Factors Governing the Different Functions of Zn2+-Sites with Identical Ligands in Proteins

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Table S1. Non-redundant Zn-CC(C/H)x (x = D, E or H_2O) sites in the PDB (2019, February).[a]

Cluster #	PDB IDs	Representative Zn-ligands	# of Zn-sites	Protein description
	Archaea			
1	**1g5c_a**, 3ten_a, 3ten_b, 3ten_c, 3ten_d, 3ten_e, 3ten_f, 3ten_g, 3ten_h, 1g5c_b, 1g5c_c, 1g5c_d, 1g5c_e, 1g5c_f	CCHw	14	β-carbonic anhydrase
2	**1h2b_b**, 1jvb_a*, 1nto_a*, 1nto_b*, 1nto_c*, 1nto_d*, 1nto_e*, 1nto_h*, 1nvg_a*, 1r37_a, 1r37_b, 2eer_a, 2eer_b, 3i4c_a*, 3i4c_b*, 3i4c_c*, 3i4c_d*, 3i4c_e*, 3i4c_h*, 2h6e_a	CCCD	34	Alcohol dehydrogenase
3	**3wid_a**, 3wid_b, 3wid_c, 3wid_d, 3wie_a, 3wie_b, 3wie_c, 3wie_d, 3wic_a, 3wic_b, 3wic_c, 3wic_d	CCCD	12	Glucose 1-dehydrogenase
4	**4ay7_b**	CCHE	1	Methyltransferase
5	***1zt2_a***, 1zt2_c	CCCD	2	DNA primase small subunit
6	***2gvi_a***	CCCD	1	Conserved hypothetical protein
7	**2oso_a**, 2osd_a	CCHE	2	Hypothetical protein mj1460
	Bacteria			
1	**1ctt_a**, 1aln_a	CCHw	2	Cytidine deaminase
2	**1fbx_a**, 1fbx_b, 1fbx_c, 1fbx_d, 1fbx_e, 1fbx_f, 1fbx_h, 1fbx_i, 1fbx_j, 1fbx_l, 1fbx_n, 1fbx_o	CCHw	12	GTP cyclohydrolase i
3	**1l6s_a**, 1w5o_a, 1b4e_a, 1i8j_a, 1i8j_b, 1l6s_b, 1l6y_a, 1l6y_b	CCCw	8	δ-aminolevulinic acid dehydratase
4	**1li5_a**, 3sp1_a, 3sp1_b, 3tqo_a, 1li5_b	CCHE	5	Cysteinyl-tRNA synthetase
5	**1uuf_a**	CCHw	1	Alcohol dehydrogenase-like protein yahk
6	**1wkq_a**, 1wkq_b	CCHw	2	Guanine deaminase
7	**1wwr_a**, 2hvv_a, 2hvv_b, 5c2o_a, 5c2o_b, 1wwr_b, 1wwr_c, 1wwr_d	CCHw	8	tRNA-specific adenosine

8	1ym3_a	CCHD	1	β–carbonic anhydrase
9	2b3j_a, 2b3j_b, 2b3j_c, 2b3j_d	CCHw	4	tRNA-specific adenosine deaminase
10	2bz1_a	CCCw	1	GTP cyclohydrolase ii
11	2fgy_a, 2fgy_b	CCHw	2	β–carbonic anhydrase
12	2g0d_a, 2g02_a	CCHw	2	Nisin biosynthesis protein NisC
13	2g84_a, 2g84_b, 4hrq_a, 4hrq_b, 4lc5_a, 4lc5_b, 4lcn_a, 4lcn_b, 4lco_a, 4lco_b, 4lcp_a, 4lcp_b, 4ld2_a, 4ld2_b	CCHw	14	Cytidine and deoxycytidylate deaminase
14	2hxv_a, 3zpc_b, 2b3z_a, 2b3z_b, 3ex8_b, 3ocq_a, 1z3a_a, 1z3a_b	CCHw	8	Riboflavin biosynthesis protein RibD
15	3bq6_a, 3t0c_a, 3bq6_b, 1xpg_a, 1xpg_b	CCHE	5	homocysteine methyltransferase
16	3dmo_a, 3mpz_a, 3mpz_b, 3mpz_c, 3mpz_d, 2d30_a, 2d30_b, 3dmo_b, 3dmo_c, 3dmo_d, 4f3w_a, 4f3w_b, 4f3w_c, 4f3w_d, 3ijf_x, 4wif_b, 4wig_a, 4wig_b	CCCw	18	Cytidine deaminase
17	3s2e_a, 4eex_a, 4eex_b, 4eez_a, 4eez_b, 4z6k_d, 3s1l_a, 3s1l_b, 3s1l_c, 3s1l_d, 3s2e_b, 3s2e_c, 3s2e_d, 3s2e_g, 3s2e_h, 3s2f_a, 3s2f_b, 3s2f_c, 3s2f_d, 3s2g_a, 3s2g_b, 3s2g_c, 3s2i_a, 3s2i_b, 3s2i_d, 3pii_a, 4gkv_a, 4gkv_b, 4gkv_c, 4gkv_d	CCHE	30	Alcohol dehydrogenase
18	3vrk_a, 1ylk_a, 1ylk_b, 1ylk_d, 3las_a, 3las_b	CCHw	6	Carbonyl sulfide hydrolase
19	3wrg_a, 3wre_a	CCCE	2	Non-reducing end βl-arabinofuranosidase
20	5cxk_a, 2a8c_a, 2a8c_b, 2a8c_c, 2a8c_d, 2a8c_e, 2a8c_f, 2a8d_a, 2a8d_b, 2a8d_c, 2a8d_d, 2a8d_e, 2a8d_f, 3e24_a, 3e28_b, 3e28_c, 3e28_d, 3e2a_a, 3e2a_b, 3e2a_c, 3e2a_d,	CCHD	74	β-carbonic anhydrase

	3e2a_e, 3e2a_f, 3e2w_a, 3e2w_b, 3e2w_c, 3e2w_d, 3e2x_a, 3e2x_b, 3e31_a, 3e31_b, 3e3f_b, 3e3g_a, 3e3g_b, 3e3g_c, 3e3g_d, 3e3g_e, 3e3g_f, 3e3i_a, 3e3i_b, 3e3i_c, 3e3i_d, 3e3i_e, 3e3i_f, 3e3i_g, 3e3i_h, 3e3i_i, 3e3i_j, 3e3i_k, 3e3i_l, 4waj_a, 4waj_b, 4wak_a, 4wak_b, 4wam_b, 5cxk_b, 5cxk_c, 5cxk_d, 5cxk_e, 5cxk_f, 5cxk_g, 5cxk_h, 1i6o_a, 1i6o_b, 1i6p_a, 1t75_a, 1t75_b, 1t75_d, 1t75_e, 2esf_a, 2esf_b, 4znz_a, 4rxy_a, 5bq1_a			
21	**5k1s_d**	CCHE	1	Zinc-binding dehydrogenase
22	**5swc_a**, 5swc_b, 5swc_c, 5swc_d, 5swc_e, 5swc_f	CCHw	6	β-carbonic anhydrase
23	***4o6o_b***	CCCw	1	Recombination protein RecR
24	***5fru_a***, 5kbe_b, 5kbg_b, 5kbh_a, 5kbh_b, 5kbi_a, 5fru_b, 5frv_a, 5frv_b, 5frw_a, 5frw_b, 5frx_a, 5fry_a, 5fry_b, 5frz_a, 5frz_b, 5fs0_a, 5fs0_b	CCCE	18	Positive phenol-degradative gene regulator
25	**2hf1_a**, 2hf1_b	CCCD	2	Putative tetraacyldisaccharide-1-p 4-kinase
26	**2qq4_a**, 2qq4_b, 2qq4_c, 2qq4_d, 2qq4_e, 2qq4_f	CCCD	6	Iron-sulfur biosynthesis protein
27	**3di4_a**, 3di4_b	CCCw	2	DUF1989 family protein
28	**3oru_a**, 3siy_a, 3siy_b, 3siy_c, 3siy_d	CCCw	5	DUF1989 family protein
29	**3p1v_a**, 4df9_a, 4df9_b, 4df9_c, 4df9_d, 4df9_e, 4df9_f, 3p1v_b	CCCE	8	Metallo-endopeptidase
30	**4esn_a**, 4esn_b	CCCw	2	DUF1312 family protein
31	**4qbg_b**, 4typ_b, 3dl0_a, 3dl0_b	CCCD	4	Adenylate kinase

	Eukaryotes			
1	**1ekj_c**	CCHw	1	Pisum sativum β carbonic anhydrase
2	**1h7n_a**, 1h7p_a, 1h7r_a, 1w31_a, 1h7o_a, 1eb3_a, 1gjp_a, 5hnr_a	CCCw	8	5-aminolaevulinic acid dehydratase
3	**1is8_c,** 1is8_b, 1is8_e,1is8_f, 1is8_g, 1is8_h	CCHw	6	Cytidine deaminase
4	**1mgo_a**, 4dl9_a, 4dl9_b, 4dla_a, 4dla_b, 4dlb_a, 3uko_a, 3uko_b, 4gl4_a, 4gl4_b, 4jji_b, 4l0q_a, 4l0q_b, 1e3e_a, 1e3e_b, 1e3l_a, 1e3l_b, 4rqu_b, 1adf_a, 1adg_a, 1cdo_b, 1hso_a, 1hso_b, 1hsz_a, 1ht0_a, 1ht0_b, 1ju9_a, 1ju9_b, 1mc5_b, 1mgo_b, 1qlh_a, 1qlj_a, 1ye3_a, 5adh_a, 8adh_a, 1m6h_a, 1m6h_b, 1ma0_a, 1ma0_b, 1mp0_a, 1teh_b, 2few_a, 2fzw_b	CCHw	43	Alcohol dehydrogenase E chain
5	**1r5t_a**, 1zab_a, 1zab_b, 1zab_c, 1zab_d, 2fr6_a, 2fr6_c, 2fr6_d, 1r5t_b, 1r5t_c, 1r5t_d, 1mq0_b	CCCw	12	Cytidine deaminase
6	**1zy7_a**, 1zy7_b, 5ed1_d, 5hp2_d, 5hp3_d	CCHw	5	adenosine deaminase
7	**2w3q_a**	CCHw	1	β-carbonic anhydrase 2
8	**2w4l_a**, 2w4l_b, 2w4l_c, 2w4l_d, 2w4l_e, 2w4l_f	CCHw	6	Deoxycytidylate deaminase
9	**2z3g_a**, 2z3g_b, 2z3g_c, 2z3g_d, 2z3h_d	CCCw	5	Blasticidin S Deaminase
10	**3boc_a**	CCHw	1	Carbonic anhydrase of marine diatoms
11	**3dh1_a**	CCHw	1	tRNA-specific adenosine deaminase 2
12	**3e6u_d**	CCHw	1	Eukaryotic lanthionine synthetase C-like protein 1
13	**3eyx_a**, 1ddz_a*, 1ddz_b*, 3uco_a, 3uco_b, 3eyx_b	CCHw	8	β-carbonic anhydrase

14	**3v4k_a**, 5jj4_a, 5jj4_b, 5jj4_c, 3ir2_a, 3ir2_b, 3v4k_b, 5hx5_a, 4rov_a, 4rov_b, 4row_a, 5k81_a, 5k81_b, 5k81_c, 5k81_d, 5k81_e, 5k81_f, 5k83_a, 5k83_b, 5k83_c, 5k83_d, 5k83_e, 5k83_f, 2nyt_a, 2nyt_c, 3vow_b, 3wus_a, 3wus_b, 3e1u_a, 3iqs_a, 5cqd_a, 5cqd_c, 5cqi_a, 5cqk_a	CCHw	34	DNA dC→dU-editing enzyme APOBEC-3G
15	**4l6o_a**, 3ppg_a, 4l61_a, 4l64_a, 4ztx_a, 1u1h_a, 1u1j_a	CCHw	7	homocysteine methyltransferase (Met6p)
16	**4w6z_b**, 4w6z_d	CCHE	2	Yeast alcohol dehydrogenase
17	**5b5z_a**, 5b5y_a, 5b5y_b, 5b5z_b, 5b60_a	CCHw	5	β-carbonic anhydrases
18	**5fi3_a**, 5h81_a, 5h81_b, 5h82_a, 5h82_b, 1yqd_a, 1yqd_b, 1yqx_b, 5h83_a, 5h83_b, 5fi3_b, 5fi5_a, 5fi5_b	CCHE	13	Tetrahydroalstonine synthase
19	**5k5w_a**, 5k5w_b	CCHw	2	β-carbonic anhydrases
20	*1du3_k*	CCCw	1	TRAIL-DR5 complex
21	*1rut_x**, 4jcj_b, 4jcj_c*, 4kfz_a*, 4kfz_b*, 2ypa_c*, 2xjy_a*, 2xjz_b*, 2xjz_c*, 2xjz_d*, 2xjz_e*, 2lxd_a, 2l4z_a, 1m3v_a, 1j2o_a, 2l6y_b, 2l6z_c, 2mbv_a	CCCD	28	LIM domain-binding protein 1
22	*2dar_a*, 2dlo_a, 2dj7_a	CCHE	3	Pdz and lim domain protein 5
23	*2rgt_a**, 2jtn_a*, 2rgt_b*, 3mmk_a*, 3mmk_b*	CCCD	10	Lim domain-binding protein
24	**3dpl_d**, 1u6g_b, 3rtr_b, 3rtr_d, 3rtr_f, 3rtr_h, 2lgv_a, 1ldj_b	CCHD	8	E3 ubiquitin-protein ligase RBX1
25	*3hcu_a*	CCHD	1	Tnf receptor-associated factor 6 (TRAF6)
26	*3vhs_a*	CCHw	1	Atpase wrnip1
27	*4hi8_b*, 3f6q_b, 3ixe_b, 4hi9_b	CCCD	4	Integrin-linked protein kinase

28	**4xba_a**, 3szq_a, 3sp4_a, 3sp4_b, 3spd_a, 3spd_b, 3spd_c, 3spd_d, 3spl_a, 3spl_b, 3spl_c, 3spl_d, 4ykl_b	CCHE	13	Aprataxin-like protein
29	**4ybg_a**	CCHE	1	Drosophila melanogaster maelstrom
30	**5af0_c**, 5af0_b, 5af0_d	CCHE	3	Mael domain from bombyx mori maelstrom
	Virus			
1	**1vq2_a**, 4p9c_b, 4p9c_g, 4p9c_h, 4p9c_i, 4p9c_l, 4p9d_a, 4p9d_b, 4p9d_c, 4p9d_d, 4p9d_e, 4p9d_f, 4p9e_a	CCHE	13	Deoxycytidylate deaminase
2	**2g9t_e**, 2g9t_a, 2g9t_b, 2g9t_c, 2g9t_d, 2g9t_f, 2g9t_g, 2g9t_h, 2g9t_i, 2g9t_j, 2g9t_k, 2g9t_l, 2g9t_m, 2g9t_n, 2g9t_o, 2g9t_p, 2g9t_q, 2g9t_r, 2g9t_s, 2g9t_t, 2g9t_u, 2g9t_w, 2ga6_e, 2ga6_g, 2ga6_q, 2ga6_s, 2ga6_t, 2ga6_v, 2ga6_w, 2xyr_b	CCCw	30	Sars coronavirus nsp10
3	**2wbt_a**, 2wbt_b	CCHE	2	A double C_2H_2 zinc finger protein
4	**3q7c_a**, 3r3l_a, 3r3l_b, 3r3l_c, 3mwp_a, 3mwp_b, 3mwp_c, 3mwt_a, 3mwt_b, 3mwt_c, 3mx2_a, 3mx2_c, 3mx5_a, 3mx5_b, 3mx5_c, 3q7b_a, 4o6h_c, 4o6h_d, 4o6h_e, 4o6i_a, 4o6i_b, 4gv3_a, 4gv6_a, 4g9z_a, 4gv9_a, 4gve_a	CCHE	26	Nucleoprotein structure of Lassa fever virus
5	**3sv6_a**, 3o8b_a, 3o8b_b, 3o8c_b, 1cu1_a, 3m5n_b, 3m5n_c, 3m5n_d, 3m5o_a, 3sv7_a, 3sv8_a, 3sv9_a, 4a1x_a, 4a1x_b, 2f9v_a, 2f9v_c, 1rtl_a, 1rtl_b, 2a4g_a, 2a4g_c, 2a4q_a, 2a4q_c, 2a4r_a, 2a4r_c, 2fm2_a, 2fm2_c,	CCCw	74	HCV NS3 protease domain/ NS4a peptide complex

	2o8m_a, 2o8m_b, 2obo_a, 2obo_c, 2obq_a, 2obq_c, 2oc0_a, 2oc0_c, 2oc1_a, 2oc1_c, 2oc7_c, 2oc8_c, 2oin_a, 3eyd_a, 3eyd_c, 3kf2_a, 3kf2_b, 3kn2_a, 3kn2_c, 3knx_a, 3knx_c, 3lon_a, 3lon_c, 3lox_a, 3lox_c, 2f9u_a, 2f9u_c, 2gvf_a, 2gvf_c, 1a1r_a, 1a1r_b, 1n1l_a, 1n1l_b, 2xcf_a, 2xcf_b, 2xcn_b, 2xni_a, 3kee_a, 3kee_b, 3kee_c, 3kee_d, 4ktc_a, 1dxp_a, 1dxp_b, 1dy9_b, 1jxp_a, 4jmy_a, 4jmy_b			
6	***4hhj_a***, 4k6m_b*, 5tfr_a, 5tfr_b, 5ccv_a, 5u0b_a, 5u0b_b, 5tmh_a, 5tmh_b, 4v0q_a, 4v0r_a, 5dto_a, 5jjr_a, 2hfz_a, 4hdh_a, 4hdh_b, 5u0c_a, 5u0c_b, 5u0c_d, 5u0c_e, 5u0c_f, 5u0c_g, 5u0c_h, 4c11_a, 4c11_b, 3vws_a, 5f3t_a, 5f3z_a, 5f41_a, 5hmw_a, 5hmx_a, 5hmy_a, 5hmz_a, 5hn0_a, 5i3p_a, 5i3q_a, 5k5m_a, 4mtp_a, 4mtp_b, 4mtp_c, 5wz3_a*, 5u04_a*	CCHE	45	RNA-directed RNA polymerase (NS5)

[a]The representative PDB IDs in each cluster are shown in bold; those with structural Zn-sites are in italics, and those with Zn-sites of unknown function are underlined. PDB entries with two Zn sites are labeled " * ".

Table S2. Second-shell residues that form hydrogen bonds with the bound water molecule in Zn-CC(C/H)w sites in archaea, bacteria, eukaryotes and viruses.

PDB	Zn ligands	Structural/Catalytic	2nd shell of Zn-bound water
Archaea			
1g5c_a	CCHw	Catalytic	D34
Bacteria			
2g84_a	CCHw	Catalytic	E79
1fbx_a	CCHw	Catalytic	E111
2hxv_a	CCHw	Catalytic	E51
1wwr_a	CCHw	Catalytic	E54
3vrk_a	CCHw	Catalytic	D46
5swc_a	CCHw	Catalytic	D41
2b3j_a	CCHw	Catalytic	E55
1wkq_a	CCHw	Catalytic	E55
2fgy_a	CCHw	Catalytic	D175
1ctt_a	CCHw	Catalytic	E104
3dmo_a	CCCw	Catalytic	E55
1l6s_a	CCCw	Catalytic	D117
2bz1_a	CCCw	Structural	−
4o6o_b	CCCw	Structural	−
2g0d_a	*CCHw*	*Catalytic*	−
Eukaryota			
3v4k_a	CCHw	Catalytic	E259
1is8_c	CCHw	Catalytic	E133
4l6o_a	CCHw	Catalytic	D738
2w4l_a	CCHw	Catalytic	E86
3eyx_a	CCHw	Catalytic	D59
5b5z_a	CCHw	Catalytic	D48
1zy7_a	CCHw	Catalytic	E396
3dh1_a	CCHw	Catalytic	E73
5k5w_a	CCHw	Catalytic	D122
3e6u_d	CCHw	Structural	−
2w3q_a	CCHw	Catalytic	D70
3vhs_a	CCHw	Structural	−
3boc_a	CCHw	Catalytic	D265
1ekj_c	CCHw	Catalytic	D162
1r5t_a	CCCw	Catalytic	E63
1h7n_a	CCCw	Catalytic	D131
2z3g_a	CCCw	Catalytic	E56
1du3_k	CCCw	Structural	−
Virus			
3sv6_a	CCCw	Structural	−
2g9t_e	CCCw	Structural	−

Table S3. PDB entries of proteins with consensus sequence/structural motifs of Zn-CC(C/H)w sites

PDB ID	Zn ligands	($\underline{H/C}$)AEx$_2$(A/V)x$_{35}$P$\underline{C}$xx($\underline{C/H}$)
1r5t_a	CCCw	C61, E63, C96, C99
1wkq_a	CCHw	H53, E55, C83, C86
1wwr_a	CCHw	H52, E54, C82, C85
2b3j_a	CCHw	H53, E55, C83, C86
2g84_a	CCHw	H77, E79, C112, C115
2hxv_a	CCHw	H49, E51, C77, C86
2w4l_a	CCHw	H84, E86, C110, C113,
2z3g_a	CCCw	C54, E56, C88, C91
3dh1_a	CCHw	H71, E73, C107, C110
3dmo_a	CCCw	C53, E55, C88, C91
		$\underline{C}$xDxRx$_{77}$$\underline{H}xx\underline{C}$
1ekj_c	CCHw	C160, D162, H220, C223
1g5c_a	CCHw	C32, D34, H87, C90
2fgy_a	CCHw	C173, D175, H242, C253
2w3q_a	CCHw	C68, D70, H124, C127
3eyx_a	CCHw	C57, D59, H112, C115
3vrk_a	CCHw	C44, D46, H97, C100
5swc_a	CCHw	C39, D41, H98, C101

Table S4. Conserved domains for catalytic and structural Zn-CC(C/H)x sites.

Conserved Domain[a]	Superfamily Description
Catalytic	
A_deamin	Adenosine-deaminase (editase) domain
ALAD_PBGS	δ-aminolevulinic acid dehydratase (ALAD) , also called porphobilinogen synthase (PBGS)
APOBEC_N	APOBEC-like N-terminal domain
β-CA	β-Carbonic Anhydrase
Cdd	Cytidine deaminase (Nucleotide transport and metabolism)
CsoSCA	Carboxysome Shell Carbonic Anhydrase
Cytidine_deaminase-like	Cytidine and deoxycytidylate deaminase
DHBP_synthase	3,4-DiHydroxy-2-Butanone 4-Phosphate
FrmA	Zn-dependent alcohol dehydrogenase
GTP cyclohydrolase II	GTP cyclohydrolase II catalyzes the first committed step in the biosynthesis of riboflavin
LanC_like	Lanthionine synthetase C-like protein
MafB19-deam	MafB19-like deaminase
Metallohydrolase-like MBL-fold	Mainly hydrolytic enzymes and related proteins which carry out various biological functions
MutL	MutL protein
P-loop_NTPase	P-loop containing Nucleoside Triphosphate Hydrolases
PRK05222	5-methyltetrahydropteroyltriglutamate--homocysteine S-methyltransferase
S-methyl_trans	Homocysteine S-methyltransferase
Tfold	Tunnelling fold
tRNA_synt_1e	tRNA-synt 1e domain containing protein
TS_Pyrimidine_HMase	Thymidylate synthase and pyrimidine hydroxymethylase
UR0-D_CIMS_like	The URO-D_CIMS_like protein superfamily includes bacterial and eukaryotic uroporphyrinogen decarboxylases (URO-D), coenzyme M methyltransferases and other putative bacterial methyltransferases, as well as cobalamine (B12) independent methionine synthases.
Structural	
Arena_nucleocapsid	Arenavirus nucleocapsid N-terminal domain
AE_Prim_S_like	Domain similar to that found in the small subunit of archaeal and eukaryotic DNA primases
Csc2_I-D	CRISPR/Cas system-associated protein Csc2
Flavi_NS5	Flavivirus RNA-directed RNA polymerase
FmdE	Molybdenum formylmethanofuran dehydrogenase operon
HIT_like	histidine triad motif-containing proteins
IscU_like	Iron-sulfur cluster scaffold-like proteins
LIM	LIM domain
Maelstrom	piRNA pathway germ-plasm component
MOZ_SAS	This region of these proteins has been suggested to be homologous to acetyltransferases
NSP10	RNA synthesis protein NSP10
OprD	Outer membrane porin, OprD family
Peptidase_C19	Peptidase C19 contains ubiquitinyl hydrolases
Peptidase_S29	Hepatitis C virus NS3 protease
PHA00733	Hypothetical protein
PRK12267	methionyl-tRNA synthetase
RecR	RecR protein
RING_Ubox	Really Interesting New Gene and U-box domains
SET	SET domains are protein lysine methyltransferase enzymes.
TNF	Tumor necrosis factor
V4R	vinyl 4 reductase domain
XylR_N	Activator of aromatic catabolism
Zf-C2HE	C2HE / C2H2 / C2HC zinc-binding finger

ZnF_Rad18	Rad18-like CCHC zinc finger
Catalytic & Structural	
MDR	Medium chain reductase/dehydrogenases (MDR)/zinc-dependent alcohol dehydrogenase-like family

[a]Conserved protein domain family name according to the CDD.[32]

Table S5. The mean BVS values of catalytic/structural Zn-CC(C/H)(D/E) sites.

Set	# of Zn-sites	Mean BVS ± standard deviation	PDB IDs[b]
Structural Zn sites[a]			
1	39	1.80 ± 0.28	4hhj_a, 4k6m_b*, 5tfr_a, 5tfr_b, 5ccv_a, 5u0b_a, 5u0b_b, 5tmh_a, 5tmh_b, 4v0q_a, 4v0r_a, 5dto_a, 2hfz_a, 4hdh_a, 4hdh_b, 5u0c_a, 5u0c_b, 5u0c_d, 5u0c_e, 5u0c_f, 5u0c_g, 5u0c_h, 4c11_a, 4c11_b, 3vws_a, 5f3t_a, 5f3z_a, 5f41_a, 5hmw_a, 5hmx_a, 5hmy_a, 5hmz_a, 5hn0_a, 5i3p_a, 5i3q_a, 4mtp_a, 4mtp_b, 4mtp_c
2	26	2.08 ± 0.27	3q7c_a, 3r3l_a, 3r3l_b, 3r3l_c, 3mwp_a, 3mwp_b, 3mwp_c, 3mwt_a, 3mwt_b, 3mwt_c, 3mx2_a, 3mx2_c, 3mx5_a, 3mx5_b, 3mx5_c, 3q7b_a, 4o6h_c, 4o6h_d, 4o6h_e, 4o6i_a, 4o6i_b, 4gv3_a, 4gv6_a, 4g9z_a, 4gv9_a, 4gve_a
4	19	2.18 ± 0.22	1rut_x*, 4jcj_c*, 4kfz_a*, 4kfz_b*, 2xjy_a*, 2xjz_e*, 2lxd_a, 2l4z_a, 1m3v_a, 1j2o_a, 2l6y_b, 2l6z_c, 2mbv_a
3	18	2.12 ± 0.21	5fru_a, 5fru_b, 5frv_a, 5frv_b, 5frw_a, 5frw_b, 5frx_a, 5fry_a, 5fry_b, 5frz_a, 5frz_b, 5fs0_a, 5fs0_b, 5kbe_b, 5kbg_b, 5kbh_a, 5kbh_b, 5kbi_a
5	13	1.88 ± 0.14	4xba_a, 3szq_a, 3sp4_a, 3sp4_b, 3spd_a, 3spd_b, 3spd_c, 3spd_d, 3spl_a, 3spl_b, 3spl_c, 3spl_d, 4ykl_b
6	10	1.70 ± 0.42	2rgt_a*, 2jtn_a*, 2rgt_b*, 3mmk_a*, 3mmk_b*
7	7	1.96 ± 0.33	1u6g_b, 3rtr_b, 3rtr_d, 3rtr_f, 3rtr_h, 2lgv_a, 1ldj_b
8	4	1.98 ± 0.07	4hi8_b, 3f6q_b, 3ixe_b, 4hi9_b
9	*3*	*1.74 ± 0.03*	*5af0_c, 5af0_b, 5af0_d*
10	3	2.06 ± 0.2	2dar_a, 2dlo_a, 2dj7_a
11	2	2.60 ± 0.3	1zt2_a, 1zt2_c
12	2	2.04 ± 0.5	2wbt_a, 2wbt_b
13	1	2.13	4ybg_a
14	15	2.09 ± 0.04	1jvb_a*, 1nto_a*, 1nto_b*, 1nto_c*, 1nto_d*, 1nto_e*, 1nto_h*, 1nvg_a*, 3i4c_a*, 3i4c_b*, 3i4c_c*, 3i4c_d*, 3i4c_e*, 3i4c_h*, 2h6e_a*
Catalytic Zn sites[c]			
Set	# of Zn-sites	Mean BVS ± standard deviation	PDB IDs[b]

1	64	2.07 ± 0.29	5cxk_a, 2a8c_a, 2a8c_b, 2a8c_c, 2a8c_d, 2a8c_e, 2a8c_f, 2a8d_a, 2a8d_b, 2a8d_c, 2a8d_d, 2a8d_e, 2a8d_f, 3e24_a, 3e28_b, 3e28_c, 3e28_d, 3e2a_a, 3e2a_b, 3e2a_c, 3e2a_d, 3e2a_e, 3e2a_f, 3e2w_a, 3e2w_b, 3e2w_c, 3e2w_d, 3e3f_b, 3e3g_a, 3e3g_c, 3e3g_d, 3e3g_e, 3e3g_f, 3e3i_a, 3e3i_b, 3e3i_c, 3e3i_d, 3e3i_e, 3e3i_f, 3e3i_g, 3e3i_h, 3e3i_i, 3e3i_j, 3e3i_k, 3e3i_l, 4wak_a, 4wak_b, 4wam_b, 5cxk_b, 5cxk_c, 5cxk_d, 5cxk_e, 5cxk_f, 5cxk_g, 5cxk_h, 1i6o_a, 1i6o_b, 1i6p_a, 1t75_a, 1t75_b, 1t75_d, 1t75_e, 2esf_a, 2esf_b
2	34	1.81 ± 0.12	1h2b_b, 1jvb_a*, 1nto_a*, 1nto_b*, 1nto_c*, 1nto_d*, 1nto_e*, 1nto_h*, 1nvg_a*, 1r37_a, 1r37_b, 2eer_a, 2eer_b, 3i4c_a*, 3i4c_b*, 3i4c_c*, 3i4c_d*, 3i4c_e*, 3i4c_h*, 2h6e_a*
3	19	1.56± 0.34	3s2e_a, 4eex_b, 4eez_b, 3s1l_a, 3s1l_b, 3s1l_c, 3s1l_d, 3s2e_b, 3s2e_c, 3s2e_d, 3s2f_a, 3s2f_b, 3s2f_c, 3s2f_d, 3s2g_a, 3s2g_b, 3s2g_c, 3s2i_b, 3s2i_d
4	12	1.74 ± 0.35	4dl9_a, 4dl9_b, 4gl4_a, 4gl4_b, 4jji_b, 4l0q_a, 4l0q_b, 3uko_a, 3uko_b, 1ma0_a, 1ma0_b, 1mp0_a,
5	*10*	*2.10 ±0.07*	*5fi3_a, 5fi3_b, 5fi5_a, 5fi5_b, 5h81_a, 5h81_b, 5h82_a, 5h82_b, 5h83_a, 5h83_b*
6	5	2.06 ± 0.13	3wid_a, 3wid_b, 3wid_c, 3wid_d, 3wie_b
7	*4*	*2.21 ±0.20*	*1ddz_a*, 1ddz_b**
8	2	1.70 ± 0.01	3bq6_a, 3bq6_b
9	2	2.10 ± 0.67	1li5_a, 1li5_b
10	2	1.82 ± 0.08	2nyt_a, 2nyt_c
11	2	1.50 ± 0.64	3ppg_a, 4ztx_a
12	1	1.95	3wrg_a
13	1	1.85	1ym3_a
14	1	1.16	4w6z_b
15	1	1.16	4ay7_b
16	1	1.89	1vq2_a

[a]Structural Zn-sites whose mean BVS minus standard deviation is <2 are highlighted in italics.
[b]PDB entries with 2 Zn sites are labeled " * ".
[c]Catalytic Zn-sites whose mean BVS minus standard deviation is >2 are highlighted in italics.

Electronic energies of all the stationary points

Energies of the system with 2nd-shell Asp (M11/6-31+G(3d,p)):
CCCw_asp 10 E(RM11) = -3474.72450375
CCCh_asp 10 E(RM11) = -3474.70976436
CCCw_asp 30 E(RM11) = -3474.74371904
CCCh_asp 30 E(RM11) = -3474.73166128
CCHw_asp 10 E(RM11) = -3262.69244708
CCHh_asp 10 E(RM11) = -3262.69307205
CCHw_asp 30 E(RM11) = -3262.70460028
CCHh_asp 30 E(RM11) = -3262.70409909

Energies of the system without 2nd-shell Asp (M11/6-31+G(3d,p)):
CCCw 10 E(RM11) = -3246.16122955
CCCh 10 E(RM11) = -3245.67448959
CCCw 30 E(RM11) = -3246.16847326
CCCh 30 E(RM11) = -3245.69502804
CCHw 10 E(RM11) = -3034.12420361
CCHh 10 E(RM11) = -3033.65097894
CCHw 30 E(RM11) = -3034.12887833
CCHh 30 E(RM11) = -3033.66370854

SI information II. The Cartesian coordinates of all the structures used in the figure, fully optimized using M06-2X/SDD at epsilon 10 and 30.

CCCh_asp_epsi10.xyz
e/opt.log   Energy: -1922.87050938
Zn1 110.171363 -21.753443 90.345171
C2 108.650870 -20.114460 92.724686
C3 106.206210 -17.355160 89.791384
C4 107.050647 -18.593157 89.633895
O5 108.216157 -18.583123 89.187200
O6 106.419734 -19.713114 90.031074
C7 111.964257 -23.200494 87.988251
S8 111.794344 -23.477040 89.847540
C9 107.900904 -22.596891 88.093902
S10 107.801271 -22.396941 89.961426
O11 110.509018 -20.365215 89.020809
O12 113.023138 -20.328761 89.298861
H13 107.809635 -20.786521 92.534258
H14 106.721099 -16.493382 89.368365
H15 106.013980 -17.183601 90.854565
H16 105.242053 -17.498977 89.297912
H17 113.021326 -23.233096 87.711247
H18 106.960379 -23.005320 87.717654
H19 108.716665 -23.281340 87.847922

H20 108.097167 -21.629691 87.626049
H21 111.552686 -22.219952 87.737570
H22 113.151421 -21.232852 89.651943
H23 112.011056 -20.216745 89.134985
H24 111.425924 -23.981810 87.445643
H25 109.807306 -19.684670 88.988250
S26 110.277127 -21.061814 92.646976
H27 108.540033 -19.670864 93.717671
H28 108.644159 -19.317402 91.974585
H29 106.961070 -20.604164 90.002206

CCCh_asp_epsi30.xyz
e/opt.log   Energy: -1922.87081436
Zn1 110.110123 -21.723847 90.234822
C2 108.651685 -20.003049 92.676164
C3 106.255599 -17.377087 89.936109
C4 107.039520 -18.631160 89.654627
O5 108.166430 -18.639948 89.116752
O6 106.404757 -19.749858 90.052864
C7 112.085948 -23.268541 88.050788
S8 111.777765 -23.443243 89.903864
C9 107.831728 -22.620859 88.007886
S10 107.773209 -22.451406 89.881150
O11 110.472464 -20.365951 88.882522
O12 112.954974 -20.281868 89.395109
H13 107.795189 -20.631815 92.419012
H14 106.753262 -16.515287 89.493330
H15 106.177324 -17.239203 91.018935
H16 105.242683 -17.473815 89.538698
H17 113.157152 -23.352501 87.852277
H18 106.899086 -23.062979 87.651923
H19 108.668404 -23.265066 87.726497
H20 107.971920 -21.638382 87.552106
H21 111.730063 -22.290639 87.719299
H22 113.072120 -21.189006 89.745082
H23 111.964725 -20.189403 89.130135
H24 111.557981 -24.056447 87.508730
H25 109.756984 -19.700294 88.832012
S26 110.253031 -20.982024 92.524014
H27 108.543487 -19.651363 93.705070
H28 108.670131 -19.139243 92.005126
H29 106.923254 -20.644715 89.968097

CCCh_epsi10.xyz
opt.log Energy: -1693.88191892
Zn1 0.564297 -0.597159 -1.563574
O2 -1.208992 -1.337310 -1.964359

C3 2.268072 2.076740 -2.486550
H4 2.518836 2.938759 -3.110292
H5 -1.474181 -2.117464 -1.443939
S6 0.727314 1.237784 -3.162783
H7 3.106595 1.374736 -2.486388
H8 2.088323 2.408391 -1.459234
S9 0.722455 0.304965 0.679610
C10 -0.081264 1.995342 0.471016
H11 -1.126655 1.958570 0.785830
H12 0.454688 2.728570 1.080191
H13 -0.039873 2.292592 -0.581678
S14 2.339154 -2.229814 -1.776723
C15 1.930635 -2.979853 -3.455489
H16 1.756260 -2.188724 -4.189939
H17 2.769326 -3.597509 -3.787213
H18 1.034548 -3.601482 -3.386709
H19 -2.041678 -0.016874 -1.967038
O20 -2.400895 0.938796 -2.010399
H21 -1.636967 1.517943 -2.209341

CCCh_epsi30
opt.log Energy: -1693.88212180
Zn1 0.499583 -0.607538 -1.572745
O2 -1.264930 -1.346953 -2.019044
C3 2.227796 2.068365 -2.483600
H4 2.474603 2.932247 -3.105593
H5 -1.528259 -2.167702 -1.565105
S6 0.688700 1.227425 -3.161636
H7 3.070341 1.371484 -2.486730
H8 2.047606 2.399524 -1.456636
S9 0.646912 0.274191 0.683691
C10 -0.011428 2.028135 0.495333
H11 -1.013172 2.103487 0.924988
H12 0.654244 2.723871 1.013180
H13 -0.057931 2.290354 -0.566234
S14 2.276102 -2.249283 -1.728445
C15 1.982587 -2.977214 -3.440854
H16 1.861251 -2.177605 -4.176513
H17 2.841687 -3.591379 -3.721496
H18 1.084755 -3.599681 -3.442524
H19 -2.092259 -0.030470 -1.988654
O20 -2.441532 0.929661 -2.011436
H21 -1.676654 1.506080 -2.214947

CCCw_asp_epsi10
a/opt.log   Energy: -1922.88566364

```
Zn1 110.547918 -21.980406 89.896842
C2 106.776997 -18.116832 87.403685
C3 107.999268 -19.009279 87.298784
O4 108.750893 -19.058498 88.379497
O5 108.251990 -19.662701 86.242244
C6 112.958777 -23.040890 87.984226
S7 112.749969 -22.952220 89.855454
C8 107.537888 -22.389812 88.569250
S9 108.838651 -23.548094 89.288560
O10 110.556840 -20.664284 88.294308
O11 113.037216 -19.778021 89.072742
H12 107.071693 -17.125227 87.756830
H13 106.087591 -18.540441 88.141379
H14 106.273512 -18.037109 86.439401
H15 113.891512 -23.559662 87.751611
H16 107.167564 -21.707902 89.339866
H17 106.705685 -22.987723 88.188592
H18 107.961452 -21.800508 87.751811
H19 112.997120 -22.028487 87.571686
H20 113.289134 -20.584930 89.573211
H21 112.129554 -19.939952 88.710753
H22 112.125638 -23.587067 87.533506
S23 110.134846 -20.704149 91.857491
C24 108.252957 -20.750547 91.917126
H25 107.923271 -20.494518 92.927063
H26 107.837966 -20.030472 91.207365
H27 107.898799 -21.753405 91.661002
H28 109.720148 -19.893530 88.343178
H29 110.551155 -21.103334 87.422537

CCCw_asp_epsi30
a/opt.log       Energy: -1922.88546300
Zn1 110.551921 -21.970106 89.854509
C2 106.837412 -18.079882 87.274902
C3 108.025819 -19.018328 87.209445
O4 108.797096 -19.028424 88.280471
O5 108.238308 -19.749240 86.196382
C6 112.978804 -23.068966 87.975942
S7 112.750092 -22.947049 89.843226
C8 107.409005 -22.387496 88.819251
S9 108.824223 -23.535124 89.305076
O10 110.557705 -20.685330 88.233420
O11 113.030554 -19.781403 89.006548
H12 107.159358 -17.093069 87.616065
H13 106.117790 -18.466125 88.004475
H14 106.354313 -18.001296 86.300244
H15 113.922348 -23.575652 87.762581
```

H16 106.592126 -22.485580 89.538558
H17 107.046519 -22.655537 87.824001
H18 107.749916 -21.348350 88.805713
H19 113.003210 -22.064823 87.543157
H20 113.292083 -20.582172 89.511886
H21 112.132405 -19.963192 88.629472
H22 112.159391 -23.637804 87.529119
S23 110.161278 -20.634500 91.781964
C24 108.287832 -20.740337 91.946622
H25 108.017530 -20.666224 93.002605
H26 107.811806 -19.926184 91.395074
H27 107.938452 -21.696419 91.547304
H28 109.739812 -19.891806 88.263811
H29 110.538893 -21.146582 87.373177

CCCw_epsi10
opt.log Energy: -1694.35853259
Zn1 0.559041 -1.010730 -0.597740
O2 -1.213139 -0.188228 -1.272891
C3 1.668990 2.009489 -0.919396
H4 0.753029 2.271702 -1.454930
H5 -1.554491 0.601046 -0.729797
S6 2.303172 0.333580 -1.499050
H7 2.432658 2.765078 -1.118572
H8 1.458315 1.982703 0.154393
S9 0.247414 -0.439358 1.756624
C10 1.940333 0.211467 2.251364
H11 2.561353 0.329645 1.358966
H12 1.828326 1.174825 2.753864
H13 2.414369 -0.497651 2.932597
H14 -1.872507 -0.683891 -1.783641
S15 0.491229 -3.269467 -1.304331
C16 1.770677 -3.225194 -2.686835
H17 2.721717 -2.842754 -2.309116
H18 1.914582 -4.241204 -3.061444
H19 1.429840 -2.585398 -3.503605
O20 -1.658886 1.611496 0.420641
H21 -1.613898 2.581528 0.386574
H22 -1.018126 1.199316 1.070325

CCCw_epsi30
opt.log Energy: -1694.35866094
Zn1 0.553314 -1.012383 -0.572879
O2 -1.230943 -0.241028 -1.268415
C3 1.696424 2.025405 -0.898932
H4 0.792085 2.327055 -1.433056
H5 -1.555861 0.570680 -0.744851

S6 2.278908 0.340233 -1.506300
H7 2.484866 2.759157 -1.081410
H8 1.479922 1.985846 0.172937
S9 0.246753 -0.427970 1.775944
C10 1.945497 0.209983 2.269332
H11 2.569910 0.315271 1.377837
H12 1.840639 1.179140 2.761568
H13 2.411494 -0.496460 2.958785
H14 -1.907246 -0.741345 -1.752336
S15 0.622565 -3.303076 -1.189206
C16 1.733428 -3.215034 -2.709701
H17 2.653589 -2.675286 -2.474498
H18 1.982738 -4.232529 -3.018895
H19 1.220904 -2.706118 -3.528665
O20 -1.641873 1.611782 0.369537
H21 -1.610094 2.580673 0.299628
H22 -1.003019 1.234005 1.037577

CCHh_asp_epsi10
e/opt.log   Energy: -1710.83817097
Zn1 109.878872 -21.675976 90.159424
C2 108.827482 -20.373198 92.730763
C3 109.112697 -19.374760 93.636061
N4 109.879335 -20.464488 91.815881
C5 110.782227 -19.535699 92.152694
N6 110.348319 -18.858479 93.253948
C7 106.520097 -17.460646 89.201510
C8 107.540177 -18.431049 88.648805
O9 108.670800 -18.493867 89.344046
O10 107.326020 -19.119188 87.615429
C11 112.135198 -23.163944 88.309641
S12 111.838907 -23.061473 90.167782
C13 107.554403 -22.563513 88.032713
S14 107.681944 -22.512079 89.914913
O15 110.216018 -20.246632 88.758155
O16 112.704042 -19.927196 89.772234
H17 107.962292 -21.011279 92.663609
H18 108.563092 -19.002519 94.482114
H19 111.701502 -19.344381 91.617259
H20 110.841294 -18.100848 93.708498
H21 106.985201 -16.483925 89.356999
H22 106.171083 -17.822887 90.173251
H23 105.673053 -17.368841 88.521507
H24 113.072057 -23.695751 88.131827
H25 106.605731 -23.034782 87.765481
H26 108.373052 -23.153546 87.612311
H27 107.579871 -21.547155 87.632466

H28 110.139313 -20.520027 87.825584
H29 112.211245 -22.158583 87.885873
H30 112.833217 -20.853692 90.077251
H31 111.833563 -19.902386 89.288454
H32 111.319946 -23.703571 87.822726
H33 109.426952 -19.322639 89.025790

CCHh_asp_epsi30
e/opt.log   Energy: -1710.83824746
Zn1 109.851513 -21.648222 90.146996
C2 108.852997 -20.394927 92.760862
C3 109.156461 -19.414511 93.680100
N4 109.880565 -20.458265 91.815436
C5 110.786702 -19.530631 92.150157
N6 110.377427 -18.881724 93.276734
C7 106.540750 -17.355979 89.201923
C8 107.510268 -18.374191 88.643568
O9 108.657972 -18.458448 89.307413
O10 107.244001 -19.078088 87.632668
C11 112.116191 -23.130241 88.272941
S12 111.794368 -23.063726 90.129049
C13 107.564575 -22.713118 88.068889
S14 107.640412 -22.466957 89.937404
O15 110.186151 -20.227413 88.736723
O16 112.683729 -19.924917 89.737249
H17 107.992041 -21.040215 92.708072
H18 108.628697 -19.065780 94.549756
H19 111.692905 -19.323086 91.599349
H20 110.878830 -18.133001 93.737724
H21 107.026663 -16.378164 89.258961
H22 106.258643 -17.645724 90.218554
H23 105.648774 -17.292363 88.578580
H24 113.051264 -23.665859 88.097818
H25 106.619801 -23.201425 87.820723
H26 108.390260 -23.345868 87.734364
H27 107.613276 -21.744503 87.566442
H28 110.133445 -20.513815 87.806292
H29 112.206087 -22.117323 87.870930
H30 112.808571 -20.849079 90.049885
H31 111.808618 -19.895060 89.262674
H32 111.303918 -23.652559 87.763474
H33 109.404122 -19.304819 88.985290

CCHh_epsi10
opt.log Energy: -1481.83779491
Zn1 -0.039481 -0.494911 -0.884885
O2 -0.070530 -2.419728 -1.134212

C3 2.010047 1.546223 -2.492918
H4 2.143772 2.544654 -2.915939
H5 -0.311688 -2.819656 -1.986181
S6 0.212136 1.028776 -2.698287
H7 2.668101 0.845830 -3.012172
H8 2.270752 1.559172 -1.431075
C9 -2.639009 -0.759188 0.717111
C10 -2.701534 1.104381 -0.456294
H11 -2.299201 -1.693907 1.143913
C12 -3.871278 1.058364 0.273085
H13 -2.345992 1.849639 -1.148448
H14 -4.702673 1.738366 0.329964
N15 -1.946771 -0.035603 -0.170246
N16 -3.813596 -0.124610 1.006810
H17 -4.518903 -0.459158 1.650333
S18 1.381415 -0.052338 1.013330
C19 0.712468 1.657261 1.426339
H20 -0.366075 1.608857 1.602383
H21 1.207466 2.031178 2.325652
H22 0.905289 2.345491 0.598158
H23 -0.374234 -2.855409 0.317981
O24 -0.508851 -2.871632 1.332285
H25 0.011369 -2.126054 1.701314

CCHh_epsi30
opt.log Energy: -1481.83594706
Zn1 -0.129615 -0.384876 -0.915605
O2 -0.100845 -2.250191 -1.453178
C3 2.137013 1.572946 -2.292866
H4 2.425785 2.540493 -2.709323
H5 -0.438434 -2.520014 -2.324542
S6 0.277802 1.350438 -2.498747
H7 2.676141 0.781282 -2.817601
H8 2.399453 1.540464 -1.231968
C9 -2.386430 -0.110832 1.118971
C10 -3.143051 0.535163 -0.841398
H11 -1.743108 -0.466996 1.906360
C12 -4.183747 0.682826 0.051661
H13 -3.115513 0.748542 -1.896431
H14 -5.192037 1.032959 -0.080107
N15 -2.029817 0.037739 -0.160850
N16 -3.685818 0.270565 1.284068
H17 -4.197224 0.256293 2.157446
S18 1.194161 -0.246415 1.099946
C19 0.860535 1.552129 1.538401
H20 -0.210813 1.712131 1.692582
H21 1.396944 1.806034 2.455234

H22 1.201279 2.202939 0.728584
H23 -0.382180 -2.910853 -0.065412
O24 -0.489455 -3.137145 0.922428
H25 -0.128021 -2.389622 1.440347

CCHw_asp_epsi10
a/opt.log   Energy: -1710.83424484
Zn1 109.519693 -21.943718 89.689835
C2 109.534354 -19.813440 91.980207
C3 110.118712 -19.579357 93.209681
N4 109.952407 -21.070947 91.526661
C5 110.762989 -21.583665 92.455295
N6 110.886941 -20.706673 93.493959
C7 105.885718 -18.771474 88.466768
C8 107.385313 -18.765917 88.708763
O9 107.848341 -18.375147 89.831475
O10 108.128143 -19.207878 87.726714
C11 112.672902 -22.647057 89.474254
S12 111.117704 -23.703500 89.602131
C13 106.879245 -22.323396 87.721580
S14 107.195404 -22.312828 89.578274
O15 110.123960 -20.427133 88.520691
O16 111.705458 -18.821218 89.952470
H17 108.861333 -19.204097 91.387727
H18 110.046808 -18.743766 93.883632
H19 111.246263 -22.545461 92.391693
H20 111.443294 -20.853056 94.326366
H21 105.372526 -18.111720 89.168807
H22 105.535049 -19.799400 88.623013
H23 105.661756 -18.484993 87.436852
H24 113.545882 -23.302884 89.439129
H25 105.810233 -22.475829 87.552857
H26 107.434214 -23.134836 87.244821
H27 107.185856 -21.363538 87.299659
H28 109.313379 -19.862558 88.135288
H29 112.758615 -21.984809 90.341381
H30 111.243930 -18.694271 90.803908
H31 112.189164 -18.021950 89.679944
H32 110.812003 -19.850769 88.946517
H33 112.640411 -22.037716 88.568647

CCHw_asp_epsi30
a/opt.log   Energy: -1710.83517465
Zn1 109.502981 -21.907279 89.716875
C2 109.575354 -19.767040 91.952372

C3 110.173869 -19.504070 93.169038
N4 109.947800 -21.055365 91.548345
C5 110.747521 -21.556851 92.493453
N6 110.905808 -20.643939 93.494402
C7 105.739636 -18.789959 88.433891
C8 107.225811 -18.772680 88.749409
O9 107.632105 -18.419664 89.905849
O10 108.021541 -19.155991 87.783850
C11 112.675679 -22.664284 89.469938
S12 111.083547 -23.671434 89.504978
C13 106.949915 -22.341989 87.686037
S14 107.194178 -22.366567 89.554309
O15 110.038766 -20.337473 88.590265
O16 111.762462 -18.833175 89.921676
H17 108.915856 -19.159538 91.342922
H18 110.134820 -18.640616 93.809700
H19 111.204411 -22.532583 92.472322
H20 111.462962 -20.774966 94.329311
H21 105.168500 -18.276250 89.208883
H22 105.417965 -19.837269 88.382982
H23 105.553563 -18.331892 87.459148
H24 113.525253 -23.347588 89.405107
H25 105.908228 -22.589192 87.466948
H26 107.599182 -23.079581 87.207940
H27 107.180147 -21.343601 87.307427
H28 109.220882 -19.782764 88.213712
H29 112.768969 -22.065166 90.380580
H30 111.482850 -18.708504 90.848189
H31 112.662223 -18.499270 89.762220
H32 110.750809 -19.770706 88.993221
H33 112.682407 -21.997755 88.604699

CCHw_epsi10
opt.log Energy: -1482.30845883
Zn1 -0.360071 -0.004930 -0.120632
O2 -0.268821 -1.719726 -1.226009
H3 -0.469187 -1.560488 -2.213648
C4 2.014993 1.193266 -2.081730
H5 2.612224 1.450994 -1.204841
H6 0.182370 -2.547742 -0.999665
S7 0.209503 1.637797 -1.779423
H8 2.376641 1.755707 -2.944281
H9 2.108564 0.122888 -2.281479
C10 -3.149176 0.492347 1.040253
C11 -3.260558 -0.039065 -1.095013
H12 -2.787109 0.706672 2.031021
C13 -4.551420 0.199080 -0.676856

H14 -2.889853 -0.325169 -2.066774
H15 -5.488322 0.162529 -1.203567
N16 -2.397742 0.148041 -0.010129
N17 -4.460812 0.532553 0.671938
H18 -5.235960 0.767223 1.279035
S19 0.752280 -0.089543 1.928278
C20 1.936641 1.366746 1.758890
H21 2.068319 1.823181 2.741731
H22 2.903532 1.019715 1.389465
H23 1.528112 2.106937 1.066364
O24 -0.815293 -0.756489 -3.455131
H25 -0.894829 -0.946300 -4.404103
H26 -0.559025 0.181776 -3.228693

CCHw_epsi30
opt.log Energy: -1482.30849458
Zn1 -0.346121 -0.012898 -0.108824
O2 -0.246141 -1.707298 -1.238215
H3 -0.463643 -1.551047 -2.223136
C4 2.014391 1.217470 -2.085119
H5 2.613648 1.469613 -1.208001
H6 -0.125392 -2.626955 -0.955593
S7 0.205708 1.638504 -1.767900
H8 2.365682 1.794725 -2.942143
H9 2.116976 0.151085 -2.299731
C10 -3.147884 0.483694 1.047650
C11 -3.240403 -0.046472 -1.089118
H12 -2.796484 0.698971 2.041956
C13 -4.535464 0.185566 -0.680095
H14 -2.862523 -0.330443 -2.058953
H15 -5.468610 0.145002 -1.213166
N16 -2.385984 0.143726 0.002723
N17 -4.456262 0.518240 0.669233
H18 -5.237425 0.748105 1.270877
S19 0.772174 -0.077549 1.941950
C20 1.955501 1.377656 1.756221
H21 2.092396 1.842172 2.734550
H22 2.920626 1.028868 1.383932
H23 1.542832 2.112004 1.059957
O24 -0.810831 -0.753398 -3.467642
H25 -0.814186 -0.955099 -4.417938
H26 -0.557580 0.183759 -3.238476