wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MX2
Title	:	UBX-L domain of VCIP135
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Deposited on	:	2014-12-07

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

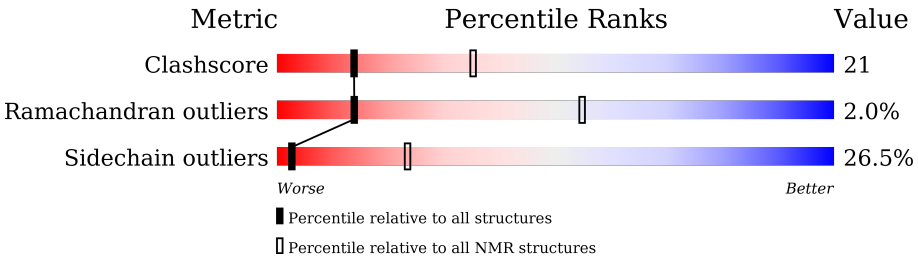
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027790
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 85%.

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	81	47% 47% 5% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:7-A:86 (80)	0.20	15

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 and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1327 atoms, of which 673 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Deubiquitinating protein VCIP135.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1327	417	673	112	121	4	0

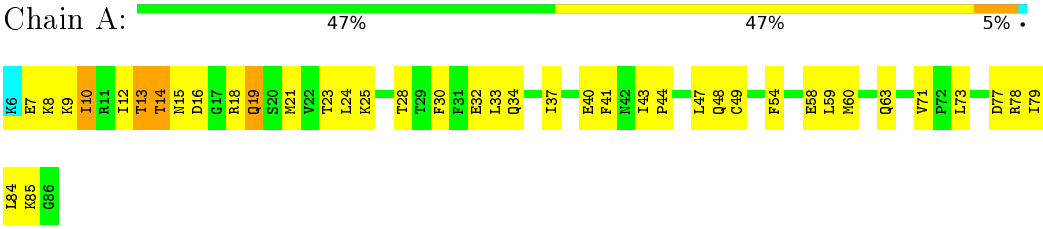
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Deubiquitinating protein VCIP135

Chain A:

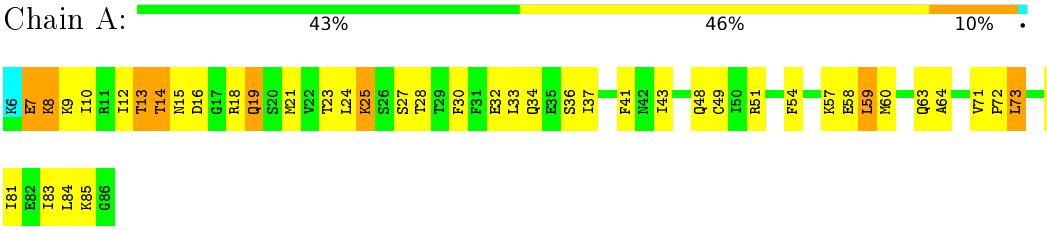


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: Deubiquitinating protein VCIP135

Chain A:



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 least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	
CNS	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)	2mx2_cs.cif
Number of chemical shift lists	1
Total number of shifts	1033
Number of shifts mapped to atoms	1006
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	645	660	659	27±5
All	All	12900	13200	13180	541

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 21.

5 of 111 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD22	1:A:84:LEU:O	0.79	1.77	17	1
1:A:8:LYS:HG3	1:A:10:ILE:HD11	0.75	1.57	19	4
1:A:15:ASN:OD1	1:A:83:ILE:HD12	0.73	1.82	20	13
1:A:49:CYS:HB2	1:A:84:LEU:HD21	0.72	1.61	17	18
1:A:13:THR:HG23	1:A:19:GLN:HB3	0.70	1.61	14	20

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	79/81 (98%)	69±1 (87±2%)	9±1 (11±2%)	2±1 (2±1%)	14 55
All	All	1580/1620 (98%)	1376 (87%)	172 (11%)	32 (2%)	14 55

All 5 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	59	LEU	16
1	A	64	ALA	10
1	A	24	LEU	3
1	A	7	GLU	2
1	A	62	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	73/74 (99%)	54±2 (73±3%)	19±2 (27±3%)	3 23
All	All	1460/1480 (99%)	1073 (73%)	387 (27%)	3 23

5 of 36 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	13	THR	20
1	A	10	ILE	20
1	A	34	GLN	20
1	A	9	LYS	20
1	A	21	MET	20

6.3.3 RNA (i)

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 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 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: 2mx2_cs.cif

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	1033
Number of shifts mapped to atoms	1006
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	223

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

- Residue not found in structure. First 5 (of 27) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	HIS	HD2	6.955	0.0	1
A	4	HIS	CD2	64.111	0.0	1
A	4	HIS	CA	56.572	0.0	1
A	1	GLY	HA2	3.791	0.0	1
A	1	GLY	CA	71.841	0.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	86	0.32 ± 0.26	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	80	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	70	-0.05 ± 0.57	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 85%, i.e. 880 atoms were assigned a chemical shift out of a possible 1038. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	300/384 (78%)	150/152 (99%)	80/160 (50%)	70/72 (97%)
Sidechain	523/594 (88%)	330/354 (93%)	184/212 (87%)	9/28 (32%)
Aromatic	57/60 (95%)	31/32 (97%)	26/26 (100%)	0/2 (0%)
Overall	880/1038 (85%)	511/538 (95%)	290/398 (73%)	79/102 (77%)

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	46	TYR	CD1	49.37	139.11 – 126.41	-65.7
1	A	52	TYR	CD1	49.44	139.11 – 126.41	-65.6
1	A	46	TYR	CD2	49.37	140.11 – 125.31	-56.3
1	A	52	TYR	CD2	49.44	140.11 – 125.31	-56.3
1	A	41	PHE	CD2	75.03	137.34 – 125.84	-49.2
1	A	30	PHE	CD2	75.21	137.34 – 125.84	-49.0
1	A	54	PHE	CD2	75.56	137.34 – 125.84	-48.7
1	A	31	PHE	CD2	75.75	137.34 – 125.84	-48.6
1	A	54	PHE	CE2	73.94	136.81 – 124.71	-47.0
1	A	41	PHE	CD1	75.03	137.63 – 125.43	-46.3
1	A	41	PHE	CE2	74.73	136.81 – 124.71	-46.3
1	A	30	PHE	CD1	75.21	137.63 – 125.43	-46.2
1	A	54	PHE	CD1	75.56	137.63 – 125.43	-45.9
1	A	31	PHE	CD1	75.75	137.63 – 125.43	-45.7
1	A	30	PHE	CE2	75.56	136.81 – 124.71	-45.6
1	A	31	PHE	CE2	75.78	136.81 – 124.71	-45.4
1	A	52	TYR	CE1	61.69	124.14 – 111.74	-45.4
1	A	46	TYR	CE1	62.64	124.14 – 111.74	-44.6
1	A	52	TYR	CE2	61.69	124.68 – 111.18	-41.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	46	TYR	CE2	62.64	124.68 – 111.18	-41.0
1	A	79	ILE	CG2	75.14	24.63 – 10.43	40.6
1	A	12	ILE	CG2	74.92	24.63 – 10.43	40.4
1	A	50	ILE	CG2	74.88	24.63 – 10.43	40.4
1	A	43	ILE	CG2	74.68	24.63 – 10.43	40.2
1	A	37	ILE	CG2	74.26	24.63 – 10.43	39.9
1	A	10	ILE	CG2	73.87	24.63 – 10.43	39.7
1	A	83	ILE	CG2	73.76	24.63 – 10.43	39.6
1	A	81	ILE	CG2	73.65	24.63 – 10.43	39.5
1	A	54	PHE	CE1	73.94	137.92 – 123.42	-39.1
1	A	41	PHE	CE1	74.73	137.92 – 123.42	-38.6
1	A	30	PHE	CE1	75.56	137.92 – 123.42	-38.0
1	A	31	PHE	CE1	75.78	137.92 – 123.42	-37.9
1	A	41	PHE	CZ	73.48	137.04 – 121.44	-35.7
1	A	30	PHE	CZ	74.03	137.04 – 121.44	-35.4
1	A	31	PHE	CZ	74.45	137.04 – 121.44	-35.1
1	A	8	LYS	CE	70.47	46.00 – 37.80	34.8
1	A	22	VAL	CG2	76.26	29.20 – 13.40	34.8
1	A	85	LYS	CE	70.17	46.00 – 37.80	34.5
1	A	6	LYS	CE	70.16	46.00 – 37.80	34.5
1	A	54	PHE	CZ	75.56	137.04 – 121.44	-34.4
1	A	71	VAL	CG2	75.66	29.20 – 13.40	34.4
1	A	25	LYS	CE	70.11	46.00 – 37.80	34.4
1	A	68	LYS	CE	70.08	46.00 – 37.80	34.4
1	A	9	LYS	CE	70.07	46.00 – 37.80	34.3
1	A	57	LYS	CE	70.06	46.00 – 37.80	34.3
1	A	4	HIS	CE1	54.22	149.70 – 125.30	-34.1
1	A	43	ILE	CD1	70.99	21.91 – 5.01	34.0
1	A	75	HIS	CE1	54.81	149.70 – 125.30	-33.9
1	A	37	ILE	CD1	70.72	21.91 – 5.01	33.9
1	A	12	ILE	CD1	70.50	21.91 – 5.01	33.8
1	A	50	ILE	CD1	70.09	21.91 – 5.01	33.5
1	A	81	ILE	CD1	70.02	21.91 – 5.01	33.5
1	A	79	ILE	CD1	69.95	21.91 – 5.01	33.4
1	A	83	ILE	CD1	69.86	21.91 – 5.01	33.4
1	A	10	ILE	CD1	69.75	21.91 – 5.01	33.3
1	A	18	ARG	CD	72.01	47.57 – 38.77	32.8
1	A	78	ARG	CD	71.74	47.57 – 38.77	32.5
1	A	11	ARG	CD	71.60	47.57 – 38.77	32.3
1	A	51	ARG	CD	71.53	47.57 – 38.77	32.2
1	A	39	ARG	CD	71.40	47.57 – 38.77	32.1
1	A	38	ALA	CB	74.48	28.03 – 9.93	30.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	64	ALA	CB	73.96	28.03 – 9.93	30.4
1	A	60	MET	CE	73.32	26.97 – 7.37	28.6
1	A	66	MET	CE	73.04	26.97 – 7.37	28.5
1	A	21	MET	CE	72.48	26.97 – 7.37	28.2
1	A	70	PRO	CG	56.00	32.66 – 21.76	26.4
1	A	62	PRO	CG	55.90	32.66 – 21.76	26.3
1	A	45	PRO	CG	55.84	32.66 – 21.76	26.3
1	A	56	PRO	CG	55.71	32.66 – 21.76	26.1
1	A	44	PRO	CG	55.59	32.66 – 21.76	26.0
1	A	61	PRO	CG	55.39	32.66 – 21.76	25.9
1	A	34	GLN	CG	62.73	39.38 – 28.18	25.8
1	A	72	PRO	CG	55.20	32.66 – 21.76	25.7
1	A	29	THR	CG2	50.28	27.15 – 15.95	25.6
1	A	23	THR	CG2	50.16	27.15 – 15.95	25.5
1	A	28	THR	CG2	50.15	27.15 – 15.95	25.5
1	A	14	THR	CG2	49.77	27.15 – 15.95	25.2
1	A	63	GLN	CG	61.99	39.38 – 28.18	25.2
1	A	13	THR	CG2	49.54	27.15 – 15.95	25.0
1	A	74	GLN	CG	61.59	39.38 – 28.18	24.8
1	A	73	LEU	CG	55.31	32.55 – 21.05	24.8
1	A	80	THR	CG2	49.29	27.15 – 15.95	24.8
1	A	8	LYS	CD	58.10	34.86 – 23.06	24.7
1	A	19	GLN	CG	61.41	39.38 – 28.18	24.7
1	A	51	ARG	CG	56.80	33.23 – 21.23	24.6
1	A	68	LYS	CG	53.22	30.67 – 19.17	24.6
1	A	48	GLN	CG	61.33	39.38 – 28.18	24.6
1	A	59	LEU	CG	55.01	32.55 – 21.05	24.5
1	A	25	LYS	CG	53.11	30.67 – 19.17	24.5
1	A	33	LEU	CG	54.88	32.55 – 21.05	24.4
1	A	9	LYS	CG	52.89	30.67 – 19.17	24.3
1	A	6	LYS	CG	52.88	30.67 – 19.17	24.3
1	A	84	LEU	CG	54.75	32.55 – 21.05	24.3
1	A	85	LYS	CG	52.70	30.67 – 19.17	24.2
1	A	8	LYS	CG	52.65	30.67 – 19.17	24.1
1	A	55	PRO	CG	53.48	32.66 – 21.76	24.1
1	A	32	GLU	CG	65.60	42.24 – 29.94	24.0
1	A	24	LEU	CG	54.38	32.55 – 21.05	24.0
1	A	55	PRO	CB	60.38	37.79 – 25.89	24.0
1	A	25	LYS	CD	57.21	34.86 – 23.06	23.9
1	A	57	LYS	CD	57.10	34.86 – 23.06	23.9
1	A	45	PRO	CB	60.21	37.79 – 25.89	23.8
1	A	9	LYS	CD	57.07	34.86 – 23.06	23.8

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	62	PRO	CB	60.19	37.79 – 25.89	23.8
1	A	56	PRO	CB	60.18	37.79 – 25.89	23.8
1	A	68	LYS	CD	57.06	34.86 – 23.06	23.8
1	A	6	LYS	CD	57.00	34.86 – 23.06	23.8
1	A	70	PRO	CB	60.03	37.79 – 25.89	23.7
1	A	39	ARG	CG	55.59	33.23 – 21.23	23.6
1	A	85	LYS	CD	56.83	34.86 – 23.06	23.6
1	A	47	LEU	CG	53.92	32.55 – 21.05	23.6
1	A	18	ARG	NE	122.10	92.63 – 76.73	23.5
1	A	11	ARG	CG	55.44	33.23 – 21.23	23.5
1	A	78	ARG	CG	55.41	33.23 – 21.23	23.5
1	A	57	LYS	CG	51.86	30.67 – 19.17	23.4
1	A	58	GLU	CG	64.78	42.24 – 29.94	23.3
1	A	44	PRO	CB	59.58	37.79 – 25.89	23.3
1	A	67	GLU	CG	64.76	42.24 – 29.94	23.3
1	A	35	GLU	CG	64.54	42.24 – 29.94	23.1
1	A	18	ARG	CG	54.95	33.23 – 21.23	23.1
1	A	7	GLU	CG	64.45	42.24 – 29.94	23.1
1	A	39	ARG	NE	121.22	92.63 – 76.73	23.0
1	A	69	GLU	CG	64.01	42.24 – 29.94	22.7
1	A	66	MET	CG	60.53	38.33 – 25.73	22.6
1	A	82	GLU	CG	63.70	42.24 – 29.94	22.5
1	A	60	MET	CG	60.28	38.33 – 25.73	22.4
1	A	86	GLY	CA	74.18	51.81 – 38.91	22.3
1	A	61	PRO	CB	58.36	37.79 – 25.89	22.3
1	A	17	GLY	CA	73.92	51.81 – 38.91	22.1
1	A	65	GLY	CA	73.46	51.81 – 38.91	21.8
1	A	21	MET	CG	59.45	38.33 – 25.73	21.8
1	A	40	GLU	CG	62.75	42.24 – 29.94	21.7
1	A	76	GLY	CA	72.79	51.81 – 38.91	21.3
1	A	72	PRO	CB	56.95	37.79 – 25.89	21.1
1	A	53	GLY	CA	72.15	51.81 – 38.91	20.8
1	A	1	GLY	CA	71.84	51.81 – 38.91	20.5
1	A	71	VAL	CG1	49.66	28.40 – 14.60	20.4
1	A	22	VAL	CG1	49.23	28.40 – 14.60	20.1
1	A	33	LEU	CD1	55.31	32.77 – 16.57	18.9
1	A	73	LEU	CD1	54.85	32.77 – 16.57	18.6
1	A	59	LEU	CD1	54.61	32.77 – 16.57	18.5
1	A	77	ASP	CB	69.99	49.06 – 32.66	17.8
1	A	84	LEU	CD1	53.11	32.77 – 16.57	17.6
1	A	47	LEU	CD1	52.90	32.77 – 16.57	17.4
1	A	37	ILE	CG1	58.32	36.54 – 18.94	17.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	8	LYS	CB	63.56	41.68 – 23.88	17.3
1	A	19	GLN	CB	60.95	38.36 – 19.96	17.3
1	A	57	LYS	CB	63.50	41.68 – 23.88	17.3
1	A	7	GLU	CB	59.74	38.65 – 21.35	17.2
1	A	3	ASP	CB	68.94	49.06 – 32.66	17.1
1	A	51	ARG	CB	61.99	39.81 – 21.51	17.1
1	A	75	HIS	CD2	62.20	137.40 – 103.40	-17.1
1	A	82	GLU	CB	59.20	38.65 – 21.35	16.9
1	A	16	ASP	CB	68.44	49.06 – 32.66	16.8
1	A	22	VAL	CB	63.11	41.76 – 23.66	16.8
1	A	18	ARG	CB	61.28	39.81 – 21.51	16.7
1	A	4	HIS	CD2	64.11	137.40 – 103.40	-16.6
1	A	58	GLU	CB	58.63	38.65 – 21.35	16.5
1	A	74	GLN	CB	59.54	38.36 – 19.96	16.5
1	A	83	ILE	CG1	56.73	36.54 – 18.94	16.5
1	A	32	GLU	CB	58.48	38.65 – 21.35	16.5
1	A	25	LYS	CB	61.90	41.68 – 23.88	16.4
1	A	9	LYS	CB	61.90	41.68 – 23.88	16.4
1	A	24	LEU	CD1	50.94	32.77 – 16.57	16.2
1	A	11	ARG	CB	60.33	39.81 – 21.51	16.2
1	A	50	ILE	CG1	56.17	36.54 – 18.94	16.2
1	A	78	ARG	CB	60.21	39.81 – 21.51	16.1
1	A	40	GLU	CB	57.92	38.65 – 21.35	16.1
1	A	59	LEU	CD2	51.45	32.60 – 15.60	16.1
1	A	73	LEU	CB	72.50	51.69 – 32.89	16.1
1	A	81	ILE	CG1	55.84	36.54 – 18.94	16.0
1	A	85	LYS	CB	61.10	41.68 – 23.88	15.9
1	A	69	GLU	CB	57.46	38.65 – 21.35	15.9
1	A	35	GLU	CB	57.44	38.65 – 21.35	15.9
1	A	6	LYS	CB	60.97	41.68 – 23.88	15.8
1	A	73	LEU	CD2	50.99	32.60 – 15.60	15.8
1	A	15	ASN	CB	65.39	47.13 – 30.23	15.8
1	A	24	LEU	CD2	50.94	32.60 – 15.60	15.8
1	A	33	LEU	CD2	50.81	32.60 – 15.60	15.7
1	A	24	LEU	CB	71.80	51.69 – 32.89	15.7
1	A	48	GLN	CB	57.87	38.36 – 19.96	15.6
1	A	63	GLN	CB	57.87	38.36 – 19.96	15.6
1	A	84	LEU	CD2	50.42	32.60 – 15.60	15.5
1	A	79	ILE	CG1	54.98	36.54 – 18.94	15.5
1	A	34	GLN	CB	57.62	38.36 – 19.96	15.5
1	A	42	ASN	CB	64.81	47.13 – 30.23	15.5
1	A	10	ILE	CG1	54.93	36.54 – 18.94	15.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	67	GLU	CB	56.68	38.65 – 21.35	15.4
1	A	47	LEU	CD2	50.27	32.60 – 15.60	15.4
1	A	39	ARG	CB	58.36	39.81 – 21.51	15.1
1	A	12	ILE	CG1	54.33	36.54 – 18.94	15.1
1	A	71	VAL	CB	59.91	41.76 – 23.66	15.0
1	A	68	LYS	CB	59.52	41.68 – 23.88	15.0
1	A	43	ILE	CB	69.21	48.82 – 28.42	15.0
1	A	84	LEU	CB	70.35	51.69 – 32.89	14.9
1	A	43	ILE	CG1	53.81	36.54 – 18.94	14.8
1	A	79	ILE	CB	68.71	48.82 – 28.42	14.7
1	A	10	ILE	CB	68.56	48.82 – 28.42	14.7
1	A	59	LEU	CB	69.88	51.69 – 32.89	14.7
1	A	47	LEU	CB	69.74	51.69 – 32.89	14.6
1	A	52	TYR	CB	70.58	50.05 – 28.55	14.5
1	A	12	ILE	CB	68.11	48.82 – 28.42	14.5
1	A	54	PHE	CB	70.01	50.37 – 29.47	14.4
1	A	41	PHE	CB	69.76	50.37 – 29.47	14.3
1	A	50	ILE	CB	67.67	48.82 – 28.42	14.2
1	A	33	LEU	CB	69.05	51.69 – 32.89	14.2
1	A	75	HIS	CB	59.56	40.69 – 19.69	14.0
1	A	81	ILE	CB	66.89	48.82 – 28.42	13.9
1	A	37	ILE	CB	65.94	48.82 – 28.42	13.4
1	A	83	ILE	CB	65.93	48.82 – 28.42	13.4
1	A	4	HIS	CB	58.17	40.69 – 19.69	13.3
1	A	30	PHE	CB	67.56	50.37 – 29.47	13.2
1	A	31	PHE	CB	66.85	50.37 – 29.47	12.9
1	A	21	MET	CB	61.69	44.20 – 21.80	12.8
1	A	66	MET	CB	59.68	44.20 – 21.80	11.9
1	A	60	MET	CB	59.47	44.20 – 21.80	11.8
1	A	46	TYR	CB	64.34	50.05 – 28.55	11.6
1	A	63	GLN	NE2	125.14	120.91 – 102.81	7.3
1	A	74	GLN	NE2	124.93	120.91 – 102.81	7.2
1	A	34	GLN	NE2	124.72	120.91 – 102.81	7.1
1	A	19	GLN	NE2	123.81	120.91 – 102.81	6.6
1	A	15	ASN	ND2	125.31	124.24 – 101.34	5.5
1	A	61	PRO	HA	2.70	6.05 – 2.75	-5.2

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: