METAL SITES IN PROTEIN STRUCTURES DETERMINED AT RESOLUTION 1.25 A OR BETTER

For further explanation see 'description'.
Where two or more equivalent sites are present in the asymmetric unit, only the first is listed here, although all have been used in evaluating average distances.

donors	metal	sequence diffs						his	cn	pdb	cn2	rms	resln	metal	startaa	carbi	other donors	E.C. No.
ODODD	Ca	3	2	3	1	-1	-1	-1	7	1b9o	0	0.1	1.1	CA 124	LYSA 79	.....	WW	
CCCC	Fe	3	30	3	-1	-1	-1	-1	4	1bq8	0	0.1	1.1	FE A 55	CYSA 6	....		
CCCC	Fe	3	30	3	-1	-1	-1	-1	4	1bq9	0	0.1	1.2	FE 55	CYSA 6	....		
CCCC	Fe	3	30	3	-1	-1	-1	-1	4	1brf	0	0.1	0.9	FE 54	CYSA 5	....		
OO	K	3	-1	-1	-1	-1	-1	-1 ..	6	1c1d	0	0.4	1.3	K 850	ASPA 118	..	WWWW	
OOO	K	2	2	-1	-1	-1	-1	-1 ...	5	1c1d	0	0.2	1.3	K 851	LEUB 170	...	WW	
O##RE	K	2	1	0	160	-1	-1	-1	6	1c1d	0	0.4	1.3	K 853	VALA 136	....b	W	
#H	Na	18	-1	-1	-1	-1	-1	-1 .d	4	1c1d	0	0.4	1.3	NA 855	LEUB 201	..	WW	
HM	Fe	35	-1	-1	-1	-1	-1	e.	6	1c75	0	0.1	1.0	FE A 93	HISA 36	..	NNNN	
HHD	Zn	4	6	-1	-1	-1	-1	-1 ee.	4	1c7k	0	0.1	1.0	ZN A 133	HISA 83	...	W	3.4.24.-
DT	Ca	2	-1	-1	-1	-1	-1	-1 ..	6	1c7k	0	0.1	1.0	CA A 134	ASPA 76	b.	WWWW	3.4.24.-
OO	Na	3	-1	-1	-1	-1	-1	-1 ..	6	1c9o	1	0.1	1.2	NA 101	VALA 20	..	WWWW	
QDONOO	Ca	39	34	2	2	2	-1	-1	6	1cse	0	0.1	1.2	CA 430	GLNE 2	.b....		3.4.21.62
HM	Fe	42	-1	-1	-1	-1	-1	-1 e.	6	1ctj	0	0.1	1.1	FE 91	HIS 19	..	NNNN	
CC	Fe	30	-1	-1	-1	-1	-1	-1 ..	5	1czp	0	0.3	1.2	FE2 599	CYSA 49	..	XSS	
HEH	Fe	2	133	-1	-1	-1	-1	-1 e.e	6	1ds1	0	0.1	1.1	FE A 341	HISA 144	...	OOW	
HH	Fe	51	-1	-1	-1	-1	-1	-1 ee	6	1e29	0	0.1	1.2	FE A 136	HISA 41	..	NNNN	
NN	Ca	1	-1	-1	-1	-1	-1	-1 ..	8	1e29	0	0.1	1.2	CA Z 225	ASNA 49	..	WWWWWW	
OD	Ca	0	-1	-1	-1	-1	-1	-1 ..	6	1e29	0	0.3	1.2	CA Z 226	ASPA 35	..	WWWW	
DDD	Mn	5	32	-1	-1	-1	-1	-1 ...	6	1e9g	0	0.2	1.1	MN B2005	ASPB 115	...	OWW	3.6.1.1
DD	Mn	5	-1	-1	-1	-1	-1	-1 ..	6	1e9g	0	0.1	1.1	MN B2008	ASPB 147	..	OOWW	3.6.1.1
DOOOD	Ca	1	7	2	2	-1	-1	-1	6	1ea7	0	0.1	0.9	CA A 311	ASPA 287	.....	W	
ODOQD	Ca	3	2	2	3	-1	-1	-1	6	1ea7	0	0.1	0.9	CA A 312	THRA 214	.....	W	
OOO	Ca	2	3	-1	-1	-1	-1	-1 ...	5	1ea7	0	0.1	0.9	CA A 315	GLYA 181	...	WW	
HHD	Zn	4	11	-1	-1	-1	-1	-1 ee.	5	1eb6	0	0.2	1.0	ZN A 178	HISA 128	..b	WW	3.4.24.39
OE	Na	3	-1	-1	-1	-1	-1	-1 ..	2	1et1	0	0.5	0.9	NA A 101	SERB 1	.b		
DDDOE	Ca	2	2	2	5	-1	-1	-1	6	1exr	0	0.1	1.0	CA A1000	ASPA 20	....b	W	
DDNOE	Ca	2	2	2	5	-1	-1	-1	7	1exr	0	0.2	1.0	CA A1001	ASPA 56	....b	WW	
DDDOE	Ca	2	2	2	5	-1	-1	-1	6	1exr	0	0.1	1.0	CA A1002	ASPA 129	....b	W	
DDNOE	Ca	2	2	2	5	-1	-1	-1	6	1exr	0	0.1	1.0	CA A1004	ASPA 93	....b	W	
DD	Mg	2	-1	-1	-1	-1	-1	-1 ..	6	1f9y	1	0.2	0.9	MG 161	ASPA 95	..	OOWW	2.7.6.3
DOOOD	Ca	1	15	2	2	-1	-1	-1	6	1ga6	0	0.1	1.0	CA A 374	ASPA 328	.....	W	3.4.23.37
QDONOO	Ca	39	34	2	2	2	-1	-1	6	1gci	0	0.1	0.8	CA 277	GLN 2	.b....		3.4.21.62
HEC	Fe	24	188	-1	-1	-1	-1	-1 e..	5	1gnl	0	0.2	1.3	FE7A1545	HISA 240	...	OO	
HH	Fe	42	-1	-1	-1	-1	-1	-1 ee	6	1gu2	0	0.1	1.2	FE A 125	HISA 53	..	NNNN	
HH	Co	2	-1	-1	-1	-1	-1	-1 ed	2	1gwm	0	0.1	1.1	CO A1154	HISA 150	..		
HH	Fe	12	-1	-1	-1	-1	-1	-1 ee	6	1gyo	0	0.1	1.2	FE A 111	HISA 28	..	NNNN	
HH	Fe	15	-1	-1	-1	-1	-1	-1 ee	6	1gyo	0	0.1	1.2	FE A 112	HISA 41	..	NNNN	
HH	Fe	53	-1	-1	-1	-1	-1	-1 ee	6	1gyo	0	0.1	1.2	FE A 113	HISA 31	..	NNNN	
HH	Fe	31	-1	-1	-1	-1	-1	-1 ee	6	1gyo	0	0.1	1.2	FE A 114	HISA 73	..	NNNN	
DE	Ca	4	-1	-1	-1	-1	-1	-1 ..	5	1h5v	0	0.2	1.1	CA A 305	ASPA 120	b.	WWW	3.2.1.4
EO	Mg	7	-1	-1	-1	-1	-1	-1 ..	4	1hbn	0	0.1	1.2	MG A1558	GLUA 117	..	WW	
OO	Na	3	-1	-1	-1	-1	-1	-1 ..	6	1hbn	0	0.2	1.2	NA A1559	LYSA 11	..	WWWW	
OOTO	Na	3	0	1	-1	-1	-1	-1	6	1hbn	0	0.1	1.2	NA A1561	ALAA 544	....	WW	
OOO	Na	2	2	-1	-1	-1	-1	-1 ...	7	1hbn	0	0.5	1.2	NA A1562	PROA 58	...	WWWW	
OO	Na	2	-1	-1	-1	-1	-1	-1 ..	6	1hbn	0	0.1	1.2	NA B1448	ASPB 99	..	WWWW	
ED	Mg	1	-1	-1	-1	-1	-1	-1 ..	3	1hbn	0	0.4	1.2	MG F1250	GLUF 34	..	W	
CCCC	Zn	3	3	8	-1	-1	-1	-1	4	1het	0	0.2	1.1	ZN A 401	CYSA 97	....		1.1.1.1
EOOE	Ca	2	3	5	-1	-1	-1	-1	6	1hj9	0	0.1	0.9	CA A1001	GLUA 70	....	WW	3.4.21.4
DD	Mg	2	-1	-1	-1	-1	-1	-1 ..	6	1hq2	1	0.2	1.3	MG A 161	ASPA 95	..	OOWW	2.7.6.3
EDDH	Mn	2	9	5	-1	-1	-1	-1 ...e	6	1i3h	0	0.1	1.2	MN A 239	GLUA 8	....	WW	
DOND	Ca	2	2	5	-1	-1	-1	-1	6	1i3h	0	0.1	1.2	CA A 240	ASPA 10	b...	WW	
OOOD	Ca	32	2	2	-1	-1	-1	-1	6	1i76	0	0.1	1.2	CA A 996	ASPA 137	....	WW	3.4.24.34
DOOODE	Ca	1	2	2	18	3	-1	-1	6	1i76	0	0.1	1.2	CA A 997	ASPA 154	.....		3.4.24.34
HDH	Zn	2	13	-1	-1	-1	-1	-1 e.e	3	1i76	0	0.1	1.2	ZN A 998	HISA 147	...		3.4.24.34;
HHH	Zn	4	6	-1	-1	-1	-1	-1 eee	5	1i76	0	0.3	1.2	ZN A 999	HISA 197	...	OO	3.4.24.34
OOD	Ca	2	23	-1	-1	-1	-1	-1 ...	7	1ic6	0	0.2	1.0	CA 280	PROA 175	..b	WWWW	3.4.21.64
CCCC	Zn	3	30	3	-1	-1	-1	-1	4	1irn	0	0.1	1.2	ZN 1	CYS 6	....		
CCCC	Fe	3	30	3	-1	-1	-1	-1	4	1iro	0	0.1	1.1	FE 1	CYS 6	....		
HHDH	Mn	55	86	4	-1	-1	-1	-1 ee.e	5	1ix9	0	0.2	0.9	MN B 206	HISB 26	....	O	1.15.1.1
HHDH	Mn	55	86	4	-1	-1	-1	-1 ee.e	5	1ixb	0	0.1	0.9	MN A 206	HISA 26	....	O	1.15.1.1
HH	Fe	36	-1	-1	-1	-1	-1	-1 ee	6	1j0o	0	0.1	1.1	FE A1004	HISA 70	..	NNNN	
HH	Fe	17	-1	-1	-1	-1	-1	-1 ee	6	1j0o	0	0.1	1.1	FE A1002	HISA 35	..	NNNN	
HH	Fe	12	-1	-1	-1	-1	-1	-1 ee	6	1j0o	0	0.1	1.1	FE A1001	HISA 22	..	NNNN	
HH	Fe	58	-1	-1	-1	-1	-1	-1 ee	6	1j0o	0	0.1	1.1	FE A1003	HISA 25	..	NNNN	
HH	Fe	36	-1	-1	-1	-1	-1	-1 ee	6	1j0p	0	0.1	0.9	FE A1004	HISA 70	..	NNNN	
HH	Fe	17	-1	-1	-1	-1	-1	-1 ee	6	1j0p	0	0.1	0.9	FE A1002	HISA 35	..	NNNN	
HH	Fe	12	-1	-1	-1	-1	-1	-1 ee	6	1j0p	0	0.1	0.9	FE A1001	HISA 22	..	NNNN	
HH	Fe	58	-1	-1	-1	-1	-1	-1 ee	6	1j0p	0	0.1	0.9	FE A1003	HISA 25	..	NNNN	
EOOE	Ca	2	3	5	-1	-1	-1	-1	6	1j8a	0	0.1	1.2	CA 501	GLUA 70	....	WW	3.4.21.4
HHC	Zn	4	68	-1	-1	-1	-1	-1 ee.	4	1j98	0	0.1	1.2	ZN A 300	HISA 54	...	W	
EDDH	Mn	2	9	5	-1	-1	-1	-1 ...e	6	1jbc	0	0.2	1.2	MN 238	GLU 8	....	WW	
DOND	Ca	2	2	5	-1	-1	-1	-1	6	1jbc	0	0.1	1.2	CA 239	ASP 10	b...	WW	
NOSOD	K	23	0	27	2	-1	-1	-1	7	1jf8	0	0.2	1.1	K 133	ASNA 13	.....	WW	
HHH	Zn	4	6	-1	-1	-1	-1	-1 eee	5	1jk3	1	0.1	1.1	ZN 400	HISA 218	...	OO	3.4.24.65
DOOODE	Ca	1	2	2	18	3	-1	-1	6	1jk3	0	0.2	1.1	CA 402	ASPA 175	.....		3.4.24.65
OOOD	Ca	32	2	2	-1	-1	-1	-1	6	1jk3	0	0.1	1.1	CA 403	ASPA 158	....	WW	3.4.24.65
DOEO	Ca	75	0	2	-1	-1	-1	-1	6	1jk3	0	0.1	1.1	CA 404	ASPA 124	b...	WW	3.4.24.65

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CC     Fe  30  -1  -1  -1  -1  -1  -1 ..    5 1jm1  0 0.3 1.1  FE1  501  CYSA 140 ..      | XSS
HH     Fe  31  -1  -1  -1  -1  -1  -1 dd    5 1jm1  0 0.3 1.1  FE2  501  HISA 142 ..      | XSS
HH     Fe  23  -1  -1  -1  -1  -1  -1 ee    6 1jni  0 0.1 1.3  FE A 110  HISA  79 ..      | NNNN
HH     Fe  18  -1  -1  -1  -1  -1  -1 ee    6 1jni  0 0.1 1.3  FE A 111  HISA  44 ..      | NNNN
CCCC   Zn   3  17   3  -1  -1  -1  -1 ....  4 1k3x  0 0.1 1.3  ZN A 501  CYSA 237 ....    |       3.2.2.-
EH     Mg 116  -1  -1  -1  -1  -1  -1 .d    6 1k4i  0 0.3 1.0  MG  1003  GLUA  37 ..      | OWWW  5.4.99.-
EH     Mn 116  -1  -1  -1  -1  -1  -1 .d    6 1k4o  0 0.1 1.1  MN  1003  GLUA  37 ..      | OOOW  5.4.99.-
EE     Zn   2  -1  -1  -1  -1  -1  -1 ..    6 1k4p  0 0.1 1.0  ZN  1003  GLUA 181 ..      | WWWW  5.4.99.-
EH     Zn 116  -1  -1  -1  -1  -1  -1 .d    5 1k4p  0 0.2 1.0  ZN  1004  GLUA  37 ..      | OWW   5.4.99.-
DOOOD  Ca   1  15   2   2  -1  -1  -1 ..... 6 1kdv  0 0.1 1.1  CA A3001  ASPA 328 .....   |    W  3.4.23.33
DOOOD  Ca   1  15   2   2  -1  -1  -1 ..... 6 1kdy  0 0.1 1.1  CA A3001  ASPA 328 .....   |    W  3.4.23.33
EE     Mg  12  -1  -1  -1  -1  -1  -1 ..    6 1kjq  1 0.4 1.0  MG     2  GLUA 267 ..      | OOWW  2.1.2.-
NOO    Na   1   2  -1  -1  -1  -1  -1 ...   6 1kjq  0 0.3 1.0  NA     7  ASNA 100 ...     | WWW   2.1.2.-
DE     Mg 112  -1  -1  -1  -1  -1  -1 ..    6 1kqp  0 0.1 1.0  MG  5001  ASPA  50 ..      | OOOW  6.3.5.1
EE     Zn   6  -1  -1  -1  -1  -1  -1 ..    2 1l0i  2 0.2 1.2  ZN A1008  GLUA  47 ..      |
DEH    Zn  35 104  -1  -1  -1  -1  -1 ..e   5 1lok  0 0.2 1.2  ZN A 901  ASPA 117 .b.     |  NO   3.4.11.10
HDD    Zn  20  62  -1  -1  -1  -1  -1 e..   5 1lok  0 0.2 1.2  ZN A 902  HISA  97 ..b     |  OO   3.4.11.10
NOSOOS K    2   0   1   1   2  -1  -1 ......7 1lqp  0 0.2 1.2   K  3001  ASNB  92 ......  |     W 2.5.1.18
HHE    Mn -99  46  -1  -1  -1  -1  -1 ee.   5 1lqp  0 0.2 1.2  MN  3003  HISA   7 ...     |  OO   2.5.1.18
HEH    Mn  46 -99  -1  -1  -1  -1  -1 e.e   5 1lqp  0 0.2 1.2  MN  3004  HISA  64 ...     |  OO   2.5.1.18
HHH    Zn   2  23  -1  -1  -1  -1  -1 eed   5 1lug  1 0.4 0.9  ZN A1001  HISA  94 ...     |  SN   4.2.1.1
HH     Fe  46  -1  -1  -1  -1  -1  -1 ee    6 1m1q  0 0.2 1.0  FE A 801  HISA  19 ..      | NNNN
HH     Fe  27  -1  -1  -1  -1  -1  -1 ee    6 1m1q  0 0.1 1.0  FE A 804  HISA  52 ..      | NNNN
HH     Fe  30  -1  -1  -1  -1  -1  -1 ee    6 1m1q  0 0.2 1.0  FE A 802  HISA   9 ..      | NNNN
HH     Fe  13  -1  -1  -1  -1  -1  -1 ee    6 1m1q  0 0.1 1.0  FE A 803  HISA  49 ..      | NNNN
HH     Fe  46  -1  -1  -1  -1  -1  -1 ee    6 1m1r  0 0.1 1.0  FE A 801  HISA  19 ..      | NNNN
HH     Fe  27  -1  -1  -1  -1  -1  -1 ee    6 1m1r  0 0.1 1.0  FE A 804  HISA  52 ..      | NNNN
HH     Fe  30  -1  -1  -1  -1  -1  -1 ee    6 1m1r  0 0.2 1.0  FE A 802  HISA   9 ..      | NNNN
HH     Fe  13  -1  -1  -1  -1  -1  -1 ee    6 1m1r  0 0.1 1.0  FE A 803  HISA  49 ..      | NNNN
CC     Fe  13  -1  -1  -1  -1  -1  -1 ..    5 1m2b  0 0.2 1.3  FE1A 301  CYSA   9 ..      | XSS
SC     Fe   4  -1  -1  -1  -1  -1  -1 ..    5 1m2b  0 0.3 1.3  FE2A 301  SERA  55 ..      | XSS
CC     Fe  13  -1  -1  -1  -1  -1  -1 ..    5 1m2d  0 0.2 1.0  FE1A 201  CYSA   9 ..      | XSS
CS     Fe   4  -1  -1  -1  -1  -1  -1 ..    5 1m2d  0 0.3 1.0  FE2A 201  CYSA  55 ..      | XSS
HEH    Zn   3 124  -1  -1  -1  -1  -1 d.d   4 1m4l  0 0.1 1.3  ZN A1308  HISA  69 .b.     |  W    3.4.17.1
HM     Fe  48  -1  -1  -1  -1  -1  -1 e.    6 1m70  0 0.2 1.3  FE A 199  HISA  18 ..      | NNNN
HM     Fe  44  -1  -1  -1  -1  -1  -1 e.    6 1m70  0 0.1 1.3  FE A 200  HISA 123 ..      | NNNN
HHHD   Zn   8   9   3  -1  -1  -1  -1 ddd.  4 1mfm  1 0.1 1.0  ZN A 154  HISA  63 ....    |       1.15.1.1
CHC    Zn  21 107  -1  -1  -1  -1  -1 .e.   4 1mgo  0 0.1 1.2  ZN A 375  CYSA  46 ...     |  W    1.1.1.1
CCCC   Zn   3   3   8  -1  -1  -1  -1 ....  4 1mgo  0 0.1 1.2  ZN A 376  CYSA  97 ....    |       1.1.1.1
HH     Fe  25  -1  -1  -1  -1  -1  -1 ee    6 1mj4  0 0.1 1.2  FE A 502  HISA  40 ..      | NNNN  1.8.3.1
EEDD   Mg  36  28  42  -1  -1  -1  -1 ....  6 1mnz  0 0.3 1.0  MG A 389  GLUA 181 ....    |   NO  5.3.1.5
EHDD   Ca   3  35   2  -1  -1  -1  -1 .e..  5 1mnz  1 0.3 1.0  CA A 390  GLUA 217 ..b.    |   W   5.3.1.5
HHH    Zn   2  23  -1  -1  -1  -1  -1 eed   4 1moo  0 0.2 1.0  ZN A 262  HISA  94 ...     |  W    4.2.1.1
OO     Zn -99  -1  -1  -1  -1  -1  -1 ..    2 1mro  2 0.8 1.2  ZN   801  CYSA 218 ..      |       1.8.-.-
HE     Zn  -1  -1  -1  -1  -1  -1  -1 e.    2 1mwq  0 0.1 1.0  ZN A 303  HISA   0 ..      |
CC     Fe  37  -1  -1  -1  -1  -1  -1 ..    5 1n60  0 0.2 1.2  FE1 4907  CYSA 102 ..      | XSS   1.2.99.2
CC     Fe  32  -1  -1  -1  -1  -1  -1 ..    5 1n60  0 0.3 1.2  FE2 4907  CYSA 105 ..      | XSS   1.2.99.2
CC     Fe   5  -1  -1  -1  -1  -1  -1 ..    5 1n60  0 0.2 1.2  FE1 4908  CYSA  42 ..      | XSS   1.2.99.2
CC     Fe  12  -1  -1  -1  -1  -1  -1 ..    5 1n60  0 0.3 1.2  FE2 4908  CYSA  50 ..      | XSS   1.2.99.2
CC     Fe  37  -1  -1  -1  -1  -1  -1 ..    5 1n62  0 0.2 1.1  FE1 3907  CYSA 102 ..      | XSS   1.2.99.2
CC     Fe  32  -1  -1  -1  -1  -1  -1 ..    5 1n62  0 0.2 1.1  FE2 3907  CYSA 105 ..      | XSS   1.2.99.2
CC     Fe   5  -1  -1  -1  -1  -1  -1 ..    5 1n62  0 0.2 1.1  FE1 3908  CYSA  42 ..      | XSS   1.2.99.2
CC     Fe  12  -1  -1  -1  -1  -1  -1 ..    5 1n62  0 0.3 1.1  FE2 3908  CYSA  50 ..      | XSS   1.2.99.2
CC     Fe  37  -1  -1  -1  -1  -1  -1 ..    5 1n63  0 0.3 1.2  FE1 3907  CYSA 102 ..      | XSS   1.2.99.2
CC     Fe  32  -1  -1  -1  -1  -1  -1 ..    5 1n63  0 0.3 1.2  FE2 3907  CYSA 105 ..      | XSS   1.2.99.2
CC     Fe   5  -1  -1  -1  -1  -1  -1 ..    5 1n63  0 0.3 1.2  FE1 3908  CYSA  42 ..      | XSS   1.2.99.2
CC     Fe  12  -1  -1  -1  -1  -1  -1 ..    5 1n63  0 0.3 1.2  FE2 3908  CYSA  50 ..      | XSS   1.2.99.2
CHC    Zn  21 107  -1  -1  -1  -1  -1 .e.   4 1n8k  1 0.1 1.1  ZN A 375  CYSA  46 ...     |  N    1.1.1.1
CCCC   Zn   3   3   8  -1  -1  -1  -1 ....  4 1n8k  0 0.1 1.1  ZN A 376  CYSA  97 ....    |       1.1.1.1
NOSOOS K    2   0   1   1   2  -1  -1 ......7 1nki  0 0.2 0.9   K  3001  ASNB  92 ......  |     W 2.5.1.18
HHE    Mn -99  46  -1  -1  -1  -1  -1 ee.   5 1nki  0 0.1 0.9  MN  4003  HISA   7 ...     |  OO   2.5.1.18
HEH    Mn  46 -99  -1  -1  -1  -1  -1 e.e   5 1nki  0 0.2 0.9  MN  4004  HISA  64 ...     |  OO   2.5.1.18
EDDH   Mn   2   9   5  -1  -1  -1  -1 ...e  6 1nls  0 0.1 0.9  MN   239  GLU    8 ....    |   WW
DOND   Ca   2   2   5  -1  -1  -1  -1 ....  6 1nls  0 0.1 0.9  CA   240  ASP   10 b...    |   WW
YY     Fe   1  -1  -1  -1  -1  -1  -1 ..    5 1nnf  1 0.3 1.1  FE A 401  TYRA 195 ..      | ONO
DOD    Mg   2 160  -1  -1  -1  -1  -1 ...   6 1o08  0 0.2 1.2  MG  2800  ASPA1008 ...     |  XWW  5.4.2.6
CE     Fe  88  -1  -1  -1  -1  -1  -1 ..    5 1oa0  0 0.3 1.3  FE4A 601  CYSA 399 ..      | XSS
HEC    Fe  24 188  -1  -1  -1  -1  -1 e..   4 1oa0  0 0.1 1.3  FE7A 601  HISA 240 ...     |  S
E#     Na   1  -1  -1  -1  -1  -1  -1 ..    3 1od8  0 0.4 1.0  NA A1305  GLUA   2 ..      | W     3.2.1.8
HDH    Fe   2  54  -1  -1  -1  -1  -1 e.e   6 1odm  0 0.2 1.1  FE A1336  HISA 214 ...     |  SWW  1.21.3.1
HH     Cu  35  -1  -1  -1  -1  -1  -1 ee    3 1oe1  0 0.1 1.0  CU A 502  HISA  94 ..      | W
HCHM   Cu  41   9   5  -1  -1  -1  -1 d.d.  4 1oe2  0 0.2 1.1  CU A 501  HISA  89 ....    |
EHH    Cu   2  35  -1  -1  -1  -1  -1 .ee   4 1oe2  0 0.2 1.1  CU A 502  GLUA  92 ...     |  W
EDDD   Ca   4   2   3  -1  -1  -1  -1 ....  6 1oxc  0 0.1 1.2  CA    11  GLUA  95 b..b    |   OO
ODNDO  Ca  80   2   1 -99  -1  -1  -1 ..... 7 1oxc  0 0.3 1.2  CA    12  ASNA  21 .b...   |    OO
OODND  Ca -99  80   2   1  -1  -1  -1 ..... 7 1oxc  0 0.3 1.2  CA    14  GLYA 114 ..b..   |    OO
HCC    Zn  29   3  -1  -1  -1  -1  -1 d..   4 1p6o  0 0.1 1.1  ZN   400  HISB 262 ...     |  O    3.5.4.1
QE     Ca -99  -1  -1  -1  -1  -1  -1 ..    6 1p6o  0 0.2 1.1  CA   403  GLNA 150 .b      | WWWW  3.5.4.1
OOD    Ca   2  23  -1  -1  -1  -1  -1 ...   7 1p7v  0 0.1 1.1  CA   480  PROA 175 ..b     |  WWWW 3.4.21.64
OOD    Ca   2  23  -1  -1  -1  -1  -1 ...   7 1p7w  0 0.1 1.0  CA   480  PROA 175 ..b     |  WWWW 3.4.21.64
OOO    Mg   1   2  -1  -1  -1  -1  -1 ...   3 1pi3  0 0.6 1.2  MG   531  ASNA 117 ...     |       4.1.1.7
DO     Ca  29  -1  -1  -1  -1  -1  -1 ..    6 1pi3  0 0.2 1.2  CA   532  ASPA 428 ..      | OOWW  4.1.1.7
ENND   Ca  99  55  54  -1  -1  -1  -1 ....  7 1pjx  0 0.1 0.9  CA   491  GLUA  21 ....    |   WWW 3.1.8.2
DOH    Ca  41   1  -1  -1  -1  -1  -1 ..d   6 1pjx  0 0.2 0.9  CA   492  ASPA 232 ...     |  WWW  3.1.8.2
OENOD  Ca   2  32   2 130  -1  -1  -1 ..... 6 1pmh  0 0.1 1.1  CA   300  ASPX  10 ....b   |    W  3.2.1.78
DNO    Ca  27   2  -1  -1  -1  -1  -1 ...   6 1po7  0 0.3 1.2  CA A 532  ASPA 428 ...     |  OOW  4.1.1.7
HH     Co -99  -1  -1  -1  -1  -1  -1 ee    6 1pyz  0 0.2 1.3  CO   101  HISA   5 ..      | NNNN
HHH    Cu   2  72  -1  -1  -1  -1  -1 dee   3 1q0e  0 0.1 1.1  CU A 152  HISA  44 ...     |       1.15.1.1
HHHD   Zn   8   9   3  -1  -1  -1  -1 ddd.  4 1q0e  1 0.1 1.1  ZN A 153  HISA  61 ....    |       1.15.1.1
DD     Mg   2  -1  -1  -1  -1  -1  -1 ..    6 1q0n  1 0.2 1.3  MG   161  ASPA  95 ..      | OOWW  2.7.6.3
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ED	Mg	29	-1	-1	-1	-1	-1	-1	..	6	1q6o	0	0.2	1.2	MG	7300	GLUA	33	..		OOWW	4.1.2.-
DO	Ca	29	-1	-1	-1	-1	-1	-1	..	5	1q6z	0	0.4	1.0	CA	A 532	ASPA	428	..		OOW	4.1.1.7
OOSO	Na	4	8	1	-1	-1	-1	-1	....	6	1qio	0	0.2	1.2	NA	130	SERA	60	....		WW	3.2.1.17
HHE	Zn	40	36	-1	-1	-1	-1	-1	ee.	4	1qtw	0	0.1	1.0	ZN	301	HISA	69	...		W	3.1.21.2
HDH	Zn	47	2	-1	-1	-1	-1	-1	e.e	5	1qtw	0	0.2	1.0	ZN	302	HISA	182	.b.		WW	3.1.21.2
EDHE	Zn	34	37	45	-1	-1	-1	-1	..d.	5	1qtw	0	0.2	1.0	ZN	303	GLUA	145	....		W	3.1.21.2
OOO	K	1	2	-1	-1	-1	-1	-1	...	6	1qv0	0	0.3	1.1	K	403	PHEA	155	...		WWW	1.13.12.5
HDDH	Zn	2	112	267	-1	-1	-1	-1	e..e	6	1qwn	0	0.3	1.2	ZN	2005	HISA	90	....		OO	3.2.1.114
DHEE	Co	64	34	31	-1	-1	-1	-1	.e..	6	1qxy	0	0.2	1.0	CO	1001	ASPA	104	....		OO	3.4.11.18
DDE	Co	11	129	-1	-1	-1	-1	-1	...	5	1qxy	0	0.2	1.0	CO	1002	ASPA	93	b..		ON	3.4.11.18
OOO	Ca	2	3	-1	-1	-1	-1	-1	. .	6	1r0r	0	0.5	1.1	CA	301	ALAE	37	...		WWW	3.4.21.62
QDONOO	Ca	39	34	2	2	2	-1	-1	.....	6	1r0r	0	0.1	1.1	CA	302	GLNE	2	.b....			3.4.21.62
DQ	Mn	35	-1	-1	-1	-1	-1	-1	..	3	1r2m	0	0.1	1.0	MN	1001	ASPA	25	..		W	
ST	Mg	18	-1	-1	-1	-1	-1	-1	..	6	1r2q	0	0.1	1.0	MG	300	SERA	34	..		OOWW	
CCCH	Zn	2	3	26	-1	-1	-1	-1	...d	4	1r5y	0	0.1	1.2	ZN	A 400	CYSA	318	....			2.4.2.29
HHHD	Fe	2	151	99	-1	-1	-1	-1	eee.	5	1ra0	0	0.3	1.1	FE	A 500	HISA	61	....		O	3.5.4.1
CCCC	Fe	3	30	3	-1	-1	-1	-1	....	4	1rb9	0	0.1	0.9	FE	54	CYS	6	....			
DOD	Mg	2	121	-1	-1	-1	-1	-1	...	6	1rmw	0	0.2	0.0	MG	1013	ASPA	44	...		OWW	3.1.3.2
DEH	Zn	35	104	-1	-1	-1	-1	-1	..e	5	1rtq	0	0.2	0.9	ZN	701	ASPA	117	.b.		WW	3.4.11.10
HDD	Zn	20	62	-1	-1	-1	-1	-1	e..	4	1rtq	0	0.2	0.9	ZN	702	HISA	97	..b		W	3.4.11.10
TS	Na	2	-1	-1	-1	-1	-1	-1	..	6	1rtq	0	0.1	0.9	NA	705	THRA	268	..		WWWW	3.4.11.10
OTO	Na	2	230	-1	-1	-1	-1	-1	..	6	1rwh	0	0.2	1.3	NA	900	HISA	233	...		WWW	4.2.2.4, 4.2
DDSOEE	Ca	2	2	2	2	3	-1	-1	.....	6	1rwy	0	0.1	1.0	CA	A 421	ASPA	51	.....b			
DDDOE	Ca	2	2	2	5	-1	-1	-1	.....	6	1rwy	0	0.1	1.0	CA	A 422	ASPA	90	....b		W	
DYYH	Fe	32	93	61	-1	-1	-1	-1	...e	6	1ryo	0	0.2	1.2	FE	A 329	ASPA	63	....		OO	
EHDD	Mn	3	35	2	-1	-1	-1	-1	.e..	5	1s5m	0	0.3	1.0	MN	A2002	GLUA	216	b.b.		W	5.3.1.5
OH	Na	13	-1	-1	-1	-1	-1	-1	.d	3	1s5m	1	0.4	1.0	NA	2005	LEUA	57	..		W	5.3.1.5
EEDD	Mn	36	28	42	-1	-1	-1	-1	....	6	1s5n	0	0.2	0.9	MN	A2001	GLUA	180	....		OO	5.3.1.5
OH	Na	13	-1	-1	-1	-1	-1	-1	.d	3	1s5n	1	0.4	0.9	NA	2005	LEUA	57	..		W	5.3.1.5
HCH	Cu	39	3	-1	-1	-1	-1	-1	d.d	3	1sf5	0	0.1	1.1	CU	A 107	HISA	53	...			
HCHM	Cu	39	3	3	-1	-1	-1	-1	d.d.	4	1sfd	0	0.4	1.0	CU	A 107	HISA	53	....			
HCH	Cu	39	3	-1	-1	-1	-1	-1	d.d	3	1sfh	1	0.1	1.0	CU	A 107	HISA	53	...			
HCHM	Cu	39	3	3	-1	-1	-1	-1	d.d.	4	1sfh	0	0.4	1.0	CU	B 107	HISB	53	....			
HC	Fe	34	-1	-1	-1	-1	-1	-1	e.	5	1su7	0	0.3	1.1	FE1A	639	HISA	261	..		XSS	1.2.99.2
DOOOD	Ca	1	17	2	2	-1	-1	-1	.....	6	1t1e	0	0.1	1.2	CA	A 700	ASPA	505	.....		W	
DOOOD	Ca	1	17	2	2	-1	-1	-1	.....	6	1t1g	0	0.1	1.2	CA	A 358	ASPA	316	.....		W	
EH	Zn	17	-1	-1	-1	-1	-1	-1	.e	3	1t8k	1	0.1	1.1	ZN	202	GLUA	58	..		N	
ODDD	Ca	1	60	2	-1	-1	-1	-1	....	7	1tjx	0	0.2	1.0	CA	1419	META	302	...b		WWW	
DDDOD	Ca	6	54	1	1	-1	-1	-1	.....	6	1tjx	0	0.1	1.0	CA	1420	ASPA	303	b.b..		W	
EOH	Mg	436	54	-1	-1	-1	-1	-1	..e	6	1ubk	0	0.1	1.2	MG	L1005	GLUL	62	...		WWW	1.12.2.1
CCCC	Ni	3	462	3	-1	-1	-1	-1	....	5	1ubk	1	0.2	1.2	NI	L1004	CYSL	81	....		X	1.12.2.1
CC	Fe	465	-1	-1	-1	-1	-1	-1	..	3	1ubk	2	0.2	1.2	FE	L1004	CYSL	84	..		X	1.12.2.1
EOH	Mg	436	54	-1	-1	-1	-1	-1	..e	6	1ubl	0	0.1	1.2	MG	L1005	GLUL	62	...		WWW	1.12.2.1
CCCC	Ni	3	462	3	-1	-1	-1	-1	....	5	1ubl	1	0.2	1.2	NI	L1004	CYSL	81	....		X	1.12.2.1
CC	Fe	465	-1	-1	-1	-1	-1	-1	..	3	1ubl	3	0.2	1.2	FE	L1004	CYSL	84	..		X	1.12.2.1
ODDD	Ca	1	60	2	-1	-1	-1	-1	....	7	1uow	0	0.2	1.0	CA	A1419	META	302	...b		WWW	
DDDOD	Ca	6	54	1	1	-1	-1	-1	.....	6	1uow	0	0.1	1.0	CA	A1420	ASPA	303	b.b..		W	
EOOE	Ca	2	3	5	-1	-1	-1	-1	....	6	1utn	0	0.1	1.1	CA	A6000	GLUA	70	....		WW	3.4.21.4
EOOE	Ca	2	3	5	-1	-1	-1	-1	....	6	1uto	0	0.1	1.1	CA	A1248	GLUA	70	....		WW	3.4.21.4
EOOE	Ca	2	3	5	-1	-1	-1	-1	....	6	1utq	0	0.1	1.1	CA	A1247	GLUA	70	....		WW	3.4.21.4
EDDD	Ca	4	2	3	-1	-1	-1	-1	....	6	1uzv	0	0.1	1.0	CA	A 997	GLUA	95	b..b		OO	
ODNDO	Ca	80	2	1	-99	-1	-1	-1	.....	7	1uzv	0	0.3	1.0	CA	A 998	ASNA	21	.b...		OO	
OODND	Ca	-99	80	2	1	-1	-1	-1	.....	7	1uzv	0	0.3	1.0	CA	B 998	GLYA	114	..b..		OO	
OOO	Na	4	9	-1	-1	-1	-1	-1	...	7	1v7t	0	0.3	1.1	NA	406	SERA	60	...		NOOW	3.2.1.17
OOSO	Na	4	8	1	-1	-1	-1	-1	....	6	1v7t	0	0.1	1.1	NA	408	SERB	260	....		WW	3.2.1.17
CCCC	Zn	3	27	3	-1	-1	-1	-1	....	4	1vfy	0	0.1	1.1	ZN	300	CYSA	192	....			
CCCH	Zn	3	21	3	-1	-1	-1	-1	...d	4	1vfy	0	0.1	1.1	ZN	301	CYSA	176	....			
EOT	Na	193	0	-1	-1	-1	-1	-1	...	5	1vk1	0	0.3	1.2	NA	302	GLUA	30	b..		WW	
OOOD	Ca	2	2	17	-1	-1	-1	-1	....	6	1vl9	0	0.1	1.0	CA	124	TYRA	28	...b		WW	3.1.1.4
OTOT	Ca	2	-99	2	-1	-1	-1	-1	....	6	1vzi	0	0.4	1.1	CA	A1127	CYSA	87	....		WW	1.15.1.2
CCCC	Fe	3	16	1	-1	-1	-1	-1	....	4	1vzi	0	0.1	1.1	FE	A1131	CYSA	9	....			1.15.1.2
HHHCH	Fe	20	6	41	3	-1	-1	-1	eee.d	5	1vzi	0	0.2	1.1	FE	A1132	HISA	48	.....			1.15.1.2
EEOOD	Ca	2	17	90	0	-1	-1	-1	.....	6	1w0n	0	0.1	0.8	CA	A1132	GLUA	16	.b...		W	3.2.1.8
OD	Mg	81	-1	-1	-1	-1	-1	-1	..	6	1w0n	0	0.1	0.8	MG	A1133	TYRA	40	..		WWWW	3.2.1.8
HCC	Zn	30	3	-1	-1	-1	-1	-1	d..	4	1wkq	0	0.1	1.2	ZN	A 201	HISA	53	...		W	3.5.4.3
CC	Fe	5	-1	-1	-1	-1	-1	-1	..	5	1wri	0	0.3	1.2	FE1A	96	CYSA	37	..		XSS	
CC	Fe	30	-1	-1	-1	-1	-1	-1	..	5	1wri	0	0.3	1.2	FE2A	96	CYSA	45	..		XSS	
HM	Fe	62	-1	-1	-1	-1	-1	-1	e.	6	1ycc	0	0.1	1.2	FE	1	HIS	18	..		NNNN	
#O	Zn	0	-1	-1	-1	-1	-1	-1	..	3	2bf9	0	0.2	1.0	ZN	A 37	GLYA	1	..		W	
DDSOEE	Ca	2	2	2	2	3	-1	-1	.....	6	2pvb	0	0.1	0.9	CA	A 110	ASPA	51	.....b			
DDDOE	Ca	2	2	2	5	-1	-1	-1	.....	6	2pvb	0	0.1	0.9	CA	A 111	ASPA	90	....b		W	
DD E	Mg	19	-1	-1	-11	-1	-1	-1	.. .	5	2tps	0	0.2	1.3	MG	A2005	ASPA	93	.. b		WW	2.5.1.3
CCCC	Fe	3	30	3	-1	-1	-1	-1	....	4	4rxn	0	0.1	1.2	FE	1	CYS	6	....			
CCCC	Fe	3	30	3	-1	-1	-1	-1	....	4	5rxn	0	0.1	1.2	FE	1	CYS	6	....			
CCCC	Fe	3	30	3	-1	-1	-1	-1	....	4	8rxn	0	0.1	1.0	FE	A 55	CYSA	6	....			
EOOE	Ca	2	3	5	-1	-1	-1	-1	....	6	1s0q	0	0.1	1.0	CA	A 959	GLUA	711	....		WW	3.4.21.4
EOOE	Ca	2	3	5	-1	-1	-1	-1	....	6	1s0r	0	0.1	1.0	CA	A 224	GLUA	52	....		WW	3.4.21.4
HDDH	Zn	2	112	267	-1	-1	-1	-1	e..e	5	1tqw	0	0.1	1.2	ZN	1400	HISA	90	....		O	3.2.1.114
DT	Ca	2	-1	-1	-1	-1	-1	-1	..	6	1yfq	0	0.3	1.1	CA	801	ASPA	313	b.		WWWW	none
NO	Ca	1	-1	-1	-1	-1	-1	-1	..	6	1yfq	0	0.2	1.1	CA	803	ASNA	184	..		WWWW	none

Notes for table of metal sites

donors are the amino-acid donor groups in the order in which they occur in polypeptide chain, using normal one letter codes for amino-acids, O for main chain carbonyl oxygen, # for terminal -NH2.

sequence diffs : sd1 to sd7 are the seqdifs (-99 signifies donors are from two different polypeptide chains, -1 is given when the second donor is water or other non-amino-acid donor);
(warning :when the residue numbers of donors have been assigned negative values in the PDB file these may be in error);

his indicates for each donor histidine whether coordination is by ND or NE (each non-histidine donor is represented by a dot)

cn is the total number of donor groups, including water molecules and small molecule ligands, treating carboxylate always as one group (coordination number,as it would be defined by a chemist, is then number of donor groups + number of bidentate carboxylate groups).

pdb is the pdbcode

cn2 is the change in coordination number if the coordination sphere is extended by 0.20 A; this number is also used to give coded information about whether the metal might be on a rotation axis - if the number is < 20 then the metal atom is not near a rotation axis ; - if 20- 29 then 20 has been added, signifying that a 2-fold axis is possible; - if 30-39 then 30 has
been added, signifying that a 3-fold axis is possible; to establish with certainty it is necessary to look at the spacegroup and coordinates.

rms is the r.m.s. deviation of metal to donor atom distances within the coordination sphere from target distances - a useful indicator of quality (0 is good, 0.5 is poor).

resln is the resolution (A) of the structure determination.

metal is the name of the metal in the pdb file,

startaa is the name in the pdb file of the first donor amino acid,

carbi indicates bidentate carboxylate groups, e.g. ..b. indicates that the third of four donor groups appears to be a bidentate carboxylate.

other dons : indicates the type of other donor groups present; W is a water molecule, O, N, X indicate O, N, or other donors in non-protein (small) molecules or ions, other 'donors' may
occasionally be close metal atoms.

E.C. number is the E.C. enzyme number,when it is given in the PDB file

The constitution of metal coordination groups is carefully defined; an atom is defined as a donor when its distance from the metal atom is within target distance + 0.75 Å; the target distances are those derived in Harding, Acta Cryst. D57, 401-411 (2001), and the software used for the listing of the coordination groups has been developed from software described there. This type of listing is further discussed in Harding, Acta Cryst. D60, 849-859 (2004) and at http://tanna.bch.ed.ac.uk