

Supplementary Information
Conformational Entropy of Intrinsically
Disordered Proteins from Amino Acid Triads

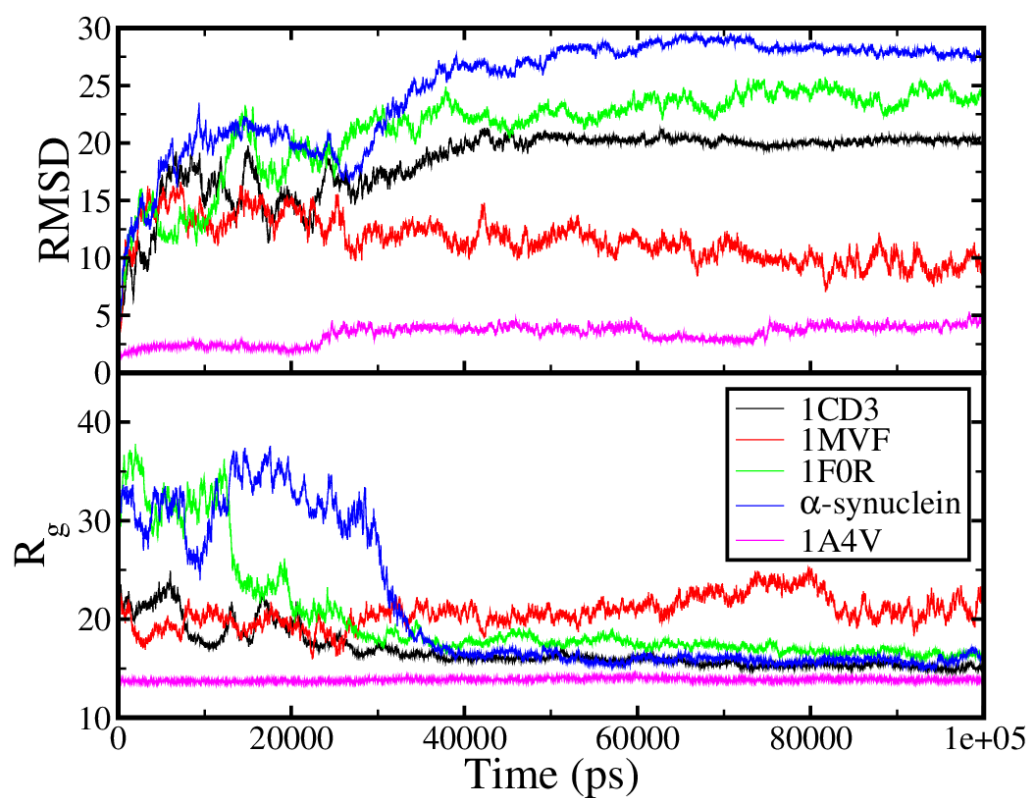
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Department of Chemistry,

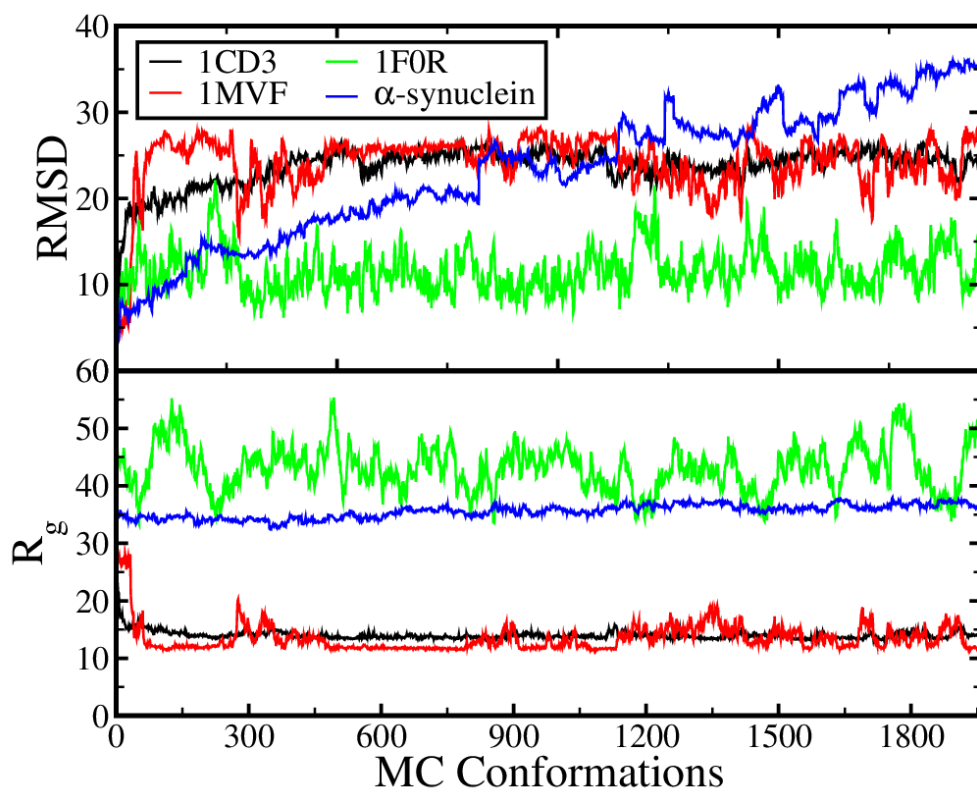
University of Delhi,

Delhi: 110007, India.

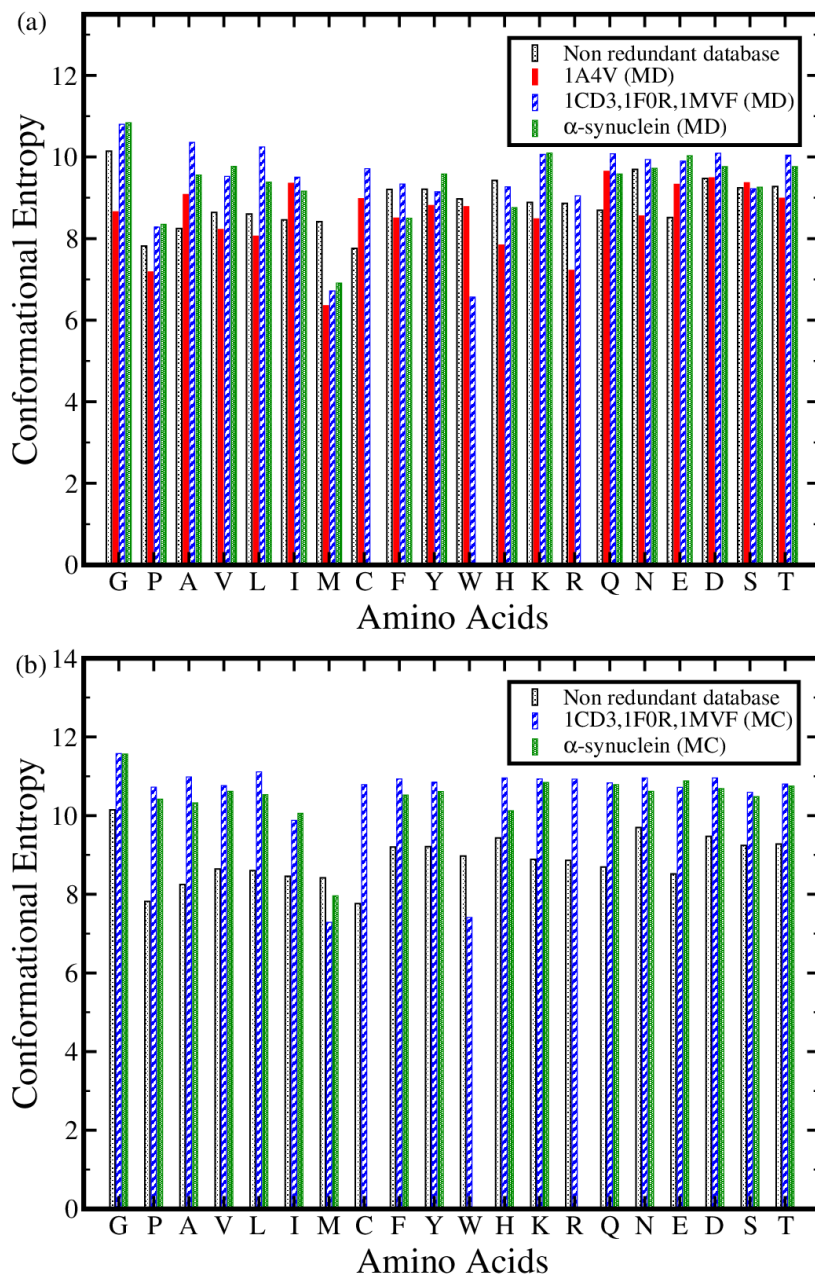
*Email: pbiswas@chemistry.du.ac.in



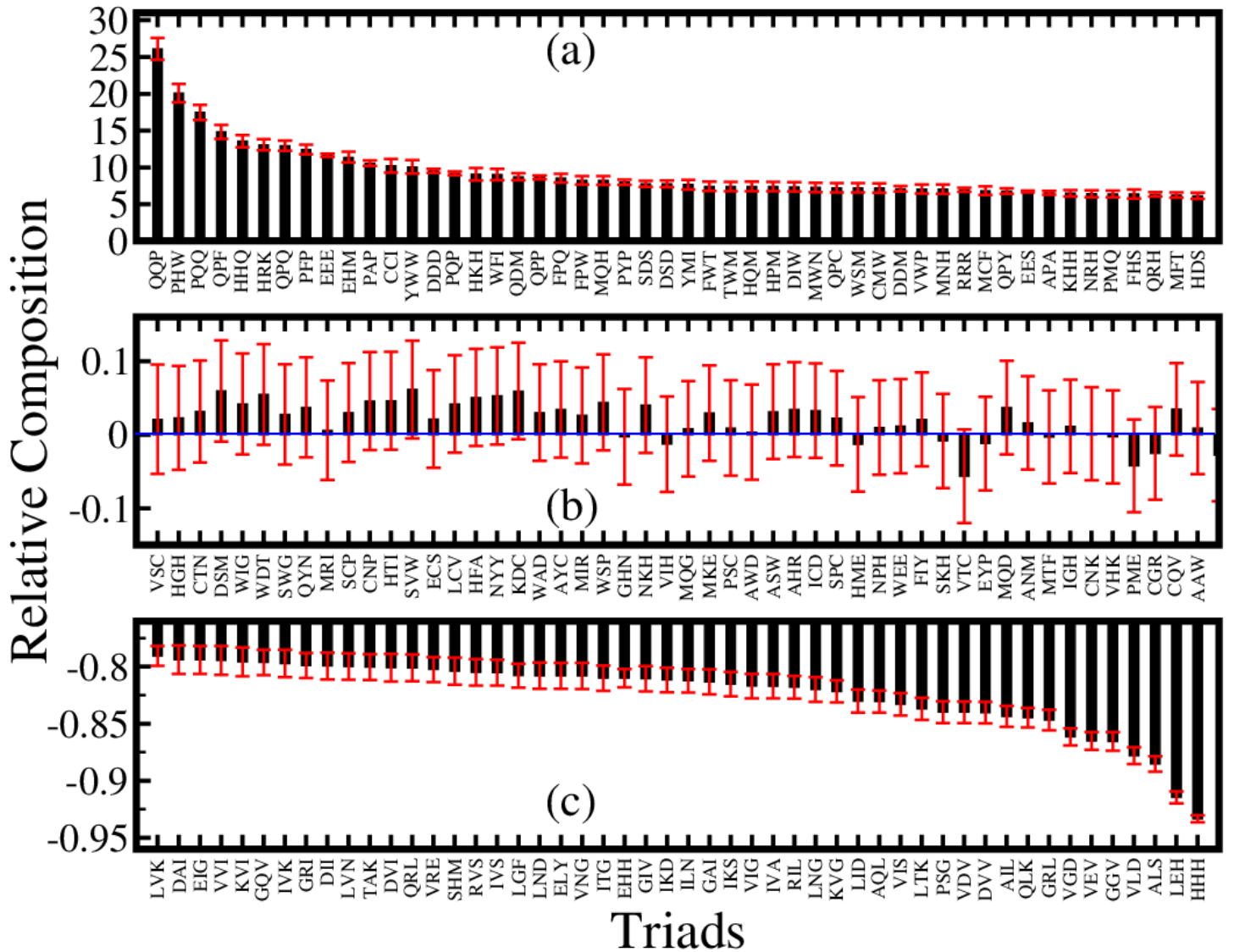
Supplementary Figure S1. RMSD (adapted with permission from DOI:10.1021/jp511961c. Copyright 2015 American Chemical Society.) and Radius of gyration (R_g) as a function of MD simulation time.



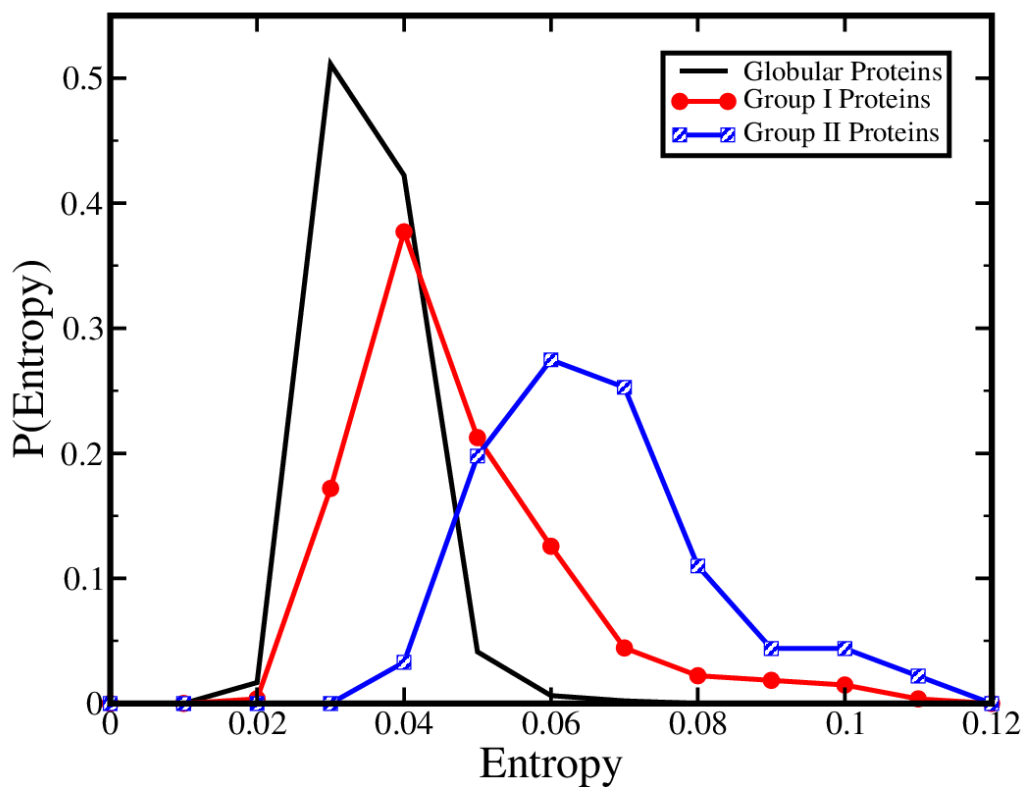
Supplementary Figure S2. RMSD and Radius of gyration (R_g) as a function of MC generated conformations.



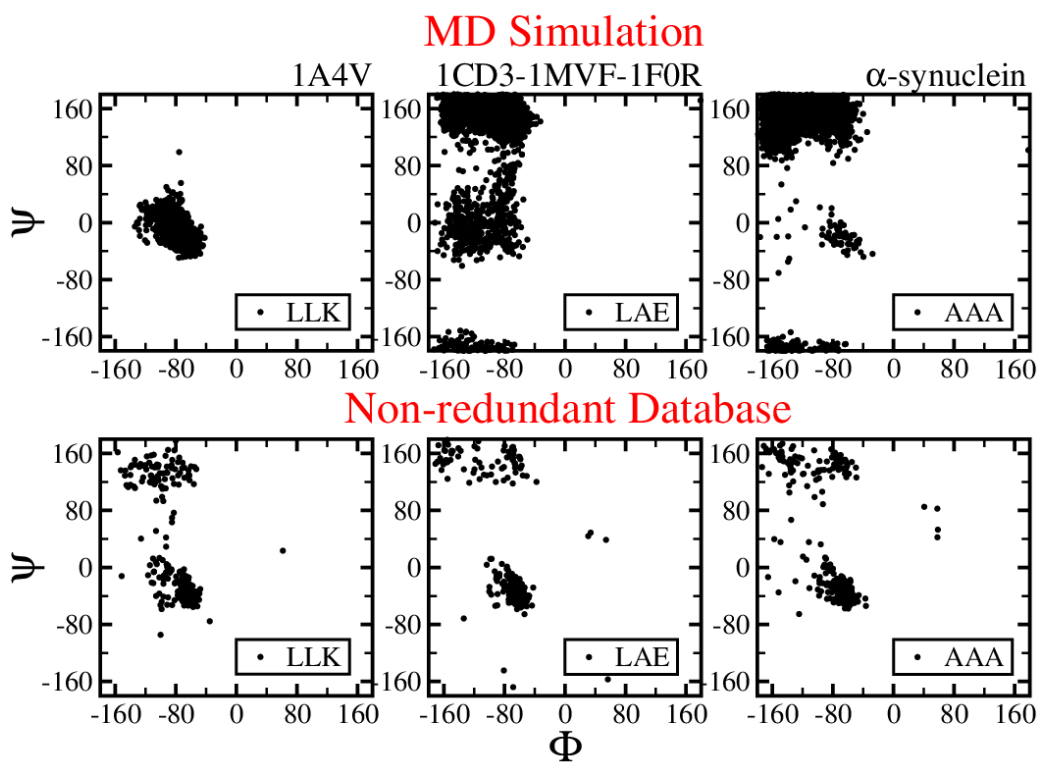
Supplementary Figure S3. Residue-wise conformational entropy for ensembles of (a) Molecular dynamics, (b) Monte Carlo generated conformations.



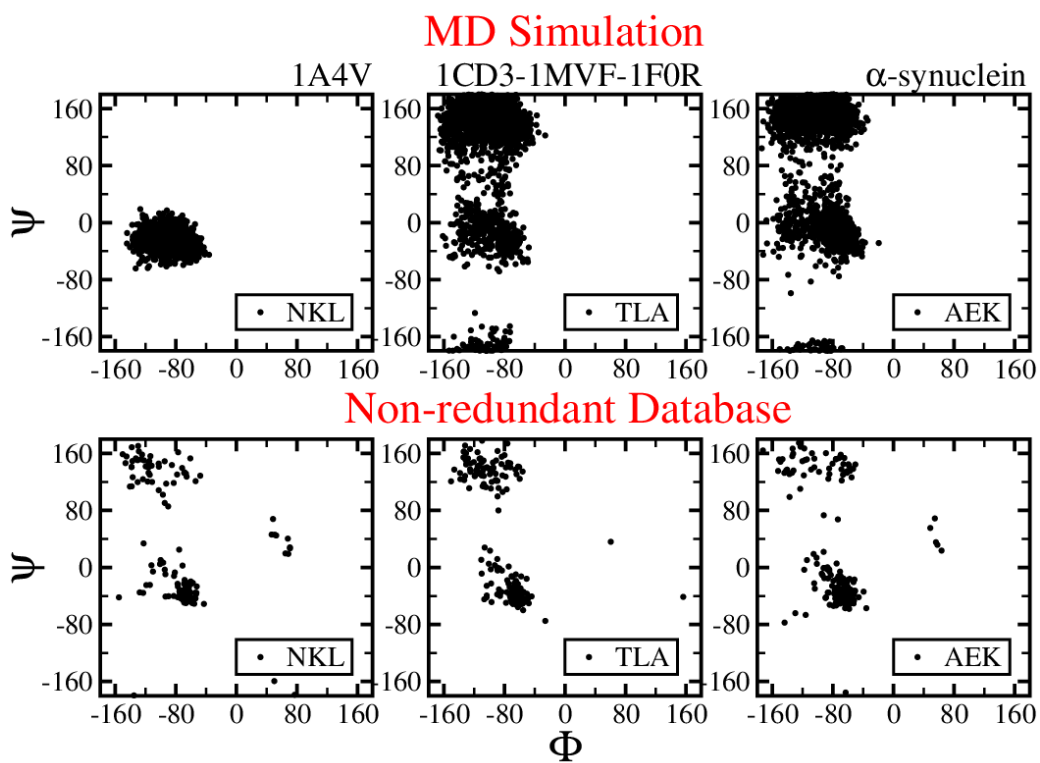
Supplementary Figure S4. The relative composition of (a) top 50 most preferred triads, (b) 50 triads with no clear preference and (c) 50 least preferred triads in Group II proteins w.r.t to the Globular proteins. 99% confidence intervals for 2000 bootstrap resampling iterations are also shown. Out of all possible 8000 triads, 2795 triads are not considered in this analysis of which 2756 triads do not exist only in Group II proteins, 2 triads do not exist only in Globular proteins and 37 triads are not present in both Group II and Globular proteins.



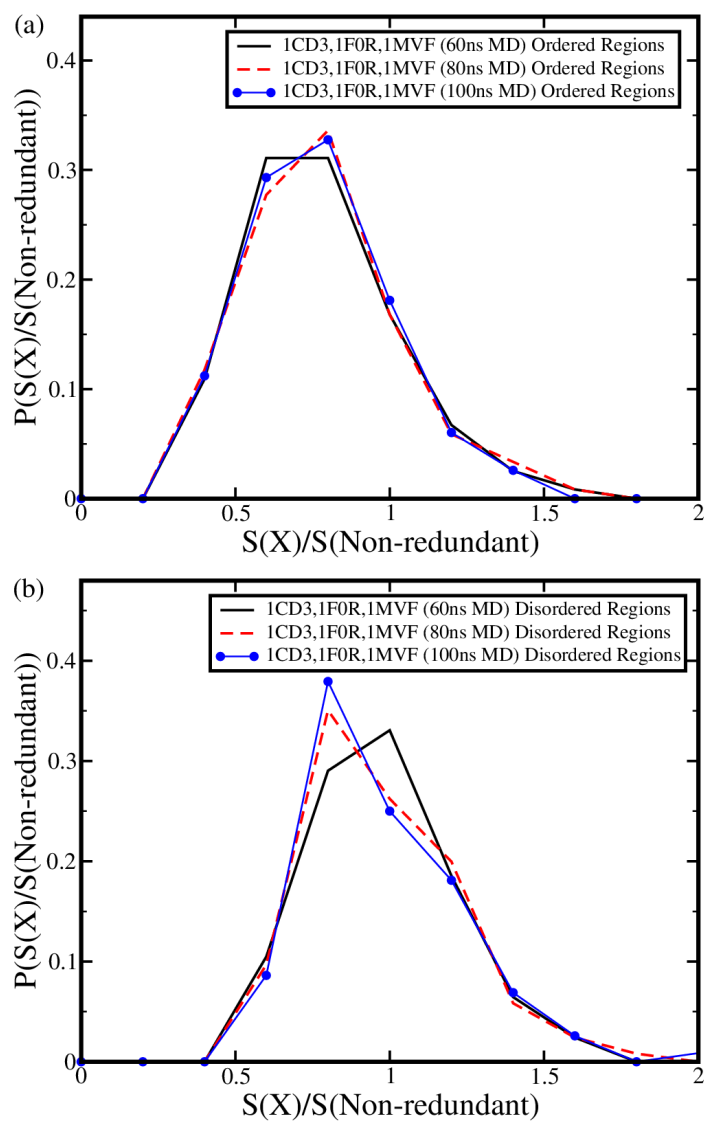
Supplementary Figure S5. Distribution of normalized relative composition calculated using triads of amino acid for data set of globular, Group I and Group II proteins. The globular proteins record the lowest normalized relative composition, while Group II proteins depict the highest value.



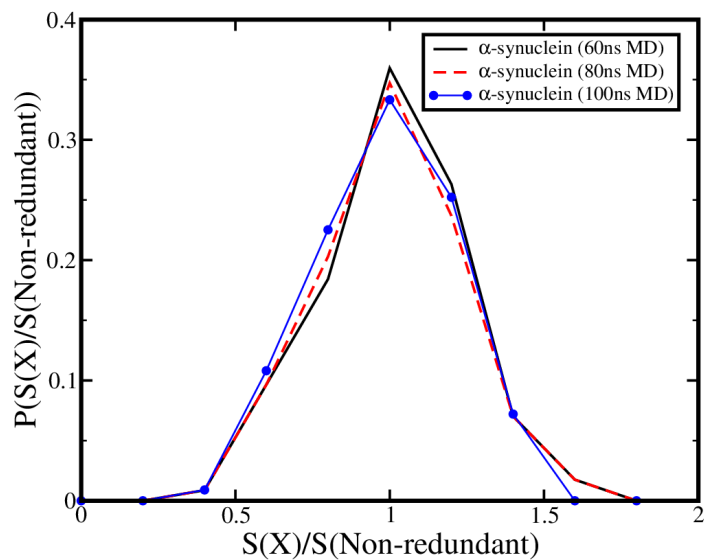
Supplementary Figure S6. $\phi - \psi$ angles of the triad *LLK* in globular (1A4V), *LAE* in IDPRs (1CD3, 1MVF and 1F0R) and *AAA* in IDP (α -synuclein). The $\phi - \psi$ angles are extracted from the MD simulation generated conformational ensemble and non-redundant database.



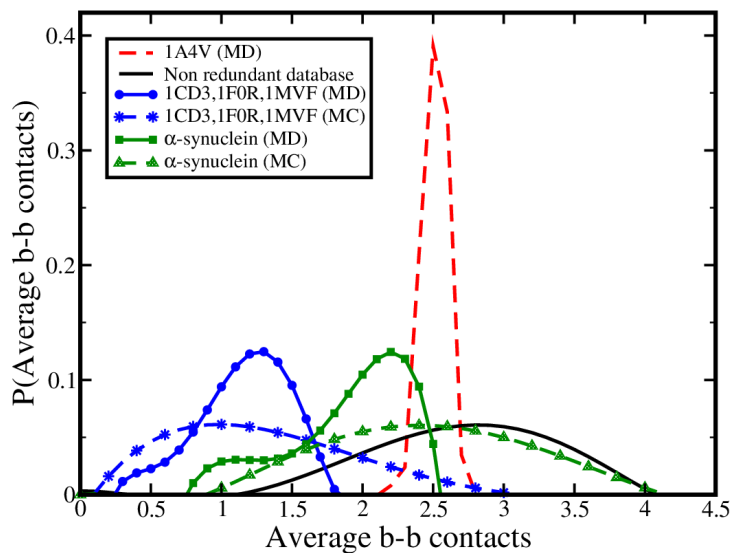
Supplementary Figure S7. $\phi - \psi$ angles of the triad *NKL* in globular (1A4V), *TLA* in IDPRs (1CD3, 1MVF and 1F0R) and *AEK* in IDP (α -synuclein). The $\phi - \psi$ angles are extracted from the MD simulation generated conformational ensemble and non-redundant database.



Supplementary Figure S8. Conformational entropy calculated using triads relative to non-redundant database for Molecular Dynamics generated ensembles of conformation for (a) ordered and (b) disordered regions of partially disordered proteins (1CD3, 1F0R and 1MVF).



Supplementary Figure S9. Conformational entropy calculated using triads relative to non-redundant database for Molecular Dynamics generated ensembles of conformation for α -synuclein.



Supplementary Figure S10. Distribution of average native contacts.

Supplementary Table S1. Selected proteins for MD and MC simulations.

| Protein | PDB ID | Ordered /Disordered | Disordered Residues (Total Residues) | Structure |
|----------------------------|--------|--------------------------|---|---|
| α -lactalbumin | 1A4V | Ordered | — (123) | Extracted from RCSB |
| Scaffolding Protein GPB | 1CD3 | Partially Disordered | 9-60 (120) | Initial template is extracted from RCSB. Disordered region is modeled by MODELLER |
| PemI-like Protein | 1MVF | Partially Disordered | 1-3, 48-82 (82) | Initial template is extracted from RCSB. Disordered region is modeled by MODELLER |
| Human Factor Xa | 1F0R | Partially Disordered | 1-82 (134) | Initial template is extracted from RCSB. Disordered region is modeled by MODELLER |
| α -synuclein | — | Completely Disordered | 1-140 (140) | Complete protein is modeled by MODELLER |

Supplementary Table S2. Relative entropy
 $(= (S(X_1X_2X_3) - S(X_1GX_3)) / S(X_1GX_3))$ of triads $(X_1X_2X_3)$ w.r.t
 X_1GX_3 where entropy of a specific triad is found to be higher than the
entropy of X_1GX_3 .

| Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval | Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval |
|--------|-------------------------------------|------------------------|--------|-------------------------------------|------------------------|
| WVM | 0.48 | 0.157 | WLM | 0.33 | 0.278 |
| HLM | 0.31 | 0.012 | HSM | 0.28 | 0.013 |
| WDM | 0.25 | 0.282 | PNC | 0.24 | 0.011 |
| HHM | 0.24 | 0.021 | HVM | 0.23 | 0.012 |
| HHH | 0.23 | 0.005 | DDK | 0.21 | 0.004 |
| DNK | 0.21 | 0.004 | PLC | 0.21 | 0.012 |
| NNR | 0.20 | 0.005 | PIC | 0.17 | 0.011 |
| DKK | 0.16 | 0.003 | TNC | 0.16 | 0.012 |
| PKC | 0.16 | 0.011 | TEC | 0.16 | 0.011 |
| FEW | 0.16 | 0.008 | NNK | 0.15 | 0.004 |
| NNQ | 0.15 | 0.004 | NDK | 0.15 | 0.004 |
| NDR | 0.14 | 0.004 | PDC | 0.14 | 0.011 |
| DNH | 0.14 | 0.005 | DYK | 0.14 | 0.004 |
| DNT | 0.14 | 0.003 | NNV | 0.13 | 0.003 |
| DFT | 0.13 | 0.003 | DFS | 0.13 | 0.003 |
| DNS | 0.12 | 0.003 | NDV | 0.12 | 0.004 |
| FDW | 0.12 | 0.009 | TAC | 0.12 | 0.009 |
| MDG | 0.12 | 0.005 | DFK | 0.12 | 0.003 |
| FAW | 0.12 | 0.008 | PFD | 0.11 | 0.004 |
| NLH | 0.11 | 0.006 | PVC | 0.11 | 0.011 |
| NSR | 0.11 | 0.005 | CSL | 0.10 | 0.006 |
| DKS | 0.10 | 0.003 | DDT | 0.10 | 0.003 |
| DYS | 0.10 | 0.003 | NTK | 0.10 | 0.004 |
| DSK | 0.10 | 0.003 | DDW | 0.10 | 0.005 |
| FSW | 0.10 | 0.008 | DSS | 0.09 | 0.003 |
| WLH | 0.09 | 0.008 | FNW | 0.09 | 0.009 |
| DTT | 0.09 | 0.003 | NYK | 0.09 | 0.004 |
| DIS | 0.09 | 0.003 | PLD | 0.09 | 0.003 |
| DRS | 0.08 | 0.003 | CDI | 0.08 | 0.005 |
| DYT | 0.08 | 0.003 | MNR | 0.08 | 0.007 |
| DLK | 0.08 | 0.003 | HDM | 0.08 | 0.011 |
| LSC | 0.08 | 0.005 | FDC | 0.08 | 0.007 |
| DNQ | 0.08 | 0.004 | WDI | 0.08 | 0.006 |
| DNR | 0.08 | 0.004 | HDY | 0.08 | 0.006 |
| CDL | 0.07 | 0.005 | TVC | 0.07 | 0.010 |

| Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval | Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval |
|--------|-------------------------------------|------------------------|--------|-------------------------------------|------------------------|
| PAC | 0.07 | 0.011 | VDM | 0.07 | 0.004 |
| DLT | 0.07 | 0.003 | CLP | 0.07 | 0.008 |
| ENQ | 0.07 | 0.004 | DST | 0.07 | 0.003 |
| NSK | 0.07 | 0.004 | TSC | 0.07 | 0.010 |
| DDR | 0.06 | 0.004 | DIT | 0.06 | 0.003 |
| PNE | 0.06 | 0.003 | DYH | 0.06 | 0.005 |
| NLR | 0.06 | 0.004 | NSV | 0.06 | 0.003 |
| TKC | 0.06 | 0.013 | RRC | 0.06 | 0.008 |
| MDY | 0.06 | 0.006 | DTQ | 0.06 | 0.004 |
| CDC | 0.06 | 0.035 | NFK | 0.06 | 0.004 |
| MNG | 0.06 | 0.005 | NFR | 0.05 | 0.004 |
| NNE | 0.05 | 0.004 | NKK | 0.05 | 0.004 |
| DVS | 0.05 | 0.003 | DDS | 0.05 | 0.003 |
| DAT | 0.05 | 0.003 | MDI | 0.05 | 0.005 |
| NRV | 0.05 | 0.003 | PVD | 0.05 | 0.003 |
| DHR | 0.05 | 0.004 | NSQ | 0.04 | 0.004 |
| PFE | 0.04 | 0.003 | DDQ | 0.04 | 0.004 |
| DLH | 0.04 | 0.004 | DQT | 0.04 | 0.004 |
| NLK | 0.04 | 0.003 | NNH | 0.04 | 0.006 |
| PNF | 0.04 | 0.003 | DAS | 0.04 | 0.003 |
| NSM | 0.04 | 0.006 | KNK | 0.04 | 0.002 |
| NKV | 0.04 | 0.003 | NRR | 0.04 | 0.004 |
| DIK | 0.04 | 0.003 | NFH | 0.04 | 0.006 |
| NDN | 0.04 | 0.004 | DTK | 0.04 | 0.003 |
| DVT | 0.04 | 0.003 | DNW | 0.04 | 0.004 |
| MSF | 0.04 | 0.006 | HFM | 0.04 | 0.018 |
| MDE | 0.04 | 0.006 | CSC | 0.04 | 0.036 |
| EDK | 0.04 | 0.003 | NYH | 0.04 | 0.006 |
| DQK | 0.04 | 0.004 | PTD | 0.03 | 0.004 |
| DFR | 0.03 | 0.004 | DVK | 0.03 | 0.003 |
| MAG | 0.03 | 0.005 | PYE | 0.03 | 0.003 |
| PND | 0.03 | 0.004 | DSH | 0.03 | 0.005 |
| HAM | 0.03 | 0.011 | MQG | 0.03 | 0.004 |
| DKT | 0.03 | 0.003 | PNV | 0.03 | 0.003 |
| DAH | 0.03 | 0.005 | SNK | 0.03 | 0.002 |
| MRG | 0.03 | 0.005 | PNA | 0.03 | 0.003 |

| Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval | Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval |
|--------|-------------------------------------|------------------------|--------|-------------------------------------|------------------------|
| MNI | 0.02 | 0.005 | DHK | 0.02 | 0.004 |
| PTC | 0.02 | 0.016 | PDD | 0.02 | 0.004 |
| DCS | 0.02 | 0.004 | NYR | 0.02 | 0.005 |
| DTC | 0.02 | 0.007 | NTR | 0.02 | 0.004 |
| DVR | 0.02 | 0.003 | TNK | 0.02 | 0.003 |
| DWK | 0.02 | 0.004 | ENV | 0.02 | 0.002 |
| DLS | 0.02 | 0.003 | CDP | 0.02 | 0.008 |
| MDF | 0.02 | 0.006 | QNV | 0.02 | 0.003 |
| SHM | 0.02 | 0.005 | DHS | 0.02 | 0.004 |
| LDI | 0.02 | 0.002 | NLQ | 0.02 | 0.004 |
| GNM | 0.01 | 0.004 | CHT | 0.01 | 0.007 |
| HYY | 0.01 | 0.006 | PID | 0.01 | 0.004 |
| PYD | 0.01 | 0.004 | NKQ | 0.01 | 0.004 |
| NAH | 0.01 | 0.006 | PDT | 0.01 | 0.003 |
| DRR | 0.01 | 0.004 | KNE | 0.01 | 0.003 |
| NRH | 0.01 | 0.006 | DRK | 0.01 | 0.004 |
| CSR | 0.01 | 0.007 | DTS | 0.01 | 0.003 |
| ENK | 0.01 | 0.003 | NRK | 0.01 | 0.004 |
| MLG | 0.01 | 0.004 | DVC | 0.01 | 0.005 |
| NIC | 0.01 | 0.007 | HNY | 0.01 | 0.006 |
| YSM | 0.01 | 0.006 | NDQ | 0.01 | 0.004 |
| DYN | 0.01 | 0.003 | NNT | 0.01 | 0.003 |
| MDK | 0.01 | 0.005 | | | |

Supplementary Table S3. Relative entropy
 $(= (S(X_1X_2X_3) - S(X_1GX_3)) / S(X_1GX_3))$ of triads $(X_1X_2X_3)$ which are
least entropic (top 100 triads) w.r.t X_1GX_3 .

| Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval | Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval |
|--------|-------------------------------------|------------------------|--------|-------------------------------------|------------------------|
| HEC | -0.93 | 0.015 | WCL | -0.93 | 0.010 |
| IWM | -0.93 | 0.009 | HMC | -0.93 | 0.015 |
| MEC | -0.93 | 0.015 | NMC | -0.93 | 0.012 |
| QCD | -0.93 | 0.008 | KMW | -0.93 | 0.009 |
| CPW | -0.93 | 0.014 | MRW | -0.94 | 0.012 |
| WYC | -0.94 | 0.051 | QCY | -0.94 | 0.008 |
| WNW | -0.94 | 0.012 | NCC | -0.94 | 0.012 |
| CMP | -0.94 | 0.012 | WCF | -0.94 | 0.011 |
| CYP | -0.94 | 0.011 | FCW | -0.94 | 0.011 |
| KMC | -0.94 | 0.010 | MCQ | -0.94 | 0.011 |
| WMI | -0.95 | 0.010 | WFC | -0.95 | 0.036 |
| CWK | -0.95 | 0.009 | FCC | -0.95 | 0.010 |
| MWI | -0.95 | 0.010 | NWM | -0.95 | 0.010 |
| CCK | -0.95 | 0.010 | MWR | -0.95 | 0.010 |
| MWG | -0.95 | 0.009 | SCM | -0.95 | 0.010 |
| KCM | -0.95 | 0.007 | WCQ | -0.95 | 0.009 |
| NCW | -0.95 | 0.009 | ICW | -0.95 | 0.009 |
| CWE | -0.96 | 0.008 | CMK | -0.96 | 0.008 |
| WWP | -0.96 | 0.009 | SCN | -0.96 | 0.008 |
| EMW | -0.96 | 0.008 | FCM | -0.96 | 0.008 |
| MCT | -0.96 | 0.008 | MHM | -0.96 | 0.008 |
| LMC | -0.96 | 0.008 | TCW | -0.96 | 0.008 |
| SMC | -0.96 | 0.008 | CDH | -0.96 | 0.008 |
| CMG | -0.96 | 0.008 | GMC | -0.96 | 0.007 |
| WEC | -0.96 | 0.033 | WTC | -0.97 | 0.036 |
| WCY | -0.97 | 0.006 | RMW | -0.97 | 0.006 |
| MCF | -0.97 | 0.006 | MQC | -0.97 | 0.011 |
| PWC | -0.97 | 0.009 | WHW | -0.97 | 0.009 |
| WLC | -0.97 | 0.029 | CTM | -0.97 | 0.010 |
| FMM | -0.97 | 0.005 | HPC | -0.97 | 0.009 |
| WSC | -0.97 | 0.030 | CDW | -0.97 | 0.008 |
| MWE | -0.98 | 0.005 | FMC | -0.98 | 0.007 |
| WAW | -0.98 | 0.007 | CPM | -0.98 | 0.008 |
| MCY | -0.98 | 0.007 | HWM | -0.98 | 0.008 |
| HKC | -0.98 | 0.008 | MIM | -0.98 | 0.006 |
| MPW | -0.98 | 0.006 | CEW | -0.98 | 0.007 |

| Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval | Triads | Relative Entropy w.r.t X_1GX_3 | Confidence Interval |
|--------|-------------------------------------|------------------------|--------|-------------------------------------|------------------------|
| CMQ | -0.98 | 0.006 | WCH | -0.98 | 0.006 |
| CCQ | -0.98 | 0.006 | CTC | -0.98 | 0.012 |
| MCV | -0.98 | 0.005 | PWW | -0.98 | 0.005 |
| WWA | -0.98 | 0.005 | CMY | -0.99 | 0.005 |
| QMW | -0.99 | 0.005 | CWG | -0.99 | 0.005 |
| CWT | -0.99 | 0.004 | MWP | -0.99 | 0.005 |
| WCE | -0.99 | 0.004 | SWC | -0.99 | 0.005 |
| WMY | -0.99 | 0.004 | YYC | -0.99 | 0.004 |
| MWA | -0.99 | 0.004 | CCM | -0.99 | 0.006 |
| PCH | -0.99 | 0.003 | YCH | -0.99 | 0.003 |
| CHM | -0.99 | 0.005 | TCC | -0.99 | 0.004 |
| WPW | -0.99 | 0.004 | CYW | -0.99 | 0.004 |
| MPM | -0.99 | 0.003 | CKC | -0.99 | 0.007 |
| KCC | -0.99 | 0.003 | CMM | -0.99 | 0.004 |

PDB IDs of 1917 Globular Proteins:

2DY7A, 4A5VA, 1BR0A, 2H2MA, 1GH9A, 2L52A, 3HVVA, 1JO6A, 2RQ5A, 2BZTA, 2KVL A, 2DGYA, 3C12A, 1DHNA, 2LS01, 2KMVA, 2LAVA, 1HE9A, 1ICXA, 2IWCA, 1JLNA, 3FS5A, 2EYIA, 2KXFA, 2W0IA, 2KNAA, 2OJ4A, 2CQWA, 2EZLA, 2KYWA, 2M2DA, 2JSPA, 3MZZA, 1GTAA, 1WOTA, 1IRLA, 2KAFA, 2LSEA, 2D1UA, 2PP4A, 1BYWA, 2HWTA, 1JW3A, 2W0NA, 2B0AA, 2JMLA, 1H7DA, 1M9GA, 2SILA, 1ABZA, 2KO6A, 2K0SA, 2JA4A, 1BKBA, 2E6JA, 1ZITA, 2YVNA, 1D6BA, 1K42A, 1L3YA, 1BW3A, 2LC2A, 1WFOA, 2K07A, 2DI0A, 2BO5A, 2IF1A, 2DZLA, 2DN8A, 1QJ9A, 2L9QA, 1ZHVA, 1YDUA, 1TH5A, 2DGZA, 2ROVA, 2LNAA, 1NGLA, 1IFGA, 2EDUA, 2NS5A, 1WMTA, 1Z33A, 1TZQA, 1UB9A, 2FYJA, 1IRZA, 2L9MA, 1A8OA, 1ZLBA, 2LRUA, 2JY9A, 2LTUA, 1SS6A, 1EXGA, 1J7GA, 1WHQA, 1L1PA, 1WXPA, 2KY9A, 1B64A, 2E00A, 1RLFA, 2JMSA, 1VDLA, 1K40A, 2E6ZA, 1TM9A, 2L7SA, 6XIAA, 1VD0A, 1T0GA, 2L0RA, 4BHCA, 1EDGA, 3APPA, 2EKHA, 1CX1A, 1YQ8A, 2VXDA, 2K0NA, 2A55A, 1IFPA, 1TAPA, 2KLUA, 1YT4A, 1GP8A, 1UGLA, 1BNOA, 2KRXA, 1R3BA, 2KMLA, 1X1FA, 3B02A, 1G8AA, 2EAOA, 2HTJA, 1P1DA, 2C0WA, 1AHCA, 2J4MA, 2KVPA, 1XRDA, 2DAFA, 1OVQA, 2JQXA, 1CDBA, 2YWXA, 1YZSA, 2JR0A, 1OLRA, 1UQVA, 2KCWA, 1LPLA, 2CRLA, 2LU3A, 1ALDA, 2LONA, 1QJTA, 2M3KA, 1U3NA, 2LBOA, 1DUJA, 2LC3A, 4DOMA, 2OYZA, 1BIPA, 2KA0A, 2L8OA, 2KRKA, 2KW7A, 2CQUA, 1EQ1A, 2FQHA, 3IHOA, 2KIAA, 1BRZA, 3V5BA, 2LEMA, 2D9ZA, 1JWEA, 2KXSA, 1KVPA, 1J57A, 2D8MA, 2DW3A, 2LXFA, 1CEMA, 2YSEA, 2KNJA, 1GJSA, 3FH2A, 3MXXA, 2DBCA, 1KUUA, 1TGOA, 1WH0A, 2AH5A, 2LQKA, 1Y2YA, 2V0FA, 1TQZA, 1QR9A, 2RA1A, 1FTSA, 3D4MA, 4E5RA, 1V49A, 1JXCA, 2LTLA, 2LNTA, 1Q50A, 2KONA, 2K3PA, 1HKGA, 1DTZA, 2KXYA, 1DVOA, 2WCYA, 2LJPA, 2L4WA, 1DDFA, 2V14A, 1WJ4A, 2BIDA, 2EDMA, 1WFMA, 1POUA, 1H8MA, 2KUMA, 2K0MA, 1Y7XA, 2PETA, 1YWXA, 2KSWA, 1DROA, 1QQFA, 3AAPA, 1L2PA, 2KMGA, 1UAPA, 2M5OA, 1OJQA, 2JXTA, 3LD1A, 1BD8A, 2JO1A, 2KMFA, 1N5HA, 2KCKA, 1SXMA, 1X58A, 1Q48A, 1C2AA, 1FQQA, 2YU3A, 2E5EA, 1G6EA, 1USSA, 3JV1A, 1VFIA, 2K88A, 2K2EA, 1NEQA, 1ZTSA, 2B68A, 2LCUA, 2OF3A, 2KBZA, 1F7WA, 1H09A, 2L0KA, 1T4YA, 2CTXA, 2XV9A, 1FUSA, 1X3AA, 2CR9A, 1C3GA, 2K3AA, 2M09A, 1Q1OA, 2EQNA, 1K8HA, 2YUIA, 1PLRA, 1EYHA, 3VPYA, 1ZRXA, 1BU2A, 2M4FA, 2LXNA, 2JNSA, 1C3YA, 2RRUA, 1ZLGA, 2ADZA, 4DNUA, 1EZAA, 1X4PA, 2XXSA, 1SG5A, 1WS6A, 3PG4A, 2LFPA, 1BEOA, 1DQCA, 2KMZA, 1P4SA, 2Z9TA, 2JVJA, 1D2PA, 4B50A, 1P3CA, 2KZ4A, 1HA8A, 4FCUA, 1W9RA, 1NYOA, 1KV4A, 2L82A, 3E9UA, 2E3EA, 2K75A, 2KGS A, 1OH1A, 2YSZA, 1WJ5A, 1PBUA, 1PMDA, 2JOQA, 2EDOA, 1WISA, 2KPTA, 2L06A, 2GQCA, 1POQA, 2AYYA, 2KMUA, 2KCOA, 1R5SA, 2JTCA, 1H6TA, 2KHVA, 1V5MA, 2LG1A, 1AD6A, 2BNHA, 3IV4A, 2AC4A, 2YUYA, 1J8SA, 1DQ0A, 2VU5A, 1ZLMA, 2R0SA, 2KWHA,

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2LORA, 2DMEA, 2JZFA, 1G03A, 2KZSA, 2G0UA, 2BAAA, 2KSVA, 2A4HA, 1CDHA, 1YWLA, 2KSFA, 2RM5A, 2M4GA, 3F9VA, 2LPDA, 1WINA, 1EMWA, 2COOA, 2RSOA, 2F3IA, 2LYCA, 1SLLA, 2YUGA, 2DA6A, 2K18A, 2LLMA, 2LF6A, 2KPYA, 1GLNA, 1I2UA, 2JN9A, 1FYBA, 2JSFA, 1ANUA, 1XIXA, 1PNEA, 2FMRA, 2FCBA, 1K5KA, 2CU1A, 2GPQA, 2JQ3A, 4AKAA, 2JZ4A, 1CFIA, 2LEQA, 2LMZA, 2KOUA, 2KB9A, 2LIOA, 1PWKA, 1XEEA, 1X67A, 1N7LA, 2LLNA, 2L1SA, 3KJEA, 1GO9A, 2KKXA, 2BYEA, 1DT4A, 1LL8A, 2RSGA, 2V6CA, 2YQKA, 2L3UA, 2CJNA, 3A7LA, 3UCIA, 1YXEA, 2EZIA, 2KVSA, 1ZXFA, 2JTOA, 1SURA, 2L25A, 2LPIA, 2KPMA, 2K5GA, 1WRGA, 2K3DA, 2K8OA, 1CWYA, 2KUA, 1G7EA, 1WCLA, 1X1EA, 1I6ZA, 1MN3A, 2AGMA, 1FEXA, 2KEPA, 1MD6A, 1RW2A, 2M26A, 2LLVA, 2ROQA, 1DV5A, 2HEQA, 2K2BA, 1SKFA, 1D3LA, 2FJ6A, 1NE3A, 1TVMA, 2BICA, 2LGZA, 3SH4A, 2D56A, 2KYA, 1PMRA, 2KWAA, 1AK6A, 2CWYA, 2E0GA, 2PXGA, 1R4GA, 1GGVA, 1FASA, 1JCUA, 1P6TA, 2L7WA, 2CRFA, 1GOKA, 3RA2A, 2KK7A, 2LR4A, 2L8KA, 1HNRA, 1ZC1A, 1OGWA, 2IMUA, 2AXLA, 2KCNA, 2KYHA, 1QZMA, 1G7OA, 2K5IA, 2KVTA, 2KHEA, 1LWBA, 1XPNA, 2KLBA, 1N81A, 2DKZA, 2LRGA, 2L2EA, 1ND9A, 1WG7A, 1WH8A, 1HP8A, 4A02A, 2JWYA, 2GMGA, 1BUYA, 2K4KA, 2K3IA, 1WHNA, 1WQKA, 2KPPA, 1YR1A, 2HNA, 1HDLA, 2YS4A, 2QU4A, 2L57A, 1PVEA, 1HKYA, 1DTVA, 1IO2A, 1IB8A, 2KJRA, 2KW8A, 2RQYA, 1AUZA, 2JHBA, 1V2YA, 2KZ5A, 2JPNA, 1I1SA, 2SNVA, 1MF7A, 2KE3A, 1KMXA, 2OQPA, 1EIKA, 2KQPA, 1AHOA, 1MHNA, 1HGVA, 2YS0A, 1VIBA, 3PM2A, 2L04A, 2BKDN, 1A6CA, 2FC3A, 1IS1A, 1A8QA, 1OMPA, 1PM6A, 3HAKA, 2JTYA, 1RHDA, 2JQYA, 1NXIA, 1WK1A, 1T45A, 2LQ4p, 2FJLA, 1C44A, 1YPCI, 4HJCA, 2L1PA, 6RHNA, 1LNSA, 2LCYA, 1RQSA, 1X4TA, 2D46A, 2IUEA, 1QXXA, 1SAPA, 1G62A, 2E63A, 1VDIA, 1QTTA, 2CR7A, 1GM0A, 1T8CA, 3HSFA, 1XU6A, 1UFZA, 2K49A, 2JWGA, 1JBJA, 2RH3A, 1TDPA, 1WWIA, 2KPUA, 1SORA, 1AGXA, 1SBXA, 1KJ6A, 1L6HA, 2E8PA, 2BBXA, 1H4AX, 2GPRA, 1IVZA, 2PTLA, 4DNIA, 2IN2A, 2LMDA, 2LRSA, 1X0HA, 2K7MA, 1VCCA, 2C83A, 1N3HA, 2EE5A, 2KLQA, 3O04A, 2JOVA, 2BFHA, 1VGPA, 1V61A, 2L9DA, 1X3OA, 2F76X, 1HCDA, 2NOCA, 1MR4A, 2E70A, 1M42A, 4ACJA, 2EQOA, 2BVBA, 1AJEA, 2KVAA, 1GYFA, 2NRGA, 1NOAA, 4A53A, 2LL0A, 3DJ9A, 1SSKA, 1RC9A, 2K5PA, 2EKIA, 1IW4A, 1X5BA, 1QW1A, 1QW2A, 2K6GA, 2B3WA, 2KK2A, 2SGAA, 1AKZA, 2JMBA, 1MIXA, 2D5UA, 1HIOA, 2KQ6A, 8OHMA, 1CTOA, 2DJPA, 2E7MA, 2QMVA, 2LYXA, 1YYCA, 2GLEA, 1X0OA, 2KYTA, 2K5EA, 2EVNA, 2LRDA, 2LW3A, 2FJZA, 2K1AA, 1PBNA, 3T7FA, 2DJ1A, 2KT8A, 3JZ9A, 1T2IA, 1WJUA, 1LMZA, 1WITA, 2LQ8A, 2AYAA, 1K19A, 2L08A, 1PRZA, 1Z8SA, 2R6QA, 2K9DA, 2NSNA, 2ARAA, 2VQ4A, 1LKNA, 1G7DA, 1HREA, 1H3QA, 2DI7A, 2KOKA, 3A4CA, 2DAQA, 2JHYA, 2G69A, 2ESKA, 1PC0A, 1J7XA, 1OTPA, 1XAAA, 2KA5A, 2RNNA, 2FZ0A, 1K8VA, 1GYVA, 1BSHA, 1AKOA, 2PNEA, 2QZQA, 2KK4A, 1WYMA,

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1UJRA, 1EHSA, 1YU5X, 2DAWA, 1IUFA, 1PGYA, 1J0TA, 2GGFA, 2DO8A,
2P25A, 1W0BA, 2KD1A, 1IMTA, 2YRQA, 1ALYA, 1FHOA, 2K73A, 2UWQA,
2RSXA, 3UFCX, 2JOZA, 2JZAA, 2M4YA, 2CRUA, 1MJZA, 2HJQA, 2JNKA,
2JOBA, 2JPSA, 1O5TA, 2L5QA, 2YWOA, 1BI5A, 1IEZA, 1URFA, 1T0VA,
1QKLA, 3FI1A, 1YVCA, 3ETPA, 2V1NA, 2LJKA, 1V5SA, 3JYLA, 3CO1A,
2RR8A, 1QTSA, 2LQGA, 2DIUA, 2K8PA, 2JVGA, 2DIRA, 1KIVA, 2K4ZA,
1QK9A, 2BZEA, 1AIWA, 2HVMA, 1BDSA, 4E2UA, 2KZ0A, 1RHXA, 1T17A,
1YSYA, 2C55A, 2KCQA, 2KZ3A, 1GQZA, 1OWAA, 1YUBA, 1EGXA, 1FHLA,
2KJQA, 4J5QA, 2YV0X, 1LQCA, 2J9VA, 1A63A, 1Q59A, 2CR2A, 1HHNA,
1K8BA, 1GVPA, 2K24A, 2YGSA, 3DJNB, 2RSTA, 1FGPA, 2K5SA, 2KRCA,
1ZDVA, 1EHXA, 2HE7A, 2CP8A, 1APCA, 2KHQA, 3R6DA, 2EQXA, 2YRVA,
2KEQA, 4AQZA, 2PPNA, 1MSCA, 1WH2A, 1F5XA, 1GVLA, 1QTOA,
1UDMA, 2LSHA, 2HZDA, 2DIQA, 1UOYA, 1WM3A, 2LVXA, 2KT6A, 2ICTA,
3DPAA, 1IADA, 1UKFA, 1WGBA, 2RRLA, 1M2EA, 1B75A, 2CPTA, 3M66A,
2L81A, 1L7YA, 3E7RL, 2I8LA, 2KC5A, 1RYKA, 1GHTA, 2LV4A, 2AKKA,
3PFMA, 3LFOA, 2DKQA, 2LNMA, 2DUNA, 1EOVA, 1CKRA, 1UFGA,
2KJIA, 1LQ7A, 1G5ZA, 2LQ3A, 2FXTA, 2X43S, 1BVHA, 1XKEA, 1WHRA,
2JZ6A, 1SE7A, 4J4RA, 2V31A, 2CG7A, 1GYZA, 1NFAA, 2JSNA, 2JZTA,
1ZAQA, 2LN7A, 1G9PA, 1BHEA, 1KOEK, 2KQZA, 2DLXA, 2M6YA, 1UG7A,
1Q38A, 1TJDA, 2RKQA, 2GF5A, 2VKCA, 2K5QA, 3IH4A, 2XK0A, 2CASA,
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2L1QA, 2L2CA, 2JVMA, 1HKAA, 2LKGA, 1E8RA, 1N6ZA, 2B9KA, 1V9VA,
2BK2A, 1C01A, 2KKVA, 2ENQA, 2QT4A, 3MX7A, 2KNIA, 2KRHA, 1WXMA,
1I2TA, 1QM9A, 1ATAA, 2KJXA, 1WRYA, 1K0HA, 2FB9A, 1N91A, 2FMCA,
3N0KA, 2DHZA, 2D49A, 2OKTA, 2KWYA, 1PV0A, 4AOGA, 1BQCA, 1GO5A,
1Z9BA, 1ZHCA, 3ZPMA, 2DHSA, 1NHLLA, 2WQGA, 2KUQA, 1E0HA, 1N88A,
1I60A, 1MWPA, 4ETXA, 3ZSLA, 2LY8A, 1WJKA, 3QYUA, 2M4VA, 1BZKA,
1T50A, 2K4NA, 1WJRA, 2CKXA, 1CKVA, 1EJ5A, 1ZUGA, 2KL2A, 1ERDA,
2KGFA, 1TJEA, 1LXLA, 2M47A, 1JI6A, 1R36A, 2JOYA, 2KEYA, 1WXAA,
2DOAA, 4JZCA, 1X52A, 1WKIA, 1XWEA, 2L1AA, 2UWRA, 1CEJA, 2L1TA,
1XNEA, 1P4XA, 2JXWA, 2Z4DA, 1A9VA, 1F6WA, 1WICA, 1YO4A, 4ULLA,
1O6XA, 3KB5A, 1KS9A, 1CZ4A, 2GBSA, 2JWHA, 1DVNA, 2K0RA, 2K5RA,
2YUDA, 1UHUA, 1JYTA, 1UG8A, 1V63A, 2KK1A, 2KLLA, 2DAVA, 1YALA,
1BGFA, 2RRDA, 2LOJA, 3SEBA, 2KNQA, 4AR0A, 2LN3A, 1ESXA, 1RZWA,
1MV3A, 2KIWA, 2JYEA, 2DA7A, 2KQ1A, 3MTVA, 1AYDA, 3T5BA, 1AGGA,

2H85A, 2K0QA, 1WF9A, 1EDXA, 3H8NA, 1FMYA, 1WGPA, 1COUA, 2YTUA, 1QHKA, 2C0SA, 1RIPA, 2CRVA, 2K4FA, 2K27A, 1Q2UA, 1A6SA, 1OQAA, 1S7IA, 2RM4A, 1RY3A, 2LAOA, 3VORA, 1YNXA, 2Q34A, 1MJCA, 1HJ0A, 1IP9A, 3F7MA, 1N3KA, 1WIXA, 2LAEA, 1A3HA, 2RNOA, 1WU3I, 3DQPA, 1WGWA, 2LWYA, 3H7ZA, 3LIGA, 1PC2A, 1R8NA, 1SB6A, 2E60A, 1WH4A, 1MP1A, 2K4EA, 2L95A, 2TMPA, 1YUWA, 3NSMA, 1VZSA, 1WWBX, 2K19A, 2COSA, 2RLOA, 2JV8A, 1YW5A, 2M0XA, 1ZU2A, 1U5MA, 2K13X, 1Q5FA, 2W0GA, 1OJGA, 2FE9A, 1AOYA, 3ONJA, 2LTFA, 2LD3A, 2ERFA, 2KQ2A, 2CTQA, 1BBYA, 1WWUA, 1LMIA, 1AA3A, 2LUWA, 1Y6IA, 2PLFA, 1PDBA, 2JMUA, 1WGSA, 2LG7A, 2OT2A, 1PJBA, 2OHEA, 2LIEA, 2KT9A, 2JA9A

PDB IDs of 138 Group I Proteins:

2ZKQq, 4KZYe, 2H4MC, 3IOZB, 4IJ3C, 3IFNP, 3ZMSC, 3BBO6, 4KP3E, 3TPMB, 3DBOA, 3KL4B, 3GZ2P, 4C2M4, 2JDII, 4GMNB, 2M14B, 2RPQB, 4DEYB, 2MBHB, 2O8GI, 3SL9C, 4BXZX, 4BPE9, 4FBWC, 4A1GE, 2P58B, 3T0YB, 2GRXC, 2XG1Y, 3N7NE, 2PQNB, 2I32E, 1Z56A, 1ONVB, 2JZ3A, 2L0YB, 3ZEYR, 1XOUA, 3IYNN, 2WSCE, 4BPE0, 3QV1G, 1OEDC, 4H62K, 2F93B, 4C3ID, 4HB1A, 3S6PE, 4C0TA, 4G91A, 2NPIC, 1AYM4, 3SJHB, 1QZ7B, 1YTVM, 2XPIB, 4BKGA, 2WSCN, 3T5XB, 3FFDP, 3TVTB, 2CLYA, 2XQNA, 4C2MD, 1CQTI, 4B6HC, 3IZRb, 1YD7A, 4B4TS, 4GOWA, 2KXCB, 2WWBC, 2XB2G, 3KYSB, 1DP5B, 4BZIF, 2PRGC, 3W3WB, 2QNAB, 1H8BB, 3BTPB, 2WSCH, 4BXTA, 3IAXB, 4HQJE, 2ZNLB, 3J3Bb, 2WZLA, 3EVYA, 3TDNA, 4E05I, 1FH1A, 4KZYf, 4BYNq, 4KBBC, 3IECE, 3ZEDD, 4BQ6C, 4KIX6, 3F1IC, 3MN7S, 3UTMC, 3ABDX, 4C5HB, 1SCFA, 3M4WE, 2K3JA, 3J3Ah, 2CKZA, 1I7WB, 1UF2K, 4ACOA, 3KNDB, 2KSEA, 4AXGC, 3PMKN, 2LOXB, 3EX7D, 4I6MD, 3PVLB, 1XF5P, 4C2M2, 3E50C, 3V62C, 4HSUB, 1BYYA, 4JPBA, 4AYBQ, 4CCFA, 1H6WA, 3J3Bu, 4JHDC, 1VSZR, 4FTBD, 3QHED, 4GXBB, 2JYVA

DisProt IDs of 91 Group II Proteins:

DP00001, DP00002, DP00005, DP00006, DP00008, DP00015, DP00017, DP00024, DP00027, DP00028, DP00038, DP00039, DP00040, DP00041, DP00042, DP00057, DP00058, DP00068, DP00069, DP00070, DP00116, DP00122, DP00124, DP00128, DP00132, DP00140, DP00143, DP00145, DP00146, DP00147, DP00148_C004, DP00158, DP00163, DP00170, DP00174, DP00180_C003, DP00185, DP00186, DP00193, DP00198, DP00199, DP00205, DP00214, DP00216, DP00219, DP00222, DP00227, DP00232, DP00242, DP00253, DP00288, DP00303, DP00330, DP00332, DP00347, DP00357, DP00359, DP00367, DP00372, DP00387, DP00421, DP00441, DP00465, DP00510, DP00521, DP00531, DP00532, DP00535, DP00538, DP00540, DP00544, DP00546, DP00550, DP00560_C007, DP00563, DP00564, DP00584,

DP00586, DP00592, DP00606, DP00613, DP00626, DP00650, DP00657, DP00663,
DP00664, DP00665, DP00674_C001, DP00675_C002, DP00694, DP00723