62 (85%)	45/49 (92%)	3/9 (33%)
Overall	761/999 (76%)	424/511 (83%)	260/382 (68%)	77/106 (73%)

7.1.4 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	47	LYS	CE	89.98	46.00 – 37.80	58.6
1	A	14	LYS	CE	89.58	46.00 – 37.80	58.1
1	A	36	ARG	CD	91.28	47.57 – 38.77	54.7
1	A	58	ARG	CD	90.58	47.57 – 38.77	53.9
1	A	72	ARG	CD	90.08	47.57 – 38.77	53.3
1	A	34	PHE	CE2	70.42	136.81 – 124.71	-49.9
1	A	75	PRO	CD	98.58	55.31 – 45.41	48.7
1	A	39	PRO	CD	98.38	55.31 – 45.41	48.5
1	A	25	PRO	CD	98.28	55.31 – 45.41	48.4
1	A	13	PRO	CD	98.18	55.31 – 45.41	48.3
1	A	26	PRO	CD	98.08	55.31 – 45.41	48.2
1	A	27	PRO	CD	97.58	55.31 – 45.41	47.7
1	A	69	PRO	CD	96.88	55.31 – 45.41	47.0
1	A	28	PRO	CD	96.78	55.31 – 45.41	46.9
1	A	47	LYS	CG	77.38	30.67 – 19.17	45.6
1	A	75	PRO	CG	76.28	32.66 – 21.76	45.0
1	A	39	PRO	CG	76.18	32.66 – 21.76	44.9
1	A	27	PRO	CG	75.38	32.66 – 21.76	44.2
1	A	28	PRO	CG	75.28	32.66 – 21.76	44.1
1	A	13	PRO	CG	75.18	32.66 – 21.76	44.0
1	A	46	THR	CG2	70.78	27.15 – 15.95	44.0
1	A	69	PRO	CG	75.08	32.66 – 21.76	43.9
1	A	26	PRO	CG	74.68	32.66 – 21.76	43.6
1	A	60	THR	CG2	69.68	27.15 – 15.95	43.0

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	31	PHE	CD2	82.62	137.34 – 125.84	-42.6
1	A	14	LYS	CG	73.88	30.67 – 19.17	42.6
1	A	62	THR	CG2	68.98	27.15 – 15.95	42.3
1	A	12	LEU	CG	75.28	32.55 – 21.05	42.2
1	A	19	GLN	CG	80.98	39.38 – 28.18	42.1
1	A	10	LEU	CG	74.78	32.55 – 21.05	41.7
1	A	25	PRO	CG	72.58	32.66 – 21.76	41.6
1	A	34	PHE	CE1	70.42	137.92 – 123.42	-41.6
1	A	18	PHE	CD2	83.92	137.34 – 125.84	-41.5
1	A	25	PRO	CB	81.08	37.79 – 25.89	41.4
1	A	34	PHE	CD2	84.22	137.34 – 125.84	-41.2
1	A	36	ARG	CG	76.58	33.23 – 21.23	41.1
1	A	14	LYS	CD	77.48	34.86 – 23.06	41.1
1	A	45	LEU	CG	73.88	32.55 – 21.05	40.9
1	A	35	LEU	CG	73.88	32.55 – 21.05	40.9
1	A	72	ARG	CG	76.18	33.23 – 21.23	40.8
1	A	13	PRO	CB	80.18	37.79 – 25.89	40.6
1	A	75	PRO	CB	79.88	37.79 – 25.89	40.4
1	A	37	LEU	CG	73.08	32.55 – 21.05	40.2
1	A	31	PHE	CD1	82.62	137.63 – 125.43	-40.1
1	A	58	ARG	CG	75.28	33.23 – 21.23	40.0
1	A	28	PRO	CB	79.38	37.79 – 25.89	39.9
1	A	31	PHE	CE2	82.62	136.81 – 124.71	-39.8
1	A	39	PRO	CB	79.08	37.79 – 25.89	39.7
1	A	56	GLU	CG	84.58	42.24 – 29.94	39.4
1	A	44	GLU	CG	84.48	42.24 – 29.94	39.3
1	A	16	GLU	CG	84.48	42.24 – 29.94	39.3
1	A	64	GLU	CG	84.48	42.24 – 29.94	39.3
1	A	51	GLU	CG	84.18	42.24 – 29.94	39.1
1	A	49	GLU	CG	84.18	42.24 – 29.94	39.1
1	A	69	PRO	CB	78.28	37.79 – 25.89	39.0
1	A	18	PHE	CD1	83.92	137.63 – 125.43	-39.0
1	A	15	MET	CG	81.18	38.33 – 25.73	39.0
1	A	68	PHE	CD2	86.82	137.34 – 125.84	-38.9
1	A	18	PHE	CE2	83.72	136.81 – 124.71	-38.9
1	A	26	PRO	CB	78.08	37.79 – 25.89	38.9
1	A	34	PHE	CD1	84.22	137.63 – 125.43	-38.8
1	A	22	TYR	CE1	70.12	124.14 – 111.74	-38.6
1	A	68	PHE	CE2	84.12	136.81 – 124.71	-38.5
1	A	27	PRO	CB	77.68	37.79 – 25.89	38.5
1	A	76	TYR	CE1	70.72	124.14 – 111.74	-38.1
1	A	29	GLY	CA	94.48	51.81 – 38.91	38.1

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	20	GLU	CG	82.88	42.24 – 29.94	38.0
1	A	22	TYR	CD1	84.82	139.11 – 126.41	-37.7
1	A	76	TYR	CD1	84.92	139.11 – 126.41	-37.7
1	A	57	GLY	CA	93.88	51.81 – 38.91	37.6
1	A	47	LYS	CD	73.08	34.86 – 23.06	37.4
1	A	66	GLY	CA	93.48	51.81 – 38.91	37.3
1	A	34	PHE	CZ	71.42	137.04 – 121.44	-37.1
1	A	11	GLY	CA	92.98	51.81 – 38.91	36.9
1	A	33	GLY	CA	92.88	51.81 – 38.91	36.8
1	A	32	GLY	CA	92.68	51.81 – 38.91	36.7
1	A	68	PHE	CD1	86.82	137.63 – 125.43	-36.6
1	A	40	GLY	CA	92.58	51.81 – 38.91	36.6
1	A	17	VAL	CG1	71.98	28.40 – 14.60	36.6
1	A	23	GLY	CA	92.18	51.81 – 38.91	36.3
1	A	22	TYR	CE2	70.12	124.68 – 111.18	-35.4
1	A	73	VAL	CG1	69.78	28.40 – 14.60	35.0
1	A	76	TYR	CE2	70.72	124.68 – 111.18	-35.0
1	A	43	VAL	CG1	69.38	28.40 – 14.60	34.7
1	A	65	VAL	CG1	68.68	28.40 – 14.60	34.2
1	A	42	ILE	CG2	65.48	24.63 – 10.43	33.8
1	A	77	VAL	CG1	67.88	28.40 – 14.60	33.6
1	A	31	PHE	CE1	82.62	137.92 – 123.42	-33.1
1	A	24	ILE	CG2	64.48	24.63 – 10.43	33.1
1	A	18	PHE	CE1	83.72	137.92 – 123.42	-32.4
1	A	22	TYR	CD2	84.82	140.11 – 125.31	-32.4
1	A	76	TYR	CD2	84.92	140.11 – 125.31	-32.3
1	A	68	PHE	CE1	84.12	137.92 – 123.42	-32.1
1	A	17	VAL	CG2	71.18	29.20 – 13.40	31.6
1	A	54	TRP	CZ2	66.62	121.76 – 106.66	-31.5
1	A	55	TRP	CZ2	66.72	121.76 – 106.66	-31.5
1	A	67	TRP	CZ2	66.72	121.76 – 106.66	-31.5
1	A	68	PHE	CZ	80.40	137.04 – 121.44	-31.3
1	A	55	TRP	CZ3	72.62	129.20 – 113.60	-31.3
1	A	67	TRP	CZ3	73.22	129.20 – 113.60	-30.9
1	A	54	TRP	CZ3	73.22	129.20 – 113.60	-30.9
1	A	35	LEU	CD1	73.88	32.77 – 16.57	30.4
1	A	31	PHE	CZ	82.02	137.04 – 121.44	-30.3
1	A	77	VAL	CG2	68.88	29.20 – 13.40	30.1
1	A	43	VAL	CG2	68.88	29.20 – 13.40	30.1
1	A	65	VAL	CG2	68.48	29.20 – 13.40	29.9
1	A	10	LEU	CD1	72.88	32.77 – 16.57	29.8
1	A	16	GLU	CB	81.48	38.65 – 21.35	29.8

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	4	ASP	CB	89.08	49.06 – 32.66	29.4
1	A	45	LEU	CD1	72.18	32.77 – 16.57	29.3
1	A	41	ASP	CB	88.88	49.06 – 32.66	29.3
1	A	73	VAL	CG2	67.48	29.20 – 13.40	29.2
1	A	12	LEU	CD2	73.48	32.60 – 15.60	29.0
1	A	38	ASN	CB	87.58	47.13 – 30.23	28.9
1	A	45	LEU	CD2	73.28	32.60 – 15.60	28.9
1	A	56	GLU	CB	79.98	38.65 – 21.35	28.9
1	A	37	LEU	CD2	72.98	32.60 – 15.60	28.8
1	A	54	TRP	CE3	71.42	129.06 – 111.96	-28.7
1	A	44	GLU	CB	79.38	38.65 – 21.35	28.5
1	A	64	GLU	CB	79.38	38.65 – 21.35	28.5
1	A	59	ASN	CB	86.68	47.13 – 30.23	28.4
1	A	8	ASN	CB	86.58	47.13 – 30.23	28.3
1	A	12	LEU	CD1	70.58	32.77 – 16.57	28.3
1	A	53	ASN	CB	86.48	47.13 – 30.23	28.3
1	A	47	LYS	CB	82.98	41.68 – 23.88	28.2
1	A	35	LEU	CD2	71.98	32.60 – 15.60	28.2
1	A	58	ARG	CB	82.18	39.81 – 21.51	28.2
1	A	73	VAL	CB	83.58	41.76 – 23.66	28.1
1	A	37	LEU	CD1	70.18	32.77 – 16.57	28.1
1	A	14	LYS	CB	82.68	41.68 – 23.88	28.0
1	A	49	GLU	CB	78.28	38.65 – 21.35	27.9
1	A	67	TRP	CE3	72.92	129.06 – 111.96	-27.8
1	A	43	VAL	CB	83.08	41.76 – 23.66	27.8
1	A	65	VAL	CB	83.08	41.76 – 23.66	27.8
1	A	63	ASN	CB	85.68	47.13 – 30.23	27.8
1	A	9	GLU	CB	77.98	38.65 – 21.35	27.7
1	A	10	LEU	CD2	71.18	32.60 – 15.60	27.7
1	A	20	GLU	CB	77.58	38.65 – 21.35	27.5
1	A	19	GLN	CB	79.68	38.36 – 19.96	27.5
1	A	24	ILE	CD1	59.78	21.91 – 5.01	27.4
1	A	71	ASN	CB	84.68	47.13 – 30.23	27.2
1	A	51	GLU	CB	77.08	38.65 – 21.35	27.2
1	A	35	LEU	CB	93.18	51.69 – 32.89	27.1
1	A	37	LEU	CB	92.98	51.69 – 32.89	27.0
1	A	5	LYS	CB	80.68	41.68 – 23.88	26.9
1	A	6	LYS	CB	80.68	41.68 – 23.88	26.9
1	A	42	ILE	CD1	58.88	21.91 – 5.01	26.9
1	A	55	TRP	CE3	74.72	129.06 – 111.96	-26.8
1	A	42	ILE	CG1	74.78	36.54 – 18.94	26.7
1	A	48	ALA	CB	67.28	28.03 – 9.93	26.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	61	ALA	CB	67.18	28.03 – 9.93	26.6
1	A	24	ILE	CG1	74.38	36.54 – 18.94	26.5
1	A	77	VAL	CB	80.58	41.76 – 23.66	26.4
1	A	2	ALA	CB	66.78	28.03 – 9.93	26.4
1	A	50	ALA	CB	66.78	28.03 – 9.93	26.4
1	A	1	ARG	CB	78.58	39.81 – 21.51	26.2
1	A	17	VAL	CB	79.98	41.76 – 23.66	26.1
1	A	3	GLN	CB	77.08	38.36 – 19.96	26.0
1	A	30	ALA	CB	66.08	28.03 – 9.93	26.0
1	A	36	ARG	CB	78.28	39.81 – 21.51	26.0
1	A	72	ARG	CB	78.28	39.81 – 21.51	26.0
1	A	55	TRP	CD1	76.02	136.18 – 116.78	-26.0
1	A	55	TRP	CB	82.08	40.02 – 19.92	25.9
1	A	45	LEU	CB	90.28	51.69 – 32.89	25.5
1	A	10	LEU	CB	90.28	51.69 – 32.89	25.5
1	A	55	TRP	CH2	76.62	133.06 – 114.56	-25.5
1	A	67	TRP	CH2	76.72	133.06 – 114.56	-25.5
1	A	15	MET	CE	66.68	26.97 – 7.37	25.3
1	A	54	TRP	CH2	77.32	133.06 – 114.56	-25.1
1	A	12	LEU	CB	89.18	51.69 – 32.89	24.9
1	A	67	TRP	CB	79.38	40.02 – 19.92	24.6
1	A	67	TRP	CD1	78.92	136.18 – 116.78	-24.5
1	A	54	TRP	CD1	79.12	136.18 – 116.78	-24.4
1	A	54	TRP	CB	78.78	40.02 – 19.92	24.3
1	A	52	HIS	CB	80.78	40.69 – 19.69	24.1
1	A	24	ILE	CB	87.68	48.82 – 28.42	24.0
1	A	21	TYR	CB	89.58	50.05 – 28.55	23.4
1	A	34	PHE	CB	88.78	50.37 – 29.47	23.4
1	A	18	PHE	CB	88.68	50.37 – 29.47	23.3
1	A	74	HIS	CB	79.18	40.69 – 19.69	23.3
1	A	38	ASN	CA	97.68	63.05 – 44.05	23.2
1	A	78	HIS	CB	78.58	40.69 – 19.69	23.0
1	A	42	ILE	CB	84.88	48.82 – 28.42	22.7
1	A	15	MET	CB	83.38	44.20 – 21.80	22.5
1	A	68	PHE	CB	86.58	50.37 – 29.47	22.3
1	A	76	TYR	CB	86.78	50.05 – 28.55	22.1
1	A	22	TYR	CB	85.18	50.05 – 28.55	21.3
1	A	31	PHE	CB	84.38	50.37 – 29.47	21.3
1	A	78	HIS	CE1	89.52	149.70 – 125.30	-19.7
1	A	74	HIS	CE1	89.62	149.70 – 125.30	-19.6
1	A	52	HIS	CE1	90.72	149.70 – 125.30	-19.2
1	A	52	HIS	CD2	70.82	137.40 – 103.40	-14.6

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	74	HIS	CD2	72.02	137.40 – 103.40	-14.2
1	A	78	HIS	CD2	72.82	137.40 – 103.40	-14.0
1	A	56	GLU	HB3	-0.79	3.10 – 0.90	-12.7
1	A	56	GLU	HG3	0.58	3.31 – 1.21	-8.0
1	A	70	CYS	CB	72.18	64.28 – 1.38	6.3
1	A	27	PRO	HA	2.37	6.05 – 2.75	-6.2
1	A	23	GLY	H	4.40	11.63 – 5.03	-6.0
1	A	28	PRO	HD3	1.68	5.52 – 1.72	-5.1

7.1.5 Random Coil Index (RCI) plots

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.

Random coil index (RCI) for chain A: