Data Processing for STL used for Protein Modeling

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(Summary)

・Input File is a PDB(text).

・In a PDB, ATOM-fields indicate coordinates of each component atom in angstrom unit. After expanding the size by one hundred million, each numerical value becomes in mm unit. The model is due to this size.

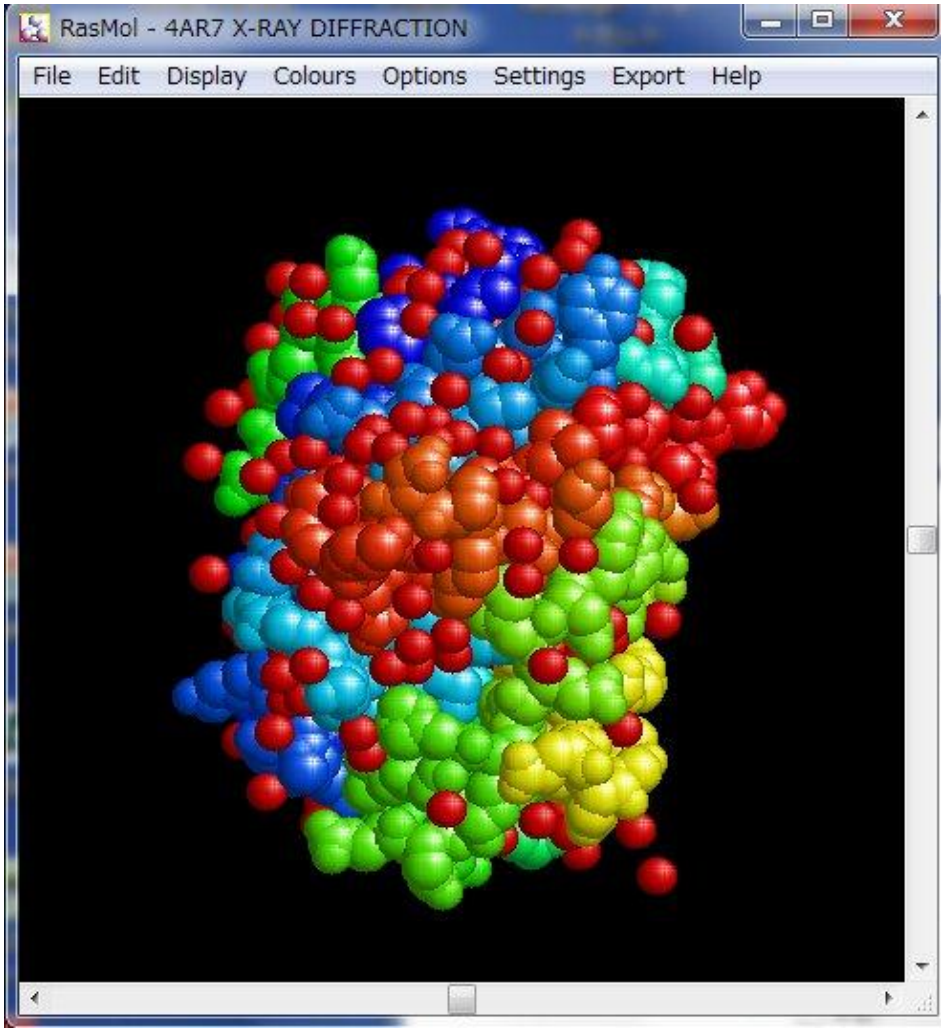
・RasWin can be used for 3D viewing.

・First we change the expanded coordinates into point-clouds with our CG soft called NfDesign and set sphere metaball of radius 1.4mm at each point.

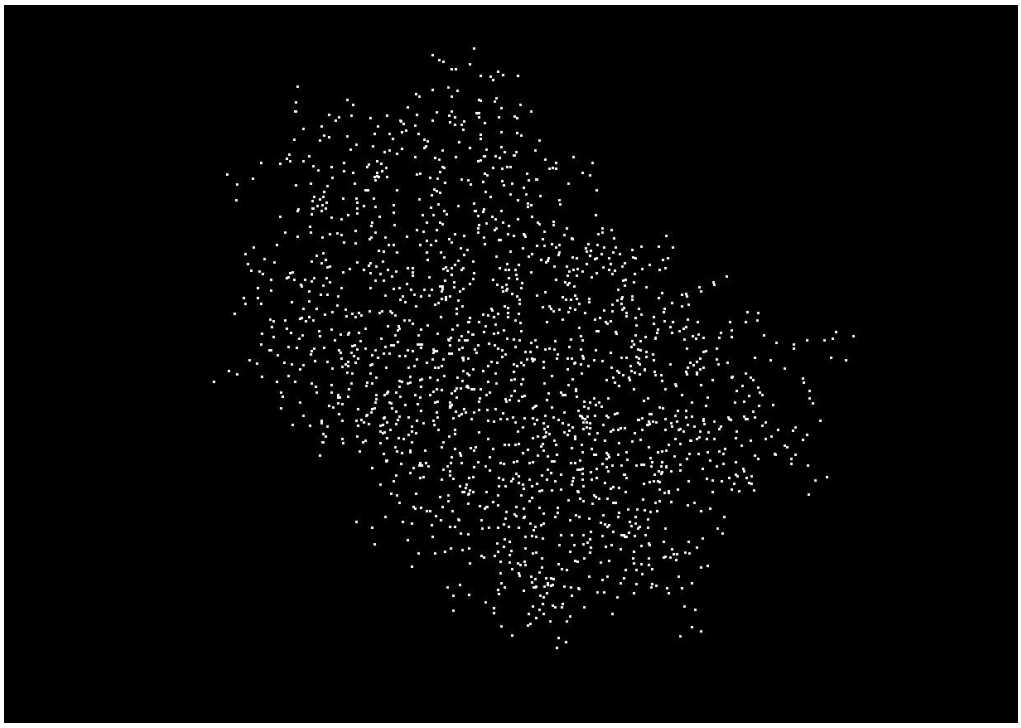
・After processing, STL data(text or binary) can be output.

（Process）

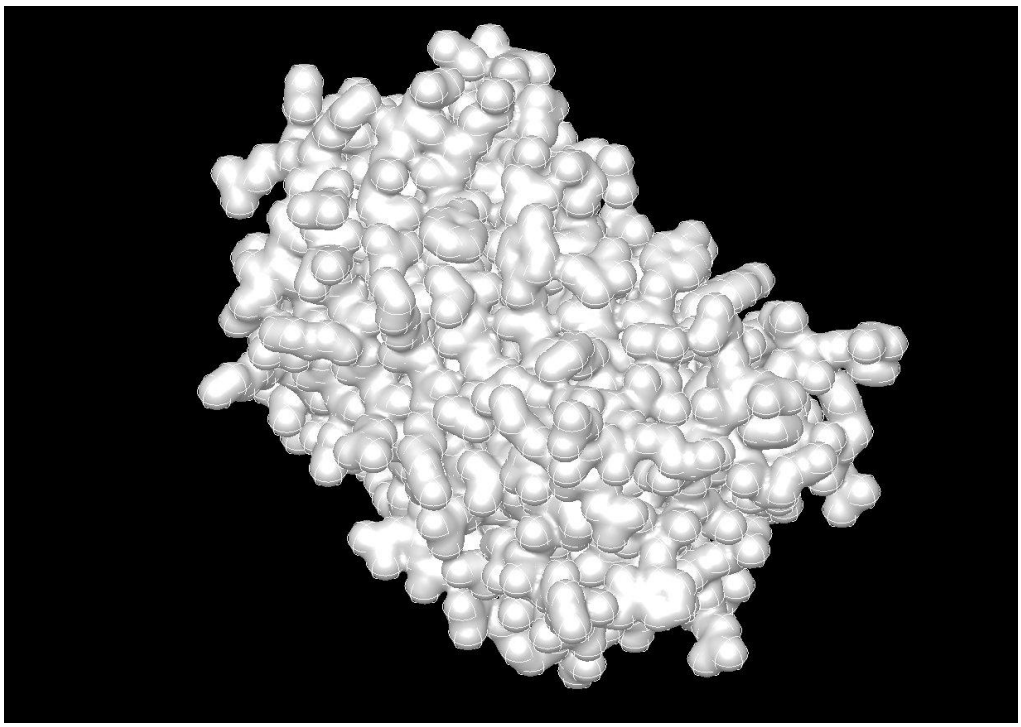
・RasWin displays 4AR7.pdb accessed from Protein Data Bank.



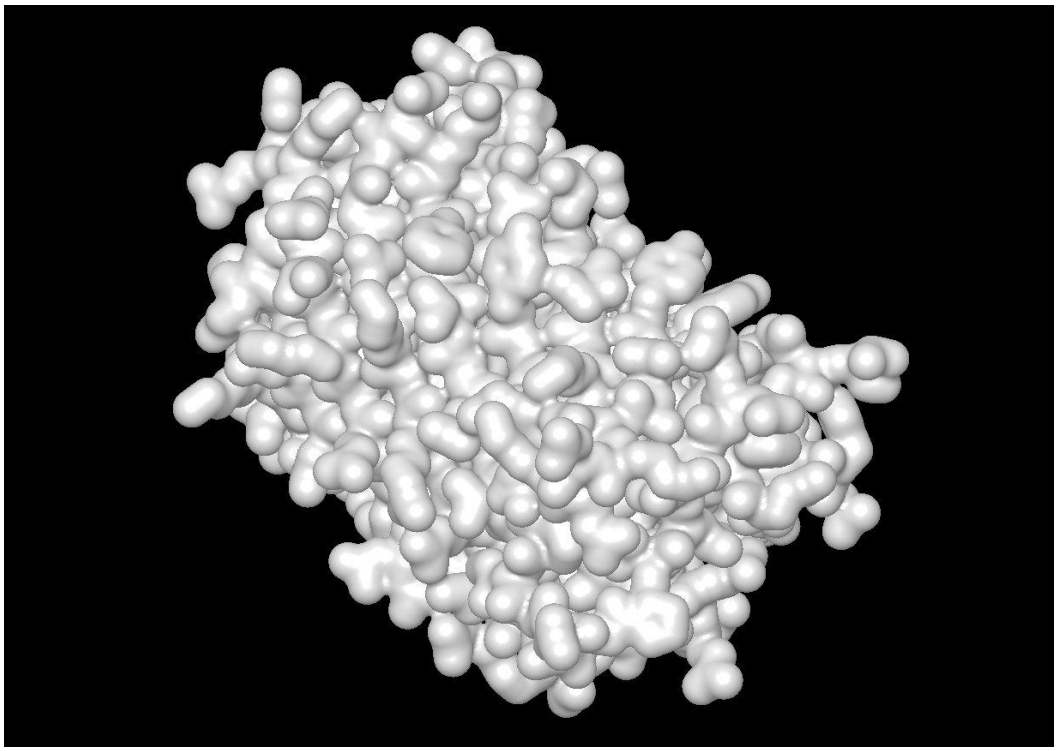
・NfDesign indicates point-clouds of　ATOM coordinates as 3D.
Points are expanded by one hundred million.(oblique viewpoint)



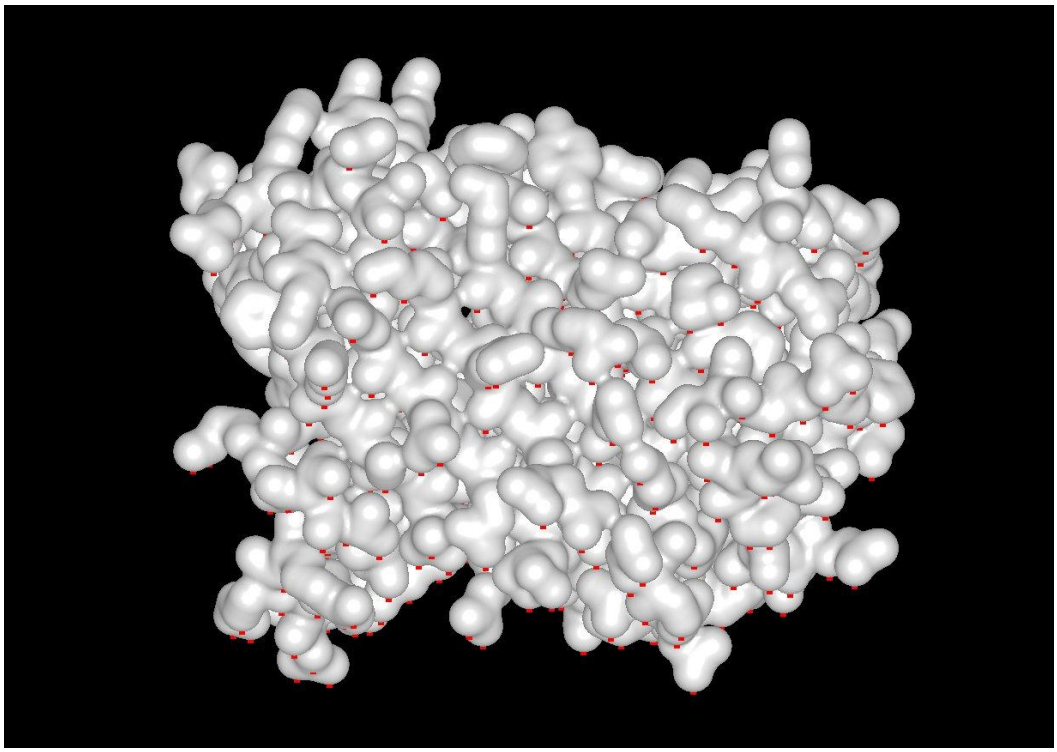
・A metaball of 1.4mm radius is set at each point.
Overlap metaballs are automatically merged.(oblique viewpoint)



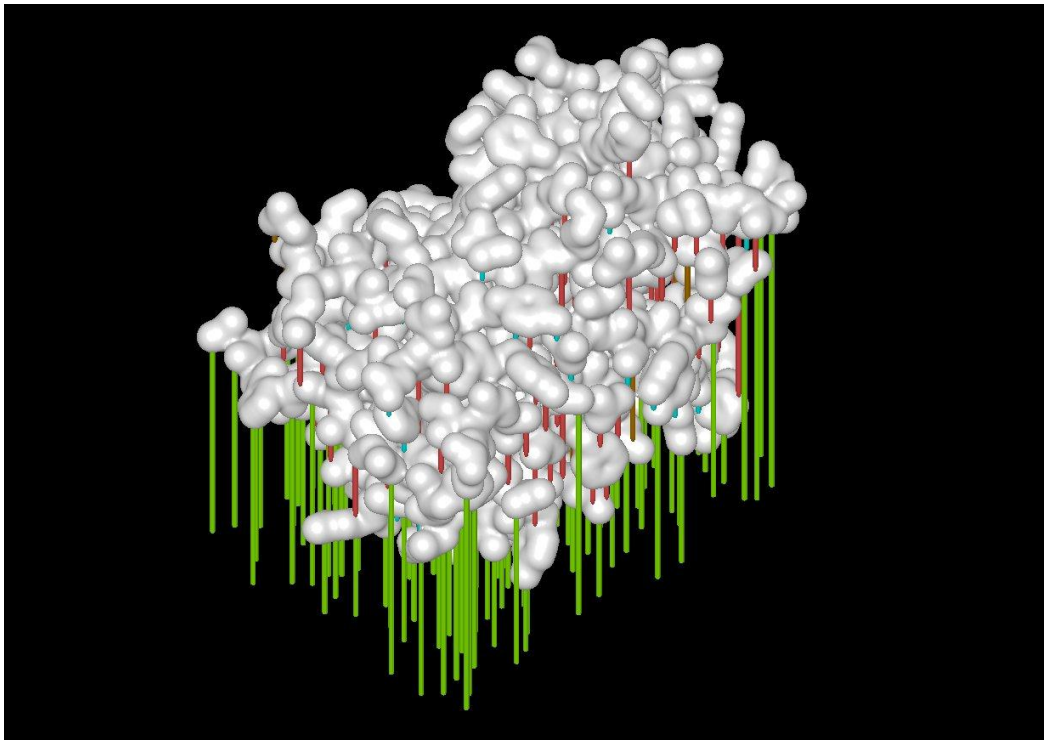
・Metaballs are changed to triangle-meshes.(oblique viewpoint)



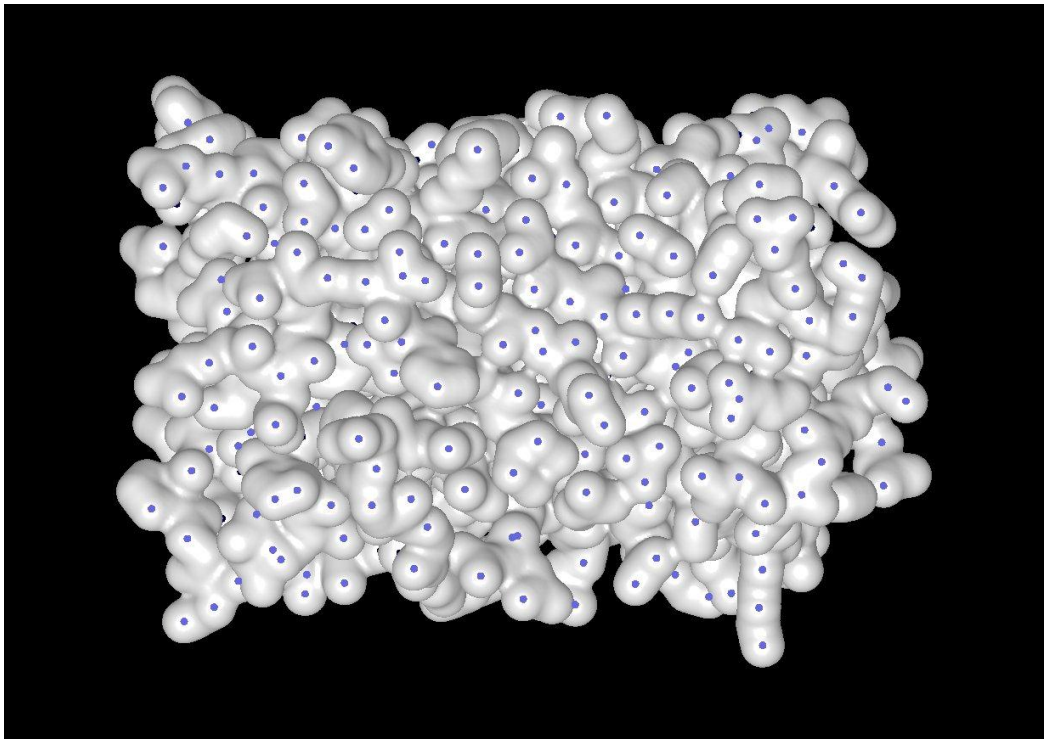
・We have found the positions of support with other programs and have set red points there.(side viewpoint)



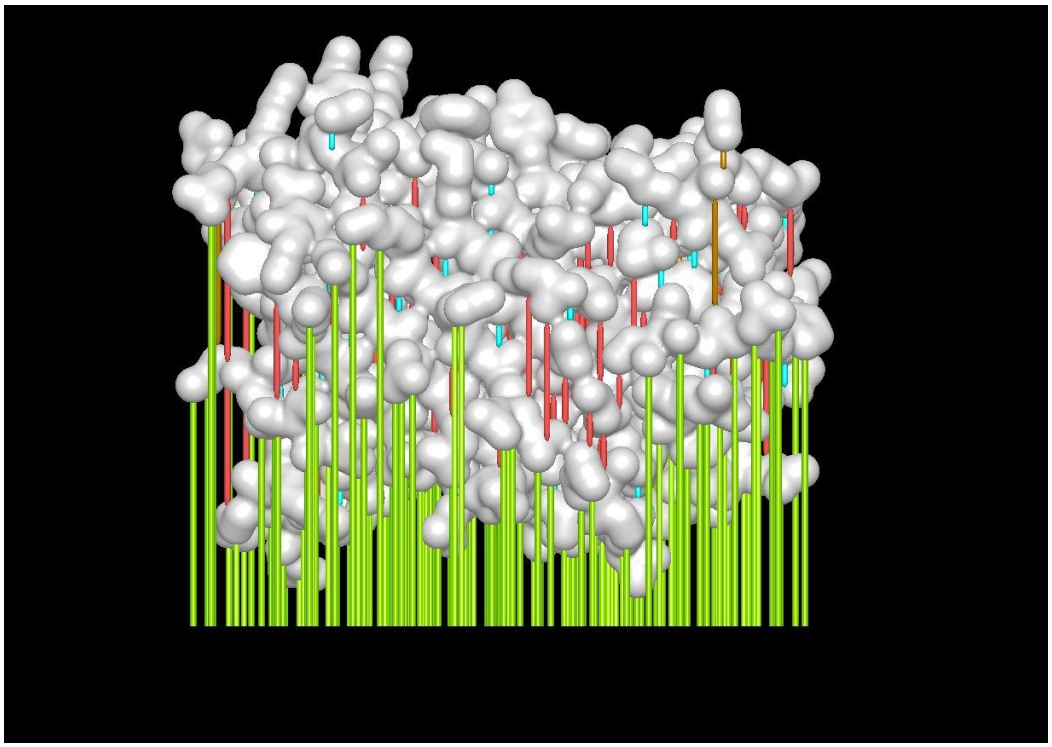
・After several steps with NfDesign, the bottom supports(green) and middle supports are finished as indicated as follows;　　(oblique viewpoint)



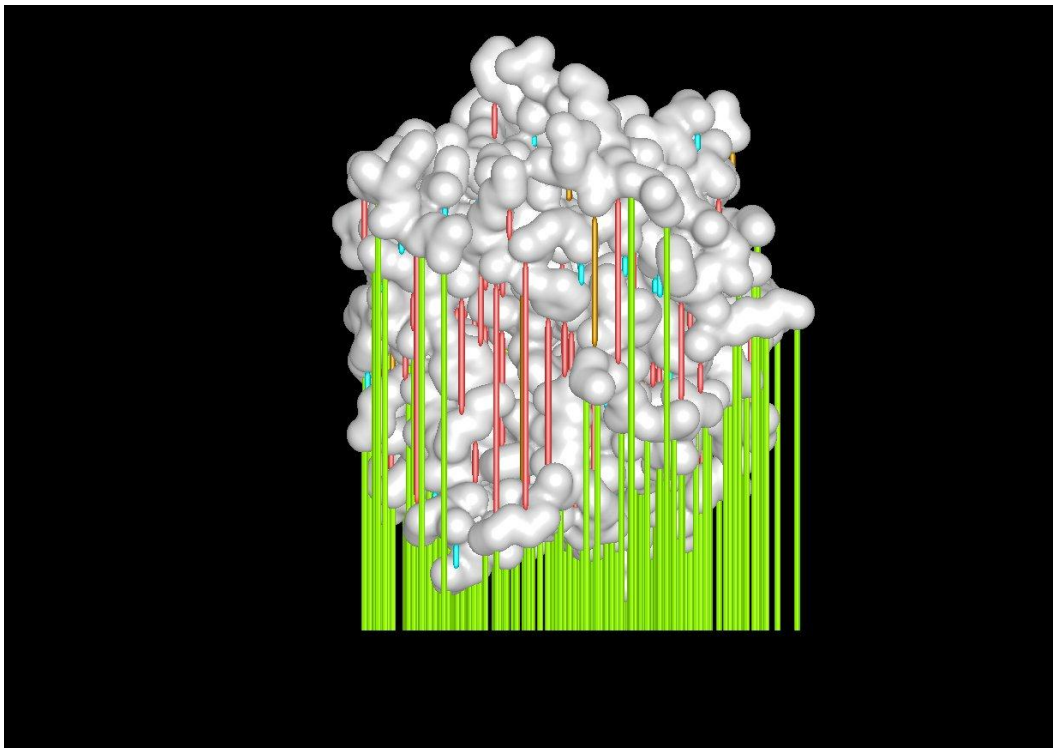
・The Bottom View of the Model and Supports; The color of bottom supports is changed.



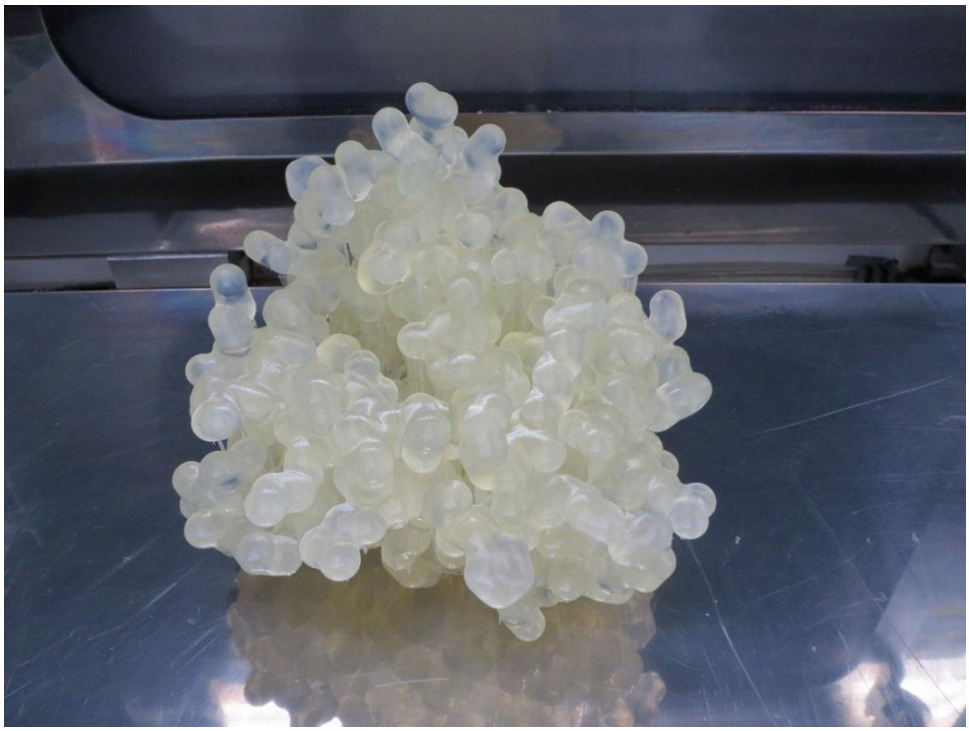
・The Side View of the Model and Supports;



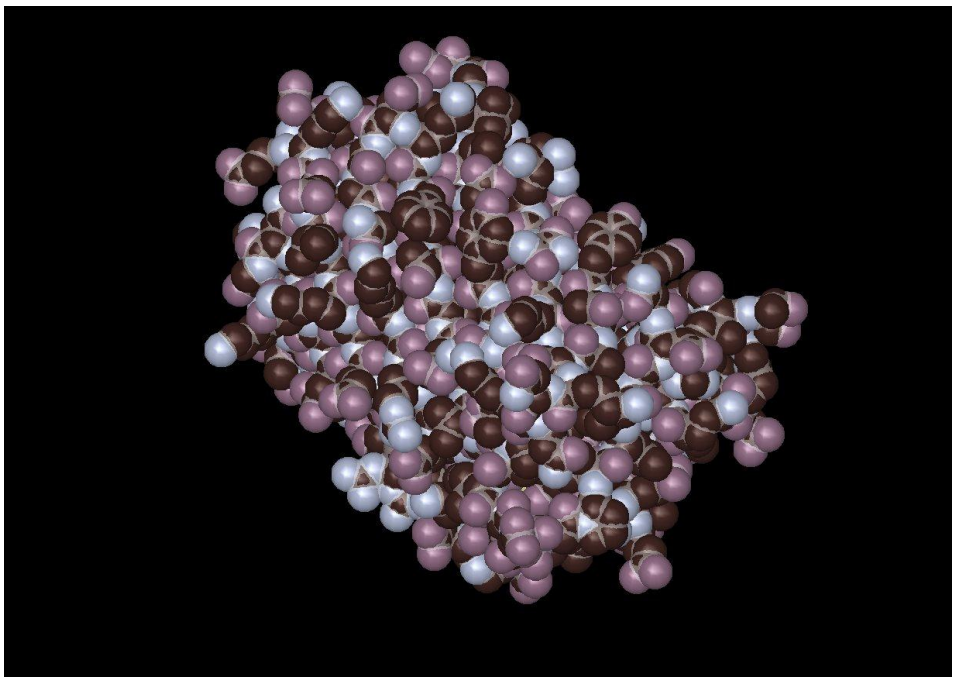
・The Front View of the Model and Supports;



・A Real Model Photo (other than this Sample Here)

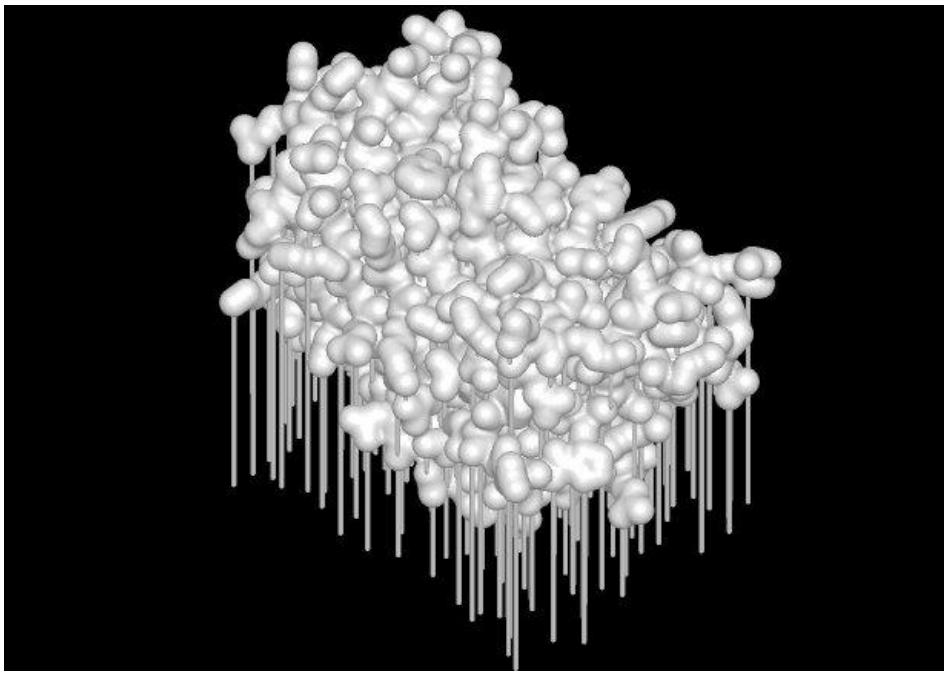


・The real model is composed in the same resin and it is difficult to find the sort of atoms. NfDesign can generate the following 3D model where the same sort of atoms has the same color and users can select any viewpoints, isometric or perspective. Color setting is indicated at the next page.



; C ; N ; O ; S

・All the images here are due to NfDesign except the first RasWin image.
NfDesign can get and output STL(binary and text) format.
The following is an image of STL within NfDesign.



・After finishing the model and supports, we can find the continuity of the object.
Errors found can be corrected with NfDesign.

・The size can freely be set. If expanded by 400 million, radius 5.6mm spheres are set.

・The thicknesses of the supports can freely be set as far as circumstances permit.

・We have set 1.4mm radius spheres(at multiplied by 100 million) so far, and this way has counted nothing. If users want different radius to the sort of atoms, it is available.