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## Pulse_program	dim	spec_type	Sync	Spec_name	Label	Proc	Ext	Cmp	Y-axis_P0_P1	Z-axis_P0_P1
HSQC	2D	hsqc	N	"15N-HSQC"	HN N X	1 2 3	EXX	DRX	-90.0 180.0	- -
CHSQC	2D	chsqc	AW	"13C-HSQC aliph"	HC C X	1 2 3	EXX	DRX	-90.0 180.0	- -
CHSQC_ARO	2D	chsqcar	AR	"13C-HSQC arom"	HC C X	1 2 3	EXX	DRX	-90.0 180.0	- -
CBCACONH	3D	cbcaconh	N	"CBCA(CO)NH"	HN N C	1 3 2	EXX	DCC	22.0 -29.0	0.0 0.0
CCCONNH	3D	ccconnh	N	"CC(CO)NH"	HN N C	1 3 2	EXX	DCC	6.0 -20.0	0.0 0.0
HBHACONH	3D	hbhaconh	N	"HBHA(CO)NH"	HN N H	1 3 2	EEX	DCC	0.0 0.0	0.0 0.0
HCCCONNH	3D	hccconnh	N	"H(CC)(CO)NH"	HN N H	1 3 2	EEX	DCC	0.0 0.0	0.0 0.0
HNCA	3D	hnca	N	"HNCA"	HN N C	1 3 2	EXX	DCC	0.0 0.0	0.0 0.0

Fig. S1. Example of PP_list.txt file for make_macro. This file lists the spectrum type of the pulse programs that have been used for multi-dimensional NMR experiments. The name of the pulse program should match with the experiment name described in the header of the pulse program file in the standard Bruker format. The file name of the template NMRPipe macro file should include the name. For example, "CBCACONH" macro file name should be CBCACONH.conv for FID conversion, xy_CBCACONH.com for xy-dimension Fourier transformation and z_CBCACONH.com for z-dimension Fourier transformation and conversion to NMRView format. Each spectrum type should have a unique name as specified in the third column in the list. Other columns, dim: dimension of the spectrum, Sync: sync-jump type in KUJIRA setting, Label: labels for all axis, Proc: processed axis order, Ext: extraction applied (E) or not (X), Y-axis_, Z-axis_P0_P1 phase correction for y- and z-dimension, respectively.

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```
name targ   C13_15N_Ubiquitin
name work   current
name macro  macros
name templ  template
name fid    fid
name ft     ft
name nv     nv
name plist  bruker_PP.list

proc vender Bruker
proc group  KUJG
proc carib  auto
proc pdata  "2 1"

ft   swap  -noswap
exx1 N      5.5
exx2 N     11.0
exx1 AW    -2.0
exx2 AW     9.0
exx1 AL    -2.0
exx2 AL     6.0
exx1 AR     5.0
exx2 AR     9.0
```

Fig. S2 Example of a pref.txt file for make_macro. This file specifies the name of the target sample (targ), the name of the pulse program list (plist). The parameters, "exx1" and "exx2" indicate extraction points (ppm) for the first and second dimensions of corresponding spectrum types with sync-jump type N (^{1}H-^{15}N), AW (^{1}H-^{13}C of aliphatic and aromatic groups), AL (^{1}H-^{13}C of aliphatic groups) or AR (^{1}H-^{13}C of aromatic groups).

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```
Entry          RIKEN_entry_ID           1 "BMRB_demo"
Entry          molecular_system         1 "Single polypeptide"
Entry          non_standard_residue     1 "no"
Entry          metal_ligand             1 "no"
Entry          structural_genomics      1 "yes"
Entry          shift_file               1 "demo.str"
Entry          title                    1 "Solution structure of 13C/15N labeled protein"
Entry          Release                  1 "Hold for publication"
Entry          entry_author             1 "Kobayashi, N."
Entry          entry_author             2 "Harano, Y."
Entry          entry_author             3 "Nakatani, E."
Entry          entry_author             4 "Fujiwara, T."
Entry          entry_author             5 "Akutsu, H."
Contact        contact_author           1 "Naohiro Kobayashi"
Contact        contact_Department       1 "Institute for Protein Research, Osaka University"
Contact        contact_address          1 "2-3, Yamadaoka, Suita, Osaka 230-0045, Japan"
Contact        contact_email            1 "xxxxx@protein.osaka-u.ac.jp"
Contact        contact_phone            1 "+81-99-999-9999"
Contact        contact_fax              1 "+81-99-999-9999"
Citations      PubMedId                 1 "."
Citations      title                    1 "Solution structure of 13C/15N labeled protein"
Citations      status                   1 "in preparation"
Citations      type                     1 "journal"
Citations      Journal_name             1 "To be Published"
Citations      citation_author          1 "Kobayashi, N."
Citations      citation_author          2 "Harano, Y."
Citations      citation_author          3 "Nakatani, E."
Citations      citation_author          4 "Fujiwara, T."
Citations      citation_author          5 "Akutsu, H."
Entity         name                     1 "domain_1"
Entity         type                     1 "polymer"
Entity         polymer                  1 "polypeptide(L)"
Entity         sequence                 1 "FSDLKFDHIASLGSVVSIAHSLIVAHSLLINWLIRSSPSYLIGAHSLIVAHSLMILWLHSL"
Entity         length                   1 "93"
Entity         ambiguous_conformer      1 "no"
Entity         ambiguous_chem_site      1 "no"
Entity         non_standard_monomer     1 "no"
Entity         non_standard_chiral      1 "no"
Entity         non_standard_linker      1 "no"
Entity         paramagnetic_metals      1 "no"
```

Fig. S3. Example of a BESS intermediate format (*.pre and *.fin) file. This file describes 22-25 mandatory items required for BMRB deposition of a single chain protein. The first and second columns construct a simple category tree and the third column indicates the item number. The final column describes the detail of each item.

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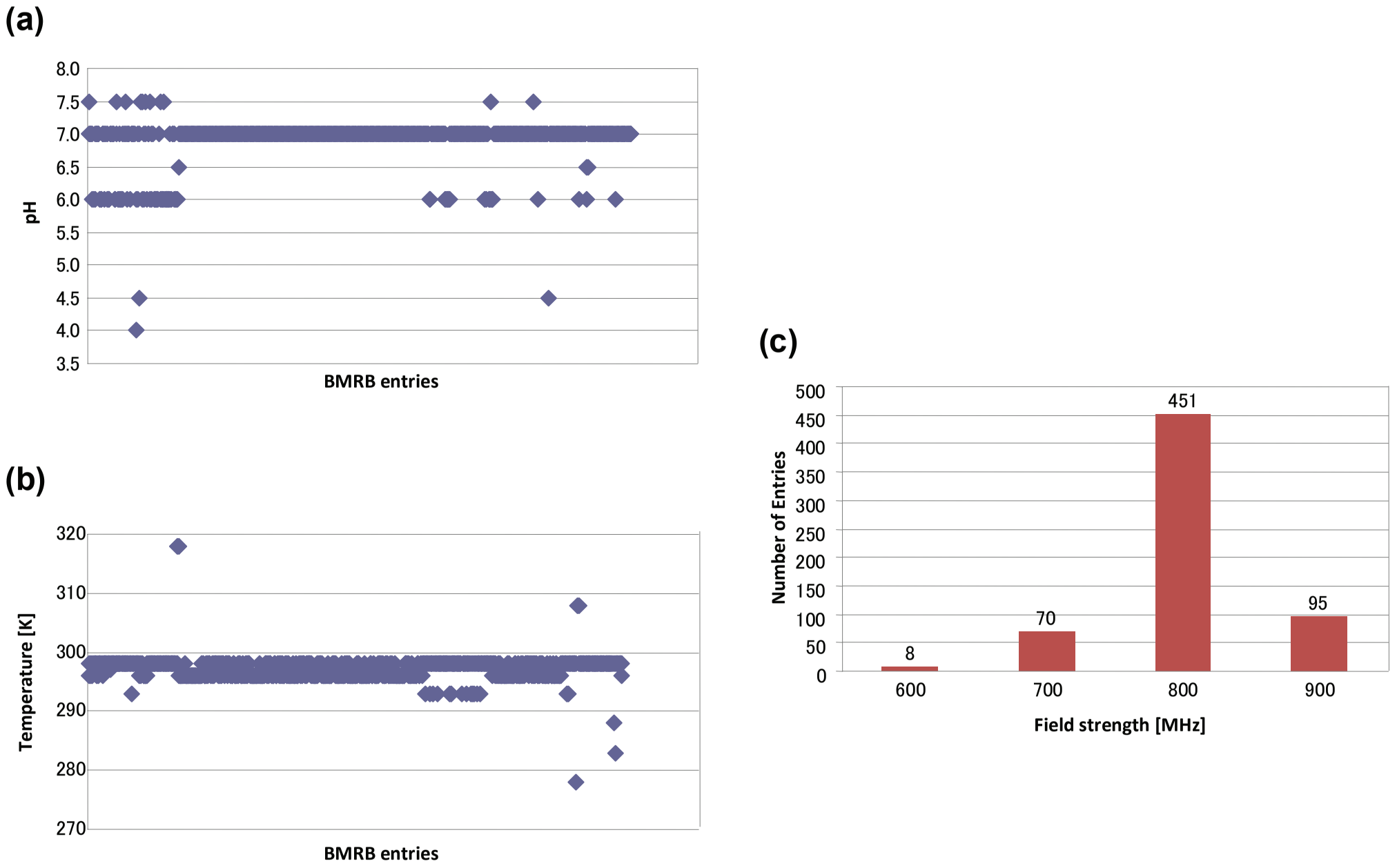

Fig. S4. Distributions of over 600 entries with respect to sample pH (a), temperature in K (b) and filed strength in MHz (c). The row axis in panels (a) and (b) correspond to each entry for the deposition.

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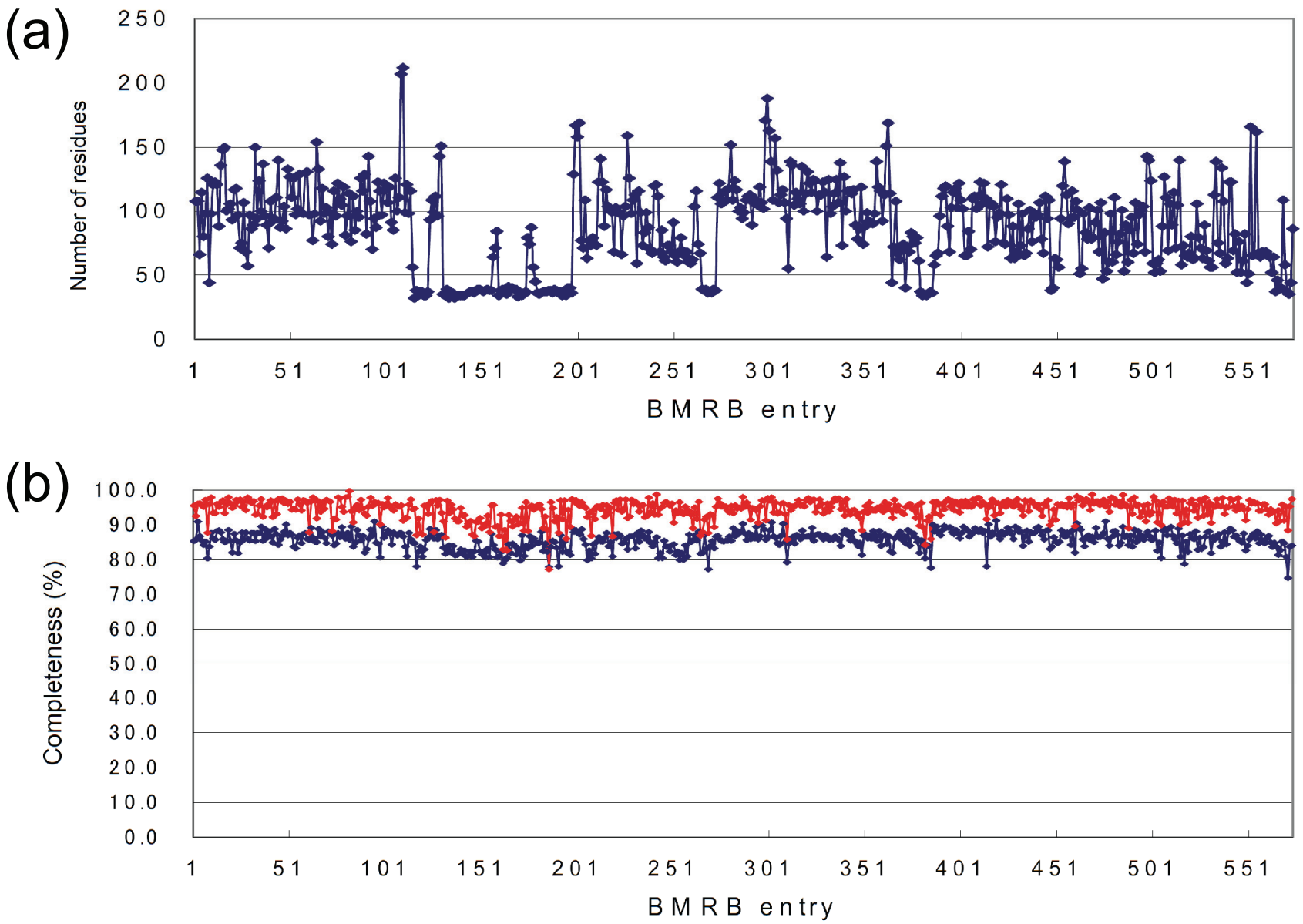

Fig. S5. (a) Chain length variation of the 553 RSGI entries. The entries not released at present are not shown. (b) The completeness of the signal assignments including ^{1}H, ^{15}N and ^{13}C atoms plotted for the 553 RSGI entries for backbone including HN, N, C', Cα and Hα atoms (red) and for all atoms (blue) observable in NMR structural studies.