

TABLE I

Proteins highly druggable (HD) with structures modeled from a template that was co-crystallised in the presence of an inhibitor or a drug-like compound (MD+)

Locus tag	Gene	Gene product	DS
AWH67_RS00420	<i>thiE</i>	thiamine phosphate synthase	1
AWH67_RS01825	-----	cytochrome c family protein	1
AWH67_RS04570	-----	acyl-CoA dehydrogenase	1
AWH67_RS01650	<i>fabI</i>	enoyl-[acyl-carrier-protein] reductase	0.99
AWH67_RS01730	<i>infB</i>	translation initiation factor IF-2	0.99
AWH67_RS01235	<i>prfC</i>	peptide chain release factor 3	0.99
AWH67_RS04810	<i>gcvP</i>	glycine dehydrogenase (aminomethyl-transferring)	0.99
AWH67_RS01195	-----	LPS export ABC transporter ATP-binding protein	0.98
AWH67_RS04335	<i>nuoM</i>	NADH-quinone oxidoreductase subunit M	0.98
AWH67_RS00525	-----	ABC transporter ATP-binding protein	0.98
AWH67_RS02850	<i>dxs</i>	1-deoxy-D-xylulose-5-phosphate synthase	0.98
AWH67_RS05345	-----	DUF1009 domain-containing protein	0.98
AWH67_RS02660	<i>thiE</i>	thiamine phosphate synthase	0.97
AWH67_RS04105	<i>folA</i>	dihydrofolate reductase	0.97
AWH67_RS03780	<i>lgt</i>	prolipoprotein diacylglycerol transferase	0.97
AWH67_RS01010	<i>phaAB</i>	monovalent cation/H <sup>+</sup> antiporter subunit A	0.97
AWH67_RS03605	-----	ABC transporter substrate-binding protein	0.97
AWH67_RS01025	<i>lpdA1</i>	dihydrolipoyl dehydrogenase	0.96
AWH67_RS02300	<i>serS</i>	serine--tRNA ligase	0.96
AWH67_RS02640	<i>thiC</i>	phosphomethylpyrimidine synthase	0.96
AWH67_RS02270	-----	peptidylprolyl isomerase	0.96
AWH67_RS03970	<i>murE</i>	UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase	0.95
AWH67_RS03610	-----	ABC transporter substrate-binding protein	0.95
AWH67_RS02235	<i>pdhA</i>	pyruvate dehydrogenase (acetyl-transferring) E1 component subunit alpha	0.95
AWH67_RS03355	<i>pyrD</i>	quinone-dependent dihydroorotate dehydrogenase	0.94
AWH67_RS04295	<i>nuoE</i>	NADH-quinone oxidoreductase subunit	0.94
AWH67_RS02305	<i>rlmJ</i>	23S rRNA (adenine(2030)-N(6))-methyltransferase	0.94
AWH67_RS05465	-----	NADPH:quinone oxidoreductase	0.93
AWH67_RS04150	<i>cycA</i>	D-serine/D-alanine/glycine transporter	0.93
AWH67_RS03525	<i>gidC</i>	membrane protein insertase	0.92
AWH67_RS05265	-----	penicillin-binding protein	0.92
AWH67_RS02020	<i>bioY</i>	biotin transporter	0.91
AWH67_RS02100	<i>tuf</i>	elongation factor Tu	0.91
AWH67_RS02505	<i>panC</i>	pantoate--beta-alanine ligase	0.91
AWH67_RS05820	<i>glnA</i>	type I glutamate--ammonia ligase	0.91
AWH67_RS02795	-----	HAD family phosphatase	0.90
AWH67_RS02025	<i>pheP</i>	amino acid permease	0.90
AWH67_RS02215	<i>lipA</i>	lipoyl synthase	0.88
AWH67_RS02915	<i>ispE</i>	4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol kinase	0.88
AWH67_RS02820	<i>ispH</i>	4-hydroxy-3-methylbut-2-enyl diphosphate reductase	0.88
AWH67_RS01255	<i>tsaE</i>	tRNA (adenosine(37)-N6)-threonylcarbamoyltransferase complex ATPase subunit type 1	0.88
AWH67_RS01475	<i>afeB</i>	manganese transporter	0.86
AWH67_RS03135	<i>usp</i>	universal stress protein	0.86
AWH67_RS00295	<i>dnaG</i>	DNA primase	0.86
AWH67_RS02890	<i>purD</i>	phosphoribosylamine--glycine ligase	0.86
AWH67_RS05775	-----	MFS transporter	0.86
AWH67_RS04220	-----	MFS transporter	0.86
AWH67_RS00840	-----	DNA-binding protein	0.85
AWH67_RS01270	<i>folC</i>	bifunctional folylpolyglutamate synthase/dihydrofolate synthase	0.85
AWH67_RS02790	<i>ccrMIM</i>	site-specific DNA-methyltransferase	0.85
AWH67_RS03180	<i>mgtE</i>	magnesium transporter	0.85
AWH67_RS05670	<i>purN</i>	phosphoribosylglycinamide formyltransferase	0.85
AWH67_RS03740	<i>yhcF</i>	redox-regulated ATPase	0.84
AWH67_RS01750	<i>trmB</i>	tRNA (guanosine(46)-N7)-methyltransferase	0.84
AWH67_RS02770	<i>ppdK</i>	pyruvate, phosphate dikinase	0.84
AWH67_RS02665	<i>thiD</i>	hydroxymethylpyrimidine/phosphomethylpyrimidine kinase	0.84
AWH67_RS04635	<i>cobT</i>	nicotinate-nucleotide--dimethylbenzimidazole phosphoribosyltransferase	0.84

Locus tag	Gene	Gene product	DS
AWH67_RS02805	-----	PAS domain S-box protein	0.84
AWH67_RS02395	<i>acpP</i>	acyl carrier protein	0.83
AWH67_RS05400	<i>gor</i>	glutathione-disulfide reductase	0.83
AWH67_RS04580	<i>pyrC</i>	dihydroorotase	0.83
AWH67_RS00580	<i>ispG</i>	4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase (flavodoxin)	0.83
AWH67_RS00500	<i>ikt</i>	transketolase	0.82
AWH67_RS03115	<i>ugpC</i>	sn-glycerol-3-phosphate import ATP-binding protein	0.82
AWH67_RS01870	<i>pstB</i>	phosphate ABC transporter ATP-binding protein	0.82
AWH67_RS00330	<i>dut</i>	dUTP diphosphatase	0.81
AWH67_RS00950	<i>dac</i>	D-alanyl-D-alanine carboxypeptidase	0.81
AWH67_RS04025	<i>ftsZ</i>	cell division protein	0.81
AWH67_RS05575	-----	MerR family transcriptional regulator	0.81
AWH67_RS04000	<i>murC</i>	UDP-N-acetylmuramate--L-alanine ligase	0.81
AWH67_RS02005	<i>aroP</i>	amino acid permease	0.80
AWH67_RS01035	<i>sucA</i>	2-oxoglutarate dehydrogenase E1 component	0.80
AWH67_RS02680	-----	PAS domain S-box protein	0.80
AWH67_RS04690	<i>purL</i>	phosphoribosylformylglycinamidine synthase subunit	0.79
AWH67_RS01600	<i>acnA</i>	aconitate hydratase	0.79
AWH67_RS04645	-----	hybrid sensor histidine kinase/response regulator	0.791
AWH67_RS03325	-----	16S rRNA (uracil(1498)-N(3))-methyltransferase	0.79
AWH67_RS03955	<i>rsmH</i>	ribosomal RNA small subunit methyltransferase H	0.79
AWH67_RS03575	<i>etfA</i>	electron transfer flavoprotein subunit alpha/FixB family protein	0.78
AWH67_RS05895	<i>secY</i>	preprotein translocase subunit	0.78
AWH67_RS05420	-----	ATP-dependent helicase	0.78
AWH67_RS01705	-----	class I SAM-dependent methyltransferase	0.78
AWH67_RS01510	<i>aroA</i>	3-phosphoshikimate 1-carboxyvinyltransferase	0.78
AWH67_RS03700	-----	N-acetyltransferase	0.77
AWH67_RS03085	-----	ABC transporter ATP-binding protein	0.77
AWH67_RS04890	-----	iron ABC transporter ATP-binding protein	0.77
AWH67_RS03075	<i>nrdI</i>	class Ib ribonucleoside-diphosphate reductase assembly flavoprotein	0.76
AWH67_RS05700	<i>rimL</i>	50S ribosomal protein L7/L12-serine acetyltransferase	0.76
AWH67_RS04315	<i>nuoI</i>	NADH-quinone oxidoreductase subunit I	0.76
AWH67_RS04490	<i>tmk</i>	dTMP kinase	0.75
AWH67_RS02160	<i>trmFO</i>	FADH(2)-oxidising methylenetetrahydrofolate--tRNA-(uracil(54)-C(5))- methyltransferase	0.746
AWH67_RS05705	<i>recG</i>	DNA helicase	0.74
AWH67_RS05740	<i>argS</i>	arginine--tRNA ligase	0.74
AWH67_RS01350	-----	radical SAM protein	0.74
AWH67_RS02410	<i>uppP</i>	undecaprenyl-diphosphatase	0.74
AWH67_RS04300	<i>nouF</i>	NADH-quinone oxidoreductase subunit F	0.73
AWH67_RS03045	<i>secA</i>	preprotein translocase subunit	0.73
AWH67_RS04575	<i>pyrB</i>	aspartate carbamoyltransferase	0.73
AWH67_RS04705	-----	MFS transporter	0.73
AWH67_RS01215	<i>rlmN</i>	23S rRNA (adenine(2503)-C(2))-methyltransferase	0.72
AWH67_RS01935	<i>tadA</i>	nucleoside deaminase	0.72
AWH67_RS03730	<i>trmL</i>	tRNA (cytidine(34)-2'-O)-methyltransferase	0.72
AWH67_RS04365	<i>lolD</i>	ABC transporter ATP-binding protein	0.71
AWH67_RS00495	<i>gap</i>	type I glyceraldehyde-3-phosphate dehydrogenase	0.71
AWH67_RS01405	<i>lepA</i>	elongation factor 4	0.71
AWH67_RS00720	<i>sdhC</i>	succinate dehydrogenase, cytochrome b556 subunit	0.7
AWH67_RS01335	-----	alpha/beta hydrolase	0.7
AWH67_RS02905	<i>tsaC</i>	threonylcarbamoyl-AMP synthase	0.7
AWH67_RS03335	<i>folD</i>	bifunctional methylenetetrahydrofolate dehydrogenase/methenyltetrahydrofolate cyclohydrolase	0.7
AWH67_RS01755	<i>metK</i>	methionine adenosyltransferase	0.7

DS: druggability score.

TABLE II

List of prioritised protein targets of *Bartonella bacilliformis* USM-LMMB07 proteins filtering by druggability scores, impact to gut microbiome and human host

Locus tag	Gene	Gene product	DS	Human off target	Gut microb (%)
AWH67_RS02160	<i>trmFO</i>	FADH(2)-oxidising methylenetetrahydrofolate--tRNA-(uracil(54)-C(5))- methyltransferase	0.75	1	31.86
AWH67_RS01090	<i>parB</i>	chromosome partitioning protein	0.82	1	33.19
AWH67_RS05895	<i>secY</i>	preprotein translocase subunit	0.78	1	32.30
AWH67_RS03000	-----	aspartate kinase	0.74	1.	30.97
AWH67_RS05565	<i>fabH</i>	3-oxoacyl-ACP synthase III	0.89	1	29.65
AWH67_RS01180	<i>ihfB</i>	integration host factor subunit beta	0.76	1	30.09
AWH67_RS05890	<i>adk</i>	adenylate kinase	0.78	0.64	27.88
AWH67_RS01565	<i>argD</i>	acetylornithine transaminase	0.85	0.65	25.66
AWH67_RS01195	-----	LPS export ABC transporter ATP-binding protein	0.98	0.70	24.78
AWH67_RS04595	<i>topA</i>	type I DNA topoisomerase	0.71	0.75	25.66
AWH67_RS03730	<i>trmL</i>	tRNA (cytidine(34)-2'-O)-methyltransferase	0.72	1	23.45
AWH67_RS01845	<i>moeB</i>	molybdopterin-synthase adenyltransferase	0.75	0.60	24.34
AWH67_RS02690	-----	DNA-binding response regulator	0.78	1	23.89
AWH67_RS02005	<i>aroP</i>	amino acid permease	0.80	0.75	22.57
AWH67_RS04665	<i>purB</i>	adenylosuccinate lyase	0.86	0.73	22.57
AWH67_RS02025	<i>PheP</i>	amino acid permease	0.90	0.76	22.12
AWH67_RS04575	<i>pyrB</i>	aspartate carbamoyltransferase	0.73	0.65	20.80
AWH67_RS01020	<i>lysI</i>	saccharopine dehydrogenase	0.73	1	21.24
AWH67_RS03940	<i>chvD</i>	energy-dependent translational throttle protein	0.93	0.72	21.24
AWH67_RS04890	-----	iron ABC transporter ATP-binding protein	0.77	0.70	20.80
AWH67_RS05820	<i>glnA</i>	type I glutamate--ammonia ligase	0.91	0.76	19.47
AWH67_RS05315	<i>cdsA</i>	phosphatidate cytidyltransferase	0.90	0.62	18.14
AWH67_RS04685	<i>PurQ</i>	phosphoribosylformylglycinamide synthase subunit	0.89	0.75	17.70
AWH67_RS04690	<i>purL</i>	phosphoribosylformylglycinamide synthase subunit	0.79	0.77	17.26
AWH67_RS05805	<i>ssb</i>	single-stranded DNA-binding protein	0.87	0.65	18.14
AWH67_RS04150	<i>cycA</i>	D-serine/D-alanine/glycine transporter	0.93	0.78	16.37
AWH67_RS00340	<i>exbB</i>	biopolymer transporter	0.95	1	16.81
AWH67_RS03955	<i>rsmH</i>	ribosomal RNA small subunit methyltransferase H	0.79	0.61	15.04
AWH67_RS04550	-----	cold-shock protein	0.73	1	15.93
AWH67_RS02790	<i>ccrMM</i>	site-specific DNA-methyltransferase	0.85	1	15.04
AWH67_RS00880	<i>lysA</i>	diaminopimelate decarboxylase	0.96	0.70	15.04
AWH67_RS05705	<i>recG</i>	DNA helicase	0.74	0.74	14.16
AWH67_RS05055	<i>flil</i>	flagellar protein export ATPase	0.77	0.69	14.60
AWH67_RS02820	<i>ispH</i>	4-hydroxy-3-methylbut-2-enyl diphosphate reductase	0.88	1	13.27
AWH67_RS04000	<i>murC</i>	UDP-N-acetylmuramate--L-alanine ligase	0.81	1	12.83
AWH67_RS01215	<i>rlmN</i>	23S rRNA (adenine(2503)-C(2))-methyltransferase	0.72	1	13.27
AWH67_RS05270	<i>clpS</i>	ATP-dependent Clp protease adapter	0.81	1	12.83
AWH67_RS04450	-----	SUF system Fe-S cluster assembly protein	0.80	1	12.39
AWH67_RS02595	-----	iron ABC transporter permease	0.99	1	11.95
AWH67_RS04880	-----	iron ABC transporter permease	0.84	1	11.95
AWH67_RS03900	<i>dnaG</i>	DNA primase	0.77	1	11.95
AWH67_RS03075	<i>nrdI</i>	class Ib ribonucleoside-diphosphate reductase assembly flavoprotein	0.76	1	11.06
AWH67_RS01510	<i>aroA</i>	3-phosphoshikimate 1-carboxyvinyltransferase	0.78	1	10.18
AWH67_RS01885	-----	aminopeptidase	0.96	1	11.50
AWH67_RS03025	-----	L-cystine transporter	0.95	0.72	11.50
AWH67_RS01985	<i>mutL</i>	DNA mismatch repair protein	0.84	0.66	11.50
AWH67_RS04105	<i>folA</i>	dihydrofolate reductase	0.97	0.68	9.29
AWH67_RS04490	<i>tmk</i>	dTMP kinase	0.75	1	9.29
AWH67_RS01475	<i>afeB</i>	manganese transporter	0.86	0.71	10.18
AWH67_RS05335	<i>fabZ</i>	beta-hydroxyacyl-ACP dehydratase	0.92	1	9.73
AWH67_RS00805	<i>htpX</i>	zinc metalloprotease	0.86	1	10.18
AWH67_RS03935	-----	bifunctional nicotinamidase/pyrazinamidase	0.86	1	9.73
AWH67_RS03645	-----	DegT/DnrJ/EryC1/StrS aminotransferase family protein	0.80	1	10.18
AWH67_RS00395	<i>rpmE</i>	50S ribosomal protein L31	0.80	1	10.18
AWH67_RS04140	<i>pdxJ</i>	pyridoxine 5'-phosphate synthase	0.72	1	9.73
AWH67_RS01155	-----	BAX inhibitor (BI)-1/YccA family protein	0.74	0.71	9.73
AWH67_RS02675	<i>pepN</i>	aminopeptidase N	0.96	0.75	9.29
AWH67_RS03175	-----	M3 family peptidase	0.98	0.70	9.29

Locus tag	Gene	Gene product	DS	Human off target (%)	Gut microb (%)
AWH67_RS01895	-----	dipeptidase	0.79	0.73	9.29
AWH67_RS00405	-----	inositol monophosphatase	0.73	0.66	8.85
AWH67_RS04095	-----	MFS transporter	0.90	1	8.85
AWH67_RS01650	<i>fabI</i>	enoyl-[acyl-carrier-protein] reductase	0.99	0.71	7.08
AWH67_RS05410	<i>nadE</i>	NAD <sup>+</sup> synthase	0.73	1	8.41
AWH67_RS03545	<i>pyrF</i>	orotidine-5'-phosphate decarboxylase	0.88	1	7.52
AWH67_RS02870	<i>fabI</i>	enoyl-[acyl-carrier-protein] reductase	0.77	0.73	7.52
AWH67_RS00435	<i>ruvC</i>	crossover junction endodeoxyribonuclease	0.70	1	7.52
AWH67_RS02305	<i>rmlJ</i>	23S rRNA (adenine(2030)-N(6))-methyltransferase	0.94	1	5.75
AWH67_RS06240	<i>fliY</i>	flagellar motor switch protein	0.75	1	7.08
AWH67_RS05735	-----	deoxyguanosinetriphosphate triphosphohydrolase	0.87	1	6.19
AWH67_RS02550	<i>rpoZ</i>	DNA-directed RNA polymerase subunit omega	0.82	1	6.64
AWH67_RS03105	<i>ugpA</i>	sn-glycerol-3-phosphate ABC transporter permease	0.96	1	6.19
AWH67_RS06105	<i>secD</i>	protein translocase subunit	0.77	1	6.19
AWH67_RS00185	<i>maf2</i>	septum formation protein	0.85	0.64	5.31
AWH67_RS02935	-----	polyprenyl synthetase family protein	0.83	0.72	5.75
AWH67_RS04735	<i>dnaE</i>	DNA polymerase III subunit alpha	0.88	1	5.31
AWH67_RS04630	<i>grp</i>	Lrp/AsnC family transcriptional regulator	0.84	1	5.31
AWH67_RS05540	<i>ribH</i>	6,7-dimethyl-8-ribityllumazine synthase	0.71	1	4.87
AWH67_RS01345	<i>dapE</i>	succinyl-diaminopimelate desuccinylase	0.75	0.78	4.87
AWH67_RS02695	<i>htrA</i>	PDZ domain-containing protein	0.73	0.66	5.31
AWH67_RS02660	<i>thiE</i>	thiamine phosphate synthase	0.97	1	3.54
AWH67_RS00895	-----	TlpA family protein disulfide reductase	0.82	1	4.42
AWH67_RS05575	-----	MerR family transcriptional regulator	0.81	1	3.98
AWH67_RS02030	<i>gpsA</i>	glycerol-3-phosphate dehydrogenase (NAD(P)(+))	0.94	0.75	4.87
AWH67_RS02905	<i>tsaC</i>	threonylcarbamoyl-AMP synthase	0.70	0.69	3.54
AWH67_RS01945	-----	16S rRNA (guanine(966)-N(2))-methyltransferase	0.98	1	3.98
AWH67_RS03525	<i>gidC</i>	membrane protein insertase	0.92	1	3.98
AWH67_RS00440	<i>ruvA</i>	Holliday junction branch migration protein	0.77	1	4.42
AWH67_RS05515	<i>argC</i>	N-acetyl-gamma-glutamyl-phosphate reductase	0.72	1	3.98
AWH67_RS04335	<i>nuoM</i>	NADH-quinone oxidoreductase subunit M	0.98	0.61	3.10
AWH67_RS01720	<i>truB</i>	tRNA pseudouridine(55) synthase	0.79	0.67	3.98
AWH67_RS01255	<i>tsaE</i>	tRNA (adenosine(37)-N6)-threonylcarbamoyltransferase complex ATPase subunit type 1	0.88	1	3.54
AWH67_RS00580	<i>ispG</i>	4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase (flavodoxin)	0.83	1	3.10
AWH67_RS02995	<i>nhaA</i>	Na <sup>+</sup> /H <sup>+</sup> antiporter	0.80	1	3.98
AWH67_RS01890	<i>mutM</i>	formamidopyrimidine-DNA glycosylase	0.93	1	3.54
AWH67_RS00210	<i>purK</i>	5-(carboxyamino)imidazole ribonucleotide synthase	0.87	1	3.10
AWH67_RS02680	-----	PAS domain S-box protein	0.80	1	2.65
AWH67_RS05445	-----	heat-shock protein	0.71	1	3.54
AWH67_RS05740	<i>argS</i>	arginine--tRNA ligase	0.74	0.67	2.21
AWH67_RS05775	-----	MFS transporter	0.86	1	2.21
AWH67_RS02020	<i>bioY</i>	biotin transporter	0.91	1	1.77
AWH67_RS02410	<i>uppP</i>	undecaprenyl-diphosphatase	0.74	1	1.33
AWH67_RS00825	-----	carbonic anhydrase	0.84	1	2.21
AWH67_RS06050	<i>gltJ1</i>	amino acid ABC transporter permease	0.74	1	2.65
AWH67_RS04320	<i>nuoJ</i>	NADH-quinone oxidoreductase subunit J	0.71	1	2.21
AWH67_RS01010	<i>phaAB</i>	monovalent cation/H <sup>+</sup> antiporter subunit A	0.97	0.66	2.21
AWH67_RS04050	-----	aminopeptidase P family protein	0.99	0.62	2.65
AWH67_RS02570	-----	transglycosylase	0.90	1	2.21
AWH67_RS02665	<i>thiD</i>	hydroxymethylpyrimidine/phosphomethylpyrimidine kinase	0.84	1	0.88
AWH67_RS00135	-----	terminase	0.84	1	2.21
AWH67_RS04340	<i>nuoN</i>	NADH-quinone oxidoreductase subunit	1	0.78	1.77
AWH67_RS02405	<i>fabD</i>	[acyl-carrier-protein] S-malonyltransferase	0.91	0.68	1.77
AWH67_RS04795	-----	rhodanese domain-containing protein	0.75	0.66	1.77
AWH67_RS03780	<i>lgt</i>	prolipoprotein diacylglycerol transferase	0.97	1	0.88
AWH67_RS01015	<i>nspC</i>	carboxynorspermidine decarboxylase	0.90	1	1.33
AWH67_RS03835	-----	TrkH family potassium uptake protein	0.90	1	1.77
AWH67_RS03180	<i>mgtE</i>	magnesium transporter	0.85	1	0.88
AWH67_RS00080	-----	hypothetical protein	0.76	1	1.77

Locus tag	Gene	Gene product	DS	Human off target (%)	Gut microb (%)
AWH67_RS05700	<i>rimL</i>	50S ribosomal protein L7/L12-serine acetyltransferase	0.76	1	0.88
AWH67_RS01375	-----	DNA-binding response regulator	0.74	1	1.77
AWH67_RS01675	-----	peptidoglycan endopeptidase	0.73	1	1.77
AWH67_RS01270	<i>folC</i>	bifunctional folylpolyglutamate synthase/dihydrofolate synthase	0.85	0.70	0.44
AWH67_RS05400	<i>gor</i>	glutathione-disulfide reductase	0.83	0.64	0
AWH67_RS03970	<i>murE</i>	UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase	0.95	1	0
AWH67_RS00420	<i>thiE</i>	thiamine phosphate synthase	1	1	0
AWH67_RS02270	-----	peptidylprolyl isomerase	0.96	1	0
AWH67_RS00680	-----	efflux RND transporter periplasmic adaptor subunit	0.94	1	1.33
AWH67_RS01415	-----	TIGR00730 family Rossmann fold protein	0.93	1	1.33
AWH67_RS02795	-----	HAD family phosphatase	0.90	1	0.44
AWH67_RS02915	<i>ispE</i>	4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol kinase	0.88	1	0
AWH67_RS01750	<i>trmB</i>	tRNA (guanosine(46)-N7)-methyltransferase	0.84	1	0
AWH67_RS02925	-----	S49 family peptidase	0.84	1	1.33
AWH67_RS05130	<i>flhA</i>	flagellar biosynthesis protein	0.83	1	1.33
AWH67_RS00950	<i>dac</i>	D-alanyl-D-alanine carboxypeptidase	0.81	1	0.44
AWH67_RS03665	-----	DNA-binding response regulator	0.80	1	1.33
AWH67_RS03325	-----	16S rRNA (uracil(1498)-N(3))-methyltransferase	0.79	1	0
AWH67_RS01355	<i>rdgB</i>	non-canonical purine NTP pyrophosphatase	0.93	0.72	0.44
AWH67_RS04580	<i>pyrC</i>	dihydroorotase	0.83	0.75	0.44
AWH67_RS03085	-----	ABC transporter ATP-binding protein	0.77	0.69	0.44
AWH67_RS04205	<i>lipB</i>	lipoate-protein ligase B	0.73	0.65	0.88
AWH67_RS00720	<i>sdhC</i>	succinate dehydrogenase, cytochrome b556 subunit	0.70	0.60	0
AWH67_RS04570	-----	acyl-CoA dehydrogenase	1	1	0
AWH67_RS05345	-----	DUF1009 domain-containing protein	0.98	1	0
AWH67_RS00535	<i>thiN</i>	thiamine diphosphokinase	0.94	1	0.44
AWH67_RS05265	-----	penicillin-binding protein	0.92	1	0
AWH67_RS03135	<i>usp</i>	universal stress protein	0.86	1	0
AWH67_RS04220	-----	MFS transporter	0.86	1	0
AWH67_RS00840	-----	DNA-binding protein	0.85	1	0
AWH67_RS04635	<i>cobT</i>	nicotinate-nucleotide--dimethylbenzimidazole phosphoribosyltransferase	0.84	1	0
AWH67_RS01690	-----	asparaginase	0.81	1	0.88
AWH67_RS00750	<i>xerC</i>	tyrosine recombinase	0.79	1	0.88
AWH67_RS04645	-----	hybrid sensor histidine kinase/response regulator	0.79	1	0
AWH67_RS01705	-----	class I SAM-dependent methyltransferase	0.78	1	0
AWH67_RS03700	-----	N-acetyltransferase	0.77	1	0
AWH67_RS01745	<i>rimP</i>	ribosome maturation factor	0.75	1	0.88
AWH67_RS00525	-----	ABC transporter ATP-binding protein	0.98	0.70	0
AWH67_RS05465	-----	NADPH:quinone oxidoreductase	0.93	0.72	0
AWH67_RS00295	<i>dnaG</i>	DNA primase	0.86	0.76	0
AWH67_RS01825	-----	cytochrome c family protein	1	0.62	0
AWH67_RS04560	<i>gatC</i>	Asp-tRNA(Asn)/Glu-tRNA(Gln) amidotransferase GatCAB subunit C	0.81	0.70	0.44
AWH67_RS02375	<i>rsmA</i>	16S rRNA (adenine(1518)-N(6)/adenine(1519)-N(6))- dimethyltransferase	0.83	0.62	0.44
AWH67_RS01335	-----	alpha/beta hydrolase	0.70	0.67	0
AWH67_RS05475	-----	beta-ketoacyl-ACP synthase II	0.97	1	0
AWH67_RS03605	-----	ABC transporter substrate-binding protein	0.97	1	0
AWH67_RS03610	-----	ABC transporter substrate-binding protein	0.95	1	0
AWH67_RS01975	<i>lpxK</i>	tetraacyldisaccharide 4'-kinase	0.93	1	0
AWH67_RS00715	<i>sdhD</i>	succinate dehydrogenase, hydrophobic membrane anchor protein	0.92	1	0
AWH67_RS01150	-----	diguanylate cyclase	0.91	1	0
AWH67_RS01100	<i>rsmG</i>	ribosomal RNA small subunit methyltransferase G	0.88	1	0
AWH67_RS03995	<i>murG</i>	undecaprenyldiphospho-muramoylpentapeptide beta-N- acetylglucosaminyltransferase	0.73	1	0
AWH67_RS04040	<i>recN</i>	DNA repair protein	0.85	1	0.44
AWH67_RS02805	-----	PAS domain S-box protein	0.84	1	0
AWH67_RS01245	<i>addA</i>	double-strand break repair helicase	0.82	1	0.44
AWH67_RS01230	<i>lisS</i>	lysine--tRNA ligase	0.80	1	0
AWH67_RS05370	-----	amino acid ABC transporter	0.78	1	0.44
AWH67_RS05235	<i>rplJ</i>	50S ribosomal protein L10	0.97	0.77	0.44
AWH67_RS03530	<i>rnpA</i>	ribonuclease P protein component	0.74	1	0.44

Locus tag	Gene	Gene product	DS	Human off target	Gut microb (%)
AWH67_RS04440	<i>sufD</i>	Fe-S cluster assembly protein	0.73	1	0.44
AWH67_RS01000	<i>phaD</i>	monovalent cation/H <sup>+</sup> antiporter subunit D	0.97	0.75	0.44
AWH67_RS04985	-----	autotransporter outer membrane beta-barrel domain-containing protein	0.70	1	0.44
AWH67_RS01955	<i>cysQ</i>	3'(2'),5'-biphosphate nucleotidase	0.93	0.76	0
AWH67_RS05195	<i>hisS</i>	histidine--tRNA ligase	0.88	0.70	0
AWH67_RS04425	-----	cysteine desulfurase	0.83	0.69	0
AWH67_RS05835	-----	RluA family pseudouridine synthase	0.80	0.68	0
AWH67_RS04705	-----	MFS transporter	0.73	0.70	0
AWH67_RS00130	-----	phage portal protein	0.99	1	0
AWH67_RS03305	-----	efflux RND transporter periplasmic adaptor subunit	0.99	1	0
AWH67_RS00835	-----	glutamine amidotransferase	0.97	1	0
AWH67_RS02360	<i>lptD</i>	LPS-assembly protein	0.97	1	0
AWH67_RS02775	<i>dsbA</i>	DsbA family protein	0.97	1	0
AWH67_RS02325	-----	autotransporter outer membrane beta-barrel domain-containing protein	0.97	1	0
AWH67_RS05490	-----	hypothetical protein	0.94	1	0
AWH67_RS01120	-----	phosphoenolpyruvate synthase regulatory protein	0.94	1	0
AWH67_RS04870	-----	autotransporter outer membrane beta-barrel domain-containing protein	0.94	1	0
AWH67_RS04995	-----	autotransporter outer membrane beta-barrel domain-containing protein	0.92	1	0
AWH67_RS01550	-----	Smr domain-containing protein	0.91	1	0
AWH67_RS02355	<i>lptG</i>	LPS export ABC transporter permease	0.90	1	0
AWH67_RS02015	<i>ecfT</i>	energy-coupling factor transporter transmembrane protein	0.90	1	0
AWH67_RS04930	<i>flgK</i>	flagellar hook-associated protein	0.87	1	0
AWH67_RS04940	-----	DNA-binding response regulator	0.87	1	0
AWH67_RS03695	-----	metallophosphoesterase	0.86	1	0
AWH67_RS03150	-----	sigma-54-dependent Fis family transcriptional regulator	0.86	1	0
AWH67_RS02200	<i>ntfY</i>	PAS domain-containing sensor histidine kinase	0.86	1	0
AWH67_RS01280	-----	cysteine biosynthesis protein	0.85	1	0
AWH67_RS01770	<i>corC</i>	HlyC/CorC family transporter	0.85	1	0
AWH67_RS02580	-----	TonB-dependent hemoglobin/transferrin/lactoferrin family receptor	0.83	1	0
AWH67_RS02435	<i>dnaB</i>	replicative DNA helicase	0.83	1	0
AWH67_RS00510	<i>zapA</i>	cell division protein	0.81	1	0
AWH67_RS00640	-----	hypothetical protein	0.81	1	0
AWH67_RS03710	-----	DUF4159 domain-containing protein	0.81	1	0
AWH67_RS00910	<i>holA</i>	DNA polymerase III subunit delta	0.80	1	0
AWH67_RS04990	-----	autotransporter outer membrane beta-barrel domain-containing protein	0.80	1	0
AWH67_RS00980	-----	hypothetical protein	0.79	1	0
AWH67_RS04165	-----	hypothetical protein	0.77	1	0
AWH67_RS03560	-----	pyrroline-5-carboxylate reductase	0.77	1	0
AWH67_RS02350	<i>lptF</i>	LPS export ABC transporter permease	0.77	1	0
AWH67_RS01495	<i>ndvB</i>	protein ndvB	0.75	1	0
AWH67_RS05075	<i>fliM</i>	flagellar motor switch protein	0.74	1	0
AWH67_RS03870	<i>tetA</i>	tetracycline resistance MFS efflux pump	0.98	0.75	0
AWH67_RS02510	<i>recO</i>	DNA repair protein	0.73	1	0
AWH67_RS04080	-----	hypothetical protein	0.73	1	0
AWH67_RS00430	-----	DUF1465 domain-containing protein	0.73	1	0
AWH67_RS05000	-----	hypothetical protein	0.72	1	0

DS: druggability score, human off target: this score reflects the results of a blastp search of the pathogen protein in the human proteome database with the scale 1 - max (alignment identity), so when a protein has no hit in the human proteome, the value is 1. Gut microbiome: percentage of the 226 representative microorganisms of human intestinal flora sequenced by the Human Microbiome Project that have at least one hit with any pathogen protein.