wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2K2D
BMRB ID	:	15701
Title	:	Solution NMR structure of C-terminal domain of human pirh2. Northeast Structural Genomics Consortium (NESG) target HT2C
Authors	:	Lemak, A.; Sheng, Y.; Karra, M.; Srisailam, S.; Laister, R.C.; Duan, S.; Arrowsmith, C.H.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-03-31

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
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:

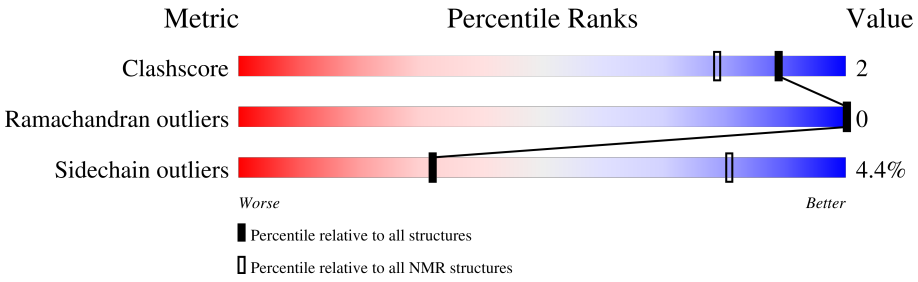
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 92%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	79	44% • 14% 41%

2 Ensemble composition and analysis

This entry contains 15 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:34-A:69 (36)	0.56	2

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 10, 12, 14, 15
2	5, 9, 11, 13

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 714 atoms, of which 352 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RING finger and CHY zinc finger domain-containing protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	47	713	216	352	68	71	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q96PM5
A	2	SER	-	expression tag	UNP Q96PM5
A	3	HIS	-	expression tag	UNP Q96PM5
A	4	MET	-	expression tag	UNP Q96PM5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

4 Residue-property plots (i)

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: RING finger and CHY zinc finger domain-containing protein 1

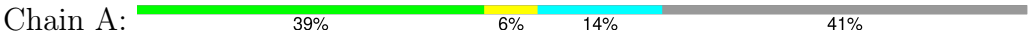
Chain A:

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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: RING finger and CHY zinc finger domain-containing protein 1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 15 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 solution	
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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	877
Number of shifts mapped to atoms	554
Number of unparsed shifts	0
Number of shifts with mapping errors	323
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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

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	274	267	266	1±1
All	All	4125	4005	3990	15

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

5 of 7 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:GLY:HA3	1:A:64:TYR:HB3	0.60	1.71	5	1
1:A:38:ILE:HD12	1:A:66:THR:HG21	0.51	1.83	9	6
1:A:38:ILE:O	1:A:46:ARG:HA	0.51	2.05	13	2
1:A:40:CYS:HA	1:A:66:THR:HG22	0.45	1.88	9	1
1:A:39:LEU:HG	1:A:46:ARG:HB3	0.43	1.91	4	3

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	36/79 (46%)	34±1 (94±4%)	2±1 (6±4%)	0±0 (0±0%)	100	100
All	All	540/1185 (46%)	507 (94%)	33 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	32/70 (46%)	31±1 (96±2%)	1±1 (4±3%)	32	81
All	All	480/1050 (46%)	459 (96%)	21 (4%)	32	81

5 of 9 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	CYS	5
1	A	40	CYS	5
1	A	39	LEU	3
1	A	42	ASP	2
1	A	50	GLN	2

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	877
Number of shifts mapped to atoms	554
Number of unparsed shifts	0
Number of shifts with mapping errors	323
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 323) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLY	HA2	4.44	0.0300	2
1	A	1	GLY	HA3	3.72	0.0300	2
1	A	1	GLY	CA	44.81	0.4000	1
1	A	2	SER	H	8.7	0.0300	1
1	A	2	SER	N	121.24	0.4000	1
1	A	4	MET	HA	4.3	0.0300	1
1	A	4	MET	HB2	2.11	0.0300	2
1	A	4	MET	HB3	1.94	0.0300	2
1	A	4	MET	HG2	2.3	0.0300	2
1	A	4	MET	HG3	2.3	0.0300	2
1	A	4	MET	C	172.22	0.4000	1
1	A	4	MET	CA	55.62	0.4000	1
1	A	4	MET	CB	29.6	0.4000	1
1	A	4	MET	CG	33.97	0.4000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	MET	H	7.98	0.0300	1
1	A	5	MET	HA	4.11	0.0300	1
1	A	5	MET	HB2	2.09	0.0300	2
1	A	5	MET	HB3	1.89	0.0300	2
1	A	5	MET	HG2	2.26	0.0300	2
1	A	5	MET	HG3	2.26	0.0300	2
1	A	5	MET	CA	57.64	0.4000	1
1	A	5	MET	CB	30.34	0.4000	1
1	A	5	MET	CG	34.52	0.4000	1
1	A	5	MET	N	126.78	0.4000	1
1	A	6	HIS	HA	4.57	0.0300	1
1	A	6	HIS	HB2	3.03	0.0300	2
1	A	6	HIS	HB3	3.03	0.0300	2
1	A	6	HIS	HD2	6.93	0.0300	1
1	A	6	HIS	HE1	7.5	0.0300	1
1	A	6	HIS	CA	56.65	0.4000	1
1	A	6	HIS	CB	31.07	0.4000	1
1	A	6	HIS	CD2	117.1	0.4000	1
1	A	6	HIS	CE1	134.9	0.4000	1
1	A	7	SER	HA	4.12	0.0300	1
1	A	7	SER	HB2	3.87	0.0300	2
1	A	7	SER	HB3	3.87	0.0300	2
1	A	7	SER	CA	60.9	0.4000	1
1	A	7	SER	CB	63.39	0.4000	1
1	A	8	ALA	HA	4.27	0.0300	1
1	A	8	ALA	HB1	1.36	0.0300	1
1	A	8	ALA	HB2	1.36	0.0300	1
1	A	8	ALA	HB3	1.36	0.0300	1
1	A	8	ALA	C	175.24	0.4000	1
1	A	8	ALA	CA	52.89	0.4000	1
1	A	8	ALA	CB	19.15	0.4000	1
1	A	9	LEU	H	8.03	0.0300	1
1	A	9	LEU	HA	4.21	0.0300	1
1	A	9	LEU	HB2	1.57	0.0300	2
1	A	9	LEU	HB3	1.57	0.0300	2
1	A	9	LEU	HD11	0.78	0.0300	2
1	A	9	LEU	HD12	0.78	0.0300	2
1	A	9	LEU	HD13	0.78	0.0300	2
1	A	9	LEU	HD21	0.84	0.0300	2
1	A	9	LEU	HD22	0.84	0.0300	2
1	A	9	LEU	HD23	0.84	0.0300	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	LEU	HG	1.47	0.0300	1
1	A	9	LEU	C	171.29	0.4000	1
1	A	9	LEU	CA	55.69	0.4000	1
1	A	9	LEU	CB	42.37	0.4000	1
1	A	9	LEU	CD1	24.92	0.4000	1
1	A	9	LEU	CD2	23.32	0.4000	1
1	A	9	LEU	CG	27.0	0.4000	1
1	A	9	LEU	N	120.26	0.4000	1
1	A	11	MET	H	8.07	0.0300	1
1	A	11	MET	HA	4.36	0.0300	1
1	A	11	MET	HB2	2.39	0.0300	2
1	A	11	MET	HB3	2.39	0.0300	2
1	A	11	MET	HG2	1.95	0.0300	2
1	A	11	MET	HG3	1.95	0.0300	2
1	A	11	MET	C	174.36	0.4000	1
1	A	11	MET	CA	56.0	0.4000	1
1	A	11	MET	CB	31.89	0.4000	1
1	A	11	MET	CG	32.6	0.4000	1
1	A	11	MET	N	120.32	0.4000	1
1	A	12	THR	H	8.12	0.0300	1
1	A	12	THR	HA	4.01	0.0300	1
1	A	12	THR	HB	4.17	0.0300	1
1	A	12	THR	HG21	1.21	0.0300	1
1	A	12	THR	HG22	1.21	0.0300	1
1	A	12	THR	HG23	1.21	0.0300	1
1	A	12	THR	C	173.19	0.4000	1
1	A	12	THR	CA	65.05	0.4000	1
1	A	12	THR	CB	69.04	0.4000	1
1	A	12	THR	CG2	21.6	0.4000	1
1	A	12	THR	N	113.77	0.4000	1
1	A	13	ARG	H	7.88	0.0300	1
1	A	13	ARG	HA	4.06	0.0300	1
1	A	13	ARG	HB2	1.68	0.0300	2
1	A	13	ARG	HB3	1.68	0.0300	2
1	A	13	ARG	HD2	3.08	0.0300	2
1	A	13	ARG	HD3	3.08	0.0300	2
1	A	13	ARG	HG2	1.47	0.0300	2
1	A	13	ARG	HG3	1.47	0.0300	2
1	A	13	ARG	C	174.72	0.4000	1
1	A	13	ARG	CA	57.9	0.4000	1
1	A	13	ARG	CB	30.11	0.4000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	ARG	CD	43.41	0.4000	1
1	A	13	ARG	CG	26.91	0.4000	1
1	A	13	ARG	N	120.97	0.4000	1
1	A	14	TYR	H	7.8	0.0300	1
1	A	14	TYR	HA	4.33	0.0300	1
1	A	14	TYR	HB2	2.84	0.0300	2
1	A	14	TYR	HB3	2.84	0.0300	2
1	A	14	TYR	HD1	6.82	0.0300	1
1	A	14	TYR	HD2	6.82	0.0300	1
1	A	14	TYR	HE1	6.64	0.0300	1
1	A	14	TYR	HE2	6.64	0.0300	1
1	A	14	TYR	C	174.09	0.4000	1
1	A	14	TYR	CA	59.72	0.4000	1
1	A	14	TYR	CB	38.21	0.4000	1
1	A	14	TYR	CD1	130.5	0.4000	1
1	A	14	TYR	CD2	130.5	0.4000	1
1	A	14	TYR	CE1	115.4	0.4000	1
1	A	14	TYR	CE2	115.4	0.4000	1
1	A	14	TYR	N	120.4	0.4000	1
1	A	15	TRP	H	8.12	0.0300	1
1	A	15	TRP	HA	4.61	0.0300	1
1	A	15	TRP	HB2	3.45	0.0300	2
1	A	15	TRP	HB3	3.35	0.0300	2
1	A	15	TRP	HD1	7.19	0.0300	1
1	A	15	TRP	HE1	10.33	0.0300	1
1	A	15	TRP	HE3	7.52	0.0300	1
1	A	15	TRP	HH2	7.09	0.0300	1
1	A	15	TRP	HZ2	7.5	0.0300	1
1	A	15	TRP	HZ3	7.2	0.0300	1
1	A	15	TRP	C	174.13	0.4000	1
1	A	15	TRP	CA	57.94	0.4000	1
1	A	15	TRP	CB	29.62	0.4000	1
1	A	15	TRP	CD1	124.3	0.4000	1
1	A	15	TRP	CE3	118.5	0.4000	1
1	A	15	TRP	CZ2	112.1	0.4000	1
1	A	15	TRP	CZ3	122.1	0.4000	1
1	A	15	TRP	N	120.37	0.4000	1
1	A	15	TRP	NE1	129.21	0.4000	1
1	A	16	ARG	H	7.86	0.0300	1
1	A	16	ARG	HA	4.19	0.0300	1
1	A	16	ARG	HB2	1.8	0.0300	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	ARG	HB3	1.8	0.0300	2
1	A	16	ARG	HD2	3.19	0.0300	2
1	A	16	ARG	HD3	3.19	0.0300	2
1	A	16	ARG	HG2	1.59	0.0300	2
1	A	16	ARG	HG3	1.59	0.0300	2
1	A	16	ARG	CA	57.59	0.4000	1
1	A	16	ARG	CB	30.64	0.4000	1
1	A	16	ARG	CD	43.38	0.4000	1
1	A	16	ARG	CG	27.02	0.4000	1
1	A	16	ARG	N	119.77	0.4000	1
1	A	17	GLN	HA	4.12	0.0300	1
1	A	17	GLN	HB2	2.05	0.0300	2
1	A	17	GLN	HB3	2.05	0.0300	2
1	A	17	GLN	HG2	2.35	0.0300	2
1	A	17	GLN	HG3	2.35	0.0300	2
1	A	17	GLN	C	174.83	0.4000	1
1	A	17	GLN	CA	57.41	0.4000	1
1	A	17	GLN	CB	28.56	0.4000	1
1	A	17	GLN	CG	33.96	0.4000	1
1	A	18	LEU	H	8.04	0.0300	1
1	A	18	LEU	HA	4.06	0.0300	1
1	A	18	LEU	HB2	1.3	0.0300	2
1	A	18	LEU	HB3	1.3	0.0300	2
1	A	18	LEU	HD11	0.64	0.0300	2
1	A	18	LEU	HD12	0.64	0.0300	2
1	A	18	LEU	HD13	0.64	0.0300	2
1	A	18	LEU	HD21	0.5	0.0300	2
1	A	18	LEU	HD22	0.5	0.0300	2
1	A	18	LEU	HD23	0.5	0.0300	2
1	A	18	LEU	HG	1.18	0.0300	1
1	A	18	LEU	C	174.38	0.4000	1
1	A	18	LEU	CA	56.65	0.4000	1
1	A	18	LEU	CB	41.63	0.4000	1
1	A	18	LEU	CD1	24.47	0.4000	1
1	A	18	LEU	CD2	23.98	0.4000	1
1	A	18	LEU	CG	26.77	0.4000	1
1	A	18	LEU	N	122.82	0.4000	1
1	A	19	ASP	H	8.24	0.0300	1
1	A	19	ASP	HA	4.44	0.0300	1
1	A	19	ASP	HB2	2.69	0.0300	2
1	A	19	ASP	HB3	2.63	0.0300	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	ASP	C	174.53	0.4000	1
1	A	19	ASP	CA	56.0	0.4000	1
1	A	19	ASP	CB	40.87	0.4000	1
1	A	19	ASP	N	119.1	0.4000	1
1	A	20	ASP	H	8.08	0.0300	1
1	A	20	ASP	HA	4.44	0.0300	1
1	A	20	ASP	HB2	2.69	0.0300	2
1	A	20	ASP	HB3	2.63	0.0300	2
1	A	20	ASP	CA	56.0	0.4000	1
1	A	20	ASP	CB	40.87	0.4000	1
1	A	20	ASP	N	121.04	0.4000	1
1	A	21	GLU	HA	4.21	0.0300	1
1	A	21	GLU	HB2	2.03	0.0300	2
1	A	21	GLU	HB3	1.95	0.0300	2
1	A	21	GLU	HG2	2.26	0.0300	2
1	A	21	GLU	HG3	2.18	0.0300	2
1	A	21	GLU	C	174.11	0.4000	1
1	A	21	GLU	CA	57.07	0.4000	1
1	A	21	GLU	CB	30.19	0.4000	1
1	A	21	GLU	CG	36.45	0.4000	1
1	A	22	VAL	H	7.99	0.0300	1
1	A	22	VAL	HA	4.02	0.0300	1
1	A	22	VAL	HB	2.05	0.0300	1
1	A	22	VAL	HG11	0.89	0.0300	2
1	A	22	VAL	HG12	0.89	0.0300	2
1	A	22	VAL	HG13	0.89	0.0300	2
1	A	22	VAL	C	173.34	0.4000	1
1	A	22	VAL	CA	62.47	0.4000	1
1	A	22	VAL	CB	32.52	0.4000	1
1	A	22	VAL	CG1	21.05	0.4000	1
1	A	22	VAL	N	120.03	0.4000	1
1	A	23	ALA	H	8.21	0.0300	1
1	A	23	ALA	HA	4.26	0.0300	1
1	A	23	ALA	HB1	1.36	0.0300	1
1	A	23	ALA	HB2	1.36	0.0300	1
1	A	23	ALA	HB3	1.36	0.0300	1
1	A	23	ALA	C	174.93	0.4000	1
1	A	23	ALA	CA	52.66	0.4000	1
1	A	23	ALA	CB	19.11	0.4000	1
1	A	23	ALA	N	126.48	0.4000	1
1	A	24	GLN	H	8.24	0.0300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	GLN	HA	4.34	0.0300	1
1	A	24	GLN	HB2	2.18	0.0300	2
1	A	24	GLN	HB3	1.97	0.0300	2
1	A	24	GLN	HE21	6.85	0.0300	2
1	A	24	GLN	HE22	7.46	0.0300	2
1	A	24	GLN	HG2	2.39	0.0300	2
1	A	24	GLN	HG3	2.39	0.0300	2
1	A	24	GLN	C	173.0	0.4000	1
1	A	24	GLN	CA	55.65	0.4000	1
1	A	24	GLN	CB	29.65	0.4000	1
1	A	24	GLN	CG	33.85	0.4000	1
1	A	24	GLN	N	118.91	0.4000	1
1	A	24	GLN	NE2	111.77	0.4000	1
1	A	25	THR	H	7.83	0.0300	1
1	A	25	THR	HA	4.62	0.0300	1
1	A	25	THR	HB	4.15	0.0300	1
1	A	25	THR	HG21	1.23	0.0300	1
1	A	25	THR	HG22	1.23	0.0300	1
1	A	25	THR	HG23	1.23	0.0300	1
1	A	25	THR	CA	59.88	0.4000	1
1	A	25	THR	CB	69.79	0.4000	1
1	A	25	THR	CG2	21.14	0.4000	1
1	A	25	THR	N	117.99	0.4000	1
1	A	26	PRO	HA	4.5	0.0300	1
1	A	26	PRO	HB2	2.25	0.0300	2
1	A	26	PRO	HB3	1.83	0.0300	2
1	A	26	PRO	HD2	3.76	0.0300	2
1	A	26	PRO	HD3	3.72	0.0300	2
1	A	26	PRO	HG2	1.97	0.0300	2
1	A	26	PRO	HG3	1.97	0.0300	2
1	A	26	PRO	C	174.21	0.4000	1
1	A	26	PRO	CA	62.76	0.4000	1
1	A	26	PRO	CB	32.04	0.4000	1
1	A	26	PRO	CD	50.94	0.4000	1
1	A	26	PRO	CG	27.35	0.4000	1
1	A	27	MET	H	8.58	0.0300	1
1	A	27	MET	HA	4.71	0.0300	1
1	A	27	MET	HB2	1.93	0.0300	2
1	A	27	MET	HB3	1.93	0.0300	2
1	A	27	MET	HE1	1.86	0.0300	1
1	A	27	MET	HE2	1.86	0.0300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	MET	HE3	1.86	0.0300	1
1	A	27	MET	HG2	2.36	0.0300	2
1	A	27	MET	HG3	2.61	0.0300	2
1	A	27	MET	CA	52.82	0.4000	1
1	A	27	MET	CB	32.71	0.4000	1
1	A	27	MET	CE	17.17	0.4000	1
1	A	27	MET	CG	32.71	0.4000	1
1	A	27	MET	N	120.94	0.4000	1
1	A	28	PRO	HA	4.44	0.0300	1
1	A	28	PRO	HB2	2.41	0.0300	2
1	A	28	PRO	HB3	1.92	0.0300	2
1	A	28	PRO	HD2	3.88	0.0300	2
1	A	28	PRO	HD3	3.55	0.0300	2
1	A	28	PRO	HG2	2.03	0.0300	2
1	A	28	PRO	HG3	2.03	0.0300	2
1	A	28	PRO	C	174.69	0.4000	1
1	A	28	PRO	CA	63.11	0.4000	1
1	A	28	PRO	CB	32.3	0.4000	1
1	A	28	PRO	CD	50.68	0.4000	1
1	A	28	PRO	CG	27.95	0.4000	1
1	A	29	SER	H	8.6	0.0300	1
1	A	29	SER	HA	4.12	0.0300	1
1	A	29	SER	HB2	3.87	0.0300	2
1	A	29	SER	HB3	3.87	0.0300	2
1	A	29	SER	CA	60.9	0.4000	1
1	A	29	SER	CB	63.39	0.4000	1
1	A	29	SER	N	117.27	0.4000	1
1	A	30	GLU	HA	4.11	0.0300	1
1	A	30	GLU	HB2	1.78	0.0300	2
1	A	30	GLU	HB3	1.78	0.0300	2
1	A	30	GLU	HG2	1.96	0.0300	2
1	A	30	GLU	HG3	1.89	0.0300	2
1	A	30	GLU	C	173.93	0.4000	1
1	A	30	GLU	CA	58.0	0.4000	1
1	A	30	GLU	CB	28.99	0.4000	1
1	A	30	GLU	CG	35.97	0.4000	1
1	A	31	TYR	H	7.9	0.0300	1
1	A	31	TYR	HA	4.64	0.0300	1
1	A	31	TYR	HB2	3.29	0.0300	2
1	A	31	TYR	HB3	2.74	0.0300	2
1	A	31	TYR	HD1	7.0	0.0300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	TYR	HD2	7.0	0.0300	1
1	A	31	TYR	HE1	6.73	0.0300	1
1	A	31	TYR	HE2	6.73	0.0300	1
1	A	31	TYR	C	173.37	0.4000	1
1	A	31	TYR	CA	57.61	0.4000	1
1	A	31	TYR	CB	39.0	0.4000	1
1	A	31	TYR	CD1	130.3	0.4000	1
1	A	31	TYR	CD2	130.3	0.4000	1
1	A	31	TYR	CE1	115.5	0.4000	1
1	A	31	TYR	CE2	115.5	0.4000	1
1	A	31	TYR	N	117.75	0.4000	1
1	A	32	GLN	H	7.75	0.0300	1
1	A	32	GLN	HA	4.15	0.0300	1
1	A	32	GLN	HB2	2.04	0.0300	2
1	A	32	GLN	HB3	2.04	0.0300	2
1	A	32	GLN	HG2	2.35	0.0300	2
1	A	32	GLN	HG3	2.35	0.0300	2
1	A	32	GLN	C	173.1	0.4000	1
1	A	32	GLN	CA	57.22	0.4000	1
1	A	32	GLN	CB	29.19	0.4000	1
1	A	32	GLN	CG	33.67	0.4000	1
1	A	32	GLN	N	119.88	0.4000	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	76	-0.24 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	71	-0.31 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	62	2.77 ± 0.22	Should be applied
^{15}N	63	-0.91 ± 0.42	Should be applied

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 92%, i.e. 430 atoms were assigned a chemical shift out of a possible 467. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	171/182 (94%)	70/74 (95%)	69/72 (96%)	32/36 (89%)
Sidechain	239/258 (93%)	163/168 (97%)	71/80 (89%)	5/10 (50%)
Aromatic	20/27 (74%)	10/13 (77%)	10/12 (83%)	0/2 (0%)
Overall	430/467 (92%)	243/255 (95%)	150/164 (91%)	37/48 (77%)

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: