Chronic lymphocytic leukemia (CLL) is the most common adult leukemia with still unclear etiology. Indications of antigenic pressure have been hinted, using sequence and structure-based reasoning. The accuracy of such approaches, and in particular of the ones derived from 3D models obtained from the patients’ antibody amino acid sequences, is intimately connected to both the reliability of the models and the quality of the methods used to compare and group them. The proposed work provides a sophisticated method for the classification of CLL patients based on clustering the amino acid sequences of the clonotypic B-cell receptor immunoglobulin, which is the ideal clone-specific marker, critical for clonal behavior and patient outcome. A novel CLL patient clustering method is hereby proposed, combining bioinformatics methods with the extraction of 3D object descriptors, used in machine learning applications. The proposed methodology achieved an efficient and highly informative grouping of CLL patients in accordance to their biological and clinical properties.