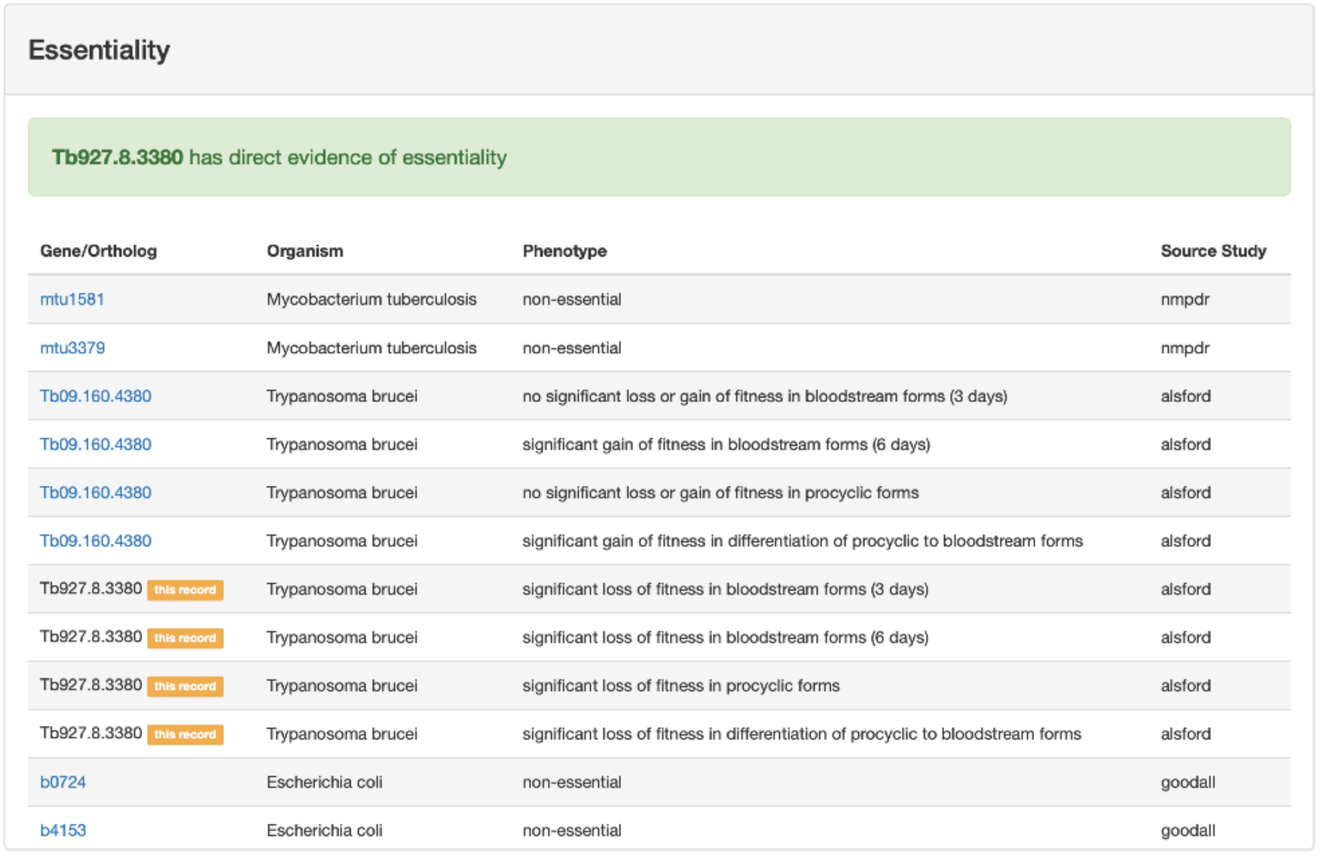
- Click on Tb927.8.3380 and scroll down to Essentiality Data
- Suppose that we discover a SDH inhibitor in our SBDD campaign against the ubiquinone binding site of *P. Aeruginosa*. Based on these data, which other species would be most worth testing its efficacy against? Which would be least worth testing?
- The inhibitor should be tested against *T. brucei* and *T. gondii*. It probably won't be effective against *M. tuberculosis* and *P. berghei*.

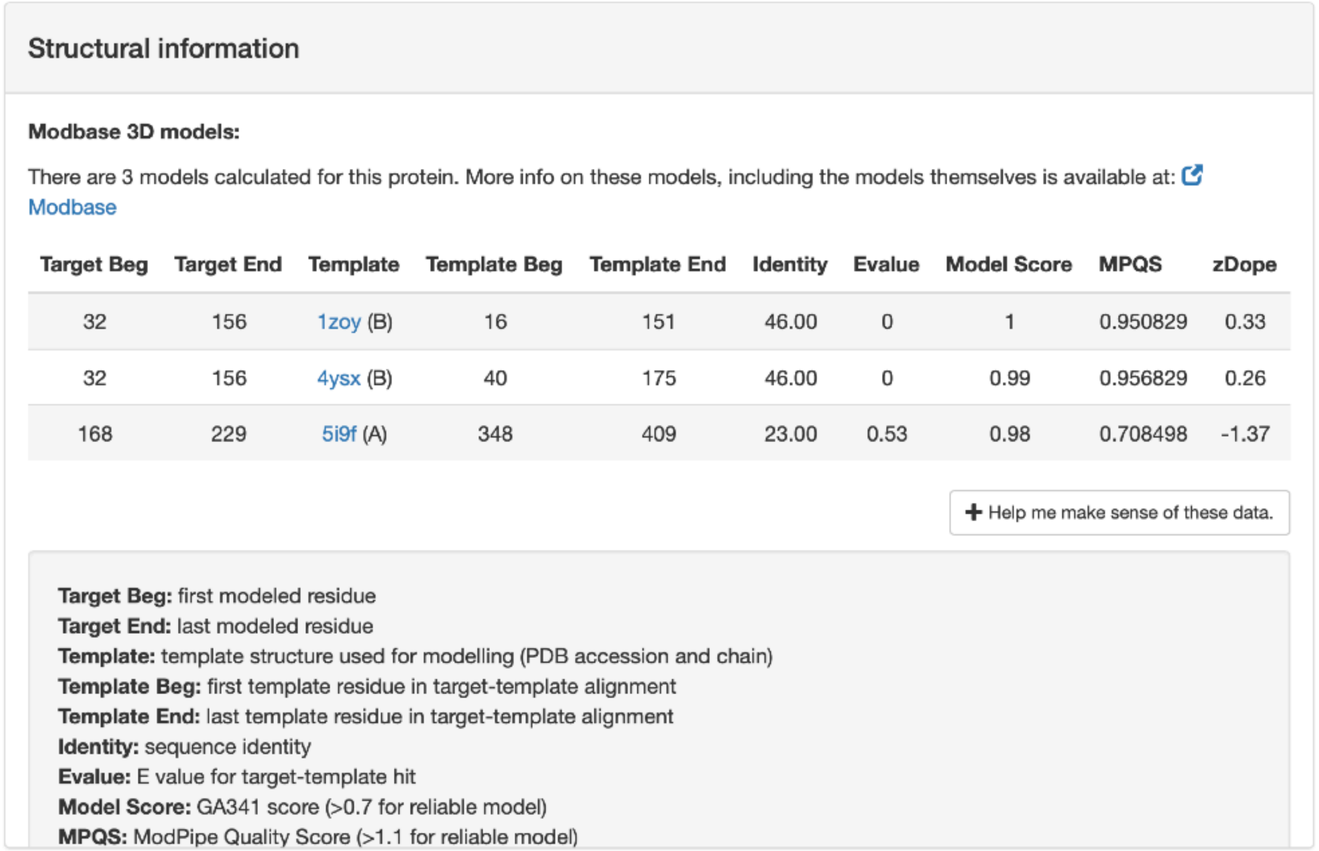


Essentiality

Tb927.8.3380 has direct evidence of essentiality

Gene/Ortholog	Organism	Phenotype	Source Study
mtu1581	Mycobacterium tuberculosis	non-essential	nmpdr
mtu3379	Mycobacterium tuberculosis	non-essential	nmpdr
Tb09.160.4380	Trypanosoma brucei	no significant loss or gain of fitness in bloodstream forms (3 days)	alsford
Tb09.160.4380	Trypanosoma brucei	significant gain of fitness in bloodstream forms (6 days)	alsford
Tb09.160.4380	Trypanosoma brucei	no significant loss or gain of fitness in procyclic forms	alsford
Tb09.160.4380	Trypanosoma brucei	significant gain of fitness in differentiation of procyclic to bloodstream forms	alsford
Tb927.8.3380 this record	Trypanosoma brucei	significant loss of fitness in bloodstream forms (3 days)	alsford
Tb927.8.3380 this record	Trypanosoma brucei	significant loss of fitness in bloodstream forms (6 days)	alsford
Tb927.8.3380 this record	Trypanosoma brucei	significant loss of fitness in procyclic forms	alsford
Tb927.8.3380 this record	Trypanosoma brucei	significant loss of fitness in differentiation of procyclic to bloodstream forms	alsford
b0724	Escherichia coli	non-essential	goodall
b4153	Escherichia coli	non-essential	goodall

- Also take a look at “Structural information”
- There is no crystal structures and the homology models from Modbase are not high quality. The homology model could be a guide, but I would not base an SBDD campaign against a *T. brucei* homology model.



Structural information

Modbase 3D models:

There are 3 models calculated for this protein. More info on these models, including the models themselves is available at: Modbase

Target Beg	Target End	Template	Template Beg	Template End	Identity	Evalue	Model Score	MPQS	zDope
32	156	1zoy (B)	16	151	46.00	0	1	0.950829	0.33
32	156	4ysx (B)	40	175	46.00	0	0.99	0.956829	0.26
168	229	5i9f (A)	348	409	23.00	0.53	0.98	0.708498	-1.37

+ Help me make sense of these data.

Target Beg: first modeled residue
Target End: last modeled residue
Template: template structure used for modelling (PDB accession and chain)
Template Beg: first template residue in target-template alignment
Template End: last template residue in target-template alignment
Identity: sequence identity
Evalue: E value for target-template hit
Model Score: GA341 score (>0.7 for reliable model)
MPQS: ModPipe Quality Score (>1.1 for reliable model)