

Structural Analysis of Hypothetical Proteins from *Helicobacter pylori*: An Approach to Estimate Functions of Unknown or Hypothetical Proteins

Supplementary Information

Table S1. The protein structures from *H. pylori* determined up to date.

PDB ID	Chain ID	AA	Structure MW	Chain MW	Ligand MW	Macromolecule Name	Classification	Ligand Name	Ligand ID	Macromol. Type	Exp. Method	Rel. Date	Center Name
1E9Y	A	238	88526.37	26571.90		Urease subunit alpha	Hydrolase			Protein	X-ray	2001-11-01	
	B	569	88526.37	61762.00	75.07	Urease subunit beta	Hydrolase	Acetohydroxamic acid	HAE	Protein	X-ray	2001-11-01	
	B	569	88526.37	61762.00	190.20	Urease subunit beta	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2001-11-01	
	B	569	88526.37	61762.00	58.70	Urease subunit beta	Hydrolase	Nickel (ii) ion	NI	Protein	X-ray	2001-11-01	
1E9Z	A	238	88435.30	26571.90		Urease subunit alpha	Hydrolase			Protein	X-ray	2001-11-01	
	B	569	88435.30	61746.00	190.20	Urease subunit beta	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2001-11-01	
	B	569	88435.30	61746.00	58.70	Urease subunit beta	Hydrolase	Nickel (ii) ion	NI	Protein	X-ray	2001-11-01	
1FUE	A	163	17761.55	17305.20	456.35	Flavodoxin	Electron transport	Flavin mononucleotide	FMN	Protein	X-ray	2002-02-06	
1G6O	A	330	77214.21	37914.60	427.20	Cag-alpha	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2001-01-24	MCSG ^a
	A	330	77214.21	37914.60	196.11	Cag-alpha	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2001-01-24	MCSG
	B	330	77214.21	37914.60	427.20	Cag-alpha	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2001-01-24	MCSG
	B	330	77214.21	37914.60	196.11	Cag-alpha	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2001-01-24	MCSG
	B	330	77214.21	37914.60	106.12	Cag-alpha	Hydrolase	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2001-01-24	MCSG
1J2Y	A	167	18689.55	18499.40	190.15	3-dehydroquinate dehydratase	Lyase	1,3,4-trihydroxy-5-oxo-cyclohexanecarboxylic acid	DQA	Protein	X-ray	2003-06-24	
1J2Z	A	270	30547.34	29896.70	96.06	Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2004-01-27	
	A	270	30547.34	29896.70	308.43	Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase	Transferase	2-hydroxymethyl-6-octylsulfanyl-tetrahydro-pyran-3,4,5-triol	SOG	Protein	X-ray	2004-01-27	
	A	270	30547.34	29896.70	150.09	Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase	Transferase	L(+)-tartaric acid	TLA	Protein	X-ray	2004-01-27	
1J6X	A	160	37837.97	18704.40	196.11	Autoinducer-2protein luxs	Signaling protein	Selenomethionine	MSE	Protein	X-ray	2001-06-08	
	A	160	37837.97	18704.40	65.38	Autoinducer-2protein luxs	Signaling protein	Zinc ion	ZN	Protein	X-ray	2001-06-08	

1J14	B	160	37837.97	18704.40	196.11	Autoinducer-2protein luxs	Signaling protein	Selenomethionine	MSE	Protein	X-ray	2001-06-08
	B	160	37837.97	18704.40	65.38	Autoinducer-2protein luxs	Signaling protein	Zinc ion	ZN	Protein	X-ray	2001-06-08
	A	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	A	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	A	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	B	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	B	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	B	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	C	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	C	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	C	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	D	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	D	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	D	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	E	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	E	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	E	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	F	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	F	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	F	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	G	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	G	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	G	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	H	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	H	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	H	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	I	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	I	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09
	I	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09
	J	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09
	J	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09

	J	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09	
	K	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09	
	K	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09	
	K	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09	
	L	144	205615.45	16960.60	55.85	Neutrophil-activating protein a	Metal transport	Fe (iii) ion	FE	Protein	X-ray	2002-10-09	
	L	144	205615.45	16960.60	118.18	Neutrophil-activating protein a	Metal transport	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2002-10-09	
	L	144	205615.45	16960.60		Neutrophil-activating protein a	Metal transport	Unknown atom or ion	UNX	Protein	X-ray	2002-10-09	
1KLX	A	138	15367.80	15367.80		Cysteineprotein B	Hydrolase			Protein	X-ray	2002-09-11	
1MW7	A	240	27161.20	27161.20		Hypothetical protein hp0162	SG ^b , unknown function			Protein	X-ray	2003-01-28	NSGC ^c
1NLY	A	330	77410.55	37914.60	523.24	Virb11 homolog	Hydrolase	Phosphothiophosphoric acid-adenylate ester	ATG	Protein	X-ray	2003-05-06	
	A	330	77410.55	37914.60	24.31	Virb11 homolog	Hydrolase	Magnesium ion	MG	Protein	X-ray	2003-05-06	
	A	330	77410.55	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	B	330	77410.55	37914.60	414.49	Virb11 homolog	Hydrolase	Nonaethylene glycol	2PE	Protein	X-ray	2003-05-06	
	B	330	77410.55	37914.60	523.24	Virb11 homolog	Hydrolase	Phosphothiophosphoric acid-adenylate ester	ATG	Protein	X-ray	2003-05-06	
	B	330	77410.55	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	B	330	77410.55	37914.60	96.06	Virb11 homolog	Hydrolase	Sulfate ion	SO4	Protein	X-ray	2003-05-06	
1NLZ	A	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	B	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	C	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	D	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	E	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	F	330	227487.61	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
1OPX	A	330	76435.81	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
1OPX	A	330	76435.81	37914.60	96.06	Virb11 homolog	Hydrolase	Sulfate ion	SO4	Protein	X-ray	2003-05-06	
	B	330	76435.81	37914.60	414.49	Virb11 homolog	Hydrolase	Nonaethylene glycol	2PE	Protein	X-ray	2003-05-06	
	B	330	76435.81	37914.60	196.11	Virb11 homolog	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2003-05-06	
	B	330	76435.81	37914.60	96.06	Virb11 homolog	Hydrolase	Sulfate ion	SO4	Protein	X-ray	2003-05-06	
1OT0	A	20	2396.99	2396.99	16.02	50sprotein L1	Antibiotic	Amino group	NH2	Protein	NMR	2004-09-07	
1OUV	A	273	29972.10	29972.10		Conservedprotein	Hydrolase			Protein	X-ray	2004-03-30	

1PU6	A	218	50786.53	25218.30	78.13	3-methyladenine dna glycosylase	Hydrolase	Beta-mercaptoethanol	BME	Protein	X-ray	2003-10-07
	A	218	50786.53	25218.30	35.45	3-methyladenine dna glycosylase	Hydrolase	Chloride ion	CL	Protein	X-ray	2003-10-07
	A	218	50786.53	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	B	218	50786.53	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	B	218	50786.53	25218.30	118.18	3-methyladenine dna glycosylase	Hydrolase	(4s)-2-methyl-2,4-pentanediol	MPD	Protein	X-ray	2003-10-07
1PU7	A	218	50921.24	25218.30	164.19	3-methyladenine dna glycosylase	Hydrolase	6-amino-3,9-dimethyl-9h-purin-3-ium	39A	Protein	X-ray	2003-10-07
	A	218	50921.24	25218.30	78.13	3-methyladenine dna glycosylase	Hydrolase	Beta-mercaptoethanol	BME	Protein	X-ray	2003-10-07
	A	218	50921.24	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	B	218	50921.24	25218.30	164.19	3-methyladenine dna glycosylase	Hydrolase	6-amino-3,9-dimethyl-9h-purin-3-ium	39A	Protein	X-ray	2003-10-07
	B	218	50921.24	25218.30	78.13	3-methyladenine dna glycosylase	Hydrolase	Beta-mercaptoethanol	BME	Protein	X-ray	2003-10-07
1PU8	B	218	50921.24	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	A	218	50911.16	25218.30	78.13	3-methyladenine dna glycosylase	Hydrolase	Beta-mercaptoethanol	BME	Protein	X-ray	2003-10-07
	A	218	50911.16	25218.30	159.15	3-methyladenine dna glycosylase	Hydrolase	3h-imidazo[2,1-i]purine	EA1	Protein	X-ray	2003-10-07
	A	218	50911.16	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	B	218	50911.16	25218.30	78.13	3-methyladenine dna glycosylase	Hydrolase	Beta-mercaptoethanol	BME	Protein	X-ray	2003-10-07
1QWL	B	218	50911.16	25218.30	159.15	3-methyladenine dna glycosylase	Hydrolase	3h-imidazo[2,1-i]purine	EA1	Protein	X-ray	2003-10-07
	B	218	50911.16	25218.30	190.20	3-methyladenine dna glycosylase	Hydrolase	Lysine nz-carboxylic acid	KCX	Protein	X-ray	2003-10-07
	A	505	118768.41	58730.70	616.50	Kata catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2004-03-30
	A	505	118768.41	58730.70	32.00	Kata catalase	Oxidoreductase	Oxygen molecule	OXY	Protein	X-ray	2004-03-30
	B	505	118768.41	58730.70	42.02	Kata catalase	Oxidoreductase	Azide ion	AZI	Protein	X-ray	2004-03-30
1QWM	B	505	118768.41	58730.70	616.50	Kata catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2004-03-30
	A	505	120393.35	58730.70	42.02	Kata catalase	Oxidoreductase	Azide ion	AZI	Protein	X-ray	2004-03-30
	A	505	120393.35	58730.70	46.03	Kata catalase	Oxidoreductase	Formic acid	FMT	Protein	X-ray	2004-03-30
	A	505	120393.35	58730.70	616.50	Kata catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2004-03-30
	B	505	120393.35	58730.70	46.03	Kata catalase	Oxidoreductase	Formic acid	FMT	Protein	X-ray	2004-03-30
1S2X	B	505	120393.35	58730.70	616.50	Kata catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2004-03-30
	A	206	23998.70	23938.60	60.10	Cag-Z	Unknown function	Isopropyl alcohol	IPA	Protein	X-ray	2004-07-27
1UHD	A	206	23998.70	23938.60	196.11	Cag-Z	Unknown function	Selenomethionine	MSE	Protein	X-ray	2004-07-27
	A	96	13339.46	10533.20	90.08	Aspartate 1-decarboxylase alpha chain	Lyase	Lactic acid	LAC	Protein	X-ray	2004-07-13
1UHE	B	24	13339.46	2806.26		Aspartate 1-decarboxylase beta chain	Lyase			Protein	X-ray	2004-07-13
	A	97	13744.94	10737.50	201.18	Aspartate 1-decarboxylase alpha chain	Lyase	N~2~-(2-amino-1-methyl-2-	NSN	Protein	X-ray	2004-07-13

oxoethylidene)asparaginate											
	B	24	13744.94	2806.26	Aspartate 1-decarboxylase beta chain	Lyase			Protein	X-ray	2004-07-13
1UM0	A	365	162446.59	40155.30	456.35	Chorismate synthase	Lyase	Flavin mononucleotide	FMN	Protein	X-ray 2004-06-01
	B	365	162446.59	40155.30	456.35	Chorismate synthase	Lyase	Flavin mononucleotide	FMN	Protein	X-ray 2004-06-01
	C	365	162446.59	40155.30	456.35	Chorismate synthase	Lyase	Flavin mononucleotide	FMN	Protein	X-ray 2004-06-01
	D	365	162446.59	40155.30	456.35	Chorismate synthase	Lyase	Flavin mononucleotide	FMN	Protein	X-ray 2004-06-01
1UM8	A	376	42519.20	42092.00	427.20	ATP-dependent Clp protease ATP-binding subunit clpx	Chaperone	Adenosine-5'-diphosphate	ADP	Protein	X-ray 2003-12-23
1UMF	A	365	160621.20	40155.30		Chorismate synthase	Lyase			Protein	X-ray 2004-06-01
	B	365	160621.20	40155.30		Chorismate synthase	Lyase			Protein	X-ray 2004-06-01
	C	365	160621.20	40155.30		Chorismate synthase	Lyase			Protein	X-ray 2004-06-01
	D	365	160621.20	40155.30		Chorismate synthase	Lyase			Protein	X-ray 2004-06-01
1X93	A	55	13142.92	6571.46		Hypothetical protein HP0222	Transcription			Protein	NMR 2005-03-22
	B	55	13142.92	6571.46		Hypothetical protein HP0222	Transcription			Protein	NMR 2005-03-22
1XNG	A	268	63146.42	30376.30	507.18	NH(3)-dependent NAD(+) synthetase	Ligase	Adenosine-5'-triphosphate	ATP	Protein	X-ray 2005-04-05
	A	268	63146.42	30376.30	665.42	NH(3)-dependent NAD(+) synthetase	Ligase	Nicotinic acid adenine dinucleotide	DND	Protein	X-ray 2005-04-05
	A	268	63146.42	30376.30	24.31	NH(3)-dependent NAD(+) synthetase	Ligase	Magnesium ion	MG	Protein	X-ray 2005-04-05
	B	268	63146.42	30376.30	507.18	NH(3)-dependent NAD(+) synthetase	Ligase	Adenosine-5'-triphosphate	ATP	Protein	X-ray 2005-04-05
	B	268	63146.42	30376.30	665.42	NH(3)-dependent NAD(+) synthetase	Ligase	Nicotinic acid adenine dinucleotide	DND	Protein	X-ray 2005-04-05
	B	268	63146.42	30376.30	24.31	NH(3)-dependent NAD(+) synthetase	Ligase	Magnesium ion	MG	Protein	X-ray 2005-04-05
1XNH	A	268	30376.30	30376.30		NH(3)-dependent NAD(+) synthetase	Ligase			Protein	X-ray 2005-04-05
1YG0	A	66	7203.31	7203.31		Copproteins	Metal transport			Protein	NMR 2006-01-24
1YGZ	A	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
	B	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
	C	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
	D	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
	E	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
	F	173	116914.20	19485.70	196.11	Inorganic pyrophosphatase	Hydrolase	Selenomethionine	MSE	Protein	X-ray 2005-11-01
1Z8M	A	88	10394.30	10394.30		Conservedprotein HP0894	SG, Unknown function			Protein	NMR 2005-11-01
1ZHC	A	76	9130.38	9130.38		Hypothetical protein HP1242	Unknown function			Protein	NMR 2005-12-06
1ZKE	A	83	56798.00	9450.13		Hypothetical protein HP1531	SG, unknown function			Protein	X-ray 2005-06-28 MCSG

	B	83	56798.00	9450.13	24.31	Hypothetical protein HP1531	SG, unknown function	Magnesium ion	MG	Protein	X-ray	2005-06-28	MCSG
	C	83	56798.00	9450.13	24.31	Hypothetical protein HP1531	SG, unknown function	Magnesium ion	MG	Protein	X-ray	2005-06-28	MCSG
	D	83	56798.00	9450.13	24.31	Hypothetical protein HP1531	SG, unknown function	Magnesium ion	MG	Protein	X-ray	2005-06-28	MCSG
	E	83	56798.00	9450.13	24.31	Hypothetical protein HP1531	SG, unknown function	Magnesium ion	MG	Protein	X-ray	2005-06-28	MCSG
	F	83	56798.00	9450.13		Hypothetical protein HP1531	SG, unknown function			Protein	X-ray	2005-06-28	MCSG
1ZOF	A	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	B	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	C	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	D	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	E	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	F	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	G	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	H	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	I	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
	J	198	222768.00	22276.80		Alkyl hydroperoxide-reductase	Oxidoreductase			Protein	X-ray	2005-11-29	
1ZUH	A	168	19265.50	19265.50		Shikimate kinase	Transferase			Protein	X-ray	2006-05-31	
1ZUI	A	168	19534.62	19265.50	94.97	Shikimate kinase	Transferase	Phosphate ion	PO4	Protein	X-ray	2006-05-31	
	A	168	19534.62	19265.50	174.15	Shikimate kinase	Transferase	(3r,4s,5r)-3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid	SKM	Protein	X-ray	2006-05-31	
2A6M	A	155	36212.60	18106.30		Ishp608 transposase	Transcription/dna			Protein	X-ray	2005-10-25	
	B	155	36212.60	18106.30		Ishp608 transposase	Transcription/dna			Protein	X-ray	2005-10-25	
2A6O	A	155	49699.42	18106.30		Ishp608 Transposase	Transcription/dna			Protein	X-ray	2005-10-25	
	B	155	49699.42	18106.30		Ishp608 Transposase	Transcription/dna			DNA			
										Protein	X-ray	2005-10-25	
										DNA			
	C	22	49699.42	6743.41		5'- d(*cp*cp*cp*cp*tp*ap*gp*cp*tp*tp*t p*ap*gp*cp*tp*ap*tp*gp*gp*gp*gp*a)-3'	Transcription/dna			Protein	X-ray	2005-10-25	
										DNA			
	D	22	49699.42	6743.41		5'- d(*cp*cp*cp*cp*tp*ap*gp*cp*tp*tp*t	Transcription/dna			Protein	X-ray	2005-10-25	
										DNA			

p*ap*gp*cp*tp*ap*tp*gp*gp*gp*gp*a												
)-3'												
2A9E	A	505	118913.44	58794.70	59.04	Kata Catalase	Oxidoreductase	Acetate ion	ACT	Protein	X-ray	2006-06-20
	A	505	118913.44	58794.70	616.50	Kata Catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2006-06-20
	A	505	118913.44	58794.70	165.21	Kata Catalase	Oxidoreductase	S-oxymethionine	MHO	Protein	X-ray	2006-06-20
	A	505	118913.44	58794.70	16.00	Kata Catalase	Oxidoreductase	Oxygen atom	O	Protein	X-ray	2006-06-20
	B	505	118913.44	58794.70	616.50	Kata Catalase	Oxidoreductase	Protoporphyrin ix containing fe	HEM	Protein	X-ray	2006-06-20
	B	505	118913.44	58794.70	165.21	Kata Catalase	Oxidoreductase	S-oxymethionine	MHO	Protein	X-ray	2006-06-20
	B	505	118913.44	58794.70	16.00	Kata Catalase	Oxidoreductase	Oxygen atom	O	Protein	X-ray	2006-06-20
2ATZ	A	180	22049.45	21480.20	507.18	H. Pylori predicted coding region hp0184	SG, unknown function	2'-deoxyguanosine-5'-triphosphate	DGT	Protein	X-ray	2005-10-11 MCSG
	A	180	22049.45	21480.20	62.07	H. Pylori predicted coding region hp0184	SG, unknown function	1,2-ethanediol	EDO	Protein	X-ray	2005-10-11 MCSG
	A	180	22049.45	21480.20	196.11	H. Pylori predicted coding region hp0184	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2005-10-11 MCSG
2B7N	A	273	93342.24	30850.90	167.12	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Quinolinic acid	NTM	Protein	X-ray	2006-02-14
	A	273	93342.24	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14
	B	273	93342.24	30850.90	167.12	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Quinolinic acid	NTM	Protein	X-ray	2006-02-14
	B	273	93342.24	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14
	C	273	93342.24	30850.90	167.12	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Quinolinic acid	NTM	Protein	X-ray	2006-02-14
	C	273	93342.24	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14
2B7P	A	273	93339.28	30850.90	166.13	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Phthalic acid	PHT	Protein	X-ray	2006-02-14
	A	273	93339.28	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14

	B	273	93339.28	30850.90	166.13	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Phthalic acid	PHT	Protein	X-ray	2006-02-14
	B	273	93339.28	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14
	C	273	93339.28	30850.90	166.13	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Phthalic acid	PHT	Protein	X-ray	2006-02-14
	C	273	93339.28	30850.90	96.06	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Sulfate ion	SO4	Protein	X-ray	2006-02-14
2B7Q	A	273	93558.32	30850.90	335.21	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Nicotinate mononucleotide	NCN	Protein	X-ray	2006-02-21
	B	273	93558.32	30850.90	335.21	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Nicotinate mononucleotide	NCN	Protein	X-ray	2006-02-21
	C	273	93558.32	30850.90	335.21	Probable nicotinate-nucleotide pyrophosphorylase	Transferase	Nicotinate mononucleotide	NCN	Protein	X-ray	2006-02-21
2BHV	A	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
	B	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
	C	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
	D	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
	E	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
	F	246	163102.81	27183.80		Comb10	Bacterial protein			Protein	X-ray	2005-03-16
2BMV	A	164	17668.11	17512.50	120.15	Flavodoxin	Electron transport	Benzamidine	BEN	Protein	X-ray	2006-06-22
	A	164	17668.11	17512.50	35.45	Flavodoxin	Electron transport	Chloride ion	CL	Protein	X-ray	2006-06-22
2BO3	A	94	11101.70	11101.70		Hypothetical protein hp0242	SG,unknown function			Protein	X-ray	2006-06-22
2BQX	A	173	19298.10	19298.10		Inorganic pyrophosphatase	Hydrolase			Protein	X-ray	2006-10-18
2BQY	A	173	19474.06	19298.10	175.96	Inorganic pyrophosphatase	Hydrolase	Pyrophosphate 2-	POP	Protein	X-ray	2006-10-18
2C4V	A	167	18691.53	18499.40	192.12	3-dehydroquinate dehydratase	Lyase	Citric acid	CIT	Protein	X-ray	2006-02-22
2C4W	A	176	20056.08	19390.40	343.32	3-dehydroquinate dehydratase	Lyase	N-tetrazol-5-yl 9-oxo-9h-xanthene-2 sulphonamide	GAJ	Protein	X-ray	2006-02-22
	A	176	20056.08	19390.40	92.09	3-dehydroquinate dehydratase	Lyase	Glycerol	GOL	Protein	X-ray	2006-02-22
	A	176	20056.08	19390.40	69.09	3-dehydroquinate dehydratase	Lyase	Imidazole	IMD	Protein	X-ray	2006-02-22
2C57	A	180	241596.66	19958.90	174.15	3-dehydroquinate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22

	B	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	C	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	D	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	E	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	F	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	G	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	H	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	I	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	J	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	K	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
	L	180	241596.66	19958.90	174.15	3-dehydroquininate dehydratase	Lyase	2,3 -anhydro-quinic acid	FA1	Protein	X-ray	2006-02-22
2CA9	A	148	34939.26	17170.40	46.03	Putative nickel-responsive regulator	Transcriptional regulation	Formic acid	FMT	Protein	X-ray	2006-07-17
	A	148	34939.26	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
	B	148	34939.26	17170.40	46.03	Putative nickel-responsive regulator	Transcriptional regulation	Formic acid	FMT	Protein	X-ray	2006-07-17
	B	148	34939.26	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
2CAD	A	148	35169.41	17170.40	46.03	Putative nickel-responsive regulator	Transcriptional regulation	Formic acid	FMT	Protein	X-ray	2006-07-17
	A	148	35169.41	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
	A	148	35169.41	17170.40	58.70	Putative nickel-responsive regulator	Transcriptional regulation	Nickel (ii) ion	NI	Protein	X-ray	2006-07-17
	B	148	35169.41	17170.40	192.12	Putative nickel-responsive regulator	Transcriptional regulation	Citric acid	CIT	Protein	X-ray	2006-07-17
	B	148	35169.41	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
	B	148	35169.41	17170.40	58.70	Putative nickel-responsive regulator	Transcriptional regulation	Nickel (ii) ion	NI	Protein	X-ray	2006-07-17

2CAJ	A	148	35046.22	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
	B	148	35046.22	17170.40	35.45	Putative nickel-responsive regulator	Transcriptional regulation	Chloride ion	CL	Protein	X-ray	2006-07-17
	B	148	35046.22	17170.40	92.09	Putative nickel-responsive regulator	Transcriptional regulation	Glycerol	GOL	Protein	X-ray	2006-07-17
	B	148	35046.22	17170.40	58.70	Putative nickel-responsive regulator	Transcriptional regulation	Nickel (ii) ion	NI	Protein	X-ray	2006-07-17
2CMG	A	262	61171.80	30585.90		Spermidine synthase	Transferase			Protein	X-ray	2007-05-08
	B	262	61171.80	30585.90		Spermidine synthase	Transferase			Protein	X-ray	2007-05-08
2CMH	A	262	91757.70	30585.90		Spermidine synthase	Transferase			Protein	X-ray	2007-05-08
	B	262	91757.70	30585.90		Spermidine synthase	Transferase			Protein	X-ray	2007-05-08
	C	262	91757.70	30585.90		Spermidine synthase	Transferase			Protein	X-ray	2007-05-08
2CMU	A	342	39349.10	39349.10	196.11	Putative peptidyl-arginine deiminase	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2006-05-24
2D2R	A	245	57152.20	28576.10		Undecaprenyl pyrophosphate synthase	Transferase			Protein	X-ray	2006-09-26
	B	245	57152.20	28576.10		Undecaprenyl pyrophosphate synthase	Transferase			Protein	X-ray	2006-09-26
2DTN	A	245	57326.14	28576.10		Undecaprenyl pyrophosphate synthase	Transferase			Protein	X-ray	2007-06-26
	B	245	57326.14	28576.10	173.94	Undecaprenyl pyrophosphate synthase	Transferase	Diphosphate	DPO	Protein	X-ray	2007-06-26
2DYU	A	334	74661.40	37330.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	B	334	74661.40	37330.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
2DYV	A	334	74661.40	37330.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	B	334	74661.40	37330.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
2E2K	A	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	B	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	C	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	D	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	E	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	F	334	223888.19	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
2E2L	A	334	224023.31	37314.70	45.04	Formamidase	Hydrolase	Formamide	ARF	Protein	X-ray	2007-02-13
	B	334	224023.31	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13
	C	334	224023.31	37314.70	45.04	Formamidase	Hydrolase	Formamide	ARF	Protein	X-ray	2007-02-13

	D	334	224023.31	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13	
	E	334	224023.31	37314.70		Formamidase	Hydrolase			Protein	X-ray	2007-02-13	
	F	334	224023.31	37314.70	45.04	Formamidase	Hydrolase	Formamide	ARF	Protein	X-ray	2007-02-13	
2EVV	A	207	95692.83	23807.10	92.09	Hypothetical protein HP0218	SG, unknown function	Glycerol	GOL	Protein	X-ray	2005-12-13	MCSG
	A	207	95692.83	23807.10	196.11	Hypothetical protein HP0218	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2005-12-13	MCSG
	B	207	95692.83	23807.10	92.09	Hypothetical protein HP0218	SG, unknown function	Glycerol	GOL	Protein	X-ray	2005-12-13	MCSG
	B	207	95692.83	23807.10	196.11	Hypothetical protein HP0218	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2005-12-13	MCSG
	B	207	95692.83	23807.10	96.06	Hypothetical protein HP0218	SG, unknown function	Sulfate ion	SO4	Protein	X-ray	2005-12-13	MCSG
	C	207	95692.83	23807.10	92.09	Hypothetical protein HP0218	SG, unknown function	Glycerol	GOL	Protein	X-ray	2005-12-13	MCSG
	C	207	95692.83	23807.10	196.11	Hypothetical protein HP0218	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2005-12-13	MCSG
	D	207	95692.83	23807.10	92.09	Hypothetical protein HP0218	SG, unknown function	Glycerol	GOL	Protein	X-ray	2005-12-13	MCSG
	D	207	95692.83	23807.10	196.11	Hypothetical protein HP0218	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2005-12-13	MCSG
2EW5	A	181	21434.93	21008.60	58.93	Peptide deformylase	Hydrolase	Cobalt (ii) ion	CO	Protein	X-ray	2006-10-24	
	A	181	21434.93	21008.60	367.40	Peptide deformylase	Hydrolase	4-((1e)-3-oxo-3-[(2-phenylethyl)amino]prop-1-en-1-yl)-1,2-phenylene diacetate	Y12	Protein	X-ray	2006-10-24	
2EW6	A	181	21366.86	21008.60	58.93	Peptide deformylase	Hydrolase	Cobalt (ii) ion	CO	Protein	X-ray	2006-10-24	
	A	181	21366.86	21008.60	299.33	Peptide deformylase	Hydrolase	(2e)-3-(3,4-dihydroxyphenyl)-n-[2-(4-hydroxyphenyl)ethyl]acrylamide	Y13	Protein	X-ray	2006-10-24	
2EW7	A	181	21067.53	21008.60	58.93	Peptide deformylase	Hydrolase	Cobalt (ii) ion	CO	Protein	X-ray	2006-10-24	
2F6S	A	201	47249.90	23464.60	196.11	Cellprotein, putative	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2006-01-10	MCSG
	A	201	47249.90	23464.60	94.97	Cellprotein, putative	SG, unknown function	Phosphate ion	PO4	Protein	X-ray	2006-01-10	MCSG
	A	201	47249.90	23464.60	65.38	Cellprotein, putative	SG, unknown function	Zinc ion	ZN	Protein	X-ray	2006-01-10	MCSG
	B	201	47249.90	23464.60	196.11	Cellprotein, putative	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2006-01-10	MCSG
	B	201	47249.90	23464.60	94.97	Cellprotein, putative	SG, unknown function	Phosphate ion	PO4	Protein	X-ray	2006-01-10	MCSG
	B	201	47249.90	23464.60	65.38	Cellprotein, putative	SG, unknown function	Zinc ion	ZN	Protein	X-ray	2006-01-10	MCSG
2FN6	A	375	85108.34	42459.20	94.97	Aminotransferase	Transferase	Phosphate ion	PO4	Protein	X-ray	2006-01-24	MKBSGI ^d
	B	375	85108.34	42459.20	94.97	Aminotransferase	Transferase	Phosphate ion	PO4	Protein	X-ray	2006-01-24	MKBSGI
2FNI	A	375	85412.69	42459.20	247.14	Aminotransferase	Transferase	Pyridoxal-5'-phosphate	PLP	Protein	X-ray	2006-01-24	MKBSGI
	B	375	85412.69	42459.20	247.14	Aminotransferase	Transferase	Pyridoxal-5'-phosphate	PLP	Protein	X-ray	2006-01-24	MKBSGI
2FNU	A	375	86629.46	42459.20	248.18	Aminotransferase	Transferase	4'-deoxy-4'-aminopyridoxal-5'	PMP	Protein	X-ray	2006-01-24	MKBSGI

							phosphate						
	A	375	86629.46	42459.20	607.36	Aminotransferase	Transferase	Uridine-diphosphate-n-acetylglucosamine	UD1	Protein	X-ray	2006-01-24	MKBSGI
	B	375	86629.46	42459.20	248.18	Aminotransferase	Transferase	4'-deoxy-4'-aminopyridoxal-5'-phosphate	PMP	Protein	X-ray	2006-01-24	MKBSGI
	B	375	86629.46	42459.20	607.36	Aminotransferase	Transferase	Uridine-diphosphate-n-acetylglucosamine	UD1	Protein	X-ray	2006-01-24	MKBSGI
2G3V	A	208	104975.36	25537.10	196.11	Cagprotein 13	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	B	208	104975.36	25537.10	196.11	Cagprotein 13	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	C	208	104975.36	25537.10	196.11	Cagprotein 13	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	D	208	104975.36	25537.10	196.11	Cagprotein 13	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	E	7	104975.36	706.74	196.11	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	E	7	104975.36	706.74	103.12	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Unknown	UNK	Protein	X-ray	2007-03-06	
	F	7	104975.36	706.74	196.11	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	F	7	104975.36	706.74	103.12	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Unknown	UNK	Protein	X-ray	2007-03-06	
	G	7	104975.36	706.74	196.11	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	G	7	104975.36	706.74	103.12	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Unknown	UNK	Protein	X-ray	2007-03-06	
2GLL	H	7	104975.36	706.74	196.11	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Selenomethionine	MSE	Protein	X-ray	2007-03-06	
	H	7	104975.36	706.74	103.12	(Unk)(unk)(unk)(unk)(unk)(mse)(unk)	Unknown function	Unknown	UNK	Protein	X-ray	2007-03-06	
	A	171	118844.75	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13	
	A	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
	B	171	118844.75	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13	
	B	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
	C	171	118844.75	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13	
	C	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	

					dehydratase							
	D	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
	E	171	118844.75	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	E	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
	F	171	118844.75	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	F	171	118844.75	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
2GLM	A	171	119207.54	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	A	171	119207.54	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
	A	171	119207.54	19611.80	482.94	(3R)-hydroxymyristoyl-acylprotein	Lyase	2-chloro-5-(5-((e)-[(2z)-3-(2-methoxyethyl)-4-oxo-2-(phenylimino)-1,3-thiazolidin-5-ylidene]methyl)-2-furyl)benzoic acid	SCB	Protein	X-ray	2007-03-13
					dehydratase							
	B	171	119207.54	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	B	171	119207.54	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
	C	171	119207.54	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	C	171	119207.54	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							
	D	171	119207.54	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
					dehydratase							
	D	171	119207.54	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
					dehydratase							

	E	171	119207.54	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
	F	171	119207.54	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
2GLP	A	171	119915.14	19611.80	415.04	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	N'-[(1e)-(3,5-dibromo-2,4- dihydroxyphenyl)methylene]nicotinohy drazide	BDE	Protein	X-ray	2007-03-13
	A	171	119915.14	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
	A	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
	B	171	119915.14	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
	B	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
	C	171	119915.14	19611.80	415.04	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	N'-[(1e)-(3,5-dibromo-2,4- dihydroxyphenyl)methylene]nicotinohy drazide	BDE	Protein	X-ray	2007-03-13
	C	171	119915.14	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
	C	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
	D	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
	E	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
	F	171	119915.14	19611.80	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2007-03-13
	F	171	119915.14	19611.80	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13
2GLV	A	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13

					dehydratase							
B	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
C	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
D	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
E	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
F	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
G	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
H	171	234661.83	19519.70		(3R)-hydroxymyristoyl-acylprotein	Lyase			Protein	X-ray	2007-03-13	
					dehydratase							
I	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
J	171	234661.83	19519.70		(3R)-hydroxymyristoyl-acylprotein	Lyase			Protein	X-ray	2007-03-13	
					dehydratase							
K	171	234661.83	19519.70	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2007-03-13	
					dehydratase							
L	171	234661.83	19519.70		(3R)-hydroxymyristoyl-acylprotein	Lyase			Protein	X-ray	2007-03-13	
					dehydratase							
2GN4	A	344	80546.24	38725.10	745.43	UDP-glcnaC6 dehydratase	Lyase	Nadph dihydro-nicotinamide-adenine-dinucleotide phosphate	NDP	Protein	X-ray	2006-05-09
	A	344	80546.24	38725.10	607.36	UDP-glcnaC6 dehydratase	Lyase	Uridine-diphosphate-n-acetylglucosamine	UD1	Protein	X-ray	2006-05-09
	B	344	80546.24	38725.10	195.23	UDP-glcnaC6 dehydratase	Lyase	2-(n-morpholino)-ethanesulfonic acid	MES	Protein	X-ray	2006-05-09
	B	344	80546.24	38725.10	745.43	UDP-glcnaC6 dehydratase	Lyase	Nadph dihydro-nicotinamide-adenine-dinucleotide phosphate	NDP	Protein	X-ray	2006-05-09
	B	344	80546.24	38725.10	607.36	UDP-glcnaC6 dehydratase	Lyase	Uridine-diphosphate-n-	UD1	Protein	X-ray	2006-05-09

							acetylglucosamine						
2GN6	A	344	80346.97	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	A	344	80346.97	38725.10	607.36	UDP-glcnaC6 dehydratase	Lyase	Uridine-diphosphate-n-acetylglucosamine	UD1	Protein	X-ray	2006-05-09	
	B	344	80346.97	38725.10	195.23	UDP-glcnaC6 dehydratase	Lyase	2-(n-morpholino)-ethanesulfonic acid	MES	Protein	X-ray	2006-05-09	
	B	344	80346.97	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	B	344	80346.97	38725.10	607.36	UDP-glcnaC6 dehydratase	Lyase	Uridine-diphosphate-n-acetylglucosamine	UD1	Protein	X-ray	2006-05-09	
2GN8	A	344	79940.58	38725.10	195.23	UDP-glcnaC6 dehydratase	Lyase	2-(n-morpholino)-ethanesulfonic acid	MES	Protein	X-ray	2006-05-09	
	A	344	79940.58	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	A	344	79940.58	38725.10	404.16	UDP-glcnaC6 dehydratase	Lyase	Uridine-5'-diphosphate	UDP	Protein	X-ray	2006-05-09	
	B	344	79940.58	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	B	344	79940.58	38725.10	404.16	UDP-glcnaC6 dehydratase	Lyase	Uridine-5'-diphosphate	UDP	Protein	X-ray	2006-05-09	
2GN9	A	344	80264.87	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	A	344	80264.87	38725.10	566.30	UDP-glcnaC6 dehydratase	Lyase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	195.23	UDP-glcnaC6 dehydratase	Lyase	2-(n-morpholino)-ethanesulfonic acid	MES	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	566.30	UDP-glcnaC6 dehydratase	Lyase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2006-05-09	
2GNA	A	344	80264.87	38725.10	566.30	UDP-glcnaC6 dehydratase	Lyase	Galactose-uridine-5'-diphosphate	GDU	Protein	X-ray	2006-05-09	
	A	344	80264.87	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	566.30	UDP-glcnaC6 dehydratase	Lyase	Galactose-uridine-5'-diphosphate	GDU	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	195.23	UDP-glcnaC6 dehydratase	Lyase	2-(n-morpholino)-ethanesulfonic acid	MES	Protein	X-ray	2006-05-09	
	B	344	80264.87	38725.10	743.41	UDP-glcnaC6 dehydratase	Lyase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2006-05-09	

2GTS	A	86	10626.50	10626.50	196.11	Hypothetical protein HP0062	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2006-05-30	MCSG
2H0U	A	217	26346.45	25890.10	456.35	NADPH-flavin oxidoreductase	Oxidoreductase	Flavin mononucleotide	FMN	Protein	X-ray	2006-06-13	MCSG
	A	217	26346.45	25890.10	196.11	NADPH-flavin oxidoreductase	Oxidoreductase	Selenomethionine	MSE	Protein	X-ray	2006-06-13	MCSG
2H1Y	A	321	71607.20	35803.60		Malonylprotein transacylase	Transferase			Protein	X-ray	2007-05-22	
	B	321	71607.20	35803.60		Malonylprotein transacylase	Transferase			Protein	X-ray	2007-05-22	
2H9Z	A	86	10205.80	10205.80		Hypothetical protein HP0495	SG, unknown function			Protein	NMR	2007-05-01	
2HQN	A	109	12481.40	12481.40		Putative transcriptional regulator	Signaling protein			Protein	NMR	2007-05-08	
2HQO	A	123	27757.80	13878.90		Putative transcriptional regulator	Signaling protein			Protein	NMR	2007-05-08	
	B	123	27757.80	13878.90		Putative transcriptional regulator	Signaling protein			Protein	NMR	2007-05-08	
2HQR	A	223	50946.60	25473.30		Putative transcriptional regulator	Signaling protein			Protein	NMR	2007-05-08	
	B	223	50946.60	25473.30		Putative transcriptional regulator	Signaling protein			Protein	NMR	2007-05-08	
2I9I	A	254	29526.70	29526.70		Hypothetical protein	SG, unknown function			Protein	X-ray	2006-09-26	NYSRCSG ^e
2IQF	A	505	118913.44	58794.70	59.04	Catalase	Oxidoreductase	Acetate ion	ACT	Protein	X-ray	2007-08-28	
	A	505	118913.44	58794.70	616.50	Catalase	Oxidoreductase	Protoporphyrin IX containing Fe	HEM	Protein	X-ray	2007-08-28	
	A	505	118913.44	58794.70	165.21	Catalase	Oxidoreductase	S-oxymethionine	MHO	Protein	X-ray	2007-08-28	
	A	505	118913.44	58794.70	16.00	Catalase	Oxidoreductase	Oxygen atom	O	Protein	X-ray	2007-08-28	
	B	505	118913.44	58794.70	616.50	Catalase	Oxidoreductase	Protoporphyrin IX containing Fe	HEM	Protein	X-ray	2007-08-28	
	B	505	118913.44	58794.70	165.21	Catalase	Oxidoreductase	S-oxymethionine	MHO	Protein	X-ray	2007-08-28	
	B	505	118913.44	58794.70	16.00	Catalase	Oxidoreductase	Oxygen atom	O	Protein	X-ray	2007-08-28	
2JFX	A	255	57359.06	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2007-07-03	
	B	255	57359.06	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2007-07-03	
2JFY	A	255	57359.06	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-02-19	
	B	255	57359.06	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-02-19	
2JFZ	A	255	58238.09	28532.40	439.52	Glutamate racemase	Isomerase	5-methyl-7-(2-methylpropyl)-2-(naphthalen-1-ylmethyl)-3-pyridin-4-yl-2h-pyrazolo[3,4-d]pyrimidine-4,6(5h,7h)-dione	003	Protein	X-ray	2007-07-03	
	A	255	58238.09	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2007-07-03	
	B	255	58238.09	28532.40	439.52	Glutamate racemase	Isomerase	5-methyl-7-(2-methylpropyl)-2-(naphthalen-1-ylmethyl)-3-pyridin-4-yl-2h-pyrazolo[3,4-d]pyrimidine-					

								4,6(5h,7h)-dione					
2JGQ	B	255	58238.09	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2007-07-03	
	A	233	53777.39	26612.00	94.97	Triosephosphate isomerase	Isomerase	Phosphate ion	PO4	Protein	X-ray	2008-02-26	
	A	233	53777.39	26612.00	363.45	Triosephosphate isomerase	Isomerase	1-[(3-cyclohexylpropanoyl)(2-hydroxyethyl)amino]-1-deoxy-d-allitol	QGA	Protein	X-ray	2008-02-26	
2JOQ	B	233	53777.39	26612.00	94.97	Triosephosphate isomerase	Isomerase	Phosphate ion	PO4	Protein	X-ray	2008-02-26	
	A	91	10673.20	10673.20		Hypothetical protein HP_0495	SG, unknown function			Protein	NMR	2007-04-03	OCSP ⁵
	A	91	10673.20			Hypothetical protein HP_0495	SG, unknown function			Protein	NMR	2007-04-03	NSGC
2K0Z	A	110	12948.60	12948.60		Uncharacterized protein hp1203	SG, unknown function			Protein	NMR	2008-03-04	NSGC
2K1O	A	66	15603.66	7801.83		Putative	Gene regulation			Protein	NMR	2008-10-07	
	B	66	15603.66	7801.83		Putative	Gene regulation			Protein	NMR	2008-10-07	
2K4J	A	115	13303.10	13303.10		Putative TRANSCRIPTIONAL REGULATOR	Transcription			Protein	NMR	2008-12-30	
2K6P	A	92	10472.30	10472.30		Uncharacterized protein HP_1423	Unknown function			Protein	NMR	2009-06-16	
2KDX	A	119	13430.88	13365.50	65.38	Hydrogenase/ureaseprotein hypa	Metal-binding protein	Zinc ion	ZN	Protein	NMR	2009-10-20	
2KI2	A	90	10470.00	10470.00		Ss-dnaprotein 12RNP2	Rnaprotein/ss-dnaprotein			Protein	NMR	2009-10-20	
2KR7	A	151	17039.20	17039.20		FKBP-type peptidyl-prolyl cis-trans isomerase slyd	Isomerase			Protein	NMR	2010-12-15	
2NQO	A	376	121834.00	40506.70		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2006-11-21	
	B	188	121834.00	20410.30		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2006-11-21	
	C	376	121834.00	40506.70		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2006-11-21	
	D	188	121834.00	20410.30		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2006-11-21	
2NZW	A	371	129659.87	43123.90		Alpha1,3-fucosyltransferase	Transferase			Protein	X-ray	2007-01-23	
	B	371	129659.87	43123.90	96.06	Alpha1,3-fucosyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2007-01-23	
	C	371	129659.87	43123.90	96.06	Alpha1,3-fucosyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2007-01-23	
2NZX	A	371	130797.36	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
	B	371	130797.36	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
	C	371	130797.36	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
2NZY	C	371	130797.36	43123.90	96.06	Alpha1,3-fucosyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2007-01-23	
	A	371	131385.89	43123.90	164.16	Alpha1,3-fucosyltransferase	Transferase	Alpha-l-fucose	FUC	Protein	X-ray	2007-01-23	

	A	371	131385.89	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
	B	371	131385.89	43123.90	164.16	Alpha1,3-fucosyltransferase	Transferase	Alpha-l-fucose	FUC	Protein	X-ray	2007-01-23	
	B	371	131385.89	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
	B	371	131385.89	43123.90	96.06	Alpha1,3-fucosyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2007-01-23	
	C	371	131385.89	43123.90	164.16	Alpha1,3-fucosyltransferase	Transferase	Alpha-l-fucose	FUC	Protein	X-ray	2007-01-23	
	C	371	131385.89	43123.90	443.20	Alpha1,3-fucosyltransferase	Transferase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2007-01-23	
	C	371	131385.89	43123.90	96.06	Alpha1,3-fucosyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2007-01-23	
2ORM	A	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
	B	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
	C	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
	D	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
	E	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
	F	67	44336.70	7389.45		Probable tautomerase HP0924	Isomerase			Protein	X-ray	2008-02-12	
2OTR	A	98	11502.60	11502.60		Hypothetical protein HP0892	SG, unknown function			Protein	NMR	2007-12-18	
2OUF	A	94	11148.60	11148.60	196.11	Hypothetical protein	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2007-02-27	MCSG
2PD3	A	275	123878.30	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17	
	A	275	123878.30	30016.60	289.55	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Triclosan	TCL	Protein	X-ray	2007-04-17	
	B	275	123878.30	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17	
	B	275	123878.30	30016.60	289.55	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Triclosan	TCL	Protein	X-ray	2007-04-17	
	C	275	123878.30	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17	
	C	275	123878.30	30016.60	289.55	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Triclosan	TCL	Protein	X-ray	2007-04-17	
	D	275	123878.30	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17	
	D	275	123878.30	30016.60	289.55	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Triclosan	TCL	Protein	X-ray	2007-04-17	

2PD4	A	275	123740.52	30016.60	255.10	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Diclosan	DCN	Protein	X-ray	2007-04-17
	A	275	123740.52	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17
	B	275	123740.52	30016.60	255.10	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Diclosan	DCN	Protein	X-ray	2007-04-17
	B	275	123740.52	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17
	C	275	123740.52	30016.60	255.10	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Diclosan	DCN	Protein	X-ray	2007-04-17
	C	275	123740.52	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17
	D	275	123740.52	30016.60	255.10	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Diclosan	DCN	Protein	X-ray	2007-04-17
	D	275	123740.52	30016.60	663.43	Enoyl-[acyl-carrier-protein] reductase [NADH]	Oxidoreductase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2007-04-17
2PLN	A	137	15663.10	15663.10	196.11	Response regulator	Signaling protein	Selenomethionine	MSE	Protein	X-ray	2007-05-01
2PT7	A	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	B	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	C	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	D	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	E	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	F	330	260955.98	37633.20		Cag-alfa	Hydrolase/protein binding			Protein	X-ray	2007-11-13
	G	152	260955.98	17578.40		Hypothetical protein	Hydrolase/protein binding			Protein	X-ray	2007-11-13

	H	152	260955.98	17578.40		Hypothetical protein	Hydrolase/protein binding			Protein	X-ray	2007-11-13	
2PVP	A	367	83921.40	41960.70		D-alanine-D-alanine ligase	Ligase			Protein	X-ray	2008-04-01	
	B	367	83921.40	41960.70		D-alanine-D-alanine ligase	Ligase			Protein	X-ray	2008-04-01	
2PZH	A	135	63418.00	15854.50		Hypothetical protein HP_0496	Hydrolase			Protein	X-ray	2008-04-08	
	B	135	63418.00	15854.50		Hypothetical protein HP_0496	Hydrolase			Protein	X-ray	2008-04-08	
	C	135	63418.00	15854.50		Hypothetical protein HP_0496	Hydrolase			Protein	X-ray	2008-04-08	
	D	135	63418.00	15854.50		Hypothetical protein HP_0496	Hydrolase			Protein	X-ray	2008-04-08	
2Q0K	A	311	70212.93	33577.50	785.56	Thioredoxin reductase	Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2007-07-03	
	A	311	70212.93	33577.50	743.41	Thioredoxin reductase	Oxidoreductase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2007-07-03	
	B	311	70212.93	33577.50	785.56	Thioredoxin reductase	Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2007-07-03	
	B	311	70212.93	33577.50	743.41	Thioredoxin reductase	Oxidoreductase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2007-07-03	
2Q0L	A	311	70212.93	33577.50	785.56	Thioredoxin reductase	Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2007-07-03	
	A	311	70212.93	33577.50	743.41	Thioredoxin reductase	Oxidoreductase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2007-07-03	
	B	311	70212.93	33577.50	785.56	Thioredoxin reductase	Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2007-07-03	
	B	311	70212.93	33577.50	743.41	Thioredoxin reductase	Oxidoreductase	Nadp nicotinamide-adenine-dinucleotide phosphate	NAP	Protein	X-ray	2007-07-03	
2QGH	A	425	47813.44	47474.20	92.09	Diaminopimelate decarboxylase	Lyase	Glycerol	GOL	Protein	X-ray	2008-05-27	
	A	425	47813.44	47474.20	247.14	Diaminopimelate decarboxylase	Lyase	Pyridoxal-5'-phosphate	PLP	Protein	X-ray	2008-05-27	
2QH5	A	308	69996.80	34998.40		Mannose-6-phosphate isomerase	Isomerase			Protein	X-ray	2007-07-17	NYSRCSG
	B	308	69996.80	34998.40		Mannose-6-phosphate isomerase	Isomerase			Protein	X-ray	2007-07-17	NYSRCSG
2QM6	A	377	122270.46	40577.80		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
	B	188	122270.46	20410.30		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
	C	377	122270.46	40577.80		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
	D	188	122270.46	20410.30		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
2QMC	A	377	122801.09	40577.80		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
	B	188	122801.09	20380.30	442.44	Gamma-glutamyltranspeptidase	Transferase	S-(p-nitrobenzyl)glutathione	GTB	Protein	X-ray	2008-02-12	

	C	377	122801.09	40577.80		Gamma-glutamyltranspeptidase	Transferase			Protein	X-ray	2008-02-12	
2QMO	D	188	122801.09	20380.30	442.44	Gamma-glutamyltranspeptidase	Transferase	S-(p-nitrobenzyl)glutathione	GTB	Protein	X-ray	2008-02-12	
	A	220	24888.11	24817.20	35.45	Dethiobiotin synthetase	Ligase	Chloride ion	CL	Protein	X-ray	2007-07-31	MCSG
	A	220	24888.11	24817.20	196.11	Dethiobiotin synthetase	Ligase	Selenomethionine	MSE	Protein	X-ray	2007-07-31	MCSG
2QV3	A	457	49391.60	49391.60		Vacuolating cytotoxin	Toxin			Protein	X-ray	2007-10-23	
2R62	A	268	58219.20	29109.60		Cell division protease ftsh homolog	Hydrolase			Protein	X-ray	2008-09-09	
2R65	B	268	58219.20	29109.60		Cell division protease ftsh homolog	Hydrolase			Protein	X-ray	2008-09-09	
	A	268	147684.02	29109.60	427.20	Cell division protease ftsh homolog	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2008-09-09	
	B	268	147684.02	29109.60	427.20	Cell division protease ftsh homolog	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2008-09-09	
2RD3	C	268	147684.02	29109.60	427.20	Cell division protease ftsh homolog	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2008-09-09	
	D	268	147684.02	29109.60	427.20	Cell division protease ftsh homolog	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2008-09-09	
	E	268	147684.02	29109.60	427.20	Cell division protease ftsh homolog	Hydrolase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2008-09-09	
	A	223	51330.60	25665.30		Transcriptional regulator	Hydrolase			Protein	X-ray	2008-09-30	
	D	223	51330.60	25665.30		Transcriptional regulator	Hydrolase			Protein	X-ray	2008-09-30	
2UVP	A	186	87079.82	21640.10	59.04	Hoba	Unknown function	Acetate ion	ACT	Protein	X-ray	2007-08-21	
2VHG	B	186	87079.82	21626.00	40.08	Hoba	Unknown function	Calcium ion	CA	Protein	X-ray	2007-08-21	
	B	186	87079.82	21626.00	92.09	Hoba	Unknown function	Glycerol	GOL	Protein	X-ray	2007-08-21	
	C	186	87079.82	21626.00	59.04	Hoba	Unknown function	Acetate ion	ACT	Protein	X-ray	2007-08-21	
	C	186	87079.82	21626.00	40.08	Hoba	Unknown function	Calcium ion	CA	Protein	X-ray	2007-08-21	
	D	186	87079.82	21626.00	92.09	Hoba	Unknown function	Glycerol	GOL	Protein	X-ray	2007-08-21	
	A	159	55926.58	18392.60	54.94	Transposase orfa	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19	
										DNA			
	B	159	55926.58	18392.60		Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
										DNA			
2VIC	C	31	55926.58	9543.22		Right end 31-mer	Dna-binding protein			Protein	X-ray	2008-02-19	
										DNA			
	D	31	55926.58	9543.22		Right end 31-mer	Dna-binding protein			Protein	X-ray	2008-02-19	
										DNA			
2VIC	A	159	52901.54	18392.60	54.94	Transposase orfa	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19	
										DNA			

	B	159	52901.54	18392.60	Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	C	26	52901.54	8003.23	5'- d(*ap*ap*ap*gp*cp*cp*cp*tp*ap *gp*cp*tp*tp*tp*ap*gp*cp*tp*ap*t p*gp*gp*gp*g)-3'	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	D	26	52901.54	8003.23	54.94	5'- d(*ap*ap*ap*gp*cp*cp*cp*tp*ap *gp*cp*tp*tp*tp*ap*gp*cp*tp*ap*t p*gp*gp*gp*g)-3'	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19
									DNA			
2VIIH	A	159	52791.66	18392.60	Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	B	159	52791.66	18392.60	Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	C	26	52791.66	8003.23	5'- d(*ap*ap*ap*gp*cp*cp*cp*tp*ap *gp*cp*tp*tp*tp*ap*gp*cp*tp*ap*t p*gp*gp*gp*g)-3'	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	D	26	52791.66	8003.23	5'- d(*ap*ap*ap*gp*cp*cp*cp*tp*ap *gp*cp*tp*tp*tp*ap*gp*cp*tp*ap*t p*gp*gp*gp*g)-3'	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
2VJU	A	159	58556.01	18392.60	54.94	Transposase orfa	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19
									DNA			
	B	159	58556.01	18392.60	Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
	C	35	58556.01	10803.00	54.94	Right end 35-mer	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19
									DNA			
	D	35	58556.01	10803.00	54.94	Right end 35-mer	Dna-binding protein	Manganese (ii) ion	MN	Protein	X-ray	2008-02-19
									DNA			
2VJV	A	159	56431.03	18392.60	Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	

									DNA			
B	159	56431.03	18392.60		Transposase orfa	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
C	26	56431.03	8003.23	24.31	5'- d(*da*da*da*dg*dc*dc*dc*dc*dt*da* dg*dc*ctp*dt *dt*dt*da*dg*dc*dt*da*dt*dg*dg*dg* dgp)-3'	Dna-binding protein	Magnesium ion	MG	Protein	X-ray	2008-02-19	
									DNA			
D	26	56431.03	8003.23	24.31	5'- d(*da*da*da*dg*dc*dc*dc*dc*dt*da* dg*dc*ctp*dt *dt*dt*da*dg*dc*dt*da*dt*dg*dg*dg* dgp)-3'	Dna-binding protein	Magnesium ion	MG	Protein	X-ray	2008-02-19	
									DNA			
E	6	56431.03	1783.23	24.31	5'-d(*dt*da*dt*dt*da*dcp)-3'	Dna-binding protein	Magnesium ion	MG	Protein	X-ray	2008-02-19	
									DNA			
F	6	56431.03	1783.23		5'-d(*dt*da*dt*dt*da*dcp)-3'	Dna-binding protein			Protein	X-ray	2008-02-19	
									DNA			
2VW9	A	134	40539.90	14969.00	SINGLE-strandedprotein	Dna-binding protein			Protein	X-ray	2009-06-02	
									DNA			
	B	134	40539.90	14969.00	SINGLE-strandedprotein	Dna-binding protein			Protein	X-ray	2009-06-02	
									DNA			
	C	35	40539.90	10601.90	Poly-dt	Dna-binding protein			Protein	X-ray	2009-06-02	
									DNA			
2W4I	A	255	115465.07	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-12-09
	B	255	115465.07	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-12-09
	B	255	115465.07	28532.40	373.47	Glutamate racemase	Isomerase	1-[(3s)-5-phenyl-3-thiophen-2-yl-3h-1,4-benzodiazepin-2-yl]azetidin-3-ol	VGA	Protein	X-ray	2008-12-09
	E	255	115465.07	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-12-09
	E	255	115465.07	28532.40	373.47	Glutamate racemase	Isomerase	1-[(3s)-5-phenyl-3-thiophen-2-yl-3h-1,4-benzodiazepin-2-yl]azetidin-3-ol	VGA	Protein	X-ray	2008-12-09
	F	255	115465.07	28532.40	147.13	Glutamate racemase	Isomerase	D-glutamic acid	DGL	Protein	X-ray	2008-12-09

2W5U	A	164	36291.90	17540.50	456.35	Flavodoxin	Electron transport	Flavin mononucleotide	FMN	Protein	X-ray	2009-12-22
	A	164	36291.90	17540.50	298.20	Flavodoxin	Electron transport	[2-(5-amino-4-cyano-1h-pyrazol-1-yl)-5-(trifluoromethyl)phenyl](hydroxy)oxoammonium	IC3	Protein	X-ray	2009-12-22
	B	164	36291.90	17540.50	456.35	Flavodoxin	Electron transport	Flavin mononucleotide	FMN	Protein	X-ray	2009-12-22
2WCQ	A	159	36846.45	18231.10	192.12	TNF-alpha protein	Immune system	Citric acid	CIT	Protein	X-ray	2009-05-12
	B	159	36846.45	18231.10	192.12	TNF-alpha protein	Immune system	Citric acid	CIT	Protein	X-ray	2009-05-12
2WCR	A	159	36589.99	18231.10	69.09	TNF-alpha protein	Immune system	Imidazole	IMD	Protein	X-ray	2009-05-12
	A	159	36589.99	18231.10	58.70	TNF-alpha protein	Immune system	Nickel (ii) ion	NI	Protein	X-ray	2009-05-12
	B	159	36589.99	18231.10		TNF-alpha protein	Immune system			Protein	X-ray	2009-05-12
2WGL	A	254	87363.00	29121.00	196.11	Urease protein UREF	Metal protein	Selenomethionine	MSE	Protein	X-ray	2009-05-26
	B	254	87363.00	29121.00	196.11	Urease protein UREF	Metal protein	Selenomethionine	MSE	Protein	X-ray	2009-05-26
	C	254	87363.00	29121.00	196.11	Urease protein UREF	Metal protein	Selenomethionine	MSE	Protein	X-ray	2009-05-26
2WKS	A	167	113098.72	18499.40	350.39	3-dehydroquinase dehydratase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24
	B	167	113098.72	18499.40	350.39	3-dehydroquinase dehydratase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24
	C	167	113098.72	18499.40	350.39	3-dehydroquinase dehydratase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24
	D	167	113098.72	18499.40	350.39	3-dehydroquinase dehydratase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24
	E	167	113098.72	18499.40	350.39	3-dehydroquinase dehydratase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24

								methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid				
	F	167	113098.72	18499.40	350.39	3-dehydroquinatase	Lyase	(1r,4s,5r)-1,4,5-trihydroxy-3-[(5-methyl-1-benzothiophen-2-yl)methoxy]cyclohex-2-ene-1-carboxylic acid	CB6	Protein	X-ray	2009-11-24
2WLT	A	332	35740.80	35607.70		L-asparaginase	Hydrolase			Protein	X-ray	2009-11-24
2WP0	A	180	68052.84	21039.40	35.45	Hoba	Dnaprotein	Chloride ion	CL	Protein	X-ray	2009-11-17
	A	180	68052.84	21039.40	92.09	Hoba	Dnaprotein	Glycerol	GOL	Protein	X-ray	2009-11-17
	A	180	68052.84	21039.40	22.99	Hoba	Dnaprotein	Sodium ion	NA	Protein	X-ray	2009-11-17
	B	180	68052.84	21039.40	35.45	Hoba	Dnaprotein	Chloride ion	CL	Protein	X-ray	2009-11-17
	B	180	68052.84	21039.40	92.09	Hoba	Dnaprotein	Glycerol	GOL	Protein	X-ray	2009-11-17
	B	180	68052.84	21039.40	22.99	Hoba	Dnaprotein	Sodium ion	NA	Protein	X-ray	2009-11-17
	C	112	68052.84	12632.60		Chromosomalprotein DNAA	Dnaprotein			Protein	X-ray	2009-11-17
	D	112	68052.84	12632.60		Chromosomalprotein DNAA	Dnaprotein			Protein	X-ray	2009-11-17
2WT4	A	332	35740.80	35607.70		L-asparaginase	Hydrolase			Protein	X-ray	2009-11-24
2WVB	A	148	34270.61	17020.20	46.03	Putative nickel-responsive regulator	Transcription	Formic acid	FMT	Protein	X-ray	2010-01-19
	A	148	34270.61	17020.20	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	B	148	34270.61	17020.20		Putative nickel-responsive regulator	Transcription			Protein	X-ray	2010-01-19
2WVC	A	148	34999.18	17008.20	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	A	148	34999.18	17008.20	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	B	148	34999.18	17008.20	46.03	Putative nickel-responsive regulator	Transcription	Formic acid	FMT	Protein	X-ray	2010-01-19
	B	148	34999.18	17008.20	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	B	148	34999.18	17008.20	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
2WVD	A	148	69746.12	17154.30	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	A	148	69746.12	17154.30	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	B	148	69746.12	17154.30	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	B	148	69746.12	17154.30	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	C	148	69746.12	17154.30	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	C	148	69746.12	17154.30	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19

2WVE	D	148	69746.12	17154.30	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	D	148	69746.12	17154.30	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	A	148	35449.64	17189.40	192.12	Putative nickel-responsive regulator	Transcription	Citric acid	CIT	Protein	X-ray	2010-01-19
	A	148	35449.64	17189.40	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	A	148	35449.64	17189.40	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	A	148	35449.64	17189.40	122.14	Putative nickel-responsive regulator	Transcription	2-amino-2-hydroxymethyl-propane-1,3-diol	TRS	Protein	X-ray	2010-01-19
2WVF	B	148	35449.64	17189.40	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	B	148	35449.64	17189.40	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	A	148	35016.47	17008.20	46.03	Putative nickel-responsive regulator	Transcription	Formic acid	FMT	Protein	X-ray	2010-01-19
	A	148	35016.47	17008.20	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	A	148	35016.47	17008.20	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2010-01-19
	A	148	35016.47	17008.20	96.06	Putative nickel-responsive regulator	Transcription	Sulfate ion	SO4	Protein	X-ray	2010-01-19
	B	148	35016.47	17008.20	46.03	Putative nickel-responsive regulator	Transcription	Formic acid	FMT	Protein	X-ray	2010-01-19
	B	148	35016.47	17008.20	92.09	Putative nickel-responsive regulator	Transcription	Glycerol	GOL	Protein	X-ray	2010-01-19
	B	148	35016.47	17008.20	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2010-01-19
2XB9	A	167	56310.93	18499.40	310.30	3-dehydroquinatase	Lyase	(1r,2r,4s,5r)-1,4,5-trihydroxy-2-(4-methoxybenzyl)-3-oxocyclohexanecarboxylic acid	XNW	Protein	X-ray	2010-09-15
	B	167	56310.93	18499.40	310.30	3-dehydroquinatase	Lyase	(1r,2r,4s,5r)-1,4,5-trihydroxy-2-(4-methoxybenzyl)-3-oxocyclohexanecarboxylic acid	XNW	Protein	X-ray	2010-09-15
	C	167	56310.93	18499.40	192.12	3-dehydroquinatase	Lyase	Citric acid	CIT	Protein	X-ray	2010-09-15
2XD9	A	167	56309.10	18499.40	270.30	3-dehydroquinatase	Lyase	(4r,6r,7s)-4,6,7-trihydroxy-2-[(1e)-prop-1-en-1-yl]-4,5,6,7-tetrahydro-1-benzothiophene-4-carboxylic acid	XD9	Protein	X-ray	2010-11-24
	B	167	56309.10	18499.40	270.30	3-dehydroquinatase	Lyase	(4r,6r,7s)-4,6,7-trihydroxy-2-[(1e)-prop-1-en-1-yl]-4,5,6,7-tetrahydro-1-benzothiophene-4-carboxylic acid	XD9	Protein	X-ray	2010-11-24
	C	167	56309.10	18499.40	270.30	3-dehydroquinatase	Lyase	(4r,6r,7s)-4,6,7-trihydroxy-2-[(1e)-prop-1-en-1-yl]-4,5,6,7-tetrahydro-1-	XD9	Protein	X-ray	2010-11-24

2XDA	A	167	18797.75	18499.40	298.35	3-dehydroquinatase	Lyase	benzothiophene-4-carboxylic acid	JPS	Protein	X-ray	2010-11-24
								(4r,6r,7s)-2-(2-cyclopropylethyl)-4,6,7-trihydroxy-4,5,6,7-tetrahydro-1-benzothiophene-4-carboxylic acid				
2XIG	A	150	71706.68	17682.50	65.38	Ferricprotein	Transcription	Zinc ion	ZN	Protein	X-ray	2011-01-19
	B	150	71706.68	17682.50	192.12	Ferricprotein	Transcription	Citric acid	CIT	Protein	X-ray	2011-01-19
	B	150	71706.68	17682.50	65.38	Ferricprotein	Transcription	Zinc ion	ZN	Protein	X-ray	2011-01-19
	C	150	71706.68	17682.50	65.38	Ferricprotein	Transcription	Zinc ion	ZN	Protein	X-ray	2011-01-19
	D	150	71706.68	17682.50	65.38	Ferricprotein	Transcription	Zinc ion	ZN	Protein	X-ray	2011-01-19
2XRH	A	100	11635.31	11512.20	123.11	Protein hp0721	Unknown function	Nicotinic acid	NIO	Protein	X-ray	2011-09-28
2Y3Y	A	91	43569.14	10428.90	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-08-17
	B	91	43569.14	10428.90	238.30	Putative nickel-responsive regulator	Transcription	4-(2-hydroxyethyl)-1-piperazine	EPE	Protein	X-ray	2011-08-17
								ethanesulfonic acid				
	B	91	43569.14	10428.90	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-08-17
	C	91	43569.14	10428.90	238.30	Putative nickel-responsive regulator	Transcription	4-(2-hydroxyethyl)-1-piperazine	EPE	Protein	X-ray	2011-08-17
								ethanesulfonic acid				
	C	91	43569.14	10428.90	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-08-17
	C	91	43569.14	10428.90	106.12	Putative nickel-responsive regulator	Transcription	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-08-17
	D	91	43569.14	10428.90	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-08-17
	Q	11	43569.14	823.77		Undecapeptide-gssgsasgag	Transcription			Protein	X-ray	2011-08-17
2ZL0	A	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22
						proteolytic subunit						
	B	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22
						proteolytic subunit						
	C	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22
						proteolytic subunit						
	D	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22
						proteolytic subunit						
	E	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22
						proteolytic subunit						
	F	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22

					proteolytic subunit					
G	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
H	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
I	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
J	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
K	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
L	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
M	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
N	196	301669.22	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
2ZL2	A	196	309119.72	21547.80	ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
B	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
C	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
D	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
E	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
F	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					
G	196	309119.72	21547.80		ATP-dependent Clp protease	Hydrolase		Protein	X-ray	2008-04-22
					proteolytic subunit					

	H	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	I	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	J	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	K	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	L	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	M	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	N	196	309119.72	21547.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	O	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	P	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	Q	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	R	7	309119.72	613.75	103.12	A peptide substrate-NVLGFTQ for Chain R and S	Hydrolase	Unknown	UNK	Protein	X-ray	2008-04-22
	S	7	309119.72	613.75	103.12	A peptide substrate-NVLGFTQ for Chain R and S	Hydrolase	Unknown	UNK	Protein	X-ray	2008-04-22
	T	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	U	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	V	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	W	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
	X	7	309119.72	777.87		A peptide substrate-NVLGFTQ	Hydrolase			Protein	X-ray	2008-04-22
2ZL3	A	196	301445.22	21531.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	B	196	301445.22	21531.80		ATP-dependent Clp protease proteolytic subunit	Hydrolase			Protein	X-ray	2008-04-22
	C	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase			Protein	X-ray	2008-04-22

					proteolytic subunit				
D	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
E	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
F	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
G	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
H	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
I	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
J	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
K	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
L	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
M	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
N	196	301445.22	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
2ZL4	1	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
2ZL4	2	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
2ZL4	A	196	305677.84	21531.80	ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
B	196	305677.84	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				
C	196	305677.84	21531.80		ATP-dependent Clp protease	Hydrolase	Protein	X-ray	2008-04-22
					proteolytic subunit				

D	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
E	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
F	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
G	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
H	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
I	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
J	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
K	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
L	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
M	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
N	196	305677.84	21531.80	ATP-dependent Clp protease proteolytic subunit	Hydrolase	Protein	X-ray	2008-04-22
O	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
P	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
Q	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
R	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
S	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
T	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
U	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
V	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22
W	4	305677.84	302.33	Peptide substrate AAAA	Hydrolase	Protein	X-ray	2008-04-22

3AH5	X	4	305677.84	302.33		Peptide substrate AAAA	Hydrolase			Protein	X-ray	2008-04-22
	Y	4	305677.84	302.33		Peptide substrate AAAA	Hydrolase			Protein	X-ray	2008-04-22
	Z	4	305677.84	302.33		Peptide substrate AAAA	Hydrolase			Protein	X-ray	2008-04-22
	A	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
	A	216	158692.48	25178.90	96.06	Thymidylate synthase thyx	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-04-20
	A	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20
	B	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
	B	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20
	C	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
	C	216	158692.48	25178.90	96.06	Thymidylate synthase thyx	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-04-20
	C	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20
	D	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
	D	216	158692.48	25178.90	96.06	Thymidylate synthase thyx	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-04-20
	D	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20
	E	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
	E	216	158692.48	25178.90	96.06	Thymidylate synthase thyx	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-04-20
	E	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20
	F	216	158692.48	25178.90	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-04-20
F	216	158692.48	25178.90	96.06	Thymidylate synthase thyx	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-04-20	
F	216	158692.48	25178.90	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-04-20	
3AKJ	A	325	75308.00	37654.00		Ctka	Transferase			Protein	X-ray	2010-12-01
	B	325	75308.00	37654.00		Ctka	Transferase			Protein	X-ray	2010-12-01
3AKK	A	325	152422.03	37654.00	427.20	Ctka	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-12-01
	A	325	152422.03	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray	2010-12-01
	B	325	152422.03	37654.00	427.20	Ctka	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-12-01
	B	325	152422.03	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray	2010-12-01
	C	325	152422.03	37654.00	427.20	Ctka	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-12-01
	C	325	152422.03	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray	2010-12-01
	D	325	152422.03	37654.00	427.20	Ctka	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-12-01
	D	325	152422.03	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray	2010-12-01
3AKL	A	325	152731.94	37654.00	506.20	Ctka	Transferase	Phosphoaminophosphonic acid-	ANP	Protein	X-ray	2010-12-01

	A	325	152731.94	37654.00	24.31	Ctka	Transferase	adenylate ester Magnesium ion	MG	Protein	X-ray 2010-12-01
	B	325	152731.94	37654.00	506.20	Ctka	Transferase	Phosphoaminophosphonic acid- adenylate ester	ANP	Protein	X-ray 2010-12-01
	B	325	152731.94	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray 2010-12-01
	C	325	152731.94	37654.00	427.20	Ctka	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray 2010-12-01
	C	325	152731.94	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray 2010-12-01
	D	325	152731.94	37654.00	506.20	Ctka	Transferase	Phosphoaminophosphonic acid- adenylate ester	ANP	Protein	X-ray 2010-12-01
	D	325	152731.94	37654.00	24.31	Ctka	Transferase	Magnesium ion	MG	Protein	X-ray 2010-12-01
3B7J	A	159	110639.91	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray 2008-09-02
	A	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray 2008-09-02
	B	159	110639.91	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray 2008-09-02
	B	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray 2008-09-02
	B	159	110639.91	18206.30	174.16	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	5-hydroxynaphthalene-1,4-dione	JUG	Protein	X-ray 2008-09-02
	C	159	110639.91	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray 2008-09-02
	C	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray 2008-09-02
	C	159	110639.91	18206.30	174.16	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	5-hydroxynaphthalene-1,4-dione	JUG	Protein	X-ray 2008-09-02
	D	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray 2008-09-02
	E	159	110639.91	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray 2008-09-02
	E	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray 2008-09-02

					dehydratase								
	F	159	110639.91	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2008-09-02	
					dehydratase								
	F	159	110639.91	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2008-09-02	
					dehydratase								
3BGH	A	236	55233.49	27376.60	96.06	Putative neuraminyllactose-binding hemagglutinin homolog	SG, unknown function	Sulfate ion	SO4	Protein	X-ray	2007-12-11	NYSRCSG
	B	236	55233.49	27376.60	96.06	Putative neuraminyllactose-binding hemagglutinin homolog	SG, unknown function	Sulfate ion	SO4	Protein	X-ray	2007-12-11	NYSRCSG
3BVE	A	181	126021.88	20957.60		Ferritin	Oxidoreductase			Protein	X-ray	2009-01-13	
	B	181	126021.88	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
	C	181	126021.88	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
	D	181	126021.88	20957.60		Ferritin	Oxidoreductase			Protein	X-ray	2009-01-13	
	E	181	126021.88	20957.60		Ferritin	Oxidoreductase			Protein	X-ray	2009-01-13	
	F	181	126021.88	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
3BVF	A	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	A	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
	B	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	B	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
	C	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	C	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
	D	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	D	181	127580.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
	D	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
	E	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	E	181	127580.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
	E	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
	F	181	127580.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	
	F	181	127580.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13	
	F	181	127580.73	20957.60	60.10	Ferritin	Oxidoreductase	Isopropyl alcohol	IPA	Protein	X-ray	2009-01-13	
3BVI	A	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13	

	B	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	C	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	D	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	D	181	126859.58	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	E	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	E	181	126859.58	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	F	181	126859.58	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
3BVK	A	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	B	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	B	181	126803.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	C	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	C	181	126803.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	D	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	E	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	F	181	126803.73	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	F	181	126803.73	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
3BVL	A	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	B	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	B	181	126915.43	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	C	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	D	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	D	181	126915.43	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
	E	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	F	181	126915.43	20957.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-01-13
	F	181	126915.43	20957.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-01-13
3C4U	A	307	67778.94	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2008-08-26
	A	307	67778.94	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
	B	307	67778.94	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2008-08-26
	B	307	67778.94	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
3C52	A	307	68201.20	33801.10	40.08	Fructose-bisphosphate aldolase	Lyase	Calcium ion	CA	Protein	X-ray	2008-08-26
	A	307	68201.20	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2008-08-26

	A	307	68201.20	33801.10	171.05	Fructose-bisphosphate aldolase	Lyase	Phosphoglycolohydroxamic acid	PGH	Protein	X-ray	2008-08-26
	A	307	68201.20	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
	B	307	68201.20	33801.10	40.08	Fructose-bisphosphate aldolase	Lyase	Calcium ion	CA	Protein	X-ray	2008-08-26
	B	307	68201.20	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2008-08-26
	B	307	68201.20	33801.10	171.05	Fructose-bisphosphate aldolase	Lyase	Phosphoglycolohydroxamic acid	PGH	Protein	X-ray	2008-08-26
	B	307	68201.20	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
3C56	A	307	68351.18	33801.10	309.11	Fructose-bisphosphate aldolase	Lyase	3-(hydroxyl[(phosphonoxy)acetyl]amino }propyl dihydrogen phosphate	PH4	Protein	X-ray	2008-08-26
	A	307	68351.18	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
	B	307	68351.18	33801.10	309.11	Fructose-bisphosphate aldolase	Lyase	3-(hydroxyl[(phosphonoxy)acetyl]amino }propyl dihydrogen phosphate	PH4	Protein	X-ray	2008-08-26
	B	307	68351.18	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2008-08-26
3C5Q	A	425	47960.63	47474.20	92.09	Diaminopimelate decarboxylase	Lyase	Glycerol	GOL	Protein	X-ray	2008-05-27
	A	425	47960.63	47474.20	247.14	Diaminopimelate decarboxylase	Lyase	Pyridoxal-5'-phosphate	PLP	Protein	X-ray	2008-05-27
3CEI	A	213	49303.55	24547.90	55.85	Superoxide dismutase	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2008-06-10
	A	213	49303.55	24547.90	96.06	Superoxide dismutase	Oxidoreductase	Sulfate ion	SO4	Protein	X-ray	2008-06-10
	B	213	49303.55	24547.90	55.85	Superoxide dismutase	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2008-06-10
3CF8	A	159	110775.93	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	A	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	A	159	110775.93	18206.30	302.24	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	3,5,7,3',4'-pentahydroxyflavone	QUE	Protein	X-ray	2008-12-09
	B	159	110775.93	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	B	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	C	159	110775.93	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09

	C	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	C	159	110775.93	18206.30	302.24	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	3,5,7,3',4'-pentahydroxyflavone	QUE	Protein	X-ray	2008-12-09
	D	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	E	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	F	159	110775.93	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
3CF9	A	159	110471.62	18206.30	270.24	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	5,7-dihydroxy-2-(4-hydroxyphenyl)-4h-chromen-4-one	AGI	Protein	X-ray	2008-12-09
	A	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	B	159	110471.62	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	B	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	C	159	110471.62	18206.30	270.24	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	5,7-dihydroxy-2-(4-hydroxyphenyl)-4h-chromen-4-one	AGI	Protein	X-ray	2008-12-09
	C	159	110471.62	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	C	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	D	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	E	159	110471.62	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	E	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	F	159	110471.62	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09

dehydratase												
3CLH	A	343	79810.02	39176.20	663.43	3-dehydroquinase synthase	Lyase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2009-03-24
	A	343	79810.02	39176.20	65.38	3-dehydroquinase synthase	Lyase	Zinc ion	ZN	Protein	X-ray	2009-03-24
	B	343	79810.02	39176.20	663.43	3-dehydroquinase synthase	Lyase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2009-03-24
	B	343	79810.02	39176.20	65.38	3-dehydroquinase synthase	Lyase	Zinc ion	ZN	Protein	X-ray	2009-03-24
3CWX	A	176	62332.80	20777.60	196.11	Protein cagd	Unknown function	Selenomethionine	MSE	Protein	X-ray	2008-12-30
	B	176	62332.80	20777.60	196.11	Protein cagd	Unknown function	Selenomethionine	MSE	Protein	X-ray	2008-12-30
	C	176	62332.80	20777.60	196.11	Protein cagd	Unknown function	Selenomethionine	MSE	Protein	X-ray	2008-12-30
3CWY	A	176	20841.15	20777.60	63.55	Protein cagd	Unknown function	Copper (ii) ion	CU	Protein	X-ray	2008-12-30
	A	176	20841.15	20777.60	196.11	Protein cagd	Unknown function	Selenomethionine	MSE	Protein	X-ray	2008-12-30
3CXN	A	274	94110.00	31339.30	196.11	Ureaseprotein uref	Chaperone	Selenomethionine	MSE	Protein	X-ray	2009-05-12
	B	274	94110.00	31339.30	92.09	Ureaseprotein uref	Chaperone	Glycerol	GOL	Protein	X-ray	2009-05-12
	B	274	94110.00	31339.30	196.11	Ureaseprotein uref	Chaperone	Selenomethionine	MSE	Protein	X-ray	2009-05-12
	C	274	94110.00	31339.30	196.11	Ureaseprotein uref	Chaperone	Selenomethionine	MSE	Protein	X-ray	2009-05-12
	B	138	63760.40	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	C	138	63760.40	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	D	138	63760.40	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	E	138	63760.40	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	A	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	B	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
3CYQ	C	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	D	138	255628.14	15940.10	293.27	Chemotaxis protein motb	Membrane protein	Beta-n-acetylmuramic acid	AMU	Protein	X-ray	2008-07-08
	E	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	F	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	G	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	H	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	I	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	J	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	K	138	255628.14	15940.10	293.27	Chemotaxis protein motb	Membrane protein	Beta-n-acetylmuramic acid	AMU	Protein	X-ray	2008-07-08
	L	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	M	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08

3D04	N	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	O	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	P	138	255628.14	15940.10		Chemotaxis protein motb	Membrane protein			Protein	X-ray	2008-07-08
	A	159	110744.01	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	A	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	A	159	110744.01	18206.30	286.28	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	(2s)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-2,3-dihydro-4h-chromen-4-one	SAK	Protein	X-ray	2008-12-09
	B	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	C	159	110744.01	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	C	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	C	159	110744.01	18206.30	286.28	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	(2s)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-2,3-dihydro-4h-chromen-4-one	SAK	Protein	X-ray	2008-12-09
	D	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	E	159	110744.01	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	E	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
	F	159	110744.01	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2008-12-09
	F	159	110744.01	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2008-12-09
3DOY	A	159	111068.44	18206.30	448.50	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	4-chloro-n'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]benzohy	2BE	Protein	X-ray	2009-05-05

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A	159	111068.44	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
A	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
B	159	111068.44	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
B	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
C	159	111068.44	18206.30	448.50	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	4-chloro-n'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]benzohydrazide	2BE	Protein	X-ray	2009-05-05	
C	159	111068.44	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
C	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
D	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
E	159	111068.44	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
E	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
F	159	111068.44	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
3DOZ	A	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	A	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	B	159	111157.34	18206.30	492.95	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	3-bromo-n'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]benzohydrazide	3BE	Protein	X-ray	2009-05-05

	B	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	B	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	C	159	111157.34	18206.30	492.95	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	3-bromo-n'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]benzohydrazide	3BE	Protein	X-ray	2009-05-05
	C	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	C	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	D	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	E	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	F	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
3DP0	A	159	110755.71	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	A	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	B	159	110755.71	18206.30	464.11	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	N'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]naphthalene-2-carbohydrazide	2BC	Protein	X-ray	2009-05-05
	B	159	110755.71	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	B	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	C	159	110755.71	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	C	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05

					dehydratase							
	D	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	E	159	110755.71	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
					dehydratase							
	E	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	F	159	110755.71	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
3DP1	A	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	B	159	110939.45	18206.30	444.08	(3R)-hydroxymyristoyl-acylprotein	Lyase	N'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]-4-methoxybenzohydrazide	2RB	Protein	X-ray	2009-05-05
					dehydratase							
	B	159	110939.45	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
					dehydratase							
	B	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	C	159	110939.45	18206.30	444.08	(3R)-hydroxymyristoyl-acylprotein	Lyase	N'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]-4-methoxybenzohydrazide	2RB	Protein	X-ray	2009-05-05
					dehydratase							
	C	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	D	159	110939.45	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
					dehydratase							
	D	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							
	E	159	110939.45	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
					dehydratase							
	E	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
					dehydratase							

	F	159	110939.45	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	F	159	110939.45	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
3DP2	A	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	A	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	B	159	111157.34	18206.30	492.95	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	4-bromo-n'-[(1e)-(3,5-dibromo-2,4- dihydroxyphenyl)methylidene]benzohy drazide	4BE	Protein	X-ray	2009-05-05
	B	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	B	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	C	159	111157.34	18206.30	492.95	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	4-bromo-n'-[(1e)-(3,5-dibromo-2,4- dihydroxyphenyl)methylidene]benzohy drazide	4BE	Protein	X-ray	2009-05-05
	C	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	D	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	D	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	E	159	111157.34	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05
	E	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
	F	159	111157.34	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05
3DP3	A	159	111111.77	18206.30	470.16	(3R)-hydroxymyristoyl-acylprotein	Lyase	4-tert-butyl-n'-[(1e)-(3,5-dibromo-2,4-	4BB	Protein	X-ray	2009-05-05

dehydratase						dihydroxyphenyl)methylidene]benzohydrate						
dehydratase						drazide						
A	159	111111.77	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
dehydratase												
A	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
B	159	111111.77	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
dehydratase												
B	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
C	159	111111.77	18206.30	470.16	(3R)-hydroxymyristoyl-acylprotein	Lyase	4-tert-butyl-n'-[(1e)-(3,5-dibromo-2,4-dihydroxyphenyl)methylidene]benzohydrate	4BB	Protein	X-ray	2009-05-05	
dehydratase												
C	159	111111.77	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
dehydratase												
C	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
D	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
E	159	111111.77	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-05-05	
dehydratase												
E	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
F	159	111111.77	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-05-05	
dehydratase												
3ED0	A	159	110832.08	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein	Lyase	Benzamidine	BEN	Protein	X-ray	2009-07-21
dehydratase												
A	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
dehydratase												
A	159	110832.08	18206.30	270.24	(3R)-hydroxymyristoyl-acylprotein	Lyase	3-methyl-1,6,8-trihydroxyanthraquinone	EMO	Protein	X-ray	2009-07-21	
dehydratase												

	B	159	110832.08	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-07-21	
	B	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
	C	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
	C	159	110832.08	18206.30	270.24	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	3-methyl-1,6,8-trihydroxyanthraquinone	EMO	Protein	X-ray	2009-07-21	
	D	159	110832.08	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-07-21	
	D	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
	E	159	110832.08	18206.30	120.15	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Benzamidine	BEN	Protein	X-ray	2009-07-21	
	E	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
	F	159	110832.08	18206.30	35.45	(3R)-hydroxymyristoyl-acylprotein dehydratase	Lyase	Chloride ion	CL	Protein	X-ray	2009-07-21	
3EGM	A	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
	A	181	126613.58	20916.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-07-28	
	B	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
	B	181	126613.58	20916.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-07-28	
	C	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
	D	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
	D	181	126613.58	20916.60	92.09	Ferritin	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2009-07-28	
	E	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
3EZS	F	181	126613.58	20916.60	55.85	Ferritin	Oxidoreductase	Fe (iii) ion	FE	Protein	X-ray	2009-07-28	
	A	376	87435.69	43374.60	62.07	Aminotransferase aspb	Transferase	1,2-ethanediol	EDO	Protein	X-ray	2008-11-18	JCSG ⁸
	A	376	87435.69	43374.60	196.11	Aminotransferase aspb	Transferase	Selenomethionine	MSE	Protein	X-ray	2008-11-18	JCSG
	A	376	87435.69	43374.60	94.97	Aminotransferase aspb	Transferase	Phosphate ion	PO4	Protein	X-ray	2008-11-18	JCSG
	B	376	87435.69	43374.60	62.07	Aminotransferase aspb	Transferase	1,2-ethanediol	EDO	Protein	X-ray	2008-11-18	JCSG

3F42	B	376	87435.69	43374.60	196.11	Aminotransferase aspb	Transferase	Selenomethionine	MSE	Protein	X-ray	2008-11-18	JCSG
	B	376	87435.69	43374.60	94.97	Aminotransferase aspb	Transferase	Phosphate ion	PO4	Protein	X-ray	2008-11-18	JCSG
	A	99	22671.87	11211.80	62.07	Protein HP0035	SG, unknown function	1,2-ethanediol	EDO	Protein	X-ray	2008-11-18	MCSG
	A	99	22671.87	11211.80	196.11	Protein HP0035	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2008-11-18	MCSG
	B	99	22671.87	11211.80	62.07	Protein HP0035	SG, unknown function	1,2-ethanediol	EDO	Protein	X-ray	2008-11-18	MCSG
	B	99	22671.87	11211.80	196.11	Protein HP0035	SG, unknown function	Selenomethionine	MSE	Protein	X-ray	2008-11-18	MCSG
3FC3	A	200	52768.99	22768.40	22.99	Restriction endonuclease Hpy99I	Hydrolase/dna	Sodium ion	NA	Protein	X-ray	2009-03-31	
										DNA			
	A	200	52768.99	22768.40	194.23	Restriction endonuclease Hpy99I	Hydrolase/dna	Tetraethylene glycol	PG4	Protein	X-ray	2009-03-31	
										DNA			
	A	200	52768.99	22768.40	65.38	Restriction endonuclease Hpy99I	Hydrolase/dna	Zinc ion	ZN	Protein	X-ray	2009-03-31	
										DNA			
3FNM	B	200	52768.99	22768.40	22.99	Restriction endonuclease Hpy99I	Hydrolase/dna	Sodium ion	NA	Protein	X-ray	2009-03-31	
										DNA			
	B	200	52768.99	22768.40	65.38	Restriction endonuclease Hpy99I	Hydrolase/dna	Zinc ion	ZN	Protein	X-ray	2009-03-31	
										DNA			
	C	11	52768.99	3358.24		5'- (*dcp*ntp*dcp*dgp*dap*dcp*dgp*ntp *dap*dgp*da)-3'	Hydrolase/dna			Protein	X-ray	2009-03-31	
										DNA			
3FX7	D	11	52768.99	3349.23		5'- (*ntp*dap*dcp*dgp*ntp*dcp*dgp*dap *dgp*ntp*dc)-3'	Hydrolase/dna			Protein	X-ray	2009-03-31	
										DNA			
	A	377	122333.35	40577.80		Gamma-glutamyltranspeptidase (Ggt) Large subunit	Transferase			Protein	X-ray	2009-05-19	
	B	188	122333.35	20410.30	178.57	Gamma-glutamyltranspeptidase (Ggt) Small subunit	Transferase	(2s)-amino[(5s)-3-chloro-4,5-dihydroisoxazol-5-yl]acetic acid	AVN	Protein	X-ray	2009-05-19	
	C	377	122333.35	40577.80		Gamma-glutamyltranspeptidase (Ggt) Large subunit	Transferase			Protein	X-ray	2009-05-19	
	D	188	122333.35	20410.30	178.57	Gamma-glutamyltranspeptidase (Ggt) Small subunit	Transferase	(2s)-amino[(5s)-3-chloro-4,5-dihydroisoxazol-5-yl]acetic acid	AVN	Protein	X-ray	2009-05-19	
3FX7	A	94	23207.80	11603.90		Putativeprotein	Unknown function			Protein	X-ray	2009-09-01	

[illegible]

	A	200	52813.04	22768.40	65.38	Restriction endonuclease Hpy99I	Hydrolase/dna	Zinc ion	ZN	Protein DNA	X-ray	2009-04-28
	B	200	52813.04	22768.40	22.99	Restriction endonuclease Hpy99I	Hydrolase/dna	Sodium ion	NA	Protein DNA	X-ray	2009-04-28
	B	200	52813.04	22768.40	65.38	Restriction endonuclease Hpy99I	Hydrolase/dna	Zinc ion	ZN	Protein DNA	X-ray	2009-04-28
	C	11	52813.04	3358.24		5'- (*dcp*ntp*dcp*dgp*dap*dcp*dgp*ntp *dap*dgp*da)-3'	Hydrolase/dna			Protein DNA	X-ray	2009-04-28
	D	11	52813.04	3349.23		5'- (*ntp*dap*dcp*dgp*ntp*dcp*dgp*dap *dgp*ntp*dc)-3'	Hydrolase/dna			Protein DNA	X-ray	2009-04-28
3GUQ	A	166	19047.00	19047.00		Putativeprotein	Toxin			Protein	X-ray	2009-09-22
3GWG	A	129	14585.43	14344.70	24.31	Chemotaxis protein chey homolog	Signaling protein	Magnesium ion	MG	Protein	X-ray	2010-03-09
	A	129	14585.43	14344.70	96.06	Chemotaxis protein chey homolog	Signaling protein	Sulfate ion	SO4	Protein	X-ray	2010-03-09
3GXV	A	123	34049.48	14291.50		Replicative DNA helicase	Hydrolase/replication			Protein	X-ray	2010-01-26
	B	123	34049.48	14291.50		Replicative DNA helicase	Hydrolase/replication			Protein	X-ray	2010-01-26
	C	22	34049.48	2490.00		Replicative DNA helicase	Hydrolase/replication			Protein	X-ray	2010-01-26
	D	26	34049.48	2976.48		Replicative DNA helicase	Hydrolase/replication			Protein	X-ray	2010-01-26
3H1E	A	129	14555.38	14344.70	66.01	Chemotaxis protein chey homolog	Signaling protein	Beryllium trifluoride ion	BEF	Protein	X-ray	2010-03-09
	A	129	14555.38	14344.70	24.31	Chemotaxis protein chey homolog	Signaling protein	Magnesium ion	MG	Protein	X-ray	2010-03-09
	A	129	14555.38	14344.70	96.06	Chemotaxis protein chey homolog	Signaling protein	Sulfate ion	SO4	Protein	X-ray	2010-03-09
3H1F	A	129	14517.12	14300.70	24.31	Chemotaxis protein chey homolog	Signaling protein	Magnesium ion	MG	Protein	X-ray	2010-03-09
	A	129	14517.12	14300.70	96.06	Chemotaxis protein chey homolog	Signaling protein	Sulfate ion	SO4	Protein	X-ray	2010-03-09
3H1G	A	129	14555.43	14314.70	24.31	Chemotaxis protein chey homolog	Signaling protein	Magnesium ion	MG	Protein	X-ray	2010-03-09
	A	129	14555.43	14314.70	96.06	Chemotaxis protein chey homolog	Signaling protein	Sulfate ion	SO4	Protein	X-ray	2010-03-09
3HPE	A	164	38000.38	18662.60	337.59	Conservedprotein	Transport protein	(13z)-docos-13-enamide	ERU	Protein	X-ray	2010-04-14
	B	164	38000.38	18662.60	337.59	Conservedprotein	Transport protein	(13z)-docos-13-enamide	ERU	Protein	X-ray	2010-04-14
3HR7	A	168	38723.12	19265.50	96.06	Shikimate kinase	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-06-16
	B	168	38723.12	19265.50	96.06	Shikimate kinase	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-06-16
3HVM	A	330	37614.50	37614.50		Agmatine deiminase	Hydrolase			Protein	X-ray	2010-01-19

3IBX	A	221	51022.20	25511.10	Putative thiaminase II	Hydrolase			Protein	X-ray	2009-11-17	
	D	221	51022.20	25511.10	Putative thiaminase II	Hydrolase			Protein	X-ray	2009-11-17	
3IEC	A	319	201373.20	36920.10	Serine/threonine-protein kinase MARK2	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	B	319	201373.20	36920.10	Serine/threonine-protein kinase MARK2	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	C	319	201373.20	36920.10	Serine/threonine-protein kinase MARK2	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	D	319	201373.20	36920.10	Serine/threonine-protein kinase MARK2	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	E	125	201373.20	13423.20	Cytotoxicity-associated immunodominant antigen	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	F	125	201373.20	13423.20	Cytotoxicity-associated immunodominant antigen	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	G	125	201373.20	13423.20	Cytotoxicity-associated immunodominant antigen	Signaling protein/toxin			Protein	X-ray	2009-12-08	
	H	125	201373.20	13423.20	Cytotoxicity-associated immunodominant antigen	Signaling protein/toxin			Protein	X-ray	2009-12-08	
3IMP	A	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	B	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	C	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	D	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	E	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	F	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	G	138	191540.41	15940.10	35.45	Chemotaxis protein motb	Membrane protein	Chloride ion	CL	Protein	X-ray	2010-08-04
	G	138	191540.41	15940.10	58.70	Chemotaxis protein motb	Membrane protein	Nickel (ii) ion	NI	Protein	X-ray	2010-08-04
	H	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	I	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	J	138	191540.41	15940.10	Chemotaxis protein motb	Membrane protein			Protein	X-ray	2010-08-04	
	K	138	191540.41	15940.10	35.45	Chemotaxis protein motb	Membrane protein	Chloride ion	CL	Protein	X-ray	2010-08-04
	K	138	191540.41	15940.10	58.70	Chemotaxis protein motb	Membrane protein	Nickel (ii) ion	NI	Protein	X-ray	2010-08-04

3IQC	L	138	191540.41	15940.10	Chemotaxis protein motb		Membrane protein			Protein	X-ray	2010-08-04		
	A	131	29940.20	14970.10	Flagellar protein		Chaperone			Protein	X-ray	2010-06-30		
	B	131	29940.20	14970.10	Flagellar protein		Chaperone			Protein	X-ray	2010-06-30		
3ISH	A	311	103089.17	33577.50	785.56	Thioredoxin reductase		Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2009-10-06	
	B	311	103089.17	33577.50	785.56	Thioredoxin reductase		Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2009-10-06	
	C	311	103089.17	33577.50	785.56	Thioredoxin reductase		Oxidoreductase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2009-10-06	
3JUJ	A	281	128348.80	32087.20	UDP-glucose pyrophosphorylase (galu)		Transferase				Protein	X-ray	2010-03-31	
	B	281	128348.80	32087.20	UDP-glucose pyrophosphorylase (galu)		Transferase				Protein	X-ray	2010-03-31	
	C	281	128348.80	32087.20	UDP-glucose pyrophosphorylase (galu)		Transferase				Protein	X-ray	2010-03-31	
	D	281	128348.80	32087.20	UDP-glucose pyrophosphorylase (galu)		Transferase				Protein	X-ray	2010-03-31	
3JUK	A	281	130905.68	32087.20	24.31	UDP-glucose pyrophosphorylase (galu)		Transferase	Magnesium ion	MG	Protein	X-ray	2010-03-31	
	A	281	130905.68	32087.20	566.30	UDP-glucose pyrophosphorylase (galu)		Transferase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2010-03-31	
	B	281	130905.68	32087.20	24.31	UDP-glucose pyrophosphorylase (galu)		Transferase	Magnesium ion	MG	Protein	X-ray	2010-03-31	
	B	281	130905.68	32087.20	566.30	UDP-glucose pyrophosphorylase (galu)		Transferase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2010-03-31	
	C	281	130905.68	32087.20	24.31	UDP-glucose pyrophosphorylase (galu)		Transferase	Magnesium ion	MG	Protein	X-ray	2010-03-31	
	C	281	130905.68	32087.20	566.30	UDP-glucose pyrophosphorylase (galu)		Transferase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2010-03-31	
	D	281	130905.68	32087.20	24.31	UDP-glucose pyrophosphorylase (galu)		Transferase	Magnesium ion	MG	Protein	X-ray	2010-03-31	
	D	281	130905.68	32087.20	566.30	UDP-glucose pyrophosphorylase (galu)		Transferase	Uridine-5'-diphosphate-glucose	UPG	Protein	X-ray	2010-03-31	
3K1H	A	158	17989.70	17989.70	Putativeprotein		Chaperone			Protein	X-ray	2010-06-30		
3K1I	A	131	70472.80	14970.10	Flagellar protein		Chaperone			Protein	X-ray	2010-06-30		
	B	131	70472.80	14970.10	Flagellar protein		Chaperone			Protein	X-ray	2010-06-30		
	C	178	70472.80	20266.30	Putativeprotein		Chaperone			Protein	X-ray	2010-06-30		
	D	178	70472.80	20266.30	Putativeprotein		Chaperone			Protein	X-ray	2010-06-30		
	3K5W	A	475	52510.07	52415.10	196.11	Carbohydrate kinase		Transferase	Selenomethionine	MSE	Protein	X-ray	2009-12-08
	A	475	52510.07	52415.10	94.97	Carbohydrate kinase		Transferase	Phosphate ion	PO4	Protein	X-ray	2009-12-08	NYSRCSG
3KU7	A	80	18431.50	9215.75	Cell division topological specificity factor		Cell cycle				Protein	X-ray	2010-05-05	
	B	80	18431.50	9215.75	Cell division topological specificity factor		Cell cycle				Protein	X-ray	2010-05-05	
3KWL	A	514	60116.00	60116.00	196.11	Uncharacterized protein		Unknown function	Selenomethionine	MSE	Protein	X-ray	2010-12-01	
3L9Z	A	170	19412.70	19412.70	Ureaseprotein uree		Metalprotein				Protein	X-ray	2010-08-25	MKBSGI

3LA0	A	170	77650.80	19412.70		Ureaseprotein uree	Metalprotein	Unknown atom or ion	UNX	Protein	X-ray	2010-08-25	MKBSGI
	B	170	77650.80	19412.70		Ureaseprotein uree	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	C	170	77650.80	19412.70		Ureaseprotein uree	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	D	170	77650.80	19412.70		Ureaseprotein uree	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
3LGH	A	148	68940.71	17170.40	24.31	Nickel-responsive regulator	Metalprotein	Magnesium ion	MG	Protein	X-ray	2010-09-15	
	A	148	68940.71	17170.40	58.70	Nickel-responsive regulator	Metalprotein	Nickel (ii) ion	NI	Protein	X-ray	2010-09-15	
	B	148	68940.71	17170.40	58.70	Nickel-responsive regulator	Metalprotein	Nickel (ii) ion	NI	Protein	X-ray	2010-09-15	
	C	148	68940.71	17170.40	58.70	Nickel-responsive regulator	Metalprotein	Nickel (ii) ion	NI	Protein	X-ray	2010-09-15	
	D	148	68940.71	17170.40	58.70	Nickel-responsive regulator	Metalprotein	Nickel (ii) ion	NI	Protein	X-ray	2010-09-15	
3LLW	A	311	142026.94	35290.60	96.06	Geranyltranstransferase (ispa)	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-03-31	NYSRCSG
	B	311	142026.94	35290.60	96.06	Geranyltranstransferase (ispa)	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-03-31	NYSRCSG
	C	311	142026.94	35290.60	96.06	Geranyltranstransferase (ispa)	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-03-31	NYSRCSG
	D	311	142026.94	35290.60	96.06	Geranyltranstransferase (ispa)	Transferase	Sulfate ion	SO4	Protein	X-ray	2010-03-31	NYSRCSG
3M1Y	A	217	98561.19	24565.60	35.45	Phosphoserine phosphatase (serb)	Hydrolase	Chloride ion	CL	Protein	X-ray	2010-03-23	NYSRCSG
	A	217	98561.19	24565.60	24.31	Phosphoserine phosphatase (serb)	Hydrolase	Magnesium ion	MG	Protein	X-ray	2010-03-23	NYSRCSG
	A	217	98561.19	24565.60	196.11	Phosphoserine phosphatase (serb)	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2010-03-23	NYSRCSG
	B	217	98561.19	24565.60	35.45	Phosphoserine phosphatase (serb)	Hydrolase	Chloride ion	CL	Protein	X-ray	2010-03-23	NYSRCSG
	B	217	98561.19	24565.60	24.31	Phosphoserine phosphatase (serb)	Hydrolase	Magnesium ion	MG	Protein	X-ray	2010-03-23	NYSRCSG
	B	217	98561.19	24565.60	196.11	Phosphoserine phosphatase (serb)	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2010-03-23	NYSRCSG
	C	217	98561.19	24565.60	35.45	Phosphoserine phosphatase (serb)	Hydrolase	Chloride ion	CL	Protein	X-ray	2010-03-23	NYSRCSG
	C	217	98561.19	24565.60	24.31	Phosphoserine phosphatase (serb)	Hydrolase	Magnesium ion	MG	Protein	X-ray	2010-03-23	NYSRCSG
	C	217	98561.19	24565.60	196.11	Phosphoserine phosphatase (serb)	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2010-03-23	NYSRCSG
	D	217	98561.19	24565.60	35.45	Phosphoserine phosphatase (serb)	Hydrolase	Chloride ion	CL	Protein	X-ray	2010-03-23	NYSRCSG
	D	217	98561.19	24565.60	24.31	Phosphoserine phosphatase (serb)	Hydrolase	Magnesium ion	MG	Protein	X-ray	2010-03-23	NYSRCSG
	D	217	98561.19	24565.60	196.11	Phosphoserine phosphatase (serb)	Hydrolase	Selenomethionine	MSE	Protein	X-ray	2010-03-23	NYSRCSG
3M21	A	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	
	B	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	
	C	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	
	D	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	
	E	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	
	F	67	44336.70	7389.45		Probable tautomerase HP_0924	Isomerase			Protein	X-ray	2010-09-01	

3MCD	A	80	18431.50	9215.75		Cell division topological specificity factor	Cell cycle			Protein	X-ray	2010-05-05	
	B	80	18431.50	9215.75		Cell division topological specificity factor	Cell cycle			Protein	X-ray	2010-05-05	
3MLE	A	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	A	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	A	242	167606.38	27148.30	35.45	Dethiobiotin synthetase	Ligase	Chloride ion	CL	Protein	X-ray	2010-05-19	MCSG
	A	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	A	242	167606.38	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2010-05-19	MCSG
	A	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
	B	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	B	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	B	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	B	242	167606.38	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2010-05-19	MCSG
	B	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
	C	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	C	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	C	242	167606.38	27148.30	35.45	Dethiobiotin synthetase	Ligase	Chloride ion	CL	Protein	X-ray	2010-05-19	MCSG
	C	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	C	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
	D	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	D	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	D	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	D	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
	E	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	E	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	E	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	E	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
	F	242	167606.38	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2010-05-19	MCSG
	F	242	167606.38	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2010-05-19	MCSG
	F	242	167606.38	27148.30	35.45	Dethiobiotin synthetase	Ligase	Chloride ion	CL	Protein	X-ray	2010-05-19	MCSG

	F	242	167606.38	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2010-05-19	MCSG
	F	242	167606.38	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2010-05-19	MCSG
	F	242	167606.38	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2010-05-19	MCSG
3MLG	A	189	43924.40	21962.20		Putativeprotein,Protein	Unknown function			Protein	X-ray	2010-05-12	
	B	189	43924.40	21962.20		Putativeprotein,Protein	Unknown function			Protein	X-ray	2010-05-12	
3MLI	A	100	47758.96	11919.70		Putativeprotein	Unknown function			Protein	X-ray	2010-05-12	
	B	100	47758.96	11919.70		Putativeprotein	Unknown function			Protein	X-ray	2010-05-12	
	C	100	47758.96	11919.70		Putativeprotein	Unknown function			Protein	X-ray	2010-05-12	
	D	100	47758.96	11919.70	40.08	Putativeprotein	Unknown function	Calcium ion	CA	Protein	X-ray	2010-05-12	
3MRS	A	168	19179.40	19179.40		Shikimate kinase	Transferase			Protein	X-ray	2011-05-04	
3MUF	A	168	19946.84	19265.50	427.20	Shikimate kinase	Transferase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2011-05-04	
	A	168	19946.84	19265.50	254.13	Shikimate kinase	Transferase	Shikimate-3-phosphate	S3P	Protein	X-ray	2011-05-04	
3MYD	A	365	40972.80	40972.80		Flagellarprotein flha	Protein transport			Protein	X-ray	2010-05-26	
3N2E	A	168	58742.29	19004.30	489.47	Shikimate kinase	Transferase	7-amino-4-hydroxy-3-[(e)-(5-hydroxy-7-sulfonaphthalen-2-yl)diazenyl]naphthalene-2-sulfonic acid	OSA	Protein	X-ray	2011-05-18	
3N2E	A	168	58742.29	19004.30	150.09	Shikimate kinase	Transferase	L(+)-tartaric acid	TLA	Protein	X-ray	2011-05-18	
	B	168	58742.29	19004.30	489.47	Shikimate kinase	Transferase	7-amino-4-hydroxy-3-[(e)-(5-hydroxy-7-sulfonaphthalen-2-yl)diazenyl]naphthalene-2-sulfonic acid	OSA	Protein	X-ray	2011-05-18	
	B	168	58742.29	19004.30	150.09	Shikimate kinase	Transferase	L(+)-tartaric acid	TLA	Protein	X-ray	2011-05-18	
	C	168	58742.29	19004.30		Shikimate kinase	Transferase			Protein	X-ray	2011-05-18	
3N3Y	A	216	104173.55	24872.60	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-05-25	
	A	216	104173.55	24872.60	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-05-25	
	B	216	104173.55	24872.60	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-05-25	
	B	216	104173.55	24872.60	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-05-25	
	C	216	104173.55	24872.60	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-05-25	
	C	216	104173.55	24872.60	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-05-25	
	D	216	104173.55	24872.60	785.56	Thymidylate synthase thyx	Transferase	Flavin-adenine dinucleotide	FAD	Protein	X-ray	2011-05-25	

	D	216	104173.55	24872.60	308.18	Thymidylate synthase thyx	Transferase	2'-deoxyuridine 5'-monophosphate	UMP	Protein	X-ray	2011-05-25
3N9R	A	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	A	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	A	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	A	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	B	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	B	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	B	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	B	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	e	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	e	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	e	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	e	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	j	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	j	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	j	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	j	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	K	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	K	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	K	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	K	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	P	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	P	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	P	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	P	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17

	U	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	U	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	U	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	U	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
	Z	307	273344.62	33801.10	35.45	Fructose-bisphosphate aldolase	Lyase	Chloride ion	CL	Protein	X-ray	2010-11-17
	Z	307	273344.62	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase	Sodium ion	NA	Protein	X-ray	2010-11-17
	Z	307	273344.62	33801.10	243.15	Fructose-bisphosphate aldolase	Lyase	2-[hydroxy(4-hydroxybutyl)amino]-2-oxoethyl dihydrogen phosphate	TD3	Protein	X-ray	2010-11-17
	Z	307	273344.62	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase	Zinc ion	ZN	Protein	X-ray	2010-11-17
3N9S	A	307	68505.37	33801.10	40.08	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Calcium ion	CA	Protein	X-ray	2010-11-17
	A	307	68505.37	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Sodium ion	NA	Protein	X-ray	2010-11-17
	A	307	68505.37	33801.10	323.13	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	4-(hydroxy[(phosphonoxy)acetyl]amino)butyl dihydrogen phosphate	TD4	Protein	X-ray	2010-11-17
	A	307	68505.37	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Zinc ion	ZN	Protein	X-ray	2010-11-17
	B	307	68505.37	33801.10	40.08	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Calcium ion	CA	Protein	X-ray	2010-11-17
	B	307	68505.37	33801.10	22.99	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Sodium ion	NA	Protein	X-ray	2010-11-17
	B	307	68505.37	33801.10	323.13	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	4-(hydroxy[(phosphonoxy)acetyl]amino)butyl dihydrogen phosphate	TD4	Protein	X-ray	2010-11-17
	B	307	68505.37	33801.10	65.38	Fructose-bisphosphate aldolase	Lyase/lyase inhibitor	Zinc ion	ZN	Protein	X-ray	2010-11-17
3NA7	A	256	30127.29	29799.30	238.30	HP0958	Gene regulation, chaperone	4-(2-hydroxyethyl)-1-piperazine ethanesulfonic acid	EPE	Protein	X-ray	2010-09-22
	A	256	30127.29	29799.30	24.31	HP0958	Gene regulation, chaperone	Magnesium ion	MG	Protein	X-ray	2010-09-22
	A	256	30127.29	29799.30	65.38	HP0958	Gene regulation, chaperone	Zinc ion	ZN	Protein	X-ray	2010-09-22
3NM4	A	230	50594.75	25050.10	62.07	MTA/SAH nucleosidase	Hydrolase	1,2-ethanediol	EDO	Protein	X-ray	2010-11-24
	A	230	50594.75	25050.10	122.14	MTA/SAH nucleosidase	Hydrolase	2-amino-2-hydroxymethyl-propane-1,3-diol	TRS	Protein	X-ray	2010-11-24

3NM5	B	230	50594.75	25050.10	62.07	MTA/SAH nucleosidase	Hydrolase	1,2-ethanediol	EDO	Protein	X-ray	2010-11-24	
	A	230	50634.69	25050.10	267.24	MTA/SAH nucleosidase	Hydrolase	(1s)-1-(7-amino-1h-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-d-ribitol	FMC	Protein	X-ray	2010-11-24	
	B	230	50634.69	25050.10	267.24	MTA/SAH nucleosidase	Hydrolase	(1s)-1-(7-amino-1h-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-d-ribitol	FMC	Protein	X-ray	2010-11-24	
	B	230	25555.64	25050.10	135.13	MTA/SAH nucleosidase	Hydrolase	Adenine	ADE	Protein	X-ray	2010-11-24	
	B	230	25555.64	25050.10	62.07	MTA/SAH nucleosidase	Hydrolase	1,2-ethanediol	EDO	Protein	X-ray	2010-11-24	
	B	230	25555.64	25050.10	122.14	MTA/SAH nucleosidase	Hydrolase	2-amino-2-hydroxymethyl-propane-1,3-diol	TRS	Protein	X-ray	2010-11-24	
3NV7	A	157	18171.08	17726.80	60.05	Phosphopantetheine adenylyltransferase	Transferase	Acetic acid	ACY	Protein	X-ray	2011-07-13	
	A	157	18171.08	17726.80	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-07-13	
3NXZ	A	170	77714.34	19412.70	63.55	UreaseProtein ureE	Metalprotein	Copper (ii) ion	CU	Protein	X-ray	2010-08-25	MKBSGI
	B	170	77714.34	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	C	170	77714.34	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	D	170	77714.34	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
3NY0	A	170	77709.50	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	B	170	77709.50	19412.70	58.70	UreaseProtein ureE	Metalprotein	Nickel (ii) ion	NI	Protein	X-ray	2010-08-25	MKBSGI
	C	170	77709.50	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
	D	170	77709.50	19412.70		UreaseProtein ureE	Metalprotein			Protein	X-ray	2010-08-25	MKBSGI
3O1Q	A	254	85956.00	28652.00		UreaseProtein ureF	Metalprotein			Protein	X-ray	2010-08-18	
	B	254	85956.00	28652.00		UreaseProtein ureF	Metalprotein			Protein	X-ray	2010-08-18	
	C	254	85956.00	28652.00		UreaseProtein ureF	Metalprotein			Protein	X-ray	2010-08-18	
3OQG	A	180	47812.51	21130.20	35.45	Hpy188I	Hydrolase/dna	Chloride ion	CL	Protein	X-ray	2010-10-20	
										DNA			
	A	180	47812.51	21130.20	196.11	Hpy188I	Hydrolase/dna	Selenomethionine	MSE	Protein	X-ray	2010-10-20	
										DNA			
	A	180	47812.51	21130.20	22.99	Hpy188I	Hydrolase/dna	Sodium ion	NA	Protein	X-ray	2010-10-20	
										DNA			
	B	180	47812.51	21130.20	196.11	Hpy188I	Hydrolase/dna	Selenomethionine	MSE	Protein	X-ray	2010-10-20	

	B	180	47812.51	21130.20	22.99	Hpy188I	Hydrolase/dna	Sodium ion	NA	DNA Protein	X-ray	2010-10-20
	C	9	47812.51	2739.85		DNA 5'- D(*GP*AP*TP*CP*TP*GP*AP*AP* C)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
	D	9	47812.51	2730.83		DNA 5'- D(*GP*TP*TP*CP*AP*GP*AP*TP* C)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
3OR3	A	180	47903.22	21130.20	40.08	Restriction endonuclease hpy188i	Hydrolase/dna	Calcium ion	CA	DNA Protein	X-ray	2010-10-20
	A	180	47903.22	21130.20	35.45	Restriction endonuclease hpy188i	Hydrolase/dna	Chloride ion	CL	DNA Protein	X-ray	2010-10-20
	A	180	47903.22	21130.20	196.11	Restriction endonuclease hpy188i	Hydrolase/dna	Selenomethionine	MSE	DNA Protein	X-ray	2010-10-20
	B	180	47903.22	21130.20	35.45	Restriction endonuclease hpy188i	Hydrolase/dna	Chloride ion	CL	DNA Protein	X-ray	2010-10-20
	B	180	47903.22	21130.20	196.11	Restriction endonuclease hpy188i	Hydrolase/dna	Selenomethionine	MSE	DNA Protein	X-ray	2010-10-20
	C	5	47903.22	1495.04		5'-D(*GP*AP*TP*CP*T)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
	D	5	47903.22	1495.04		5'-D(*GP*TP*TP*CP*A)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
	E	4	47903.22	1199.85		5'-D(P*GP*AP*AP*C)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
	F	4	47903.22	1190.84		5'-D(P*GP*AP*TP*C)-3'	Hydrolase/dna			DNA Protein	X-ray	2010-10-20
3OTW	A	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	DNA Protein	X-ray	2011-09-14
	A	163	116401.20	18520.60	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	DNA Protein	X-ray	2011-09-14

	B	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	Protein	X-ray	2011-09-14	
	B	163	116401.20	18520.60	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-09-14	
	C	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	Protein	X-ray	2011-09-14	
	C	163	116401.20	18520.60	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-09-14	
	D	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	Protein	X-ray	2011-09-14	
	D	163	116401.20	18520.60	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-09-14	
	E	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	Protein	X-ray	2011-09-14	
	E	163	116401.20	18520.60	96.06	Phosphopantetheine adenylyltransferase	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-09-14	
	F	163	116401.20	18520.60	767.53	Phosphopantetheine adenylyltransferase	Transferase	Coenzyme a	COA	Protein	X-ray	2011-09-14	
3P9Z	A	229	26411.45	26309.40	102.05	Uroporphyrinogen III cosynthase (HemD)	Ligase	Malonate ion	MLI	Protein	X-ray	2010-11-03	MCSG
	A	229	26411.45	26309.40	196.11	Uroporphyrinogen III cosynthase (HemD)	Ligase	Selenomethionine	MSE	Protein	X-ray	2010-11-03	MCSG
3PHG	A	269	60278.40	30139.20		Shikimate dehydrogenase	Oxidoreductase			Protein	X-ray	2011-11-09	
	B	269	60278.40	30139.20		Shikimate dehydrogenase	Oxidoreductase			Protein	X-ray	2011-11-09	
3PHH	A	269	30313.35	30139.20	174.15	Shikimate dehydrogenase	Oxidoreductase	(3r,4s,5r)-3,4,5-trihydroxycyclohex-1- ene-1-carboxylic acid	SKM	Protein	X-ray	2011-11-09	
3PHI	A	269	62117.56	30139.20	745.43	Shikimate dehydrogenase	Oxidoreductase	Nadph dihydro-nicotinamide-adenine- dinucleotide phosphate	NDP	Protein	X-ray	2011-11-09	
	A	269	62117.56	30139.20	174.15	Shikimate dehydrogenase	Oxidoreductase	(3r,4s,5r)-3,4,5-trihydroxycyclohex-1- ene-1-carboxylic acid	SKM	Protein	X-ray	2011-11-09	
	B	269	62117.56	30139.20	745.43	Shikimate dehydrogenase	Oxidoreductase	Nadph dihydro-nicotinamide-adenine-	NDP	Protein	X-ray	2011-11-09	

							dinucleotide phosphate					
	B	269	62117.56	30139.20	174.15	Shikimate dehydrogenase	Oxidoreductase	(3r,4s,5r)-3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid	SKM	Protein	X-ray	2011-11-09
3PHJ	A	269	60626.70	30139.20	174.15	Shikimate dehydrogenase	Oxidoreductase	3-dehydroshikimate	DHK	Protein	X-ray	2011-11-09
	B	269	60626.70	30139.20	174.15	Shikimate dehydrogenase	Oxidoreductase	3-dehydroshikimate	DHK	Protein	X-ray	2011-11-09
3PHT	A	148	34324.00	17103.30	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-11-23
	B	148	34324.00	17103.30	58.70	Putative nickel-responsive regulator	Transcription	Nickel (ii) ion	NI	Protein	X-ray	2011-11-23
3Q1O	A	310	143464.69	35175.50	246.09	Geranyltranstransferase (IspA)	Transferase	3-methylbut-3-enyl trihydrogen diphosphate	IPE	Protein	X-ray	2011-01-12 NYSRCSG
	A	310	143464.69	35175.50	24.31	Geranyltranstransferase (IspA)	Transferase	Magnesium ion	MG	Protein	X-ray	2011-01-12 NYSRCSG
	A	310	143464.69	35175.50	96.06	Geranyltranstransferase (IspA)	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-01-12 NYSRCSG
	B	310	143464.69	35175.50	246.09	Geranyltranstransferase (IspA)	Transferase	3-methylbut-3-enyl trihydrogen diphosphate	IPE	Protein	X-ray	2011-01-12 NYSRCSG
	B	310	143464.69	35175.50	24.31	Geranyltranstransferase (IspA)	Transferase	Magnesium ion	MG	Protein	X-ray	2011-01-12 NYSRCSG
	B	310	143464.69	35175.50	96.06	Geranyltranstransferase (IspA)	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-01-12 NYSRCSG
	C	310	143464.69	35175.50	246.09	Geranyltranstransferase (IspA)	Transferase	3-methylbut-3-enyl trihydrogen diphosphate	IPE	Protein	X-ray	2011-01-12 NYSRCSG
	C	310	143464.69	35175.50	24.31	Geranyltranstransferase (IspA)	Transferase	Magnesium ion	MG	Protein	X-ray	2011-01-12 NYSRCSG
	C	310	143464.69	35175.50	96.06	Geranyltranstransferase (IspA)	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-01-12 NYSRCSG
	D	310	143464.69	35175.50	246.09	Geranyltranstransferase (IspA)	Transferase	3-methylbut-3-enyl trihydrogen diphosphate	IPE	Protein	X-ray	2011-01-12 NYSRCSG
	D	310	143464.69	35175.50	24.31	Geranyltranstransferase (IspA)	Transferase	Magnesium ion	MG	Protein	X-ray	2011-01-12 NYSRCSG
3QBU	A	326	150530.31	37567.20	65.38	PutativeProtein	Hydrolase	Zinc ion	ZN	Protein	X-ray	2011-05-25
	B	326	150530.31	37567.20	65.38	PutativeProtein	Hydrolase	Zinc ion	ZN	Protein	X-ray	2011-05-25
	C	326	150530.31	37567.20	65.38	PutativeProtein	Hydrolase	Zinc ion	ZN	Protein	X-ray	2011-05-25
	D	326	150530.31	37567.20	65.38	PutativeProtein	Hydrolase	Zinc ion	ZN	Protein	X-ray	2011-05-25
3QDL	A	210	98414.38	24101.20	456.35	Oxygen-insensitive NADPH nitroreductase	Oxidoreductase	Flavin mononucleotide	FMN	Protein	X-ray	2012-01-18
3QDL	A	210	98414.38	24101.20	92.09	Oxygen-insensitive NADPH nitroreductase	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2012-01-18
	B	210	98414.38	24101.20	456.35	Oxygen-insensitive NADPH	Oxidoreductase	Flavin mononucleotide	FMN	Protein	X-ray	2012-01-18

					nitroreductase								
	C	210	98414.38	24101.20	456.35	Oxygen-insensitive NADPH	Oxidoreductase	Flavin mononucleotide	FMN	Protein	X-ray	2012-01-18	
						nitroreductase							
	D	210	98414.38	24101.20	456.35	Oxygen-insensitive NADPH	Oxidoreductase	Flavin mononucleotide	FMN	Protein	X-ray	2012-01-18	
						nitroreductase							
	D	210	98414.38	24101.20	92.09	Oxygen-insensitive NADPH	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2012-01-18	
						nitroreductase							
3QHP	A	166	37157.20	18578.60		TypeProtein J (CapJ)	Transferase			Protein	X-ray	2011-06-29	
	B	166	37157.20	18578.60		TypeProtein J (CapJ)	Transferase			Protein	X-ray	2011-06-29	
3QXC	A	242	28684.82	27148.30	507.18	Dethiobiotin synthetase	Ligase	Adenosine-5'-triphosphate	ATP	Protein	X-ray	2011-03-30	MCSG
	A	242	28684.82	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG
	A	242	28684.82	27148.30	92.09	Dethiobiotin synthetase	Ligase	Glycerol	GOL	Protein	X-ray	2011-03-30	MCSG
	A	242	28684.82	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28684.82	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2011-03-30	MCSG
	A	242	28684.82	27148.30	106.12	Dethiobiotin synthetase	Ligase	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-03-30	MCSG
3QXH	A	242	28188.65	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2011-03-30	MCSG
	A	242	28188.65	27148.30	427.20	Dethiobiotin synthetase	Ligase	Adenosine-5'-diphosphate	ADP	Protein	X-ray	2011-03-30	MCSG
	A	242	28188.65	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG
	A	242	28188.65	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28188.65	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2011-03-30	MCSG
3QXJ	A	242	28316.41	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG
	A	242	28316.41	27148.30	523.18	Dethiobiotin synthetase	Ligase	Guanosine-5'-triphosphate	GTP	Protein	X-ray	2011-03-30	MCSG
	A	242	28316.41	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28316.41	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2011-03-30	MCSG
3QXS	A	242	28423.56	27148.30	506.20	Dethiobiotin synthetase	Ligase	Phosphoaminophosphonic acid-adenylate ester	ANP	Protein	X-ray	2011-03-30	MCSG
	A	242	28423.56	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG
	A	242	28423.56	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28423.56	27148.30	62.01	Dethiobiotin synthetase	Ligase	Nitrate ion	NO3	Protein	X-ray	2011-03-30	MCSG
3QXX	A	242	28358.81	27148.30	159.23	Dethiobiotin synthetase	Ligase	8-aminooctanoic acid	8AC	Protein	X-ray	2011-03-30	MCSG
	A	242	28358.81	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG

	A	242	28358.81	27148.30	443.20	Dethiobiotin synthetase	Ligase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2011-03-30	MCSG
	A	242	28358.81	27148.30	92.09	Dethiobiotin synthetase	Ligase	Glycerol	GOL	Protein	X-ray	2011-03-30	MCSG
	A	242	28358.81	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28358.81	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2011-03-30	MCSG
3QY0	A	242	28728.17	27148.30	62.07	Dethiobiotin synthetase	Ligase	1,2-ethanediol	EDO	Protein	X-ray	2011-03-30	MCSG
	A	242	28728.17	27148.30	443.20	Dethiobiotin synthetase	Ligase	Guanosine-5'-diphosphate	GDP	Protein	X-ray	2011-03-30	MCSG
	A	242	28728.17	27148.30	24.31	Dethiobiotin synthetase	Ligase	Magnesium ion	MG	Protein	X-ray	2011-03-30	MCSG
	A	242	28728.17	27148.30	94.97	Dethiobiotin synthetase	Ligase	Phosphate ion	PO4	Protein	X-ray	2011-03-30	MCSG
3RPF	A	148	51184.51	16988.50	62.07	Molybdopterin synthase catalytic subunit	Transferase	1,2-ethanediol	EDO	Protein	X-ray	2011-06-29	MCSG
	A	148	51184.51	16988.50	196.11	Molybdopterin synthase catalytic subunit	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
	A	148	51184.51	16988.50	96.06	Molybdopterin synthase catalytic subunit	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-06-29	MCSG
	B	148	51184.51	16988.50	62.07	Molybdopterin synthase catalytic subunit	Transferase	1,2-ethanediol	EDO	Protein	X-ray	2011-06-29	MCSG
	B	148	51184.51	16988.50	196.11	Molybdopterin synthase catalytic subunit	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
	B	148	51184.51	16988.50	96.06	Molybdopterin synthase catalytic subunit	Transferase	Sulfate ion	SO4	Protein	X-ray	2011-06-29	MCSG
	C	74	51184.51	8383.56	196.11	Molybdopterin converting factor, subunit 1 (MoaD)	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
	D	74	51184.51	8383.56	196.11	Molybdopterin converting factor, subunit 1 (MoaD)	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
3RRL	A	235	97219.09	25806.50	196.11	Succinyl-CoA:3-ketoacid-coenzyme A transferase subunit A	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
	B	207	97219.09	22757.00	196.11	Succinyl-CoA:3-ketoacid-coenzyme A transferase subunit B	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
	C	235	97219.09	25806.50	92.09	Succinyl-CoA:3-ketoacid-coenzyme A transferase subunit A	Transferase	Glycerol	GOL	Protein	X-ray	2011-06-29	MCSG
	C	235	97219.09	25806.50	196.11	Succinyl-CoA:3-ketoacid-coenzyme A	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG

transferase subunit A													
	D	207	97219.09	22757.00	196.11	Succinyl-CoA:3-ketoacid-coenzyme A	Transferase	Selenomethionine	MSE	Protein	X-ray	2011-06-29	MCSG
transferase subunit B													
3SF5	A	254	118438.17	28652.00	92.09	UreaseProtein ureF	Chaperone	Glycerol	GOL	Protein	X-ray	2011-11-02	
	A	254	118438.17	28652.00	106.12	UreaseProtein ureF	Chaperone	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-11-02	
	B	265	118438.17	29757.30	106.12	UreaseProtein ureH	Chaperone	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-11-02	
	B	265	118438.17	29757.30	96.06	UreaseProtein ureH	Chaperone	Sulfate ion	SO4	Protein	X-ray	2011-11-02	
	C	254	118438.17	28652.00	92.09	UreaseProtein ureF	Chaperone	Glycerol	GOL	Protein	X-ray	2011-11-02	
	C	254	118438.17	28652.00	106.12	UreaseProtein ureF	Chaperone	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-11-02	
	C	254	118438.17	28652.00	96.06	UreaseProtein ureF	Chaperone	Sulfate ion	SO4	Protein	X-ray	2011-11-02	
	D	265	118438.17	29757.30	106.12	UreaseProtein ureH	Chaperone	Di(hydroxyethyl)ether	PEG	Protein	X-ray	2011-11-02	
	D	265	118438.17	29757.30	96.06	UreaseProtein ureH	Chaperone	Sulfate ion	SO4	Protein	X-ray	2011-11-02	
3SXP	A	362	209058.16	41148.20	663.43	ADP-L-glycero-D-mannoheptose-6-epimerase	Isomerase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2012-02-08	
	B	362	209058.16	41148.20	663.43	ADP-L-glycero-D-mannoheptose-6-epimerase	Isomerase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2012-02-08	
	C	362	209058.16	41148.20	663.43	ADP-L-glycero-D-mannoheptose-6-epimerase	Isomerase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2012-02-08	
	D	362	209058.16	41148.20	663.43	ADP-L-glycero-D-mannoheptose-6-epimerase	Isomerase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2012-02-08	
	E	362	209058.16	41148.20	663.43	ADP-L-glycero-D-mannoheptose-6-epimerase	Isomerase	Nicotinamide-adenine-dinucleotide	NAD	Protein	X-ray	2012-02-08	
3T9J	A	164	19068.87	19006.80	62.07	Neutrophil-activating protein	Metal transport	1,2-ethanediol	EDO	Protein	X-ray	2012-02-08	
3TA8	A	164	19366.77	19006.80	62.07	Neutrophil-activating protein	Metal transport	1,2-ethanediol	EDO	Protein	X-ray	2012-02-08	
	A	164	19366.77	19006.80	55.85	Neutrophil-activating protein	Metal transport	Fe (III) ion	FE	Protein	X-ray	2012-02-08	
3TC1	A	315	72308.81	36130.10	24.31	Octaprenyl Pyrophosphate Synthase	Transferase	Magnesium ion	MG	Protein	X-ray	2011-08-31	
	B	315	72308.81	36130.10	24.31	Octaprenyl Pyrophosphate Synthase	Transferase	Magnesium ion	MG	Protein	X-ray	2011-08-31	
3TDG	A	273	30991.95	30571.50	46.03	PutativeProtein	Oxidoreductase	Formic acid	FMT	Protein	X-ray	2011-11-09	
	A	273	30991.95	30571.50	92.09	PutativeProtein	Oxidoreductase	Glycerol	GOL	Protein	X-ray	2011-11-09	
	A	273	30991.95	30571.50	282.33	PutativeProtein	Oxidoreductase	Hexaethylene glycol	P6G	Protein	X-ray	2011-11-09	
3TJ8	A	170	39394.36	19437.70	46.03	UreaseProtein ureE	metalProtein	Formic acid	FMT	Protein	X-ray	2011-11-02	

3TJ9	B	170	39394.36	19437.70	46.03	UreaseProtein ureE	metalProtein	Formic acid	FMT	Protein	X-ray	2011-11-02
	B	170	39394.36	19437.70	58.70	UreaseProtein ureE	metalProtein	Nickel (ii) ion	NI	Protein	X-ray	2011-11-02
	A	170	77927.58	19437.70	46.03	UreaseProtein ureE	metalProtein	Formic acid	FMT	Protein	X-ray	2011-11-02
	A	170	77927.58	19437.70	65.38	UreaseProtein ureE	metalProtein	Zinc ion	ZN	Protein	X-ray	2011-11-02
	B	170	77927.58	19437.70		UreaseProtein ureE	metalProtein			Protein	X-ray	2011-11-02
	C	170	77927.58	19437.70	65.38	UreaseProtein ureE	metalProtein	Zinc ion	ZN	Protein	X-ray	2011-11-02
3TJA	D	170	77927.58	19437.70		UreaseProtein ureE	metalProtein			Protein	X-ray	2011-11-02
	A	170	78170.48	19437.70	35.45	UreaseProtein ureE	metalProtein	Chloride ion	CL	Protein	X-ray	2011-11-02
	A	170	78170.48	19437.70	96.06	UreaseProtein ureE	metalProtein	Sulfate ion	SO4	Protein	X-ray	2011-11-02
	B	170	78170.48	19437.70	96.06	UreaseProtein ureE	metalProtein	Sulfate ion	SO4	Protein	X-ray	2011-11-02
	C	170	78170.48	19437.70	96.06	UreaseProtein ureE	metalProtein	Sulfate ion	SO4	Protein	X-ray	2011-11-02
	D	170	78170.48	19437.70	96.06	UreaseProtein ureE	Metalprotein	Sulfate ion	SO4	Protein	X-ray	2011-11-02
3TWO	A	348	79226.37	38737.00	745.43	Mannitol dehydrogenase	Oxidoreductase	Nadph dihydro-nicotinamide-adenine-dinucleotide phosphate	NDP	Protein	X-ray	2011-10-12
	A	348	79226.37	38737.00	65.38	Mannitol dehydrogenase	Oxidoreductase	Zinc ion	ZN	Protein	X-ray	2011-10-12
	B	348	79226.37	38737.00	745.43	Mannitol dehydrogenase	Oxidoreductase	Nadph dihydro-nicotinamide-adenine-dinucleotide phosphate	NDP	Protein	X-ray	2011-10-12
	B	348	79226.37	38737.00	65.38	Mannitol dehydrogenase	Oxidoreductase	Zinc ion	ZN	Protein	X-ray	2011-10-12
	A	160	37445.60	18722.80	196.11	ImmunoglobulinProteinProtein D	Rnaprotein	Selenomethionine	MSE	Protein	X-ray	2012-02-08
	B	160	37445.60	18722.80	196.11	ImmunoglobulinProteinProtein D	Rnaprotein	Selenomethionine	MSE	Protein	X-ray	2012-02-08
3USW	A	258	29018.70	29018.70		FlagellarProtein	Motor protein			Protein	X-ray	2011-12-14
3USY	A	234	52240.80	26120.40		FlagellarProtein	Motor protein			Protein	X-ray	2011-12-14
	B	234	52240.80	26120.40		FlagellarProtein	Motor protein			Protein	X-ray	2011-12-14

^a Midwest Center for SG; ^b Structural Genomics; ^c Northeast SG Consortium; ^d Montreal-Kingston Bacterial Structural Genomics Initiative; ^e New York SGX Research Center for SG; ^f Ontario Centre for Structural Proteomics; ^g Joint Center for SG.