Validation report of Level(s)
0, A

I^{2}PC Validation server

March 2, 2022
6:55am

Abstract

The map seems to be well centered. There is no problem with the suggested threshold. There seems to be a problem with the map's background (see Sec. 2.3). There seems to be a problem with its local B-factor (see Sec. 2.6). There seems to be a problem with the map hand (see Sec. 2.8). There seems to be a problem with its MapQ scores (see Sec. 4.1). The EMRinger score is negative, it seems that the model side chains do not match the map (see Sec. 4.4). DAQ detects some mismatch between the map and its model (see Sec. 4.5).

The average resolution of the map estimated by various methods goes from 1.1Å to 6.4Å with an average of 3.9Å. The resolution provided by the user was 3.8Å.

The overall score (passing tests) of this report is 6 out of 13 evaluable items.

0.a Mass analysis	Sec. 2.1	OK
0.b Mask analysis	Sec. 2.2	OK
0.c Background analysis	Sec. 2.3	2 warnings
0.d B-factor analysis	Sec. 2.4	OK
0.e DeepRes	Sec. 2.5	1 warnings
0.f LocBfactor	Sec. 2.6	1 warnings
0.g LocOccupancy	Sec. 2.7	OK
0.h DeepHand	Sec. 2.8	2 warnings
A.a MapQ	Sec. 4.1	1 warnings
A.d Map-Model Guinier	Sec. 4.2	OK
A.e Phenix validation	Sec. 4.3	OK
A.f EMRinger	Sec. 4.4	1 warnings
A.g DAQ	Sec. 4.5	1 warnings

Summary of the warnings across sections.

If it is empty below this point, it means that there are no warnings.

Section 2.3 (0.c Background analysis)

1. **The null hypothesis that the background mean is 0 has been rejected because the p-value of the comparison is smaller than 0.001**
2. **There is a significant proportion of outlier values in the background (cdf5 ratio=8586.32)**

Section 2.5 (0.e DeepRes)

1. **The reported resolution, 3.84 Å, is particularly with respect to the local resolution distribution. It occupies the 0.09 percentile**

Section 2.6 (0.f LocBfactor)

1. **The median B-factor is out of the interval [-300,0]**

Section 2.8 (0.h DeepHand)

1. **The volume seems to be flipped.**
2. **The orientation of the volume is uncertain.**

Section 4.1 (A.a MapQ)

1. **The median Q-score is less than 0.1.**

Section 4.4 (A.f EMRinger)

1. **The EMRinger score is smaller than 1, it is 0.748.**

Section 4.5 (A.g DAQ)

1. **The average DAQ is smaller than 0.5.**

Contents

1 Input data

Input map: /home/coss/data/Dropbox/Aplicaciones/ShareLaTeX/MapValidation/-EMDB22838/emd_22838.map
SHA256 hash: 2ae2d0b9aed1e9c2fab2e32a643720f604861daf3e03307d44056083415153b4
Voxel size: 1.058000 (Å)
Visualization threshold: 0.200000
Resolution estimated by user: 3.840000

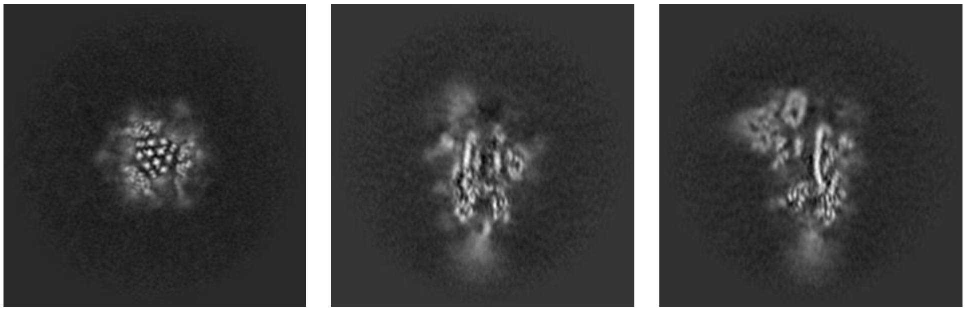
Orthogonal slices of the input map

Explanation:

In the orthogonal slices of the map, the noise outside the protein should not have any structure (stripes going out, small blobs, particularly high or low densities, ...)

Results:

See Fig. 1.



(a) X Slice 150 (b) Y Slice 150 (c) Z Slice 150

Figure 1: Central slices of the input map in the three dimensions

Orthogonal slices of maximum variance of the input map

Results:

See Fig. 2.

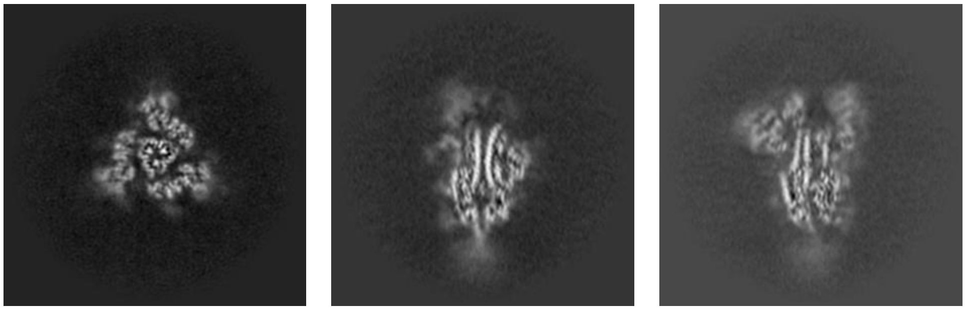

(a) X Slice 135 (b) Y Slice 146 (c) Z Slice 157

Figure 2: Slices of maximum variation in the three dimensions

Orthogonal projections of the input map

Explanation:
In the projections there should not be stripes (this is an indication of directional overweighting, or angular attraction), and there should not be a dark halo around or inside the structure (this is an indication of incorrect CTF correction or the reconstruction of a biased map).

Results:
See Fig. 3.

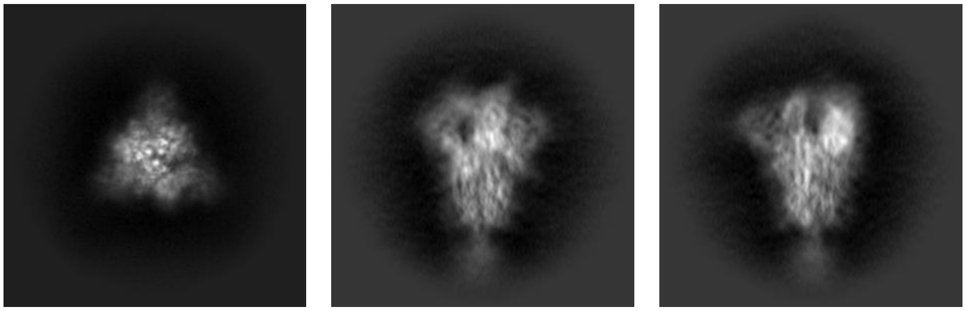

(a) X Projection (b) Y Projection (c) Z Projection

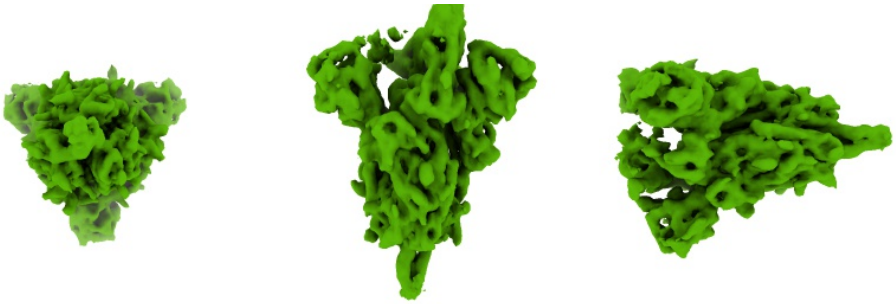
Figure 3: Projections in the three dimensions

Isosurface views of the input map

Explanation:

An isosurface is the surface of all points that have the same gray value. In these views there should not be many artifacts or noise blobs around the map.

Results:
See Fig. 4.



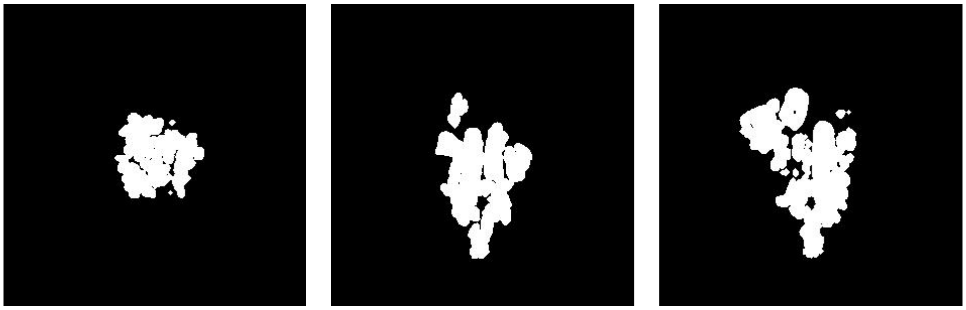
(a) View 1 (b) View 2 (c) View 3

Figure 4: Isosurface at threshold=0.200000. Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

Orthogonal slices of maximum variance of the mask

Explanation:
The mask has been calculated at the suggested threshold 0.200000, the largest connected component was selected, and then dilated by 2Å.

Results:
See Fig. 5.



(a) X Slice 150 (b) Y Slice 150 (c) Z Slice 150

Figure 5: Slices of maximum variation in the three dimensions of the mask

2 Level 0 analysis

2.1 Level 0.a Mass analysis

Explanation:
The reconstructed map must be relatively well centered in the box, and there should be at least 30Å (the exact size depends on the CTF) on each side to make sure that the CTF can be appropriately corrected.

Results:
The space from the left and right in X are 82.52 and 50.78 Å, respectively. There is a decentering ratio (abs(Right-Left)/Size)% of 10.00%

The space from the left and right in Y are 82.52 and 101.57 Å, respectively. There is a decentering ratio (abs(Right-Left)/Size)% of 6.00%

The space from the left and right in Z are 92.05 and 87.81 Å, respectively. There is a decentering ratio (abs(Right-Left)/Size)% of 1.33%

The center of mass is at (x,y,z)=(148.88,144.32,145.88). The decentering of the center of mass (abs(Center)/Size)% is 0.37, 1.89, and 1.37, respectively.%

Automatic criteria: The validation is OK if 1) the decentering and center of mass less than 20% of the map dimensions in all directions, and 2) the extra space on each direction is more than 20% of the map dimensions.

STATUS: OK

2.2 Level 0.b Mask analysis

Explanation:
The map at the suggested threshold should have most of its mass concentrated in a single connected component. It is normal that after thresholding there are a few thousands of very small, disconnected noise blobs. However, there total mass should not exceed 10%. The raw mask (just thresholding) and the mask constructed for the analysis (thresholding + largest connected component + dilation) should significantly overlap. Overlap is defined by the overlapping coefficient (size(Raw AND Constructed)/size(Raw)) that is a number between 0 and 1, the closer to 1, the more they agree.

Results:

Raw mask: At threshold 0.200000, there are 24 connected components with a total number of voxels of 236482 and a volume of 280062.58 Å^3 (see Fig. 6). The size and percentage of the total number of voxels for the raw mask are listed below (up to 95% of the mass or the first 100 clusters, whatever happens first), the list contains (No. voxels (volume in Å^3), percentage, cumulatedPercentage):

, (236064 (279567.55), 99.82, 99.82)

Number of components to reach 95% of the mass: 2

The average size of the remaining 22 components is 19.00 voxels (1.18 Å^3). Their size go from 273 voxels (323.31 Å^3) to 1 voxels (1.18 Å^3).

The slices of the raw mask can be seen in Fig. 6.

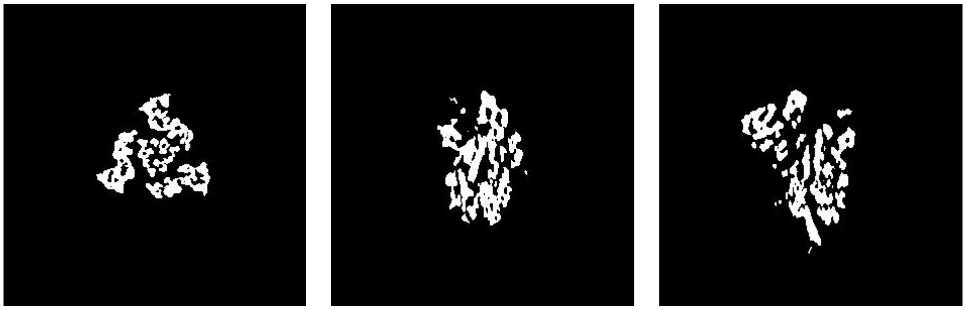

(a) X Slice 137 (b) Y Slice 138 (c) Z Slice 153

Figure 6: Maximum variance slices in the three dimensions of the raw mask

The following table shows the variation of the mass enclosed at different thresholds (see Fig. 7):

Threshold	**Voxel mass**	**Molecular mass(kDa)**	**# Aminoacids**
0.0333	961872.00	943.77	8579.74
0.0665	692613.00	679.58	6178.00
0.0998	518448.00	508.69	4624.47
0.1330	399920.00	392.39	3567.22
0.1663	310352.00	304.51	2768.29
0.1996	237318.00	232.85	2116.84
0.2328	178114.00	174.76	1588.75
0.2661	132228.00	129.74	1179.45
0.2994	96304.00	94.49	859.02
0.3326	69000.00	67.70	615.47
0.3659	48618.00	47.70	433.66
0.3991	33917.00	33.28	302.53
0.4324	23468.00	23.03	209.33
0.4657	16279.00	15.97	145.21
0.4989	11193.00	10.98	99.84
0.5322	7656.00	7.51	68.29
0.5654	5010.00	4.92	44.69
0.5987	3108.00	3.05	27.72
0.6320	1832.00	1.80	16.34
0.6652	917.00	0.90	8.18
0.6985	372.00	0.36	3.32
0.7318	120.00	0.12	1.07
0.7650	32.00	0.03	0.29
0.7983	6.00	0.01	0.05

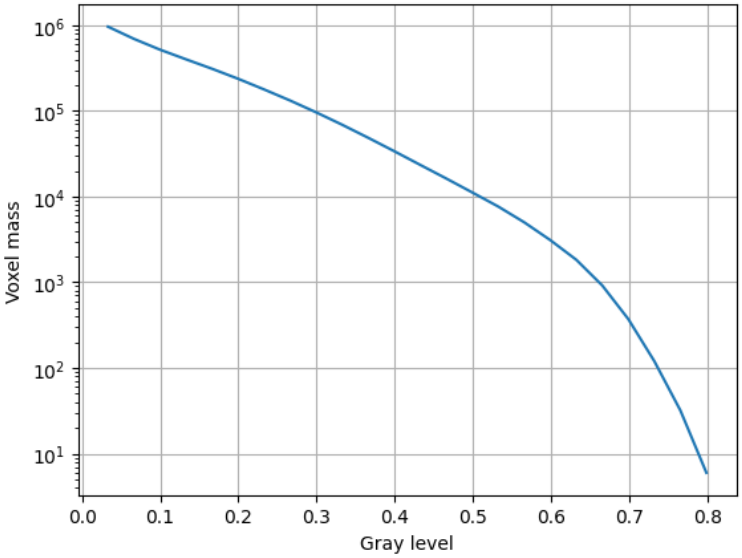


Figure 7: Voxel mass as a function of the gray level.

Constructed mask: After keeping the largest component of the previous mask and dilating it by 2Å, there is a total number of voxels of 528227 and a volume of 625572.43 Å^3. The overlap between the raw and constructed mask is 1.00.

Automatic criteria: The validation is OK if 1) to keep 95% of the mass we need to keep at most 5 connected components; and 2) the average volume of the blobs outside the given threshold has a size smaller than 5Å^3; and 3) the overlap between the raw mask and the mask constructed for the analysis is larger than 75%.

STATUS: OK

2.3 Level 0.c Background analysis

Explanation:
Background is defined as the region outside the macromolecule mask. The background mean should be zero, and the number of voxels with a very low or very high value (below 5 standard deviations of the noise) should be very

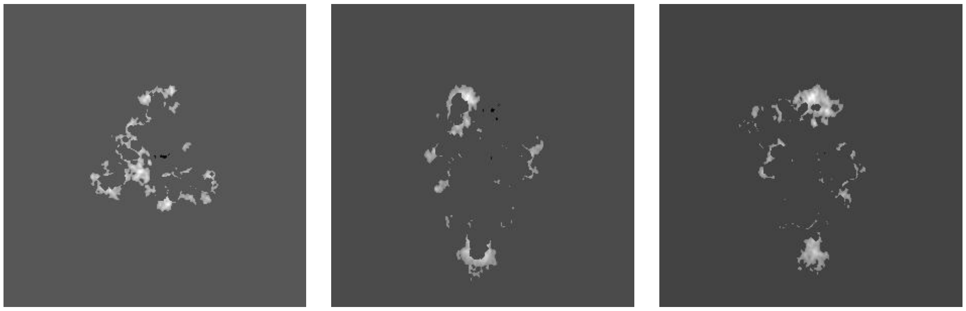
small and they should be randomly distributed without any specific structure. Sometimes, you can see some structure due to the symmetry of the structure.

Results:

The null hypothesis that the background mean is 0 was tested with a one-sample Student's t-test. The resulting t-statistic and p-value were -1661.72 and 0.000000, respectively.

The mean and standard deviation (sigma) of the background were -0.005457 and 0.016896. The percentage of background voxels whose absolute value is larger than 5 times the standard deviation is 0.49 % (see Fig. 8). The same percentage from a Gaussian would be 0.000057% (ratio between the two percentages: 8586.319777).

Slices of the background beyond 5*sigma can be seen in Fig. 8.



(a) X Slice 106 (b) Y Slice 152 (c) Z Slice 135

Figure 8: Maximum variance slices in the three dimensions of the parts of the background beyond 5*sigma

Automatic criteria: The validation is OK if 1) the p-value of the null hypothesis that the background has 0 mean is larger than 0.001; and 2) the number of voxels above or below 5 sigma is smaller than 20 times the amount expected for a Gaussian with the same standard deviation whose mean is 0.

WARNINGS: 2 warnings

1. **The null hypothesis that the background mean is 0 has been rejected because the p-value of the comparison is smaller than 0.001**
2. **There is a significant proportion of outlier values in the background (cdf5 ratio=8586.32)**

2.4 Level 0.d B-factor analysis

Explanation:
The B-factor line [Rosenthal and Henderson, 2003] fitted between 15Åand the resolution reported should have a slope that is between 0 and 300 Å^2.

Results:
Fig. 9 shows the logarithm (in natural units) of the structure factor (the module squared of the Fourier transform) of the experimental map, its fitted line, and the corrected map. The estimated B-factor was -155.5. The fitted line was $\log(|F|^2) = -38.9/R^2 + (-10.5)$.

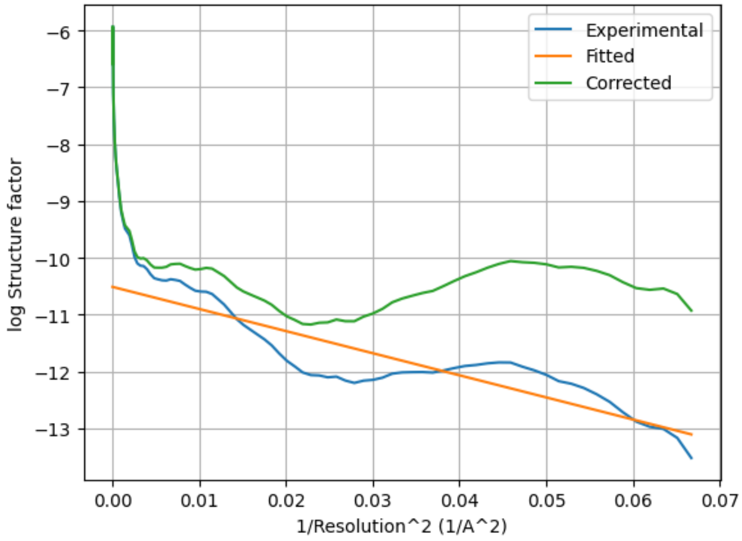


Figure 9: Guinier plot. The X-axis is the square of the inverse of the resolution in Å.

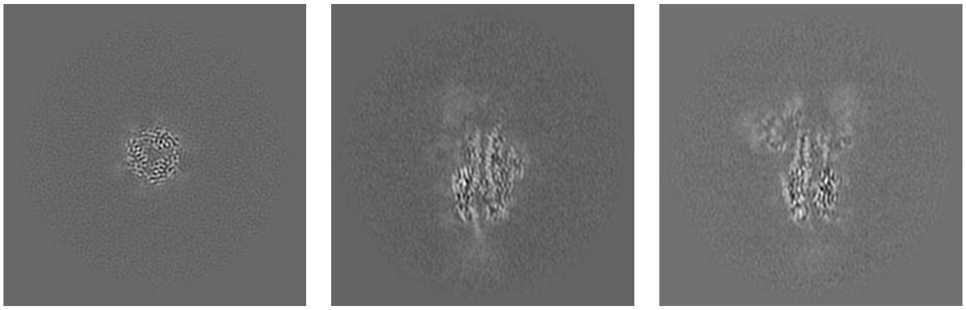

(a) X Slice 192 (b) Y Slice 145 (c) Z Slice 157

Figure 10: Slices of maximum variation in the three dimensions of the B-factor corrected map

Automatic criteria: The validation is OK if the B-factor is in the range [-300,0].

STATUS: OK

2.5 Level 0.e Local resolution with DeepRes

Explanation:
DeepRes [Ramírez-Aportela et al., 2019] measures the local resolution using a neural network that has been trained on the appearance of atomic structures at different resolutions. Then, by comparing the local appearance of the input map to the appearance of the atomic structures a local resolution label can be assigned.

Results:

Fig. 11 shows the histogram of the local resolution according to DeepRes. Some representative percentiles are:

Percentile	**Resolution(Å)**
2.5%	4.41
25%	5.54
50%	6.38
75%	7.27
97.5%	9.16

The reported resolution, 3.84 Å, is at the percentile 0.1. Fig. 12 shows some representative views of the local resolution.

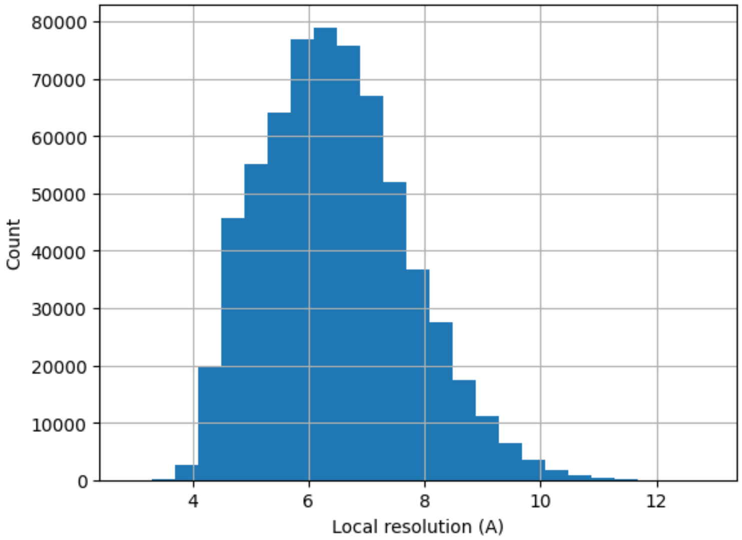
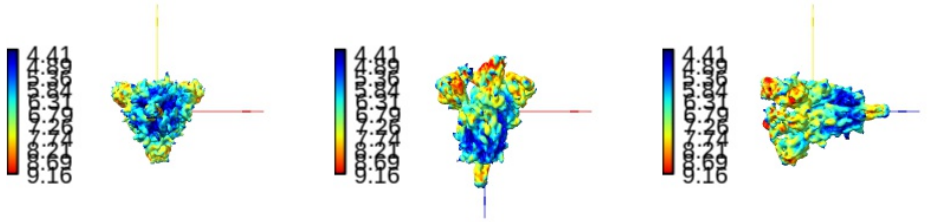


Figure 11: Histogram of the local resolution according to deepres.



(a) View 1 (b) View 2 (c) View 3

Figure 12: Local resolution according to DeepRes. Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

Automatic criteria: The validation is OK if the percentile of the user provided resolution is larger than 0.1% of the percentile of the local resolution as estimated by DeepRes.

WARNINGS: 1 warnings

1. **The reported resolution, 3.84 Å, is particularly with respect to the local resolution distribution. It occupies the 0.09 percentile**

2.6 Level 0.f Local B-factor

Explanation:
LocBfactor [Kaur et al., 2021] estimates a local resolution B-factor by decomposing the input map into a local magnitude and phase term using the spiral transform.

Results:

Fig. 13 shows the histogram of the local B-factor according to LocBfactor. Some representative percentiles are:

Percentile	**Local B-factor (Å^{-2})**
2.5%	-444.04
25%	-367.63
50%	-327.21
75%	-285.93
97.5%	-206.83

Fig. 14 shows some representative views of the local B-factor.

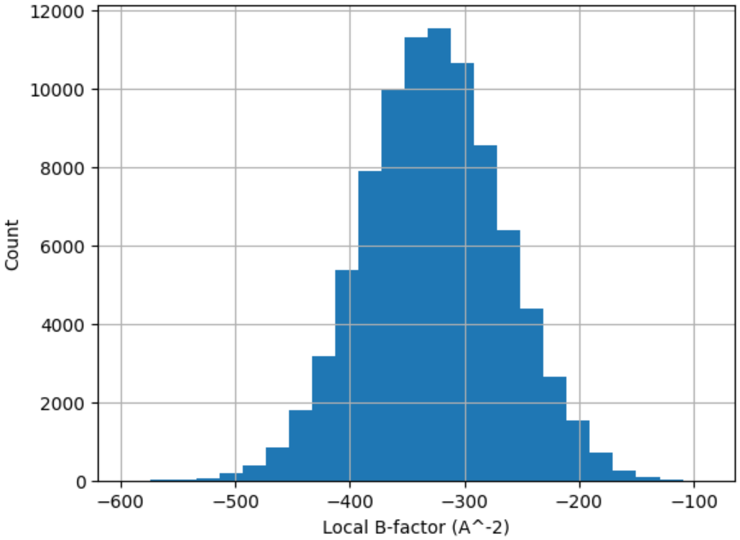
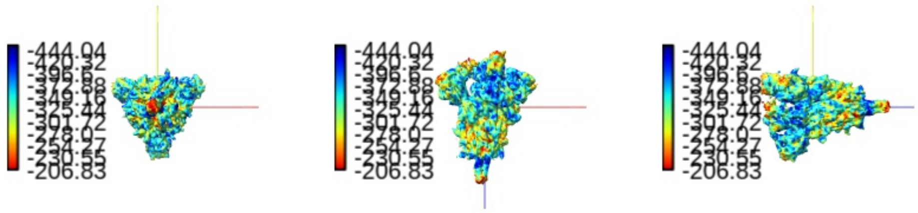


Figure 13: Histogram of the local B-factor according to LocBfactor.



(a) View 1 (b) View 2 (c) View 3

Figure 14: Local B-factor according to LocBfactor. Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

Automatic criteria: The validation is OK if the median B-factor is in the range [-300,0].

WARNINGS: 1 warnings

1. **The median B-factor is out of the interval [-300,0]**

2.7 Level 0.g Local Occupancy

Explanation:
LocOccupancy [Kaur et al., 2021] estimates the occupancy of a voxel by the macromolecule.

Results:

Fig. 15 shows the histogram of the local occupancy according to LocOccupancy. Some representative percentiles are:

Percentile	**Local Occupancy [0-1]**
2.5%	0.08
25%	0.58
50%	0.83
75%	1.00
97.5%	1.00

Fig. 16 shows some representative views of the local occupancy.

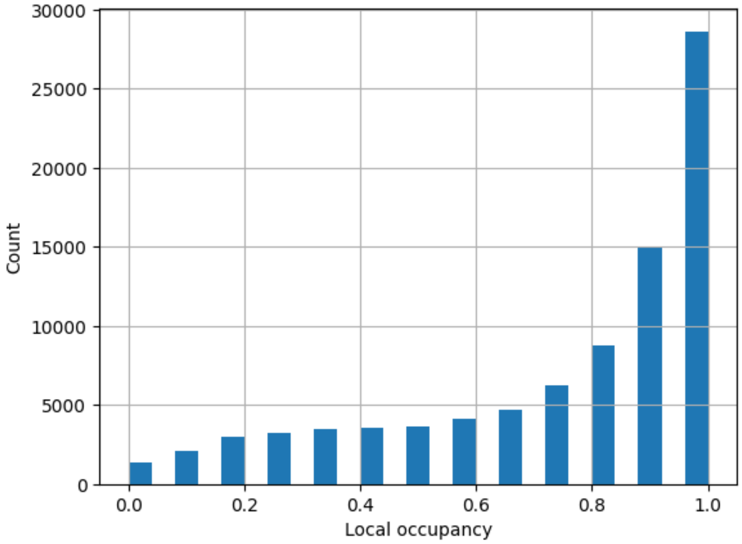
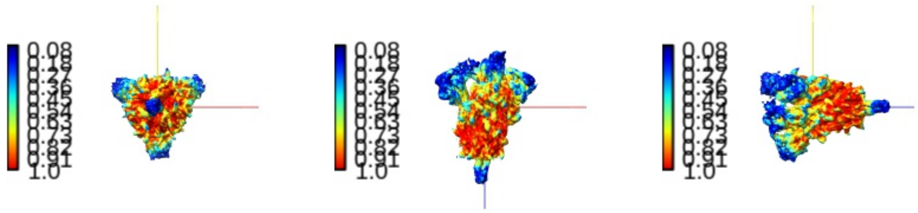


Figure 15: Histogram of the local occupancy according to LocOccupancy.



(a) View 1 (b) View 2 (c) View 3

Figure 16: Local occupancy according to LocOccupancy. Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

Automatic criteria: The validation is OK if the median occupancy is larger than 50%.

STATUS: OK

2.8 Level 0.h Hand correction

Explanation:
Deep Hand determines the correction of the hand for those maps with a resolution smaller than 5Å. The method calculates a value between 0 (correct hand) and 1 (incorrect hand) using a neural network to assign its hand.

Results:

Deep hand assigns a score of 0.552 to the input volume.
Automatic criteria: The validation is OK if the deep hand score is smaller than 0.5.

WARNINGS: 2 warnings

1. **The volume seems to be flipped.**
2. **The orientation of the volume is uncertain.**

3 Atomic model

Atomic model: /home/coss/data/Dropbox/Aplicaciones/ShareLaTeX/MapValidation/-EMDB22838/7kec_updated.pdb

See Fig. 17.

(a) View 1 (b) View 2 (c) View 3

Figure 17: Input atomic model Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

4 Level A analysis

4.1 Level A.a MapQ

Explanation:
MapQ [Pintilie et al., 2020] computes the local correlation between the map and each one of its atoms assumed to have a Gaussian shape.

Results:

Fig. 18 shows the histogram of the Q-score according calculated by MapQ. Some representative percentiles are:

Percentile	**MapQ score [0-1]**
2.5%	-0.35
25%	0.00
50%	0.00
75%	0.00
97.5%	0.33

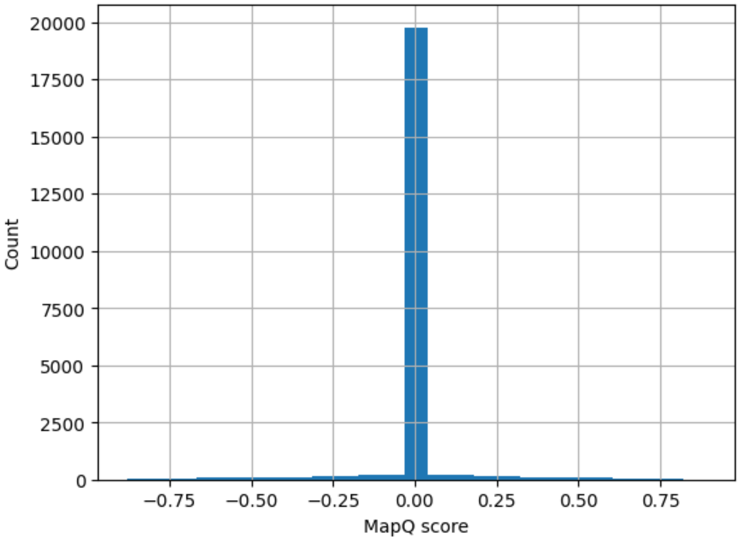


Figure 18: Histogram of the Q-score.

The following table shows the average Q score and estimated resolution for each chain.

Chain	Average Q score [0-1]	Estimated Resol. (Å)
A	-0.00	6.3
A	0.00	0.0
B	-0.00	6.3
B	-0.01	0.0
C	-0.00	6.3
C	0.00	0.0
D	0.00	0.0
E	0.00	0.0
F	0.00	0.0
G	0.00	0.0
H	0.00	0.0
I	-0.00	0.0
J	0.00	0.0
K	0.00	0.0
L	0.05	0.0
M	0.15	0.0
N	0.10	0.0
O	0.00	0.0

Automatic criteria: The validation is OK if the median Q-score is larger than 0.1.

WARNINGS: 1 warnings

1. **The median Q-score is less than 0.1.**

4.2 Level A.d Map-Model Guinier analysis

Explanation:
We compared the Guinier plot [Rosenthal and Henderson, 2003] of the atomic model and the experimental map. We made the mean of both profiles to be equal (and equal to the mean of the atomic model) to make sure that they had comparable scales.

Results:
Fig. 19 shows the logarithm (in natural units) of the structure factor (the module squared of the Fourier transform) of the atom model and the exper-

imental map. The correlation between the two profiles was 0.982.

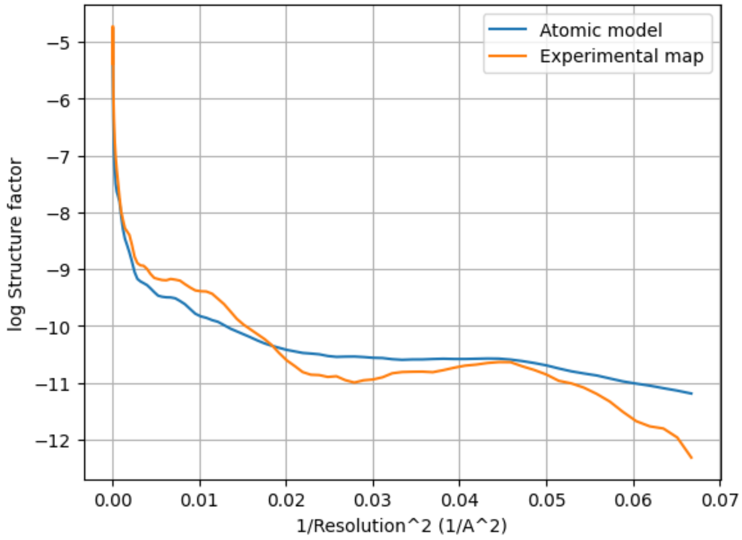


Figure 19: Guinier plot of the atom model and experimental map. The X-axis is the square of the inverse of the resolution in Å.

Automatic criteria: The validation is OK if the correlation between the two Guinier profiles is larger than 0.5.

STATUS: OK

4.3 Level A.e Phenix validation

Explanation:
Phenix provides a number of tools to assess the agreement between the experimental map and its atomic model [Afonine et al., 2018]. There are several cross-correlations to assess the quality of the fitting:

- CC (mask): Model map vs. experimental map correlation coefficient calculated considering map values inside a mask calculated around the macromolecule.
- CC (box): Model map vs. experimental map correlation coefficient calculated considering all grid points of the box.

- CC (volume) and CC (peaks) compare only map regions with the highest density values and regions below a certain contouring threshold level are ignored. CC (volume): The map region considered is defined by the N highest points inside the molecular mask. CC (peaks): In this case, calculations consider the union of regions defined by the N highest peaks in the model-calculated map and the N highest peaks in the experimental map.
- Local real-space correlation coefficients CC (main chain) and CC (side chain) involve the main skeleton chain and side chains, respectively.

There are also multiple ways of measuring the resolution:

- d99: Resolution cutoff beyond which Fourier map coefficients are negligibly small. Calculated from the full map.
- d_model: Resolution cutoff at which the model map is the most similar to the target (experimental) map. For d_model to be meaningful, the model is expected to fit the map as well as possible. d_model (B factors = 0) tries to avoid the blurring of the map.
- d_FSC_model; Resolution cutoff up to which the model and map Fourier coefficients are similar at FSC values of 0, 0.143, 0.5.

In addition to these resolution measurements the overall isotropic B factor is another indirect measure of the quality of the map.

Results:

To avoid ringing in Fourier space a smooth mask with a radius of 7.7 Å has been applied.

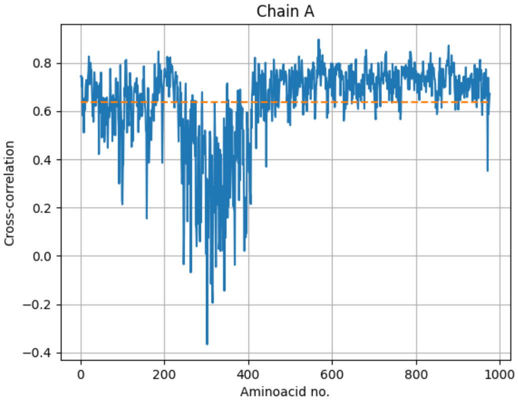
Overall correlation coefficients:

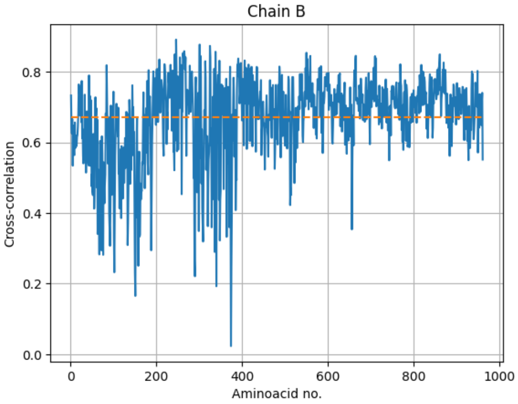
CC (mask) = 0.619
CC (box) = 0.737
CC (volume) = 0.659
CC (peaks) = 0.616
CC (main chain) = 0.654
CC (side chain) = 0.670

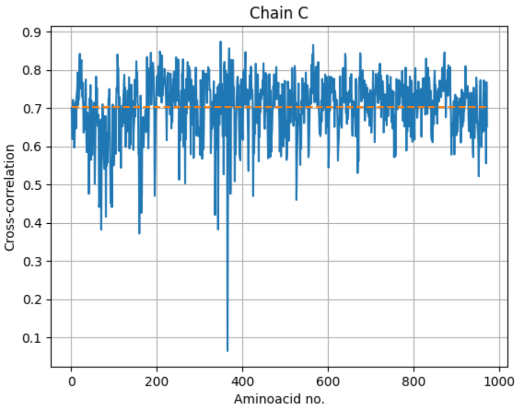
Correlation coefficients per chain:

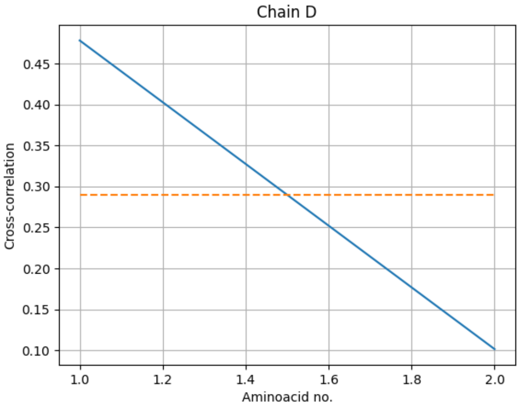
Chain	**Cross-correlation**
A	0.647861
B	0.674413
C	0.692197
D	0.280030
E	0.728180
F	0.746660
G	0.737342
H	0.719959
I	0.710197
J	0.709352
K	0.686594
L	0.703614
M	0.700790
N	0.698624
O	0.694403

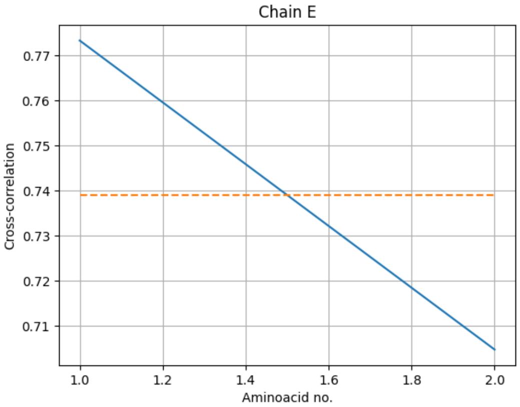
We now show the correlation profiles of the different chain per residue.

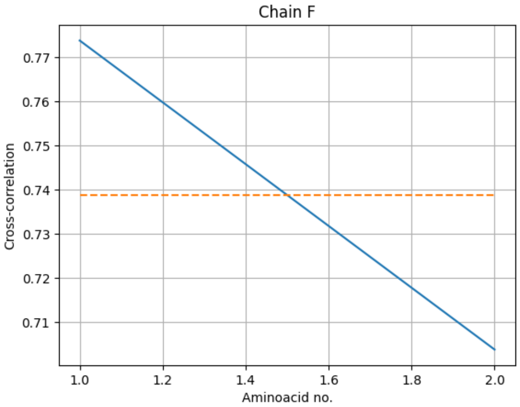


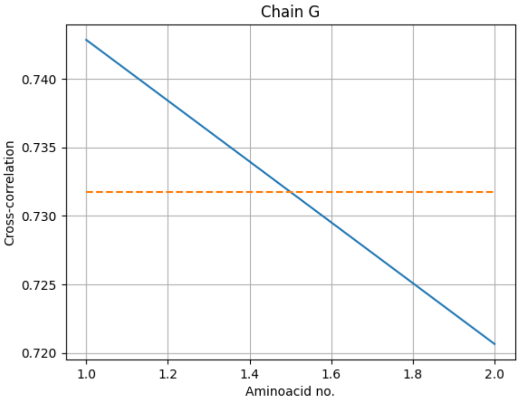


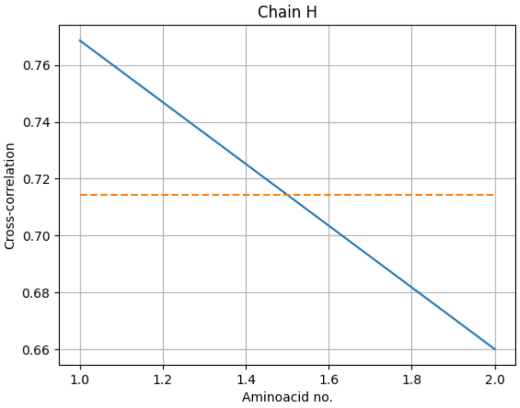

Chain C
Cross-correlation
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
200
400
600
800
1000
Aminoacid no.

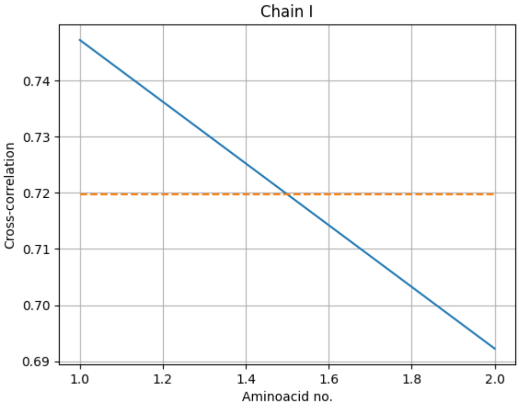

Chain D
Cross-correlation
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

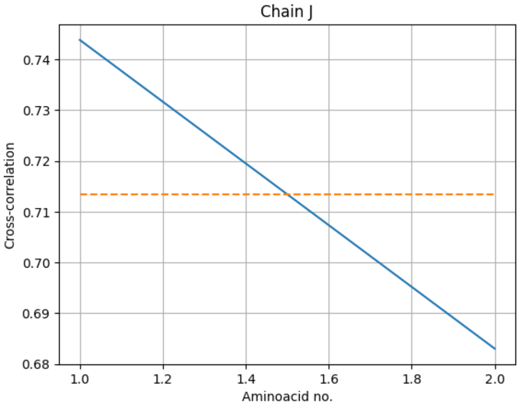

Chain E
Cross-correlation
0.71
0.72
0.73
0.74
0.75
0.76
0.77
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

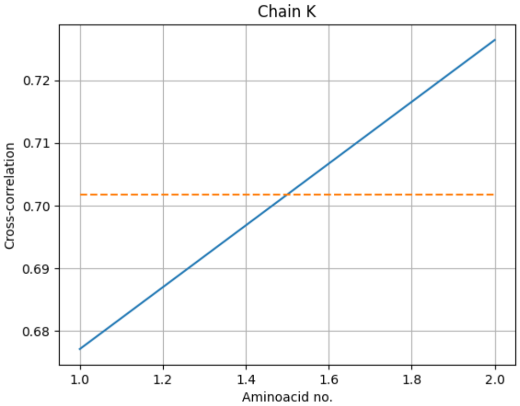

Chain F
Cross-correlation
0.71
0.72
0.73
0.74
0.75
0.76
0.77
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

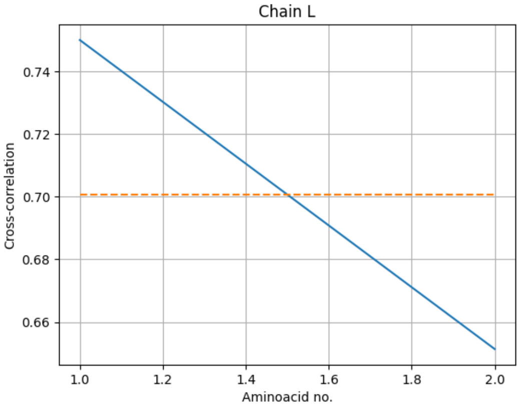

Chain G
Cross-correlation
0.720
0.725
0.730
0.735
0.740
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

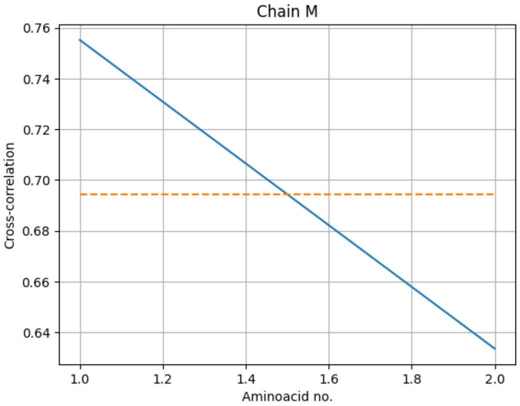

Chain H
Cross-correlation
0.66
0.68
0.70
0.72
0.74
0.76
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

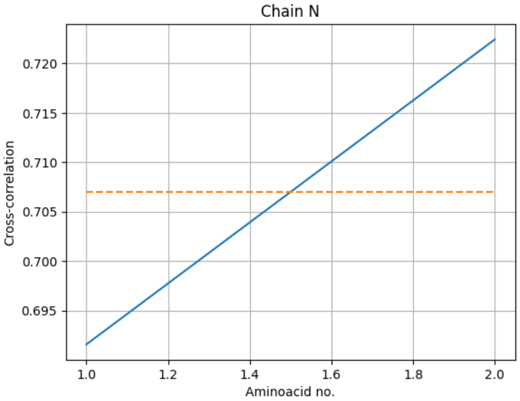

Chain I
Cross-correlation
0.74
0.73
0.72
0.71
0.70
0.69
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.


Chain J
Cross-correlation
0.74
0.73
0.72
0.71
0.70
0.69
0.68
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.


Chain K
Cross-correlation
0.72
0.71
0.70
0.69
0.68
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.


Chain L
Cross-correlation
0.74
0.72
0.70
0.68
0.66
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.


Chain M
Cross-correlation
0.76
0.74
0.72
0.70
0.68
0.66
0.64
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.


Chain N
Cross-correlation
0.720
0.715
0.710
0.705
0.700
0.695
1.0
1.2
1.4
1.6
1.8
2.0
Aminoacid no.

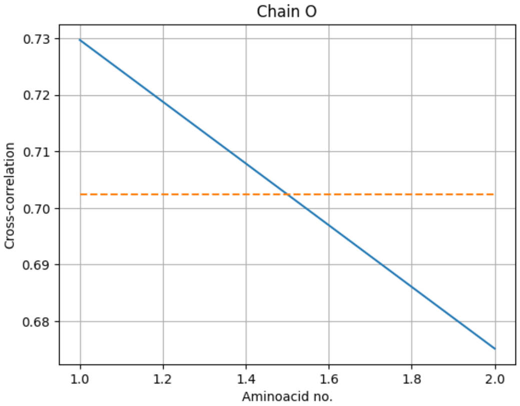


Fig. 20 shows the histogram of all cross-correlations evaluated at the residues. The percentage of residues whose correlation is below 0.5 is 8.7 %.

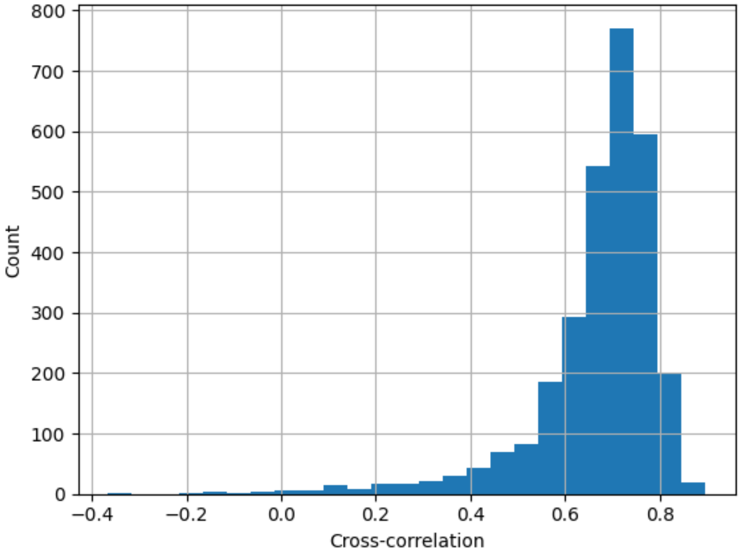


Figure 20: Histogram of the cross-correlation between the map and model evaluated for all residues.

Resolutions estimated from the model:

Resolution (Å)	**Masked**	**Unmasked**
d99	4.8	4.7
d_model	3.9	3.9
d_model (B-factor=0)	8.2	8.2
FSC_model=0	3.7	3.8
FSC_model=0.143	3.8	3.8
FSC_model=0.5	4.2	4.4

Overall isotropic B factor:

B factor	**Masked**	**Unmasked**
Overall B-iso	235.0	255.0

Fig. 21 shows the FSC between the input map and the model.

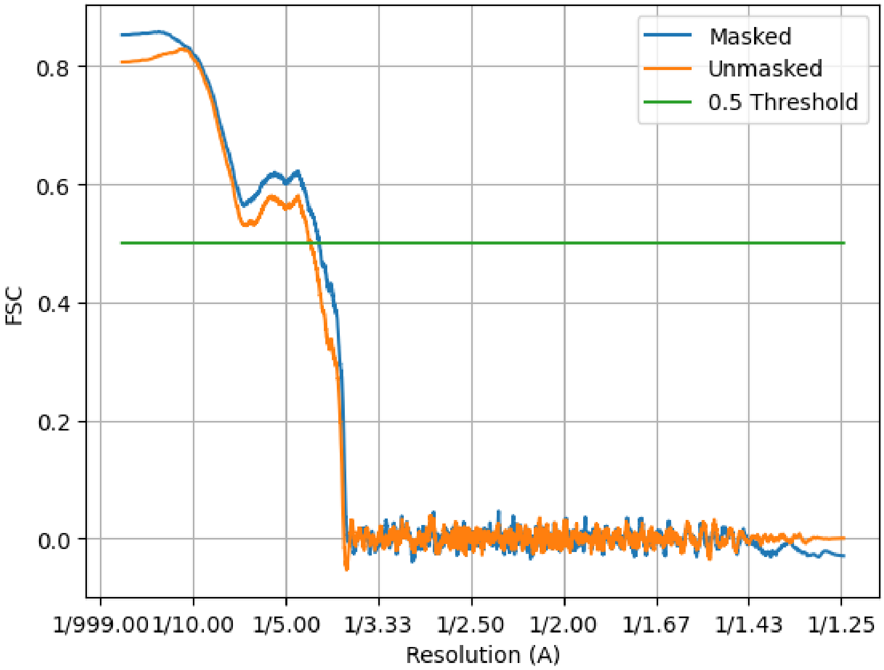


Figure 21: FSC between the input map and model with and without a mask constructed from the model. The X-axis is the square of the inverse of the resolution in Å.

Automatic criteria: The validation is OK if 1) the percentage of residues whose correlation is smaller than 0.5 is smaller than 10%, and 2) the resolution reported by the user is larger than 0.8 times the resolution estimated between the map and model at FSC=0.5.

STATUS: OK

4.4 Level A.f EMRinger validation

Explanation:
EMringer [Barad et al., 2015] compares the side chains of the atomic model to the CryoEM map. The following features are reported:

- Optimal Threshold: Electron potential map cutoff value at which the maximum EMRinger score was obtained.
- Rotamer Ratio: Fraction of rotameric residues at the Optimal threshold value.
- Max Zscore: Z-score computed to determine the significance of the distribution at the Optimal threshold value.
- Model Length: Total of non-gamma-branched, non-proline aminoacids with a non-H gamma atom used in global EMRinger score computation.
- EMRinger Score: Maximum EMRinger score calculated at the Optimal Threshold.

A rotameric residue is one in which EMRinger peaks that fall within defined rotamers based on chi1, this often suggests a problem with the modelling of the backbone. In general, the user should look at the profiles and identify regions that may need improvement.
Results:

General results:

Optimal threshold	0.537408
Rotamer ratio	1.000
Max. Zscore	2.91
Model length	1514
EMRinger Score	0.748

Fig. 22 shows the EMRinger score and fraction of rotameric residues as a function of the map threshold. The optimal threshold was selected looking for the maximum EMRinger score in this plot.

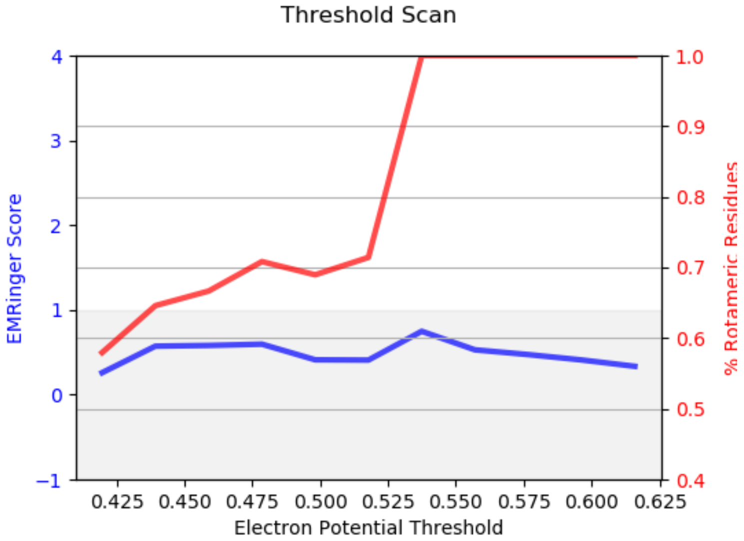


Figure 22: EMRinger score and fraction of rotameric residues as a function of the map threshold.

Fig. 23 shows the histogram for rotameric (blue) and non-rotameric (red) residues at the optimal threshold.

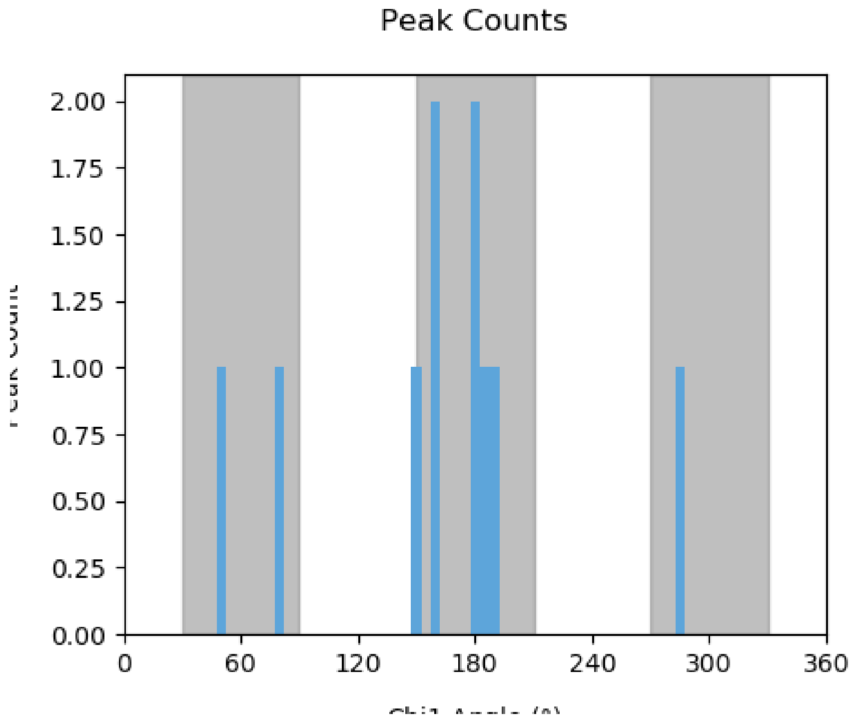
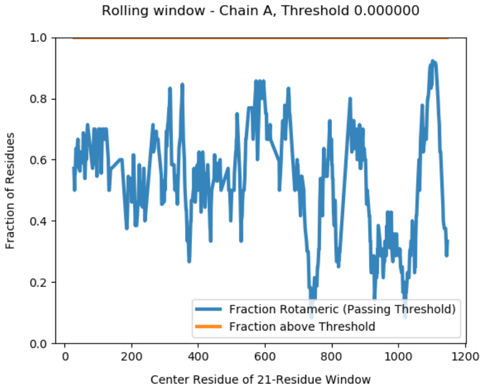
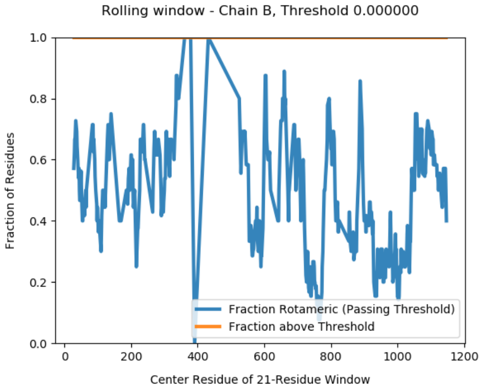
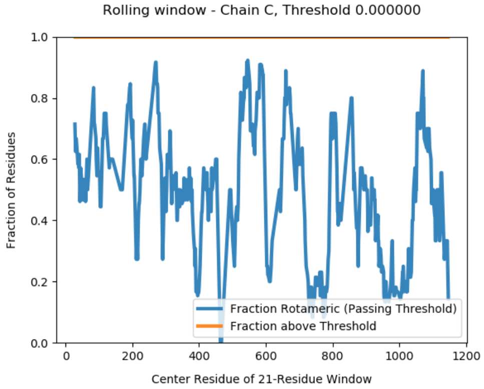


Figure 23: Histogram for rotameric (blue) and non-rotameric (red) residues at the optimal threshold as a function of the angle Chi1.

The following plots show the rolling window EMRinger analysis of the different chains to distinguish regions of improved model quality. This analysis was performed on rolling sliding 21-residue windows along the primary sequence of the protein chains.







Automatic criteria: The validation is OK if the EMRinger score and Max. Zscore are larger than 1.

WARNINGS: 1 warnings

1. **The EMRinger score is smaller than 1, it is 0.748.**

4.5 Level A.g DAQ validation

Explanation:
DAQ [Terashi et al., 2022] is a computational tool using deep learning that can estimate the residue-wise local quality for protein models from cryo-Electron Microscopy maps. The method calculates the likelihood that a given density feature corresponds to an aminoacid, atom, and secondary structure. These likelihoods are combined into a score that ranges from -1 (bad quality) to 1 (good quality).

Results:
Fig. 24 shows the histogram of the DAQ values. The mean and standard deviation were 0.2 and 0.2, respectively.

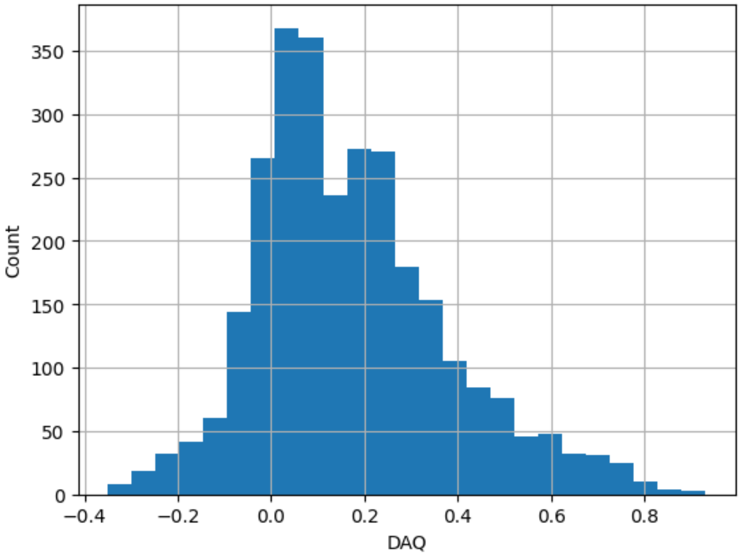
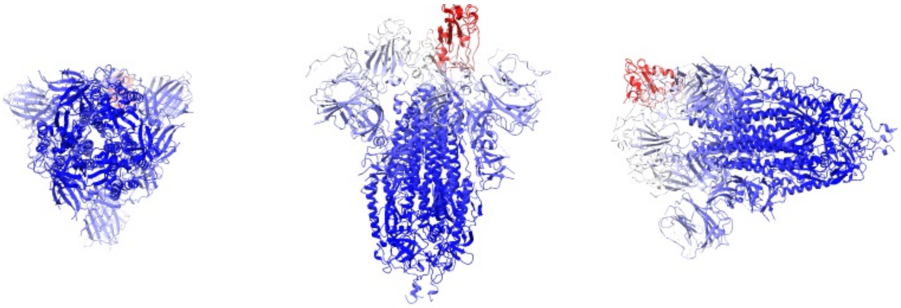


Figure 24: Histogram of the DAQ values.

The atomic model colored by DAQ can be seen in Fig. 25.



(a) View 1 (b) View 2 (c) View 3

Figure 25: Atomic model colored by DAQ Views generated by ChimeraX at a the following X, Y, Z angles: View 1 (0,0,0), View 2 (90, 0, 0), View 3 (0, 90, 0).

Automatic criteria: The validation is OK if the average DAQ score is larger than 0.5.

WARNINGS: 1 warnings

1. **The average DAQ is smaller than 0.5.**

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[Terashi et al., 2022] Terashi, G., Wang, X., Subramaniya, S.R.M.V., Tesmer, J.J.G. and Kihara, D. (2022). Residue-Wise Local Quality Estimation for Protein Models from Cryo-EM Maps. (submitted).