

The role of conformational fluctuations in the recognition of the Josephin domain of ataxin-3 with ubiquitin

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Supplementary Information

Table S1. Values of HN RDC in Phages at high salt

| Phages 500mM NaCl | | |
|--------------------------|------|--------|
| Seq.No. | Res. | RDC |
| 2 | GLU | -3.96 |
| 3 | SER | 7.16 |
| 4 | ILE | -0.75 |
| 5 | PHE | 15.01 |
| 7 | GLU | 15.7 |
| 8 | LYS | 9.89 |
| 9 | GLN | 5.16 |
| 11 | GLY | 4.57 |
| 12 | SER | 9.47 |
| 13 | LEU | 11.82 |
| 15 | ALA | -5.48 |
| 17 | HIS | -2.53 |
| 18 | CYS | -9.32 |
| 20 | ASN | 3.53 |
| 21 | ASN | -14.07 |
| 23 | LEU | 0.18 |
| 25 | GLY | -9.17 |
| 27 | TYR | 7.80 |
| 28 | PHE | -4.73 |
| 29 | SER | -3.37 |
| 32 | GLU | -2.20 |
| 34 | SER | 7.71 |
| 35 | SER | -15.96 |
| 36 | ILE | -9.53 |
| 38 | HIS | -5.76 |
| 47 | ARG | -2.73 |
| 51 | GLY | 2.02 |
| 53 | VAL | 1.50 |
| 54 | THR | 6.72 |

| | | |
|-----|-----|--------|
| 55 | SER | -7.96 |
| 57 | ASP | 4.70 |
| 60 | THR | 4.13 |
| 62 | LEU | -0.06 |
| 64 | GLN | 1.99 |
| 66 | SER | -4.99 |
| 67 | GLY | 2.53 |
| 68 | ASN | -6.89 |
| 71 | ASP | -2.99 |
| 72 | SER | 6.17 |
| 79 | VAL | 1.88 |
| 80 | ILE | -3.02 |
| 81 | SER | -9.60 |
| 83 | ALA | -0.66 |
| 84 | LEU | -6.26 |
| 88 | GLY | -5.40 |
| 90 | GLU | -5.21 |
| 91 | LEU | -9.81 |
| 92 | ILE | -12.77 |
| 93 | LEU | -6.28 |
| 94 | PHE | 20.41 |
| 96 | SER | 0.68 |
| 98 | GLU | 1.85 |
| 99 | TYR | -2.15 |
| 100 | GLN | -8.92 |
| 102 | LEU | 13.39 |
| 103 | ARG | 0.02 |
| 105 | ASP | 0.04 |
| 107 | ILE | 17.65 |
| 108 | ASN | 0.49 |
| 110 | ARG | -12.53 |
| 111 | SER | 9.85 |
| 112 | PHE | 6.99 |
| 113 | ILE | 9.73 |
| 115 | ASN | 27.84 |
| 116 | TYR | 17.57 |
| 117 | LYS | 18.28 |
| 118 | GLU | 14.58 |
| 119 | HIS | 5.76 |
| 120 | TRP | 21.8 |
| 121 | PHE | 18.25 |
| 122 | THR | 29.84 |
| 123 | VAL | -1.00 |
| 124 | ARG | 4.30 |
| 126 | LEU | 0.61 |
| 127 | GLY | -2.56 |
| 128 | LYS | -2.19 |
| 129 | GLN | 8.99 |
| 130 | TRP | 6.26 |
| 131 | PHE | -2.38 |
| 132 | ASN | -7.89 |
| 133 | LEU | 3.62 |
| 135 | SER | -2.17 |
| 137 | LEU | 5.52 |
| 138 | THR | 7.05 |

| | | |
|-----|-----|--------|
| 142 | LEU | 0.08 |
| 143 | ILE | 0.40 |
| 144 | SER | 0.54 |
| 145 | ASP | -13.86 |
| 146 | THR | -4.07 |
| 148 | LEU | -12.30 |
| 149 | ALA | -5.22 |
| 150 | LEU | -12.51 |
| 151 | PHE | -9.69 |
| 154 | GLN | -16.29 |
| 155 | LEU | -8.46 |
| 158 | GLU | -8.64 |
| 159 | GLY | 16.16 |
| 161 | SER | 24.14 |
| 162 | ILE | 17.00 |
| 163 | PHE | 14.95 |
| 164 | VAL | -3.09 |
| 165 | VAL | -13.15 |
| 166 | LYS | -10.59 |
| 167 | GLY | 4.09 |
| 168 | ASP | -3.41 |
| 169 | LEU | 8.27 |
| 171 | ASP | -1.42 |
| 172 | CYS | 12.17 |
| 173 | GLU | 10.48 |
| 174 | ALA | -6.73 |
| 175 | ASP | 3.95 |
| 176 | GLN | 11.01 |
| 177 | LEU | -1.25 |
| 181 | ILE | 0.89 |
| 182 | ARG | 4.34 |

Table S2. RDC collected in phages at low ionic strength.

| Phages no salt | | |
|-----------------------|------|-------|
| Seq.No. | Res. | RDC |
| 2 | GLU | 0.54 |
| 3 | SER | -0.03 |
| 4 | ILE | 0.15 |
| 5 | PHE | 0.01 |
| 7 | GLU | 0.57 |
| 8 | LYS | 1.13 |
| 9 | GLN | 4.22 |
| 10 | GLU | -1.8 |
| 11 | GLY | 0.56 |
| 12 | SER | 0.28 |
| 13 | LEU | -0.76 |
| 15 | ALA | -0.59 |
| 17 | HIS | -0.43 |
| 19 | LEU | 11.96 |
| 21 | ASN | 1.25 |

| | | |
|-----|-----|-------|
| 23 | LEU | -0.97 |
| 25 | GLY | -0.11 |
| 27 | TYR | -0.52 |
| 28 | PHE | 0.08 |
| 34 | SER | 0.23 |
| 35 | SER | 2.74 |
| 36 | ILE | -0.45 |
| 38 | HIS | 0.04 |
| 46 | MET | -2.39 |
| 51 | GLY | 0.19 |
| 52 | GLY | 9.3 |
| 53 | VAL | 0.25 |
| 54 | THR | -0.06 |
| 55 | SER | -5.9 |
| 56 | GLU | 1.03 |
| 57 | ASP | -2.65 |
| 59 | ARG | -0.08 |
| 60 | THR | 0.08 |
| 62 | LEU | -0.35 |
| 64 | GLN | 0.75 |
| 66 | SER | -0.76 |
| 67 | GLY | -2.14 |
| 68 | ASN | -1.83 |
| 71 | ASP | 0.27 |
| 72 | SER | 1.3 |
| 79 | VAL | -1.32 |
| 80 | ILE | -0.31 |
| 81 | SER | -0.78 |
| 83 | ALA | 0.05 |
| 86 | VAL | -2.02 |
| 90 | GLU | 0.77 |
| 91 | LEU | 1.08 |
| 93 | LEU | -0.02 |
| 96 | SER | -1.48 |
| 98 | GLU | 1.29 |
| 99 | TYR | -0.62 |
| 100 | GLN | 4.41 |
| 102 | LEU | -0.85 |
| 105 | ASP | -0.49 |
| 107 | ILE | 0.13 |
| 110 | ARG | -0.36 |
| 111 | SER | -0.19 |
| 112 | PHE | 0.71 |
| 113 | ILE | 0.2 |
| 115 | ASN | 1.27 |
| 116 | TYR | 0.96 |
| 117 | LYS | 0.62 |
| 118 | GLU | -0.43 |
| 119 | HIS | 0.48 |
| 120 | TRP | 1.64 |
| 121 | PHE | -0.64 |
| 122 | THR | 0.32 |
| 123 | VAL | 0.83 |
| 124 | ARG | 1 |
| 126 | LEU | -0.21 |

| | | |
|-----|-----|-------|
| 128 | LYS | -0.38 |
| 130 | TRP | 1.09 |
| 132 | ASN | -0.89 |
| 133 | LEU | -1.08 |
| 135 | SER | 8.68 |
| 136 | LEU | -3.09 |
| 138 | THR | -0.06 |
| 139 | GLY | 0.2 |
| 142 | LEU | -0.06 |
| 143 | ILE | -0.43 |
| 145 | ASP | -0.27 |
| 146 | THR | 0.03 |
| 148 | LEU | 0.24 |
| 149 | ALA | -0.14 |
| 150 | LEU | 0.23 |
| 151 | PHE | -1.79 |
| 154 | GLN | -0.27 |
| 155 | LEU | -1.34 |
| 158 | GLU | -0.73 |
| 159 | GLY | -0.03 |
| 161 | SER | 0.36 |
| 162 | ILE | 0.44 |
| 163 | PHE | 0.42 |
| 164 | VAL | 0.08 |
| 165 | VAL | 0.03 |
| 166 | LYS | -0.05 |
| 167 | GLY | -0.06 |
| 168 | ASP | -0.69 |
| 169 | LEU | -0.29 |
| 171 | ASP | -0.84 |
| 172 | CYS | 0 |
| 173 | GLU | 0.23 |
| 174 | ALA | -0.83 |
| 175 | ASP | -2.95 |
| 176 | GLN | -0.5 |
| 177 | LEU | 0.17 |
| 181 | ILE | -1.46 |
| 182 | ARG | -0.08 |

Table S3. RDC collected in gels

| Gels | | |
|---------|------|------|
| Seq.No. | Res. | RDC |
| 4 | ILE | 8.5 |
| 7 | GLU | -2.1 |
| 11 | GLY | 6.2 |
| 24 | GLN | 2.3 |
| 25 | GLY | -3.7 |
| 38 | HIS | -0.7 |
| 51 | GLY | 2.3 |

| | | |
|-----|-----|-------|
| 54 | THR | 5.1 |
| 60 | THR | -1.4 |
| 67 | GLY | 10 |
| 72 | SER | 4.6 |
| 79 | VAL | 8.6 |
| 93 | ALA | -0.3 |
| 94 | LEU | -1.7 |
| 111 | SER | -14.3 |
| 112 | PHE | 1 |
| 116 | PHE | -1.2 |
| 118 | GLU | 2.2 |
| 121 | PHE | 4.1 |
| 123 | VAL | -5.43 |
| 124 | ARG | 2.2 |
| 126 | LEU | 6.2 |
| 127 | GLY | 6.6 |
| 131 | PHE | 2.1 |
| 132 | ASN | 0.3 |
| 138 | THR | 8.1 |
| 139 | LEU | 7.7 |
| 142 | LEU | -1 |
| 143 | ILE | 2.1 |
| 145 | ASP | -4.3 |
| 149 | ALA | -4.2 |
| 150 | LEU | 1.2 |
| 159 | GLY | -2.4 |
| 161 | SER | 0.2 |
| 163 | PHE | -7 |
| 164 | VAL | -3.6 |
| 165 | VAL | 5.3 |
| 167 | GLY | -4.8 |
| 169 | LEU | -7 |

Table S4. RDC collected in doped bicelles.

| doped Bicelles | | |
|-----------------------|------|-------|
| Seq.No. | Res. | RDC |
| 2 | GLU | -0.29 |
| 3 | SER | 0.17 |
| 4 | ILE | -0.24 |
| 5 | PHE | -5.50 |
| 8 | LYS | -0.38 |
| 9 | GLN | 2.38 |
| 10 | GLU | -0.24 |
| 11 | GLY | -2.56 |
| 13 | LEU | -0.79 |
| 15 | ALA | 0.50 |
| 17 | HIS | 0.03 |
| 19 | LEU | -0.64 |
| 21 | ASN | 0.13 |

| | | |
|-----|-----|-------|
| 23 | LEU | -7.32 |
| 25 | GLY | 0.27 |
| 27 | TYR | -0.39 |
| 28 | PHE | -0.94 |
| 34 | SER | -0.23 |
| 35 | SER | 0.70 |
| 36 | ILE | 0.87 |
| 38 | HIS | -2.29 |
| 46 | MET | -2.07 |
| 51 | GLY | -0.53 |
| 53 | VAL | -1.21 |
| 54 | THR | -2.10 |
| 55 | SER | -4.83 |
| 56 | GLU | 2.29 |
| 59 | ARG | -1.92 |
| 60 | THR | 0.18 |
| 64 | GLN | -0.29 |
| 66 | SER | -1.18 |
| 67 | GLY | 2.62 |
| 68 | ASN | 1.07 |
| 72 | SER | 0.63 |
| 79 | VAL | 0.25 |
| 80 | ILE | -0.29 |
| 81 | SER | -0.28 |
| 83 | ALA | -0.03 |
| 86 | VAL | 0.62 |
| 90 | GLU | 0.50 |
| 91 | LEU | 0.04 |
| 93 | LEU | 0.07 |
| 96 | SER | -1.16 |
| 98 | GLU | 1.35 |
| 99 | TYR | 0.07 |
| 100 | GLN | -0.23 |
| 102 | LEU | -0.31 |
| 105 | ASP | -0.33 |
| 107 | ILE | -2.14 |
| 110 | ARG | -1.22 |
| 111 | SER | -0.15 |
| 112 | PHE | -0.26 |
| 113 | ILE | -0.99 |
| 115 | ASN | 0.38 |
| 116 | TYR | 0.70 |
| 117 | LYS | 0.42 |
| 118 | GLU | 0.84 |
| 119 | HIS | 3.12 |
| 120 | TRP | 0.02 |
| 121 | PHE | -0.67 |
| 122 | THR | -0.09 |
| 123 | VAL | 0.95 |
| 124 | ARG | 0.23 |
| 126 | LEU | 0.15 |
| 128 | LYS | -0.20 |
| 130 | TRP | 0.01 |
| 132 | ASN | -0.26 |
| 135 | SER | 5.53 |

| | | |
|-----|-----|-------|
| 136 | LEU | -1.04 |
| 138 | THR | -0.17 |
| 139 | GLY | 0.18 |
| 142 | LEU | -0.02 |
| 143 | ILE | 0.46 |
| 145 | ASP | 0.06 |
| 146 | THR | -0.50 |
| 148 | LEU | 0.28 |
| 149 | ALA | 0.10 |
| 150 | LEU | 0.21 |
| 151 | PHE | 0.22 |
| 154 | GLN | -0.41 |
| 155 | LEU | -0.63 |
| 158 | GLU | -1.06 |
| 159 | GLY | -0.45 |
| 161 | SER | -0.08 |
| 162 | ILE | -0.23 |
| 163 | PHE | -0.4 |
| 164 | VAL | -0.07 |
| 165 | VAL | 0.11 |
| 166 | LYS | -0.17 |
| 167 | GLY | -0.27 |
| 168 | ASP | -0.01 |
| 169 | LEU | -1.50 |
| 171 | ASP | 0.14 |
| 172 | CYS | 0.15 |
| 173 | GLU | 0.27 |
| 175 | ASP | 3.95 |
| 176 | GLN | -5.28 |
| 177 | LEU | -3.33 |
| 181 | ILE | 0.17 |
| 182 | ARG | -0.08 |