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(71) Applicants: **ILLUMINA, INC.** [US/US]; 5200 Illumina Way, San Diego, California 92122 (US). **ILLUMINA CAMBRIDGE LIMITED** [GB/GB]; 19 Granta Park, Great Abington, Cambridge CB21 6DF (GB).

(72) Inventors: **HAMP, Tobias**; 19 Granta Park, Great Abington, Cambridge CB21 6DF (GB). **GAO, Hong**; 5200 Illumina Way, San Diego, California 92122 (US). **FARH, Kai-How**; 5200 Illumina Way, San Diego, California 92122 (US).

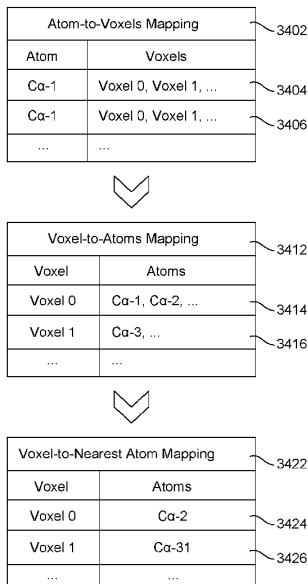
(74) Agent: **KHAN, Sikander M.** et al.; Haynes Beffel & Wolfeld LLP, P.O. Box 366, 637 Main Street, Half Moon Bay, California 94019 (US).

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(54) Title: EFFICIENT VOXELIZATION FOR DEEP LEARNING

Figure 34



(57) Abstract: The technology disclosed relates to efficiently determining which atoms in a protein are nearest to voxels in a grid. The atoms have three-dimensional (3D) atom coordinates, and the voxels have 3D voxel coordinates. The technology disclosed generates an atom-to-voxels mapping that maps, to each of the atoms, a containing voxel selected based on matching 3D atom coordinates of a particular atom of the protein to the 3D voxel coordinates in the grid. The technology disclosed generates a voxel-to-atoms mapping that maps, to each of the voxels, a subset of the atoms. The subset of the atoms mapped to a particular voxel in the grid includes those atoms in the protein that are mapped to the particular voxel by the atom-to-voxels mapping. The technology disclosed includes using the voxel-to-atoms mapping to determine, for each of the voxels, a nearest atom in the protein.

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