

Table D for deposit : Mg sites with links to ATP and to protein

*cngp* lists the amino-acid side chain donor groups, O represents main chain carbonyl oxygen,  
*sd1*, *sd2* are sequence separations of first and second donors, second and third donors,  
*CN* is coordination number, *resln* is structure resolution,  
*rms* is r.m.s deviation of metal-donor atom distances from target values, a quality indicator,  
*npd\_1*, *npd\_2* etc are full names from PDB files of all non-protein donor groups (MO3, MO4 etc are old PDB usage for hydrated metal ions),  
*class* is from PDB header,

<i>cngp</i>	<i>sd1</i>	<i>sd2</i>	<i>CN</i>	<i>rms</i>	<i>resln</i>	<i>pdb</i>	<i>npd_1</i>	<i>npd_2</i>	<i>npd_3</i>	<i>npd_4</i>	<i>npd_5</i>	<i>class</i>
D	-1	-1	3	0.39	2.50	2aqx	ATP_O3G_2462_	ATP_O2A_2462_	-	-	-	TRANSFERASE
D	-1	-1	6	0.09	1.60	1kj9	ATP_O1G_1_	HOH_O_123_	HOH_O_129_	HOH_O_133_	HOH_O_252_	TRANSFERASE
D	-1	-1	4	0.14	2.50	2aqx	ATP_O3G_1462_	ATP_O2A_1462_	HOH_O_105_	-	-	TRANSFERASE
D	-1	-1	4	0.19	2.50	2aqx	ATP_O1G_2462_	ATP_O1B_2462_	-	-	-	TRANSFERASE
D	-1	-1	6	0.23	2.25	1y8q	ATP_O2G_801_	ATP_O2B_801_	HOH_O_220_	HOH_O_414_	HOH_O_727_	LIGASE
D	-1	-1	3	0.26	2.40	1der	ATP_O1B_1_J	ATP_O2A_1_J	-	-	-	CHAPERONIN
D	-1	-1	6	0.36	2.10	1u5r	ATP_O2B_411_	HOH_O_18_	HOH_O_46_	HOH_O_316_	-	TRANSFERASE
D	-1	-1	2	0.37	2.30	1q97	ATP_O3B_485_	-	-	-	-	TRANSFERASE
D	-1	-1	4	0.49	2.30	1q97	ATP_O1G_485_	ATP_O2G_485_	ATP_O1A_485_	-	-	TRANSFERASE
DD	2	-1	6	0.35	2.00	1dy3	ATP_O2B_200_A	ATP_O1A_200_A	HOH_O_78_Z	HOH_O_140_Z	-	PYROPHOSPHORYLASE
DD	2	-1	6	0.47	2.00	1dy3	ATP_O1G_200_A	ATP_O2B_200_A	87Y_O16_201_A	HOH_O_141_Z	-	PYROPHOSPHORYLASE
DD	98	-1	6	0.12	2.11	1mb9	ATP_O2G_702_	ATP_O2A_702_	ATP_O3A_702_	HOH_O_655_	-	HYDROLASE
DE	16	-1	3	0.54	2.20	2cja	ATP_O2A_1507_B	-	-	-	-	LIGASE
DE	99	-1	5	0.37	2.40	1n56	ATP_O1A_1803_	HOH_O_648_	HOH_O_1023_	-	-	TRANSFERASE/DNA
DOD	1	97	7	0.35	2.40	1n56	ATP_O1G_1803_	ATP_O1A_1803_	HOH_O_666_	-	-	TRANSFERASE/DNA
E	-1	-1	6	0.10	1.60	1kj9	ATP_O3G_1_	ATP_O2B_1_	EDO_O1_15_	HOH_O_35_	-	TRANSFERASE
E	-1	-1	3	0.39	2.15	1yfr	ATP_O1B_1500_	ATP_O1A_1500_	-	-	-	LIGASE
E	-1	-1	3	0.61	2.40	2i4o	ATP_O3G_402_	ATP_O2B_402_	-	-	-	LIGASE
ED	2	-1	5	0.28	2.20	1tfw	ATP_O3G_1501_	ATP_O2B_1501_	ATP_O1A_1501_	-	-	TRANSFERASE/RNA
ED	24	-1	6	0.11	2.10	1a49	OXL_O1_2333_D	OXL_O4_2333_D	ATP_O2G_2335_D	HOH_O_6439_	-	TRANSFERASE
ED	24	-1	5	0.17	2.10	1a49	OXL_O1_1733_C	OXL_O4_1733_C	ATP_O2G_1735_C	-	-	TRANSFERASE
EE	12	-1	6	0.11	1.60	1kj9	ATP_O2G_5_	ATP_O2A_5_	HOH_O_420_	-	-	TRANSFERASE
EQ	3	-1	4	0.41	2.40	2i4o	ATP_O2B_402_	ATP_O2A_402_	-	-	-	LIGASE
EQ	3	-1	5	0.39	2.40	2i4o	MG_MG_302_	ATP_O2B_401_	ATP_O2A_401_	-	-	LIGASE
Hn	163	-1	3	0.39	2.00	1yun	ATP_O1B_1220_	-	-	-	-	TRANSFERASE
N	-1	-1	6	0.15	2.40	2bu2	ATP_O2G_1386_A	ATP_O2B_1386_A	ATP_O1A_1386_A	HOH_O_40_Z	HOH_O_87_Z	TRANSFERASE
N	-1	-1	6	0.31	2.20	1tc0	ATP_O1B_601_	ATP_O2A_601_	HOH_O_75_	HOH_O_109_	HOH_O_110_	CHAPERONE
N	-1	-1	3	0.32	2.50	1tid	ATP_O1G_201_	ATP_O1B_201_	-	-	-	TRANSCRIPTION
N	-1	-1	6	0.43	2.50	1tid	ATP_O1G_200_	ATP_O1B_200_	ATP_O1A_200_	HOH_O_2_	HOH_O_49_	TRANSCRIPTION
N	-1	-1	3	0.45	2.00	1csn	ATP_O1G_299_	ATP_O2A_299_	-	-	-	PHOSPHOTRANSFERASE

ND	13	-1	6	0.08	2.40	1s9j	ATP_O1B_535_	ATP_O2A_535_	HOH_O_97_	HOH_O_98_	-	TRANSFERASE
ND	13	-1	6	0.11	2.20	1qmq	ATP_O2G_381_A	ATP_O3B_381_A	ATP_O2A_381_A	HOH_O_111_Z	-	COMPLEX(PROTEINKINASE/CYCL
ND	13	-1	6	0.37	2.10	1u5r	ATP_O2G_412_	ATP_O2A_412_	HOH_O_31_	HOH_O_225_	-	TRANSFERASE
O	-1	-1	3	0.49	1.70	1xng	ATP_O1G_304_	ATP_O2B_304_	-	-	-	LIGASE
O	-1	-1	6	0.34	1.70	1xng	ATP_O1G_303_	ATP_O2B_303_	ATP_O2A_303_	HOH_O_55_	HOH_O_161_	LIGASE
R	-1	-1	3	0.46	2.50	1xdp	ATP_O2A_704_	HOH_O_94_	-	-	-	TRANSFERASE
RR	30	-1	4	0.40	2.50	1xdp	ATP_O1G_701_	-	-	-	-	TRANSFERASE
S	-1	-1	6	0.03	1.85	2iyw	ATP_O1G_201_A	ATP_O1B_201_A	HOH_O_10_Z	HOH_O_200_Z	HOH_O_204_Z	TRANSFERASE
S	-1	-1	6	0.06	1.70	1e2q	ATP_O3G_302_A	ATP_O1B_302_A	HOH_O_21_Z	HOH_O_22_Z	HOH_O_23_Z	THYMIDYLATEKINASE
S	-1	-1	6	0.10	2.27	1w7a	ATP_O2G_1801_A	ATP_O2B_1801_A	MO3_O1_1802_A	MO3_O2_1802_A	MO3_O3_1802_A	DNABINDING
S	-1	-1	6	0.14	2.50	1xef	ATP_O3G_800_	ATP_O2B_800_	HOH_O_160_	HOH_O_165_	HOH_O_171_	TRANSPORTPROTEIN
S	-1	-1	6	0.28	2.50	2c8v	ATP_O3G_5292_A	ATP_O1B_5292_A	HOH_O_4_Z	HOH_O_13_Z	HOH_O_97_Z	XIDOREDUCTASE
S	-1	-1	2	0.69	2.40	1kvk	ATP_O3G_535_	-	-	-	-	TRANSFERASE
SQ	28	-1	6	0.06	1.50	2cbz	ATP_O1G_1873_A	ATP_O2B_1873_A	HOH_O_187_Z	HOH_O_278_Z	-	TRANSPORT
SQ	103	-1	6	0.04	1.60	1f2u	ATP_O1G_901_A	ATP_O1B_901_A	HOH_O_48_	HOH_O_51_	-	REPLICATION
SQ	105	-1	6	0.10	2.50	1xex	ATP_O1G_1001_	ATP_O1B_1001_	HOH_O_30_	HOH_O_109_	-	CELLCYCLE
T	-1	-1	5	0.08	2.40	1e79	ATP_O2G_600_A	ATP_O2B_600_A	HOH_O_72_Z	HOH_O_73_Z	-	ATPPHOSPHORYLASE
T	-1	-1	6	0.16	1.80	2bek	ATP_O3G_500_A	ATP_O2B_500_A	HOH_O_62_Z	HOH_O_183_Z	HOH_O_321_Z	CHROMOSOMESEGREGATION
T	-1	-1	6	0.16	1.94	1svm	ATP_O1G_800_A	ATP_O2B_800_A	HOH_O_5_	HOH_O_803_	HOH_O_804_	VIRUS/VIRALPROTEIN
T	-1	-1	6	0.19	2.40	1ii0	ATP_O2G_1591_	ATP_O1B_1591_	HOH_O_2073_	HOH_O_2102_	HOH_O_2209_	HYDROLASE
T	-1	-1	6	0.22	2.20	1ytm	ATP_O3G_1541_	ATP_O2B_1541_	HOH_O_9_	HOH_O_229_	HOH_O_351_	LYASE
T	-1	-1	6	0.30	1.80	1os1	ATP_O3G_541_	ATP_O2B_541_	HOH_O_674_	HOH_O_716_	HOH_O_738_	LYASE
TDE	38	61	6	0.16	1.80	1a82	ATP_O3G_802_	ATP_O1B_802_	HOH_O_444_	-	-	BIOTINBIOSYNTHESIS
TE	86	-1	6	0.13	2.10	1g64	ATP_O2B_1000_	ATP_O2A_1000_	HOH_O_1380_	HOH_O_1381_	-	TRANSFERASE
TE	86	-1	6	0.14	2.10	1g64	ATP_O2B_999_	ATP_O2A_999_	HOH_O_1331_	HOH_O_1332_	-	TRANSFERASE
TQ	28	-1	6	0.07	2.05	2bbs	ATP_O2G_1_	ATP_O2B_1_	HOH_O_7_	HOH_O_202_	-	TRANSPORTPROTEIN
X	-1	-1	6	0.18	2.20	1tc0	ATP_O1B_301_	ATP_O2A_301_	HOH_O_38_	HOH_O_50_	HOH_O_125_	CHAPERONE

The following proteins have  $\geq 75\%$  sequence identity to proteins in the list above, as established with PISCES (G. Wang and R. L. Dunbrack, Jr. PISCES: a protein sequence culling server. *Bioinformatics*, 19:1589-1591, 2003) and the sites appear very similar.

E	-1	-1	6	0.16	1.60	1kj8	ATP_O3G_1_	ATP_O2B_1_	HOH_O_29_	HOH_O_231_	-	TRANSFERASE
E	-1	-1	3	0.51	1.60	1kj8	ATP_O3G_5_	HOH_O_726_	-	-	-	TRANSFERASE
EE	12	-1	6	0.08	1.60	1kj8	ATP_O2G_1_	ATP_O2A_1_	HOH_O_22_	-	-	TRANSFERASE
EE	12	-1	7	0.41	1.60	1kj8	ATP_O2G_5_	ATP_O3B_5_	ATP_O2A_5_	HOH_O_539_	-	TRANSFERASE
ND	13	-1	6	0.32	2.10	1u5r	ATP_O3G_411_	ATP_O2A_411_	HOH_O_218_	HOH_O_261_	-	TRANSFERASE
T	-1	-1	4	0.26	2.30	1xmj	ATP_O2G_1_	ATP_O2B_1_	HOH_O_105_	-	-	MEMBRANEPROTEIN,HYDROLAS
TQ	28	-1	6	0.13	2.25	1xmi	ATP_O2G_4_	ATP_O2B_4_	HOH_O_687_	HOH_O_709_	-	MEMBRANEPROTEIN,HYDROLAS
TQ	28	-1	4	0.15	2.35	1r0z	ATP_O2G_404_	ATP_O2B_404_	-	-	-	TRANSPORTPROTEIN
TQ	28	-1	5	0.17	2.20	1r0x	ATP_O2G_4_	ATP_O2B_4_	HOH_O_378_	-	-	TRANSPORTPROTEIN

Distribution of coordination numbers in whole set

		<i>Number</i>
CN =	1	0
	2	2
	3	11
	4	7
	5	6
	6	38
	7	2

note that these include carboxylate groups