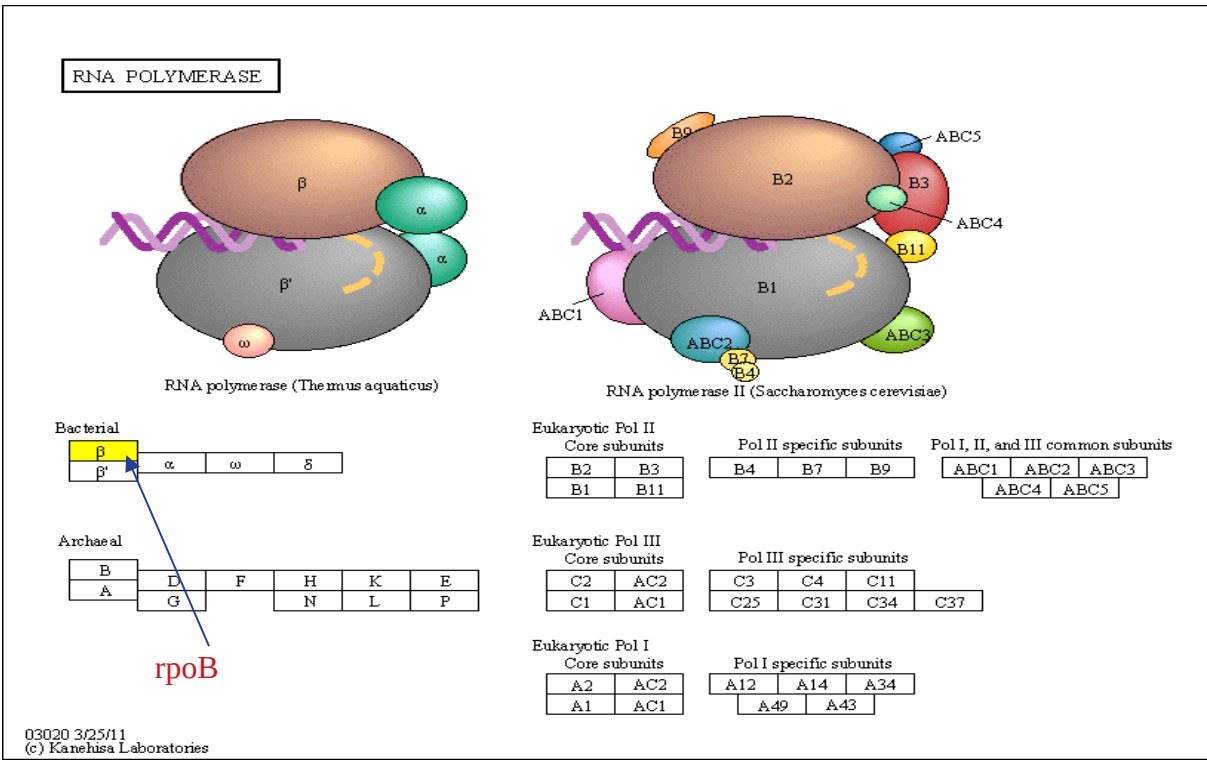


Figure E6.1. Mapping of non-homologous interacting partners of MAP mimicry proteins (nHIPMMP) on the MAP metabolic pathway (source KEGG). KEGG ID is in parenthesis.

(1) MAP protein: P42384

| S. No. | nHIPMMP | Color code |
|--------|---------|------------|
| 1. | grpE | Red |
| 2. | gyrB | Green |
| 3. | rpoB | Yellow |

(i) RNA polymerase (mpa03020)



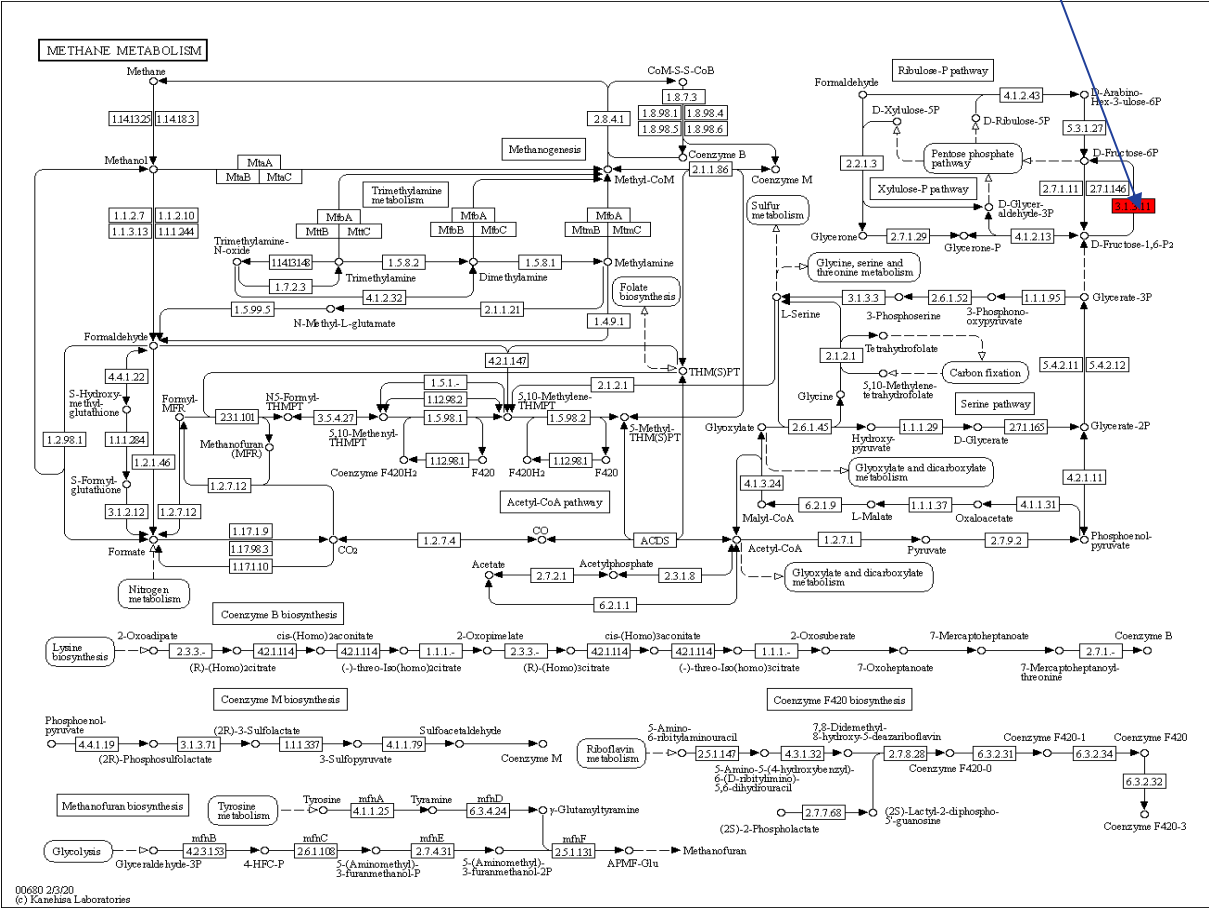
KEGG mapped protein: rpoB

(2) MAP protein: Q73WG6

| S. No. | nHIPMMP | Color code |
|--------|----------|------------|
| 1. | MAP_2692 | Red |
| 2. | MAP_2694 | Green |

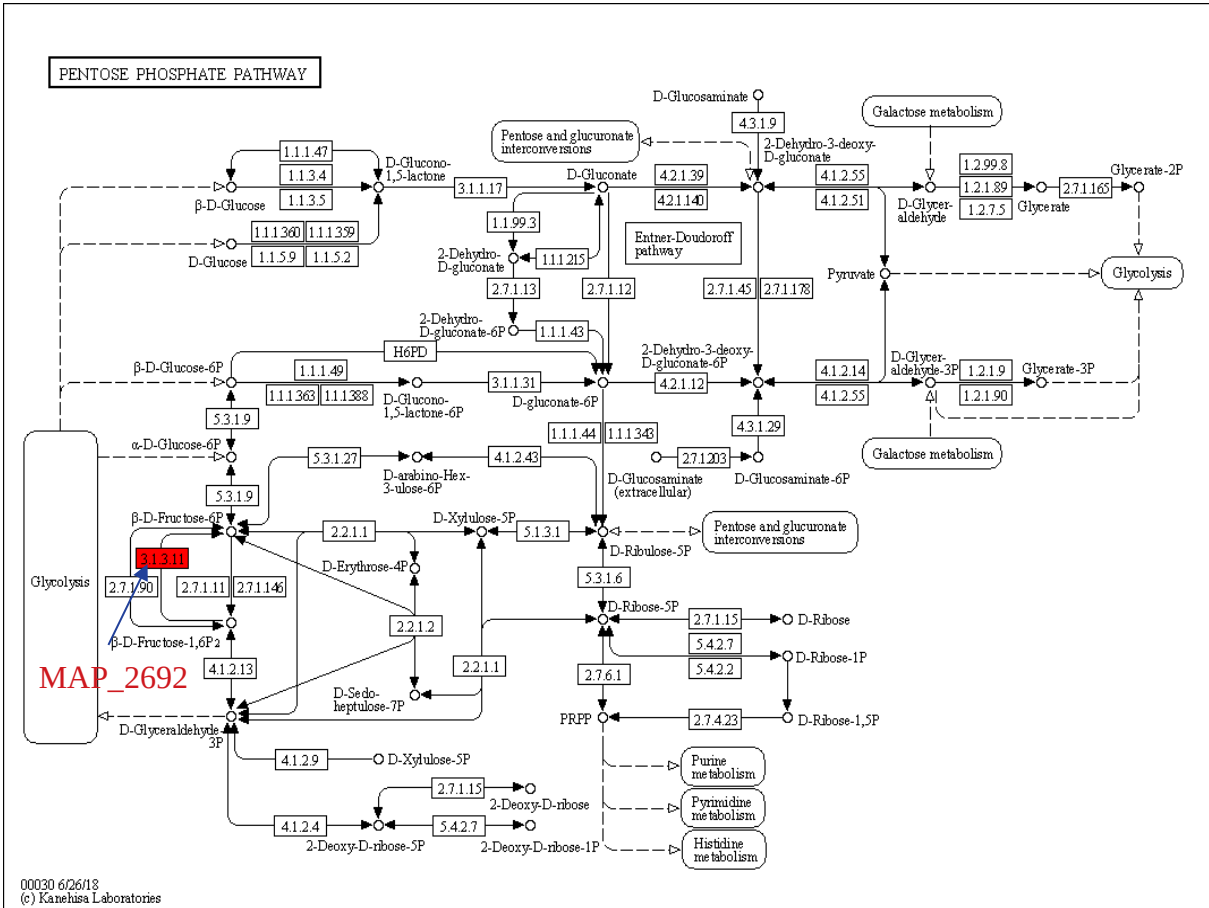
(i) Methane metabolism (mpa00680)

MAP_2692



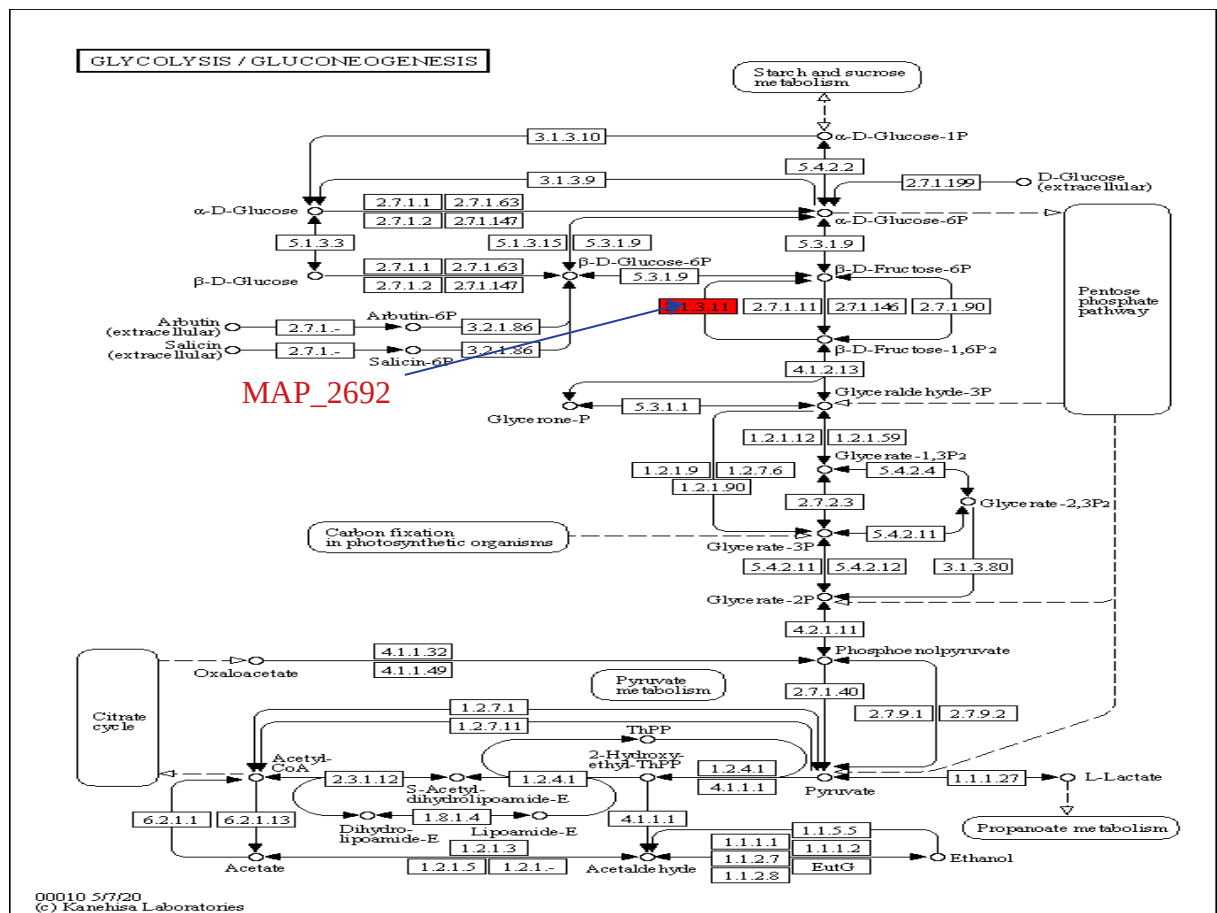
KEGG mapped protein: MAP_2692

(ii) Pentose phosphate pathway (mpa00030)



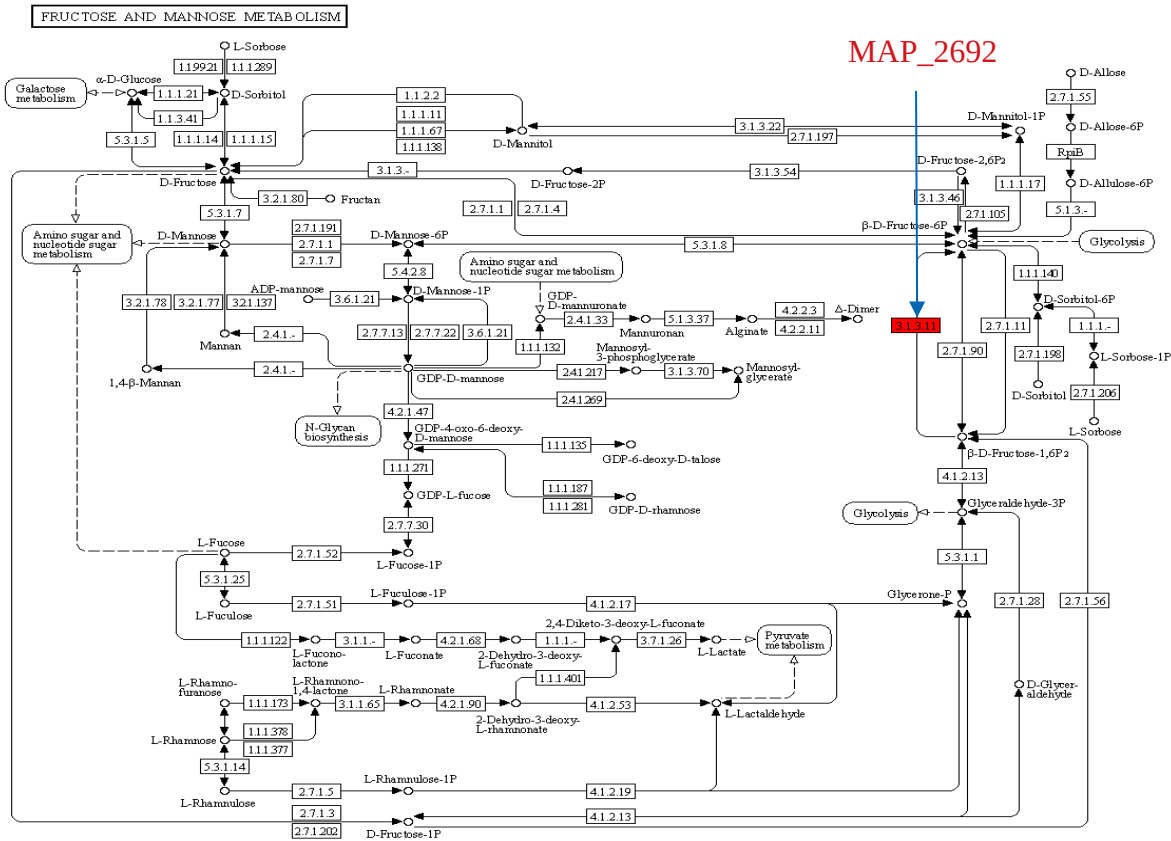
KEGG mapped protein: MAP_2692

(iii) Glycolysis / Gluconeogenesis (mpa00010)



KEGG mapped protein: MAP_2692

(iv) Fructose and mannose metabolism (mpa00051)



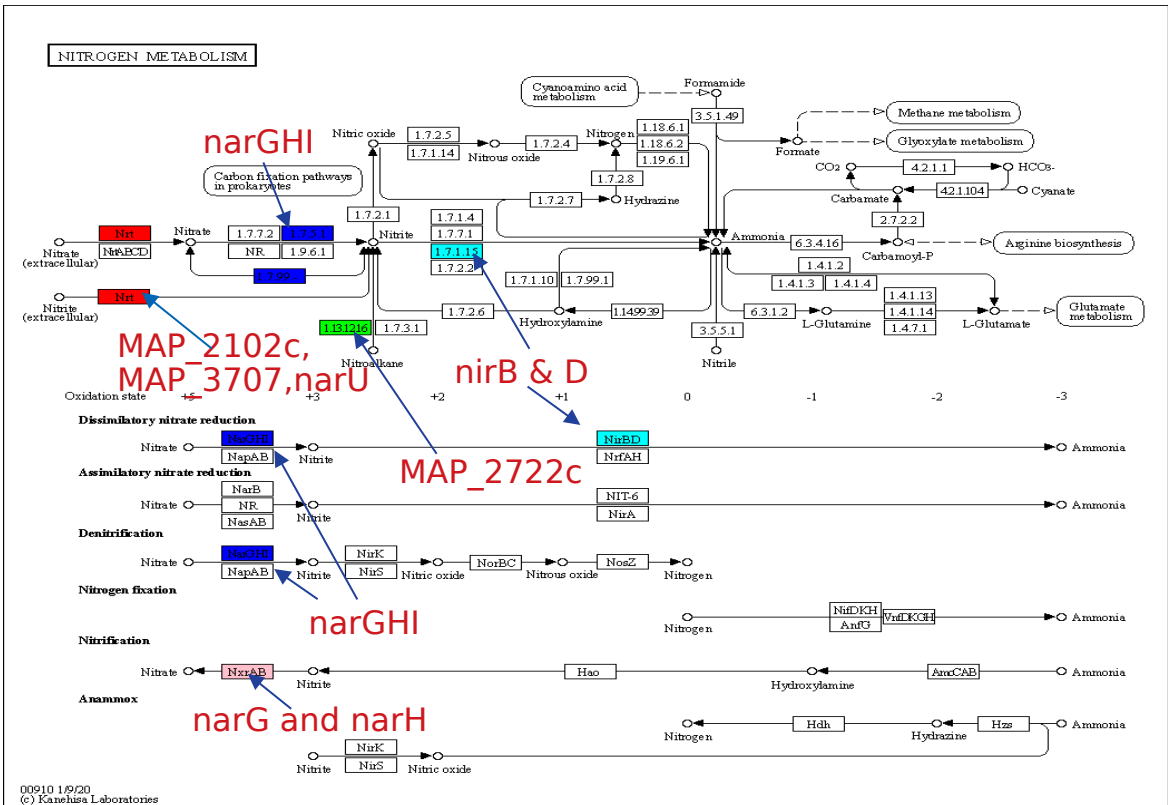
KEGG mapped protein: MAP_2692

00051 3/27/20
(c) Kanehisa Laboratories

(3) MAP protein: Q73WP1

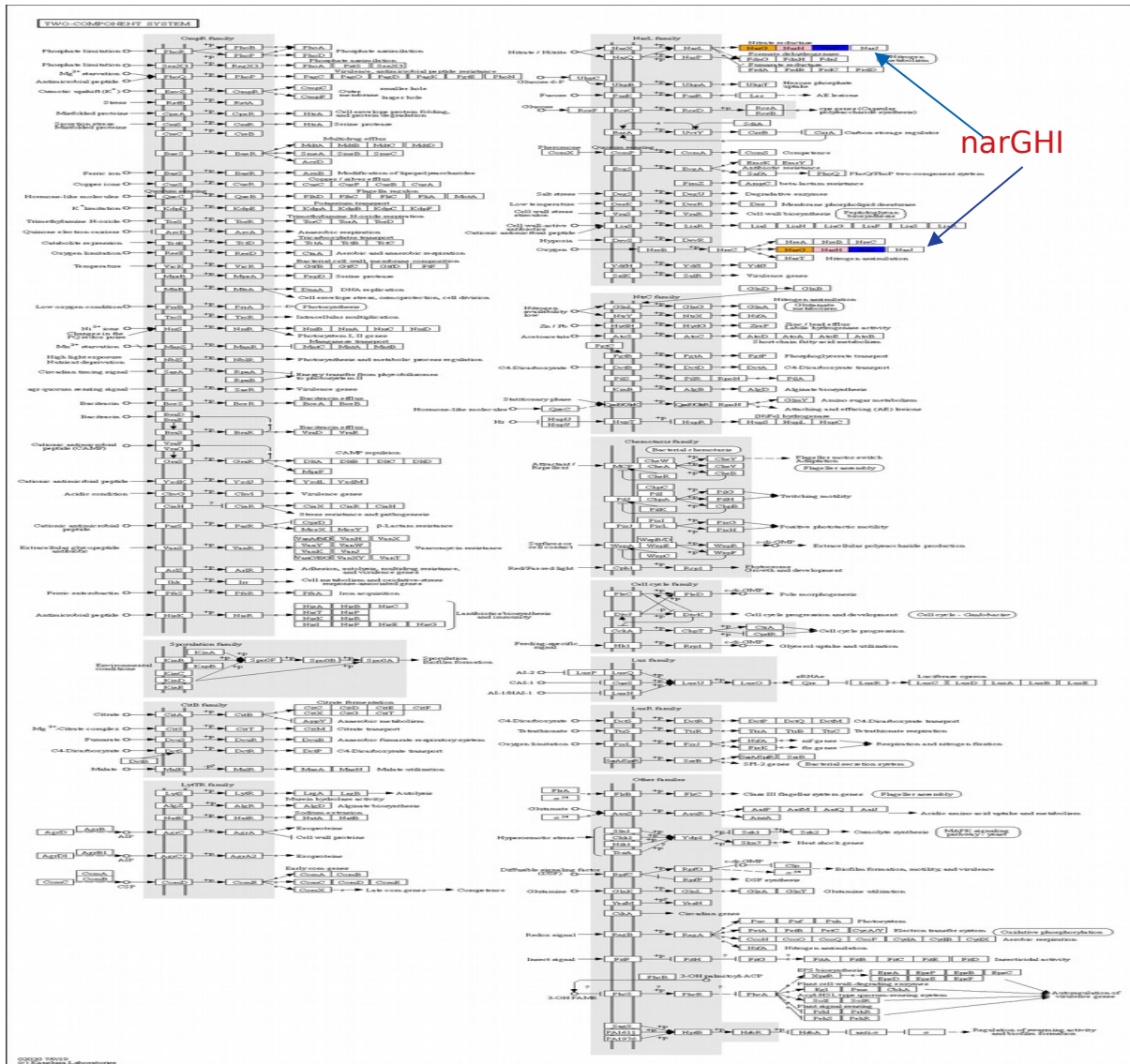
| S. No. | nHIPMMP | Color code |
|--------|-----------|------------|
| 1. | MAP_2102c | Red |
| 2. | MAP_2722c | Green |
| 3. | MAP_3707c | Yellow |
| 4. | narG | Orange |
| 5. | narH | Pink |
| 6. | narI | Blue |
| 7. | narJ | Teal |
| 8. | narU | Voilet |
| 9. | nirB | cyan |
| 10. | nirD | Grey |

(i) Nitrogen metabolism (mpa00910)



KEGG mapped protein: MAP_2102c, MAP_2722c, MAP_3707c, narG, narH, narI, narU, nirB, nirD

(ii) Two-component system (mpa02020)

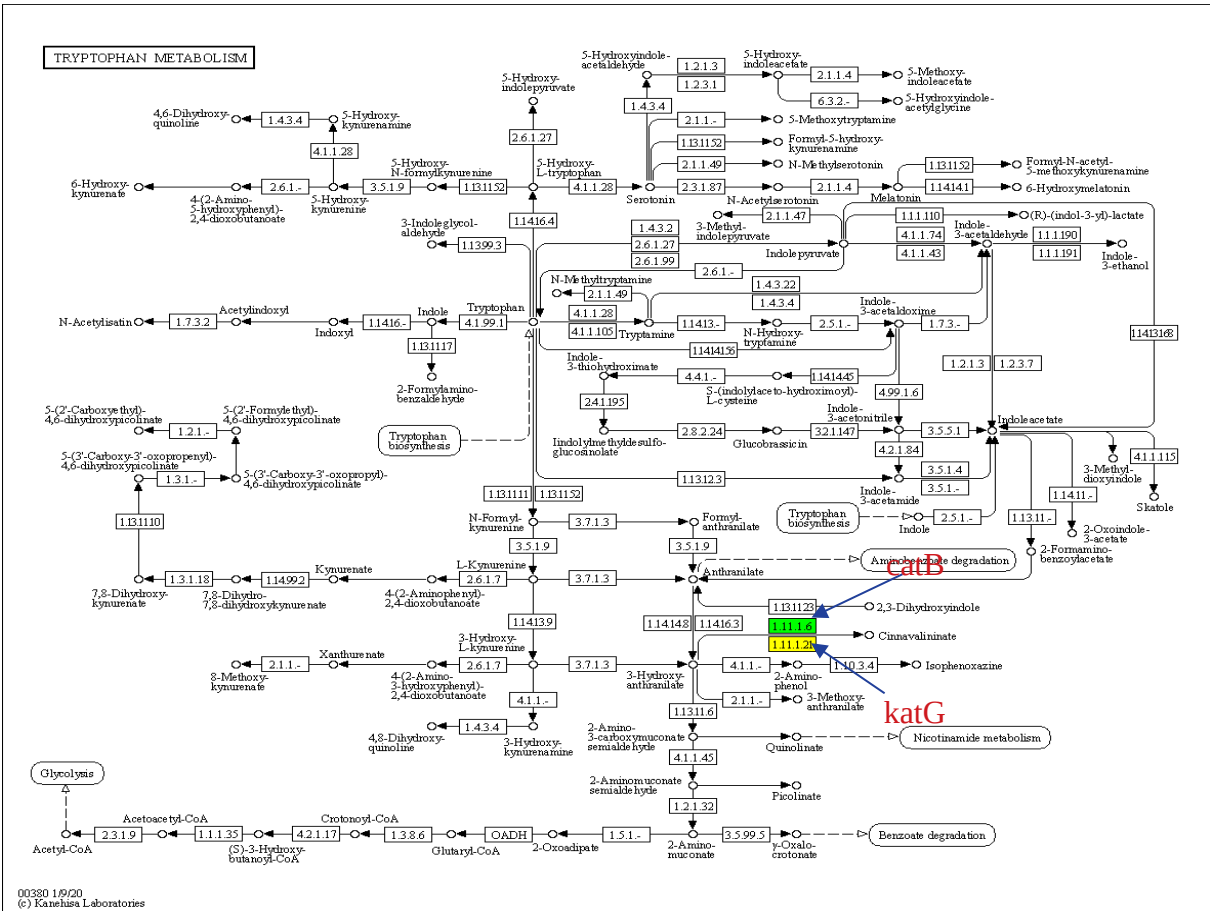


KEGG mapped protein: narG, narH, narI

(4) MAP protein: Q73ZL3

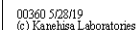
| S. No. | nHIPMMP | Color code |
|--------|---------|------------|
| 1. | ahpD | Red |
| 2. | catB | Green |
| 3. | katG | Yellow |
| 4. | oxyR | Orange |
| 5. | sodC | Pink |
| 6. | tpx | Voilet |
| 7. | trxB2 | Grey |

(i) Tryptophan metabolism (mpa00380)



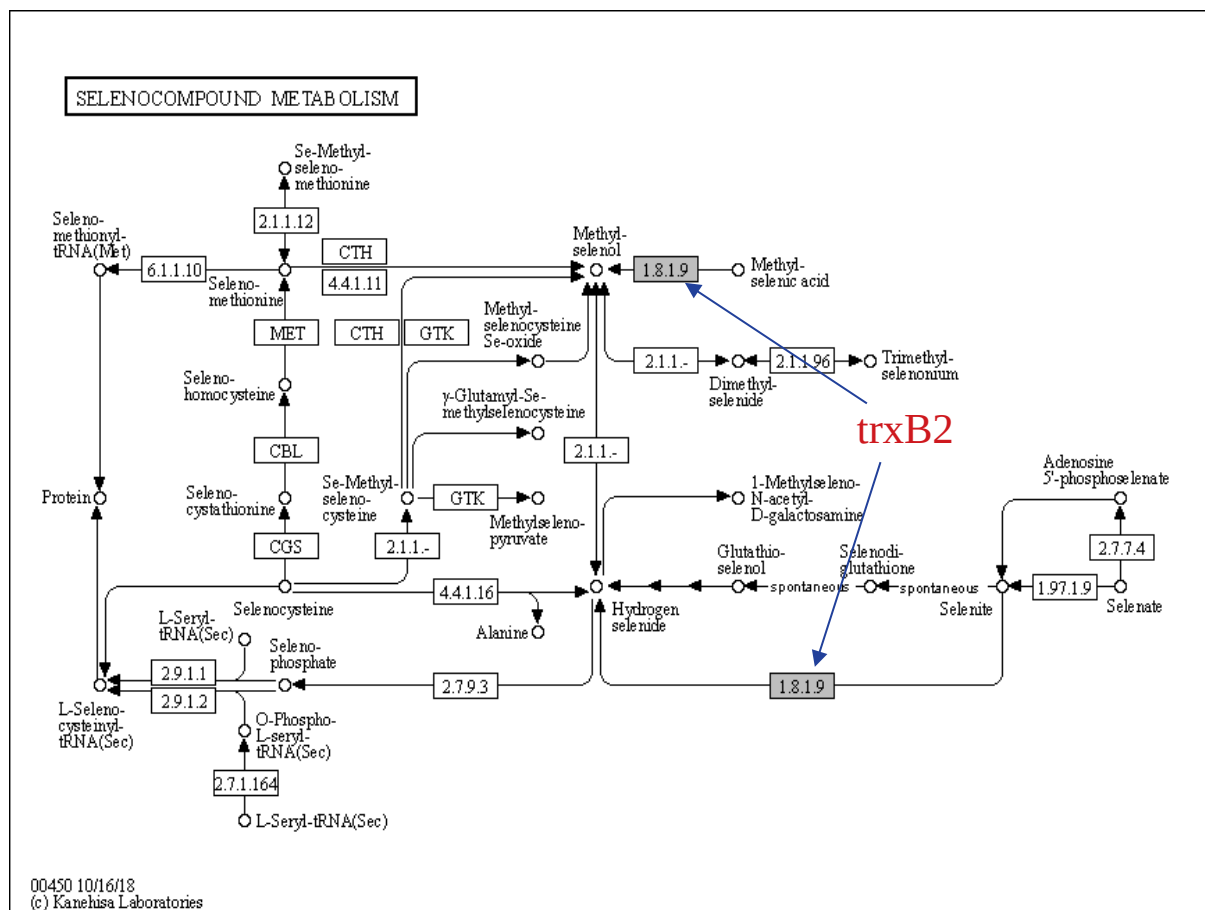
KEGG mapped protein: catB, katG

(ii) Phenylalanine metabolism (mpa00360)



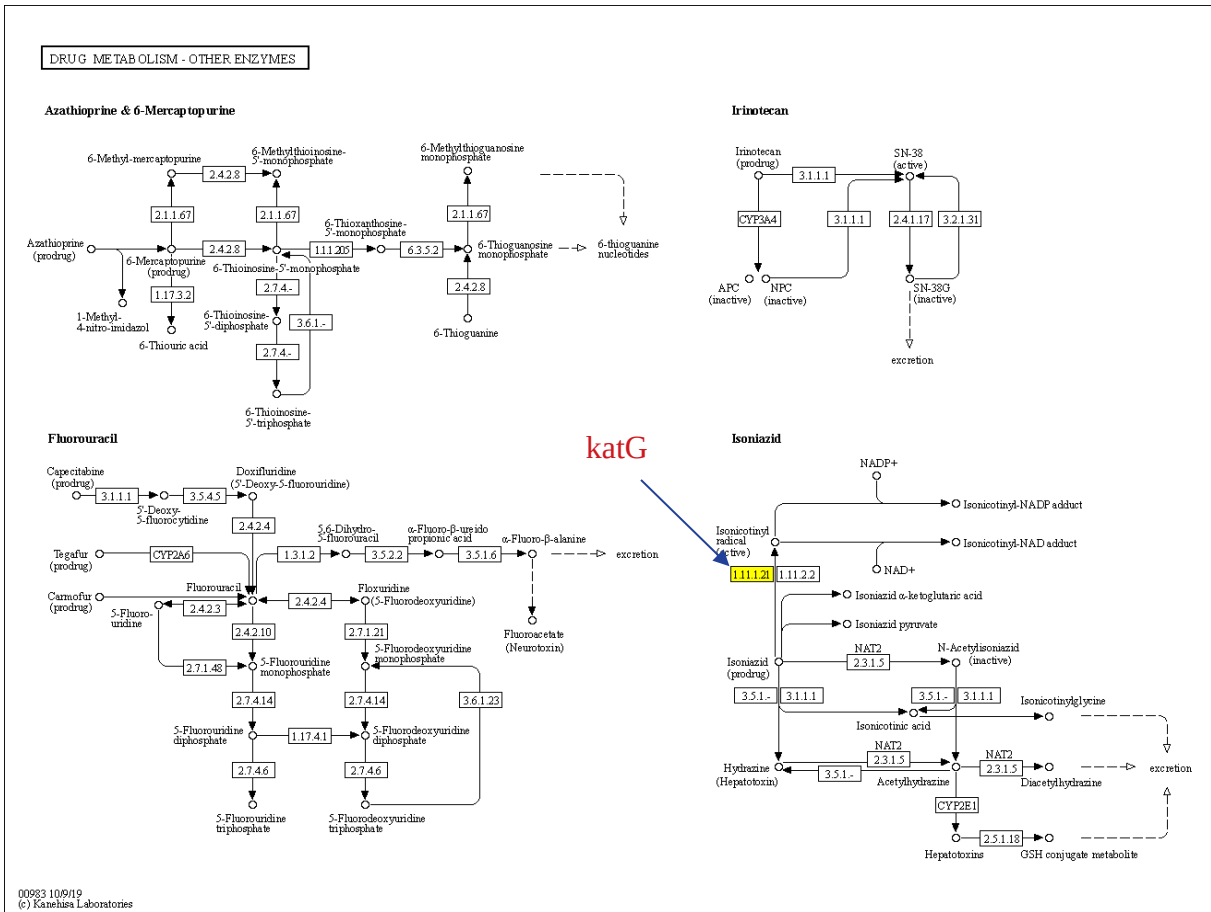
KEGG mapped protein: katG

(iii) Selenocompound metabolism (mpa00450)



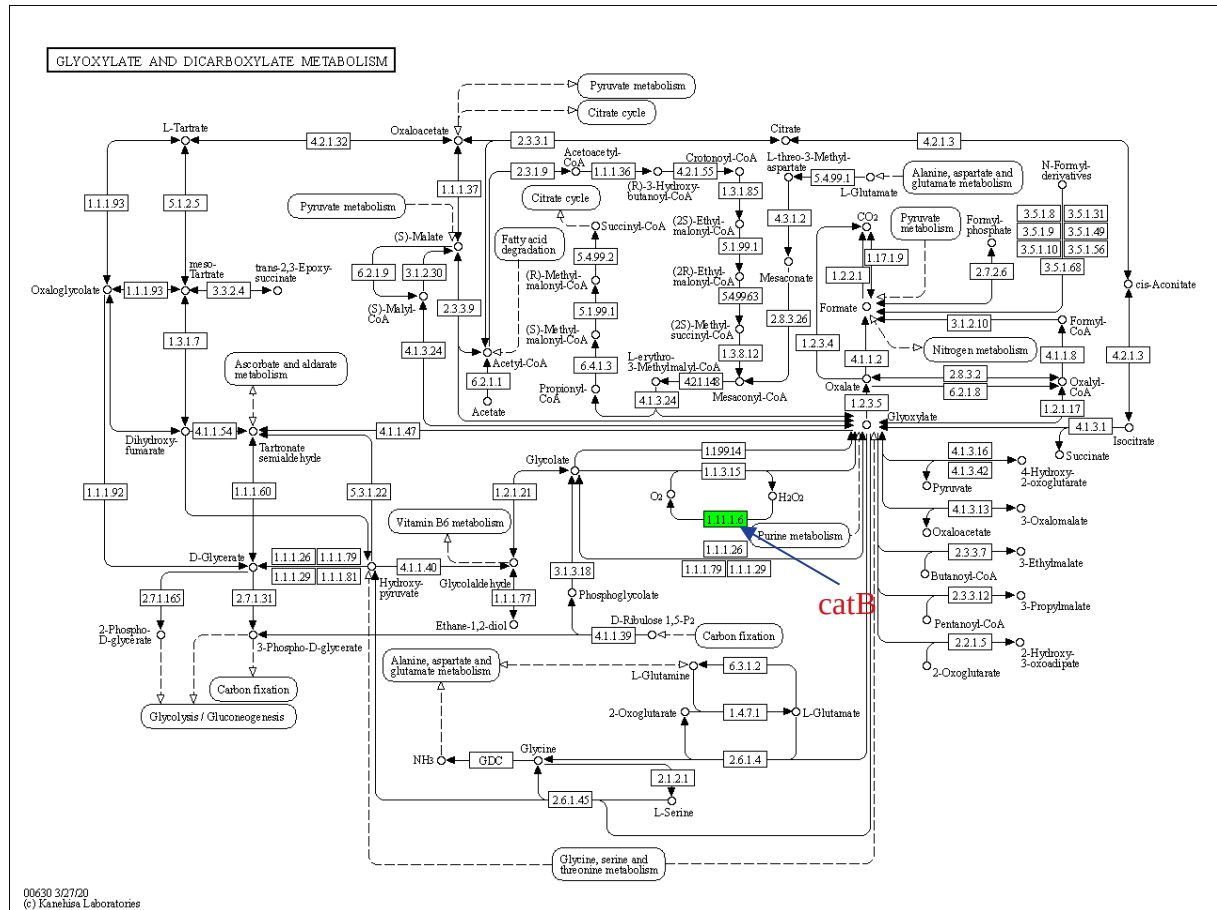
KEGG mapped protein: taxB2

(iv) Drug metabolism - other enzymes (mpa00983)



KEGG mapped protein: katG

(v) Glyoxylate and dicarboxylate metabolism (mpa00630)

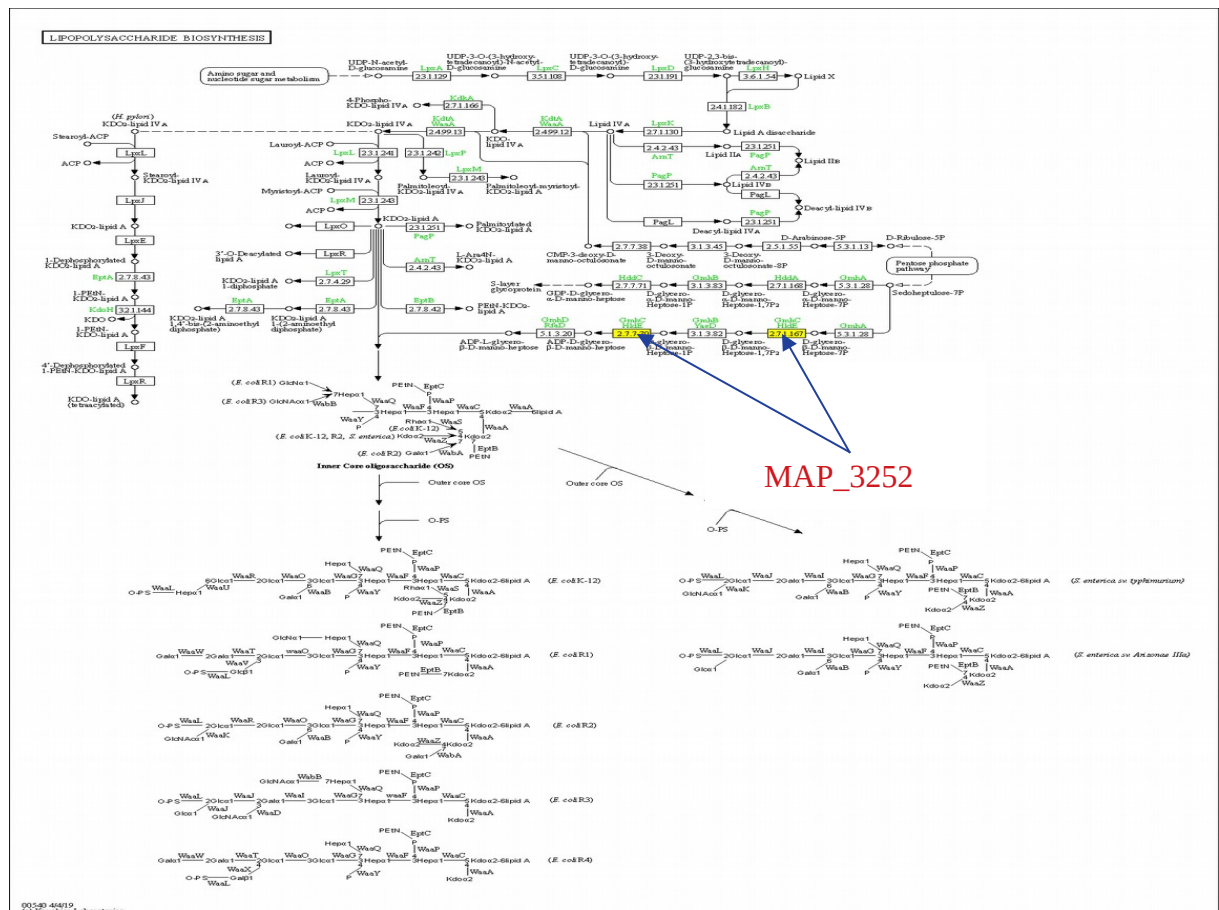


KEGG mapped protein: catB

(5) MAP protein: Q740V8

| S. No. | nHIPMMP | Color code |
|--------|----------|------------|
| 1. | MAP_1234 | Red |
| 2. | MAP_1235 | Green |
| 3. | MAP_3252 | Yellow |

(i) Lipopolysaccharide biosynthesis (mpa00540)

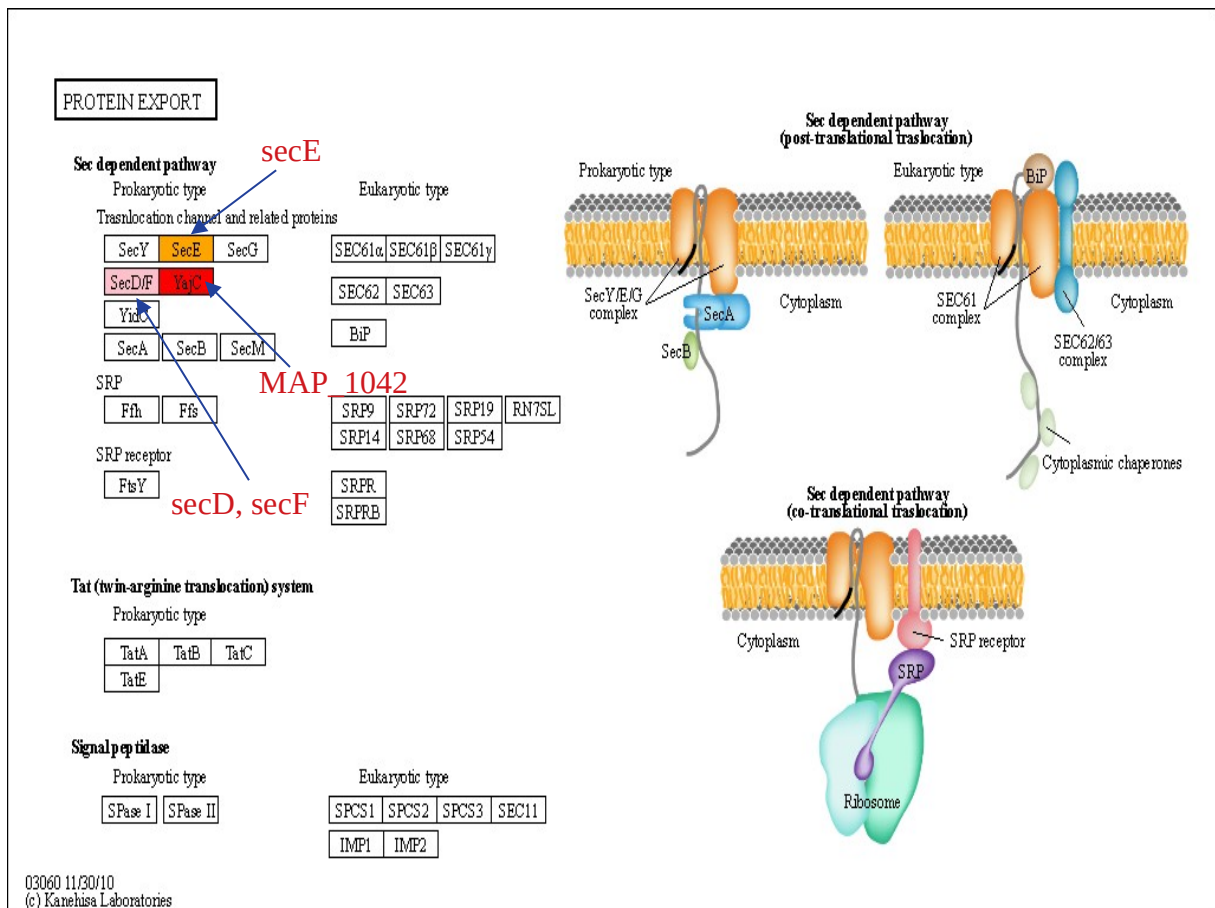


KEGG mapped protein: MAP_3252

(6) MAP protein: Q741P6

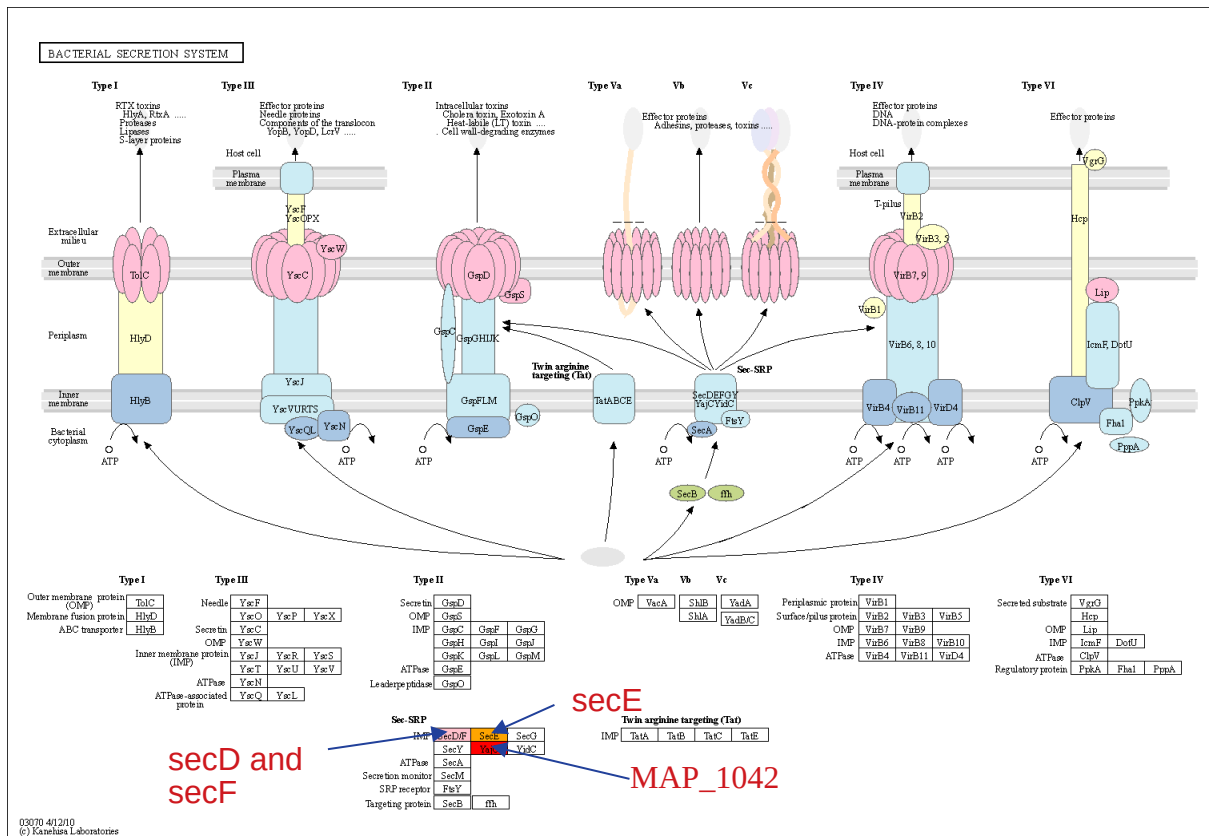
| S. No. | nHIPMMP | Color code |
|--------|----------|------------|
| 1. | MAP_1042 | Red |
| 2. | MAP_1045 | Green |
| 3. | relA | Yellow |
| 4. | secD | Pink |
| 5. | secE | Orange |
| 6. | secF | Grey |
| 7. | secY | Voilet |
| 8. | yidC | Blue |

(i) Protein export (mpa03060)



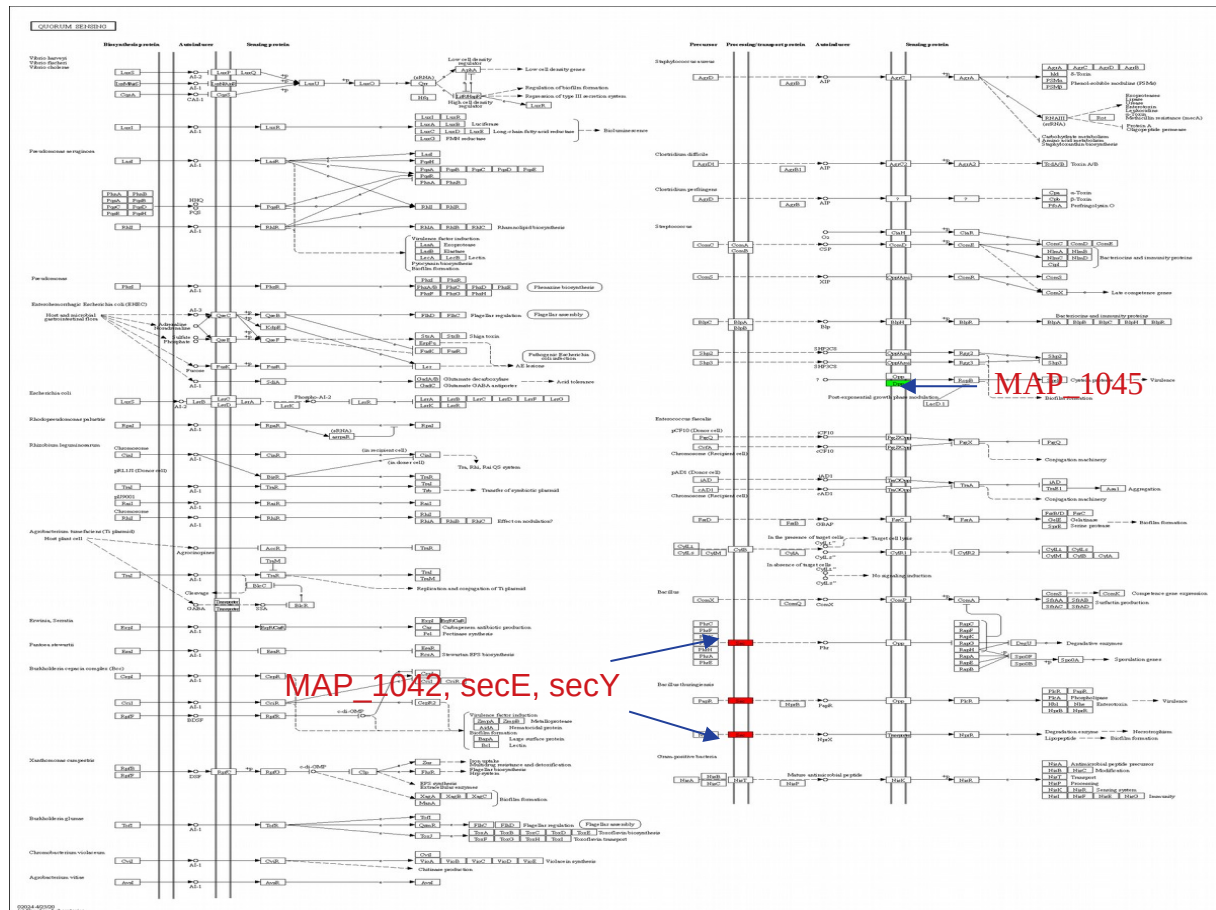
KEGG mapped protein: secD, secE, secF, MAP_1042

(ii) Bacterial secretion system (mpa03070)



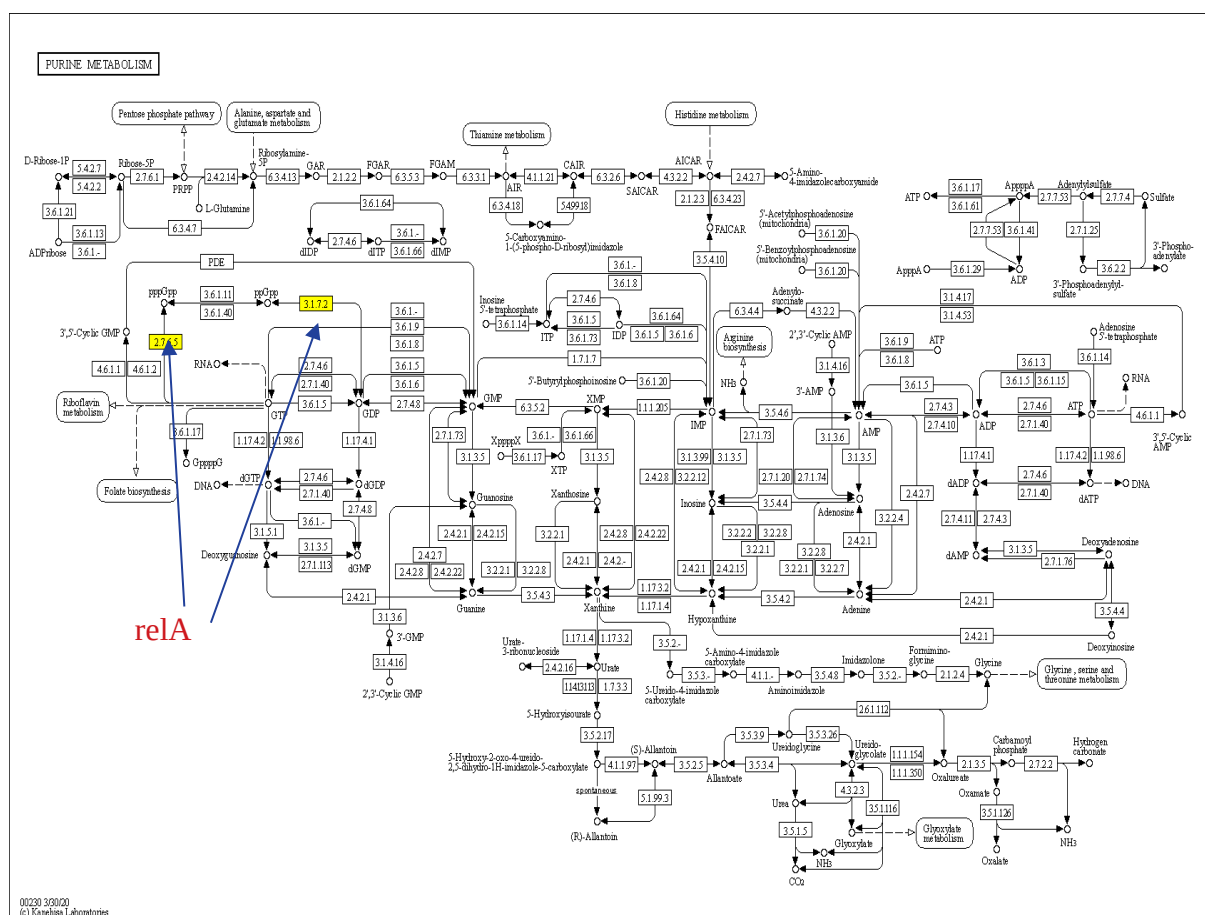
KEGG mapped protein: secD, secE, secF, MAP_1042

(iii) Quorum sensing (mpa02024)



KEGG mapped protein: secE, secY, MAP_1045, MAP_1042

(iv) Purine metabolism (mpa00230)



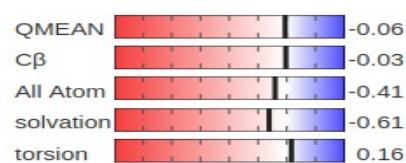
KEGG mapped protein: relA

Figure E6.2. Quality assessment of katG, narH and rpoB modeled structure using Qualitative Model Energy Analysis (QMEAN) score, MolProbity score, and Ramachandran plot. The root-mean-square deviation (RMSD) between the 3D homology structure and template structure are also shown.

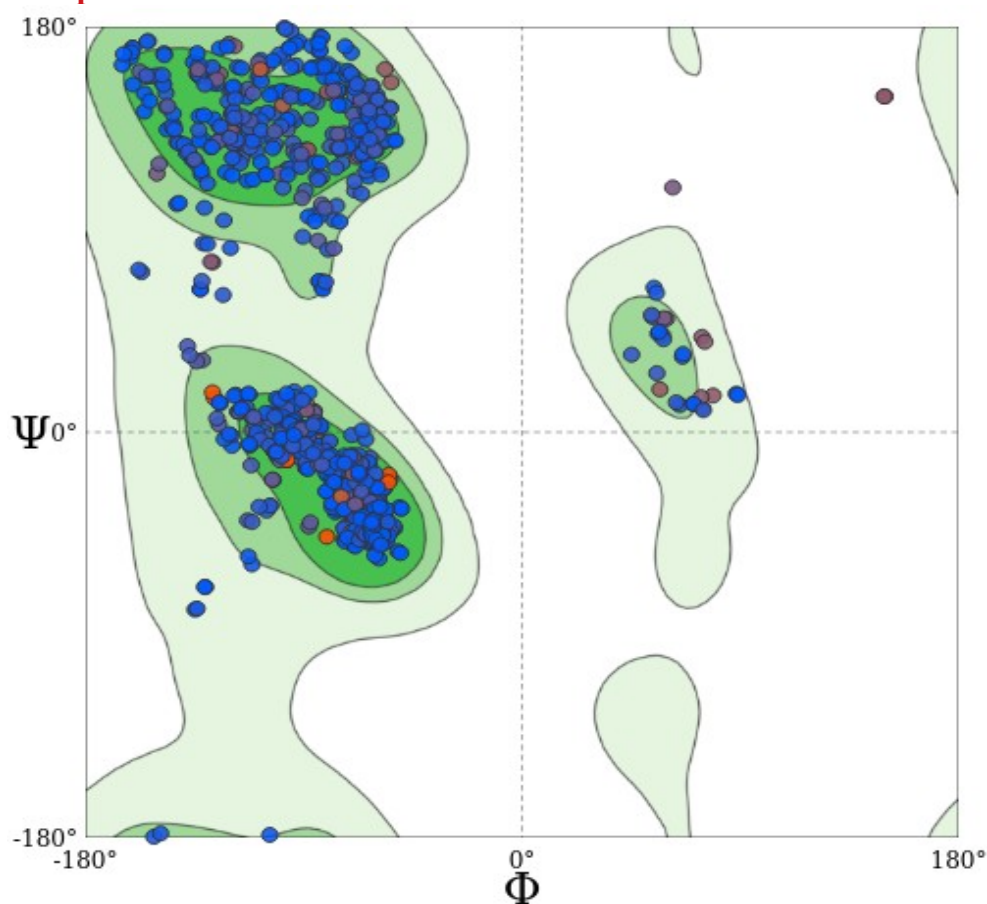
(1) Target: katG

| Parameters | Scores |
|-----------------------|------------|
| Template used | 5SXX.1.A |
| Template identity | 65.14% |
| Qmean value | -0.06 |
| MolProbity Score | 1.09 |
| Clash Score | 1.43 |
| Ramachandran Favoured | 97.25% |
| Ramachandran Outliers | 0.49% |
| Rotamer Outliers | 1.25% |
| Bad Bonds | 5 / 11431 |
| Bad Angles | 78 / 15586 |
| Twisted Non-Proline | 2 / 1334 |

Quality Estimate

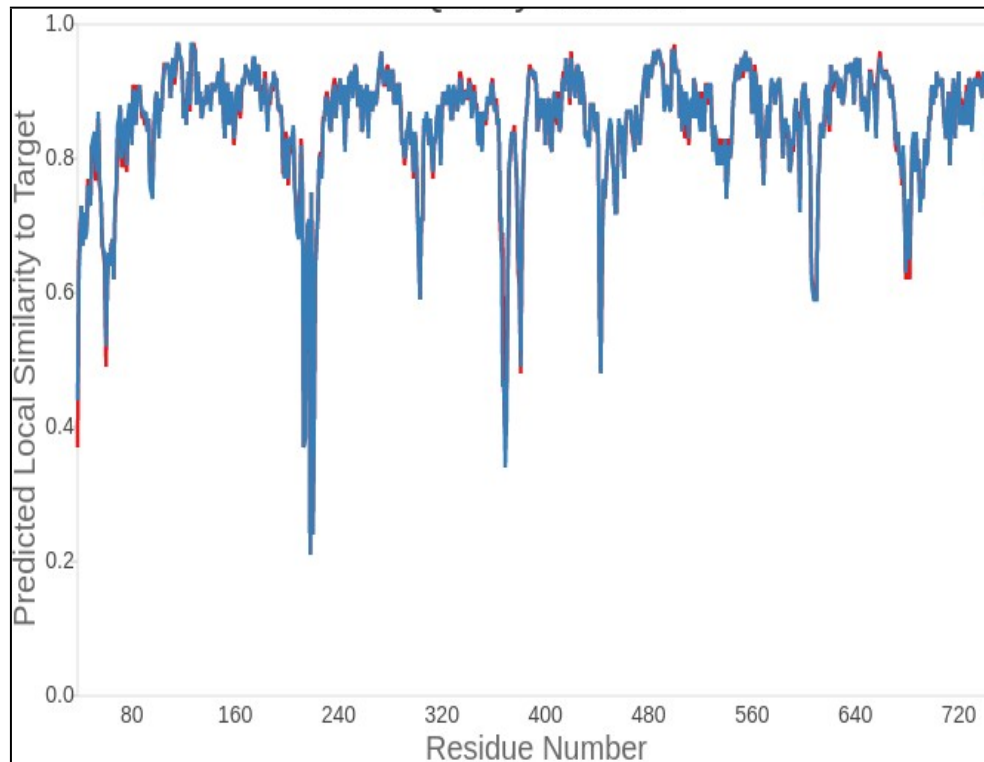


Ramachandran plot of katG model structure

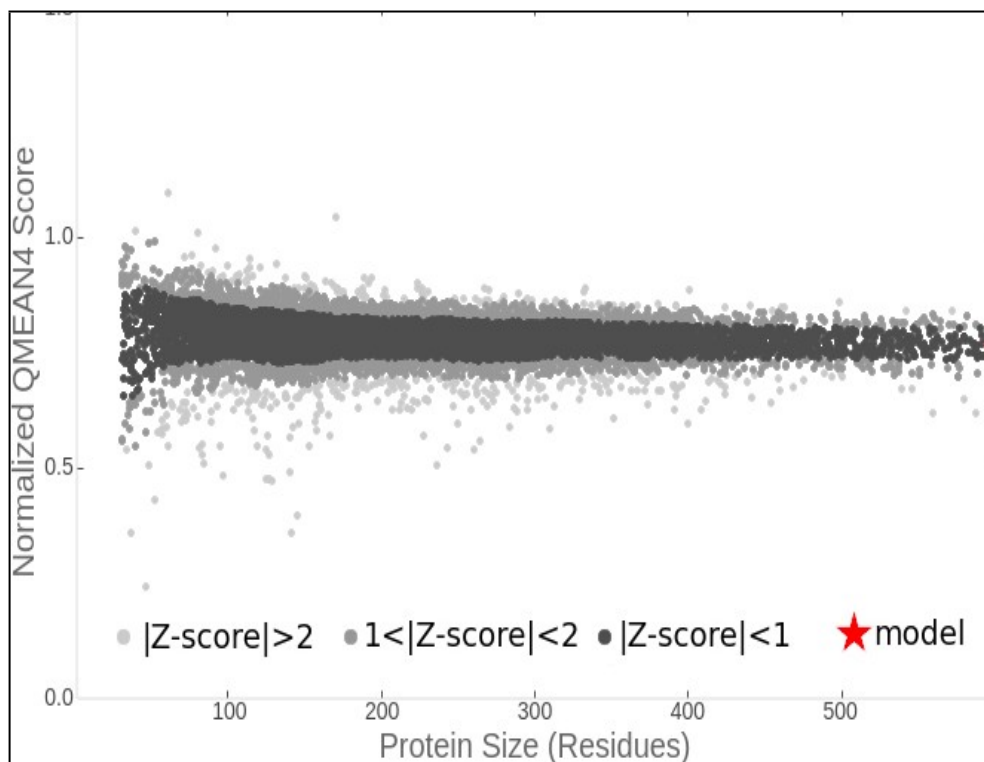


Swiss-model structure assessment

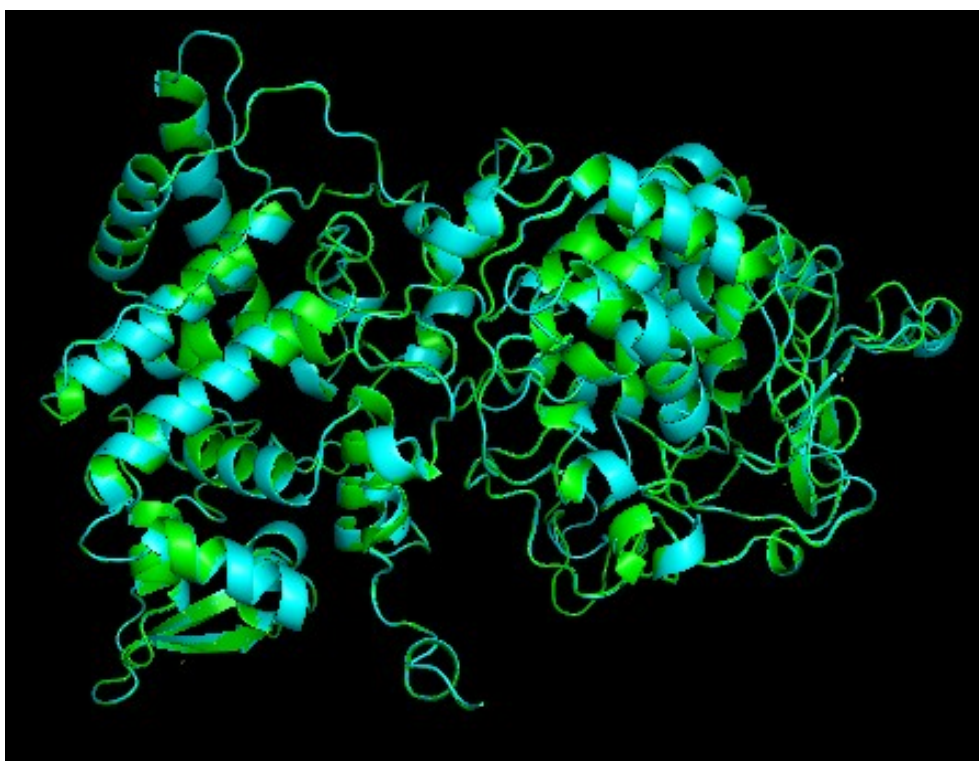
(i) Local quality estimate of katG model structure



(ii) Comparison between Non-redundant set of PDB structure & katG model structure



Structure superimposition of katG model structure and 5SXX (template) using pymol



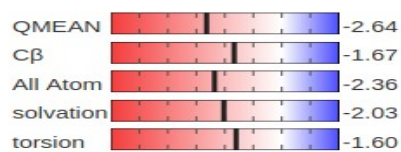
RMSD value between katG and template: 0.118

Color code: katG-Cyan & 5SXX-Green

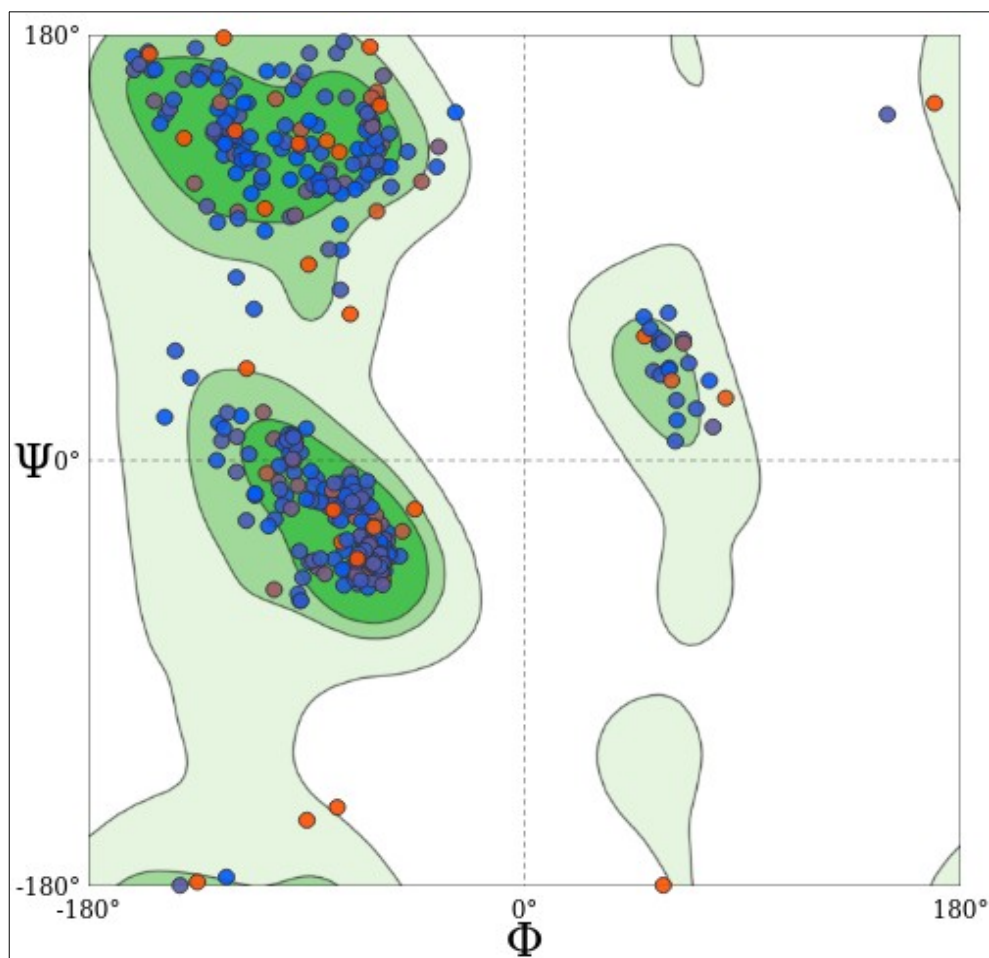
(2) Target: narH

| Parameters | Scores |
|-----------------------|-----------|
| Template used | 1Y5N.2.E |
| Template identity | 58.46% |
| Qmean value | -2.64 |
| MolProbity Score | 1.14 |
| Clash Score | 0.40 |
| Ramachandran Favoured | 94.61% |
| Ramachandran Outliers | 1.04% |
| Bad Bonds | 0 / 3924 |
| Bad Angles | 27 / 5332 |
| Cis Non-Proline | 1 / 450 |
| Cis Prolines | 2 / 33 |

Quality Estimate

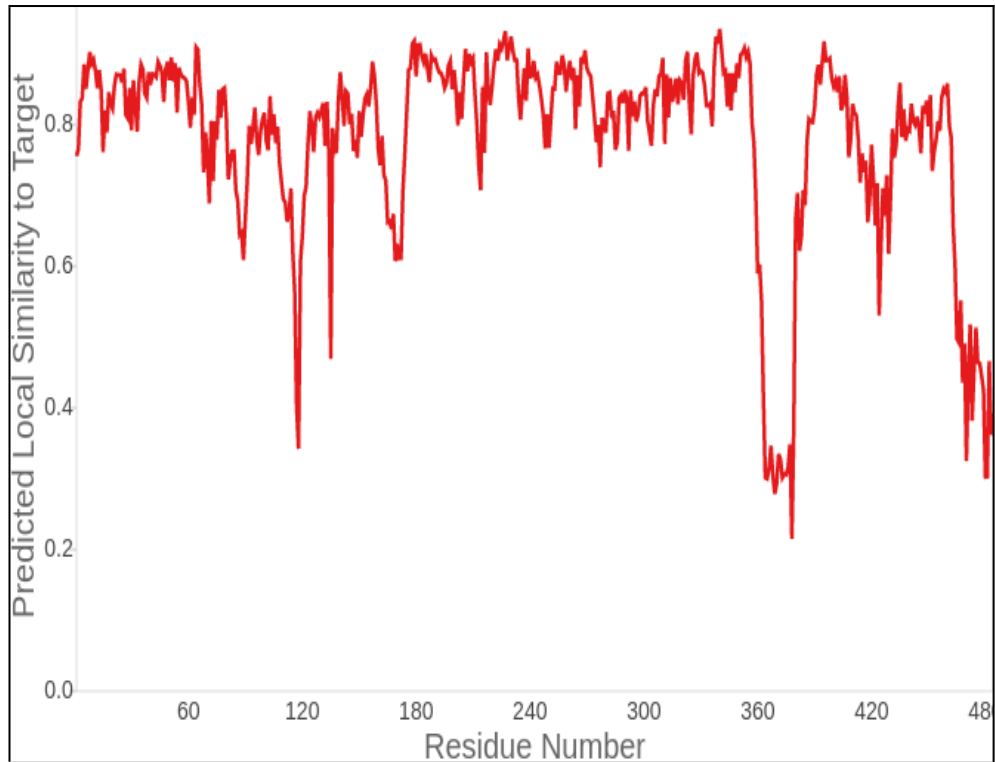


Ramachandran plot of narH model structure

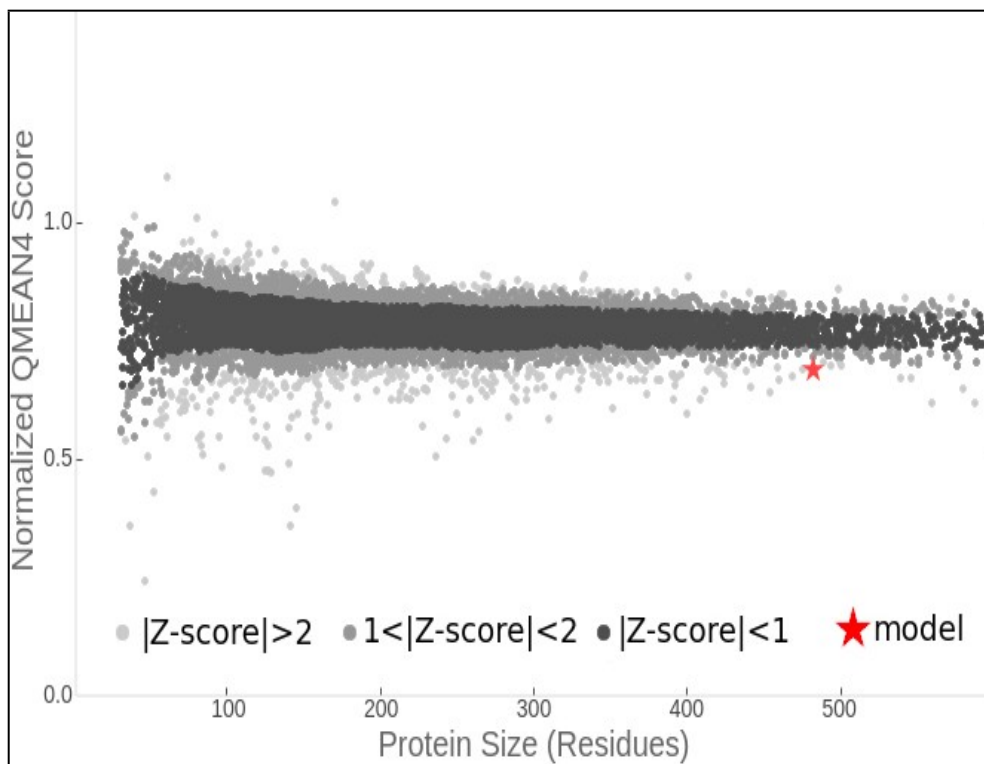


Swiss-model structure assessment

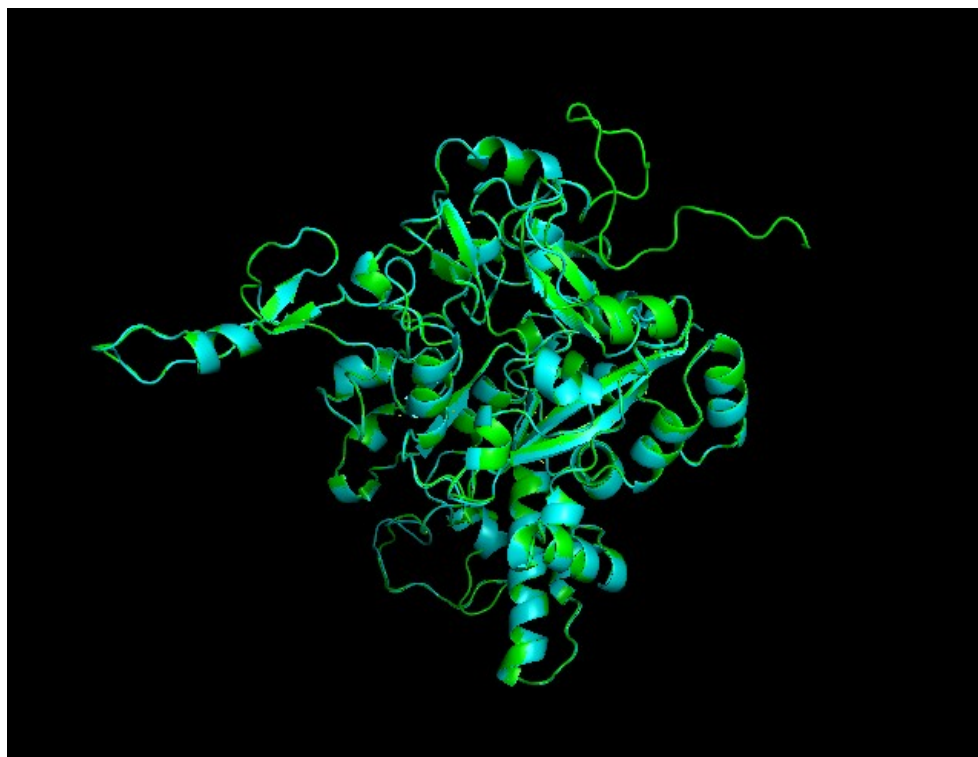
(i) Local quality estimate of narH model structure



(ii) Comparison between Non-redundant set of PDB structure & narH model structure



Structure superimposition of narH model structure and 1Y5N (template) using pymol



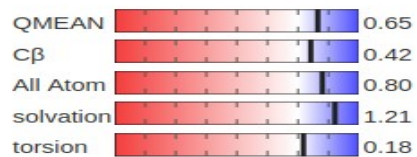
RMSD value between narH and template: 0.187

Color code:- narH-Cyan & 1Y5N-Green

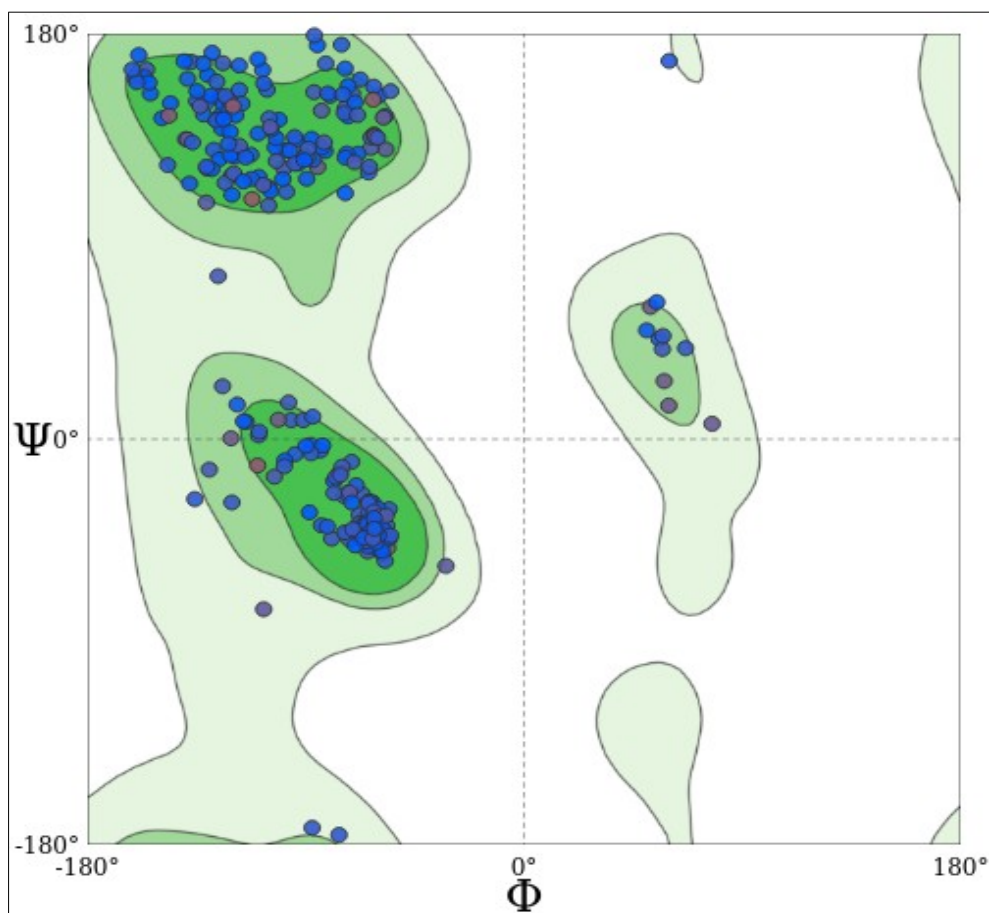
(3) Target: rpoB

| Parameters | Scores |
|-----------------------|-----------|
| Template used | 4KBM.1.A |
| Template identity | 95.35% |
| Qmean value | 0.65 |
| MolProbity Score | 0.78 |
| Clash Score | 0.33 |
| Ramachandran Favoured | 97.88% |
| Ramachandran Outliers | 0.53% |
| Bad Bonds | 2 / 3071 |
| Bad Angles | 22 / 4155 |
| Cis Non-Proline | 1 / 360 |
| Cis Prolines | 1 / 19 |

Quality Estimate

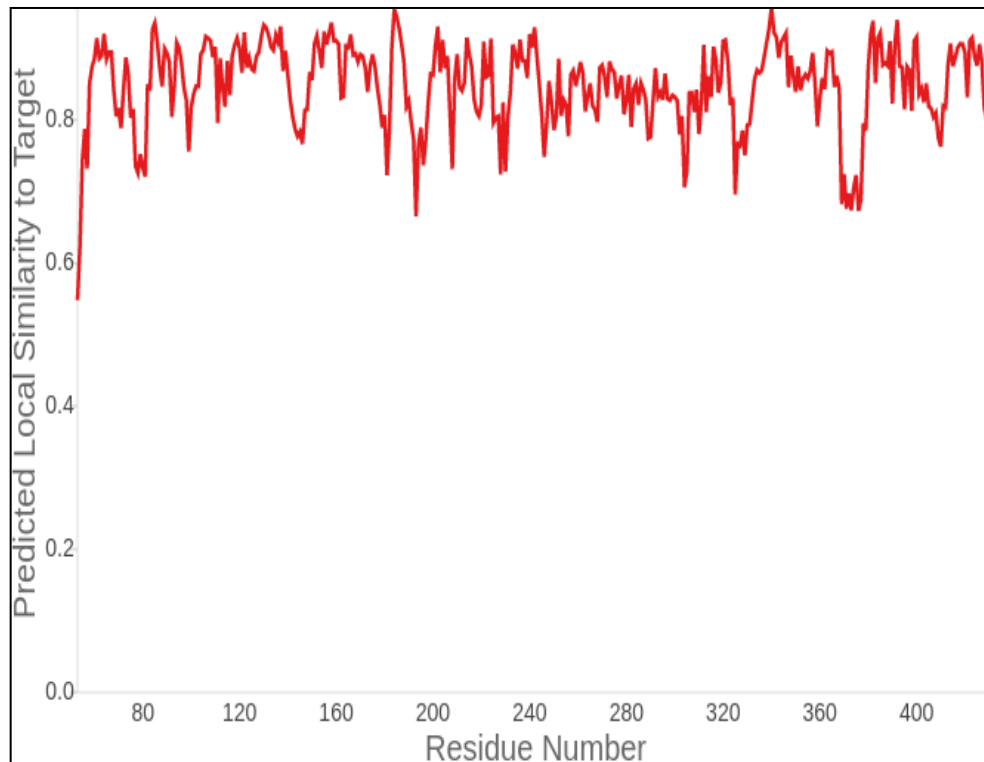


Ramachandran plot of rpoB model structure

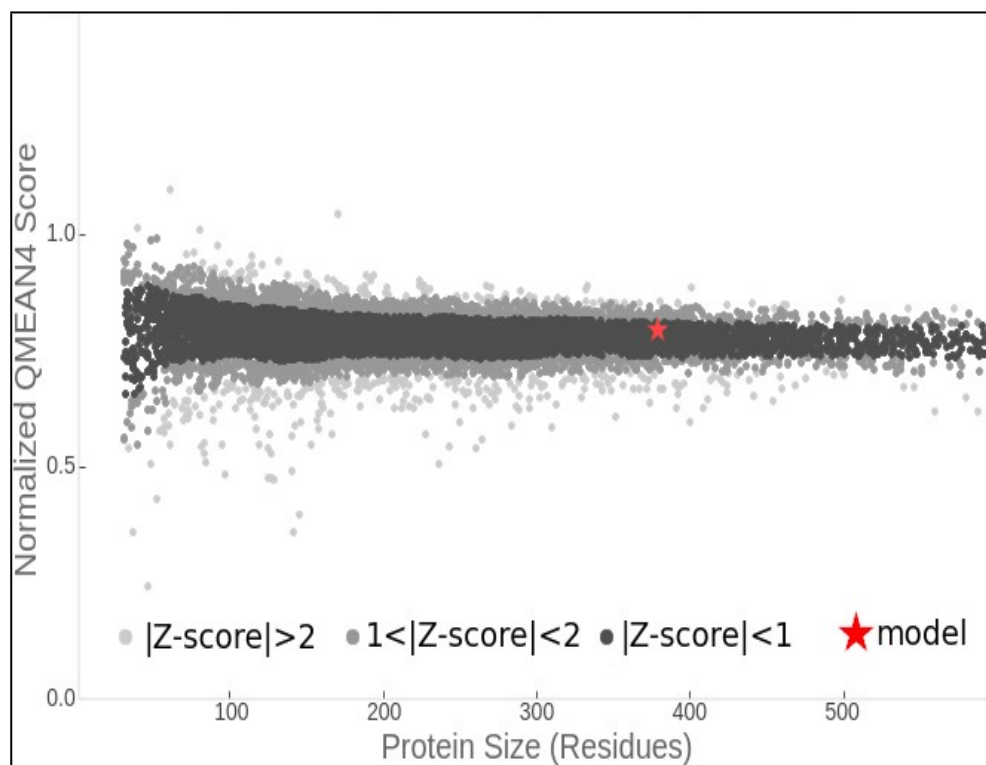


Swiss-model structure assessment

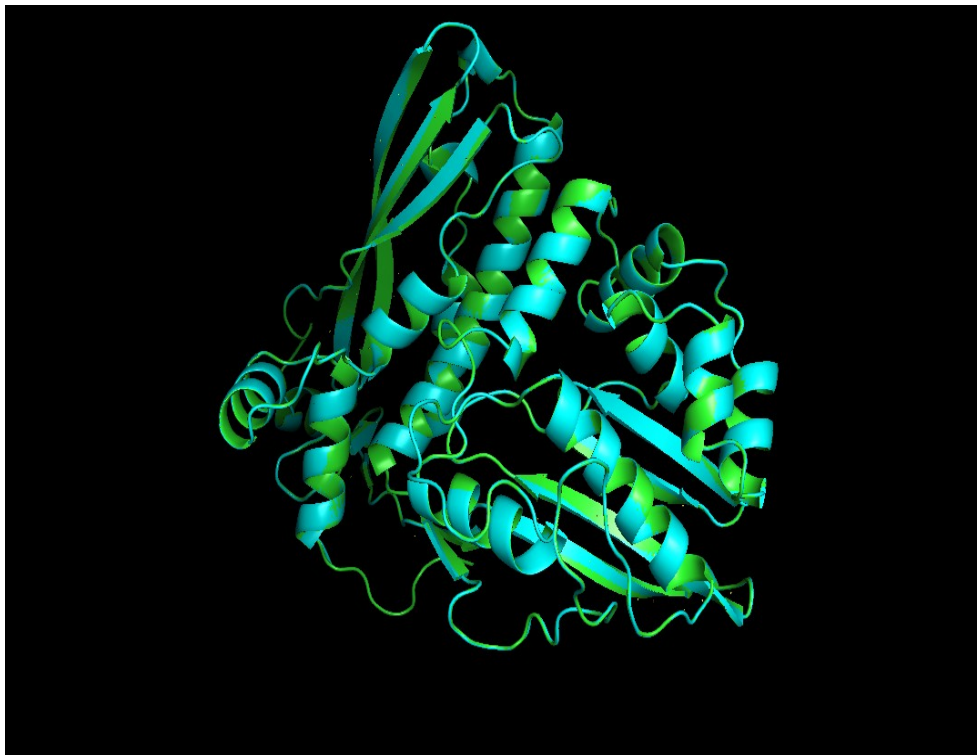
(i) Local quality estimate of rpoB model structure



(ii) Comparison between Non-redundant set of PDB structure & rpoB model structure



Structure superimposition of rpoB model structure and 4KBM (template) using pymol

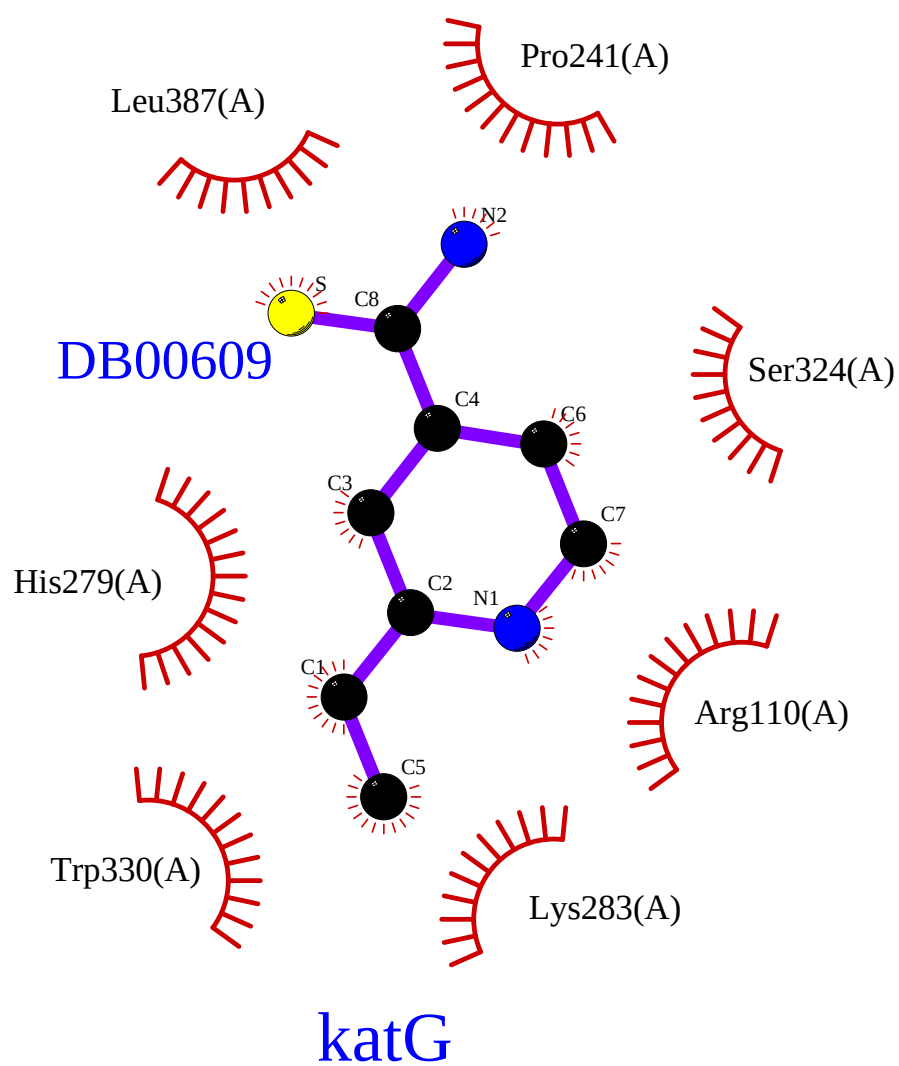


RMSD value between rpoB and template: 0.051

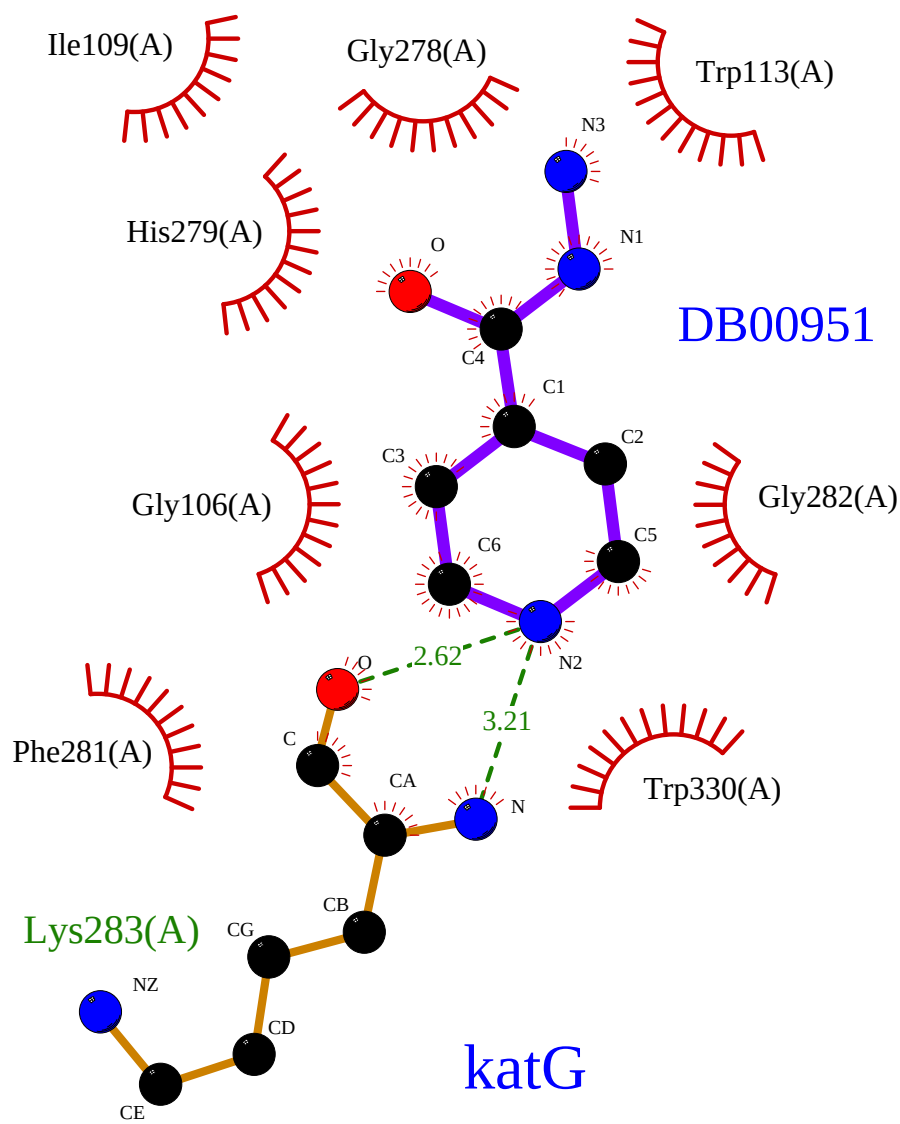
Color code: rpoB-Cyan & 4KBM-Green

Figure S3. The interaction pattern of the proposed drug with the target proteins.

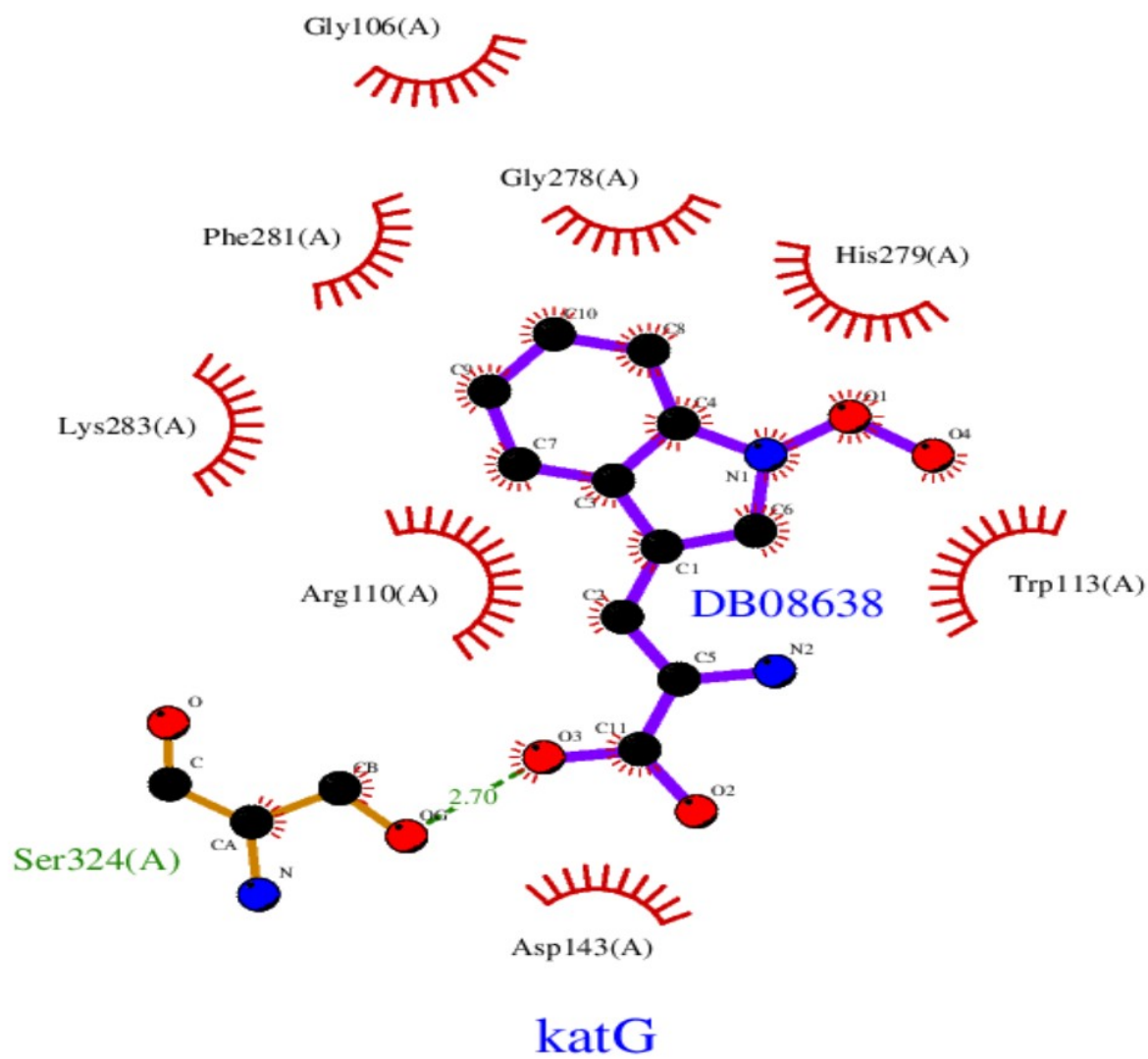
(i) Interaction pattern of katG with DB00609



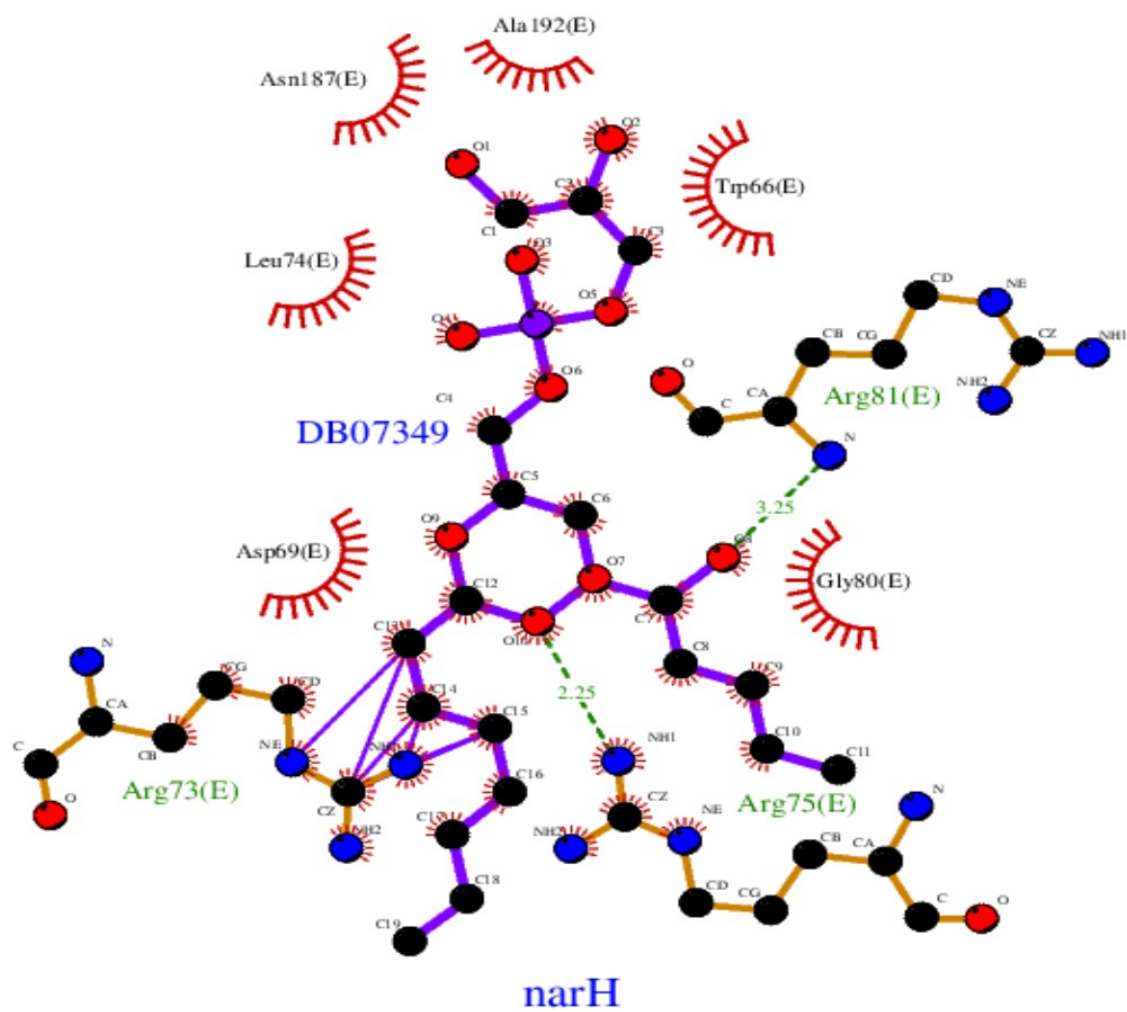
(ii) Interaction pattern of katG with DB00951



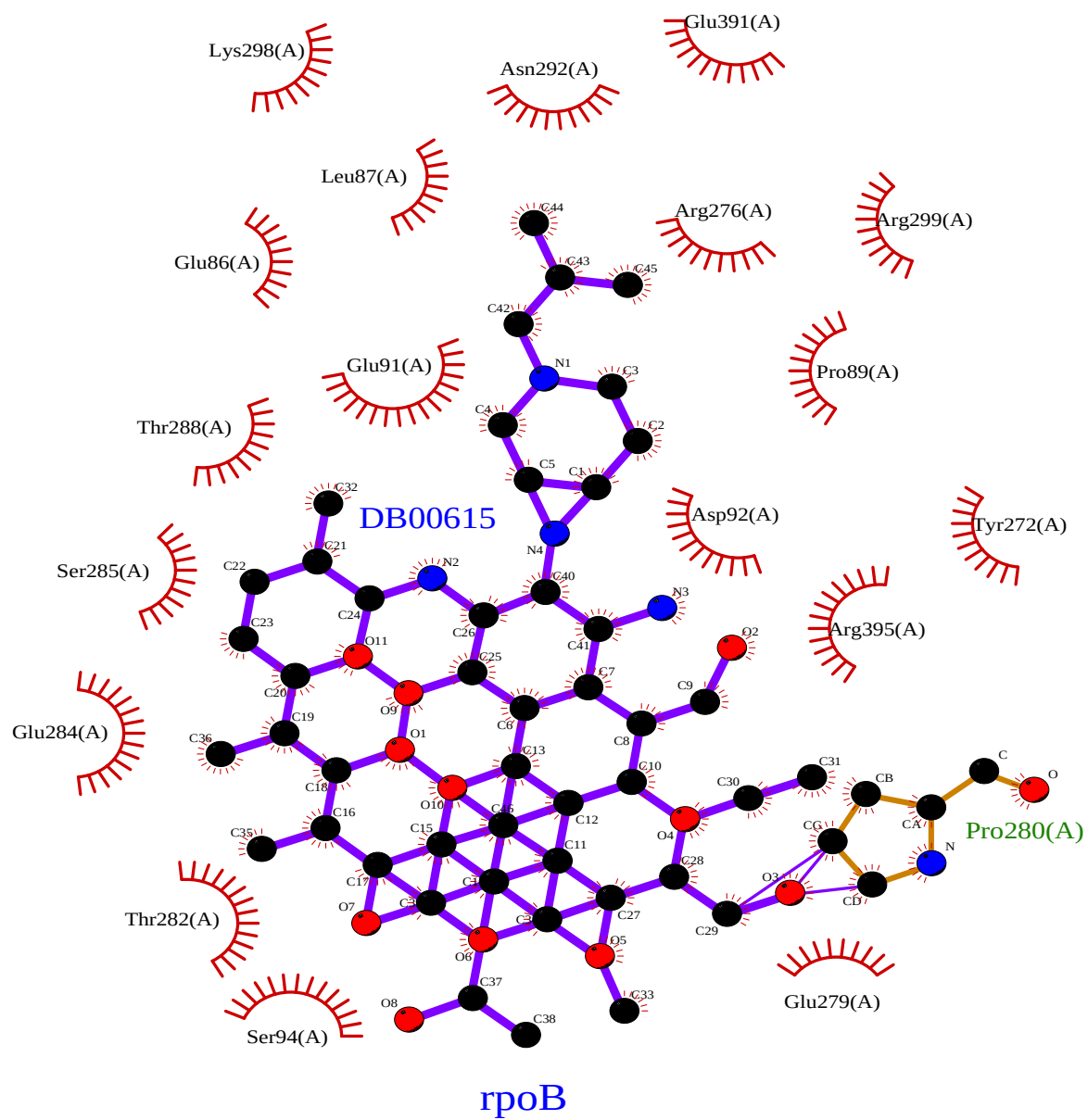
(iii) Interaction pattern of katG with DB08638



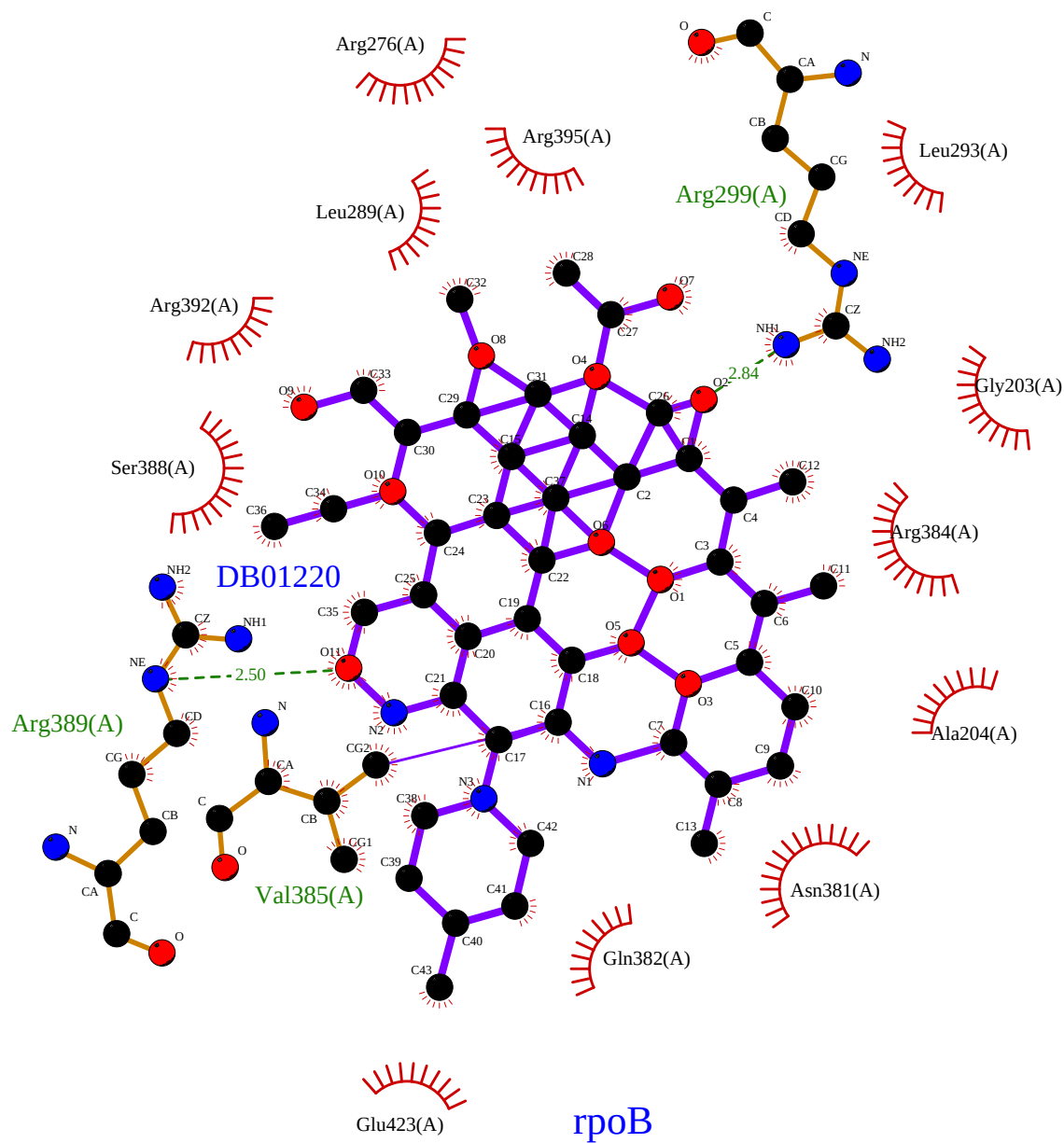
(iv) Interaction pattern of narH with DB07349



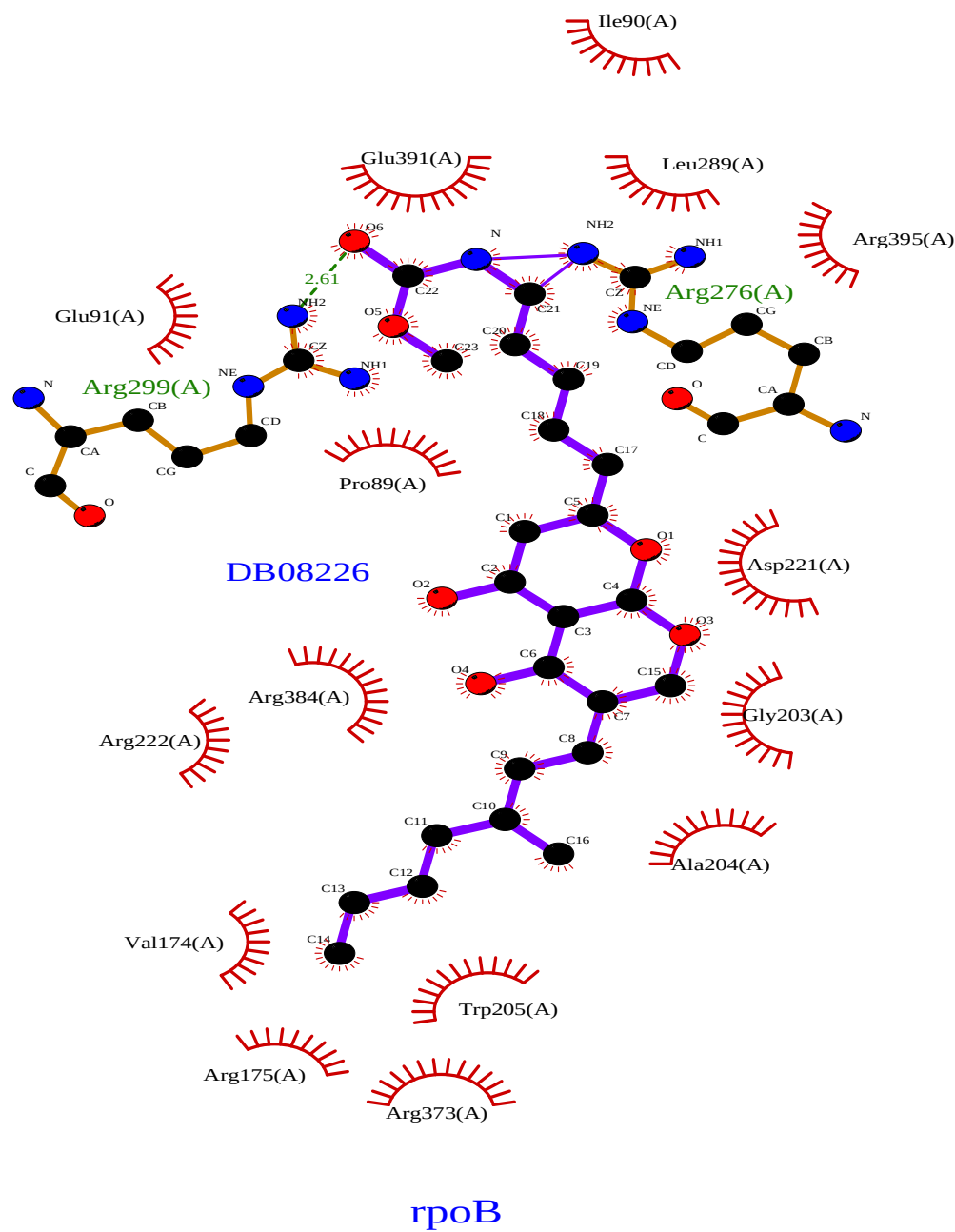
(v) Interaction pattern of rpoB with DB00615



(vi) Interaction pattern of rpoB with DB01220



(vii) Interaction pattern of rpoB with DB08226



(viii) Interaction pattern of rpoB and DB08266

