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Pattern prediction and coordination geometry analysis from cadmium binding proteins- A computational approach

R. Jesu Jaya Sudan *et al.*,

Supplementary material

Cadmium coordination table obtained from cadmium bound structures

PDB ID	**cngpname**	**position**	**nspan**	**np**	**nw**	**nn**	**dons**	**met**	**sd1**	**sd2**	**sd3**	**sd4**	**sd5**	**sd6**	**sd7**	**cn**	**res**	**Sec.Str**	**Fold/Architecture**
1A5Z	1A5Z_A	238	3	2	0	0	EE	CD	3	-	-	-	-	-	-	2	2.1	HH	3-Layer(aba) Sandwich
1AAZ	1AAZ_B	75	-	1	2	0	H	CD	-1	-1	-	-	-	-	-	3	2	S	3-Layer(aba) Sandwich
1AQB	1AQB_A	140	2	2	0	0	DH	CD	2	-	-	-	-	-	-	2	1.65	TT	lipocalins
1BHQ	1BHQ_1	142	100	3	2	0	SSD	CD	2	98	-1	-1	-	-	-	5	2.7	TTT	3-Layer(aba) Sandwich
1CDP	1CDP_A	90	11	5	1	0	DDDKE	CD	2	2	2	5	-1	-	-	6	1.6	TTTTH	EF Hand-like
1CFZ	1CFZ_A	16	77	3	1	0	EDH	CD	46	31	-1	-	-	-	-	4	2.2	HSH	3-Layer(aba) Sandwich
1CON	1CON_A	8	16	4	2	0	EDDH	CD	2	9	5	-1	-1	-	-	6	2	SSTS	Sandwich
1CYJ	1CYJ_A	71	-	1	0	0	E	CD	-	-	-	-	-	-	-	1	1.9	H	Cytochrome
1DCD	1DCD_A	9	20	4	0	0	CCCC	CD	3	16	1	-	-	-	-	4	2	STST	Uncharacterized
1DPE	1DPE_A	55	11	2	2	0	EH	CD	11	-1	-1	-	-	-	-	4	2	SS	Alpha-Beta Complex
1DV3	1DV3_A	124	4	3	3	0	DHH	CD	2	2	-1	-1	-1	-	-	6	2.5	TTS	Irregular
1DYP	1DYP_A	241	-	1	1	2	E	CD	-1	-1	-1	-	-	-	-	4	1.54	S	concanavalin like glucanases
1EE3	1EE3_P	69	127	3	2	0	HEH	CD	3	124	-1	-1	-	-	-	5	1.7	TTS	hydrolase like
1ESF	1ESF_A	1	226	4	0	0	SHHD	CD	186	38	2	-	-	-	-	4	1.9	TSSS	OB fold
1ET7	1ET7_A	-	-	-	2	0	-	CD	-1	-1	-	-	-	-	-	2	1.7	-	immunoglobin beta like sandwich
1EU1	1EU1_A	87	4	2	0	0	DD	CD	4	-	-	-	-	-	-	2	1.3	HH	rossmann fold
1EXQ	1EXQ_A	65	27	3	0	0	CHE	CD	2	25	-	-	-	-	-	3	1.6	SST	Ribonuclease H like motif
1FA7	1FA7_A	5	51	2	2	0	HE	CD	51	-1	-1	-	-	-	-	4	1.9	SS	glyoxylase
1FE0	1FE0_A	12	3	2	0	0	CC	CD	3	-	-	-	-	-	-	2	1.75	TH	Ferridoxin like
1FNU	1FNU_A	90	-	1	2	0	C	CD	-1	-1	-	-	-	-	-	3	1.94	T	OB fold

1FYE	1FYE_A	224	3	2	2	0	EH	CD	3	-1	-1	-	-	-	-	4	1.2	TS	Flavodoxin
1G0C	1G0C_A	276	45	2	0	0	EE	CD	45	-	-	-	-	-	-	2	1.9	HH	TIM barrel
1G3W	1G3W_A	79	19	3	1	3	HEH	CD	4	15	-1	-1	-1	-1	-	7	2.4	HHH	orthogonal bundle
1G8F	1G8F_A	168	68	3	0	4	DHH	CD	67	1	-1	-1	-1	-1	-	7	1.95	THH	rossmann fold
1GL1	1GL1_A	245	-	1	1	0	N	CD	-1	-	-	-	-	-	-	2	2.1	T	Beta Barrel
1GYN	1GYN_A	110	154	2	4	0	HH	CD	154	-1	-1	-1	-1	-	-	6	2	TT	TIM barrel
1HB6	1HB6_A	14	-	1	0	0	H	CD	-	-	-	-	-	-	-	1	2	T	Up-down Bundle
1HK7	1HK7_A	406	3	2	1	0	EE	CD	3	-1	-	-	-	-	-	3	2.5	HT	Uncharacterized
1HSL	1HSL_A	1	204	2	1	0	AE	CD	204	-1	-	-	-	-	-	3	1.89	TH	Periplasmic binding protein
1I0D	1IOD_A	201	29	2	3	1	HH	CD	29	-1	-1	-1	-1	-	-	6	1.3	SS	TIM barrel
1IB4	1IB4_A	202	29	2	0	0	HD	CD	29	-	-	-	-	-	-	2	2	TT	3 Solenoid
1IJ2	1IJ2_A	18	-	1	1	0	H	CD	-1	-	-	-	-	-	-	2	1.7	H	coiled coil
1JK4	1JK4_A	76	-	1	0	0	D	CD	-	-	-	-	-	-	-	1	2.3	T	Sandwich
1KCQ	1KCQ_A	258	-	1	2	0	E	CD	-1	-1	-	-	-	-	-	3	1.65	T	Gelsolin like
1KUF	1KUF_A	144	10	3	3	0	HHH	CD	4	6	-	-	-	-	-	3	1.35	HHT	Zincin like
1LNE	1LNE_E	142	24	3	2	0	HHE	CD	4	20	-1	-1	-	-	-	5	1.7	HHH	Zincin like
1M8R	1M8R_A	28	21	4	0	0	YGGD	CD	2	2	17	-	-	-	-	4	1.9	TTTH	phospholipase
1MOX	1MOX_A	495	3	2	0	1	ED	CD	3	-1	-	-	-	-	-	3	2.5	TS	Alpha-Beta Horseshoe
1MQO	1MQO_A	116	80	4	0	3	HHDH	CD	2	2	76	-1	-1	-1	-	7	1.35	TTTT	Metallohydrolase
1N0I	1NOI_A	183	81	2	2	0	HE	CD	81	-1	-1	-	-	-	-	4	2	TT	3-Layer(aba) Sandwich
1N2Z	1N2Z_A	245	-	1	2	2	E	CD	-1	-1	-1	-1	-	-	-	5	2	T	3-Layer(aba) Sandwich
1NCX	1NCX_A	106	11	4	1	0	DNDE	CD	2	2	7	-1	-	-	-	5	1.8	TTTH	EF hand like
1NG1	1NGI_A	11	22	2	0	0	EE	CD	22	-	-	-	-	-	-	2	2.03	HH	Up-down Bundle
1NP8	1NP8_A	68	11	5	1	0	DDTKE	CD	2	2	2	5	-1	-	-	6	2	TTTTH	EF Hand-like
1NPE	1NPE_A	1010	24	3	3	0	SDV	CD	3	21	-1	-1	-1	-	-	6	2.3	STT	6 Propellor
1OEB	1OEB_A	24	18	2	1	0	EH	CD	18	-	-	-	-	-	-	2	1.76	ST	SH3 like barrel
1OEE	1OEE_A	144	11	3	3	0	HHH	CD	9	2	-1	-1	-1	-	-	6	2.1	TTS	Beta Barrel

1ON3	1ON3_A	388	-	1	2	0	H	CD	-1	-1	-	-	-	-	-	3	1.9	H	ClpP crotonase
1OO2	1OO2_C	72	-	1	2	0	E	CD	-1	-1	-	-	-	-	-	3	1.56	S	immunoglobin beta like sandwich
1P8Z	1P8Z_G	109	7	3	0	0	DGA	CD	5	2	-	-	-	-	-	3	2.6	HTT	2-Layer Sandwich
1P9E	1P9E_B	147	108	4	2	0	HHHD	CD	2	85	21	-1	-1	-	-	6	2.4	TTTT	Metallohydrolase
1PE1	1PE1_A	1011	222	4	1	0	CHED	CD	174	37	11	-1	-	-	-	5	1.74	TTSH	TIM barrel
1PL3	1PL3_A	21	3	2	2	3	PD	CD	3	-1	-1	-1	-1	-1	-	7	1.9	TT	immunoglobin beta like sandwich
1Q7Z	1Q7Z_A	207	66	4	0	0	CNCC	CD	27	38	1	-	-	-	-	4	1.7	STST	TIM barrel
1QJW	1QJW_A	146	-	1	1	0	E	CD	-1	-	-	-	-	-	-	2	1.9	H	TIM barrel
1R0I	1R0I_A	6	36	4	0	0	CCCC	CD	3	30	3	-	-	-	-	4	1.5	STTT	Rubredoxin
1RJ4	1RJ4_A	113	-	1	0	1	E	CD	-1	-	-	-	-	-	-	2	2	H	Up-down Bundle
1RWI	1RWI_A	244	-	1	1	0	D	CD	-1	-	-	-	-	-	-	2	1.8	T	6-bladed beta propeller
1RZM	1RZM_A	102	207	4	0	0	CHED	CD	170	26	11	-	-	-	-	4	2.2	THST	TIM barrel
1TQ5	1TQ5_A	57	44	3	2	0	HHH	CD	2	42	-1	-1	-	-	-	5	1.76	SSS	double stranded beta helix
1UVO	1UVO_A	59	10	5	1	0	ENQDE	CD	2	3	2	3	-1	-	-	6	1.85	TSTTT	Trypsin like serine proteases
1UXJ	1UXJ_A	243	34	2	1	0	DE	CD	34	-1	-	-	-	-	-	3	1.75	TS	rossmann fold
1VCF	1VCF_A	135	1	2	0	0	DD	CD	1	-	-	-	-	-	-	2	2.6	HH	TIM barrel
1VQQ	1VQQ_A	232	-	1	0	0	H	CD	-	-	-	-	-	-	-	1	1.8	T	Cystatin
1VSJ	1VSJ_A	64	57	2	4	0	DD	CD	57	-1	-1	-1	-1	-	-	6	2.1	ST	2-Layer Sandwich
1W1B	1W1B_1	124	4	2	3	0	HH	CD	4	-1	-1	-1	-	-	-	5	2.1	ST	Alpha-Beta Barrel
1W77	1W77_A	121	70	2	1	0	EE	CD	70	-1	-	-	-	-	-	3	2	TH	Uncharacterized
1W9H	1W9H_A	159	268	2	1	2	QL	CD	268	-1	-1	-1	-	-	-	5	1.95	HT	rossmann fold
1WB4	1WB4	823	66	3	1	0	CHM	CD	63	3	-1	-	-	-	-	4	1.4	THH	rossmann fold
1WQG	1WQG_A	10	4	2	1	0	EE	CD	4	-1	-	-	-	-	-	3	2.15	HH	orthogonal bundle
1XAU	1XAU_A	107	-	1	4	0	H	CD	-1	-1	-1	-1	-	-	-	5	1.8	T	immunoglobin beta like sandwich

1XZO	1XZO_A	55	-	1	2	1	H	CD	-1	-1	-1	-	-	-	-	4	1.7	H	Thioredoxin
1Y47	1Y47_A	10	29	3	0	0	EEH	CD	26	3	-	-	-	-	-	3	2.7	HHH	Up-down Bundle
1Y66	1Y66_A	29	-	1	0	0	E	CD	-	-	-	-	-	-	-	1	1.65	H	Uncharacterized
1YJ1	1JY1_A	-	-	-	1	2	-	CD	-1	-1	-1	-	-	-	-	3	1.3	-	Ubiquitin
1Z16	1Z16_A	147	5	2	0	0	KE	CD	5	-	-	-	-	-	-	2	1.72	TH	rossmann fold
1Z98	1Z98_A	28	3	2	2	0	DE	CD	3	-1	-1	-	-	-	-	4	2.1	TT	Up-down Bundle
1ZND	1ZND_A	139	-	1	3	0	E	CD	-1	-1	-1	-	-	-	-	4	1.6	H	lipocalins
1ZPS	1ZPS_A	85	4	3	2	0	DDD	CD	2	2	-1	-1	-	-	-	5	1.7	STS	His I like
1ZWW	1ZWW_A	108	-	1	0	0	C	CD	-	-	-	-	-	-	-	1	2.3	T	Uncharacterized
2A97	2A97_A	383	-	1	1	0	D	CD	-1	-	-	-	-	-	-	2	1.8	S	Zincin like
2AVP	2AVP_A	18	1	2	2	0	DE	CD	1	-1	-1	-	-	-	-	4	2.04	HH	TPR domain-based design
2B3P	2B3P_A	102	-	1	0	2	D	CD	-1	-1	-	-	-	-	-	3	1.4	T	beta barrel
2BJD	2BJD_A	36	-	1	3	0	H	CD	-1	-1	-1	-	-	-	-	4	1.27	H	Uncharacterized
2BMZ	2BMZ_A	41	13	2	1	0	DH	CD	13	-1	-	-	-	-	-	3	2.4	SS	Aligned Prism
2BT7	2BT7_A	158	-	1	0	0	H	CD	-	-	-	-	-	-	-	1	2.35	T	Uncharacterized
2C3G	3C3G_A	15	33	2	1	0	DD	CD	33	-1	-	-	-	-	-	3	2	TS	Uncharacterized
2CN2	2CN2_A	55	361	3	3	0	IDE	CD	359	2	-1	-1	-1	-	-	6	2.1	SSS	Uncharacterized
2CU3	2CU3_A	7	-	1	0	0	E	CD	-	-	-	-	-	-	-	1	1.7	S	ubiquitin like
2DVZ	2DVZ_A	225	-	1	2	0	D	CD	-1	-1	-	-	-	-	-	3	2.3	T	Uncharacterized
2ENR	2ENR_A	8	16	4	2	0	EEDH	CD	2	9	5	-1	-1	-	-	6	2.35	SSTS	Sandwich
2EV0	2EV0_A	11	91	4	2	0	EHEE	CD	66	22	3	-1	-1	-	-	6	1.65	HHHH	DNA binding 3 helical bundle
2F91	2F91_A	70	10	5	1	0	EDVEE	CD	2	3	2	3	-1	-	-	6	2	TSTTT	Trypsin like serine proteases
2FU4	2FU4_A	33	48	2	0	2	HE	CD	48	-1	-1	-	-	-	-	4	1.8	TS	Uncharacterized
2GSM	2GSM_B	280	5	3	0	0	EHH	CD	3	2	-	-	-	-	-	3	2	HTT	Up-down Bundle
2HZ1	2HZ1_A	33	44	2	0	0	HH	CD	44	-	-	-	-	-	-	2	1.8	HT	3-Layer(aba) Sandwich
2IGI	2IGI_A	11	-	1	4	1	D	CD	-1	-1	-1	-1	-1	-	-	6	1.7	S	Ribonuclease H like motif

2J4K	2J4K_A	104	-	1	0	0	H	CD	-	-	-	-	-	-	-	1	2.2	T	Uncharacterized
2JHF	2JHF_A	46	128	3	1	0	CHC	CD	21	107	-1	-	-	-	-	4	1	TTT	Rossmann fold
2OA9	2OA9_A	59	175	2	0	0	HE	CD	175	-	-	-	-	-	-	2	1.5	SH	Uncharacterized
2P5Q	2P5Q_A	22	81	2	3	0	ED	CD	81	-1	-1	-1	-	-	-	5	2	TT	Uncharacterized
2PZI	2PZI_A	105	26	4	0	0	CCCC	CD	3	20	3	-	-	-	-	4	2.4	STST	Uncharacterized
2Q88	2Q88_A	250	-	1	3	0	E	CD	-1	-1	-1	-	-	-	-	4	1.9	H	Uncharacterized
2QTF	2QTF_A	92	-	1	2	0	E	CD	-1	-1	-	-	-	-	-	3	2	H	Uncharacterized
2V2P	2V2P_A	80	-	1	1	0	D	CD	-1	-	-	-	-	-	-	2	1.15	T	Ferritin like
2V4B	2V4B_A	261	204	3	2	0	EDD	CD	83	121	-1	-1	-	-	-	5	2	STT	Uncharacterized
2VG9	2VG9_A	120	-	1	1	0	D	CD	-1	-	-	-	-	-	-	2	2	T	Sandwich
2VLI	2VLI_A	145	5	2	0	1	EH	CD	5	-1	-	-	-	-	-	3	1.95	TS	Uncharacterized
2W5F	2W5F_A	169	-	1	0	2	D	CD	-1	-1	-	-	-	-	-	3	1.9	T	TIM barrel
2WXU	2WXU_A	46	1	2	3	0	HE	CD	1	-1	-1	-1	-	-	-	5	1.8	HH	orthogonal bundle
2X7K	2X7K_A	31	58	2	2	0	HD	CD	58	-1	-1	-	-	-	-	4	1.15	TT	Uncharacterized
2X7W	2X7W_A	144	116	4	1	0	EDHE	CD	34	37	45	-1	-	-	-	5	2.36	SSST	Uncharacterized
2ZGD	2ZGD_A	30	9	3	0	0	EQE	CD	6	3	-	-	-	-	-	3	1.9	HHH	alpha horseshoe
2ZQO	2ZQO_A	241	-	1	2	1	H	CD	-1	-1	-1	-	-	-	-	4	1.8	S	beta-trefoil
3A02	3A02_A	126	4	2	0	1	EQ	CD	4	-1	-	-	-	-	-	3	1	HH	Homeobox
3A04	3A04_A	343	3	2	0	0	EE	CD	3	-	-	-				2	1.97	HH	orthogonal bundle
3AFP	3AFP_B	62	3	2	1	0	EE	CD	3	-1	-	-	-	-	-	3	2.05	HH	Uncharacterized
3AMS	3AMS_A	27	259	3	2	0	DED	CD	183	76	-1	-1	-	-	-	5	2.08	SST	Uncharacterized
3AO4	3AO4_A	65	27	3	0	0	CHE	CD	2	25	-	-	-	-	-	3	1.97	SST	Uncharacterized
3B40	3B40_A	48	3	2	0	0	EE	CD	3	-	-	-	-	-	-	2	2	TH	Alpha-Beta Barrel
3BOE	3BOE_A	263	62	3	1	1	CHC	CD	52	10	-1	-1	-	-	-	5	1.4	TST	CdCA1
3C7M	3C7M_A	113	-	1	1	2	D	CD	-1	-	-	-	-	-	-	2	1.55	T	Uncharacterized
3CEL	3CEL_A	65	190	2	0	0	EE	CD	125	-	-	-	-	-	-	2	2	HT	Distorted Sandwich
3DZE	3DZE_A	101	-	1	3	0	C	CD	-1	-1	-1	-	-	-	-	4	1.15	H	Uncharacterized
3EIG	3EIG_A	183	-	1	1	1	E	CD	-1	-1	-	-	-	-	-	3	1.7	S	3 layer sandwich

3FGH	3FGH_A	166	-	1	1	2	E	CD	-1	-1	-1	-	-	-	-	4	1.35	H	orthogonal bundle
3FQN	3FQN_A	30	-	1	3	0	D	CD	-1	-1	-1	-	-	-	-	4	1.65	T	immunoglobin beta like sandwich
3HEQ	3HEQ_A	140	7	2	2	0	HD	CD	7	-1	-1	-	-	-	-	4	1.8	TH	orthogonal bundle
3IIS	3IIS_M	5	-	1	1	0	D	CD	-1	-	-	-	-	-	-	2	1.4	H	Uncharacterized
3IP1	3IP1_A	131	14	4	0	0	CCCC	CD	3	3	8	-	-	-	-	4	2.09	TTTH	Uncharacterized
3JQX	3JQX_A	908	31	5	0	0	EETDD	CD	2	21	6	2	-	-	-	5	2.2	TTSTS	Uncharacterized
3KBS	3KBS_A	217	40	4	1	0	EHDD	CD	3	35	2	-1	-	-	-	5	1.8	THTT	TIM barrel
3KD0	3KD0_A	32	42	2	0	3	CM	CD	42	-1	-1	-1	-	-	-	5	1.7	TT	Uncharacterized
3LKW	3LKW_A	23	5	2	1	0	HH	CD	5	-1	-	-	-	-	-	3	2	TT	Uncharacterized
3M31	3M31_A	64	347	2	0	0	EE	CD	347	-	-	-	-	-	-	2	1.85	HH	Uncharacterized
3MMW	3MMW_A	96	2	2	2	0	HE	CD	2	-1	-1	-	-	-	-	4	1.85	TT	Uncharacterized
3P5U	3P5U_A	162	-	1	2	0	H	CD	-1	-1	-	-	-	-	-	3	1.5	S	Uncharacterized
3PK1	3PK1_A	225	-	1	0	0	E	CD	-	-	-	-	-	-	-	1	2.49	T	Uncharacterized
3PO0	3PO0_A	55	1	2	0	0	DH	CD	1	-	-	-	-	-	-	2	1.55	TT	Uncharacterized
4MT2	4MT2_A	50	10	4	0	0	CCCC	CD	7	2	1	-	-	-	-	4	2	TTTT	Irregular

pid- Protein ID as given in Protein data bank followed by the chain ID
position - position of the first residue in the chelate loop
nspan- represents the length span of the chelate loop
np- represents the number of donor atoms
nw- represents the number of water molecule
nn- represents the number of non protein donors
don- indicate the donor atoms specified as single letter codes
met - metal ion,
sd1 to sd7 - positioning of the residues from the first residue of the chelate
cn- coordination number,
res- resolution
sec.str-secondary structural elements
Fold/Architecture- Structural classification according to CATH and SCOP database