

Consistency and Clarity in Chemical Concepts

Concept	Definitions from ODBMB	Definitions from Gold Book	Characteristic feature	Proposed definitions based on concept diagram
primary structure	The first order of complexity of structural organization exhibited by polypeptide and protein molecules, and by polynucleotide and nucleic-acid molecules. When applied to a segment of a polypeptide chain, or to a polypeptide or protein molecule, it refers to the linear sequence of the amino-acid residues of the polypeptide chain(s), without regard to spatial arrangement, apart from configuration at the α -carbon atoms (and excluding positions of any disulfide bonds).	In the context of macromolecules such as proteins, constitutional formula, usually abbreviated to a statement of the sequence and if appropriate cross-linking of chains.	LEVEL: sequence of building blocks	Sequence of building blocks in a linear macromolecule, such as the sequence of amino acid residues in a polypeptide chain.
secondary structure	Arrangement of the polypeptide structure into locally-organized, hydrogen-bonded structures, in particular α -helices and β sheets	The conformational arrangement (α -helix, β -pleated sheet, etc.) of the backbone segments of a macromolecule such as a polypeptide chain of a protein without regard to the conformation of the side chains or the relationship to other segments.	LEVEL: localized segments	Part of the conformation of a polypeptide (or other macromolecule) specifying the internal spatial arrangement of individual backbone segments without regard to the conformation of side chains or the relationship to other segments. <i>Comment:</i> The segments are typically organized via hydrogen bonds. Examples of secondary structure elements are α -helices and β -pleated sheets in polypeptides.
tertiary structure	The level of protein structure at which an entire polypeptide chain has folded into a 3-D structure. The tertiary structure results from interactions between amino-acid residues that may be widely separated in the primary structure, but may be brought into proximity by the folding of the polypeptide chain.	The spatial organization (including conformation) of an entire protein molecule or other molecule consisting of a single chain.	LEVEL: entire molecule	Part of the conformation of an entire polypeptide (or other macromolecule consisting of a single chain) specifying the spatial arrangements of all backbone segments relative to each other. <i>Comment:</i> The tertiary structure results from interactions between amino-acid residues that may be widely separated in the primary structure, but may be brought into proximity by the folding of the polypeptide chain.
α -helix	A helical, or spiral conformation of a polypeptide chain in which successive turns of the helix are held together by hydrogen bonds between the amide peptide links, the carbonyl group of any given residue being hydrogen-bonded to the imino group of the third residue behind it in the chain. An α -helix has 3.6 residues per turn, and the pitch is 5.4 Å per turn. The helix may be left- or right handed, the latter being much more common.	Not defined.	GEOMETRY: helix	Secondary structure element consisting of a helical conformation in which turns of the helix are held together by hydrogen bonds between the amide links in such a way that the carbonyl group in every amide link is bonded by a hydrogen bond to the imino group in the amide link three residues behind the first amide link. <i>Comment:</i> An α -helix has 3.6 residues per turn, and the pitch of the helix is 5.4 Å. The helix may be left- or right-handed, the latter being much more common.
β -pleated sheet	An approximately planar array of two or more adjacent β -strands such that hydrogen bonds may be formed between C=O groups of one β -strand and NH groups of another.	Not defined.	GEOMETRY: planar sheet of strands	Secondary structure element consisting of a planar array formed by two or more adjacent β -strands via hydrogen bonds between carbonyl groups of one β -strand and imino groups of another.

Table 3. Definitions from ODBMB and Gold Book of selected molecular structure concepts illustrated in figure 2.