METHOD AND SYSTEM FOR FAST PROTEIN VISUALIZATION USING PRE-CALCULATED IMAGE SIMILARITY INDEX AND ATOM DEPTH

Field of the Invention

[0001] The present invention generally relates to methods and systems for visualization of protein three-dimension structures, and more particularly to a method and system for fast protein visualization using image similarity index and atom depth.

Background of the Invention

[0002] Many protein three-dimension structures are available now. It is predictable that more and more protein three-dimension structures will be elucidated. The ever-increasingly available structures facilitate protein modeling, drug design, and analysis of protein-protein interactions. This is because the 3D structure of a protein determines its interaction with other molecules, hence its functions. For example, haemoglobin, being in a cup shape has the ability to carry oxygen molecules in the blood stream.

[0003] The utilization of protein 3D structures, however, requires fast visualization. Currently, there are many well-established ways of visualizing the 3D protein structures. For example, Can et al. disclose a fast protein visualization using Java 3D that improves rendering speed by modifying the scene-graph structure. See, Can et al., "FPV: Fast Protein Visualization Using Java 3D," Bioinformatics, 19, 0-10. Huitema and van Liere disclose a fast visualization of protein surfaces using a zonal map. See, Huitema and van Liere, Time critical computing and rendering of molecular surfaces using a zonal map, in : Proceedings of the EG Workshop on Virtual Environments, 2000, pp. 115-124. Nonetheless, the growing number of new structure data in the Protein Data Bank means that researchers studying the interaction between protein molecules need new tools that are capable of loading and displaying this huge amount of data rapidly.

[0004] Atom depth has been used as a geometric descriptor of the interior of a protein 3D structure. While its definition may vary according to different practicing group, the atom depth has been shown its usefulness in many aspects. For example, atom depth

has been found to be correlated with several molecular, residue and atomic properties such as average protein domain size, protein stability, free energy of formation of protein complexes, amino acid type hydrophobicity, residue conservation and hydrogen/deuterium amide proton exchange rates. See, Pintar et al., Atom Depth In Protein Structure and Funcation, TRENDS in Biochemical Sciences, 28: 593-597 (2003). However, there is no disclosure in the prior art that the atom depth is related to the visualization of protein 3D structures.

Summary of the Invention

[0005] Therefore, one of the objectives of the present invention is to provide a method and system for rendering fast visualization of protein 3D structures. The method and system of the present invention improves the speed of visualization using pre-calculated image similarity index and atom depth.

[0006] In one aspect, the present invention provides a method for rendering fast visualization of protein three dimension structures. In one embodiment, the method comprises the steps of providing a file of the three dimension structure of a protein, calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area, calculating image similarity indexes of images with different atom numbers in comparison with the original image, generating a rendering table that correlates the image similarity indexes with the atom depths, and displaying the three dimension structure with an accuracy that is input by a user. In a further embodiment of the method, the steps of calculating atom depth, calculating image similarity indexes, and generating a rendering table can be done prior to visualization so that the rendering table is part of the file of the three dimension structure of a protein. In yet another further embodiment of the method, the rendering table is generated by following pseudo-code:

```
For Y_rotation_angle = principal viewing angles(eg. 0, 90,-90) do
    For X_rotation_angle = principal viewing angles (eg. 0,90,180,270) do
      For atom depth threshold = 0 to max do
            Generate a image for all atoms with atom depth less than the
            threshold value
            Compare generated  image with original image to get image
            similarity index
      End for
    End for
```

End for

[0007] In another aspect of the present invention, there is provided a database of protein three dimension structure files, wherein each protein three dimension structure file comprises a rendering table that correlates image similarity indexes and atom depths; thereby the protein three dimension structure files enable fast visualization upon selection of an image similarity index for viewing by a user.

[0008] In yet another aspect of the present invention, there is provided a system for fast visualization of protein three dimension structures. In one embodiment, the system comprises a computer readable medium; a computer program embedded within the computer readable medium, wherein the computer program enables fast visualization of protein three dimension structures; wherein the computer program comprises: means for providing a file of the three dimension structure of a protein; means for calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area; means for calculating image similarity indexes of images with different atom numbers in comparison with the original image; and means generating a rendering table that correlates the image similarity indexes with the atom depths; and a display means for displaying the three dimension structure with an accuracy that is input by a user. In a further embodiment of the system, the steps of calculating atom depth, calculating image similarity indexes, and generating a rendering table can be done prior to visualization so that the rendering table is part of the file of the three dimension structure of a protein.

[0009] The objectives and advantages of the invention will become apparent from the following detailed description of preferred embodiments thereof in connection with the accompanying drawings.

Brief Description of the Drawings

[0010] Preferred embodiments according to the present invention will now be described with reference to the Figures, in which like reference numerals denote like elements.

[0011] FIG 1 shows a flowchart of the method of rending fast visualization of protein three-dimension structures in accordance with one embodiment of the present invention.

[0012] FIG 2 shows a functional block diagram of the system in accordance with one embodiment of the present invention.

[0013] FIG 3 shows one exemplary annotation of a PDB file with rendering table information in accordance with one embodiment of the present invention.

[0014] FIG 4 shows the different images rendered using different atom depth.

[0015] FIG 5 shows the results of rendering for different viewing angles when a similarity index of 50.0 is chosen.

[0016] FIG 6 shows real time visualization for different protein-protein interaction positions between the Dengue 2 Virus Envelope protein domain 3 (colored in light gray) and Sugar Binding Protein (colored in dark gray) using atom depth of 6.0. (696 atoms were rendered compared to a total of 1822 atoms).

Detailed Description of the Invention

[0017] The present invention may be understood more readily by reference to the following detailed description of certain embodiments of the invention.

[0018] Throughout this application, where publications are referenced, the disclosures of these publications are hereby incorporated by reference, in their entireties, into this application in order to more fully describe the state of art to which this invention pertains.

[0019] In the following detailed description, specific details are set forth in order to provide a thorough understanding of the invention. However, it will be understood by those skilled in the relevant art that the present invention may be practiced without these specific details. In other instances, well-known methods, procedures, components, and materials have not been described in detail so as not to obscure the present invention.

[0020] In one aspect of the present invention, there is provided a method of rendering fast visualization of protein three-dimension structures. Briefly, the method improves the speed of visualization of protein three-dimension structures by displaying fewer atoms. The method is based on the realization that atoms buried deep within three-dimension structures contribute less to the surface configuration of one protein than do the ones exposed on the surfaces. In other words, the contribution of one atom to the surface configuration of one protein is related to its position within the three-dimension structure.

Thus, the method defines a solvent-accessible surface area of the three-dimension structure of one protein, then calculates the atom depth of each atom of the protein from the nearest solvent-accessible atom, and then provides a rendering table that correlates the atom depth threshold with the similarity index threshold; thereby, according to the image similarity index threshold supplied by a user, the images of protein three-dimension structures can be output with constant image accuracies regardless of view angle.

[0021] As discussed earlier, the terms of "solvent-accessible surface area" and "atom depth" can be defined differently. While the present invention is not limited to any particular definitions of these terms, the following definitions are given for the convenience of illustrating of the principles of the present invention.

[0022] For a protein's three-dimension structure, "solvent-accessible surface area" as used herein refers to the continuous surface that can be reached by the center of charge of a solvent molecule.

[0023] "Atom depth" as used herein is defined as the distance of an atom within one protein's three-dimension structure to its nearest surface atom of the solvent-accessible surface area.

[0024] "Similarity index" as used herein denotes a measurement of the similarity of the new image generated by an atom depth threshold in comparison with the original image.

[0025] Now referring to FIG 1, there is provided a flowchart of the method of rending fast visualization of protein three-dimension structures in accordance with one embodiment of the present invention. The method **10** obtains files of three-dimension structures of proteins **11**. The files can be obtained from locally stored folders or public or private database via web, e.g., http://www.rcsb.org/pdb. Each file usually includes structural information such as the atom number, atom type, residue name, residue number, atomic coordinates, occupancy, temperature factor etc. For each file, the method then calculates the solvent-accessible surface area through any of the publicly available software (e.g., POPS [http://mathbio.nimr.mrc.ac.uk/~ffranca/POPS/], GETAREA1.1 [http://www.scsb.utmb.edu/cgi-bin/get_a_form.tcl]) **12.** Then the method calculates the atom depth for each atom **13**. A predefined threshold for the solvent accessible surface area is used to decide which of the atoms are surface atoms. Surface atoms will be

assigned the atom depth value of 0. For any non-surface atom, the distance to the nearest surface atom is denoted as the atom depth.

[0026] Then the method provides a rendering table for each protein **14**. The rendering table correlates the atom depth with similarity indexes at different view angles. The image similarity indexes of one protein molecule are generated for a fixed number of view angles known as the reference view angles. The number of reference view angles needed depends on the shape of the protein molecules. For globular protein molecules, 12 view angles are generally sufficient. From each of the reference view angle, images are generated using different atom depth thresholds. The newly generated images are then compared with the original image to calculate the image similarity index which measures the percentage of pixels with the same intensity in the 2 images excluding the background pixels. The data for the image similarity index is stored into a rendering table as shown in Table 3. For viewing angle not belonging to the reference view angle, the image similarity index will be interpolated from the data of the 2 closest reference view angle. Experimental result shows that the interpolated data is a good estimate of the actual data.

[0027] Create the Rendering Table according to the pseudo code below:

```
For Y_rotation_angle = principal viewing angles(eg. 0, 90,-90) do
    For X_rotation_angle = principal viewing angles (eg. 0,90,180,270) do
      For atom depth threshold = 0 to max do
            Generate a image for all atoms with atom depth less than the
            threshold value
            Compare generated  image with original image to get image
            similarity index
      End for
    End for
End for
```

[0028] Then the rendering table allows displaying a three-dimension structure of one protein with a pre-defined accuracy according to a user's input **15**. When the user supplies an image similarity index, a corresponding atom depth threshold will be identified within the rendering table. For example, if the viewing angle is 90 degrees and the similarity index is 95.0, the threshold value of 6.0 will be chosen according to Table 3. If the viewing angle is 45 degrees, the image similarity data for view angle 45 degrees will be generated using a simple interpolation of the data for 0 and 90 degrees. If the similarity index is 95.0, the threshold for viewing angle 45 degrees is 6.5 as shown in Table 1. For

each atom, if the atom depth is less the threshold, the atom will be rendered. If the atom depth is more than the threshold, the atom will not be rendered.

[0029] In another aspect of the present invention, there is provided a system for rendering fast visualization of protein three-dimension structures. FIG 2 shows a functional block diagram of the system in accordance with one embodiment of the present invention. The system **20** comprises an input means **25** for enabling a user to input information such as protein ID and similarity index, a display means **26** for displaying the three-dimension structures of proteins, and a microprocessor **21** for taking instructions from the input means, executing the fast visualization programs, and outputting the three-dimension images. The microprocessor **21** further comprises a ROM/RAM memory module **22** for storing protein files and intermediate data, a program module **23** for supporting the microprocessor to obtain protein files via internet, and a fast protein visualization program **24** embedded within the microprocessor. The input means may be any electronic item that is suitable for inputting information to the microprocessor. The displaying means may be any electronic item that is able to display a three-dimension structure. The microprocessor may be a PC, PDA, or notebook.

[0030] In yet another aspect of the present invention, there is provided a database of protein three-dimension structure files, wherein each file is annotated with a rendering table. In order for the new PDB files with atom depths and rendering table to be compatible with conventional PDB viewer, the PDB "USER" record is used as explained in Couch et al., "Annotating PDB Files with Scene Information," J. Mol. Graph. (1995) 13,153-158. In one embodiment, four new annotation records are employed to implement the fast rendering.

[0031] USER ATOMDEPTH atom_number atom_depth: The atom number and the atom depth are recorded here;

[0032] USER XROTATION principal view angles: The principal view angles from rotating the X axis;

[0033] USER YROTATION principal view angles: The principal view angles from rotating the Y axis; and

[0034] USER RDATA atom_depth_threshold similarity index1, similarity index2,.....: The rendering data are recorded here, atom depth threshold is given together with the similarity index for each combination of the principal view angles.

[0035] One exemplary annotation is shown in FIG 3.

[0036] Examples

[0037] The following examples are provided for the sole purpose of illustrating the principles of the present invention. They are by no means intended to limit the scope of the present invention.

[0038] Data

[0039] The pdb data files for protein molecules were obtained from the PDB database, http://www.rcsb.org/pdb/.

[0040] Results

[0041] FIG 4 shows the different images rendered using different atom depths. As the image similarity index increases, atom depth increases resulting in better images at higher rendering time and vice versa. The image similarity index allows the user to trade image accuracy for speed of rendering.

[0042] FIG 5 shows the result of rendering for different viewing angles when a similarity index of 50.0 is chosen. Different atom depths for different view angles will be selected to give image similarity of 50.0.

[0043] Table 1 shows the interpolated data for Y rotation =45 degrees and the actual data. It can be seen that the interpolated data closely resembles the actual data as the maximum error between the interpolated and actual data is only 2%. The minimum error rates demonstrated that we could accurately interpolate the image similarity index for any view angle and obtain constant image accuracy.

[0044] Table 1. Comparison of interpolated data with actual data

Atom Depth	Y rot = 0 deg	Y rot = 90 deg	Interpolated Data for Y rot =45 deg	Actual data for Y rot = 45 deg	Error between interpolated and actual data (%)
14.50	100.00	100.00	100	100	0
14.00	100.00	100.00	99.99783	100	0.002166
13.50	99.98	100.00	99.98917	100	0.010828
13.00	99.95	100.00	99.97618	99.98582	0.009643
12.50	99.90	100.00	99.95024	99.9844	0.03417
12.00	99.85	100.00	99.92136	99.96597	0.04462
11.50	99.74	100.00	99.86794	99.91491	0.047014
11.00	99.64	100.00	99.81741	99.85535	0.038001
10.50	99.48	99.98	99.73168	99.7731	0.041522
10.00	99.30	99.94	99.62027	99.65398	0.033827
9.50	99.05	99.88	99.46069	99.5845	0.12432
9.00	98.75	99.81	99.27665	99.49374	0.218194
8.50	98.37	99.71	99.04452	99.21437	0.171195
8.00	97.79	99.51	98.64976	98.86552	0.218235
7.50	96.93	99.20	98.06705	98.34792	0.28558
7.00	95.90	98.44	97.17177	97.42899	0.264009
6.50	94.40	97.24	95.81943	96.67882	0.888908
6.00	91.76	95.20	93.47743	94.73744	1.329998
5.50	88.85	92.97	90.90654	92.3834	1.598619
5.00	84.86	89.72	87.28948	89.07923	2.009168
4.50	78.70	84.12	81.41109	82.92468	1.825267
4.00	73.29	79.18	76.23214	77.97411	2.234026
3.50	66.30	73.24	69.76995	71.3289	2.185578
3.00	60.24	67.50	63.87075	65.21973	2.068366
2.50	53.37	60.47	56.92201	57.56201	1.111834
2.00	45.02	51.03	48.02668	48.67762	1.33725
1.50	39.79	45.47	42.63369	43.24915	1.423057
1.00	31.83	37.25	34.54327	34.83841	0.847148
0.5	31.83	37.25	34.54327	34.83841	0.847148

[0045] Table 2 shows the potential gain in rendering speed at the different similarity index. Consider the viewing angle at X rotation = 0 degree & Y rotation = 0 degree, a similarity index of 95.0 will lead to an atom depth of 6.5. From Table 2, an atom depth of 6.5 will give a rendering gain of about 1.4 times over the original image. A lost of 5% in image quality will give rise to a 1.4 times improvement in rendering speed. From Table 2, the atom gain is seen to be a good estimate of the time gain even though the atoms have different radii.

[0046] Table 2. Number of atoms and speed gain at different similarity index for X rotation = 0 deg, Y rotation =0 deg

Similarity Index	Atom Depth	No atoms	Time (s)	Atom gain	Time gain	Time gain (%)
100	14.5	11521	186	1	1	0
99	9.5	10495	171	1.097761	1.087719	8.77
98	8	9570	155	1.203866	1.2	20
97	7.5	9194	147	1.2531	1.265306	26.53
96	7	8773	144	1.313234	1.291667	29.166
95	6.5	8217	134	1.402093	1.38806	38.80
90	5.5	6945	112	1.658891	1.660714	66.07
85	5	6203	108	1.857327	1.722222	72.22
80	4.5	5319	88	2.166009	2.113636	111.36
75	4	4631	76	2.4878	2.447368	144.73
70	4	4631	76	2.4878	2.447368	144.73
65	3.5	3872	66	2.975465	2.818182	181.81
60	3	3308	56	3.482769	3.321429	232.14
55	2.5	2703	45	4.262301	4.133333	313.33
50	2.5	2703	45	4.262301	4.133333	313.33
45	2	1895	32	6.079683	5.8125	481.25
40	1.5	1450	23	7.945517	8.086957	708.69
35	1	967	17	11.91417	10.94118	994.11
30	1	967	17	11.91417	10.94118	994.11

[0047] Time gain is defined to be the ratio for time taken to render all the atoms over the time taken to render the atoms satisfying the similarity index threshold. Atom gain is defined to be the ratio for the total number of atoms over the number of atoms satisfying the similarity index threshold.

[0048] Table 3. Rendering Table for 1ova.pdb

	X rotation = 0 degree				X rotation = 90 degrees				X rotation = -90 degrees			
Atom Depth	Y rot = 0	Y rot = 90	Y rot = 180	Y rot = 270	Y rot = 0	Y rot = 90	Y rot = 180	Y rot = 270	Y rot = 0	Y rot = 90	Y rot = 180	Y rot = 270
14.50	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
14.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
13.50	99.98	100.00	100.00	100.00	100.00	100.00	100.00	100.00	99.97	99.97	99.97	99.97
13.00	99.95	100.00	99.97	100.00	99.99	99.99	99.99	99.99	99.94	99.94	99.94	99.94
12.50	99.90	100.00	99.95	99.99	99.96	99.96	99.96	99.96	99.92	99.92	99.92	99.92
12.00	99.85	100.00	99.91	99.97	99.93	99.93	99.93	99.93	99.84	99.83	99.83	99.83
11.50	99.74	100.00	99.83	99.97	99.91	99.91	99.91	99.91	99.80	99.80	99.80	99.79
11.00	99.64	100.00	99.77	99.97	99.87	99.86	99.86	99.86	99.67	99.66	99.66	99.65
10.50	99.48	99.98	99.74	99.95	99.74	99.72	99.73	99.72	99.36	99.36	99.37	99.36
10.00	99.30	99.94	99.71	99.88	99.56	99.56	99.55	99.55	99.26	99.25	99.26	99.24
9.50	99.05	99.88	99.55	99.80	99.33	99.32	99.32	99.32	98.97	98.95	98.96	98.93
9.00	98.75	99.81	99.16	99.38	99.05	99.05	99.06	99.05	98.59	98.57	98.59	98.55
8.50	98.37	99.71	98.92	98.95	98.40	98.37	98.38	98.39	97.97	97.93	97.96	97.93
8.00	97.79	99.51	98.63	98.48	97.51	97.47	97.50	97.48	97.25	97.25	97.24	97.22
7.50	96.93	99.20	98.19	97.88	96.55	96.53	96.54	96.53	96.41	96.37	96.41	96.39
7.00	95.90	98.44	97.27	97.18	95.22	95.20	95.20	95.17	95.72	95.69	95.76	95.69
6.50	94.40	97.24	96.09	96.03	93.58	93.56	93.56	93.52	94.19	94.09	94.19	94.12
6.00	91.76	95.20	94.08	94.38	90.59	90.51	90.53	90.48	92.21	92.06	92.19	92.09
5.50	88.85	92.97	90.79	91.26	85.86	85.80	85.79	85.74	89.13	88.97	89.09	88.97
5.00	84.86	89.72	87.12	87.34	81.62	81.51	81.52	81.47	84.86	84.67	84.87	84.72
4.50	78.70	84.12	81.15	81.61	75.79	75.66	75.64	75.62	78.54	78.29	78.48	78.40
4.00	73.29	79.18	75.59	75.96	70.16	70.02	70.00	70.02	72.30	72.04	72.24	72.06
3.50	66.30	73.24	69.37	69.25	64.31	64.11	64.15	64.15	66.16	65.94	66.15	65.97
3.00	60.24	67.50	63.64	62.73	59.23	57.99	58.04	58.05	59.08	58.83	59.01	58.84
2.50	53.37	60.47	56.76	54.30	51.19	50.90	50.96	50.99	52.03	51.71	51.94	51.74
2.00	45.02	51.03	47.86	45.23	42.18	41.75	41.77	41.70	43.73	43.24	43.55	43.30
1.50	39.79	45.47	41.56	38.64	36.07	35.66	35.70	35.64	37.91	37.36	37.73	37.47
1.00	31.83	37.25	34.21	31.33	28.79	28.47	28.50	28.44	30.09	29.66	29.92	29.74
0.50	31.83	37.25	34.21	31.33	28.79	28.47	28.50	28.44	30.09	29.66	29.92	29.74
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

[0049] The visualization rendered with fewer atoms was applied to study protein-protein interactions and found that it was applicable in such studies. For example, FIG 6 shows real time visualization for different protein-protein interaction positions between the Dengue 2 Virus Envelope protein domain 3 (colored in light gray) and Sugar Binding Protein (colored in dark gray) using atom depth of 6.0. (696 atoms were rendered compared to a total of 1822 atoms).

[0050] While the present invention has been described with reference to particular embodiments, it will be understood that the embodiments are illustrative and that the invention scope is not so limited. Alternative embodiments of the present invention will become apparent to those having ordinary skill in the art to which the present invention pertains. Such alternate embodiments are considered to be encompassed within the spirit and scope of the present invention. Accordingly, the scope of the present invention is described by the appended claims and is supported by the foregoing description.

CLAIMS

What is claimed is:

1. A method for rendering fast visualization of protein three dimension structures, said method comprising the steps of:

providing a file of the three dimension structure of a protein; wherein when the file is presented with all atoms of the protein, it is considered as original image for comparison;

calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area;

generating a plurality of images with different atom depth thresholds for a predetermined number of view angles; wherein the different atom depth thresholds determine the number of atoms that are shown in each of the plurality of images;

calculating image similarity indexes of images between each of the plurality of images with different atom depth thresholds and the original image at each of the predetermined number of view angles;

generating a rendering table that correlates the image similarity indexes with the atom depths; and

displaying the three dimension structure with an accuracy that is input by a user.

2. The method of claim 1, wherein the steps of calculating atom depth, calculating image similarity indexes, and generating a rendering table can be done prior to visualization so that the rendering table is part of the file of the three dimension structure of a protein.

3. The method of claim 1, wherein the rendering table is generated by following pseudo-code:

```
For Y_rotation_angle = principal viewing angles(eg. 0, 90,-90) do
    For X_rotation_angle = principal viewing angles (eg. 0,90,180,270) do
      For atom depth threshold = 0 to max do
            Generate a image for all atoms with atom depth less than the
            threshold value
```

```
                    Compare generated  image with original image to get image
                    similarity index
                End for
            End for
        End for
```

4. A database of protein three dimension structure files, wherein each protein three dimension structure file comprises a rendering table that correlates image similarity indexes and atom depths; thereby the protein three dimension structure files enable fast visualization upon selection of an image similarity index for viewing by a user;

wherein the image similarity indexes are obtained by generating a plurality of images with different atom depth thresholds for a predetermined number of view angles; wherein the different atom depth thresholds determine the number of atoms that are shown in each of the plurality of images; and

calculating image similarity indexes of images between each of the plurality of images with different atom depth thresholds and original image at each of the predetermined number of view angles.

5. The database of claim 4, wherein the rendering table is generated by following pseudo-code:

```
For Y_rotation_angle = principal viewing angles(eg. 0, 90,-90) do
    For X_rotation_angle = principal viewing angles (eg. 0,90,180,270) do
        For atom depth threshold = 0 to max do
                Generate a image for all atoms with atom depth less than the
                threshold value
                Compare generated  image with original image to get image
                similarity index
        End for
    End for
End for
```

6. A system for fast visualization of protein three dimension structures, said system comprising:

a computer readable medium;

a computer program embedded within the computer readable medium, wherein the computer program enables fast visualization of protein three dimension structures;

wherein the computer program comprises:

means for providing a file of the three dimension structure of a protein;

means for calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area;

means for generating a plurality of images with different atom depth thresholds for a predetermined number of view angles; wherein the different atom depth thresholds determine the number of atoms that are shown in each of the plurality of images;

means for calculating image similarity indexes of images between each of the plurality of images with different atom depth thresholds and the original image at each of the predetermined number of view angles; and

means generating a rendering table that correlates the image similarity indexes with the atom depths; and

a display means for displaying the three dimension structure with an accuracy that is input by a user.

7. The system of claim 6, wherein the steps of calculating atom depth, calculating image similarity indexes, and generating a rendering table can be done prior to visualization so that the rendering table is part of the file of the three dimension structure of a protein.

8. The system of claim 7, wherein the rendering table is generated by following pseudo-code:

```
For Y_rotation_angle = principal viewing angles(eg. 0, 90,-90) do
    For X_rotation_angle = principal viewing angles (eg. 0,90,180,270) do
      For atom depth threshold = 0 to max do
            Generate a image for all atoms with atom depth less than the
            threshold value
            Compare generated  image with original image to get image
            similarity index
      End for
    End for
End for
```

METHOD AND SYSTEM FOR FAST PROTEIN VISUALIZATION USING PRE-CALCULATED IMAGE SIMILARITY INDEX AND ATOM DEPTH

ABSTRACT

The present invention provides a method and system for rendering fast visualization of protein 3D structures. The method and system of the present invention improves the speed of visualization using pre-calculated image similarity index and atom depth. In one embodiment, the method comprises the steps of providing a file of the three dimension structure of a protein, calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area, calculating image similarity indexes of images with different atom numbers in comparison with the original image, generating a rendering table that correlates the image similarity indexes with the atom depths, and displaying the three dimension structure with an accuracy that is input by a user. In one embodiment, the system comprises a computer readable medium; a computer program embedded within the computer readable medium, wherein the computer program enables fast visualization of protein three dimension structures; wherein the computer program comprises: means for providing a file of the three dimension structure of a protein; means for calculating atom depth of each atom within the three dimension structure using a solvent accessible surface area; means for calculating image similarity indexes of images with different atom numbers in comparison with the original image; and means generating a rendering table that correlates the image similarity indexes with the atom depths; and a display means for displaying the three dimension structure with an accuracy that is input by a user.

FIG 5