Step-by-Step Instructions to Reproduce the Examples in the Tutorials

Uniform Hollow Cylinder model:

1. Go to **Domain View** pane on the top-left corner, choose **Uniform Hollow Cylinder** and press **Add**.

2. It is recommended to go to **3D Graph** to see the structures you are going to compute.

3. Increase the **Level of Detail** to maximum (this option can be found at the **Preferences** pane).

4. In **Domain View**, Select the **Uniform Hollow Cylinder** model that you have already added.

5. Go to **Parameter Editor** pane, change the **Height** (in nm units) to 15.

6. Go to **Settings** and choose **Suggest Parameters.**

7. In **Suggest Parameters** pane, write: **x**=2, **y**=2 (the cylinder diameter is 2 nm), **z**=15 (the Height) and **q Max**=10 (in units of nm^{-1}).

8. On the left side of the **Suggest Parameters** pane you should get: **Grid Size=**110**, Integration Method=**Adaptive Gauss Kronrod, **Integration Iterations:** 1E6, **Convergence:** 0.001, **Generated Points:**1000, **Update Interval**: 500 ms. If not, follow the instructions again.

9. Enter the proposed parameters to the **Preferences** pane.
10. Go to the **2D Graph** and click **Generate** in the **Controls** pane.
11. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

Two Geometric Thingymabobs:

1. Go to **Domain View** pane on the top-left corner, choose **Uniform Hollow Cylinder** and press **Add**.

2. It is recommended to go to **3D Graph** to see the structures you are about to compute.

3. Go to **Domain View**, choose **Sphere,** and press **Add**.

4. In the **Preferences** pane, increase the **Level of Detail** to maximum.

5. In **Domain View**, select the **Sphere** model that you have already added.

6. Go to **Symmetry Editor** and change **Z**=7, go to **Parameter Editor** and change the **Radius** of **Layer 2** to: 2.

7. In **Domain View**, select the **Uniform Hollow Cylinder** model you have already added.

8. In the **Parameter Editor** pane, press **Add Layer**.

9. In the **Parameter Editor** pane, go to the electron density, **E.D.,** of the 3rd layer, click on the current number and change it to 450.

10. Go to **Settings** and choose **Suggest Parameters.**

11. In **Suggest Parameters**, write: **x**=4, **y**=4 (the diameter is 4), **z**=14 (the height) and **q Max**=5.

12. On the left side of the **Suggest Parameters** pane you should get: **Grid Size =**60**, Integration Method =**Monte Carlo **Integration Iterations:** 1E6, **Convergence:**0.001, **Generated Points:** 500, **Update Interval**: 500 ms. If not, repeat the instructions.

13. Enter the proposed parameters to the **Preferences** pane.

14. Go to the **2D Graph** and click **Generate** in the **Controls** pane.

15. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

Singel Small PDB and Fit part a:

1. Go to **Domain View** pane on the top-left corner, choose **PDB file,** also ensure that **Center PDB** option is ticked before pressing **Add.** Load the **PDB file** of **Lysozyme.**
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.
3. Increase the **Level of Detail** to maximum (this option can be found at the **Preferences** pane). If the **3D Graph** becomes slower, reduce the **Level of Detail**.

   Note: you may skip steps 4 and 5 and go directly to step 6, using the proposed parameters from step 5.

4. Go to **Domain View**, choose **Uniform Hollow Cylinder,** and press **Add**.
5. Try to change the parameters of the **Uniform Hollow Cylinder** so that it will envelope the Lysozyme structure. On the left side of **Suggest Parameters** pane you should get: **x=**4**, y=**4, **z=**4**, q Max=**10**.**
6. Delete the **Uniform Hollow Cylinder** model**.**
7. On the left side of **Suggest Parameters** you should get**: Grid Size=**50**, Integration Method =**Monte Carlo, **Integration Iterations:** 1E6, **Convergence:** 0.001, **Generated Points:** 1000, **Updated Interval**: 500 ms.
8. Enter the proposed parameters to the **Preferences** pane.
9. In **Domain View**, select the **PDB file** of **Lysozyme** you have already added.
10. In **Parameter Editor** pane, change the **Outer Solvent ED** to 364, **Solvation Thickness** to 0.3 and choose the **Fill Holes** option**.**
11. Go to the **2D Graph** and click **Generate** in the **Controls** pane.
12. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

PDB file part b:

1. Go to **Domain View** pane on the top-left corner, choose **PDB file**. Make sure that **Center PDB** option is ticked before pressing **Add.** Insert the **PDB file** of **Lysozyme** twice**.**
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.

3. Increase the **Level of Detail** to maximum (this option can be found at the **Preferences** pane). If the **3D Graph** becomes slow, reduce the **Level of Detail**.

4. Go to **Domain View**, choose **Manual Symmetry,** and press **Add**. The program allows you to *import locations from file*, choose **No.**

5. To add a layer, go to **Domain View**, choose **Manual Symmetry,** and press **Add Layer**.

6. Go to **Entities** pane in **Domain View**, and drag one of the **PDB File** of **Lysozyme** into **Manual Symmetry.**

7. In **Manual Symmetry,** choose the **PDB File** of **Lysozyme,** which will be later used as the outer solvent.

8. In **Parameter Editor**, change the **Solvent ED** to 0, **Outer Solvent ED** to 1, **Solvation Thickness** to 0.3, and tick the **Fill Holes** and **Solvent Only** options**.**
9. Go to **Domain View**, choose **Manual Symmetry.**

10. In **Parameter Editor**, change the **Scale** to 4 and choose the **Mutable** options**.**
11. Right click **Scale** and choose **Edit Constrains,** change the **Absolute minimum** to 3 and the **Absolute maximum** to 5.
12. In **Controls** pane, choose the **Mutable** option for **Domain Scale** and **Domain Constant.**

13. go to the **2D Graph** and click **Generate** in the **Controls** pane.
14. When the calculation is done click **Fit** in the **Controls** pane.
15. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

Symmetry Files part a:

1. Go to **Domain View** pane on the top-left corner, choose **Sphere** and press **Add**.
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.

3. Increase the **Level of Detail** to maximum (this option can be found in the **Preferences** pane). If the **3D Graph** becomes slow, reduce the **Level of Detail**.

4. In **Domain View**, Choose **sphere**.
5. Go to **Parameter Editor** and change the **Radius** of layer 2 to 0.5 and the **E.D.** to 900.
6. Go to **Domain View**, choose **Manual Symmetry,** and press **Add**. The program allows you to *import locations from file*, choose **No.**

Note: It is possible to skip steps 7-10 by importing locations file called *.dol file, which is located in the fourth example folder, when the **Manual Symmetry** allows you to *import locations from file*.

7. Go to **Entities** pane in **Domain View** and drag the **Sphere** into **Manual Symmetry.**
8. Go to **Domain View**, choose **Manual Symmetry.**
9. Go to **Parameter Editor,** add 7 layers with the parameters:
   alpha=0, **beta**=0**, gamma**=0 and **z**=0.
   Specific parameters for each layer are:
   Layer 1: x=0, **y**=0 ; **Layer 2: x**=1**, y**=0 ; **Layer 3: x**=-1**, y**=0 ;
   Layer 4: x=0.5**, y**=0.866025404 **; Layer 5: x**=0.5 **, y**=-0.866025404 ;
   Layer 6: x=-0.5 **, y**=0.866025404 **; Layer 7: x**=-0.5 **, y**=-0.866025404 **.**
10. Go to **Domain View**, choose **Symmetric Layered Slabs** and press **Add**.
11. Try to change your **Symmetric Layered Slabs** model parameters so that it will envelope the **Manual Symmetry**. On the left side of **Suggest Parameters** pane you should get: **x=**2.5**, y=**2.5, **z=**1**, q Max=**10**.**
12. Delete the **Symmetric Layered Slabs** model**.**
13. On the left side of **Suggest Parameters** pane you should get**: Grid Size=**30**, Integration Method=**Monte Carlo, **Integration Iterations:** 1E6, **Convergence:** 0.001, **Generated Points:** 1000, **Updated Interval**: 500 ms. If not repeat the instructions.

14. Enter the proposed parameters to the **Preferences** pane.
15. Go to the **2D Graph** and click **Generate** in the **Controls** pane.

16. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

Symmetry_Files Part b:

Note: this is another way to compute the same model as in **Symmetry_Files part a**.

1. Go to **Domain View** pane on the top-left corner, choose **Sphere**, and press **Add**.
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.

3. Increase the **Level of Detail** to maximum (this option can be found at the **Preferences** pane). If the **3D Graph** become slower, reduce the **Level of Detail**.

4. In **Domain View**, Choose **sphere**.
5. Go to **Parameter Editor** and change the **Radius** of layer 2 to 0.4 and the **E.D.** to 400
6. Go to **Domain View**, choose **Space-Filling Symmetry**, and press **Add**.
7. Go to **Entities** pane in **Domain View**, and drag the **Sphere** to **Manual Symmetry.**
8. Go to **Domain View**, choose **Space-Filling Symmetry**.
9. Go to **Parameter Editor,** change:
   Vector 1 to: **Distance=**1, **Angle**=90, **Repetitions**=9;
   Vector 2 to: **Distance=**1, **Angle**=90, **Repetitions**=9;
   Vector 3 to: **Distance=**1, **Angle**=120, **Repetitions**=1;
10. Go to **Symmetry Editor** and change **Gamma** to 120 and **x** to 4.
11. Go to **Domain View**, choose **Symmetric Layered Slabs**, and press **Add**.
12. Try to change your **Symmetric Layered Slabs** model parameters so that it will envelope the **Manual Symmetry**. On the left side of **Suggest Parameters** pane you should get: **x=**8**, y=**12, **z=**1**, q Max=**10**.**
13. Delete the **Symmetric Layered Slabs** model**.**
14. On the left side of **Suggest Parameters** pane, you should get**: Grid Size=**100**, Integration Method=** Adaptive Gauss Kronrod, **Integration Iterations:**1E6, **Convergence:** 0.001, **Generated Points:** 1000, **Updated Interval**: 500 ms. If not repeat the instructions.

15. Enter the suggested parameters to the **Preferences** pane.
16. Go to the **2D Graph** and click **Generate** in the **Controls** pane.
17. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

PDB_Symmetry_Files Part a:

1. Go to **Domain View** pane on the top-left corner, choose the **PDB file**: **3j6f_Dimer_2_2_Added_H_GCentered.pdb**. Make sure **Center PDB** option is ticked before pressing **Add.**
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.
3. Reduce the **Level of Detail** to minimum (this option can be found at the **Preferences** pane).
4. Go to **Domain View**, choose **Scripted Symmetry**, and press **Add**.
5. Choose the **Left_Hand_Helix** model, located in the relevant tutorial folder.
6. Go to **Domain View**, choose the **Left Hand Helix** model.
7. Go to **Parameter Editor,** change the parameters:
   Radius=11.9, **Pitch=**12.2, **Units per Pitch**=14, **Units in Pitch**=14, **Units to Skip in Pitch**=0, **Discrete Height**=3, **# Helix Starts**=3.
8. Go to the **Entities** pane in **Domain View**, and drag the **PDB file**: **3j6f** into **Scripted Symmetry.**
9. Choose the **PDB file**: **3j6f** in **Domain View**, go to **Symmetry Editor** and change **gamma** to 270.
10. On the left side of **Suggest Parameters** pane you should get**: Grid Size =**180**, Integration Method=**Monte Carlo, **Integration Iterations:** 1E6, **Convergence:** 0.001 **Generated Points:** 500, Updated **Interval**: 500 ms. If not repeat the instructions.
11. Enter the proposed parameters to the **Preferences** pane.
12. Go to the **2D Graph** and click **Generate** in the **Controls** pane.
13. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.

PDB file with symmetry Part b:

Note: Run this example only on GPU or Remote D+. This is another way to compute the same model as **PDB_Symmetry_Files Part a**.

1. Go to **Domain View** pane on the top-left corner, choose **PDB file**: **3j6f_Dimer_2_2_Added_H_GCentered.pdb**. Make sure to select the **Center PDB** option before pressing **Add**.
2. It is recommended to go to **3D Graph** to see the structures you are about to compute.
3. Reduce the **Level of Detail** to minimum (this option can be found at the **Preferences** pane).
4. Choose **PDB file**: **3j6f** in **Domain View.**
5. Go to **Domain View**, choose **Uniform Hollow Cylinder**, and press **Add**.
6. Try to change the Cylinder parameters so that it will envelope the **PDB file 3j6f**. Make sure you insert the following parameters into **Suggest parameters: x=**6**, y=**6, **z=**8**, q=**5**.**
7. Delete the **Uniform Hollow Cylinder** model**.**
8. On the left side of the **Suggest Parameters** pane you should get**: Grid Size =**50**, Integration Method=** Adaptive (VEGAS) Monte Carlo, **Integration Iterations:** 1E6, **Convergence:** 0.001, **Generated Points:** 500, **Updated Interval**: 500 ms . If not repeat the instructions.
9. Enter the proposed parameters to the **Preferences** pane.
10. Go to **Domain View**, choose **Scripted Symmetry**, and press **Add**. Choose the **Left_Hand_Helix** model, located in the relevant tutorial folder.
11. Go to **Domain View**, choose the **Left Hand Helix** model.
14. Go to **Parameter Editor,** insert the following parameters: **Radius=**11.9, **Pitch=**12.2, **Units per Pitch**=14, **Units in Pitch**=14, **Units to Skip in Pitch**=0, **Discrete Height**=3, **# Helix Starts**=3.
12. Go to the **Entities** pane inside **Domain View** and drag the **PDB file 3j6f** into **Scripted Symmetry.**
13. Choose **PDB file 3j6f** in **Domain View**, go to **Symmetry Editor**, and change **gamma** to 270.
14. In **Symmetry Editor**, make sure the option **Use Grid From Here** is ticked only next to the **PDB file** of and not next to the **Left Hand Helix** model**.**
15. Go to the **2D Graph** and click **Generate** in the **Controls** pane.

16. Go to **File** menu and choose **Export 1D Graph,** save the computed scattering curve as an *.out file.