

マニュアルはネット上にも他の人のがあるので探してみてください。

1. タンパク質構造データの取得

<http://www.rcsb.org/pdb/home/home.do> へ行き、目的のタンパク質構造で検索する。

The screenshot shows the RCSB PDB homepage. The search bar at the top right contains the text "Histamine H1", with a black arrow pointing to it. Below the search bar, a dropdown menu displays search results. Under the "UniProt Molecule Name" section, it lists "Histamine H1 receptor (1)" with a "Find all" link. Under the "Ontology Terms" section, it lists "HS: HISTAMINE RECEPTOR H1 [Geno ... (1)", "D27.505...425.400: Histam... [... (5)", and "D27.505...425.400: Histam... [... (5)". Under the "Sequence Cluster Name" section, it lists "Histamine H1 ..." with a "Find all" link. The main content area features a "Welcome" message, a "Wellcome Trust Image Awards" section with three images, and a "RAF Protein Kinases" section with a 3D protein structure. The footer includes "Latest Entries" (As of Tuesday Mar 22), "New Features" (February 2016 Release), and "News" (Improving Download Services).

RCSB PDB - Search Results

www.rcsb.org/pdb/results/results.do?grid=2604B0CF&tabtoShow=Current

RCSB PDB Deposit Search Visualize Analyze Download Learn More

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RCSB PDB An Information Portal to 117240 Biological Macromolecular Structures

Search by PDB ID, author, macromolecule, sequence, or ligands

Advanced Search | Browse by Annotations | Search History (1) | Previous Results (1)

1 Structure 1 Citation 4 Ligands

Search Parameter:
Text Search for: histamine h1

Refinements

ORGANISM
Enterobacteria phage T4 s... (1)

UNIPROT MOLECULE NAME
Endolysin (1)
Histamine H1 receptor (1)
Refine Query

TAXONOMY
Eukaryota/Viruses (1)

EXPERIMENTAL METHOD
X-ray (1)

X-RAY RESOLUTION
3.1 and more (1)
Refine Query

RELEASE DATE
Jun 2011 (1)
Refine Query

POLYMER TYPE
Protein (1)

ENZYME CLASSIFICATION
3.2.1.17: Lysozyme (1)

Currently showing 1 - 1 of 1 Page: 1 of 1 Displaying 25 Results

View: Detailed Reports: Select one... Sort: Sort by... Download Files

3RZE

Structure of the human histamine H1 receptor in complex with doxepin

Shimamura, T., Han, G.W., Shiroishi, M., Weyand, S., Tsujimoto, H., Winter, G., Katritch, V., Abagyan, R., Cherezov, V., Liu, W., Kobayashi, T., Stevens, R., Iwata, S., GPCR Network, Joint Center for Innovative Membrane Protein Technologies

Structure of the human histamine H1 receptor complex with doxepin.
(2011) Nature 475: 65-70

Released: 2011-06-15
Method: X-RAY DIFFRACTION
Resolution: 3.10 Å
Residue Count: 452

Macromolecule Content
Histamine H1 receptor, Lysozym ... (protein)
Unique Ligands: 4
OLC 5EH D7V PO4

Membrane Protein [Input](#)
Group Name: ALPHA-HELICAL
Sub Group: G Protein-Coupled Receptors (GPCRs)
Master Protein Name: Histamine H1 receptor, complexed with doxepin

3D View

1

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RCSB PDB - 3RZE: Stru

www.rcsb.org/pdb/explore/explore.do?structureId=3RZE

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RCSB PDB An Information Portal to 117240 Biological Macromolecular Structures

Search by PDB ID, author, macromolecule, sequence, or ligands

Advanced Search | Browse by Annotations | Search History (1) | Previous Results (1)

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment Literature

Biological Assembly 1

3RZE

Structure of the human histamine H1 receptor in complex with doxepin

DOI: 10.2210/pdb3rze/pdb

Classification: HYDROLASE

Deposited: 2011-05-11 Released: 2011-06-15

Deposition author(s): Shimamura, T., Han, G.W., Shiroishi, M., Weyand, S., Tsujimoto, H., Winter, G., Katritch, V., Abagyan, R., Cherezov, V., Liu, W., Kobayashi, T., Stevens, R., Iwata, S., GPCR Network, Joint Center for Innovative Membrane Protein Technologies

Organism: Homo sapiens | Enterobacteria phage T4 sensu lato

Expression System: Pichia pastoris

Mutation(s): 2

Structural Biology Knowledgebase: 3RZE (5 models >22 annotations) [SERRA.org](#)

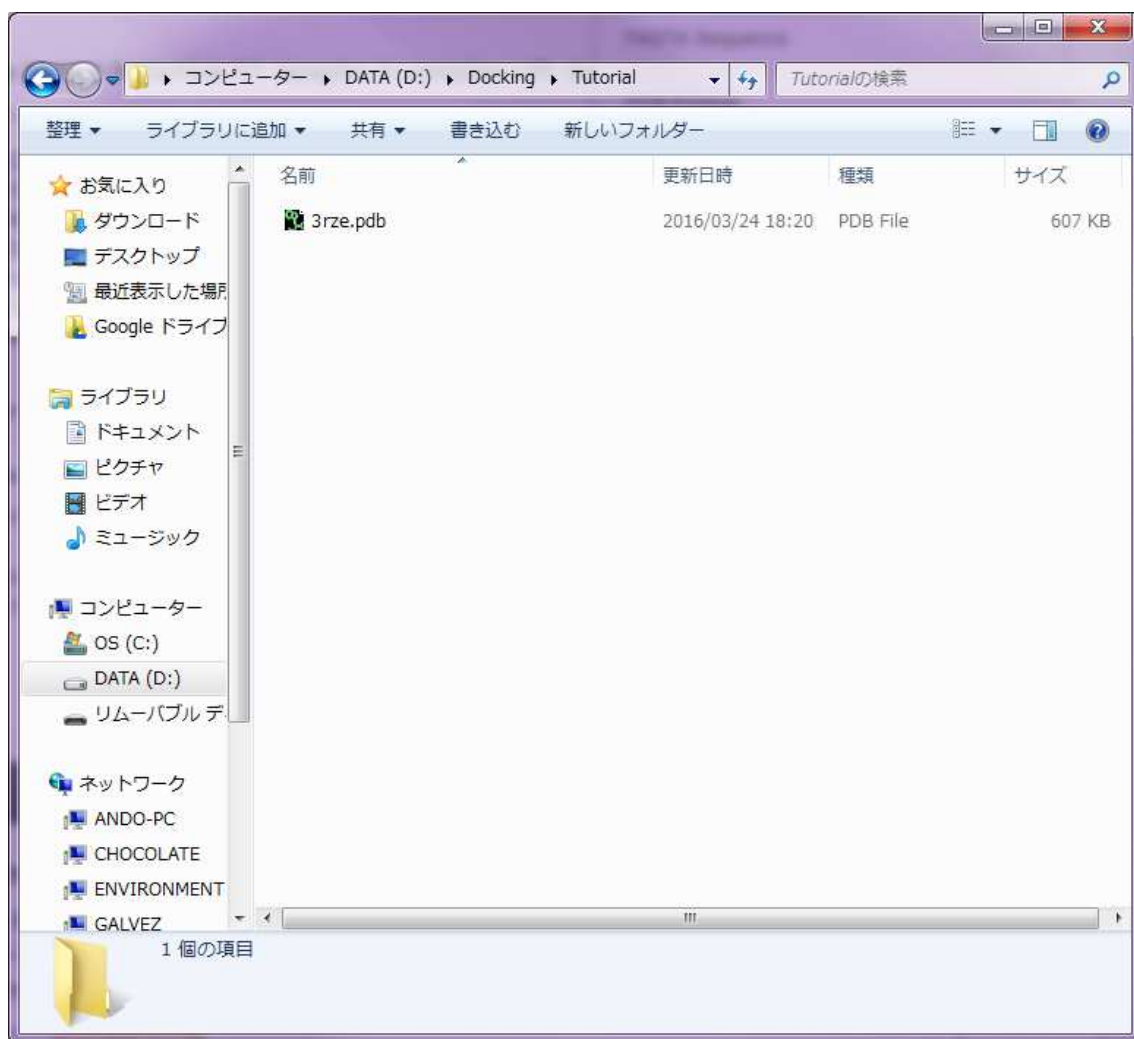
Experimental Data Snapshot

wwPDB Validation

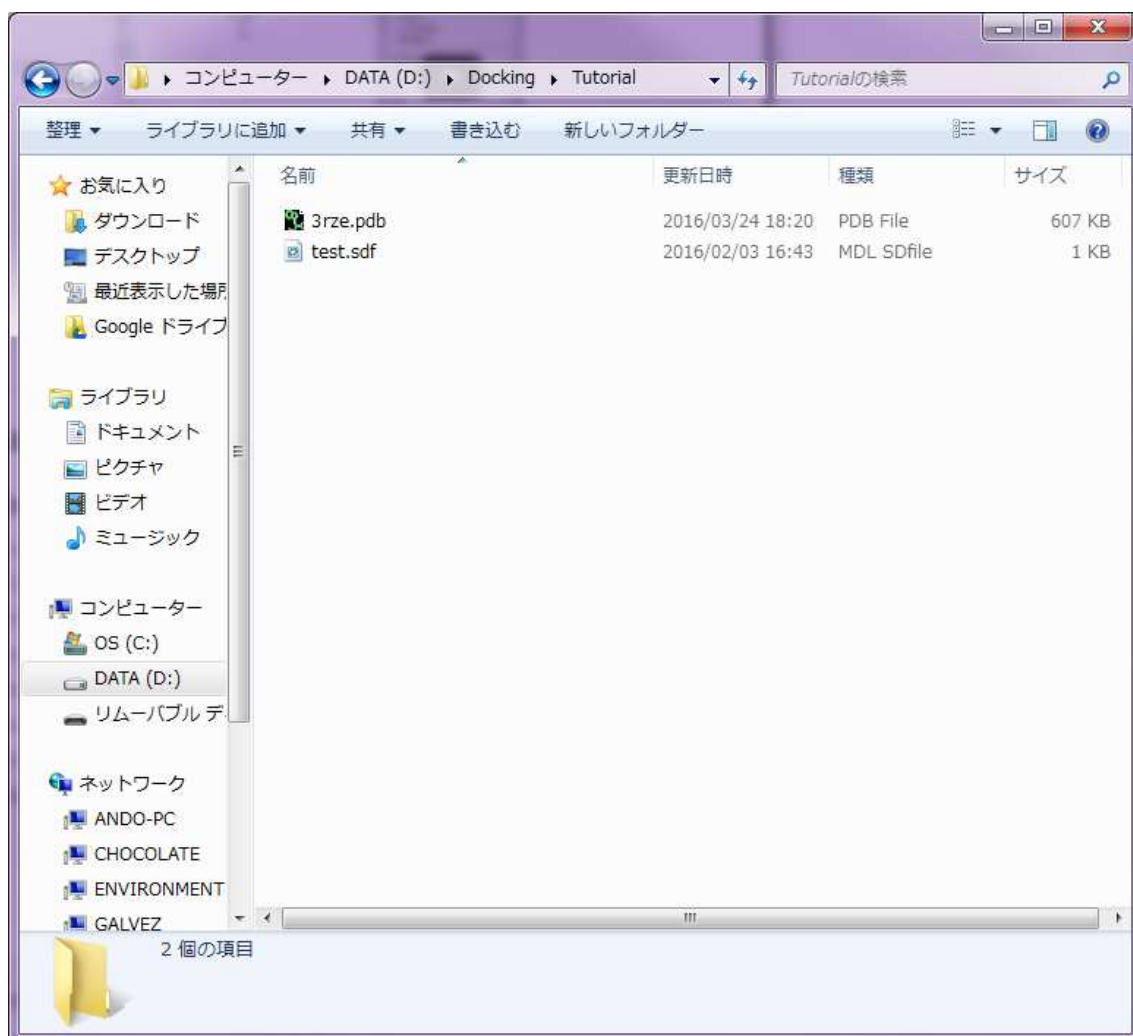
Display Files Download Files

FASTA Sequence
PDB Format
PDB Format (gz)
PDBx/mmCIF Format
PDBx/mmCIF Format (gz)
PDBML/XML Format (gz)
Structure Factors (mmCIF)
Structure Factors (mmCIF - gz)
Biological Assembly (PDB format - gz) (A+S)

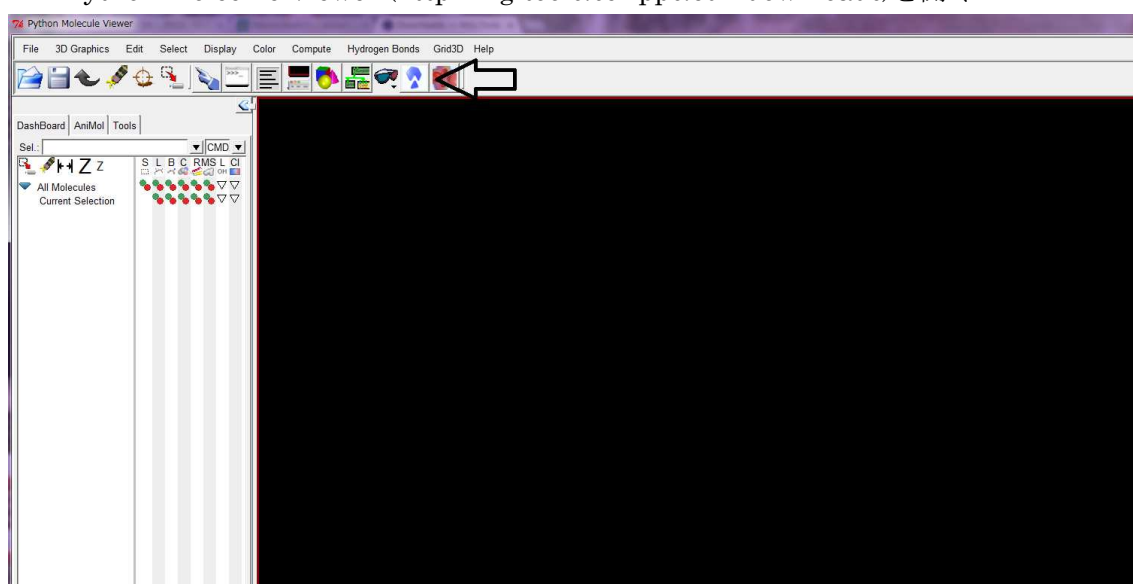
PDB Format を選択しダウンロードする。



2. ドッキングしたい構造を用意する。

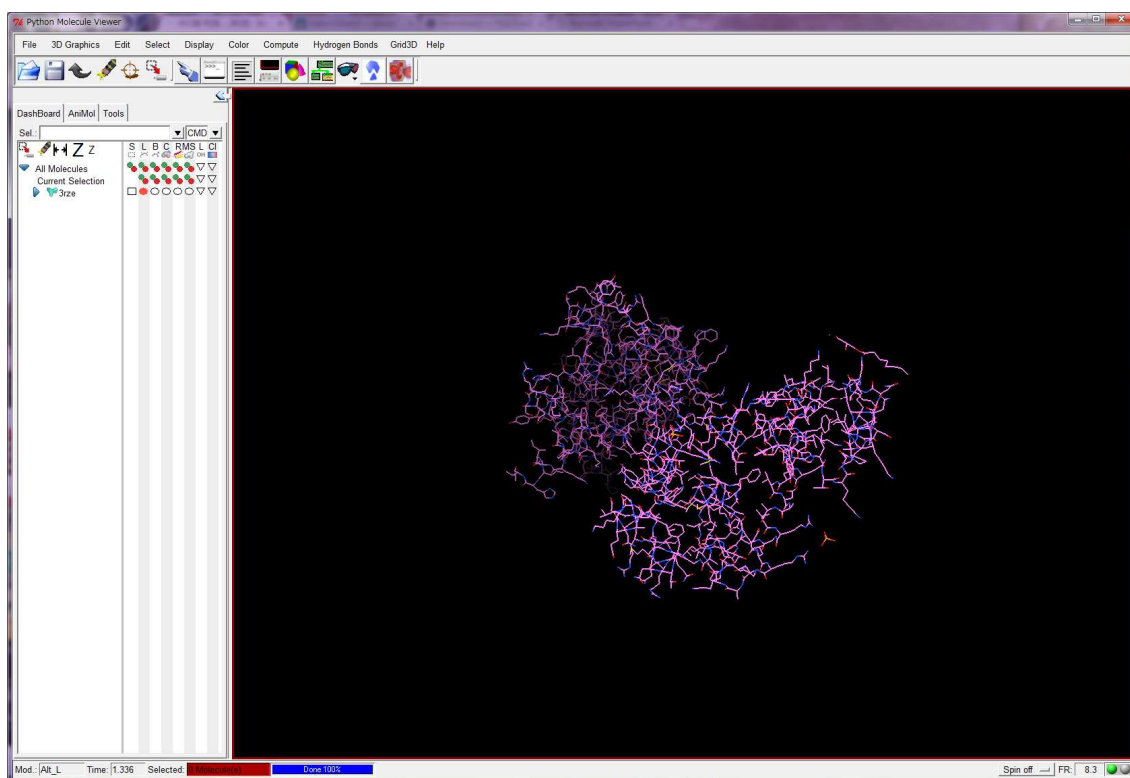


3. Python Molecule Viewer (<http://mglttools.scripps.edu/downloads>)を開く

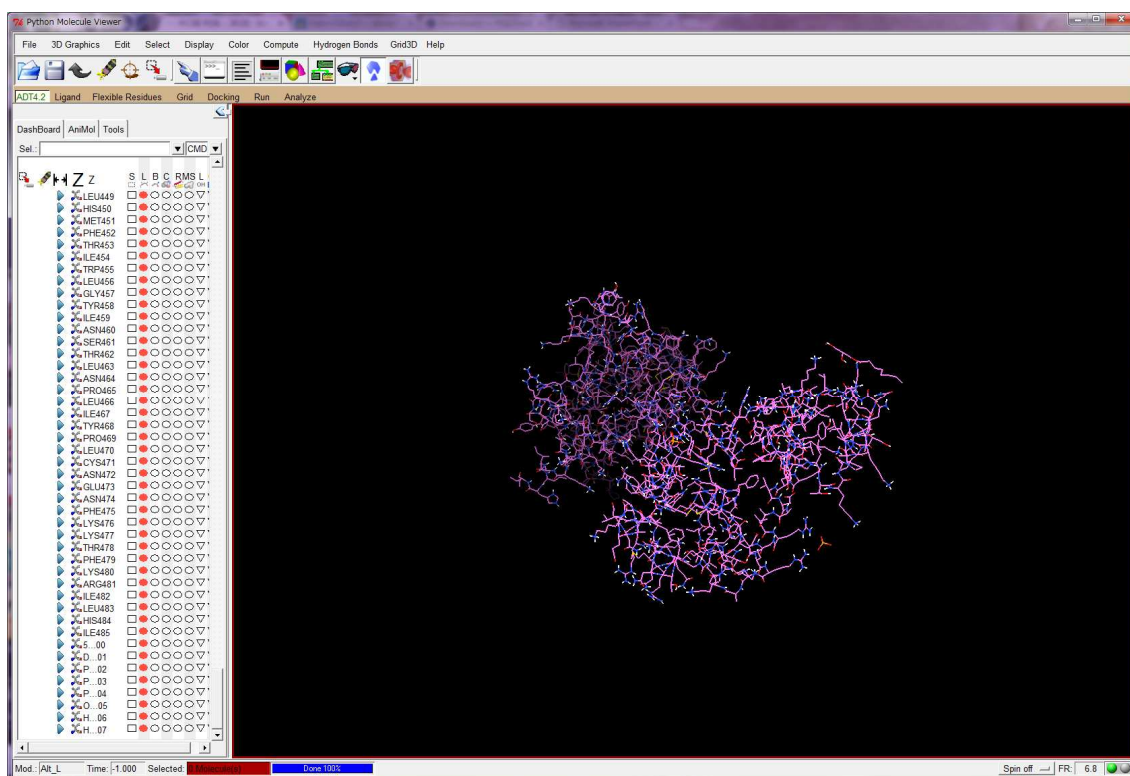


Auto Dock Tools(<http://mglttools.scripps.edu/downloads>)のボタンを押す

ダウンロードしたタンパク質を開く。



Edit>Hydrogens>add で水素を付加する。



邪魔なリガンドは選択して削除する。この場合 5EH,D7V,PO4,OLC。タンパク質データをダウンロードした際のページで確認が可能。

RCSB PDB - 3RZE: Str

www.rcsb.org/pdb/explore/explore.do?structureId=3rze

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB Login

Small Molecules

Ligands 4 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
OLC Query on OLC Download SDF File Download CCD File	A	(2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate 1-Oleoyl-R-glycerol (Synonym) C ₂₁ H ₄₀ O ₄ RZRNAVUHWFMIP-GDCKJWNLSA-N		 Ligand Explorer Binding Pocket (JSmol) Electron Density (JSmol)
5EH Query on 5EH Download SDF File Download CCD File	A	(3E)-3-(dibenzo[b,e]oxepin-11(6H)-ylidene)-N,N-dimethylpropan-1-amine C ₁₉ H ₂₁ N O ODQWQRRAPPTVAG-GZTJUZNOSA-N		 Ligand Explorer Binding Pocket (JSmol) Electron Density (JSmol)
D7V Query on D7V Download SDF File Download CCD File	A	(3Z)-3-(dibenzo[b,e]oxepin-11(6H)-ylidene)-N,N-dimethylpropan-1-amine C ₁₉ H ₂₁ N O ODQWQRRAPPTVAG-BOPTXTBSA-N		 Ligand Explorer Binding Pocket (JSmol)
PO4 Query on PO4 Download SDF File Download CCD File	A	PHOSPHATE ION O ₄ P NBIIXXVUZAFBLC-UHFFFAOYSA-K		 Ligand Explorer Binding Pocket (JSmol) Electron Density (JSmol)

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION

Resolution: 3.1 Å

R-Value Free: 0.249

R-Value Work: 0.214

Space Group: I 4 2 2

Electron Density Server: EDS

Unit Cell

Length (Å)	Angle (°)
a = 88.14	α = 90.00
b = 88.14	β = 90.00

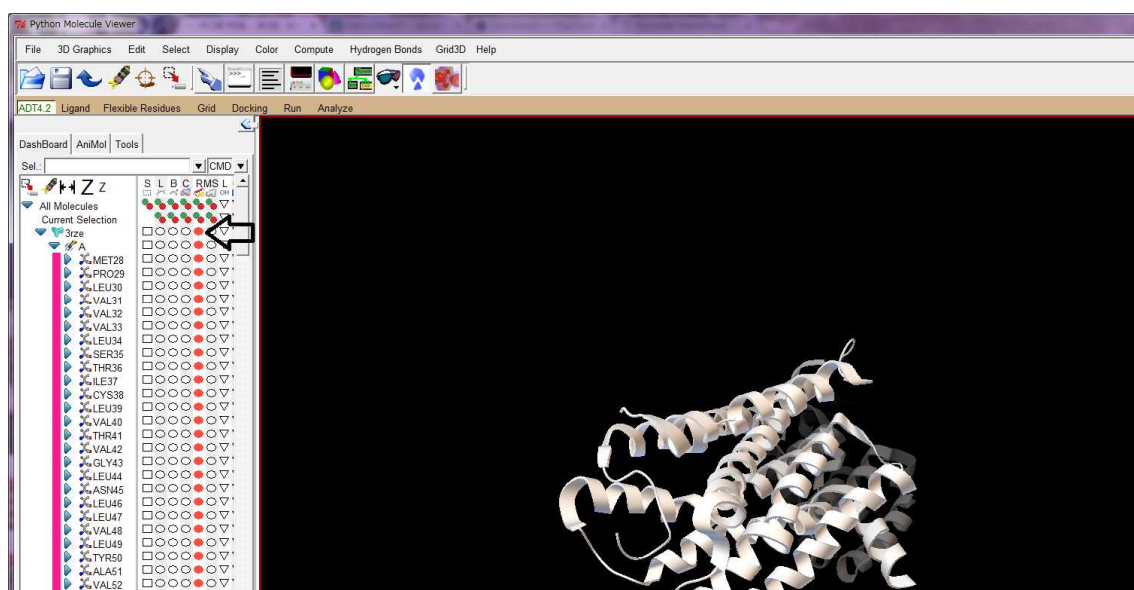
Structure Validation

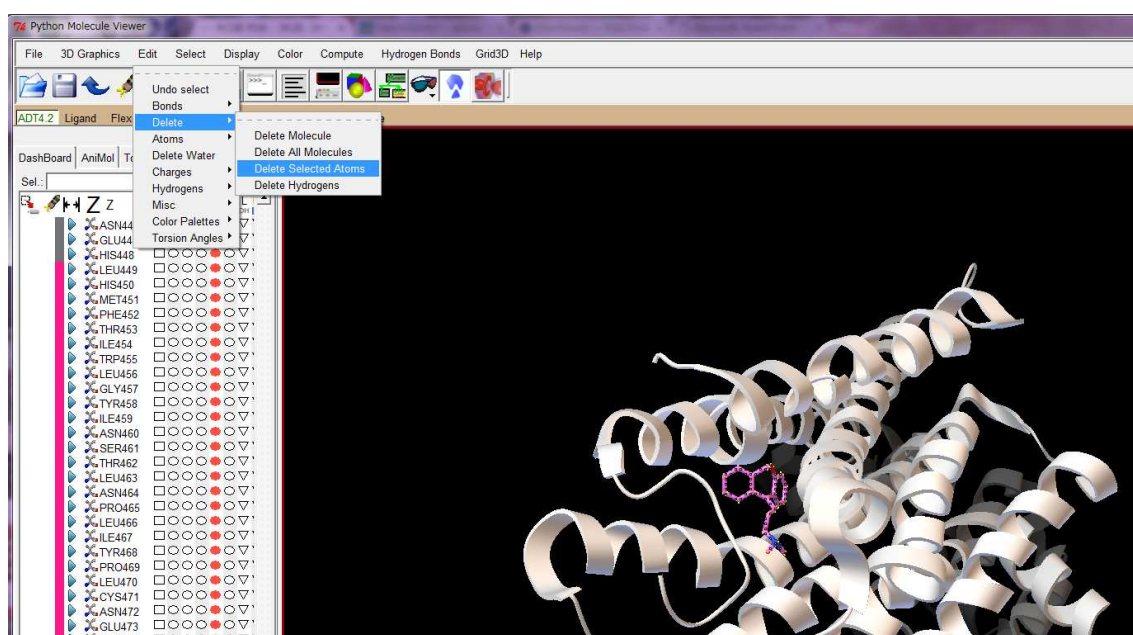
View Full Validation Report or Ramachandran Plots

Metric	Percentile Ranks	Value
Rfree		0.278
Clashscore		9
Ramachandran outliers		1.2%
Sidechain outliers		11.2%

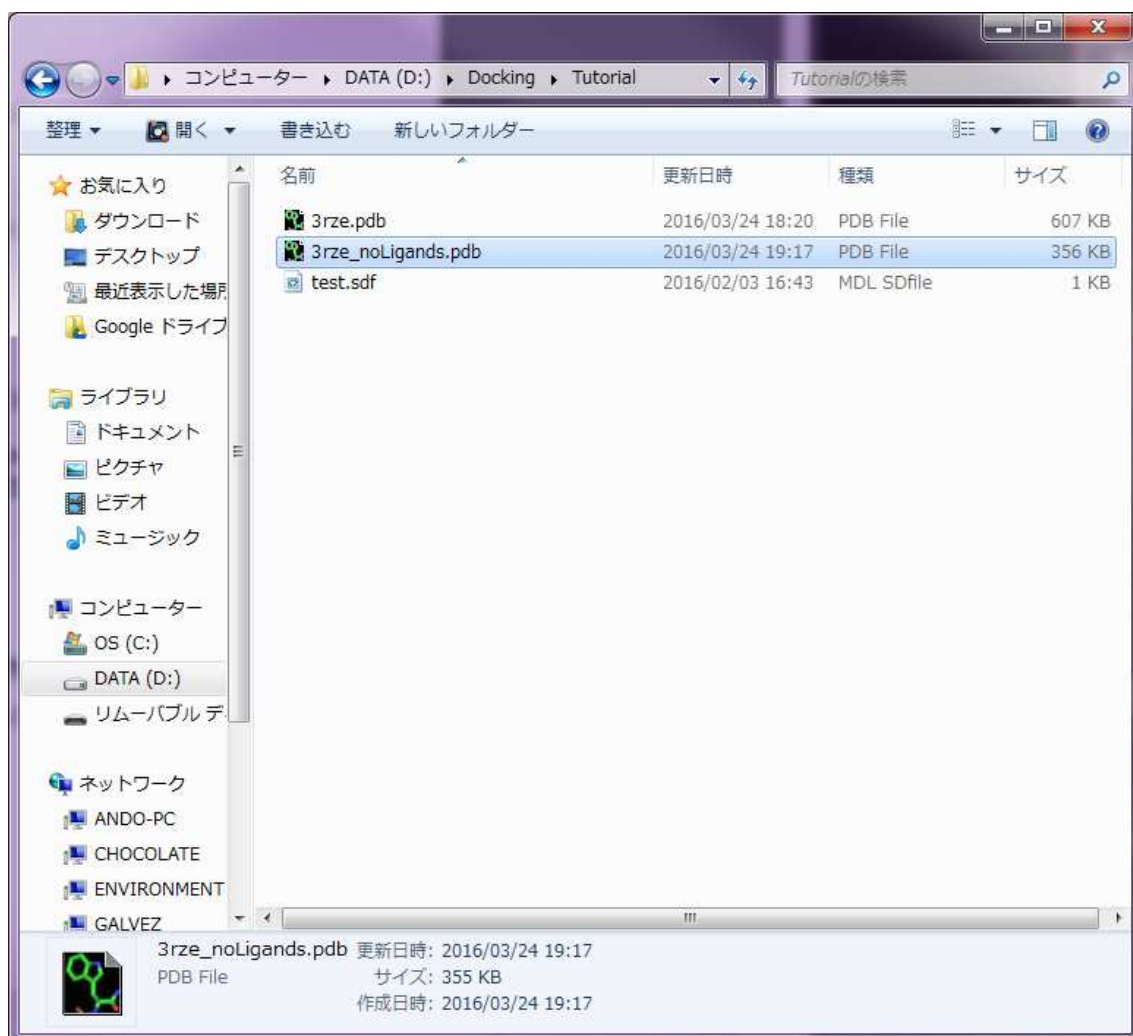
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リボン表記にしておくと見やすい。



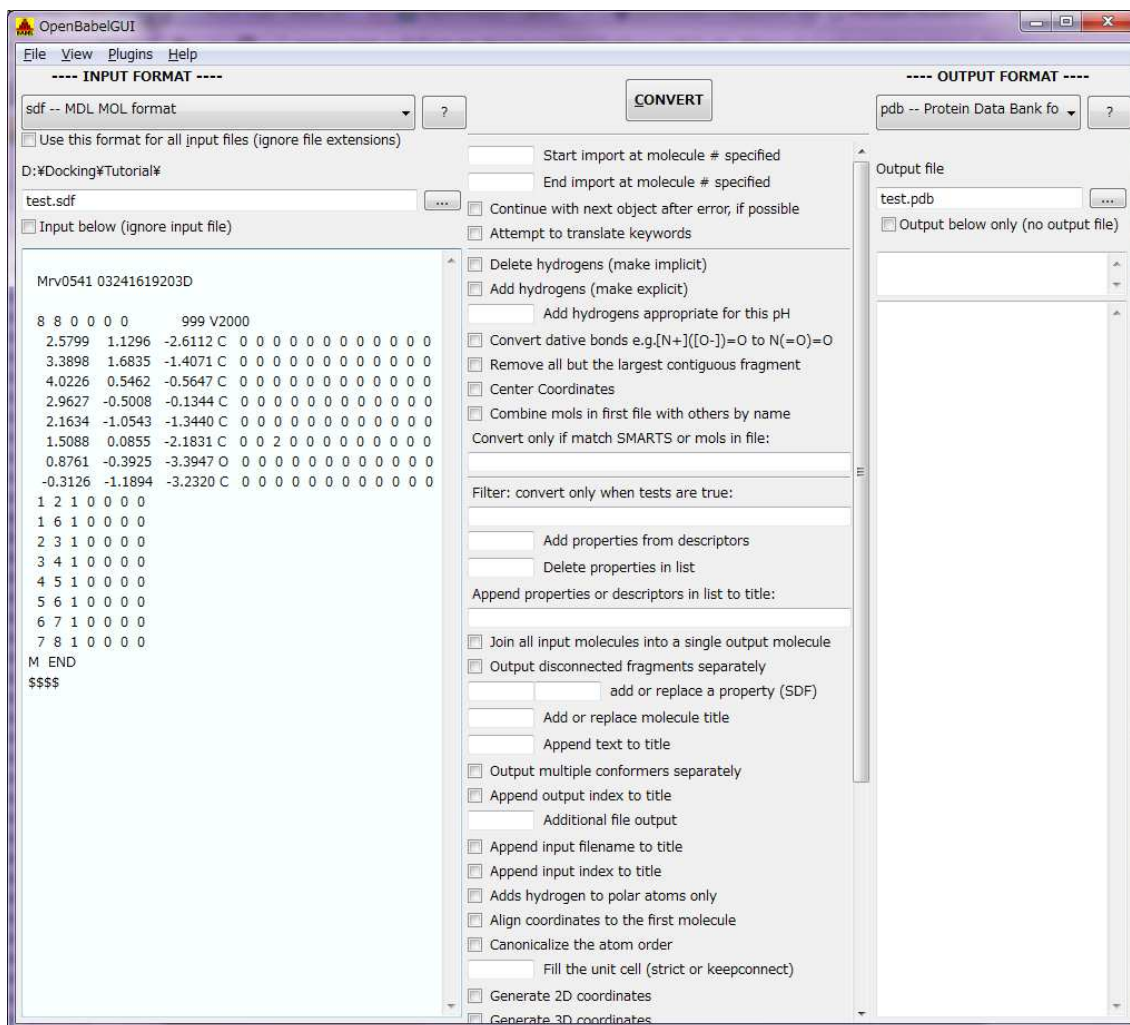


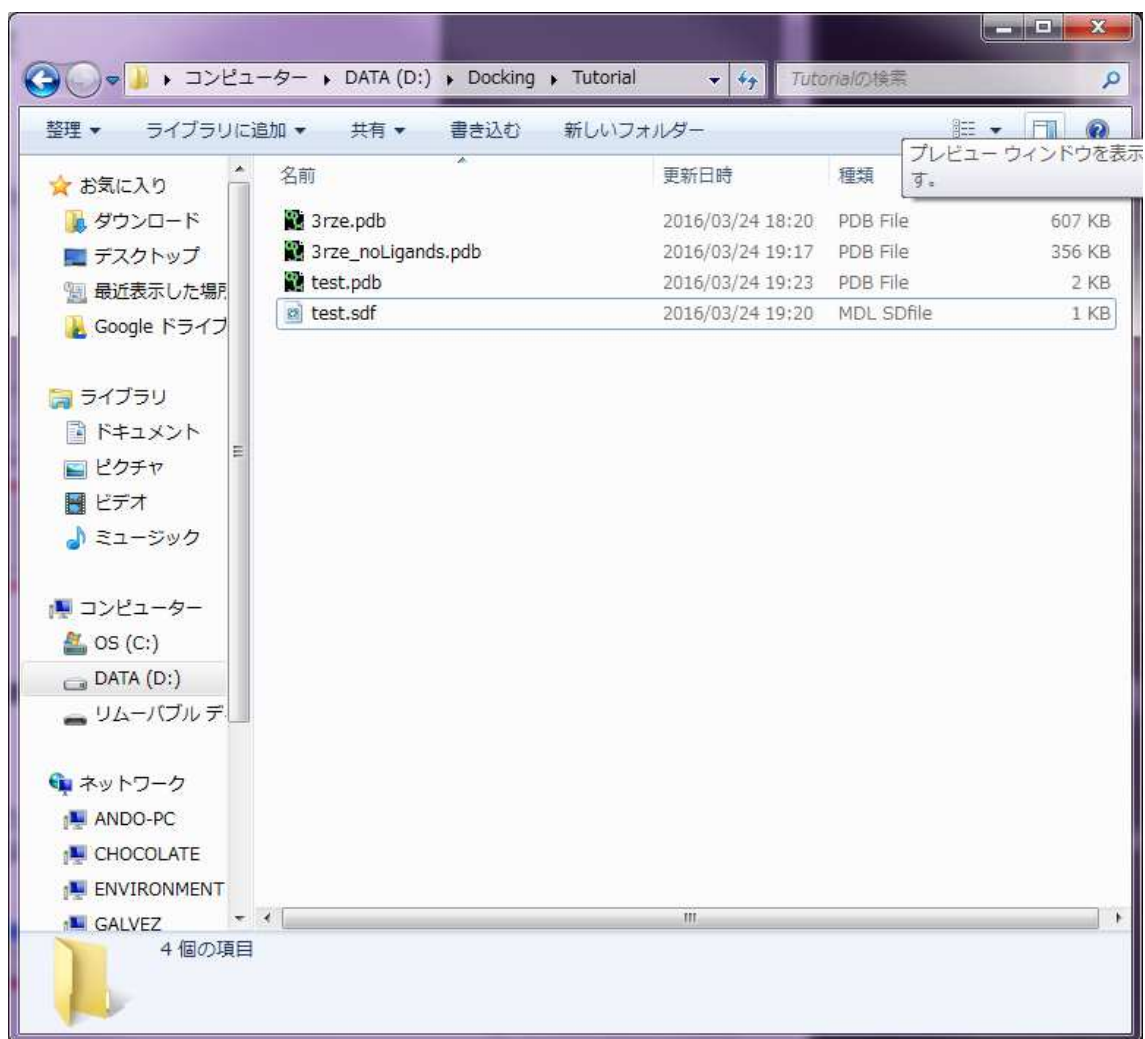
削除したら保存する。



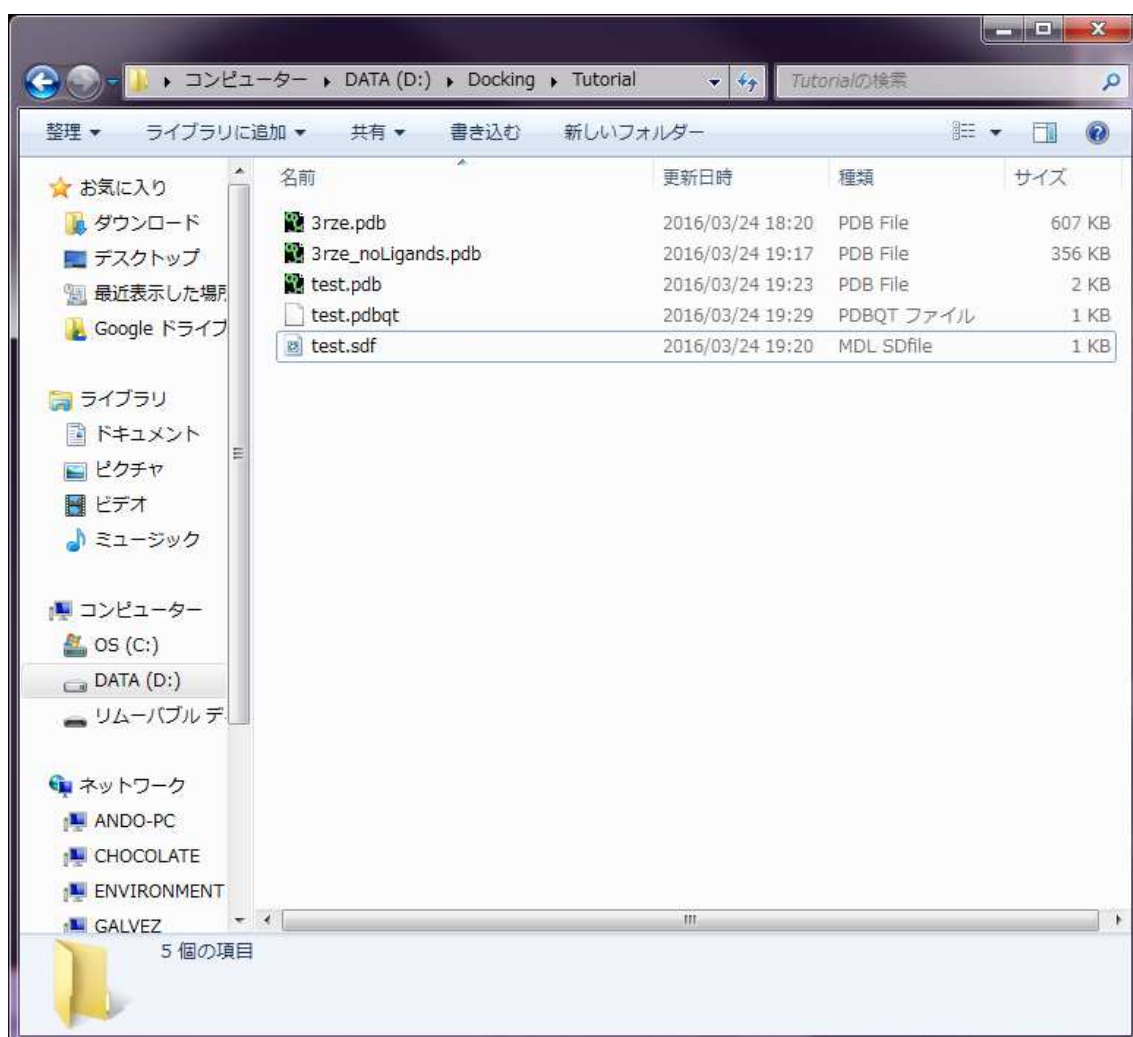
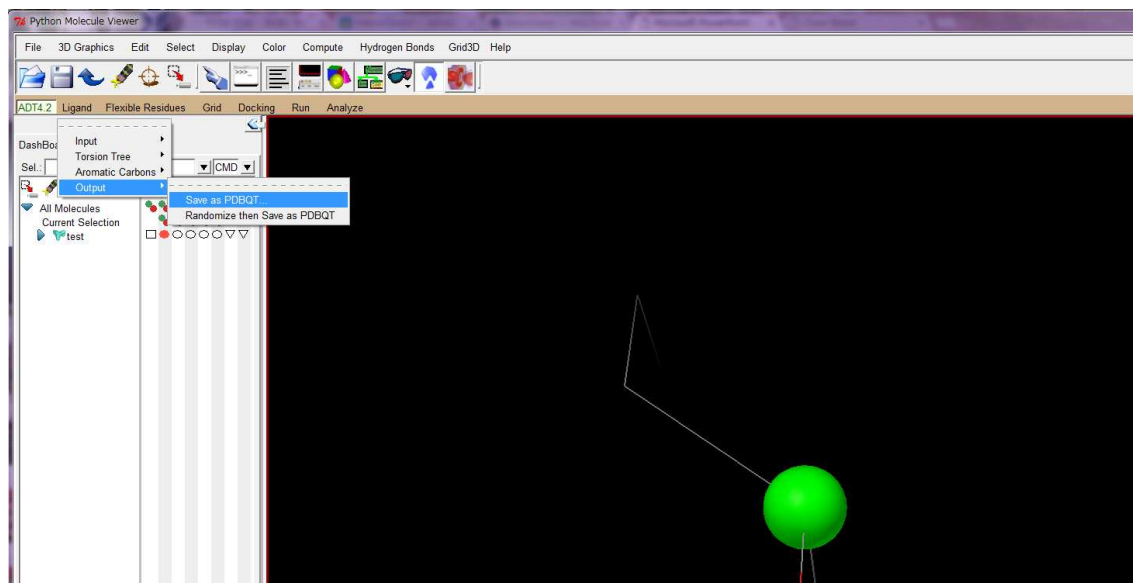
(<https://www.chemaxon.com/products/marvin/marvinsketch/>)で三次元配座に変える。

さらに OpenBabel(http://openbabel.org/wiki/Main_Page)で pdb 形式に変換する。





5. ドッキングしたい構造を Python Molecule Viewer で読み込み pdbqt 形式に変換する。
Ligand>Input>Open で読み込み
Ligand>TorsionTree>DetectRoot を選択
Pdbqt 形式で保存

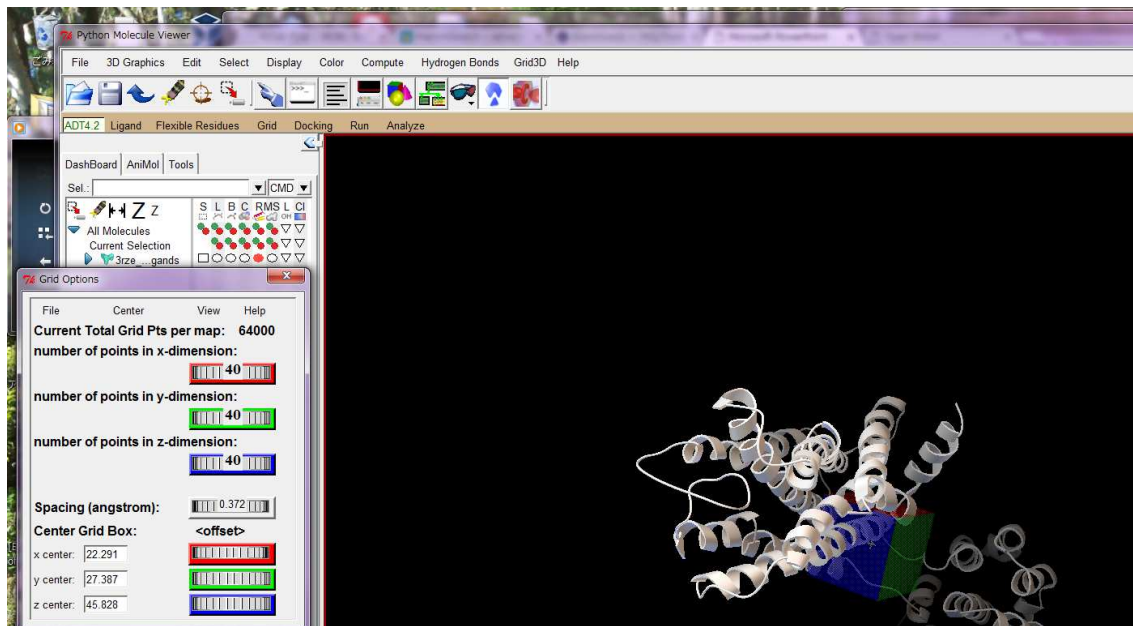


6. タンパク質データを読み込み pdbqt 形式で保存する。

Grid>Macromolecule>Open で pdb ファイルを選択すると自動的に作成される。

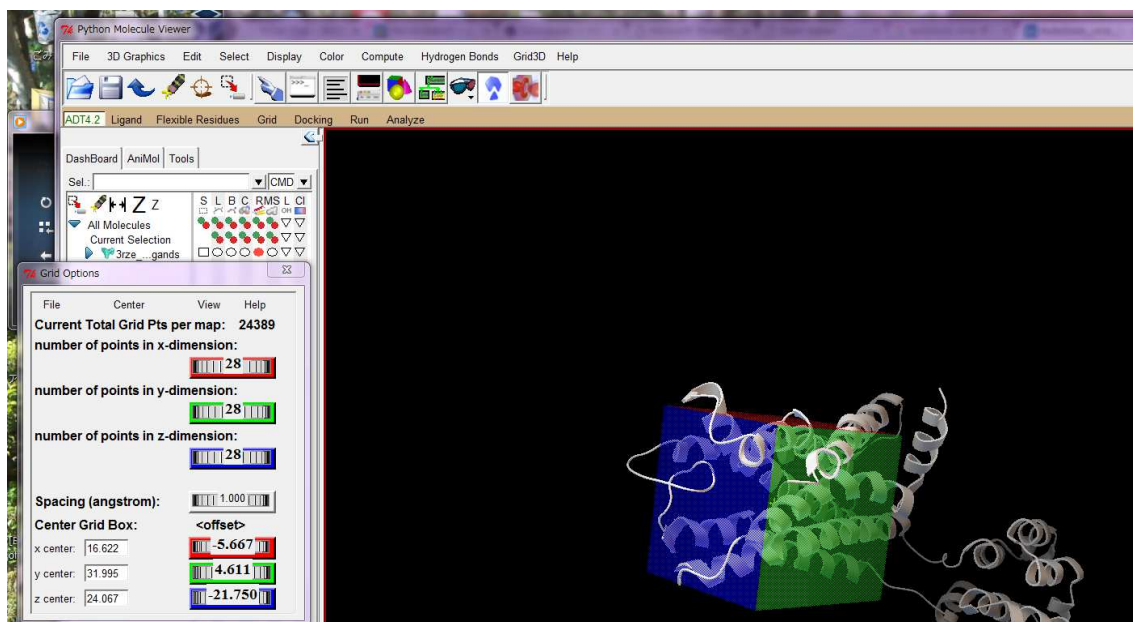
表示をリボン形式にしてグリッドを設定する。設定範囲はもともとリガンドが存在したあたりにするといいい。

Grid>GridBox を選択するとウィンドウが現れる。

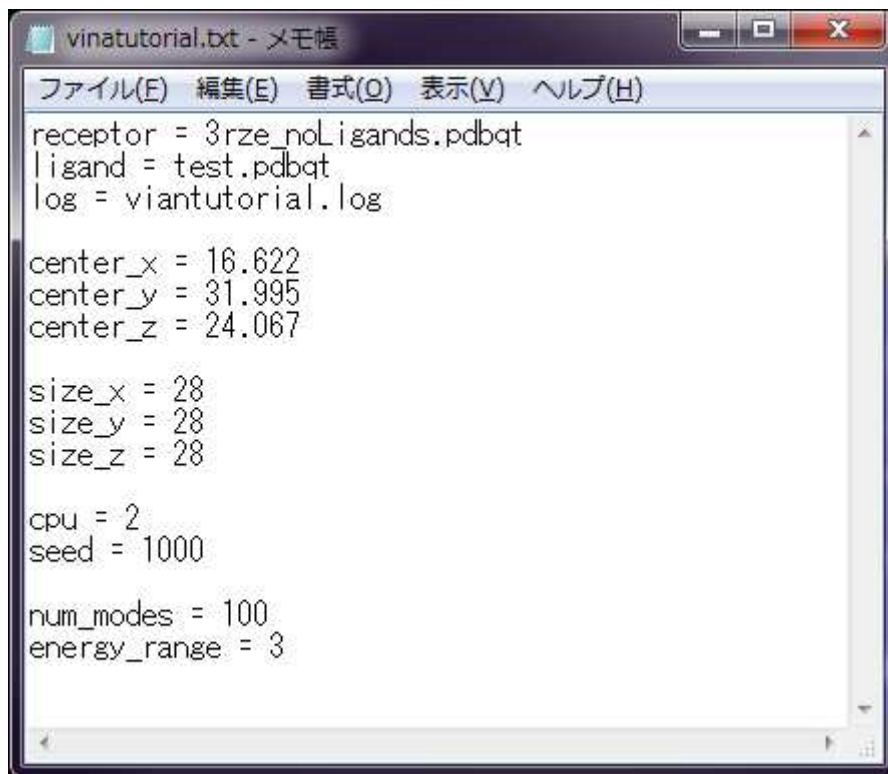


Spacing を 1 にし、グリッドサイズと位置を選択する。

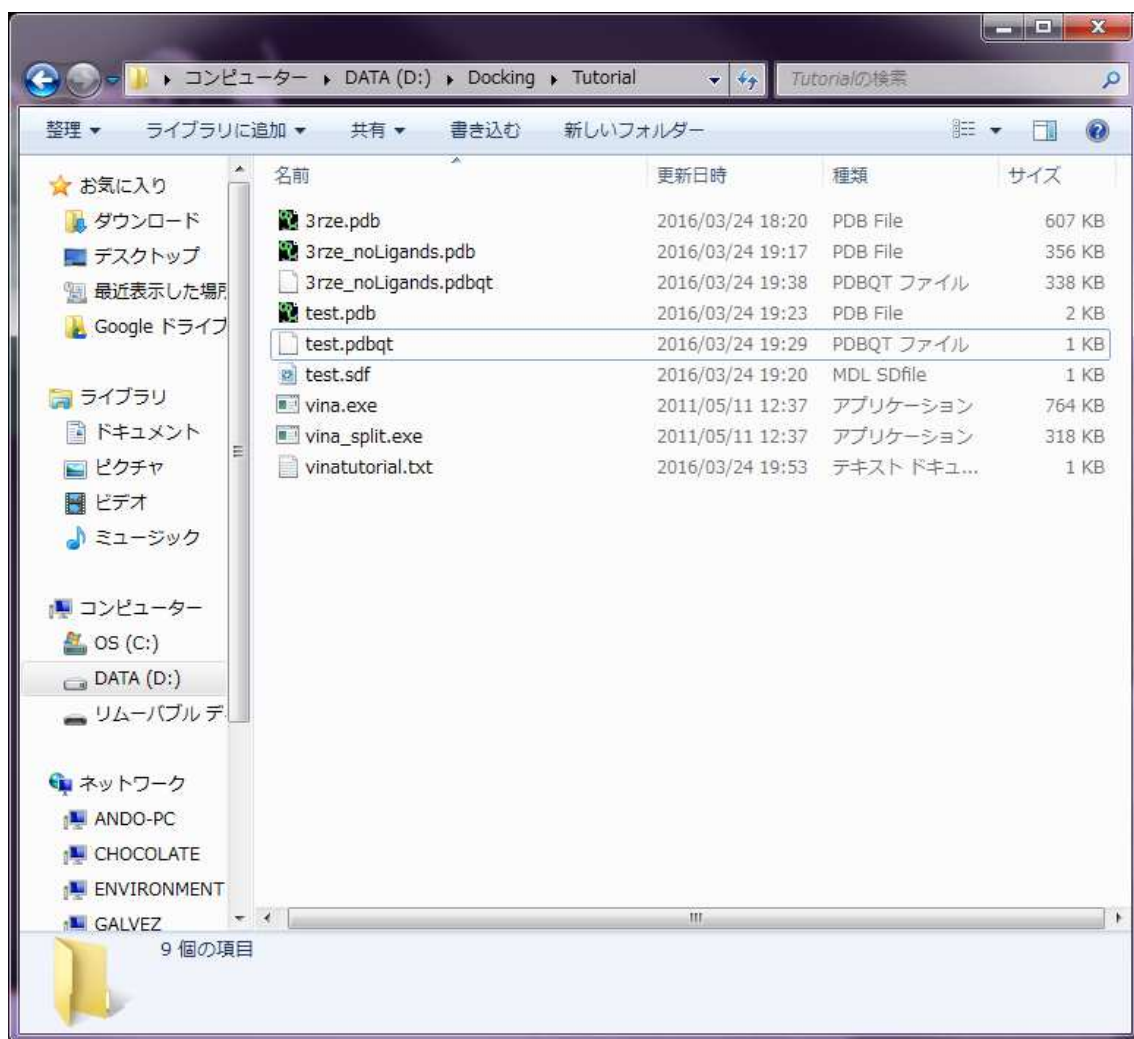
大きさは 27000Angstrom³ 以下でなくてははいけない。



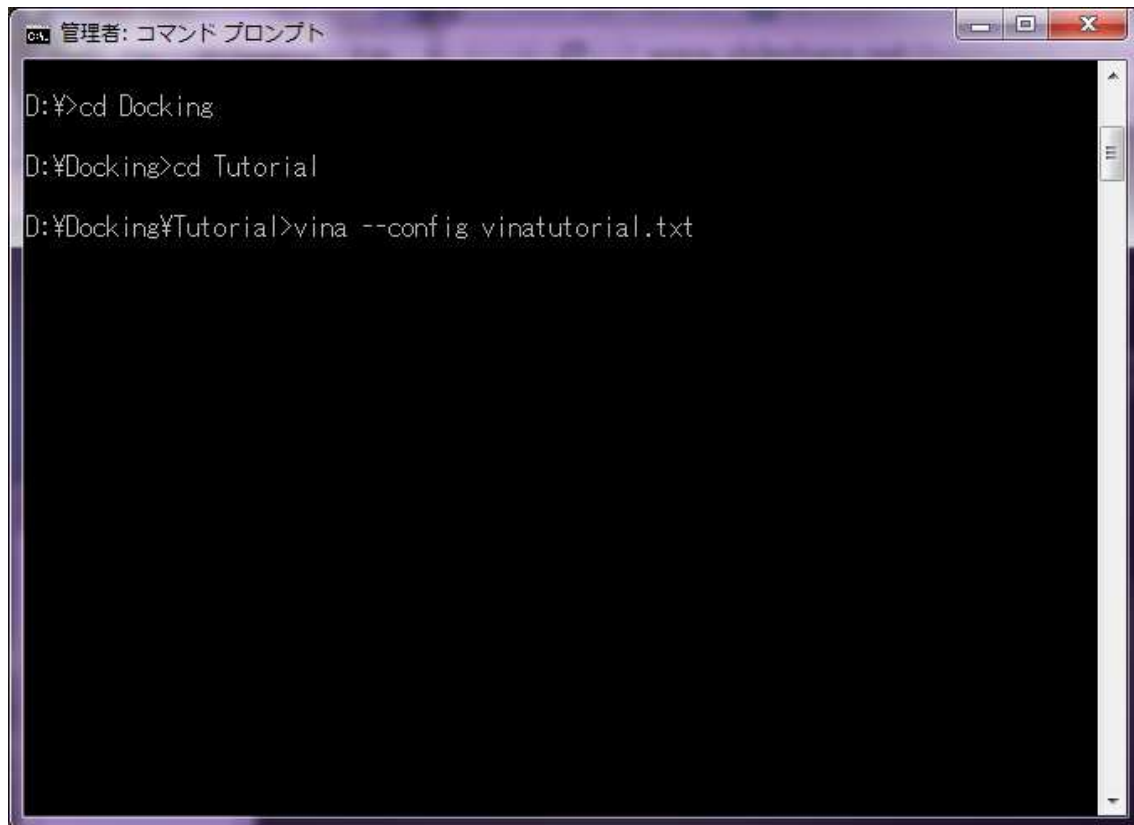
設定した値を自分でテキストファイルに書き込む。



7. vina.exe と vina_split.exe(<http://vina.scripps.edu/download.html>)をフォルダにコピー



8. コマンドプロンプトを起動してファイルがあるディレクトリで
vina --config (作成した設定ファイル)と入力して実行



```
管理者: コマンド プロンプト
D:¥>cd Docking
D:¥Docking>cd Tutorial
D:¥Docking¥Tutorial>vina --config vinatutorial.txt
```

9. Log ファイルが作成される。Affinity が結合エネルギー

```
viantutorial.log - メモ帳
ファイル(F) 編集(E) 書式(O) 表示(V) ヘルプ(H)
#####
# If you used AutoDock Vina in your work, please cite:
#
# O. Trott, A. J. Olson,
# AutoDock Vina: improving the speed and accuracy of docking
# with a new scoring function, efficient optimization and
# multithreading, Journal of Computational Chemistry 31 (2010)
# 455-461
#
# DOI 10.1002/jcc.21334
#
# Please see http://vina.scripps.edu for more information.
#####
Output will be test_out.pdbqt
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1000
Performing search ... done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1   |    -5.6   |    0.000   |    0.000
  2   |    -5.3   |    2.151   |    4.266
  3   |    -5.3   |    1.160   |    1.317
  4   |    -5.2   |    2.553   |    5.237
  5   |    -5.1   |    2.680   |    5.001
  6   |    -5.1   |    4.224   |    5.388
  7   |    -4.8   |    3.865   |    5.447
  8   |    -4.8   |    1.512   |    3.907
  9   |    -4.7   |    9.058   |   10.527
 10   |    -4.7   |    2.215   |    4.092
 11   |    -4.7   |    9.748   |   10.856
 12   |    -4.7   |    2.589   |    3.459
 13   |    -4.6   |   10.098   |   11.136
 14   |    -4.6   |    2.353   |    3.670
 15   |    -4.6   |    3.499   |    4.687
 16   |    -4.3   |   10.500   |   11.812
 17   |    -4.2   |    9.943   |   11.293
 18   |    -3.9   |    1.580   |    3.738
 19   |    -3.4   |   10.518   |   11.918
 20   |    -3.3   |   15.140   |   16.139
Writing output ... done.
```