Figure S2: Global communication networks for 25 additional proteins
Global communication networks (GCNs) integrate tertiary (contact rearrangement) and quaternary networks. Quaternary nodes, substrate and effector sites, quaternary interfaces, and quaternary node – ligand site interactions are repre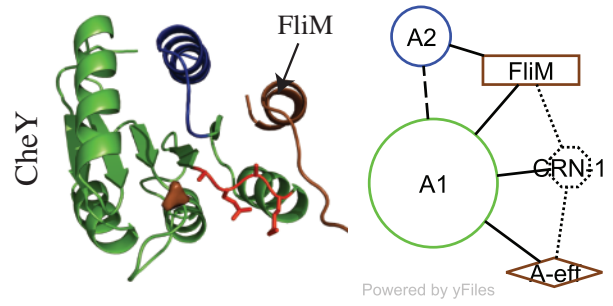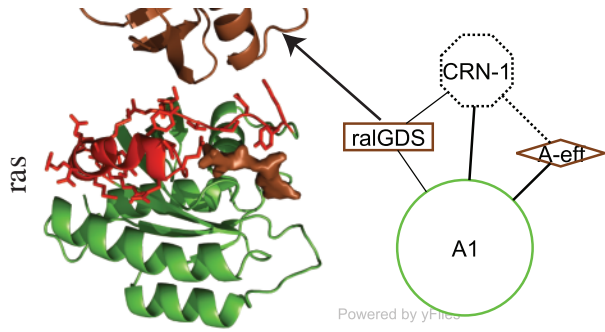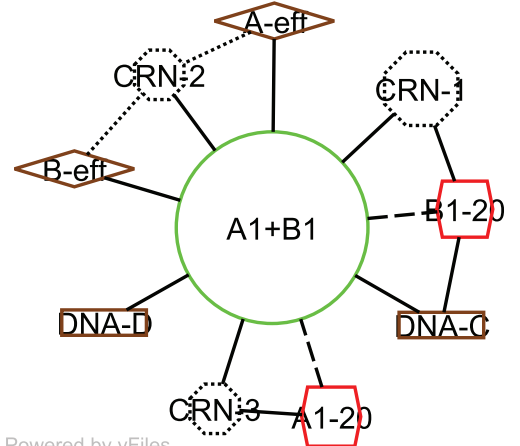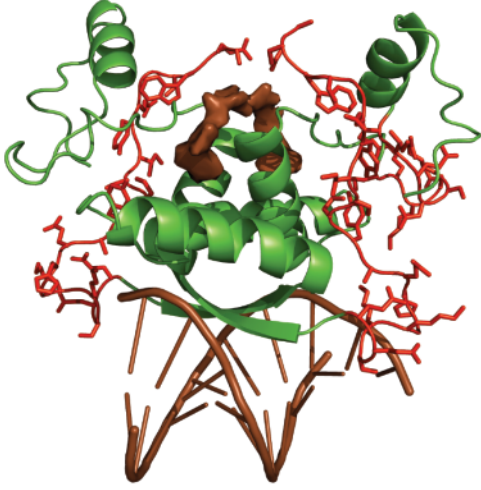sented as in figure 2 of the main text. Each quaternary node is mapped to its position in the three-dimensional structure of the active state by the node's outline color. Square nodes represent segments present only in the active state structure. Tertiary nodes comprising 10 or more residues or contacting a ligand site are represented as octagons with the area proportional to the number of residues; these nodes are numbered by size from large to small. Modifications to both tertiary and quaternary node areas have been made to account for the participation of some residues in both tertiary and quaternary nodes. Quaternary node-tertiary node edges indicate intersections (shared residues) between these two types of nodes, and an edge between a tertiary node and a ligand site indicates that the ligand site participates in the CRN cluster corresponding to the tertiary node. Finally, the density of dashing of a quaternary edge is proportional to the interfacial contact rearrangement f_{CR}. Solid: $f_{CR} < 10\%$ (conserved interface); dashed: $10\% \leq f_{CR} \leq 50\%$ (moderately rearranged); dotted: $f_{CR} > 50\%$ (extensively rearranged). See the methods for the full details of the GCN representation and associated calculations. Graphs drawn by yEd graph editor (www.yworks.com). Specific residues comprised by each quaternary node are available in the supplemental data sets. For the GCN of ras, ralGDS is connected to rigid-body cluster A1 and tertiary node CRN-1 because residues from both of those nodes bind ralGDS in 1LFD.pdb. Similarly or the GCN of CheY, a peptide fragment of FliM is connected to rigid-body clusters A1 and A2 and tertiary node CRN-1 because residues from both of those nodes bind the FliM fragment in 1F4V.pdb.

ras

CRN-1

ralGDS

A-eff

A1

CheY

A2

FliM

A1

CRN-1

A-eff

Gt

CRN-1

A-eff

A341-349

A1

IRK

CRN-2

A1

A-eff

A-subs

A2

CRN-1

A6

AraC

A-eff

CRN-2

B-eff

CRN-1

A1

B1

A168-171

B168-171
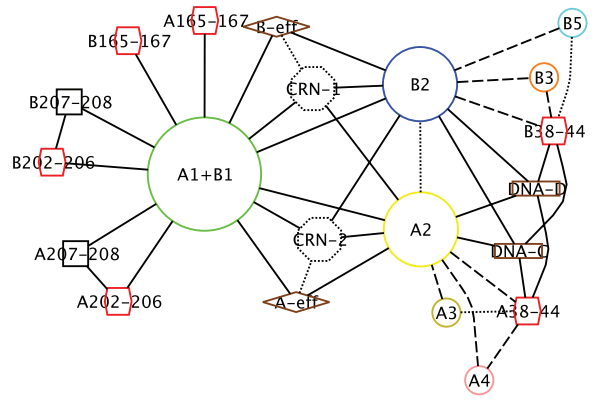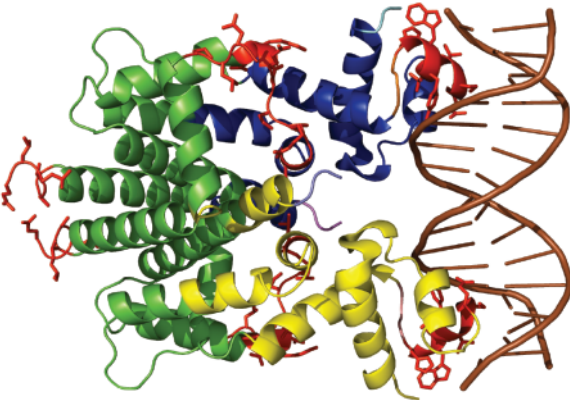
Arg repressor

A-eff

B-eff

CRN-2

E82-85

F-eff

CRN-1
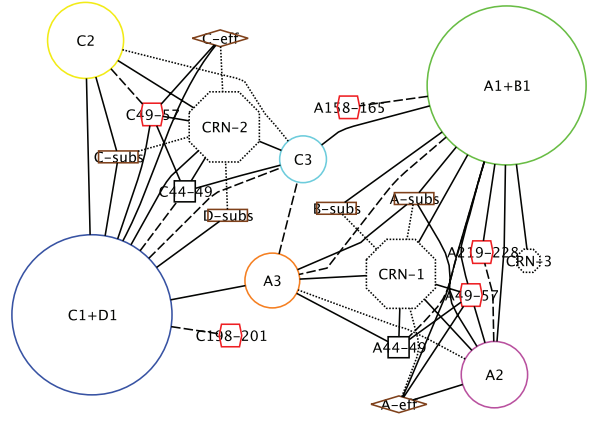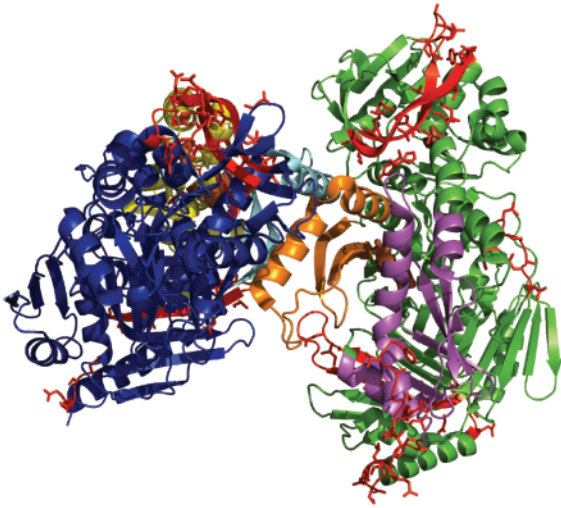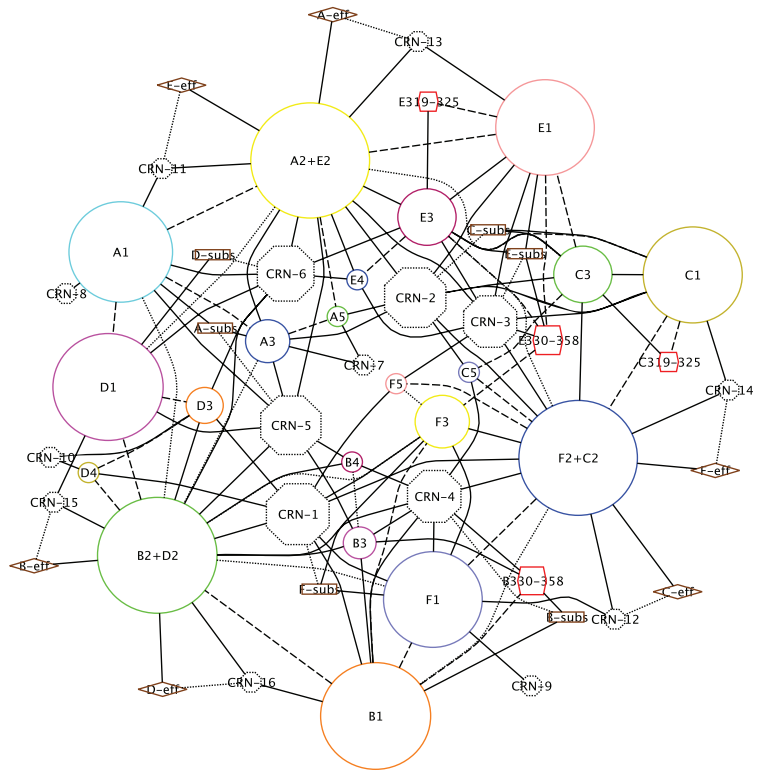
C1+A1+F1+E1+B1+D1
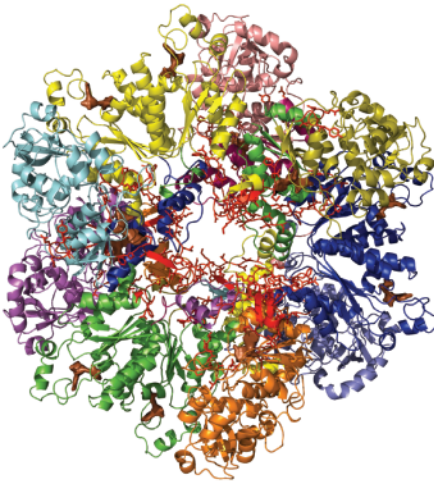
F-eff

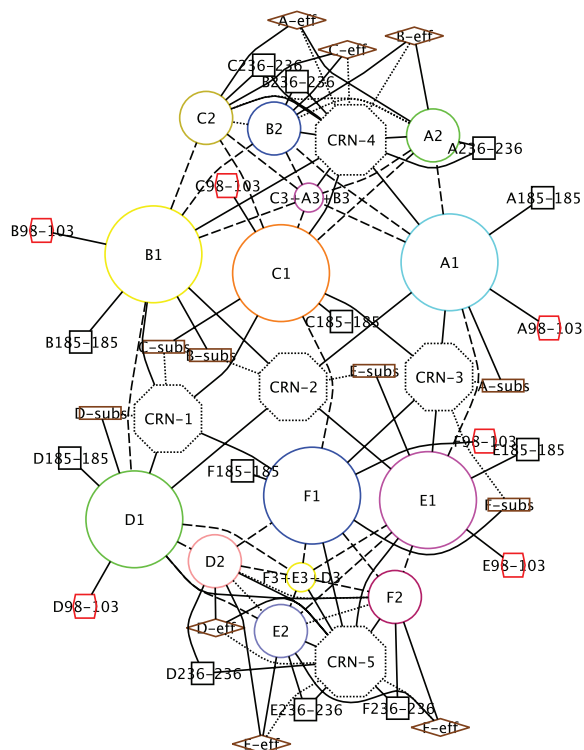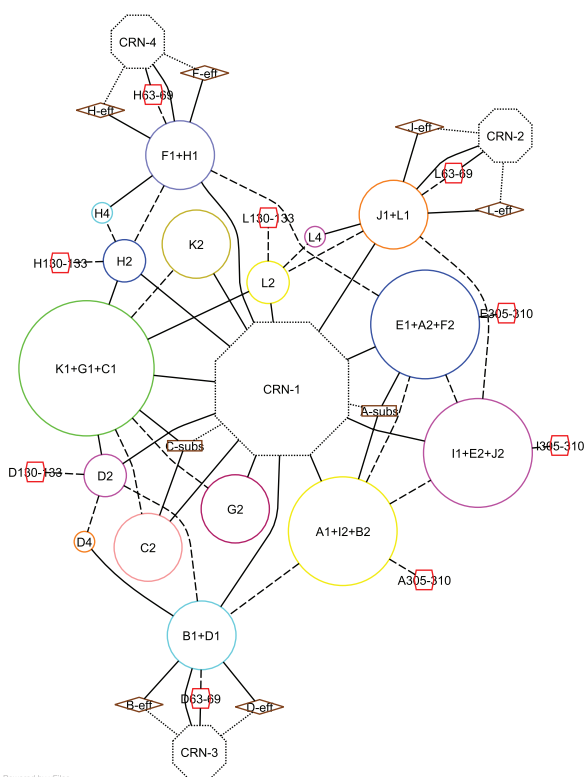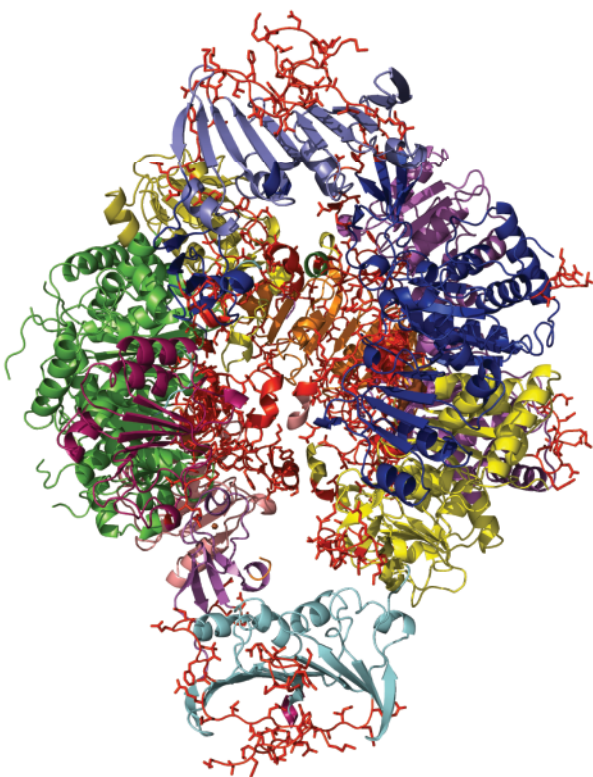D-eff

C-eff

D2
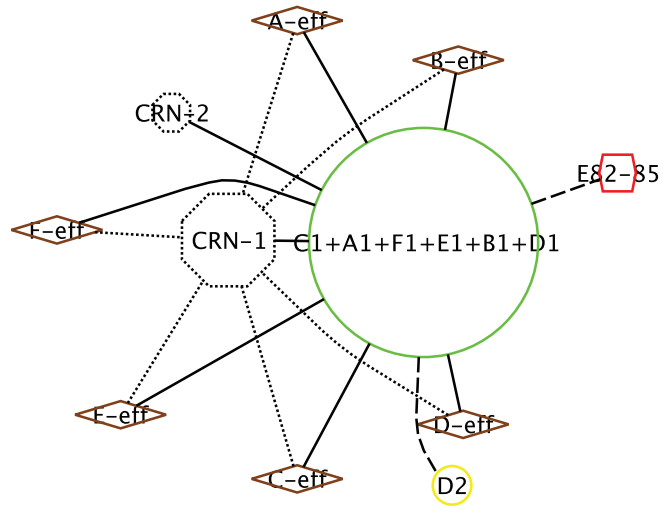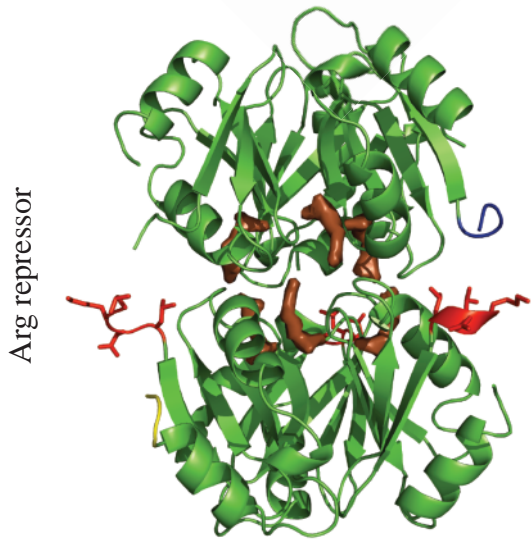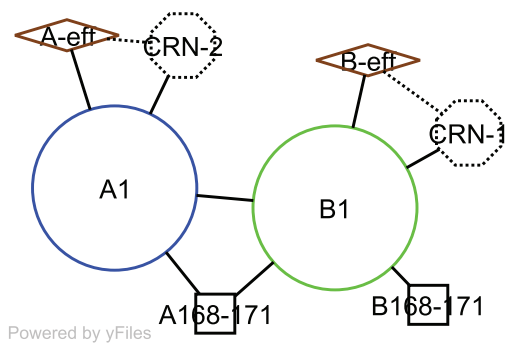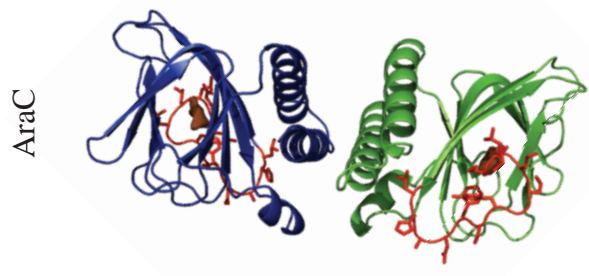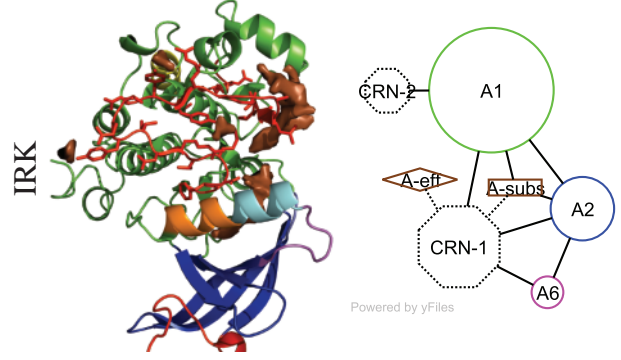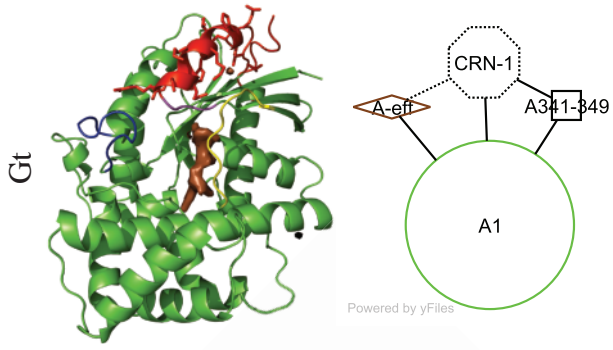
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Met repressor
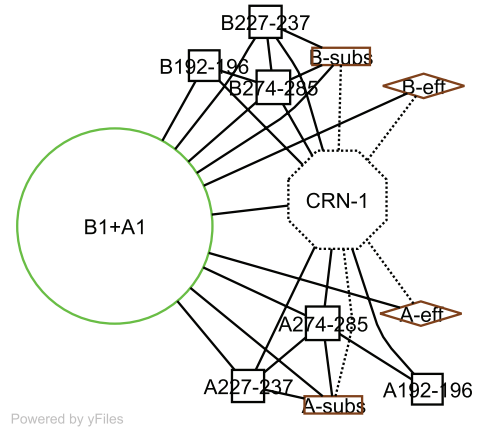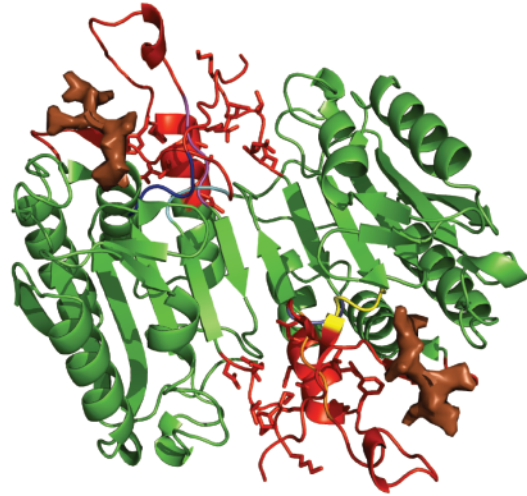
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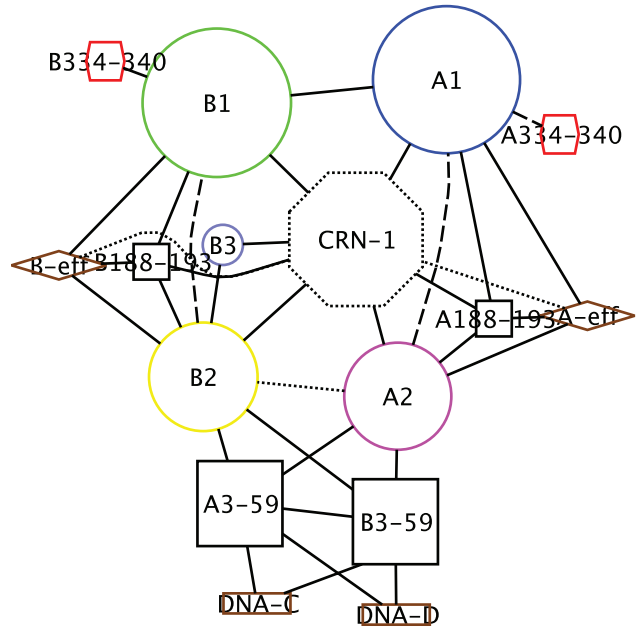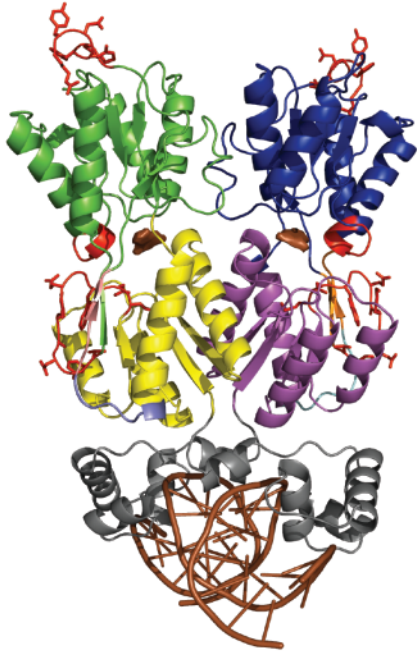
Tet repressor

anthranilate synthase

ATP sulfurylase

ATP -PRT

ATCase

caspase

B227-237
B192-196
B274-285
B-subs
B-eff
B1+A1
CRN-1
A274-285
A-eff
A227-237
A-subs
A192-196

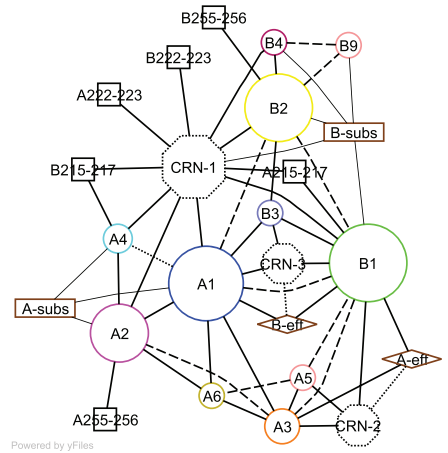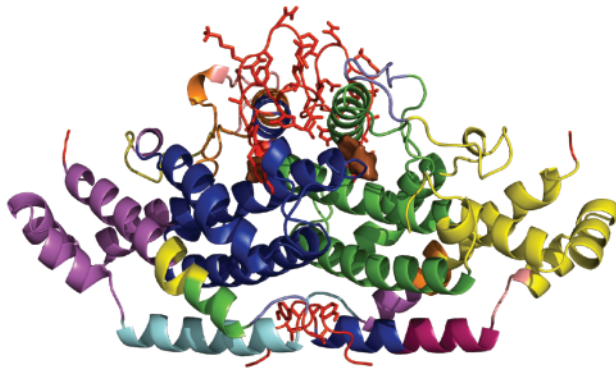*Powered by yFiles*

chorismate mutase

B255-256
B4
B9
B222-223
B2
A222-223
B-subs
CRN-1
B215-217
A215-217
B3
A4
CRN-3
B1
A1
A-subs
B-eff
A2
A-eff
A5
A6
A255-256
A3
CRN-2

Powered by yFiles

DAHP synthase

CRN-2
B-subs
A1
B2
A2
A-subs
B1
A93-101
B1-
CRN-1
A-eff
A1-
B-eff
D1-
C-eff
C1-
C6
C3+D6
B-eff
C312-320
D3+C5
D-eff
D5
C2
C4
C1
D1
D2
CRN-4
CRN-3
D4
C-subs
D-subs
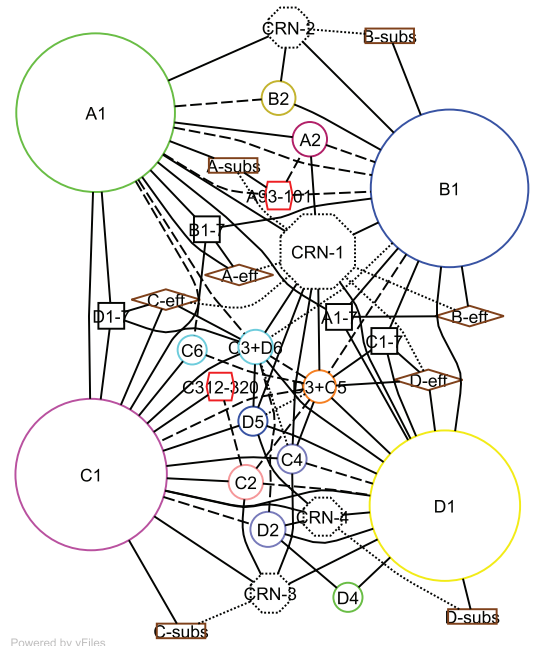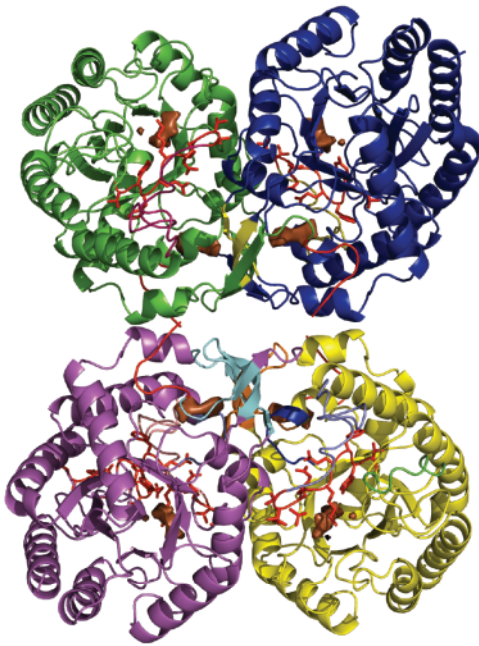
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FBPase-1

GTP cyclohydrolase I

glcN-6-P deaminase

CRN-14
F-subs
F2
D-eff
F-eff
CRN-2
B2
D2
CRN-12
CRN-13
CRN-3
D-subs
F1
B-eff
B-subs
D1
B1
F3+D3+B3
CRN-5
CRN-4
CRN-8
E4
C2
C4
CRN-10
CRN-6
E1
A4
C3+A3+E3
C-subs
E-subs
E-eff
C1
CRN-7
CRN-1
CRN-11
E2
A1
A2
CRN-9
A-eff
A-subs
C-eff
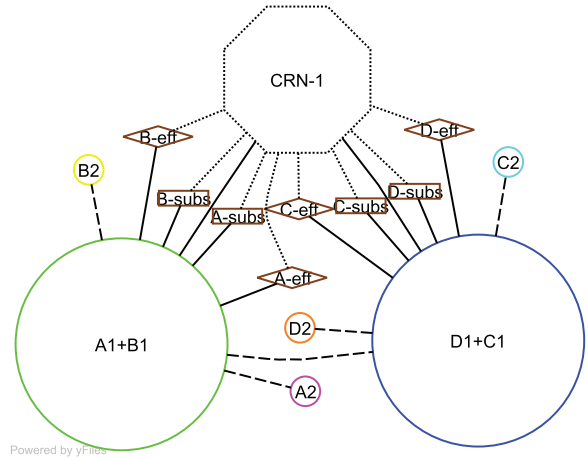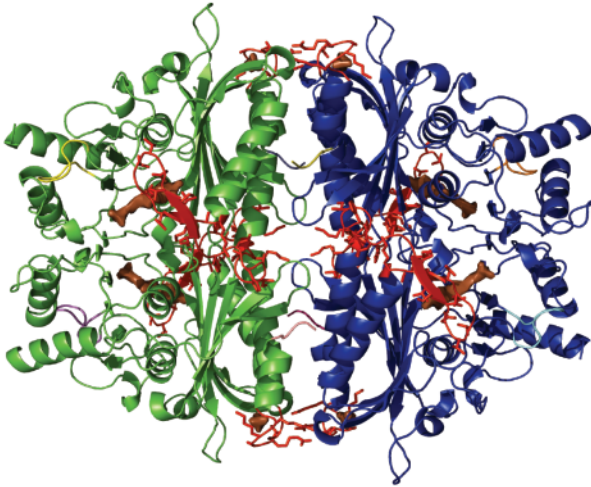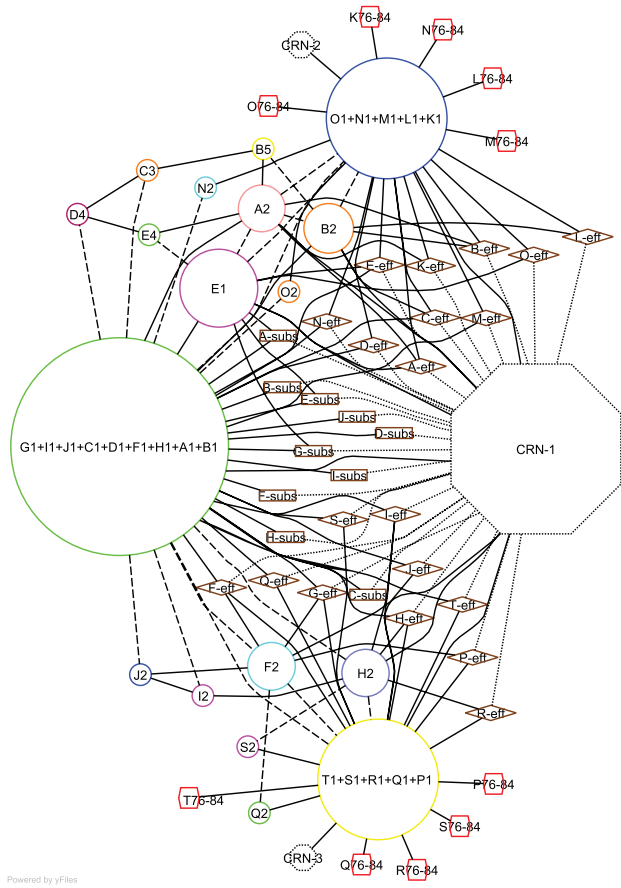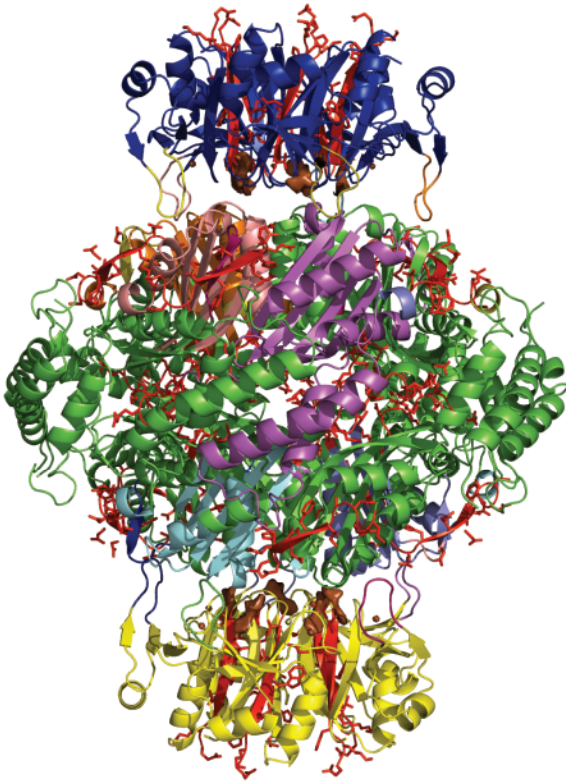
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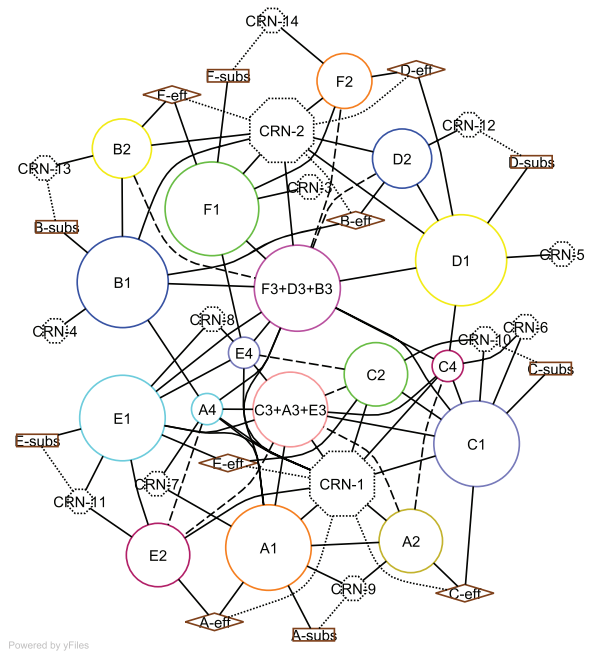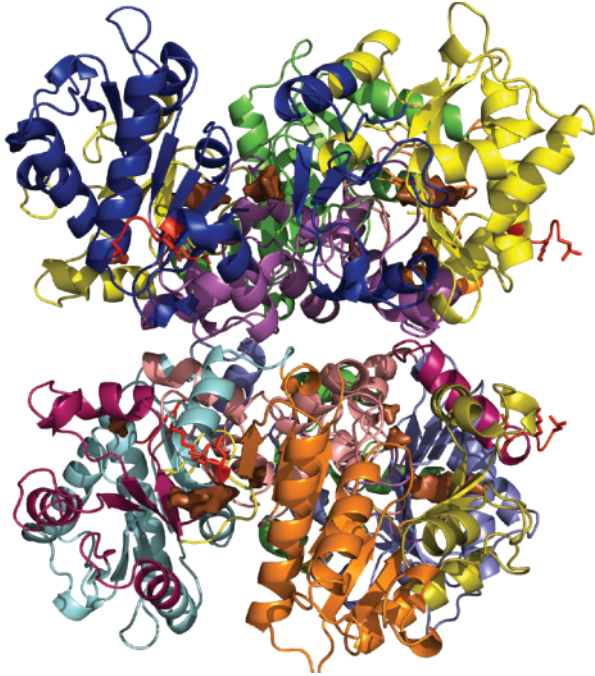
glycogen phosphorylase

A-eff
CRN-2
CRN-3
CRN-4
A10-18
A3
B10-18
B-eff
B3
A1
B1
A5
B2
A282-286
A-subs
A2
B282-286
CRN-1
B-subs

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hemoglobin

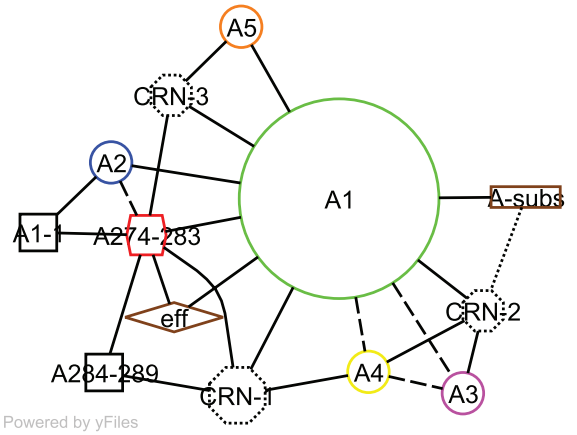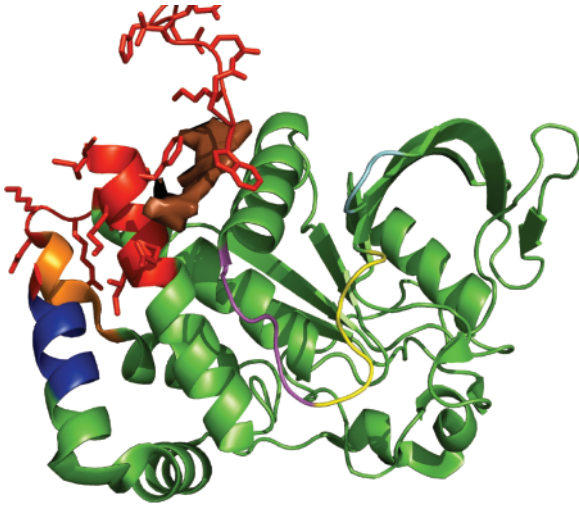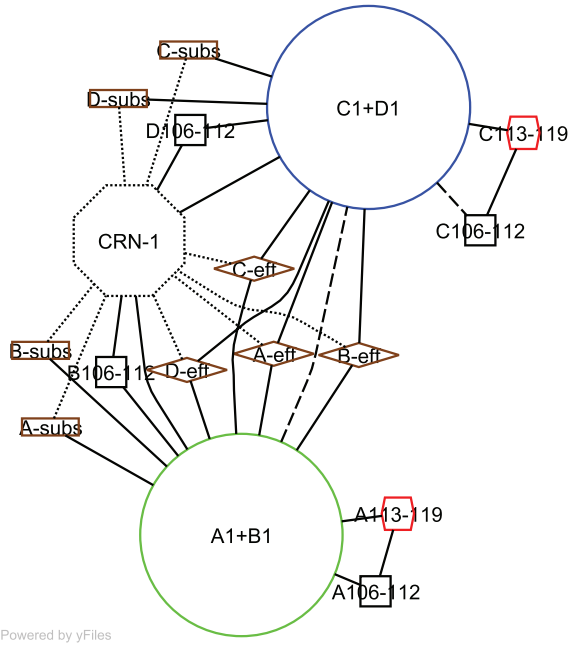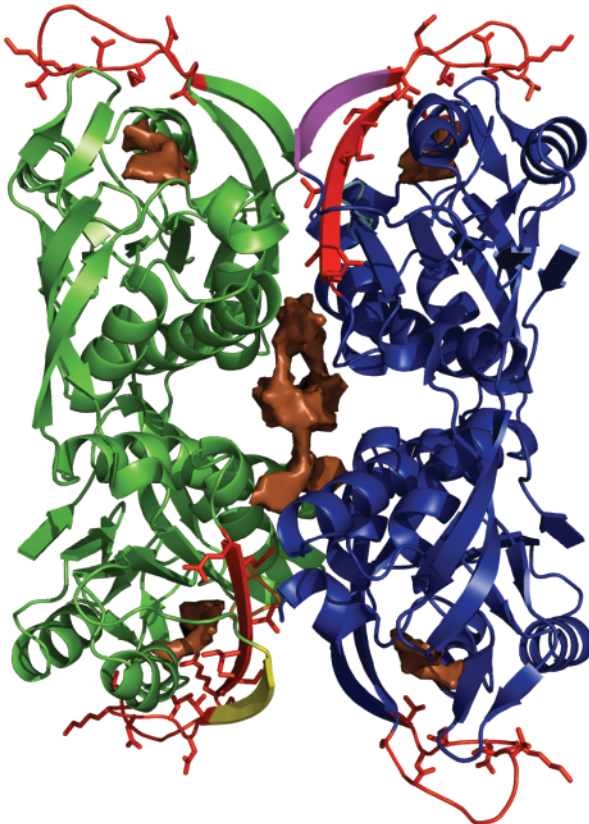D-eff
D2
CRN-1
A-eff
D4
C1+D1
A1+B1
C3
C-eff
B2
B3
CRN-2
B-eff

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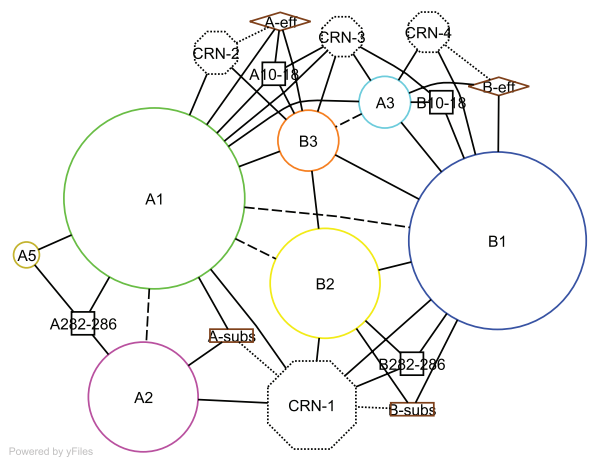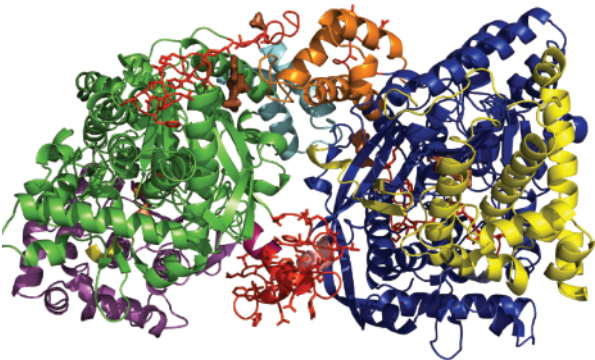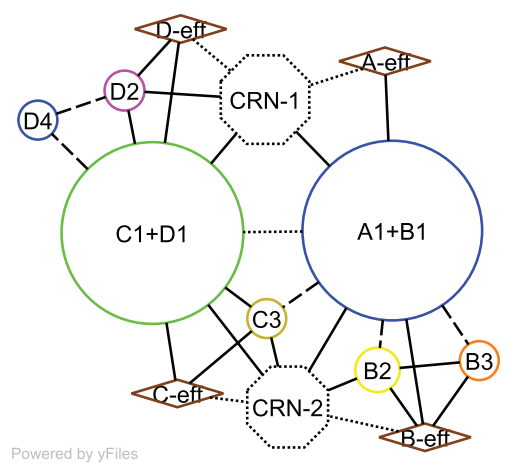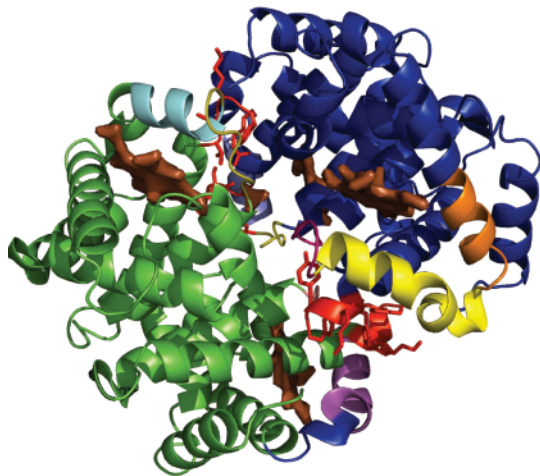
lactate DH
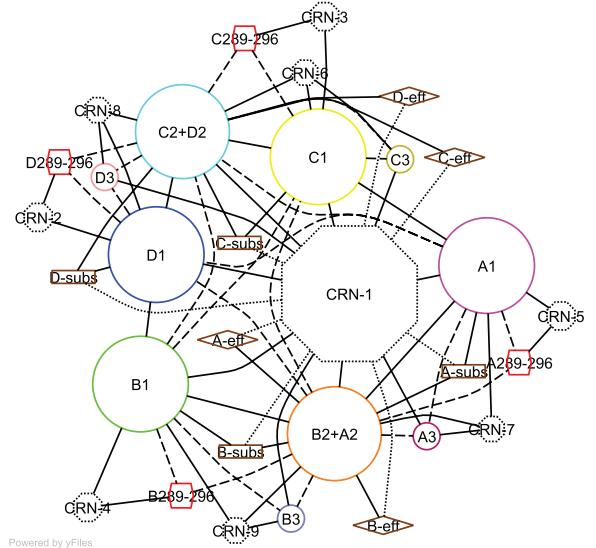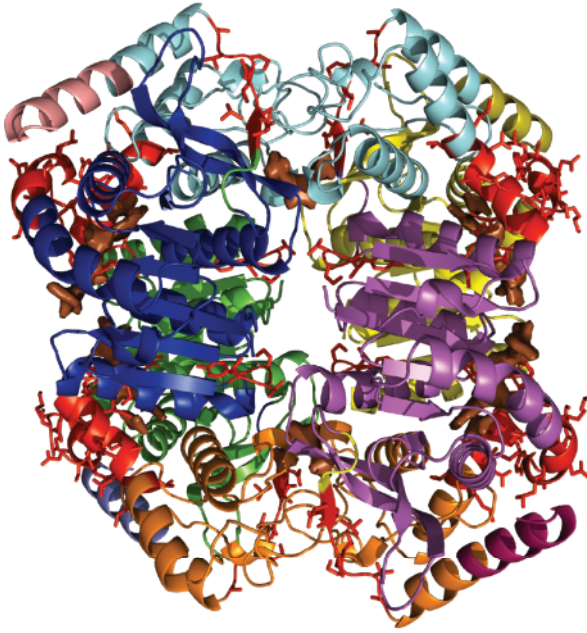
phosphoglycerate DH

PTP1B

uracil PRT

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End Figure S2.