Additional rxns:

ALDD2x ALDD2x: acald\_c + h2o\_c + nad\_c --> ac\_c + 2 h\_c + nadh\_c added!

rxn11663 rxn11663: nad\_c + phthr\_c --> co2\_c + cpd08449 + nadh\_c added!

PDX5PS2 PDX5PS2: cpd08449 + dxyl5p\_c --> 2 h2o\_c + h\_c + pdx5p\_c + pi\_c added!

Missing rxns:

PDX5PS

Edits finished in iML1515 on 6/27/2024

1. Reaction: CDGS
   * No gene reaction rule, done by QueE (b2777) – added to model
     1. Gene wasn’t in iML1515 🡪 gene added to model
2. Reaction: AACTOOR
   * No gene reaction rule, done by TynA (b1386) – added to model
3. PYRt2rpp
   * No gene reaction rule, done by: – added to model
     1. CstA (b0598)
     2. BtsT (b4354)
4. HEX4
   * No gene reaction rule, done by Mak (b0394) – added to model

\*\*OTHER EDITS\*\*

Use what Chris finds when he compares iML1515 to \*our model (“iML1515\_PLP\_Jun27\_JTB” for now)/check stoichiometry to write up exact changes, but summary:

“Side Reactions”:

1. “GTHS\_2” – “Glutathione synthetase (aberrant)”
   * gg4abut\_c 🡪 ophth\_c
     1. Metabolite: ophth\_c added to model
2. “GLUCYS\_2” – “Gamma-glutamylcysteine synthetase (aberrant)”
   * C02356\_c 🡪 gg4abut\_c
     1. Metabolite: gg4abut\_c added to model
3. "RE2034C" – “(S)-2-aminobutanoate aminotransferase”
   * Reversible reaction: production of “C02356\_c” ((S)-2-aminobutanoate aminotransferase) from 2obut\_c + glu\_\_L\_c
   * Taken from iCHOv1 model
     1. Metabolite: C02356\_c added to model
4. “RE2040C” – “Gamma-glutamyl-GABA Lyase”
   * Reversible reaction: 5oxpro\_c + C02356\_c 🡪 gg4abut\_c
   * Taken from iCHOv1 model (\*CHANGE: in their model gg4abut\_c = “CE1661\_c” 🡪 changed to match the “gg4abut\_c” in our model
     1. Metabolite: 5oxpro\_c added to model
5. “CITMSec” – “Citramalate/2-Isopropylmalate synthase (aberrant)”

Taken from iAF987 model (Rxn: CITMS; Enzyme: CimA) 🡪 (Rxn\*: CITMSec; Enzyme\*: LeuA (b0074)LeuA production of citramalate using pyr\_c (instead of 3mob\_c) when pyruvate levels are high (\*prediction)

**TPP reactions added to model on 6/27/2024:**

1A. DXPS (already in model – fine as is)

* -1.0 g3p\_c, -1.0 h\_c, -1.0 pyr\_c 🡪 1.0 co2\_c, **1.0 dxyl5p\_c**

1B. “**THISCOSH**”

* Descriptive name: ThiS-COSH formation
* Model: \*our model
* Reaction: thiscoo\_c + atp\_c + L\_\_cys\_c + iscssh\_c 🡪 1.0 ppi\_c + L\_\_ala\_c + amp\_c + iscs\_c + **thiscos\_c**
* Stoichiometry:
  + **-1.0 thiscoo\_c**, -1.0 atp\_c, -1.0 cys\_\_L\_c, -1.0 iscssh\_c 🡪 1.0 ppi\_c, 1.0 ala\_\_L\_c, 1.0 amp\_c, 1.0 iscs\_c, **1.0 thiscos\_c**
* Default bounds: (Lower: 0, Upper: 1000)
* Objective coefficient:
* Subsystem: Cofactor and Prosthetic Group Biosynthesis – JTB TPP synthesis
* Gene Reaction Rule: (b4407 and b3992 and b0423 and b2530)
* Genes: b4407 (thiS), b3992 (thiF), b0423 (thiI), b2530 (iscS)
* “Metabolites” that were added (in similar format to “iscs\_c”/”iscssh\_c”):
  + “thiscoo\_c”
    - Descriptive name = “ThiS sulfur carrier protein”
    - Model = \*our model
    - Formula: “C4H6N2O3”
    - charge = -1
    - Compartment = c – cytosol
    - Reaction: THISCOSH; BTS5 ((1.0 thiscoo\_c for BTS5) plus b4407 (thiS) rxn rule\*\*)
  + “thiscos\_c”
    - Descriptive name = “ThiS-COSH”
    - Model = \*our model
    - Formula: “C4H7N2O2S”
    - charge = 0
    - Compartment = c – cytosol
    - Reaction: THISCOSH; BTS5 ((-1.0 thiscos\_c for BTS5) plus b4407 (thiS) rxn rule \*\*)

1C. **“DHGLYS”**

* Descriptive name: Dehydroglycine synthase
* Model: \*our model
* Reaction: tyr\_\_L\_c+ nadph\_c + amet\_c 🡪 **dhgly\_c** + h\_c + nadp\_c + met\_\_L\_c + dad\_5\_c + 4crsol\_c
* Stoichiometry:
  + -1.0 tyr\_\_L\_c, -1.0 nadph\_c, -1.0 amet\_c 🡪 **1.0 dhgly\_c**, 1.0 h\_c, 1.0 nadp\_c, 1.0 met\_\_L\_c, 1.0 dad\_5\_c, 1.0 4crsol\_c
* Default bounds: (0, 1000)
* Objective coefficient:
* Subsystem: Cofactor and Prosthetic Group Biosynthesis – JTB TPP synthesis
* Gene Reaction Rule: b3990
* Genes: b3990 (thiH)

1D. “**THZPSN\_THIG**”

* Descriptive name: Thiazole phosphate synthase/thiol sulfurtransferase
* Model: \*our model
* Reaction: **thiscos\_c** + **dxyl5p\_c** + **dhgly\_c** 🡪 2.0 h2o\_c + **thiscoo\_c** + **C20246\_c**
* Stoichiometry:
  + **-1.0 thiscos\_c**, -**1.0 dxyl5p\_c**, -**1.0 dhgly\_c** 🡪 2.0 h2o\_c, 1.0 thiscoo\_c, **1.0 C20246\_c**
* Default bounds: (0, 1000)
* Objective coefficient:
* Subsystem: Cofactor and Prosthetic Group Biosynthesis – JTB TPP synthesis
* Gene Reaction Rule: b3991
* Genes: b3991 (thiG)
* Metabolite that was added:
  + “C20246\_c”
  + Descriptive name = “2-[(2R,5Z)-2-carboxy-4-methylthiazol-5(2H)-ylidene]ethyl phosphate”
  + Model = \*our model
  + Formula: C7H7NO6PS
  + charge = -3
  + Compartment = c – cytosol
  + Reaction: THZPSN\_THIG,

2A. “**AMPMS2\_2**” – AMPMS2 needs edited (iML1515 has NAD+/NADH as cofactor; biocyc says it’s amet\_c… 🡪 Put both in to see if it makes a difference)

* Descriptive name: Phosphomethylpyrimidine synthase
* Model: \*our model
* Reaction: air\_c + amet\_c 🡪 **4ampm\_c** + dad\_5\_c + met\_\_L\_c + 3.0 h\_c + co2\_c + for\_c
* Stoichiometry:
  + -1.0 air\_c, -1.0 amet\_c 🡪 1.0 **4ampm\_c**, 1.0 dad\_5\_c, 1.0 met\_\_L\_c, 3.0 h\_c, 1.0 co2\_c, 1.0 for\_c
* Default bounds: (0,1000)
* Objective coefficient:
* Subsystem: Cofactor and Prosthetic Group Biosynthesis – JTB TPP synthesis Gene Reaction Rule: b3994
* Genes: b3994 (thiC)

2B. PMPK (already in model – fine as is; b2103 (thiD))

* -1.0 **4ampm\_c**, -1.0 atp\_c 🡪 1.0 adp\_c, **1.0 2mahmp\_c**

2C. “**TMPS**” –

* Descriptive name: Thiamine phosphate synthase
* Model: \*our model
* Reaction: **2mahmp\_c** + 2.0 h\_c + **C20246\_c** 🡪 **thmmp\_c** + ppi\_c + co2\_c
* Stoichiometry:
  + -**1.0 2mahmp\_c**, -2.0 h\_c, -1.0 **C20246\_c** 🡪 **1.0 thmmp\_c**, 1.0 ppi\_c, 1.0 co2\_c
* Default bounds: (0, 1000)
* Objective coefficient:
* Subsystem: Cofactor and Prosthetic Group Biosynthesis – JTB TPP synthesis
* Gene Reaction Rule: b3993
* Genes: b3993 (thiE)
  + \*\*NOTE: in KEGG this reaction takes C20247 🡪 thmmp\_c; the differences is:
  + <https://www.genome.jp/entry/R09977> - C20246 is reduced (C7H7NO6PS 🡪 C7H10NO6PS ) via this reaction:
* ID Definition
* ----------------------------------------------------------------------------------------------------
* [5.3.99.10](https://www.genome.jp/entry/5.3.99.10) thiazole tautomerase; tenI (gene name)
  + - There is no identified gene that does this reaction in E. coli (and the C20246 metabolite links clearly show the metabolite is annotated as intended) so I’m just keeping C20246 in place for the model reaction

2D. TMPK (already in model – fine as is; b0417 (thiL))

* -1.0 thmmp\_c, -1.0 atp\_c 🡪 1.0 adp\_c, **1.0 thmpp\_c**