Supplementary Information

Rapid protein assignments and structures from raw NMR spectra with the deep learning technique ARTINA

Piotr Klukowski[1]*, Roland Riek[1]*, Peter Güntert[1,2,3]*

[1] Laboratory of Physical Chemistry, ETH Zurich, Vladimir-Prelog-Weg 2, 8093 Zurich, Switzerland

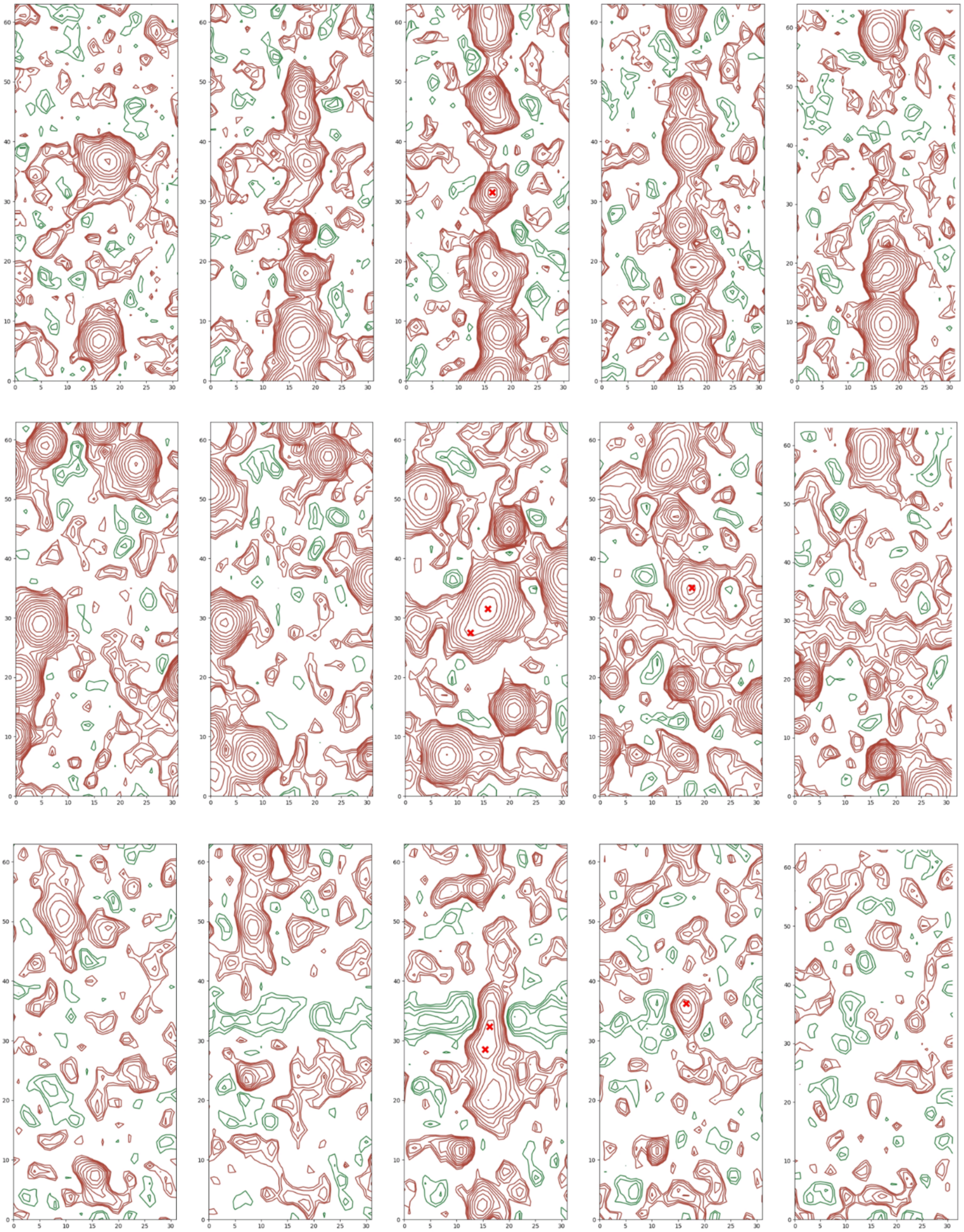
[2] Institute of Biophysical Chemistry, Goethe University Frankfurt, Max-von-Laue-Str. 9, 60438 Frankfurt am Main, Germany

[3] Department of Chemistry, Tokyo Metropolitan University, 1-1 Minami-Osawa, Hachioji, 192-0397 Tokyo, Japan

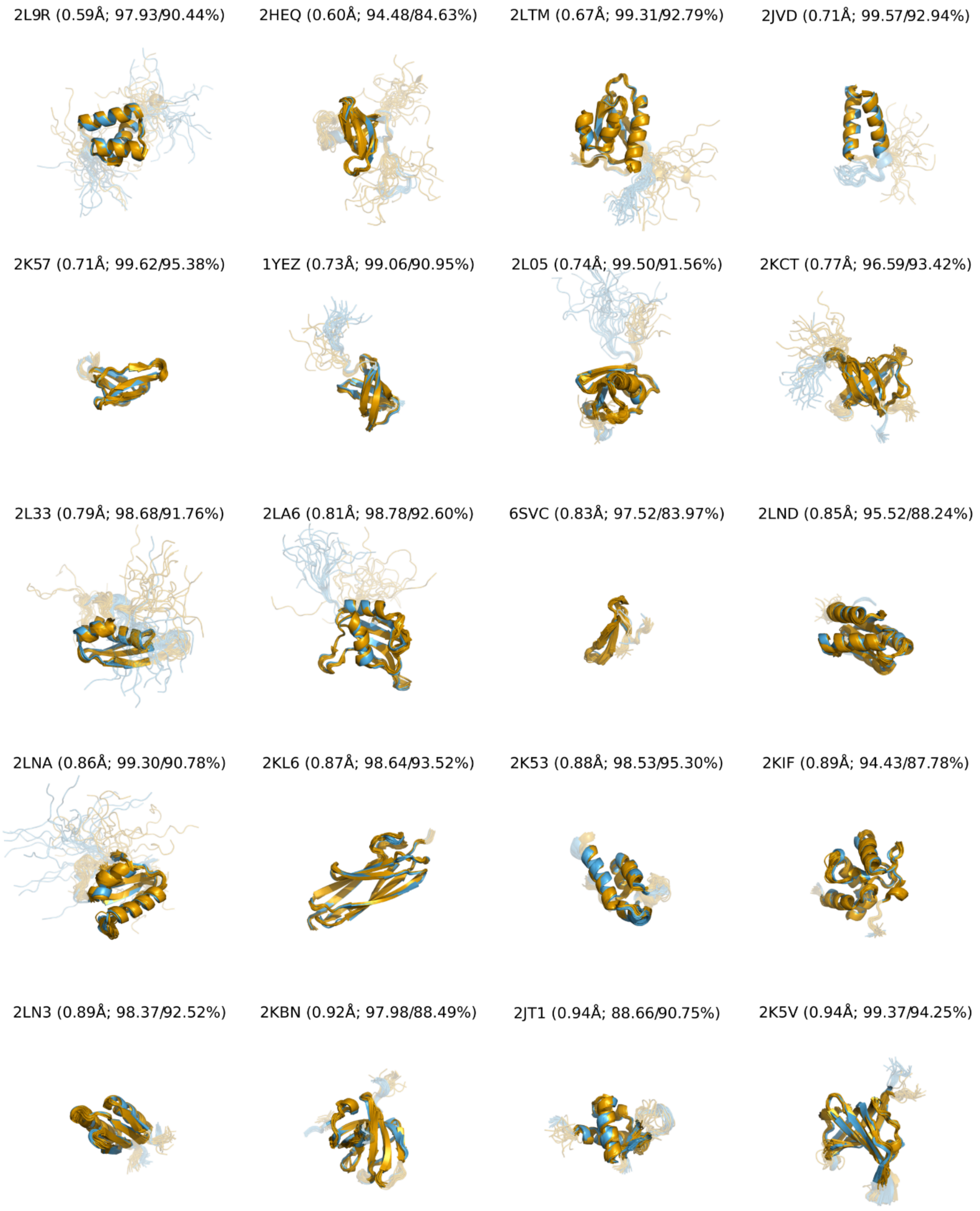
* e-mail: piotr.klukowski@phys.chem.ethz.ch; roland.riek@phys.chem.ethz.ch; peter.guentert@phys.chem.ethz.ch

Contents

Supplementary Figure 1 Examples of generated spectrum fragments for deconvolution model training. Each row presents one generated spectrum fragment of size 64 × 32 × 5 that was used for the deconvolution model training. Ground truth positions of signal components are marked by red crosses.



Supplementary Figure 2 Visualization of 100 protein structures determined with ARTINA (blue) overlaid with corresponding PDB depositions (orange). Each panel contains information about PDB code, RMSD between ARTINA structure and PDB deposition, and backbone/side-chain chemical shift assignment accuracy. Well-defined and disordered regions (Supplementary Table 4) are shown in and strong and light colors, respectively.



2L9R (0.59Å; 97.93/90.44%)

2HEQ (0.60Å; 94.48/84.63%)

2LTM (0.67Å; 99.31/92.79%)

2JVD (0.71Å; 99.57/92.94%)

2K57 (0.71Å; 99.62/95.38%)

1YEZ (0.73Å; 99.06/90.95%)

2L05 (0.74Å; 99.50/91.56%)

2KCT (0.77Å; 96.59/93.42%)

2L33 (0.79Å; 98.68/91.76%)

2LA6 (0.81Å; 98.78/92.60%)

6SVC (0.83Å; 97.52/83.97%)

2LND (0.85Å; 95.52/88.24%)

2LNA (0.86Å; 99.30/90.78%)

2KL6 (0.87Å; 98.64/93.52%)

2K53 (0.88Å; 98.53/95.30%)

2KIF (0.89Å; 94.43/87.78%)

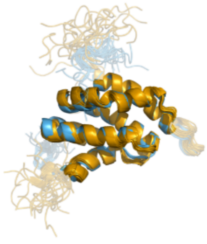
2LN3 (0.89Å; 98.37/92.52%)

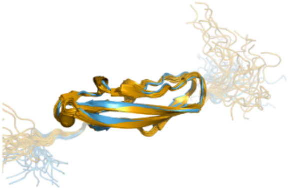
2KBN (0.92Å; 97.98/88.49%)

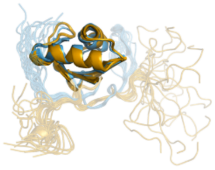
2JT1 (0.94Å; 88.66/90.75%)

2K5V (0.94Å; 99.37/94.25%)

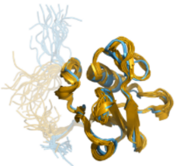
Supplementary Figure 2 (continued)

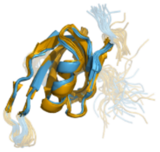

1VDY (0.95Å; 95.48/88.37%)

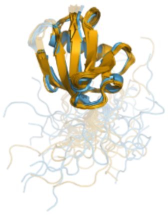

2KPN (0.97Å; 96.95/91.16%)

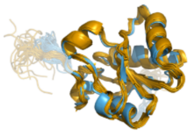

2MQL (0.98Å; 83.59/70.55%)

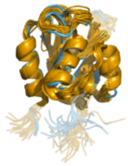

2K3A (0.99Å; 96.79/84.40%)

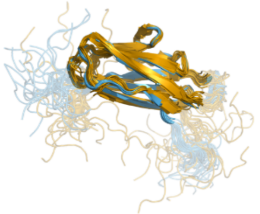

1WQU (0.99Å; 98.05/86.80%)

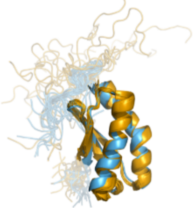

2K50 (1.00Å; 97.39/89.74%)


2KJR (1.02Å; 99.76/91.62%)

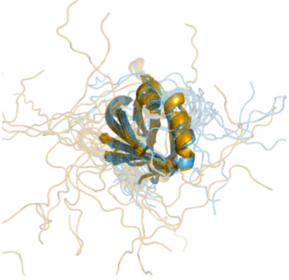

1VEE (1.03Å; 97.81/90.30%)

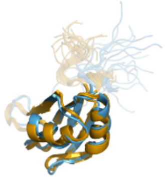

2K1G (1.05Å; 97.22/92.18%)

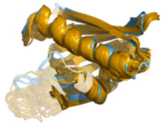

2L3B (1.05Å; 93.97/86.19%)


2M5O (1.08Å; 92.48/90.20%)

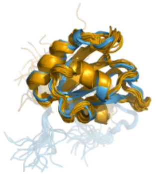

2K52 (1.10Å; 97.17/93.54%)

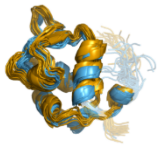

2M4F (1.11Å; 90.80/81.83%)

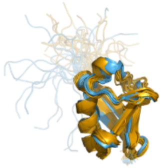

2MB0 (1.11Å; 97.69/88.46%)

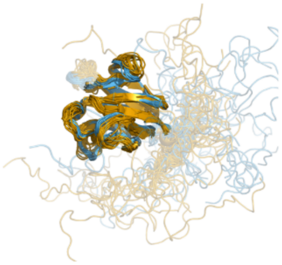

2N4B (1.14Å; 98.94/90.25%)


6SOW (1.16Å; 88.97/78.57%)


2LXU (1.19Å; 99.40/91.33%)

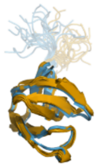

MDM2 (1.24Å; 98.08/84.88%)


2KK8 (1.25Å; 99.18/90.26%)

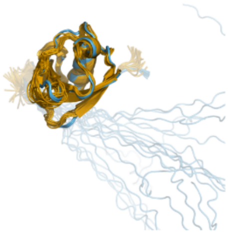

2KKL (1.26Å; 94.06/80.60%)

Supplementary Figure 2 (continued)

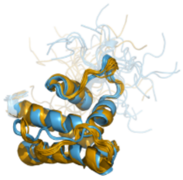
2KRS (1.26Å; 98.47/96.18%)



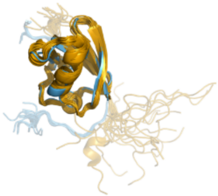
1T0Y (1.27Å; 97.27/85.04%)



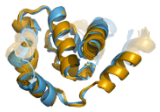
2L3G (1.28Å; 98.04/93.19%)



2KD0 (1.37Å; 97.24/91.96%)

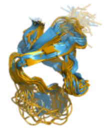


6GT7 (1.39Å; 96.93/79.31%)

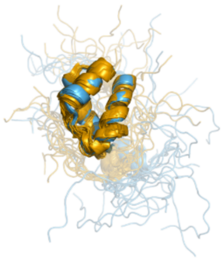


1PQX (1.40Å; 99.03/86.51%)

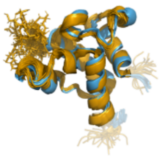
2LX7 (1.41Å; 98.54/87.84%)



2LK2 (1.42Å; 96.08/86.08%)



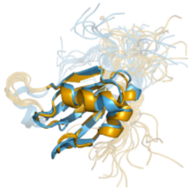
2LL8 (1.42Å; 98.04/91.42%)



2JRM (1.43Å; 97.21/92.14%)

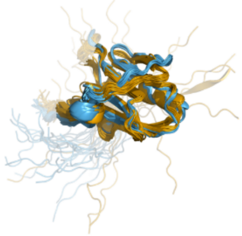
2K3D (1.44Å; 98.96/89.76%)

2LEA (1.45Å; 96.17/83.33%)

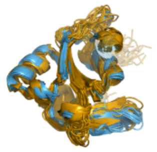


2K5D (1.47Å; 99.25/92.40%)

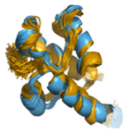
2KKZ (1.47Å; 96.50/87.83%)



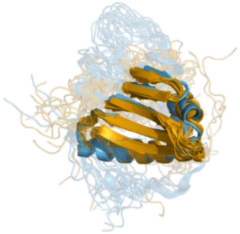
2JQN (1.52Å; 97.81/90.68%)



2LML (1.53Å; 97.44/91.71%)

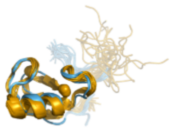


2LAK (1.54Å; 92.15/78.69%)

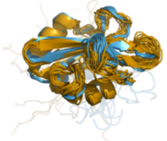


2LVB (1.56Å; 89.27/84.11%)

2MA6 (1.56Å; 98.94/89.36%)

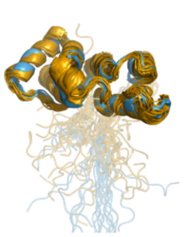


2MK2 (1.56Å; 99.58/91.97%)

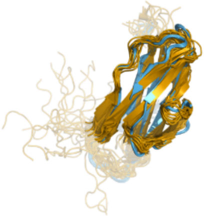


Supplementary Figure 2 (continued)

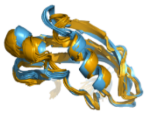
2L06 (1.57Å; 96.46/84.28%)



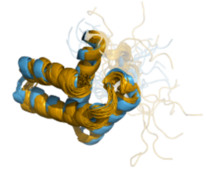
2L7Q (1.57Å; 96.11/82.62%)



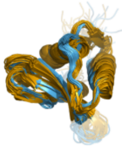
MH04 (1.57Å; 98.58/88.57%)



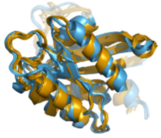
2KIW (1.59Å; 93.99/80.94%)



2K0M (1.60Å; 96.87/92.08%)

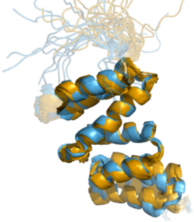


KRAS4B (1.60Å; 98.00/76.81%)

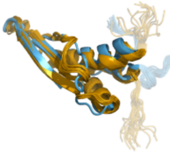


2K75 (1.65Å; 98.77/88.36%)

2LAH (1.71Å; 93.23/85.67%)

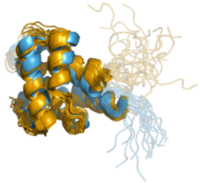


2MDR (1.72Å; 93.17/82.89%)



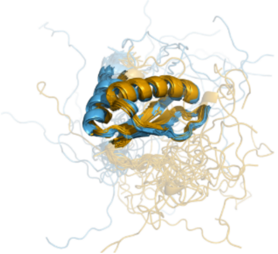
2JVO (1.77Å; 96.64/76.42%)

2JN8 (1.83Å; 95.45/89.68%)

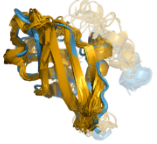


2K1S (1.83Å; 98.83/92.02%)

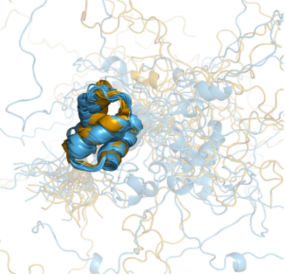
2KHD (1.87Å; 97.29/87.63%)



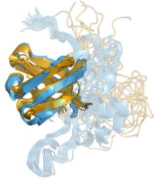
2KVO (1.87Å; 98.17/90.00%)



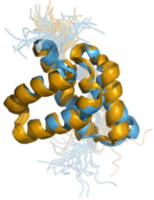
2RN7 (1.93Å; 94.35/81.02%)



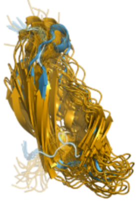
2FB7 (1.94Å; 95.95/81.18%)



2KD1 (1.99Å; 98.31/90.36%)

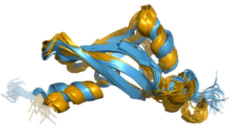


6FIP (2.05Å; 97.86/79.15%)



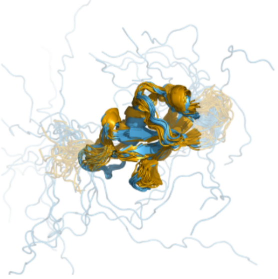
2ERR (2.09Å; 96.36/78.40%)

2KRT (2.09Å; 97.01/82.72%)

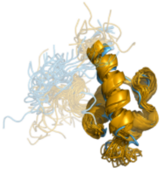


Supplementary Figure 2 (continued)

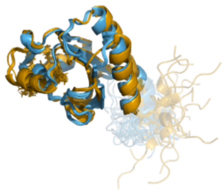
1SE9 (2.10Å; 88.55/82.13%)



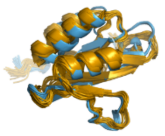
2L1P (2.13Å; 96.29/87.04%)



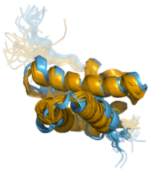
2M7U (2.14Å; 85.70/73.47%)



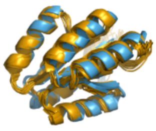
2KFP (2.23Å; 97.39/79.51%)



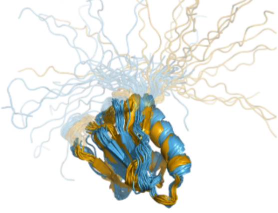
2KOB (2.24Å; 88.18/82.29%)



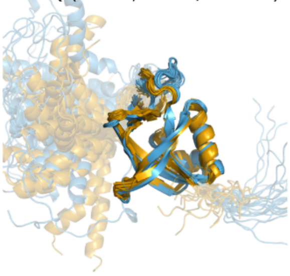
2LRH (2.30Å; 94.91/77.45%)



2LTL (2.37Å; 96.44/90.46%)

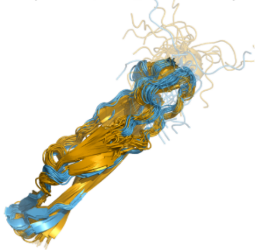


2G0Q (2.38Å; 93.99/84.33%)



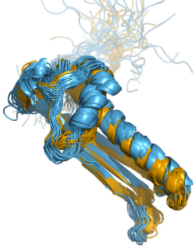
2LTA (2.39Å; 95.17/81.57%)

2LFI (2.42Å; 89.30/76.07%)

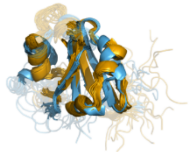


2LGH (2.43Å; 98.03/88.92%)

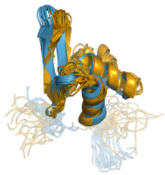
2JXP (2.58Å; 97.08/89.62%)



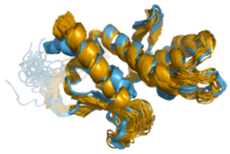
2KL5 (2.58Å; 79.41/68.59%)



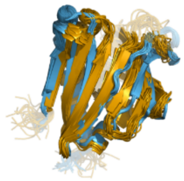
2KZV (2.62Å; 95.84/81.67%)



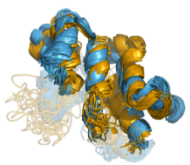
2B3W (2.67Å; 93.39/80.09%)



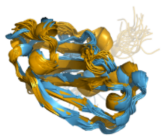
2LF2 (2.68Å; 97.56/85.86%)



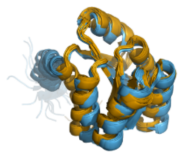
2L8V (2.79Å; 93.82/76.58%)



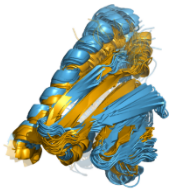
2KCD (3.13Å; 91.30/79.24%)



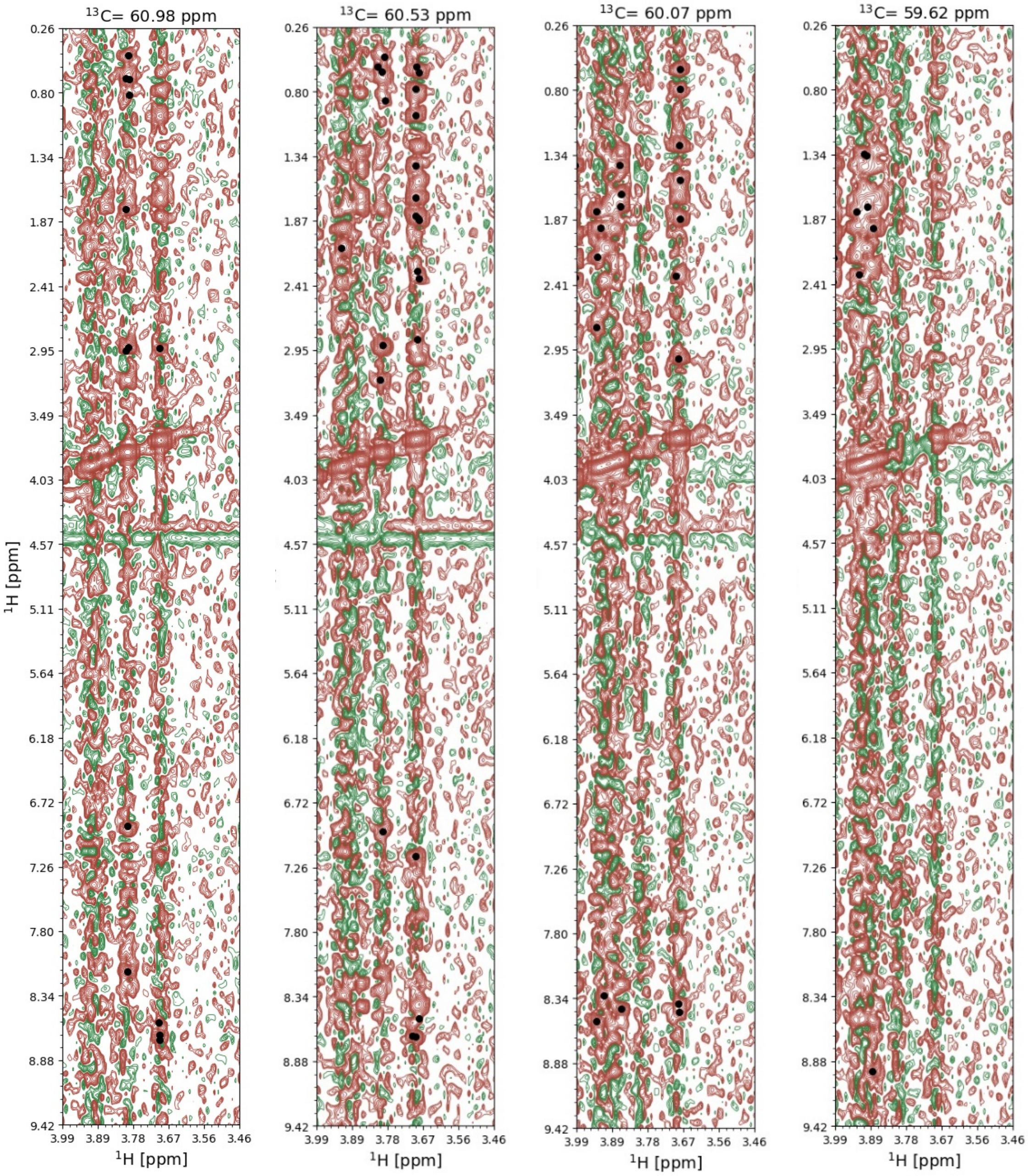
2L82 (3.55Å; 97.87/81.05%)



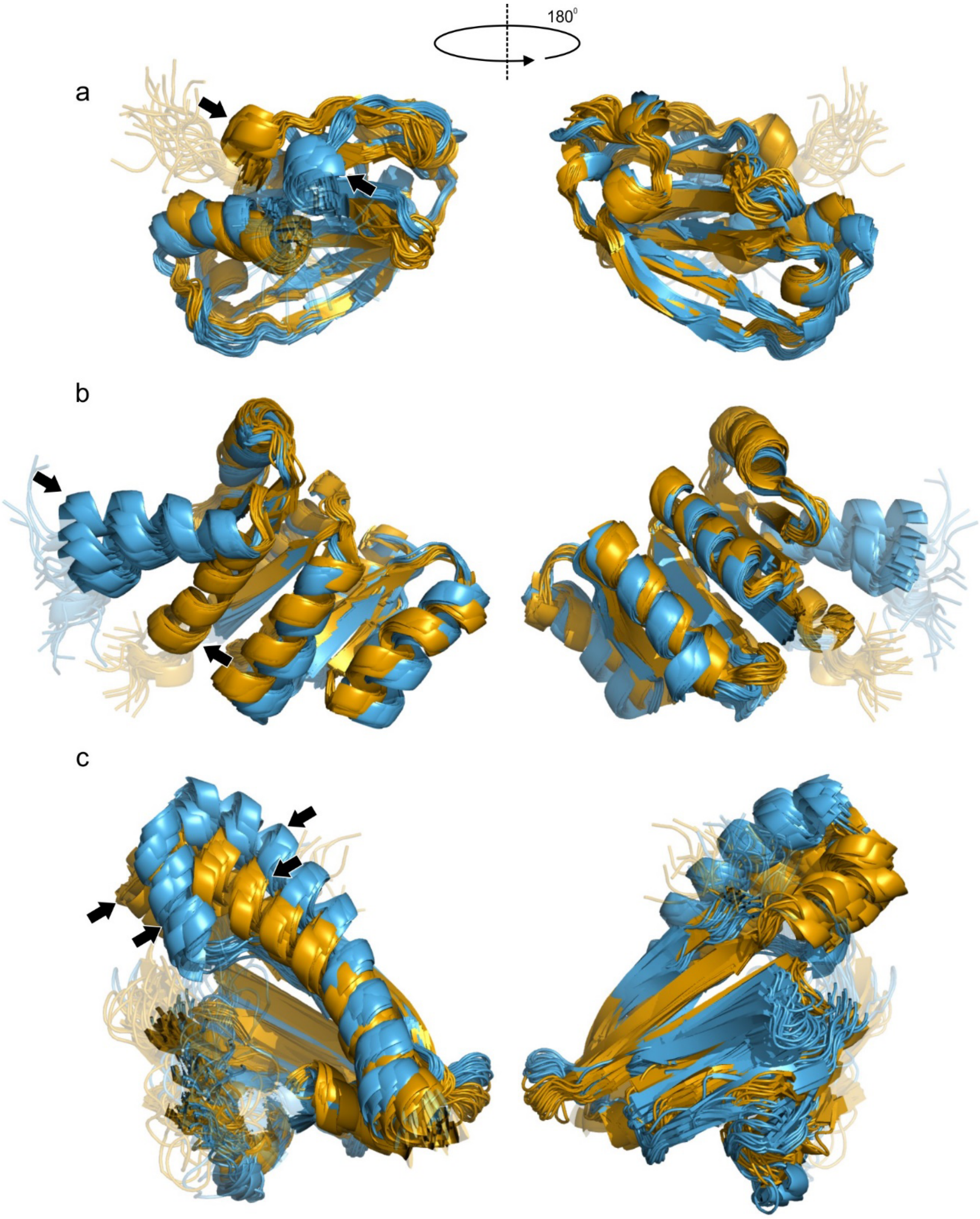
2M47 (4.72Å; 92.86/80.32%)



Supplementary Figure 3 Robustness of peak picking to background artefacts. A fragment of four consecutive layers of a ^{13}C-resolved [^{1}H, ^{1}H]-NOESY spectrum of a 20% ^{13}C-labelled protein of protein 6SOW[39] is shown. Final signal coordinates (after deconvolution) with classifier response > 0.5 are marked in black.



Supplementary Figure 4 The three proteins with backbone RMSD > 3 Å between the automatically determined structure (blue) and the PDB deposition (orange). a Protein 2KCD. The α-helix at residues 105–109 is displaced. **b** Protein 2L82. The α-helix at residues 138–153 is displaced. **c** Protein 2M47. The main reason for the high RMSD is a displacement of the last two α-helices at residues 111–157.



Supplementary Table 1 Supported NMR spectrum types.

Spectrum category	Supported spectrum types
2D	^{13}C-HSQC, ^{15}N-HSQC, NOESY (homonuclear), TOCSY (homonuclear), CACO, CBHEaro, CBHDaro
3D for backbone assignment	HNCA, HNHA, CBCANH, HNcoCA, HNCO, HNcaCO, CBCAcoNH, HBHAcoNH, CBCACOcaHA
3D for side-chain assignment	HCCH-TOCSY, ^{15}N-TOCSY, HCCH-COSY, CcoNH, HCcoNH, CCH-TOCSY
3D/4D NOESY	3D ^{13}C-resolved [^{1}H,^{1}H]-NOESY, 3D ^{15}N-resolved [^{1}H,^{1}H]-NOESY, 4D CC-NOESY

Further information about spectra can be provided to ARTINA by the use of tags. For instance, the ALI or ARO tags can be used to indicate that a ^{13}C-NOESY spectrum is expected to contain only aliphatic or aromatic signals. The tags POS and NEG can be used to restrict peak picking to positive and negative signals.

Supplementary Table 2 Proteins and spectra used for automated structure determination experiments.

ID	Protein	Residues	Number of spectra			
			Backbone	Side-chain	NOESY	Total
1	6SVC	35	2	1	3	6
2	2JVD	54	6	3	2	11
3	2K57	55	6	6	2	14
4	6SOW	58	5	2	3	10
5	2LX7	60	7	7	4	18
6	2MA6	61	5	7	4	16
7	2JRM	65	5	4	3	12
8	1YEZ	68	8	5	3	16
9	2L9R	69	5	1	3	9
10	2K52	74	7	4	3	14
11	2KRS	74	5	7	4	16
12	2K53	76	4	4	3	11
13	2JT1	77	6	1	3	10
14	2JVO	77	4	4	2	10
15	2ERR	81	3	2	2	7
16	2L1P	83	4	2	3	9
17	2LN3	83	5	3	3	11
18	2HEQ	84	6	3	4	13
19	2KK8	84	5	4	3	12
20	2KD0	85	6	4	3	13
21	2LML	86	6	5	4	15
22	2K3D	87	6	2	4	12
23	2LK2	89	7	6	4	17
24	MH04	90	7	3	2	12
25	1PQX	91	4	5	3	12
26	2L33	91	4	3	3	10
27	2KZV	92	7	6	4	17
28	2KCT	94	6	6	3	15
29	2MDR	94	4	3	3	10
30	2FB7	95	5	4	2	11
31	2MB0	95	2	3	3	8
32	2L05	95	6	4	3	13
33	2KJR	95	5	4	3	12
34	2M5O	97	5	1	3	9
35	MDM2	97	3	2	2	7
36	2LNA	99	6	7	4	17
37	2LA6	99	5	2	3	10
38	6FIP	99	6	5	2	13
39	2LEA	100	4	3	3	10
40	2LL8	101	6	6	3	15
41	2KPN	103	7	4	3	14
42	2K0M	104	7	4	3	14
43	2K5V	104	8	4	3	15
44	2MQL	105	2	4	3	9
45	2K75	106	6	6	3	15
46	2LTM	107	5	3	3	11
47	2KOB	108	7	5	4	16
48	2KHD	108	7	7	3	17
49	2RN7	108	5	4	3	12
50	2LXU	108	5	5	4	14
51	2KIF	108	1	1	3	5
52	2KBN	109	6	5	4	15
53	2MK2	109	7	4	3	14
54	2K50	110	8	3	3	14
55	2KL5	110	3	2	3	8
56	2LTA	110	5	2	3	10
57	2KIW	111	7	7	4	18
58	2LVB	112	4	1	3	8
59	2LND	112	5	3	3	11
60	1WQU	114	8	6	2	16
61	2KL6	114	8	5	3	16
62	6GT7	115	5	3	3	11
63	2JN8	115	7	8	3	18
64	2K5D	116	7	4	3	14
65	2KD1	118	6	4	3	13
66	2LTL	119	4	3	3	10
67	2KVO	120	7	7	4	18
68	1T0Y	120	6	5	3	14
69	2KCD	120	8	6	5	19
70	2KRT	121	7	5	3	15
71	2LFI	122	5	5	3	13
72	2JQN	122	5	3	3	11
73	2L7Q	124	6	4	3	13
74	2KFP	125	7	6	4	17
75	1SE9	126	6	3	3	12
76	2L3G	126	5	3	3	11
77	2L3B	130	7	4	4	15
78	2LRH	134	5	3	3	11
79	1VEE	134	8	5	3	16
80	2K1G	136	7	7	3	17
81	2KKZ	140	7	5	3	15
82	1VDY	140	8	7	2	17
83	2KKL	140	7	7	4	18
84	2N4B	142	6	5	4	15
85	2L8V	143	7	4	4	15
86	2LGH	144	7	6	4	17
87	2K1S	149	6	6	4	16
88	2M4F	151	8	6	2	16
89	2JXP	155	8	7	2	17
90	2L06	155	6	6	3	15
91	2LAH	160	4	3	3	10
92	2LAK	160	7	6	4	17
93	2L82	162	4	2	3	9
94	2M47	163	7	7	3	17
95	2K3A	163	8	6	3	17
96	2M7U	165	5	3	3	11
97	2B3W	168	8	7	5	20
98	KRAS4B	169	6	5	3	14
99	2G0Q	173	7	2	3	12
100	2LF2	175	7	7	4	18

Supplementary Table 3 Metadata for PDB reference structures. Extracted from PDB entries.

Protein number	1
PDB code	6SVC, doi:10.2210/pdb6SVC/pdb
BMRB code	34432, doi:10.13018/BMR34432
PDB Header	PEPTIDE BINDING PROTEIN
Protein name	PROTEIN ALLOSTERY OF WW DOMAIN AT ATOMIC RESOLUTION: APO STRUCTURE
Deposition date	18.09.2019
PDB title	PROTEIN ALLOSTERY OF THE WW DOMAIN AT ATOMIC RESOLUTION: APO STRUCTURE
PDB authors	D.STROTZ, J.ORTS, M.FRIEDMANN, P.GUNTERT, B.VOGELI, R.RIEK
Last author	RIEK
Reference	ANGEW.CHEM.INT.ED.ENGL. 59, 22132 (2020), doi:10.1002/ANIE.202008734
Reference authors	D.STROTZ, J.ORTS, H.KADAVATH, M.FRIEDMANN, D.GHOSH, S.OLSSON, C.N.CHI, A.POKHARNA, P.GUNTERT, B.VOGELI, R.RIEK
Reference title	PROTEIN ALLOSTERY AT ATOMIC RESOLUTION
Software listed	CCPNMR, CYANA, NMRDRAW, NMRPIPE
Spectrometer	BRUKER (700 MHZ)

Protein number	2
PDB code	2JVD, doi:10.2210/pdb2JVD/pdb
BMRB code	15476, doi:10.13018/BMR15476
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	FOLDED N-TERMINAL FRAGMENT OF UPF0291 PROTEIN YNZC FROM BACILLUS SUBTILIS
Deposition date	18.09.2007
PDB title	SOLUTION NMR STRUCTURE OF THE FOLDED N-TERMINAL FRAGMENT OF UPF0291 PROTEIN YNZC FROM BACILLUS SUBTILIS. NORTHEAST STRUCTURAL GENOMICS TARGET SR384-1-46
PDB authors	J.M.ARAMINI, S.SHARMA, Y.J.HUANG, L.ZHAO, L.A.OWENS, K.STOKES, M.JIANG, R.XIAO, M.C.BARAN, G.V.T.SWAPNA, T.B.ACTON, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	PROTEINS 72, 526 (2008), doi:10.1002/PROT.22064
Reference authors	J.M.ARAMINI, S.SHARMA, Y.J.HUANG, G.V.SWAPNA, C.K.HO, K.SHETTY, K.CUNNINGHAM, L.C.MA, L.ZHAO, L.A.OWENS, M.JIANG, R.XIAO, J.LIU, M.C.BARAN, T.B.ACTON, B.ROST, G.T.MONTELIONE
Reference title	SOLUTION NMR STRUCTURE OF THE SOS RESPONSE PROTEIN YNZC FROM BACILLUS SUBTILIS
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PROCHECK, PSVS, SPARKY, TOPSPIN, VNMR
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	3
PDB code	2K57, doi:10.2210/pdb2K57/pdb
BMRB code	15825, doi:10.13018/BMR15825
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	PUTATIVE LIPOPROTEIN FROM PSEUDOMONAS SYRINGAE GENE LOCUS PSPTO2350
Deposition date	25.06.2008
PDB title	SOLUTION NMR STRUCTURE OF PUTATIVE LIPOPROTEIN FROM PSEUDOMONAS SYRINGAE GENE LOCUS PSPTO2350. NORTHEAST STRUCTURAL GENOMICS TARGET PSR76A
PDB authors	D.HANG, J.A.ARAMINI, P.ROSSI, D.WANG, M.JIANG, M.MAGLAQUI, R.XIAO, J.LIU, M.C.BARAN, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PDBSTAT, PROCHECK, PSVS, RPF(AUTOSTRUCTURE), SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	4
PDB code	6SOW, doi:10.2210/pdb6SOW/pdb
BMRB code	34430, doi:10.13018/BMR34430
PDB Header	PROTEIN BINDING
Protein name	STAPHYLOCOCCAL PROTEIN A, C DOMAIN
Deposition date	30.08.2019
PDB title	NMR SOLUTION STRUCTURE OF STAPHYLOCOCCAL PROTEIN A, C DOMAIN
PDB authors	S.M.BACKLUND, H.IWAI
Last author	IWAI
Reference	MOLECULES 2, 6 (2021), doi:10.3390/MOLECULES26030747
Reference authors	H.A.HEIKKINEN, S.M.BACKLUND, H.IWAI
Reference title	NMR STRUCTURE DETERMINATIONS OF SMALL PROTEINS USING ONLY ONE FRACTIONALLY 20% 13 C- AND UNIFORMLY 100% 15 N-LABELED SAMPLE
Software listed	AMBER, CCPNMR, CYANA, PSVS, TALOS
Spectrometer	BRUKER (850 MHZ)

Protein number	5
PDB code	2LX7, doi:10.2210/pdb2LX7/pdb

BMRB code	18662, doi:10.13018/BMR18662
PDB Header	PROTEIN BINDING
Protein name	SH3 DOMAIN OF GROWTH ARREST-SPECIFIC PROTEIN 7 (GAS7) (FRAGMENT 1-60) FROM HOMO SAPIENS
Deposition date	15.08.2012
PDB title	SOLUTION NMR STRUCTURE OF SH3 DOMAIN OF GROWTH ARREST-SPECIFIC PROTEIN 7 (GAS7) (FRAGMENT 1-60) FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET HR8574A
PDB authors	Y.YANG, T.A.RAMELOT, L.DAN, E.KOHAN, H.JANJUA, R.XIAO, T.ACTON, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PINE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	6
PDB code	2MA6, doi:10.2210/pdb2MA6/pdb
BMRB code	19329, doi:10.13018/BMR19329
PDB Header	LIGASE
Protein name	RING FINGER DOMAIN FROM KIP1 UBIQUITINATION-PROMOTING E3 COMPLEX PROTEIN 1 (KPC1/RNF123) FROM HOMO SAPIENS
Deposition date	28.06.2013
PDB title	SOLUTION NMR STRUCTURE OF THE RING FINGER DOMAIN FROM THE KIP1 UBIQUITINATION-PROMOTING E3 COMPLEX PROTEIN 1 (KPC1/RNF123) FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET HR8700A
PDB authors	T.A.RAMELOT, Y.YANG, H.JANJUA, E.KOHAN, H.WANG, R.XIAO, T.B.ACTON, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, FMCGUI, NMRPIPE, PINE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	7
PDB code	2JRM, doi:10.2210/pdb2JRM/pdb
BMRB code	15339, doi:10.13018/BMR15339
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	RIBOSOME MODULATION FACTOR VP1593 FROM VIBRIO PARAHAEMOLYTICUS
Deposition date	27.06.2007
PDB title	SOLUTION NMR STRUCTURE OF RIBOSOME MODULATION FACTOR VP1593 FROM VIBRIO PARAHAEMOLYTICUS. NORTHEAST STRUCTURAL GENOMICS TARGET VPR55
PDB authors	Y.TANG, P.ROSSI, G.SWAPNA, H.WANG, M.JIANG, K.CUNNINGHAM, L.OWENS, L.MA, R.XIAO, J.LIU, M.C.BARAN, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, X-PLOR
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	8
PDB code	1YEZ, doi:10.2210/pdb1YEZ/pdb
BMRB code	6505, doi:10.13018/BMR6505
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	CONSERVED PROTEIN FROM GENE LOCUS MM1357 OF METHANOSARCINA MAZEI
Deposition date	29.12.2004
PDB title	SOLUTION STRUCTURE OF THE CONSERVED PROTEIN FROM THE GENE LOCUS MM1357 OF METHANOSARCINA MAZEI. NORTHEAST STRUCTURAL GENOMICS TARGET MAR30
PDB authors	P.ROSSI, J.M.ARAMINI, G.V.T.SWAPNA, Y.P.HUANG, R.XIAO, C.K.HO, L.C.MA, T.B.ACTON, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, SPARKY, VNMR, XWINNMR
Spectrometer	BRUKER, VARIAN (600 MHZ, 500 MHZ)

Protein number	9
PDB code	2L9R, doi:10.2210/pdb2L9R/pdb
BMRB code	17484, doi:10.13018/BMR17484
PDB Header	TRANSCRIPTION
Protein name	HOMEOBOX DOMAIN OF HOMEOBOX PROTEIN NKX-3.1 FROM HOMO SAPIENS

Deposition date	22.02.2011
PDB title	SOLUTION NMR STRUCTURE OF HOMEOBOX DOMAIN OF HOMEOBOX PROTEIN NKX-3.1 FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR6470A
PDB authors	G.LIU, R.XIAO, H.-W.LEE, K.HAMILTON, C.CICCOSANTI, H.B.WANG, T.B.ACTON, J.K.EVERETT, Y.J.HUANG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	10
PDB code	2K52, doi:10.2210/pdb2K52/pdb
BMRB code	15821, doi:10.13018/BMR15821
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	UNCHARACTERIZED PROTEIN MJ1198 FROM METHANOCALDOCOCCUS JANNASCHII
Deposition date	24.06.2008
PDB title	STRUCTURE OF UNCHARACTERIZED PROTEIN MJ1198 FROM METHANOCALDOCOCCUS JANNASCHII. NORTHEAST STRUCTURAL GENOMICS TARGET MJR117B
PDB authors	P.ROSSI, M.MAGLAQUI, E.L.FOOTE, K.HAMILTON, C.CICCOSANTI, R.XIAO, R.NAIR, G.SWAPNA, J.K.EVERETT, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PROCHECK, PSVS, RPF(AUTOSTRUCTURE), SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	11
PDB code	2KRS, doi:10.2210/pdb2KRS/pdb
BMRB code	16647, doi:10.13018/BMR16647
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	SH3 DOMAIN FROM CPF_0587 (FRAGMENT 415-479) FROM CLOSTRIDIUM PERFRINGENS
Deposition date	22.12.2009
PDB title	SOLUTION NMR STRUCTURE OF SH3 DOMAIN FROM CPF_0587 (FRAGMENT 415-479) FROM CLOSTRIDIUM PERFRINGENS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET CPR74A
PDB authors	T.A.RAMELOT, J.R.CORT, M.MAGLAQUI, C.CICCOSANTI, H.JANJUA, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	12
PDB code	2K53, doi:10.2210/pdb2K53/pdb
BMRB code	15822, doi:10.13018/BMR15822
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	A3DK08 PROTEIN FROM CLOSTRIDIUM THERMOCELLUM
Deposition date	24.06.2008
PDB title	NMR SOLUTION STRUCTURE OF A3DK08 PROTEIN FROM CLOSTRIDIUM THERMOCELLUM: NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CMR9
PDB authors	G.V.T.SWAPNA, W.HUANG, M.JIANG, E.L.FOOTE, R.XIAO, R.NAIR, J.EVERETT, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	13
PDB code	2JT1, doi:10.2210/pdb2JT1/pdb
BMRB code	15386, doi:10.13018/BMR15386
PDB Header	TRANSCRIPTION
Protein name	PEFI (PLASMID-ENCODED FIMBRIAE REGULATORY) PROTEIN FROM SALMONELLA TYPHIMURIUM
Deposition date	17.07.2007
PDB title	SOLUTION NMR STRUCTURE OF PEFI (PLASMID-ENCODED FIMBRIAE REGULATORY) PROTEIN FROM SALMONELLA TYPHIMURIUM. NORTHEAST STRUCTURAL GENOMICS TARGET STR82

PDB authors	J.M.ARAMINI, P.ROSSI, H.WANG, C.NWOSU, K.CUNNINGHAM, L.-C.MA, R.XIAO, J.LIU, M.C.BARAN, G.V.T.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	PROTEINS 79, 335 (2011), doi:10.1002/PROT.22869
Reference authors	J.M.ARAMINI, P.ROSSI, J.R.CORT, L.C.MA, R.XIAO, T.B.ACTON, G.T.MONTELIONE
Reference title	SOLUTION NMR STRUCTURE OF THE PLASMID-ENCODED FIMBRIAE REGULATORY PROTEIN PEFI FROM SALMONELLA ENTERICA SEROVAR TYPHIMURIUM
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PDBSTAT, PROCHECK, PSVS, SPARKY, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	14
PDB code	2JVO, doi:10.2210/pdb2JVO/pdb
BMRB code	15485, doi:10.13018/BMR15485
PDB Header	RNA BINDING PROTEIN
Protein name	SEGMENTAL ISOTOPE LABELING OF NPL3
Deposition date	24.09.2007
PDB title	SEGMENTAL ISOTOPE LABELING OF NPL3
PDB authors	L.SKRISOVSKA, F.H.-T.ALLAIN
Last author	ALLAIN
Reference	J.MOL.BIOL. 375, 151 (2008), doi:10.1016/J.JMB.2007.09.030
Reference authors	L.SKRISOVSKA, F.H.ALLAIN
Reference title	IMPROVED SEGMENTAL ISOTOPE LABELING METHODS FOR THE NMR STUDY OF MULTIDOMAIN OR LARGE PROTEINS: APPLICATION TO THE RRMS OF NPL3P AND HNRNP L
Software listed	ATNOS/CANDID, SPARKY, XWINNMR
Spectrometer	BRUKER (900 MHZ, 600 MHZ, 500 MHZ)

Protein number	15
PDB code	2ERR, doi:10.2210/pdb2ERR/pdb
BMRB code	6895, doi:10.13018/BMR6895
PDB Header	RNA BINDING PROTEIN
Protein name	RNA BINDING DOMAIN OF HUMAN FOX-1 IN COMPLEX WITH UGCAUGU
Deposition date	25.10.2005
PDB title	NMR STRUCTURE OF THE RNA BINDING DOMAIN OF HUMAN FOX-1 IN COMPLEX WITH UGCAUGU
PDB authors	F.H.ALLAIN, S.D.AUWETER
Last author	AUWETER
Reference	EMBO J. 25, 163 (2006), doi:10.1038/SJ.EMBOJ.7600918
Reference authors	S.D.AUWETER, R.FASAN, L.REYMOND, J.G.UNDERWOOD, D.L.BLACK, S.PITSCH, F.H.ALLAIN
Reference title	MOLECULAR BASIS OF RNA RECOGNITION BY THE HUMAN ALTERNATIVE SPLICING FACTOR FOX-1
Software listed	AMBER, CYANA
Spectrometer	BRUKER (900 MHZ, 600 MHZ, 500 MHZ)

Protein number	16
PDB code	2L1P, doi:10.2210/pdb2L1P/pdb
BMRB code	17092, doi:10.13018/BMR17092
PDB Header	DNA BINDING PROTEIN
Protein name	N-TERMINAL DOMAIN OF DNA-BINDING PROTEIN SATB1 FROM HOMO SAPIENS
Deposition date	02.08.2010
PDB title	NMR SOLUTION STRUCTURE OF THE N-TERMINAL DOMAIN OF DNA-BINDING PROTEIN SATB1 FROM HOMO SAPIENS: NORTHEAST STRUCTURAL GENOMICS TARGET HR4435B(179-250)
PDB authors	G.V.T.SWAPNA, A.F.MONTELIONE, R.SHASTRY, C.CICCOSANTI, H.JANJUA, R.XIAO, T.B.ACTON, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	17
PDB code	2LN3, doi:10.2210/pdb2LN3/pdb
BMRB code	18145, doi:10.13018/BMR18145
PDB Header	DE NOVO PROTEIN
Protein name	DE NOVO DESIGNED PROTEIN, IF3-LIKE FOLD
Deposition date	15.12.2011
PDB title	SOLUTION NMR STRUCTURE OF DE NOVO DESIGNED PROTEIN, IF3-LIKE FOLD, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET OR135 (CASD TARGET)
PDB authors	G.LIU, R.KOGA, N.KOGA, R.XIAO, H.LEE, H.JANJUA, E.KOHAN, T.B.ACTON, J.K.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	NATURE 491, 222 (2012), doi:10.1038/NATURE11600
Reference authors	N.KOGA, R.TATSUMI-KOGA, G.LIU, R.XIAO, T.B.ACTON, G.T.MONTELIONE, D.BAKER
Reference title	PRINCIPLES FOR DESIGNING IDEAL PROTEIN STRUCTURES

Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	18
PDB code	2HEQ, doi:10.2210/pdb2HEQ/pdb
BMRB code	7175, doi:10.13018/BMR7175
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	BACILLUS SUBTILIS PROTEIN YORP
Deposition date	21.06.2006
PDB title	NMR STRUCTURE OF BACILLUS SUBTILIS PROTEIN YORP, NORTHEAST STRUCTURAL GENOMICS TARGET SR399
PDB authors	T.A.RAMELOT, J.R.CORT, D.WANG, H.JANJUA, K.CUNNINGHAM, L.-C.MA, R.XIAO, J.LIU, M.BARAN, G.V.T.SWAPNA, T.B.ACTON, B.ROST, G.M.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, NMRPIPE, SPARKY, VNMR, X-PLOR_NIH
Spectrometer	VARIAN (750 MHZ, 600 MHZ)

Protein number	19
PDB code	2KK8, doi:10.2210/pdb2KK8/pdb
BMRB code	16355, doi:10.13018/BMR16355
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	A PUTATIVE UNCHARACTERIZED PROTEIN OBTAINED FROM ARABIDOPSIS THALIANA
Deposition date	16.06.2009
PDB title	NMR SOLUTION STRUCTURE OF A PUTATIVE UNCHARACTERIZED PROTEIN OBTAINED FROM ARABIDOPSIS THALIANA: NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET AR3449A
PDB authors	R.MANI, S.V.T.GURLA, R.SHASTRY, C.CICCOSANTI, E.FOOTE, M.JIANG, R.XIAO, R.NAIR, J.EVERETT, Y.HUANG, T.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ, 500 MHZ)

Protein number	20
PDB code	2KD0, doi:10.2210/pdb2KD0/pdb
BMRB code	16101, doi:10.13018/BMR16101
PDB Header	SIGNALING PROTEIN
Protein name	O64736 PROTEIN FROM ARABIDOPSIS THALIANA
Deposition date	31.12.2008
PDB title	NMR SOLUTION STRUCTURE OF O64736 PROTEIN FROM ARABIDOPSIS THALIANA. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM MEGA TARGET AR3445A
PDB authors	G.V.T.SWAPNA, R.SHASTRY, E.FOOTE, C.CICCOSANTI, M.JIANG, R.XIAO, R.NAIR, J.EVERETT, Y.HUANG, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, SPARKY
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	21
PDB code	2LML, doi:10.2210/pdb2LML/pdb
BMRB code	16860, doi:10.13018/BMR16860
PDB Header	TRANSPORT PROTEIN
Protein name	HOLO ACYL CARRIER PROTEIN FROM GEOBACTER METALLIREDUCENS REFINED WITH NH RDCS
Deposition date	05.12.2011
PDB title	SOLUTION NMR STRUCTURE OF HOLO ACYL CARRIER PROTEIN FROM GEOBACTER METALLIREDUCENS REFINED WITH NH RDCS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET GMR141
PDB authors	T.A.RAMELOT, M.J.SMOLA, H.LEE, L.ZHAO, C.CICCOSANTI, E.L.FOOTE, K.HAMILTON, R.NAIR, B.ROST, G.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	BIOCHEMISTRY 50, 1442 (2011), doi:10.1021/BI101932S
Reference authors	T.A.RAMELOT, M.J.SMOLA, H.W.LEE, C.CICCOSANTI, K.HAMILTON, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY
Reference title	SOLUTION STRUCTURE OF 4'-PHOSPHOPANTETHEINE - GMACP3 FROM GEOBACTER METALLIREDUCENS: A SPECIALIZED ACYL CARRIER PROTEIN WITH ATYPICAL STRUCTURAL FEATURES AND A PUTATIVE ROLE IN LIPOPOLYSACCHARIDE BIOSYNTHESIS
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, FMCGUI, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	22
PDB code	2K3D, doi:10.2210/pdb2K3D/pdb
BMRB code	15750, doi:10.13018/BMR15750
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	FOLDED 79 RESIDUE FRAGMENT OF LIN0334 FROM LISTERIA INNOCUA
Deposition date	02.05.2008
PDB title	SOLUTION NMR STRUCTURE OF THE FOLDED 79 RESIDUE FRAGMENT OF LIN0334 FROM LISTERIA INNOCUA. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET LKR15
PDB authors	T.A.RAMELOT, L.ZHAO, M.JIANG, E.L.FOOTE, R.XIAO, J.LIU, M.C.BARAN, G.V.T.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	23
PDB code	2LK2, doi:10.2210/pdb2LK2/pdb
BMRB code	17971, doi:10.13018/BMR17971
PDB Header	TRANSCRIPTION
Protein name	HOMEOBOX DOMAIN (171-248) OF HUMAN HOMEOBOX PROTEIN TGIF1
Deposition date	30.09.2011
PDB title	SOLUTION NMR STRUCTURE OF HOMEOBOX DOMAIN (171-248) OF HUMAN HOMEOBOX PROTEIN TGIF1, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR4411B
PDB authors	Y.YANG, T.A.RAMELOT, J.R.CORT, R.SHASTRY, C.CICCOSANTI, K.HAMILTON, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	ASDP, AUTOASSIGN, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	24
PDB code	(MH04)
BMRB code	
PDB Header	
Protein name	
Deposition date	
PDB title	
PDB authors	
Last author	
Reference	
Reference authors	
Reference title	
Software listed	
Spectrometer	

Protein number	25
PDB code	1PQX, doi:10.2210/pdb1PQX/pdb
BMRB code	5844, doi:10.13018/BMR5844
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	STAPHYLOCOCCUS AUREUS PROTEIN SAV1430
Deposition date	19.06.2003
PDB title	SOLUTION NMR STRUCTURE OF STAPHYLOCOCCUS AUREUS PROTEIN SAV1430. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET ZR18
PDB authors	M.C.BARAN, J.M.ARAMINI, R.XIAO, Y.J.HUANG, T.B.ACTON, L.SHIH, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOPROC, AUTOSTRUCTURE, NMRPIPE, SPARKY, VNMR, X-PLOR
Spectrometer	VARIAN (600 MHZ, 500 MHZ)

Protein number	26
PDB code	2L33, doi:10.2210/pdb2L33/pdb
BMRB code	17169, doi:10.13018/BMR17169
PDB Header	TRANSCRIPTION REGULATOR
Protein name	DRBM 2 DOMAIN OF INTERLEUKIN ENHANCER- BINDING FACTOR 3 FROM HOMO SAPIENS
Deposition date	03.09.2010
PDB title	SOLUTION NMR STRUCTURE OF DRBM 2 DOMAIN OF INTERLEUKIN ENHANCER- BINDING FACTOR 3 FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR4527E

PDB authors	G.LIU, H.JANJUA, R.XIAO, T.B.ACTON, A.CICCOSANTI, R.B.SHASTRY, J.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	27
PDB code	2KZV, doi:10.2210/pdb2KZV/pdb
BMRB code	17020, doi:10.13018/BMR17020
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	CV_0373(175-257) PROTEIN FROM CHROMOBACTERIUM VIOLACEUM
Deposition date	25.06.2010
PDB title	SOLUTION NMR STRUCTURE OF CV_0373(175-257) PROTEIN FROM CHROMOBACTERIUM VIOLACEUM, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CVR118A
PDB authors	Y.YANG, T.A.RAMELOT, D.WANG, C.CICCOSANTI, L.MAO, H.JANJUA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	28
PDB code	2KCT, doi:10.2210/pdb2KCT/pdb
BMRB code	16096, doi:10.13018/BMR16096
PDB Header	CHAPERONE
Protein name	OB-FOLD DOMAIN OF HEME CHAPERONE CCME FROM DESULFOVIBRIO VULGARIS
Deposition date	29.12.2008
PDB title	SOLUTION NMR STRUCTURE OF THE OB-FOLD DOMAIN OF HEME CHAPERONE CCME FROM DESULFOVIBRIO VULGARIS. NORTHEAST STRUCTURAL GENOMICS TARGET DVR115G
PDB authors	J.M.ARAMINI, P.ROSSI, H.LEE, A.LEMAK, H.WANG, E.L.FOOTE, M.JIANG, R.XIAO, R.NAIR, G.V.T.SWAPNA, T.B.ACTON, B.ROST, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PDBSTAT, PINE, PSVS, SPARKY, TOPSPIN, VNMRJ
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	29
PDB code	2MDR, doi:10.2210/pdb2MDR/pdb
BMRB code	19502, doi:10.13018/BMR19502
PDB Header	HYDROLASE
Protein name	THIRD DOUBLE-STRANDED RNA-BINDING DOMAIN (DSRBD3) OF HUMAN ADENOSINE-DEAMINASE ADAR1
Deposition date	17.09.2013
PDB title	SOLUTION STRUCTURE OF THE THIRD DOUBLE-STRANDED RNA-BINDING DOMAIN (DSRBD3) OF HUMAN ADENOSINE-DEAMINASE ADAR1
PDB authors	P.BARRAUD, S.BANERJEE, W.I.MOHAMED, M.F.JANTSCH, F.H.ALLAIN
Last author	ALLAIN
Reference	PROC.NATL.ACAD.SCI.USA 111, E1852 (2014), doi:10.1073/PNAS.1323698111
Reference authors	P.BARRAUD, S.BANERJEE, W.I.MOHAMED, M.F.JANTSCH, F.H.ALLAIN
Reference title	A BIMODULAR NUCLEAR LOCALIZATION SIGNAL ASSEMBLED VIA AN EXTENDED DOUBLE-STRANDED RNA-BINDING DOMAIN ACTS AS AN RNA-SENSING SIGNAL FOR TRANSPORTIN 1
Software listed	ATNOS, CING, CNS, CYANA, PROCHECKNMR, SPARKY, TOPSPIN
Spectrometer	BRUKER (900 MHZ, 750 MHZ, 700 MHZ, 600 MHZ, 500 MHZ)

Protein number	30
PDB code	2FB7, doi:10.2210/pdb2FB7/pdb
BMRB code	7084, doi:10.13018/BMR7084
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	PROTEIN FROM ZEBRA FISH DR.13312
Deposition date	08.12.2005
PDB title	NMR SOLUTION STRUCTURE OF PROTEIN FROM ZEBRA FISH DR.13312
PDB authors	R.C.TYLER, J.SONG, J.L.MARKLEY, CENTER FOR EUKARYOTIC STRUCTURAL GENOMICS (CESG)
Last author	MARKLEY
Reference	
Reference authors	
Reference title	
Software listed	ARIA, CNS, NMRPIPE, NMRVIEW

Spectrometer	VARIAN (600 MHZ)

Protein number	31
PDB code	2MB0, doi:10.2210/pdb2MB0/pdb
BMRB code	19382, doi:10.13018/BMR19382
PDB Header	SPLICING/RNA
Protein name	HNRNP G RRM IN COMPLEX WITH RNA 5'-AUCAAA-3'
Deposition date	22.07.2013
PDB title	SOLUTION STRUCTURE OF HNRNP G RRM IN COMPLEX WITH THE RNA 5'-AUCAAA-3'
PDB authors	A.MOURSY, F.H.-T.ALLAIN, A.CLERY
Last author	CLERY
Reference	NUCLEIC ACIDS RES. 42, 6659 (2014), doi:10.1093/NAR/GKU244
Reference authors	A.MOURSY, F.H.ALLAIN, A.CLERY
Reference title	CHARACTERIZATION OF THE RNA RECOGNITION MODE OF HNRNP G EXTENDS ITS ROLE IN SMN2 SPLICING REGULATION
Software listed	AMBER
Spectrometer	BRUKER (900 MHZ, 700 MHZ, 600 MHZ, 500 MHZ)

Protein number	32
PDB code	2L05, doi:10.2210/pdb2L05/pdb
BMRB code	17030, doi:10.13018/BMR17030
PDB Header	TRANSFERASE
Protein name	RAS-BINDING DOMAIN OF SERINE/THREONINE- PROTEIN KINASE B-RAF FROM HOMO SAPIENS
Deposition date	30.06.2010
PDB title	SOLUTION NMR STRUCTURE OF THE RAS-BINDING DOMAIN OF SERINE/THREONINE- PROTEIN KINASE B-RAF FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR4694F
PDB authors	J.M.ARAMINI, H.JANJUA, C.CICCOSANTI, R.SHASTRY, Y.J.HUANG, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PINE, PSVS, SPARKY, TALOS+, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	33
PDB code	2KJR, doi:10.2210/pdb2KJR/pdb
BMRB code	16338, doi:10.13018/BMR16338
PDB Header	CHAPERONE
Protein name	N-TERMINAL UBIQUITIN-LIKE DOMAIN FROM TUBULIN-BINDING COFACTOR B, CG11242, FROM DROSOPHILA MELANOGASTER
Deposition date	08.06.2009
PDB title	SOLUTION NMR STRUCTURE OF THE N-TERMINAL UBIQUITIN-LIKE DOMAIN FROM TUBULIN-BINDING COFACTOR B, CG11242, FROM DROSOPHILA MELANOGASTER. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET FR629A (RESIDUES 8- 92)
PDB authors	T.A.RAMELOT, J.R.CORT, R.SHASTRY, C.CICCOSANTI, M.JIANG, R.NAIR, B.ROST, G.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 500 MHZ)

Protein number	34
PDB code	2M5O, doi:10.2210/pdb2M5O/pdb
BMRB code	19068, doi:10.13018/BMR19068
PDB Header	BIOSYNTHETIC PROTEIN
Protein name	SOLUTION NMR STRUCTURE CTD DOMAIN OF NFU1 IRON-SULFUR CLUSTER SCAFFOLD HOMOLOG FROM HOMO SAPIENS
Deposition date	01.03.2013
PDB title	SOLUTION NMR STRUCTURE CTD DOMAIN OF NFU1 IRON-SULFUR CLUSTER SCAFFOLD HOMOLOG FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET HR2876C
PDB authors	G.LIU, R.XIAO, H.JANJUA, K.HAMILTON, R.SHASTRY, E.KOHAN, T.B.ACTON, J.K.EVERETT, K.PEDERSON, Y.J.HUANG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG), MITOCHONDRIAL PROTEIN PARTNERSHIP (MPP)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	35
PDB code	(MDM2)
BMRB code	
PDB Header	
Protein name	
Deposition date	
PDB title	
PDB authors	
Last author	
Reference	
Reference authors	
Reference title	
Software listed	
Spectrometer	

Protein number	36
PDB code	2LNA, doi:10.2210/pdb2LNA/pdb
BMRB code	18156, doi:10.13018/BMR18156
PDB Header	HYDROLASE
Protein name	MITOCHONDRIAL INNER MEMBRANE DOMAIN (RESIDUES 164-251), FTSH_EXT, FROM PARAPLEGIN-LIKE PROTEIN AFG3L2 FROM HOMO SAPIENS
Deposition date	20.12.2011
PDB title	SOLUTION NMR STRUCTURE OF THE MITOCHONDRIAL INNER MEMBRANE DOMAIN (RESIDUES 164-251), FTSH_EXT, FROM THE PARAPLEGIN-LIKE PROTEIN AFG3L2 FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR6741A
PDB authors	T.A.RAMELOT, Y.YANG, H.LEE, H.JANUA, E.KOHAN, R.SHASTRY, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG), MITOCHONDRIAL PROTEIN PARTNERSHIP (MPP)
Last author	KENNEDY
Reference	FEBS LETT. 587, 3522 (2013), doi:10.1016/J.FEBSLET.2013.09.009
Reference authors	T.A.RAMELOT, Y.YANG, I.D.SAHU, H.W.LEE, R.XIAO, G.A.LORIGAN, G.T.MONTELIONE, M.A.KENNEDY
Reference title	NMR STRUCTURE AND MD SIMULATIONS OF THE AAA PROTEASE INTERMEMBRANE SPACE DOMAIN INDICATES PERIPHERAL MEMBRANE LOCALIZATION WITHIN THE HEXAOLIGOMER
Software listed	AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PINE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	37
PDB code	2LA6, doi:10.2210/pdb2LA6/pdb
BMRB code	17508, doi:10.13018/BMR17508
PDB Header	RNA BINDING PROTEIN
Protein name	RRM DOMAIN OF RNA-BINDING PROTEIN FUS FROM HOMO SAPIENS
Deposition date	04.03.2011
PDB title	SOLUTION NMR STRUCTURE OF RRM DOMAIN OF RNA-BINDING PROTEIN FUS FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR6430A
PDB authors	G.LIU, R.XIAO, H.JANJUA, C.CICCOSANTI, H.WANG, H.LEE, T.B.ACTON, J.K.EVERETT, Y.J.HUANG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	38
PDB code	6FIP, doi:10.2210/pdb6FIP/pdb
BMRB code	34235, doi:10.13018/BMR34235
PDB Header	TRANSPORT PROTEIN
Protein name	PSEUDOMONAS AERUGINOSA TONB CTD
Deposition date	19.01.2018
PDB title	SOLUTION NMR STRUCTURE OF PSEUDOMONAS AERUGINOSA TONB CTD
PDB authors	J.S.OEEMIG, O.H.SAMULI OLLILA, H.A.HEIKKINEN, H.IWAI
Last author	IWAI
Reference	PEERJ 6, E5412 (2018), doi:10.7717/PEERJ.5412
Reference authors	J.S.OEEMIG, O.H.S.OLLILA, H.IWAI
Reference title	NMR STRUCTURE OF THE C-TERMINAL DOMAIN OF TONB PROTEIN FROMPSEUDOMONAS AERUGINOSA
Software listed	AMBER, CCPNMR, CYANA, NMRPIPE
Spectrometer	VARIAN (800 MHZ)

Protein number	39
PDB code	2LEA, doi:10.2210/pdb2LEA/pdb
BMRB code	17705, doi:10.13018/BMR17705
PDB Header	RNA BINDING PROTEIN
Protein name	HUMAN SRSF2 (SC35) RRM
Deposition date	15.06.2011
PDB title	SOLUTION STRUCTURE OF HUMAN SRSF2 (SC35) RRM

PDB authors	G.M.DAUBNER, A.CLERY, S.JAYNE, J.STEVENIN, F.H.-T.ALLAIN
Last author	ALLAIN
Reference	EMBO J. 31, 162 (2012), doi:10.1038/EMBOJ.2011.367
Reference authors	G.M.DAUBNER, A.CLERY, S.JAYNE, J.STEVENIN, F.H.ALLAIN
Reference title	A SYN-ANTI CONFORMATIONAL DIFFERENCE ALLOWS SRSF2 TO RECOGNIZE GUANINES AND CYTOSINES EQUALLY WELL
Software listed	AMBER, CYANA, SPARKY
Spectrometer	BRUKER (900 MHZ, 700 MHZ, 600 MHZ, 500 MHZ)

Protein number	40
PDB code	2LL8, doi:10.2210/pdb2LL8/pdb
BMRB code	18032, doi:10.13018/BMR18032
PDB Header	TRANSFERASE
Protein name	SPECIALIZED HOLO-ACYL CARRIER PROTEIN RPA2022 FROM RHODOPSEUDOMONAS PALUSTRIS REFINED WITH NH RDCS
Deposition date	31.10.2011
PDB title	SOLUTION NMR STRUCTURE OF THE SPECIALIZED HOLO-ACYL CARRIER PROTEIN RPA2022 FROM RHODOPSEUDOMONAS PALUSTRIS REFINED WITH NH RDCS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET RPR324
PDB authors	T.A.RAMELOT, S.NI, P.ROSSI, Y.YANG, H.WANG, C.CICCOSANTI, M.MAGLAQUI, H.JANJUA, R.NAIR, B.ROSET, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	BIOCHEMISTRY 51, 7239 (2012), doi:10.1021/BI300546B
Reference authors	T.A.RAMELOT, P.ROSSI, F.FOROUHAR, H.W.LEE, Y.YANG, S.NI, S.UNSER, S.LEW, J.SEETHARAMAN, R.XIAO, T.B.ACTON, J.K.EVERETT, J.H.PRESTEGARD, J.F.HUNT, G.T.MONTELIONE, M.A.KENNEDY
Reference title	STRUCTURE OF A SPECIALIZED ACYL CARRIER PROTEIN ESSENTIAL FOR LIPID A BIOSYNTHESIS WITH VERY LONG-CHAIN FATTY ACIDS IN OPEN AND CLOSED CONFORMATIONS
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, FMCGUI, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	41
PDB code	2KPN, doi:10.2210/pdb2KPN/pdb
BMRB code	16561, doi:10.13018/BMR16561
PDB Header	HYDROLASE
Protein name	A BACTERIAL IG-LIKE (BIG_3) DOMAIN FROM BACILLUS CEREUS
Deposition date	16.10.2009
PDB title	SOLUTION NMR STRUCTURE OF A BACTERIAL IG-LIKE (BIG_3) DOMAIN FROM BACILLUS CEREUS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET BCR147A
PDB authors	J.M.ARAMINI, D.WANG, C.T.CICCOSANTI, H.JANJUA, B.ROST, T.B.ACTON, R.XIAO, G.V.T.SWAPNA, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PINE, PSVS, SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	42
PDB code	2K0M, doi:10.2210/pdb2K0M/pdb
BMRB code	15652, doi:10.13018/BMR15652
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	UNCHARACTERIZED PROTEIN FROM RHODOSPIRILLUM RUBRUM GENE LOCUS RRU_A0810
Deposition date	04.02.2008
PDB title	SOLUTION NMR STRUCTURE OF THE UNCHARACTERIZED PROTEIN FROM RHODOSPIRILLUM RUBRUM GENE LOCUS RRU_A0810. NORTHEAST STRUCTURAL GENOMICS TARGET RRR43
PDB authors	P.ROSSI, H.WANG, M.JIANG, E.L.FOOTE, R.XIAO, J.LIU, G.SWAPNA, T.B.ACTON, M.C.BARAN, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PROCHECKNMR, PSVS, SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ)

Protein number	43
PDB code	2K5V, doi:10.2210/pdb2K5V/pdb
BMRB code	15849, doi:10.13018/BMR15849
PDB Header	DNA BINDING PROTEIN
Protein name	SECOND OB-FOLD DOMAIN OF REPLICATION PROTEIN A FROM METHANOCOCCUS MARIPALUDIS
Deposition date	30.06.2008
PDB title	SOLUTION NMR STRUCTURE OF THE SECOND OB-FOLD DOMAIN OF REPLICATION PROTEIN A FROM METHANOCOCCUS MARIPALUDIS. NORTHEAST STRUCTURAL GENOMICS TARGET MRR110B

PDB authors	J.M.ARAMINI, M.MAGLAQUI, M.JIANG, C.CICCOSANTI, R.XIAO, R.NAIR, J.K.EVERETT, G.VT.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	44
PDB code	2MQL, doi:10.2210/pdb2MQL/pdb
BMRB code	25038, doi:10.13018/BMR25038
PDB Header	RNA BINDING PROTEIN
Protein name	STRUCTURAL INVESTIGATION OF HNRNP L
Deposition date	24.06.2014
PDB title	STRUCTURAL INVESTIGATION OF HNRNP L
PDB authors	M.BLATTER, F.ALLAIN
Last author	ALLAIN
Reference	J.MOL.BIOL. 427, 3001 (2015), doi:10.1016/J.JMB.2015.05.020
Reference authors	M.BLATTER, S.DUNIN-HORKAWICZ, I.GRISHINA, C.MARIS, S.THORE, T.MAIER, A.BINDEREIF, J.M.BUJNICKI, F.H.ALLAIN
Reference title	THE SIGNATURE OF THE FIVE-STRANDED VRRM FOLD DEFINED BY FUNCTIONAL, STRUCTURAL AND COMPUTATIONAL ANALYSIS OF THE HNRNP L PROTEIN
Software listed	AMBER, CYANA, SPARKY, TOPSPIN
Spectrometer	BRUKER (900 MHZ, 700 MHZ)

Protein number	45
PDB code	2K75, doi:10.2210/pdb2K75/pdb
BMRB code	15902, doi:10.13018/BMR15902
PDB Header	DNA BINDING PROTEIN
Protein name	OB DOMAIN OF TA0387 FROM THERMOPLASMA ACIDOPHILUM
Deposition date	01.08.2008
PDB title	SOLUTION NMR STRUCTURE OF THE OB DOMAIN OF TA0387 FROM THERMOPLASMA ACIDOPHILUM. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET TAR80B
PDB authors	T.A.RAMELOT, K.DING, D.LEE, M.JIANG, C.CICCOSANTI, R.XIAO, R.NAIR, J.K.EVERETT, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	46
PDB code	2LTM, doi:10.2210/pdb2LTM/pdb
BMRB code	18489, doi:10.13018/BMR18489
PDB Header	ELECTRON TRANSPORT
Protein name	NFU1 IRON-SULFUR CLUSTER SCAFFOLD HOMOLOG FROM HOMO SAPIENS
Deposition date	29.05.2012
PDB title	SOLUTION NMR STRUCTURE OF NFU1 IRON-SULFUR CLUSTER SCAFFOLD HOMOLOG FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET HR2876B
PDB authors	G.LIU, R.XIAO, H.JANJUA, K.HAMILTON, R.SHASTRY, E.KOHAN, T.B.ACTON, J.K.EVERETT, H.LEE, Y.J.HUANG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG), MITOCHONDRIAL PROTEIN PARTNERSHIP (MPP)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	47
PDB code	2KOB, doi:10.2210/pdb2KOB/pdb
BMRB code	16498, doi:10.13018/BMR16498
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	CLOLEP_01837 (FRAGMENT 61-160) FROM CLOSTRIDIUM LEPTUM
Deposition date	15.09.2009
PDB title	SOLUTION NMR STRUCTURE OF CLOLEP_01837 (FRAGMENT 61-160) FROM CLOSTRIDIUM LEPTUM. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET QLR8A
PDB authors	T.A.RAMELOT, D.LEE, C.CICCOSANTI, M.JIANG, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	

Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	48
PDB code	2KHD, doi:10.2210/pdb2KHD/pdb
BMRB code	16238, doi:10.13018/BMR16238
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	VC_A0919 FROM VIBRIO CHOLERAE
Deposition date	02.04.2009
PDB title	SOLUTION NMR STRUCTURE OF VC_A0919 FROM VIBRIO CHOLERAE. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET VCR52
PDB authors	T.A.RAMELOT, J.R.CORT, H.WANG, C.CICCOSANTI, M.JIANG, J.LIU, B.ROST, G.V.T.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 750 MHZ, 600 MHZ)

Protein number	49
PDB code	2RN7, doi:10.2210/pdb2RN7/pdb
BMRB code	11017, doi:10.13018/BMR11017
PDB Header	UNKNOWN FUNCTION
Protein name	TNPE PROTEIN FROM SHIGELLA FLEXNERI
Deposition date	08.12.2007
PDB title	NMR SOLUTION STRUCTURE OF TNPE PROTEIN FROM SHIGELLA FLEXNERI. NORTHEAST STRUCTURAL GENOMICS TARGET SFR125
PDB authors	T.A.RAMELOT, J.R.CORT, A.SEMESI, M.GARCIA, A.A.YEE, C.H.ARROWSMITH, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, NMRPIPE, SPARKY, VNMR, X-PLOR
Spectrometer	VARIAN (750 MHZ, 600 MHZ)

Protein number	50
PDB code	2LXU, doi:10.2210/pdb2LXU/pdb
BMRB code	18698, doi:10.13018/BMR18698
PDB Header	RNA BINDING PROTEIN
Protein name	EUKARYOTIC RNA RECOGNITION MOTIF, RRM1, FROM HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN H FROM HOMO SAPIENS
Deposition date	31.08.2012
PDB title	SOLUTION NMR STRUCTURE OF THE EUKARYOTIC RNA RECOGNITION MOTIF, RRM1, FROM THE HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN H FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET HR8614A
PDB authors	T.A.RAMELOT, Y.YANG, K.PEDERSON, R.SHASTRY, E.KOHAN, H.JANJUA, R.XIAO, T.B.ACTON, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, FMCGUI, NMRPIPE, PALES, PINE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	51
PDB code	2KIF, doi:10.2210/pdb2KIF/pdb
BMRB code	16272, doi:10.13018/BMR16272
PDB Header	TRANSFERASE
Protein name	AN O6-METHYLGUANINE DNA METHYLTRANSFERASE FAMILY PROTEIN FROM VIBRIO PARAHAEMOLYTICUS
Deposition date	03.05.2009
PDB title	SOLUTION NMR STRUCTURE OF AN O6-METHYLGUANINE DNA METHYLTRANSFERASE FAMILY PROTEIN FROM VIBRIO PARAHAEMOLYTICUS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET VPR247
PDB authors	J.M.ARAMINI, R.L.BELOTE, C.T.CICCOSANTI, M.JIANG, B.ROST, R.NAIR, G.V.T.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	J.BIOL.CHEM. 285, 13736 (2010), doi:10.1074/JBC.M109.093591
Reference authors	J.M.ARAMINI, J.L.TUBBS, S.KANUGULA, P.ROSSI, A.ERTEKIN, M.MAGLAQUI, K.HAMILTON, C.T.CICCOSANTI, M.JIANG, R.XIAO, T.T.SOONG, B.ROST, T.B.ACTON, J.K.EVERETT, A.E.PEGG, J.A.TAINER, G.T.MONTELIONE

Reference title	STRUCTURAL BASIS OF O6-ALKYLGUANINE RECOGNITION BY A BACTERIAL ALKYLTRANSFERASE-LIKE DNA REPAIR PROTEIN
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PINE, PSVS, SPARKY, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	52
PDB code	2KBN, doi:10.2210/pdb2KBN/pdb
BMRB code	16051, doi:10.13018/BMR16051
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	OB DOMAIN (RESIDUES 67-166) OF MM0293 FROM METHANOSARCINA MAZEI
Deposition date	03.12.2008
PDB title	SOLUTION NMR STRUCTURE OF THE OB DOMAIN (RESIDUES 67-166) OF MM0293 FROM METHANOSARCINA MAZEI. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET MAR214A
PDB authors	T.A.RAMELOT, K.DING, M.MAGLIQUI, M.JIANG, C.CICCOSANTI, R.XIAO, J.LUI, J.K.EVERETT, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, PSVS, SPARKY, TOPSPIN, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	53
PDB code	2MK2, doi:10.2210/pdb2MK2/pdb
BMRB code	19749, doi:10.13018/BMR19749
PDB Header	HYDROLASE
Protein name	N-TERMINAL DOMAIN (SH2 DOMAIN) OF HUMAN INOSITOL POLYPHOSPHATE PHOSPHATASE-LIKE PROTEIN 1 (INPPL1) (FRAGMENT 20-117)
Deposition date	23.01.2014
PDB title	SOLUTION NMR STRUCTURE OF N-TERMINAL DOMAIN (SH2 DOMAIN) OF HUMAN INOSITOL POLYPHOSPHATE PHOSPHATASE-LIKE PROTEIN 1 (INPPL1) (FRAGMENT 20-117), NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR9134A
PDB authors	Y.YANG, T.A.RAMELOT, H.JANJUA, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PINE, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	54
PDB code	2K50, doi:10.2210/pdb2K50/pdb
BMRB code	15819, doi:10.13018/BMR15819
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	REPLICATION FACTOR A RELATED PROTEIN FROM METHANOBACTERIUM THERMOAUTOTROPHICUM
Deposition date	23.06.2008
PDB title	SOLUTION NMR STRUCTURE OF THE REPLICATION FACTOR A RELATED PROTEIN FROM METHANOBACTERIUM THERMOAUTOTROPHICUM. NORTHEAST STRUCTURAL GENOMICS TARGET TR91A
PDB authors	P.ROSSI, R.XIAO, M.MAGLAQUI, E.L.FOOTE, C.CICCOSANTI, G.SWAPNA, T.B.ACTON, B.ROST, J.K.EVERETT, M.JIANG, R.NAIR, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PROCHECK, PSVS, RPF(AUTOSTRUCTURE), SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	55
PDB code	2KL5, doi:10.2210/pdb2KL5/pdb
BMRB code	16384, doi:10.13018/BMR16384
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	PROTEIN YUTD FROM B.SUBTILIS
Deposition date	30.06.2009
PDB title	SOLUTION NMR STRUCTURE OF PROTEIN YUTD FROM B.SUBTILIS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SR232
PDB authors	G.LIU, K.HAMILTON, R.XIAO, C.CICCOSANTI, C.J.HO, J.EVERETT, R.NAIR, T.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, TOPSPIN, VNMRJ, XEASY

Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	56
PDB code	2LTA, doi:10.2210/pdb2LTA/pdb
BMRB code	18465, doi:10.13018/BMR18465
PDB Header	DE NOVO PROTEIN
Protein name	DE NOVO DESIGNED PROTEIN, ROSSMANN 3X1 FOLD
Deposition date	15.05.2012
PDB title	SOLUTION NMR STRUCTURE OF DE NOVO DESIGNED PROTEIN, ROSSMANN 3X1 FOLD, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET OR157
PDB authors	G.LIU, R.KOGA, N.KOGA, R.XIAO, K.PEDERSON, K.HAMILTON, E.KOHAN, T.B.ACTON, G.KORNHABER, J.K.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	NATURE 491, 222 (2012), doi:10.1038/NATURE11600
Reference authors	N.KOGA, R.TATSUMI-KOGA, G.LIU, R.XIAO, T.B.ACTON, G.T.MONTELIONE, D.BAKER
Reference title	PRINCIPLES FOR DESIGNING IDEAL PROTEIN STRUCTURES
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	57
PDB code	2KIW, doi:10.2210/pdb2KIW/pdb
BMRB code	16298, doi:10.13018/BMR16298
PDB Header	DNA BINDING PROTEIN
Protein name	DOMAIN N-TERMINAL TO INTEGRASE DOMAIN OF SH1003 FROM STAPHYLOCOCCUS HAEMOLYTICUS
Deposition date	12.05.2009
PDB title	SOLUTION NMR STRUCTURE OF THE DOMAIN N-TERMINAL TO THE INTEGRASE DOMAIN OF SH1003 FROM STAPHYLOCOCCUS HAEMOLYTICUS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SHR105F (64-166)
PDB authors	Y.YANG, T.A.RAMELOT, R.L.BELOTE, E.L.FOOTE, H.JANJUA, R.NAIR, B.ROST, G.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	58
PDB code	2LVB, doi:10.2210/pdb2LVB/pdb
BMRB code	18561, doi:10.13018/BMR18561
PDB Header	DE NOVO PROTEIN
Protein name	SOLUTION NMR STRUCTURE DE NOVO DESIGNED PFK FOLD PROTEIN
Deposition date	30.06.2012
PDB title	SOLUTION NMR STRUCTURE DE NOVO DESIGNED PFK FOLD PROTEIN, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET OR250
PDB authors	G.LIU, N.KOGA, R.KOGA, R.XIAO, K.HAMILTON, E.KOHAN, T.B.ACTON, G.KORNHABER, J.K.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	NATURE 491, 222 (2012), doi:10.1038/NATURE11600
Reference authors	N.KOGA, R.TATSUMI-KOGA, G.LIU, R.XIAO, T.B.ACTON, G.T.MONTELIONE, D.BAKER
Reference title	PRINCIPLES FOR DESIGNING IDEAL PROTEIN STRUCTURES
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	59
PDB code	2LND, doi:10.2210/pdb2LND/pdb
BMRB code	18161, doi:10.13018/BMR18161
PDB Header	DE NOVO PROTEIN
Protein name	DE NOVO DESIGNED PROTEIN, PFK FOLD
Deposition date	23.12.2011
PDB title	SOLUTION NMR STRUCTURE OF DE NOVO DESIGNED PROTEIN, PFK FOLD, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET OR134
PDB authors	G.LIU, N.KOGA, R.KOGA, R.XIAO, H.LEE, H.JANJUA, E.KOHAN, T.B.ACTON, J.K.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	60
PDB code	1WQU, doi:10.2210/pdb1WQU/pdb
BMRB code	6331, doi:10.13018/BMR6331
PDB Header	TRANSFERASE
Protein name	HUMAN FES SH2 DOMAIN
Deposition date	02.10.2004
PDB title	SOLUTION STRUCTURE OF THE HUMAN FES SH2 DOMAIN
PDB authors	A.SCOTT, D.PANTOJA-UCEDA, S.KOSHIBA, M.INOUE, T.KIGAWA, T.TERADA, M.SHIROUZU, A.TANAKA, S.SUGANO, S.YOKOYAMA, P.GUNTERT, RIKEN STRUCTURAL GENOMICS/PROTEOMICS INITIATIVE (RSGI)
Last author	GUNTERT
Reference	J.BIOMOL.NMR 31, 357 (2005), doi:10.1007/S10858-005-0946-6
Reference authors	A.SCOTT, D.PANTOJA-UCEDA, S.KOSHIBA, M.INOUE, T.KIGAWA, T.TERADA, M.SHIROUZU, A.TANAKA, S.SUGANO, S.YOKOYAMA, P.GUNTERT
Reference title	SOLUTION STRUCTURE OF THE SRC HOMOLOGY 2 DOMAIN FROM THE HUMAN FELINE SARCOMA ONCOGENE FES
Software listed	CYANA, NMRPIPE, NMRVIEW, OPALP
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	61
PDB code	2KL6, doi:10.2210/pdb2KL6/pdb
BMRB code	16385, doi:10.13018/BMR16385
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	CARDB DOMAIN OF PF1109 FROM PYROCOCCUS FURIOSUS
Deposition date	30.06.2009
PDB title	SOLUTION NMR STRUCTURE OF THE CARDB DOMAIN OF PF1109 FROM PYROCOCCUS FURIOSUS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET PFR193A
PDB authors	J.M.ARAMINI, D.LEE, C.CICCOSANTI, K.HAMILTON, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, G.V.T.SWAPNA, J.K.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PINE, PSVS, SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	62
PDB code	6GT7, doi:10.2210/pdb6GT7/pdb
BMRB code	34287, doi:10.13018/BMR34287
PDB Header	TRANSFERASE
Protein name	FREE HELIX BUNDLE DOMAIN FROM FUNCTIONAL PRN1 PRIMASE
Deposition date	15.06.2018
PDB title	NMR STRUCTURE OF THE FREE HELIX BUNDLE DOMAIN FROM THE FUNCTIONAL PRN1 PRIMASE
PDB authors	J.BOUDET, G.LIPPS, F.ALLAIN
Last author	ALLAIN
Reference	CELL 176, 154 (2019), doi:10.1016/J.CELL.2018.11.031
Reference authors	J.BOUDET, J.C.DEVILLIER, T.WIEGAND, L.SALMON, B.H.MEIER, G.LIPPS, F.H.ALLAIN
Reference title	A SMALL HELICAL BUNDLE PREPARES PRIMER SYNTHESIS BY BINDING TWO NUCLEOTIDES THAT ENHANCE SEQUENCE-SPECIFIC RECOGNITION OF THE DNA TEMPLATE
Software listed	AMBER, CANDID, CYANA, SPARKY
Spectrometer	BRUKER (900 MHZ, 700 MHZ, 600 MHZ)

Protein number	63
PDB code	2JN8, doi:10.2210/pdb2JN8/pdb
BMRB code	15089, doi:10.13018/BMR15089
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	Q8ZRJ2 FROM SALMONELLA TYPHIMURIUM
Deposition date	29.12.2006
PDB title	SOLUTION NMR STRUCTURE OF Q8ZRJ2 FROM SALMONELLA TYPHIMURIUM. NORTHEAST STRUCTURAL GENOMICS TARGET STR65
PDB authors	J.M.ARAMINI, J.R.CORT, C.K.HO, K.CUNNINGHAM, L.-C.MA, R.XIAO, J.LIU, M.C.BARAN, G.V.T.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, BRUKER, NMRPIPE, PDBSTAT, PSVS, SPARKY, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (750 MHZ, 600 MHZ, 500 MHZ)

Protein number	64
PDB code	2K5D, doi:10.2210/pdb2K5D/pdb
BMRB code	15829, doi:10.13018/BMR15829
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	SAG0934 FROM STREPTOCOCCUS AGALACTIAE
Deposition date	26.06.2008

PDB title	SOLUTION NMR STRUCTURE OF SAG0934 FROM STREPTOCOCCUS AGALACTIAE. NORTHEAST STRUCTURAL GENOMICS TARGET SAR32[1-108]
PDB authors	J.M.ARAMINI, P.ROSSI, L.ZHAO, E.L.FOOTE, M.JIANG, R.XIAO, S.SHARMA, G.VT.SWAPNA, R.NAIR, J.K.EVERETT, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	65
PDB code	2KD1, doi:10.2210/pdb2KD1/pdb
BMRB code	16102, doi:10.13018/BMR16102
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	INTEGRASE-LIKE DOMAIN FROM BACILLUS CEREUS ORDERED LOCUS BC_1272
Deposition date	31.12.2008
PDB title	SOLUTION NMR STRUCTURE OF THE INTEGRASE-LIKE DOMAIN FROM BACILLUS CEREUS ORDERED LOCUS BC_1272. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET BCR268F
PDB authors	P.ROSSI, H.LEE, M.MAGLAQUI, E.L.FOOTE, W.A.BUCHWALD, M.JIANG, G.V.T.SWAPNA, R.NAIR, R.XIAO, T.B.ACTON, B.ROST, J.H.PRESTEGARD, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PDBSTAT, PINE, PROCHECK, PSVS, SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	66
PDB code	2LTL, doi:10.2210/pdb2LTL/pdb
BMRB code	18487, doi:10.13018/BMR18487
PDB Header	ELECTRON TRANSPORT
Protein name	NIFU-LIKE PROTEIN FROM SACCHAROMYCES CEREVISIAE
Deposition date	29.05.2012
PDB title	SOLUTION NMR STRUCTURE OF NIFU-LIKE PROTEIN FROM SACCHAROMYCES CEREVISIAE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG) TARGET YR313A
PDB authors	G.LIU, R.XIAO, K.HAMILTON, H.JANJUA, R.SHASTRY, E.KOHAN, T.B.ACTON, J.K.EVERETT, H.LEE, Y.J.HUANG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG), MITOCHONDRIAL PROTEIN PARTNERSHIP (MPP)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PINE, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	67
PDB code	2KVO, doi:10.2210/pdb2KVO/pdb
BMRB code	16782, doi:10.13018/BMR16782
PDB Header	PHOTOSYNTHESIS
Protein name	PHOTOSYSTEM II REACTION CENTER PSB28 PROTEIN FROM SYNECHOCYSTIS SP.(STRAIN PCC 6803)
Deposition date	22.03.2010
PDB title	SOLUTION NMR STRUCTURE OF PHOTOSYSTEM II REACTION CENTER PSB28 PROTEIN FROM SYNECHOCYSTIS SP.(STRAIN PCC 6803), NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SGR171
PDB authors	Y.YANG, T.A.RAMELOT, J.R.CORT, D.WANG, C.CICCOSANTI, K.HAMILTON, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	PROTEINS 79, 340 (2011), doi:10.1002/PROT.22876
Reference authors	Y.YANG, T.A.RAMELOT, J.R.CORT, D.WANG, C.CICCOSANTI, K.HAMILTON, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY
Reference title	SOLUTION NMR STRUCTURE OF PHOTOSYSTEM II REACTION CENTER PROTEIN PSB28 FROM SYNECHOCYSTIS SP. STRAIN PCC 6803
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	68
PDB code	1T0Y, doi:10.2210/pdb1T0Y/pdb
BMRB code	6176, doi:10.13018/BMR6176
PDB Header	CHAPERONE
Protein name	A UBIQUITIN-LIKE DOMAIN FROM TUBULIN-BINDING COFACTOR B

Deposition date	13.04.2004
PDB title	SOLUTION STRUCTURE OF A UBIQUITIN-LIKE DOMAIN FROM TUBULIN-BINDING COFACTOR B
PDB authors	B.L.LYTLE, F.C.PETERSON, S.H.QUI, M.LUO, B.F.VOLKMAN, J.L.MARKLEY, CENTER FOR EUKARYOTIC STRUCTURAL GENOMICS (CESG)
Last author	MARKLEY
Reference	J.BIOL.CHEM. 279, 46787 (2004), doi:10.1074/JBC.M409422200
Reference authors	B.L.LYTLE, F.C.PETERSON, S.H.QIU, M.LUO, Q.ZHAO, J.L.MARKLEY, B.F.VOLKMAN
Reference title	SOLUTION STRUCTURE OF A UBIQUITIN-LIKE DOMAIN FROM TUBULIN-BINDING COFACTOR B
Software listed	CYANA, NMRPIPE, SPSCAN, X-PLOR_NIH, XEASY, XWINNMR
Spectrometer	BRUKER (600 MHZ)

Protein number	69
PDB code	2KCD, doi:10.2210/pdb2KCD/pdb
BMRB code	16072, doi:10.13018/BMR16072
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	SSP0047 FROM STAPHYLOCOCCUS SAPROPHYTICUS
Deposition date	19.12.2008
PDB title	SOLUTION NMR STRUCTURE OF SSP0047 FROM STAPHYLOCOCCUS SAPROPHYTICUS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SYR6
PDB authors	T.A.RAMELOT, K.DING, C.X.CHEN, M.JIANG, C.CICCOSANTI, R.XIAO, J.LIU, M.C.BARAN, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 750 MHZ, 600 MHZ)

Protein number	70
PDB code	2KRT, doi:10.2210/pdb2KRT/pdb
BMRB code	16648, doi:10.13018/BMR16648
PDB Header	LIPID BINDING PROTEIN
Protein name	A CONSERVED HYPOTHETICAL MEMBRANE LIPOPROTEIN OBTAINED FROM UREAPLASMA PARVUM
Deposition date	22.12.2009
PDB title	SOLUTION NMR STRUCTURE OF A CONSERVED HYPOTHETICAL MEMBRANE LIPOPROTEIN OBTAINED FROM UREAPLASMA PARVUM: NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET UUR17A (139-239)
PDB authors	R.MANI, G.SWAPNA, H.JANJUA, C.CICCOSANTI, Y.HUANG, D.PATEL, R.XIAO, T.ACTON, J.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, PINE
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ, 500 MHZ)

Protein number	71
PDB code	2LFI, doi:10.2210/pdb2LFI/pdb
BMRB code	17754, doi:10.13018/BMR17754
PDB Header	METAL BINDING PROTEIN
Protein name	A MUCBP DOMAIN (FRAGMENT 187-294) OF PROTEIN LBA1460 FROM LACTOBACILLUS ACIDOPHILUS
Deposition date	30.06.2011
PDB title	SOLUTION NMR STRUCTURE OF A MUCBP DOMAIN (FRAGMENT 187-294) OF THE PROTEIN LBA1460 FROM LACTOBACILLUS ACIDOPHILUS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET LAR80A
PDB authors	E.A.FELDMANN, T.A.RAMELOT, Y.YANG, H.LEE, C.CICCOSANTI, H.JANJUA, R.NAIR, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	72
PDB code	2JQN, doi:10.2210/pdb2JQN/pdb
BMRB code	15281, doi:10.13018/BMR15281
PDB Header	STRUCTURAL GENOMICS
Protein name	CC0527 FROM CAULOBACTER CRESCENTUS
Deposition date	05.06.2007
PDB title	SOLUTION NMR STRUCTURE OF CC0527 FROM CAULOBACTER CRESCENTUS. NORTHEAST STRUCTURAL GENOMICS TARGET CCR55
PDB authors	J.M.ARAMINI, P.ROSSI, H.N.B.MOSELEY, D.WANG, C.NWOSU, K.CUNNINGHAM, L.MA, R.XIAO, J.LIU, M.C.BARAN, G.V.T.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)

Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	73
PDB code	2L7Q, doi:10.2210/pdb2L7Q/pdb
BMRB code	17370, doi:10.13018/BMR17370
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	CONJUGATE TRANSPOSON PROTEIN BVU_1572(27- 141) FROM BACTEROIDES VULGATUS
Deposition date	20.12.2010
PDB title	SOLUTION NMR STRUCTURE OF CONJUGATE TRANSPOSON PROTEIN BVU_1572(27- 141) FROM BACTEROIDES VULGATUS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET BVR155
PDB authors	Y.YANG, T.A.RAMELOT, J.R.CORT, D.WANG, C.CICCOSANTI, H.JANJUA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	PROTEINS 80, 667 (2012), doi:10.1002/PROT.23235
Reference authors	T.A.RAMELOT, Y.YANG, R.XIAO, T.B.ACTON, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY
Reference title	SOLUTION NMR STRUCTURE OF BT_0084, A CONJUGATIVE TRANSPOSON LIPOPROTEIN FROM BACTEROIDES THETAIOTAMICRON
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	74
PDB code	2KFP, doi:10.2210/pdb2KFP/pdb
BMRB code	16186, doi:10.13018/BMR16186
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	PSPTO_3016 FROM PSEUDOMONAS SYRINGAE
Deposition date	24.02.2009
PDB title	SOLUTION NMR STRUCTURE OF PSPTO_3016 FROM PSEUDOMONAS SYRINGAE. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET PSR293
PDB authors	E.A.FELDMANN, T.A.RAMELOT, L.ZHAO, K.HAMILTON, C.CICCOSANTI, R.XIAO, R.NAIR, J.K.EVERETT, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	J.STRUCT.FUNCT.GENOM. 13, 155 (2012), doi:10.1007/S10969-012-9140-8
Reference authors	E.A.FELDMANN, J.SEETHARAMAN, T.A.RAMELOT, S.LEW, L.ZHAO, K.HAMILTON, C.CICCOSANTI, R.XIAO, T.B.ACTON, J.K.EVERETT, L.TONG, G.T.MONTELIONE, M.A.KENNEDY
Reference title	SOLUTION NMR AND X-RAY CRYSTAL STRUCTURES OF PSEUDOMONAS SYRINGAE PSPTO_3016 FROM PROTEIN DOMAIN FAMILY PF04237 (DUF419) ADOPT A "DOUBLE WING" DNA BINDING MOTIF
Software listed	AUTOASSIGN, AUTOSTRUCTURE, NMRPIPE, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	75
PDB code	1SE9, doi:10.2210/pdb1SE9/pdb
BMRB code	6128, doi:10.13018/BMR6128
PDB Header	PLANT PROTEIN
Protein name	AT3G01050, A UBIQUITIN-FOLD PROTEIN FROM ARABIDOPSIS THALIANA
Deposition date	16.02.2004
PDB title	STRUCTURE OF AT3G01050, A UBIQUITIN-FOLD PROTEIN FROM ARABIDOPSIS THALIANA
PDB authors	B.F.VOLKMAN, B.L.LYTLE, F.C.PETERSON, CENTER FOR EUKARYOTIC STRUCTURAL GENOMICS (CESG)
Last author	PETERSON
Reference	NAT.METHODS 1, 149 (2004), doi:10.1038/NMETH716
Reference authors	D.A.VINAROV, B.L.LYTLE, F.C.PETERSON, E.M.TYLER, B.F.VOLKMAN, J.L.MARKLEY
Reference title	CELL-FREE PROTEIN PRODUCTION AND LABELING PROTOCOL FOR NMR-BASED STRUCTURAL PROTEOMICS
Software listed	CYANA, NMRPIPE, SPSCAN, X-PLOR_NIH, XEASY, XWINNMR
Spectrometer	BRUKER (600 MHZ)

Protein number	76
PDB code	2L3G, doi:10.2210/pdb2L3G/pdb
BMRB code	17192, doi:10.13018/BMR17192
PDB Header	SIGNALING PROTEIN
Protein name	CH DOMAIN OF RHO GUANINE NUCLEOTIDE EXCHANGE FACTOR 7 FROM HOMO SAPIENS
Deposition date	13.09.2010
PDB title	SOLUTION NMR STRUCTURE OF CH DOMAIN OF RHO GUANINE NUCLEOTIDE EXCHANGE FACTOR 7 FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR4495E
PDB authors	G.LIU, R.XIAO, H.JANJUA, T.B.ACTON, A.CICCOSANTI, R.SHASTRY, J.EVERETT, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	

Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	77
PDB code	2L3B, doi:10.2210/pdb2L3B/pdb
BMRB code	17176, doi:10.13018/BMR17176
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	BT_0084 LIPOPROTEIN FROM BACTEROIDES THETAIOTAOMICRON
Deposition date	10.09.2010
PDB title	SOLUTION NMR STRUCTURE OF THE BT_0084 LIPOPROTEIN FROM BACTEROIDES THETAIOTAOMICRON, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET BTR376
PDB authors	T.A.RAMELOT, Y.YANG, D.WANG, C.CICCOSANTI, H.JANJUA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	PROTEINS 867 2012, doi:10.1002/PROT.23235
Reference authors	T.A.RAMELOT, Y.YANG, R.XIAO, T.B.ACTON, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY
Reference title	SOLUTION NMR STRUCTURE OF BT_0084, A CONJUGATIVE TRANSPOSON LIPOPROTEIN FROM BACTEROIDES THETAIOTAMICRON
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	78
PDB code	2LRH, doi:10.2210/pdb2LRH/pdb
BMRB code	18372, doi:10.13018/BMR18372
PDB Header	DE NOVO PROTEIN
Protein name	DE NOVO DESIGNED PROTEIN, P-LOOP NTPASE FOLD
Deposition date	30.03.2012
PDB title	SOLUTION NMR STRUCTURE OF DE NOVO DESIGNED PROTEIN, P-LOOP NTPASE FOLD, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET OR137
PDB authors	G.LIU, N.KOGA, R.KOGA, R.XIAO, H.LEE, H.JANJUA, E.KOHAN, T.B.ACTON, J.K.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PSVS, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	79
PDB code	1VEE, doi:10.2210/pdb1VEE/pdb
BMRB code	5929, doi:10.13018/BMR5929
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	HYPOTHETICAL RHODANESE DOMAIN AT4G01050 FROM ARABIDOPSIS THALIANA
Deposition date	30.03.2004
PDB title	NMR STRUCTURE OF THE HYPOTHETICAL RHODANESE DOMAIN AT4G01050 FROM ARABIDOPSIS THALIANA
PDB authors	D.PANTOJA-UCEDA, B.LOPEZ-MENDEZ, S.KOSHIBA, M.INOUE, T.KIGAWA, T.TERADA, M.SHIROUZU, A.TANAKA, M.SEKI, K.SHINOZAKI, S.YOKOYAMA, P.GUNTERT, RIKEN STRUCTURAL GENOMICS/PROTEOMICS INITIATIVE (RSGI)
Last author	GUNTERT
Reference	PROTEIN SCI. 14, 224 (2005), doi:10.1110/PS.041138705
Reference authors	D.PANTOJA-UCEDA, B.LOPEZ-MENDEZ, S.KOSHIBA, M.INOUE, T.KIGAWA, T.TERADA, M.SHIROUZU, A.TANAKA, M.SEKI, K.SHINOZAKI, S.YOKOYAMA, P.GUNTERT
Reference title	SOLUTION STRUCTURE OF THE RHODANESE HOMOLOGY DOMAIN AT4G01050(175-295) FROM ARABIDOPSIS THALIANA
Software listed	CYANA, OPALP
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	80
PDB code	2K1G, doi:10.2210/pdb2K1G/pdb
BMRB code	15603, doi:10.13018/BMR15603
PDB Header	LIPOPROTEIN
Protein name	LIPOPROTEIN SPR FROM ESCHERICHIA COLI K12
Deposition date	03.03.2008
PDB title	SOLUTION NMR STRUCTURE OF LIPOPROTEIN SPR FROM ESCHERICHIA COLI K12. NORTHEAST STRUCTURAL GENOMICS TARGET ER541-37-162
PDB authors	J.M.ARAMINI, P.ROSSI, L.ZHAO, M.JIANG, M.MAGLAQUI, R.XIAO, J.LIU, M.C.BARAN, G.V.T.SWAPNA, Y.J.HUANG, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	BIOCHEMISTRY 47, 9715 (2008), doi:10.1021/BI8010779
Reference authors	J.M.ARAMINI, P.ROSSI, Y.J.HUANG, L.ZHAO, M.JIANG, M.MAGLAQUI, R.XIAO, J.LOCKE, R.NAIR, B.ROST, T.B.ACTON, M.INOUYE, G.T.MONTELIONE

Reference title	SOLUTION NMR STRUCTURE OF THE NLPC/P60 DOMAIN OF LIPOPROTEIN SPR FROM ESCHERICHIA COLI: STRUCTURAL EVIDENCE FOR A NOVEL CYSTEINE PEPTIDASE CATALYTIC TRIAD
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	81
PDB code	2KKZ, doi:10.2210/pdb2KKZ/pdb
BMRB code	16376, doi:10.13018/BMR16376
PDB Header	ANTIVIRAL PROTEIN
Protein name	MONOMERIC W187R MUTANT OF A/UDORN NS1 EFFECTOR DOMAIN
Deposition date	29.06.2009
PDB title	SOLUTION NMR STRUCTURE OF THE MONOMERIC W187R MUTANT OF A/UDORN NS1 EFFECTOR DOMAIN. NORTHEAST STRUCTURAL GENOMICS TARGET OR8C[W187R]
PDB authors	J.M.ARAMINI, L.MA, H.LEE, L.ZHAO, K.CUNNINGHAM, C.CICCOSANTI, H.JANJUA, Y.FANG, R.XIAO, R.M.KRUG, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, MOLPROBITY, NMRPIPE, PDBSTAT, PSVS, SPARKY, TALOS, TOPSPIN
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	82
PDB code	1VDY, doi:10.2210/pdb1VDY/pdb
BMRB code	5928, doi:10.13018/BMR5928
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	HYPOTHETICAL ENTH-VHS DOMAIN AT3G16270 FROM ARABIDOPSIS THALIANA
Deposition date	25.03.2004
PDB title	NMR STRUCTURE OF THE HYPOTHETICAL ENTH-VHS DOMAIN AT3G16270 FROM ARABIDOPSIS THALIANA
PDB authors	B.LOPEZ-MENDEZ, D.PANTOJA-UCEDA, T.TOMIZAWA, S.KOSHIBA, T.KIGAWA, M.SHIROUZU, T.TERADA, M.INOUE, T.YABUKI, M.AOKI, E.SEKI, T.MATSUDA, H.HIROTA, M.YOSHIDA, A.TANAKA, T.OSANAI, M.SEKI, K.SHINOZAKI, S.YOKOYAMA, P.GUNTERT, RIKEN STRUCTURAL GENOMICS/PROTEOMICS INITIATIVE (RSGI)
Last author	GUNTERT
Reference	
Reference authors	
Reference title	
Software listed	CYANA, OPALP
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	83
PDB code	2KKL, doi:10.2210/pdb2KKL/pdb
BMRB code	16364, doi:10.13018/BMR16364
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	FHA DOMAIN OF MB1858 FROM MYCOBACTERIUM BOVIS
Deposition date	25.06.2009
PDB title	SOLUTION NMR STRUCTURE OF FHA DOMAIN OF MB1858 FROM MYCOBACTERIUM BOVIS. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET MBR243C (24- 155)
PDB authors	Y.YANG, T.A.RAMELOT, D.WANG, E.L.FOOTE, M.JIANG, R.NAIR, B.ROST, G.SWAPNA, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	84
PDB code	2N4B, doi:10.2210/pdb2N4B/pdb
BMRB code	17611, doi:10.13018/BMR17611
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	RALSTONIA METALLIDURANS RMET_5065 DETERMINED BY COMBINING EVOLUTIONARY COUPLINGS (EC) AND SPARSE NMR DATA
Deposition date	17.06.2015
PDB title	EC-NMR STRUCTURE OF RALSTONIA METALLIDURANS RMET_5065 DETERMINED BY COMBINING EVOLUTIONARY COUPLINGS (EC) AND SPARSE NMR DATA. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CRR115
PDB authors	Y.TANG, Y.J.HUANG, T.A.HOPF, C.SANDER, D.MARKS, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	NAT.METHODS 12, 751 (2015), doi:10.1038/NMETH.3455
Reference authors	Y.TANG, Y.J.HUANG, T.A.HOPF, C.SANDER, D.S.MARKS, G.T.MONTELIONE

Reference title	PROTEIN STRUCTURE DETERMINATION BY COMBINING SPARSE NMR DATA WITH EVOLUTIONARY COUPLINGS
Software listed	ASDP, CYANA, EC-NMR, EVFOLD-PLM, REDUCE, ROSETTA, TALOS+
Spectrometer	

Protein number	85
PDB code	2L8V, doi:10.2210/pdb2L8V/pdb
BMRB code	17429, doi:10.13018/BMR17429
PDB Header	PHOTOSYNTHESIS
Protein name	PHYCOBILISOME LINKER POLYPEPTIDE DOMAIN OF CPCC (20-153) FROM THERMOSYNECHOCOCCUS ELONGATUS
Deposition date	26.01.2011
PDB title	SOLUTION NMR STRUCTURE OF THE PHYCOBILISOME LINKER POLYPEPTIDE DOMAIN OF CPCC (20-153) FROM THERMOSYNECHOCOCCUS ELONGATUS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET TER219A
PDB authors	T.A.RAMELOT, Y.YANG, J.R.CORT, D.LEE, C.CICCOSANTI, K.HAMILTON, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	86
PDB code	2LGH, doi:10.2210/pdb2LGH/pdb
BMRB code	17809, doi:10.13018/BMR17809
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	AHSA1-LIKE PROTEIN AHA_2358 FROM AEROMONAS HYDROPHILA REFINED WITH NH RDCS
Deposition date	26.07.2011
PDB title	SOLUTION NMR STRUCTURE OF THE AHSA1-LIKE PROTEIN AHA_2358 FROM AEROMONAS HYDROPHILA REFINED WITH NH RDCS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET AHR99
PDB authors	T.A.RAMELOT, Y.YANG, H.LEE, D.WANG, C.CICCOSANTI, H.JANJUA, R.NAIR, T.B.ACTON, R.XIAO, J.K.EVERETT, J.H.PRESTEGARD, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	87
PDB code	2K1S, doi:10.2210/pdb2K1S/pdb
BMRB code	15683, doi:10.13018/BMR15683
PDB Header	LIPOPROTEIN
Protein name	FOLDED C-TERMINAL FRAGMENT OF YIAD FROM ESCHERICHIA COLI
Deposition date	14.03.2008
PDB title	SOLUTION NMR STRUCTURE OF THE FOLDED C-TERMINAL FRAGMENT OF YIAD FROM ESCHERICHIA COLI. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET ER553
PDB authors	T.A.RAMELOT, L.ZHAO, K.HAMILTON, M.MAGLAQUI, R.XIAO, J.LIU, M.C.BARAN, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, NMRPIPE, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	88
PDB code	2M4F, doi:10.2210/pdb2M4F/pdb
BMRB code	19001, doi:10.13018/BMR19001
PDB Header	IMMUNE SYSTEM
Protein name	OUTER SURFACE PROTEIN E
Deposition date	05.02.2013
PDB title	SOLUTION STRUCTURE OF OUTER SURFACE PROTEIN E
PDB authors	A.BHATTACHARJEE, J.S.OEEMIG, R.KOLODZIEJCZYK, T.MERI, T.KAJANDER, H.IWAI, T.JOKIRANTA, A.GOLDMAN
Last author	GOLDMAN
Reference	J.BIOL.CHEM. 288, 18685 (2013), doi:10.1074/JBC.M113.459040
Reference authors	A.BHATTACHARJEE, J.S.OEEMIG, R.KOLODZIEJCZYK, T.MERI, T.KAJANDER, M.J.LEHTINEN, H.IWAI, T.S.JOKIRANTA, A.GOLDMAN
Reference title	STRUCTURAL BASIS FOR COMPLEMENT EVASION BY LYME DISEASE PATHOGEN BORRELIA BURGDORFERI
Software listed	AMBER, CCPNMR_ANALYSIS, CING, CYANA, NMRPIPE, VNMRJ

Spectrometer	VARIAN (800 MHZ, 600 MHZ)

Protein number	89
PDB code	2JXP, doi:10.2210/pdb2JXP/pdb
BMRB code	15568, doi:10.13018/BMR15568
PDB Header	LIPOPROTEIN
Protein name	UNCHARACTERIZED LIPOPROTEIN B FROM NITROSOMONAS EUROPAEA
Deposition date	27.11.2007
PDB title	SOLUTION NMR STRUCTURE OF UNCHARACTERIZED LIPOPROTEIN B FROM NITROSOMONAS EUROPAEA. NORTHEAST STRUCTURAL GENOMICS TARGET NER45A
PDB authors	P.ROSSI, D.WANG, H.JANJUA, L.OWENS, R.XIAO, M.C.BARAN, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PROCHECK, PSVS, RPF, SPARKY, TOPSPIN, XEASY
Spectrometer	BRUKER (800 MHZ)

Protein number	90
PDB code	2L06, doi:10.2210/pdb2L06/pdb
BMRB code	17031, doi:10.13018/BMR17031
PDB Header	PROTEIN BINDING
Protein name	PBS LINKER POLYPEPTIDE DOMAIN (FRAGMENT 254-400) OF PHYCOBILISOME LINKER PROTEIN APCE FROM SYNECHOCYSTIS SP. PCC 6803
Deposition date	30.06.2010
PDB title	SOLUTION NMR STRUCTURE OF THE PBS LINKER POLYPEPTIDE DOMAIN (FRAGMENT 254-400) OF PHYCOBILISOME LINKER PROTEIN APCE FROM SYNECHOCYSTIS SP. PCC 6803. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SGR209C
PDB authors	T.A.RAMELOT, Y.YANG, J.R.CORT, K.HAMILTON, C.CICCOSANTI, D.LEE, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CYANA, NMRPIPE, PDBSTAT, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR
Spectrometer	BRUKER, VARIAN (850 MHZ, 750 MHZ, 600 MHZ, 500 MHZ)

Protein number	91
PDB code	2LAH, doi:10.2210/pdb2LAH/pdb
BMRB code	17524, doi:10.13018/BMR17524
PDB Header	CELL CYCLE, APOPTOSIS
Protein name	MITOTIC CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1 N-TERMINAL DOMAIN FROM HOMO SAPIENS
Deposition date	14.03.2011
PDB title	SOLUTION NMR STRUCTURE OF MITOTIC CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1 N-TERMINAL DOMAIN FROM HOMO SAPIENS, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET HR5460A (METHODS DEVELOPMENT)
PDB authors	G.LIU, R.XIAO, H.LEE, K.HAMILTON, T.B.ACTON, C.CICCOSANTI, J.K.EVERETT, R.T.SHASTRY, Y.J.HUANG, G.T.MONTELIONE, N.NORTHEAST STRUCTURAL GENOMICS CONSORTIUM, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	92
PDB code	2LAK, doi:10.2210/pdb2LAK/pdb
BMRB code	17530, doi:10.13018/BMR17530
PDB Header	STRUCTURE GENOMICS, UNKNOWN FUNCTION
Protein name	AHSA1-LIKE PROTEIN RHE_CH02687 (1-152) FROM RHIZOBIUM ETLI
Deposition date	16.03.2011
PDB title	SOLUTION NMR STRUCTURE OF THE AHSA1-LIKE PROTEIN RHE_CH02687 (1-152) FROM RHIZOBIUM ETLI, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET RER242
PDB authors	Y.YANG, T.A.RAMELOT, J.R.CORT, D.WANG, C.CICCOSANTI, H.JANJUA, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	93
PDB code	2L82, doi:10.2210/pdb2L82/pdb
BMRB code	17390, doi:10.13018/BMR17390
PDB Header	DE NOVO PROTEIN
Protein name	DE NOVO DESIGNED PROTEIN, P-LOOP NTPASE FOLD
Deposition date	31.12.2010
PDB title	SOLUTION NMR STRUCTURE OF DE NOVO DESIGNED PROTEIN, P-LOOP NTPASE FOLD, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET OR32
PDB authors	G.LIU, N.KOGA, R.KOGA, R.XIAO, K.HAMILTON, H.JANJUA, S.TONG, T.B.ACTON, J.EVERETT, D.BAKER, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PALES, PINE, REDCAT, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (800 MHZ, 600 MHZ)

Protein number	94
PDB code	2M47, doi:10.2210/pdb2M47/pdb
BMRB code	18989, doi:10.13018/BMR18989
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	POLYKETIDE_CYC-LIKE PROTEIN CGL2372 FROM CORYNEBACTERIUM GLUTAMICUM
Deposition date	30.01.2013
PDB title	SOLUTION NMR STRUCTURE OF THE POLYKETIDE_CYC-LIKE PROTEIN CGL2372 FROM CORYNEBACTERIUM GLUTAMICUM, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CGR160
PDB authors	Y.YANG, T.A.RAMELOT, D.LEE, C.CICCOSANTI, A.SAPIN, H.JANJUA, R.NAIR, B.ROST, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PINE, PSVS, SPARKY, TALOS+, TOPSPIN, VNMRJ, XEASY
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Protein number	95
PDB code	2K3A, doi:10.2210/pdb2K3A/pdb
BMRB code	15335, doi:10.13018/BMR15335
PDB Header	HYDROLASE
Protein name	STAPHYLOCOCCUS SAPROPHYTICUS CHAP (CYSTEINE, HISTIDINE-DEPENDENT AMIDOHYDROLASES/PEPTIDASES) DOMAIN PROTEIN
Deposition date	29.04.2008
PDB title	NMR SOLUTION STRUCTURE OF STAPHYLOCOCCUS SAPROPHYTICUS CHAP (CYSTEINE, HISTIDINE-DEPENDENT AMIDOHYDROLASES/PEPTIDASES) DOMAIN PROTEIN. NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SYR11
PDB authors	P.ROSSI, J.M.ARAMINI, C.X.CHEN, C.NWOSU, K.C.CUNNINGHAM, L.A.OWENS, R.XIAO, J.LIU, M.C.BARAN, G.SWAPNA, T.B.ACTON, B.ROST, G.T.MONTELIONE, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	MONTELIONE
Reference	PROTEINS 74, 515 (2008), doi:10.1002/PROT.22267
Reference authors	P.ROSSI, J.M.ARAMINI, R.XIAO, C.X.CHEN, C.NWOSU, L.A.OWENS, M.MAGLAQUI, R.NAIR, M.FISCHER, T.B.ACTON, B.HONIG, B.ROST, G.T.MONTELIONE
Reference title	STRUCTURAL ELUCIDATION OF THE CYS-HIS-GLU-ASN PROTEOLYTIC RELAY IN THE SECRETED CHAP DOMAIN ENZYME FROM THE HUMAN PATHOGEN STAPHYLOCOCCUS SAPROPHYTICUS
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, MOLMOL, MOLPROBITY, NMRPIPE, PDBSTAT, PROCHECK, PROSA, PSVS, SPARKY, TOPSPIN, VERIFY3D, X-PLOR
Spectrometer	BRUKER (800 MHZ, 600 MHZ)

Protein number	96
PDB code	2M7U, doi:10.2210/pdb2M7U/pdb
BMRB code	19213, doi:10.13018/BMR19213
PDB Header	SIGNALING PROTEIN
Protein name	BLUE LIGHT-ABSORBING STATE OF TEPIXJ, AN ACTIVE CYANOBACTERIOCHROME DOMAIN
Deposition date	01.05.2013
PDB title	BLUE LIGHT-ABSORBING STATE OF TEPIXJ, AN ACTIVE CYANOBACTERIOCHROME DOMAIN
PDB authors	G.CORNILESCU, C.C.CORNILESCU, S.E.BURGIE, J.M.WALKER, J.L.MARKLEY, A.T.ULIJASZ, R.D.VIERSTRA
Last author	VIERSTRA
Reference	
Reference authors	
Reference title	
Software listed	NMRPIPE, PIPP, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (900 MHZ, 800 MHZ, 700 MHZ, 600 MHZ)

Protein number	97
PDB code	2B3W, doi:10.2210/pdb2B3W/pdb
BMRB code	6782, doi:10.13018/BMR6782
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	E.COLI PROTEIN YBIA
Deposition date	21.09.2005
PDB title	NMR STRUCTURE OF THE E.COLI PROTEIN YBIA, NORTHEAST STRUCTURAL GENOMICS TARGET ET24
PDB authors	T.A.RAMELOT, J.R.CORT, R.XIAO, L.Y.SHIH, T.B.ACTON, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOSTRUCTURE, CNS, NMRPIPE, SPARKY, VNMR, X-PLOR
Spectrometer	VARIAN (800 MHZ, 750 MHZ, 600 MHZ)

Protein number	98
PDB code	(KRAS4B)
BMRB code	
PDB Header	
Protein name	
Deposition date	
PDB title	
PDB authors	
Last author	
Reference	
Reference authors	
Reference title	
Software listed	
Spectrometer	

Protein number	99
PDB code	2G0Q, doi:10.2210/pdb2G0Q/pdb
BMRB code	7007, doi:10.13018/BMR7007
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	AT5G39720.1 FROM ARABIDOPSIS THALIANA
Deposition date	13.02.2006
PDB title	SOLUTION STRUCTURE OF AT5G39720.1 FROM ARABIDOPSIS THALIANA
PDB authors	B.F.VOLKMAN, F.C.PETERSON, B.L.LYTLE, CENTER FOR EUKARYOTIC STRUCTURAL GENOMICS (CESG)
Last author	LYTLE
Reference	ACTA CRYSTALLOGR.,SECT.F 62, 490 (2006), doi:10.1107/S1744309106015946
Reference authors	B.L.LYTLE, F.C.PETERSON, E.M.TYLER, C.L.NEWMAN, D.A.VINAROV, J.L.MARKLEY, B.F.VOLKMAN
Reference title	SOLUTION STRUCTURE OF ARABIDOPSIS THALIANA PROTEIN AT5G39720.1, A MEMBER OF THE AIG2-LIKE PROTEIN FAMILY
Software listed	GARANT, NMRPIPE, SPSCAN, X-PLOR_NIH, XEASY, XWINNMR
Spectrometer	BRUKER (600 MHZ)

Protein number	100
PDB code	2LF2, doi:10.2210/pdb2LF2/pdb
BMRB code	17736, doi:10.13018/BMR17736
PDB Header	STRUCTURAL GENOMICS, UNKNOWN FUNCTION
Protein name	AHSA1-LIKE PROTEIN CHU_1110 FROM CYTOPHAGA HUTCHINSONII
Deposition date	28.06.2011
PDB title	SOLUTION NMR STRUCTURE OF THE AHSA1-LIKE PROTEIN CHU_1110 FROM CYTOPHAGA HUTCHINSONII, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CHR152
PDB authors	Y.YANG, T.A.RAMELOT, D.LEE, C.CICCOSANTI, T.B.ACTON, R.XIAO, J.K.EVERETT, G.T.MONTELIONE, M.A.KENNEDY, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM (NESG)
Last author	KENNEDY
Reference	
Reference authors	
Reference title	
Software listed	AUTOASSIGN, AUTOSTRUCTURE, CNS, CYANA, NMRPIPE, PDBSTAT, PINE_SERVER, PSVS, SPARKY, TOPSPIN, VNMR, X-PLOR_NIH
Spectrometer	BRUKER, VARIAN (850 MHZ, 600 MHZ)

Supplementary Table 4 Results of automated structure determination of 100 proteins.

ID	Protein	Chemical shift assignment		Ramachandran plot statistics				Structure calculation and comparison to PDB reference				
		Backbone accuracy [%]	Side-chain accuracy [%]	Most favoured [%]	Additionally allowed [%]	Generously allowed [%]	Disallowed [%]	Number of distance restraints	CYANA target function [Å^2]	Residue range for RMSD calculation	Backbone RMSD to reference [Å]	Side-chain RMSD to reference [Å]
1	6SVC	97.52	83.97	96.40	3.60	0.00	0.00	1066	1.80	7-29	0.83	1.53
2	2JVD	99.57	92.94	89.80	10.20	0.00	0.00	1182	0.30	4-37	0.71	1.29
3	2K57	99.62	95.38	88.20	11.80	0.00	0.00	1176	0.35	5-52	0.71	1.22
4	6SOW	88.97	78.57	87.70	12.30	0.00	0.00	1111	2.32	8-55	1.16	2.04
5	2LX7	98.54	87.84	91.40	8.60	0.00	0.00	484	0.32	5-59	1.41	2.02
6	2MA6	98.94	89.36	67.40	30.00	2.60	0.00	953	3.25	10-57	1.56	2.09
7	2JRM	97.21	92.14	87.30	12.60	0.00	0.10	1312	0.50	6-47	1.43	2.55
8	1YEZ	99.06	90.95	89.10	10.90	0.00	0.00	1063	0.58	15-25,29-66	0.73	1.20
9	2L9R	97.93	90.44	89.20	10.80	0.00	0.00	1322	0.37	13-56	0.59	1.18
10	2K52	97.17	93.54	91.00	9.00	0.00	0.00	2018	2.68	7-70	1.10	1.81
11	2KRS	98.47	96.18	88.00	12.00	0.00	0.00	1378	0.35	2-61	1.26	1.50
12	2K53	98.53	95.30	93.40	6.60	0.00	0.00	1183	0.60	8-28,39-66	0.88	1.29
13	2JT1	88.66	90.75	91.60	8.40	0.00	0.00	1240	0.11	5-57,66-69	0.94	1.39
14	2JVO	96.64	76.42	77.90	22.00	0.10	0.00	2263	10.44	6-71	1.77	2.49
15	2ERR	96.36	78.40	87.30	12.70	0.00	0.00	1578	13.61	2-75	2.09	3.16
16	2L1P	96.29	87.04	83.90	13.40	2.60	0.00	2075	2.10	19-78	2.13	2.94
17	2LN3	98.37	92.52	87.20	12.70	0.10	0.00	1947	1.15	6-72	0.89	1.34
18	2HEQ	94.48	84.63	80.40	17.80	1.80	0.00	1822	3.20	17-20,34-68	0.60	1.48
19	2KK8	99.18	90.26	84.40	15.60	0.00	0.00	1818	2.24	10-82	1.25	2.04
20	2KD0	97.24	91.96	85.80	14.20	0.00	0.00	2215	4.43	13-81	1.37	2.02
21	2LML	97.44	91.71	91.30	8.70	0.00	0.00	1197	0.67	3-78	1.53	1.90
22	2K3D	98.96	89.76	85.90	14.10	0.00	0.00	1922	2.00	2-81	1.44	2.13
23	2LK2	96.08	86.08	82.90	17.10	0.00	0.00	1152	0.94	14-65	1.42	1.98
24	MH04	98.58	88.57	89.00	11.00	0.00	0.00	1522	0.86	6-87	1.57	2.35
25	1PQX	99.03	86.51	81.70	16.00	2.30	0.00	1977	10.18	13-19,28-34,38-65,70-81	1.40	2.02
26	2L33	98.68	91.76	79.70	20.10	0.20	0.00	2092	1.37	19-36,46-79	0.79	1.32
27	2KZV	95.84	81.67	85.50	14.50	0.00	0.00	1440	0.41	9-80	2.62	3.13
28	2KCT	96.59	93.42	83.20	16.70	0.10	0.10	2431	4.45	11-37,44-83	0.77	1.32
29	2MDR	93.17	82.89	85.00	13.90	0.80	0.30	2307	3.06	9-89	1.72	3.04
30	2FB7	95.95	81.18	79.90	20.00	0.10	0.00	1218	1.51	20-52,74-87	1.94	2.52
31	2MB0	97.69	88.46	83.50	16.50	0.00	0.00	2701	9.63	8-41,49-85	1.11	1.81
32	2L05	99.50	91.56	85.10	14.10	0.10	0.80	2336	2.07	19-89	0.74	1.23
33	2KJR	99.76	91.62	79.90	20.10	0.00	0.00	2109	1.04	15-23,28-94	1.02	1.35
34	2M5O	92.48	90.20	77.40	22.60	0.10	0.00	2476	7.18	17-91	1.08	1.59
35	MDM2	98.08	84.88	87.40	12.30	0.30	0.00	1452	1.29	9-92	1.24	1.87
36	2LNA	99.30	90.78	78.80	19.90	1.20	0.00	2569	4.06	16-49,59-94	0.86	1.45
37	2LA6	98.78	92.60	83.60	16.40	0.00	0.00	2370	6.62	15-97	0.81	1.34
38	6FIP	97.86	79.15	85.20	14.80	0.10	0.00	2381	17.06	11-93	2.05	2.88
39	2LEA	96.17	83.33	75.40	24.50	0.10	0.00	2542	7.98	15-45,55-88	1.45	2.00
40	2LL8	98.04	91.42	89.90	10.10	0.00	0.00	2237	2.64	4-90	1.42	1.79
41	2KPN	96.95	91.16	79.80	20.00	0.20	0.00	2287	2.33	12-84	0.97	1.58
42	2K0M	96.87	92.08	88.00	12.00	0.00	0.10	1508	0.69	7-70,76-93	1.60	2.09
43	2K5V	99.37	94.25	89.20	10.80	0.00	0.00	1974	1.10	2-29,38-78,83-94	0.94	1.50
44	2MQL	83.59	70.55	72.10	25.10	2.80	0.10	2836	22.17	15-84	0.98	1.56
45	2K75	98.77	88.36	90.10	9.90	0.10	0.00	1881	0.77	3-92	1.65	1.98
46	2LTM	99.31	92.79	85.60	14.40	0.00	0.00	2696	2.68	14-99	0.67	1.46
47	2KOB	88.18	82.29	84.90	15.10	0.00	0.00	1840	2.66	3-93	2.24	2.93
48	2KHD	97.29	87.63	87.90	12.00	0.10	0.00	1059	0.04	31-97	1.87	2.22
49	2RN7	94.35	81.02	84.10	15.80	0.10	0.00	459	0.54	10-55	1.93	2.26
50	2LXU	99.40	91.33	82.90	17.10	0.00	0.00	2115	1.40	9-95	1.19	1.81

Supplementary Table 4 continued

ID	Protein	Chemical shift assignment		Ramachandran plot statistics				Structure calculation and comparison to PDB reference				
		Backbone accuracy [%]	Side-chain accuracy [%]	Most favored [%]	Additionally allowed [%]	Generously allowed [%]	Disallowed [%]	Number of distance restraints	CYANA target function [Å^2]	Residue range for RMSD calculation	Backbone RMSD to reference [Å]	Side-chain RMSD to reference [Å]
51	2KIF	94.43	87.78	81.80	18.20	0.10	0.00	3056	3.64	3-97	0.89	1.51
52	2KBN	97.98	88.49	88.80	11.20	0.00	0.00	2347	0.45	5-29,34-54,58-76,81-94	0.92	1.46
53	2MK2	99.58	91.97	85.50	14.40	0.10	0.00	2049	2.62	14-108	1.56	2.13
54	2K50	97.39	89.74	84.40	15.40	0.00	0.20	2157	0.86	10-34,42-85,92-105	1.00	1.57
55	2KL5	79.41	68.59	72.40	25.50	2.20	0.00	1878	5.90	12-53,58-66,76-86,93-99	2.58	3.38
56	2LTA	95.17	81.57	91.10	8.90	0.00	0.00	1989	0.73	4-98	2.39	2.90
57	2KIW	93.99	80.94	87.50	12.50	0.00	0.00	1964	1.10	2-81	1.59	2.08
58	2LVB	89.27	84.11	92.70	7.30	0.00	0.00	1711	0.86	3-102	1.56	2.17
59	2LND	95.52	88.24	92.90	7.10	0.00	0.00	2605	1.29	3-48,52-101	0.85	1.44
60	1WQU	98.05	86.80	79.60	20.20	0.20	0.10	3785	9.51	8-106	0.99	1.53
61	2KL6	98.64	93.52	86.00	14.00	0.00	0.00	2752	1.99	6-106	0.87	1.38
62	6GT7	96.93	79.31	89.10	10.90	0.00	0.00	3069	4.21	7-30,40-87,94-113	1.39	2.00
63	2JN8	95.45	89.68	83.00	16.80	0.30	0.00	1863	1.12	12-26,31-109	1.83	2.36
64	2K5D	99.25	92.40	75.50	24.30	0.20	0.00	2425	1.44	19-50,55-84,98-107	1.47	1.87
65	2KD1	98.31	90.36	83.60	16.30	0.00	0.10	2550	6.35	7-89	1.99	3.02
66	2LTL	96.44	90.46	89.00	11.00	0.00	0.00	1667	1.07	19-35,39-41,46-110	2.37	2.85
67	2KVO	98.17	90.00	79.20	20.80	0.00	0.00	2112	3.88	3-23,28-103	1.87	2.18
68	1T0Y	97.27	85.04	76.10	23.80	0.10	0.00	2521	1.60	4-83	1.27	1.96
69	2KCD	91.30	79.24	83.40	16.60	0.00	0.00	1421	10.14	3-108	3.13	3.59
70	2KRT	97.01	82.72	81.80	18.20	0.00	0.00	1844	0.83	6-114	2.09	2.73
71	2LFI	89.30	76.07	85.90	14.10	0.00	0.00	1661	0.80	2-104	2.42	2.89
72	2JQN	97.81	90.68	88.50	11.50	0.00	0.00	1904	1.09	3-111	1.52	1.86
73	2L7Q	96.11	82.62	83.80	16.20	0.00	0.00	2125	1.74	12-37,46-101,105-114	1.57	2.15
74	2KFP	97.39	79.51	82.30	17.70	0.00	0.00	2650	8.46	3-115	2.23	2.89
75	1SE9	88.55	82.13	76.80	22.80	0.30	0.10	1507	1.85	17-84,94-101	2.10	2.59
76	2L3G	98.04	93.19	83.90	16.10	0.00	0.00	2870	2.34	13-123	1.28	1.95
77	2L3B	93.97	86.19	83.20	16.80	0.00	0.00	2185	0.81	14-38,45-113	1.05	1.63
78	2LRH	94.91	77.45	90.60	9.40	0.00	0.00	3261	5.26	3-122	2.30	2.75
79	1VEE	97.81	90.30	78.20	21.70	0.10	0.00	3627	5.14	6-123	1.03	1.41
80	2K1G	97.22	92.18	79.00	20.90	0.00	0.00	3366	14.38	5-78,83-122	1.05	1.68
81	2KKZ	96.50	87.83	82.40	16.80	0.80	0.00	2513	2.36	5-80,86-118	1.47	2.12
82	1VDY	95.48	88.37	84.60	15.40	0.00	0.00	3833	9.13	9-102,113-128	0.95	1.43
83	2KKL	94.06	80.60	71.40	28.40	0.10	0.00	2127	2.09	33-90,96-125	1.26	2.09
84	2N4B	98.94	90.25	85.00	14.50	0.60	0.00	3659	10.49	2-26,40-54,66-134	1.14	1.95
85	2L8V	93.82	76.58	85.00	15.00	0.00	0.00	1989	2.82	4-22,37-65,73-129	2.79	3.35
86	2LGH	98.03	88.92	83.50	16.40	0.00	0.00	2831	3.18	2-109,113-135	2.43	2.70
87	2K1S	98.83	92.02	86.50	13.50	0.00	0.00	2811	2.63	3-140	1.83	2.05
88	2M4F	90.80	81.83	82.30	16.90	0.80	0.00	3427	6.07	23-46,51-57,63-94,103-114,120-129,136-148	1.11	1.75
89	2JXP	97.08	89.62	86.50	13.50	0.00	0.00	2279	0.91	16-144	2.58	2.91
90	2L06	96.46	84.28	84.50	15.40	0.10	0.00	3374	13.42	15-38,45-141	1.57	2.05
91	2LAH	93.23	85.67	84.90	15.10	0.00	0.00	3573	10.34	14-25,33-158	1.71	2.22
92	2LAK	92.15	78.69	81.30	18.00	0.70	0.00	2180	4.21	10-37,68-77,93-139	1.54	1.82
93	2L82	97.87	81.05	85.40	14.40	0.20	0.00	3596	3.72	3-151	3.55	3.86
94	2M47	92.86	80.32	89.20	10.80	0.00	0.00	1930	1.46	5-25,40-56,66-156	4.72	5.42
95	2K3A	96.79	84.40	72.30	27.60	0.10	0.00	1680	0.81	57-102,108-127,138-153	0.99	1.34
96	2M7U	85.70	73.47	79.50	19.10	1.40	0.00	3243	15.64	12-151	2.14	2.96
97	2B3W	93.39	80.09	81.70	16.70	0.90	0.80	4315	23.41	16-162	2.67	3.37
98	KRAS4B	98.00	76.81	89.00	11.00	0.00	0.00	4678	10.89	4-24,37-59,66-163	1.60	2.30
99	2G0Q	93.99	84.33	79.30	20.30	0.00	0.40	3113	4.53	18-54,60-126	2.38	3.03
100	2LF2	97.56	85.86	86.10	13.80	0.10	0.00	3421	4.30	6-44,53-69,76-105,111-165	2.68	3.09

Residue ranges for RMSD calculation were determined by CYRANGE applied to the region between the first residue of the first secondary structure element and the last residue of the final secondary structure element of the reference PDB structure.

Supplementary Table 5 Structure accuracy prediction. Actual and predicted backbone RMSD between ARTINA and reference PDB structures. See Supplementary Figure 2 for details.

ID	Protein	RMSD to reference (Å)	Predicted RMSD to reference (Å)	Difference (Å)
1	6SVC	0.83	1.67	0.84
2	2JVD	0.71	0.56	-0.15
3	2K57	0.71	1.00	0.29
4	6SOW	1.16	2.44	1.28
5	2LX7	1.41	3.22	1.81
6	2MA6	1.56	2.00	0.44
7	2JRM	1.43	1.33	-0.10
8	1YEZ	0.73	0.78	0.05
9	2L9R	0.59	0.67	0.08
10	2K52	1.10	1.00	-0.10
11	2KRS	1.26	0.78	-0.48
12	2K53	0.88	0.78	-0.10
13	2JT1	0.94	0.67	-0.27
14	2JVO	1.77	0.78	-0.99
15	2ERR	2.09	2.78	0.69
16	2L1P	2.13	1.33	-0.80
17	2LN3	0.89	0.89	-0.00
18	2HEQ	0.60	0.89	0.29
19	2KK8	1.25	1.56	0.31
20	2KD0	1.37	0.78	-0.59
21	2LML	1.53	1.11	-0.42
22	2K3D	1.44	2.00	0.56
23	2LK2	1.42	0.67	-0.75
24	MH04	1.57	2.00	0.43
25	1PQX	1.40	0.56	-0.84
26	2L33	0.79	0.67	-0.12
27	2KZV	2.62	1.89	-0.73
28	2KCT	0.77	1.33	0.56
29	2MDR	1.72	1.67	-0.05
30	2FB7	1.94	1.56	-0.38
31	2MB0	1.11	1.00	-0.11
32	2L05	0.74	0.89	0.15
33	2KJR	1.02	0.89	-0.13
34	2M5O	1.08	1.11	0.03
35	MDM2	1.24	1.11	-0.13
36	2LNA	0.86	1.00	0.14
37	2LA6	0.81	0.78	-0.03
38	6FIP	2.05	3.00	0.95
39	2LEA	1.45	0.89	-0.56
40	2LL8	1.42	1.22	-0.20
41	2KPN	0.97	1.00	0.03
42	2K0M	1.60	1.22	-0.38
43	2K5V	0.94	0.89	-0.05
44	2MQL	0.98	0.33	-0.65
45	2K75	1.65	1.11	-0.54
46	2LTM	0.67	1.00	0.33
47	2KOB	2.24	1.78	-0.46
48	2KHD	1.87	2.44	0.57
49	2RN7	1.93	2.33	0.40
50	2LXU	1.19	1.11	-0.08
51	2KIF	0.89	1.00	0.11
52	2KBN	0.92	1.00	0.08
53	2MK2	1.56	1.78	0.22
54	2K50	1.00	1.00	0.00
55	2KL5	2.58	2.11	-0.47
56	2LTA	2.39	2.22	-0.17
57	2KIW	1.59	1.22	-0.37
58	2LVB	1.56	1.11	-0.45
59	2LND	0.85	1.11	0.26
60	1WQU	0.99	1.00	0.01
61	2KL6	0.87	1.33	0.46
62	6GT7	1.39	1.33	-0.06
63	2JN8	1.83	1.67	-0.16
64	2K5D	1.47	1.67	0.20
65	2KD1	1.99	2.78	0.79
66	2LTL	2.37	3.89	1.52
67	2KVO	1.87	2.22	0.35
68	1T0Y	1.27	1.00	-0.27
69	2KCD	3.13	3.00	-0.13
70	2KRT	2.09	1.89	-0.20
71	2LFI	2.42	3.11	0.69
72	2JQN	1.52	1.67	0.15
73	2L7Q	1.57	1.22	-0.35
74	2KFP	2.23	2.33	0.10
75	1SE9	2.10	2.00	-0.10
76	2L3G	1.28	2.00	0.72
77	2L3B	1.05	1.33	0.28
78	2LRH	2.30	3.00	0.70
79	1VEE	1.03	0.56	-0.47
80	2K1G	1.05	1.00	-0.05
81	2KKZ	1.47	2.00	0.53
82	1VDY	0.95	1.00	0.05
83	2KKL	1.26	1.11	-0.15
84	2N4B	1.14	1.00	-0.14
85	2L8V	2.79	2.56	-0.23
86	2LGH	2.43	2.78	0.35
87	2K1S	1.83	2.00	0.17
88	2M4F	1.11	1.33	0.22
89	2JXP	2.58	3.33	0.75
90	2L06	1.57	1.67	0.10
91	2LAH	1.71	2.44	0.73
92	2LAK	1.54	1.33	-0.21
93	2L82	3.55	2.67	-0.88
94	2M47	4.72	3.11	-1.61
95	2K3A	0.99	1.33	0.34
96	2M7U	2.14	2.56	0.42
97	2B3W	2.67	2.89	0.22
98	KRAS4B	1.60	1.22	-0.38
99	2G0Q	2.38	2.44	0.06
100	2LF2	2.68	2.33	-0.35

Supplementary Table 6 ANSURR structure evaluation scores. Correlation and RMSD scores given are the average of the corresponding scores calculated by ANSURR version 2.0.55 for the individual conformers of the structure calculated by ARTINA and the reference structure in the PDB, respectively.

ID	Protein	ARTINA		Reference	
		Correlation score (%)	RMSD score (%)	Correlation score (%)	RMSD score (%)
1	6SVC	18.6	34.6	21.4	12.2
2	2JVD	72.0	83.5	94.5	74.2
3	2K57	16.3	49.3	18.3	51.0
4	6SOW	44.7	63.2	60.6	84.5
5	2LX7	28.7	4.5	35.1	19.3
6	2MA6	21.8	2.4	61.9	70.7
7	2JRM	88.7	90.6	75.8	63.5
8	1YEZ	49.1	71.0	49.9	76.5
9	2L9R	92.0	33.0	77.4	90.9
10	2K52	4.1	7.4	23.5	81.4
11	2KRS	43.5	49.7	19.7	6.4
12	2K53	60.4	39.6	59.5	77.2
13	2JT1	77.1	24.1	93.1	71.7
14	2JVO	1.4	55.1	10.3	88.6
15	2ERR	29.4	34.9	25.8	86.7
16	2L1P	91.4	50.4	77.1	40.1
17	2LN3	64.7	89.6	56.9	85.4
18	2HEQ	82.3	63.0	91.8	69.5
19	2KK8	41.4	16.1	23.9	52.1
20	2KD0	59.1	43.1	17.1	40.5
21	2LML	36.7	37.4	73.9	87.9
22	2K3D	36.2	51.6	52.1	32.9
23	2LK2	96.7	36.7	97.7	44.1
24	MH04	51.3	24.4	18.1	25.5
25	1PQX	33.9	25.2	72.7	13.2
26	2L33	80.0	46.3	89.5	64.8
27	2KZV	89.8	45.8	64.2	11.8
28	2KCT	85.0	48.8	88.3	57.9
29	2MDR	38.6	57.4	36.0	36.1
30	2FB7	73.8	10.2	44.8	18.4
31	2MB0	49.4	52.1	43.1	56.9
32	2L05	68.9	45.1	54.9	62.5
33	2KJR	49.1	32.9	31.9	7.3
34	2M5O	71.0	42.8	92.5	91.5
35	MDM2	64.3	26.0	65.1	17.3
36	2LNA	73.3	43.8	69.9	64.9
37	2LA6	45.6	31.4	76.6	79.2
38	6FIP	54.9	33.2	57.3	44.0
39	2LEA	39.1	16.1	30.8	34.1
40	2LL8	14.4	77.9	45.3	90.4
41	2KPN	92.8	26.5	65.6	33.3
42	2K0M	24.0	45.8	24.9	72.2
43	2K5V	33.7	7.6	33.2	51.4
44	2MQL	40.8	36.4	61.9	21.0
45	2K75	15.2	9.4	28.7	20.0
46	2LTM	43.5	56.1	20.7	67.1
47	2KOB	63.3	32.6	80.9	75.2
48	2KHD	79.5	19.3	77.2	23.4
49	2RN7	91.1	24.1	88.6	41.7
50	2LXU	79.4	42.2	68.9	77.7
51	2KIF	26.4	58.4	53.6	85.9
52	2KBN	44.6	20.8	54.0	15.3
53	2MK2	72.2	31.2	64.9	46.1
54	2K50	46.9	15.3	65.5	65.2
55	2KL5	68.2	20.4	31.4	66.0
56	2LTA	21.3	45.9	38.0	92.7
57	2KIW	71.4	78.2	94.2	38.9
58	2LVB	30.2	70.1	51.7	96.3
59	2LND	43.0	84.7	55.3	96.7
60	1WQU	29.7	36.7	7.1	38.3
61	2KL6	42.1	18.9	31.9	55.5
62	6GT7	14.1	76.4	27.9	67.8
63	2JN8	67.1	47.5	90.5	47.1
64	2K5D	80.2	27.0	77.9	42.9
65	2KD1	71.5	35.6	65.2	71.3
66	2LTL	61.4	8.6	78.7	60.0
67	2KVO	27.3	40.1	68.5	22.2
68	1T0Y	95.3	42.3	56.9	64.6
69	2KCD	12.6	16.1	50.2	20.0
70	2KRT	28.0	29.6	23.1	62.7
71	2LFI	22.8	3.9	56.4	75.9
72	2JQN	5.1	35.1	36.7	40.7
73	2L7Q	83.5	9.7	60.5	51.7
74	2KFP	43.5	34.5	47.2	12.9
75	1SE9	78.1	11.5	82.0	44.6
76	2L3G	68.7	32.2	74.8	76.9
77	2L3B	49.2	12.6	68.2	59.6
78	2LRH	10.3	88.2	25.1	95.1
79	1VEE	0.9	37.6	1.1	50.5
80	2K1G	35.5	64.0	77.0	73.8
81	2KKZ	74.2	23.9	71.3	91.1
82	1VDY	3.7	26.9	5.7	50.8
83	2KKL	55.1	29.9	46.8	6.5
84	2N4B	22.1	23.3	48.0	62.4
85	2L8V	31.6	31.9	23.7	39.4
86	2LGH	48.4	36.5	65.8	85.1
87	2K1S	57.1	48.9	58.2	77.1
88	2M4F	81.5	26.5	76.9	46.5
89	2JXP	48.1	12.7	52.1	46.6
90	2L06	49.8	57.0	52.9	49.7
91	2LAH	24.8	63.1	19.8	92.2
92	2LAK	59.0	11.9	47.3	6.1
93	2L82	24.4	91.0	35.8	98.5
94	2M47	13.8	8.3	36.6	60.7
95	2K3A	81.0	28.0	74.7	61.0
96	2M7U	58.8	33.2	37.1	13.6
97	2B3W	73.2	24.4	55.9	55.5
98	KRAS4B	3.8	43.9	2.8	40.8
99	2G0Q	87.6	27.6	34.2	68.4
100	2LF2	31.8	29.4	28.6	35.2

Supplementary Table 7 RPF structure evaluation scores.

ID	Protein	Recall	Precision	F-measure	DP-score
1	6SVC	0.91	0.87	0.89	0.70
2	2JVD	0.93	0.93	0.93	0.77
3	2K57	0.94	0.86	0.90	0.75
4	6SOW	0.82	0.84	0.83	0.64
5	2LX7	0.86	0.84	0.85	0.52
6	2MA6	0.83	0.83	0.83	0.55
7	2JRM	0.86	0.88	0.87	0.67
8	1YEZ	0.85	0.82	0.83	0.65
9	2L9R	0.93	0.86	0.89	0.83
10	2K52	0.91	0.82	0.86	0.75
11	2KRS	0.93	0.90	0.92	0.78
12	2K53	0.89	0.89	0.89	0.66
13	2JT1	0.92	0.88	0.90	0.72
14	2JVO	0.81	0.90	0.85	0.70
15	2ERR	0.88	0.89	0.88	0.69
16	2L1P	0.81	0.88	0.85	0.68
17	2LN3	0.92	0.88	0.90	0.74
18	2HEQ	0.73	0.69	0.71	0.55
19	2KK8	0.87	0.88	0.88	0.64
20	2KD0	0.83	0.91	0.87	0.67
21	2LML	0.94	0.89	0.91	0.68
22	2K3D	0.85	0.90	0.87	0.68
23	2LK2	0.90	0.88	0.89	0.65
24	MH04	0.85	0.88	0.86	0.60
25	1PQX	0.80	0.86	0.83	0.65
26	2L33	0.88	0.88	0.88	0.74
27	2KZV	0.85	0.87	0.86	0.65
28	2KCT	0.85	0.88	0.87	0.75
29	2MDR	0.80	0.87	0.83	0.66
30	2FB7	0.78	0.81	0.79	0.57
31	2MB0	0.90	0.90	0.90	0.83
32	2L05	0.85	0.88	0.86	0.72
33	2KJR	0.89	0.90	0.89	0.74
34	2M5O	0.84	0.88	0.86	0.68
35	MDM2	0.93	0.87	0.90	0.65
36	2LNA	0.85	0.90	0.87	0.73
37	2LA6	0.89	0.87	0.88	0.72
38	6FIP	0.67	0.79	0.73	0.51
39	2LEA	0.79	0.88	0.83	0.68
40	2LL8	0.88	0.90	0.89	0.72
41	2KPN	0.89	0.87	0.88	0.78
42	2K0M	0.94	0.85	0.89	0.73
43	2K5V	0.94	0.92	0.93	0.81
44	2MQL	0.80	0.89	0.84	0.68
45	2K75	0.91	0.85	0.88	0.69
46	2LTM	0.91	0.87	0.89	0.79
47	2KOB	0.90	0.85	0.87	0.65
48	2KHD	0.92	0.85	0.88	0.64
49	2RN7	0.92	0.67	0.78	0.63
50	2LXU	0.92	0.88	0.90	0.73
51	2KIF	0.88	0.90	0.89	0.76
52	2KBN	0.91	0.88	0.89	0.72
53	2MK2	0.87	0.88	0.87	0.70
54	2K50	0.90	0.84	0.87	0.76
55	2KL5	0.83	0.79	0.81	0.63
56	2LTA	0.86	0.79	0.82	0.70
57	2KIW	0.89	0.85	0.87	0.61
58	2LVB	0.92	0.85	0.89	0.70
59	2LND	0.81	0.85	0.83	0.66
60	1WQU	0.87	0.92	0.89	0.80
61	2KL6	0.94	0.84	0.89	0.80
62	6GT7	0.90	0.84	0.87	0.76
63	2JN8	0.88	0.84	0.86	0.65
64	2K5D	0.87	0.92	0.89	0.74
65	2KD1	0.87	0.86	0.87	0.65
66	2LTL	0.90	0.85	0.87	0.63
67	2KVO	0.85	0.81	0.83	0.61
68	1T0Y	0.87	0.85	0.86	0.76
69	2KCD	0.90	0.79	0.84	0.53
70	2KRT	0.91	0.71	0.80	0.80
71	2LFI	0.78	0.83	0.81	0.53
72	2JQN	0.94	0.84	0.88	0.77
73	2L7Q	0.88	0.82	0.85	0.69
74	2KFP	0.80	0.87	0.83	0.59
75	1SE9	0.82	0.78	0.80	0.59
76	2L3G	0.92	0.86	0.89	0.77
77	2L3B	0.81	0.83	0.82	0.67
78	2LRH	0.80	0.86	0.82	0.63
79	1VEE	0.89	0.91	0.90	0.76
80	2K1G	0.87	0.88	0.88	0.80
81	2KKZ	0.90	0.82	0.86	0.68
82	1VDY	0.89	0.92	0.90	0.82
83	2KKL	0.84	0.88	0.86	0.65
84	2N4B	0.80	0.90	0.85	0.65
85	2L8V	0.86	0.77	0.81	0.62
86	2LGH	0.87	0.90	0.89	0.70
87	2K1S	0.80	0.84	0.82	0.61
88	2M4F	0.83	0.88	0.85	0.66
89	2JXP	0.90	0.82	0.86	0.73
90	2L06	0.89	0.87	0.88	0.72
91	2LAH	0.90	0.79	0.84	0.80
92	2LAK	0.90	0.84	0.87	0.72
93	2L82	0.82	0.83	0.82	0.70
94	2M47	0.89	0.81	0.85	0.69
95	2K3A	0.88	0.77	0.82	0.70
96	2M7U	0.80	0.71	0.75	0.72
97	2B3W	0.81	0.85	0.83	0.68
98	KRAS4B	0.92	0.88	0.90	0.83
99	2G0Q	0.86	0.80	0.83	0.72
100	2LF2	0.84	0.88	0.86	0.68

Calculated by the RPF web server at https://montelionelab.chem.rpi.edu/rpf/ running ASDP version 2.3. All scores are between 0 and 1, with higher values indicating better agreement between data and structure. Recall measures the fraction of NOE cross peaks that are retrieved by the query structures, while Precision measures the fraction of retrieved proton pair interactions in the query structure that are relevant, weighted by interproton distance. The F-measure score provides an assessment of the overall fit between the query model structure(s) and the experimental data, assuming that the input data are near complete; the Discriminating Power DP-score measures how the query structure is distinguished from a freely rotating chain model.[32] Scores depend on the NOESY peak lists, chemical shift assignments, and structures.

Supplementary Table 8 Consensus structure bundles. NMR structure bundles calculated by ARTINA and by using consensus distance restraints with the *multnoeassign* command of CYANA. RMSD values are the average of the 20 backbone RMSDs between the individual conformers and their mean coordinates for the residue given in Supplementary Table 4.

ID	Protein	ARTINA		Consensus	
		Target function value (Å^2)	**RMSD to mean (Å)**	**Target function value (Å^2)**	**RMSD to mean (Å)**
1	6SVC	1.80	0.04	0.61	0.12
2	2JVD	0.30	0.14	0.03	0.33
3	2K57	0.35	0.15	0.29	0.25
4	6SOW	2.32	0.10	0.45	0.40
5	2LX7	0.32	0.80	0.32	0.95
6	2MA6	3.25	0.14	1.95	0.41
7	2JRM	0.50	0.13	0.20	0.37
8	1YEZ	0.58	0.14	0.37	0.35
9	2L9R	0.37	0.21	0.36	0.30
10	2K52	2.68	0.17	0.84	0.48
11	2KRS	0.35	0.18	0.21	0.40
12	2K53	0.60	0.38	0.42	0.33
13	2JT1	0.11	0.29	0.10	0.35
14	2JVO	10.44	0.05	3.66	0.16
15	2ERR	13.61	0.46	8.86	0.62
16	2L1P	2.10	0.08	0.27	0.25
17	2LN3	1.15	0.14	0.09	0.27
18	2HEQ	3.20	0.03	0.82	0.30
19	2KK8	2.24	0.29	0.82	0.78
20	2KD0	4.43	0.07	1.63	0.24
21	2LML	0.67	0.48	0.57	0.69
22	2K3D	2.00	0.12	0.94	0.44
23	2LK2	0.94	0.36	0.45	0.43
24	MH04	0.86	0.46	0.54	0.81
25	1PQX	10.18	0.13	8.54	0.29
26	2L33	1.37	0.16	0.16	0.30
27	2KZV	0.41	0.46	0.30	0.81
28	2KCT	4.45	0.11	2.67	0.21
29	2MDR	3.06	0.12	0.86	0.42
30	2FB7	1.51	0.29	0.37	0.69
31	2MB0	9.63	0.09	4.22	0.25
32	2L05	2.07	0.17	0.53	0.53
33	2KJR	1.04	0.15	0.39	0.45
34	2M5O	7.18	0.07	3.54	0.24
35	MDM2	1.29	0.72	0.63	1.07
36	2LNA	4.06	0.14	1.06	0.61
37	2LA6	6.62	0.11	4.89	0.19
38	6FIP	17.06	0.13	6.79	1.39
39	2LEA	7.98	0.09	1.13	0.35
40	2LL8	2.64	0.24	1.08	0.44
41	2KPN	2.33	0.14	0.72	0.56
42	2K0M	0.69	0.43	0.53	0.57
43	2K5V	1.10	0.22	0.48	0.40
44	2MQL	22.17	0.09	5.11	0.18
45	2K75	0.77	0.41	0.21	0.65
46	2LTM	2.68	0.07	0.96	0.25
47	2KOB	2.66	0.33	1.16	0.55
48	2KHD	0.04	0.48	0.01	0.73
49	2RN7	1.80	1.02	0.61	0.12
50	2LXU	0.30	0.27	0.03	0.33
51	2KIF	3.64	0.14	0.68	0.41
52	2KBN	0.45	0.22	1.58	0.42
53	2MK2	2.62	0.39	0.21	0.71
54	2K50	0.86	0.25	1.04	0.40
55	2KL5	5.90	0.44	0.26	1.12
56	2LTA	0.73	0.46	1.96	0.63
57	2KIW	1.10	0.28	0.37	0.63
58	2LVB	0.86	0.50	0.41	0.52
59	2LND	1.29	0.15	1.12	0.62
60	1WQU	9.51	0.14	0.30	0.30
61	2KL6	1.99	0.17	2.90	0.56
62	6GT7	4.21	0.13	0.63	0.36
63	2JN8	1.12	0.39	1.73	0.72
64	2K5D	1.44	0.19	0.38	0.49
65	2KD1	6.35	0.26	0.46	0.63
66	2LTL	1.07	0.77	1.99	2.42
67	2KVO	3.88	0.22	0.66	0.75
68	1T0Y	1.60	0.15	1.73	0.46
69	2KCD	10.14	0.57	0.24	1.50
70	2KRT	0.83	0.58	5.44	0.90
71	2LFI	0.80	0.73	0.30	2.02
72	2JQN	1.09	0.58	0.43	0.72
73	2L7Q	1.74	0.23	1.02	0.55
74	2KFP	8.46	0.23	0.26	0.57
75	1SE9	1.85	0.48	4.15	1.05
76	2L3G	2.34	0.21	0.70	0.63
77	2L3B	0.81	0.30	0.76	0.55
78	2LRH	5.26	0.18	0.32	0.80
79	1VEE	5.14	0.13	0.76	0.26
80	2K1G	14.38	0.12	1.90	0.29
81	2KKZ	2.36	0.35	3.50	0.86
82	1VDY	9.13	0.13	0.69	0.47
83	2KKL	2.09	0.42	4.31	0.89
84	2N4B	10.49	0.10	0.44	0.38
85	2L8V	2.82	0.80	5.82	1.27
86	2LGH	3.18	0.56	1.06	0.83
87	2K1S	2.63	0.26	1.37	0.72
88	2M4F	6.07	0.18	0.59	0.54
89	2JXP	0.91	1.28	0.86	4.17
90	2L06	13.42	0.25	0.31	0.51
91	2LAH	10.34	0.35	5.11	0.89
92	2LAK	4.21	0.38	6.29	0.81
93	2L82	3.72	0.55	2.02	0.86
94	2M47	1.46	1.59	0.56	2.39
95	2K3A	0.81	0.25	0.78	0.45
96	2M7U	15.64	0.25	0.42	0.93
97	2B3W	23.41	0.33	7.67	0.89
98	KRAS4B	10.89	0.22	7.11	0.65
99	2G0Q	4.53	0.55	1.86	1.25
100	2LF2	4.30	0.38	1.13	0.82

Supplementary Table 9 Results of restrained energy refinement. CYANA structure bundles calculated by ARTINA were energy-refined in explicit water using OPALp. Backbone RMSDs to the reference PDB structure before and after energy refinement show a standard deviation of 0.07 Å, maximal deviation of 0.16 Å, and linear correlation coefficient of 0.998.

ID	Protein	CYANA		OPALp		ID	Protein	ARTINA		OPAlp	
		AMBER energy (kcal/mol)	**RMSD to reference (Å)**	**AMBER energy (kcal/mol)**	**RMSD to reference (Å)**			**AMBER energy (kcal/mol)**	**RMSD to reference (Å)**	**AMBER energy (kcal/mol)**	**RMSD to reference (Å)**
1	6SVC	-664	0.83	-974	0.91	51	2KIF	-2906	0.89	-3905	0.81
2	2JVD	-1590	0.71	-2044	0.59	52	2KBN	-3061	0.92	-3974	0.87
3	2K57	-1547	0.71	-2270	0.61	53	2MK2	-2936	1.56	-4013	1.49
4	6SOW	-1892	1.16	-2369	1.09	54	2K50	-3051	1.00	-3976	0.85
5	2LX7	-1981	1.41	-2372	1.37	55	2KL5	-3039	2.58	-4149	2.56
6	2MA6	-1200	1.56	-1740	1.40	56	2LTA	-3214	2.39	-4298	2.36
7	2JRM	-1733	1.43	-2309	1.38	57	2KIW	-2779	1.59	-3733	1.56
8	1YEZ	-1961	0.73	-2463	0.61	58	2LVB	-3533	1.56	-4492	1.52
9	2L9R	-1319	0.59	-1877	0.54	59	2LND	-3512	0.85	-4359	0.81
10	2K52	-2597	1.10	-3242	1.06	60	1WQU	-3058	0.99	-4019	0.89
11	2KRS	-2228	1.26	-2809	1.19	61	2KL6	-3287	0.87	-4413	0.78
12	2K53	-2055	0.88	-2753	0.87	62	6GT7	-3421	1.39	-4474	1.34
13	2JT1	-2064	0.94	-2792	0.87	63	2JN8	-3285	1.83	-4290	1.77
14	2JVO	-1912	1.77	-2573	1.77	64	2K5D	-3500	1.47	-4544	1.43
15	2ERR	-2788	2.09	-3397	2.04	65	2KD1	-2298	1.99	-3492	1.99
16	2L1P	-2259	2.13	-2932	2.14	66	2LTL	-3266	2.37	-4322	2.38
17	2LN3	-2501	0.89	-3284	0.82	67	2KVO	-3111	1.87	-4156	1.76
18	2HEQ	-1952	0.60	-2780	0.57	68	1T0Y	-3261	1.27	-4412	1.23
19	2KK8	-2369	1.25	-3099	1.20	69	2KCD	-2950	3.13	-4099	3.14
20	2KD0	-1865	1.37	-2553	1.29	70	2KRT	-4018	2.09	-5052	2.04
21	2LML	-2331	1.53	-3095	1.44	71	2LFI	-3451	2.42	-4437	2.45
22	2K3D	-2347	1.44	-3094	1.43	72	2JQN	-3560	1.52	-4547	1.48
23	2LK2	-2288	1.42	-3056	1.37	73	2L7Q	-3272	1.57	-4451	1.45
24	MH04	-2942	1.57	-3645	1.56	74	2KFP	-3419	2.23	-4485	2.15
25	1PQX	-2398	1.40	-3198	1.31	75	1SE9	-2800	2.10	-4006	2.07
26	2L33	-2613	0.79	-3353	0.80	76	2L3G	-4106	1.28	-5120	1.17
27	2KZV	-2599	2.62	-3276	2.60	77	2L3B	-3838	1.05	-4904	1.01
28	2KCT	-2484	0.77	-3225	0.73	78	2LRH	-3853	2.30	-5364	2.26
29	2MDR	-2770	1.72	-3540	1.74	79	1VEE	-3642	1.03	-4911	0.93
30	2FB7	-2359	1.94	-3153	1.89	80	2K1G	-4044	1.05	-5109	1.02
31	2MB0	-2934	1.11	-3905	1.03	81	2KKZ	-3854	1.47	-5136	1.38
32	2L05	-2134	0.74	-3053	0.69	82	1VDY	-4235	0.95	-5516	0.87
33	2KJR	-2797	1.02	-3557	1.03	83	2KKL	-3245	1.26	-4606	1.23
34	2M5O	-1612	1.08	-2526	1.04	84	2N4B	-4485	1.14	-5526	1.07
35	MDM2	-2857	1.24	-3644	1.24	85	2L8V	-4036	2.79	-5337	2.81
36	2LNA	-3227	0.86	-4005	0.76	86	2LGH	-3831	2.43	-5001	2.39
37	2LA6	-2771	0.81	-3645	0.78	87	2K1S	-5004	1.83	-6232	1.74
38	6FIP	-2719	2.05	-3637	2.04	88	2M4F	-4357	1.11	-5942	1.06
39	2LEA	-2738	1.45	-3599	1.38	89	2JXP	-4596	2.58	-5895	2.55
40	2LL8	-2611	1.42	-3403	1.34	90	2L06	-4389	1.57	-5848	1.47
41	2KPN	-2678	0.97	-3623	0.87	91	2LAH	-4976	1.71	-6375	1.67
42	2K0M	-3002	1.60	-3776	1.52	92	2LAK	-4201	1.54	-5388	1.43
43	2K5V	-2818	0.94	-3728	0.84	93	2L82	-5405	3.55	-7021	3.55
44	2MQL	-1780	0.98	-2762	0.93	94	2M47	-3907	4.72	-5279	4.72
45	2K75	-3142	1.65	-4036	1.57	95	2K3A	-4339	0.99	-5567	0.92
46	2LTM	-3030	0.67	-3870	0.57	96	2M7U	-4846	2.14	-6344	2.12
47	2KOB	-2974	2.24	-3982	2.19	97	2B3W	-4335	2.67	-5976	2.68
48	2KHD	-2886	1.87	-3686	1.80	98	KRAS4B	-5147	1.60	-6814	1.64
49	2RN7	-3214	1.93	-4240	1.92	99	2G0Q	-3999	2.38	-5697	2.36
50	2LXU	-3344	1.19	-4281	1.08	100	2LF2	-5149	2.68	-6737	2.68

Supplementary Table 10 Chemical shift assignment accuracy of protein core residues. Chemical shift assignment accuracy (%) is reported for core residues of the given amino acid types. The penultimate column (ARO) presents the accuracy calculated for His, Phe, Tyr, and Trp shifts. Core residues are those with a solvent-accessible surface area (SASA) in the protein of up to 20% of the corresponding SASA of the isolated residue. SASAs were calculated with Biopython 1.7.9.

Protein	**ALA**	**ARG**	**ASN**	**ASP**	**CYS**	**GLU**	**GLN**	**GLY**	**HIS**	**ILE**	**LEU**	**LYS**	**MET**	**PHE**	**PRO**	**SER**	**THR**	**TRP**	**TYR**	**VAL**	**ARO**	**RMSD**
6SVC	100.0	-	80.0	-	-	-	-	100.0	-	-	69.2	-	-	-	95.2	100.0	-	100.0	92.3	-	95.6	0.83
2JVD	100.0	-	-	-	-	97.0	93.3	-	-	100.0	100.0	94.1	-	-	-	-	-	-	-	-	-	0.71
2K57	100.0	-	100.0	100.0	-	100.0	100.0	100.0	-	100.0	100.0	-	-	87.5	100.0	100.0	100.0	-	85.7	100.0	86.7	0.71
6SOW	100.0	100.0	91.7	-	-	-	93.3	-	-	95.2	88.6	-	-	78.0	92.3	100.0	-	-	-	-	78.0	1.16
2LX7	85.7	-	-	-	100.0	93.9	-	100.0	-	100.0	100.0	100.0	-	71.0	91.7	-	94.7	95.0	-	100.0	80.4	1.41
2MA6	100.0	-	-	100.0	100.0	-	-	100.0	92.3	100.0	100.0	-	-	87.5	-	88.2	-	80.0	-	100.0	86.2	1.56
2JRM	100.0	-	-	100.0	71.4	-	-	90.0	-	-	100.0	-	-	-	-	100.0	-	95.0	100.0	-	96.3	1.43
1YEZ	100.0	-	-	100.0	-	-	-	100.0	-	98.8	92.9	-	-	87.5	100.0	100.0	100.0	-	100.0	97.7	91.3	0.73
2L9R	100.0	88.1	100.0	-	-	100.0	97.6	-	-	100.0	97.1	94.1	100.0	84.4	-	-	100.0	85.0	-	95.5	84.6	0.59
2K52	100.0	-	95.5	95.8	-	100.0	100.0	91.7	-	88.0	97.6	-	84.6	93.3	100.0	-	100.0	-	100.0	100.0	96.6	1.10
2KRS	100.0	100.0	-	100.0	-	100.0	-	97.6	-	100.0	100.0	-	100.0	-	100.0	100.0	-	100.0	100.0	97.7	100.0	1.26
2K53	100.0	-	95.0	100.0	100.0	95.0	-	100.0	-	100.0	100.0	100.0	94.4	100.0	-	100.0	100.0	-	100.0	100.0	100.0	0.88
2JT1	85.7	93.8	-	100.0	-	-	86.7	100.0	80.0	90.0	95.2	-	-	-	91.7	-	77.8	95.0	100.0	83.3	93.2	0.94
2JVO	87.5	84.6	-	-	-	90.0	-	100.0	90.9	84.6	94.9	-	50.0	70.5	27.3	95.2	100.0	-	-	94.1	73.0	1.77
2ERR	100.0	81.8	-	71.4	-	90.0	-	88.0	83.3	93.8	94.9	-	100.0	84.2	12.5	100.0	100.0	-	-	92.0	84.0	2.09
2L1P	92.9	-	-	-	100.0	-	92.9	50.0	-	92.9	87.1	82.4	-	93.8	-	91.7	100.0	97.5	92.9	100.0	95.7	2.13
2LN3	100.0	93.8	-	100.0	-	100.0	-	100.0	-	100.0	93.9	92.2	100.0	81.3	-	82.4	88.9	-	-	100.0	81.3	0.89
2HEQ	95.2	-	100.0	100.0	100.0	93.9	-	83.3	83.3	100.0	87.8	88.2	-	75.0	100.0	100.0	100.0	-	74.1	93.9	76.4	0.60
2KK8	-	-	100.0	100.0	100.0	81.8	90.5	-	-	95.2	92.8	100.0	90.9	84.6	-	100.0	92.0	-	100.0	96.1	92.6	1.25
2KD0	100.0	-	-	-	100.0	-	100.0	100.0	-	100.0	90.4	100.0	-	100.0	95.8	95.8	91.9	-	-	98.2	100.0	1.37
2LML	100.0	-	100.0	87.5	-	100.0	-	100.0	85.7	100.0	100.0	100.0	-	83.3	-	100.0	76.0	60.0	100.0	100.0	81.3	1.53
2K3D	100.0	-	82.9	100.0	-	-	71.4	100.0	-	94.2	100.0	100.0	100.0	87.1	-	97.0	96.4	-	97.6	93.9	91.1	1.44
2LK2	92.9	62.5	-	-	100.0	90.9	-	83.3	100.0	100.0	94.5	100.0	90.9	100.0	100.0	90.6	90.0	91.9	-	100.0	94.5	1.42
MH04	100.0	-	100.0	100.0	-	93.9	78.6	100.0	-	98.6	100.0	-	88.5	83.3	94.4	-	77.8	100.0	100.0	96.1	90.8	1.57
1PQX	100.0	-	100.0	100.0	-	-	100.0	100.0	80.0	96.4	97.6	94.1	84.6	68.8	-	91.7	94.4	95.0	100.0	96.6	82.9	1.40
2L33	100.0	-	95.0	-	-	100.0	-	100.0	-	-	95.4	100.0	79.2	95.3	100.0	-	100.0	-	100.0	100.0	96.4	0.79
2KZV	97.1	-	-	100.0	-	100.0	-	91.7	88.9	92.9	85.4	-	88.5	73.9	91.7	88.2	84.2	-	92.9	97.7	79.7	2.62
2KCT	100.0	87.5	-	100.0	-	100.0	-	97.2	-	100.0	94.0	-	-	100.0	100.0	-	95.6	-	100.0	98.7	100.0	0.77
2MDR	96.3	-	-	100.0	-	100.0	53.8	96.0	-	100.0	92.3	100.0	-	79.5	86.4	84.6	-	-	92.3	100.0	85.5	1.72
2FB7	100.0	-	-	100.0	-	-	-	91.7	-	90.6	90.0	92.6	-	70.0	-	93.8	94.3	-	100.0	100.0	85.0	1.94
2MB0	97.2	-	100.0	89.5	-	100.0	100.0	96.0	-	97.4	100.0	100.0	91.7	80.8	-	100.0	100.0	-	100.0	97.4	83.3	1.11
2L05	100.0	93.8	-	100.0	100.0	90.9	-	100.0	83.3	100.0	97.6	-	-	81.3	100.0	100.0	96.3	100.0	100.0	98.9	91.9	0.74
2KJR	100.0	-	91.7	87.5	-	100.0	93.3	100.0	71.4	100.0	92.9	94.1	100.0	75.0	-	100.0	94.7	-	92.9	100.0	79.5	1.02
2M5O	-	-	-	100.0	100.0	-	100.0	86.7	-	99.0	90.5	100.0	76.9	81.3	-	87.5	100.0	-	92.9	97.7	86.7	1.08
MDM2	100.0	-	100.0	83.3	0.0	-	100.0	100.0	70.0	91.5	97.8	-	100.0	64.0	100.0	100.0	95.8	-	63.1	100.0	64.0	1.24
2LNA	-	87.5	91.7	100.0	-	100.0	93.3	100.0	-	100.0	94.6	-	-	72.5	-	-	100.0	86.8	92.9	100.0	80.1	0.86
2LA6	100.0	-	73.8	100.0	-	90.9	-	95.8	-	99.0	100.0	-	-	89.5	100.0	95.8	100.0	-	100.0	100.0	90.8	0.81
6FIP	100.0	-	-	93.8	-	100.0	-	100.0	-	95.9	85.7	-	84.6	76.6	91.7	87.5	100.0	60.0	69.2	94.5	72.2	2.05
2LEA	100.0	63.6	90.0	96.4	-	100.0	-	93.1	-	92.3	93.2	68.8	51.2	96.4	88.9	90.5	97.4	-	-	98.6	96.4	1.45
2LL8	100.0	87.5	91.7	100.0	100.0	100.0	-	-	85.7	100.0	99.0	-	-	88.9	100.0	93.8	89.3	70.0	71.4	97.7	82.9	1.42
2KPN	96.4	-	-	100.0	-	-	93.3	100.0	91.7	100.0	97.6	-	-	100.0	100.0	-	97.8	-	93.1	99.0	94.7	0.97
2K0M	100.0	100.0	100.0	100.0	87.5	100.0	100.0	100.0	90.0	96.4	98.6	94.1	96.2	75.0	-	20.0	-	63.2	92.3	100.0	77.9	1.60
2K5V	97.1	-	91.7	100.0	-	100.0	80.0	100.0	-	96.4	100.0	94.1	-	87.5	-	100.0	100.0	-	100.0	100.0	91.3	0.94
2MQL	91.7	-	90.0	100.0	71.4	90.0	30.8	90.0	54.5	79.0	80.0	-	85.7	53.6	63.6	76.2	-	-	70.8	89.0	60.3	0.98
2K75	100.0	-	91.7	100.0	-	-	86.7	95.8	-	96.0	85.4	-	-	75.0	-	97.2	100.0	-	76.9	99.0	75.9	1.65
2LTM	100.0	100.0	100.0	83.3	-	-	100.0	100.0	-	100.0	91.8	98.0	69.6	86.3	95.8	100.0	100.0	85.0	100.0	98.2	87.6	0.67
2KOB	100.0	85.7	90.9	100.0	87.5	-	70.0	33.3	37.5	99.2	76.5	88.2	-	59.1	91.7	60.0	88.9	95.0	64.3	100.0	65.8	2.24
2KHD	100.0	75.0	-	-	-	100.0	-	100.0	-	100.0	85.7	91.2	-	77.1	-	-	100.0	-	100.0	100.0	85.5	1.87
2RN7	100.0	-	-	-	100.0	-	100.0	-	-	100.0	64.3	-	92.3	-	-	93.3	100.0	75.0	-	100.0	75.0	1.93
2LXU	100.0	-	83.3	100.0	100.0	98.2	93.3	95.7	-	97.6	98.2	98.0	96.2	81.3	100.0	100.0	100.0	-	-	99.0	81.3	1.19

Supplementary Table 10 continued

Protein	ALA	ARG	ASN	ASP	CYS	GLU	GLN	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL	ARO	RMSD
2KIF	100.0	96.4	90.9	100.0	-	90.0	92.9	100.0	-	91.3	95.2	90.6	-	75.6	100.0	90.5	100.0	97.4	92.3	100.0	87.7	0.89
2KBN	95.2	-	97.0	100.0	-	90.9	78.2	93.3	-	97.9	95.9	80.0	-	100.0	83.3	100.0	100.0	90.0	100.0	96.1	96.0	0.92
2MK2	100.0	93.8	-	100.0	93.8	100.0	-	94.4	71.4	96.4	95.7	-	-	94.1	100.0	94.1	100.0	100.0	92.9	100.0	91.8	1.56
2K50	100.0	85.7	100.0	96.8	-	100.0	-	86.7	85.7	96.4	93.9	100.0	76.9	100.0	79.2	88.9	94.4	90.0	-	100.0	95.1	1.00
2KL5	88.9	46.2	21.4	92.9	8.3	95.0	44.4	90.0	-	76.9	71.9	81.3	-	83.0	-	-	16.7	-	80.0	100.0	81.7	2.58
2LTA	92.9	-	-	87.5	-	100.0	100.0	-	-	97.4	91.4	87.1	-	100.0	-	68.8	100.0	70.0	100.0	95.5	88.0	2.39
2KIW	95.9	92.9	83.3	93.8	-	-	-	-	-	95.2	85.7	-	-	66.1	100.0	95.2	55.6	73.7	100.0	98.5	78.9	1.59
2LVB	100.0	-	100.0	100.0	-	90.9	100.0	61.5	-	96.9	92.9	78.8	61.5	89.6	83.3	84.4	100.0	-	92.6	97.0	90.7	1.56
2LND	94.3	-	95.2	100.0	-	77.3	89.3	63.2	-	98.0	95.2	-	69.2	87.5	100.0	94.6	94.4	-	97.4	97.0	92.0	0.85
1WQU	100.0	87.5	-	100.0	-	95.5	96.4	92.9	100.0	98.2	79.5	-	-	77.1	95.8	93.9	100.0	95.0	100.0	97.7	91.6	0.99
2KL6	100.0	75.0	93.5	100.0	-	100.0	-	100.0	100.0	100.0	83.3	94.1	-	96.9	95.8	100.0	93.1	76.9	95.3	99.4	90.5	0.87
6GT7	100.0	-	50.0	95.7	100.0	85.0	-	80.0	100.0	94.5	86.0	66.7	90.9	66.7	81.3	91.7	88.5	97.2	97.4	89.9	93.0	1.39
2JN8	97.6	93.8	100.0	75.0	-	100.0	100.0	100.0	55.6	100.0	97.1	94.1	38.5	87.5	100.0	75.0	100.0	97.5	100.0	86.4	87.5	1.83
2K5D	100.0	75.0	-	100.0	-	100.0	93.3	-	-	100.0	100.0	88.2	-	84.4	-	96.9	100.0	95.0	96.6	98.2	91.4	1.47
2KD1	100.0	93.3	81.8	-	-	90.9	-	93.3	90.9	96.8	95.8	100.0	84.6	75.0	-	84.4	100.0	85.0	79.2	97.7	82.0	1.99
2LTL	91.7	-	95.0	74.3	100.0	-	90.4	100.0	-	99.4	93.1	96.0	95.8	75.6	-	92.9	90.6	64.7	-	100.0	72.6	2.37
2KVO	100.0	-	100.0	87.5	-	100.0	71.4	96.7	-	100.0	88.1	88.2	89.2	75.7	97.2	97.5	94.7	90.0	100.0	98.5	83.9	1.87
1T0Y	100.0	-	100.0	100.0	-	90.0	100.0	100.0	100.0	97.6	89.1	94.1	100.0	92.9	-	92.3	100.0	-	97.6	96.8	97.1	1.27
2KCD	100.0	-	73.9	100.0	-	100.0	18.2	94.1	75.0	99.0	81.9	50.0	100.0	81.0	79.2	100.0	100.0	40.0	67.5	100.0	68.2	3.13
2KRT	85.7	-	85.7	87.5	-	81.8	78.6	100.0	-	93.6	77.9	90.0	100.0	90.9	25.0	100.0	100.0	-	100.0	100.0	93.5	2.09
2LFI	95.2	-	91.7	81.3	-	90.5	38.0	91.3	60.0	84.3	90.2	-	-	58.5	-	81.3	96.3	85.3	69.2	98.5	68.7	2.42
2JQN	96.4	-	-	100.0	-	100.0	76.7	95.5	90.0	100.0	87.9	94.1	-	82.5	91.7	95.8	100.0	100.0	100.0	100.0	90.4	1.52
2L7Q	100.0	50.0	83.3	91.7	-	95.5	70.5	100.0	-	94.6	90.2	-	100.0	85.2	91.7	91.4	94.7	60.0	88.8	100.0	84.3	1.57
2KFP	91.9	-	91.7	100.0	-	-	-	96.7	100.0	98.4	85.5	81.8	95.8	87.5	52.2	100.0	79.3	70.3	90.9	96.9	84.8	2.23
1SE9	100.0	100.0	-	100.0	-	100.0	100.0	100.0	-	82.1	94.3	74.4	90.9	75.0	75.0	93.3	100.0	100.0	100.0	92.4	87.9	2.10
2L3G	100.0	-	95.5	93.8	92.3	93.9	100.0	96.7	-	92.7	95.6	-	-	89.7	100.0	96.9	97.3	90.0	100.0	96.6	91.3	1.28
2L3B	100.0	82.4	-	100.0	100.0	90.9	75.0	100.0	-	95.2	94.7	-	100.0	89.6	83.3	79.2	93.3	-	93.5	100.0	91.6	1.05
2LRH	85.7	-	93.9	91.7	-	87.7	96.4	-	-	96.4	90.6	89.7	89.7	64.1	-	88.9	90.0	-	100.0	88.3	78.3	2.30
1VEE	100.0	77.8	100.0	100.0	-	-	100.0	95.8	-	100.0	95.7	94.1	-	88.7	89.2	89.6	96.4	100.0	98.2	100.0	94.9	1.03
2K1G	100.0	89.3	91.7	93.8	87.5	100.0	83.6	98.1	79.2	100.0	100.0	-	84.6	84.4	100.0	97.9	100.0	100.0	96.2	100.0	90.2	1.05
2KKZ	95.2	44.4	94.3	100.0	100.0	87.9	-	90.0	76.9	98.0	92.8	88.2	77.8	83.3	79.2	91.3	100.0	65.0	-	100.0	77.8	1.47
1VDY	100.0	89.5	100.0	100.0	100.0	90.9	100.0	66.7	-	97.3	84.9	92.6	92.3	88.6	100.0	89.5	89.7	-	96.4	100.0	91.7	0.95
2KKL	89.3	-	91.7	84.4	-	45.5	50.0	91.2	28.6	96.4	91.2	-	-	84.2	-	90.9	89.3	-	-	93.2	75.6	1.26
2N4B	100.0	88.2	87.5	100.0	-	97.0	93.3	100.0	80.0	100.0	100.0	-	100.0	82.3	100.0	100.0	95.7	80.0	90.5	97.0	83.0	1.14
2L8V	95.1	71.4	41.7	93.8	-	86.4	50.0	100.0	80.0	91.4	76.1	70.6	-	50.0	91.7	78.8	94.7	-	82.0	97.2	67.9	2.79
2LGH	98.4	88.2	55.9	100.0	100.0	100.0	92.0	100.0	91.7	97.6	96.3	100.0	100.0	82.5	100.0	100.0	100.0	79.1	100.0	98.9	82.8	2.43
2K1S	100.0	93.8	95.2	87.5	-	100.0	100.0	95.7	-	97.1	92.9	-	55.3	100.0	100.0	95.7	95.5	-	78.3	99.2	87.2	1.83
2M4F	100.0	-	100.0	100.0	-	92.1	-	100.0	-	100.0	97.3	97.1	92.3	70.1	-	87.5	100.0	75.0	72.7	100.0	71.8	1.11
2JXP	100.0	37.5	-	100.0	-	94.5	90.6	100.0	-	98.2	89.6	100.0	80.0	95.1	-	93.8	100.0	-	96.4	99.1	95.7	2.58
2L06	98.6	43.8	91.7	100.0	-	93.2	91.7	100.0	80.0	98.9	93.4	64.7	84.6	81.4	72.2	84.8	100.0	-	76.2	100.0	79.2	1.57
2LAH	97.2	92.3	97.5	100.0	87.5	90.0	84.6	80.0	78.6	93.6	90.5	100.0	75.0	74.3	90.9	81.8	93.8	94.3	92.3	96.7	84.2	1.71
2LAK	100.0	75.0	45.5	93.3	100.0	90.5	81.8	90.5	78.6	96.4	96.7	-	92.3	37.5	88.9	95.1	94.7	66.7	67.9	96.5	63.9	1.54
2L82	100.0	74.1	100.0	95.9	-	76.0	98.1	100.0	-	96.9	92.3	-	-	77.5	100.0	78.3	95.8	89.5	97.4	87.4	83.8	3.55
2M47	97.6	-	100.0	87.5	100.0	54.5	76.9	90.2	-	81.1	78.3	100.0	76.9	83.3	78.9	89.6	92.9	62.9	91.7	96.6	75.7	4.72
2K3A	100.0	-	97.0	-	87.5	95.5	85.7	90.0	57.1	98.2	100.0	-	100.0	-	83.3	94.6	100.0	91.7	93.5	100.0	87.3	0.99
2M7U	89.3	61.1	75.0	73.9	50.0	84.2	85.7	96.2	68.2	88.3	75.8	-	83.3	89.5	63.6	65.2	84.8	83.8	91.7	87.2	85.0	2.14
2B3W	92.8	91.1	73.9	95.5	-	75.8	75.9	82.1	80.8	100.0	84.4	79.4	72.2	77.2	95.8	87.5	81.4	71.8	53.8	96.0	71.6	2.67
KRAS4B	94.4	77.8	80.0	97.1	95.2	84.6	78.4	94.3	100.0	79.1	84.0	63.2	90.0	81.4	68.4	64.3	86.2	-	92.6	95.7	87.7	1.60
2G0Q	100.0	87.0	100.0	93.3	75.0	69.7	85.7	95.2	100.0	90.0	82.5	92.3	83.9	87.5	78.6	90.9	94.6	65.0	82.9	94.1	85.0	2.38
2LF2	100.0	87.5	83.3	100.0	87.5	86.4	93.3	95.1	100.0	99.3	89.7	-	87.5	89.7	100.0	92.0	91.8	61.2	96.2	100.0	82.4	2.68
Mean	97.7	81.8	89.2	95.7	88.4	92.8	85.4	93.6	81.3	96.1	91.6	90.3	86.6	82.2	88.3	91.0	94.2	83.6	91.4	97.5	85.2	1.55
Median	100.0	87.5	93.5	100.0	100.0	95.0	92.4	96.7	83.3	97.6	93.1	94.1	90.0	83.3	94.8	93.8	96.4	88.2	96.2	98.6	85.5	1.44

Supplementary Table 11 Quantitative analysis of sources of backbone RMSD in automatically determined structures. Each row presents backbone the RMSD to reference [Å] of an automatically determined protein structure. The quantity was calculated for 7 different residue ranges. The broadest one (**REF**) has been determined by CYRANGE[27] and corresponds to the values reported in Supplementary Table 4 and Figure 4. Remaining residue ranges cover the same fragments of the sequence as REF with the exclusion of: (**A**) the first secondary structure element, (**B**) the last secondary structure element, (**C**) α-helices, (**D**) β-sheets, (**E**) α-helices and β-sheets, and (**F**) flexible loops. The last column (**G**) presents difference between REF and the minimum value of A–F. Proteins that benefit by more than 0.5 Å RMSD decrease from the exclusion of one group of residues are highlighted in green. If a residue range contains less than 10 residues, its RMSD is not calculated.

ID	Protein	REF	A	B	C	D	E	F	G
1	6SVC	0.83	0.84	0.78	0.83	-	-	0.54	0.29
2	2JVD	0.71	0.58	0.68	-	0.71	-	0.69	0.13
3	2K57	0.71	0.74	0.69	0.71	0.66	0.68	0.60	0.11
4	6SOW	1.16	0.57	1.20	-	1.16	-	1.20	0.59
5	2LX7	1.41	1.43	1.43	1.41	1.59	1.59	0.70	0.71
6	2MA6	1.56	1.56	1.51	1.54	1.44	1.37	1.38	0.19
7	2JRM	1.43	1.46	1.58	1.87	1.43	-	1.04	0.39
8	1YEZ	0.73	0.70	0.74	0.73	0.86	0.86	0.63	0.10
9	2L9R	0.59	0.56	0.60	-	0.59	-	0.6	0.03
10	2K52	1.10	1.16	1.13	1.10	1.35	1.37	0.81	0.29
11	2KRS	1.26	1.28	1.22	1.26	1.43	1.40	1.16	0.10
12	2K53	0.88	0.88	0.92	0.80	0.88	-	0.85	0.08
13	2JT1	0.94	0.86	0.95	0.74	0.98	-	0.84	0.20
14	2JVO	1.77	1.76	1.73	1.83	1.63	1.73	1.67	0.14
15	2ERR	2.09	2.13	2.14	2.27	1.97	2.44	1.89	0.20
16	2L1P	2.13	2.25	2.07	2.96	2.13	2.96	1.5	0.63
17	2LN3	0.89	0.87	0.91	0.79	0.92	0.84	0.85	0.10
18	2HEQ	0.60	0.62	0.61	0.60	0.76	0.63	0.43	0.17
19	2KK8	1.25	1.23	1.26	1.28	1.16	1.39	1.08	0.17
20	2KD0	1.37	1.42	1.40	1.15	1.57	1.37	1.30	0.22
21	2LML	1.53	1.46	1.50	1.39	1.53	1.39	1.57	0.14
22	2K3D	1.44	1.28	1.44	1.32	1.54	1.49	1.33	0.16
23	2LK2	1.42	1.49	1.36	1.21	1.42	1.21	1.13	0.29
24	MH04	1.57	1.57	1.58	1.58	1.85	1.97	0.97	0.60
25	1PQX	1.40	1.44	1.39	1.24	1.61	1.62	1.19	0.21
26	2L33	0.79	0.72	0.77	0.70	0.90	-	0.70	0.09
27	2KZV	2.62	2.82	2.70	3.07	2.84	3.33	1.98	0.64
28	2KCT	0.77	0.71	0.78	0.77	0.79	0.79	0.65	0.12
29	2MDR	1.72	1.73	1.70	1.77	1.79	1.96	1.13	0.59
30	2FB7	1.94	2.02	2.01	1.94	2.5	2.5	1.41	0.53
31	2MB0	1.11	1.14	1.11	1.04	1.18	1.06	1.08	0.07
32	2L05	0.74	0.76	0.73	0.75	0.66	0.69	0.73	0.08
33	2KJR	1.02	1.05	1.02	1.06	1.08	1.26	0.83	0.19
34	2M5O	1.08	1.12	1.08	1.02	1.13	1.26	0.93	0.15
35	MDM2	1.24	1.22	1.19	1.17	1.26	1.20	1.08	0.16
36	2LNA	0.86	0.86	0.84	0.85	0.92	1.00	0.77	0.09
37	2LA6	0.81	0.82	0.81	0.81	0.87	0.91	0.56	0.25
38	6FIP	2.05	2.07	2.08	1.98	2.37	2.29	1.72	0.33
39	2LEA	1.45	1.36	1.47	1.51	1.36	1.42	1.34	0.11
40	2LL8	1.42	1.42	1.50	1.47	1.42	1.47	1.32	0.10

Supplementary Table 11 continued

ID	Protein	REF	A	B	C	D	E	F	G
41	2KPN	0.97	0.98	1.04	0.83	1.19	0.93	0.93	0.14
42	2K0M	1.60	1.62	1.57	1.38	1.82	1.45	1.52	0.22
43	2K5V	0.94	0.95	0.85	0.94	1.18	0.93	0.92	0.09
44	2MQL	0.98	1.01	0.98	0.96	1.10	1.14	0.82	0.16
45	2K75	1.65	1.65	1.64	1.65	1.73	1.76	1.47	0.18
46	2LTM	0.67	0.68	0.65	0.66	0.72	0.69	0.62	0.05
47	2KOB	2.24	2.20	2.28	2.08	2.24	2.23	2.20	0.16
48	2KHD	1.87	1.88	1.13	1.11	1.99	0.83	1.78	1.04
49	2RN7	1.93	1.12	2.12	-	1.93	-	1.81	0.81
50	2LXU	1.19	1.21	1.24	1.29	1.22	1.45	0.96	0.23
51	2KIF	0.89	0.90	0.90	0.98	0.92	1.02	0.79	0.10
52	2KBN	0.92	0.88	0.92	0.92	1.00	0.92	0.91	0.04
53	2MK2	1.56	1.58	1.57	1.57	1.80	1.91	1.11	0.45
54	2K50	1.00	1.00	0.91	1.00	0.90	0.88	1.01	0.12
55	2KL5	2.58	2.63	2.69	2.09	3.25	2.93	2.15	0.49
56	2LTA	2.39	2.47	2.32	2.18	2.65	2.88	1.92	0.47
57	2KIW	1.59	1.63	1.56	1.69	1.59	1.86	1.47	0.12
58	2LVB	1.56	1.57	1.65	1.83	1.56	2.36	1.20	0.36
59	2LND	0.85	0.86	0.82	0.66	0.84	0.69	0.87	0.19
60	1WQU	0.99	0.99	0.99	0.96	1.04	1.04	0.89	0.10
61	2KL6	0.87	0.89	0.88	0.87	1.09	1.09	0.63	0.24
62	6GT7	1.39	1.36	1.29	1.16	1.39	1.16	1.40	0.23
63	2JN8	1.83	1.74	1.87	2.17	1.83	2.22	1.61	0.22
64	2K5D	1.47	1.49	1.54	1.47	1.77	1.77	0.96	0.51
65	2KD1	1.99	1.97	1.89	1.94	1.99	2.04	1.91	0.10
66	2LTL	2.37	2.32	2.10	2.33	2.40	2.72	2.09	0.28
67	2KVO	1.87	1.89	2.00	2.01	2.11	2.64	1.33	0.54
68	1T0Y	1.27	1.29	1.30	1.31	1.43	1.71	0.88	0.39
69	2KCD	3.13	2.98	2.40	2.40	3.61	2.75	3.22	0.73
70	2KRT	2.09	1.92	2.00	1.94	2.41	2.18	1.90	0.19
71	2LFI	2.42	2.34	2.40	2.42	2.64	2.59	2.28	0.14
72	2JQN	1.52	1.55	1.51	1.50	1.65	1.57	1.37	0.15
73	2L7Q	1.57	1.35	1.58	1.57	1.61	1.60	1.53	0.22
74	2KFP	2.23	2.29	2.24	2.21	2.44	2.56	1.71	0.52
75	1SE9	2.10	2.19	2.20	2.19	2.48	2.93	1.10	1.00
76	2L3G	1.28	1.32	1.33	1.72	1.28	1.76	0.84	0.44
77	2L3B	1.05	0.97	1.02	1.05	0.96	0.96	1.07	0.09
78	2LRH	2.3	2.35	1.45	1.50	2.57	1.85	2.25	0.85
79	1VEE	1.03	1.03	1.03	1.02	1.09	1.10	0.89	0.14
80	2K1G	1.05	1.05	1.08	1.06	1.12	1.24	0.92	0.13
81	2KKZ	1.47	1.43	1.46	1.51	1.50	1.72	1.32	0.15
82	1VDY	0.95	0.88	1.01	1.12	0.95	1.20	0.83	0.12
83	2KKL	1.26	1.29	1.28	1.26	1.50	1.50	0.85	0.41
84	2N4B	1.14	1.17	1.13	1.17	1.22	1.40	0.94	0.20
85	2L8V	2.79	2.80	2.79	2.79	2.79	2.80	2.54	0.25
86	2LGH	2.43	2.49	2.58	2.67	2.83	3.57	1.67	0.76
87	2K1S	1.83	1.76	1.87	1.81	2.00	2.29	1.56	0.27
88	2M4F	1.11	1.14	1.13	1.16	1.48	1.93	0.83	0.28
89	2JXP	2.58	2.60	2.46	2.22	3.11	2.63	2.51	0.36
90	2L06	1.57	1.58	1.58	1.74	1.57	1.79	1.43	0.14
91	2LAH	1.71	1.75	1.64	1.90	1.71	1.95	1.63	0.08
92	2LAK	1.54	1.54	1.61	1.33	1.34	1.52	1.53	0.21
93	2L82	3.55	3.61	1.04	1.08	3.97	1.24	3.83	2.51
94	2M47	4.72	4.88	4.79	3.77	4.8	4.33	4.71	0.95
95	2K3A	0.99	0.97	1.00	1.02	1.05	1.14	0.89	0.10
96	2M7U	2.14	2.19	2.18	1.96	2.31	2.27	1.92	0.22
97	2B3W	2.67	2.62	2.60	2.91	2.59	2.77	2.50	0.17
98	KRAS4B	1.60	1.61	1.61	1.57	1.67	1.58	1.56	0.04
99	2G0Q	2.38	2.44	2.48	2.50	3.08	3.67	1.14	1.24
100	2LF2	2.68	2.71	2.24	2.37	3.03	3.00	2.51	0.44

Supplementary Table 12 Quality metrics of 26 protein structures determined without and with 4D CC-NOESY spectra.

Protein	Backbone RMSD to reference [Å]		Heavy-atom RMSD to reference [Å]		Backbone chemical shift assignment accuracy [%]		Side-chain chemical shift assignment accuracy [%]	
	without CCNOESY	with CCNOESY	without CCNOESY	with CCNOESY	without CCNOESY	with CCNOESY	without CCNOESY	with CCNOESY
2B3W	2.25	2.67	3.05	3.37	95.28	93.39	81.41	80.09
2HEQ	0.50	0.60	1.27	1.48	95.30	94.48	84.03	84.63
2K1S	1.49	1.83	1.82	2.05	98.39	98.83	92.14	92.02
2K3D	1.54	1.44	2.33	2.13	98.96	98.96	88.89	89.76
2K75	1.65	1.65	2.03	1.98	98.36	98.77	88.36	88.36
2KBN	1.09	0.92	1.76	1.46	98.18	97.98	89.49	88.49
2KCD	1.77	3.13	2.48	3.59	97.22	91.30	86.86	79.24
2KFP	2.03	2.23	2.65	2.89	97.02	97.39	81.96	79.51
2KIW	2.78	1.59	3.23	2.08	94.96	93.99	79.50	80.94
2KKL	1.80	1.26	2.45	2.09	94.06	94.06	81.67	80.60
2KOB	2.27	2.24	2.77	2.93	91.18	88.18	85.05	82.29
2KRS	1.02	1.26	1.35	1.50	98.47	98.47	96.40	96.18
2KVO	2.24	1.87	2.58	2.18	98.35	98.17	90.27	90.00
2KZV	2.04	2.62	2.68	3.13	96.58	95.84	83.45	81.67
2L3B	1.23	1.05	1.74	1.63	93.79	93.97	86.31	86.19
2L8V	7.49	2.79	7.87	3.35	93.63	93.82	76.32	76.58
2LAK	1.49	1.54	1.82	1.82	92.59	92.15	80.73	78.69
2LF2	3.79	2.68	4.10	3.09	97.80	97.56	86.58	85.86
2LGH	1.54	2.43	1.99	2.70	97.43	98.03	88.44	88.92
2LK2	0.90	1.42	1.66	1.98	96.81	96.08	87.44	86.08
2LML	1.15	1.53	1.54	1.90	97.44	97.44	91.53	91.71
2LNA	0.89	0.86	1.51	1.45	98.14	99.30	91.57	90.78
2LX7	1.42	1.41	1.93	2.02	97.81	98.54	88.59	87.84
2LXU	1.64	1.19	2.33	1.81	99.20	99.40	92.77	91.33
2MA6	1.52	1.56	2.09	2.09	98.59	98.94	89.36	89.36
2N4B	1.26	1.14	2.04	1.95	98.94	98.94	89.81	90.25
Median	**1.54**	**1.55**	**2.07**	**2.07**	**97.43**	**97.50**	**87.90**	**87.01**
Mean	**1.88**	**1.73**	**2.43**	**2.26**	**96.71**	**96.31**	**86.88**	**86.05**

Rows presenting proteins with more than 1 Å difference in backbone RMSD to reference are highlighted in green (if better without 4D CC-NOESY) or red (if better with 4D CC-NOESY).

Supplementary Table 13 Accuracy of automated chemical shift assignment using all input spectra. Chemical shift assignment accuracy (%) is reported for the 45 proteins in the automated chemical shift assignment experiment (see Results section).

Protein	**All shifts**	**Backbone**	**Side-chain**	**ALA**	**ARG**	**ASN**	**ASP**	**CYS**	**GLU**	**GLN**	**GLY**	**HIS**	**ILE**	**LEU**	**LYS**	**MET**	**PHE**	**PRO**	**SER**	**THR**	**TRP**	**TYR**	**VAL**
2JVD	95.8	99.6	93.2	100.0	100.0	91.7	-	-	98.7	91.1	100.0	-	100.0	100.0	90.8	100.0	75.0	-	95.8	100.0	-	92.9	100.0
2K57	95.9	99.6	93.2	100.0	95.8	100.0	95.8	-	100.0	98.2	100.0	-	100.0	100.0	95.3	-	65.6	100.0	100.0	97.8	-	78.6	100.0
2LX7	93.1	98.2	89.6	100.0	93.1	-	100.0	100.0	96.4	90.0	93.2	57.1	100.0	99.1	100.0	80.0	74.5	97.2	100.0	89.5	85.0	100.0	100.0
1YEZ	94.7	99.7	91.0	100.0	93.9	-	100.0	-	93.9	85.7	100.0	-	100.0	85.7	90.0	0.0	81.7	97.2	100.0	100.0	-	100.0	97.7
2K52	92.5	95.8	90.3	100.0	87.0	97.7	95.0	-	97.7	100.0	96.7	-	91.0	87.4	91.6	91.7	82.6	91.7	100.0	100.0	-	88.1	100.0
2JT1	89.2	92.8	86.7	100.0	90.0	87.5	100.0	-	92.5	86.7	100.0	80.0	92.9	85.7	80.9	100.0	-	87.5	75.9	94.4	95.0	92.9	84.1
2HEQ	87.5	95.0	82.0	95.0	96.9	97.0	96.8	100.0	95.5	-	85.4	61.3	100.0	91.7	92.9	-	50.0	95.0	87.5	100.0	55.0	71.1	92.7
2KD0	95.2	98.6	92.7	100.0	92.9	100.0	100.0	100.0	100.0	97.1	100.0	83.3	100.0	97.8	90.6	87.5	71.9	95.8	95.8	94.5	-	-	100.0
2LK2	90.8	97.5	86.1	100.0	83.1	91.7	96.8	100.0	87.0	92.2	83.3	91.3	98.2	89.7	85.0	96.0	90.5	97.9	89.3	96.4	86.5	95.1	100.0
MH04	92.9	98.8	88.7	98.6	86.4	100.0	100.0	-	92.4	84.5	100.0	-	97.1	97.1	95.2	80.8	85.7	96.7	90.0	80.0	80.0	96.4	97.7
2KZV	87.2	95.4	81.3	97.6	77.1	100.0	100.0	-	95.5	90.5	91.7	67.4	92.9	86.3	86.3	78.6	76.1	91.3	89.3	89.5	71.1	92.9	100.0
2L05	94.8	99.5	91.7	100.0	91.7	87.0	100.0	100.0	98.5	93.3	100.0	83.3	100.0	100.0	94.1	93.9	87.5	83.9	100.0	97.2	77.5	100.0	100.0
6FIP	88.6	98.5	81.8	100.0	78.1	100.0	90.9	-	100.0	96.4	100.0	0.0	96.9	92.9	86.3	84.6	72.4	95.8	93.8	100.0	70.0	61.5	100.0
2KPN	92.2	96.7	88.6	97.1	81.3	63.6	97.2	-	96.0	86.7	92.3	90.9	100.0	95.2	82.4	52.4	81.3	100.0	90.6	98.3	-	89.7	98.7
2K0M	91.7	95.3	89.1	94.6	96.4	100.0	97.9	68.8	97.3	100.0	97.6	72.7	97.1	94.0	95.7	92.3	63.0	95.7	89.2	100.0	57.9	87.5	98.7
2K5V	94.2	98.9	90.8	97.1	90.6	90.0	100.0	-	91.9	86.7	98.3	-	92.0	93.7	93.6	79.2	85.4	100.0	97.2	100.0	100.0	100.0	100.0
2KOB	81.8	87.4	77.8	100.0	72.5	85.3	85.4	87.5	83.1	73.3	66.7	25.0	100.0	84.2	76.2	0.0	56.7	91.7	71.3	88.9	95.0	71.4	100.0
2KHD	90.6	96.9	85.6	100.0	73.7	83.3	100.0	100.0	86.7	92.0	97.1	66.7	98.5	90.5	90.2	-	66.2	100.0	96.7	100.0	-	100.0	99.0
2MK2	94.0	99.2	90.0	100.0	87.7	100.0	100.0	100.0	98.2	94.0	97.9	76.2	96.4	95.1	100.0	81.8	95.7	97.9	90.4	100.0	80.0	87.5	97.9
2K50	92.3	98.0	88.3	100.0	94.3	100.0	100.0	-	96.6	-	96.7	80.6	98.2	91.1	95.1	63.4	87.1	65.0	93.9	91.7	90.0	-	97.7
2KIW	85.5	96.3	78.2	95.2	92.8	87.5	93.8	-	92.7	90.0	100.0	67.7	98.4	83.3	69.6	68.0	69.4	75.0	92.5	82.2	68.4	94.0	94.9
1WQU	90.5	98.6	84.9	100.0	93.4	100.0	100.0	-	95.5	87.8	95.0	86.1	98.6	80.5	77.9	-	75.0	96.9	95.2	100.0	97.5	95.2	97.9
2KL6	94.1	98.1	91.3	100.0	84.4	92.4	100.0	-	93.0	86.7	97.9	83.3	96.4	92.9	97.5	85.7	72.9	100.0	100.0	97.8	89.7	87.7	98.5
6GT7	85.1	96.7	78.1	100.0	90.6	58.8	95.5	100.0	76.6	100.0	86.7	90.0	94.2	88.7	77.0	100.0	76.2	79.2	94.4	83.3	64.6	88.2	94.9
2K5D	94.8	98.5	92.1	100.0	90.4	89.6	96.6	-	100.0	93.3	97.2	-	100.0	94.4	91.6	96.4	81.3	100.0	95.8	98.4	60.0	96.5	98.0
2KVO	91.3	96.7	87.3	100.0	77.0	93.6	92.5	-	96.1	90.5	93.3	75.0	100.0	89.8	90.4	94.0	75.5	79.2	96.9	96.9	90.0	90.5	98.5
2KCD	81.2	86.7	77.6	100.0	95.2	75.9	100.0	50.0	77.0	81.2	91.3	67.5	99.2	72.7	83.5	92.0	60.7	83.3	96.9	94.9	55.0	68.0	100.0
2L7Q	86.8	94.5	81.5	100.0	64.1	82.3	96.3	-	93.2	69.2	97.9	50.0	96.4	84.5	89.7	68.0	85.5	88.3	93.0	97.3	92.5	82.9	94.5
2KFP	86.2	96.8	79.6	97.3	68.2	91.2	100.0	-	89.6	90.5	94.4	81.0	98.4	90.1	75.1	95.8	82.1	76.8	93.8	86.2	86.0	74.3	96.9
2L3B	88.8	94.0	85.0	90.5	79.3	61.1	90.9	50.0	81.8	80.6	97.6	86.7	94.6	93.3	93.1	78.6	90.0	88.1	90.3	97.8	-	90.0	98.5
1VEE	92.9	98.0	89.1	100.0	93.5	100.0	100.0	-	98.5	100.0	93.4	-	100.0	98.0	84.6	-	76.7	96.5	85.8	95.3	97.5	83.9	100.0
2K1G	89.7	95.4	85.6	100.0	92.4	87.0	97.5	25.0	90.9	86.4	92.2	70.8	97.6	85.7	95.8	63.3	72.7	100.0	91.3	98.0	82.5	90.0	100.0
2KKZ	89.7	95.2	86.0	91.5	86.9	84.3	100.0	100.0	90.9	88.9	88.7	61.5	98.9	90.3	88.2	67.1	84.0	83.0	93.7	100.0	80.0	100.0	100.0
1VDY	90.2	95.5	86.4	100.0	91.9	84.6	100.0	100.0	78.5	100.0	71.7	95.2	99.1	84.3	90.1	84.6	78.9	96.6	87.3	93.1	100.0	92.9	100.0
2KKL	82.3	90.2	76.3	95.2	66.4	83.3	76.1	-	84.4	78.0	90.8	44.9	97.6	81.8	96.1	-	66.1	90.1	86.3	89.4	-	78.6	95.1
2L8V	82.2	93.1	74.6	97.9	77.8	83.3	98.4	-	83.6	70.0	96.7	88.9	92.9	76.8	74.6	-	65.3	89.4	72.3	97.2	89.5	72.1	84.7
2LGH	90.5	96.2	86.1	98.2	79.3	58.8	100.0	100.0	98.3	93.3	97.2	74.1	85.5	100.0	96.0	94.1	80.9	100.0	98.4	97.8	73.8	78.6	100.0
2M4F	85.1	91.1	80.4	96.4	100.0	90.7	93.8	-	87.2	46.2	97.6	44.4	93.9	98.2	78.9	76.9	70.3	-	76.8	94.4	70.0	65.4	99.1
2JXP	89.5	93.9	86.1	97.6	86.7	100.0	100.0	-	72.7	89.9	82.9	64.3	98.1	89.3	89.6	77.8	87.5	86.1	92.5	100.0	-	88.1	99.2
2LAK	84.2	91.7	78.6	93.7	79.0	45.5	100.0	100.0	82.2	92.0	91.5	72.9	100.0	90.2	94.1	77.8	65.4	81.2	92.4	85.5	63.2	62.7	93.6
2M47	84.6	91.6	79.0	98.2	83.0	93.8	74.1	100.0	84.7	79.5	91.2	66.7	85.6	89.2	96.1	53.8	86.7	76.1	80.3	92.9	58.1	95.8	85.8
2K3A	86.8	94.2	80.0	89.5	87.5	84.8	96.9	87.5	87.9	69.2	83.0	63.6	88.1	90.8	63.3	76.9	87.5	91.7	89.5	88.6	90.0	91.7	98.3
2B3W	82.2	89.6	77.4	96.2	79.4	80.7	94.5	-	83.1	82.6	94.1	61.4	98.8	88.6	81.9	74.2	81.1	94.3	83.0	57.7	65.4	52.6	96.5
KRAS4B	85.2	97.7	77.5	96.3	76.2	85.0	95.2	85.7	88.5	90.3	96.4	78.4	81.6	80.6	78.7	80.0	74.3	70.7	81.5	85.6	-	89.8	96.0
2LF2	89.1	96.6	83.5	96.9	71.4	90.3	98.9	87.5	96.8	93.3	95.4	81.0	98.4	90.6	77.2	85.0	85.8	96.7	93.0	95.4	69.3	88.5	100.0
Median	**89.7**	**96.6**	**86.0**	**100.0**	**87.0**	**90.0**	**98.7**	**100.0**	**92.7**	**90.0**	**96.4**	**72.9**	**98.2**	**90.3**	**90.1**	**80.4**	**76.5**	**94.3**	**92.5**	**96.9**	**80.0**	**89.7**	**98.7**

Supplementary Table 14 Accuracy of automated chemical shift assignment using all except NOESY-type input spectra. Chemical shift assignment accuracy (%) is reported for the 45 proteins in the automated chemical shift assignment experiment (see Results section).

Protein	All shifts	Backbone	Side-chain	ALA	ARG	ASN	ASP	CYS	GLU	GLN	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
2JVD	91.4	100.0	85.4	100.0	100.0	70.8	-	-	100.0	80.0	100.0	-	100.0	100.0	83.2	100.0	66.7	-	95.8	77.8	-	80.0	100.0
2K57	92.5	98.9	88.0	100.0	89.6	84.2	95.8	-	100.0	87.7	100.0	-	100.0	100.0	95.3	-	53.1	100.0	100.0	97.8	-	60.7	100.0
2LX7	85.8	93.8	80.4	100.0	93.1	-	100.0	87.5	83.6	65.0	84.7	85.7	100.0	99.1	100.0	100.0	57.4	94.4	100.0	89.5	55.0	85.2	100.0
1YEZ	92.3	98.7	87.5	100.0	92.7	-	100.0	-	87.8	78.6	100.0	-	100.0	85.7	90.0	100.0	69.0	97.2	95.8	100.0	-	100.0	97.7
2K52	85.4	94.1	79.7	85.7	84.8	77.3	85.0	-	96.6	67.9	86.7	-	99.1	69.5	96.4	83.3	63.0	79.2	100.0	100.0	-	61.9	100.0
2JT1	75.6	99.1	58.6	100.0	61.7	75.0	100.0	-	79.2	65.0	100.0	80.0	73.8	70.5	63.2	90.9	-	79.2	79.3	88.9	50.0	80.0	78.4
2HEQ	75.1	87.0	66.2	87.5	75.0	63.6	87.1	100.0	71.2	-	64.6	35.5	92.9	82.3	76.5	-	66.7	86.7	87.5	88.6	40.0	76.8	92.7
2KD0	92.9	97.5	89.5	100.0	92.9	90.9	100.0	100.0	100.0	91.4	90.5	66.7	100.0	92.8	91.2	95.8	62.5	95.8	94.4	94.5	-	-	100.0
2LK2	84.0	96.1	75.6	100.0	74.2	68.8	93.5	100.0	83.3	77.8	88.9	84.8	98.2	86.8	80.0	72.0	85.7	97.9	92.9	96.4	67.6	75.6	100.0
MH04	87.3	98.6	79.1	94.3	80.0	84.8	100.0	-	97.0	86.9	100.0	-	98.6	82.9	94.0	76.9	63.3	88.3	93.3	88.0	45.0	80.0	98.9
2KZV	77.0	91.0	66.9	97.6	63.5	75.8	89.1	-	90.9	52.4	83.3	69.6	89.3	66.1	79.4	92.9	60.9	95.7	81.3	78.9	57.9	78.6	93.2
2L05	81.8	95.5	73.1	100.0	82.3	60.9	100.0	100.0	90.9	53.3	86.7	66.7	97.1	87.3	77.3	87.9	75.0	46.2	91.7	100.0	55.0	78.6	100.0
6FIP	85.7	99.4	76.2	100.0	75.0	100.0	89.1	-	87.3	91.1	100.0	11.1	91.8	92.9	82.9	85.9	81.5	94.4	100.0	100.0	35.0	88.9	95.5
2KPN	87.9	96.3	81.3	97.1	87.5	86.4	95.8	-	87.9	66.7	94.9	68.2	100.0	89.3	75.9	61.9	58.3	89.6	87.5	96.6	-	76.2	97.4
2K0M	82.5	91.1	76.3	95.9	77.5	86.4	97.9	56.3	85.1	82.1	95.2	50.0	95.7	81.0	92.2	84.6	47.1	95.7	89.2	100.0	15.8	78.6	96.0
2K5V	89.5	98.5	83.1	97.1	81.3	75.0	100.0	-	88.9	66.7	93.3	-	91.1	97.6	90.9	87.5	64.6	100.0	97.2	100.0	60.0	73.2	100.0
2KOB	74.5	85.6	66.3	100.0	81.3	50.5	93.8	12.5	80.0	73.3	66.7	31.3	87.8	82.0	75.5	0.0	54.5	70.8	72.5	96.3	30.0	52.5	100.0
2KHD	83.0	92.5	75.4	100.0	71.9	69.4	100.0	93.8	80.6	80.0	88.6	62.5	58.2	88.9	89.2	-	54.9	100.0	93.3	100.0	-	69.0	96.0
2MK2	85.0	98.7	74.5	100.0	76.2	72.7	97.5	75.0	90.9	73.5	93.8	69.0	89.3	86.9	100.0	72.7	74.5	97.9	78.8	85.2	70.0	75.0	94.8
2K50	85.6	95.6	78.4	100.0	87.9	75.8	89.1	-	88.8	-	93.3	58.1	97.3	93.8	93.7	48.8	69.6	48.3	93.9	91.7	40.0	-	100.0
2KIW	78.3	95.2	67.0	95.2	90.4	66.7	93.8	-	87.3	70.0	100.0	51.6	92.1	85.7	62.9	64.0	61.3	77.8	83.6	77.8	73.7	76.2	89.9
1WQU	83.4	97.9	73.6	100.0	92.1	81.8	100.0	-	87.5	72.4	90.0	81.9	97.1	78.8	64.7	-	50.0	94.8	94.0	100.0	80.0	54.8	91.8
2KL6	85.9	95.5	79.2	100.0	53.1	73.7	90.6	-	85.2	66.7	97.9	83.3	98.2	94.6	86.6	95.2	45.8	98.3	100.0	95.6	46.2	67.9	98.0
6GT7	61.0	95.4	40.0	90.9	59.4	52.9	81.8	76.9	58.9	50.0	60.0	60.0	62.5	59.4	51.5	63.6	57.1	58.3	83.3	72.2	62.5	52.9	65.3
2K5D	88.0	96.4	81.8	100.0	86.5	68.8	90.9	-	96.6	66.7	88.9	-	100.0	86.5	88.2	64.3	68.8	97.2	95.8	100.0	75.0	63.2	98.0
2KVO	84.4	95.2	76.5	100.0	62.1	76.6	92.5	-	91.5	69.0	91.7	50.0	100.0	89.8	87.5	68.0	64.3	77.1	93.8	96.9	70.0	57.1	98.5
2KCD	76.3	85.6	70.1	100.0	81.0	60.2	88.9	62.5	86.2	61.4	91.3	65.0	99.2	67.4	80.0	100.0	50.0	80.0	93.8	94.9	60.0	61.6	100.0
2L7Q	61.1	72.9	52.7	95.2	34.4	49.4	86.3	-	66.7	32.4	91.7	50.0	81.0	64.3	62.9	68.0	43.1	86.7	83.7	78.4	5.0	25.9	96.4
2KFP	75.3	91.1	65.4	94.6	56.5	59.6	90.0	-	90.9	64.9	97.2	81.0	98.4	91.4	61.7	87.5	53.6	67.4	87.5	82.8	43.9	50.0	95.3
2L3B	68.7	83.1	57.8	90.5	51.2	50.0	78.4	25.0	69.1	46.8	92.9	53.3	94.6	59.3	70.3	71.4	68.6	78.6	83.3	97.8	-	53.0	83.1
1VEE	84.4	96.4	75.3	100.0	87.0	77.3	98.6	-	93.9	85.7	86.8	-	100.0	93.4	72.8	-	68.5	91.8	80.0	90.6	55.0	58.9	100.0
2K1G	82.6	94.6	74.1	100.0	86.4	72.5	100.0	0.0	83.1	72.7	79.2	70.8	97.6	85.7	92.4	67.3	61.0	100.0	82.6	92.0	40.0	73.8	100.0
2KKZ	71.2	83.5	62.8	83.0	76.2	60.2	78.6	100.0	70.2	75.6	79.2	30.8	81.1	61.0	71.6	52.9	59.6	50.0	82.5	79.2	70.0	85.7	97.4
1VDY	81.4	91.8	73.8	100.0	65.4	53.8	100.0	100.0	76.9	82.1	63.0	76.2	98.2	87.9	78.7	84.6	47.4	91.5	80.0	93.1	100.0	82.1	99.1
2KKL	57.8	69.4	49.0	86.7	32.9	57.1	67.0	-	72.5	49.2	80.3	30.6	50.0	48.3	88.2	-	34.7	64.8	64.4	51.1	-	100.0	64.0
2L8V	73.5	89.5	61.9	93.8	65.7	70.0	85.9	-	84.9	50.0	86.7	72.2	78.6	74.0	74.6	-	65.4	74.5	58.5	97.2	50.0	59.3	82.3
2LGH	82.0	92.6	73.7	84.7	74.1	50.0	93.1	100.0	89.2	75.2	93.1	67.2	84.3	98.1	94.0	85.3	61.8	100.0	96.9	95.5	47.6	92.9	99.1
2M4F	84.5	94.2	76.9	96.4	93.8	72.9	93.8	-	82.0	69.2	96.4	61.1	96.6	95.5	76.8	76.9	69.2	-	89.3	97.8	80.0	62.8	96.4
2JXP	79.3	86.7	73.4	96.0	78.8	63.6	80.0	-	54.0	66.1	74.3	75.0	91.6	79.4	84.3	55.6	68.8	86.1	78.8	100.0	-	71.4	95.9
2LAK	78.0	89.1	69.7	90.1	69.8	18.2	97.3	100.0	77.8	84.0	89.6	55.7	100.0	93.8	94.1	61.1	53.3	77.9	93.9	89.1	40.4	62.2	76.4
2M47	76.4	86.7	68.3	98.2	74.1	77.1	74.1	79.2	77.3	66.7	93.0	50.0	76.0	88.3	94.2	69.2	62.7	55.7	73.2	86.6	39.0	75.0	89.4
2K3A	82.8	94.5	72.1	91.0	87.5	73.3	100.0	87.5	83.8	73.1	83.0	70.5	84.5	93.9	95.9	84.6	6.3	91.7	82.4	86.2	75.0	67.8	98.3
2B3W	76.6	92.3	66.3	97.1	68.9	68.4	90.9	-	87.7	75.7	92.2	61.4	100.0	85.0	77.8	71.0	57.9	54.3	87.2	73.1	48.7	48.7	96.5
KRAS4B	66.9	85.7	55.4	92.6	52.3	55.0	76.2	95.2	73.8	54.0	96.4	70.3	59.2	77.1	55.1	80.0	60.8	31.7	57.4	73.3	-	48.1	89.3
2LF2	78.7	89.7	70.5	95.9	64.8	66.7	70.5	25.0	92.5	70.0	92.3	57.1	95.6	86.2	72.4	70.0	70.8	58.3	82.5	92.7	49.1	71.2	97.4
Median	**82.5**	**94.2**	**73.7**	**97.6**	**76.2**	**70.0**	**93.3**	**87.5**	**86.2**	**70.0**	**91.7**	**65.0**	**96.6**	**86.5**	**82.9**	**76.9**	**61.6**	**86.7**	**87.5**	**93.1**	**52.5**	**71.4**	**97.4**