DB2: A database of single domain globular proteins

Sankar Basu[1*] & Rahul Banerjee[1]

[1] Crystallography and Molecular Biology Devision; Saha Institute of Nuclear Physics, Kolkata - 700064

[*] nemo8130@gmail.com

The database has been used for the computation of shape (S_m) and electrostatic complementarity (E_m) of buried interior residues within proteins [1], and for the construction of the Complementarity Plot [1] [2] [3]

PDB ID and chain identifier (underscored) for each polypeptide chain is given under its respective protein class. This database is a subset of a larger database discussed in detail in a previous report [4] . Hydrogen atoms were geometrically fixed to all structures by the program REDUCE [5]. In order to confirm the resonance states of histidine, polar hydrogens were reassigned by GROMACS (v.4) using its G43a1 force field [6]. 95% of the assignments were found to be identical in both programs.

all α:

1C02_B, 1C1K_A, 1EL4_A, 1ELK_B, 1EYH_A, 1EZJ_A (Ca^{+2}), 1G5N_A (Ca^{+2}), 1G8E_A, 1I8O_A, 1JKV_A (Ca^{+2}, Mn^{+3}), 1LJ9_A, 1MOJ_A (Fe^{+3}), 1MXR_B (Fe^{+3}, Hg^{+2}), 1OOH_B, 1OXJ_A, 1Q08_A (Zn^{+2}), 1Q5Z_A, 1QYZ_A, 1R1T_B, 1R5Z_B, 1R7J_A, 1SZH_A, 1TFJ_A, 1U2W_B (Zn^{+2}), 1U84_A, 1UCR_B, 1WPA_A, 1WXC_A, 1ZKR_A, 2A61_A, 2AIB_A, 2B8I_A, 2BA2_C, 2CWL_A, 2D48_A, 2D4X_A, 2DPO_A, 2E1N_B, 2ERB_A, 2F2B_A, 2FBQ_A, 2FD5_A, 2FMM_E, 2FP1_A, 2FU4_A, 2GXG_A, 2HRA_A, 2I3F_B, 2IC6_B, 2IGP_A, 2IMI_B, 2NZ7_B, 2O37_A, 2O70_F, 2OEB_A, 2OQG_C, 2PQR_B, 2QRW_K, 2QSA_A, 2RKN_A (Zn^{+2}), 3B9W_A, 3BS7_B, 3C1D_B, 3CHM_A, 3DHZ_B (Fe^{+2}).

all β:

1DJR_H, 1DMH_B (Fe^{+3}), 1EZG_B, 1F7D_A, 1I0R_B, 1I4U_A, 1IBY_B (Cu^{+2}), 1J71_A, 1K12_A (Ca^{+2}), 1KJL_A, 1KT6_A, 1KZQ_B, 1LR5_C (Zn^{+2}), 1LSL_A, 1LXZ_A, 1LYQ_B, 1NTV_A, 1NYK_B, 1NYW_B, 1OU8_B, 1P3C_A, 1PXD_A, 1QB5_E, 1QXM_A, 1R77_B, 1R8O_A, 1ROC_A, 1RU4_A (Ca^{+2}), 1S1D_A (Ca^{+2}), 1SE0_A (Zn^{+2}), 1T2W_C, 1TH7_L, 1V8H_A, 1VM9_A, 1WD3_A, 1WLG_B, 1WLI_B, 1WS7_A, 1XU1_B, 1YFQ_A (Ca^{+2}), 1YOA_A, 1Z3T_A, 1ZVT_B, 2A6V_A, 2AYD_A (Zn^{+2}), 2D37_A, 2DCY_C, 2DP9_A, 2DUR_A (Ca^{+2}), 2EI5_A, 2ERF_A, 2ET1_A (Mn^{+2}), 2F6E_A, 2G9F_A, 2GGV_B, 2GH2_A (Fe^{+3}), 2HAL_A, 2ICC_A, 2IQY_A (Ca^{+2}), 2O8L_A, 2OFZ_A, 2OR7_B, 2PA7_A, 2PCX_A (Zn^{+2}), 2R5O_A, 2RJ2_A, 3BOV_A, 3BU1_A, 3D9X_C, 3F5R_A.

α | β:

1DJ0_A, 1EKG_A, 1EQ6_A, 1F1U_A, 1F46_B, 1F5M_B, 1G1T_A (Ca^{+2}), 1G2R_A, 1IQZ_A, 1J1G_A, 1J1Y_A, 1J27_A, 1J3W_B, 1JD5_A (Zn^{+2}), 1JYH_A, 1JYO_B, 1K2A_A, 1KJO_A (Zn^{+2}, Ca^{+2}), 1KQB_C, 1KUX_A, 1LN4_A, 1LO7_A, 1LQP_B, 1M4D_A, 1M4J_B, 1NE9_A, 1NWA_A, 1NWW_B, 1OZ9_A, 1PC4_A, 1PPV_B (Mg^{+2}, Mn^{+2}), 1R29_A, 1R45_A, 1RC9_A, 1RKI_A, 1RWZ_A, 1S5U_E, 1TA8_A, 1TKE_A, 1TP6_A, 1TR0_I, 1TU1_A, 1TUA_A, 1TUH_A, 1TUV_A, 1WRI_A, 1XBI_A, 1XMT_A, 1XPP_D, 1Y60_D, 1YAR_D, 1YGT_A, 1YPY_A, 1YWM_A, 1Z4R_A, 1ZDY_A, 1ZHQ_G, 1ZHX_A, 1ZT3_A, 2A15_A, 2AAL_A, 2ACY_A, 2B18_A, 2BBE_A, 2CVE_A, 2DT4_A, 2E11_B, 2E12_A, 2E8G_B, 2EA1_A, 2FHZ_A, 2FJR_B, 2FL4_A, 2FVV_A, 2FYG_A (Zn^{+2}), 2G64_A (Zn^{+2}), 2G8O_A, 2GEB_A (Ca^{+2}), 2GH5_B, 2GHT_A, 2GMN_B (Zn^{+2}), 2GU3_A, 2GWM_A, 2H2Z_A, 2I2Q_A, 2I7D_A, 2IF6_A, 2IG8_B, 2NR7_A, 2NTT_B, 2O28_A, 2OH5_A, 2P0W_A, 2P2O_B, 2P3H_A, 2PLQ_A, 2PU3_A, 2Q0L_B, 2QKP_B, 2Z51_A, 3BJK_C, 3BK8_A, 3C8I_B, 3COU_A, 3DA4_A, 3DHA_A (Zn^{+2}).

α + β:

1C7N_C, 1DGF_B, 1DJE_A, 1DQZ_B, 1EQC_A, 1EU8_A, 1F8M_B, 1G5T_A, 1G8A_A, 1I2A_A, 1I2K_A, 1I5G_A, 1I6W_B, 1I9C_B, 1IM5_A (Zn^{+2}), 1INL_C, 1IZC_A, 1JAY_B, 1JJF_A, 1JKE_C (Zn^{+2}), 1JX6_A (Ca^{+2}), 1K4M_B, 1K7C_A, 1LOK_A (Zn^{+2}), 1LUA_B, 1LWD_B, 1N3Y_A, 1NF9_A, 1O04_G, 1OOE_B, 1OZN_A, 1P6O_B (Zn^{+2}, Ca^{+2}), 1Q7L_A (Zn^{+2}), 1RKU_B, 1SG0_B (Zn^{+2}), 1SW5_B, 1T1V_B, 1TJY_A, 1TP9_B, 1TVP_A, 1UB3_B, 1UC7_A, 1UEH_B, 1UG6_A, 1UK8_A, 1V2X_A, 1V37_A, 1VFL_A (Zn^{+2}), 1WN5_B, 1WO8_A, 1WOU_A, 1WPN_A, 1WX1_B, 1XBY_A, 1XQ6_B, 1XS5_A, 1XX1_B, 1Y1P_A, 1Y1T_A, 1Y6V_A, 1YB6_A, 1YD0_A, 1YN9_B, 1YQZ_B, 1YZX_B, 1ZL0_A, 1ZOI_C, 1ZR6_A (Zn^{+2}), 1ZX0_C, 1ZZG_A, 1ZZW_B, 2A14_A, 2A1I_A, 2ACF_C, 2AEU_A, 2AGD_B, 2AP1_A (Zn^{+2}), 2AVD_B, 2B1K_A, 2B3F_B, 2B82_A, 2CYG_A, 2E5F_A, 2FB9_A, 2FLA_A, 2FQX_A, 2FY6_A, 2G84_A (Zn^{+2}), 2GSO_A (Zn^{+2}), 2H1C_A, 2H1V_A, 2HC9_A (Zn^{+2}), 2HL6_B, 2HOR_A, 2HPJ_A, 2HRC_B, 2HU9_A, 2HXU_A (Mg^{+2}), 2HY5_B, 2HZL_B, 2I49_A, 2I56_C (Zn^{+2}), 2NZX_C, 2OUI_B, 2P51_A (Mg^{+2}), 2PS1_A, 2QDX_A, 2QUL_B (Mn^{+2}), 2REM_C, 2RHJ_A, 2YW3_D, 2Z1Y_B, 2Z6R_B, 3B4U_B, 3B8X_B, 3BJE_B (Ca^{+2}), 3BOE_A, 3C9H_B, 3CQ5_B, 3D2H_A, 3DAF_A (Fe^{+2}), 3E96_B, 3ES7_B (Mg^{+2}), 3EVF_A.

Multidomain:

1DLJ_A, 1EEJ_B, 1F60_A, 1FP2_A, 1FW1_A, 1G8L_B, 1HM9_B (Ca^{+2}), 1HYO_B (Ca^{+2}), 1IG3_A, 1JAK_A, 1K7I_A (Zn^{+2}, Ca^{+2}), 1KTB_A, 1LBV_A, 1M1H_A, 1OWL_A, 1P1M_A, 1RA0_A (Fe^{+3}), 1RQP_C, 1SZN_A, 1T0F_A, 1T2D_A, 1T4B_B, 1U60_C, 1VBK_A, 1YU0_A (Ca^{+2}), 1Z6F_A, 1ZJC_A (Co^{+2}), 2CZ1_B, 2GA2_A (Mn^{+2}), 2GDQ_B, 2GGO_A, 2GZ1_B, 2GZJ_F (Zn^{+2}), 2PUZ_B (Fe^{+3}), 3ETJ_A (Mg^{+2}).

References:

1. Basu S, Bhattacharyya D, Banerjee R. Self-Complementarity within Proteins: Bridging the Gap between Binding and Folding. Biophys J. 2012;102: 2605–2614. doi:10.1016/j.bpj.2012.04.029

2. Basu S, Bhattacharyya D, Banerjee R. SARAMA: A Standalone Suite of Programs for the Complementarity Plot—A Graphical Structure Validation Tool for Proteins. J Bioinforma Intell Control. 2013;2: 321–323. doi:10.1166/jbic.2013.1059

3. Basu S, Bhattacharyya D, Banerjee R. Applications of complementarity plot in error detection and structure validation of proteins. Indian J Biochem Biophys. 2014;51: 188–200.

4. Basu S, Bhattacharyya D, Banerjee R. Mapping the distribution of packing topologies within protein interiors shows predominant preference for specific packing motifs. BMC Bioinformatics. 2011;12: 195. doi:10.1186/1471-2105-12-195

5. Reduce Software : Kinemage Website [Internet]. [cited 12 Jun 2016]. Available: http://kinemage.biochem.duke.edu/software/reduce.php

6. Molecular Dynamics Simulations - Gromacs [Internet]. [cited 12 Jun 2016]. Available: http://www.gromacs.org/Documentation/Terminology/Molecular_Dynamics_Simulations

Please cite Ref(1) if you use the database in your publication.