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12/2/2025

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 ₃ OH)	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 (C8H9NO2)	24
Uric acid (C5H4N4O3)	21
Nicotinamide (C6H6N2O)	19
Riboflavin (C17H20N4O6)	56
Folic acid (C19H19N7O6)	64
Ubiquitin (C378H629N105O118S)	1347
Cytochrome c (C513H826N140O154S3Fe)	1807
Insulin (C256H381N65O77S6)	883
Lysozyme (C613H959N193O185S10)	2190
Trypsin inhibitor (BPTI) (C278H434N82O84S6)	986
Ribonuclease A (C507H770N148O157S8)	1786
Histone H4 (C472H756N132O141S3)	1664
Myoglobin (C738H1160N202O218S2Fe)	2580
Beta-lactoglobulin (C817H1285N221O251S8)	2867
Calmodulin (C357H565N95O102S4)	1245
Cold Shock Protein (CspA) (C335H545N91O95S3)	1177
Protein G B1 domain (C272H432N82O86S4)	973
Protein L (C346H558N98O102S4)	1224
Engrailed homeodomain (C292H466N84O88S3)	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.