Supporting Information for:

NMR Hyperfine Shifts in Blue Copper Proteins: a Quantum Chemical Investigation

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Full Citation of Gaussian 03 in Ref.21:

Gaussian 03, Revision B.03; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.;Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc., Pittsburgh PA, 2003.

Table S1. Large Models Used in the Calculations

Model	Geometry optimization	Protein	Residues
Calc3	No	Am	Cys 93 + Met 99 + His 96 + His 54 + Asn 55
		Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47
		Rc	Cys 138 + Met 148 + His 143 + His 85 + Ser 86
Calc4	Cys-SCH_2	Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47
		Rc	Cys 138 + Met 148 + His 143 + His 85 + Ser 86
Calc5	Cys-SCH_2 + Cu	Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47
		Rc	Cys 138 + Met 148 + His 143 + His 85 + Ser 86
Calc6	Cys-SCH_2 + Cu + other first coordination shell atoms	Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41 + Gly 39
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38 + Pro 36
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47 + Ala 45
		Rc	Cys 138 + Met 148 + His 143 + His 85 + Ser 86
Calc7	Cys-SCH_2 + Cu + other first coordination shell atoms	Am	Cys 93 + Met 99 + His 96 + His 54 + Asn 55 + Pro 53 + Glu 50
		Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45 + Ser 113 + Phe 114 + Thr 10 + Asp 11
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41 + Gly 39 + Asn 9 + water
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38 + Pro 36 + Ala 33 + Gly 34
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47 + Ala 45 + Thr 90 + Val 91 + water + water
		Rc	Cys 138 + Gln 139 + ILE 140 + Met 148 + His 143 + His 85 + Ser 86 + Gly 84 + Phe 83 + Asn 80
Calc8	No	Am	Cys 93 + Met 99 + His 96 + His 54 + Asn 55 + Pro 53 + Glu 50
		Az	Cys 112 + Met 121 + His 117 + His 46 + Asn 47 + Gly 45 + Ser 113 + Phe 114 + Thr 10 + Asp 11
		Pa	Cys 78 + Met 86 + His 81 + His 40 + Asn 41 + Gly 39 + Asn 9 + water
		Pc	Cys 84 + Met 92 + His 87 + His 37 + Asn 38 + Pro 36 + Ala 33 + Gly 34
		St	Cys 89 + Gln 99 + His 94 + His 46 + Asn 47 + Ala 45 + Thr 90 + Val 91 + water + water
		Rc	Cys 138 + Gln 139 + ILE 140 + Met 148 + His 143 + His 85 + Ser 86 + Gly 84 + Phe 83 + Asn 80

Table S2: The structure of the Calc3 model used for Am (PDB format)

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HETATM    1  N          53      16.576   2.131  10.730
HETATM    2  CA         53      16.032   0.778  10.889
HETATM    3  C          53      17.088  -0.066  11.587
HETATM    4  O          53      18.259   0.312  11.595
HETATM    5  CB         53      15.717   0.099   9.533
HETATM    6  CG         53      14.652   0.774   8.668
HETATM    7  ND1        53      13.378   0.752   9.010
HETATM    8  CD2        53      14.875   1.404   7.479
HETATM    9  CE1        53      12.769   1.374   8.031
HETATM   10  NE2        53      13.650   1.758   7.132
HETATM   11  H          53      17.552   2.241  10.493
HETATM   12  HA         53      15.104   0.854  11.455
HETATM   13 1HB         53      16.637  -0.009   8.958
HETATM   14 2HB         53      15.284  -0.865   9.801
HETATM   15  HD2        53      15.815   1.571   6.954
HETATM   16  HE1        53      11.695   1.547   7.970
HETATM   17  HE2        53      13.420   2.259   6.286
HETATM   18  N          54      16.689  -1.195  12.175
HETATM   19  CA         54      17.658  -2.107  12.766
HETATM   20  C          54      17.132  -3.509  12.492
HETATM   21  O          54      16.177  -3.673  11.717
HETATM   22  CB         54      17.815  -1.868  14.279
HETATM   23  HCG        54      16.991  -2.312  14.838
HETATM   24  H          54      15.705  -1.419  12.211
HETATM   25  HA         54      18.650  -1.954  12.340
HETATM   26 1HB         54      18.694  -2.347  14.662
HETATM   27 2HB         54      17.817  -0.791  14.428
HETATM   28  N          92      12.070  -5.197  12.800
HETATM   29  CA         92      12.663  -3.894  13.049
HETATM   30  C          92      12.038  -3.356  14.340
HETATM   31  O          92      10.802  -3.216  14.406
HETATM   32  CB         92      12.355  -2.989  11.877
HETATM   33  SG         92      13.050  -1.337  12.135
HETATM   34  H          92      11.181  -5.246  12.323
HETATM   35  HA         92      13.746  -3.950  13.159
HETATM   36 1HB         92      11.275  -2.913  11.751
HETATM   37 2HB         92      12.806  -3.418  10.982
HETATM   38  N          95       9.539  -0.454  13.939
HETATM   39  CA         95       8.594  -0.728  12.857
HETATM   40  C          95       8.327  -2.235  12.826
HETATM   41  O          95       8.796  -2.906  11.895
HETATM   42  CB         95       9.185  -0.271  11.501
HETATM   43  CG         95       9.817   1.123  11.475
HETATM   44  ND1        95      11.075   1.281  11.084
HETATM   45  CD2        95       9.227   2.301  11.843
HETATM   46  CE1        95      11.312   2.566  11.199
HETATM   47  NE2        95      10.220   3.160  11.645
HETATM   48  H          95      10.372  -1.020  14.015
HETATM   49  HA         95       7.666  -0.182  13.027
HETATM   50 1HB         95       9.912  -1.006  11.155
HETATM   51 2HB         95       8.326  -0.199  10.834
HETATM   52  HD2        95       8.214   2.485  12.202
HETATM   53  HE1        95      12.254   3.062  10.965
HETATM   54  HE2        95      10.148   4.153  11.816
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HETATM   55 CU    CU   107      12.489  -0.076  10.541
HETATM   56  N          98       7.803  -4.718   9.857
HETATM   57  CA         98       8.923  -5.104   8.994
HETATM   58  C          98       9.471  -6.398   9.570
HETATM   59  O          98      10.028  -6.383  10.678
HETATM   60  CB         98      10.057  -4.083   9.015
HETATM   61  CG         98       9.659  -2.748   8.476
HETATM   62  SD         98      11.028  -1.572   8.525
HETATM   63  CE         98      12.299  -2.353   7.559
HETATM   64  H          98       7.980  -4.058  10.601
HETATM   65  HA         98       8.568  -5.188   7.967
HETATM   66 1HB         98      10.424  -3.968  10.035
HETATM   67 2HB         98      10.840  -4.467   8.362
HETATM   68 1HG         98       9.312  -2.860   7.449
HETATM   69 2HG         98       8.858  -2.357   9.104
HETATM   70 1HE         98      13.179  -1.711   7.529
HETATM   71 2HE         98      12.562  -3.309   8.011
HETATM   72 3HE         98      11.935  -2.518   6.545
HETATM   73  H          73      17.590  -4.361  12.972
HETATM   74  H          74      16.366   2.677  11.553
HETATM   75  H          75       9.049  -0.456  14.822
HETATM   76  H          76       7.740  -2.705  13.601
HETATM   77  H          77      12.017  -5.714  13.666
HETATM   78  H          78      12.662  -3.101  15.184
HETATM   79  H          79       7.370  -5.547  10.238
HETATM   80  H          80       9.377  -7.323   9.020
CONECT    1   11    2   74
CONECT    2    1   12    3    5
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    7    5    8
CONECT    7    6    9   55
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   24   19
CONECT   19   18   25   20   22
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   23   26   27
CONECT   23   22
CONECT   24   18
CONECT   25   19
CONECT   26   22
CONECT   27   22
CONECT   28   34   29   77
CONECT   29   28   35   30   32
CONECT   30   29   31   78
CONECT   31   30
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CONECT   32   33   29   36   37
CONECT   33   32   55
CONECT   34   28
CONECT   35   29
CONECT   36   32
CONECT   37   32
CONECT   38   48   39   75
CONECT   39   38   49   40   42
CONECT   40   39   41   76
CONECT   41   40
CONECT   42   39   43   50   51
CONECT   43   44   42   45
CONECT   44   43   46   55
CONECT   45   43   47   52
CONECT   46   44   47   53
CONECT   47   45   46   54
CONECT   48   38
CONECT   49   39
CONECT   50   42
CONECT   51   42
CONECT   52   45
CONECT   53   46
CONECT   54   47
CONECT   55    7   33   44   62
CONECT   56   64   57   79
CONECT   57   56   65   58   60
CONECT   58   57   59   80
CONECT   59   58
CONECT   60   57   61   66   67
CONECT   61   60   62   68   69
CONECT   62   61   63   55
CONECT   63   62   70   71   72
CONECT   64   56
CONECT   65   57
CONECT   66   60
CONECT   67   60
CONECT   68   61
CONECT   69   61
CONECT   70   63
CONECT   71   63
CONECT   72   63
CONECT   73   20
CONECT   74    1
CONECT   75   38
CONECT   76   40
CONECT   77   28
CONECT   78   30
CONECT   79   56
CONECT   80   58
END
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Table S3: The structure of the Calc3 model used for Az (PDB format)

```
HETATM    1  N       A  45      10.834  28.132  10.253
HETATM    2  CA      A  45      11.984  28.847   9.738
HETATM    3  C       A  45      13.067  27.873   9.320
HETATM    4  O       A  45      13.179  26.786   9.896
HETATM    5  H       A  45      10.661  28.114  11.248
HETATM    6 1HA      A  45      11.684  29.447   8.879
HETATM    7 2HA      A  45      12.376  29.495  10.522
HETATM    8  N       A  46      13.843  28.237   8.304
HETATM    9  CA      A  46      14.955  27.410   7.855
HETATM   10  C       A  46      16.185  28.278   7.634
HETATM   11  O       A  46      16.080  29.416   7.177
HETATM   12  CB      A  46      14.605  26.708   6.537
HETATM   13  CG      A  46      13.353  25.890   6.588
HETATM   14  ND1     A  46      13.217  24.831   7.472
HETATM   15  CD2     A  46      12.257  25.900   5.779
HETATM   16  CE1     A  46      12.042  24.231   7.138
HETATM   17  NE2     A  46      11.472  24.887   6.097
HETATM   18  H       A  46      13.657  29.110   7.831
HETATM   19  HA      A  46      15.157  26.661   8.621
HETATM   20 1HB      A  46      14.523  27.449   5.741
HETATM   21 2HB      A  46      15.417  26.007   6.343
HETATM   22  HD2     A  46      12.059  26.629   4.993
HETATM   23  HE1     A  46      11.622  23.355   7.633
HETATM   24  HE2     A  46      10.602  24.644   5.645
HETATM   25  N       A  47      17.349  27.754   7.983
HETATM   26  CA      A  47      18.595  28.302   7.471
HETATM   27  C       A  47      19.320  27.195   6.719
HETATM   28  O       A  47      18.806  26.075   6.604
HETATM   29  CB      A  47      19.474  28.841   8.617
HETATM   30  H       A  47      17.372  26.964   8.612
HETATM   31  HA      A  47      18.385  29.138   6.804
HETATM   32 1HB      A  47      20.375  29.292   8.202
HETATM   33 2HB      A  47      18.882  29.583   9.153
HETATM   34  N       A 112      19.845  22.291   8.154
HETATM   35  CA      A 112      19.112  23.392   8.769
HETATM   36  C       A 112      19.217  23.222  10.276
HETATM   37  O       A 112      19.002  22.120  10.778
HETATM   38  CB      A 112      17.651  23.331   8.338
HETATM   39  SG      A 112      16.579  24.525   9.198
HETATM   40  H       A 112      19.447  21.363   8.191
HETATM   41  HA      A 112      19.523  24.355   8.464
HETATM   42 1HB      A 112      17.268  22.322   8.493
HETATM   43 2HB      A 112      17.629  23.601   7.282
HETATM   44  N       A 117      14.901  20.251  12.929
HETATM   45  CA      A 117      14.831  20.117  11.479
HETATM   46  C       A 117      15.897  19.207  10.881
HETATM   47  O       A 117      15.694  18.646   9.802
HETATM   48  CB      A 117      14.904  21.490  10.807
HETATM   49  CG      A 117      13.645  22.289  10.919
HETATM   50  ND1     A 117      13.444  23.422  10.174
HETATM   51  CD2     A 117      12.546  22.133  11.714
HETATM   52  CE1     A 117      12.283  23.921  10.522
HETATM   53  NE2     A 117      11.714  23.134  11.482
HETATM   54  H       A 117      15.334  21.064  13.343
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HETATM   55  HA      A 117      13.869  19.643  11.282
HETATM   56 1HB      A 117      15.733  22.058  11.229
HETATM   57 2HB      A 117      15.056  21.304   9.744
HETATM   58  HD2     A 117      12.382  21.320  12.421
HETATM   59  HE1     A 117      11.839  24.826  10.108
HETATM   60  HE2     A 117      10.823  23.288  11.932
HETATM   61 CU    CU A 199      14.539  24.127   8.740
HETATM   62  H          62      15.307  19.415  13.325
HETATM   63  H          63      16.830  19.053  11.402
HETATM   64  H          64      10.836  27.188   9.894
HETATM   65  H          65      20.787  22.268   8.519
HETATM   66  H          66      19.479  24.063  10.901
HETATM   67  H          67      20.289  27.388   6.283
HETATM   68  H          68      19.781  28.043   9.294
HETATM   69  N       A 121      16.342  17.634   7.133
HETATM   70  CA      A 121      16.843  18.704   6.293
HETATM   71  C       A 121      18.351  18.714   6.325
HETATM   72  O       A 121      18.962  19.492   7.057
HETATM   73  CB      A 121      16.299  20.048   6.771
HETATM   74  CG      A 121      14.795  20.141   6.699
HETATM   75  SD      A 121      14.195  21.812   6.939
HETATM   76  CE      A 121      14.681  22.524   5.353
HETATM   77  H       A 121      16.716  17.516   8.064
HETATM   78  HA      A 121      16.509  18.537   5.269
HETATM   79 1HB      A 121      16.626  20.229   7.795
HETATM   80 2HB      A 121      16.696  20.808   6.098
HETATM   81 1HG      A 121      14.454  19.768   5.734
HETATM   82 2HG      A 121      14.393  19.533   7.509
HETATM   83 1HE      A 121      14.385  23.573   5.320
HETATM   84 2HE      A 121      15.762  22.447   5.236
HETATM   85 3HE      A 121      14.189  21.982   4.545
HETATM   86  H          86      16.401  16.758   6.633
HETATM   87  H          87      18.902  18.029   5.697
CONECT    1    5    2   64
CONECT    2    1    6    7    3
CONECT    3    2    4    8
CONECT    4    3
CONECT    5    1
CONECT    6    2
CONECT    7    2
CONECT    8    3   18    9
CONECT    9    8   19   10   12
CONECT   10    9   11   25
CONECT   11   10
CONECT   12    9   13   20   21
CONECT   13   14   12   15
CONECT   14   13   16   61
CONECT   15   13   17   22
CONECT   16   14   17   23
CONECT   17   15   16   24
CONECT   18    8
CONECT   19    9
CONECT   20   12
CONECT   21   12
CONECT   22   15
CONECT   23   16
CONECT   24   17
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CONECT   25   10   30   26
CONECT   26   25   31   27   29
CONECT   27   26   28   67
CONECT   28   27
CONECT   29   26   32   33   68
CONECT   30   25
CONECT   31   26
CONECT   32   29
CONECT   33   29
CONECT   34   40   35   65
CONECT   35   34   41   36   38
CONECT   36   35   37   66
CONECT   37   36
CONECT   38   39   35   42   43
CONECT   39   38   61
CONECT   40   34
CONECT   41   35
CONECT   42   38
CONECT   43   38
CONECT   44   54   45   62
CONECT   45   44   55   46   48
CONECT   46   45   47   63
CONECT   47   46
CONECT   48   45   49   56   57
CONECT   49   50   48   51
CONECT   50   49   52   61
CONECT   51   49   53   58
CONECT   52   50   53   59
CONECT   53   51   52   60
CONECT   54   44
CONECT   55   45
CONECT   56   48
CONECT   57   48
CONECT   58   51
CONECT   59   52
CONECT   60   53
CONECT   61   14   39   50 75
CONECT   62   44
CONECT   63   46
CONECT   64    1
CONECT   65   34
CONECT   66   36
CONECT   67   27
CONECT   68   29
CONECT   69   77   70   86
CONECT   70   69   78   71   73
CONECT   71   70   72   87
CONECT   72   71
CONECT   73   70   74   79   80
CONECT   74   73   75   81   82
CONECT   75   74   76
CONECT   76   75   83   84   85
CONECT   77   69
CONECT   78   70
CONECT   79   73
CONECT   80   73
CONECT   81   74
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CONECT   82   74
CONECT   83   76
CONECT   84   76
CONECT   85   76
CONECT   86   69
CONECT   87   71
END
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Table S4: The structure of the Calc3 model used for Pa (PDB format)

```
HETATM    1  N   UNK     1      34.462  16.297  -2.840
HETATM    2  C   UNK     1      33.644  15.575  -1.868
HETATM    3  C   UNK     1      34.433  14.519  -1.127
HETATM    4  O   UNK     1      35.501  14.057  -1.555
HETATM    5  C   UNK     1      32.474  14.883  -2.602
HETATM    6  C   UNK     1      31.596  15.827  -3.374
HETATM    7  N   UNK     1      30.793  16.807  -2.836
HETATM    8  C   UNK     1      31.483  15.901  -4.725
HETATM    9  C   UNK     1      30.181  17.427  -3.827
HETATM   10  N   UNK     1      30.573  16.907  -4.987
HETATM   11  H   UNK     1      34.933  15.778  -3.567
HETATM   12  H   UNK     1      33.282  16.303  -1.142
HETATM   13  H   UNK     1      32.867  14.120  -3.274
HETATM   14  H   UNK     1      31.845  14.439  -1.830
HETATM   15  H   UNK     1      32.007  15.288  -5.458
HETATM   16  H   UNK     1      29.464  18.240  -3.713
HETATM   17  H   UNK     1      30.259  17.198  -5.902
HETATM   18  N   UNK     1      33.925  14.074   0.003
HETATM   19  C   UNK     1      34.465  12.968   0.777
HETATM   20  C   UNK     1      33.271  12.313   1.473
HETATM   21  O   UNK     1      32.125  12.690   1.247
HETATM   22  C   UNK     1      35.522  13.398   1.784
HETATM   23  H   UNK     1      33.099  14.535   0.358
HETATM   24  H   UNK     1      34.982  12.273   0.116
HETATM   25  H   UNK     1      36.113  12.532   2.083
HETATM   26  H   UNK     1      36.136  14.141   1.276
HETATM   27  N   UNK     1      29.061  14.229   3.644
HETATM   28  C   UNK     1      30.225  14.813   2.985
HETATM   29  C   UNK     1      30.645  15.974   3.886
HETATM   30  O   UNK     1      29.815  16.859   4.127
HETATM   31  C   UNK     1      29.895  15.231   1.576
HETATM   32  S   UNK     1      31.194  16.282   0.882
HETATM   33  H   UNK     1      28.150  14.625   3.462
HETATM   34  H   UNK     1      31.047  14.107   2.868
HETATM   35  H   UNK     1      28.948  15.771   1.570
HETATM   36  H   UNK     1      29.818  14.333   0.963
HETATM   37  N   UNK     1      30.089  19.668   2.719
HETATM   38  C   UNK     1      28.743  19.924   2.261
HETATM   39  C   UNK     1      27.631  19.420   3.171
HETATM   40  O   UNK     1      26.477  19.432   2.770
HETATM   41  C   UNK     1      28.546  19.327   0.852
HETATM   42  C   UNK     1      29.543  19.880  -0.138
HETATM   43  N   UNK     1      30.307  19.032  -0.928
HETATM   44  C   UNK     1      29.888  21.162  -0.414
HETATM   45  C   UNK     1      31.074  19.830  -1.682
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HETATM   46  N   UNK     1      30.849  21.102  -1.391
HETATM   47  H   UNK     1      30.422  18.714   2.725
HETATM   48  H   UNK     1      28.653  21.010   2.259
HETATM   49  H   UNK     1      28.645  18.243   0.900
HETATM   50  H   UNK     1      27.548  19.602   0.510
HETATM   51  H   UNK     1      29.482  22.062   0.049
HETATM   52  H   UNK     1      31.785  19.481  -2.431
HETATM   53  H   UNK     1      31.308  21.895  -1.817
HETATM   54 CU   UNK     1      30.465  17.118  -0.939
HETATM   55  N   UNK     1      24.408  17.224   2.157
HETATM   56  C   UNK     1      24.984  16.069   1.441
HETATM   57  C   UNK     1      25.231  14.932   2.419
HETATM   58  O   UNK     1      26.216  14.871   3.158
HETATM   59  C   UNK     1      26.268  16.516   0.738
HETATM   60  C   UNK     1      26.816  15.404  -0.159
HETATM   61  S   UNK     1      27.987  16.104  -1.359
HETATM   62  C   UNK     1      28.401  14.581  -2.218
HETATM   63  H   UNK     1      24.998  17.975   2.487
HETATM   64  H   UNK     1      24.292  15.700   0.684
HETATM   65  H   UNK     1      26.063  17.401   0.136
HETATM   66  H   UNK     1      27.015  16.747   1.497
HETATM   67  H   UNK     1      27.325  14.660   0.454
HETATM   68  H   UNK     1      25.991  14.933  -0.694
HETATM   69  H   UNK     1      29.120  14.794  -3.009
HETATM   70  H   UNK     1      28.835  13.873  -1.513
HETATM   71  H   UNK     1      27.498  14.153  -2.654
HETATM   72  H   UNK     1      35.130  16.877  -2.353
HETATM   73  H   UNK     1      33.439  11.508   2.173
HETATM   74  H   UNK     1      35.086  13.817   2.691
HETATM   75  H   UNK     1      29.220  14.195   4.641
HETATM   76  H   UNK     1      31.641  16.021   4.302
HETATM   77  H   UNK     1      30.216  20.075   3.635
HETATM   78  H   UNK     1      27.860  19.055   4.161
HETATM   79  H   UNK     1      23.827  16.895   2.915
HETATM   80  H   UNK     1      24.504  14.134   2.469
CONECT    1    2   11   72
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   54
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   25   26   74
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CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   75
CONECT   28   27   29   31   34
CONECT   29   28   30   76
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
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CONECT   80   57
END
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Table S5: The structure of the Calc3 model used for Pc (PDB format)

```
ATOM      1  N   UNK     1       4.103  34.339  15.185  1.00  0.00
ATOM      2  C   UNK     1       4.992  33.545  15.990  1.00  0.00
ATOM      3  C   UNK     1       5.176  32.169  15.301  1.00  0.00
ATOM      4  O   UNK     1       4.427  31.772  14.434  1.00  0.00
ATOM      5  C   UNK     1       4.395  33.294  17.344  1.00  0.00
ATOM      6  C   UNK     1       4.163  34.407  18.291  1.00  0.00
ATOM      7  N   UNK     1       5.162  35.218  18.775  1.00  0.00
ATOM      8  C   UNK     1       2.952  34.795  18.848  1.00  0.00
ATOM      9  C   UNK     1       4.572  36.081  19.598  1.00  0.00
ATOM     10  N   UNK     1       3.236  35.857  19.674  1.00  0.00
ATOM     11  H   UNK     1       3.437  33.878  14.758  1.00  0.00
ATOM     12  H   UNK     1       5.838  33.996  16.025  1.00  0.00
ATOM     13  H   UNK     1       3.447  32.920  17.176  1.00  0.00
ATOM     14  H   UNK     1       4.944  32.577  17.764  1.00  0.00
ATOM     15  H   UNK     1       2.063  34.452  18.734  1.00  0.00
ATOM     16  H   UNK     1       5.044  36.764  20.072  1.00  0.00
ATOM     17  H   UNK     1       2.630  36.345  20.187  1.00  0.00
ATOM     18  N   UNK     1       6.198  31.468  15.812  1.00  0.00
ATOM     19  C   UNK     1       6.450  30.074  15.388  1.00  0.00
ATOM     20  C   UNK     1       7.065  29.344  16.612  1.00  0.00
ATOM     21  O   UNK     1       7.373  29.977  17.639  1.00  0.00
ATOM     22  C   UNK     1       7.216  29.930  14.115  1.00  0.00
ATOM     23  H   UNK     1       6.688  31.779  16.493  1.00  0.00
ATOM     24  H   UNK     1       5.553  29.723  15.172  1.00  0.00
ATOM     25  H   UNK     1       7.272  28.907  13.865  1.00  0.00
ATOM     26  H   UNK     1       6.755  30.319  13.352  1.00  0.00
ATOM     27  N   UNK     1      10.796  30.916  19.636  1.00  0.00
ATOM     28  C   UNK     1      10.020  31.569  18.549  1.00  0.00
ATOM     29  C   UNK     1      11.116  32.329  17.768  1.00  0.00
ATOM     30  O   UNK     1      11.756  33.220  18.363  1.00  0.00
ATOM     31  C   UNK     1       8.950  32.469  19.093  1.00  0.00
ATOM     32  S   UNK     1       8.211  33.486  17.848  1.00  0.00
ATOM     33  H   UNK     1      11.089  31.512  20.273  1.00  0.00
ATOM     34  H   UNK     1       9.572  30.918  18.020  1.00  0.00
ATOM     35  H   UNK     1       8.217  31.999  19.529  1.00  0.00
ATOM     36  H   UNK     1       9.394  33.098  19.763  1.00  0.00
ATOM     37  N   UNK     1      11.296  36.270  17.651  1.00  0.00
ATOM     38  C   UNK     1      11.306  36.871  18.972  1.00  0.00
ATOM     39  C   UNK     1      12.266  36.245  19.959  1.00  0.00
ATOM     40  O   UNK     1      12.106  36.448  21.183  1.00  0.00
ATOM     41  C   UNK     1       9.880  36.740  19.559  1.00  0.00
ATOM     42  C   UNK     1       8.845  37.461  18.738  1.00  0.00
ATOM     43  N   UNK     1       7.577  36.945  18.572  1.00  0.00
ATOM     44  C   UNK     1       8.935  38.696  18.126  1.00  0.00
ATOM     45  C   UNK     1       6.944  37.818  17.826  1.00  0.00
ATOM     46  N   UNK     1       7.709  38.881  17.542  1.00  0.00
ATOM     47  H   UNK     1      11.006  35.404  17.600  1.00  0.00
ATOM     48  H   UNK     1      11.438  37.847  18.912  1.00  0.00
ATOM     49  H   UNK     1       9.710  35.772  19.725  1.00  0.00
ATOM     50  H   UNK     1       9.947  37.122  20.472  1.00  0.00
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ATOM      51  H   UNK     1       9.672  39.307  18.064  1.00  0.00
ATOM      52  H   UNK     1       6.019  37.728  17.527  1.00  0.00
ATOM      53  H   UNK     1       7.461  39.639  17.027  1.00  0.00
ATOM      54  N   UNK     1      11.565  35.142  23.943  1.00  0.00
ATOM      55  C   UNK     1      10.455  34.174  23.708  1.00  0.00
ATOM      56  C   UNK     1      11.047  32.771  23.434  1.00  0.00
ATOM      57  O   UNK     1      11.195  32.324  22.289  1.00  0.00
ATOM      58  C   UNK     1       9.557  34.671  22.579  1.00  0.00
ATOM      59  C   UNK     1       8.275  33.872  22.515  1.00  0.00
ATOM      60  S   UNK     1       7.019  34.631  21.519  1.00  0.00
ATOM      61  C   UNK     1       5.801  33.261  21.553  1.00  0.00
ATOM      62  H   UNK     1      11.864  35.581  23.255  1.00  0.00
ATOM      63  H   UNK     1       9.970  34.104  24.548  1.00  0.00
ATOM      64  H   UNK     1       9.358  35.619  22.729  1.00  0.00
ATOM      65  H   UNK     1      10.006  34.653  21.680  1.00  0.00
ATOM      66  H   UNK     1       8.325  32.957  22.118  1.00  0.00
ATOM      67  H   UNK     1       7.876  33.784  23.448  1.00  0.00
ATOM      68  H   UNK     1       6.370  32.432  21.623  1.00  0.00
ATOM      69  H   UNK     1       5.203  33.494  22.203  1.00  0.00
ATOM      70  H   UNK     1       5.477  33.177  20.590  1.00  0.00
ATOM      71 Cu   UNK     1       7.050  34.960  18.716  1.00  0.00
ATOM      72  H   UNK     1      12.217  36.341  17.242  1.00  0.00
ATOM      73  H   UNK     1      13.082  35.629  19.610  1.00  0.00
ATOM      74  H   UNK     1       7.227  28.277  16.572  1.00  0.00
ATOM      75  H   UNK     1       8.176  30.417  14.288  1.00  0.00
ATOM      76  H   UNK     1      11.588  30.431  19.239  1.00  0.00
ATOM      77  H   UNK     1      11.323  32.095  16.734  1.00  0.00
ATOM      78  H   UNK     1      12.332  34.670  24.401  1.00  0.00
ATOM      79  H   UNK     1      11.342  32.159  24.273  1.00  0.00
ATOM      80  H   UNK     1       4.639  34.861  14.507  1.00  0.00
CONECT     1    2   11   80
CONECT     2    1    3    5   12
CONECT     3    2    4   18
CONECT     4    3
CONECT     5    2    6   13   14
CONECT     6    5    7    8
CONECT     7    6    9   71
CONECT     8    6   10   15
CONECT     9    7   10   16
CONECT    10    8    9   17
CONECT    11    1
CONECT    12    2
CONECT    13    5
CONECT    14    5
CONECT    15    8
CONECT    16    9
CONECT    17   10
CONECT    18    3   19   23
CONECT    19   18   20   22   24
CONECT    20   19   21   74
CONECT    21   20
CONECT    22   19   25   26   75
CONECT    23   18
CONECT    24   19
CONECT    25   22
CONECT    26   22
CONECT    27   28   33   76
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CONECT   28   27   29   31   34
CONECT   29   28   30   77
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   71
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   72
CONECT   38   37   39   41   48
CONECT   39   38   40   73
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   71
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54   55   62   78
CONECT   55   54   56   58   63
CONECT   56   55   57   79
CONECT   57   56
CONECT   58   55   59   64   65
CONECT   59   58   60   66   67
CONECT   60   59   61   71
CONECT   61   60   68   69   70
CONECT   62   54
CONECT   63   55
CONECT   64   58
CONECT   65   58
CONECT   66   59
CONECT   67   59
CONECT   68   61
CONECT   69   61
CONECT   70   61
CONECT   71    7   32   43   60
CONECT   72   37
CONECT   73   39
CONECT   74   20
CONECT   75   22
CONECT   76   27
CONECT   77   29
CONECT   78   54
CONECT   79   56
CONECT   80    1
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
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Table S6: The structure of the Calc3 model used for St (PDB format)

ATOM	1	N	UNK	1	26.904	26.900	40.895	1.00	0.00
ATOM	2	C	UNK	1	27.565	27.152	39.606	1.00	0.00
ATOM	3	C	UNK	1	26.474	27.805	38.715	1.00	0.00
ATOM	4	O	UNK	1	25.343	27.298	38.697	1.00	0.00
ATOM	5	C	UNK	1	27.903	25.772	38.955	1.00	0.00
ATOM	6	S	UNK	1	28.606	26.113	37.282	1.00	0.00
ATOM	7	H	UNK	1	26.257	26.130	40.989	1.00	0.00
ATOM	8	H	UNK	1	28.463	27.760	39.715	1.00	0.00
ATOM	9	H	UNK	1	28.646	25.256	39.563	1.00	0.00
ATOM	10	H	UNK	1	27.013	25.147	38.883	1.00	0.00
ATOM	11	N	UNK	1	33.083	25.534	34.695	1.00	0.00
ATOM	12	C	UNK	1	32.040	25.855	35.747	1.00	0.00
ATOM	13	C	UNK	1	32.496	27.154	36.414	1.00	0.00
ATOM	14	O	UNK	1	33.515	27.736	36.081	1.00	0.00
ATOM	15	C	UNK	1	32.207	24.725	36.859	1.00	0.00
ATOM	16	C	UNK	1	31.822	23.389	36.314	1.00	0.00
ATOM	17	N	UNK	1	30.515	23.077	36.011	1.00	0.00
ATOM	18	C	UNK	1	32.583	22.308	35.952	1.00	0.00
ATOM	19	C	UNK	1	30.468	21.831	35.518	1.00	0.00
ATOM	20	N	UNK	1	31.696	21.352	35.483	1.00	0.00
ATOM	21	H	UNK	1	34.067	25.698	34.852	1.00	0.00
ATOM	22	H	UNK	1	31.031	25.921	35.340	1.00	0.00
ATOM	23	H	UNK	1	33.244	24.696	37.194	1.00	0.00
ATOM	24	H	UNK	1	31.553	24.962	37.698	1.00	0.00
ATOM	25	H	UNK	1	33.667	22.218	36.019	1.00	0.00
ATOM	26	H	UNK	1	29.568	21.304	35.200	1.00	0.00
ATOM	27	H	UNK	1	31.951	20.429	35.163	1.00	0.00
ATOM	28	N	UNK	1	31.769	27.553	37.459	1.00	0.00
ATOM	29	C	UNK	1	32.239	28.694	38.251	1.00	0.00
ATOM	30	C	UNK	1	31.679	28.485	39.674	1.00	0.00
ATOM	31	O	UNK	1	31.049	27.430	39.910	1.00	0.00
ATOM	32	C	UNK	1	31.824	30.024	37.674	1.00	0.00
ATOM	33	H	UNK	1	30.911	27.078	37.700	1.00	0.00
ATOM	34	H	UNK	1	33.328	28.730	38.252	1.00	0.00
ATOM	35	H	UNK	1	32.182	30.827	38.318	1.00	0.00
ATOM	36	H	UNK	1	32.272	30.091	36.683	1.00	0.00
ATOM	37	N	UNK	1	23.450	23.921	35.214	1.00	0.00
ATOM	38	C	UNK	1	24.181	23.139	36.230	1.00	0.00
ATOM	39	C	UNK	1	23.540	23.241	37.604	1.00	0.00
ATOM	40	O	UNK	1	23.415	22.259	38.346	1.00	0.00
ATOM	41	C	UNK	1	25.626	23.626	36.270	1.00	0.00
ATOM	42	C	UNK	1	26.353	23.381	34.987	1.00	0.00
ATOM	43	N	UNK	1	27.688	23.596	34.859	1.00	0.00
ATOM	44	C	UNK	1	25.923	22.936	33.782	1.00	0.00
ATOM	45	C	UNK	1	28.106	23.305	33.640	1.00	0.00
ATOM	46	N	UNK	1	27.030	22.896	32.957	1.00	0.00
ATOM	47	H	UNK	1	23.925	24.646	34.696	1.00	0.00
ATOM	48	H	UNK	1	24.146	22.086	35.952	1.00	0.00
ATOM	49	H	UNK	1	25.644	24.691	36.500	1.00	0.00
ATOM	50	H	UNK	1	26.138	23.057	37.046	1.00	0.00
ATOM	51	H	UNK	1	24.902	22.663	33.515	1.00	0.00
ATOM	52	H	UNK	1	29.126	23.383	33.264	1.00	0.00
ATOM	53	H	UNK	1	27.028	22.604	31.990	1.00	0.00
ATOM	54	Cu	UNK	1	28.919	24.149	36.393	1.00	0.00

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ATOM      55  N   UNK     1       24.282  21.109  40.914  1.00  0.00
ATOM      56  C   UNK     1       25.612  21.639  41.237  1.00  0.00
ATOM      57  C   UNK     1       25.404  22.887  42.119  1.00  0.00
ATOM      58  O   UNK     1       25.502  24.019  41.674  1.00  0.00
ATOM      59  C   UNK     1       26.449  22.008  40.030  1.00  0.00
ATOM      60  C   UNK     1       27.888  22.320  40.345  1.00  0.00
ATOM      61  C   UNK     1       28.748  22.572  39.121  1.00  0.00
ATOM      62  O   UNK     1       28.231  22.829  38.026  1.00  0.00
ATOM      63  N   UNK     1       30.053  22.462  39.274  1.00  0.00
ATOM      64  H   UNK     1       23.798  21.411  40.081  1.00  0.00
ATOM      65  H   UNK     1       26.168  20.851  41.744  1.00  0.00
ATOM      66  H   UNK     1       26.404  21.203  39.297  1.00  0.00
ATOM      67  H   UNK     1       26.020  22.928  39.634  1.00  0.00
ATOM      68  H   UNK     1       27.936  23.185  41.007  1.00  0.00
ATOM      69  H   UNK     1       28.295  21.432  40.828  1.00  0.00
ATOM      70  H   UNK     1       30.434  22.220  40.178  1.00  0.00
ATOM      71  H   UNK     1       30.666  22.621  38.487  1.00  0.00
ATOM      72  H   UNK     1       26.466  27.750  41.221  1.00  0.00
ATOM      73  H   UNK     1       26.696  28.681  38.124  1.00  0.00
ATOM      74  H   UNK     1       32.809  25.944  33.814  1.00  0.00
ATOM      75  H   UNK     1       31.827  29.228  40.444  1.00  0.00
ATOM      76  H   UNK     1       30.740  30.113  37.606  1.00  0.00
ATOM      77  H   UNK     1       22.606  24.297  35.622  1.00  0.00
ATOM      78  H   UNK     1       23.182  24.202  37.944  1.00  0.00
ATOM      79  H   UNK     1       23.674  21.215  41.714  1.00  0.00
ATOM      80  H   UNK     1       25.164  22.755  43.164  1.00  0.00
CONECT     1    2    7   72
CONECT     2    1    3    5    8
CONECT     3    2    4   73
CONECT     4    3
CONECT     5    2    6    9   10
CONECT     6    5   54
CONECT     7    1
CONECT     8    2
CONECT     9    5
CONECT    10    5
CONECT    11   12   21   74
CONECT    12   11   13   15   22
CONECT    13   12   14   28
CONECT    14   13
CONECT    15   12   16   23   24
CONECT    16   15   17   18
CONECT    17   16   19   54
CONECT    18   16   20   25
CONECT    19   17   20   26
CONECT    20   18   19   27
CONECT    21   11
CONECT    22   12
CONECT    23   15
CONECT    24   15
CONECT    25   18
CONECT    26   19
CONECT    27   20
CONECT    28   13   29   33
CONECT    29   28   30   32   34
CONECT    30   29   31   75
CONECT    31   30
```

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CONECT   32   29   35   36   76
CONECT   33   28
CONECT   34   29
CONECT   35   32
CONECT   36   32
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    6   17   43   62
CONECT   55   56   64   79
CONECT   56   55   57   59   65
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   66   67
CONECT   60   59   61   68   69
CONECT   61   60   62   63
CONECT   62   54   61
CONECT   63   61   70   71
CONECT   64   55
CONECT   65   56
CONECT   66   59
CONECT   67   59
CONECT   68   60
CONECT   69   60
CONECT   70   63
CONECT   71   63
CONECT   72    1
CONECT   73    3
CONECT   74   11
CONECT   75   30
CONECT   76   32
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
```

Table S7: The structure of the Calc4 model used for Az (PDB format)

```
HETATM    1  N       A  45      10.834  28.132  10.253
```

```
HETATM    2  CA      A  45      11.984  28.847   9.738
HETATM    3  C       A  45      13.067  27.873   9.320
HETATM    4  O       A  45      13.179  26.786   9.896
HETATM    5  H       A  45      10.661  28.114  11.248
HETATM    6 1HA      A  45      11.684  29.447   8.879
HETATM    7 2HA      A  45      12.376  29.495  10.522
HETATM    8  N       A  46      13.843  28.237   8.304
HETATM    9  CA      A  46      14.955  27.410   7.855
HETATM   10  C       A  46      16.185  28.278   7.634
HETATM   11  O       A  46      16.080  29.416   7.177
HETATM   12  CB      A  46      14.605  26.708   6.537
HETATM   13  CG      A  46      13.353  25.890   6.588
HETATM   14  ND1     A  46      13.217  24.831   7.472
HETATM   15  CD2     A  46      12.257  25.900   5.779
HETATM   16  CE1     A  46      12.042  24.231   7.138
HETATM   17  NE2     A  46      11.472  24.887   6.097
HETATM   18  H       A  46      13.657  29.110   7.831
HETATM   19  HA      A  46      15.157  26.661   8.621
HETATM   20 1HB      A  46      14.523  27.449   5.741
HETATM   21 2HB      A  46      15.417  26.007   6.343
HETATM   22  HD2     A  46      12.059  26.629   4.993
HETATM   23  HE1     A  46      11.622  23.355   7.633
HETATM   24  HE2     A  46      10.602  24.644   5.645
HETATM   25  N       A  47      17.349  27.754   7.983
HETATM   26  CA      A  47      18.595  28.302   7.471
HETATM   27  C       A  47      19.320  27.195   6.719
HETATM   28  O       A  47      18.806  26.075   6.604
HETATM   29  CB      A  47      19.474  28.841   8.617
HETATM   30  H       A  47      17.372  26.964   8.612
HETATM   31  HA      A  47      18.385  29.138   6.804
HETATM   32 1HB      A  47      20.375  29.292   8.202
HETATM   33 2HB      A  47      18.882  29.583   9.153
HETATM   34  N       A 112      19.845  22.291   8.154
HETATM   35  CA      A 112      19.112  23.392   8.769
HETATM   36  C       A 112      19.217  23.222  10.276
HETATM   37  O       A 112      19.002  22.120  10.778
HETATM   38  CB      A 112      17.667  23.315   8.298
HETATM   39  SG      A 112      16.624  24.556   9.142
HETATM   40  H       A 112      19.447  21.363   8.191
HETATM   41  HA      A 112      19.523  24.355   8.464
HETATM   42 1HB      A 112      17.262  22.322   8.510
HETATM   43 2HB      A 112      17.629  23.490   7.219
HETATM   44  N       A 117      14.901  20.251  12.929
HETATM   45  CA      A 117      14.831  20.117  11.479
HETATM   46  C       A 117      15.897  19.207  10.881
HETATM   47  O       A 117      15.694  18.646   9.802
HETATM   48  CB      A 117      14.904  21.490  10.807
HETATM   49  CG      A 117      13.645  22.289  10.919
HETATM   50  ND1     A 117      13.444  23.422  10.174
HETATM   51  CD2     A 117      12.546  22.133  11.714
HETATM   52  CE1     A 117      12.283  23.921  10.522
HETATM   53  NE2     A 117      11.714  23.134  11.482
HETATM   54  H       A 117      15.334  21.064  13.343
HETATM   55  HA      A 117      13.869  19.643  11.282
HETATM   56 1HB      A 117      15.733  22.058  11.229
HETATM   57 2HB      A 117      15.056  21.304   9.744
HETATM   58  HD2     A 117      12.382  21.320  12.421
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HETATM   59  HE1      A 117       11.839  24.826  10.108
HETATM   60  HE2      A 117       10.823  23.288  11.932
HETATM   61 CU    CU A 199       14.539  24.127   8.740
HETATM   62  H           62       15.307  19.415  13.325
HETATM   63  H           63       16.830  19.053  11.402
HETATM   64  H           64       10.836  27.188   9.894
HETATM   65  H           65       20.787  22.268   8.519
HETATM   66  H           66       19.479  24.063  10.901
HETATM   67  H           67       20.289  27.388   6.283
HETATM   68  H           68       19.781  28.043   9.294
HETATM   69  N        A 121       16.342  17.634   7.133
HETATM   70  CA       A 121       16.843  18.704   6.293
HETATM   71  C        A 121       18.351  18.714   6.325
HETATM   72  O        A 121       18.962  19.492   7.057
HETATM   73  CB       A 121       16.299  20.048   6.771
HETATM   74  CG       A 121       14.795  20.141   6.699
HETATM   75  SD       A 121       14.195  21.812   6.939
HETATM   76  CE       A 121       14.681  22.524   5.353
HETATM   77  H        A 121       16.716  17.516   8.064
HETATM   78  HA       A 121       16.509  18.537   5.269
HETATM   79 1HB       A 121       16.626  20.229   7.795
HETATM   80 2HB       A 121       16.696  20.808   6.098
HETATM   81 1HG       A 121       14.454  19.768   5.734
HETATM   82 2HG       A 121       14.393  19.533   7.509
HETATM   83 1HE       A 121       14.385  23.573   5.320
HETATM   84 2HE       A 121       15.762  22.447   5.236
HETATM   85 3HE       A 121       14.189  21.982   4.545
HETATM   86  H           86       16.401  16.758   6.633
HETATM   87  H           87       18.902  18.029   5.697
CONECT    1    5    2   64
CONECT    2    1    6    7    3
CONECT    3    2    4    8
CONECT    4    3
CONECT    5    1
CONECT    6    2
CONECT    7    2
CONECT    8    3   18    9
CONECT    9    8   19   10   12
CONECT   10    9   11   25
CONECT   11   10
CONECT   12    9   13   20   21
CONECT   13   14   12   15
CONECT   14   13   16   61
CONECT   15   13   17   22
CONECT   16   14   17   23
CONECT   17   15   16   24
CONECT   18    8
CONECT   19    9
CONECT   20   12
CONECT   21   12
CONECT   22   15
CONECT   23   16
CONECT   24   17
CONECT   25   10   30   26
CONECT   26   25   31   27   29
CONECT   27   26   28   67
CONECT   28   27
```

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CONECT   29   26   32   33   68
CONECT   30   25
CONECT   31   26
CONECT   32   29
CONECT   33   29
CONECT   34   40   35   65
CONECT   35   34   41   36   38
CONECT   36   35   37   66
CONECT   37   36
CONECT   38   39   35   42   43
CONECT   39   38   61
CONECT   40   34
CONECT   41   35
CONECT   42   38
CONECT   43   38
CONECT   44   54   45   62
CONECT   45   44   55   46   48
CONECT   46   45   47   63
CONECT   47   46
CONECT   48   45   49   56   57
CONECT   49   50   48   51
CONECT   50   49   52   61
CONECT   51   49   53   58
CONECT   52   50   53   59
CONECT   53   51   52   60
CONECT   54   44
CONECT   55   45
CONECT   56   48
CONECT   57   48
CONECT   58   51
CONECT   59   52
CONECT   60   53
CONECT   61   14   39   50 75
CONECT   62   44
CONECT   63   46
CONECT   64    1
CONECT   65   34
CONECT   66   36
CONECT   67   27
CONECT   68   29
CONECT   69   77   70   86
CONECT   70   69   78   71   73
CONECT   71   70   72   87
CONECT   72   71
CONECT   73   70   74   79   80
CONECT   74   73   75   81   82
CONECT   75   74   76
CONECT   76   75   83   84   85
CONECT   77   69
CONECT   78   70
CONECT   79   73
CONECT   80   73
CONECT   81   74
CONECT   82   74
CONECT   83   76
CONECT   84   76
CONECT   85   76
```

```
CONECT   86   69
CONECT   87   71
END
```

Table S8: The structure of the Calc4 model used for Pa (PDB format)

```
HETATM    1  N   UNK     1      34.462  16.297  -2.840
HETATM    2  C   UNK     1      33.644  15.575  -1.868
HETATM    3  C   UNK     1      34.433  14.519  -1.127
HETATM    4  O   UNK     1      35.501  14.057  -1.555
HETATM    5  C   UNK     1      32.474  14.883  -2.602
HETATM    6  C   UNK     1      31.596  15.827  -3.374
HETATM    7  N   UNK     1      30.793  16.807  -2.836
HETATM    8  C   UNK     1      31.483  15.901  -4.725
HETATM    9  C   UNK     1      30.181  17.427  -3.827
HETATM   10  N   UNK     1      30.573  16.907  -4.987
HETATM   11  H   UNK     1      34.933  15.778  -3.567
HETATM   12  H   UNK     1      33.282  16.303  -1.142
HETATM   13  H   UNK     1      32.867  14.120  -3.274
HETATM   14  H   UNK     1      31.845  14.439  -1.830
HETATM   15  H   UNK     1      32.007  15.288  -5.458
HETATM   16  H   UNK     1      29.464  18.240  -3.713
HETATM   17  H   UNK     1      30.259  17.198  -5.902
HETATM   18  N   UNK     1      33.925  14.074   0.003
HETATM   19  C   UNK     1      34.465  12.968   0.777
HETATM   20  C   UNK     1      33.271  12.313   1.473
HETATM   21  O   UNK     1      32.125  12.690   1.247
HETATM   22  C   UNK     1      35.522  13.398   1.784
HETATM   23  H   UNK     1      33.099  14.535   0.358
HETATM   24  H   UNK     1      34.982  12.273   0.116
HETATM   25  H   UNK     1      36.113  12.532   2.083
HETATM   26  H   UNK     1      36.136  14.141   1.276
HETATM   27  N   UNK     1      29.061  14.229   3.644
HETATM   28  C   UNK     1      30.225  14.813   2.985
HETATM   29  C   UNK     1      30.645  15.974   3.886
HETATM   30  O   UNK     1      29.815  16.859   4.127
HETATM   31  C   UNK     1      29.858  15.305   1.605
HETATM   32  S   UNK     1      31.264  16.213   0.865
HETATM   33  H   UNK     1      28.150  14.625   3.462
HETATM   34  H   UNK     1      31.047  14.107   2.868
HETATM   35  H   UNK     1      29.008  15.986   1.678
HETATM   36  H   UNK     1      29.593  14.456   0.969
HETATM   37  N   UNK     1      30.089  19.668   2.719
HETATM   38  C   UNK     1      28.743  19.924   2.261
HETATM   39  C   UNK     1      27.631  19.420   3.171
HETATM   40  O   UNK     1      26.477  19.432   2.770
HETATM   41  C   UNK     1      28.546  19.327   0.852
HETATM   42  C   UNK     1      29.543  19.880  -0.138
HETATM   43  N   UNK     1      30.307  19.032  -0.928
HETATM   44  C   UNK     1      29.888  21.162  -0.414
HETATM   45  C   UNK     1      31.074  19.830  -1.682
HETATM   46  N   UNK     1      30.849  21.102  -1.391
HETATM   47  H   UNK     1      30.422  18.714   2.725
HETATM   48  H   UNK     1      28.653  21.010   2.259
HETATM   49  H   UNK     1      28.645  18.243   0.900
```

```
HETATM   50  H   UNK     1      27.548  19.602   0.510
HETATM   51  H   UNK     1      29.482  22.062   0.049
HETATM   52  H   UNK     1      31.785  19.481  -2.431
HETATM   53  H   UNK     1      31.308  21.895  -1.817
HETATM   54 CU   UNK     1      30.465  17.118  -0.939
HETATM   55  N   UNK     1      24.408  17.224   2.157
HETATM   56  C   UNK     1      24.984  16.069   1.441
HETATM   57  C   UNK     1      25.231  14.932   2.419
HETATM   58  O   UNK     1      26.216  14.871   3.158
HETATM   59  C   UNK     1      26.268  16.516   0.738
HETATM   60  C   UNK     1      26.816  15.404  -0.159
HETATM   61  S   UNK     1      27.987  16.104  -1.359
HETATM   62  C   UNK     1      28.401  14.581  -2.218
HETATM   63  H   UNK     1      24.998  17.975   2.487
HETATM   64  H   UNK     1      24.292  15.700   0.684
HETATM   65  H   UNK     1      26.063  17.401   0.136
HETATM   66  H   UNK     1      27.015  16.747   1.497
HETATM   67  H   UNK     1      27.325  14.660   0.454
HETATM   68  H   UNK     1      25.991  14.933  -0.694
HETATM   69  H   UNK     1      29.120  14.794  -3.009
HETATM   70  H   UNK     1      28.835  13.873  -1.513
HETATM   71  H   UNK     1      27.498  14.153  -2.654
HETATM   72  H   UNK     1      35.130  16.877  -2.353
HETATM   73  H   UNK     1      33.439  11.508   2.173
HETATM   74  H   UNK     1      35.086  13.817   2.691
HETATM   75  H   UNK     1      29.220  14.195   4.641
HETATM   76  H   UNK     1      31.641  16.021   4.302
HETATM   77  H   UNK     1      30.216  20.075   3.635
HETATM   78  H   UNK     1      27.860  19.055   4.161
HETATM   79  H   UNK     1      23.827  16.895   2.915
HETATM   80  H   UNK     1      24.504  14.134   2.469
CONECT    1    2   11   72
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   54
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   25   26   74
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
```

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CONECT   27   28   33   75
CONECT   28   27   29   31   34
CONECT   29   28   30   76
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
END
```

Table S9: The structure of the Calc4 model used for Pc (PDB format)

```
HETATM    1  N   UNK     1       4.103  34.339  15.185
HETATM    2  C   UNK     1       4.992  33.545  15.990
HETATM    3  C   UNK     1       5.176  32.169  15.301
HETATM    4  O   UNK     1       4.427  31.772  14.434
HETATM    5  C   UNK     1       4.395  33.294  17.344
HETATM    6  C   UNK     1       4.163  34.407  18.291
HETATM    7  N   UNK     1       5.162  35.218  18.775
HETATM    8  C   UNK     1       2.952  34.795  18.848
HETATM    9  C   UNK     1       4.572  36.081  19.598
HETATM   10  N   UNK     1       3.236  35.857  19.674
HETATM   11  H   UNK     1       3.452  33.734  14.706
HETATM   12  H   UNK     1       5.938  34.075  16.098
HETATM   13  H   UNK     1       3.479  32.713  17.235
HETATM   14  H   UNK     1       5.212  32.767  17.837
HETATM   15  H   UNK     1       1.983  34.352  18.669
HETATM   16  H   UNK     1       5.090  36.860  20.137
HETATM   17  H   UNK     1       2.573  36.374  20.233
HETATM   18  N   UNK     1       6.198  31.468  15.812
HETATM   19  C   UNK     1       6.450  30.074  15.388
HETATM   20  C   UNK     1       7.065  29.344  16.612
HETATM   21  O   UNK     1       7.373  29.977  17.639
HETATM   22  C   UNK     1       7.216  29.930  14.115
HETATM   23  H   UNK     1       6.804  31.898  16.496
HETATM   24  H   UNK     1       5.512  29.597  15.106
HETATM   25  H   UNK     1       7.350  28.872  13.889
HETATM   26  H   UNK     1       6.666  30.408  13.304
HETATM   27  N   UNK     1      10.796  30.916  19.636
HETATM   28  C   UNK     1      10.020  31.569  18.549
HETATM   29  C   UNK     1      11.116  32.329  17.768
HETATM   30  O   UNK     1      11.756  33.220  18.363
HETATM   31  C   UNK     1       9.049  32.553  19.151
HETATM   32  S   UNK     1       8.281  33.488  17.781
HETATM   33  H   UNK     1      10.171  30.381  20.221
HETATM   34  H   UNK     1       9.466  30.872  17.920
HETATM   35  H   UNK     1       8.265  32.034  19.711
HETATM   36  H   UNK     1       9.587  33.236  19.811
HETATM   37  N   UNK     1      11.296  36.270  17.651
HETATM   38  C   UNK     1      11.306  36.871  18.972
HETATM   39  C   UNK     1      12.266  36.245  19.959
HETATM   40  O   UNK     1      12.106  36.448  21.183
HETATM   41  C   UNK     1       9.880  36.740  19.559
HETATM   42  C   UNK     1       8.845  37.461  18.738
HETATM   43  N   UNK     1       7.577  36.945  18.572
HETATM   44  C   UNK     1       8.935  38.696  18.126
HETATM   45  C   UNK     1       6.944  37.818  17.826
HETATM   46  N   UNK     1       7.709  38.881  17.542
HETATM   47  H   UNK     1      10.628  36.753  17.067
HETATM   48  H   UNK     1      11.637  37.900  18.835
HETATM   49  H   UNK     1       9.614  35.686  19.635
HETATM   50  H   UNK     1       9.892  37.205  20.545
HETATM   51  H   UNK     1       9.782  39.366  18.111
HETATM   52  H   UNK     1       5.928  37.695  17.482
HETATM   53  H   UNK     1       7.430  39.681  16.992
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HETATM   54  N   UNK     1      11.565  35.142  23.943
HETATM   55  C   UNK     1      10.455  34.174  23.708
HETATM   56  C   UNK     1      11.047  32.771  23.434
HETATM   57  O   UNK     1      11.195  32.324  22.289
HETATM   58  C   UNK     1       9.557  34.671  22.579
HETATM   59  C   UNK     1       8.275  33.872  22.515
HETATM   60  S   UNK     1       7.019  34.631  21.519
HETATM   61  C   UNK     1       5.801  33.261  21.553
HETATM   62  H   UNK     1      11.180  36.058  24.122
HETATM   63  H   UNK     1       9.826  34.095  24.595
HETATM   64  H   UNK     1       9.322  35.723  22.738
HETATM   65  H   UNK     1      10.088  34.547  21.635
HETATM   66  H   UNK     1       8.488  32.874  22.133
HETATM   67  H   UNK     1       7.884  33.825  23.531
HETATM   68  H   UNK     1       4.921  33.542  20.974
HETATM   69  H   UNK     1       6.249  32.366  21.121
HETATM   70  H   UNK     1       5.509  33.060  22.584
HETATM   71 CU   UNK     1       7.050  34.960  18.716
HETATM   72  H   UNK     1      12.216  36.342  17.241
HETATM   73  H   UNK     1      13.082  35.629  19.610
HETATM   74  H   UNK     1       7.227  28.277  16.572
HETATM   75  H   UNK     1       8.191  30.405  14.222
HETATM   76  H   UNK     1      11.488  30.301  19.233
HETATM   77  H   UNK     1      11.323  32.095  16.734
HETATM   78  H   UNK     1      12.109  34.844  24.740
HETATM   79  H   UNK     1      11.342  32.159  24.273
HETATM   80  H   UNK     1       4.639  34.861  14.507
CONECT    1    2   11   80
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   71
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   74
CONECT   21   20
CONECT   22   19   25   26   75
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   76
CONECT   28   27   29   31   34
CONECT   29   28   30   77
CONECT   30   29
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CONECT   31   28   32   35   36
CONECT   32   31   71
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   72
CONECT   38   37   39   41   48
CONECT   39   38   40   73
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   71
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54   55   62   78
CONECT   55   54   56   58   63
CONECT   56   55   57   79
CONECT   57   56
CONECT   58   55   59   64   65
CONECT   59   58   60   66   67
CONECT   60   59   61   71
CONECT   61   60   68   69   70
CONECT   62   54
CONECT   63   55
CONECT   64   58
CONECT   65   58
CONECT   66   59
CONECT   67   59
CONECT   68   61
CONECT   69   61
CONECT   70   61
CONECT   71    7   32   43   60
CONECT   72   37
CONECT   73   39
CONECT   74   20
CONECT   75   22
CONECT   76   27
CONECT   77   29
CONECT   78   54
CONECT   79   56
CONECT   80    1
END
```

Table S10: The structure of the Calc4 model used for St (PDB format)

```
ATOM      1  N   UNK     1      26.904  26.900  40.895  1.00  0.00
ATOM      2  C   UNK     1      27.565  27.152  39.606  1.00  0.00
```

ATOM	3	C	UNK	1	26.474	27.805	38.715	1.00	0.00
ATOM	4	O	UNK	1	25.343	27.298	38.697	1.00	0.00
ATOM	5	C	UNK	1	27.993	25.834	38.977	1.00	0.00
ATOM	6	S	UNK	1	28.596	26.121	37.262	1.00	0.00
ATOM	7	H	UNK	1	26.257	26.130	40.989	1.00	0.00
ATOM	8	H	UNK	1	28.463	27.760	39.715	1.00	0.00
ATOM	9	H	UNK	1	28.789	25.382	39.575	1.00	0.00
ATOM	10	H	UNK	1	27.141	25.150	38.930	1.00	0.00
ATOM	11	N	UNK	1	33.083	25.534	34.695	1.00	0.00
ATOM	12	C	UNK	1	32.040	25.855	35.747	1.00	0.00
ATOM	13	C	UNK	1	32.496	27.154	36.414	1.00	0.00
ATOM	14	O	UNK	1	33.515	27.736	36.081	1.00	0.00
ATOM	15	C	UNK	1	32.207	24.725	36.859	1.00	0.00
ATOM	16	C	UNK	1	31.822	23.389	36.314	1.00	0.00
ATOM	17	N	UNK	1	30.515	23.077	36.011	1.00	0.00
ATOM	18	C	UNK	1	32.583	22.308	35.952	1.00	0.00
ATOM	19	C	UNK	1	30.468	21.831	35.518	1.00	0.00
ATOM	20	N	UNK	1	31.696	21.352	35.483	1.00	0.00
ATOM	21	H	UNK	1	34.067	25.698	34.852	1.00	0.00
ATOM	22	H	UNK	1	31.031	25.921	35.340	1.00	0.00
ATOM	23	H	UNK	1	33.244	24.696	37.194	1.00	0.00
ATOM	24	H	UNK	1	31.553	24.962	37.698	1.00	0.00
ATOM	25	H	UNK	1	33.667	22.218	36.019	1.00	0.00
ATOM	26	H	UNK	1	29.568	21.304	35.200	1.00	0.00
ATOM	27	H	UNK	1	31.951	20.429	35.163	1.00	0.00
ATOM	28	N	UNK	1	31.769	27.553	37.459	1.00	0.00
ATOM	29	C	UNK	1	32.239	28.694	38.251	1.00	0.00
ATOM	30	C	UNK	1	31.679	28.485	39.674	1.00	0.00
ATOM	31	O	UNK	1	31.049	27.430	39.910	1.00	0.00
ATOM	32	C	UNK	1	31.824	30.024	37.674	1.00	0.00
ATOM	33	H	UNK	1	30.911	27.078	37.700	1.00	0.00
ATOM	34	H	UNK	1	33.328	28.730	38.252	1.00	0.00
ATOM	35	H	UNK	1	32.182	30.827	38.318	1.00	0.00
ATOM	36	H	UNK	1	32.272	30.091	36.683	1.00	0.00
ATOM	37	N	UNK	1	23.450	23.921	35.214	1.00	0.00
ATOM	38	C	UNK	1	24.181	23.139	36.230	1.00	0.00
ATOM	39	C	UNK	1	23.540	23.241	37.604	1.00	0.00
ATOM	40	O	UNK	1	23.415	22.259	38.346	1.00	0.00
ATOM	41	C	UNK	1	25.626	23.626	36.270	1.00	0.00
ATOM	42	C	UNK	1	26.353	23.381	34.987	1.00	0.00
ATOM	43	N	UNK	1	27.688	23.596	34.859	1.00	0.00
ATOM	44	C	UNK	1	25.923	22.936	33.782	1.00	0.00
ATOM	45	C	UNK	1	28.106	23.305	33.640	1.00	0.00
ATOM	46	N	UNK	1	27.030	22.896	32.957	1.00	0.00
ATOM	47	H	UNK	1	23.925	24.646	34.696	1.00	0.00
ATOM	48	H	UNK	1	24.146	22.086	35.952	1.00	0.00
ATOM	49	H	UNK	1	25.644	24.691	36.500	1.00	0.00
ATOM	50	H	UNK	1	26.138	23.057	37.046	1.00	0.00
ATOM	51	H	UNK	1	24.902	22.663	33.515	1.00	0.00
ATOM	52	H	UNK	1	29.126	23.383	33.264	1.00	0.00
ATOM	53	H	UNK	1	27.028	22.604	31.990	1.00	0.00
ATOM	54	Cu	UNK	1	28.919	24.149	36.393	1.00	0.00
ATOM	55	N	UNK	1	24.282	21.109	40.914	1.00	0.00
ATOM	56	C	UNK	1	25.612	21.639	41.237	1.00	0.00
ATOM	57	C	UNK	1	25.404	22.887	42.119	1.00	0.00
ATOM	58	O	UNK	1	25.502	24.019	41.674	1.00	0.00
ATOM	59	C	UNK	1	26.449	22.008	40.030	1.00	0.00

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ATOM      60  C   UNK     1       27.888  22.320  40.345  1.00  0.00
ATOM      61  C   UNK     1       28.748  22.572  39.121  1.00  0.00
ATOM      62  O   UNK     1       28.231  22.829  38.026  1.00  0.00
ATOM      63  N   UNK     1       30.053  22.462  39.274  1.00  0.00
ATOM      64  H   UNK     1       23.798  21.411  40.081  1.00  0.00
ATOM      65  H   UNK     1       26.168  20.851  41.744  1.00  0.00
ATOM      66  H   UNK     1       26.404  21.203  39.297  1.00  0.00
ATOM      67  H   UNK     1       26.020  22.928  39.634  1.00  0.00
ATOM      68  H   UNK     1       27.936  23.185  41.007  1.00  0.00
ATOM      69  H   UNK     1       28.295  21.432  40.828  1.00  0.00
ATOM      70  H   UNK     1       30.434  22.220  40.178  1.00  0.00
ATOM      71  H   UNK     1       30.666  22.621  38.487  1.00  0.00
ATOM      72  H   UNK     1       26.466  27.750  41.221  1.00  0.00
ATOM      73  H   UNK     1       26.696  28.681  38.124  1.00  0.00
ATOM      74  H   UNK     1       32.809  25.944  33.814  1.00  0.00
ATOM      75  H   UNK     1       31.827  29.228  40.444  1.00  0.00
ATOM      76  H   UNK     1       30.740  30.113  37.606  1.00  0.00
ATOM      77  H   UNK     1       22.606  24.297  35.622  1.00  0.00
ATOM      78  H   UNK     1       23.182  24.202  37.944  1.00  0.00
ATOM      79  H   UNK     1       23.674  21.215  41.714  1.00  0.00
ATOM      80  H   UNK     1       25.164  22.755  43.164  1.00  0.00
CONECT     1    2    7   72
CONECT     2    1    3    5    8
CONECT     3    2    4   73
CONECT     4    3
CONECT     5    2    6    9   10
CONECT     6    5   54
CONECT     7    1
CONECT     8    2
CONECT     9    5
CONECT    10    5
CONECT    11   12   21   74
CONECT    12   11   13   15   22
CONECT    13   12   14   28
CONECT    14   13
CONECT    15   12   16   23   24
CONECT    16   15   17   18
CONECT    17   16   19   54
CONECT    18   16   20   25
CONECT    19   17   20   26
CONECT    20   18   19   27
CONECT    21   11
CONECT    22   12
CONECT    23   15
CONECT    24   15
CONECT    25   18
CONECT    26   19
CONECT    27   20
CONECT    28   13   29   33
CONECT    29   28   30   32   34
CONECT    30   29   31   75
CONECT    31   30
CONECT    32   29   35   36   76
CONECT    33   28
CONECT    34   29
CONECT    35   32
CONECT    36   32
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CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    6   17   43   62
CONECT   55   56   64   79
CONECT   56   55   57   59   65
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   66   67
CONECT   60   59   61   68   69
CONECT   61   60   62   63
CONECT   62   54   61
CONECT   63   61   70   71
CONECT   64   55
CONECT   65   56
CONECT   66   59
CONECT   67   59
CONECT   68   60
CONECT   69   60
CONECT   70   63
CONECT   71   63
CONECT   72    1
CONECT   73    3
CONECT   74   11
CONECT   75   30
CONECT   76   32
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
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Table S11: The structure of the Calc5 model used for Az (PDB format)

```
HETATM    1  N       A  45      10.834  28.132  10.253
HETATM    2  CA      A  45      11.984  28.847   9.738
HETATM    3  C       A  45      13.067  27.873   9.320
HETATM    4  O       A  45      13.179  26.786   9.896
HETATM    5  H       A  45      10.661  28.114  11.248
HETATM    6 1HA      A  45      11.684  29.447   8.879
HETATM    7 2HA      A  45      12.376  29.495  10.522
HETATM    8  N       A  46      13.843  28.237   8.304
HETATM    9  CA      A  46      14.955  27.410   7.855
HETATM   10  C       A  46      16.185  28.278   7.634
HETATM   11  O       A  46      16.080  29.416   7.177
HETATM   12  CB      A  46      14.605  26.708   6.537
HETATM   13  CG      A  46      13.353  25.890   6.588
HETATM   14  ND1     A  46      13.217  24.831   7.472
HETATM   15  CD2     A  46      12.257  25.900   5.779
HETATM   16  CE1     A  46      12.042  24.231   7.138
HETATM   17  NE2     A  46      11.472  24.887   6.097
HETATM   18  H       A  46      13.657  29.110   7.831
HETATM   19  HA      A  46      15.157  26.661   8.621
HETATM   20 1HB      A  46      14.523  27.449   5.741
HETATM   21 2HB      A  46      15.417  26.007   6.343
HETATM   22  HD2     A  46      12.059  26.629   4.993
HETATM   23  HE1     A  46      11.622  23.355   7.633
HETATM   24  HE2     A  46      10.602  24.644   5.645
HETATM   25  N       A  47      17.349  27.754   7.983
HETATM   26  CA      A  47      18.595  28.302   7.471
HETATM   27  C       A  47      19.320  27.195   6.719
HETATM   28  O       A  47      18.806  26.075   6.604
HETATM   29  CB      A  47      19.474  28.841   8.617
HETATM   30  H       A  47      17.372  26.964   8.612
HETATM   31  HA      A  47      18.385  29.138   6.804
HETATM   32 1HB      A  47      20.375  29.292   8.202
HETATM   33 2HB      A  47      18.882  29.583   9.153
HETATM   34  N       A 112      19.845  22.291   8.154
HETATM   35  CA      A 112      19.112  23.392   8.769
HETATM   36  C       A 112      19.217  23.222  10.276
HETATM   37  O       A 112      19.002  22.120  10.778
HETATM   38  CB      A 112      17.665  23.331   8.310
HETATM   39  SG      A 112      16.670  24.596   9.182
HETATM   40  H       A 112      19.447  21.363   8.191
HETATM   41  HA      A 112      19.523  24.355   8.464
HETATM   42 1HB      A 112      17.243  22.346   8.527
HETATM   43 2HB      A 112      17.613  23.513   7.233
HETATM   44  N       A 117      14.901  20.251  12.929
HETATM   45  CA      A 117      14.831  20.117  11.479
HETATM   46  C       A 117      15.897  19.207  10.881
HETATM   47  O       A 117      15.694  18.646   9.802
HETATM   48  CB      A 117      14.904  21.490  10.807
HETATM   49  CG      A 117      13.645  22.289  10.919
HETATM   50  ND1     A 117      13.444  23.422  10.174
HETATM   51  CD2     A 117      12.546  22.133  11.714
HETATM   52  CE1     A 117      12.283  23.921  10.522
HETATM   53  NE2     A 117      11.714  23.134  11.482
HETATM   54  H       A 117      15.334  21.064  13.343
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HETATM   55  HA      A 117      13.869  19.643  11.282
HETATM   56 1HB      A 117      15.733  22.058  11.229
HETATM   57 2HB      A 117      15.056  21.304   9.744
HETATM   58  HD2     A 117      12.382  21.320  12.421
HETATM   59  HE1     A 117      11.839  24.826  10.108
HETATM   60  HE2     A 117      10.823  23.288  11.932
HETATM   61 CU    CU A 199      14.589  24.207   8.788
HETATM   62  H          62      15.307  19.415  13.325
HETATM   63  H          63      16.830  19.053  11.402
HETATM   64  H          64      10.836  27.188   9.894
HETATM   65  H          65      20.787  22.268   8.519
HETATM   66  H          66      19.479  24.063  10.901
HETATM   67  H          67      20.289  27.388   6.283
HETATM   68  H          68      19.781  28.043   9.294
HETATM   69  N       A 121      16.342  17.634   7.133
HETATM   70  CA      A 121      16.843  18.704   6.293
HETATM   71  C       A 121      18.351  18.714   6.325
HETATM   72  O       A 121      18.962  19.492   7.057
HETATM   73  CB      A 121      16.299  20.048   6.771
HETATM   74  CG      A 121      14.795  20.141   6.699
HETATM   75  SD      A 121      14.195  21.812   6.939
HETATM   76  CE      A 121      14.681  22.524   5.353
HETATM   77  H       A 121      16.716  17.516   8.064
HETATM   78  HA      A 121      16.509  18.537   5.269
HETATM   79 1HB      A 121      16.626  20.229   7.795
HETATM   80 2HB      A 121      16.696  20.808   6.098
HETATM   81 1HG      A 121      14.454  19.768   5.734
HETATM   82 2HG      A 121      14.393  19.533   7.509
HETATM   83 1HE      A 121      14.385  23.573   5.320
HETATM   84 2HE      A 121      15.762  22.447   5.236
HETATM   85 3HE      A 121      14.189  21.982   4.545
HETATM   86  H          86      16.401  16.758   6.633
HETATM   87  H          87      18.902  18.029   5.697
CONECT    1    5    2   64
CONECT    2    1    6    7    3
CONECT    3    2    4    8
CONECT    4    3
CONECT    5    1
CONECT    6    2
CONECT    7    2
CONECT    8    3   18    9
CONECT    9    8   19   10   12
CONECT   10    9   11   25
CONECT   11   10
CONECT   12    9   13   20   21
CONECT   13   14   12   15
CONECT   14   13   16   61
CONECT   15   13   17   22
CONECT   16   14   17   23
CONECT   17   15   16   24
CONECT   18    8
CONECT   19    9
CONECT   20   12
CONECT   21   12
CONECT   22   15
CONECT   23   16
CONECT   24   17
```

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CONECT   25   10   30   26
CONECT   26   25   31   27   29
CONECT   27   26   28   67
CONECT   28   27
CONECT   29   26   32   33   68
CONECT   30   25
CONECT   31   26
CONECT   32   29
CONECT   33   29
CONECT   34   40   35   65
CONECT   35   34   41   36   38
CONECT   36   35   37   66
CONECT   37   36
CONECT   38   39   35   42   43
CONECT   39   38   61
CONECT   40   34
CONECT   41   35
CONECT   42   38
CONECT   43   38
CONECT   44   54   45   62
CONECT   45   44   55   46   48
CONECT   46   45   47   63
CONECT   47   46
CONECT   48   45   49   56   57
CONECT   49   50   48   51
CONECT   50   49   52   61
CONECT   51   49   53   58
CONECT   52   50   53   59
CONECT   53   51   52   60
CONECT   54   44
CONECT   55   45
CONECT   56   48
CONECT   57   48
CONECT   58   51
CONECT   59   52
CONECT   60   53
CONECT   61   14   39   50 75
CONECT   62   44
CONECT   63   46
CONECT   64    1
CONECT   65   34
CONECT   66   36
CONECT   67   27
CONECT   68   29
CONECT   69   77   70   86
CONECT   70   69   78   71   73
CONECT   71   70   72   87
CONECT   72   71
CONECT   73   70   74   79   80
CONECT   74   73   75   81   82
CONECT   75   74   76
CONECT   76   75   83   84   85
CONECT   77   69
CONECT   78   70
CONECT   79   73
CONECT   80   73
CONECT   81   74
```

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CONECT   82   74
CONECT   83   76
CONECT   84   76
CONECT   85   76
CONECT   86   69
CONECT   87   71
END
```

Table S12: The structure of the Calc5 model used for Pa (PDB format)

```
HETATM    1  N   UNK     1      34.462  16.297  -2.840
HETATM    2  C   UNK     1      33.644  15.575  -1.868
HETATM    3  C   UNK     1      34.433  14.519  -1.127
HETATM    4  O   UNK     1      35.501  14.057  -1.555
HETATM    5  C   UNK     1      32.474  14.883  -2.602
HETATM    6  C   UNK     1      31.596  15.827  -3.374
HETATM    7  N   UNK     1      30.793  16.807  -2.836
HETATM    8  C   UNK     1      31.483  15.901  -4.725
HETATM    9  C   UNK     1      30.181  17.427  -3.827
HETATM   10  N   UNK     1      30.573  16.907  -4.987
HETATM   11  H   UNK     1      34.933  15.778  -3.567
HETATM   12  H   UNK     1      33.282  16.303  -1.142
HETATM   13  H   UNK     1      32.867  14.120  -3.274
HETATM   14  H   UNK     1      31.845  14.439  -1.830
HETATM   15  H   UNK     1      32.007  15.288  -5.458
HETATM   16  H   UNK     1      29.464  18.240  -3.713
HETATM   17  H   UNK     1      30.259  17.198  -5.902
HETATM   18  N   UNK     1      33.925  14.074   0.003
HETATM   19  C   UNK     1      34.465  12.968   0.777
HETATM   20  C   UNK     1      33.271  12.313   1.473
HETATM   21  O   UNK     1      32.125  12.690   1.247
HETATM   22  C   UNK     1      35.522  13.398   1.784
HETATM   23  H   UNK     1      33.099  14.535   0.358
HETATM   24  H   UNK     1      34.982  12.273   0.116
HETATM   25  H   UNK     1      36.113  12.532   2.083
HETATM   26  H   UNK     1      36.136  14.141   1.276
HETATM   27  N   UNK     1      29.061  14.229   3.644
HETATM   28  C   UNK     1      30.225  14.813   2.985
HETATM   29  C   UNK     1      30.645  15.974   3.886
HETATM   30  O   UNK     1      29.815  16.859   4.127
HETATM   31  C   UNK     1      29.867  15.301   1.606
HETATM   32  S   UNK     1      31.293  16.198   0.896
HETATM   33  H   UNK     1      28.150  14.625   3.462
HETATM   34  H   UNK     1      31.047  14.107   2.868
HETATM   35  H   UNK     1      29.021  15.989   1.668
HETATM   36  H   UNK     1      29.605  14.454   0.967
HETATM   37  N   UNK     1      30.089  19.668   2.719
HETATM   38  C   UNK     1      28.743  19.924   2.261
HETATM   39  C   UNK     1      27.631  19.420   3.171
HETATM   40  O   UNK     1      26.477  19.432   2.770
HETATM   41  C   UNK     1      28.546  19.327   0.852
HETATM   42  C   UNK     1      29.543  19.880  -0.138
HETATM   43  N   UNK     1      30.307  19.032  -0.928
HETATM   44  C   UNK     1      29.888  21.162  -0.414
HETATM   45  C   UNK     1      31.074  19.830  -1.682
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HETATM   46  N   UNK     1      30.849  21.102  -1.391
HETATM   47  H   UNK     1      30.422  18.714   2.725
HETATM   48  H   UNK     1      28.653  21.010   2.259
HETATM   49  H   UNK     1      28.645  18.243   0.900
HETATM   50  H   UNK     1      27.548  19.602   0.510
HETATM   51  H   UNK     1      29.482  22.062   0.049
HETATM   52  H   UNK     1      31.785  19.481  -2.431
HETATM   53  H   UNK     1      31.308  21.895  -1.817
HETATM   54 CU   UNK     1      30.473  17.068  -0.895
HETATM   55  N   UNK     1      24.408  17.224   2.157
HETATM   56  C   UNK     1      24.984  16.069   1.441
HETATM   57  C   UNK     1      25.231  14.932   2.419
HETATM   58  O   UNK     1      26.216  14.871   3.158
HETATM   59  C   UNK     1      26.268  16.516   0.738
HETATM   60  C   UNK     1      26.816  15.404  -0.159
HETATM   61  S   UNK     1      27.987  16.104  -1.359
HETATM   62  C   UNK     1      28.401  14.581  -2.218
HETATM   63  H   UNK     1      24.998  17.975   2.487
HETATM   64  H   UNK     1      24.292  15.700   0.684
HETATM   65  H   UNK     1      26.063  17.401   0.136
HETATM   66  H   UNK     1      27.015  16.747   1.497
HETATM   67  H   UNK     1      27.325  14.660   0.454
HETATM   68  H   UNK     1      25.991  14.933  -0.694
HETATM   69  H   UNK     1      29.120  14.794  -3.009
HETATM   70  H   UNK     1      28.835  13.873  -1.513
HETATM   71  H   UNK     1      27.498  14.153  -2.654
HETATM   72  H   UNK     1      35.130  16.877  -2.353
HETATM   73  H   UNK     1      33.439  11.508   2.173
HETATM   74  H   UNK     1      35.086  13.817   2.691
HETATM   75  H   UNK     1      29.220  14.195   4.641
HETATM   76  H   UNK     1      31.641  16.021   4.302
HETATM   77  H   UNK     1      30.216  20.075   3.635
HETATM   78  H   UNK     1      27.860  19.055   4.161
HETATM   79  H   UNK     1      23.827  16.895   2.915
HETATM   80  H   UNK     1      24.504  14.134   2.469
CONECT    1    2   11   72
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   54
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   25   26   74
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CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   75
CONECT   28   27   29   31   34
CONECT   29   28   30   76
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
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CONECT   80   57
END
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Table S13: The structure of the Calc5 model used for Pc (PDB format)

```
HETATM    1  N   UNK     1       4.103  34.339  15.185
HETATM    2  C   UNK     1       4.992  33.545  15.990
HETATM    3  C   UNK     1       5.176  32.169  15.301
HETATM    4  O   UNK     1       4.427  31.772  14.434
HETATM    5  C   UNK     1       4.395  33.294  17.344
HETATM    6  C   UNK     1       4.163  34.407  18.291
HETATM    7  N   UNK     1       5.162  35.218  18.775
HETATM    8  C   UNK     1       2.952  34.795  18.848
HETATM    9  C   UNK     1       4.572  36.081  19.598
HETATM   10  N   UNK     1       3.236  35.857  19.674
HETATM   11  H   UNK     1       3.452  33.734  14.706
HETATM   12  H   UNK     1       5.938  34.075  16.098
HETATM   13  H   UNK     1       3.479  32.713  17.235
HETATM   14  H   UNK     1       5.212  32.767  17.837
HETATM   15  H   UNK     1       1.983  34.352  18.669
HETATM   16  H   UNK     1       5.090  36.860  20.137
HETATM   17  H   UNK     1       2.573  36.374  20.233
HETATM   18  N   UNK     1       6.198  31.468  15.812
HETATM   19  C   UNK     1       6.450  30.074  15.388
HETATM   20  C   UNK     1       7.065  29.344  16.612
HETATM   21  O   UNK     1       7.373  29.977  17.639
HETATM   22  C   UNK     1       7.216  29.930  14.115
HETATM   23  H   UNK     1       6.804  31.898  16.496
HETATM   24  H   UNK     1       5.512  29.597  15.106
HETATM   25  H   UNK     1       7.350  28.872  13.889
HETATM   26  H   UNK     1       6.666  30.408  13.304
HETATM   27  N   UNK     1      10.796  30.916  19.636
HETATM   28  C   UNK     1      10.020  31.569  18.549
HETATM   29  C   UNK     1      11.116  32.329  17.768
HETATM   30  O   UNK     1      11.756  33.220  18.363
HETATM   31  C   UNK     1       9.050  32.553  19.151
HETATM   32  S   UNK     1       8.271  33.478  17.779
HETATM   33  H   UNK     1      10.171  30.381  20.221
HETATM   34  H   UNK     1       9.466  30.872  17.920
HETATM   35  H   UNK     1       8.266  32.035  19.712
HETATM   36  H   UNK     1       9.587  33.238  19.810
HETATM   37  N   UNK     1      11.296  36.270  17.651
HETATM   38  C   UNK     1      11.306  36.871  18.972
HETATM   39  C   UNK     1      12.266  36.245  19.959
HETATM   40  O   UNK     1      12.106  36.448  21.183
HETATM   41  C   UNK     1       9.880  36.740  19.559
HETATM   42  C   UNK     1       8.845  37.461  18.738
HETATM   43  N   UNK     1       7.577  36.945  18.572
HETATM   44  C   UNK     1       8.935  38.696  18.126
HETATM   45  C   UNK     1       6.944  37.818  17.826
HETATM   46  N   UNK     1       7.709  38.881  17.542
HETATM   47  H   UNK     1      10.628  36.753  17.067
HETATM   48  H   UNK     1      11.637  37.900  18.835
HETATM   49  H   UNK     1       9.614  35.686  19.635
HETATM   50  H   UNK     1       9.892  37.205  20.545
HETATM   51  H   UNK     1       9.782  39.366  18.111
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HETATM   52  H   UNK     1       5.928  37.695  17.482
HETATM   53  H   UNK     1       7.430  39.681  16.992
HETATM   54  N   UNK     1      11.565  35.142  23.943
HETATM   55  C   UNK     1      10.455  34.174  23.708
HETATM   56  C   UNK     1      11.047  32.771  23.434
HETATM   57  O   UNK     1      11.195  32.324  22.289
HETATM   58  C   UNK     1       9.557  34.671  22.579
HETATM   59  C   UNK     1       8.275  33.872  22.515
HETATM   60  S   UNK     1       7.019  34.631  21.519
HETATM   61  C   UNK     1       5.801  33.261  21.553
HETATM   62  H   UNK     1      11.180  36.058  24.122
HETATM   63  H   UNK     1       9.826  34.095  24.595
HETATM   64  H   UNK     1       9.322  35.723  22.738
HETATM   65  H   UNK     1      10.088  34.547  21.635
HETATM   66  H   UNK     1       8.488  32.874  22.133
HETATM   67  H   UNK     1       7.884  33.825  23.531
HETATM   68  H   UNK     1       4.921  33.542  20.974
HETATM   69  H   UNK     1       6.249  32.366  21.121
HETATM   70  H   UNK     1       5.509  33.060  22.584
HETATM   71 CU   UNK     1       7.122  35.012  18.715
HETATM   72  H   UNK     1      12.216  36.342  17.241
HETATM   73  H   UNK     1      13.082  35.629  19.610
HETATM   74  H   UNK     1       7.227  28.277  16.572
HETATM   75  H   UNK     1       8.191  30.405  14.222
HETATM   76  H   UNK     1      11.488  30.301  19.233
HETATM   77  H   UNK     1      11.323  32.095  16.734
HETATM   78  H   UNK     1      12.109  34.844  24.740
HETATM   79  H   UNK     1      11.342  32.159  24.273
HETATM   80  H   UNK     1       4.639  34.861  14.507
CONECT    1    2   11   80
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   71
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   74
CONECT   21   20
CONECT   22   19   25   26   75
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   76
CONECT   28   27   29   31   34
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CONECT   29   28   30   77
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   71
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   72
CONECT   38   37   39   41   48
CONECT   39   38   40   73
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   71
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54   55   62   78
CONECT   55   54   56   58   63
CONECT   56   55   57   79
CONECT   57   56
CONECT   58   55   59   64   65
CONECT   59   58   60   66   67
CONECT   60   59   61   71
CONECT   61   60   68   69   70
CONECT   62   54
CONECT   63   55
CONECT   64   58
CONECT   65   58
CONECT   66   59
CONECT   67   59
CONECT   68   61
CONECT   69   61
CONECT   70   61
CONECT   71    7   32   43   60
CONECT   72   37
CONECT   73   39
CONECT   74   20
CONECT   75   22
CONECT   76   27
CONECT   77   29
CONECT   78   54
CONECT   79   56
CONECT   80    1
END
```

Table S14: The structure of the Calc5 model used for St (PDB format)

ATOM	1	N	UNK	1	26.904	26.900	40.895	1.00	0.00
ATOM	2	C	UNK	1	27.565	27.152	39.606	1.00	0.00
ATOM	3	C	UNK	1	26.474	27.805	38.715	1.00	0.00
ATOM	4	O	UNK	1	25.343	27.298	38.697	1.00	0.00
ATOM	5	C	UNK	1	27.993	25.838	38.973	1.00	0.00
ATOM	6	S	UNK	1	28.604	26.147	37.265	1.00	0.00
ATOM	7	H	UNK	1	26.257	26.130	40.989	1.00	0.00
ATOM	8	H	UNK	1	28.463	27.760	39.715	1.00	0.00
ATOM	9	H	UNK	1	28.791	25.384	39.568	1.00	0.00
ATOM	10	H	UNK	1	27.144	25.152	38.919	1.00	0.00
ATOM	11	N	UNK	1	33.083	25.534	34.695	1.00	0.00
ATOM	12	C	UNK	1	32.040	25.855	35.747	1.00	0.00
ATOM	13	C	UNK	1	32.496	27.154	36.414	1.00	0.00
ATOM	14	O	UNK	1	33.515	27.736	36.081	1.00	0.00
ATOM	15	C	UNK	1	32.207	24.725	36.859	1.00	0.00
ATOM	16	C	UNK	1	31.822	23.389	36.314	1.00	0.00
ATOM	17	N	UNK	1	30.515	23.077	36.011	1.00	0.00
ATOM	18	C	UNK	1	32.583	22.308	35.952	1.00	0.00
ATOM	19	C	UNK	1	30.468	21.831	35.518	1.00	0.00
ATOM	20	N	UNK	1	31.696	21.352	35.483	1.00	0.00
ATOM	21	H	UNK	1	34.067	25.698	34.852	1.00	0.00
ATOM	22	H	UNK	1	31.031	25.921	35.340	1.00	0.00
ATOM	23	H	UNK	1	33.244	24.696	37.194	1.00	0.00
ATOM	24	H	UNK	1	31.553	24.962	37.698	1.00	0.00
ATOM	25	H	UNK	1	33.667	22.218	36.019	1.00	0.00
ATOM	26	H	UNK	1	29.568	21.304	35.200	1.00	0.00
ATOM	27	H	UNK	1	31.951	20.429	35.163	1.00	0.00
ATOM	28	N	UNK	1	31.769	27.553	37.459	1.00	0.00
ATOM	29	C	UNK	1	32.239	28.694	38.251	1.00	0.00
ATOM	30	C	UNK	1	31.679	28.485	39.674	1.00	0.00
ATOM	31	O	UNK	1	31.049	27.430	39.910	1.00	0.00
ATOM	32	C	UNK	1	31.824	30.024	37.674	1.00	0.00
ATOM	33	H	UNK	1	30.911	27.078	37.700	1.00	0.00
ATOM	34	H	UNK	1	33.328	28.730	38.252	1.00	0.00
ATOM	35	H	UNK	1	32.182	30.827	38.318	1.00	0.00
ATOM	36	H	UNK	1	32.272	30.091	36.683	1.00	0.00
ATOM	37	N	UNK	1	23.450	23.921	35.214	1.00	0.00
ATOM	38	C	UNK	1	24.181	23.139	36.230	1.00	0.00
ATOM	39	C	UNK	1	23.540	23.241	37.604	1.00	0.00
ATOM	40	O	UNK	1	23.415	22.259	38.346	1.00	0.00
ATOM	41	C	UNK	1	25.626	23.626	36.270	1.00	0.00
ATOM	42	C	UNK	1	26.353	23.381	34.987	1.00	0.00
ATOM	43	N	UNK	1	27.688	23.596	34.859	1.00	0.00
ATOM	44	C	UNK	1	25.923	22.936	33.782	1.00	0.00
ATOM	45	C	UNK	1	28.106	23.305	33.640	1.00	0.00
ATOM	46	N	UNK	1	27.030	22.896	32.957	1.00	0.00
ATOM	47	H	UNK	1	23.925	24.646	34.696	1.00	0.00
ATOM	48	H	UNK	1	24.146	22.086	35.952	1.00	0.00
ATOM	49	H	UNK	1	25.644	24.691	36.500	1.00	0.00
ATOM	50	H	UNK	1	26.138	23.057	37.046	1.00	0.00
ATOM	51	H	UNK	1	24.902	22.663	33.515	1.00	0.00
ATOM	52	H	UNK	1	29.126	23.383	33.264	1.00	0.00
ATOM	53	H	UNK	1	27.028	22.604	31.990	1.00	0.00
ATOM	54	Cu	UNK	1	28.882	24.188	36.373	1.00	0.00
ATOM	55	N	UNK	1	24.282	21.109	40.914	1.00	0.00
ATOM	56	C	UNK	1	25.612	21.639	41.237	1.00	0.00
ATOM	57	C	UNK	1	25.404	22.887	42.119	1.00	0.00

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ATOM      58  O   UNK     1       25.502  24.019  41.674  1.00  0.00
ATOM      59  C   UNK     1       26.449  22.008  40.030  1.00  0.00
ATOM      60  C   UNK     1       27.888  22.320  40.345  1.00  0.00
ATOM      61  C   UNK     1       28.748  22.572  39.121  1.00  0.00
ATOM      62  O   UNK     1       28.231  22.829  38.026  1.00  0.00
ATOM      63  N   UNK     1       30.053  22.462  39.274  1.00  0.00
ATOM      64  H   UNK     1       23.798  21.411  40.081  1.00  0.00
ATOM      65  H   UNK     1       26.168  20.851  41.744  1.00  0.00
ATOM      66  H   UNK     1       26.404  21.203  39.297  1.00  0.00
ATOM      67  H   UNK     1       26.020  22.928  39.634  1.00  0.00
ATOM      68  H   UNK     1       27.936  23.185  41.007  1.00  0.00
ATOM      69  H   UNK     1       28.295  21.432  40.828  1.00  0.00
ATOM      70  H   UNK     1       30.434  22.220  40.178  1.00  0.00
ATOM      71  H   UNK     1       30.666  22.621  38.487  1.00  0.00
ATOM      72  H   UNK     1       26.466  27.750  41.221  1.00  0.00
ATOM      73  H   UNK     1       26.696  28.681  38.124  1.00  0.00
ATOM      74  H   UNK     1       32.809  25.944  33.814  1.00  0.00
ATOM      75  H   UNK     1       31.827  29.228  40.444  1.00  0.00
ATOM      76  H   UNK     1       30.740  30.113  37.606  1.00  0.00
ATOM      77  H   UNK     1       22.606  24.297  35.622  1.00  0.00
ATOM      78  H   UNK     1       23.182  24.202  37.944  1.00  0.00
ATOM      79  H   UNK     1       23.674  21.215  41.714  1.00  0.00
ATOM      80  H   UNK     1       25.164  22.755  43.164  1.00  0.00
CONECT     1    2    7   72
CONECT     2    1    3    5    8
CONECT     3    2    4   73
CONECT     4    3
CONECT     5    2    6    9   10
CONECT     6    5   54
CONECT     7    1
CONECT     8    2
CONECT     9    5
CONECT    10    5
CONECT    11   12   21   74
CONECT    12   11   13   15   22
CONECT    13   12   14   28
CONECT    14   13
CONECT    15   12   16   23   24
CONECT    16   15   17   18
CONECT    17   16   19   54
CONECT    18   16   20   25
CONECT    19   17   20   26
CONECT    20   18   19   27
CONECT    21   11
CONECT    22   12
CONECT    23   15
CONECT    24   15
CONECT    25   18
CONECT    26   19
CONECT    27   20
CONECT    28   13   29   33
CONECT    29   28   30   32   34
CONECT    30   29   31   75
CONECT    31   30
CONECT    32   29   35   36   76
CONECT    33   28
CONECT    34   29
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CONECT   35   32
CONECT   36   32
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    6   17   43   62
CONECT   55   56   64   79
CONECT   56   55   57   59   65
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   66   67
CONECT   60   59   61   68   69
CONECT   61   60   62   63
CONECT   62   54   61
CONECT   63   61   70   71
CONECT   64   55
CONECT   65   56
CONECT   66   59
CONECT   67   59
CONECT   68   60
CONECT   69   60
CONECT   70   63
CONECT   71   63
CONECT   72    1
CONECT   73    3
CONECT   74   11
CONECT   75   30
CONECT   76   32
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
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Table S15: The structure of the Calc6 model used for Az (PDB format)

```
HETATM    1  N       A  45      10.834  28.132  10.253
HETATM    2  CA      A  45      11.984  28.847   9.738
HETATM    3  C       A  45      13.067  27.873   9.320
HETATM    4  O       A  45      13.192  26.786   9.893
HETATM    5  H       A  45      10.661  28.114  11.248
HETATM    6 1HA      A  45      11.684  29.447   8.879
HETATM    7 2HA      A  45      12.376  29.495  10.522
HETATM    8  N       A  46      13.843  28.237   8.304
HETATM    9  CA      A  46      14.955  27.410   7.855
HETATM   10  C       A  46      16.185  28.278   7.634
HETATM   11  O       A  46      16.080  29.416   7.177
HETATM   12  CB      A  46      14.605  26.708   6.537
HETATM   13  CG      A  46      13.353  25.890   6.588
HETATM   14  ND1     A  46      13.194  24.810   7.446
HETATM   15  CD2     A  46      12.257  25.900   5.779
HETATM   16  CE1     A  46      12.042  24.231   7.138
HETATM   17  NE2     A  46      11.472  24.887   6.097
HETATM   18  H       A  46      13.657  29.110   7.831
HETATM   19  HA      A  46      15.157  26.661   8.621
HETATM   20 1HB      A  46      14.523  27.449   5.741
HETATM   21 2HB      A  46      15.417  26.007   6.343
HETATM   22  HD2     A  46      12.059  26.629   4.993
HETATM   23  HE1     A  46      11.622  23.355   7.633
HETATM   24  HE2     A  46      10.602  24.644   5.645
HETATM   25  N       A  47      17.349  27.754   7.983
HETATM   26  CA      A  47      18.595  28.302   7.471
HETATM   27  C       A  47      19.320  27.195   6.719
HETATM   28  O       A  47      18.806  26.075   6.604
HETATM   29  CB      A  47      19.474  28.841   8.617
HETATM   30  H       A  47      17.372  26.964   8.612
HETATM   31  HA      A  47      18.385  29.138   6.804
HETATM   32 1HB      A  47      20.375  29.292   8.202
HETATM   33 2HB      A  47      18.882  29.583   9.153
HETATM   34  N       A 112      19.845  22.291   8.154
HETATM   35  CA      A 112      19.112  23.392   8.769
HETATM   36  C       A 112      19.217  23.222  10.276
HETATM   37  O       A 112      19.002  22.120  10.778
HETATM   38  CB      A 112      17.662  23.323   8.305
HETATM   39  SG      A 112      16.655  24.590   9.157
HETATM   40  H       A 112      19.447  21.363   8.191
HETATM   41  HA      A 112      19.523  24.355   8.464
HETATM   42 1HB      A 112      17.246  22.339   8.533
HETATM   43 2HB      A 112      17.615  23.489   7.226
HETATM   44  N       A 117      14.901  20.251  12.929
HETATM   45  CA      A 117      14.831  20.117  11.479
HETATM   46  C       A 117      15.897  19.207  10.881
HETATM   47  O       A 117      15.694  18.646   9.802
HETATM   48  CB      A 117      14.904  21.490  10.807
HETATM   49  CG      A 117      13.645  22.289  10.919
HETATM   50  ND1     A 117      13.442  23.420  10.164
HETATM   51  CD2     A 117      12.546  22.133  11.714
HETATM   52  CE1     A 117      12.283  23.921  10.522
HETATM   53  NE2     A 117      11.714  23.134  11.482
HETATM   54  H       A 117      15.334  21.064  13.343
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HETATM   55  HA      A 117      13.869  19.643  11.282
HETATM   56 1HB      A 117      15.733  22.058  11.229
HETATM   57 2HB      A 117      15.056  21.304   9.744
HETATM   58  HD2     A 117      12.382  21.320  12.421
HETATM   59  HE1     A 117      11.839  24.826  10.108
HETATM   60  HE2     A 117      10.823  23.288  11.932
HETATM   61 CU    CU A 199      14.575  24.190   8.760
HETATM   62  H          62      15.307  19.415  13.325
HETATM   63  H          63      16.830  19.053  11.402
HETATM   64  H          64      10.836  27.188   9.894
HETATM   65  H          65      20.787  22.268   8.519
HETATM   66  H          66      19.479  24.063  10.901
HETATM   67  H          67      20.289  27.388   6.283
HETATM   68  H          68      19.781  28.043   9.294
HETATM   69  N       A 121      16.342  17.634   7.133
HETATM   70  CA      A 121      16.843  18.704   6.293
HETATM   71  C       A 121      18.351  18.714   6.325
HETATM   72  O       A 121      18.962  19.492   7.057
HETATM   73  CB      A 121      16.299  20.048   6.771
HETATM   74  CG      A 121      14.795  20.141   6.699
HETATM   75  SD      A 121      14.137  21.820   6.937
HETATM   76  CE      A 121      14.681  22.524   5.353
HETATM   77  H       A 121      16.716  17.516   8.064
HETATM   78  HA      A 121      16.509  18.537   5.269
HETATM   79 1HB      A 121      16.626  20.229   7.795
HETATM   80 2HB      A 121      16.696  20.808   6.098
HETATM   81 1HG      A 121      14.454  19.768   5.734
HETATM   82 2HG      A 121      14.393  19.533   7.509
HETATM   83 1HE      A 121      14.385  23.573   5.320
HETATM   84 2HE      A 121      15.762  22.447   5.236
HETATM   85 3HE      A 121      14.189  21.982   4.545
HETATM   86  H          86      16.401  16.758   6.633
HETATM   87  H          87      18.902  18.029   5.697
CONECT    1    5    2   64
CONECT    2    1    6    7    3
CONECT    3    2    4    8
CONECT    4    3
CONECT    5    1
CONECT    6    2
CONECT    7    2
CONECT    8    3   18    9
CONECT    9    8   19   10   12
CONECT   10    9   11   25
CONECT   11   10
CONECT   12    9   13   20   21
CONECT   13   14   12   15
CONECT   14   13   16   61
CONECT   15   13   17   22
CONECT   16   14   17   23
CONECT   17   15   16   24
CONECT   18    8
CONECT   19    9
CONECT   20   12
CONECT   21   12
CONECT   22   15
CONECT   23   16
CONECT   24   17
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CONECT   25   10   30   26
CONECT   26   25   31   27   29
CONECT   27   26   28   67
CONECT   28   27
CONECT   29   26   32   33   68
CONECT   30   25
CONECT   31   26
CONECT   32   29
CONECT   33   29
CONECT   34   40   35   65
CONECT   35   34   41   36   38
CONECT   36   35   37   66
CONECT   37   36
CONECT   38   39   35   42   43
CONECT   39   38   61
CONECT   40   34
CONECT   41   35
CONECT   42   38
CONECT   43   38
CONECT   44   54   45   62
CONECT   45   44   55   46   48
CONECT   46   45   47   63
CONECT   47   46
CONECT   48   45   49   56   57
CONECT   49   50   48   51
CONECT   50   49   52   61
CONECT   51   49   53   58
CONECT   52   50   53   59
CONECT   53   51   52   60
CONECT   54   44
CONECT   55   45
CONECT   56   48
CONECT   57   48
CONECT   58   51
CONECT   59   52
CONECT   60   53
CONECT   61   14   39   50 75
CONECT   62   44
CONECT   63   46
CONECT   64    1
CONECT   65   34
CONECT   66   36
CONECT   67   27
CONECT   68   29
CONECT   69   77   70   86
CONECT   70   69   78   71   73
CONECT   71   70   72   87
CONECT   72   71
CONECT   73   70   74   79   80
CONECT   74   73   75   81   82
CONECT   75   74   76
CONECT   76   75   83   84   85
CONECT   77   69
CONECT   78   70
CONECT   79   73
CONECT   80   73
CONECT   81   74
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CONECT   82   74
CONECT   83   76
CONECT   84   76
CONECT   85   76
CONECT   86   69
CONECT   87   71
END
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Table S16: The structure of the Calc6 model used for Pa (PDB format)

```
HETATM    1  N          86      24.408  17.224   2.157
HETATM    2  CA         86      24.984  16.069   1.441
HETATM    3  C          86      25.231  14.932   2.419
HETATM    4  O          86      26.216  14.871   3.158
HETATM    5  CB         86      26.268  16.516   0.738
HETATM    6  CG         86      26.816  15.404  -0.159
HETATM    7  SD         86      27.965  16.124  -1.383
HETATM    8  CE         86      28.401  14.581  -2.218
HETATM    9  H          86      24.998  17.975   2.487
HETATM   10  HA         86      24.292  15.700   0.684
HETATM   11 1HB         86      26.063  17.401   0.136
HETATM   12 2HB         86      27.015  16.747   1.497
HETATM   13 1HG         86      27.325  14.660   0.454
HETATM   14 2HG         86      25.991  14.933  -0.694
HETATM   15 1HE         86      29.120  14.794  -3.009
HETATM   16 2HE         86      28.835  13.873  -1.513
HETATM   17 3HE         86      27.498  14.153  -2.654
HETATM   18  N          39      35.713  17.441  -5.031
HETATM   19  CA         39      35.414  18.266  -3.887
HETATM   20  C          39      34.603  17.620  -2.793
HETATM   21  O          39      34.058  18.334  -1.948
HETATM   22  H          39      36.494  16.804  -4.972
HETATM   23 1HA         39      36.341  18.657  -3.469
HETATM   24 2HA         39      34.773  19.057  -4.276
HETATM   25  N          40      34.462  16.297  -2.840
HETATM   26  CA         40      33.644  15.575  -1.868
HETATM   27  C          40      34.433  14.519  -1.127
HETATM   28  O          40      35.501  14.057  -1.555
HETATM   29  CB         40      32.474  14.883  -2.602
HETATM   30  CG         40      31.596  15.827  -3.374
HETATM   31  ND1        40      30.780  16.797  -2.822
HETATM   32  CD2        40      31.483  15.901  -4.725
HETATM   33  CE1        40      30.181  17.427  -3.827
HETATM   34  NE2        40      30.573  16.907  -4.987
HETATM   35  H          40      34.933  15.778  -3.567
HETATM   36  HA         40      33.282  16.303  -1.142
HETATM   37 1HB         40      32.867  14.120  -3.274
HETATM   38 2HB         40      31.845  14.439  -1.830
HETATM   39  HD2        40      32.007  15.288  -5.458
HETATM   40  HE1        40      29.464  18.240  -3.713
HETATM   41  HE2        40      30.259  17.198  -5.902
HETATM   42  N          41      33.925  14.074   0.003
HETATM   43  CA         41      34.465  12.968   0.777
HETATM   44  C          41      33.271  12.313   1.473
HETATM   45  O          41      32.125  12.690   1.247
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HETATM   46  CB          41       35.522  13.398   1.784
HETATM   47  H           41       33.099  14.535   0.358
HETATM   48  HA          41       34.982  12.273   0.116
HETATM   49 1HB          41       36.113  12.532   2.083
HETATM   50 2HB          41       36.136  14.141   1.276
HETATM   51  N           78       29.061  14.229   3.644
HETATM   52  CA          78       30.225  14.813   2.985
HETATM   53  C           78       30.645  15.974   3.886
HETATM   54  O           78       29.815  16.859   4.127
HETATM   55  CB          78       29.867  15.303   1.601
HETATM   56  SG          78       31.303  16.180   0.888
HETATM   57  H           78       28.150  14.625   3.462
HETATM   58  HA          78       31.047  14.107   2.868
HETATM   59 1HB          78       29.028  15.997   1.663
HETATM   60 2HB          78       29.596  14.456   0.967
HETATM   61  N           81       30.089  19.668   2.719
HETATM   62  CA          81       28.743  19.924   2.261
HETATM   63  C           81       27.631  19.420   3.171
HETATM   64  O           81       26.477  19.432   2.770
HETATM   65  CB          81       28.546  19.327   0.852
HETATM   66  CG          81       29.543  19.880  -0.138
HETATM   67  ND1         81       30.291  19.054  -0.951
HETATM   68  CD2         81       29.888  21.162  -0.414
HETATM   69  CE1         81       31.074  19.830  -1.682
HETATM   70  NE2         81       30.849  21.102  -1.391
HETATM   71  H           81       30.422  18.714   2.725
HETATM   72  HA          81       28.653  21.010   2.259
HETATM   73 1HB          81       28.645  18.243   0.900
HETATM   74 2HB          81       27.548  19.602   0.510
HETATM   75  HD2         81       29.482  22.062   0.049
HETATM   76  HE1         81       31.785  19.481  -2.431
HETATM   77  HE2         81       31.308  21.895  -1.817
HETATM   78 CU    CU    125       30.505  17.104  -0.881
HETATM   79  H           79       23.827  16.895   2.915
HETATM   80  H           80       24.504  14.134   2.469
HETATM   81  H           81       35.815  18.024  -5.849
HETATM   82  H           82       33.439  11.508   2.173
HETATM   83  H           83       35.086  13.817   2.691
HETATM   84  H           84       29.220  14.195   4.641
HETATM   85  H           85       31.641  16.021   4.302
HETATM   86  H           86       30.216  20.075   3.635
HETATM   87  H           87       27.860  19.055   4.161
CONECT    1    9    2   79
CONECT    2    1   10    3    5
CONECT    3    2    4   80
CONECT    4    3
CONECT    5    2    6   11   12
CONECT    6    5    7   13   14
CONECT    7    6    8   78
CONECT    8    7   15   16   17
CONECT    9    1
CONECT   10    2
CONECT   11    5
CONECT   12    5
CONECT   13    6
CONECT   14    6
CONECT    0    7
```

```
CONECT    0    7
CONECT   15    8
CONECT   16    8
CONECT   17    8
CONECT   18   22   19   81
CONECT   19   18   23   24   20
CONECT   20   19   21   25
CONECT   21   20
CONECT   22   18
CONECT   23   19
CONECT   24   19
CONECT   25   20   35   26
CONECT   26   25   36   27   29
CONECT   27   26   28   42
CONECT   28   27
CONECT   29   26   30   37   38
CONECT   30   31   29   32
CONECT   31   30   33   78
CONECT   32   30   34   39
CONECT   33   31   34   40
CONECT   34   32   33   41
CONECT   35   25
CONECT   36   26
CONECT   37   29
CONECT   38   29
CONECT   39   32
CONECT   40   33
CONECT   41   34
CONECT   42   27   47   43
CONECT   43   42   48   44   46
CONECT   44   43   45   82
CONECT   45   44
CONECT   46   43   49   50   83
CONECT   47   42
CONECT   48   43
CONECT   49   46
CONECT   50   46
CONECT   51   57   52   84
CONECT   52   51   58   53   55
CONECT   53   52   54   85
CONECT   54   53
CONECT   55   56   52   59   60
CONECT   56   55   78
CONECT   57   51
CONECT   58   52
CONECT   59   55
CONECT   60   55
CONECT    0   56
CONECT    0   56
CONECT   61   71   62   86
CONECT   62   61   72   63   65
CONECT   63   62   64   87
CONECT   64   63
CONECT   65   62   66   73   74
CONECT   66   67   65   68
CONECT   67   66   69   78
CONECT   68   66   70   75
```

```
CONECT   69   67   70   76
CONECT   70   68   69   77
CONECT   71   61
CONECT   72   62
CONECT   73   65
CONECT   74   65
CONECT   75   68
CONECT   76   69
CONECT   77   70
CONECT   78   31   56   67    7
CONECT   79    1
CONECT   80    3
CONECT   81   18
CONECT   82   44
CONECT   83   46
CONECT   84   51
CONECT   85   53
CONECT   86   61
CONECT   87   63
END
```

Table S17: The structure of the Calc6 model used for Pc (PDB format)

```
HETATM    1  C           1       2.364  38.230  15.334
HETATM    2  O           2       2.163  39.446  15.413
HETATM    3  N           3       2.981  37.662  14.335
HETATM    4  CA          4       3.263  36.259  14.099
HETATM    5  C           5       4.286  35.653  15.040
HETATM    6  O           6       5.181  36.295  15.583
HETATM    7  CB          7       3.774  36.173  12.649
HETATM    8  CG          8       3.412  37.521  12.008
HETATM    9  CD          9       3.467  38.507  13.169
HETATM   10  N          10       4.103  34.339  15.185
HETATM   11  CA         11       4.992  33.545  15.990
HETATM   12  C          12       5.176  32.169  15.301
HETATM   13  O          13       4.427  31.772  14.434
HETATM   14  CB         14       4.395  33.294  17.344
HETATM   15  CG         15       4.163  34.407  18.291
HETATM   16  ND1        16       5.148  35.220  18.789
HETATM   17  CD2        17       2.952  34.795  18.848
HETATM   18  CE1        18       4.572  36.081  19.598
HETATM   19  NE2        19       3.236  35.857  19.674
HETATM   20  H          20       2.573  36.374  20.233
HETATM   21  N          21       6.198  31.468  15.812
HETATM   22  CA         22       6.450  30.074  15.388
HETATM   23  C          23       7.065  29.344  16.612
HETATM   24  O          24       7.373  29.977  17.639
HETATM   25  CB         25       7.216  29.930  14.115
HETATM   26  N          26      10.796  30.916  19.636
HETATM   27  CA         27      10.020  31.569  18.549
HETATM   28  C          28      11.116  32.329  17.768
HETATM   29  O          29      11.756  33.220  18.363
HETATM   30  CB         30       9.046  32.557  19.148
HETATM   31  SG         31       8.246  33.457  17.771
HETATM   32  N          32      11.296  36.270  17.651
HETATM   33  CA         33      11.306  36.871  18.972
```

```
HETATM   34  C          34      12.266  36.245  19.959
HETATM   35  O          35      12.106  36.448  21.183
HETATM   36  CB         36       9.880  36.740  19.559
HETATM   37  CG         37       8.845  37.461  18.738
HETATM   38  ND1        38       7.602  36.938  18.544
HETATM   39  CD2        39       8.935  38.696  18.126
HETATM   40  CE1        40       6.944  37.818  17.826
HETATM   41  NE2        41       7.709  38.881  17.542
HETATM   42  H          42       7.430  39.681  16.992
HETATM   43  N          43      11.565  35.142  23.943
HETATM   44  CA         44      10.455  34.174  23.708
HETATM   45  C          45      11.047  32.771  23.434
HETATM   46  O          46      11.195  32.324  22.289
HETATM   47  CB         47       9.557  34.671  22.579
HETATM   48  CG         48       8.275  33.872  22.515
HETATM   49  SD         49       6.969  34.658  21.508
HETATM   50  CE         50       5.801  33.261  21.553
HETATM   51 CU    CU   100       7.112  35.030  18.661
HETATM   52  H          52       2.009  37.602  16.137
HETATM   53  H          53       2.353  35.686  14.276
HETATM   54  H          54       4.844  35.971  12.603
HETATM   55  H          55       3.253  35.371  12.127
HETATM   56  H          56       2.445  37.508  11.506
HETATM   57  H          57       4.168  37.787  11.269
HETATM   58  H          58       4.448  38.955  13.324
HETATM   59  H          59       2.762  39.319  12.990
HETATM   60  H          60       3.325  33.893  14.720
HETATM   61  H          61       5.938  34.075  16.098
HETATM   62  H          62       5.212  32.767  17.837
HETATM   63  H          63       3.479  32.713  17.235
HETATM   64  H          64       1.983  34.352  18.669
HETATM   65  H          65       5.090  36.860  20.137
HETATM   66  H          66       6.804  31.898  16.496
HETATM   67  H          67       5.512  29.597  15.106
HETATM   68  H          68       7.227  28.277  16.572
HETATM   69  H          69       8.191  30.405  14.222
HETATM   70  H          70       6.666  30.408  13.304
HETATM   71  H          71       7.350  28.872  13.889
HETATM   72  H          72      11.488  30.301  19.233
HETATM   73  H          73      10.171  30.381  20.221
HETATM   74  H          74       9.466  30.872  17.920
HETATM   75  H          75      11.323  32.095  16.734
HETATM   76  H          76       8.274  32.040  19.727
HETATM   77  H          77       9.587  33.253  19.789
HETATM   78  H          78      12.216  36.342  17.241
HETATM   79  H          79      10.628  36.753  17.067
HETATM   80  H          80      11.637  37.900  18.835
HETATM   81  H          81      13.082  35.629  19.610
HETATM   82  H          82       9.892  37.205  20.545
HETATM   83  H          83       9.614  35.686  19.635
HETATM   84  H          84       9.782  39.366  18.111
HETATM   85  H          85       5.928  37.695  17.482
HETATM   86  H          86      12.109  34.844  24.740
HETATM   87  H          87      11.180  36.058  24.122
HETATM   88  H          88       9.826  34.095  24.595
HETATM   89  H          89      11.342  32.159  24.273
HETATM   90  H          90      10.088  34.547  21.635
```

```
HETATM   91  H          91       9.322  35.723  22.738
HETATM   92  H          92       8.521  32.922  22.040
HETATM   93  H          93       7.893  33.716  23.524
HETATM   94  H          94       5.509  33.060  22.584
HETATM   95  H          95       6.249  32.366  21.121
HETATM   96  H          96       4.921  33.542  20.974
CONECT    1    2    3   52
CONECT    2    1
CONECT    3    1    4    9
CONECT    4    3    5    7   53
CONECT    5    4    6   10
CONECT    6    5
CONECT    7    4    8   54   55
CONECT    8    7    9   56   57
CONECT    9    3    8   58   59
CONECT   10    5   11   60
CONECT   11   10   12   14   61
CONECT   12   11   13   21
CONECT   13   12
CONECT   14   11   15   62   63
CONECT   15   14   16   17
CONECT   16   15   18   51
CONECT   17   15   19   64
CONECT   18   16   19   65
CONECT   19   17   18   20
CONECT   20   19
CONECT   21   12   22   66
CONECT   22   21   23   25   67
CONECT   23   22   24   68
CONECT   24   23
CONECT   25   22   69   70   71
CONECT   26   27   72   73
CONECT   27   26   28   30   74
CONECT   28   27   29   75
CONECT   29   28
CONECT   30   27   31   76   77
CONECT   31   30   51
CONECT   32   33   78   79
CONECT   33   32   34   36   80
CONECT   34   33   35   81
CONECT   35   34
CONECT   36   33   37   82   83
CONECT   37   36   38   39
CONECT   38   37   40   51
CONECT   39   37   41   84
CONECT   40   38   41   85
CONECT   41   39   40   42
CONECT   42   41
CONECT   43   44   86   87
CONECT   44   43   45   47   88
CONECT   45   44   46   89
CONECT   46   45
CONECT   47   44   48   90   91
CONECT   48   47   49   92   93
CONECT   49   48   50   51
CONECT   50   49   94   95   96
CONECT   51   16   31   38   49
```

```
CONECT   52    1
CONECT   53    4
CONECT   54    7
CONECT   55    7
CONECT   56    8
CONECT   57    8
CONECT   58    9
CONECT   59    9
CONECT   60   10
CONECT   61   11
CONECT   62   14
CONECT   63   14
CONECT   64   17
CONECT   65   18
CONECT   66   21
CONECT   67   22
CONECT   68   23
CONECT   69   25
CONECT   70   25
CONECT   71   25
CONECT   72   26
CONECT   73   26
CONECT   74   27
CONECT   75   28
CONECT   76   30
CONECT   77   30
CONECT   78   32
CONECT   79   32
CONECT   80   33
CONECT   81   34
CONECT   82   36
CONECT   83   36
CONECT   84   39
CONECT   85   40
CONECT   86   43
CONECT   87   43
CONECT   88   44
CONECT   89   45
CONECT   90   47
CONECT   91   47
CONECT   92   48
CONECT   93   48
CONECT   94   50
CONECT   95   50
CONECT   96   50
END
```

Table S18: The structure of the Calc6 model used for St (PDB format)

```
HETATM    1  N          45      34.887  25.474  32.582
HETATM    2  CA         45      33.676  24.664  32.497
HETATM    3  C          45      32.628  25.023  33.552
HETATM    4  O          45      31.435  24.777  33.347
HETATM    5  CB         45      34.043  23.180  32.703
HETATM    6  H          45      35.642  25.167  33.178
HETATM    7  HA         45      33.249  24.856  31.513
```

HETATM	8	1HB	45	33.141	22.571	32.640
HETATM	9	2HB	45	34.746	22.869	31.930
HETATM	10	3HB	45	34.501	23.052	33.684
HETATM	11	N	46	33.083	25.534	34.695
HETATM	12	CA	46	32.040	25.855	35.747
HETATM	13	C	46	32.496	27.154	36.414
HETATM	14	O	46	33.515	27.736	36.081
HETATM	15	CB	46	32.207	24.725	36.859
HETATM	16	CG	46	31.822	23.389	36.314
HETATM	17	ND1	46	30.494	23.064	36.023
HETATM	18	CD2	46	32.583	22.308	35.952
HETATM	19	CE1	46	30.468	21.831	35.518
HETATM	20	NE2	46	31.696	21.352	35.483
HETATM	21	H	46	34.067	25.698	34.852
HETATM	22	HA	46	31.031	25.921	35.340
HETATM	23	1HB	46	33.244	24.696	37.194
HETATM	24	2HB	46	31.553	24.962	37.698
HETATM	25	HD2	46	33.667	22.218	36.019
HETATM	26	HE1	46	29.568	21.304	35.200
HETATM	27	HE2	46	31.951	20.429	35.163
HETATM	28	N	47	31.769	27.553	37.459
HETATM	29	CA	47	32.239	28.694	38.251
HETATM	30	C	47	31.679	28.485	39.674
HETATM	31	O	47	31.049	27.430	39.910
HETATM	32	CB	47	31.824	30.024	37.674
HETATM	33	H	47	30.911	27.078	37.700
HETATM	34	HA	47	33.328	28.730	38.252
HETATM	35	1HB	47	32.182	30.827	38.318
HETATM	36	2HB	47	32.272	30.091	36.683
HETATM	37	N	89	26.904	26.900	40.895
HETATM	38	CA	89	27.565	27.152	39.606
HETATM	39	C	89	26.474	27.805	38.715
HETATM	40	O	89	25.343	27.298	38.697
HETATM	41	CB	89	27.992	25.837	38.970
HETATM	42	SG	89	28.638	26.162	37.278
HETATM	43	H	89	26.257	26.130	40.989
HETATM	44	HA	89	28.463	27.760	39.715
HETATM	45	1HB	89	28.771	25.366	39.576
HETATM	46	2HB	89	27.136	25.164	38.893
HETATM	47	N	94	23.450	23.921	35.214
HETATM	48	CA	94	24.181	23.139	36.230
HETATM	49	C	94	23.540	23.241	37.604
HETATM	50	O	94	23.415	22.259	38.346
HETATM	51	CB	94	25.626	23.626	36.270
HETATM	52	CG	94	26.353	23.381	34.987
HETATM	53	ND1	94	27.730	23.599	34.884
HETATM	54	CD2	94	25.923	22.936	33.782
HETATM	55	CE1	94	28.106	23.305	33.640
HETATM	56	NE2	94	27.030	22.896	32.957
HETATM	57	H	94	23.925	24.646	34.696
HETATM	58	HA	94	24.146	22.086	35.952
HETATM	59	1HB	94	25.644	24.691	36.500
HETATM	60	2HB	94	26.138	23.057	37.046
HETATM	61	HD2	94	24.902	22.663	33.515
HETATM	62	HE1	94	29.126	23.383	33.264
HETATM	63	HE2	94	27.028	22.604	31.990
HETATM	64	N	99	24.282	21.109	40.914

```
HETATM   65  CA         99      25.612  21.639  41.237
HETATM   66  C          99      25.404  22.887  42.119
HETATM   67  O          99      25.502  24.019  41.674
HETATM   68  CB         99      26.449  22.008  40.030
HETATM   69  CG         99      27.888  22.320  40.345
HETATM   70  CD         99      28.748  22.572  39.121
HETATM   71  OE1        99      28.234  22.856  38.029
HETATM   72  NE2        99      30.053  22.462  39.274
HETATM   73  H          99      23.798  21.411  40.081
HETATM   74  HA         99      26.168  20.851  41.744
HETATM   75 1HB         99      26.404  21.203  39.297
HETATM   76 2HB         99      26.020  22.928  39.634
HETATM   77 1HG         99      27.936  23.185  41.007
HETATM   78 2HG         99      28.295  21.432  40.828
HETATM   79 1HE2        99      30.434  22.220  40.178
HETATM   80 2HE2        99      30.666  22.621  38.487
HETATM   81 CU    CU   110      28.895  24.212  36.368
HETATM   82  H          82      34.640  26.425  32.814
HETATM   83  H          83      31.827  29.228  40.444
HETATM   84  H          84      30.740  30.113  37.606
HETATM   85  H          85      26.466  27.750  41.220
HETATM   86  H          86      26.696  28.681  38.124
HETATM   87  H          87      22.606  24.297  35.622
HETATM   88  H          88      23.182  24.202  37.944
HETATM   89  H          89      23.674  21.215  41.714
HETATM   90  H          90      25.164  22.755  43.164
CONECT    1    6    2   82
CONECT    2    1    7    3    5
CONECT    3    2    4   11
CONECT    4    3
CONECT    5    2    8    9   10
CONECT    6    1
CONECT    7    2
CONECT    8    5
CONECT    9    5
CONECT   10    5
CONECT   11    3   21   12
CONECT   12   11   22   13   15
CONECT   13   12   14   28
CONECT   14   13
CONECT   15   12   16   23   24
CONECT   16   15   17   18
CONECT   17   16   19   81
CONECT   18   16   20   25
CONECT   19   17   20   26
CONECT   20   18   19   27
CONECT   21   11
CONECT   22   12
CONECT   23   15
CONECT   24   15
CONECT   25   18
CONECT   26   19
CONECT   27   20
CONECT   28   13   33   29
CONECT   29   28   34   30   32
CONECT   30   29   31   83
CONECT   31   30
```

```
CONECT   32   29   35   36   84
CONECT   33   28
CONECT   34   29
CONECT   35   32
CONECT   36   32
CONECT   37   43   38   85
CONECT   38   37   44   39   41
CONECT   39   38   40   86
CONECT   40   39
CONECT   41   38   42   45   46
CONECT   42   41   81
CONECT   43   37
CONECT   44   38
CONECT   45   41
CONECT   46   41
CONECT    0   42
CONECT    0   42
CONECT   47   57   48   87
CONECT   48   47   58   49   51
CONECT   49   48   50   88
CONECT   50   49
CONECT   51   48   52   59   60
CONECT   52   51   53   54
CONECT   53   52   55   81
CONECT   54   52   56   61
CONECT   55   53   56   62
CONECT   56   54   55   63
CONECT   57   47
CONECT   58   48
CONECT   59   51
CONECT   60   51
CONECT   61   54
CONECT   62   55
CONECT   63   56
CONECT   64   73   65   89
CONECT   65   64   74   66   68
CONECT   66   65   67   90
CONECT   67   66
CONECT   68   65   69   75   76
CONECT   69   68   70   77   78
CONECT   70   69   71   72
CONECT   71   70   81
CONECT   72   70   79   80
CONECT   73   64
CONECT   74   65
CONECT   75   68
CONECT   76   68
CONECT   77   69
CONECT   78   69
CONECT   79   72
CONECT   80   72
CONECT   81   17   42   53   71
CONECT   82    1
CONECT   83   30
CONECT   84   32
CONECT   85   37
CONECT   86   39
```

```
CONECT   87   47
CONECT   88   49
CONECT   89   64
CONECT   90   66
END
```

Table S19: The structure of the Calc7 model used for Az (PDB format)

```
HETATM    1  CA          1       9.466  24.311   2.267
HETATM    2  C           2       8.732  24.295   3.614
HETATM    3  O           3       9.342  24.102   4.664
HETATM    4  HA          4       9.142  25.190   1.709
HETATM    5  N           5       7.407  24.425   3.559
HETATM    6  H           6       6.980  24.691   2.683
HETATM    7  H           7      10.544  24.343   2.426
HETATM    8  H           8       9.215  23.411   1.706
HETATM    9  H           9       6.840  24.261   4.378
HETATM   10  CA         10      16.843  18.704   6.293
HETATM   11  CB         11      16.299  20.048   6.771
HETATM   12  CG         12      14.795  20.141   6.699
HETATM   13  SD         13      14.126  21.819   6.935
HETATM   14  CE         14      14.681  22.524   5.353
HETATM   15  HA         15      16.509  18.537   5.269
HETATM   16 1HB         16      16.626  20.229   7.795
HETATM   17 2HB         17      16.696  20.808   6.098
HETATM   18 1HG         18      14.454  19.768   5.734
HETATM   19 2HG         19      14.393  19.533   7.509
HETATM   20 1HE         20      14.385  23.573   5.320
HETATM   21 2HE         21      15.762  22.447   5.236
HETATM   22 3HE         22      14.189  21.982   4.545
HETATM   23  N          23      10.834  28.132  10.253
HETATM   24  CA         24      11.984  28.847   9.738
HETATM   25  C          25      13.067  27.873   9.320
HETATM   26  O          26      13.200  26.793   9.905
HETATM   27  H          27      10.661  28.114  11.248
HETATM   28 1HA         28      11.684  29.447   8.879
HETATM   29 2HA         29      12.376  29.495  10.522
HETATM   30  N          30      13.843  28.237   8.304
HETATM   31  CA         31      14.955  27.410   7.855
HETATM   32  C          32      16.185  28.278   7.634
HETATM   33  O          33      16.080  29.416   7.177
HETATM   34  CB         34      14.605  26.708   6.537
HETATM   35  CG         35      13.353  25.890   6.588
HETATM   36  ND1        36      13.199  24.810   7.446
HETATM   37  CD2        37      12.257  25.900   5.779
HETATM   38  CE1        38      12.042  24.231   7.138
HETATM   39  NE2        39      11.472  24.887   6.097
HETATM   40  H          40      13.657  29.110   7.831
HETATM   41  HA         41      15.157  26.661   8.621
HETATM   42 1HB         42      14.523  27.449   5.741
HETATM   43 2HB         43      15.417  26.007   6.343
HETATM   44  HD2        44      12.059  26.629   4.993
HETATM   45  HE1        45      11.622  23.355   7.633
HETATM   46  HE2        46      10.602  24.644   5.645
HETATM   47  N          47      17.349  27.754   7.983
```

```
HETATM   48  CA         48      18.595  28.302   7.471
HETATM   49  C          49      19.320  27.195   6.719
HETATM   50  O          50      18.806  26.075   6.604
HETATM   51  CB         51      19.474  28.841   8.617
HETATM   52  H          52      17.372  26.964   8.612
HETATM   53  HA         53      18.385  29.138   6.804
HETATM   54 1HB         54      20.375  29.292   8.202
HETATM   55 2HB         55      18.882  29.583   9.153
HETATM   56  N          56      19.845  22.291   8.154
HETATM   57  CA         57      19.112  23.392   8.769
HETATM   58  C          58      19.217  23.222  10.276
HETATM   59  O          59      19.002  22.120  10.778
HETATM   60  CB         60      17.668  23.304   8.303
HETATM   61  SG         61      16.645  24.600   9.078
HETATM   62  H          62      19.447  21.363   8.191
HETATM   63  HA         63      19.523  24.355   8.464
HETATM   64 1HB         64      17.255  22.332   8.584
HETATM   65 2HB         65      17.624  23.417   7.217
HETATM   66  N          66      19.580  24.281  10.999
HETATM   67  CA         67      19.806  24.167  12.441
HETATM   68  C          68      18.627  24.632  13.293
HETATM   69  O          69      18.724  24.660  14.516
HETATM   70  H          70      19.701  25.175  10.546
HETATM   71  HA         71      19.927  23.101  12.632
HETATM   72  N          72      17.523  25.009  12.650
HETATM   73  CA         73      16.288  25.315  13.378
HETATM   74  C          74      15.877  24.044  14.137
HETATM   75  O          75      16.031  22.939  13.617
HETATM   76  CB         76      15.195  25.719  12.377
HETATM   77  H          77      17.537  25.085  11.643
HETATM   78  HA         78      16.434  26.140  14.076
HETATM   79 1HB         79      15.635  26.319  11.581
HETATM   80 2HB         80      14.782  24.788  11.989
HETATM   81  CB         81      14.904  21.490  10.807
HETATM   82  CG         82      13.645  22.289  10.919
HETATM   83  ND1        83      13.439  23.417  10.160
HETATM   84  CD2        84      12.546  22.133  11.714
HETATM   85  CE1        85      12.283  23.921  10.522
HETATM   86  NE2        86      11.714  23.134  11.482
HETATM   87 1HB         87      15.733  22.058  11.229
HETATM   88 2HB         88      15.056  21.304   9.744
HETATM   89  HD2        89      12.382  21.320  12.421
HETATM   90  HE1        90      11.839  24.826  10.108
HETATM   91  HE2        91      10.823  23.288  11.932
HETATM   92 CU    CU A 199      14.562  24.163   8.740
HETATM   93  H          93      15.453  24.120  15.127
HETATM   94  H          94      20.660  24.791  12.705
HETATM   95  H          95      10.836  27.188   9.895
HETATM   96  H          96      20.289  27.388   6.283
HETATM   97  H          97      19.781  28.044   9.294
HETATM   98  H          98      14.842  20.549  11.353
HETATM   99  H          99      14.413  26.321  12.839
HETATM  100  H         100      17.932  18.706   6.334
HETATM  101  H         101      16.462  17.909   6.934
HETATM  102  H         102      20.787  22.268   8.519
CONECT    1    4    2    7    8
CONECT    2    1    3    5
```

```
CONECT    3    2
CONECT    4    1
CONECT    5    2    6    9
CONECT    6    5
CONECT    7    1
CONECT    8    1
CONECT    9    5
CONECT   10   15   11  100  101
CONECT   11   10   12   16   17
CONECT   12   11   13   18   19
CONECT   13   12   14   92
CONECT   14   13   20   21   22
CONECT   15   10
CONECT   16   11
CONECT   17   11
CONECT   18   12
CONECT   19   12
CONECT   20   14
CONECT   21   14
CONECT   22   14
CONECT   23   27   24   95
CONECT   24   23   28   29   25
CONECT   25   24   26   30
CONECT   26   25
CONECT   27   23
CONECT   28   24
CONECT   29   24
CONECT   30   25   40   31
CONECT   31   30   41   32   34
CONECT   32   31   33   47
CONECT   33   32
CONECT   34   31   35   42   43
CONECT   35   34   36   37
CONECT   36   35   38   92
CONECT   37   35   39   44
CONECT   38   36   39   45
CONECT   39   37   38   46
CONECT   40   30
CONECT   41   31
CONECT   42   34
CONECT   43   34
CONECT   44   37
CONECT   45   38
CONECT   46   39
CONECT   47   32   52   48
CONECT   48   47   53   49   51
CONECT   49   48   50   96
CONECT   50   49
CONECT   51   48   54   55   97
CONECT   52   47
CONECT   53   48
CONECT   54   51
CONECT   55   51
CONECT   56   62   57  102
CONECT   57   56   63   58   60
CONECT   58   57   59   66
CONECT   59   58
```

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CONECT   60   57   61   64   65
CONECT   61   60   92
CONECT   62   56
CONECT   63   57
CONECT   64   60
CONECT   65   60
CONECT   66   58   70   67
CONECT   67   66   71   68   94
CONECT   68   67   69   72
CONECT   69   68
CONECT   70   66
CONECT   71   67
CONECT   72   68   77   73
CONECT   73   72   78   74   76
CONECT   74   73   75   93
CONECT   75   74
CONECT   76   73   79   80   99
CONECT   77   72
CONECT   78   73
CONECT   79   76
CONECT   80   76
CONECT   81   82   87   88   98
CONECT   82   81   83   84
CONECT   83   82   85   92
CONECT   84   82   86   89
CONECT   85   83   86   90
CONECT   86   84   85   91
CONECT   87   81
CONECT   88   81
CONECT   89   84
CONECT   90   85
CONECT   91   86
CONECT   92   13   36   61   83
CONECT   93   74
CONECT   94   67
CONECT   95   23
CONECT   96   49
CONECT   97   51
CONECT   98   81
CONECT   99   76
CONECT  100   10
CONECT  101   10
CONECT  102   56
END
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Table S20: The structure of the Calc7 model used for Pa (PDB format)

```
HETATM    1  CA          1      24.984  16.069   1.441
HETATM    2  CB          2      26.268  16.516   0.738
HETATM    3  CG          3      26.816  15.404  -0.159
HETATM    4  SD          4      27.969  16.123  -1.381
HETATM    5  CE          5      28.401  14.581  -2.218
HETATM    6  HA          6      24.292  15.700   0.684
HETATM    7 1HB          7      26.063  17.401   0.136
HETATM    8 2HB          8      27.015  16.747   1.497
HETATM    9 1HG          9      27.325  14.660   0.454
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HETATM   10 2HG         10      25.991  14.933  -0.694
HETATM   11 1HE         11      29.120  14.794  -3.009
HETATM   12 2HE         12      28.835  13.873  -1.513
HETATM   13 3HE         13      27.498  14.153  -2.654
HETATM   14  N          14      35.713  17.441  -5.031
HETATM   15  CA         15      35.414  18.266  -3.887
HETATM   16  C          16      34.603  17.620  -2.793
HETATM   17  O          17      34.073  18.336  -1.940
HETATM   18  H          18      36.494  16.804  -4.972
HETATM   19 1HA         19      36.341  18.657  -3.469
HETATM   20 2HA         20      34.773  19.057  -4.276
HETATM   21  N          21      34.462  16.297  -2.840
HETATM   22  CA         22      33.644  15.575  -1.868
HETATM   23  C          23      34.433  14.519  -1.127
HETATM   24  O          24      35.501  14.057  -1.555
HETATM   25  CB         25      32.474  14.883  -2.602
HETATM   26  CG         26      31.596  15.827  -3.374
HETATM   27  ND1        27      30.782  16.795  -2.819
HETATM   28  CD2        28      31.483  15.901  -4.725
HETATM   29  CE1        29      30.181  17.427  -3.827
HETATM   30  NE2        30      30.573  16.907  -4.987
HETATM   31  H          31      34.933  15.778  -3.567
HETATM   32  HA         32      33.282  16.303  -1.142
HETATM   33 1HB         33      32.867  14.120  -3.274
HETATM   34 2HB         34      31.845  14.439  -1.830
HETATM   35  HD2        35      32.007  15.288  -5.458
HETATM   36  HE1        36      29.464  18.240  -3.713
HETATM   37  HE2        37      30.259  17.198  -5.902
HETATM   38  N          38      33.925  14.074   0.003
HETATM   39  CA         39      34.465  12.968   0.777
HETATM   40  C          40      33.271  12.313   1.473
HETATM   41  O          41      32.125  12.690   1.247
HETATM   42  CB         42      35.522  13.398   1.784
HETATM   43  H          43      33.099  14.535   0.358
HETATM   44  HA         44      34.982  12.273   0.116
HETATM   45 1HB         45      36.113  12.532   2.083
HETATM   46 2HB         46      36.136  14.141   1.276
HETATM   47  N          47      29.061  14.229   3.644
HETATM   48  CA         48      30.225  14.813   2.985
HETATM   49  C          49      30.645  15.974   3.886
HETATM   50  O          50      29.815  16.859   4.127
HETATM   51  CB         51      29.875  15.311   1.604
HETATM   52  SG         52      31.315  16.188   0.895
HETATM   53  H          53      28.150  14.625   3.462
HETATM   54  HA         54      31.047  14.107   2.868
HETATM   55 1HB         55      29.041  16.013   1.669
HETATM   56 2HB         56      29.601  14.470   0.961
HETATM   57  CB         57      28.546  19.327   0.852
HETATM   58  CG         58      29.543  19.880  -0.138
HETATM   59  ND1        59      30.291  19.050  -0.950
HETATM   60  CD2        60      29.888  21.162  -0.414
HETATM   61  CE1        61      31.074  19.830  -1.682
HETATM   62  NE2        62      30.849  21.102  -1.391
HETATM   63 1HB         63      28.645  18.243   0.900
HETATM   64 2HB         64      27.548  19.602   0.510
HETATM   65  HD2        65      29.482  22.062   0.049
HETATM   66  HE1        66      31.785  19.481  -2.431
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HETATM   67  HE2         67       31.308  21.895  -1.817
HETATM   68 CU    CU   125       30.525  17.106  -0.884
HETATM   69  H           69       25.203  15.286   2.167
HETATM   70  H           70       24.538  16.919   1.958
HETATM   71  H           71       28.723  19.732   1.848
HETATM   72  H           72       29.220  14.195   4.641
HETATM   73  H           73       31.641  16.021   4.302
HETATM   74  H           74       35.085  13.817   2.690
HETATM   75  H           75       35.815  18.024  -5.849
HETATM   76  H           76       33.439  11.508   2.173
HETATM   77  O   HOH   263       31.785  23.434  -2.402
HETATM   78  H1  HOH   263       31.785  24.394  -2.402
HETATM   79  H2  HOH   263       32.690  23.114  -2.402
HETATM   80  CB          80       28.094  19.145  -8.318
HETATM   81  CG          81       29.552  19.242  -7.936
HETATM   82  OD1         82       29.979  18.899  -6.831
HETATM   83  ND2         83       30.335  19.718  -8.897
HETATM   84 1HB          84       28.009  18.758  -9.333
HETATM   85 2HB          85       27.648  20.138  -8.264
HETATM   86 1HD2         86       29.935  19.977  -9.788
HETATM   87 2HD2         87       31.326  19.819  -8.733
HETATM   88  H           88       27.575  18.472  -7.635
CONECT    1    6    2   69   70
CONECT    2    1    3    7    8
CONECT    3    2    4    9   10
CONECT    4    3    5   68
CONECT    5    4   11   12   13
CONECT    6    1
CONECT    7    2
CONECT    8    2
CONECT    9    3
CONECT   10    3
CONECT   11    5
CONECT   12    5
CONECT   13    5
CONECT   14   18   15   75
CONECT   15   14   19   20   16
CONECT   16   15   17   21
CONECT   17   16
CONECT   18   14
CONECT   19   15
CONECT   20   15
CONECT   21   16   31   22
CONECT   22   21   32   23   25
CONECT   23   22   24   38
CONECT   24   23
CONECT   25   22   26   33   34
CONECT   26   25   27   28
CONECT   27   26   29   68
CONECT   28   26   30   35
CONECT   29   27   30   36
CONECT   30   28   29   37
CONECT   31   21
CONECT   32   22
CONECT   33   25
CONECT   34   25
CONECT   35   28
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CONECT   36   29
CONECT   37   30
CONECT   38   23   43   39
CONECT   39   38   44   40   42
CONECT   40   39   41   76
CONECT   41   40
CONECT   42   39   45   46   74
CONECT   43   38
CONECT   44   39
CONECT   45   42
CONECT   46   42
CONECT   47   53   48   72
CONECT   48   47   54   49   51
CONECT   49   48   50   73
CONECT   50   49
CONECT   51   48   52   55   56
CONECT   52   51   68
CONECT   53   47
CONECT   54   48
CONECT   55   51
CONECT   56   51
CONECT   57   58   63   64   71
CONECT   58   57   59   60
CONECT   59   58   61   68
CONECT   60   58   62   65
CONECT   61   59   62   66
CONECT   62   60   61   67
CONECT   63   57
CONECT   64   57
CONECT   65   60
CONECT   66   61
CONECT   67   62
CONECT   68    4   27   52   59
CONECT   69    1
CONECT   70    1
CONECT   71   57
CONECT   72   47
CONECT   73   49
CONECT   74   42
CONECT   75   14
CONECT   76   40
CONECT   77   78   79
CONECT   78   77
CONECT   79   77
CONECT   80   81   84   85   88
CONECT   81   80   82   83
CONECT   82   81
CONECT   83   81   86   87
CONECT   84   80
CONECT   85   80
CONECT   86   83
CONECT   87   83
CONECT   88   80
END
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Table S21: The structure of the Calc7 model used for Pc (PDB format)

```
HETATM    1  C           1       2.364  38.230  15.334
HETATM    2  O           2       2.163  39.446  15.413
HETATM    3  N           3       2.981  37.662  14.335
HETATM    4  CA          4       3.263  36.259  14.099
HETATM    5  C           5       4.286  35.653  15.040
HETATM    6  O           6       5.183  36.298  15.575
HETATM    7  CB          7       3.774  36.173  12.649
HETATM    8  CG          8       3.412  37.521  12.008
HETATM    9  CD          9       3.467  38.507  13.169
HETATM   10  N          10       4.103  34.339  15.185
HETATM   11  CA         11       4.992  33.545  15.990
HETATM   12  C          12       5.176  32.169  15.301
HETATM   13  O          13       4.427  31.772  14.434
HETATM   14  CB         14       4.395  33.294  17.344
HETATM   15  CG         15       4.163  34.407  18.291
HETATM   16  ND1        16       5.151  35.217  18.785
HETATM   17  CD2        17       2.952  34.795  18.848
HETATM   18  CE1        18       4.572  36.081  19.598
HETATM   19  NE2        19       3.236  35.857  19.674
HETATM   20  H          20       2.573  36.374  20.233
HETATM   21  N          21       6.198  31.468  15.812
HETATM   22  CA         22       6.450  30.074  15.388
HETATM   23  C          23       7.065  29.344  16.612
HETATM   24  O          24       7.373  29.977  17.639
HETATM   25  CB         25       7.216  29.930  14.115
HETATM   26  N          26      10.796  30.916  19.636
HETATM   27  CA         27      10.020  31.569  18.549
HETATM   28  C          28      11.116  32.329  17.768
HETATM   29  O          29      11.756  33.220  18.363
HETATM   30  CB         30       9.042  32.557  19.144
HETATM   31  SG         31       8.255  33.464  17.762
HETATM   32  N          32      11.296  36.270  17.651
HETATM   33  CA         33      11.306  36.871  18.972
HETATM   34  C          34      12.266  36.245  19.959
HETATM   35  O          35      12.106  36.448  21.183
HETATM   36  CB         36       9.880  36.740  19.559
HETATM   37  CG         37       8.845  37.461  18.738
HETATM   38  ND1        38       7.602  36.937  18.543
HETATM   39  CD2        39       8.935  38.696  18.126
HETATM   40  CE1        40       6.944  37.818  17.826
HETATM   41  NE2        41       7.709  38.881  17.542
HETATM   42  H          42       7.430  39.681  16.992
HETATM   43  N          43      11.565  35.142  23.943
HETATM   44  CA         44      10.455  34.174  23.708
HETATM   45  C          45      11.047  32.771  23.434
HETATM   46  O          46      11.195  32.324  22.289
HETATM   47  CB         47       9.557  34.671  22.579
HETATM   48  CG         48       8.275  33.872  22.515
HETATM   49  SD         49       6.970  34.659  21.509
HETATM   50  CE         50       5.801  33.261  21.553
HETATM   51 CU    CU   100       7.104  35.026  18.653
HETATM   52  H          52       2.009  37.602  16.137
HETATM   53  H          53       2.353  35.686  14.276
HETATM   54  H          54       4.844  35.971  12.603
HETATM   55  H          55       3.253  35.371  12.127
HETATM   56  H          56       2.445  37.508  11.506
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HETATM   57  H          57       4.168  37.787  11.269
HETATM   58  H          58       4.448  38.955  13.324
HETATM   59  H          59       2.762  39.319  12.990
HETATM   60  H          60       3.325  33.893  14.720
HETATM   61  H          61       5.938  34.075  16.098
HETATM   62  H          62       5.212  32.767  17.837
HETATM   63  H          63       3.479  32.713  17.235
HETATM   64  H          64       1.983  34.352  18.669
HETATM   65  H          65       5.090  36.860  20.137
HETATM   66  H          66       6.804  31.898  16.496
HETATM   67  H          67       5.512  29.597  15.106
HETATM   68  H          68       7.227  28.277  16.572
HETATM   69  H          69       8.191  30.405  14.222
HETATM   70  H          70       6.666  30.408  13.304
HETATM   71  H          71       7.350  28.872  13.889
HETATM   72  H          72      11.488  30.301  19.233
HETATM   73  H          73      10.171  30.381  20.221
HETATM   74  H          74       9.466  30.872  17.920
HETATM   75  H          75      11.323  32.095  16.734
HETATM   76  H          76       8.266  32.038  19.715
HETATM   77  H          77       9.578  33.251  19.790
HETATM   78  H          78      12.216  36.342  17.241
HETATM   79  H          79      10.628  36.753  17.067
HETATM   80  H          80      11.637  37.900  18.835
HETATM   81  H          81      13.082  35.629  19.610
HETATM   82  H          82       9.892  37.205  20.545
HETATM   83  H          83       9.614  35.686  19.635
HETATM   84  H          84       9.782  39.366  18.111
HETATM   85  H          85       5.928  37.695  17.482
HETATM   86  H          86      12.109  34.844  24.740
HETATM   87  H          87      11.180  36.058  24.122
HETATM   88  H          88       9.826  34.095  24.595
HETATM   89  H          89      11.342  32.159  24.273
HETATM   90  H          90      10.088  34.547  21.635
HETATM   91  H          91       9.322  35.723  22.738
HETATM   92  H          92       8.521  32.922  22.040
HETATM   93  H          93       7.893  33.716  23.524
HETATM   94  H          94       5.509  33.060  22.584
HETATM   95  H          95       6.249  32.366  21.121
HETATM   96  H          96       4.921  33.542  20.974
HETATM   97  N          33      -1.169  36.500  21.211
HETATM   98  CA         33      -0.936  37.960  21.110
HETATM   99  C          33       0.486  38.184  20.636
HETATM  100  O          33       1.365  37.341  20.914
HETATM  101  H          33      -2.114  36.331  21.526
HETATM  102  HA         33      -1.631  38.390  20.389
HETATM  103  N          34       0.686  39.280  19.934
HETATM  104  CA         34       2.028  39.646  19.462
HETATM  105  H          34      -0.097  39.880  19.716
HETATM  106 1HA         34       1.975  40.581  18.905
HETATM  107 2HA         34       2.693  39.770  20.317
HETATM  108  H          12      -0.517  36.100  21.871
HETATM  109  H          13      -1.089  38.434  22.080
HETATM  110  H          14       2.413  38.858  18.814
CONECT    1    2    3   52
CONECT    2    1
CONECT    3    1    4    9
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CONECT    4    3    5    7   53
CONECT    5    4    6   10
CONECT    6    5
CONECT    7    4    8   54   55
CONECT    8    7    9   56   57
CONECT    9    3    8   58   59
CONECT   10    5   11   60
CONECT   11   10   12   14   61
CONECT   12   11   13   21
CONECT   13   12
CONECT   14   11   15   62   63
CONECT   15   14   16   17
CONECT   16   15   18   51
CONECT   17   15   19   64
CONECT   18   16   19   65
CONECT   19   17   18   20
CONECT   20   19
CONECT   21   12   22   66
CONECT   22   21   23   25   67
CONECT   23   22   24   68
CONECT   24   23
CONECT   25   22   69   70   71
CONECT   26   27   72   73
CONECT   27   26   28   30   74
CONECT   28   27   29   75
CONECT   29   28
CONECT   30   27   31   76   77
CONECT   31   30   51
CONECT   32   33   78   79
CONECT   33   32   34   36   80
CONECT   34   33   35   81
CONECT   35   34
CONECT   36   33   37   82   83
CONECT   37   36   38   39
CONECT   38   37   40   51
CONECT   39   37   41   84
CONECT   40   38   41   85
CONECT   41   39   40   42
CONECT   42   41
CONECT   43   44   86   87
CONECT   44   43   45   47   88
CONECT   45   44   46   89
CONECT   46   45
CONECT   47   44   48   90   91
CONECT   48   47   49   92   93
CONECT   49   48   50   51
CONECT   50   49   94   95   96
CONECT   51   16   31   38   49
CONECT   52    1
CONECT   53    4
CONECT   54    7
CONECT   55    7
CONECT   56    8
CONECT   57    8
CONECT   58    9
CONECT   59    9
CONECT   60   10
```

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CONECT   61   11
CONECT   62   14
CONECT   63   14
CONECT   64   17
CONECT   65   18
CONECT   66   21
CONECT   67   22
CONECT   68   23
CONECT   69   25
CONECT   70   25
CONECT   71   25
CONECT   72   26
CONECT   73   26
CONECT   74   27
CONECT   75   28
CONECT   76   30
CONECT   77   30
CONECT   78   32
CONECT   79   32
CONECT   80   33
CONECT   81   34
CONECT   82   36
CONECT   83   36
CONECT   84   39
CONECT   85   40
CONECT   86   43
CONECT   87   43
CONECT   88   44
CONECT   89   45
CONECT   90   47
CONECT   91   47
CONECT   92   48
CONECT   93   48
CONECT   94   50
CONECT   95   50
CONECT   96   50
CONECT   97  111   98  108
CONECT   98   97  102   99  109
CONECT   99   98  100  103
CONECT  100   99
CONECT  101   97
CONECT  102   98
CONECT  103   99  105  104
CONECT  104  103  106  107  110
CONECT  105  103
CONECT  106  104
CONECT  107  104
CONECT  108   97
CONECT  109   98
CONECT  110  104
END
```

Table S22: The structure of the Calc7 model used for St (PDB format)

```
HETATM    1  O   HOH   125      27.056  22.210  30.282
HETATM    2  H1  HOH   125      27.056  23.170  30.282
```

```
HETATM    3  H2  HOH   125      27.961  21.890  30.282
HETATM    4  O   HOH   179      33.275  19.601  34.303
HETATM    5  H1  HOH   179      33.275  20.561  34.303
HETATM    6  H2  HOH   179      34.180  19.281  34.303
HETATM    7  CB          7      26.449  22.008  40.030
HETATM    8  CG          8      27.888  22.320  40.345
HETATM    9  CD          9      28.748  22.572  39.121
HETATM   10  OE1        10      28.230  22.847  38.030
HETATM   11  NE2        11      30.053  22.462  39.274
HETATM   12 1HB         12      26.404  21.203  39.297
HETATM   13 2HB         13      26.020  22.928  39.634
HETATM   14 1HG         14      27.936  23.185  41.007
HETATM   15 2HG         15      28.295  21.432  40.828
HETATM   16 1HE2        16      30.434  22.220  40.178
HETATM   17 2HE2        17      30.666  22.621  38.487
HETATM   18  N          18      26.904  26.900  40.895
HETATM   19  CA         19      27.565  27.152  39.606
HETATM   20  C          20      26.474  27.805  38.715
HETATM   21  O          21      25.343  27.298  38.697
HETATM   22  CB         22      27.998  25.827  39.003
HETATM   23  SG         23      28.740  26.113  37.353
HETATM   24  H          24      26.257  26.130  40.989
HETATM   25  HA         25      28.463  27.760  39.715
HETATM   26 1HB         26      28.741  25.353  39.652
HETATM   27 2HB         27      27.135  25.167  38.886
HETATM   28  N          28      26.794  28.933  38.109
HETATM   29  CA         29      25.774  29.681  37.362
HETATM   30  C          30      25.826  29.367  35.880
HETATM   31  O          31      25.140  29.986  35.078
HETATM   32  H          32      27.740  29.282  38.159
HETATM   33  HA         33      24.813  29.357  37.760
HETATM   34  N          34      26.630  28.369  35.498
HETATM   35  CA         35      26.673  28.034  34.043
HETATM   36  C          36      25.454  27.250  33.670
HETATM   37  O          37      25.097  26.252  34.269
HETATM   38  CB         38      27.940  27.241  33.740
HETATM   39  CG1        39      27.897  26.576  32.374
HETATM   40  CG2        40      29.187  28.056  33.946
HETATM   41  H          41      27.188  27.860  36.169
HETATM   42  HA         42      26.687  28.951  33.454
HETATM   43  HB         43      27.979  26.432  34.470
HETATM   44 1HG1        44      28.823  26.025  32.209
HETATM   45 2HG1        45      27.052  25.888  32.331
HETATM   46 3HG1        46      27.785  27.338  31.602
HETATM   47 1HG2        47      30.061  27.447  33.717
HETATM   48 2HG2        48      29.167  28.924  33.287
HETATM   49 3HG2        49      29.237  28.388  34.983
HETATM   50  N          50      34.887  25.474  32.582
HETATM   51  CA         51      33.676  24.664  32.497
HETATM   52  C          52      32.628  25.023  33.552
HETATM   53  O          53      31.433  24.798  33.336
HETATM   54  H          54      35.642  25.167  33.178
HETATM   55  HA         55      33.249  24.856  31.513
HETATM   56  N          56      33.083  25.534  34.695
HETATM   57  CA         57      32.040  25.855  35.747
HETATM   58  C          58      32.496  27.154  36.414
HETATM   59  O          59      33.515  27.736  36.081
```

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HETATM   60  CB          60       32.207  24.725  36.859
HETATM   61  CG          61       31.822  23.389  36.314
HETATM   62  ND1         62       30.493  23.065  36.024
HETATM   63  CD2         63       32.583  22.308  35.952
HETATM   64  CE1         64       30.468  21.831  35.518
HETATM   65  NE2         65       31.696  21.352  35.483
HETATM   66  H           66       34.067  25.698  34.852
HETATM   67  HA          67       31.031  25.921  35.340
HETATM   68 1HB          68       33.244  24.696  37.194
HETATM   69 2HB          69       31.553  24.962  37.698
HETATM   70  HD2         70       33.667  22.218  36.019
HETATM   71  HE1         71       29.568  21.304  35.200
HETATM   72  HE2         72       31.951  20.429  35.163
HETATM   73  N           73       31.769  27.553  37.459
HETATM   74  CA          74       32.239  28.694  38.251
HETATM   75  C           75       31.679  28.485  39.674
HETATM   76  O           76       31.049  27.430  39.910
HETATM   77  CB          77       31.824  30.024  37.674
HETATM   78  H           78       30.911  27.078  37.700
HETATM   79  HA          79       33.328  28.730  38.252
HETATM   80 1HB          80       32.182  30.827  38.318
HETATM   81 2HB          81       32.272  30.091  36.683
HETATM   82  CB          82       25.626  23.626  36.270
HETATM   83  CG          83       26.353  23.381  34.987
HETATM   84  ND1         84       27.730  23.592  34.889
HETATM   85  CD2         85       25.923  22.936  33.782
HETATM   86  CE1         86       28.106  23.305  33.640
HETATM   87  NE2         87       27.030  22.896  32.957
HETATM   88 1HB          88       25.644  24.691  36.500
HETATM   89 2HB          89       26.138  23.057  37.046
HETATM   90  HD2         90       24.902  22.663  33.515
HETATM   91  HE1         91       29.126  23.383  33.264
HETATM   92  HE2         92       27.028  22.604  31.990
HETATM   93 CU    CU    110       28.874  24.179  36.375
HETATM   94  H           94       26.466  27.750  41.221
HETATM   95  H           95       25.936  30.753  37.472
HETATM   96  H           96       24.863  27.585  32.830
HETATM   97  H           97       34.640  26.425  32.814
HETATM   98  H           98       31.827  29.228  40.444
HETATM   99  H           99       30.740  30.113  37.606
HETATM  100  H          100       24.584  23.314  36.201
HETATM  101  H          101       25.896  21.676  40.908
HETATM  102  H          102       33.943  23.621  32.665
CONECT    1    2    3
CONECT    2    1
CONECT    3    1
CONECT    4    5    6
CONECT    5    4
CONECT    6    4
CONECT    7    8   12   13  101
CONECT    8    7    9   14   15
CONECT    9    8   10   11
CONECT   10    9   93
CONECT   11    9   16   17
CONECT   12    7
CONECT   13    7
CONECT   14    8
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CONECT   15    8
CONECT   16   11
CONECT   17   11
CONECT   18   24   19   94
CONECT   19   18   25   20   22
CONECT   20   19   21   28
CONECT   21   20
CONECT   22   19   23   26   27
CONECT   23   22   93
CONECT   24   18
CONECT   25   19
CONECT   26   22
CONECT   27   22
CONECT   28   20   32   29
CONECT   29   28   33   30   95
CONECT   30   29   31   34
CONECT   31   30
CONECT   32   28
CONECT   33   29
CONECT   34   30   41   35
CONECT   35   34   42   36   38
CONECT   36   35   37   96
CONECT   37   36
CONECT   38   35   39   40   43
CONECT   39   38   44   45   46
CONECT   40   38   47   48   49
CONECT   41   34
CONECT   42   35
CONECT   43   38
CONECT   44   39
CONECT   45   39
CONECT   46   39
CONECT   47   40
CONECT   48   40
CONECT   49   40
CONECT   50   54   51   97
CONECT   51   50   55   52  102
CONECT   52   51   53   56
CONECT   53   52
CONECT   54   50
CONECT   55   51
CONECT   56   52   66   57
CONECT   57   56   67   58   60
CONECT   58   57   59   73
CONECT   59   58
CONECT   60   57   61   68   69
CONECT   61   60   62   63
CONECT   62   61   64   93
CONECT   63   61   65   70
CONECT   64   62   65   71
CONECT   65   63   64   72
CONECT   66   56
CONECT   67   57
CONECT   68   60
CONECT   69   60
CONECT   70   63
CONECT   71   64
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CONECT   72   65
CONECT   73   58   78   74
CONECT   74   73   79   75   77
CONECT   75   74   76   98
CONECT   76   75
CONECT   77   74   80   81   99
CONECT   78   73
CONECT   79   74
CONECT   80   77
CONECT   81   77
CONECT   82   83   88   89  100
CONECT   83   82   84   85
CONECT   84   83   86   93
CONECT   85   83   87   90
CONECT   86   84   87   91
CONECT   87   85   86   92
CONECT   88   82
CONECT   89   82
CONECT   90   85
CONECT   91   86
CONECT   92   87
CONECT   93   10   23   62   84
CONECT   94   18
CONECT   95   29
CONECT   96   36
CONECT   97   50
CONECT   98   75
CONECT   99   77
CONECT  100   82
CONECT  101    7
CONECT  102   51
END
```

Table S23: The structure of the Calc7 model used for Am (PDB format)

```
HETATM    1  C1  UNK     1      -8.391  -3.121  -2.463  1.00  0.00
HETATM    2  C2  UNK     1      -7.367  -4.117  -1.947  1.00  0.00
HETATM    3  C3  UNK     1      -5.992  -3.614  -1.576  1.00  0.00
HETATM    4  C4  UNK     1      -5.061  -4.729  -1.113  1.00  0.00
HETATM    5  O5  UNK     1      -5.506  -5.848  -0.850  1.00  0.00
HETATM    6  O6  UNK     1      -3.865  -4.498  -1.030  1.00  0.00
HETATM    7  H7  UNK     1      -9.351  -3.623  -2.581  1.00  0.00
HETATM    8  H8  UNK     1      -7.789  -4.672  -1.109  1.00  0.00
HETATM    9  H9  UNK     1      -7.170  -4.738  -2.821  1.00  0.00
HETATM   10  H10 UNK     1      -5.549  -3.102  -2.431  1.00  0.00
HETATM   11  H11 UNK     1      -6.114  -2.927  -0.738  1.00  0.00
HETATM   12  H12 UNK     1      -8.491  -2.299  -1.755  1.00  0.00
HETATM   13  H13 UNK     1      -8.064  -2.731  -3.427  1.00  0.00
HETATM   14  N14 UNK     1       6.315  -3.582  -0.041  1.00  0.00
HETATM   15  C15 UNK     1       5.717  -3.545  -1.379  1.00  0.00
HETATM   16  C16 UNK     1       6.674  -2.747  -2.246  1.00  0.00
HETATM   17  O17 UNK     1       6.826  -1.536  -2.029  1.00  0.00
HETATM   18  C18 UNK     1       4.374  -2.820  -1.400  1.00  0.00
HETATM   19  C19 UNK     1       3.325  -3.495  -0.578  1.00  0.00
HETATM   20  S20 UNK     1       1.711  -2.617  -0.565  1.00  0.00
HETATM   21  C21 UNK     1       1.349  -2.547  -2.357  1.00  0.00
```

```
HETATM   22  H22 UNK     1       6.012  -2.895   0.635  1.00  0.00
HETATM   23  H23 UNK     1       5.550  -4.566  -1.721  1.00  0.00
HETATM   24  H24 UNK     1       4.508  -1.797  -1.048  1.00  0.00
HETATM   25  H25 UNK     1       4.024  -2.832  -2.431  1.00  0.00
HETATM   26  H26 UNK     1       3.176  -4.511  -0.943  1.00  0.00
HETATM   27  H27 UNK     1       3.669  -3.513   0.457  1.00  0.00
HETATM   28  H28 UNK     1       0.406  -2.019  -2.491  1.00  0.00
HETATM   29  H29 UNK     1       2.138  -2.026  -2.900  1.00  0.00
HETATM   30  H30 UNK     1       1.255  -3.563  -2.739  1.00  0.00
HETATM   31 H104 UNK     1       7.321  -3.554  -0.122  1.00  0.00
HETATM   32 H105 UNK     1       7.217  -3.230  -3.046  1.00  0.00
HETATM   33  C31 UNK     1      -5.646   0.238   1.422  1.00  0.00
HETATM   34  O32 UNK     1      -5.320  -0.075   0.282  1.00  0.00
HETATM   35  N33 UNK     1      -5.438   1.488   1.869  1.00  0.00
HETATM   36  C34 UNK     1      -4.827   2.533   1.059  1.00  0.00
HETATM   37  C35 UNK     1      -3.384   2.234   0.699  1.00  0.00
HETATM   38  O36 UNK     1      -2.635   1.734   1.541  1.00  0.00
HETATM   39  C37 UNK     1      -4.970   3.789   1.881  1.00  0.00
HETATM   40  C38 UNK     1      -6.210   3.504   2.703  1.00  0.00
HETATM   41  C39 UNK     1      -5.974   2.059   3.105  1.00  0.00
HETATM   42  H40 UNK     1      -5.317   2.625   0.090  1.00  0.00
HETATM   43  H41 UNK     1      -4.110   3.890   2.544  1.00  0.00
HETATM   44  H42 UNK     1      -5.034   4.701   1.288  1.00  0.00
HETATM   45  H43 UNK     1      -6.209   4.133   3.593  1.00  0.00
HETATM   46  H44 UNK     1      -7.151   3.683   2.184  1.00  0.00
HETATM   47  H45 UNK     1      -6.928   1.587   3.339  1.00  0.00
HETATM   48  H46 UNK     1      -5.329   1.934   3.974  1.00  0.00
HETATM   49  N47 UNK     1      -2.976   2.590  -0.523  1.00  0.00
HETATM   50  C48 UNK     1      -1.597   2.377  -0.978  1.00  0.00
HETATM   51  C49 UNK     1      -1.191   3.588  -1.805  1.00  0.00
HETATM   52  O50 UNK     1      -2.060   4.329  -2.263  1.00  0.00
HETATM   53  C51 UNK     1      -1.455   1.128  -1.883  1.00  0.00
HETATM   54  C52 UNK     1      -1.793  -0.218  -1.240  1.00  0.00
HETATM   55  N53 UNK     1      -0.984  -0.758  -0.307  1.00  0.00
HETATM   56  C54 UNK     1      -2.862  -1.004  -1.555  1.00  0.00
HETATM   57  C55 UNK     1      -1.577  -1.901  -0.043  1.00  0.00
HETATM   58  N56 UNK     1      -2.667  -2.046  -0.766  1.00  0.00
HETATM   59  H57 UNK     1      -3.638   3.020  -1.154  1.00  0.00
HETATM   60  H58 UNK     1      -0.972   2.232  -0.098  1.00  0.00
HETATM   61  H59 UNK     1      -2.055   1.261  -2.784  1.00  0.00
HETATM   62  H60 UNK     1      -0.389   1.068  -2.104  1.00  0.00
HETATM   63  H61 UNK     1      -3.664  -0.821  -2.269  1.00  0.00
HETATM   64  H62 UNK     1      -1.203  -2.625   0.680  1.00  0.00
HETATM   65  H63 UNK     1      -3.276  -2.850  -0.724  1.00  0.00
HETATM   66  N64 UNK     1       0.113   3.798  -1.995  1.00  0.00
HETATM   67  C65 UNK     1       0.572   4.871  -2.865  1.00  0.00
HETATM   68  C66 UNK     1       1.808   4.333  -3.573  1.00  0.00
HETATM   69  O67 UNK     1       2.100   3.131  -3.484  1.00  0.00
HETATM   70  C68 UNK     1       0.935   6.138  -2.044  1.00  0.00
HETATM   71  H69 UNK     1       0.787   3.208  -1.530  1.00  0.00
HETATM   72  H70 UNK     1      -0.206   5.164  -3.570  1.00  0.00
HETATM   73  H71 UNK     1       0.997   6.998  -2.711  1.00  0.00
HETATM   74  H72 UNK     1       0.136   6.257  -1.313  1.00  0.00
HETATM   75 H101 UNK     1      -6.102  -0.496   2.070  1.00  0.00
HETATM   76 H102 UNK     1       2.430   4.998  -4.154  1.00  0.00
HETATM   77 H103 UNK     1       1.901   6.050  -1.545  1.00  0.00
HETATM   78  N73 UNK     1       5.741   1.393  -1.462  1.00  0.00
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HETATM   79  C74 UNK     1       4.539   1.954  -0.869  1.00  0.00
HETATM   80  C75 UNK     1       4.944   2.562   0.478  1.00  0.00
HETATM   81  O76 UNK     1       5.474   1.834   1.339  1.00  0.00
HETATM   82  C77 UNK     1       3.462   0.906  -0.675  1.00  0.00
HETATM   83  S78 UNK     1       1.992   1.714   0.079  1.00  0.00
HETATM   84  H79 UNK     1       6.029   0.463  -1.194  1.00  0.00
HETATM   85  H80 UNK     1       4.090   2.722  -1.499  1.00  0.00
HETATM   86  H81 UNK     1       3.826   0.117  -0.011  1.00  0.00
HETATM   87  H82 UNK     1       3.202   0.466  -1.641  1.00  0.00
HETATM   88 Cu   UNK     1       0.667   0.017   0.472  1.00  0.00
HETATM   89 H106 UNK     1       6.510   2.035  -1.334  1.00  0.00
HETATM   90 H107 UNK     1       4.773   3.609   0.678  1.00  0.00
HETATM   91  N83 UNK     1       3.779   0.664   3.619  1.00  0.00
HETATM   92  C84 UNK     1       4.029  -0.770   3.483  1.00  0.00
HETATM   93  C85 UNK     1       5.314  -0.956   2.671  1.00  0.00
HETATM   94  O86 UNK     1       5.231  -1.381   1.510  1.00  0.00
HETATM   95  C87 UNK     1       2.846  -1.453   2.756  1.00  0.00
HETATM   96  C88 UNK     1       1.445  -1.082   3.249  1.00  0.00
HETATM   97  N89 UNK     1       0.530  -0.590   2.387  1.00  0.00
HETATM   98  C90 UNK     1       0.972  -1.172   4.529  1.00  0.00
HETATM   99  C91 UNK     1      -0.520  -0.361   3.134  1.00  0.00
HETATM  100  N92 UNK     1      -0.262  -0.705   4.383  1.00  0.00
HETATM  101  H93 UNK     1       3.834   1.250   2.799  1.00  0.00
HETATM  102  H94 UNK     1       4.134  -1.224   4.468  1.00  0.00
HETATM  103  H95 UNK     1       2.917  -1.261   1.685  1.00  0.00
HETATM  104  H96 UNK     1       2.951  -2.513   2.990  1.00  0.00
HETATM  105  H97 UNK     1       1.474  -1.532   5.428  1.00  0.00
HETATM  106  H98 UNK     1      -1.463   0.048   2.770  1.00  0.00
HETATM  107  H99 UNK     1      -0.926  -0.622   5.140  1.00  0.00
HETATM  108 H108 UNK     1       4.374   1.042   4.343  1.00  0.00
HETATM  109 H109 UNK     1       6.276  -0.721   3.103  1.00  0.00
CONECT    1    2    7   12   13
CONECT    2    1    3    8    9
CONECT    3    2    4   10   11
CONECT    4    3    5    6
CONECT    5    4
CONECT    6    4
CONECT    7    1
CONECT    8    2
CONECT    9    2
CONECT   10    3
CONECT   11    3
CONECT   12    1
CONECT   13    1
CONECT   14   15   22   31
CONECT   15   14   16   18   23
CONECT   16   15   17   32
CONECT   17   16
CONECT   18   15   19   24   25
CONECT   19   18   20   26   27
CONECT   20   19   21
CONECT   21   20   28   29   30
CONECT   22   14
CONECT   23   15
CONECT   24   18
CONECT   25   18
CONECT   26   19
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CONECT   27   19
CONECT   28   21
CONECT   29   21
CONECT   30   21
CONECT   31   14
CONECT   32   16
CONECT   33   34   35   75
CONECT   34   33
CONECT   35   33   36   41
CONECT   36   35   37   39   42
CONECT   37   36   38   49
CONECT   38   37
CONECT   39   36   40   43   44
CONECT   40   39   41   45   46
CONECT   41   35   40   47   48
CONECT   42   36
CONECT   43   39
CONECT   44   39
CONECT   45   40
CONECT   46   40
CONECT   47   41
CONECT   48   41
CONECT   49   37   50   59
CONECT   50   49   51   53   60
CONECT   51   50   52   66
CONECT   52   51
CONECT   53   50   54   61   62
CONECT   54   53   55   56
CONECT   55   54   57
CONECT   56   54   58   63
CONECT   57   55   58   64
CONECT   58   56   57   65
CONECT   59   49
CONECT   60   50
CONECT   61   53
CONECT   62   53
CONECT   63   56
CONECT   64   57
CONECT   65   58
CONECT   66   51   67   71
CONECT   67   66   68   70   72
CONECT   68   67   69   76
CONECT   69   68
CONECT   70   67   73   74   77
CONECT   71   66
CONECT   72   67
CONECT   73   70
CONECT   74   70
CONECT   75   33
CONECT   76   68
CONECT   77   70
CONECT   78   79   84   89
CONECT   79   78   80   82   85
CONECT   80   79   81   90
CONECT   81   80
CONECT   82   79   83   86   87
CONECT   83   82   88
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CONECT   84   78
CONECT   85   79
CONECT   86   82
CONECT   87   82
CONECT   88   83
CONECT   89   78
CONECT   90   80
CONECT   91   92  101  108
CONECT   92   91   93   95  102
CONECT   93   92   94  109
CONECT   94   93
CONECT   95   92   96  103  104
CONECT   96   95   97   98
CONECT   97   96   99
CONECT   98   96  100  105
CONECT   99   97  100  106
CONECT  100   98   99  107
CONECT  101   91
CONECT  102   92
CONECT  103   95
CONECT  104   95
CONECT  105   98
CONECT  106   99
CONECT  107  100
CONECT  108   91
CONECT  109   93
MASTER    0    0    0    0    0    0    0    0    3  109    0  109    0
END
```

Table S24: The structure of the Calc7 model used for Az from PDB # 4AZU (PDB format)

```
HETATM    1 Cu1  UNK     1      -0.418  -0.531   0.340  1.00  0.00
HETATM    2  N35 UNK     1       3.468  -1.306  -3.808  1.00  0.00
HETATM    3  C36 UNK     1       3.233  -0.465  -2.648  1.00  0.00
HETATM    4  C37 UNK     1       4.244  -0.901  -1.605  1.00  0.00
HETATM    5  O38 UNK     1       4.383  -2.110  -1.413  1.00  0.00
HETATM    6  C39 UNK     1       1.811  -0.740  -2.151  1.00  0.00
HETATM    7  S40 UNK     1       1.426   0.158  -0.601  1.00  0.00
HETATM    8  H41 UNK     1       3.183  -2.275  -3.770  1.00  0.00
HETATM    9  H42 UNK     1       3.328   0.586  -2.919  1.00  0.00
HETATM   10  H43 UNK     1       1.093  -0.439  -2.920  1.00  0.00
HETATM   11  H44 UNK     1       1.703  -1.810  -1.959  1.00  0.00
HETATM   12  N45 UNK     1       4.939  -0.006  -0.895  1.00  0.00
HETATM   13  C46 UNK     1       5.946  -0.425   0.061  1.00  0.00
HETATM   14  C47 UNK     1       5.471  -0.394   1.494  1.00  0.00
HETATM   15  O48 UNK     1       6.303  -0.623   2.390  1.00  0.00
HETATM   16  H49 UNK     1       4.760   0.979  -1.027  1.00  0.00
HETATM   17  H50 UNK     1       6.158  -1.454  -0.230  1.00  0.00
HETATM   18  N51 UNK     1       4.187  -0.102   1.773  1.00  0.00
HETATM   19  C52 UNK     1       3.722  -0.118   3.155  1.00  0.00
HETATM   20  C53 UNK     1       3.962  -1.551   3.670  1.00  0.00
HETATM   21  O54 UNK     1       3.801  -2.510   2.901  1.00  0.00
HETATM   22  C55 UNK     1       2.194   0.292   3.228  1.00  0.00
HETATM   23  H56 UNK     1       3.546   0.127   1.026  1.00  0.00
HETATM   24  H57 UNK     1       4.255   0.603   3.774  1.00  0.00
HETATM   25  H58 UNK     1       2.051   1.251   2.729  1.00  0.00
HETATM   26  H59 UNK     1       1.633  -0.495   2.726  1.00  0.00
```

HETATM	27	H90	UNK	1	6.806	0.244	0.038	1.00	0.00
HETATM	28	H91	UNK	1	4.441	-1.251	-4.073	1.00	0.00
HETATM	29	H92	UNK	1	4.268	-1.718	4.692	1.00	0.00
HETATM	30	H93	UNK	1	1.855	0.402	4.259	1.00	0.00
HETATM	31	N2	UNK	1	-2.062	2.587	4.545	1.00	0.00
HETATM	32	C3	UNK	1	-1.475	3.523	3.584	1.00	0.00
HETATM	33	C4	UNK	1	-1.010	2.825	2.298	1.00	0.00
HETATM	34	O5	UNK	1	-0.590	1.662	2.360	1.00	0.00
HETATM	35	H6	UNK	1	-1.615	2.451	5.440	1.00	0.00
HETATM	36	H7	UNK	1	-2.205	4.294	3.335	1.00	0.00
HETATM	37	H8	UNK	1	-0.596	3.966	4.052	1.00	0.00
HETATM	38	N9	UNK	1	-1.087	3.490	1.144	1.00	0.00
HETATM	39	C10	UNK	1	-0.621	2.934	-0.117	1.00	0.00
HETATM	40	C11	UNK	1	0.168	4.010	-0.850	1.00	0.00
HETATM	41	O12	UNK	1	-0.115	5.198	-0.715	1.00	0.00
HETATM	42	C13	UNK	1	-1.770	2.514	-1.051	1.00	0.00
HETATM	43	C14	UNK	1	-2.685	1.430	-0.494	1.00	0.00
HETATM	44	N15	UNK	1	-2.233	0.301	0.104	1.00	0.00
HETATM	45	C16	UNK	1	-4.044	1.515	-0.459	1.00	0.00
HETATM	46	C17	UNK	1	-3.342	-0.282	0.495	1.00	0.00
HETATM	47	N18	UNK	1	-4.404	0.430	0.169	1.00	0.00
HETATM	48	H19	UNK	1	-1.486	4.418	1.145	1.00	0.00
HETATM	49	H20	UNK	1	-0.028	2.053	0.123	1.00	0.00
HETATM	50	H21	UNK	1	-2.363	3.390	-1.315	1.00	0.00
HETATM	51	H22	UNK	1	-1.292	2.076	-1.927	1.00	0.00
HETATM	52	H23	UNK	1	-4.680	2.303	-0.859	1.00	0.00
HETATM	53	H24	UNK	1	-3.367	-1.236	1.023	1.00	0.00
HETATM	54	H25	UNK	1	-5.358	0.172	0.376	1.00	0.00
HETATM	55	N26	UNK	1	1.190	3.598	-1.579	1.00	0.00
HETATM	56	C27	UNK	1	1.913	4.479	-2.477	1.00	0.00
HETATM	57	C28	UNK	1	2.087	3.621	-3.712	1.00	0.00
HETATM	58	O29	UNK	1	1.737	2.431	-3.703	1.00	0.00
HETATM	59	C30	UNK	1	3.276	4.895	-1.886	1.00	0.00
HETATM	60	H31	UNK	1	1.480	2.633	-1.509	1.00	0.00
HETATM	61	H32	UNK	1	1.394	5.418	-2.671	1.00	0.00
HETATM	62	H33	UNK	1	3.825	5.486	-2.619	1.00	0.00
HETATM	63	H34	UNK	1	3.011	5.468	-0.998	1.00	0.00
HETATM	64	H87	UNK	1	2.517	4.046	-4.606	1.00	0.00
HETATM	65	H88	UNK	1	3.928	4.059	-1.635	1.00	0.00
HETATM	66	H89	UNK	1	-2.205	1.692	4.099	1.00	0.00
HETATM	67	C60	UNK	1	0.977	-3.458	1.001	1.00	0.00
HETATM	68	C61	UNK	1	0.015	-2.974	2.064	1.00	0.00
HETATM	69	N62	UNK	1	-0.662	-1.814	1.879	1.00	0.00
HETATM	70	C63	UNK	1	-0.170	-3.505	3.306	1.00	0.00
HETATM	71	C64	UNK	1	-1.275	-1.644	3.026	1.00	0.00
HETATM	72	N65	UNK	1	-0.974	-2.633	3.854	1.00	0.00
HETATM	73	H66	UNK	1	1.852	-2.809	0.981	1.00	0.00
HETATM	74	H67	UNK	1	0.437	-3.417	0.055	1.00	0.00
HETATM	75	H68	UNK	1	0.246	-4.419	3.731	1.00	0.00
HETATM	76	H69	UNK	1	-1.927	-0.801	3.254	1.00	0.00
HETATM	77	H70	UNK	1	-1.325	-2.705	4.798	1.00	0.00
HETATM	78	H84	UNK	1	1.326	-4.472	1.197	1.00	0.00
HETATM	79	C71	UNK	1	0.078	-4.955	-4.254	1.00	0.00
HETATM	80	C72	UNK	1	-0.139	-3.783	-3.321	1.00	0.00
HETATM	81	C73	UNK	1	-1.385	-3.956	-2.488	1.00	0.00
HETATM	82	S74	UNK	1	-1.867	-2.548	-1.429	1.00	0.00
HETATM	83	C75	UNK	1	-2.508	-1.430	-2.704	1.00	0.00

```
HETATM   84  H76 UNK     1      -0.789  -5.048  -4.909  1.00  0.00
HETATM   85  H77 UNK     1       0.725  -3.676  -2.666  1.00  0.00
HETATM   86  H78 UNK     1      -0.263  -2.888  -3.930  1.00  0.00
HETATM   87  H79 UNK     1      -2.220  -4.226  -3.134  1.00  0.00
HETATM   88  H80 UNK     1      -1.157  -4.751  -1.776  1.00  0.00
HETATM   89  H81 UNK     1      -2.823  -0.506  -2.220  1.00  0.00
HETATM   90  H82 UNK     1      -1.750  -1.205  -3.454  1.00  0.00
HETATM   91  H83 UNK     1      -3.366  -1.900  -3.184  1.00  0.00
HETATM   92  H85 UNK     1       0.977  -4.793  -4.849  1.00  0.00
HETATM   93  H86 UNK     1       0.192  -5.868  -3.670  1.00  0.00
HETATM   94  C94 UNK     1      -8.416   0.079  -1.599  1.00  0.00
HETATM   95  C95 UNK     1      -8.125  -0.450  -0.206  1.00  0.00
HETATM   96  O96 UNK     1      -6.980  -0.758   0.130  1.00  0.00
HETATM   97  H97 UNK     1      -8.729   1.116  -1.477  1.00  0.00
HETATM   98  N98 UNK     1      -9.150  -0.609   0.633  1.00  0.00
HETATM   99  H99 UNK     1     -10.080  -0.373   0.320  1.00  0.00
HETATM  100 H100 UNK     1      -7.543  -0.001  -2.245  1.00  0.00
HETATM  101 H101 UNK     1      -9.230  -0.495  -2.043  1.00  0.00
HETATM  102 H102 UNK     1      -8.998  -0.961   1.568  1.00  0.00
CONECT    1    7
CONECT    2    3    8   28
CONECT    3    2    4    6    9
CONECT    4    3    5   12
CONECT    5    4
CONECT    6    3    7   10   11
CONECT    7    1    6
CONECT    8    2
CONECT    9    3
CONECT   10    6
CONECT   11    6
CONECT   12    4   13   16
CONECT   13   12   14   17   27
CONECT   14   13   15   18
CONECT   15   14
CONECT   16   12
CONECT   17   13
CONECT   18   14   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   29
CONECT   21   20
CONECT   22   19   25   26   30
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   13
CONECT   28    2
CONECT   29   20
CONECT   30   22
CONECT   31   32   35   66
CONECT   32   31   33   36   37
CONECT   33   32   34   38
CONECT   34   33
CONECT   35   31
CONECT   36   32
CONECT   37   32
CONECT   38   33   39   48
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CONECT   39   38   40   42   49
CONECT   40   39   41   55
CONECT   41   40
CONECT   42   39   43   50   51
CONECT   43   42   44   45
CONECT   44   43   46
CONECT   45   43   47   52
CONECT   46   44   47   53
CONECT   47   45   46   54
CONECT   48   38
CONECT   49   39
CONECT   50   42
CONECT   51   42
CONECT   52   45
CONECT   53   46
CONECT   54   47
CONECT   55   40   56   60
CONECT   56   55   57   59   61
CONECT   57   56   58   64
CONECT   58   57
CONECT   59   56   62   63   65
CONECT   60   55
CONECT   61   56
CONECT   62   59
CONECT   63   59
CONECT   64   57
CONECT   65   59
CONECT   66   31
CONECT   67   68   73   74   78
CONECT   68   67   69   70
CONECT   69   68   71
CONECT   70   68   72   75
CONECT   71   69   72   76
CONECT   72   70   71   77
CONECT   73   67
CONECT   74   67
CONECT   75   70
CONECT   76   71
CONECT   77   72
CONECT   78   67
CONECT   79   80   84   92   93
CONECT   80   79   81   85   86
CONECT   81   80   82   87   88
CONECT   82   81   83
CONECT   83   82   89   90   91
CONECT   84   79
CONECT   85   80
CONECT   86   80
CONECT   87   81
CONECT   88   81
CONECT   89   83
CONECT   90   83
CONECT   91   83
CONECT   92   79
CONECT   93   79
CONECT   94   95   97  100  101
CONECT   95   94   96   98
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CONECT   96   95
CONECT   97   94
CONECT   98   95   99  102
CONECT   99   98
CONECT  100   94
CONECT  101   94
CONECT  102   98
MASTER    0    0    0    0    0    0    0    0    3  102    0  102    0
END
```

Table S25: The structure of the Calc7 model used for Az from PDB # 2CCW (PDB format)

```
HETATM    1  C1  UNK     1       8.264  -2.217  -0.119  1.00  0.00
HETATM    2  C2  UNK     1       8.071  -0.740  -0.413  1.00  0.00
HETATM    3  O3  UNK     1       6.965  -0.263  -0.619  1.00  0.00
HETATM    4  H4  UNK     1       8.586  -2.234   0.921  1.00  0.00
HETATM    5  N5  UNK     1       9.168   0.011  -0.398  1.00  0.00
HETATM    6  H6  UNK     1      10.060  -0.439  -0.244  1.00  0.00
HETATM    7  H7  UNK     1       7.367  -2.810  -0.299  1.00  0.00
HETATM    8  H8  UNK     1       9.058  -2.613  -0.753  1.00  0.00
HETATM    9  H9  UNK     1       9.112   1.010  -0.537  1.00  0.00
HETATM   10  C10 UNK     1       0.036  -3.317  -5.810  1.00  0.00
HETATM   11  C11 UNK     1       0.257  -2.696  -4.436  1.00  0.00
HETATM   12  C12 UNK     1       1.462  -1.821  -4.404  1.00  0.00
HETATM   13  S13 UNK     1       1.843  -1.063  -2.787  1.00  0.00
HETATM   14  C14 UNK     1       2.233  -2.580  -1.875  1.00  0.00
HETATM   15  H15 UNK     1       0.900  -3.944  -6.032  1.00  0.00
HETATM   16  H16 UNK     1      -0.621  -2.115  -4.155  1.00  0.00
HETATM   17  H17 UNK     1       0.419  -3.508  -3.727  1.00  0.00
HETATM   18  H18 UNK     1       2.328  -2.381  -4.759  1.00  0.00
HETATM   19  H19 UNK     1       1.246  -0.975  -5.056  1.00  0.00
HETATM   20  H20 UNK     1       2.478  -2.307  -0.849  1.00  0.00
HETATM   21  H21 UNK     1       1.385  -3.265  -1.876  1.00  0.00
HETATM   22  H22 UNK     1       3.092  -3.067  -2.337  1.00  0.00
HETATM   23  H93 UNK     1      -0.880  -3.907  -5.823  1.00  0.00
HETATM   24  H94 UNK     1      -0.042  -2.528  -6.558  1.00  0.00
HETATM   25  N23 UNK     1       2.229   3.688   3.623  1.00  0.00
HETATM   26  C24 UNK     1       1.648   2.555   4.302  1.00  0.00
HETATM   27  C25 UNK     1       1.128   1.542   3.275  1.00  0.00
HETATM   28  O26 UNK     1       0.813   1.877   2.132  1.00  0.00
HETATM   29  H27 UNK     1       1.759   4.581   3.641  1.00  0.00
HETATM   30  H28 UNK     1       2.403   2.080   4.930  1.00  0.00
HETATM   31  H29 UNK     1       0.819   2.895   4.922  1.00  0.00
HETATM   32  N30 UNK     1       1.052   0.300   3.741  1.00  0.00
HETATM   33  C31 UNK     1       0.509  -0.780   2.915  1.00  0.00
HETATM   34  C32 UNK     1      -0.423  -1.657   3.743  1.00  0.00
HETATM   35  O33 UNK     1      -0.245  -1.873   4.913  1.00  0.00
HETATM   36  C34 UNK     1       1.585  -1.677   2.306  1.00  0.00
HETATM   37  C35 UNK     1       2.577  -0.968   1.443  1.00  0.00
HETATM   38  N36 UNK     1       2.196  -0.165   0.373  1.00  0.00
HETATM   39  C37 UNK     1       3.940  -0.993   1.469  1.00  0.00
HETATM   40  C38 UNK     1       3.320   0.263  -0.188  1.00  0.00
HETATM   41  N39 UNK     1       4.379  -0.200   0.438  1.00  0.00
HETATM   42  H40 UNK     1       1.372   0.099   4.677  1.00  0.00
HETATM   43  H41 UNK     1      -0.024  -0.290   2.101  1.00  0.00
HETATM   44  H42 UNK     1       2.110  -2.207   3.101  1.00  0.00
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HETATM	45	H43	UNK	1	1.058	-2.366	1.647	1.00	0.00
HETATM	46	H44	UNK	1	4.564	-1.540	2.175	1.00	0.00
HETATM	47	H45	UNK	1	3.355	0.910	-1.064	1.00	0.00
HETATM	48	H46	UNK	1	5.342	-0.006	0.204	1.00	0.00
HETATM	49	N47	UNK	1	-1.420	-2.197	3.050	1.00	0.00
HETATM	50	C48	UNK	1	-2.242	-3.275	3.566	1.00	0.00
HETATM	51	C49	UNK	1	-2.388	-4.328	2.485	1.00	0.00
HETATM	52	O50	UNK	1	-1.811	-4.248	1.405	1.00	0.00
HETATM	53	C51	UNK	1	-3.579	-2.780	4.128	1.00	0.00
HETATM	54	H52	UNK	1	-1.613	-1.841	2.125	1.00	0.00
HETATM	55	H53	UNK	1	-1.750	-3.730	4.426	1.00	0.00
HETATM	56	H54	UNK	1	-4.088	-3.602	4.633	1.00	0.00
HETATM	57	H55	UNK	1	-3.341	-1.977	4.826	1.00	0.00
HETATM	58	H99	UNK	1	-4.245	-2.418	3.344	1.00	0.00
HETATM	59	H100	UNK	1	2.438	3.436	2.667	1.00	0.00
HETATM	60	H102	UNK	1	-3.023	-5.181	2.674	1.00	0.00
HETATM	61	N56	UNK	1	-3.476	-3.390	-2.295	1.00	0.00
HETATM	62	C57	UNK	1	-3.291	-2.400	-1.233	1.00	0.00
HETATM	63	C58	UNK	1	-4.286	-1.275	-1.443	1.00	0.00
HETATM	64	O59	UNK	1	-4.372	-0.732	-2.556	1.00	0.00
HETATM	65	C60	UNK	1	-1.864	-1.884	-1.310	1.00	0.00
HETATM	66	S61	UNK	1	-1.528	-0.699	0.033	1.00	0.00
HETATM	67	H62	UNK	1	-3.019	-3.251	-3.185	1.00	0.00
HETATM	68	H63	UNK	1	-3.459	-2.862	-0.260	1.00	0.00
HETATM	69	H64	UNK	1	-1.165	-2.722	-1.232	1.00	0.00
HETATM	70	H65	UNK	1	-1.717	-1.375	-2.266	1.00	0.00
HETATM	71	N66	UNK	1	-5.077	-0.924	-0.426	1.00	0.00
HETATM	72	C67	UNK	1	-6.035	0.162	-0.524	1.00	0.00
HETATM	73	C68	UNK	1	-5.534	1.488	0.007	1.00	0.00
HETATM	74	O69	UNK	1	-6.308	2.446	0.050	1.00	0.00
HETATM	75	H70	UNK	1	-5.006	-1.433	0.444	1.00	0.00
HETATM	76	H71	UNK	1	-6.189	0.291	-1.596	1.00	0.00
HETATM	77	N72	UNK	1	-4.283	1.573	0.382	1.00	0.00
HETATM	78	C73	UNK	1	-3.712	2.878	0.719	1.00	0.00
HETATM	79	C74	UNK	1	-3.865	3.773	-0.499	1.00	0.00
HETATM	80	O75	UNK	1	-3.651	3.300	-1.630	1.00	0.00
HETATM	81	C76	UNK	1	-2.262	2.735	1.119	1.00	0.00
HETATM	82	H77	UNK	1	-3.713	0.741	0.438	1.00	0.00
HETATM	83	H78	UNK	1	-4.233	3.319	1.569	1.00	0.00
HETATM	84	H79	UNK	1	-2.164	1.932	1.850	1.00	0.00
HETATM	85	H80	UNK	1	-1.718	2.505	0.202	1.00	0.00
HETATM	86	C81	UNK	1	-1.115	1.574	-3.022	1.00	0.00
HETATM	87	C82	UNK	1	-0.194	2.486	-2.294	1.00	0.00
HETATM	88	N83	UNK	1	0.493	2.044	-1.177	1.00	0.00
HETATM	89	C84	UNK	1	0.137	3.787	-2.501	1.00	0.00
HETATM	90	C85	UNK	1	1.194	3.072	-0.749	1.00	0.00
HETATM	91	N86	UNK	1	1.040	4.138	-1.533	1.00	0.00
HETATM	92	H87	UNK	1	-2.014	1.413	-2.426	1.00	0.00
HETATM	93	H88	UNK	1	-0.578	0.638	-3.174	1.00	0.00
HETATM	94	H89	UNK	1	-0.246	4.433	-3.291	1.00	0.00
HETATM	95	H90	UNK	1	1.825	3.059	0.140	1.00	0.00
HETATM	96	H91	UNK	1	1.499	5.031	-1.434	1.00	0.00
HETATM	97	Cu92	UNK	1	0.375	0.277	-0.302	1.00	0.00
HETATM	98	H95	UNK	1	-1.423	1.993	-3.980	1.00	0.00
HETATM	99	H96	UNK	1	-4.463	-3.544	-2.444	1.00	0.00
HETATM	100	H97	UNK	1	-4.155	4.808	-0.385	1.00	0.00
HETATM	101	H98	UNK	1	-1.867	3.639	1.580	1.00	0.00

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HETATM  102 H101 UNK     1      -6.917  -0.094   0.062  1.00  0.00
HETATM  103 O103 UNK     1       2.526   6.420  -1.148  1.00  0.00
HETATM  104 H104 UNK     1       2.495   5.708  -0.504  1.00  0.00
HETATM  105 H105 UNK     1       1.808   7.034  -0.980  1.00  0.00
CONECT    1    2    4    7    8
CONECT    2    1    3    5
CONECT    3    2
CONECT    4    1
CONECT    5    2    6    9
CONECT    6    5
CONECT    7    1
CONECT    8    1
CONECT    9    5
CONECT   10   11   15   23   24
CONECT   11   10   12   16   17
CONECT   12   11   13   18   19
CONECT   13   12   14
CONECT   14   13   20   21   22
CONECT   15   10
CONECT   16   11
CONECT   17   11
CONECT   18   12
CONECT   19   12
CONECT   20   14
CONECT   21   14
CONECT   22   14
CONECT   23   10
CONECT   24   10
CONECT   25   26   29   59
CONECT   26   25   27   30   31
CONECT   27   26   28   32
CONECT   28   27
CONECT   29   25
CONECT   30   26
CONECT   31   26
CONECT   32   27   33   42
CONECT   33   32   34   36   43
CONECT   34   33   35   49
CONECT   35   34
CONECT   36   33   37   44   45
CONECT   37   36   38   39
CONECT   38   37   40
CONECT   39   37   41   46
CONECT   40   38   41   47
CONECT   41   39   40   48
CONECT   42   32
CONECT   43   33
CONECT   44   36
CONECT   45   36
CONECT   46   39
CONECT   47   40
CONECT   48   41
CONECT   49   34   50   54
CONECT   50   49   51   53   55
CONECT   51   50   52   60
CONECT   52   51
CONECT   53   50   56   57   58
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CONECT   54   49
CONECT   55   50
CONECT   56   53
CONECT   57   53
CONECT   58   53
CONECT   59   25
CONECT   60   51
CONECT   61   62   67   99
CONECT   62   61   63   65   68
CONECT   63   62   64   71
CONECT   64   63
CONECT   65   62   66   69   70
CONECT   66   65   97
CONECT   67   61
CONECT   68   62
CONECT   69   65
CONECT   70   65
CONECT   71   63   72   75
CONECT   72   71   73   76  102
CONECT   73   72   74   77
CONECT   74   73
CONECT   75   71
CONECT   76   72
CONECT   77   73   78   82
CONECT   78   77   79   81   83
CONECT   79   78   80  100
CONECT   80   79
CONECT   81   78   84   85  101
CONECT   82   77
CONECT   83   78
CONECT   84   81
CONECT   85   81
CONECT   86   87   92   93   98
CONECT   87   86   88   89
CONECT   88   87   90   97
CONECT   89   87   91   94
CONECT   90   88   91   95
CONECT   91   89   90   96
CONECT   92   86
CONECT   93   86
CONECT   94   89
CONECT   95   90
CONECT   96   91
CONECT   97   66   88
CONECT   98   86
CONECT   99   61
CONECT  100   79
CONECT  101   81
CONECT  102   72
CONECT  103  104  105
CONECT  104  103
CONECT  105  103
MASTER    0    0    0    0    0    0    0    0    3  105    0  105    0
END
```

Table S26. Proton NMR Hyperfine Shifts in Az using Different Structures (unit: ppm).

	δ_{hf}^{expt}	δ_{hf}^{calc7}	δ_{hf}^{calc7}	δ_{hf}^{calc7}
PDB #		1NWP	4AZU	2CCW
C112 $C^{\alpha}H$	-12.8	-9.3	-11.4	-1.2
C112 $C^{\beta}H^{\beta1}$	846.5	761.6	923.8	735.1
C112 $C^{\beta}H^{\beta2}$	797.1	590.3	491.4	581.1
H117 $C^{\delta2}H$	47.1	22.3	8.0	25.4
H117 $C^{\varepsilon1}H$	39.9	35.6	25.4	35.6
H117 $N^{\varepsilon2}H$	15.3	18.2	9.0	17.2
H46 $C^{\delta2}H$	43.2	21.3	15.2	27.4
H46 $C^{\varepsilon1}H$	27.2	13.1	23.3	25.4
H46 $N^{\varepsilon2}H$	15.4	9.0	8.0	10.1
N47 NH	-40.7	-42.0	-31.8	-78.7
N47 $C^{\alpha}H$	15.2	15.2	9.0	22.3
R^2		0.99	0.91	0.99

[a] Tentative assignments of $H^{\beta1}/H^{\beta2}$ are made to let them have the same order as reported in experiment.

Table S27. Key Bond Lengths in Copper Centers of Am [a]

Structure	1AAC	1AAC-Calc7	2OV0
Cu-S^{Cys}	2.11	2.19	2.17
Cu-S^{Met}	2.90	3.02	3.07
Cu-N^{HisC}	2.03	2.01	2.05
Cu-N^{HisN}	1.95	1.98	1.99
Cu-O [b]	3.92	3.87	3.76

[a] The bond length is in Å; [b] The carbonyl O in the 5th coordination position.

Table S28. Structure of 1RCY-Calc3 model in PDB format.

```
ATOM      1  N   UNK     1      -1.419   5.476  19.885  1.00  0.00
ATOM      2  C   UNK     1      -2.027   5.122  18.601  1.00  0.00
ATOM      3  C   UNK     1      -3.483   4.646  18.747  1.00  0.00
ATOM      4  O   UNK     1      -3.914   4.251  19.832  1.00  0.00
ATOM      5  C   UNK     1      -1.221   4.006  17.923  1.00  0.00
ATOM      6  C   UNK     1       0.250   4.270  17.842  1.00  0.00
ATOM      7  N   UNK     1       0.799   4.982  16.808  1.00  0.00
ATOM      8  C   UNK     1       1.247   3.791  18.634  1.00  0.00
ATOM      9  C   UNK     1       2.105   4.921  16.982  1.00  0.00
ATOM     10  N   UNK     1       2.422   4.212  18.072  1.00  0.00
ATOM     11  H   UNK     1      -0.570   5.011  20.171  1.00  0.00
ATOM     12  H   UNK     1      -2.020   6.029  17.996  1.00  0.00
ATOM     13  H   UNK     1      -1.393   3.065  18.445  1.00  0.00
ATOM     14  H   UNK     1      -1.577   3.958  16.894  1.00  0.00
ATOM     15  H   UNK     1       1.133   3.191  19.537  1.00  0.00
ATOM     16  H   UNK     1       2.834   5.389  16.321  1.00  0.00
ATOM     17  H   UNK     1       3.353   4.023  18.415  1.00  0.00
ATOM     18  N   UNK     1      -4.232   4.684  17.648  1.00  0.00
ATOM     19  C   UNK     1      -5.617   4.213  17.651  1.00  0.00
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ATOM	20	C	UNK	1	-5.756	3.196	16.531	1.00	0.00
ATOM	21	O	UNK	1	-4.870	3.085	15.682	1.00	0.00
ATOM	22	C	UNK	1	-6.605	5.362	17.420	1.00	0.00
ATOM	23	H	UNK	1	-3.836	5.046	16.793	1.00	0.00
ATOM	24	H	UNK	1	-5.847	3.774	18.622	1.00	0.00
ATOM	25	H	UNK	1	-7.623	4.973	17.427	1.00	0.00
ATOM	26	H	UNK	1	-6.471	6.085	18.225	1.00	0.00
ATOM	27	N	UNK	1	-4.582	4.735	11.981	1.00	0.00
ATOM	28	C	UNK	1	-4.309	5.392	13.245	1.00	0.00
ATOM	29	C	UNK	1	-4.600	6.869	13.009	1.00	0.00
ATOM	30	O	UNK	1	-4.167	7.440	11.996	1.00	0.00
ATOM	31	C	UNK	1	-2.851	5.223	13.656	1.00	0.00
ATOM	32	S	UNK	1	-2.461	6.210	15.137	1.00	0.00
ATOM	33	H	UNK	1	-3.908	4.806	11.232	1.00	0.00
ATOM	34	H	UNK	1	-4.917	4.965	14.042	1.00	0.00
ATOM	35	H	UNK	1	-2.204	5.530	12.834	1.00	0.00
ATOM	36	H	UNK	1	-2.684	4.172	13.893	1.00	0.00
ATOM	37	N	UNK	1	0.554	9.902	11.237	1.00	0.00
ATOM	38	C	UNK	1	0.762	8.454	11.190	1.00	0.00
ATOM	39	C	UNK	1	0.215	7.755	9.950	1.00	0.00
ATOM	40	O	UNK	1	0.937	7.010	9.286	1.00	0.00
ATOM	41	C	UNK	1	0.242	7.793	12.469	1.00	0.00
ATOM	42	C	UNK	1	1.058	8.111	13.682	1.00	0.00
ATOM	43	N	UNK	1	0.893	7.435	14.867	1.00	0.00
ATOM	44	C	UNK	1	2.042	9.040	13.829	1.00	0.00
ATOM	45	C	UNK	1	1.769	7.963	15.705	1.00	0.00
ATOM	46	N	UNK	1	2.486	8.935	15.123	1.00	0.00
ATOM	47	H	UNK	1	-0.007	10.298	11.978	1.00	0.00
ATOM	48	H	UNK	1	1.842	8.327	11.120	1.00	0.00
ATOM	49	H	UNK	1	-0.792	8.093	12.638	1.00	0.00
ATOM	50	H	UNK	1	0.317	6.716	12.316	1.00	0.00
ATOM	51	H	UNK	1	2.406	9.731	13.069	1.00	0.00
ATOM	52	H	UNK	1	1.893	7.647	16.741	1.00	0.00
ATOM	53	H	UNK	1	3.214	9.485	15.555	1.00	0.00
ATOM	54	Cu	UNK	1	-0.225	5.992	15.360	1.00	0.00
ATOM	55	N	UNK	1	0.811	4.243	8.468	1.00	0.00
ATOM	56	C	UNK	1	0.172	3.459	9.514	1.00	0.00
ATOM	57	C	UNK	1	-1.297	3.168	9.203	1.00	0.00
ATOM	58	O	UNK	1	-2.206	3.814	9.734	1.00	0.00
ATOM	59	C	UNK	1	0.317	4.124	10.885	1.00	0.00
ATOM	60	C	UNK	1	0.023	3.178	12.030	1.00	0.00
ATOM	61	S	UNK	1	0.511	3.797	13.639	1.00	0.00
ATOM	62	C	UNK	1	0.116	2.402	14.652	1.00	0.00
ATOM	63	H	UNK	1	0.844	5.251	8.530	1.00	0.00
ATOM	64	H	UNK	1	0.693	2.502	9.546	1.00	0.00
ATOM	65	H	UNK	1	1.327	4.521	10.991	1.00	0.00
ATOM	66	H	UNK	1	-0.419	4.927	10.933	1.00	0.00
ATOM	67	H	UNK	1	-1.040	2.939	12.040	1.00	0.00
ATOM	68	H	UNK	1	0.626	2.288	11.851	1.00	0.00
ATOM	69	H	UNK	1	0.362	2.626	15.690	1.00	0.00
ATOM	70	H	UNK	1	-0.949	2.183	14.570	1.00	0.00
ATOM	71	H	UNK	1	0.691	1.538	14.321	1.00	0.00
ATOM	72	H	UNK	1	-2.110	5.397	20.618	1.00	0.00
ATOM	73	H	UNK	1	-6.634	2.569	16.479	1.00	0.00
ATOM	74	H	UNK	1	-6.426	5.840	16.457	1.00	0.00
ATOM	75	H	UNK	1	-5.491	5.018	11.644	1.00	0.00
ATOM	76	H	UNK	1	-5.187	7.422	13.728	1.00	0.00

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ATOM      77  H   UNK     1       0.207  10.221  10.344  1.00  0.00
ATOM      78  H   UNK     1      -0.811   7.914   9.652  1.00  0.00
ATOM      79  H   UNK     1       0.438   3.973   7.569  1.00  0.00
ATOM      80  H   UNK     1      -1.544   2.382   8.505  1.00  0.00
CONECT     1    2   11   72
CONECT     2    1    3    5   12
CONECT     3    2    4   18
CONECT     4    3
CONECT     5    2    6   13   14
CONECT     6    5    7    8
CONECT     7    6    9   54
CONECT     8    6   10   15
CONECT     9    7   10   16
CONECT    10    8    9   17
CONECT    11    1
CONECT    12    2
CONECT    13    5
CONECT    14    5
CONECT    15    8
CONECT    16    9
CONECT    17   10
CONECT    18    3   19   23
CONECT    19   18   20   22   24
CONECT    20   19   21   73
CONECT    21   20
CONECT    22   19   25   26   74
CONECT    23   18
CONECT    24   19
CONECT    25   22
CONECT    26   22
CONECT    27   28   33   75
CONECT    28   27   29   31   34
CONECT    29   28   30   76
CONECT    30   29
CONECT    31   28   32   35   36
CONECT    32   31   54
CONECT    33   27
CONECT    34   28
CONECT    35   31
CONECT    36   31
CONECT    37   38   47   77
CONECT    38   37   39   41   48
CONECT    39   38   40   78
CONECT    40   39
CONECT    41   38   42   49   50
CONECT    42   41   43   44
CONECT    43   42   45   54
CONECT    44   42   46   51
CONECT    45   43   46   52
CONECT    46   44   45   53
CONECT    47   37
CONECT    48   38
CONECT    49   41
CONECT    50   41
CONECT    51   44
CONECT    52   45
CONECT    53   46
```

```
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
```

Table S29. Structure of 1RCY-Calc4 model in PDB format.

```
ATOM      1  N   UNK     1      -1.419   5.476  19.885  1.00  0.00
ATOM      2  C   UNK     1      -2.027   5.122  18.601  1.00  0.00
ATOM      3  C   UNK     1      -3.483   4.646  18.747  1.00  0.00
ATOM      4  O   UNK     1      -3.914   4.251  19.832  1.00  0.00
ATOM      5  C   UNK     1      -1.221   4.006  17.923  1.00  0.00
ATOM      6  C   UNK     1       0.250   4.270  17.842  1.00  0.00
ATOM      7  N   UNK     1       0.799   4.982  16.808  1.00  0.00
ATOM      8  C   UNK     1       1.247   3.791  18.634  1.00  0.00
ATOM      9  C   UNK     1       2.105   4.921  16.982  1.00  0.00
ATOM     10  N   UNK     1       2.422   4.212  18.072  1.00  0.00
ATOM     11  H   UNK     1      -0.570   5.011  20.171  1.00  0.00
ATOM     12  H   UNK     1      -2.020   6.029  17.996  1.00  0.00
ATOM     13  H   UNK     1      -1.393   3.065  18.445  1.00  0.00
ATOM     14  H   UNK     1      -1.577   3.958  16.894  1.00  0.00
ATOM     15  H   UNK     1       1.133   3.191  19.537  1.00  0.00
ATOM     16  H   UNK     1       2.834   5.389  16.321  1.00  0.00
ATOM     17  H   UNK     1       3.353   4.023  18.415  1.00  0.00
ATOM     18  N   UNK     1      -4.232   4.684  17.648  1.00  0.00
ATOM     19  C   UNK     1      -5.617   4.213  17.651  1.00  0.00
ATOM     20  C   UNK     1      -5.756   3.196  16.531  1.00  0.00
ATOM     21  O   UNK     1      -4.870   3.085  15.682  1.00  0.00
ATOM     22  C   UNK     1      -6.605   5.362  17.420  1.00  0.00
ATOM     23  H   UNK     1      -3.836   5.046  16.793  1.00  0.00
ATOM     24  H   UNK     1      -5.847   3.774  18.622  1.00  0.00
ATOM     25  H   UNK     1      -7.623   4.973  17.427  1.00  0.00
```

```
ATOM      26  H   UNK     1       -6.471   6.085  18.225  1.00  0.00
ATOM      27  N   UNK     1       -4.582   4.735  11.981  1.00  0.00
ATOM      28  C   UNK     1       -4.309   5.392  13.245  1.00  0.00
ATOM      29  C   UNK     1       -4.600   6.869  13.009  1.00  0.00
ATOM      30  O   UNK     1       -4.167   7.440  11.996  1.00  0.00
ATOM      31  C   UNK     1       -2.844   5.179  13.603  1.00  0.00
ATOM      32  S   UNK     1       -2.382   6.151  15.085  1.00  0.00
ATOM      33  H   UNK     1       -3.908   4.806  11.232  1.00  0.00
ATOM      34  H   UNK     1       -4.917   4.965  14.042  1.00  0.00
ATOM      35  H   UNK     1       -2.211   5.503  12.771  1.00  0.00
ATOM      36  H   UNK     1       -2.663   4.118  13.793  1.00  0.00
ATOM      37  N   UNK     1        0.554   9.902  11.237  1.00  0.00
ATOM      38  C   UNK     1        0.762   8.454  11.190  1.00  0.00
ATOM      39  C   UNK     1        0.215   7.755   9.950  1.00  0.00
ATOM      40  O   UNK     1        0.937   7.010   9.286  1.00  0.00
ATOM      41  C   UNK     1        0.242   7.793  12.469  1.00  0.00
ATOM      42  C   UNK     1        1.058   8.111  13.682  1.00  0.00
ATOM      43  N   UNK     1        0.893   7.435  14.867  1.00  0.00
ATOM      44  C   UNK     1        2.042   9.040  13.829  1.00  0.00
ATOM      45  C   UNK     1        1.769   7.963  15.705  1.00  0.00
ATOM      46  N   UNK     1        2.486   8.935  15.123  1.00  0.00
ATOM      47  H   UNK     1       -0.007  10.298  11.978  1.00  0.00
ATOM      48  H   UNK     1        1.842   8.327  11.120  1.00  0.00
ATOM      49  H   UNK     1       -0.792   8.093  12.638  1.00  0.00
ATOM      50  H   UNK     1        0.317   6.716  12.316  1.00  0.00
ATOM      51  H   UNK     1        2.406   9.731  13.069  1.00  0.00
ATOM      52  H   UNK     1        1.893   7.647  16.741  1.00  0.00
ATOM      53  H   UNK     1        3.214   9.485  15.555  1.00  0.00
ATOM      54 Cu   UNK     1       -0.225   5.992  15.360  1.00  0.00
ATOM      55  N   UNK     1        0.811   4.243   8.468  1.00  0.00
ATOM      56  C   UNK     1        0.172   3.459   9.514  1.00  0.00
ATOM      57  C   UNK     1       -1.297   3.168   9.203  1.00  0.00
ATOM      58  O   UNK     1       -2.206   3.814   9.734  1.00  0.00
ATOM      59  C   UNK     1        0.317   4.124  10.885  1.00  0.00
ATOM      60  C   UNK     1        0.023   3.178  12.030  1.00  0.00
ATOM      61  S   UNK     1        0.511   3.797  13.639  1.00  0.00
ATOM      62  C   UNK     1        0.116   2.402  14.652  1.00  0.00
ATOM      63  H   UNK     1        0.844   5.251   8.530  1.00  0.00
ATOM      64  H   UNK     1        0.693   2.502   9.546  1.00  0.00
ATOM      65  H   UNK     1        1.327   4.521  10.991  1.00  0.00
ATOM      66  H   UNK     1       -0.419   4.927  10.933  1.00  0.00
ATOM      67  H   UNK     1       -1.040   2.939  12.040  1.00  0.00
ATOM      68  H   UNK     1        0.626   2.288  11.851  1.00  0.00
ATOM      69  H   UNK     1        0.362   2.626  15.690  1.00  0.00
ATOM      70  H   UNK     1       -0.949   2.183  14.570  1.00  0.00
ATOM      71  H   UNK     1        0.691   1.538  14.321  1.00  0.00
ATOM      72  H   UNK     1       -2.110   5.397  20.618  1.00  0.00
ATOM      73  H   UNK     1       -6.634   2.569  16.479  1.00  0.00
ATOM      74  H   UNK     1       -6.426   5.840  16.457  1.00  0.00
ATOM      75  H   UNK     1       -5.491   5.018  11.644  1.00  0.00
ATOM      76  H   UNK     1       -5.187   7.422  13.728  1.00  0.00
ATOM      77  H   UNK     1        0.207  10.221  10.344  1.00  0.00
ATOM      78  H   UNK     1       -0.811   7.914   9.652  1.00  0.00
ATOM      79  H   UNK     1        0.438   3.973   7.569  1.00  0.00
ATOM      80  H   UNK     1       -1.544   2.382   8.505  1.00  0.00
CONECT     1    2   11   72
CONECT     2    1    3    5   12
```

```
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9   54
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   25   26   74
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   75
CONECT   28   27   29   31   34
CONECT   29   28   30   76
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
```

```
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
```

Table S30. Structure of 1RCY-Calc5 model in PDB format.

```
ATOM      1  N   UNK     1      -1.419   5.476  19.885  1.00  0.00
ATOM      2  C   UNK     1      -2.027   5.122  18.601  1.00  0.00
ATOM      3  C   UNK     1      -3.483   4.646  18.747  1.00  0.00
ATOM      4  O   UNK     1      -3.914   4.251  19.832  1.00  0.00
ATOM      5  C   UNK     1      -1.221   4.006  17.923  1.00  0.00
ATOM      6  C   UNK     1       0.250   4.270  17.842  1.00  0.00
ATOM      7  N   UNK     1       0.799   4.982  16.808  1.00  0.00
ATOM      8  C   UNK     1       1.247   3.791  18.634  1.00  0.00
ATOM      9  C   UNK     1       2.105   4.921  16.982  1.00  0.00
ATOM     10  N   UNK     1       2.422   4.212  18.072  1.00  0.00
ATOM     11  H   UNK     1      -0.570   5.011  20.171  1.00  0.00
ATOM     12  H   UNK     1      -2.020   6.029  17.996  1.00  0.00
ATOM     13  H   UNK     1      -1.393   3.065  18.445  1.00  0.00
ATOM     14  H   UNK     1      -1.577   3.958  16.894  1.00  0.00
ATOM     15  H   UNK     1       1.133   3.191  19.537  1.00  0.00
ATOM     16  H   UNK     1       2.834   5.389  16.321  1.00  0.00
ATOM     17  H   UNK     1       3.353   4.023  18.415  1.00  0.00
ATOM     18  N   UNK     1      -4.232   4.684  17.648  1.00  0.00
ATOM     19  C   UNK     1      -5.617   4.213  17.651  1.00  0.00
ATOM     20  C   UNK     1      -5.756   3.196  16.531  1.00  0.00
ATOM     21  O   UNK     1      -4.870   3.085  15.682  1.00  0.00
ATOM     22  C   UNK     1      -6.605   5.362  17.420  1.00  0.00
ATOM     23  H   UNK     1      -3.836   5.046  16.793  1.00  0.00
ATOM     24  H   UNK     1      -5.847   3.774  18.622  1.00  0.00
ATOM     25  H   UNK     1      -7.623   4.973  17.427  1.00  0.00
ATOM     26  H   UNK     1      -6.471   6.085  18.225  1.00  0.00
ATOM     27  N   UNK     1      -4.582   4.735  11.981  1.00  0.00
ATOM     28  C   UNK     1      -4.309   5.392  13.245  1.00  0.00
ATOM     29  C   UNK     1      -4.600   6.869  13.009  1.00  0.00
ATOM     30  O   UNK     1      -4.167   7.440  11.996  1.00  0.00
ATOM     31  C   UNK     1      -2.850   5.179  13.602  1.00  0.00
```

```
ATOM      32  S   UNK     1       -2.406   6.166  15.076  1.00  0.00
ATOM      33  H   UNK     1       -3.908   4.806  11.232  1.00  0.00
ATOM      34  H   UNK     1       -4.917   4.965  14.042  1.00  0.00
ATOM      35  H   UNK     1       -2.217   5.504  12.771  1.00  0.00
ATOM      36  H   UNK     1       -2.666   4.118  13.795  1.00  0.00
ATOM      37  N   UNK     1        0.554   9.902  11.237  1.00  0.00
ATOM      38  C   UNK     1        0.762   8.454  11.190  1.00  0.00
ATOM      39  C   UNK     1        0.215   7.755   9.950  1.00  0.00
ATOM      40  O   UNK     1        0.937   7.010   9.286  1.00  0.00
ATOM      41  C   UNK     1        0.242   7.793  12.469  1.00  0.00
ATOM      42  C   UNK     1        1.058   8.111  13.682  1.00  0.00
ATOM      43  N   UNK     1        0.893   7.435  14.867  1.00  0.00
ATOM      44  C   UNK     1        2.042   9.040  13.829  1.00  0.00
ATOM      45  C   UNK     1        1.769   7.963  15.705  1.00  0.00
ATOM      46  N   UNK     1        2.486   8.935  15.123  1.00  0.00
ATOM      47  H   UNK     1       -0.007  10.298  11.978  1.00  0.00
ATOM      48  H   UNK     1        1.842   8.327  11.120  1.00  0.00
ATOM      49  H   UNK     1       -0.792   8.093  12.638  1.00  0.00
ATOM      50  H   UNK     1        0.317   6.716  12.316  1.00  0.00
ATOM      51  H   UNK     1        2.406   9.731  13.069  1.00  0.00
ATOM      52  H   UNK     1        1.893   7.647  16.741  1.00  0.00
ATOM      53  H   UNK     1        3.214   9.485  15.555  1.00  0.00
ATOM      54 Cu   UNK     1       -0.276   5.892  15.340  1.00  0.00
ATOM      55  N   UNK     1        0.811   4.243   8.468  1.00  0.00
ATOM      56  C   UNK     1        0.172   3.459   9.514  1.00  0.00
ATOM      57  C   UNK     1       -1.297   3.168   9.203  1.00  0.00
ATOM      58  O   UNK     1       -2.206   3.814   9.734  1.00  0.00
ATOM      59  C   UNK     1        0.317   4.124  10.885  1.00  0.00
ATOM      60  C   UNK     1        0.023   3.178  12.030  1.00  0.00
ATOM      61  S   UNK     1        0.511   3.797  13.639  1.00  0.00
ATOM      62  C   UNK     1        0.116   2.402  14.652  1.00  0.00
ATOM      63  H   UNK     1        0.844   5.251   8.530  1.00  0.00
ATOM      64  H   UNK     1        0.693   2.502   9.546  1.00  0.00
ATOM      65  H   UNK     1        1.327   4.521  10.991  1.00  0.00
ATOM      66  H   UNK     1       -0.419   4.927  10.933  1.00  0.00
ATOM      67  H   UNK     1       -1.040   2.939  12.040  1.00  0.00
ATOM      68  H   UNK     1        0.626   2.288  11.851  1.00  0.00
ATOM      69  H   UNK     1        0.362   2.626  15.690  1.00  0.00
ATOM      70  H   UNK     1       -0.949   2.183  14.570  1.00  0.00
ATOM      71  H   UNK     1        0.691   1.538  14.321  1.00  0.00
ATOM      72  H   UNK     1       -2.110   5.397  20.618  1.00  0.00
ATOM      73  H   UNK     1       -6.634   2.569  16.479  1.00  0.00
ATOM      74  H   UNK     1       -6.426   5.840  16.457  1.00  0.00
ATOM      75  H   UNK     1       -5.491   5.018  11.644  1.00  0.00
ATOM      76  H   UNK     1       -5.187   7.422  13.728  1.00  0.00
ATOM      77  H   UNK     1        0.207  10.221  10.344  1.00  0.00
ATOM      78  H   UNK     1       -0.811   7.914   9.652  1.00  0.00
ATOM      79  H   UNK     1        0.438   3.973   7.569  1.00  0.00
ATOM      80  H   UNK     1       -1.544   2.382   8.505  1.00  0.00
CONECT     1    2   11   72
CONECT     2    1    3    5   12
CONECT     3    2    4   18
CONECT     4    3
CONECT     5    2    6   13   14
CONECT     6    5    7    8
CONECT     7    6    9   54
CONECT     8    6   10   15
```

```
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   73
CONECT   21   20
CONECT   22   19   25   26   74
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   28   33   75
CONECT   28   27   29   31   34
CONECT   29   28   30   76
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   38   47   77
CONECT   38   37   39   41   48
CONECT   39   38   40   78
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   43   44
CONECT   43   42   45   54
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   61
CONECT   55   56   63   79
CONECT   56   55   57   59   64
CONECT   57   56   58   80
CONECT   58   57
CONECT   59   56   60   65   66
CONECT   60   59   61   67   68
CONECT   61   54   60   62
CONECT   62   61   69   70   71
CONECT   63   55
CONECT   64   56
CONECT   65   59
```

```
CONECT   66   59
CONECT   67   60
CONECT   68   60
CONECT   69   62
CONECT   70   62
CONECT   71   62
CONECT   72    1
CONECT   73   20
CONECT   74   22
CONECT   75   27
CONECT   76   29
CONECT   77   37
CONECT   78   39
CONECT   79   55
CONECT   80   57
MASTER        0    0    0    0    0    0    0    0   80    0   80    0
END
```

Table S31. Structure of 1RCY-Calc6 model in PDB format.

```
HETATM    1  N1  UNK     1       5.005  -2.083  -0.470  1.00  0.00
HETATM    2  C2  UNK     1       4.152  -0.910  -0.269  1.00  0.00
HETATM    3  C3  UNK     1       4.938   0.411  -0.334  1.00  0.00
HETATM    4  O4  UNK     1       6.161   0.429  -0.181  1.00  0.00
HETATM    5  C5  UNK     1       3.457  -0.989   1.097  1.00  0.00
HETATM    6  C6  UNK     1       2.767  -2.291   1.362  1.00  0.00
HETATM    7  N7  UNK     1       1.475  -2.525   0.946  1.00  0.00
HETATM    8  C8  UNK     1       3.195  -3.347   2.106  1.00  0.00
HETATM    9  C9  UNK     1       1.149  -3.698   1.446  1.00  0.00
HETATM   10  N10 UNK     1       2.153  -4.233   2.152  1.00  0.00
HETATM   11  H11 UNK     1       5.031  -2.799   0.240  1.00  0.00
HETATM   12  H12 UNK     1       3.422  -0.917  -1.078  1.00  0.00
HETATM   13  H13 UNK     1       4.183  -0.796   1.886  1.00  0.00
HETATM   14  H14 UNK     1       2.676  -0.230   1.083  1.00  0.00
HETATM   15  H15 UNK     1       4.173  -3.464   2.572  1.00  0.00
HETATM   16  H16 UNK     1       0.180  -4.174   1.301  1.00  0.00
HETATM   17  H17 UNK     1       2.143  -5.124   2.629  1.00  0.00
HETATM   18  N18 UNK     1       4.227   1.513  -0.560  1.00  0.00
HETATM   19  C19 UNK     1       4.856   2.834  -0.597  1.00  0.00
HETATM   20  C20 UNK     1       4.104   3.725   0.377  1.00  0.00
HETATM   21  O21 UNK     1       3.022   3.361   0.840  1.00  0.00
HETATM   22  C22 UNK     1       4.795   3.449  -1.999  1.00  0.00
HETATM   23  H23 UNK     1       3.232   1.437  -0.709  1.00  0.00
HETATM   24  H24 UNK     1       5.908   2.741  -0.326  1.00  0.00
HETATM   25  H25 UNK     1       5.270   4.430  -1.987  1.00  0.00
HETATM   26  H26 UNK     1       5.324   2.782  -2.680  1.00  0.00
HETATM   27  H72 UNK     1       5.947  -1.782  -0.680  1.00  0.00
HETATM   28  H73 UNK     1       4.520   4.679   0.665  1.00  0.00
HETATM   29  H74 UNK     1       3.762   3.571  -2.325  1.00  0.00
HETATM   30  N27 UNK     1      -0.757   4.227  -0.375  1.00  0.00
HETATM   31  C28 UNK     1       0.145   3.263  -0.975  1.00  0.00
HETATM   32  C29 UNK     1      -0.253   3.189  -2.444  1.00  0.00
HETATM   33  O30 UNK     1      -1.447   3.088  -2.766  1.00  0.00
HETATM   34  C31 UNK     1      -0.050   1.921  -0.293  1.00  0.00
HETATM   35  S32 UNK     1       0.909   0.623  -1.152  1.00  0.00
HETATM   36  H33 UNK     1      -1.705   3.950  -0.162  1.00  0.00
HETATM   37  H34 UNK     1       1.183   3.565  -0.835  1.00  0.00
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HETATM   38  H35 UNK     1      -1.108   1.643  -0.327  1.00  0.00
HETATM   39  H36 UNK     1       0.267   1.988   0.752  1.00  0.00
HETATM   40 Cu54 UNK     1       0.377  -1.235  -0.179  1.00  0.00
HETATM   41  H75 UNK     1      -0.769   5.069  -0.933  1.00  0.00
HETATM   42  H76 UNK     1       0.509   3.225  -3.209  1.00  0.00
HETATM   43  N37 UNK     1      -4.437  -1.338  -3.395  1.00  0.00
HETATM   44  C38 UNK     1      -4.268  -1.080  -1.965  1.00  0.00
HETATM   45  C39 UNK     1      -5.035   0.121  -1.421  1.00  0.00
HETATM   46  O40 UNK     1      -5.760   0.001  -0.433  1.00  0.00
HETATM   47  C41 UNK     1      -2.782  -0.993  -1.605  1.00  0.00
HETATM   48  C42 UNK     1      -2.066  -2.303  -1.697  1.00  0.00
HETATM   49  N43 UNK     1      -0.804  -2.488  -1.181  1.00  0.00
HETATM   50  C44 UNK     1      -2.498  -3.476  -2.236  1.00  0.00
HETATM   51  C45 UNK     1      -0.485  -3.736  -1.439  1.00  0.00
HETATM   52  N46 UNK     1      -1.480  -4.380  -2.065  1.00  0.00
HETATM   53  H47 UNK     1      -3.634  -1.288  -4.006  1.00  0.00
HETATM   54  H48 UNK     1      -4.719  -1.939  -1.469  1.00  0.00
HETATM   55  H49 UNK     1      -2.294  -0.266  -2.253  1.00  0.00
HETATM   56  H50 UNK     1      -2.732  -0.682  -0.561  1.00  0.00
HETATM   57  H51 UNK     1      -3.461  -3.660  -2.710  1.00  0.00
HETATM   58  H52 UNK     1       0.465  -4.196  -1.165  1.00  0.00
HETATM   59  H53 UNK     1      -1.481  -5.347  -2.356  1.00  0.00
HETATM   60  H77 UNK     1      -5.173  -0.749  -3.758  1.00  0.00
HETATM   61  H78 UNK     1      -4.942   1.082  -1.906  1.00  0.00
HETATM   62  N55 UNK     1      -5.892   1.254   2.166  1.00  0.00
HETATM   63  C56 UNK     1      -4.547   1.578   2.614  1.00  0.00
HETATM   64  C57 UNK     1      -4.205   3.053   2.399  1.00  0.00
HETATM   65  O58 UNK     1      -3.508   3.419   1.447  1.00  0.00
HETATM   66  C59 UNK     1      -3.500   0.675   1.956  1.00  0.00
HETATM   67  C60 UNK     1      -2.165   0.708   2.669  1.00  0.00
HETATM   68  S61 UNK     1      -1.052  -0.647   2.130  1.00  0.00
HETATM   69  C62 UNK     1       0.319  -0.272   3.264  1.00  0.00
HETATM   70  H63 UNK     1      -6.052   0.910   1.229  1.00  0.00
HETATM   71  H64 UNK     1      -4.525   1.393   3.688  1.00  0.00
HETATM   72  H65 UNK     1      -3.872  -0.349   1.926  1.00  0.00
HETATM   73  H66 UNK     1      -3.336   1.055   0.947  1.00  0.00
HETATM   74  H67 UNK     1      -1.700   1.683   2.526  1.00  0.00
HETATM   75  H68 UNK     1      -2.378   0.524   3.722  1.00  0.00
HETATM   76  H69 UNK     1       1.115  -0.992   3.075  1.00  0.00
HETATM   77  H70 UNK     1       0.697   0.738   3.107  1.00  0.00
HETATM   78  H71 UNK     1      -0.026  -0.375   4.293  1.00  0.00
HETATM   79  H79 UNK     1      -6.505   2.036   2.346  1.00  0.00
HETATM   80  H80 UNK     1      -4.581   3.790   3.094  1.00  0.00
CONECT    1    2   11   27
CONECT    2    1    3    5   12
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    7    8
CONECT    7    6    9
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
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CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   19   23
CONECT   19   18   20   22   24
CONECT   20   19   21   28
CONECT   21   20
CONECT   22   19   25   26   29
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27    1
CONECT   28   20
CONECT   29   22
CONECT   30   31   36   41
CONECT   31   30   32   34   37
CONECT   32   31   33   42
CONECT   33   32
CONECT   34   31   35   38   39
CONECT   35   34   40
CONECT   36   30
CONECT   37   31
CONECT   38   34
CONECT   39   34
CONECT   40   35
CONECT   41   30
CONECT   42   32
CONECT   43   44   53   60
CONECT   44   43   45   47   54
CONECT   45   44   46   61
CONECT   46   45
CONECT   47   44   48   55   56
CONECT   48   47   49   50
CONECT   49   48   51
CONECT   50   48   52   57
CONECT   51   49   52   58
CONECT   52   50   51   59
CONECT   53   43
CONECT   54   44
CONECT   55   47
CONECT   56   47
CONECT   57   50
CONECT   58   51
CONECT   59   52
CONECT   60   43
CONECT   61   45
CONECT   62   63   70   79
CONECT   63   62   64   66   71
CONECT   64   63   65   80
CONECT   65   64
CONECT   66   63   67   72   73
CONECT   67   66   68   74   75
CONECT   68   67   69
CONECT   69   68   76   77   78
CONECT   70   62
CONECT   71   63
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CONECT   72   66
CONECT   73   66
CONECT   74   67
CONECT   75   67
CONECT   76   69
CONECT   77   69
CONECT   78   69
CONECT   79   62
CONECT   80   64
MASTER    0    0    0    0    0    0    0    0    3   80    0   80    0
END
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Table S32. Structure of 1RCY-Calc7 model in PDB format.

```
HETATM    1  C1  UNK     1      -3.867   5.988  -2.448  1.00  0.00
HETATM    2  C2  UNK     1      -2.931   4.986  -1.743  1.00  0.00
HETATM    3  C3  UNK     1      -2.068   4.193  -2.703  1.00  0.00
HETATM    4  S4  UNK     1      -0.653   3.383  -1.849  1.00  0.00
HETATM    5  C5  UNK     1       0.146   2.647  -3.312  1.00  0.00
HETATM    6  H6  UNK     1      -3.277   6.545  -3.177  1.00  0.00
HETATM    7  H7  UNK     1      -2.295   5.519  -1.037  1.00  0.00
HETATM    8  H8  UNK     1      -3.569   4.269  -1.226  1.00  0.00
HETATM    9  H9  UNK     1      -2.682   3.452  -3.215  1.00  0.00
HETATM   10  H10 UNK     1      -1.640   4.893  -3.421  1.00  0.00
HETATM   11  H11 UNK     1       1.025   2.092  -2.985  1.00  0.00
HETATM   12  H12 UNK     1      -0.535   1.974  -3.831  1.00  0.00
HETATM   13  H13 UNK     1       0.451   3.447  -3.986  1.00  0.00
HETATM   14 H110 UNK     1      -4.684   5.463  -2.941  1.00  0.00
HETATM   15 H111 UNK     1      -4.280   6.678  -1.712  1.00  0.00
HETATM   16  N14 UNK     1       7.372  -1.094   2.203  1.00  0.00
HETATM   17  C15 UNK     1       5.938  -1.282   2.167  1.00  0.00
HETATM   18  C16 UNK     1       5.552  -2.288   1.092  1.00  0.00
HETATM   19  O17 UNK     1       6.137  -2.286   0.032  1.00  0.00
HETATM   20  C18 UNK     1       5.209   0.040   1.871  1.00  0.00
HETATM   21  H19 UNK     1       7.850  -0.935   1.329  1.00  0.00
HETATM   22  H20 UNK     1       5.641  -1.652   3.148  1.00  0.00
HETATM   23  H21 UNK     1       5.597   0.470   0.949  1.00  0.00
HETATM   24  H22 UNK     1       4.141  -0.151   1.763  1.00  0.00
HETATM   25  N23 UNK     1       4.552  -3.089   1.362  1.00  0.00
HETATM   26  C24 UNK     1       4.006  -4.046   0.423  1.00  0.00
HETATM   27  C25 UNK     1       2.651  -3.751  -0.155  1.00  0.00
HETATM   28  O26 UNK     1       1.659  -4.490   0.030  1.00  0.00
HETATM   29  H27 UNK     1       4.136  -3.037   2.281  1.00  0.00
HETATM   30  H28 UNK     1       4.719  -4.208  -0.386  1.00  0.00
HETATM   31  H29 UNK     1       3.845  -4.940   1.025  1.00  0.00
HETATM   32  N30 UNK     1       2.523  -2.696  -0.912  1.00  0.00
HETATM   33  C31 UNK     1       1.268  -2.169  -1.433  1.00  0.00
HETATM   34  C32 UNK     1       0.586  -3.161  -2.346  1.00  0.00
HETATM   35  O33 UNK     1       1.218  -4.008  -2.987  1.00  0.00
HETATM   36  C34 UNK     1       1.601  -0.905  -2.244  1.00  0.00
HETATM   37  C35 UNK     1       2.246   0.210  -1.502  1.00  0.00
HETATM   38  N36 UNK     1       1.559   1.063  -0.640  1.00  0.00
HETATM   39  C37 UNK     1       3.544   0.616  -1.564  1.00  0.00
HETATM   40  C38 UNK     1       2.493   1.954  -0.234  1.00  0.00
HETATM   41  N39 UNK     1       3.710   1.705  -0.752  1.00  0.00
HETATM   42  H40 UNK     1       3.368  -2.200  -1.159  1.00  0.00
HETATM   43  H41 UNK     1       0.596  -1.958  -0.602  1.00  0.00
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HETATM	44	H42	UNK	1	2.218	-1.174	-3.102	1.00	0.00
HETATM	45	H43	UNK	1	0.630	-0.508	-2.542	1.00	0.00
HETATM	46	H44	UNK	1	4.325	0.149	-2.164	1.00	0.00
HETATM	47	H45	UNK	1	2.274	2.777	0.446	1.00	0.00
HETATM	48	N46	UNK	1	-0.723	-3.015	-2.457	1.00	0.00
HETATM	49	C47	UNK	1	-1.509	-3.819	-3.396	1.00	0.00
HETATM	50	C48	UNK	1	-2.167	-2.921	-4.441	1.00	0.00
HETATM	51	O49	UNK	1	-2.179	-1.694	-4.315	1.00	0.00
HETATM	52	C50	UNK	1	-2.598	-4.643	-2.696	1.00	0.00
HETATM	53	H51	UNK	1	-1.193	-2.332	-1.880	1.00	0.00
HETATM	54	H52	UNK	1	-0.812	-4.510	-3.872	1.00	0.00
HETATM	55	H53	UNK	1	-3.003	-5.377	-3.392	1.00	0.00
HETATM	56	H54	UNK	1	-2.130	-5.137	-1.845	1.00	0.00
HETATM	57	N55	UNK	1	-5.258	0.641	-2.836	1.00	0.00
HETATM	58	C56	UNK	1	-4.365	-0.165	-2.040	1.00	0.00
HETATM	59	C57	UNK	1	-5.100	-0.605	-0.744	1.00	0.00
HETATM	60	O58	UNK	1	-5.823	0.220	-0.161	1.00	0.00
HETATM	61	C59	UNK	1	-3.114	0.658	-1.725	1.00	0.00
HETATM	62	S60	UNK	1	-1.903	-0.223	-0.664	1.00	0.00
HETATM	63	H61	UNK	1	-5.348	1.616	-2.591	1.00	0.00
HETATM	64	H62	UNK	1	-4.072	-1.030	-2.635	1.00	0.00
HETATM	65	H63	UNK	1	-2.622	0.918	-2.666	1.00	0.00
HETATM	66	H64	UNK	1	-3.407	1.577	-1.208	1.00	0.00
HETATM	67	N65	UNK	1	-4.879	-1.869	-0.354	1.00	0.00
HETATM	68	C66	UNK	1	-5.533	-2.401	0.843	1.00	0.00
HETATM	69	C67	UNK	1	-4.734	-2.267	2.132	1.00	0.00
HETATM	70	O68	UNK	1	-5.260	-2.657	3.189	1.00	0.00
HETATM	71	H69	UNK	1	-4.257	-2.457	-0.889	1.00	0.00
HETATM	72	H70	UNK	1	-6.421	-1.779	0.960	1.00	0.00
HETATM	73	N71	UNK	1	-3.504	-1.761	2.098	1.00	0.00
HETATM	74	C72	UNK	1	-2.787	-1.604	3.360	1.00	0.00
HETATM	75	C73	UNK	1	-3.576	-0.693	4.258	1.00	0.00
HETATM	76	O74	UNK	1	-3.975	0.388	3.775	1.00	0.00
HETATM	77	C75	UNK	1	-1.368	-1.068	3.191	1.00	0.00
HETATM	78	C76	UNK	1	-0.449	-2.075	2.488	1.00	0.00
HETATM	79	C77	UNK	1	-0.758	-0.709	4.554	1.00	0.00
HETATM	80	C78	UNK	1	1.015	-1.656	2.308	1.00	0.00
HETATM	81	H79	UNK	1	-3.078	-1.492	1.223	1.00	0.00
HETATM	82	H80	UNK	1	-2.686	-2.596	3.801	1.00	0.00
HETATM	83	H81	UNK	1	-1.445	-0.177	2.568	1.00	0.00
HETATM	84	H82	UNK	1	-0.437	-3.009	3.049	1.00	0.00
HETATM	85	H83	UNK	1	-0.867	-2.213	1.491	1.00	0.00
HETATM	86	H84	UNK	1	0.254	-0.329	4.411	1.00	0.00
HETATM	87	H85	UNK	1	-1.368	0.055	5.035	1.00	0.00
HETATM	88	H86	UNK	1	-0.726	-1.598	5.184	1.00	0.00
HETATM	89	H87	UNK	1	1.533	-2.446	1.759	1.00	0.00
HETATM	90	H88	UNK	1	1.121	-0.731	1.731	1.00	0.00
HETATM	91	H89	UNK	1	1.536	-1.524	3.264	1.00	0.00
HETATM	92	C90	UNK	1	-3.465	4.027	2.595	1.00	0.00
HETATM	93	C91	UNK	1	-2.604	3.014	1.825	1.00	0.00
HETATM	94	C92	UNK	1	-1.271	2.762	2.468	1.00	0.00
HETATM	95	N93	UNK	1	-0.243	2.100	1.809	1.00	0.00
HETATM	96	C94	UNK	1	-0.828	3.102	3.712	1.00	0.00
HETATM	97	C95	UNK	1	0.761	2.055	2.666	1.00	0.00
HETATM	98	N96	UNK	1	0.455	2.651	3.825	1.00	0.00
HETATM	99	H97	UNK	1	-2.832	4.858	2.905	1.00	0.00
HETATM	100	H98	UNK	1	-3.146	2.073	1.733	1.00	0.00

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HETATM  101  H99 UNK     1      -2.407   3.445   0.843  1.00  0.00
HETATM  102 H100 UNK     1      -1.394   3.636   4.476  1.00  0.00
HETATM  103 H101 UNK     1       1.724   1.590   2.453  1.00  0.00
HETATM  104 H102 UNK     1       1.058   2.748   4.629  1.00  0.00
HETATM  105 Cu   UNK     1      -0.317   1.167  -0.039  1.00  0.00
HETATM  106 H104 UNK     1       7.801  -1.872   2.685  1.00  0.00
HETATM  107 H105 UNK     1       5.372   0.738   2.693  1.00  0.00
HETATM  108 H106 UNK     1      -2.630  -3.369  -5.307  1.00  0.00
HETATM  109 H107 UNK     1      -3.421  -4.012  -2.359  1.00  0.00
HETATM  110 H108 UNK     1      -6.173   0.213  -2.853  1.00  0.00
HETATM  111 H109 UNK     1      -3.791  -0.963   5.281  1.00  0.00
HETATM  112 H112 UNK     1      -4.271   4.390   1.958  1.00  0.00
HETATM  113 H113 UNK     1      -3.891   3.546   3.475  1.00  0.00
HETATM  114 H114 UNK     1      -5.698  -3.469   0.700  1.00  0.00
HETATM  115 C115 UNK     1       6.978   2.199  -2.066  1.00  0.00
HETATM  116 C116 UNK     1       6.999   3.224  -0.938  1.00  0.00
HETATM  117 O117 UNK     1       7.913   4.056  -0.691  1.00  0.00
HETATM  118 N118 UNK     1       5.938   3.165  -0.246  1.00  0.00
HETATM  119 H119 UNK     1       6.449   2.613  -2.924  1.00  0.00
HETATM  120 H120 UNK     1       6.465   1.312  -1.695  1.00  0.00
HETATM  121 H121 UNK     1       5.222   2.493  -0.482  1.00  0.00
HETATM  122 H122 UNK     1       5.814   3.790   0.539  1.00  0.00
HETATM  123 H123 UNK     1       7.989   1.941  -2.381  1.00  0.00
CONECT    1    2    6   14   15
CONECT    2    1    3    7    8
CONECT    3    2    4    9   10
CONECT    4    3    5
CONECT    5    4   11   12   13
CONECT    6    1
CONECT    7    2
CONECT    8    2
CONECT    9    3
CONECT   10    3
CONECT   11    5
CONECT   12    5
CONECT   13    5
CONECT   14    1
CONECT   15    1
CONECT   16   17   21  106
CONECT   17   16   18   20   22
CONECT   18   17   19   25
CONECT   19   18
CONECT   20   17   23   24  107
CONECT   21   16
CONECT   22   17
CONECT   23   20
CONECT   24   20
CONECT   25   18   26   29
CONECT   26   25   27   30   31
CONECT   27   26   28   32
CONECT   28   27
CONECT   29   25
CONECT   30   26
CONECT   31   26
CONECT   32   27   33   42
CONECT   33   32   34   36   43
CONECT   34   33   35   48
```

```
CONECT   35   34
CONECT   36   33   37   44   45
CONECT   37   36   38   39
CONECT   38   37   40  105
CONECT   39   37   41   46
CONECT   40   38   41   47
CONECT   41   39   40
CONECT   42   32
CONECT   43   33
CONECT   44   36
CONECT   45   36
CONECT   46   39
CONECT   47   40
CONECT   48   34   49   53
CONECT   49   48   50   52   54
CONECT   50   49   51  108
CONECT   51   50
CONECT   52   49   55   56  109
CONECT   53   48
CONECT   54   49
CONECT   55   52
CONECT   56   52
CONECT   57   58   63  110
CONECT   58   57   59   61   64
CONECT   59   58   60   67
CONECT   60   59
CONECT   61   58   62   65   66
CONECT   62   61  105
CONECT   63   57
CONECT   64   58
CONECT   65   61
CONECT   66   61
CONECT   67   59   68   71
CONECT   68   67   69   72  114
CONECT   69   68   70   73
CONECT   70   69
CONECT   71   67
CONECT   72   68
CONECT   73   69   74   81
CONECT   74   73   75   77   82
CONECT   75   74   76  111
CONECT   76   75
CONECT   77   74   78   79   83
CONECT   78   77   80   84   85
CONECT   79   77   86   87   88
CONECT   80   78   89   90   91
CONECT   81   73
CONECT   82   74
CONECT   83   77
CONECT   84   78
CONECT   85   78
CONECT   86   79
CONECT   87   79
CONECT   88   79
CONECT   89   80
CONECT   90   80
CONECT   91   80
```

```
CONECT   92   93   99  112  113
CONECT   93   92   94  100  101
CONECT   94   93   95   96
CONECT   95   94   97  105
CONECT   96   94   98  102
CONECT   97   95   98  103
CONECT   98   96   97  104
CONECT   99   92
CONECT  100   93
CONECT  101   93
CONECT  102   96
CONECT  103   97
CONECT  104   98
CONECT  105   38   62   95
CONECT  106   16
CONECT  107   20
CONECT  108   50
CONECT  109   52
CONECT  110   57
CONECT  111   75
CONECT  112   92
CONECT  113   92
CONECT  114   68
CONECT  115  116  119  120  123
CONECT  116  115  117  118
CONECT  117  116
CONECT  118  116  121  122
CONECT  119  115
CONECT  120  115
CONECT  121  118
CONECT  122  118
CONECT  123  115
MASTER    0    0    0    0    0    0    0    0    3  123    0  123    0
END
```

Table S33. Structure of 2CAK-Calc3 model in PDB format.

```
HEADER    ELECTRON TRANSPORT                      21-DEC-05   2CAK
HETATM    1  N           1      -1.399  14.711  20.175
HETATM    2  CA          2      -1.978  14.382  18.879
HETATM    3  C           3      -3.408  13.911  19.012
HETATM    4  O           4      -3.826  13.362  20.037
HETATM    5  CB          5      -1.140  13.240  18.277
HETATM    6  CG          6       0.297  13.529  18.032
HETATM    7  ND1         7       0.791  14.276  16.983
HETATM    8  CD2         8       1.373  13.077  18.733
HETATM    9  CE1         9       2.107  14.257  17.079
HETATM   10  NE2        10       2.517  13.548  18.147
HETATM   11  H          11      -0.602  14.167  20.475
HETATM   12  HA         12      -1.973  15.271  18.249
HETATM   13 1HB         13      -1.230  12.353  18.904
HETATM   14 2HB         14      -1.561  13.088  17.283
HETATM   15  HD2        15       1.330  12.442  19.618
HETATM   16  HE1        16       2.779  14.754  16.380
HETATM   17  HE2        17       3.468  13.396  18.452
HETATM   18  N          18      -4.155  14.072  17.934
HETATM   19  CA         19      -5.524  13.556  17.865
```

```
HETATM   20  C          20      -5.640  12.508  16.761
HETATM   21  O          21      -4.736  12.339  15.940
HETATM   22  CB         22      -6.557  14.662  17.607
HETATM   23  H          23      -3.773  14.563  17.138
HETATM   24  HA         24      -5.738  13.111  18.837
HETATM   25 1HB         25      -7.559  14.271  17.780
HETATM   26 2HB         26      -6.336  15.475  18.298
HETATM   27  N          27      -4.508  13.888  12.110
HETATM   28  CA         28      -4.262  14.626  13.325
HETATM   29  C          29      -4.605  16.122  13.087
HETATM   30  O          30      -4.277  16.643  12.007
HETATM   31  CB         31      -2.818  14.517  13.769
HETATM   32  SG         32      -2.411  15.481  15.266
HETATM   33  H          33      -3.790  13.909  11.400
HETATM   34  HA         34      -4.889  14.202  14.109
HETATM   35 1HB         35      -2.566  13.469  13.932
HETATM   36 2HB         36      -2.223  14.948  12.964
HETATM   37  N          37       0.424  19.200  11.306
HETATM   38  CA         38       0.801  17.802  11.290
HETATM   39  C          39       0.243  17.068  10.065
HETATM   40  O          40       1.018  16.334   9.429
HETATM   41  CB         41       0.364  17.118  12.594
HETATM   42  CG         42       1.227  17.479  13.768
HETATM   43  ND1        43       1.168  16.777  14.955
HETATM   44  CD2        44       2.154  18.472  13.893
HETATM   45  CE1        45       2.055  17.368  15.761
HETATM   46  NE2        46       2.669  18.391  15.154
HETATM   47  H          47      -0.274  19.535  11.954
HETATM   48  HA         48       1.887  17.753  11.217
HETATM   49 1HB         49      -0.672  17.378  12.811
HETATM   50 2HB         50       0.470  16.044  12.440
HETATM   51  HD2        51       2.432  19.196  13.127
HETATM   52  HE1        52       2.254  17.056  16.786
HETATM   53  HE2        53       3.378  18.989  15.553
HETATM   54 CU   CU1 A 156      -0.196  15.306  15.498
HETATM   55  H          55      -2.118  14.674  20.884
HETATM   56  H          56      -6.532  11.902  16.698
HETATM   57  H          57      -5.387  14.183  11.709
HETATM   58  H          58       0.184  19.495  10.370
HETATM   59  H          59      -0.788  17.185   9.765
HETATM   60  N          60       0.910  13.487   8.593
HETATM   61  CA         61       0.283  12.669   9.611
HETATM   62  C          62      -1.158  12.394   9.244
HETATM   63  O          63      -2.099  13.030   9.774
HETATM   64  CB         64       0.386  13.357  10.986
HETATM   65  CG         65       0.044  12.441  12.143
HETATM   66  SD         66       0.587  13.121  13.732
HETATM   67  CE         67       0.124  11.725  14.816
HETATM   68  H          68       0.924  14.493   8.681
HETATM   69  HA         69       0.805  11.714   9.672
HETATM   70 1HB         70       1.393  13.752  11.120
HETATM   71 2HB         71      -0.350  14.161  10.992
HETATM   72 1HG         72      -1.033  12.274  12.168
HETATM   73 2HG         73       0.571  11.499  11.988
HETATM   74 1HE         74       0.385  11.963  15.847
HETATM   75 2HE         75      -0.949  11.550  14.745
HETATM   76 3HE         76       0.660  10.829  14.503
```

```
HETATM   77  H          77       0.546  13.233   7.686
HETATM   78  H          78      -1.381  11.634   8.510
HETATM   79  H          79      -6.510  15.019  16.578
HETATM   80  H          80      -5.118  16.697  13.844
CONECT    1   11    2   55
CONECT    2    1   12    3    5
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    8    7
CONECT    7    6   54    9
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   23   19
CONECT   19   18   24   20   22
CONECT   20   19   21   56
CONECT   21   20
CONECT   22   19   25   26   79
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   33   28   57
CONECT   28   27   34   29   31
CONECT   29   28   30   80
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   47   38   58
CONECT   38   37   48   39   41
CONECT   39   38   40   59
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   44   43
CONECT   43   42   54   45
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
```

```
CONECT   54    7   32   43   66
CONECT   55    1
CONECT   56   20
CONECT   57   27
CONECT   58   37
CONECT   59   39
CONECT   60   68   61   77
CONECT   61   60   69   62   64
CONECT   62   61   63   78
CONECT   63   62
CONECT   64   61   65   70   71
CONECT   65   64   66   72   73
CONECT   66   54   65   67
CONECT   67   66   74   75   76
CONECT   68   60
CONECT   69   61
CONECT   70   64
CONECT   71   64
CONECT   72   65
CONECT   73   65
CONECT   74   67
CONECT   75   67
CONECT   76   67
CONECT   77   60
CONECT   78   62
CONECT   79   22
CONECT   80   29
END
```

Table S34. Structure of 2CAK-Calc4 model in PDB format.

```
HEADER    ELECTRON TRANSPORT                        21-DEC-05   2CAK
HETATM    1  N           1      -1.399  14.711  20.175
HETATM    2  CA          2      -1.978  14.382  18.879
HETATM    3  C           3      -3.408  13.911  19.012
HETATM    4  O           4      -3.826  13.362  20.037
HETATM    5  CB          5      -1.140  13.240  18.277
HETATM    6  CG          6       0.297  13.529  18.032
HETATM    7  ND1         7       0.791  14.276  16.983
HETATM    8  CD2         8       1.373  13.077  18.733
HETATM    9  CE1         9       2.107  14.257  17.079
HETATM   10  NE2        10       2.517  13.548  18.147
HETATM   11  H         11      -0.602  14.167  20.475
HETATM   12  HA        12      -1.973  15.271  18.249
HETATM   13 1HB        13      -1.230  12.353  18.904
HETATM   14 2HB        14      -1.561  13.088  17.283
HETATM   15  HD2       15       1.330  12.442  19.618
HETATM   16  HE1       16       2.779  14.754  16.380
HETATM   17  HE2       17       3.468  13.396  18.452
HETATM   18  N         18      -4.155  14.072  17.934
HETATM   19  CA        19      -5.524  13.556  17.865
HETATM   20  C         20      -5.640  12.508  16.761
HETATM   21  O         21      -4.736  12.339  15.940
HETATM   22  CB        22      -6.557  14.662  17.607
HETATM   23  H         23      -3.773  14.563  17.138
HETATM   24  HA        24      -5.738  13.111  18.837
HETATM   25 1HB        25      -7.559  14.271  17.780
```

```
HETATM   26 2HB         26      -6.336  15.475  18.298
HETATM   27  N          27      -4.508  13.888  12.110
HETATM   28  CA         28      -4.262  14.626  13.325
HETATM   29  C          29      -4.605  16.122  13.087
HETATM   30  O          30      -4.277  16.643  12.007
HETATM   31  CB         31      -2.801  14.454  13.731
HETATM   32  SG         32      -2.351  15.456  15.202
HETATM   33  H          33      -3.790  13.909  11.400
HETATM   34  HA         34      -4.889  14.202  14.109
HETATM   35 1HB         35      -2.617  13.400  13.960
HETATM   36 2HB         36      -2.148  14.753  12.904
HETATM   37  N          37       0.424  19.200  11.306
HETATM   38  CA         38       0.801  17.802  11.290
HETATM   39  C          39       0.243  17.068  10.065
HETATM   40  O          40       1.018  16.334   9.429
HETATM   41  CB         41       0.364  17.118  12.594
HETATM   42  CG         42       1.227  17.479  13.768
HETATM   43  ND1        43       1.168  16.777  14.955
HETATM   44  CD2        44       2.154  18.472  13.893
HETATM   45  CE1        45       2.055  17.368  15.761
HETATM   46  NE2        46       2.669  18.391  15.154
HETATM   47  H          47      -0.274  19.535  11.954
HETATM   48  HA         48       1.887  17.753  11.217
HETATM   49 1HB         49      -0.672  17.378  12.811
HETATM   50 2HB         50       0.470  16.044  12.440
HETATM   51  HD2        51       2.432  19.196  13.127
HETATM   52  HE1        52       2.254  17.056  16.786
HETATM   53  HE2        53       3.378  18.989  15.553
HETATM   54 CU   CU1 A 156      -0.196  15.306  15.498
HETATM   55  H          55      -2.118  14.674  20.884
HETATM   56  H          56      -6.532  11.902  16.698
HETATM   57  H          57      -5.387  14.183  11.709
HETATM   58  H          58       0.184  19.495  10.370
HETATM   59  H          59      -0.788  17.185   9.765
HETATM   60  N          60       0.910  13.487   8.593
HETATM   61  CA         61       0.283  12.669   9.611
HETATM   62  C          62      -1.158  12.394   9.244
HETATM   63  O          63      -2.099  13.030   9.774
HETATM   64  CB         64       0.386  13.357  10.986
HETATM   65  CG         65       0.044  12.441  12.143
HETATM   66  SD         66       0.587  13.121  13.732
HETATM   67  CE         67       0.124  11.725  14.816
HETATM   68  H          68       0.924  14.493   8.681
HETATM   69  HA         69       0.805  11.714   9.672
HETATM   70 1HB         70       1.393  13.752  11.120
HETATM   71 2HB         71      -0.350  14.161  10.992
HETATM   72 1HG         72      -1.033  12.274  12.168
HETATM   73 2HG         73       0.571  11.499  11.988
HETATM   74 1HE         74       0.385  11.963  15.847
HETATM   75 2HE         75      -0.949  11.550  14.745
HETATM   76 3HE         76       0.660  10.829  14.503
HETATM   77  H          77       0.546  13.233   7.686
HETATM   78  H          78      -1.381  11.634   8.510
HETATM   79  H          79      -6.510  15.019  16.578
HETATM   80  H          80      -5.118  16.697  13.844
CONECT    1   11    2   55
CONECT    2    1   12    3    5
```

```
CONECT    3    2    4   18
CONECT    4    3
CONECT    5    2    6   13   14
CONECT    6    5    8    7
CONECT    7    6   54    9
CONECT    8    6   10   15
CONECT    9    7   10   16
CONECT   10    8    9   17
CONECT   11    1
CONECT   12    2
CONECT   13    5
CONECT   14    5
CONECT   15    8
CONECT   16    9
CONECT   17   10
CONECT   18    3   23   19
CONECT   19   18   24   20   22
CONECT   20   19   21   56
CONECT   21   20
CONECT   22   19   25   26   79
CONECT   23   18
CONECT   24   19
CONECT   25   22
CONECT   26   22
CONECT   27   33   28   57
CONECT   28   27   34   29   31
CONECT   29   28   30   80
CONECT   30   29
CONECT   31   28   32   35   36
CONECT   32   31   54
CONECT   33   27
CONECT   34   28
CONECT   35   31
CONECT   36   31
CONECT   37   47   38   58
CONECT   38   37   48   39   41
CONECT   39   38   40   59
CONECT   40   39
CONECT   41   38   42   49   50
CONECT   42   41   44   43
CONECT   43   42   54   45
CONECT   44   42   46   51
CONECT   45   43   46   52
CONECT   46   44   45   53
CONECT   47   37
CONECT   48   38
CONECT   49   41
CONECT   50   41
CONECT   51   44
CONECT   52   45
CONECT   53   46
CONECT   54    7   32   43   66
CONECT   55    1
CONECT   56   20
CONECT   57   27
CONECT   58   37
CONECT   59   39
```

```
CONECT   60   68   61   77
CONECT   61   60   69   62   64
CONECT   62   61   63   78
CONECT   63   62
CONECT   64   61   65   70   71
CONECT   65   64   66   72   73
CONECT   66   54   65   67
CONECT   67   66   74   75   76
CONECT   68   60
CONECT   69   61
CONECT   70   64
CONECT   71   64
CONECT   72   65
CONECT   73   65
CONECT   74   67
CONECT   75   67
CONECT   76   67
CONECT   77   60
CONECT   78   62
CONECT   79   22
CONECT   80   29
END
```

Table S35. Structure of 2CAK-Calc7 model in PDB format.

```
HEADER    ELECTRON TRANSPORT                      21-DEC-05   2CAK
HETATM    1  CA          1       0.283  12.669   9.611
HETATM    2  CB          2       0.386  13.357  10.986
HETATM    3  CG          3       0.044  12.441  12.143
HETATM    4  SD          4       0.631  13.115  13.753
HETATM    5  CE          5       0.124  11.725  14.816
HETATM    6  HA          6       0.805  11.714   9.672
HETATM    7 1HB          7       1.393  13.752  11.120
HETATM    8 2HB          8      -0.350  14.161  10.992
HETATM    9 1HG          9      -1.033  12.274  12.168
HETATM   10 2HG         10       0.571  11.499  11.988
HETATM   11 1HE         11       0.385  11.963  15.847
HETATM   12 2HE         12      -0.949  11.550  14.745
HETATM   13 3HE         13       0.660  10.829  14.503
HETATM   14  N          14       3.782  16.161  22.789
HETATM   15  CA         15       2.744  16.500  21.840
HETATM   16  C          16       1.436  15.812  22.202
HETATM   17  O          17       1.452  14.677  22.622
HETATM   18  CB         18       3.132  16.075  20.413
HETATM   19  H          19       3.905  15.188  23.028
HETATM   20  HA         20       2.620  17.582  21.878
HETATM   21 1HB         21       3.375  15.013  20.404
HETATM   22 2HB         22       2.296  16.263  19.739
HETATM   23  N          23       0.333  16.486  21.989
HETATM   24  CA         24      -0.995  15.951  22.201
HETATM   25  C          25      -1.819  15.646  20.982
HETATM   26  O          26      -2.901  16.223  20.733
HETATM   27  H          27       0.414  17.436  21.657
HETATM   28 1HA         28      -0.933  15.062  22.829
HETATM   29 2HA         29      -1.532  16.768  22.682
HETATM   30  N          30      -1.399  14.711  20.175
HETATM   31  CA         31      -1.978  14.382  18.879
```

```
HETATM   32  C          32      -3.408  13.911  19.012
HETATM   33  O          33      -3.826  13.362  20.037
HETATM   34  CB         34      -1.140  13.240  18.277
HETATM   35  CG         35       0.297  13.529  18.032
HETATM   36  ND1        36       0.759  14.298  16.965
HETATM   37  CD2        37       1.373  13.077  18.733
HETATM   38  CE1        38       2.107  14.257  17.079
HETATM   39  NE2        39       2.517  13.548  18.147
HETATM   40  H          40      -0.602  14.167  20.475
HETATM   41  HA         41      -1.973  15.271  18.249
HETATM   42 1HB         42      -1.230  12.353  18.904
HETATM   43 2HB         43      -1.561  13.088  17.283
HETATM   44  HD2        44       1.330  12.442  19.618
HETATM   45  HE1        45       2.779  14.754  16.380
HETATM   46  N          46      -4.155  14.072  17.934
HETATM   47  CA         47      -5.524  13.556  17.865
HETATM   48  C          48      -5.640  12.508  16.761
HETATM   49  O          49      -4.736  12.339  15.940
HETATM   50  CB         50      -6.557  14.662  17.607
HETATM   51  H          51      -3.773  14.563  17.138
HETATM   52  HA         52      -5.738  13.111  18.837
HETATM   53 1HB         53      -7.559  14.271  17.780
HETATM   54 2HB         54      -6.336  15.475  18.298
HETATM   55  N          55      -4.508  13.888  12.110
HETATM   56  CA         56      -4.262  14.626  13.325
HETATM   57  C          57      -4.605  16.122  13.087
HETATM   58  O          58      -4.277  16.643  12.007
HETATM   59  CB         59      -2.795  14.441  13.720
HETATM   60  SG         60      -2.317  15.374  15.226
HETATM   61  H          61      -3.790  13.909  11.400
HETATM   62  HA         62      -4.889  14.202  14.109
HETATM   63 1HB         63      -2.613  13.378  13.902
HETATM   64 2HB         64      -2.154  14.779  12.899
HETATM   65  N          65      -5.236  16.739  14.096
HETATM   66  CA         66      -5.627  18.145  13.978
HETATM   67  C          67      -4.610  19.147  14.507
HETATM   68  O          68      -4.866  20.358  14.388
HETATM   69  H          69      -5.443  16.230  14.944
HETATM   70  HA         70      -5.700  18.312  12.903
HETATM   71  N          71      -3.496  18.713  15.091
HETATM   72  CA         72      -2.523  19.703  15.543
HETATM   73  C          73      -2.072  20.516  14.362
HETATM   74  O          74      -1.712  19.895  13.339
HETATM   75  CB         75      -1.315  19.091  16.247
HETATM   76  CG1        76      -1.689  18.455  17.592
HETATM   77  CG2        77      -0.231  20.153  16.486
HETATM   78  CD1        78      -0.539  17.850  18.406
HETATM   79  H          79      -3.328  17.725  15.218
HETATM   80  HA         80      -3.019  20.331  16.283
HETATM   81  HB         81      -0.935  18.310  15.589
HETATM   82 1HG1        82      -2.160  19.203  18.229
HETATM   83 2HG1        83      -2.376  17.643  17.355
HETATM   84 1HG2        84       0.621  19.696  16.989
HETATM   85 2HG2        85       0.090  20.566  15.530
HETATM   86 3HG2        86      -0.635  20.951  17.109
HETATM   87 1HD1        87      -0.958  17.400  19.310
HETATM   88 2HD1        88      -0.006  17.062  17.863
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HETATM   89 3HD1        89       0.193  18.602  18.723
HETATM   90  CA         90       0.801  17.802  11.290
HETATM   91  CB         91       0.364  17.118  12.594
HETATM   92  CG         92       1.227  17.479  13.768
HETATM   93  ND1        93       1.180  16.779  14.966
HETATM   94  CD2        94       2.154  18.472  13.893
HETATM   95  CE1        95       2.055  17.368  15.761
HETATM   96  NE2        96       2.669  18.391  15.154
HETATM   97  HA         97       1.887  17.753  11.217
HETATM   98 1HB         98      -0.672  17.378  12.811
HETATM   99 2HB         99       0.470  16.044  12.440
HETATM  100  HD2       100       2.432  19.196  13.127
HETATM  101  HE1       101       2.254  17.056  16.786
HETATM  102  HE2       102       3.378  18.989  15.553
HETATM  103 CU   CU1 A 156      -0.138  15.271  15.501
HETATM  104  H         104       3.656  16.702  23.633
HETATM  105  H         105       3.999  16.648  20.085
HETATM  106  H         106      -6.532  11.902  16.698
HETATM  107  H         107      -6.510  15.019  16.578
HETATM  108  H         108      -5.387  14.183  11.709
HETATM  109  H         109      -2.060  21.595  14.396
HETATM  110  H         110      -0.761  12.515   9.340
HETATM  111  H         111       0.758  13.295   8.855
HETATM  112  H         112       0.347  17.300  10.436
HETATM  113  H         113       0.484  18.845  11.303
HETATM  114  H         114      -6.535  18.301  14.561
HETATM  115  CB        115       4.469  11.441  20.245
HETATM  116  CG        116       5.582  12.258  19.598
HETATM  117  OD1       117       6.823  12.085  19.734
HETATM  118  ND2       118       5.107  13.169  18.854
HETATM  119 1HB        119       4.152  10.654  19.561
HETATM  120 2HB        120       3.642  12.119  20.455
HETATM  121 1HD2       121       4.106  13.269  18.760
HETATM  122 2HD2       122       5.732  13.790  18.359
HETATM  123  H         123       4.812  10.973  21.168
CONECT    1    6    2  110  111
CONECT    2    1    3    7    8
CONECT    3    2    4    9   10
CONECT    4    3    5  103
CONECT    5    4   11   12   13
CONECT    6    1
CONECT    7    2
CONECT    8    2
CONECT    9    3
CONECT   10    3
CONECT   11    5
CONECT   12    5
CONECT   13    5
CONECT   14   19   15  104
CONECT   15   14   20   16   18
CONECT   16   15   17   23
CONECT   17   16
CONECT   18   15   21   22  105
CONECT   19   14
CONECT   20   15
CONECT   21   18
CONECT   22   18
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CONECT   23   16   27   24
CONECT   24   23   28   29   25
CONECT   25   24   26   30
CONECT   26   25
CONECT   27   23
CONECT   28   24
CONECT   29   24
CONECT   30   25   40   31
CONECT   31   30   41   32   34
CONECT   32   31   33   46
CONECT   33   32
CONECT   34   31   35   42   43
CONECT   35   34   37   36
CONECT   36   35  103   38
CONECT   37   35   39   44
CONECT   38   36   39   45
CONECT   39   37   38
CONECT   40   30
CONECT   41   31
CONECT   42   34
CONECT   43   34
CONECT   44   37
CONECT   45   38
CONECT   46   32   51   47
CONECT   47   46   52   48   50
CONECT   48   47   49  106
CONECT   49   48
CONECT   50   47   53   54  107
CONECT   51   46
CONECT   52   47
CONECT   53   50
CONECT   54   50
CONECT   55   61   56  108
CONECT   56   55   62   57   59
CONECT   57   56   58   65
CONECT   58   57
CONECT   59   56   60   63   64
CONECT   60   59  103
CONECT   61   55
CONECT   62   56
CONECT   63   59
CONECT   64   59
CONECT   65   57   69   66
CONECT   66   65   70   67  114
CONECT   67   66   68   71
CONECT   68   67
CONECT   69   65
CONECT   70   66
CONECT   71   67   79   72
CONECT   72   71   80   73   75
CONECT   73   72   74  109
CONECT   74   73
CONECT   75   72   76   77   81
CONECT   76   75   78   82   83
CONECT   77   75   84   85   86
CONECT   78   76   87   88   89
CONECT   79   71
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CONECT   80   72
CONECT   81   75
CONECT   82   76
CONECT   83   76
CONECT   84   77
CONECT   85   77
CONECT   86   77
CONECT   87   78
CONECT   88   78
CONECT   89   78
CONECT   90   97   91  112  113
CONECT   91   90   92   98   99
CONECT   92   91   94   93
CONECT   93   92  103   95
CONECT   94   92   96  100
CONECT   95   93   96  101
CONECT   96   94   95  102
CONECT   97   90
CONECT   98   91
CONECT   99   91
CONECT  100   94
CONECT  101   95
CONECT  102   96
CONECT  103    4   36   60   93
CONECT  104   14
CONECT  105   18
CONECT  106   48
CONECT  107   50
CONECT  108   55
CONECT  109   73
CONECT  110    1
CONECT  111    1
CONECT  112   90
CONECT  113   90
CONECT  114   66
CONECT  115  116  119  120  123
CONECT  116  115  117  118
CONECT  117  116
CONECT  118  116  121  122
CONECT  119  115
CONECT  120  115
CONECT  121  118
CONECT  122  118
CONECT  123  115
END
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Table S36. Structure of 2CAK-Calc9 model in PDB format.

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HETATM    1  C1  UNK     1      -3.857   5.989  -2.433  1.00  0.00
HETATM    2  C2  UNK     1      -2.921   4.986  -1.731  1.00  0.00
HETATM    3  C3  UNK     1      -2.059   4.195  -2.692  1.00  0.00
HETATM    4  S4  UNK     1      -0.644   3.383  -1.840  1.00  0.00
HETATM    5  C5  UNK     1       0.155   2.650  -3.305  1.00  0.00
HETATM    6  H6  UNK     1      -3.268   6.547  -3.161  1.00  0.00
HETATM    7  H7  UNK     1      -2.284   5.517  -1.023  1.00  0.00
HETATM    8  H8  UNK     1      -3.559   4.268  -1.215  1.00  0.00
HETATM    9  H9  UNK     1      -2.672   3.454  -3.205  1.00  0.00
HETATM   10  H10 UNK     1      -1.631   4.896  -3.409  1.00  0.00
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HETATM	11	H11	UNK	1	1.035	2.094	-2.980	1.00	0.00
HETATM	12	H12	UNK	1	-0.526	1.977	-3.825	1.00	0.00
HETATM	13	H13	UNK	1	0.460	3.451	-3.978	1.00	0.00
HETATM	14	H110	UNK	1	-4.674	5.465	-2.927	1.00	0.00
HETATM	15	H111	UNK	1	-4.270	6.678	-1.696	1.00	0.00
HETATM	16	N14	UNK	1	7.385	-1.101	2.200	1.00	0.00
HETATM	17	C15	UNK	1	5.951	-1.289	2.164	1.00	0.00
HETATM	18	C16	UNK	1	5.565	-2.293	1.087	1.00	0.00
HETATM	19	O17	UNK	1	6.149	-2.289	0.027	1.00	0.00
HETATM	20	C18	UNK	1	5.222	0.034	1.871	1.00	0.00
HETATM	21	H19	UNK	1	7.863	-0.940	1.325	1.00	0.00
HETATM	22	H20	UNK	1	5.654	-1.660	3.144	1.00	0.00
HETATM	23	H21	UNK	1	5.609	0.466	0.949	1.00	0.00
HETATM	24	H22	UNK	1	4.154	-0.157	1.763	1.00	0.00
HETATM	25	N23	UNK	1	4.564	-3.095	1.356	1.00	0.00
HETATM	26	C24	UNK	1	4.019	-4.050	0.415	1.00	0.00
HETATM	27	C25	UNK	1	2.663	-3.753	-0.161	1.00	0.00
HETATM	28	O26	UNK	1	1.671	-4.493	0.022	1.00	0.00
HETATM	29	H27	UNK	1	4.149	-3.044	2.275	1.00	0.00
HETATM	30	H28	UNK	1	4.731	-4.210	-0.394	1.00	0.00
HETATM	31	H29	UNK	1	3.857	-4.945	1.016	1.00	0.00
HETATM	32	N30	UNK	1	2.535	-2.697	-0.916	1.00	0.00
HETATM	33	C31	UNK	1	1.280	-2.170	-1.436	1.00	0.00
HETATM	34	C32	UNK	1	0.597	-3.160	-2.351	1.00	0.00
HETATM	35	O33	UNK	1	1.229	-4.005	-2.993	1.00	0.00
HETATM	36	C34	UNK	1	1.489	-0.887	-2.266	1.00	0.00
HETATM	37	C35	UNK	1	2.123	0.243	-1.541	1.00	0.00
HETATM	38	N36	UNK	1	1.507	1.070	-0.613	1.00	0.00
HETATM	39	C37	UNK	1	3.427	0.667	-1.655	1.00	0.00
HETATM	40	C38	UNK	1	2.476	1.946	-0.239	1.00	0.00
HETATM	41	N39	UNK	1	3.641	1.735	-0.833	1.00	0.00
HETATM	42	H40	UNK	1	3.380	-2.201	-1.162	1.00	0.00
HETATM	43	H41	UNK	1	0.608	-1.961	-0.604	1.00	0.00
HETATM	44	H42	UNK	1	2.116	-1.146	-3.128	1.00	0.00
HETATM	45	H43	UNK	1	0.511	-0.602	-2.670	1.00	0.00
HETATM	46	H44	UNK	1	4.210	0.267	-2.288	1.00	0.00
HETATM	47	H45	UNK	1	2.287	2.766	0.441	1.00	0.00
HETATM	48	N46	UNK	1	-0.755	-3.027	-2.450	1.00	0.00
HETATM	49	C47	UNK	1	-1.498	-3.816	-3.400	1.00	0.00
HETATM	50	C48	UNK	1	-2.157	-2.916	-4.443	1.00	0.00
HETATM	51	O49	UNK	1	-2.170	-1.690	-4.315	1.00	0.00
HETATM	52	C50	UNK	1	-2.587	-4.642	-2.701	1.00	0.00
HETATM	53	H51	UNK	1	-1.214	-2.232	-2.019	1.00	0.00
HETATM	54	H52	UNK	1	-0.802	-4.506	-3.878	1.00	0.00
HETATM	55	H53	UNK	1	-2.992	-5.374	-3.399	1.00	0.00
HETATM	56	H54	UNK	1	-2.119	-5.137	-1.851	1.00	0.00
HETATM	57	N55	UNK	1	-5.248	0.642	-2.830	1.00	0.00
HETATM	58	C56	UNK	1	-4.355	-0.165	-2.036	1.00	0.00
HETATM	59	C57	UNK	1	-5.089	-0.608	-0.741	1.00	0.00
HETATM	60	O58	UNK	1	-5.812	0.217	-0.155	1.00	0.00
HETATM	61	C59	UNK	1	-3.109	0.663	-1.722	1.00	0.00
HETATM	62	S60	UNK	1	-1.909	-0.222	-0.658	1.00	0.00
HETATM	63	H61	UNK	1	-5.338	1.617	-2.583	1.00	0.00
HETATM	64	H62	UNK	1	-4.061	-1.029	-2.632	1.00	0.00
HETATM	65	H63	UNK	1	-2.616	0.924	-2.663	1.00	0.00
HETATM	66	H64	UNK	1	-3.408	1.583	-1.209	1.00	0.00
HETATM	67	N65	UNK	1	-4.867	-1.872	-0.353	1.00	0.00

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HETATM   68  C66 UNK     1      -5.521  -2.406   0.843  1.00  0.00
HETATM   69  C67 UNK     1      -4.721  -2.275   2.132  1.00  0.00
HETATM   70  O68 UNK     1      -5.247  -2.667   3.189  1.00  0.00
HETATM   71  H69 UNK     1      -4.245  -2.460  -0.890  1.00  0.00
HETATM   72  H70 UNK     1      -6.409  -1.785   0.962  1.00  0.00
HETATM   73  N71 UNK     1      -3.463  -1.778   2.089  1.00  0.00
HETATM   74  C72 UNK     1      -2.774  -1.614   3.360  1.00  0.00
HETATM   75  C73 UNK     1      -3.563  -0.705   4.261  1.00  0.00
HETATM   76  O74 UNK     1      -3.962   0.377   3.779  1.00  0.00
HETATM   77  C75 UNK     1      -1.355  -1.078   3.192  1.00  0.00
HETATM   78  C76 UNK     1      -0.436  -2.083   2.486  1.00  0.00
HETATM   79  C77 UNK     1      -0.744  -0.721   4.555  1.00  0.00
HETATM   80  C78 UNK     1       1.029  -1.663   2.309  1.00  0.00
HETATM   81  H79 UNK     1      -3.135  -1.281   1.267  1.00  0.00
HETATM   82  H80 UNK     1      -2.672  -2.607   3.800  1.00  0.00
HETATM   83  H81 UNK     1      -1.432  -0.186   2.571  1.00  0.00
HETATM   84  H82 UNK     1      -0.423  -3.018   3.045  1.00  0.00
HETATM   85  H83 UNK     1      -0.855  -2.220   1.490  1.00  0.00
HETATM   86  H84 UNK     1       0.268  -0.341   4.412  1.00  0.00
HETATM   87  H85 UNK     1      -1.354   0.043   5.038  1.00  0.00
HETATM   88  H86 UNK     1      -0.712  -1.611   5.183  1.00  0.00
HETATM   89  H87 UNK     1       1.547  -2.452   1.759  1.00  0.00
HETATM   90  H88 UNK     1       1.135  -0.736   1.733  1.00  0.00
HETATM   91  H89 UNK     1       1.549  -1.533   3.266  1.00  0.00
HETATM   92 Cu   UNK     1      -0.350   1.179  -0.010  1.00  0.00
HETATM   93 H104 UNK     1       7.814  -1.879   2.680  1.00  0.00
HETATM   94 H105 UNK     1       5.385   0.730   2.694  1.00  0.00
HETATM   95 H106 UNK     1      -2.620  -3.363  -5.310  1.00  0.00
HETATM   96 H107 UNK     1      -3.410  -4.011  -2.363  1.00  0.00
HETATM   97 H108 UNK     1      -6.163   0.214  -2.848  1.00  0.00
HETATM   98 H109 UNK     1      -3.777  -0.976   5.283  1.00  0.00
HETATM   99 H114 UNK     1      -5.686  -3.475   0.699  1.00  0.00
HETATM  100  C90 UNK     1      -3.452   4.018   2.606  1.00  0.00
HETATM  101  C91 UNK     1      -2.592   3.007   1.834  1.00  0.00
HETATM  102  C92 UNK     1      -1.259   2.754   2.476  1.00  0.00
HETATM  103  N93 UNK     1      -0.233   2.095   1.818  1.00  0.00
HETATM  104  C94 UNK     1      -0.815   3.092   3.721  1.00  0.00
HETATM  105  C95 UNK     1       0.774   2.047   2.672  1.00  0.00
HETATM  106  N96 UNK     1       0.468   2.640   3.832  1.00  0.00
HETATM  107  H97 UNK     1      -2.819   4.849   2.917  1.00  0.00
HETATM  108  H98 UNK     1      -3.134   2.066   1.740  1.00  0.00
HETATM  109  H99 UNK     1      -2.395   3.440   0.853  1.00  0.00
HETATM  110 H100 UNK     1      -1.381   3.624   4.485  1.00  0.00
HETATM  111 H101 UNK     1       1.736   1.582   2.457  1.00  0.00
HETATM  112 H102 UNK     1       1.071   2.736   4.636  1.00  0.00
HETATM  113 H112 UNK     1      -4.259   4.382   1.970  1.00  0.00
HETATM  114 H113 UNK     1      -3.878   3.536   3.486  1.00  0.00
HETATM  115 C115 UNK     1       6.988   2.200  -2.063  1.00  0.00
HETATM  116 C116 UNK     1       7.010   3.224  -0.933  1.00  0.00
HETATM  117 O117 UNK     1       7.924   4.055  -0.685  1.00  0.00
HETATM  118 N118 UNK     1       5.949   3.163  -0.241  1.00  0.00
HETATM  119 H119 UNK     1       6.459   2.616  -2.920  1.00  0.00
HETATM  120 H120 UNK     1       6.476   1.312  -1.694  1.00  0.00
HETATM  121 H121 UNK     1       5.233   2.491  -0.478  1.00  0.00
HETATM  122 H122 UNK     1       5.826   3.786   0.545  1.00  0.00
HETATM  123 H123 UNK     1       8.000   1.943  -2.379  1.00  0.00
CONECT    1    2    6   14   15
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CONECT    2    1    3    7    8
CONECT    3    2    4    9   10
CONECT    4    3    5
CONECT    5    4   11   12   13
CONECT    6    1
CONECT    7    2
CONECT    8    2
CONECT    9    3
CONECT   10    3
CONECT   11    5
CONECT   12    5
CONECT   13    5
CONECT   14    1
CONECT   15    1
CONECT   16   17   21   93
CONECT   17   16   18   20   22
CONECT   18   17   19   25
CONECT   19   18
CONECT   20   17   23   24   94
CONECT   21   16
CONECT   22   17
CONECT   23   20
CONECT   24   20
CONECT   25   18   26   29
CONECT   26   25   27   30   31
CONECT   27   26   28   32
CONECT   28   27
CONECT   29   25
CONECT   30   26
CONECT   31   26
CONECT   32   27   33   42
CONECT   33   32   34   36   43
CONECT   34   33   35   48
CONECT   35   34
CONECT   36   33   37   44   45
CONECT   37   36   38   39
CONECT   38   37   40   92
CONECT   39   37   41   46
CONECT   40   38   41   47
CONECT   41   39   40
CONECT   42   32
CONECT   43   33
CONECT   44   36
CONECT   45   36
CONECT   46   39
CONECT   47   40
CONECT   48   34   49   53
CONECT   49   48   50   52   54
CONECT   50   49   51   95
CONECT   51   50
CONECT   52   49   55   56   96
CONECT   53   48
CONECT   54   49
CONECT   55   52
CONECT   56   52
CONECT   57   58   63   97
CONECT   58   57   59   61   64
```

```
CONECT   59   58   60   67
CONECT   60   59
CONECT   61   58   62   65   66
CONECT   62   61   92
CONECT   63   57
CONECT   64   58
CONECT   65   61
CONECT   66   61
CONECT   67   59   68   71
CONECT   68   67   69   72   99
CONECT   69   68   70   73
CONECT   70   69
CONECT   71   67
CONECT   72   68
CONECT   73   69   74   81
CONECT   74   73   75   77   82
CONECT   75   74   76   98
CONECT   76   75
CONECT   77   74   78   79   83
CONECT   78   77   80   84   85
CONECT   79   77   86   87   88
CONECT   80   78   89   90   91
CONECT   81   73
CONECT   82   74
CONECT   83   77
CONECT   84   78
CONECT   85   78
CONECT   86   79
CONECT   87   79
CONECT   88   79
CONECT   89   80
CONECT   90   80
CONECT   91   80
CONECT   92   38   62
CONECT   93   16
CONECT   94   20
CONECT   95   50
CONECT   96   52
CONECT   97   57
CONECT   98   75
CONECT   99   68
CONECT  100  101  107  113  114
CONECT  101  100  102  108  109
CONECT  102  101  103  104
CONECT  103  102  105
CONECT  104  102  106  110
CONECT  105  103  106  111
CONECT  106  104  105  112
CONECT  107  100
CONECT  108  101
CONECT  109  101
CONECT  110  104
CONECT  111  105
CONECT  112  106
CONECT  113  100
CONECT  114  100
CONECT  115  116  119  120  123
```

```
CONECT  116  115  117  118
CONECT  117  116
CONECT  118  116  121  122
CONECT  119  115
CONECT  120  115
CONECT  121  118
CONECT  122  118
CONECT  123  115
MASTER    0    0    0    0    0    0    0    0    3  123    0  123    0
END
```

Table S37. Fitting parameters for equation (9)

AIM property	*a*	*b*	*c*	R^2
ρ(**r**)	6.7455	-0.86593	9.60481	0.93
G(**r**)	4.61544	-0.70012	6.80167	0.97
|V(**r**)|	4.88843	-0.59674	6.83757	0.94

Table S38. Computed Fermi Contact Spin Densities for Different H-C-S-Cu Torsion Angles in a Pc Model (unit: au)

$H^{\beta 2}$-C-S-Cu (°)	$H^{\beta 1}$-C-S-Cu (°)	$\rho_{\alpha\beta}$ ($H^{\beta 1}$) (au)	$\rho_{\alpha\beta}$ ($H^{\beta 2}$) (au)
180	-63.4	0.00788	-0.00005
150	-93.4	0.01155	0.00443
120	-123.4	0.00856	0.01167
90	-153.4	0.00310	0.01466
60	176.6	-0.00003	0.00983
30	146.6	0.00262	0.00282
0	116.6	0.00771	0.00006
-30	86.6	0.01040	0.00402
-60	56.6	0.00795	0.01084
-90	26.6	0.00284	0.01367
-120	-3.4	0.00004	0.01026
-150	-33.4	0.00223	0.00347
-180	-63.4	0.00788	-0.00005

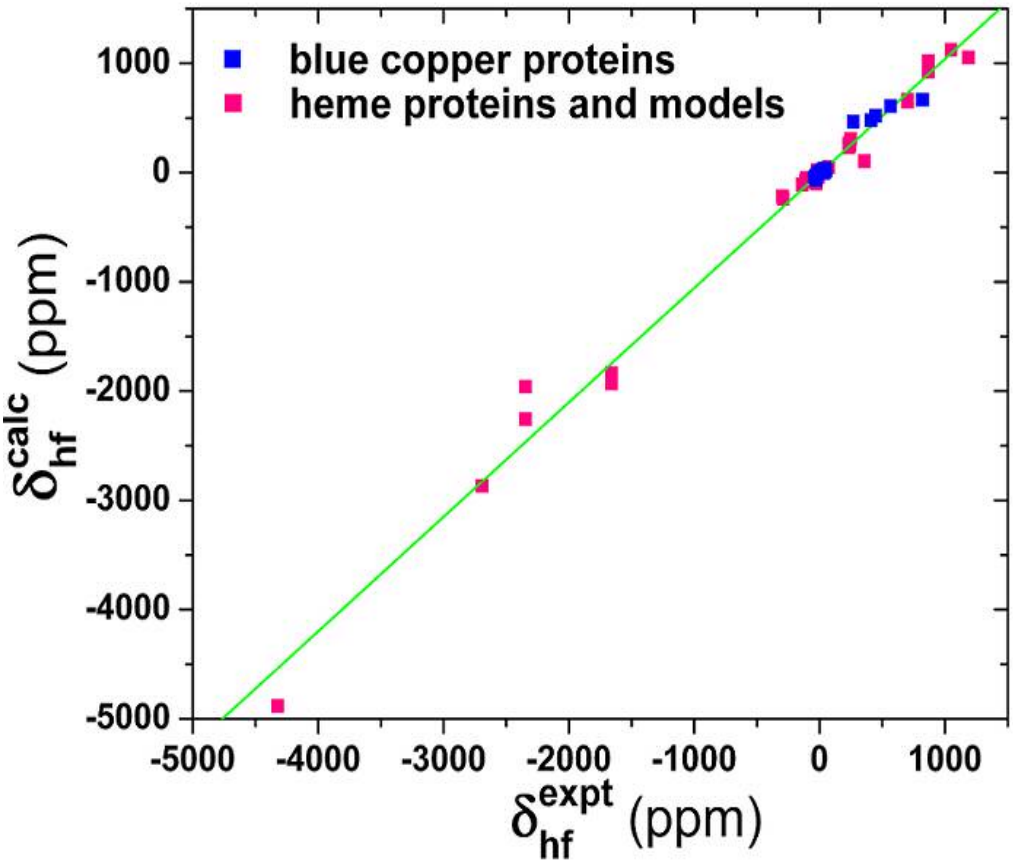

Figure S1. Calculated NMR hyperfine shifts versus experimental data in BCPs and heme proteins and models.

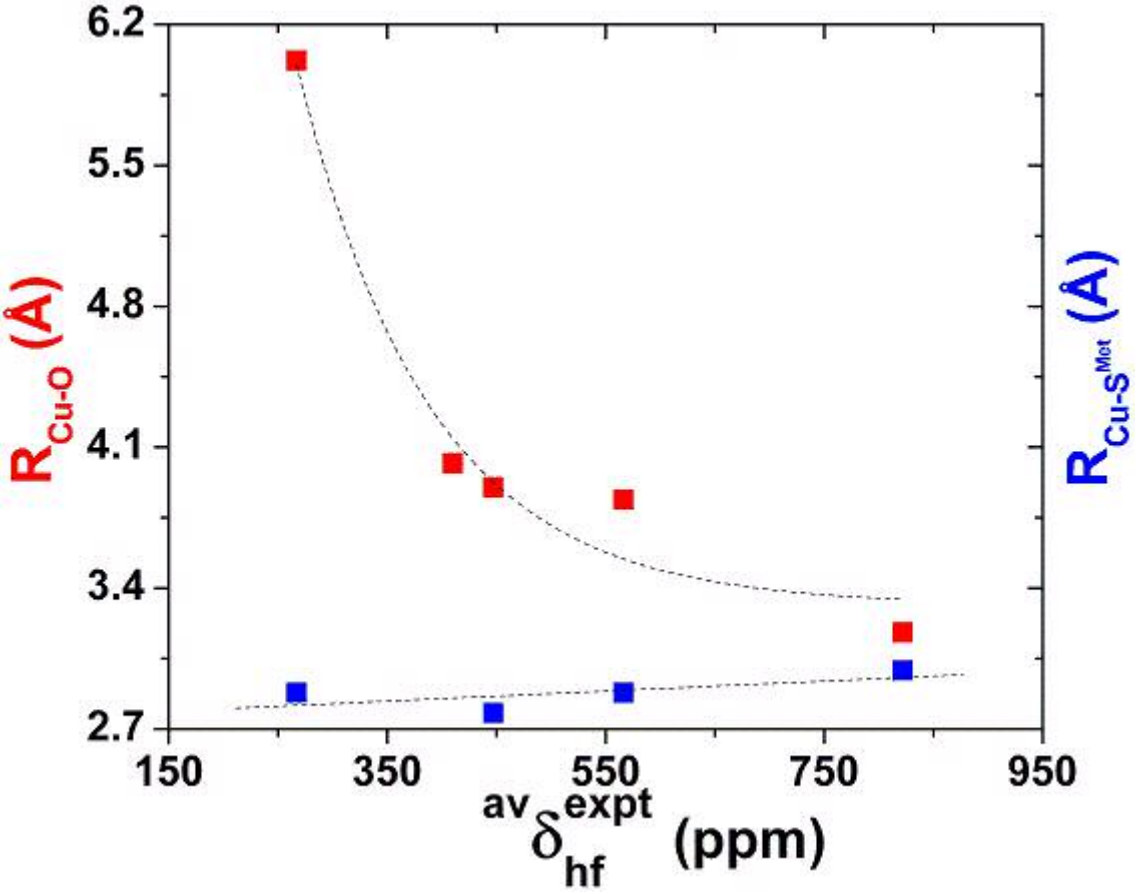

Figure S2. Plots of the optimized distances of Cu(II) and the axial ligands versus the average NMR hyperfine shifts of the Cys C^{β} protons ($^{av}\delta_{hf}^{expt}$) in BCPs.

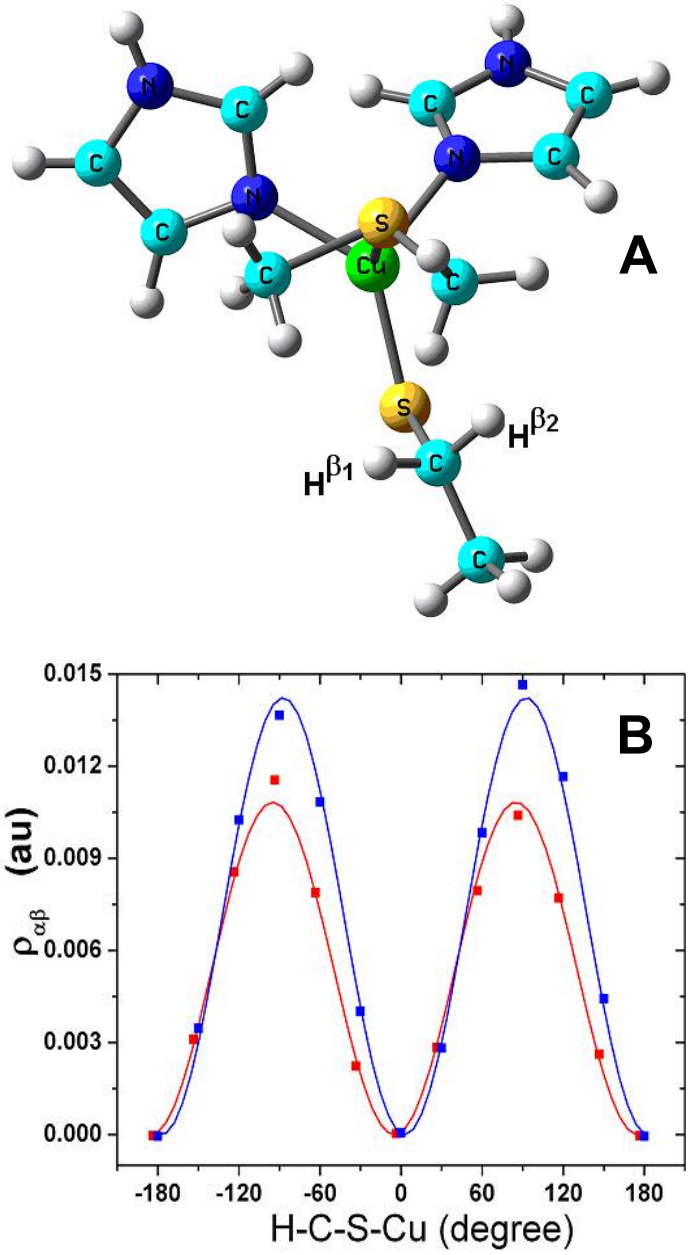

Figure S3. (A) Structure of the Pc model used in the calculations of the effect of torsion angle on hyperfine shift. (B) Calculated Karplus-type dependence of Fermi contact spin density on H-C^{β}-S-Cu angle ($H^{\beta 1}$-red, $H^{\beta 2}$-blue). They can be fitted by the following equations: $\rho_{\alpha\beta}$ ($H^{\beta 1}$) = 0.01083 $\sin^2(\theta + 4.9)$ and $\rho_{\alpha\beta}$ ($H^{\beta 2}$) = 0.01424 $\sin^2(\theta - 2.7)$ with R^2 = 0.995 and 0.996 respectively.