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Table 10. Global bond values

Molecule	Global Bond Values
Carbon monoxide (CO)	3
Water (H ₂ O)	2
Carbon dioxide (CO ₂)	4
Methane (CH ₄)	4
Ammonia (NH ₃)	3
Formaldehyde (CH ₂ O)	4
Acetone (C ₃ H ₆ O)	10
Hydrogen peroxide (H ₂ O ₂)	3
Nitric oxide (NO)	2
Methanol (CH ₄ O)	5
Sulfur dioxide (SO ₂)	3
Hydrogen cyanide (HCN)	4
Propane (C ₃ H ₈)	10
Butane (C ₄ H ₁₀)	13
Ethylene (C ₂ H ₄)	6
Formic acid (H ₂ CO ₂)	5

Hydrogen sulfide (H ₂ S)	2
Phosphine (PH ₃)	3
Oxygen (O ₂)	2
H ₂	1
Caffeine (C ₈ H ₁₀ N ₄ O ₂)	29
Nicotine (C ₁₀ H ₁₄ N ₂)	30
Aspirin (C ₉ H ₈ O ₄)	26
Ibuprofen (C ₁₃ H ₁₈ O ₂)	37
Cholesterol (C ₂₇ H ₄₆ O)	78
Glutathione (C ₁₀ H ₁₇ N ₃ O ₆ S)	40
Serotonin (C ₁₀ H ₁₂ N ₂ O)	30
Dopamine (C ₈ H ₁₁ NO ₂)	25
Vanillin (C ₈ H ₈ O ₃)	23
Thymine (C ₅ H ₆ N ₂ O ₂)	18
Cytosine (C ₄ H ₅ N ₃ O)	16
Adenine (C ₅ H ₅ N ₅)	20
Guanine (C ₅ H ₅ N ₅ O)	21
Lactic acid (C ₃ H ₆ O ₃)	12
Glucose (C ₆ H ₁₂ O ₆)	24

Acetaminophen (C ₈ H ₉ NO ₂)	24
Uric acid (C ₅ H ₄ N ₄ O ₃)	21
Nicotinamide (C ₆ H ₆ N ₂ O)	19
Riboflavin (C ₁₇ H ₂₀ N ₄ O ₆)	56
Folic acid (C ₁₉ H ₁₉ N ₇ O ₆)	64
Ubiquitin (C ₃₇₈ H ₆₂₉ N ₁₀₅ O ₁₁₈ S)	1347
Cytochrome c (C ₅₁₃ H ₈₂₆ N ₁₄₀ O ₁₅₄ S ₃ Fe)	1807
Insulin (C ₂₅₆ H ₃₈₁ N ₆₅ O ₇₇ S ₆)	883
Lysozyme (C ₆₁₃ H ₉₅₉ N ₁₉₃ O ₁₈₅ S ₁₀)	2190
Trypsin inhibitor (BPTI) (C ₂₇₈ H ₄₃₄ N ₈₂ O ₈₄ S ₆)	986
Ribonuclease A (C ₅₀₇ H ₇₇₀ N ₁₄₈ O ₁₅₇ S ₈)	1786
Histone H4 (C ₄₇₂ H ₇₅₆ N ₁₃₂ O ₁₄₁ S ₃)	1664
Myoglobin (C ₇₃₈ H ₁₁₆₀ N ₂₀₂ O ₂₁₈ S ₂ Fe)	2580
Beta-lactoglobulin (C ₈₁₇ H ₁₂₈₅ N ₂₂₁ O ₂₅₁ S ₈)	2867
Calmodulin (C ₃₅₇ H ₅₆₅ N ₉₅ O ₁₀₂ S ₄)	1245
Cold Shock Protein (CspA) (C ₃₃₅ H ₅₄₅ N ₉₁ O ₉₅ S ₃)	1177
Protein G B1 domain (C ₂₇₂ H ₄₃₂ N ₈₂ O ₈₆ S ₄)	973
Protein L (C ₃₄₆ H ₅₅₈ N ₉₈ O ₁₀₂ S ₄)	1224
Engrailed homeodomain (C ₂₉₂ H ₄₆₆ N ₈₄ O ₈₈ S ₃)	1034

Villin headpiece (HP35) (C157H258N46O51S2)	565
Hemoglobin (C2952H4664N812O832S8Fe4)	10300
Serum Albumin (C2936H4624N786O889S41)	10293
α -Amylase (C3360H5380N920O1040S30)	11860
Catalase (C3520H5600N960O1100S32Fe4)	12418
Lactase (C3600H5740N980O1120S34)	12694
Glutamine Synthetase (C3900H6240N1060O1200S36)	13746
Pyruvate Kinase (C4050H6460N1100O1240S38)	14258
DNA Polymerase I (C4350H6940N1180O1320S40)	15300
RNA Polymerase II (C4480H7140N1220O1360S42Zn8Mg2)	15772
Chaperonin GroEL (C4750H7580N1290O1430S44)	16699
ATP Synthase (F1 unit) (C4920H7840N1340O1480S46Mg2)	17298
Dynein Motor Domain (C5100H8120N1390O1530S48)	17923
Myosin Heavy Chain (C5350H8520N1460O1600S50)	18800
Kinesin (C5600H8920N1530O1670S52)	19677
Titin Fragment (C5850H9320N1600O1740S54)	20554

Reproducibility Statement:

The bond-count values listed in this table correspond to the total number of covalent bonds in each molecule and are required as direct input to the Exclusion-Zone SASA code. Since the model computes

its exclusion correction from the global bond count rather than from structural files, providing these values enables full reproducibility of all benchmark results reported in this work.