

電子顕微鏡 (単粒子解析) の構造・マップの登録

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EMDBとは

<https://www.ebi.ac.uk/pdbe/emdb/>

The Electron Microscopy Data Bank (EMDB) is a public repository for **electron microscopy density maps of macromolecular complexes and subcellular structures**. It covers a variety of techniques, including **single-particle analysis, electron tomography, and electron (2D) crystallography**.

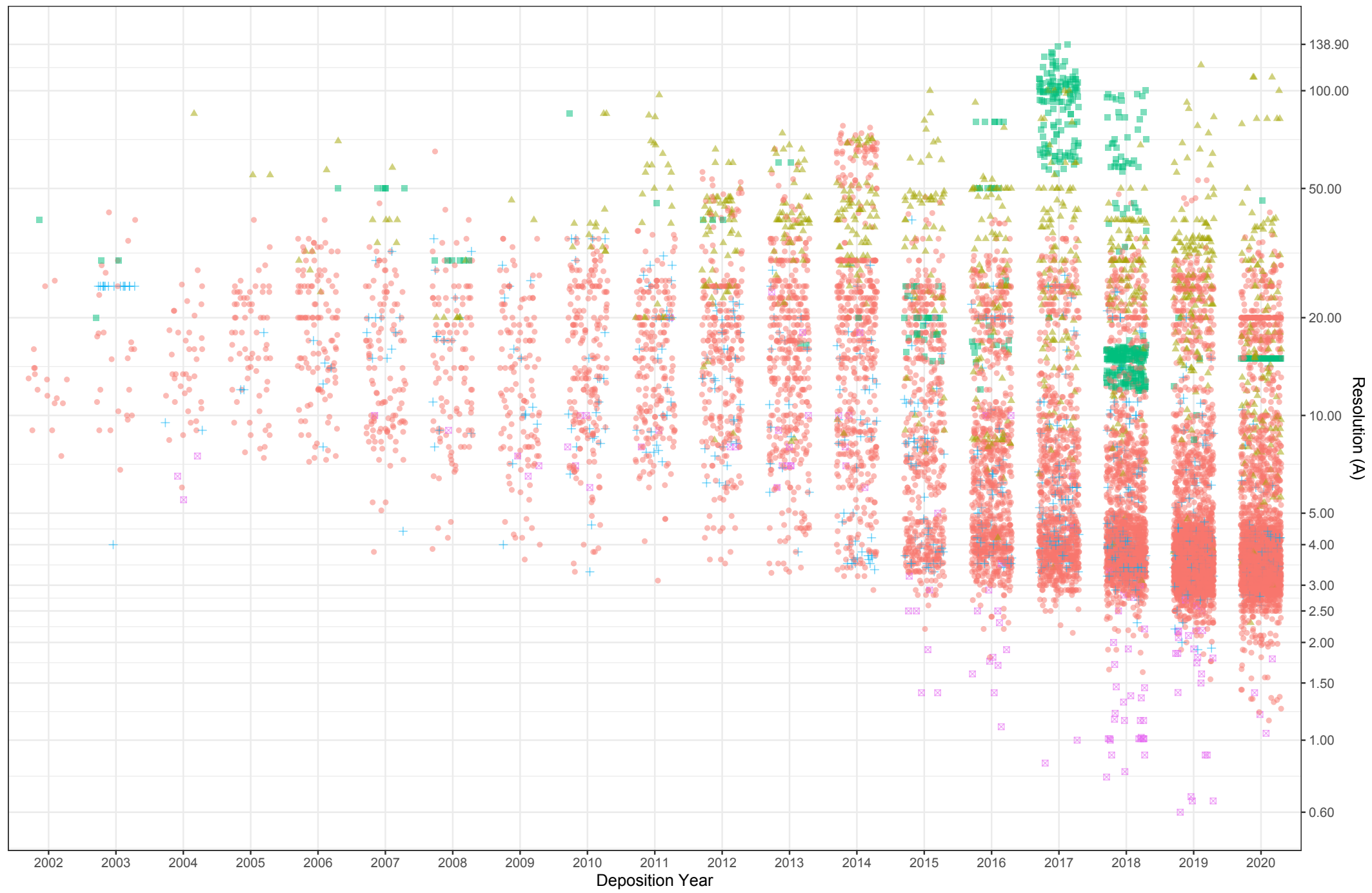
The EMDB was **founded at EBI in 2002**, under the leadership of Kim Henrick. Since 2007 it has been operated jointly by the PDBe, and the Research Collaboratory for Structural Bioinformatics (RCSB PDB) as a part of EMDataBank which is funded by a joint NIH grant to PDBe, the RCSB and the National Center for Macromolecular Imaging (NCMI).

- 単粒子, トモグラフィ, サブトモグラム平均化, ヘリカル再構成, 電子結晶学のマップを登録するデータベース
- PDBの0個以上のエントリと対応可能
- PDBと同時に登録可能 (まだPDB形式もOK)
- XMLヘッダ + MRC/CCP4マップファイルで構成
- <ftp://ftp.pdbj.org/pub/emdb/structures/EMD-xxxxx/>
 - header/
 - images/
 - fsc/
 - map/ primary map
 - masks/
 - other/ half maps and additional maps etc
 - ...

EMDB統計

As of 2021-Jan-06

method ● singleParticle ▲ subtomogramAveraging ■ tomography + helical ✖ twoDCrystal
10987 1051 887 703 149



EMDB登録に必要なデータ

- 必須
 - Primary map
 - Image of the map (500×500 pixels in .jpg, .png, etc. format)
- 推奨
 - FSC curves
 - Half maps
 - Masks
 - その他使用したmap (additional maps)
- Map fileはそれぞれpixel sizeとrecommended contour levelの情報が必要
- 試料状態・電顕・検出器・測定条件・解析方法の情報も必要

Half mapsを必ず登録してください (お願い)

Primary map

モデル構築(精密化)に使用した, 目で見て欲しいマップ

Half maps

実際の解析結果に対応 (結晶で言う F_o , $\sigma(F_o)$)

Half mapsとmaskがあればFSCカーブも再計算可能

複数の再構成を組み合わせている場合は各half mapsを登録

十分細かい分解能シェル内において以下の議論が適用

$$F_{1o} = F_t + n_1 \quad F_{2o} = F_t + n_2 \quad (F_{1o}, F_{2o}: \text{Half map 1,2のFourier係数})$$

$$F_o = \frac{F_{1o} + F_{2o}}{2} = F_t + \frac{n_1 + n_2}{2} = F_t + n \quad (F_o: \text{Full mapのFourier係数})$$

$$\sigma_n^2 = \frac{\text{var}(F_{1o} - F_{2o})}{4} \quad (F_o \text{のnoise})$$

この方法による精密化は現在開発中

$$\rightarrow \text{精密化ターゲットに利用: } p(F_o; F_c) \propto \exp\left(-\frac{|F_o - DF_c|^2}{\sigma_{U,T}^2 + \sigma_n^2}\right)$$

$$\text{var}(F_o) = \text{var}(F_t) + \text{var}(n) = \sigma_T^2 + \sigma_n^2 \quad (\text{Variance of signal} + \text{variance of noise})$$

$$\text{FSC}_{\text{half}} = \frac{\sum F_{o1} F_{o2}^*}{\sqrt{\sum |F_{o1}|^2 \sum |F_{o2}|^2}} = \frac{\sigma_T^2}{\sigma_T^2 + 2\sigma_n^2}$$

$$\text{FSC}_{\text{full}} = \frac{\sigma_T^2}{\sigma_T^2 + \sigma_n^2} = \frac{2\text{FSC}_{\text{half}}}{1 + \text{FSC}_{\text{half}}}$$

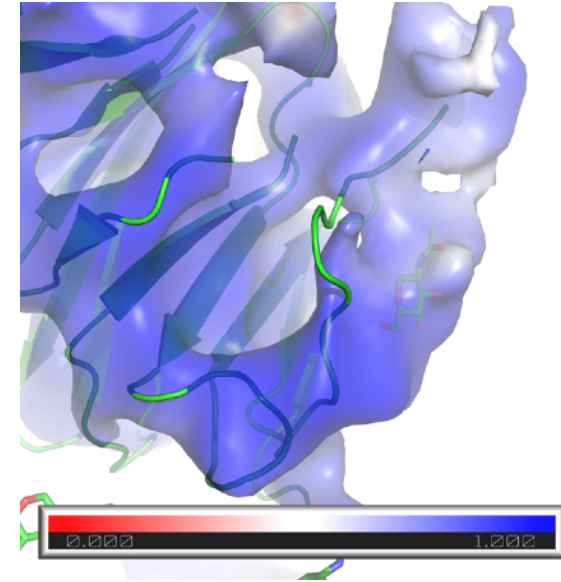
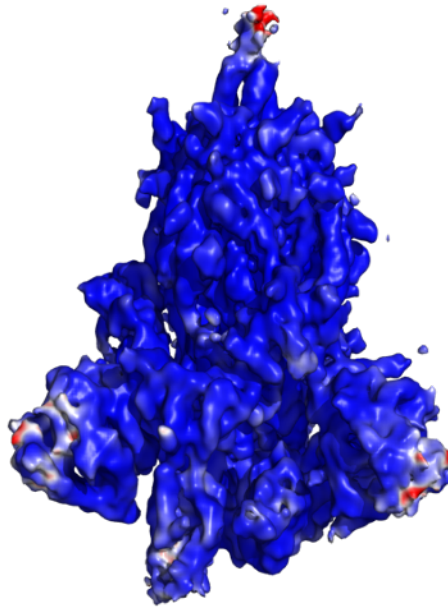
Half mapsを必ず登録してください (お願い)

利用例: half mapsを用いたvalidation

```
emda rcc --h1 emd_22162_half_map_1.map --h2 emd_22162_half_map_2.map --mdl 6x6f.pdb --res 4
```

$$RCC_{\text{full}} = \frac{2CC(\rho_{o1}, \rho_{o2})}{1 + CC(\rho_{o1}, \rho_{o2})}$$

Full-map equivalent for
real space half map CC



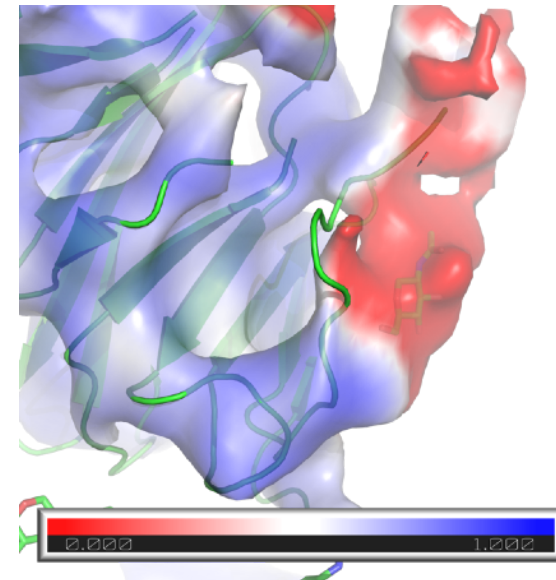
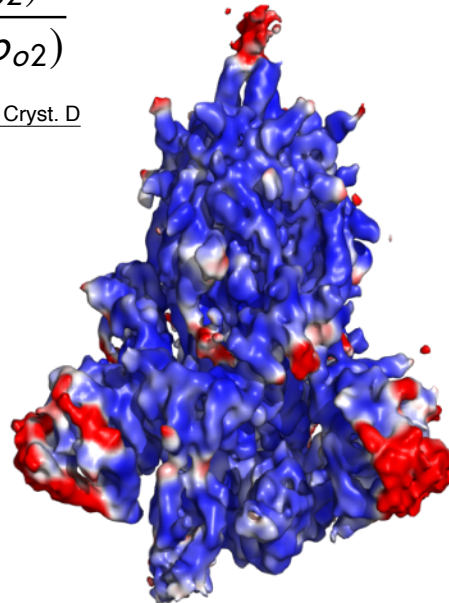
Kernel size: 5 px

$$CC(\rho_m, \rho_o) = CC(\rho_m, \rho_t) \sqrt{\frac{2CC(\rho_{o1}, \rho_{o2})}{1 + CC(\rho_{o1}, \rho_{o2})}}$$

t: true, m: model

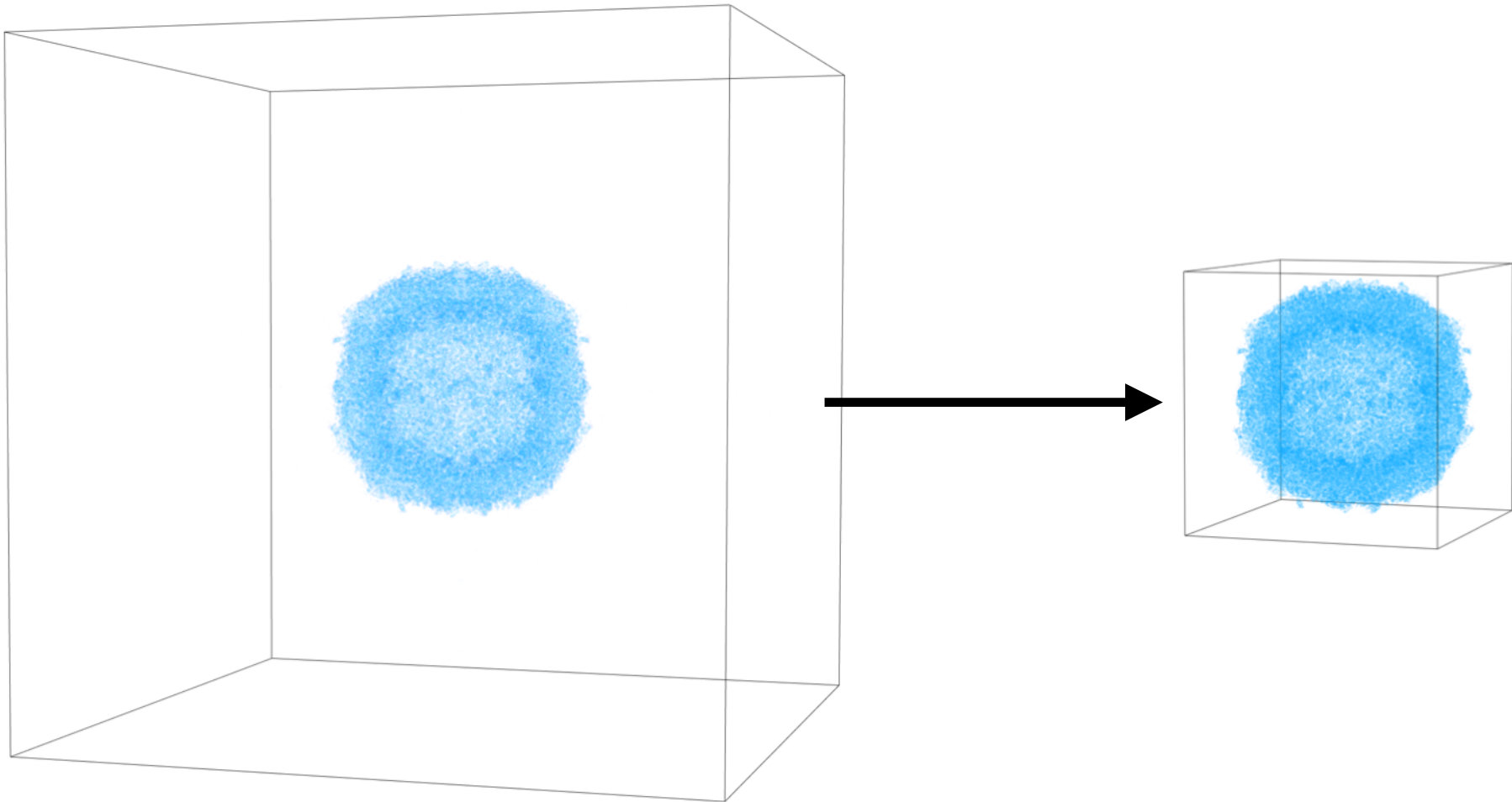
See Nicholls et al. (2018) Acta Cryst. D

$CC(\rho_m, \rho_o)$
Map-model CC



できれば小さなboxで登録を

```
relion_image_handler --i input.mrc --o output.mrc --new_box 256
```



Box size: 600 × 600 × 600
824 MB

Box size: 256 × 256 × 256
65 MB

モデル構築前に切り出してしまうことをお勧めします
(特に高分解能などでboxを大きく取っている時)

mask+10 Å程度取っておけば十分

非対称単位のみを登録を (ご提案)

- マップに対称性が適用されているならばモデルもその対称に従う必要がある
- 対称ならば独立な部分だけの座標を登録すべき
- 対称性を記述(BIOMT/_pdbx_struct_oper_list)して登録すれば拡張した全体の座標もPDBで提供される
- 現状Validation reportでは対称性を考慮してくれない問題はある... (改善していく予定)
- Annotation作業でも混乱が生じがちなので、ファイルを要求し自分できちんと確認する

7A4M

Cryo-EM structure of mouse heavy-chain apoferritin at 1.22 Å

7A4Mの概要

EMDBエントリー [11638](#)

分子名称 Ferritin heavy chain, FE (III) ION, ZINC ION, ... (4 entities in total)

機能のキーワード iron storage, metal binding protein

由来する生物種 Mus musculus (Mouse)

タンパク質・核酸の個数 1

分子量合計 [20200.85](#)

構造登録者 [Nakane, T., Kotecha, A., Sente, A., Yamashita, K., McMullan, G., Masiulis, S., Brown, P.M.G.E., Grigoras, I.T., Malinauskaitė, L., Malinauskas, T., Miehlings, J., Yu, L., Karia, D., Pechnikova, E.V., de Jong, E., Keizer, J., Bischoff, M., McCormack, J., Tiemeijer, P., Hardwick, S.W., Chirgadze, D.Y., Murshudov, G., Aricescu, A.R., Scheres, S.H.W.](#) (登録日: 2020-08-20, 公開日: 2020-10-26, 最終更新日: 2020-11-18)

主引用文献 [Nakane, T., Kotecha, A., Sente, A., McMullan, G., Masiulis, S., Brown, P.M.G.E., Grigoras, I.T., Malinauskaitė, L., Malinauskas, T., Miehlings, J., Uchanski, T., Yu, L., Karia, D., Pechnikova, E.V., de Jong, E., Keizer, J., Bischoff, M., McCormack, J., Tiemeijer, P., Hardwick, S.W., Chirgadze, D.Y., Murshudov, G., Aricescu, A.R., Scheres, S.H.W. **Single-particle cryo-EM at atomic resolution.** *Nature*, 587:152-156, 2020 \[PubMed: 33087931\]\(#\) \(主引用文献が同じPDBエントリー\) \[DOI: 10.1038/s41586-020-2829-0\]\(#\) \[Import into Mendeliev\]\(#\)](#)

実験手法 ELECTRON MICROSCOPY (1.22 Å)

構造検証レポート

Metric Percentile Ranks Value

Clashscore 2

Ramachandran outliers 0

ダウンロード

- Sequence (fasta)
- PDBx/mmCIF
- PDBML (ヘッダのみ (no-atom))
- PDB形式 (全ての情報)
- 検証レポート (PDF)
- More...

構造

非対称単位を表示

生物学的単位を表示

他のデータベース情報

wwPDB DOI Landing Page [Yorodumi](#)

7A5V

CryoEM structure of a human gamma-aminobutyric acid receptor, the GABA(A)R-beta3 homopentamer, in complex with histamine and megabody Mb25 in lipid nanodisc

7A5Vの概要

関連するPDBエントリー [4COF](#)

EMDBエントリー [11657](#)

分子名称 Gamma-aminobutyric acid receptor subunit beta-3, Gamma-aminobutyric acid receptor subunit beta-3, Megabody Mb25, 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose, ... (11 entities in total)

機能のキーワード pentameric ligand-gated ion channel, neurotransmitter receptor, gaba(a) receptor, membrane protein

由来する生物種 Homo sapiens (Human)

タンパク質・核酸の個数 2

分子量合計 [104693.2](#)

構造登録者 [Nakane, T., Kotecha, A., Sente, A., Yamashita, K., McMullan, G., Masiulis, S., Brown, P.M.G.E., Grigoras, I.T., Malinauskaitė, L., Malinauskas, T., Miehlings, J., Yu, L., Karia, D., Pechnikova, E.V., de Jong, E., Keizer, J., Bischoff, M., McCormack, J., Tiemeijer, P., Hardwick, S.W., Chirgadze, D.Y., Murshudov, G., Aricescu, A.R., Scheres, S.H.W.](#) (登録日: 2020-08-22, 公開日: 2020-11-18, 最終更新日: 2020-11-25)

主引用文献 [Nakane, T., Kotecha, A., Sente, A., McMullan, G., Masiulis, S., Brown, P.M.G.E., Grigoras, I.T., Malinauskaitė, L., Malinauskas, T., Uchanski, T., Yu, L., Karia, D., Pechnikova, E.V., de Jong, E., Keizer, J., Bischoff, M., McCormack, J., Tiemeijer, P., Hardwick, S.W., Chirgadze, D.Y., Murshudov, G., Aricescu, A.R., Scheres, S.H.W. **Single-particle cryo-EM at atomic resolution.** *Nature*, 587:152-156, 2020 \[PubMed: 33087931\]\(#\) \(主引用文献が同じPDBエントリー\) \[DOI: 10.1038/s41586-020-2829-0\]\(#\) \[Import into Mendeliev\]\(#\)](#)

実験手法 ELECTRON MICROSCOPY (1.7 Å)

ダウンロード

- Sequence (fasta)
- PDBx/mmCIF
- PDBML (ヘッダのみ (no-atom))
- PDB形式 (全ての情報)
- 検証レポート (PDF)
- More...

構造

非対称単位を表示

生物学的単位を表示

他のデータベース情報

wwPDB DOI Landing Page [Yorodumi](#)

非対称単位のみを登録を (ご提案)

```
$ rellion_refine --sym 0 --print_symmetry_ops
```

```
R(1)=
  1 0 0
  0 1 0
  0 0 1

R(2)=
  0 1 0
  0 0 1
  1 0 0

R(3)=
  0 0 1
  1 0 0
  0 1 0

R(4)=
  0 1 0
 -1 0 0
  0 0 1

⋮

R(24)=
  0 -1 0
 -1 0 0
  0 0 -1
```



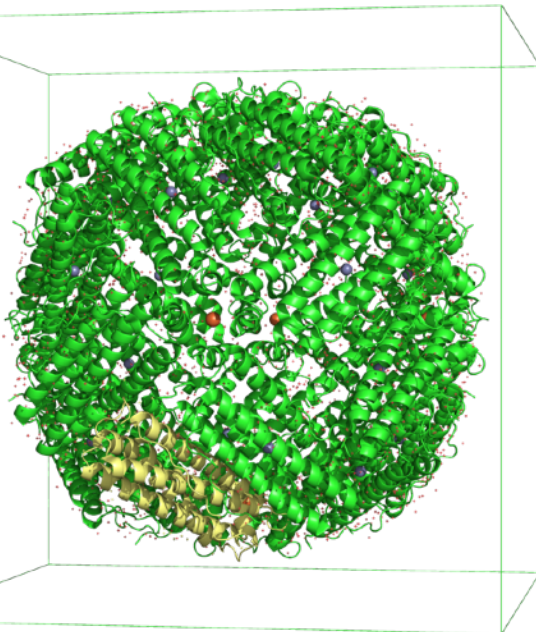
```
MATRIX1 1 1.000000 0.000000 0.000000 0.000000 0.00000 1
MATRIX2 1 0.000000 1.000000 0.000000 0.000000 0.00000 1
MATRIX3 1 0.000000 0.000000 1.000000 0.000000 0.00000 1
MATRIX1 2 0.000000 1.000000 0.000000 0.000000 0.00000
MATRIX2 2 0.000000 0.000000 1.000000 0.000000 0.00000
MATRIX3 2 1.000000 0.000000 0.000000 0.000000 0.00000
MATRIX1 3 0.000000 0.000000 1.000000 0.000000 0.00000
MATRIX2 3 1.000000 0.000000 0.000000 0.000000 0.00000
MATRIX3 3 0.000000 1.000000 0.000000 0.000000 0.00000
MATRIX1 4 0.000000 1.000000 0.000000 0.000000 0.00000
MATRIX2 4 -1.000000 0.000000 0.000000 0.000000 136.49921
MATRIX3 4 0.000000 0.000000 1.000000 0.000000 0.00000
⋮
MATRIX1 24 0.000000 -1.000000 0.000000 0.000000 136.49921
MATRIX2 24 -1.000000 0.000000 0.000000 0.000000 136.49921
MATRIX3 24 0.000000 0.000000 -1.000000 0.000000 136.49921
```

原点ではなく box の中心周りの対称操作にする必要があるため、

$$c - Mc$$

の並進が必要(M: 回転行列, c: box の中心座標)

- 非対称単位だけのモデルから全体を再現できるように、再構成で使用した対称操作を記述する
- REFMAC5の場合はNCSconstraintの機能を使ってそのまま非対称単位だけで精密化できる (要ver. 5.8.0272)
- 他の場合には同一構造になるように注意して精密化し、非対称単位だけ取り出してMATRIXを記述すればよい
- 手でやるのは大変なので以下の方法を一応用意しました (ちゃんとしたパイプラインを整備する予定...)



Box size= 136.499 Å

PDB: 7a4m

Download https://github.com/keitaroyam/yamtbx/blob/master/yamtbx/command_line/set_mtrix_records.py
 cctbx.python set_mtrix_records.py asym.pdb 0 [--box-size=136.499] [--overwrite]
 gemmi convert --expand-ncs=new asym.pdb complete.pdb

あまり嬉しくないエントリの例 (1)

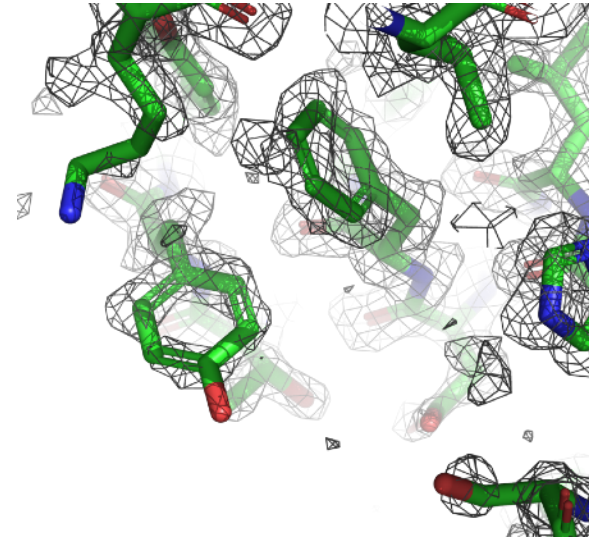
Primary mapとhalf mapsとでpixel sizeが一致しない

PDB 6v21 / EMD-21024

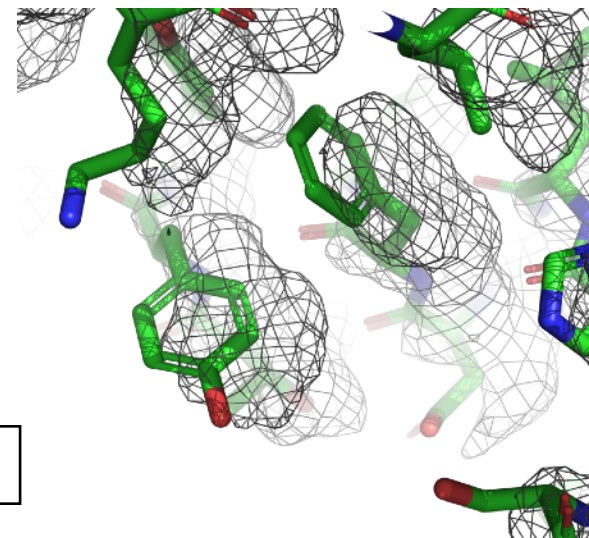
emd_21024.map
384×384×384
0.562 Å/px

emd_21024_half_map_1.map
384×384×384
0.566 Å/px

emd_21024_half_map_2.map
384×384×384
0.566 Å/px



Primary map



Half map 1

正しいpixel sizeを使って解析しているか要確認！

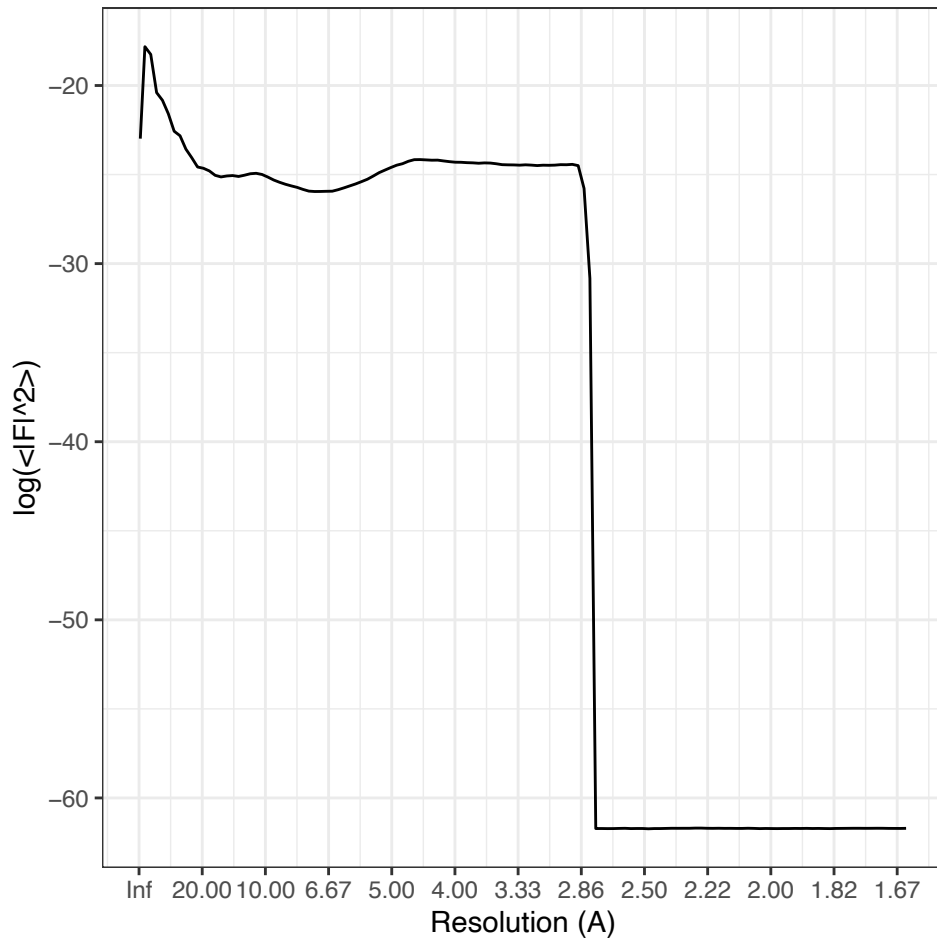
(PostProcessでpixel sizeを変えて、half mapsの方がそのままになった?)

あまり嬉しくないエントリの例 (2)

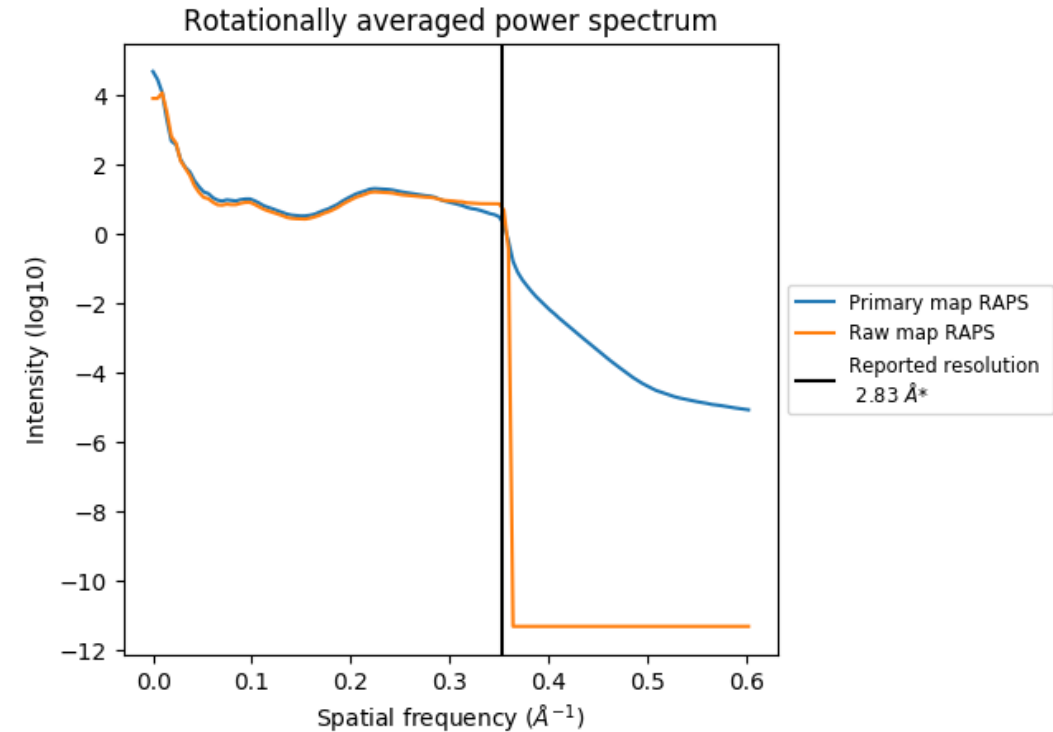
Half mapsがlow-pass/sharpenen/maskされてたりする

PDB 6k7I / EMD-9939

```
relicon_image_handler --i emd_9939_half_map_1.map:mrc --power
```



7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.353\AA^{-1}

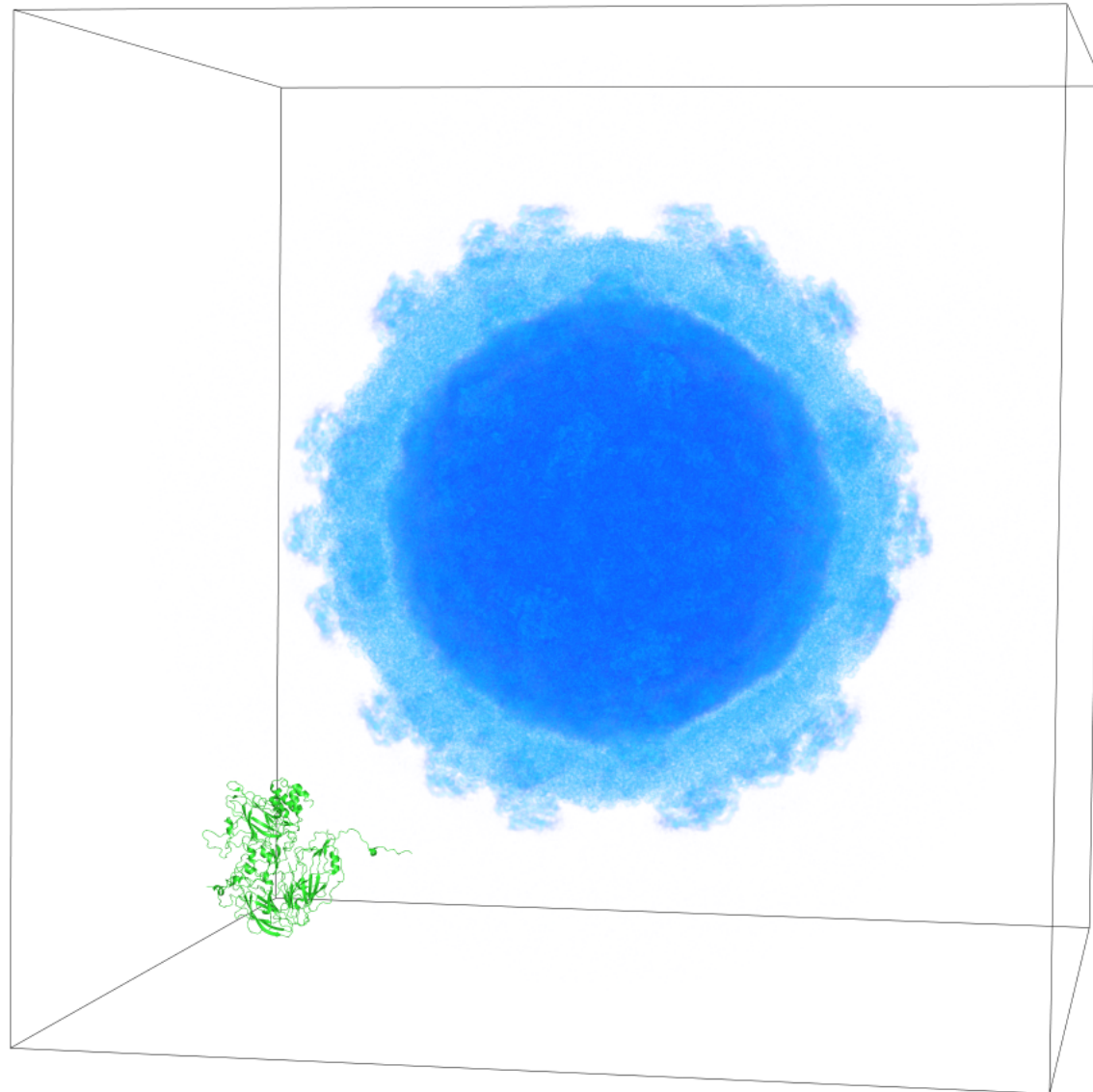
間違えてPostProcess後のhalf mapsをアップしてしまった
(差し替え依頼中)

Validation reportを見ましょう..orz
(Raw map = sum of half maps)

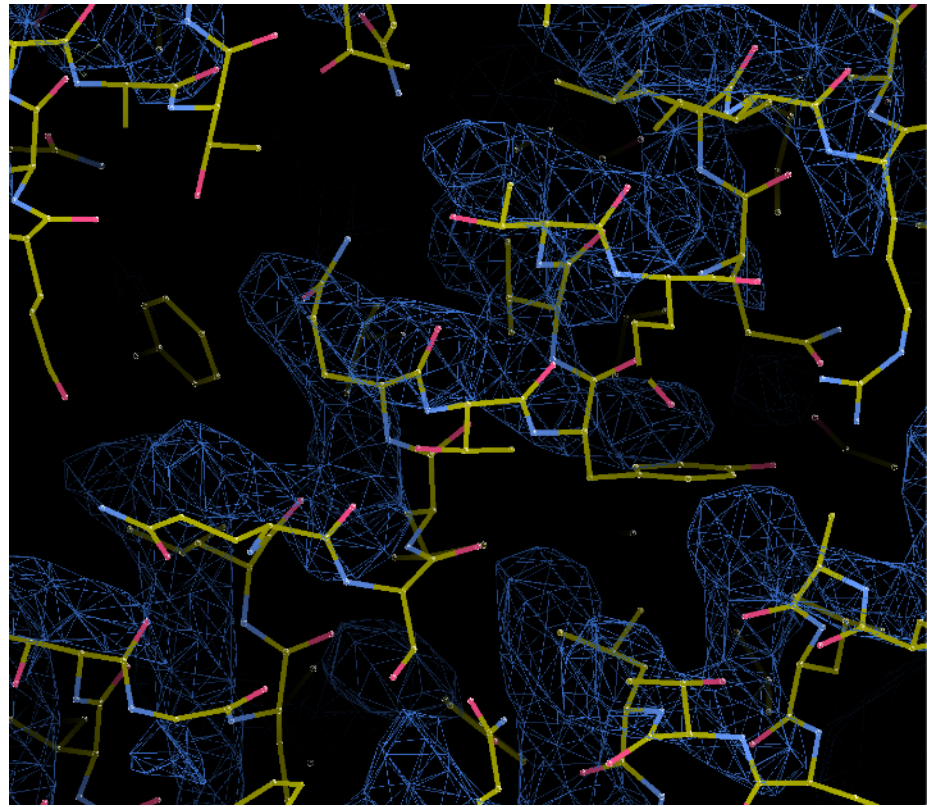
あまり嬉しくないエントリの例 (3)

完全にずれている・対称操作の記述も無し

PDB 5mm2 / EMD-3528

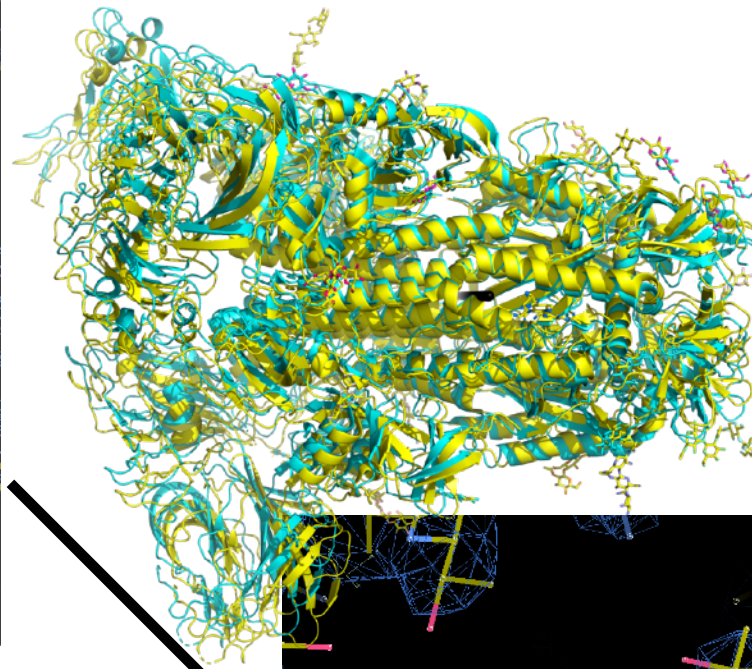


あまり嬉しくないエントリの例 (4)

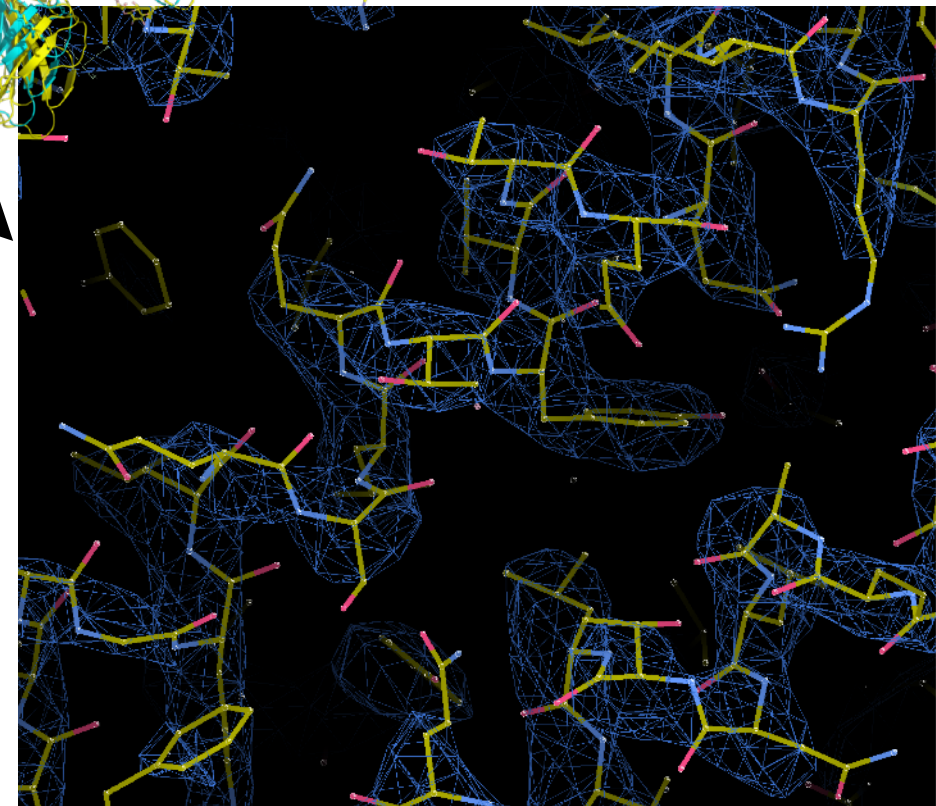


PDB 6crz / EMD-7577

微妙にずれている

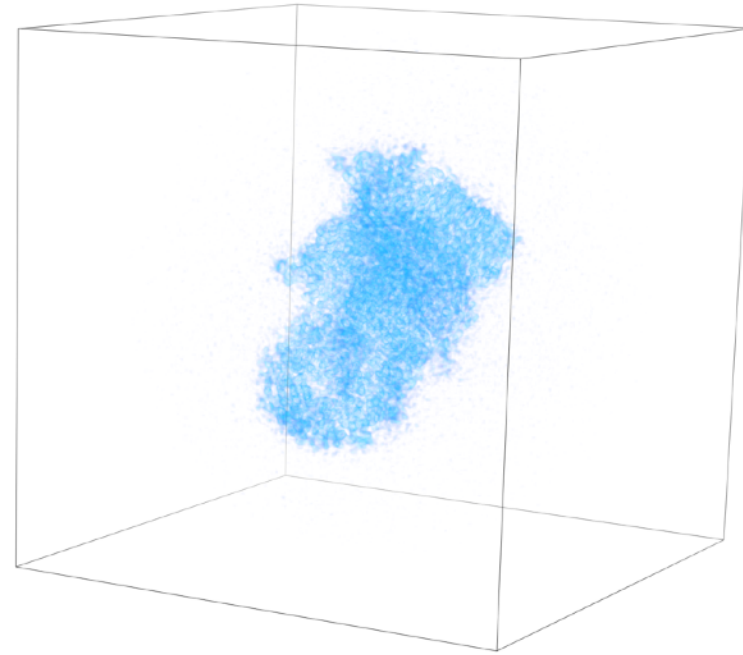


3.5° rotation
+ 1.7 Å
(Jiggle-fit by COOT)



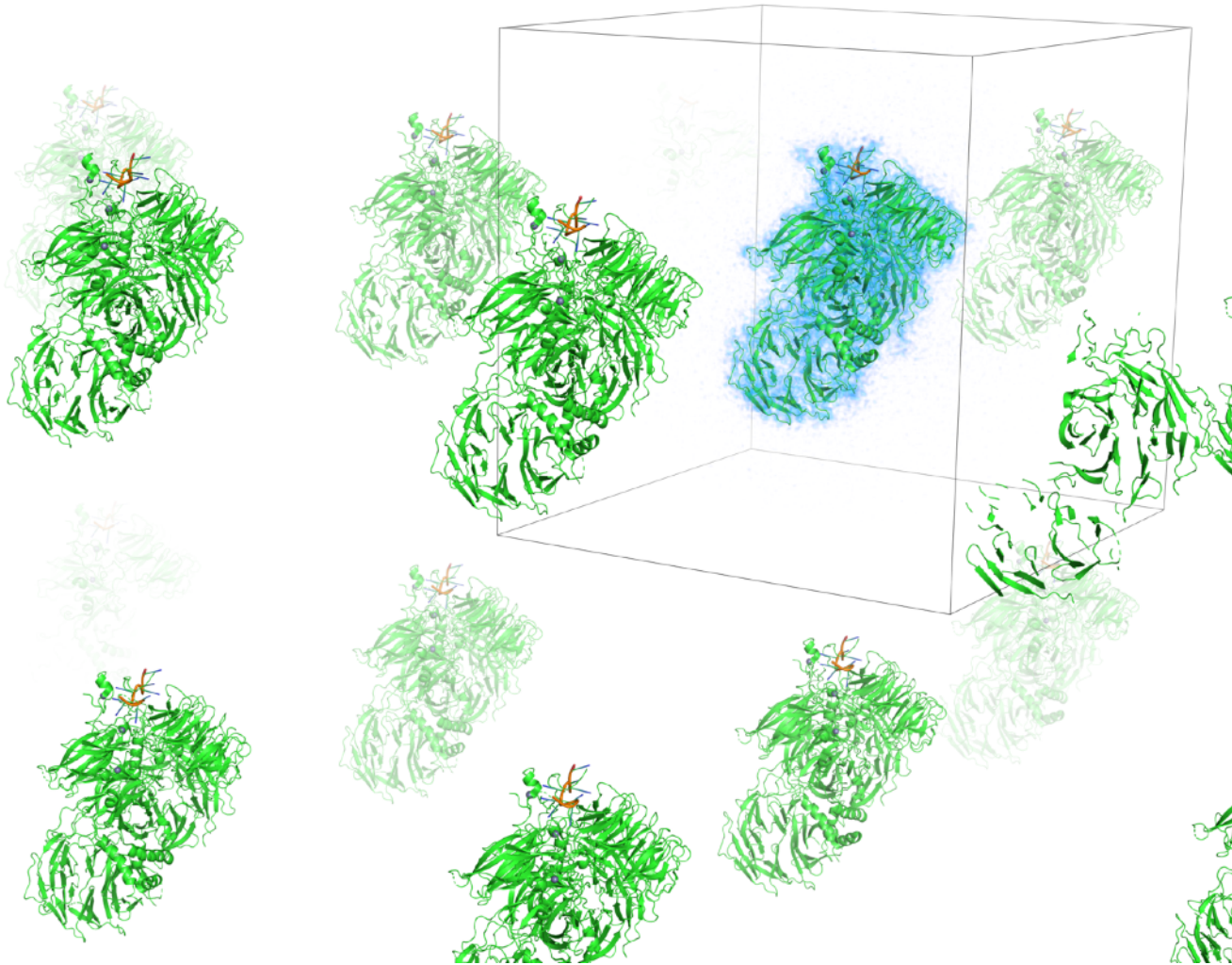
あまり嬉しくないエントリの例 (5)

PDB 6fbs / EMD-4225



あまり嬉しくないエントリの例 (5)

PDB 6fbs / EMD-4225



「並進対称性」を適用すると重なる
→結晶ではないので厳密には正しくない取り扱い
(COOTでモデル組むときにboxの外で始めてしまった?)

あまり嬉しくないエントリの例 (6)

原点がboxの中心からずれている

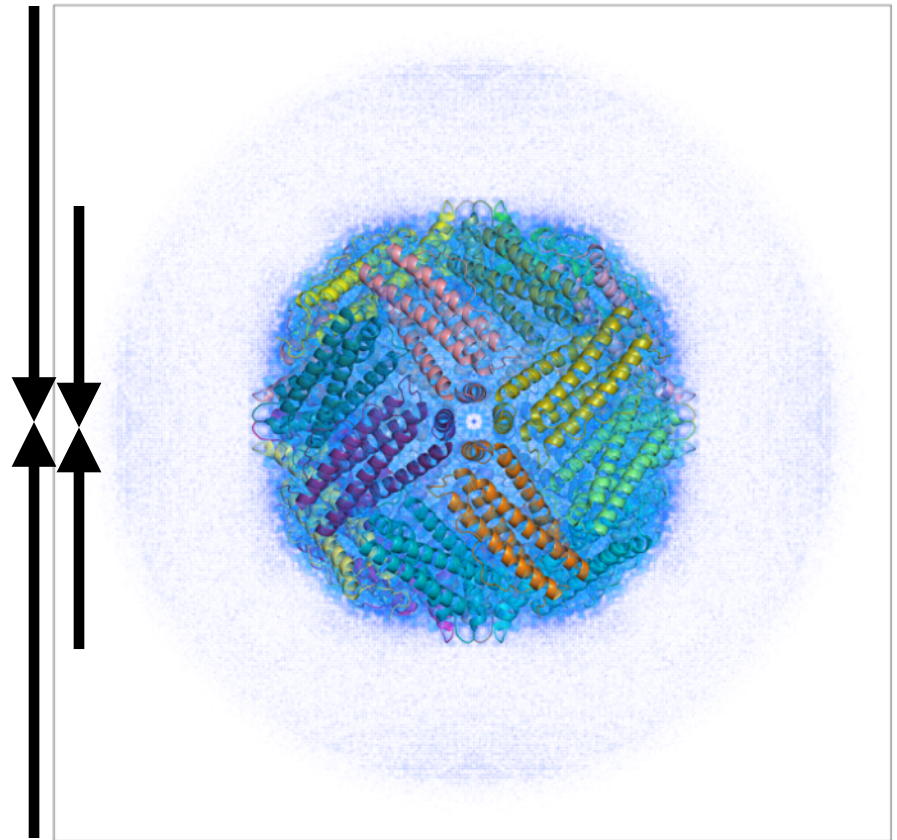
PDB 6wx6 / EMD-21951

Center of mass (protein model):
[117.504, 117.504, **116.688**]

Center of the box:
[117.504, 117.504, **117.504**]

Voxel size:
[0.816, 0.816, 0.816]

Zに-1 pxずれている



(この場合これが原因か分かりませんが)

手系を反転させるときに `relion_image_handler --flipz` 等を使うと
中心がズれてしまうので, `--invert_hand`を使いましょう

あまり嬉しくないエントリの例 (7)

Cn対称リスト (頻度)

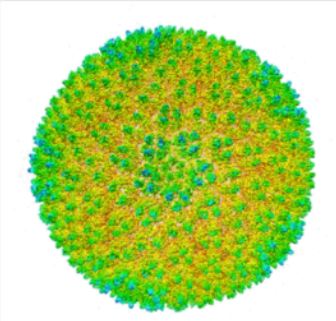
2288 C1
 385 C2
 212 C3
 206 C4
 72 C5
 86 C6
 52 C7
 10 C8
 7 C9
 2 C10
 5 C11
 12 C12
 6 C13
 13 C14
 13 C15
 5 C16
 1 C17
 1 C18
 1 C21
 2 C22
 1 C23
 5 C24
 1 C27
 1 C30
 1 C31
 1 C32
 1 C33
 1 C34
 1 C38
 1 C42
 3 C60
 1 C532

!?

EMDataResource
Unified Data Resource for 3DEM

EMD-4633 New Mol*3DViewer start new search

Title Cryo-EM structure of SH1 full particle.
Authors De Colibus L, Roine E, Walter TS, Ilca SL, Wang X, Wang N, Roseman AM, Bamford D, Huiskonen JT, Stuart DI
Method Single Particle (Reported Resolution 3.8 Å) [PDB:6qt9](#)



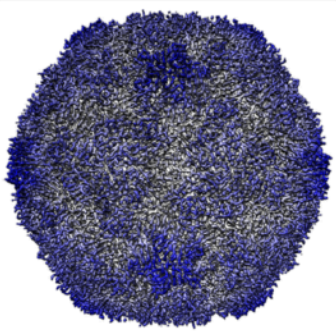
| Summary | Sample | Experiment | Map | Download | Links |
|--------------------------------|---------------------------|------------|-----|----------|-------|
| Vitrification | FEI VITROBOT MARK IV | | | | |
| Microscope | FEI POLARA 300 (300 kV) | | | | |
| Detector | GATAN K2 SUMMIT (4k x 4k) | | | | |
| Electron Dose | 1 (e/sq. Å) | | | | |
| Number of Particles | 16185 | | | | |
| Imposed Symmetry | C532 | | | | |
| Reconstruction Software | cisTEM | | | | |

<https://www.emdataresource.org/EMD-4633> 明らかに点群532 (I)の間違い

EMDataResource
Unified Data Resource for 3DEM

EMD-10220 New Mol*3DViewer start new search

Title Cryo-EM structure of rhinovirus-B5 complexed to antiviral OBR-5-340
Authors Wald J, Goessweiner-Mohr N, Blaas D, Pasin M
Method Single Particle (Reported Resolution 3.6 Å) [PDB:6sk5](#)



| Summary | Sample | Experiment | Map | Download | Links |
|---|---------------------------|------------|-----|----------|-------|
| Fitting Details: Rosetta: DiMaio, F. et al. Atomic-accuracy models from 4.5-Å cryo-electron microscopy data with density-guided iterative local refinement. Nat. Meth (2015). doi:10.1038/nmeth.3286 | | | | | |
| Vitrification | FEI VITROBOT MARK III | | | | |
| Microscope | FEI POLARA 300 (300 kV) | | | | |
| Detector | GATAN K2 SUMMIT (4k x 4k) | | | | |
| Images Collected | 2547 | | | | |
| Electron Dose | 40 (e/sq. Å) | | | | |
| Number of Particles | 46070 | | | | |
| Imposed Symmetry | C60 | | | | |
| Fitting Source Models | 1sym | | | | |

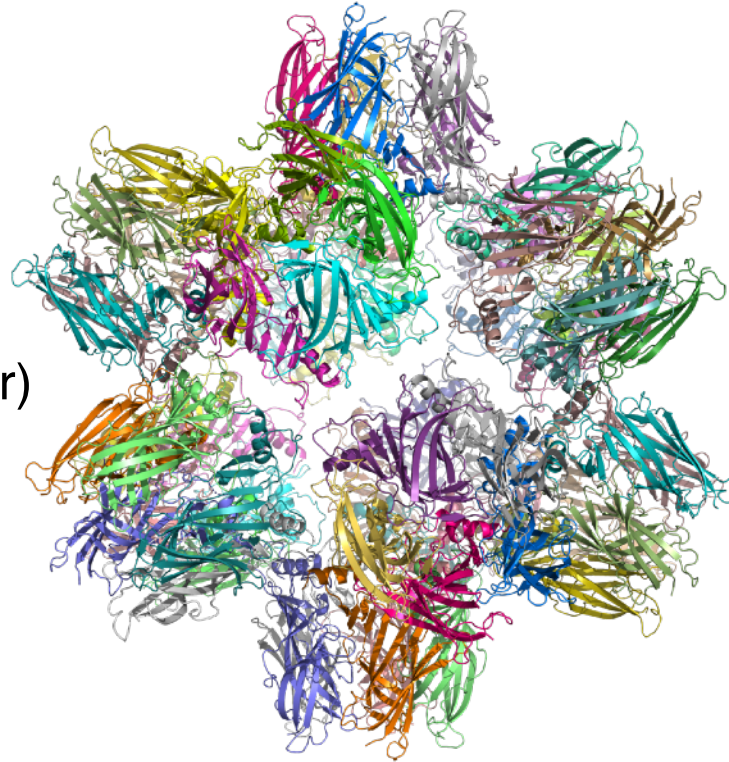
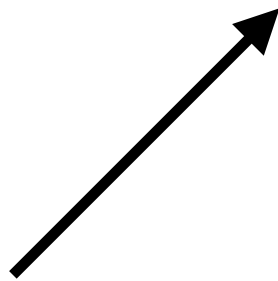
<https://www.emdataresource.org/EMD-10220> これもicosahedralの間違い (多重度60の意味?)

あまり嬉しくないエントリの例 (8)

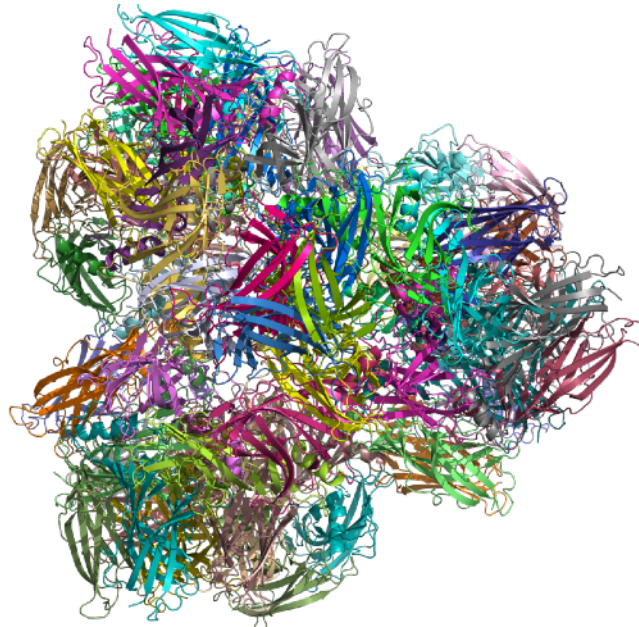
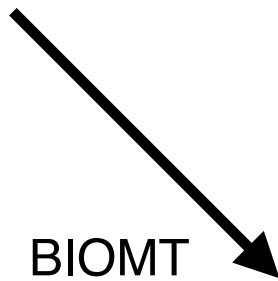
PDB 4aod



MTRIX
(`_struct_ncs_oper`)



BIOMT
(`_pdbx_struct_oper_list`)



MTRIXとBIOMTで
operatorが食い違っている

```
MTRIX1 1 1.000000 0.000000 0.000000 0.000000 1
MTRIX2 1 0.000000 1.000000 0.000000 0.000000 1
MTRIX3 1 0.000000 0.000000 1.000000 0.000000 1
MTRIX1 2 -0.638235 0.262556 0.723685 0.000000 93.23290
MTRIX2 2 0.263276 -0.808923 0.525670 145.85156
MTRIX3 2 0.723424 0.526030 0.447158 -99.61087
MTRIX1 3 0.053540 -0.688324 0.723425 130.33752
MTRIX2 3 0.688513 -0.499271 -0.526002 191.18123
MTRIX3 3 0.723245 0.526250 0.447189 -99.61156
MTRIX1 4 -0.138197 0.951057 -0.276390 66.28390
MTRIX2 4 -0.425326 -0.309014 -0.850652 369.65385
MTRIX3 4 -0.894427 -0.000002 0.447214 206.95127
MTRIX1 5 0.361983 0.262984 -0.894320 181.51684
MTRIX2 5 -0.588201 0.808715 -0.000268 111.52288
MTRIX3 5 0.723179 0.526137 0.447428 -99.64622
MTRIX1 6 -0.447790 0.850337 -0.276426 124.96839
MTRIX2 6 -0.525647 -0.000262 0.850703 96.54892
MTRIX3 6 0.723312 0.526239 0.447094 -99.60640
MTRIX1 7 0.809328 -0.587357 0.000117 111.22375
MTRIX2 7 -0.587357 -0.809328 -0.000046 342.75416
MTRIX3 7 0.000122 -0.000031 -1.000000 285.98582
MTRIX1 8 -0.671086 0.687901 0.276470 101.05413
MTRIX2 8 0.162163 0.500082 -0.850659 169.94620
MTRIX3 8 -0.723427 -0.526032 -0.447150 385.60843
MTRIX1 9 -0.361624 -0.263238 0.894390 104.46807
MTRIX2 9 -0.588261 0.808671 0.000161 111.45480
MTRIX3 9 -0.723310 -0.526077 -0.447288 385.63868
MTRIX1 10 0.447724 -0.850437 0.276224 161.09678
MTRIX2 10 -0.525930 -0.000630 0.850528 96.67429
MTRIX3 10 -0.723146 -0.526076 -0.447552 385.65377
MTRIX1 11 0.638661 -0.262488 -0.723334 192.63400
MTRIX2 11 0.263075 -0.808894 0.525816 145.85092
MTRIX3 11 -0.723121 -0.526109 -0.447555 385.65465
MTRIX1 12 -0.053475 0.688102 -0.723641 155.73938
MTRIX2 12 0.688529 -0.499455 -0.525807 191.15112
MTRIX3 12 -0.723235 -0.526365 -0.447070 385.60831
```

```
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D, E
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000 0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.000000 0.00000
REMARK 350 BIOMT1 2 0.997251 0.000950 -0.074094 12.65858
REMARK 350 BIOMT2 2 0.000950 -1.000000 -0.000035 328.65829
REMARK 350 BIOMT3 2 -0.074094 -0.000035 -0.997251 345.43041
REMARK 350 BIOMT1 3 -0.998591 -0.037548 0.037505 236.77609
REMARK 350 BIOMT2 3 -0.037548 0.000417 -0.999295 337.19833
REMARK 350 BIOMT3 3 0.037505 -0.999295 -0.001826 328.68044
REMARK 350 BIOMT1 4 -0.998660 0.036598 0.036589 224.75055
REMARK 350 BIOMT2 4 0.036598 -0.000418 0.999330 -8.32664
REMARK 350 BIOMT3 4 0.036589 0.999330 -0.000922 0.09779
REMARK 350 BIOMT1 5 0.053080 -0.687990 0.723777 103.35324
REMARK 350 BIOMT2 5 0.688179 -0.500000 -0.525747 253.60843
REMARK 350 BIOMT3 5 0.723597 0.525994 0.446920 -79.02119
REMARK 350 BIOMT1 6 -0.001347 0.688014 -0.725696 127.92609
REMARK 350 BIOMT2 6 0.724767 0.500672 0.473329 -83.61828
REMARK 350 BIOMT3 6 0.688993 -0.525323 -0.499325 257.39075
REMARK 350 BIOMT1 7 -0.000027 -0.725546 0.688173 121.82351
REMARK 350 BIOMT2 7 -0.688154 0.499328 0.526418 75.15089
REMARK 350 BIOMT3 7 -0.725565 -0.473555 -0.499301 416.56757
REMARK 350 BIOMT1 8 -0.051706 0.725522 -0.686254 121.08238
REMARK 350 BIOMT2 8 -0.724792 -0.500000 -0.474000 412.38894
REMARK 350 BIOMT3 8 -0.687024 0.472883 0.551705 79.27151
REMARK 350 BIOMT1 9 0.053080 0.688179 0.723597 -122.83448
REMARK 350 BIOMT2 9 -0.687990 -0.500000 0.525994 239.47488
REMARK 350 BIOMT3 9 0.723777 -0.525747 0.446920 93.84533
REMARK 350 BIOMT1 10 -0.000027 -0.688154 -0.725565 353.96547
REMARK 350 BIOMT2 10 -0.725546 0.499328 -0.473555 248.13124
REMARK 350 BIOMT3 10 0.688173 0.526418 -0.499301 84.59608
REMARK 350 BIOMT1 11 -0.051706 -0.724792 -0.687024 359.61844
REMARK 350 BIOMT2 11 0.725522 -0.500000 0.472883 80.86028
REMARK 350 BIOMT3 11 -0.686254 -0.474000 0.551705 234.83130
REMARK 350 BIOMT1 12 -0.001347 0.724767 0.688993 -116.56422
REMARK 350 BIOMT2 12 0.688014 0.500672 -0.525323 89.06357
REMARK 350 BIOMT3 12 -0.725696 0.473329 -0.499325 260.93594
```

登録の流れ

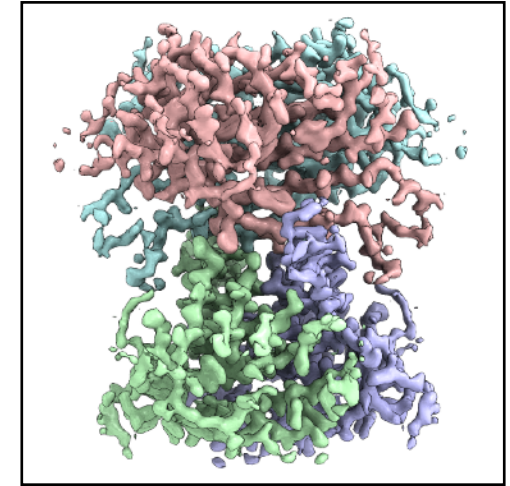
～RELION 3.1で解析した1.93 Å streptavidinの場合～

PostProcess/job798/note.txt:

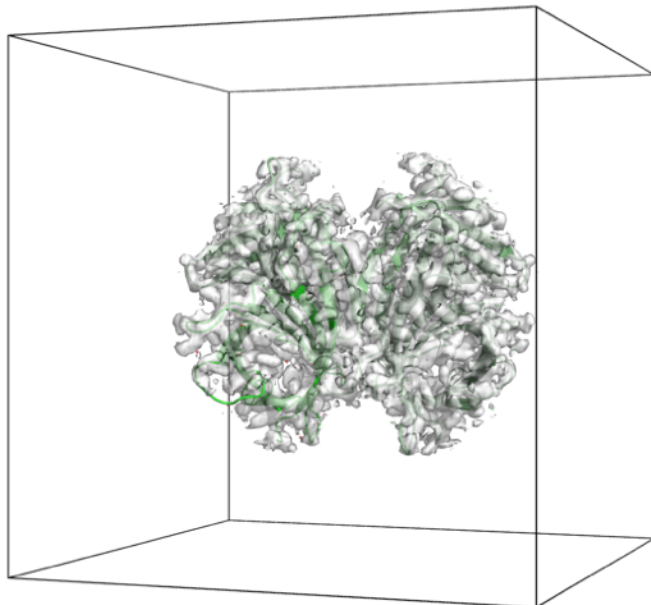
```
`which relion_postprocess` --mask MaskCreate/job790/mask.mrc
--i Refine3D/job796/run_half1_class001_unfil.mrc ...
```

| | |
|--|--------------|
| PostProcess/job798/postprocess_masked.mrc | ←Primary map |
| PostProcess/job798/postprocess_fsc.xml | ←FSC curve |
| MaskCreate/job790/mask.mrc | ←Mask |
| Refine3D/job796/run_half1_class001_unfil.mrc | ←Half map 1 |
| Refine3D/job796/run_half2_class001_unfil.mrc | ←Half map 2 |
| Refmac_1/refined.mmcif | ←精密化した構造 |

Map・maskは上記を切り出したもの

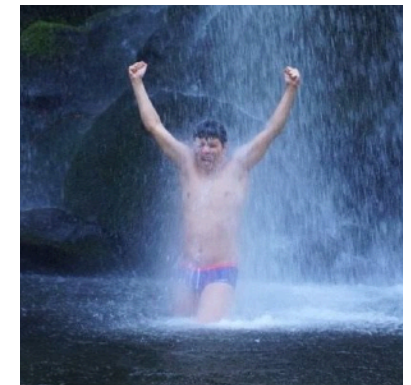


+ サムネイル画像 (500x500 px)



構造は非対称単位のみ. mmCIFに対称操作は
記述済み (REFMACによる出力)


```
loop_
_struct_ncs_oper.id
_struct_ncs_oper.code
_struct_ncs_oper.matrix[1][1]
_struct_ncs_oper.matrix[1][2]
_struct_ncs_oper.matrix[1][3]
_struct_ncs_oper.vector[1]
_struct_ncs_oper.matrix[2][1]
_struct_ncs_oper.matrix[2][2]
_struct_ncs_oper.matrix[2][3]
_struct_ncs_oper.vector[2]
_struct_ncs_oper.matrix[3][1]
_struct_ncs_oper.matrix[3][2]
_struct_ncs_oper.matrix[3][3]
_struct_ncs_oper.vector[3]
1 given 1 0 0 0 1 0 0 0 1 0
2 generate -1 0 0 87.99963 0 -1 0 87.99963 0 0 1 0
3 generate 1 0 0 0 0 -1 0 87.99963 0 0 -1 87.99963
4 generate -1 0 0 87.99963 0 1 0 0 0 0 -1 87.99963
```




解析: 東京大学 平泉将浩さん

西澤准教授・濡木教授

登録の流れ



wwPDB OneDep System

[FAQ](#)
[Tutorials](#)


Existing deposition

Deposition ID

Password


Log in

Forgot Password

Validation server

Have you checked your data at the stand-alone validation server?
validate.wwpdb.org

wwPDB regions



Start a new deposition

Welcome to the wwPDB OneDep system!

To continue with an existing deposition, please login on the left.
Please note that un-submitted sessions will expire 3 months after last login. Un-submitted sessions and uploaded files will be removed once they expire.

To start a new deposition, please complete the form below. Upon completion, you will be emailed login information specific to your new deposition.

Question about an in-progress deposition? For fastest response, login into your session and select the "Communication" page from the left hand navigation panel.

For requests such as entry release or citation updates, please login to the deposition system and send us a message through the communications section

If you have any other feedback, please write to us at deposit-help@mail.wwpdb.org
At this time this deposition system does not work with Internet Explorer versions 8 or less.

Warning: Please note the current system does not support multiple simultaneous depositions.

On initiation of a deposition session the wwPDB OneDep system will provide the Corresponding Author with a deposition session password. Responsibility for managing the access information to each deposition session, and hence the privacy of this information, rests with the Principal Investigator(s).

Your e-mail address

Password (optional, or we will provide one)
This is a shared "group password"
(6 to 16 alphanumeric characters)

Country/Region

Experimental method

X-Ray Diffraction

Electron Microscopy

- Helical
- Single particle
- Subtomogram averaging
- Tomography

Solution NMR

Neutron Diffraction

Electron Crystallography

Solid-state NMR

Fiber Diffraction

Are you depositing coordinates with this submission?

No, experimental data only

Yes

Has the associated map been deposited previously?

No

Yes

Requested accession codes

PDB EMDB BMRB

Please copy this code: **79747**

Privacy policy

Tick to indicate that you have read and accepted the wwPDB policy on personal data privacy, including what data wwPDB collects, how the data is stored and shared. www.wwpdb.org/about/privacy

Start deposition

座標もあるときは同時に
登録しましょう

登録の流れ

Map upload instructions

- Uploaded map and masks (CCP4 or MRC map formats only) will be converted to the Electron Microscopy Data Bank map format. For large maps the conversion maybe slow - we appreciate your patience.
- **If you wish to upload files larger than 1.5Gb, please try first. If it fails, please contact us through the communication tab to obtain alternate upload options.**
- Map must have positive densities (contrast), irrespective of the type of electron microscope images (negative stain, or frozen-hydrated). If the contrast density for the map is found to be negative, a scale factor of (-1) will be applied to make the density positive, following the convention recommended by [Heymann et al. J. Struct. Biol. 2005 \(2\):196-207](#)
- Image of your map (500x500 pixel, white background preferred) must be free from copyright restrictions. This image will be displayed on the atlas pages for your entry when the map is released.
- FSC curve files (XML format) can be generated via [this server](#), or using software packages such as EMAN2, RELION or Bsoft. An example of a FSC curve file is available [here](#)

ファイルを選択

| | Converted file name | Author's file name | Upload date/time (UTC) | File size | File type |
|-----------------|---|----------------------------------|------------------------|-----------|--|
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_em-volume_P1.map.V2 | postprocess_masked_cut.mrc | 2021-01-16 10:13 | 5.33 MB | EM map (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.05 Short description: FSC-weighted, sharpened and masked map by PostProcess |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_img-emdb_P1.png.V1 | EMDB_2_Streptavidin.png | 2021-01-16 10:23 | 211.49 KB | Entry image for public display |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_em-mask-volume_P1.map.V2 | mask_cut.mrc | 2021-01-16 10:25 | 5.33 MB | EM mask (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.5 Short description: |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_em-half-volume_P2.map.V2 | run_half2_class001_unfil_cut.mrc | 2021-01-16 10:26 | 5.33 MB | EM half map (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.05 Short description: |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_em-half-volume_P1.map.V2 | run_half1_class001_unfil_cut.mrc | 2021-01-16 10:26 | 5.33 MB | EM half map (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.05 Short description: |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_fsc-xml_P1.xml.V2 | postprocess_fsc.xml | 2021-01-16 10:31 | 7.29 KB | FSC file (XML format) |
| Previous upload | <input checked="" type="checkbox"/> D_1300020330_model_P1.cif.V7 | refined_fix.mmcif | 2021-01-16 10:37 | 165.49 KB | Coordinates (mmCIF format) |

- ✓ Select file type...
 - 0) Coordinates
 - Coordinates (mmCIF format)
 - Coordinates (PDB format)
 - 1) Main map (mandatory)
 - EM map (MRC/CCP4 format)
 - 2) Image for EMDB (mandatory)
 - Entry image for public display
 - 3) Additional maps
 - Additional EM map (MRC/CCP4 format)
 - 4) Masks
 - EM mask (MRC/CCP4 format)
 - 5) Half (even-odd) maps
 - EM half map (MRC/CCP4 format)
- Other Files
 - FSC file (XML format)
 - Layer line data

Process selected files

登録の流れ

Map upload instructions

- Uploaded map and masks (CCP4 or MRC map formats only) will be converted to the Electron Microscopy Data Bank map format. For large maps the conversion maybe slow - we appreciate your patience.
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- Map must have positive densities (contrast), irrespective to the type of electron microscope images (negative stain, or frozen-hydrated). If the contrast density for the map is found to be negative, a scale factor of (-1) will be applied to make the density positive, following the convention recommended by [Heymann et al. J. Struct. Biol. 2005 \(2\):196-207](#)
- Image of your map (500x500 pixel, white background preferred) must be free from copyright restrictions. This image will be displayed on the atlas pages for your entry when the map is released.
- FSC curve files (XML format) can be generated via [this server](#), or using software packages such as EMAN2, RELION or Bsoft. An example of a FSC curve file is available [here](#)

ファイルを選択

| | Converted file name | Author's file name | Upload date/time (UTC) | File size | File type | |
|-----------------|-------------------------------------|---------------------------------------|----------------------------------|------------------|-----------|--|
| Previous upload | <input checked="" type="checkbox"/> | D_1300020330_em-volume_P1.map.V2 | postprocess_masked_cut.mrc | 2021-01-16 10:13 | 5.33 MB | EM map (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.05 Short description: FSC-weighted, sharpened and masked map by PostProcess |
| Previous upload | <input checked="" type="checkbox"/> | D_13000 | | | | |
| Previous upload | <input checked="" type="checkbox"/> | D_13000 | | | | |
| Previous upload | <input checked="" type="checkbox"/> | D_13000 | | | | |
| Previous upload | <input checked="" type="checkbox"/> | D_1300020330_em-half-volume_P1.map.V2 | run_half1_class001_unfil_cut.mrc | 2021-01-16 10:26 | 5.33 MB | EM half map (MRC/CCP4 format) Pixel spacing (Å): 0.7999967 Contour level: 0.05 Short description: |
| Previous upload | <input checked="" type="checkbox"/> | D_1300020330_fsc-xml_P1.xml.V2 | postprocess_fsc.xml | 2021-01-16 10:31 | 7.29 KB | FSC file (XML format) |
| Previous upload | <input checked="" type="checkbox"/> | D_1300020330_model_P1.cif.V7 | refined_fix.mmcif | 2021-01-16 10:37 | 165.49 KB | Coordinates (mmCIF format) |

- Pixel sizeはヘッダと異なると警告が出る (ヘッダのまままでOKのオプションが欲しい...)
- Contour levelはChimeraやCOOT等で確認しておくこと (rmsdレベルで書かないように注意)
- Descriptionも書いておいたほうが良いかも
- ミスがあるとpixel, contour, descriptionは全部消える(!)

- ✓ Select file type...
- 0) Coordinates
 - Coordinates (mmCIF format)
 - Coordinates (PDB format)
 - 1) Main map (mandatory)
 - EM map (MRC/CCP4 format)
 - 2) Image for EMDB (mandatory)
 - Entry image for public display
 - 3) Additional maps
 - Additional EM map (MRC/CCP4 format)
 - 4) Masks
 - EM mask (MRC/CCP4 format)
 - 5) Half (even-odd) maps
 - EM half map (MRC/CCP4 format)
- Other Files
- FSC file (XML format)
 - Layer line data

Process selected files

Submit deposition

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
- ✓ Re-upload files
- ✓ Upload summary
- Admin
 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
 - ✓ Entry title & author
 - ✓ Citation information
- Macromolecules
 - ✓ 1) Streptavidin
- EM sample
 - ✓ Overall sample description
- EM experiment
 - ✓ Specimen preparation
 - ✓ Microscopy
 - ✓ Image recording
 - ✓ Reconstruction
 - ✓ Fitting interpretation
- ✓ Ligands
- ✓ Assembly
- ✓ Related entries
- ✓ Validation reports
- ✓ Summary & conditions

Log out

Overall sample description

Overall sample information

Choose the map or mask described in this section: **i**

Type*: **i**

Macromolecules and ligands in the sample: **i** Streptavidin

Name*: **i**

Details: **i**

Source

How was the sample obtained?*: **i**

Natural source

Organism name*: **i**

NCBI taxonomy ID*: **i**

Strain (if not provided in organism name): **i**

Organ: **i**

Tissue: **i**

Organelle: **i**

Cellular location: **i**

Molecular weight

Experimentally measured?: **i** NO YES

Molecular weight units: **i**

Molecular weight: **i**

- CELL
- COMPLEX
- ORGANELLE OR CELLULAR COMPONENT
- RIBOSOME
- TISSUE
- VIRUS

かなり不思議な分類・・・

(`_em_entity_assembly.type`に対応)

登録の流れ

Submit deposition

All Items

Mandatory items

Navigation

- Instructions
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 - Microscopy
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 - Fitting interpretation
- Ligands
- Assembly
- Related entries
- Validation reports
- Summary & conditions

Log out

Spe

Specimen

Choose a sample or sample subcomponent used for this specimen preparation*: (1) Streptavidin

Specimen state*: PARTICLE

Specimen concentration (mg/mL):

Specimen details:

- 2D ARRAY
- 3D ARRAY
- FILAMENT
- HELICAL ARRAY
- PARTICLE
- TISSUE

Buffer

pH*: 7.2

Buffer components

| Formula | Name | Concentration | Concentration units |
|---------|------|---------------|---------------------|
| | | | |

Buffer details:

Vitrification

Was the specimen vitrified?*: YES

Cryogen*: ETHANE

Chamber humidity (%): 100

Chamber temperature (K): 277

Instrument: FEI VITROBOT MARK IV

Details:

- ETHANE
- ETHANE-PROPANE
- FREON 12
- FREON 22
- HELIUM
- METHANE
- NITROGEN
- OTHER
- PROPANE

Staining

Specimen stained?*: NO YES

Embedding

Specimen embedded?*: NO YES

Shadowing

Specimen shadowed?*: NO YES

Grid

Company and model: UltrAuFoil R1.2/1.3

Material: GOLD

Grid mesh (lines/inch): 300

Film support

Material: GOLD Topology: HOLEY ARRAY Thickness: 500

Grid pretreatment

Type of pretreatment: GLOW DISCHARGE

Time (s): 120

Atmosphere: AIR

Pressure (Pa):

Details: coated grid with pentylamine before glow discharge

登録の流れ

Submit deposition

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
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- ✓ Upload summary
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 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
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- ✓ Assembly
- ✓ Related entries
- ✓ Validation reports
- ✓ Summary & conditions

Log out

Choose the specimen preparation used for this microscopy session* (1) Streptavidin ▼

Microscope model*: TFS KRIOS ▼

Illumination mode*: FLOOD BEAM ▼

Imaging mode*: BRIGHT FIELD ▼

Electron source*: FIELD EMISSION GUN ▼

Acceleration voltage (kV)*: 300

C2 aperture diameter (μm): []

Spherical aberration coefficient (Cs in mm): []

Nominal minimum defocus (nm): []

Calibrated minimum defocus (nm): []

Nominal maximum defocus (nm): []

Calibrated maximum defocus (nm): []

Nominal magnification: []

Calibrated magnification: []

Specimen holder: []

Cooling cryogen: [] ▼

Minimum temperature (K): []

Maximum temperature (K): []

Alignment procedure: [] ▼

Residual tilt (if alignment procedure is coma free, mrad): []

TFS KRIOSとFEI TITAN KRIOSが別にある...

- FLOOD BEAM
- OTHER
- SPOT SCAN

- BRIGHT FIELD
- DARK FIELD
- DIFFRACTION
- OTHER

- FIELD EMISSION GUN
- LAB6
- OTHER
- TUNGSTEN HAIRPIN

Details:



[]

Specialist optics

Phase plate information:



[] ▼

Spherical aberration corrector information:



[]

Chromatic aberration corrector information:



[]

Energy filter name:



GIF Bioquantum

Energy filter slit width (range) in electron volts (eV):



15

Software used to collect images

| Name | Version | Details |
|----------|---------|---------|
| SerialEM | [] | [] |

⌵ +

Continue to next section

登録の流れ

Submit deposition

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
- ✓ Re-upload files
- ✓ Upload summary
- ✚ Admin
 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
 - ✓ Entry title & author
 - ✓ Citation information
- ✚ Macromolecules
 - ✓ 1) Streptavidin
- ✚ EM sample
 - ✓ Overall sample description
- ✚ EM experiment
 - ✓ Specimen preparation
 - ✓ Microscopy
 - Image recording
 - ✓ Reconstruction
 - ✓ Fitting interpretation
- ✓ Ligands
- ✓ Assembly
- ✓ Related entries
- ✓ Validation reports
- ✓ Summary & conditions

Log out

Image recording

| | | |
|--|---|--|
| Microscopy settings*: | i | (1) TFS KRIOS (300kV) ▾ |
| Film/CCD/Direct electron detector model*: | i | GATAN K3 BIOQUANTUM (6k x 4k) ▾ |
| Width (pixel units): | i | <input type="text"/> |
| Height (pixel units): | i | <input type="text"/> |
| Sampling interval (μm): | i | <input type="text"/> |
| Average electron dose per image ($\text{e}^-/\text{\AA}^2$): | i | <input type="text" value="70"/> |
| Average exposure time per image (seconds): | i | <input type="text" value="1.5"/> |
| Number of grids imaged: | i | <input type="text" value="1"/> |
| Number of images: | i | <input type="text" value="2277"/> |
| Details: | i | <div style="border: 1px solid #ccc; height: 80px; width: 100%;"></div> |

Continue to next section

ここで"image"はmovieのことを意味しているようです

登録の流れ

- EMDB MAP
- INSILICO MODEL
- NONE
- ORTHOGONAL TILT
- OTHER
- PDB ENTRY
- RANDOM CONICAL TILT

Submit deposition

All items

Mandatory items

Navigation

- Instructions
- Communication
- Re-upload files
- Upload summary
- Admin
 - Contact information
 - Grant information
 - Release status
 - Entry title & author
 - Citation information
- Macromolecules
 - 1) Straptavidin
- EM sample
 - Overall sample description
- EM experiment
 - Specimen preparation
 - Microscopy
 - Image recording
 - Reconstruction**
 - Fitting interpretation
- Ligands
- Assembly
- Related entries
- Validation reports
- Summary & conditions

Log out

Reconstruction

Image processing and reconstruction

Choose the image detector used for this reconstruction: (1) GATAN K3 BIOQUANTUM (6k x 4k) v

Details:

Particle selection

Number of particles selected from the micrographs, at the start of the image processing:

Details:

Particle selection software

| Name | Version | Details |
|--------|---------|---------|
| RELION | 3.1 | |

CTF correction

Correction type*: PHASE FLIPPING AND AMPLITUDE CORRECTION v

Details:

Software used to determine and/or apply the CTF correction

| Name | Version | Details |
|---------|---------|---------|
| CTFFIND | 4.1.13 | |

- NONE
- PHASE FLIPPING AND AMPLITUDE CORRECTION
- PHASE FLIPPING ONLY

Startup model information

Startup model type*: OTHER v

Details:

Initial angle assignment

Angle assignment type*: MAXIMUM LIKELIHOOD v

Details:

Initial angular assignment software

| Name | Version | Details |
|--------|---------|---------|
| RELION | 3.1 | |

Final angle assignment

Angle assignment type*: MAXIMUM LIKELIHOOD v

Details:

Final angular assignment software

| Name | Version | Details |
|--------|---------|---------|
| RELION | 3.1 | |

- ANGULAR RECONSTITUTION
- COMMON LINE
- MAXIMUM LIKELIHOOD
- NOT APPLICABLE
- OTHER
- PROJECTION MATCHING
- RANDOM ASSIGNMENT

Final classification software

| Name | Version | Details |
|------|---------|---------|
| | | |

Final reconstruction

Number of particles used*: 19045

Number of classes used: 1

Reconstruction algorithm: v

Resolution (Å)*: 1.93

Resolution method*: FSC 0.143 CUT-OFF v

Half-map generation: EVEN/ODD MAPS REFINED TOTALLY INDEPENDENT (GOLD STANDARD) v

Details:

Applied point group symmetry

Point group: D2

Final reconstruction software

| Name | Version | Details |
|--------|---------|---------|
| RELION | 3.1 | |

登録の流れ

Submit deposition

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
- ✓ Re-upload files
- ✓ Upload summary
- ✚ Admin
 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
 - ✓ Entry title & author
 - ✓ Citation information
- ✚ Macromolecules
 - ✓ 1) Streptavidin
- ✚ EM sample
 - ✓ Overall sample description
- ✚ EM experiment
 - ✓ Specimen preparation
 - ✓ Microscopy
 - ✓ Image recording
 - ✓ Reconstruction
 - ✓ **Fitting interpretation**
- ✓ Ligands
- ✓ Assembly
- ✓ Related entries
- ✓ Validation reports
- ✓ Summary & conditions

Log out

Fitting interpretation

Fitting

Refinement protocol: ⓘ

Target criteria: ⓘ

Overall B value (Å²): ⓘ

Refinement space: ⓘ

- AB INITIO MODEL
- BACKBONE TRACE
- FLEXIBLE FIT
- OTHER
- RIGID BODY FIT

Initial model source

| PDB ID | Chain ID | Residue range |
|-----------------------------------|--------------------------------|-------------------------------|
| <input type="text" value="5N7X"/> | <input type="text" value="M"/> | <input type="text" value=""/> |

⌵ +

どうしてこういう選択肢なのか？ 選びづらい...

Model fitting software

| Name | Version | Details |
|-------------------------------------|-------------------------------|-------------------------------|
| <input type="text" value="MOLREP"/> | <input type="text" value=""/> | <input type="text" value=""/> |

⌵ +

Model refinement software

| Name | Version | Details |
|-------------------------------------|---------------------------------------|-------------------------------|
| <input type="text" value="REFMAC"/> | <input type="text" value="5.8.0272"/> | <input type="text" value=""/> |

⌵ +

Details: ⓘ

⌵ +

Continue to next section

登録の流れ

Submit deposition

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
- ✓ Re-upload files
- ✓ Upload summary
- Admin
 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
 - ✓ Entry title & author
 - ✓ Citation information
- Macromolecules
 - ✓ 1) Streptavidin
- EM sample
 - ✓ Overall sample description
- EM experiment
 - ✓ Specimen preparation
 - ✓ Microscopy
 - ✓ Image recording
 - ✓ Reconstruction
 - ✓ Fitting interpretation
- Ligands
 - ✓ Assembly
 - ✓ Related entries
 - ✓ Validation reports
 - ✓ Summary & conditions

Log out

Assembly

▼ Quaternary structure

Please provide information about the macromolecular assembly.
Please account for all protein chains including bound peptides and for each individual nucleic acid strand involved in the complex.

Assembly ID*:

Assembly details*:

Experimental evidence for the assembly

Experiments performed to support the assembly:

Additional information about the assembly:

Chains and matrices for the assembly

Does this assembly apply to all chains?: N Y

List of chain IDs in this assembly:

Can you generate the assembly without applying matrices?: N Y

Provide 3x4 rotation with translation matrices in the format:

| R1-1 | R1-2 | R1-3 | T1 |
|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| <input type="text" value="1.0"/> | <input type="text" value="0.0"/> | <input type="text" value="0.0"/> | <input type="text" value="0.0"/> |
| <input type="text" value="0.0"/> | <input type="text" value="1.0"/> | <input type="text" value="0.0"/> | <input type="text" value="0.0"/> |
| <input type="text" value="0.0"/> | <input type="text" value="0.0"/> | <input type="text" value="1.0"/> | <input type="text" value="0.0"/> |

- PDBにBIOMTを書きおいても自動で読んでくれない模様
- mmCIFに_pdbx_struct_oper_listを入れておくと読んでくれる？ (未確認)
- 手打ちは絶対にミスをするのでコピペしましょう (annotatorにMTRIXと同じ情報を入れておいてと頼んだことあり)
- MTRIX/BIOMTはannotation時におかしくなりやすい印象があります。
ファイルを要求して自分できちんと確認した方が良いです

Validation report (1)

28

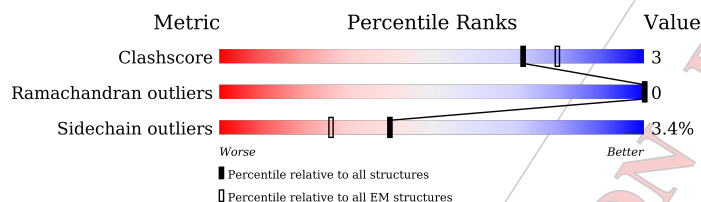
Page 2 Preliminary Full wwPDB EM Validation Report D_1300020330

1 Overall quality at a glance [i](#)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 119 | |

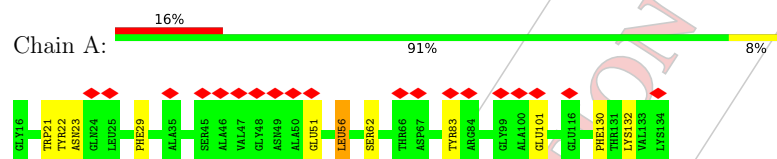
モデルのマッピングに対する評価は指定したcontour levelに依存している模様
(なのであまり意味はない...)

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3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion $< 40\%$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1:



Validation report (2)

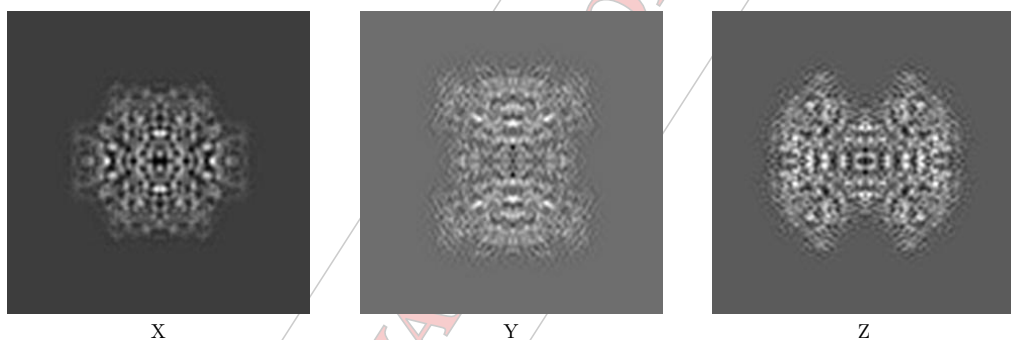
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D_1300020330. These allow visual inspection of the internal detail of the map and identification of artifacts.

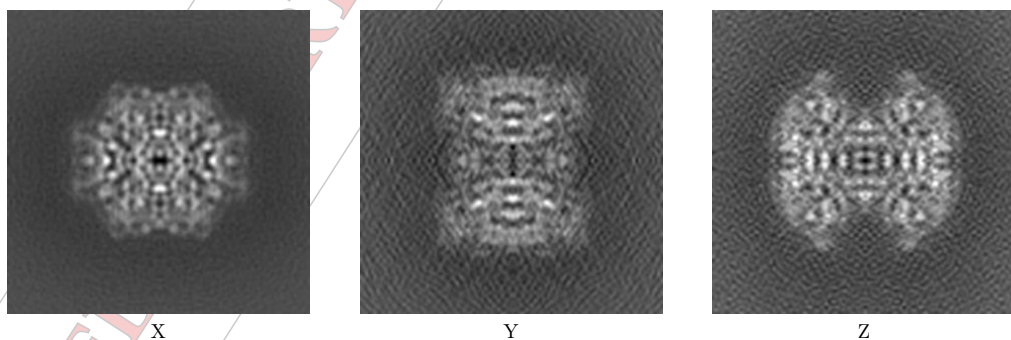
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



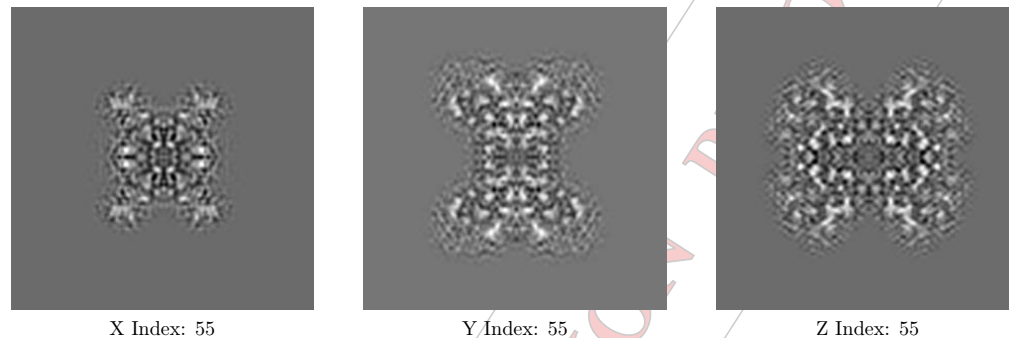
6.1.2 Raw map



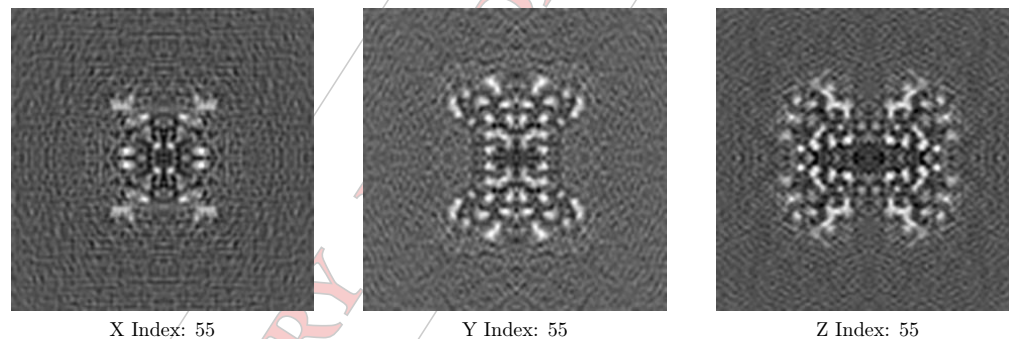
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



6.2.2 Raw map



The images above show central slices of the map in three orthogonal directions.

Raw map = half mapsを足したものの

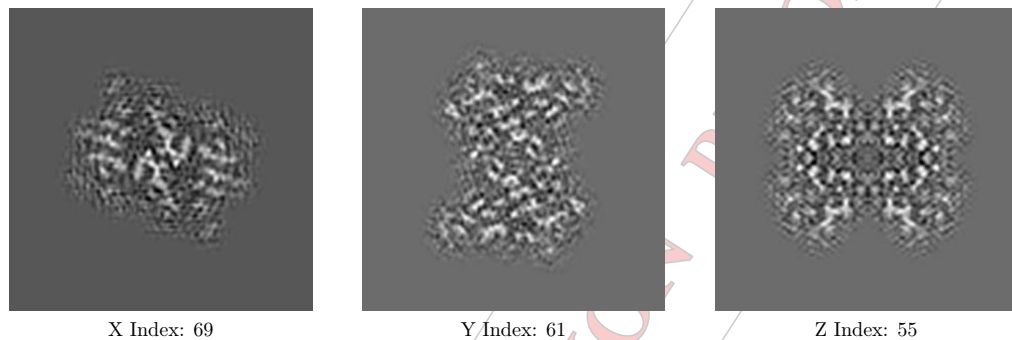
Validation report (3)

30

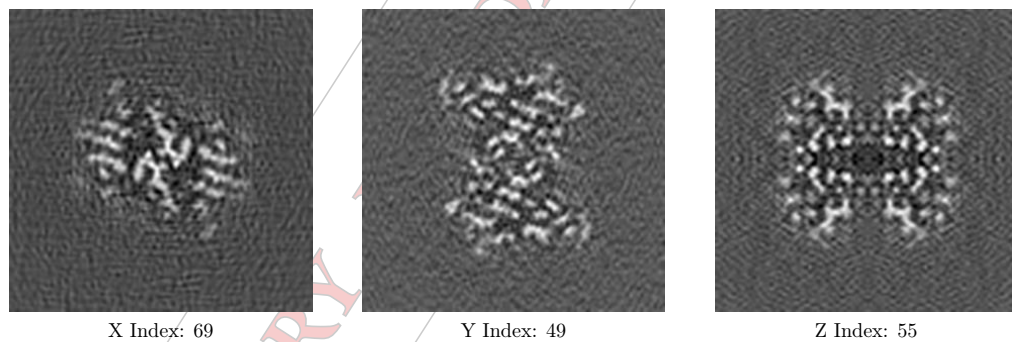
Page 11 Preliminary Full wwPDB EM Validation Report D_1300020330

6.3 Largest variance slices [i](#)

6.3.1 Primary map



6.3.2 Raw map

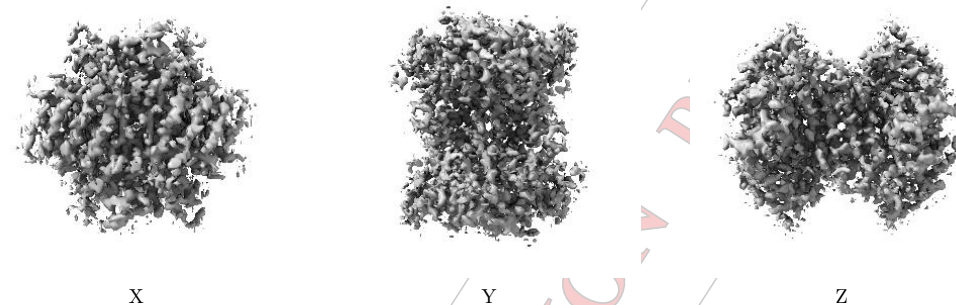


The images above show the largest variance slices of the map in three orthogonal directions.

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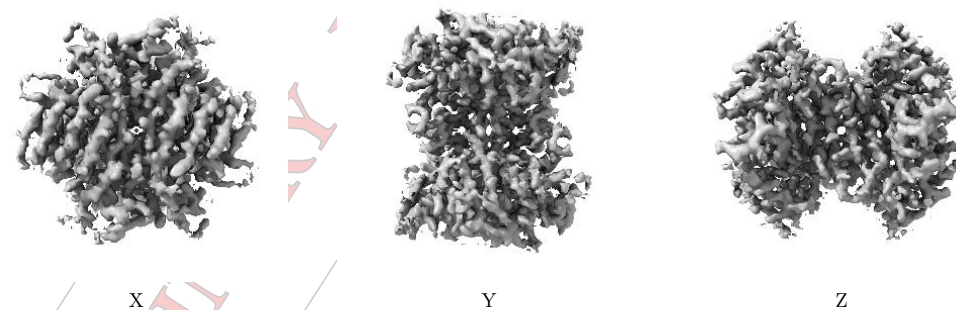
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

Validation report (4)

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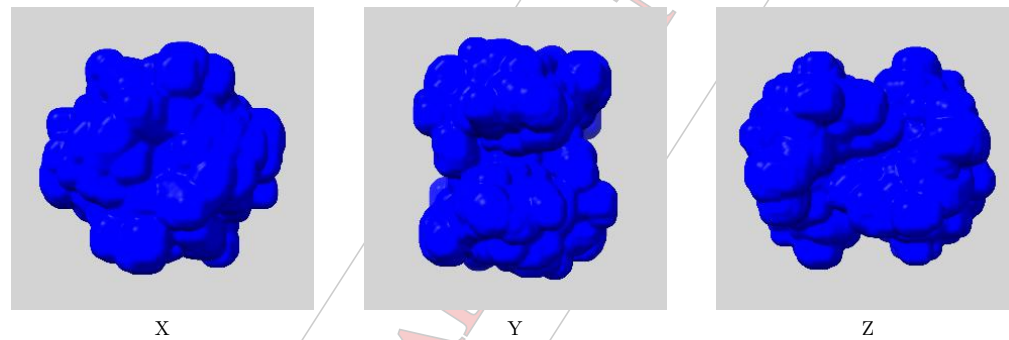
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

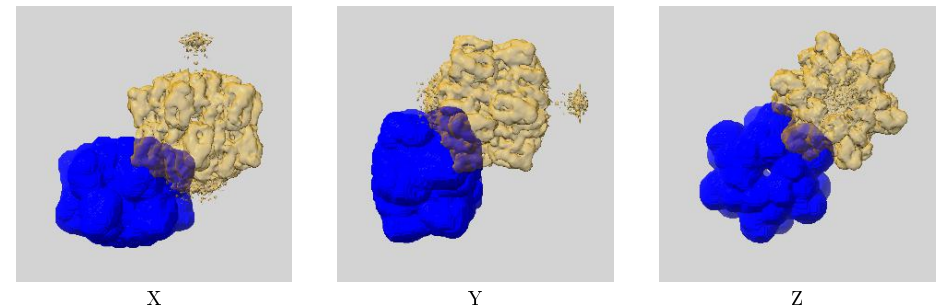
6.5.1 D_1300020330_em-mask-volume_P1.map.V2 [i](#)



Maskとmapがきちんと重なっているか

悪い例:

2.5.1 emd_4906_msk_1.map [i](#)



<https://www.emdataresource.org/EMD-4906>

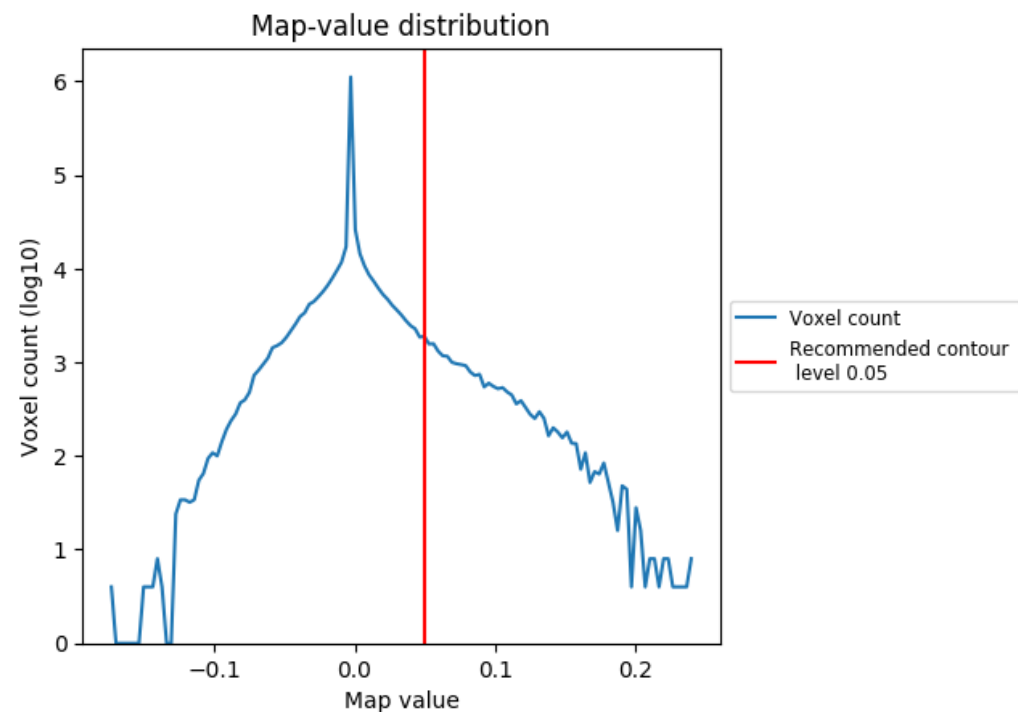
Validation report (5)

32

7 Map analysis [i](#)

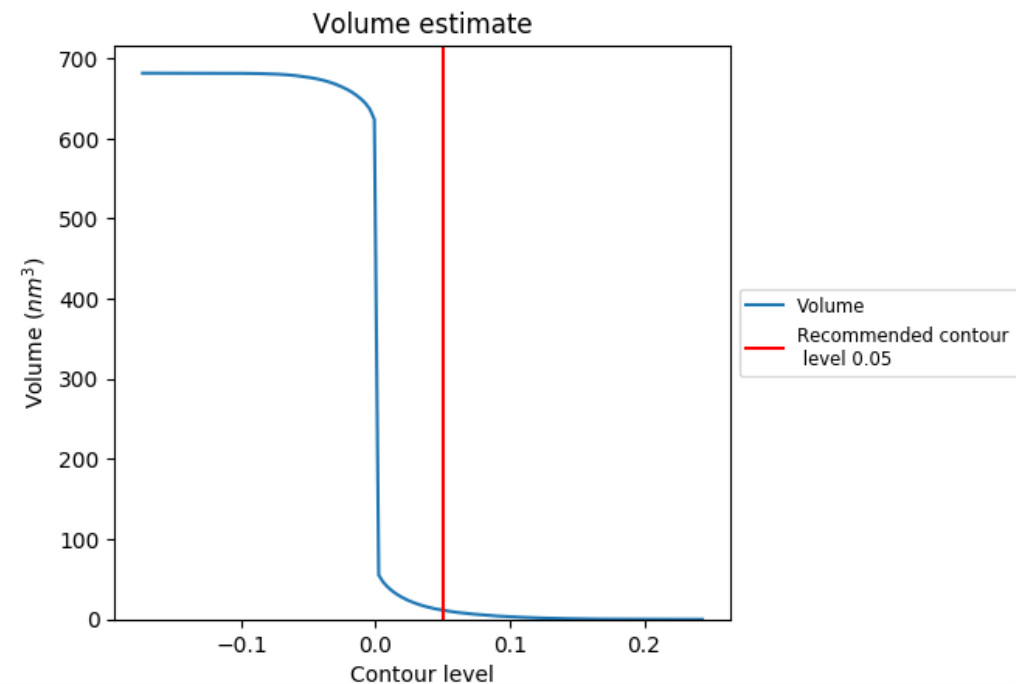
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11 nm³; this corresponds to an approximate mass of 10 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

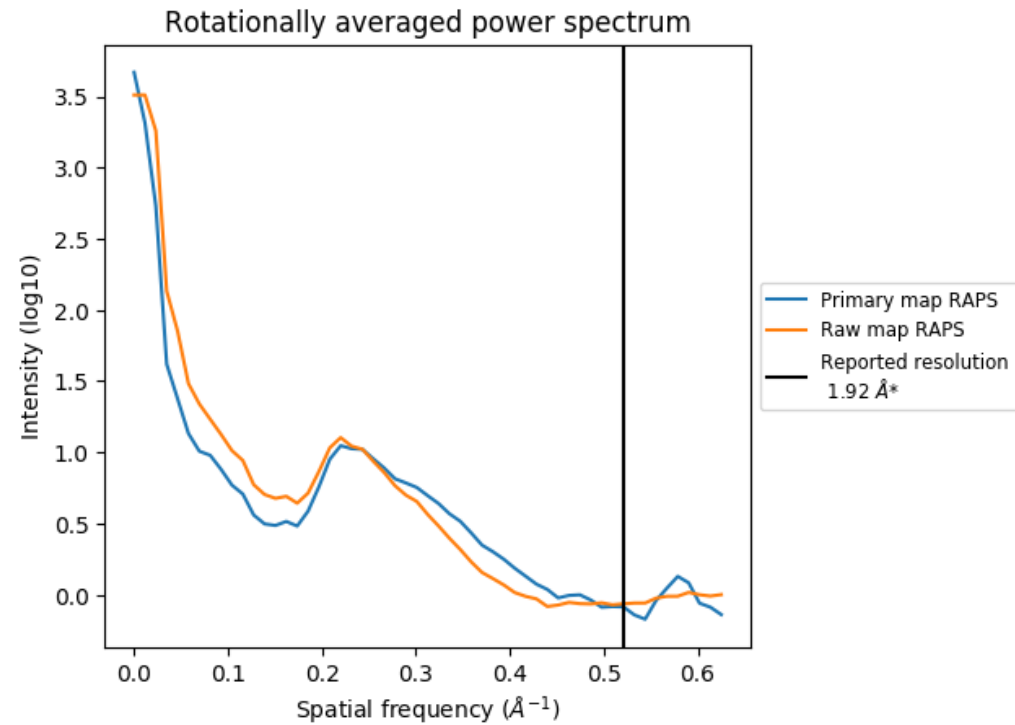
だいたい過小評価される印象
(結局recommended contour level依存)

Validation report (6)

33

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7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.521\AA^{-1}

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8.2 Resolution estimates [i](#)

| Resolution estimate (\AA) | Estimation criterion (FSC cut-off) | | |
|--------------------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | - | - | - |
| Author-provided FSC curve | 1.95 | 2.38 | 1.99 |
| Calculated* | 2.41 | 2.92 | 2.46 |

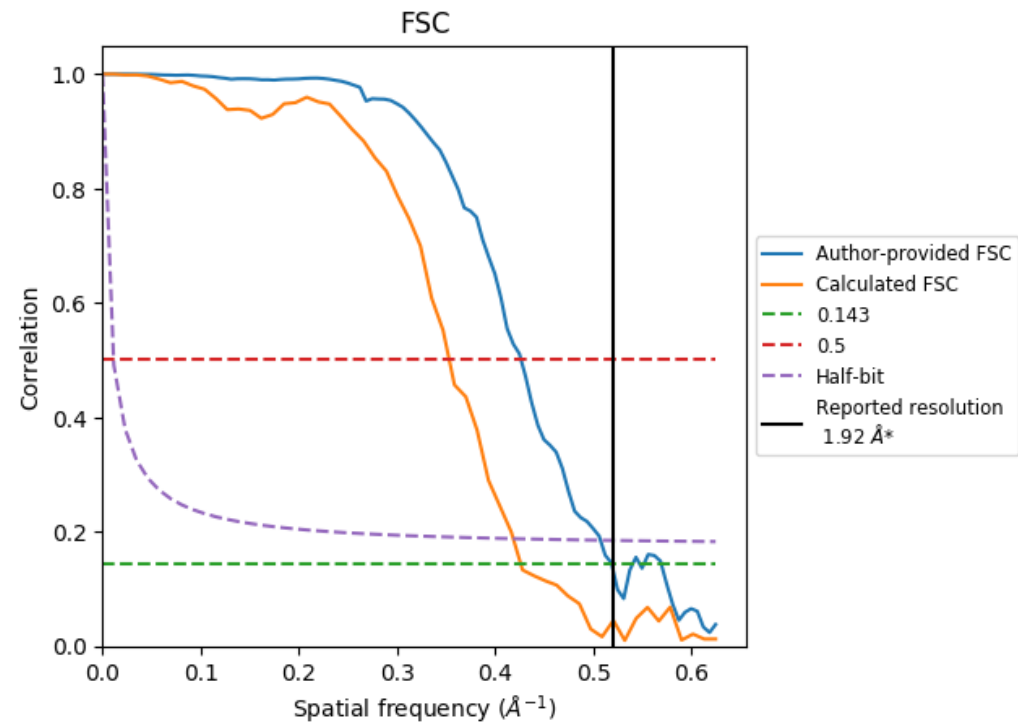
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.521\AA^{-1}

FSC計算でmaskを考慮してくれない
ので悪くなる

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

Validation report (7)

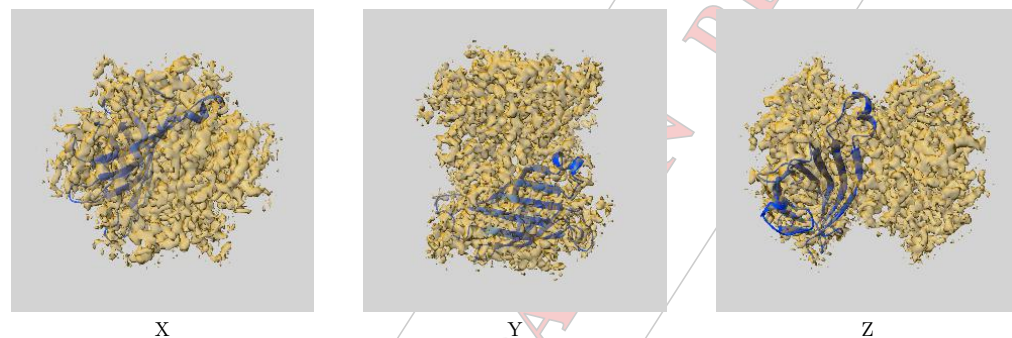
34

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9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map D_1300020330 and PDB model D_1300020330. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

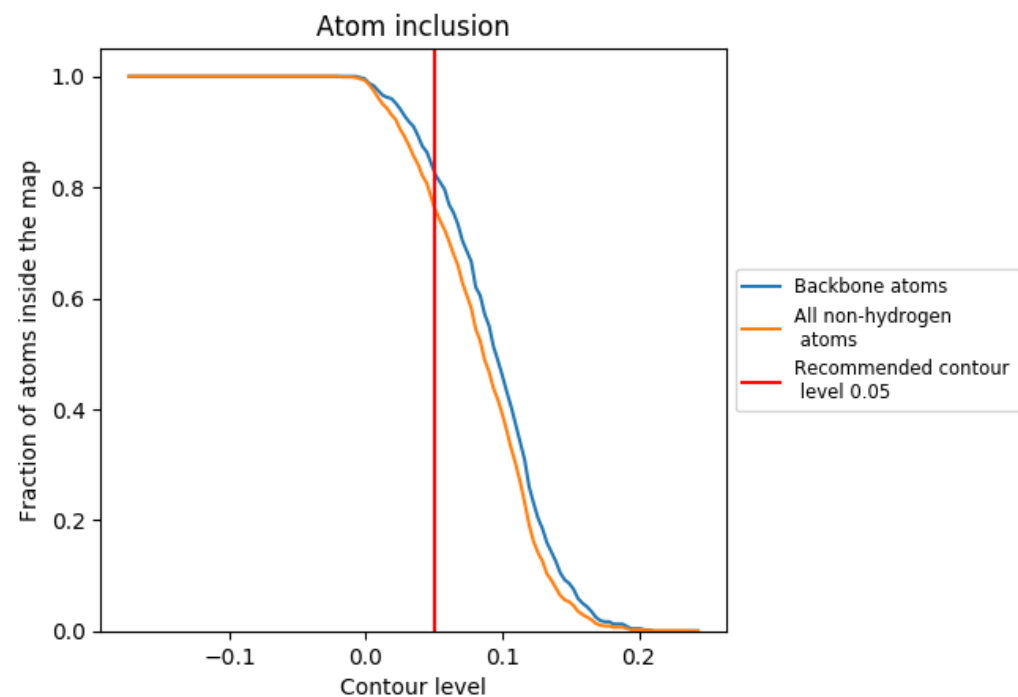


The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

MATRIX (_struct_ncs_oper)を見てくれないので非対称単位しか表示されない
(近々変わるはず)

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9.2 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

PDBjアノテータの方による登録の注意点

2020/12/01 取材：川端猛先生

1. 対応するマップと座標はできるだけ一緒に（同じdeposition_idで）登録してください
 - マップと座標を別々に登録してしまうと、マップと座標の重なりに関する検証レポートが作成できなくなってしまう。
 - データの公開時期をそろえる場合も好都合
2. マップと座標のRelease Statusはできるだけ同一にしてください
 - 特別な事情がない限り、同じStatusにしないとあとの処理が混乱。
3. マップの差し替えはできるだけrelease前に行ってください
 - release前なら、主マップ(primary map)の差し替え(replace)は可能です。Release後に主マップを入れ替えるには、Obsoleteが必要となり、EMDB IDが変更されることになってしまいます。
4. 対称性のあるウィルスカプシドなどの座標を入力する場合、対称操作の変換行列のアップロードを忘れないでください
5. マップと座標がきちんと重なっているか、UCSF Chimeraでチェックしてから、登録してください
 - マップと座標がきちんと重ならないケースがときどきあります。多くは、ピクセル幅(pixel spacing)や原点座標の設定ミスによるものです。UCSF Chimeraで重なりを確認してから、登録を行うようにしてください。

まとめ

- 特に注意すべきこと
 - Pixel sizeは正しいか
 - Map/modelにズレは無いか
 - Map同士はズれてないか
- 推奨したいこと
 - **Half maps, mask, FSC curveも登録する**
 - 対称性がある場合は非対称単位を登録する (operatorを正確に！)
 - 小さなboxで精密化・登録する
- 座標がある場合はPDBも同時に登録する
- Annotatorにファイルを要求する/ファイルをよく確認する
- Validation reportもよく確認する+網羅されていない項目もあるので自分でも可能な限り確認する

謝辭

- Takanori Nakane
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