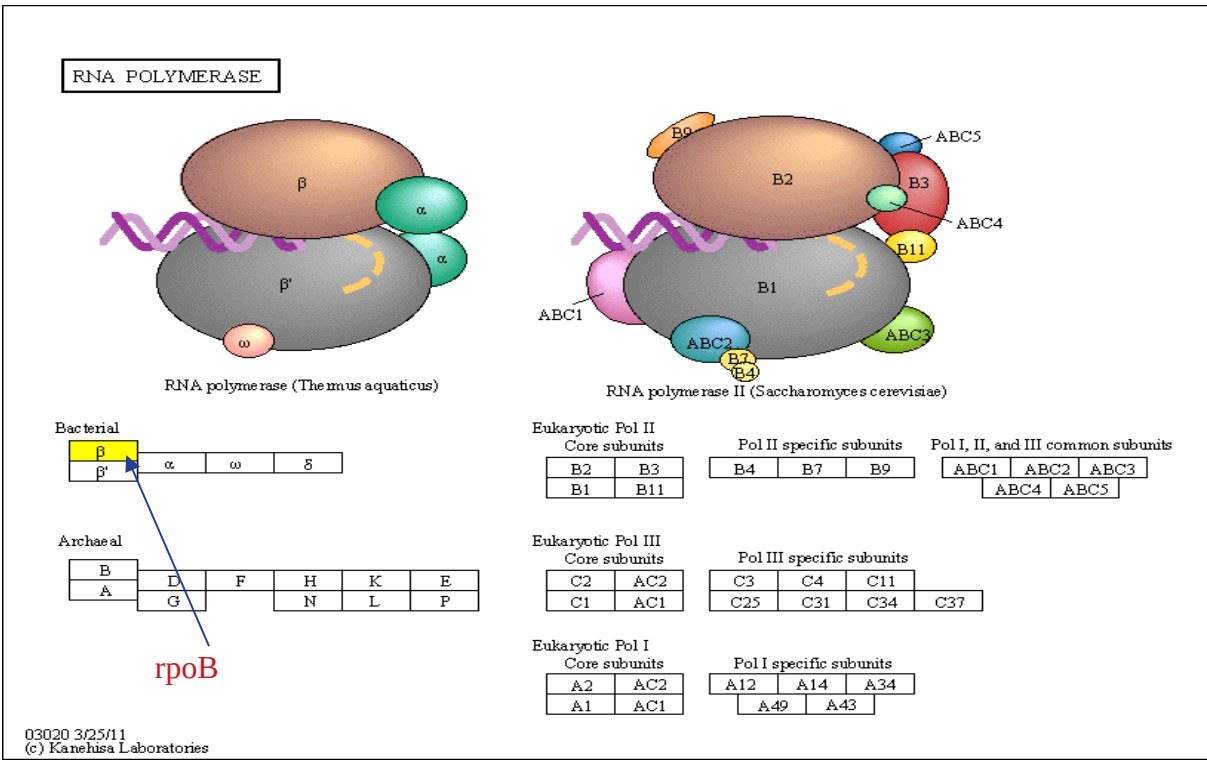


**Figure E6.1.** Mapping of non-homologous interacting partners of MAP mimicry proteins (nHIPMMP) on the MAP metabolic pathway (source KEGG). KEGG ID is in parenthesis.

**(1) MAP protein: P42384**

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

**(i) RNA polymerase (mpa03020)**



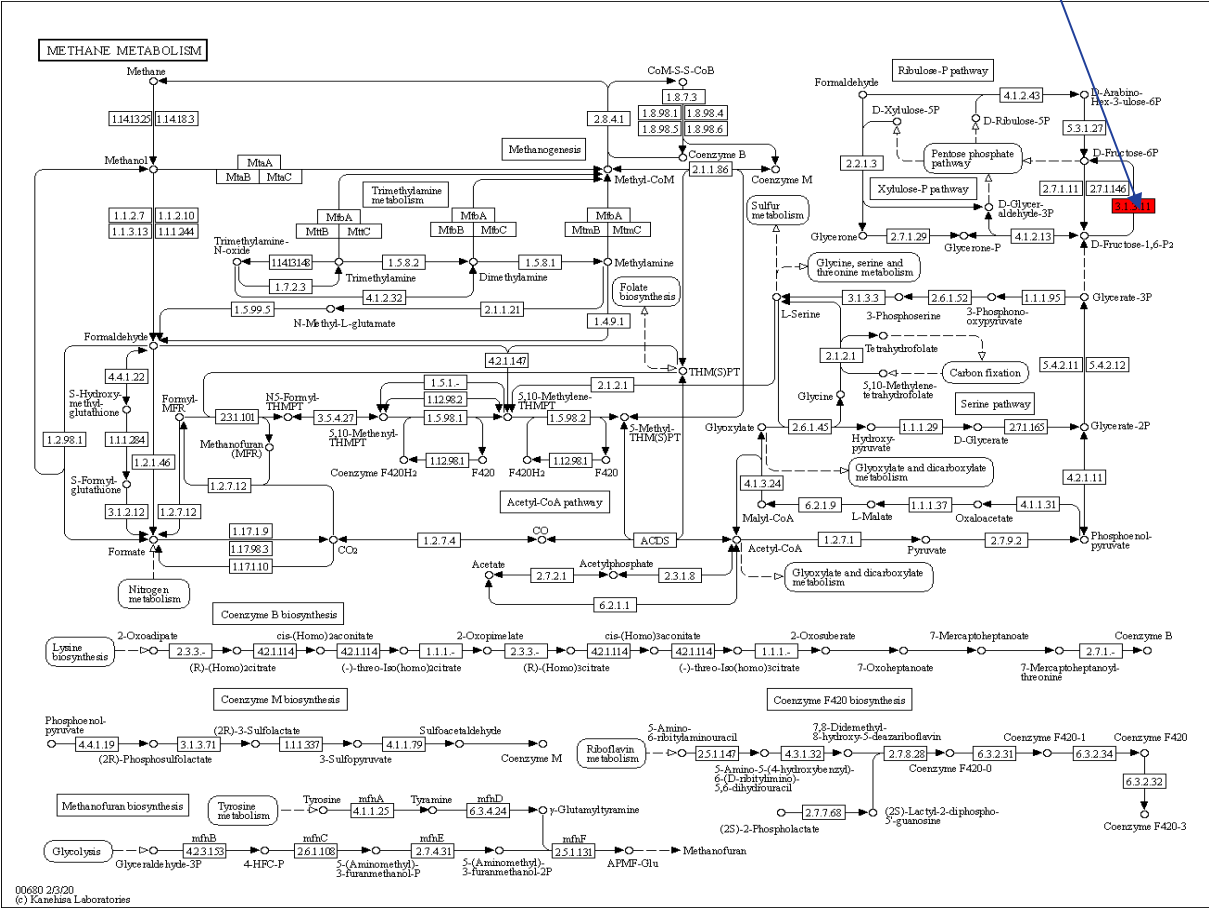
**KEGG mapped protein: rpoB**

(2) MAP protein: Q73WG6

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

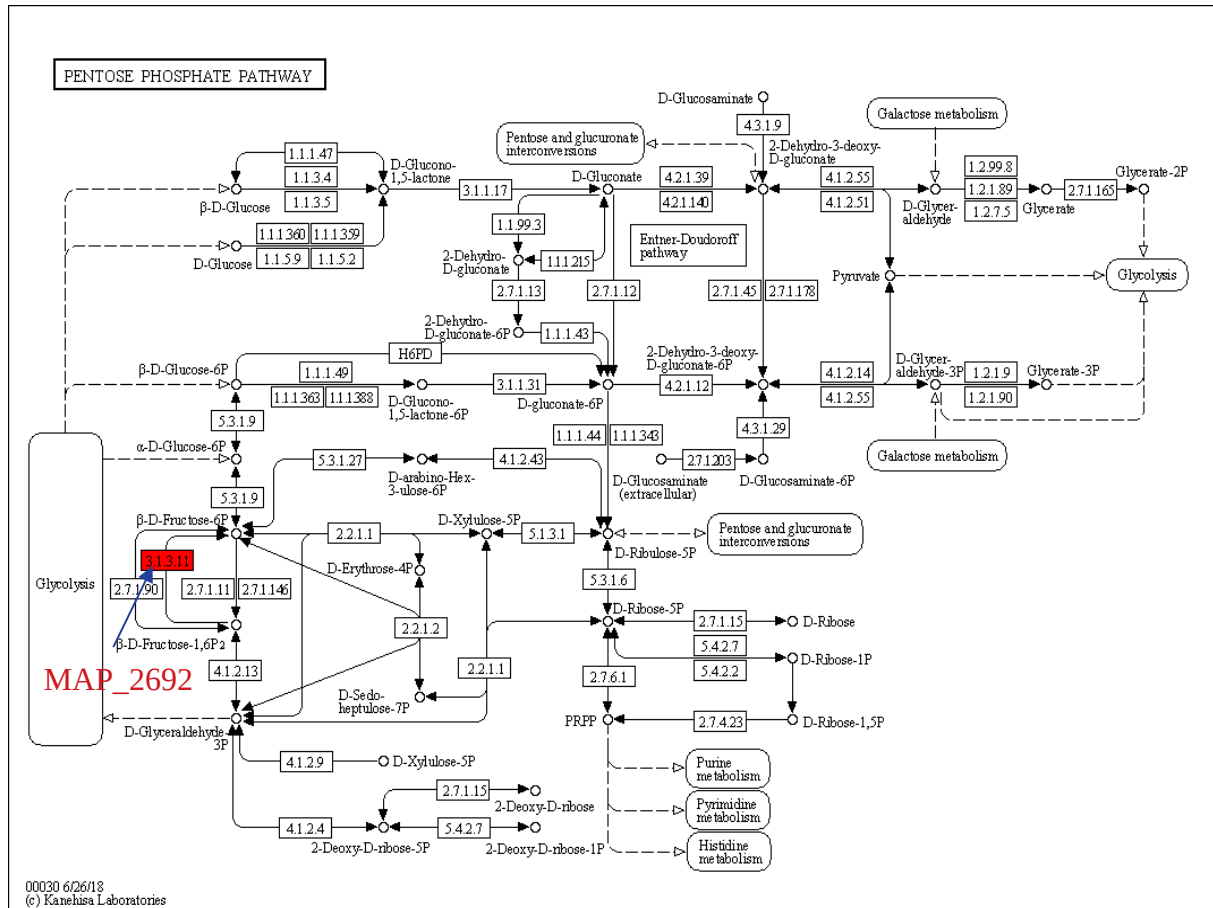
(i) Methane metabolism (mpa00680)

MAP\_2692



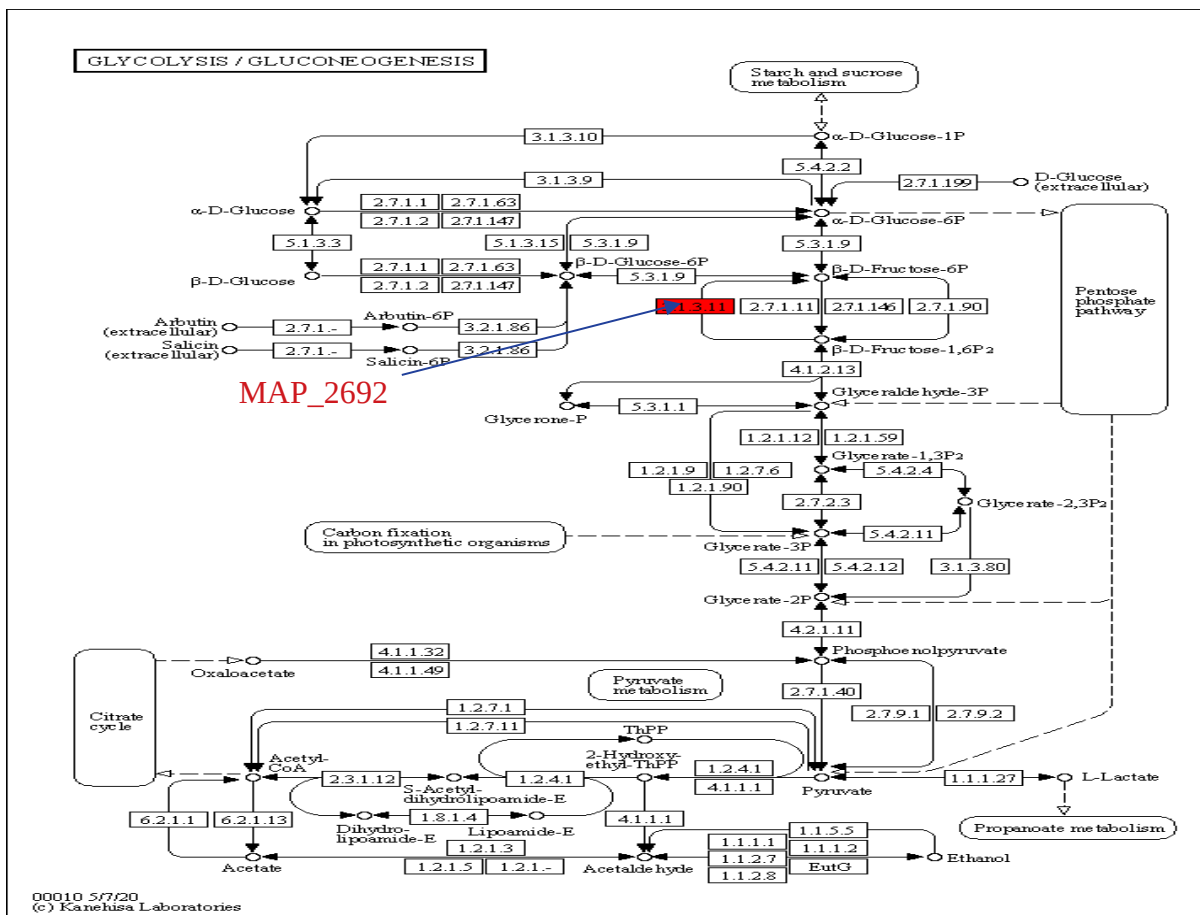
KEGG mapped protein: MAP\_2692

**(ii) Pentose phosphate pathway (mpa00030)**



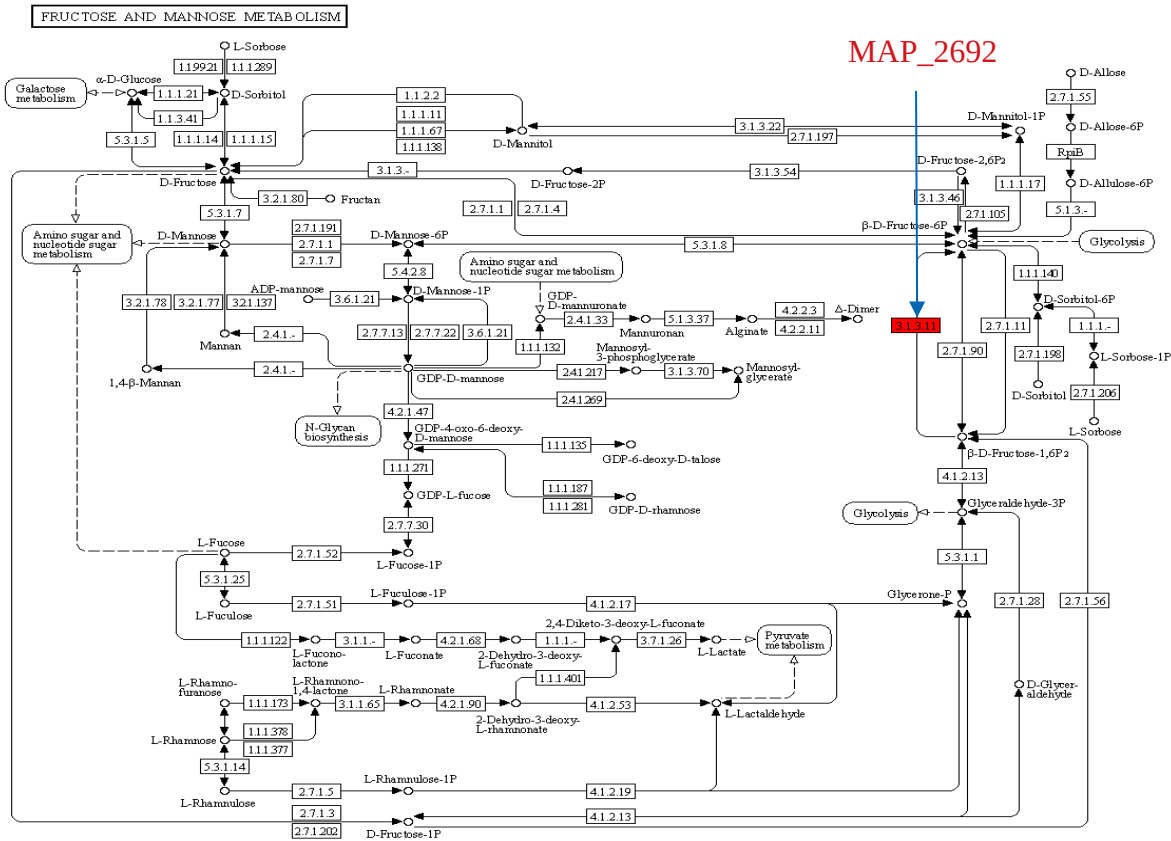
**KEGG mapped protein: MAP\_2692**

**(iii) Glycolysis / Gluconeogenesis (mpa00010)**



**KEGG mapped protein: MAP\_2692**

**(iv) Fructose and mannose metabolism (mpa00051)**

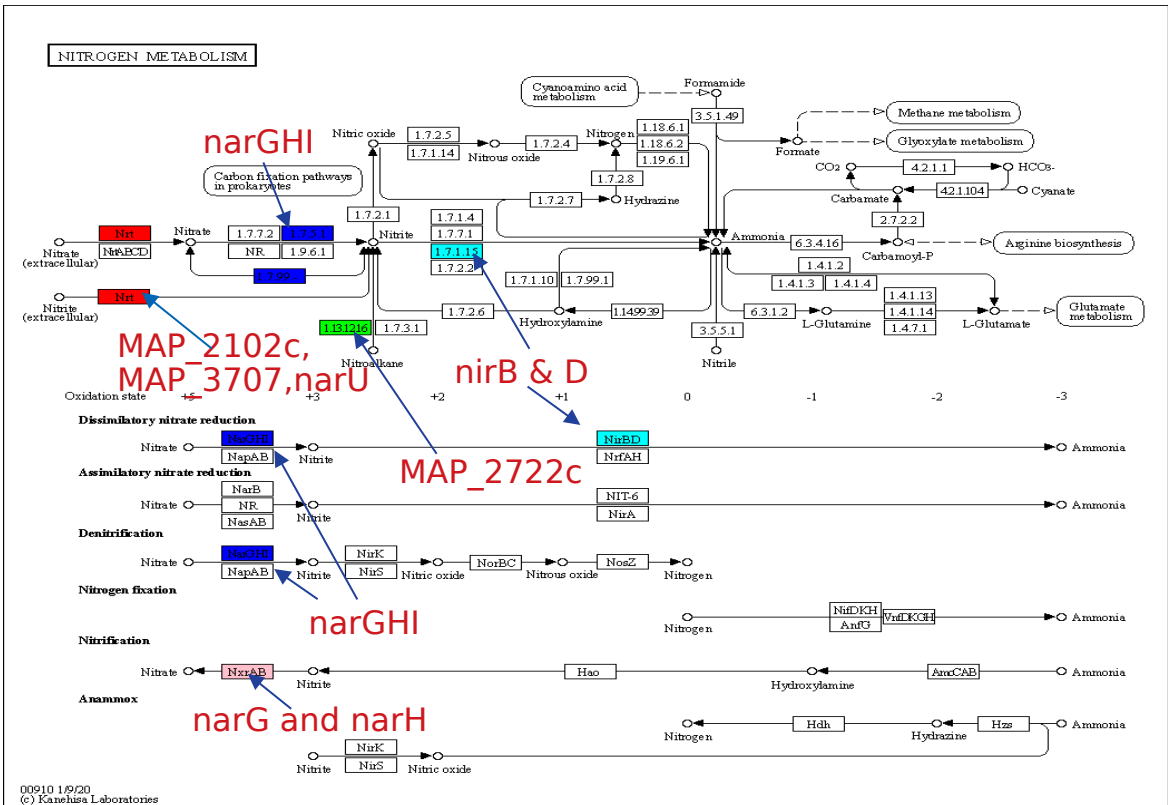


**KEGG mapped protein: MAP\_2692**

### (3) MAP protein: Q73WP1

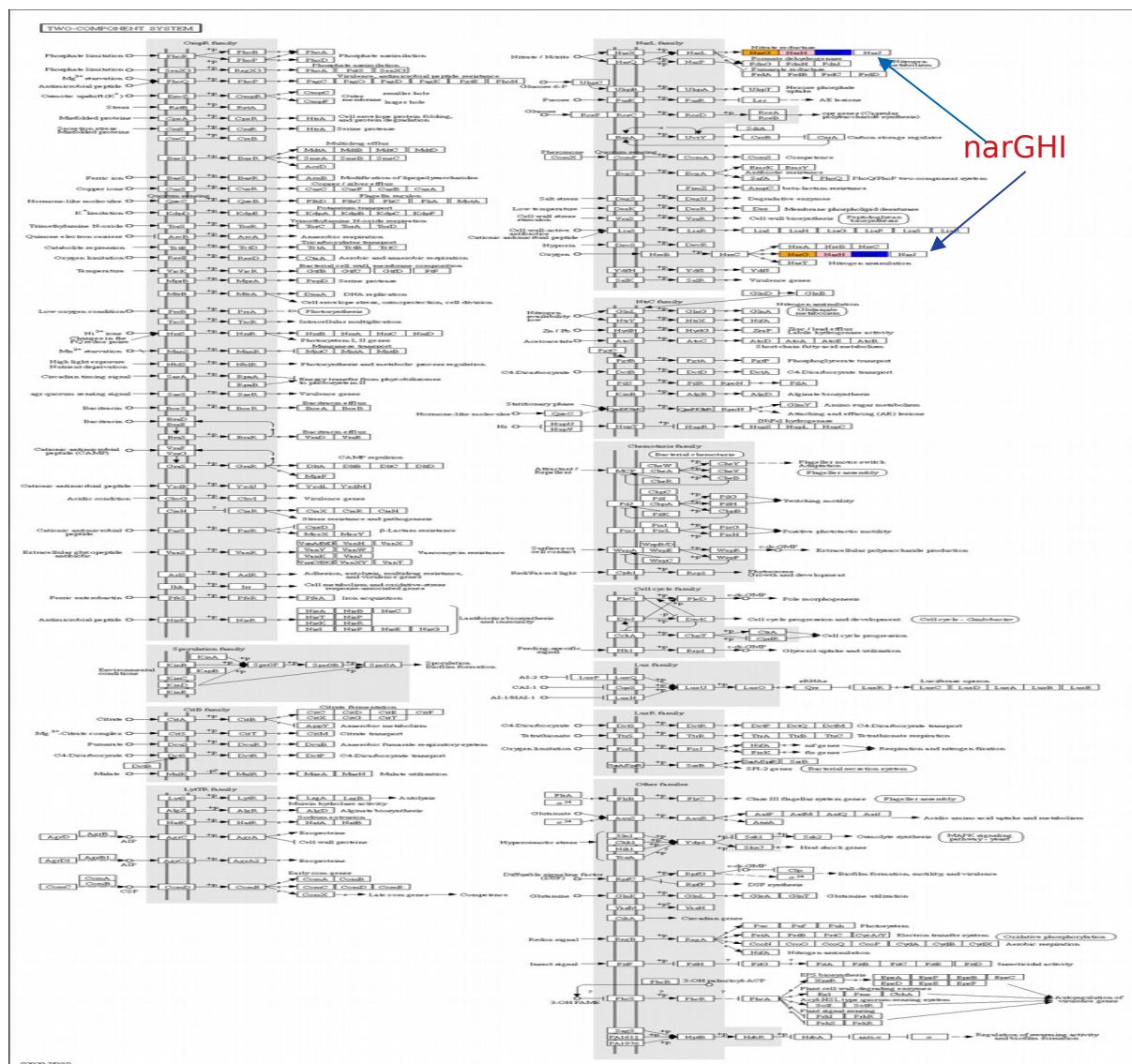
S. No.	nHIPMMP	Color code
1.	MAP_2102c	Red
2.	MAP_2722c	Green
3.	MAP_3707c	Yellow
4.	narG	Orange
5.	narH	Pink
6.	narI	Blue
7.	narJ	Teal
8.	narU	Voilet
9.	nirB	cyan
10.	nirD	Grey

### (i) Nitrogen metabolism (mpa00910)



KEGG mapped protein: MAP\_2102c, MAP\_2722c, MAP\_3707c, narG, narH, narI, narU, nirB, nirD

## (ii) Two-component system (mpa02020)

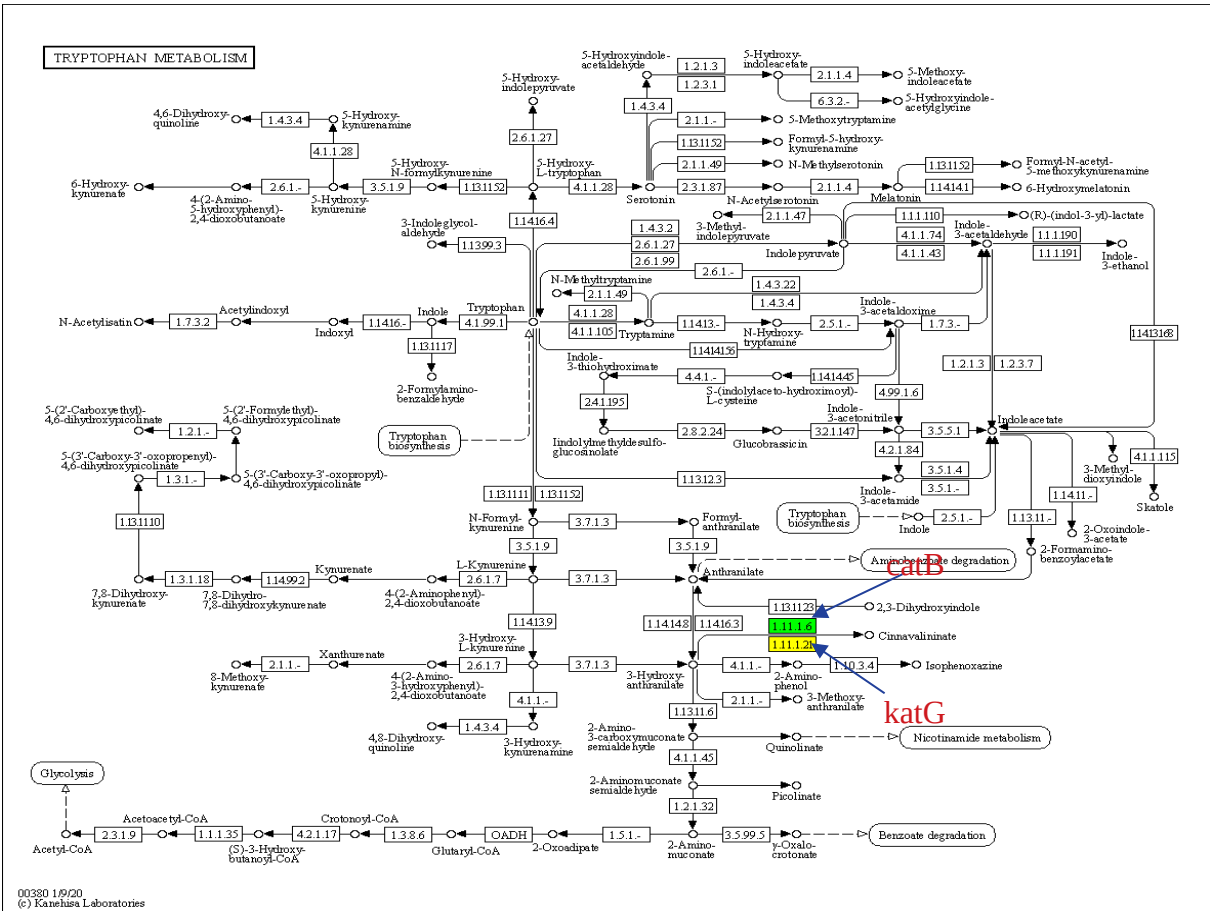


KEGG mapped protein: narG, narH, narI

(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

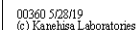
(i) Tryptophan metabolism (mpa00380)



KEGG mapped protein: catB, katG

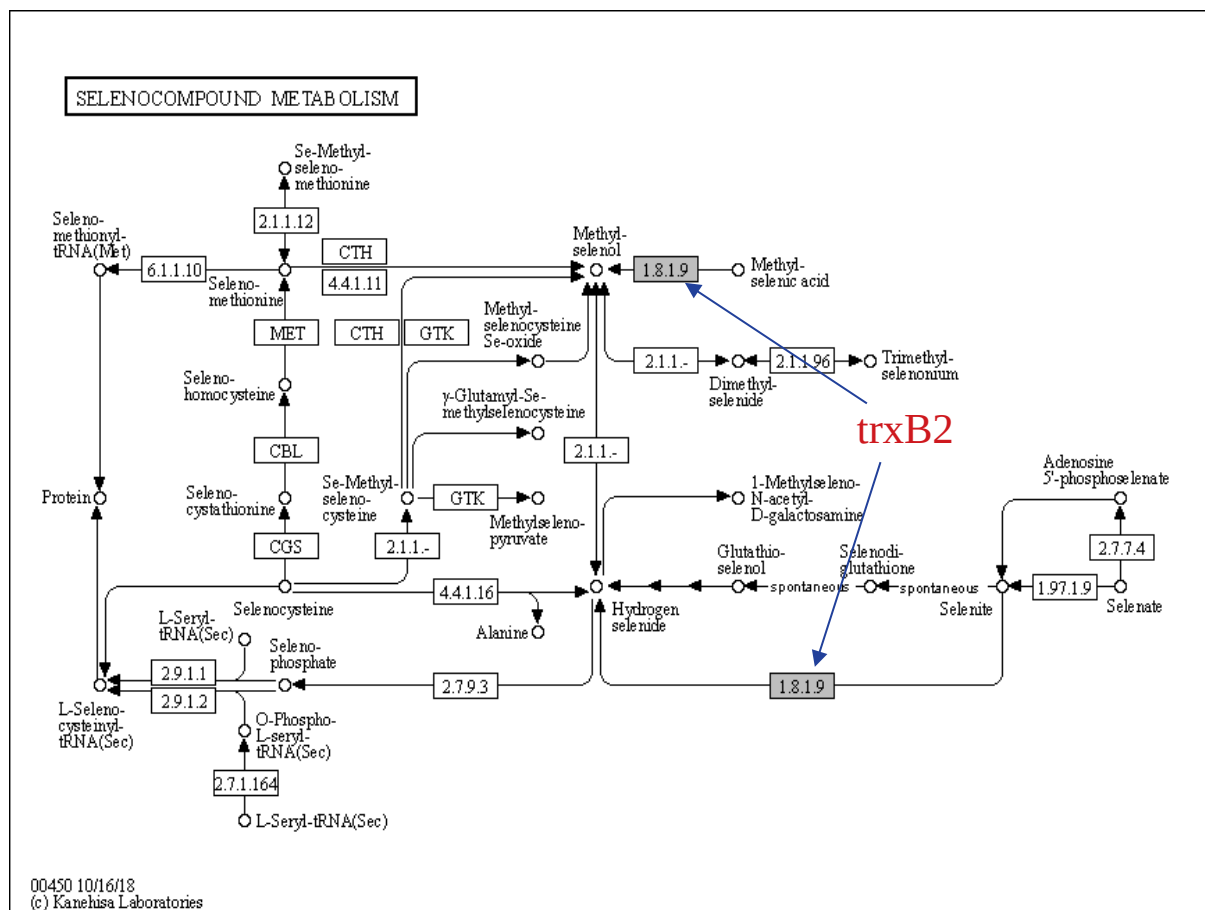


**(ii) Phenylalanine metabolism (mpa00360)**



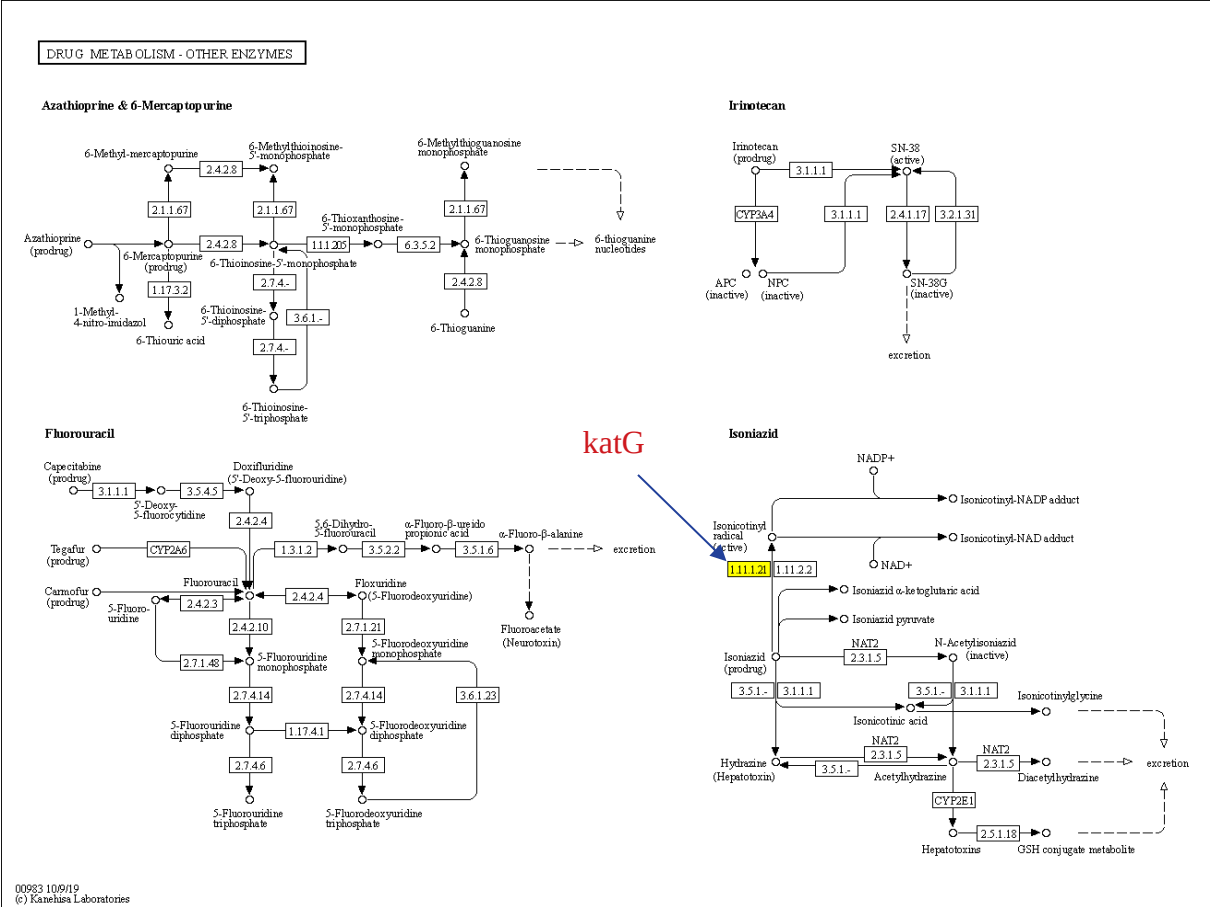
**KEGG mapped protein: katG**

**(iii) Selenocompound metabolism (mpa00450 )**



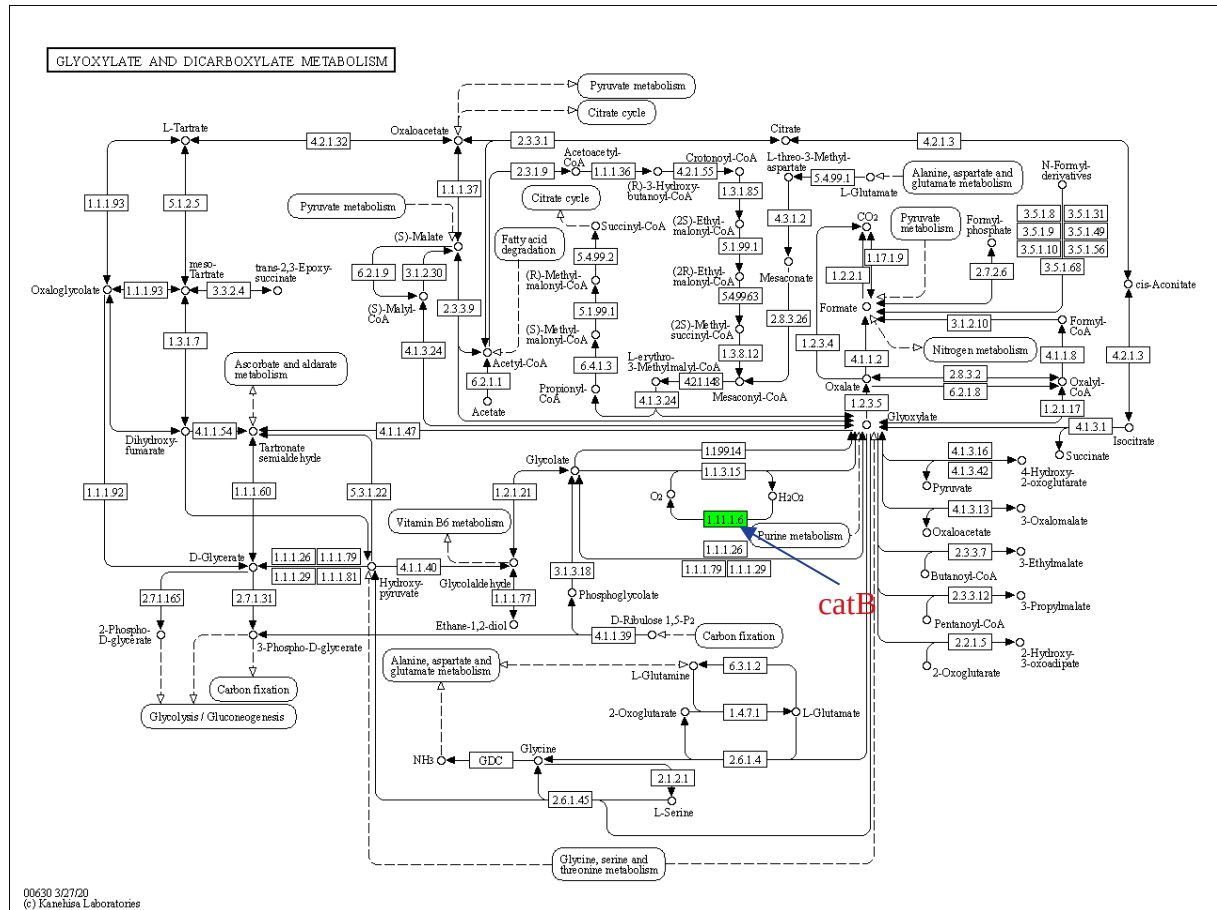
**KEGG mapped protein: taxB2**

**(iv) Drug metabolism - other enzymes (mpa00983)**



**KEGG mapped protein: katG**

## (v) Glyoxylate and dicarboxylate metabolism (mpa00630)

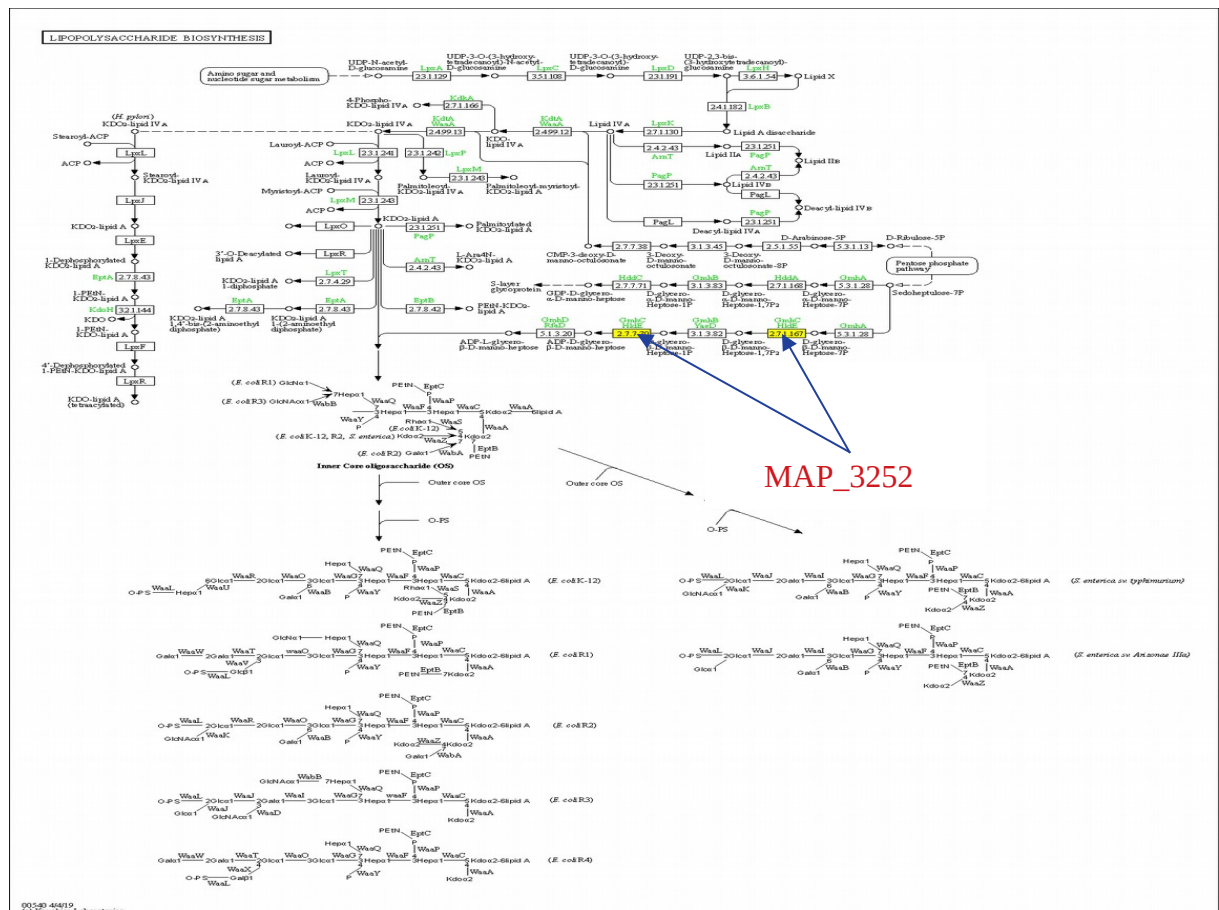


**KEGG mapped protein: catB**

## (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)

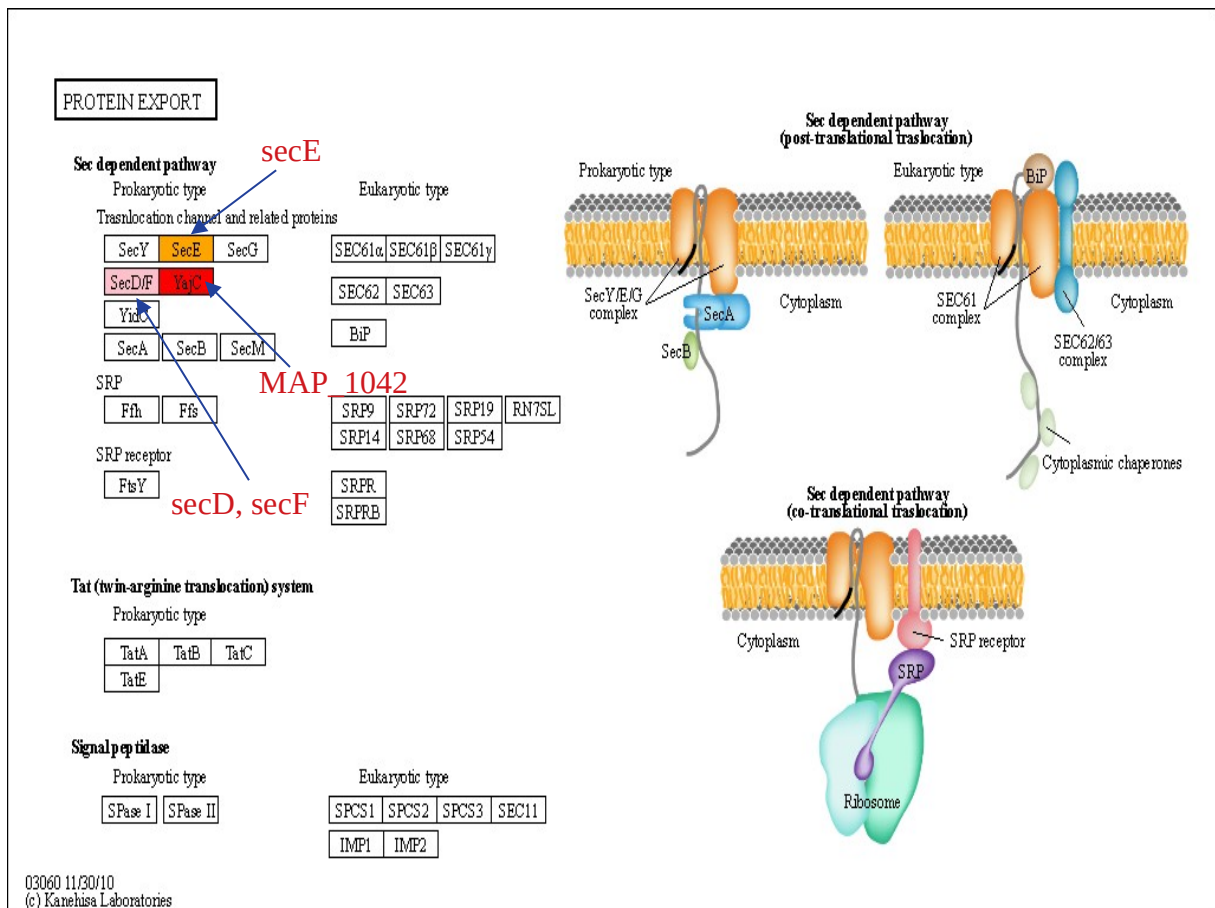


### KEGG mapped protein: MAP\_3252

## (6) MAP protein: Q741P6

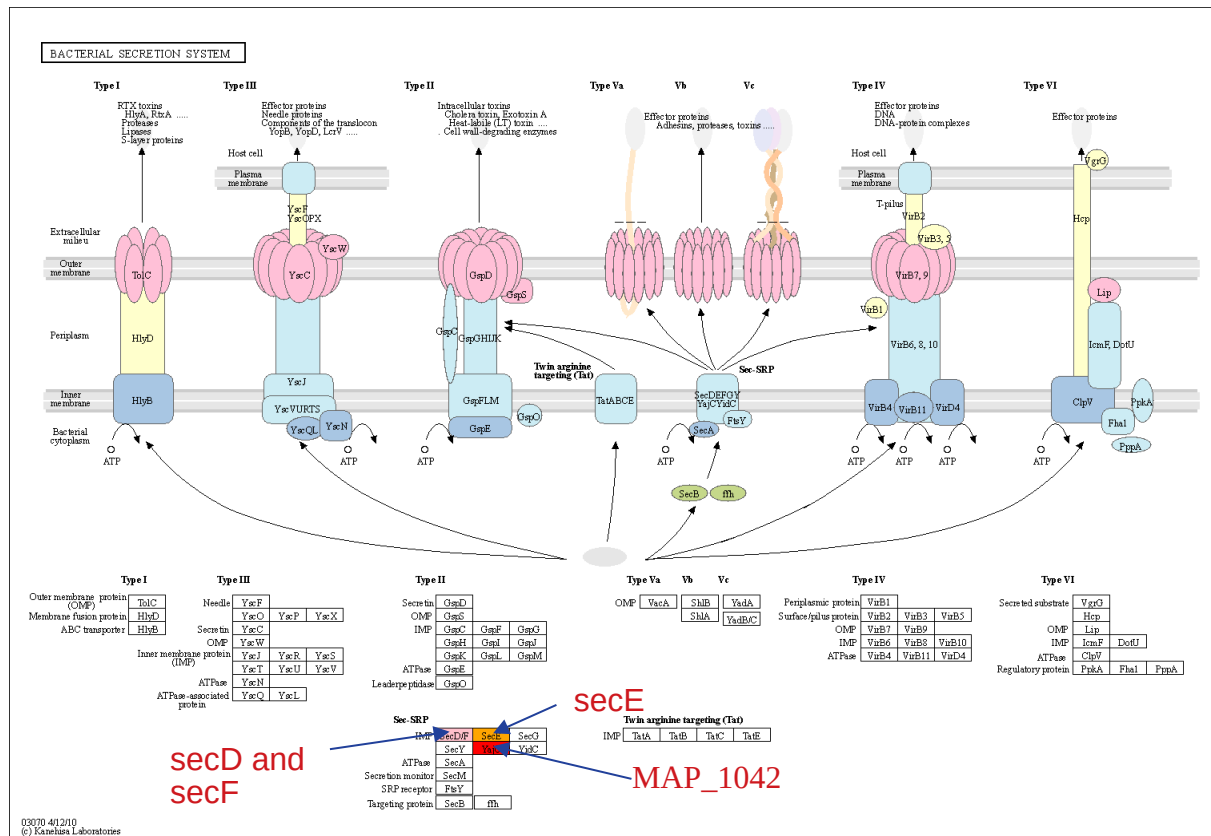
S. No.	nHIPMMP	Color code
1.	MAP_1042	Red
2.	MAP_1045	Green
3.	relA	Yellow
4.	secD	Pink
5.	secE	Orange
6.	secF	Grey
7.	secY	Voilet
8.	yidC	Blue

### (i) Protein export (mpa03060)



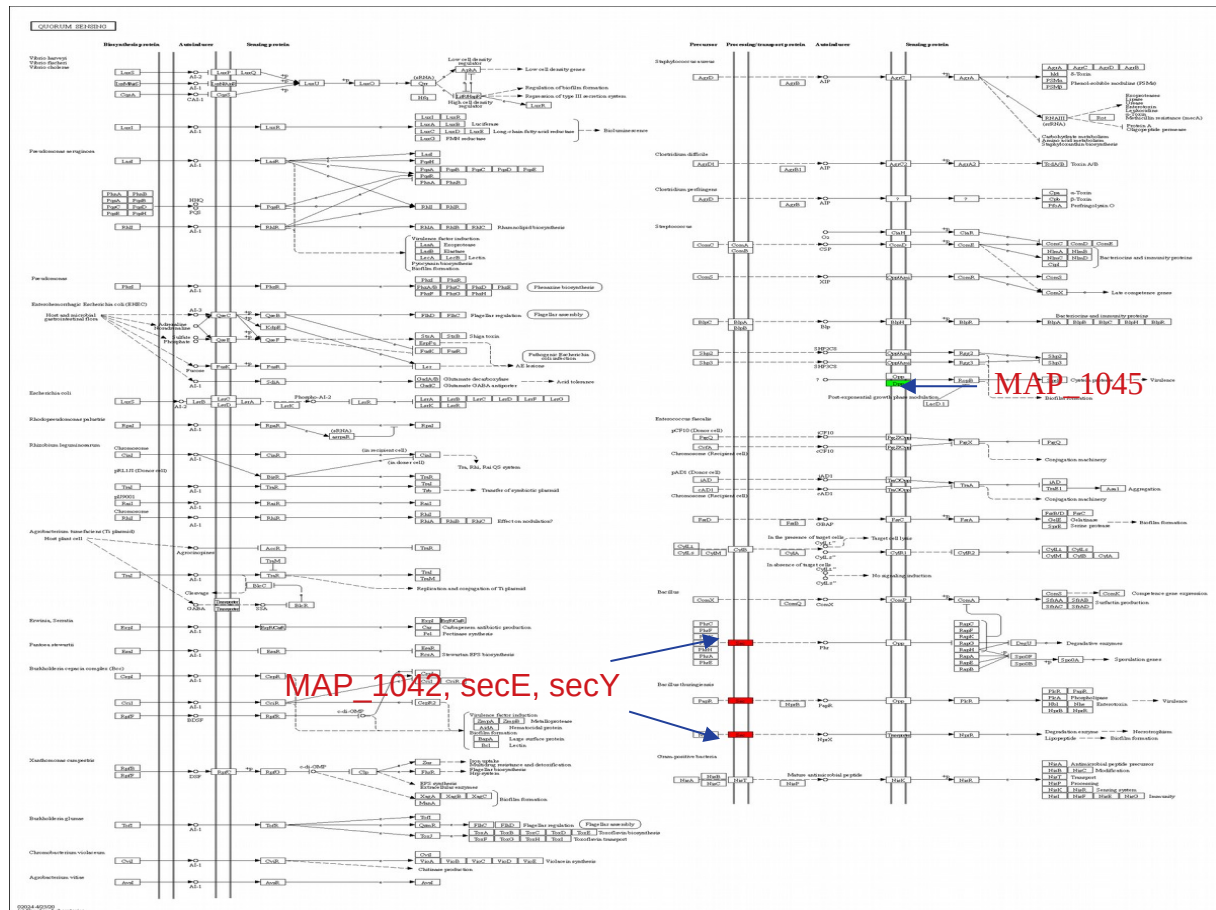
**KEGG mapped protein:** secD, secE, secF, MAP\_1042

## (ii) Bacterial secretion system (mpa03070)



KEGG mapped protein: secD, secE, secF, MAP\_1042

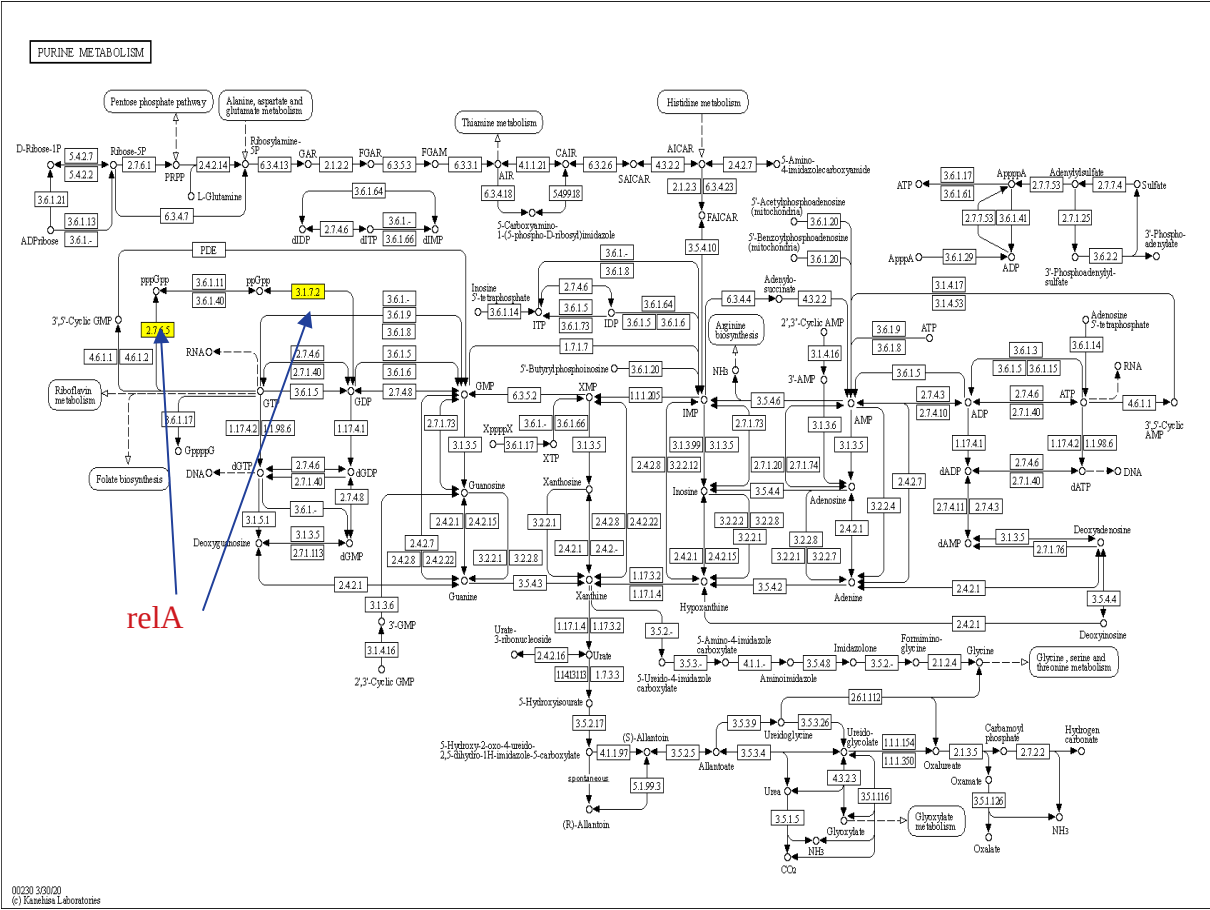
**(iii) Quorum sensing (mpa02024)**



**KEGG mapped protein:** secE, secY, MAP\_1045, MAP\_1042



**(iv) Purine metabolism (mpa00230)**

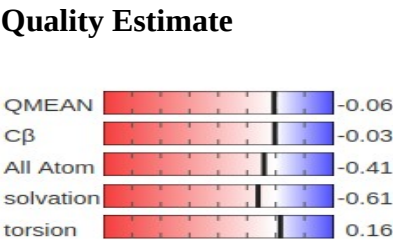


**KEGG mapped protein: relA**

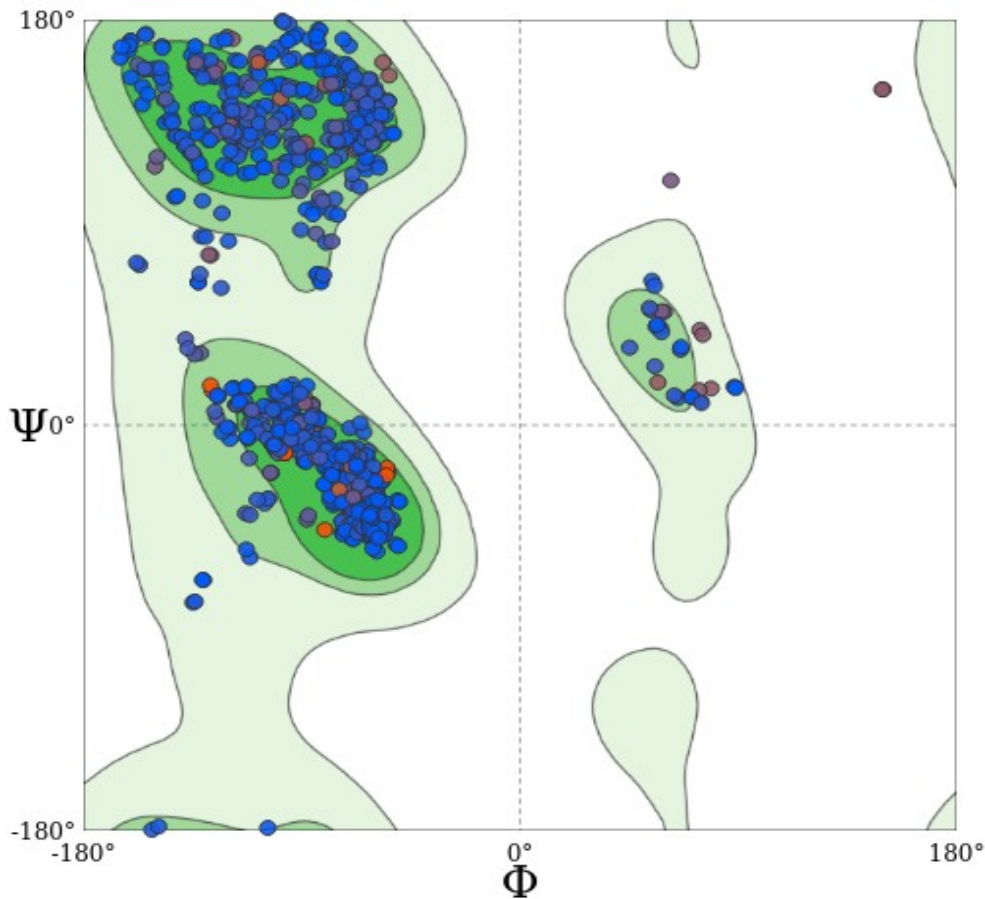
**Figure E6.2.** Quality assessment of katG, narH and rpoB modeled structure using Qualitative Model Energy Analysis (QMEAN) score, MolProbity score, and Ramachandran plot. The root-mean-square deviation (RMSD) between the 3D homology structure and template structure are also shown.

**(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

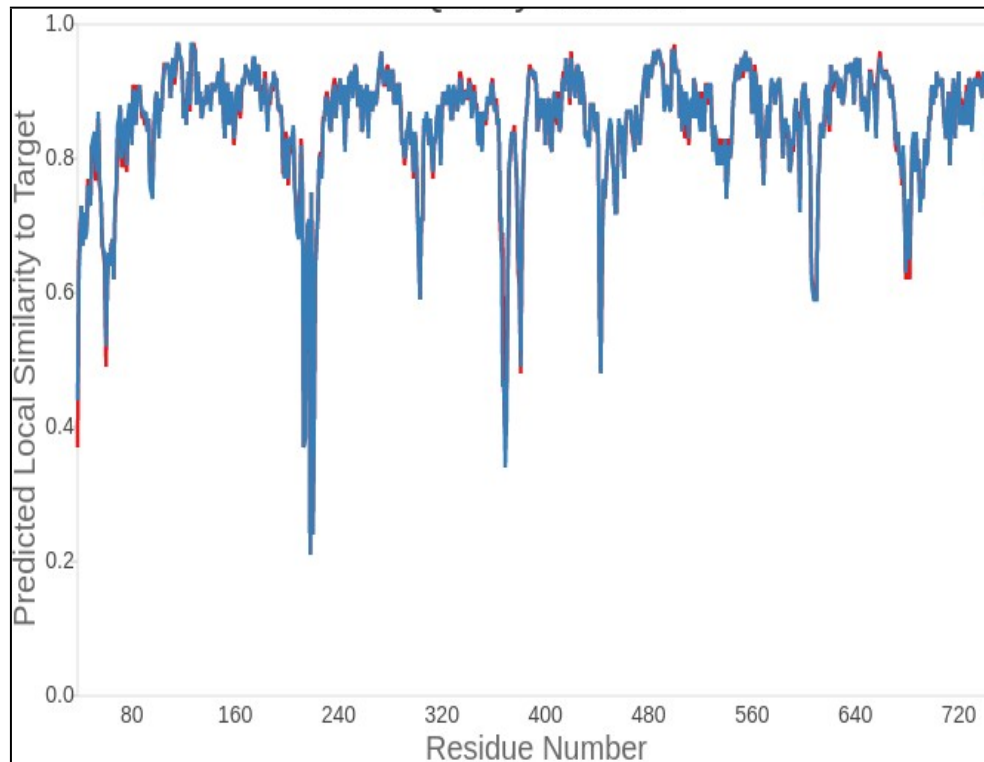


**Ramachandran plot of katG model structure**

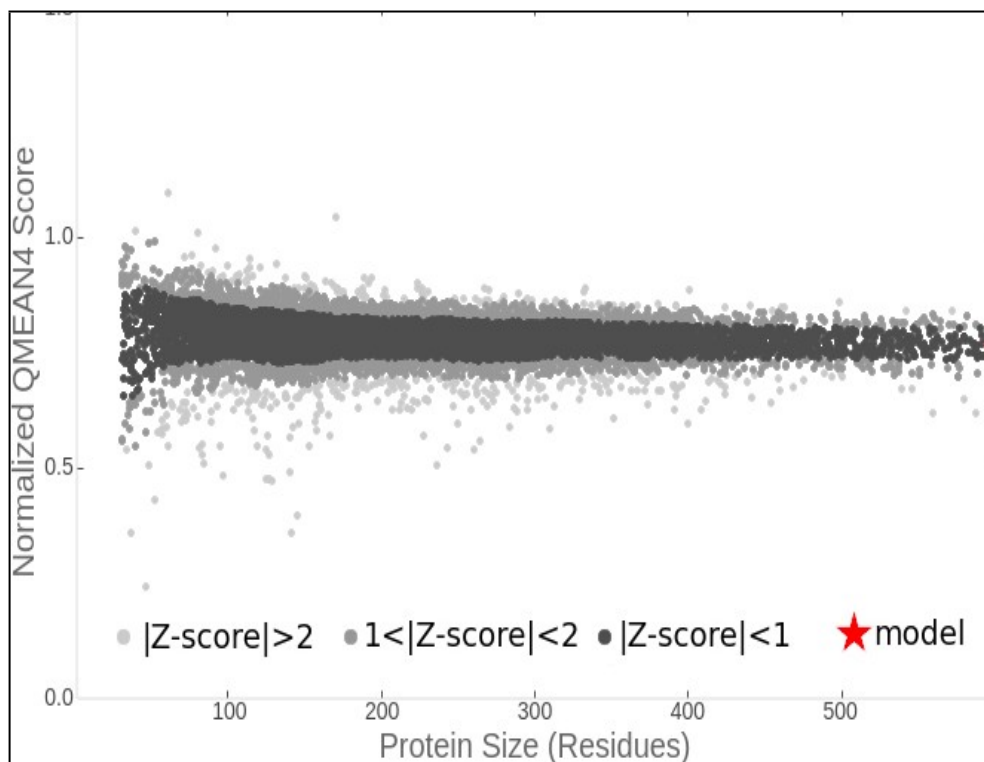


## Swiss-model structure assessment

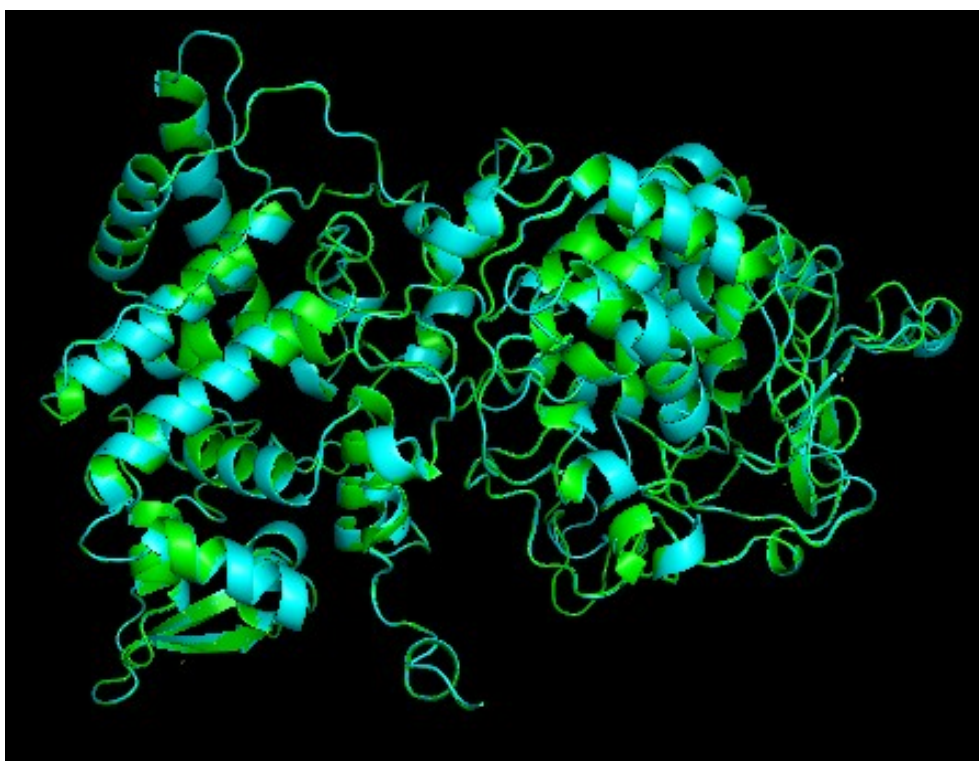
### (i) Local quality estimate of katG model structure



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



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



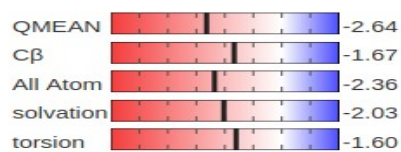
**RMSD value between katG and template: 0.118**

**Color code:** katG-Cyan & 5SXX-Green

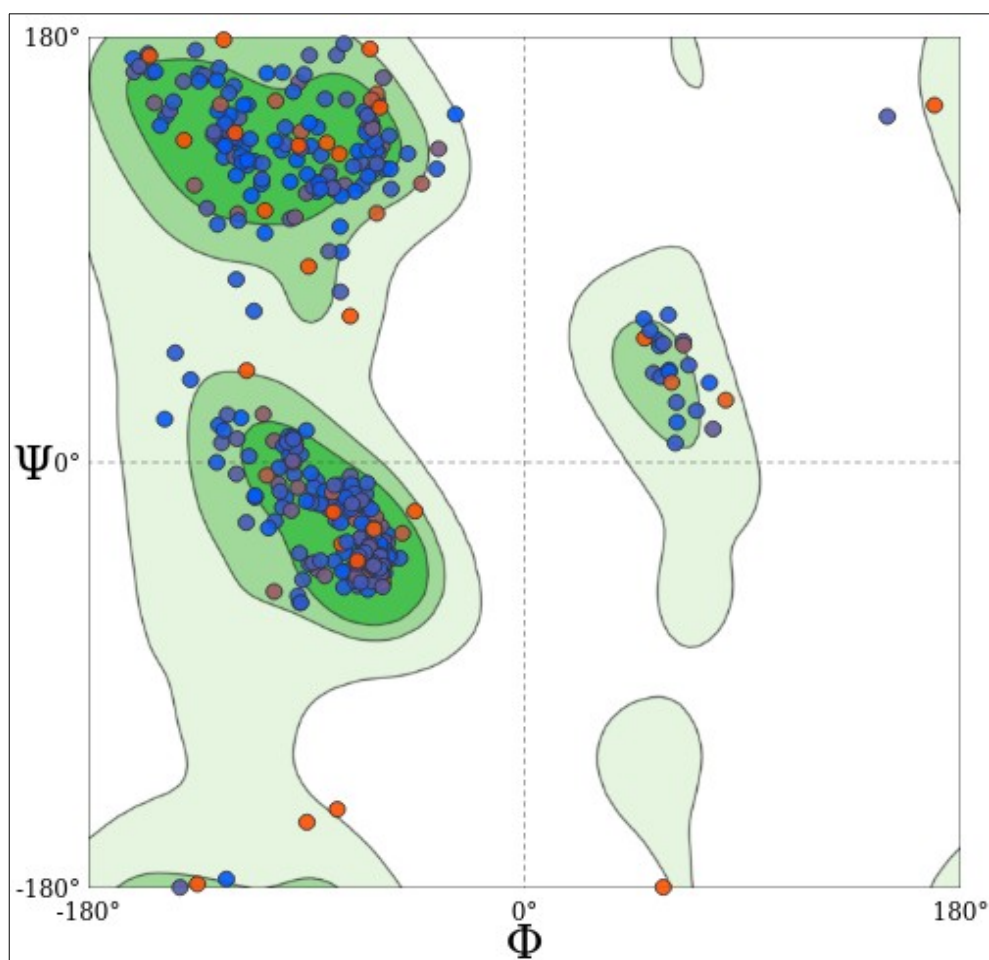
## (2) Target: narH

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

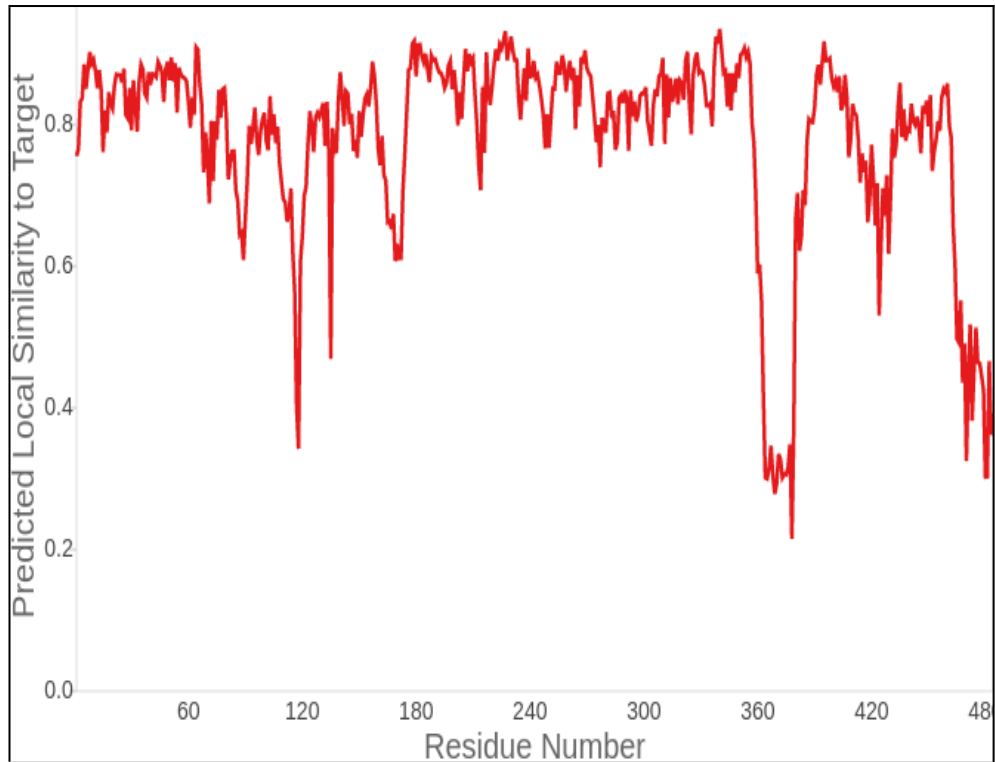


### Ramachandran plot of narH model structure

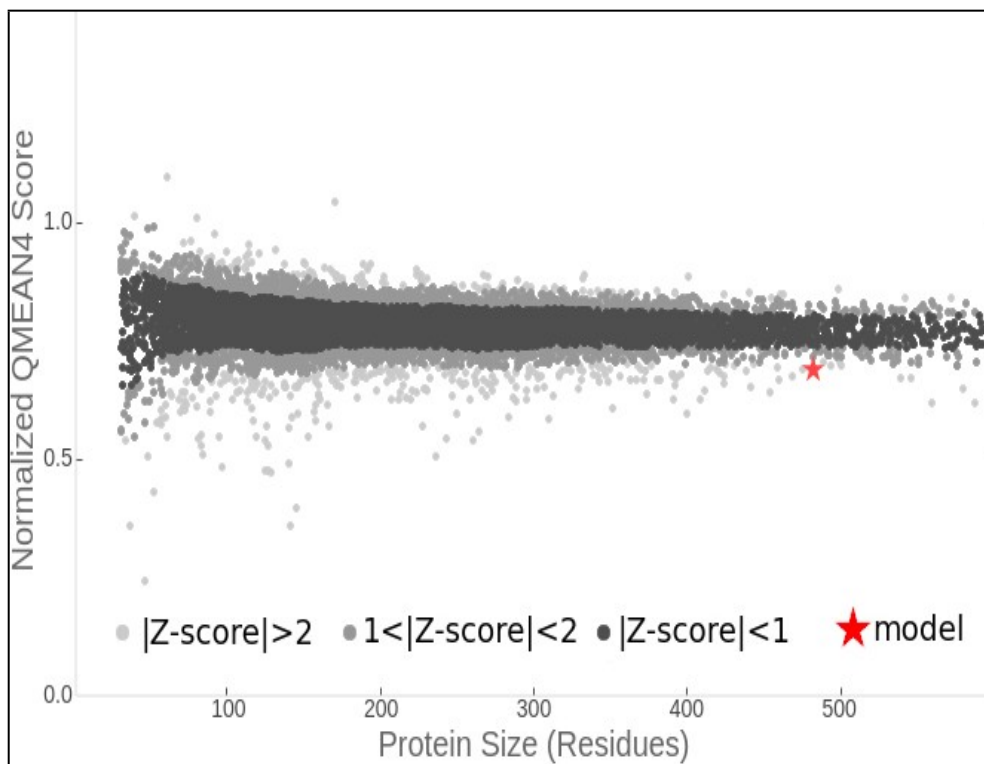


## Swiss-model structure assessment

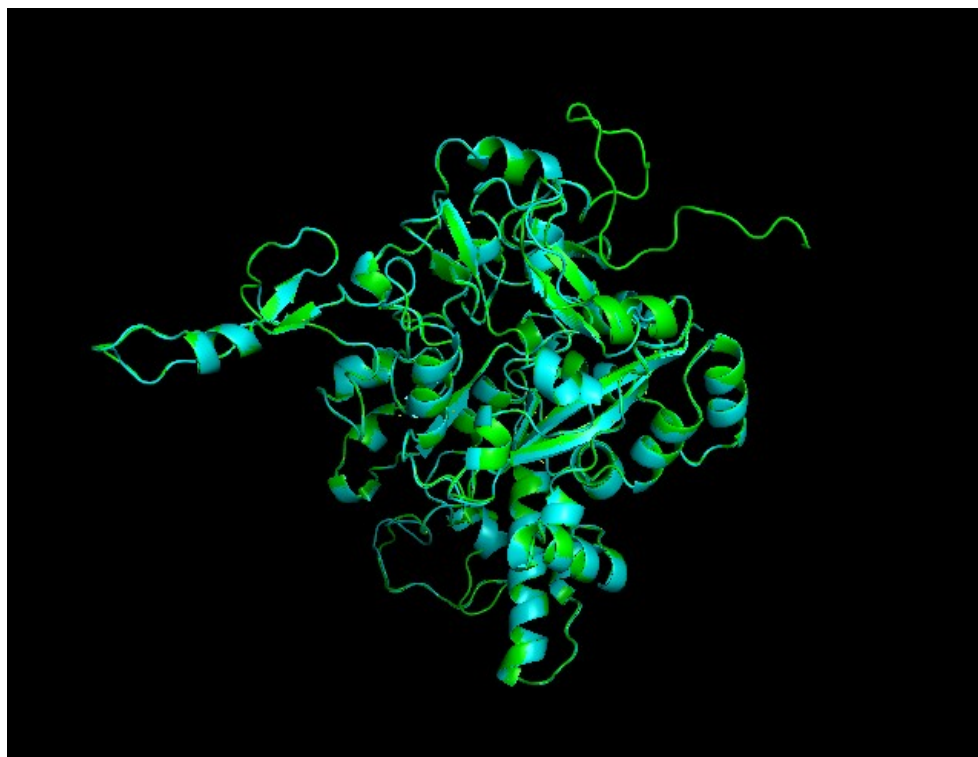
### (i) Local quality estimate of narH model structure



### (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**

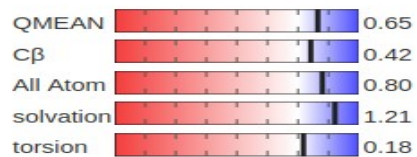
**Color code:-** narH-Cyan & 1Y5N-Green



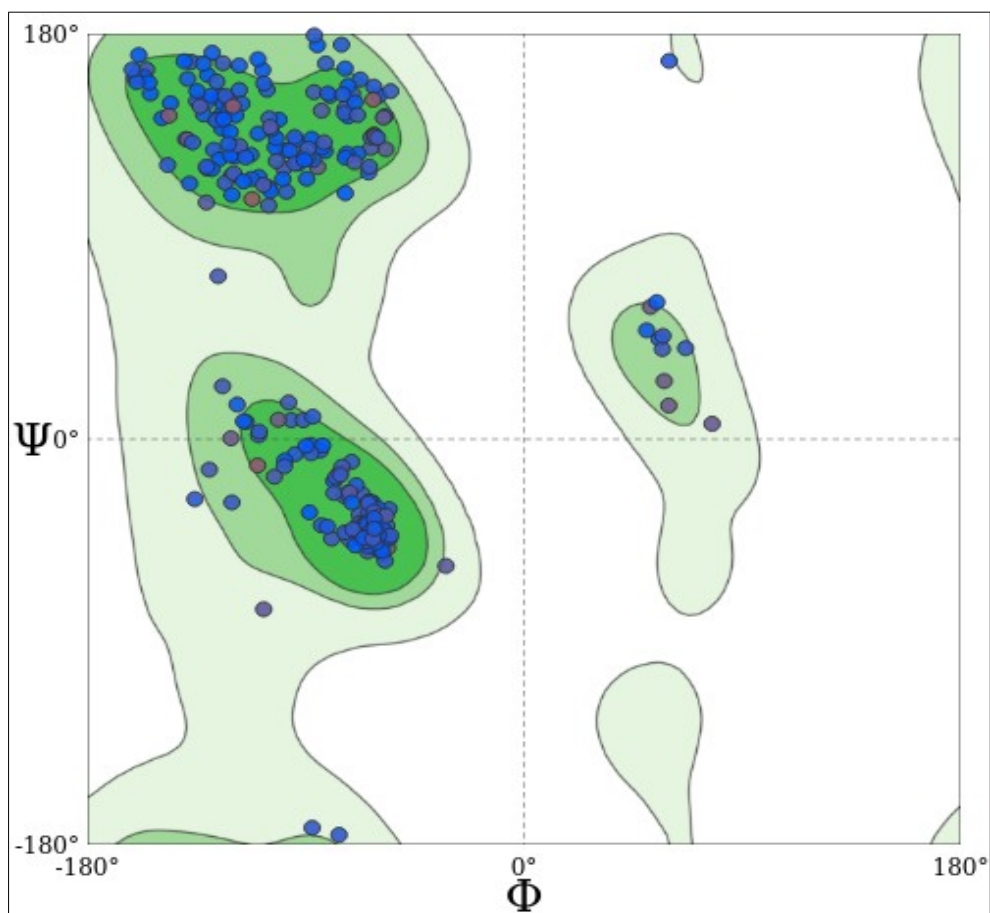
### (3) Target: rpoB

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



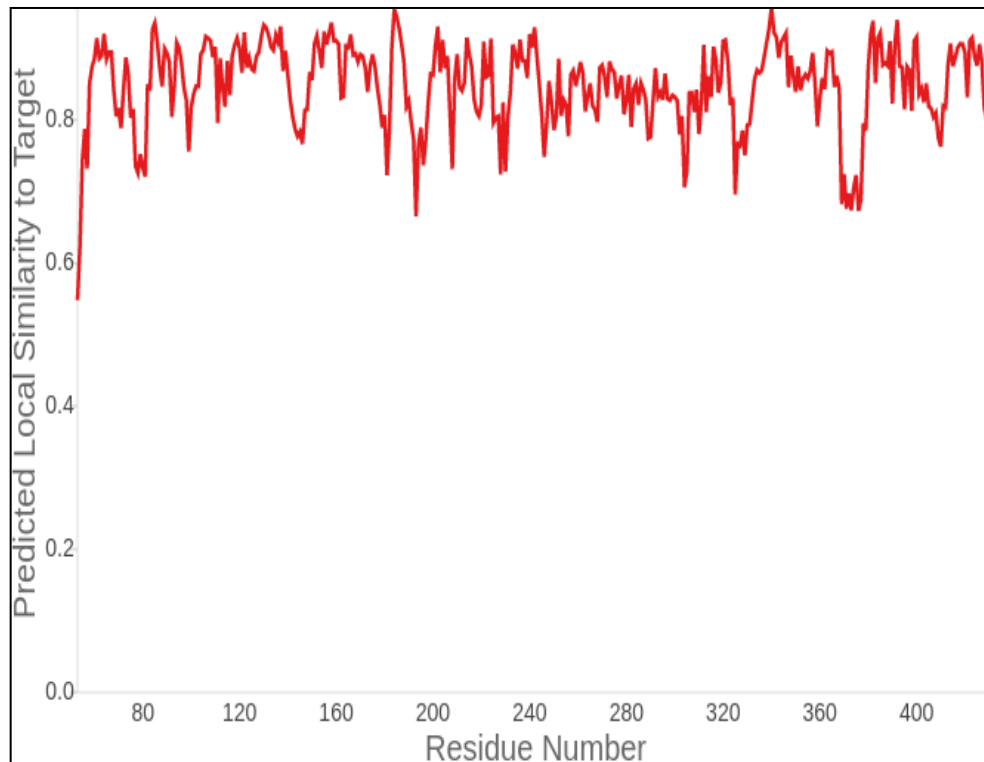
### Ramachandran plot of rpoB model structure



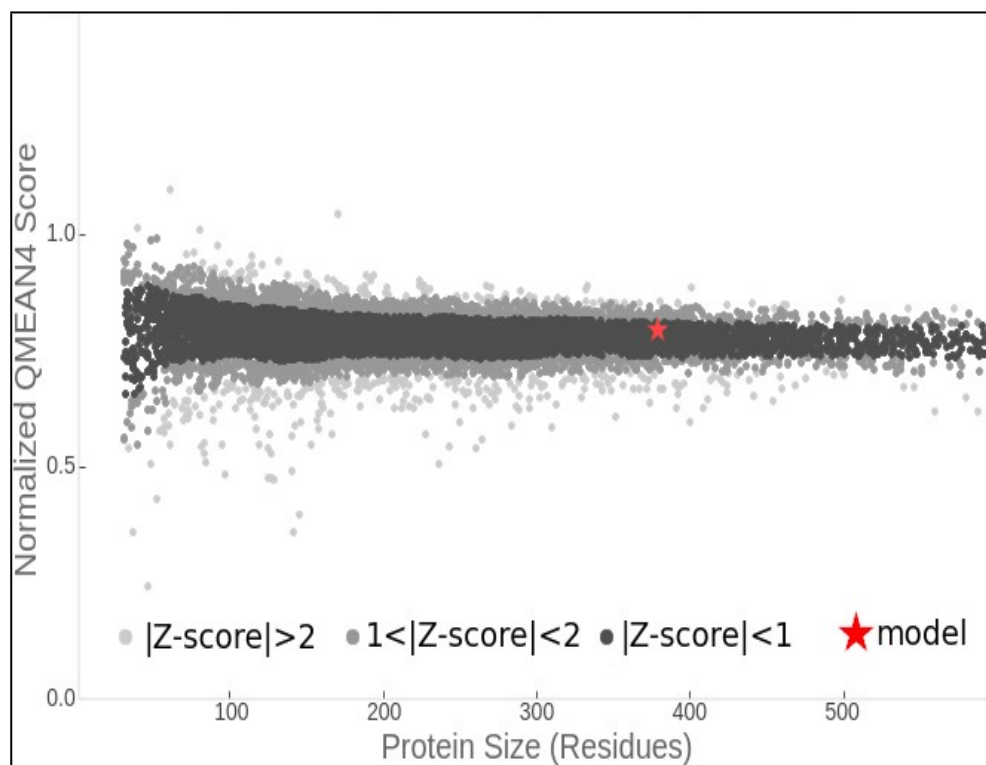


## Swiss-model structure assessment

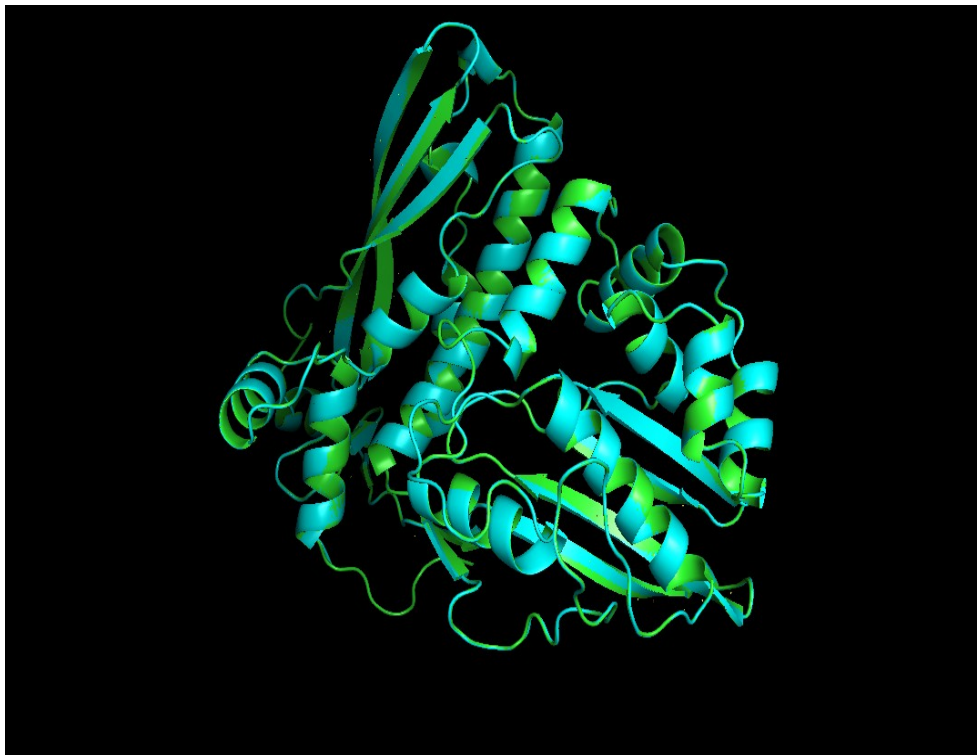
### (i) Local quality estimate of rpoB model structure



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



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

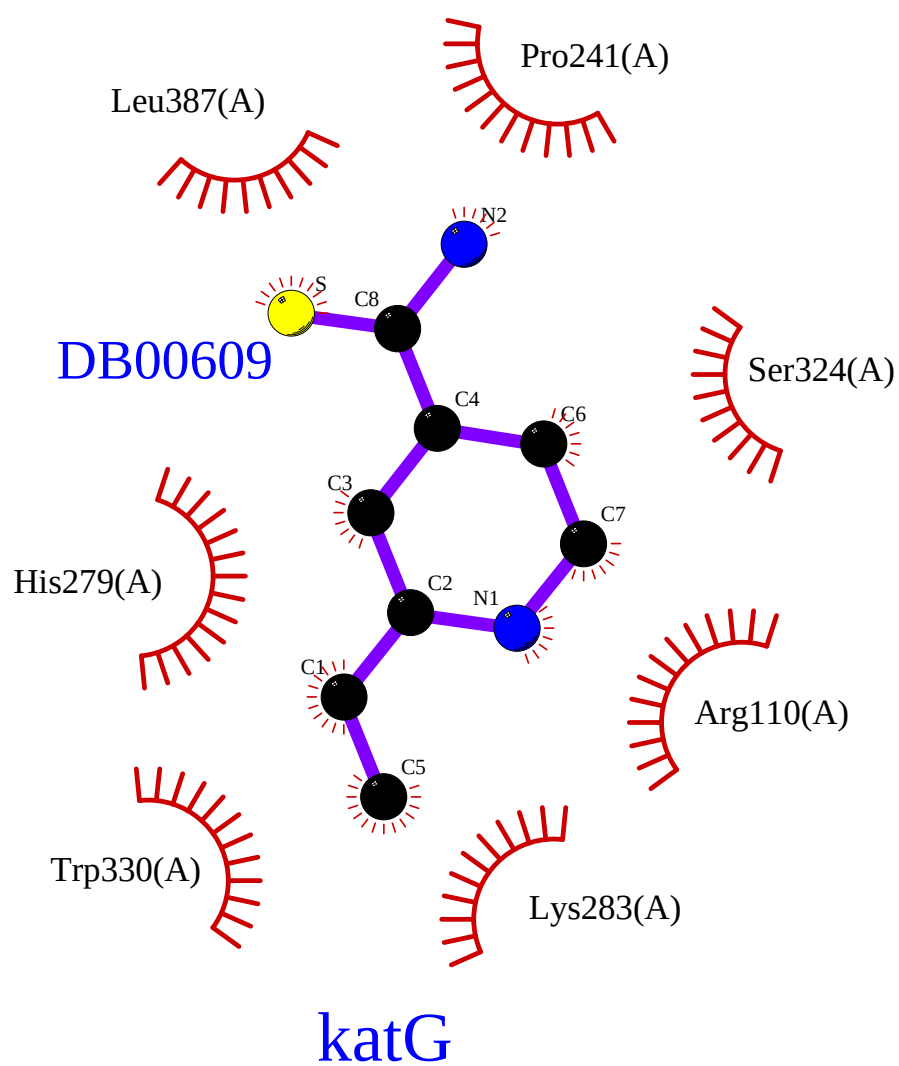


**RMSD value between rpoB and template: 0.051**

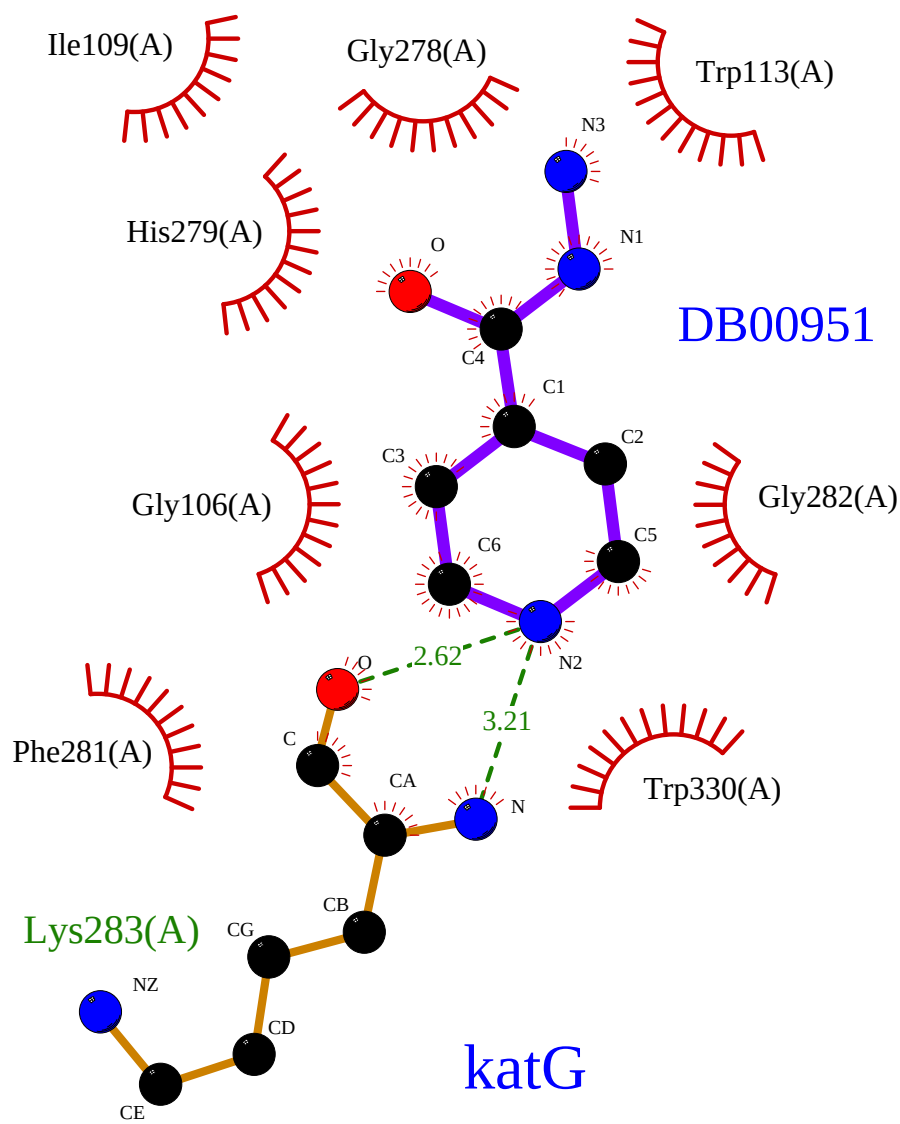
**Color code:** rpoB-Cyan & 4KBM-Green

Figure E6.3. The interaction pattern of the proposed drug with the target proteins.

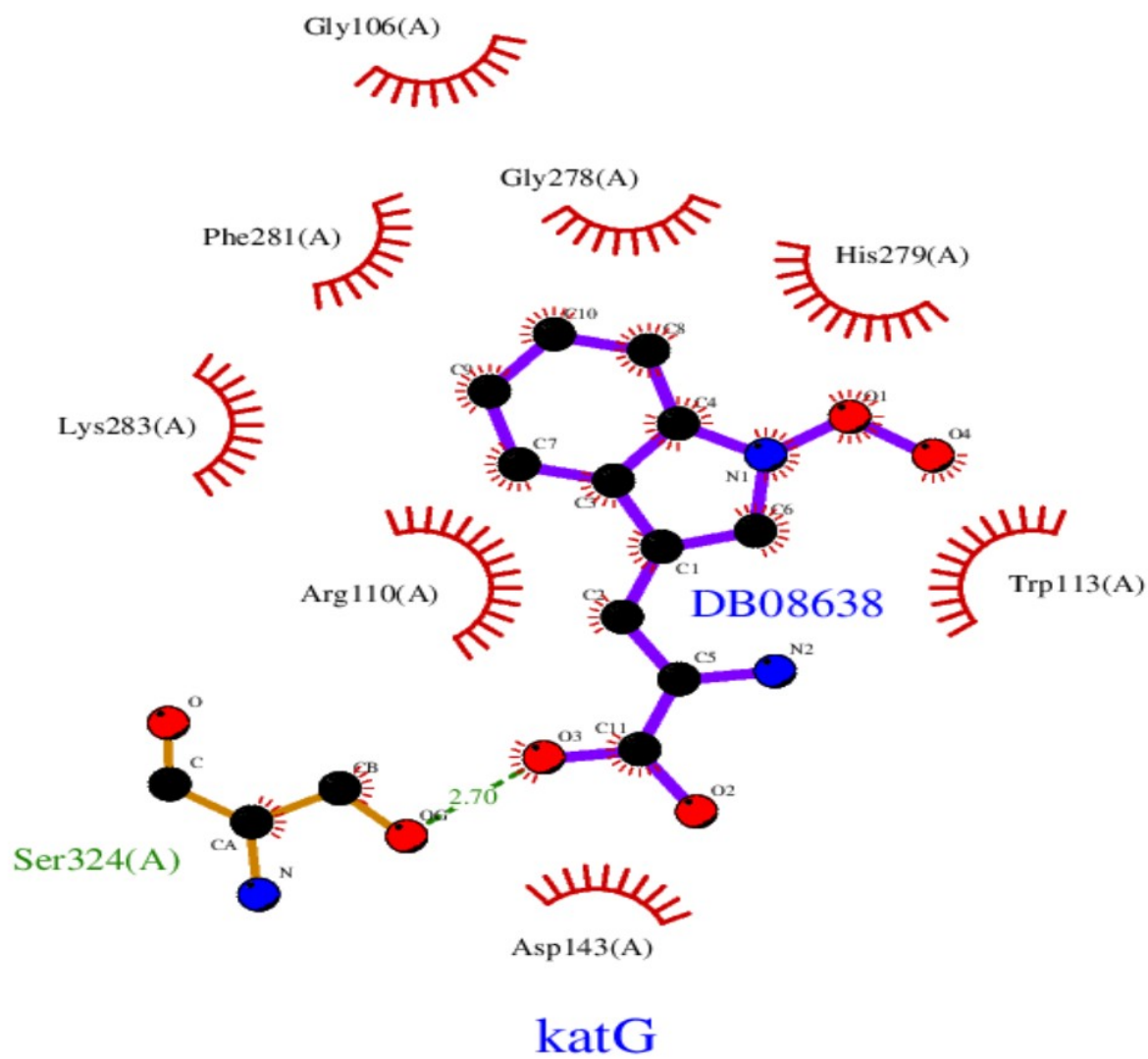
(i) Interaction pattern of katG with DB00609



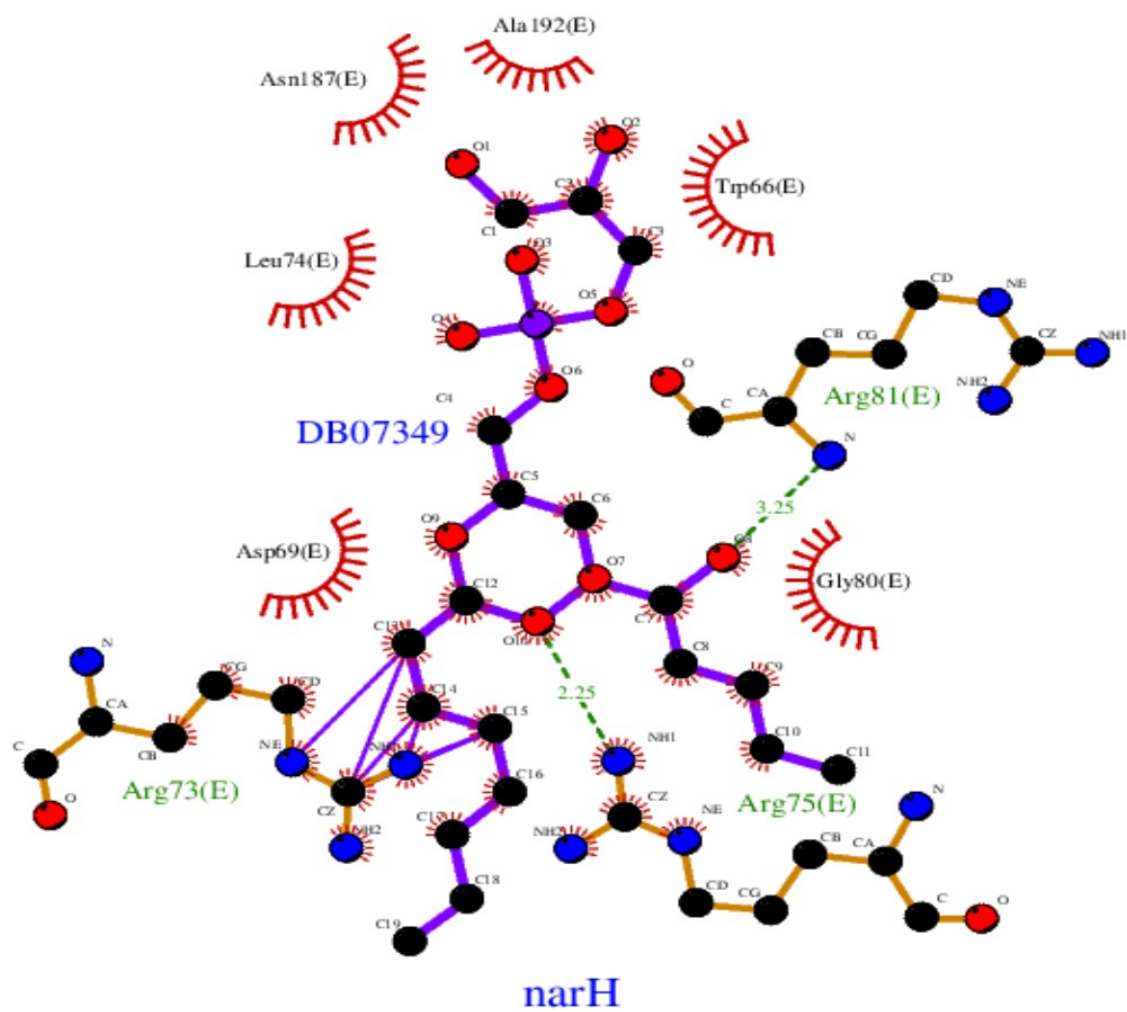
(ii) Interaction pattern of katG with DB00951



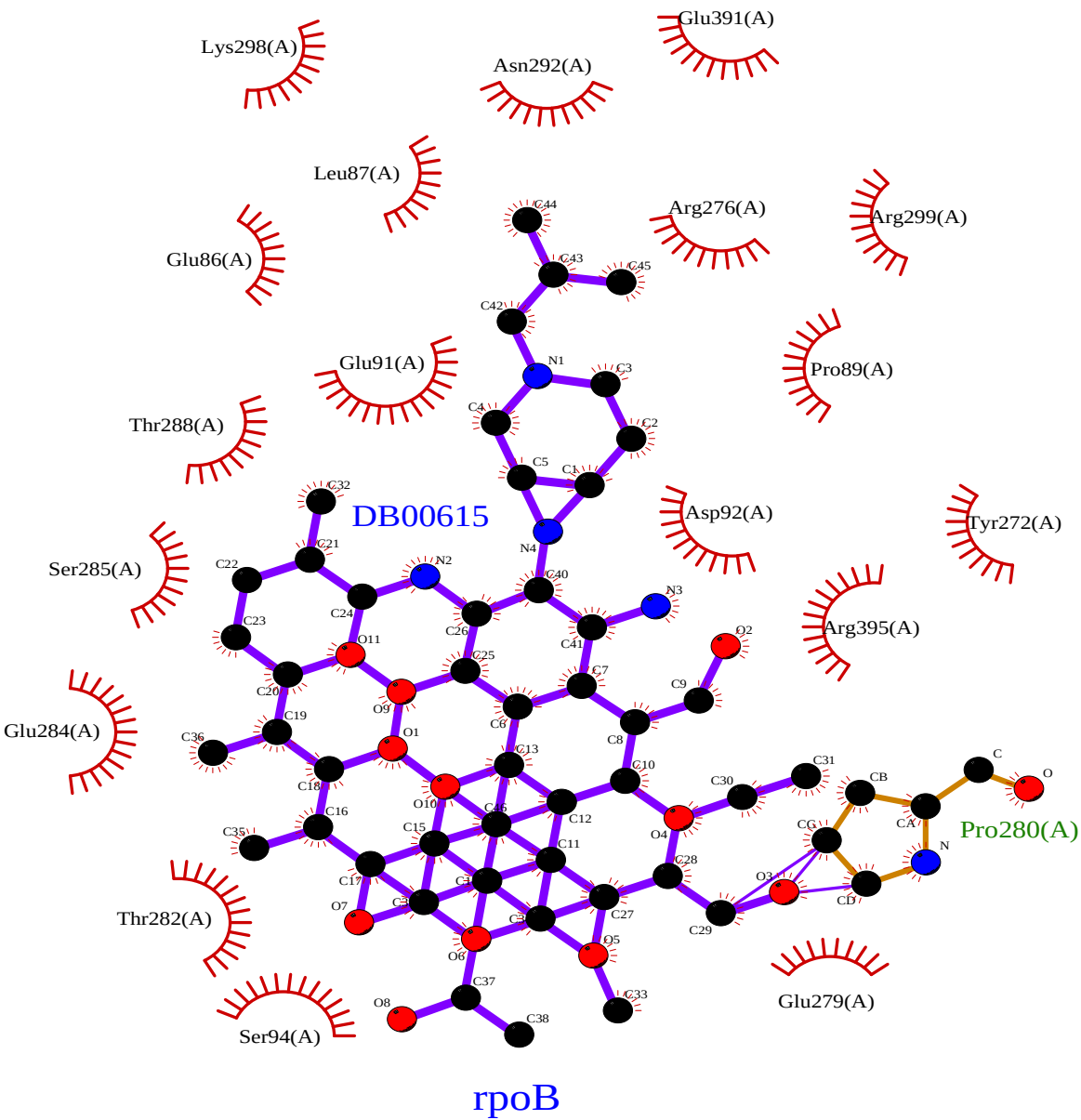
(iii) Interaction pattern of katG with DB08638



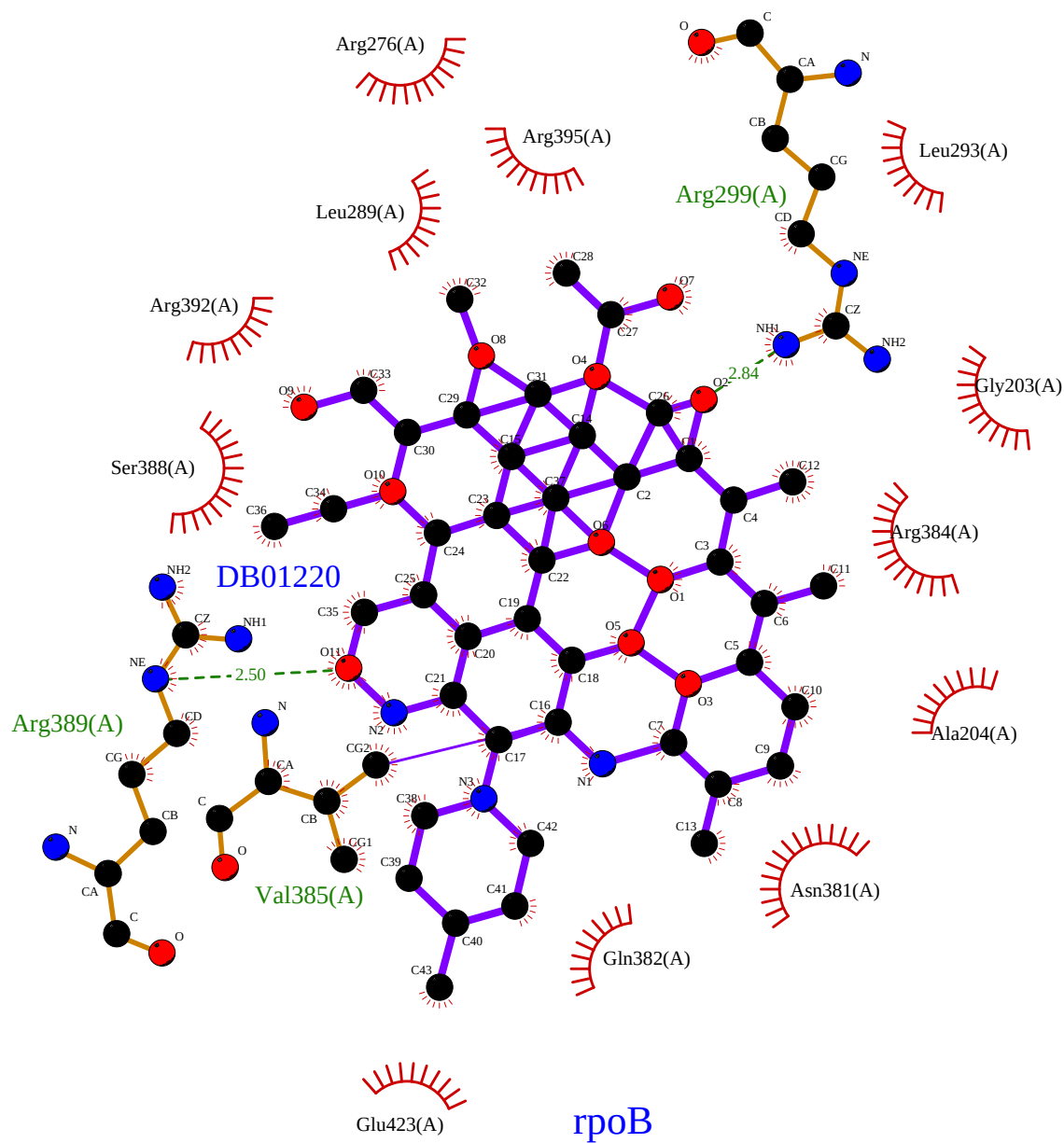
(iv) Interaction pattern of narH with DB07349



(v) Interaction pattern of rpoB with DB00615

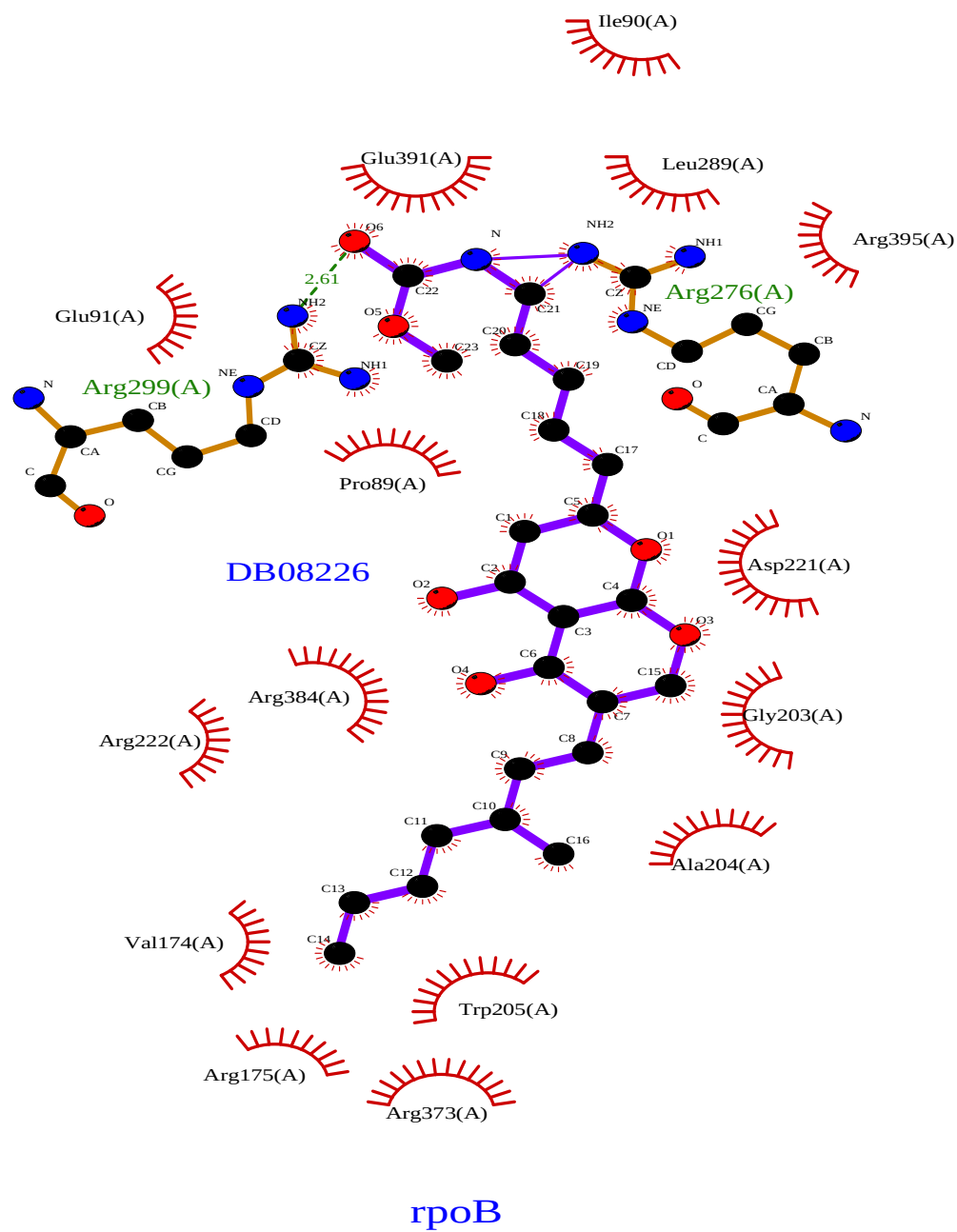


(vi) Interaction pattern of rpoB with DB01220





(vii) Interaction pattern of rpoB with DB08226



(viii) Interaction pattern of rpoB and DB08266

