

Supplementary Material

Ensemble description of the intrinsically disordered N-terminal domain of the Nipah virus P/V protein from combined NMR and SAXS

Marco Schiavina^{1,2§}, Edoardo Salladini^{4§}, Maria Grazia Murralli^{1,2§}, Giancarlo Tria^{2,3}, Isabella Felli^{1,2*}, Roberta Pierattelli^{1,2*} and Sonia Longhi^{4*}

¹Magnetic Resonance Center (CERM), University of Florence, Via Luigi Sacconi 6, 50019 Sesto Fiorentino, Italy

²Department of Chemistry “Ugo Schiff”, University of Florence, Via della Lastruccia 3-13, 50019 Sesto Fiorentino, Italy

³Florence Center for Electron Nanoscopy (FloCEN), University of Florence, Via della Lastruccia 3-13, 50019 Sesto Fiorentino, Italy

⁴Aix Marseille Univ, CNRS, Architecture et Fonction des Macromolécules Biologiques (AFMB), UMR 7257, Marseille, France

*To whom correspondence should be sent:

felli@cerm.unifi.it

roberta.pierattelli@unifi.it

sonia.longhi@afmb.univ-mrs.fr; sonia.longhi@univ-amu.fr

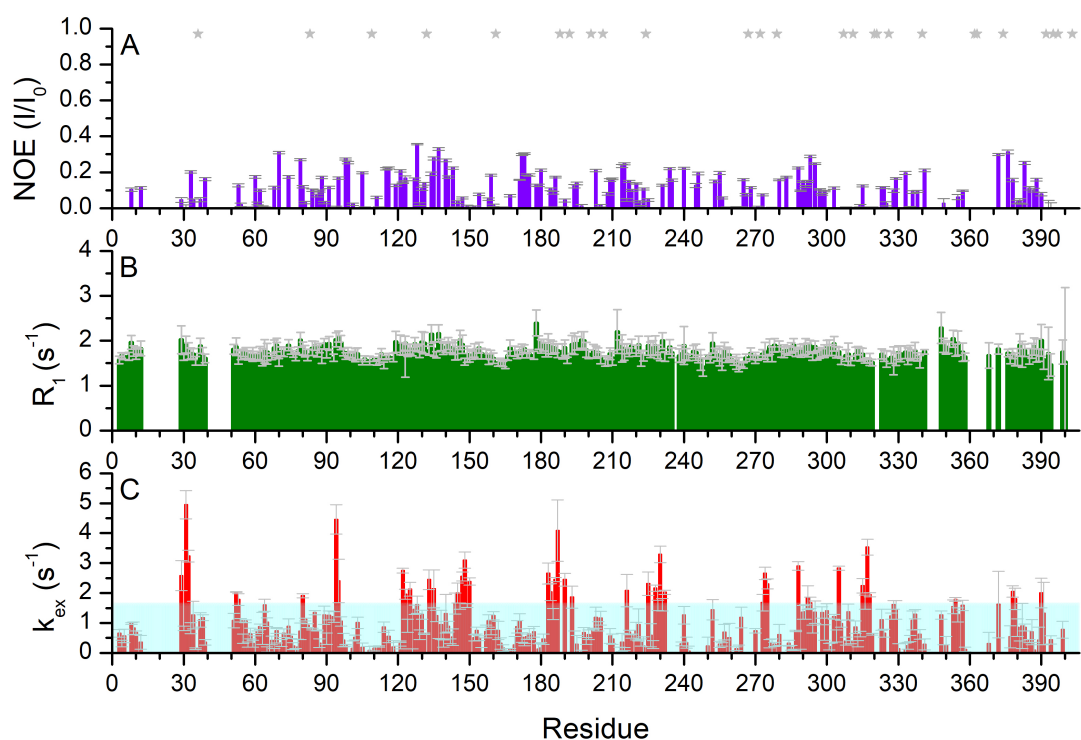
[§]These authors contributed equally to the work

Supplementary text

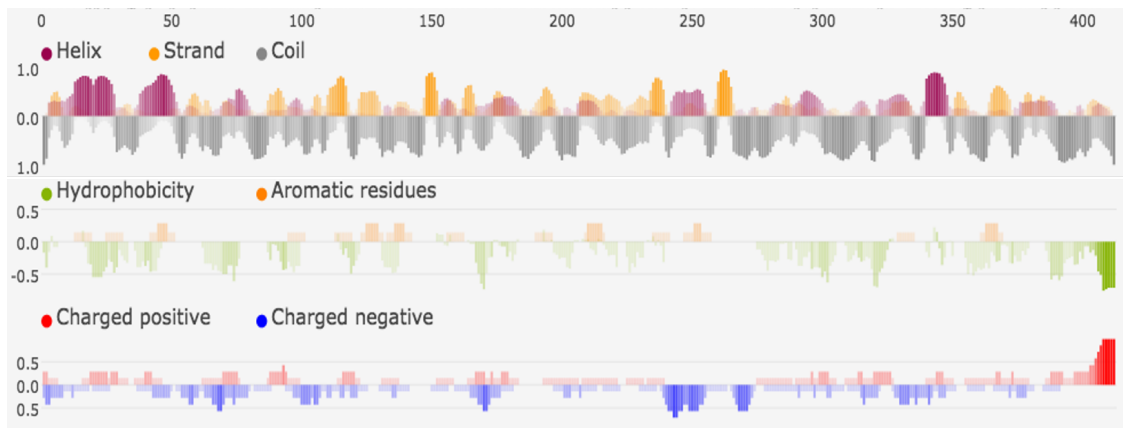
Discrepancy between experimentally observed R_g and R_g expected from Flory's power law

Flory's power law attempts at generalizing the IDP behavior while taking into account only sequence length and thus neglecting sequence specificities. Although Flory's power law remains a useful tool, the extent to which it can be generalized to all IDPs is a matter of debate, with several instances of deviations having been experimentally observed. Systematic collections of SAXS data on IDPs, such as the work of Cordeiro et al. [1], show a large scatter that indicates a lot of variation in scaling behavior. A similar study carried out Sosnick and co-workers [2] showed that several IDPs obeyed a scaling law with an exponent close to 0.6. Further, Sosnick and co-workers explained that the scaling law exponent reflects the quality of the solvent (aqueous buffer, sometimes also with denaturant) for a particular IDP and that solvent quality (and scaling exponent) can vary with the amino acid sequence. Consequently, it is not surprising to observe deviations from Flory's power law such as those we observed for NiV PNT.

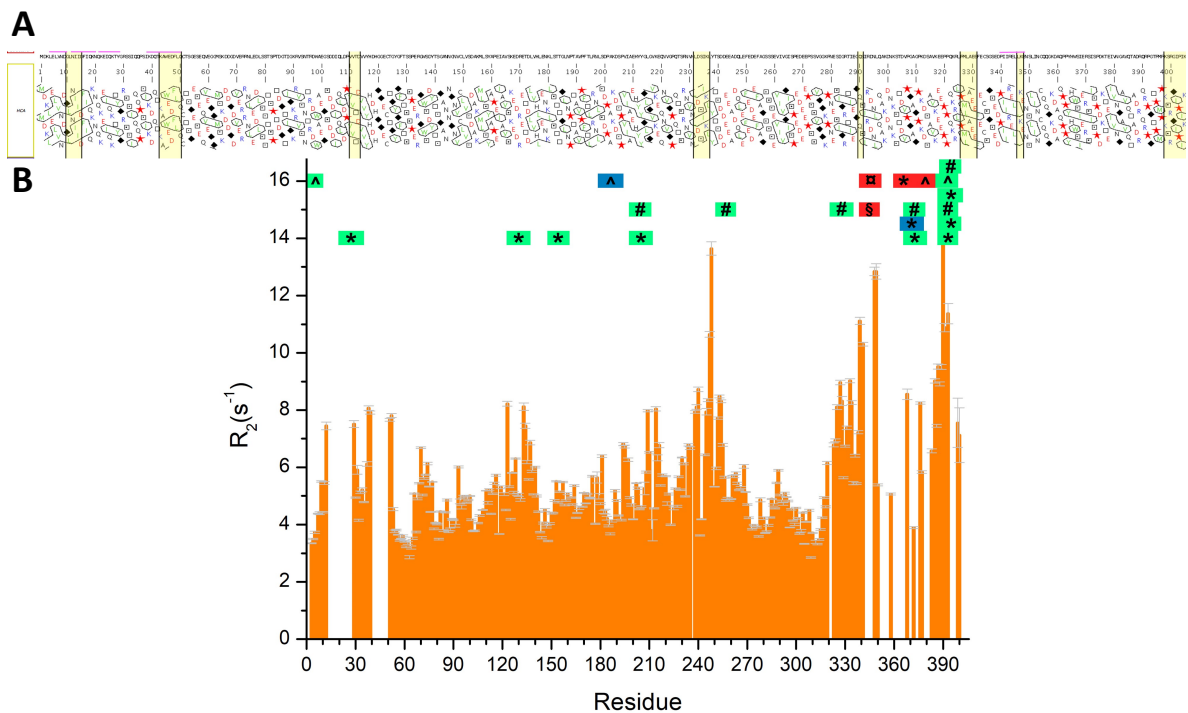
Supplementary Figures



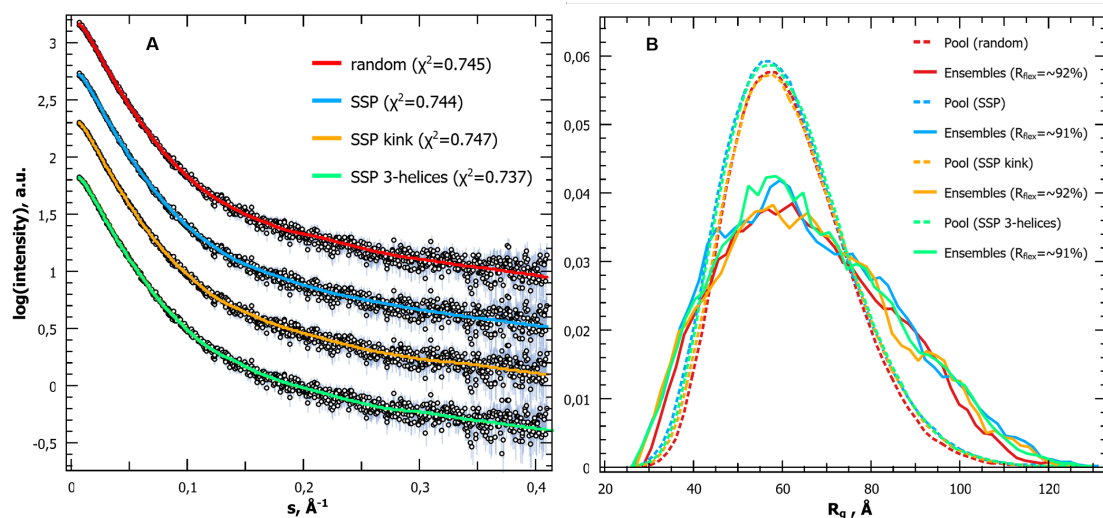
Supplementary Figure S1. (A) 1H - ^{15}N -NOE measurements, (B) ^{15}N R_1 relaxation rates and (C) k_{ex} , as derived from CLEANEX-PM experiment using the approach reported in [3], of NiV PNT, carried out at 700 MHz and 288 K on a 100 μM ^{15}N -labeled sample. The light cyan box represents the modal value of $1.38 s^{-1}$.



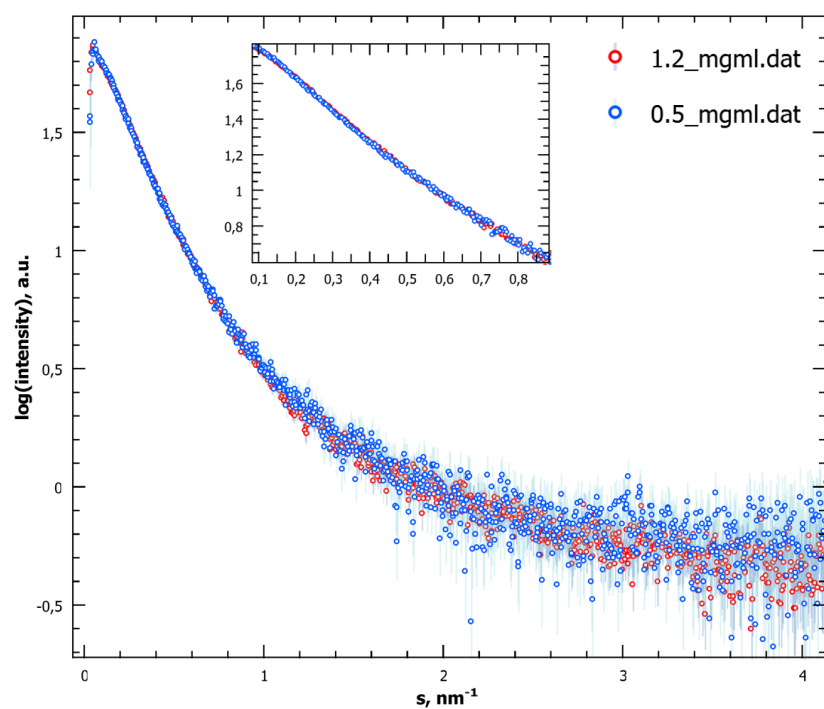
Supplementary Figure S2. Excerpt of the output generated by FELLS [4].



Supplementary Figure S3. (A) Hydrophobic cluster analysis (HCA) plot [5] of NiV PNT as obtained using MeDor [6]. Molecular Recognition Elements (MoREs), as predicted by MoRFPred [7] are shown in yellow. The α -helices, as predicted by PSIPRED [8], are shown as pink horizontal bars above the sequence. Four of them fall within the region encompassing the first 50 residues while the fifth one encompasses residues 340-348. (B) ^{15}N R_2 relaxation rates and putative Short Linear Motifs (SLiMs) as identified by the ELM database (<http://elm.eu.org/>) (see also **Supplementary Table S3**). The SLiMs are identified as follows according to the ELM classification: §, CLV (cleavage site); #, DOC (docking site); ^; LIG (ligand binding site); *, MOD (post-translational modification site), □, TRG (targeting site). The color code is representative of the conservation score (red < 0.95; blue 0.95-1; green 1).



Supplementary Figure S4. Modeling NiV PNT as a conformational ensemble. (A) Experimental scattering curve of NiV PNT and EOM 2.0 ensemble fits obtained using different initial pools as explained in **(B)**. **(B)** R_g distributions of the initial pools generated by: (*red dot*) EOM 2.0 (without restraints), (*blue dot*) Flexible-Meccano (with NMR secondary structure restraints), (*orange dot*) Flexible-Meccano (while imposing a kink centered at residue 20 providing NMR restraints), and (*green dot*) Flexible-Meccano (with α -helices imposed to residues 1-30). R_g distributions of the corresponding selected ensembles obtained using EOM 2.0 are shown as solid lines.



Supplementary Figure S5. Superimposition of the experimental scattering curves of NiV PNT collected at 0.5 mg/mL (*light blue*) and 1.2 mg/mL (*orange*). Inset: zoom on the superimposition at very low angle.

Supplementary Table S1. Acquisition parameters.

| Experiments | Dimension of acquired data | | | Spectral width (ppm) | | | NS ^a | d1 (s) ^b |
|--|----------------------------|-------------------------|-------------------------|----------------------|----------------|----------------|-----------------|---------------------|
| | t ₁ | t ₂ | t ₃ | F ₁ | F ₂ | F ₃ | | |
| ¹H detected | | | | | | | | |
| ¹ H- ¹⁵ N BEST-TROSY | 1024 (¹⁵ N) | 8192 (¹ H) | | 35 | 15 | | 2 | 0.05 |
| BT HNCO | 224 (¹³ C) | 112 (¹⁵ N) | 4096(¹ H) | 6 | 24 | 12 | 4 | 0.13 |
| BT HN(CA)CO | 224 (¹³ C) | 112 (¹⁵ N) | 4096(¹ H) | 6 | 24 | 12 | 8 | 0.13 |
| BT HNCACB | 148 (¹³ C) | 128 (¹⁵ N) | 4096(¹ H) | 34 | 25 | 12 | 4 | 0.20 |
| BT HN(CO)CACB | 220 (¹³ C) | 128 (¹⁵ N) | 4096(¹ H) | 65 | 25 | 12 | 16 | 0.20 |
| BT (H)N(COCA)NNH | 134 (¹⁵ N) | 134 (¹⁵ N) | 4096(¹ H) | 25 | 25 | 12 | 8 | 0.20 |
| BT (H)N(CA)NNH | 148 (¹⁵ N) | 128 (¹⁵ N) | 4096(¹ H) | 25 | 25 | 12 | 16 | 0.20 |
| ¹³C detected | | | | | | | | |
| CON | 1264 (¹⁵ N) | 1024 (¹³ C) | | 40 | 30 | | 8 | 2.00 |
| (H)CBCACON | 164 (¹³ C) | 128 (¹⁵ N) | 1024 (¹³ C) | 69 | 34 | 30 | 4 | 0.80 |
| (H)CBCANCO | 164 (¹³ C) | 128(¹⁵ N) | 1024 (¹³ C) | 69 | 34 | 30 | 8 | 0.80 |
| (HCA)COCON | 108 (¹³ C) | 128 (¹⁵ N) | 1024 (¹³ C) | 12 | 35 | 30 | 8 | 1.6 |
| ^a number of acquired scans | | | | | | | | |
| ^b relaxation delay in seconds | | | | | | | | |

Supplementary Table S2. Chemical shift (ppm) values for assigned residues of NiV PNT (aa 1-406) in 10 mM sodium phosphate buffer, pH 6.5, supplemented with 5 mM EDTA and 5 mM DTT at 288 K. ^1H resonances were calibrated with respect to the signal of 2,2-dimethylsilapentane-5-sulfonic acid (DSS). ^{13}C chemical shifts were referred to external DSS. ^{15}N chemical shifts were referred indirectly to the ^{13}C standard using the conversion factor derived from the ratio of NMR frequencies [9].

| Number | Type | H^{N} | N | C^{α} | C^{β} | C' |
|--------|------|-----------------------|---------|---------------------|--------------------|-------------|
| 2 | ASP | | | 54.28 | 41.361 | 175.708 |
| 3 | LYS | 8.442 | 122.574 | 56.413 | 32.901 | 176.375 |
| 4 | LEU | 8.364 | 124.439 | 55.136 | 42.051 | 177.295 |
| 5 | GLU | 8.389 | 122.708 | 56.187 | 30.119 | 176.175 |
| 6 | LEU | 8.389 | 123.935 | 54.96 | 42.217 | 177.281 |
| 7 | VAL | 8.147 | 121.906 | 62.253 | 32.653 | 175.97 |
| 8 | ASN | 8.566 | 123.424 | 52.81 | 38.905 | 174.984 |
| 9 | ASP | 8.354 | 121.881 | 54.531 | 40.954 | 176.829 |
| 10 | GLY | 8.351 | 109.211 | 45.541 | // | 174.413 |
| 11 | LEU | 8.024 | 121.695 | 55.304 | 42.398 | 177.189 |
| 12 | ASN | 8.523 | 120.187 | 53.115 | 38.681 | 175.206 |
| 13 | ILE | 8.116 | 122.14 | 61.464 | 37.802 | 176.434 |
| 28 | TYR | | | 57.809 | 38.751 | 176.383 |
| 29 | GLY | 8.33 | 110.865 | 45.188 | // | 174.11 |
| 30 | ARG | 8.189 | 121.072 | 55.965 | 30.725 | 176.561 |
| 31 | SER | 8.447 | 117.458 | 58.295 | 63.755 | 174.65 |
| 32 | SER | 8.365 | 118.503 | 58.114 | 63.675 | 174.439 |
| 33 | ILE | 8.075 | 122.448 | 61.065 | 38.431 | 176.188 |
| 34 | GLN | 8.381 | 124.958 | 55.45 | 29.448 | 175.584 |
| 35 | GLN | 8.441 | 123.814 | 53.63 | 28.727 | 173.924 |
| 36 | PRO | // | 137.762 | 63.004 | 31.969 | 176.799 |
| 37 | SER | 8.512 | 116.99 | 58.12 | 63.879 | 174.891 |
| 38 | ILE | 8.25 | 123.527 | 61.297 | 38.488 | 176.108 |
| 39 | LYS | 8.233 | 125.953 | 55.974 | 32.744 | 175.928 |
| 40 | ASP | 8.19 | 124.36 | 53.578 | 41.887 | 174.951 |
| 50 | GLN | | | 55.797 | 28.988 | 176.216 |
| 51 | CYS | 8.251 | 120.433 | 58.71 | 28.988 | 175.145 |
| 52 | THR | 8.243 | 116.528 | 61.724 | 69.66 | 174.744 |
| 53 | SER | 8.322 | 118.652 | 58.433 | 63.755 | 175.115 |
| 54 | GLY | 8.434 | 111.549 | 45.136 | // | 174.328 |
| 55 | GLU | 8.301 | 121.182 | 56.599 | 30.209 | 176.802 |
| 56 | SER | 8.388 | 117.207 | 58.48 | 63.82 | 174.581 |
| 57 | GLU | 8.442 | 123.256 | 56.548 | 30.092 | 176.422 |
| 58 | GLN | 8.396 | 122.26 | 55.494 | 29.182 | 175.944 |
| 59 | VAL | 8.244 | 122.538 | 62.016 | 32.775 | 176.366 |
| 60 | GLU | 8.612 | 125.912 | 56.769 | 29.974 | 177.126 |
| 61 | GLY | 8.559 | 111.586 | 45.352 | // | 174.837 |
| 62 | GLY | 8.304 | 109.203 | 45.208 | // | 174.204 |

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|-----|-----|-------|---------|--------|--------|---------|
| 63 | MET | 8.262 | 120.25 | 55.294 | 32.929 | 176.391 |
| 64 | SER | 8.467 | 118.256 | 58.236 | 63.705 | 174.638 |
| 65 | LYS | 8.489 | 124.246 | 56.245 | 33.084 | 182.359 |
| 66 | ASP | | 122.234 | 54.163 | 41.216 | 176.104 |
| 67 | ASP | 8.299 | 122.051 | 54.539 | 40.991 | 177.092 |
| 68 | GLY | 8.433 | 109.548 | 45.52 | // | 174.322 |
| 69 | ASP | 8.233 | 121.339 | 54.441 | 40.969 | 176.87 |
| 70 | VAL | 8.012 | 120.993 | 63.215 | 32.26 | 176.789 |
| 71 | GLU | 8.385 | 123.271 | 57.19 | 29.627 | 177.111 |
| 72 | ARG | 8.184 | 122.315 | 56.583 | 30.127 | 182.756 |
| 73 | ARG | | 122.199 | 56.473 | 30.554 | 176.481 |
| 74 | ASN | 8.468 | 119.99 | 53.402 | 38.337 | 175.743 |
| 75 | LEU | 8.209 | 122.931 | 55.915 | 41.952 | 177.977 |
| 76 | GLU | 8.298 | 121.069 | 56.82 | 30.046 | 176.498 |
| 77 | ASP | 8.241 | 121.499 | 54.525 | 41.028 | 176.729 |
| 78 | LEU | 8.254 | 123.868 | 55.469 | 41.971 | 178.059 |
| 79 | SER | 8.317 | 116.578 | 59.127 | 63.656 | 174.955 |
| 80 | SER | 8.211 | 117.849 | 58.34 | 63.375 | 174.85 |
| 81 | THR | 8.111 | 115.844 | 61.47 | 69.597 | 174.487 |
| 82 | SER | 8.332 | 120.306 | 56.297 | 63.398 | 172.887 |
| 83 | PRO | // | 138.777 | 63.239 | 32.057 | 177.483 |
| 84 | THR | 8.273 | 113.976 | 61.61 | 69.423 | 174.658 |
| 85 | ASP | 8.226 | 123.041 | 54.233 | 41.078 | 176.925 |
| 86 | GLY | 8.425 | 110.271 | 45.575 | // | 174.758 |
| 87 | THR | 8.162 | 114.355 | 62.251 | 69.569 | 175.008 |
| 88 | ILE | 8.102 | 123.563 | 61.341 | 38.479 | 176.862 |
| 89 | GLY | 8.465 | 113.381 | 45.229 | // | 173.91 |
| 90 | LYS | 8.093 | 121.528 | 55.885 | 33.148 | 176.506 |
| 91 | ARG | 8.413 | 123.779 | 55.903 | 30.882 | 176.346 |
| 92 | VAL | 8.312 | 122.73 | 62.031 | 32.444 | 176.147 |
| 93 | SER | 8.425 | 120.081 | 57.842 | 63.784 | 174.248 |
| 94 | ASN | 8.562 | 121.952 | 53.026 | 38.694 | 175.427 |
| 95 | THR | 8.141 | 114.825 | 61.859 | 69.497 | 174.541 |
| 96 | ARG | 8.297 | 123.397 | 55.901 | 30.52 | 175.879 |
| 97 | ASP | 8.276 | 122.047 | 54.167 | 40.873 | 176.008 |
| 98 | TRP | 7.982 | 122.191 | 57.283 | 29.406 | 175.815 |
| 99 | ALA | 7.981 | 126.156 | 52.146 | 19.395 | 177.258 |
| 100 | GLU | 8.132 | 120.87 | 56.836 | 30.019 | 177.123 |
| 101 | GLY | 8.441 | 111.21 | 45.364 | // | 174.334 |
| 102 | SER | 8.133 | 115.975 | 58.149 | 63.729 | 174.402 |
| 103 | ASP | | 122.637 | 54.237 | 41.132 | 175.987 |
| 104 | ASP | | 121.228 | 54.21 | 40.965 | 176.102 |
| 105 | ILE | 7.986 | 121.751 | 61.046 | 38.75 | 176.063 |
| 106 | GLN | 8.446 | 125.596 | 55.073 | 29.221 | 181.626 |
| 107 | LEU | | 125.209 | 54.615 | 42.472 | 176.888 |
| 108 | ASP | 8.358 | 123.461 | 52.441 | 40.517 | 174.337 |

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|-----|-----|-------|---------|--------|--------|---------|
| 109 | PRO | // | 136.753 | 62.929 | 31.973 | 176.774 |
| 110 | VAL | 8.235 | 121.564 | 62.47 | 32.349 | 176.515 |
| 111 | VAL | 8.291 | 125.514 | 62.194 | 32.596 | 176.31 |
| 112 | THR | 8.219 | 118.719 | 61.523 | 69.76 | 174.079 |
| 113 | ASP | 8.291 | 123.727 | 54.184 | 41.058 | 175.988 |
| 114 | VAL | 8.063 | 121.424 | 62.286 | 32.505 | 175.825 |
| 115 | VAL | 8.093 | 124.952 | 61.953 | 32.665 | 175.534 |
| 116 | TYR | 8.332 | 125.489 | 57.716 | 38.686 | 175.382 |
| 117 | HIS | 8.18 | 122.235 | 54.912 | 29.933 | 173.766 |
| 118 | ASP | | 122.463 | 54.197 | 40.977 | 176.189 |
| 119 | HIS | | 120.293 | 55.715 | 29.092 | 175.43 |
| 120 | GLY | | 110.422 | 45.644 | // | 174.805 |
| 121 | GLY | 8.337 | 109.628 | 45.128 | // | 174.298 |
| 122 | GLU | 8.378 | 121.141 | 56.562 | 30.035 | 176.717 |
| 123 | CYS | 8.495 | 120.86 | 58.416 | 27.696 | 174.899 |
| 124 | THR | 8.195 | 116.622 | 61.906 | 69.593 | 174.995 |
| 125 | GLY | 8.323 | 111.484 | 45.006 | // | 173.84 |
| 126 | TYR | 8.107 | 120.694 | 58.131 | 38.632 | 176.408 |
| 127 | GLY | 8.298 | 111.183 | 45.086 | // | 173.776 |
| 128 | PHE | 8.004 | 120.424 | 57.757 | 39.569 | 176.018 |
| 129 | THR | 8.134 | 116.324 | 61.441 | 69.839 | 174.074 |
| 130 | SER | 8.271 | 118.775 | 57.984 | 63.801 | 174.043 |
| 131 | SER | 8.321 | 119.125 | 57.208 | 63.365 | 172.969 |
| 132 | PRO | // | 138.58 | 63.552 | 31.971 | 177.151 |
| 133 | GLU | | 121.107 | 56.692 | 29.715 | 176.739 |
| 134 | ARG | | 121.976 | 56.188 | 30.518 | 176.75 |
| 135 | GLY | 8.345 | 110.23 | 45.062 | // | 173.987 |
| 136 | TRP | 8.044 | 121.536 | 57.453 | 29.54 | 176.496 |
| 137 | SER | 8.047 | 117.617 | 58.185 | 63.917 | 173.765 |
| 138 | ASP | 8.092 | 122.307 | 54.197 | 40.889 | 176.225 |
| 139 | TYR | 8.118 | 121.266 | 58.319 | 38.378 | 176.408 |
| 140 | THR | 8.029 | 115.609 | 61.747 | 69.603 | 174.747 |
| 141 | SER | 8.205 | 118.459 | 58.505 | 63.51 | 175.212 |
| 142 | GLY | 8.32 | 111.424 | 45.369 | // | 174.075 |
| 143 | ALA | 8.091 | 124.024 | 52.638 | 19.115 | 177.698 |
| 144 | ASN | 8.421 | 117.972 | 53.21 | 38.677 | 175.158 |
| 145 | ASN | 8.329 | 119.571 | 53.112 | 38.572 | 175.775 |
| 146 | GLY | 8.371 | 109.267 | 45.449 | // | 174.003 |
| 147 | ASN | 8.237 | 119.241 | 53.204 | 38.857 | 175.255 |
| 148 | VAL | 8.081 | 120.933 | 62.161 | 32.721 | 175.884 |
| 149 | CYS | 8.468 | 124.257 | 58.321 | 27.867 | 174.393 |
| 150 | LEU | 8.423 | 126.314 | 55.016 | 42.172 | 177.312 |
| 151 | VAL | 8.158 | 121.967 | 62.078 | 32.816 | 176.156 |
| 152 | SER | 8.361 | 120.016 | 58.232 | 63.87 | 174.325 |
| 153 | ASP | 8.281 | 123.517 | 54.108 | 41.092 | 176.307 |
| 154 | ALA | 8.244 | 125.15 | 53.019 | 18.777 | 178.278 |

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|-----|-----|-------|---------|--------|--------|---------|
| 155 | LYS | 8.258 | 120.081 | 56.431 | 32.591 | 176.994 |
| 156 | MET | | 120.976 | 55.322 | 32.37 | 176.359 |
| 157 | LEU | 8.138 | 123.547 | 55.142 | 42.129 | 177.225 |
| 158 | SER | 8.1 | 116.395 | 58.113 | 63.737 | 173.799 |
| 159 | TYR | 8.076 | 122.731 | 57.409 | 38.85 | 174.841 |
| 160 | ALA | 8.129 | 128.213 | 49.979 | 18.424 | 174.8 |
| 161 | PRO | // | 135.873 | 62.732 | 32.018 | 176.89 |
| 162 | GLU | 8.544 | 121.5 | 56.592 | 30.003 | 176.534 |
| 163 | ILE | 8.147 | 123.078 | 60.825 | 38.609 | 175.797 |
| 164 | ALA | 8.368 | 129.433 | 52.284 | 19.142 | 177.495 |
| 165 | VAL | 8.157 | 120.831 | 61.982 | 32.787 | 176.286 |
| 166 | SER | 8.52 | 121.029 | 57.819 | 63.919 | 174.625 |
| 167 | LYS | 8.541 | 124.676 | 56.553 | 32.953 | 182.756 |
| 168 | GLU | | 122.028 | 56.938 | 29.824 | 176.417 |
| 169 | ASP | 8.333 | 122.327 | 54.431 | 40.982 | 176.362 |
| 170 | ARG | 8.246 | 121.621 | 56.839 | 30.41 | 176.738 |
| 171 | GLU | 8.484 | 122.042 | 56.968 | 29.889 | 177.057 |
| 172 | THR | 8.073 | 114.959 | 62.256 | 69.552 | 174.429 |
| 173 | ASP | 8.304 | 123.177 | 54.472 | 40.945 | 176.351 |
| 174 | LEU | 8.116 | 122.536 | 55.469 | 42.151 | 177.748 |
| 175 | VAL | 7.939 | 120.558 | 62.556 | 32.457 | 182.359 |
| 176 | HIS | | 122.481 | 56.173 | 30.088 | 176.182 |
| 177 | LEU | 8.227 | 123.961 | 55.406 | 42.204 | 177.409 |
| 178 | GLU | 8.499 | 134.621 | 56.554 | 29.971 | 176.395 |
| 179 | ASN | 8.405 | 120.443 | 53.228 | 38.705 | 175.348 |
| 180 | LYS | 8.294 | 122.531 | 56.413 | 32.76 | 176.739 |
| 181 | LEU | 8.253 | 123.128 | 55.14 | 42.102 | 177.676 |
| 182 | SER | 8.3 | 116.992 | 58.095 | 63.522 | 175.206 |
| 183 | THR | 8.252 | 116.02 | 61.556 | 69.29 | 175.067 |
| 184 | THR | 8.101 | 116.057 | 62.007 | 69.558 | 175.195 |
| 185 | GLY | 8.38 | 111.739 | 45.067 | // | 173.865 |
| 186 | LEU | 8.057 | 121.71 | 54.623 | 42.355 | 176.968 |
| 187 | ASN | 8.527 | 121.172 | 51.204 | 38.689 | 173.492 |
| 188 | PRO | // | 137.262 | 63.39 | 32.134 | 177.22 |
| 189 | THR | 8.162 | 114.097 | 61.619 | 69.427 | 174.239 |
| 190 | ALA | 8.145 | 127.195 | 52.154 | 19.266 | 177.361 |
| 191 | VAL | 8.139 | 122.043 | 59.75 | 32.395 | 174.666 |
| 192 | PRO | // | 139.927 | 62.868 | 32.052 | |
| 193 | PHE | | | 58.154 | 39.197 | 175.924 |
| 194 | THR | 7.947 | 116.593 | 61.534 | 69.813 | 173.907 |
| 195 | LEU | 8.123 | 124.993 | 55 | 42.132 | 177.167 |
| 196 | ARG | | 122.315 | 55.824 | 30.569 | 175.788 |
| 197 | ASN | 8.483 | 120.498 | 52.924 | 38.577 | 175.346 |
| 198 | LEU | 8.306 | 123.645 | 55.305 | 41.896 | 177.464 |
| 199 | SER | 8.203 | 116.281 | 58.297 | 63.768 | 173.83 |
| 200 | ASP | 8.227 | 123.903 | 52.066 | 41.146 | 174.637 |

| | | | | | | |
|-----|-----|-------|---------|--------|--------|---------|
| 201 | PRO | // | 138.145 | 63.541 | 32.057 | 177.106 |
| 202 | ALA | 8.36 | 123.379 | 52.362 | 18.723 | 178.252 |
| 203 | LYS | 8.041 | 120.228 | 56.301 | 32.941 | 176.411 |
| 204 | ASP | 8.206 | 121.126 | 54.148 | 41.014 | 175.918 |
| 205 | SER | 8.128 | 117.61 | 56.399 | 63.239 | 172.63 |
| 206 | PRO | // | 138.517 | 62.91 | 31.969 | 176.778 |
| 207 | VAL | | 121.35 | 62.453 | 32.429 | 176.308 |
| 208 | ILE | 8.242 | 126.511 | 60.554 | 38.278 | 175.849 |
| 209 | ALA | 8.36 | 129.238 | 52.332 | 19.222 | 177.484 |
| 210 | GLU | 8.321 | 120.645 | 56.528 | 30.149 | 176.248 |
| 211 | HIS | | 119.796 | 55.277 | 29.83 | 174.076 |
| 212 | TYR | 8.12 | 122.285 | 57.706 | 38.72 | 175.408 |
| 213 | TYR | 8.227 | 123.021 | 57.803 | 38.661 | 176.068 |
| 214 | GLY | 7.733 | 109.975 | 45.072 | // | 173.918 |
| 215 | LEU | 8.105 | 121.831 | 55.214 | 42.176 | 178.114 |
| 216 | GLY | 8.497 | 110.534 | 45.13 | // | 174.137 |
| 217 | VAL | 7.925 | 120.037 | 62.28 | 32.502 | 176.389 |
| 218 | LYS | 8.42 | 125.601 | 56.192 | 32.93 | 176.609 |
| 219 | GLU | 8.42 | 122.815 | 56.832 | 30.151 | 176.342 |
| 220 | GLN | 8.384 | 121.653 | 55.771 | 29.441 | 175.633 |
| 221 | ASN | 8.539 | 120.656 | 53.27 | 38.805 | 174.975 |
| 222 | VAL | 8.118 | 120.234 | 62.007 | 32.77 | 176.279 |
| 223 | GLY | 8.337 | 112.992 | 44.404 | // | 171.87 |
| 224 | PRO | // | 134.827 | 63.163 | 31.958 | 177.368 |
| 225 | GLN | 8.643 | 121.26 | 55.782 | 29.262 | 176.419 |
| 226 | THR | 8.19 | 115.827 | 61.866 | 69.78 | 174.662 |
| 227 | SER | 8.355 | 118.693 | 58.325 | 63.645 | 174.438 |
| 228 | ARG | 8.366 | 123.369 | 55.907 | 30.727 | 175.904 |
| 229 | ASN | 8.481 | 120.856 | 53.055 | 38.566 | 175.292 |
| 230 | VAL | 8.11 | 120.821 | 62.247 | 32.704 | 175.725 |
| 231 | ASN | 8.485 | 122.351 | 53.13 | 38.61 | 175.54 |
| 232 | LEU | 8.284 | 123.655 | 55.533 | 42.087 | 177.467 |
| 233 | ASP | | 120.594 | 54.73 | 40.903 | 176.556 |
| 234 | SER | 8.039 | 115.772 | 58.502 | 63.843 | 174.554 |
| 235 | ILE | 7.957 | 122.749 | 61.256 | 38.502 | 176.443 |
| 236 | LYS | | 125.929 | 56.171 | 32.783 | 175.947 |
| 237 | LEU | | 124.132 | 54.907 | 42.494 | 176.799 |
| 238 | TYR | 8.189 | 121.293 | 57.449 | 38.949 | 175.831 |
| 239 | THR | 8.178 | 116.371 | 61.064 | 70.108 | 174.297 |
| 240 | SER | 8.372 | 118.267 | 58.283 | 63.864 | 174.407 |
| 241 | ASP | 8.446 | 122.59 | 54.318 | 41.053 | 175.912 |
| 242 | ASP | 8.216 | 120.929 | 54.193 | 40.898 | 176.093 |
| 243 | GLU | | 115.527 | 56.736 | 30.163 | 176.859 |
| 244 | GLU | 8.362 | 121.914 | 56.55 | 29.963 | 176.555 |
| 245 | ALA | 8.194 | 125.165 | 52.662 | 19.224 | 177.8 |
| 246 | ASP | 8.295 | 119.971 | 54.435 | 40.834 | 176.377 |

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|-----|-----|-------|---------|--------|--------|---------|
| 247 | GLN | 8.237 | 120.773 | 55.638 | 29.159 | 175.973 |
| 248 | LEU | 8.219 | 123.532 | 55.381 | 42.183 | 175.98 |
| 249 | GLU | | 121.615 | 56.592 | 30.067 | 176.245 |
| 250 | PHE | 8.12 | 120.831 | 57.649 | 39.701 | 176.345 |
| 251 | GLU | | 123.087 | 56.241 | 30.433 | 175.879 |
| 252 | ASP | 8.36 | 122.361 | 54.18 | 41.256 | 176.558 |
| 253 | GLU | 8.494 | 122.68 | 57.046 | 29.876 | 176.421 |
| 254 | PHE | 8.299 | 120.735 | 57.481 | 38.972 | 175.876 |
| 255 | ALA | 8.049 | 126.075 | 52.907 | 19.009 | 178.168 |
| 256 | GLY | 8.013 | 108.329 | 45.283 | // | 174.31 |
| 257 | SER | 8.199 | 116.132 | 58.444 | 64.075 | 174.836 |
| 258 | SER | 8.469 | 118.473 | 58.391 | 63.839 | 174.702 |
| 259 | SER | 8.359 | 118.399 | 58.316 | 63.747 | 174.362 |
| 260 | GLU | 8.345 | 123.4 | 56.413 | 30.456 | 176.191 |
| 261 | VAL | 8.19 | 122.998 | 62.454 | 32.674 | 175.871 |
| 262 | ILE | 8.361 | 127.308 | 60.648 | 38.301 | 176.184 |
| 263 | VAL | 8.348 | 126.627 | 62.079 | 32.587 | 176.428 |
| 264 | GLY | 8.466 | 113.609 | 45.007 | // | 173.625 |
| 265 | ILE | 8.038 | 120.671 | 60.661 | 39.021 | 176.301 |
| 266 | SER | 8.644 | 122.987 | 56.287 | 63.387 | 172.987 |
| 267 | PRO | // | 138.655 | 63.565 | 31.962 | 177.398 |
| 268 | GLU | 8.536 | 120.422 | 56.898 | 29.787 | 176.473 |
| 269 | ASP | 8.185 | 121.131 | 54.48 | 41.265 | 176.1 |
| 270 | GLU | 8.103 | 121.375 | 56.026 | 30.788 | 176.267 |
| 271 | GLU | 8.46 | 124.449 | 54.247 | 29.68 | 174.751 |
| 272 | PRO | // | 138.513 | 63.119 | 31.871 | 177.237 |
| 273 | SER | 8.505 | 116.413 | 58.255 | 63.576 | 174.978 |
| 274 | SER | 8.367 | 118.604 | 58.161 | 63.639 | 174.779 |
| 275 | VAL | 8.135 | 121.976 | 62.438 | 32.359 | 176.93 |
| 276 | GLY | 8.5 | 113.043 | 45.147 | // | 174.69 |
| 277 | GLY | 8.219 | 109.11 | 45.031 | // | 173.825 |
| 278 | LYS | 8.305 | 122.451 | 53.918 | 32.54 | 174.397 |
| 279 | PRO | // | 137.988 | 63.078 | 31.978 | 176.878 |
| 280 | ASN | 8.6 | 119.42 | 53.381 | 38.541 | 175.537 |
| 281 | GLU | 8.404 | 122.217 | 56.565 | 30.215 | 176.547 |
| 282 | SER | 8.383 | 117.274 | 58.352 | 63.567 | 174.74 |
| 283 | ILE | 8.062 | 123.031 | 61.51 | 38.573 | 176.892 |
| 284 | GLY | 8.49 | 113.129 | 45.253 | // | 174.012 |
| 285 | ARG | 8.123 | 121.187 | 55.895 | 31.165 | 176.542 |
| 286 | THR | 8.325 | 117.044 | 61.922 | 69.972 | 174.632 |
| 287 | ILE | 8.352 | 124.31 | 61.107 | 38.227 | 176.442 |
| 288 | GLU | 8.567 | 125.934 | 56.889 | 29.936 | 177.205 |
| 289 | GLY | 8.497 | 110.783 | 45.439 | // | 174.398 |
| 290 | GLN | 8.173 | 120.418 | 55.934 | 29.487 | 176.185 |
| 291 | SER | 8.456 | 117.814 | 58.628 | 63.564 | 174.811 |
| 292 | ILE | 8.183 | 123.425 | 61.611 | 38.451 | 176.599 |

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|-----|-----|-------|---------|--------|--------|---------|
| 293 | ARG | 8.296 | 124.815 | 56.477 | 30.804 | 176.301 |
| 294 | ASP | 8.266 | 121.597 | 54.505 | 40.947 | 176.235 |
| 295 | ASN | 8.324 | 119.432 | 53.37 | 38.471 | 175.657 |
| 296 | LEU | 8.222 | 122.403 | 55.598 | 41.725 | 177.737 |
| 297 | GLN | 8.221 | 120.662 | 55.717 | 29.142 | 175.956 |
| 298 | ALA | 8.209 | 125.683 | 52.578 | 19.025 | 177.973 |
| 299 | LYS | 8.268 | 120.942 | 56.287 | 32.899 | 176.389 |
| 300 | ASP | 8.279 | 121.454 | 53.914 | 41.073 | 175.989 |
| 301 | ASN | 8.332 | 120.182 | 53.089 | 38.627 | 175.386 |
| 302 | LYS | 8.347 | 122.053 | 56.266 | 32.864 | 176.951 |
| 303 | SER | 8.374 | 117.573 | 58.363 | 63.514 | 174.965 |
| 304 | THR | 8.181 | 115.721 | 61.521 | 69.42 | 174.268 |
| 305 | ASP | 8.275 | 123.777 | 54.133 | 40.935 | 175.82 |
| 306 | VAL | 8.145 | 122.636 | 59.954 | 32.581 | 174.563 |
| 307 | PRO | // | 140.658 | 63.311 | 31.913 | 177.724 |
| 308 | GLY | 8.545 | 110.626 | 45.027 | // | 173.927 |
| 309 | ALA | 8.13 | 124.251 | 52.218 | 19.635 | 178.011 |
| 310 | GLY | 8.341 | 109.241 | 44.396 | // | 171.878 |
| 311 | PRO | // | 135.131 | 62.888 | 32.075 | 177.451 |
| 312 | LYS | 8.53 | 122.165 | 56.075 | 32.816 | 176.624 |
| 313 | ASP | 8.329 | 122.028 | 54.255 | 41.265 | 176.374 |
| 314 | SER | 8.249 | 117.02 | 58.483 | 63.601 | 174.31 |
| 315 | ALA | 8.307 | 126.509 | 52.637 | 19.096 | 177.747 |
| 316 | VAL | 8.048 | 120.444 | 62.144 | 32.318 | 176.096 |
| 317 | LYS | 8.424 | 126.83 | 55.866 | 33.026 | 176.178 |
| 318 | GLU | | 123.828 | 55.971 | 30.518 | 176.086 |
| 319 | GLU | | 125.158 | 54.116 | 29.75 | 174.056 |
| 320 | PRO | // | 139.197 | 61.246 | 30.654 | 174.812 |
| 321 | PRO | // | 135.805 | 62.852 | 32.126 | 176.885 |
| 322 | GLN | | 121.633 | 55.777 | 29.431 | 176.061 |
| 323 | LYS | | 123.688 | 56.06 | 33.064 | 176.194 |
| 324 | ARG | | 123.635 | 55.638 | 30.928 | 175.959 |
| 325 | LEU | | 126.166 | 55.409 | 41.284 | 174.872 |
| 326 | PRO | // | 138.636 | 63.001 | 31.817 | 176.668 |
| 327 | MET | 8.395 | 120.954 | 55.478 | 33.111 | 176.129 |
| 328 | LEU | 8.299 | 124.244 | 54.885 | 42.33 | 177.107 |
| 329 | ALA | 8.338 | 125.304 | 52.773 | 19.083 | 177.961 |
| 330 | GLU | 8.427 | 120.055 | 56.837 | 30.035 | 176.641 |
| 331 | GLU | 8.293 | 121.607 | 57.258 | 29.999 | 176.252 |
| 332 | PHE | 8.293 | 120.807 | 57.511 | 39.718 | 175.732 |
| 333 | GLU | 8.318 | 122.971 | 56.416 | 30.171 | 176.216 |
| 334 | CYS | 8.418 | 121.018 | 58.283 | 27.958 | 174.819 |
| 335 | SER | 8.575 | 119.309 | 58.65 | 63.71 | 175.203 |
| 336 | GLY | 8.526 | 111.966 | 45.252 | // | 174.29 |
| 337 | SER | 8.183 | 115.84 | 58.538 | 63.919 | 174.546 |
| 338 | GLU | 8.51 | 123.099 | 56.333 | 30.239 | 175.924 |

| | | | | | | |
|-----|-----|-------|---------|--------|--------|---------|
| 339 | ASP | 8.329 | 124.294 | 52.309 | 41.455 | 174.957 |
| 340 | PRO | // | 137.86 | 63.873 | 32.145 | 177.714 |
| 341 | ILE | | 120.437 | 62.092 | 32.785 | |
| 347 | LYS | | | 57.066 | 32.344 | 177.426 |
| 348 | GLU | | 121.531 | 57.156 | 29.793 | 176.922 |
| 349 | ASN | 8.381 | 119.576 | 53.578 | 38.587 | 175.692 |
| 350 | SER | 8.201 | 116.632 | 59.077 | 63.517 | 174.87 |
| 351 | LEU | 8.15 | 123.758 | 55.57 | 41.94 | 177.8 |
| 352 | ILE | 8.15 | 120.115 | 61.369 | 38.281 | 176.266 |
| 353 | ASN | 8.375 | 122.042 | 53.274 | 38.504 | 175.416 |
| 354 | CYS | 8.247 | 119.98 | 58.757 | 27.778 | 174.831 |
| 355 | GLN | 8.463 | 122.809 | 56.061 | 29.038 | 176.025 |
| 356 | GLN | | 121.704 | 56.073 | 29.413 | 176.554 |
| 357 | GLY | | 110.906 | 45.12 | // | 176.553 |
| 358 | LYS | | 121.369 | 56.494 | 32.831 | 176.598 |
| 359 | ASP | | 121.099 | 54.189 | 40.889 | 175.785 |
| 360 | ALA | | 124.36 | 52.205 | 19.143 | 177.426 |
| 361 | GLN | | 121.178 | 53.258 | 28.868 | 173.577 |
| 362 | PRO | // | 139.123 | 61.159 | 30.659 | 174.715 |
| 363 | PRO | // | 135.238 | 61.311 | 30.542 | |
| 367 | SER | | | 58.121 | 63.607 | 174.359 |
| 368 | ILE | 8.16 | 122.844 | 60.766 | 38.684 | 176.047 |
| 369 | GLU | 8.394 | 121.674 | 56.045 | 29.129 | |
| 371 | SER | | | 61.897 | 70.026 | 174.335 |
| 372 | ILE | | 122.611 | 60.71 | 38.706 | 176.069 |
| 373 | SER | | 121.749 | 55.827 | 62.993 | 173.044 |
| 374 | PRO | // | 138.261 | 63.266 | 31.913 | 176.633 |
| 375 | ASP | | 120.308 | 54.029 | 40.826 | 176.37 |
| 376 | LYS | 8.26 | 122.211 | 56.16 | 32.668 | 176.704 |
| 377 | THR | 8.18 | 116.072 | 62.234 | 69.633 | 174.497 |
| 378 | GLU | 8.417 | 124.137 | 56.251 | 30.283 | 176.112 |
| 379 | ILE | 8.244 | 123.608 | 60.887 | 38.202 | 176.38 |
| 380 | VAL | 8.32 | 126.034 | 62.061 | 32.675 | 175.995 |
| 381 | ASN | 8.664 | 123.963 | 53.346 | 38.59 | 175.767 |
| 382 | GLY | 8.402 | 109.942 | 45.222 | // | 173.745 |
| 383 | ALA | 8.064 | 124.1 | 52.191 | 19.337 | 177.781 |
| 384 | VAL | | 120.325 | 62.272 | 32.571 | 176.375 |
| 385 | GLN | 8.578 | 125.355 | 55.493 | 29.494 | 176.174 |
| 386 | THR | 8.238 | 116.61 | 61.775 | 69.659 | 174.576 |
| 387 | ALA | 8.407 | 126.586 | 52.64 | 19.048 | 177.603 |
| 388 | ASP | 8.304 | 119.877 | 54.336 | 40.89 | 176.435 |
| 389 | ARG | 8.171 | 121.551 | 56.063 | 30.367 | 176.272 |
| 390 | GLN | 8.344 | 121.252 | 55.626 | 29.136 | 175.817 |
| 391 | ARG | 8.359 | 124.111 | 53.946 | 29.925 | 174.248 |
| 392 | PRO | // | 138.018 | 63.215 | 32.101 | 177.458 |
| 393 | GLY | 8.561 | 110.186 | 44.986 | // | 174.042 |

| | | | | | | |
|-----|-----|-------|---------|--------|--------|---------|
| 394 | THR | 8.033 | 117.341 | 59.909 | 69.96 | 172.713 |
| 395 | PRO | // | 139.659 | 62.975 | 32.109 | 176.659 |
| 396 | MET | 8.315 | 121.560 | 54.025 | 32.318 | 174.806 |
| 397 | PRO | // | 137.716 | 63.258 | 32.026 | |
| 398 | LYS | | | 56.289 | 32.818 | 176.829 |
| 399 | SER | 8.355 | 117.483 | 58.222 | 63.698 | 174.563 |
| 400 | ARG | 8.487 | 123.745 | 56.05 | 30.658 | 176.627 |
| 401 | GLY | 8.393 | 110.215 | 44.887 | // | |
| 402 | ILE | | | 52.868 | 41.367 | 175.221 |
| 403 | PRO | // | 136.107 | 62.932 | 31.897 | |

Supplementary Table S3. Predicted Short Linear Motifs (SLiMs) with a conservation score ≥ 0.88 as provided by the ELM database (see also **Supplementary Figure S3B**). The full report is available at:

http://elm.eu.org/cgimodel.py?fun=smartResult&userId=QiKRrpLIDz&EXPECT_CUTOFF=100&r=1&bg=on

| SLiM Code | Type | Residues | Conservation Score |
|---------------------|----------|----------|--------------------|
| LIG_WD40_WDRS_VDV_2 | DKEL | 2-6 | 1.00 |
| MOD_GSK3_1 | IQKTYGRS | 24-31 | 1.00 |
| MOD_CK2_1 | GFTSSPE | 127-133 | 1.00 |
| MOD_SUMO_rev_2 | SDAKML | 152-157 | 1.00 |
| LIG_WD40_WDRS_VDV_2 | TTGLNPTA | 183-190 | 0.97 |
| DOC_WW_Pin1_4 | AKDSPY | 202-207 | 1.00 |
| MOD_Pro_Dkin_1 | AKDSPVI | 202-208 | 1.00 |
| DOC_USP7_MATH_1 | AGDSSS | 255-259 | 1.00 |
| DOC_PP2A_B56_1 | LPMLAEE | 325-331 | 1.00 |
| CLV_PCSK_SKI1_1 | RELLK | 343-347 | 0.90 |
| TRG_Pf_PMV_PEXEL_1 | RELLKE | 343-348 | 0.90 |
| MOD_GSK3_1 | YHWSIERS | 364-371 | 0.88 |
| MOD_PIK_1 | IERSISP | 368-374 | 0.97 |
| DOC_WW_Pin1_4 | RSISPD | 370-375 | 1.00 |
| MOD_Pro_Dkin_1 | RSISPK | 370-376 | 1.00 |
| LIG_FHA_1 | DKTEIVN | 375-381 | 0.88 |
| LIG_SH3_3 | RQRPOTP | 389-395 | 1.00 |
| DOC_WW_Pin1_4 | RPGTPM | 391-395 | 1.00 |
| MOD_DYRK1A_RPXSP_1 | RPGTP | 391-395 | 1.00 |
| MOD_Pro_Dkin_1 | RPGTPMP | 391-397 | 1.00 |
| MOD_CDK_CPxxK_3 | RPGTPMPK | 391-398 | 1.00 |
| DOC_CKS1_1 | PGTPMP | 392-397 | 1.00 |

Supplementary Table S4. SAXS data-collection and scattering-derived parameters.

| Data-collection parameters | |
|---|--------------------------|
| Data source and instrument (beamline) | ESRF (BM29) |
| Instrument (detector) | PILATUS 1M |
| Beam geometry (mm ²) | 0.7 x 0.7 |
| Wavelength (Å) | 0.992 |
| Detector distance (m) | 2.847 |
| <i>s</i> range (nm ⁻¹) | 0.028-4.525 |
| Exposure time (sec) | 10 (10 frames x 1.00sec) |
| Concentration (mg ml ⁻¹) | 1.2 |
| Temperature (K) | 293 |
| Structural parameters | |
| <i>I</i> (0) (cm ⁻¹) [from <i>P</i> (<i>r</i>)] | 69.53±0.1 |
| <i>R</i> _g (nm) [from <i>P</i> (<i>r</i>)] | 6.36±0.2 |
| <i>I</i> (0) (cm ⁻¹) [from Guinier approximation] | 69.62±0.7 |
| <i>R</i> _g (nm) [from Guinier approximation] | 6.17±0.12 |
| <i>D</i> _{max} (nm) | 23±1 |
| Molecular-mass determination | |
| Molecular mass <i>M</i> _r (kDa) [from <i>water calibration</i>] | ~47 |
| Calculated monomeric <i>M</i> _r (kDa) [from <i>sequence</i>]* | ~45 |
| Software employed | |
| Primary data reduction | PIPELINE |
| Data processing | ATSAS 3.0.1 |
| Flexibility assessment | EOM 2.0 |

* as obtained using the ProtParam tool of the expasy server (<https://web.expasy.org/protparam/>)

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