Journal Name

Dynamic Article Links ►

Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/xxxxxx

ARTICLE TYPE

The MEP Pathway and the Development of Inhibitors as Potential Anti-Infective Agents- PDB Codes and Images of Enzymes in Surface Representations.

Ian Hale[a], Paul M. O'Neill[a], Neil G. Berry[a], Audrey Odom*[b], and Raman Sharma[a]*

Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
DOI: 10.1039/b000000x

Contents

Table S1 - DXS

PDB ID	Resolution	Source
2O1S	2.4	*Escherichia coli*
2O1X	2.9	*Deinococcus radiodurans*

TableS2 - IspC

PDB ID	Resolution	Source
1JVS	2.2	*Escherichia coli*
1K5H	2.5	*Escherichia coli*
1ONN	2.6	*Escherichia coli*
1ONO	2.5	*Escherichia coli*
1ONP	2.5	*Escherichia coli*
1Q0H	2.2	*Escherichia coli*
1Q0L	2.65	*Escherichia coli*
1Q0Q	1.9	*Escherichia coli*
1R0K	1.91	*Zymomonas mobilis*
1R0L	2.7	*Zymomonas mobilis*
1T1R	2.3	*Escherichia coli*
1T1S	2.4	*Escherichia coli*
2C82	1.9	*Mycobacterium Tuberculosis*
2EGH	2.2	*Escherichia coli str. K12 substr.*
2JCV	2.2	*Mycobacterium Tuberculosis*

2JCX	2.1	*Mycobacterium Tuberculosis*
2JCY	2.35	*Mycobacterium Tuberculosis*
2JCZ	2.05	*Mycobacterium Tuberculosis*
2JD0	2.3	*Mycobacterium Tuberculosis*
2JD1	2	*Mycobacterium Tuberculosis*
2JD2	2.15	*Mycobacterium Tuberculosis*
2Y1C	1.9	*Mycobacterium Tuberculosis*
2Y1D	2.05	*Mycobacterium Tuberculosis*
2Y1E	1.65	*Mycobacterium Tuberculosis*
2Y1F	1.96	*Mycobacterium Tuberculosis*
2Y1G	1.95	*Mycobacterium Tuberculosis*
3A06	2	*Thermotoga maritima*
3A14	2	*Thermotoga maritima*
3ANL	2.1	*Escherichia coli*
3ANM	2	*Escherichia coli*
3ANN	2	*Escherichia coli*
3AU8	1.86	*Plasmodium falciparum*
3AU9	1.9	*Plasmodium falciparum*
3AUA	2.15	*Plasmodium falciparum*
3IIE	2.21	*Yersinia pseudotuberculosis YPIII*
3R0I	2.1	*Escherichia coli K-12*
3RAS	2.55	*Mycobacterium tuberculosis*

Table S3 - IspD

PDB ID	Resolution	Source
1H3M	2.4	*Escherichia coli*
1I52	1.5	*Escherichia coli*
1INI	1.82	*Escherichia coli*
1INJ	1.55	*Escherichia coli*
1VGT	1.8	*Escherichia coli*
1VGU	2.8	*Escherichia coli*
1VGW	2.35	*Neisseria gonorrhoeae*
1VGZ	3	*Neisseria gonorrhoeae*
1VPA	2.67	*Thermotoga maritima*
1W55	2.3	*Campylobacter jejuni*
1W57	3.09	*Campylobacter jejuni*
1W77	2	*Arabidopsis thaliana*
2PX7	2.2	*Thermus thermophilus HB8*
2XWL	1.49	*Mycobacterium smegmatis*
2XWM	1.8	*Mycobacterium smegmatis*
2XWN	2.9	*Mycobacterium tuberculosis*
2YC3	1.4	*Arabidopsis thaliana*
2YC5	1.6	*Arabidopsis thaliana*
2YCM	1.8	*Arabidopsis thaliana*
3F1C	2.3	*Listeria monocytogenes str. 4b F2365*
3N9W	1.9	*Escherichia coli*
3OKR	2.4	*Mycobacterium tuberculosis*

3Q7U	2.1	*Mycobacterium tuberculosis*
3Q80	2	*Mycobacterium tuberculosis*

Table S4 - IspE

PDB ID	Resolution	Source
1OJ4	2.01	*Escherichia coli*
1UEK	1.7	*Thermus thermophilus*
2V2Q	2.3	*Aquifex aeolicus*
2V2T	3.05	*Mus musculus*
2V2V	2.4	*Aquifex aeolicus*
2V2Z	2.25	*Aquifex aeolicus*
2V34	2.3	*Aquifex aeolicus*
2V8P	2.1	*Aquifex aeolicus*
2VF3	2.2	*Aquifex aeolicus*
2WW4	2	*Escherichia coli*

Table S5 - IspF

PDB ID	Resolution	Source
1GX1	1.8	*Escherichia coli*
1H47	1.99	*Escherichia coli*
1H48	2.3	*Escherichia coli*
1IV1	1.65	*Thermus thermophilus*
1IV2	1.55	*Thermus thermophilus*
1IV3	1.52	*Thermus thermophilus*

1IV4	1.55	*Thermus thermophilus*
1JN1	2.9	*Haemophilus influenzae*
1JY8	2.5	*Escherichia coli*
1KNJ	2.8	*Escherichia coli*
1KNK	2.8	*Escherichia coli*
1T0A	1.6	*Shewanella oneidensis*
1U3L	2.5	*Escherichia coli*
1U3P	2.85	*Escherichia coli*
1U40	2.8	*Escherichia coli*
1U43	3.2	*Escherichia coli*
1VH8	2.35	*Haemophilus influenzae*
1VHA	2.35	*Haemophilus influenzae*
1W55	2.3	*Campylobacter jejuni*
1W57	3.09	*Campylobacter jejuni*
1YQN	3.11	*Escherichia coli*
2AMT	2.3	*Escherichia coli*
2GZL	2.5	*Escherichia coli*
2PMP	2.3	*Arabidopsis thaliana*
2UZH	2.2	*Mycobacterium smegmatis*
3B6N	2.26	*Plasmodium vivax SaI-1*
3ELC	2.5	*Escherichia coli K-12*
3EOR	2.9	*Escherichia coli K-12*
3ERN	2.1	*Escherichia coli K-12*
3ESJ	2.7	*Escherichia coli K-12*

3F0D	1.2	*Burkholderia pseudomallei*
3F0E	2.05	*Burkholderia pseudomallei*
3F0F	2.09	*Burkholderia pseudomallei*
3F0G	2.08	*Burkholderia pseudomallei*
3F6M	2.96	*Yersinia pestis*
3FBA	3.1	*Escherichia coli*
3FPI	2.8	*Yersinia pestis*
3GHZ	2.03	*Salmonella typhimurium*
3IEQ	2.1	*Burkholderia pseudomallei*
3IEW	2.1	*Burkholderia pseudomallei*
3IKE	2.3	*Burkholderia pseudomallei*
3IKF	2.07	*Burkholderia pseudomallei*
3JVH	1.69	*Burkholderia pseudomallei*
3K14	1.7	*Burkholderia pseudomallei*
3K2X	1.85	*Burkholderia pseudomallei*
3KE1	2.05	*Burkholderia pseudomallei*
3MBM	1.8	*Burkholderia pseudomallei*
3P0Z	1.95	*Burkholderia pseudomallei*
3P10	1.7	*Burkholderia pseudomallei*
3Q8H	1.75	*Burkholderia pseudomallei*
3QHD	1.7	*Burkholderia pseudomallei*
3RE3	2.64	*Francisella tularensis subsp. tularensis*
3T80	2.5	*Salmonella enterica subsp. enterica serovar Typhimurium*

Table S6 - IspG

PDB ID	Resolution	Source
2Y0F	2.5	*Thermus thermophilus*
3NOY	2.7	*Aquifex aeolicus*

Table S7 - IspH

PDB ID	Resolution	Source
3DNF	1.65	*Aquifex aeolicus*
3F7T	1.8	*Escherichia coli*
3KE8	1.7	*Escherichia coli*
3KE9	1.9	*Escherichia coli*
3KEF	1.7	*Escherichia coli*
3KEL	1.8	*Escherichia coli*
3KEM	2	*Escherichia coli*

Figure S1. Tertiary structure of IspD monomer with CTP-bound from *E. Coli* (PDB code: 1I52). The protein is shown in pale green surface representation and CTP in yellow stick representation. Mg^{2+} is represented by gray sphere. Image created in PyMol.

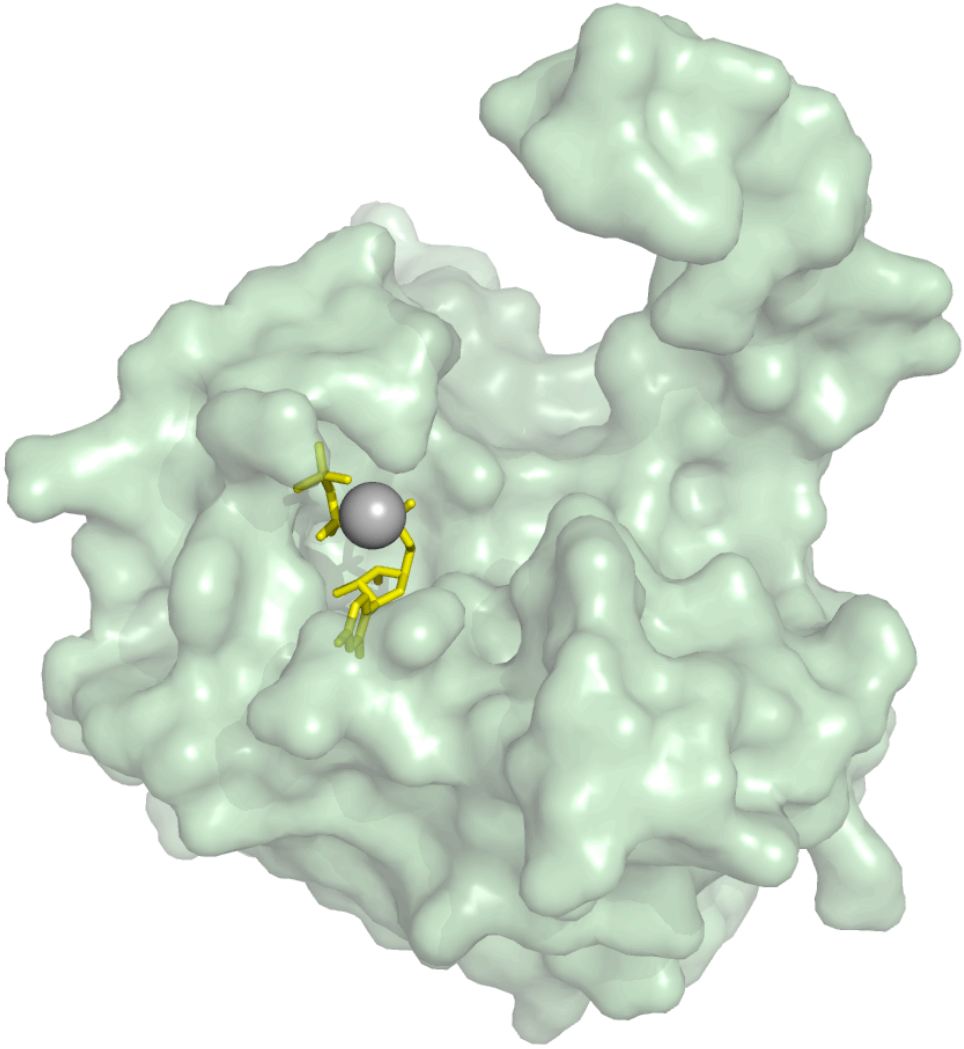

Figure S2. Tertiary structure of IspD monomer with CDP-ME bound from *E. Coli* (PDB code: 1INI). The protein is shown in pale green surface representation and CDP-ME in yellow stick representation. Mg^{2+} represented by gray sphere. Image created in PyMol.

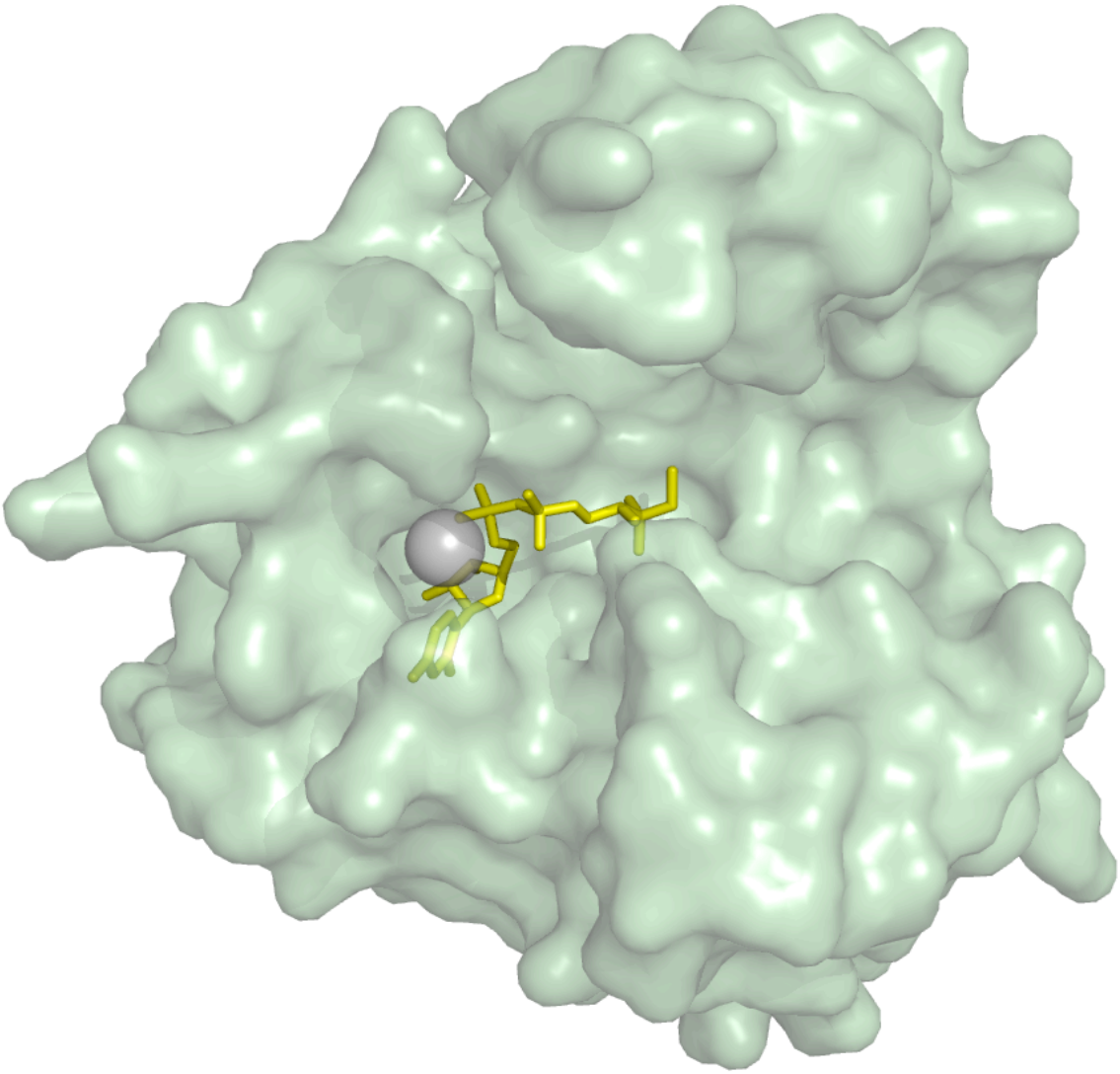

Figure S3. Tertiary structure of IspE monomer from *E. coli* with CDP-ME and AMP-PNP bound (PDB code: 1OJ4). N-terminus and C-terminus domains are depicted in red and blue surface format, respectively. AMP-PNP and CDP-ME are shown in green and yellow stick representation. Image created in PyMol.