Table 2

Hydrogen bond in 42 X-ray elucidated proteins

Protein			Hydrogen Bonds					Residues		Sites		Groups		Secondary Structure: Helix/Turn		PBS		ABS		Sheet	
		n	N:O	R:O	N:R	R:R	Sum	D	A	D	A	D	A	n	f	n	f	n	f	f	f
351C	Cytochrome C551 (oxidized), 1·6 Å (Almassy & Dickerson, 1978)	82	71	9	7	6	93	55	51	67	59	57	**49**	3	0·683	0	0	0	0	0·0	0·683
2ACT	Actinidin, 2·0 Å (Baker, 1980)	218	146	28	35	29	238	153	135	190	172	**136**	**149**	12	0·482	2	0·018	10	0·294	0·298	0·733
2APP	Penicillopepsin, 1·8 Å (James & Sielecki, 1983)	323	190	37	46	39	312	232	220	280	261	**233**	**255**	22	0·390	13	0·186	21	0·502	0·598	0·873
2AZA	Azurin (oxidized), 1·8 Å (Norris *et al.*, 1986)	129	72	16	17	20	125	89	**83**	112	101	83	85	6	0·434	4	0·202	8	0·372	0·496	0·876
1BP2	Phospholipase *A2*, 1·7 Å (Dijkstra *et al.*, 1981)	123	106	16	15	18	155	85	80	110	100	90	**84**	8	0·780	0	0	4	0·130	0·130	0·854
2CA2	Carbonic anhydrase, 1·9 Å (Eriksson *et al.*, 1988)	256	137	45	38	46	266	173	176	235	222	187	**181**	15	0·418	7	0·129	13	0·359	0·422	0·797
2CDV	Cytochrome *C3*, 1·8 Å (Higuchi *et al.*, 1984)	107	56	16	14	16	102	66	61	81	76	**61**	**61**	6	0·570	4	0·065	4	0·112	0·178	0·673
5CHA	Alpha chymotrypsin A, 1·67 Å (Blevins & Tulinsky, 1985)	237	126	26	25	14	191	140	135	176	159	141	**136**	11	0·325	12	0·017	14	0·414	0·418	0·688
5CPA	Carboxypeptidase *A* Alpha, 1·54 Å (Rees *et al.*, 1983)	307	239	42	39	48	368	233	216	284	261	**221**	223	14	0·596	11	0·189	5	0·111	0·241	0·811
1CRN	Crambin, 1·5 Å (Hendrickson & Teeter, 1981)	46	39	8	3	2	52	28	28	35	30	32	**28**	3	0·630	0	0	2	0·109	0·109	0·739
2CTS	Citrate synthase, 2·0 Å (Remington *et al.*, 1982)	437	387	49	48	40	524	320	293	389	337	328	**306**	17	0·762	2	0·009	4	0·027	0·037	0·787
5CYT	Cytochrome *c* (reduced), 1·5 Å (Takano & Dickerson, 1981)	103	75	18	10	3	106	66	66	80	72	71	**62**	7	0·718	0	0	2	0·068	0·068	0·767
4DFR	Dihydrofolate reductase, 1·7 Å (Bolin *et al.*, 1982)	159	106	18	9	18	151	104	101	128	114	109	**97**	7	0·365	8	0·283	5	0·214	0·421	0·742
1ECD	Hemoglobin (erythrocruorin), 1·4 Å (Weber *et al.*, 1978)	136	161	14	9	15	199	108	99	132	115	106	**104**	3	0·978	0	0	0	0	0	0·978
4FXN	Flavodoxin (semiquinone form), 1·8 Å (Smith *et al.*, 1977)	138	113	14	9	10	146	90	93	107	103	**94**	**94**	8	0·587	6	0·268	0	0	0·268	0·810
1GCR	Gamma-II crystallin, 1·6 Å (Wistow *et al.*, 1983)	174	91	20	24	23	158	120	112	152	135	**113**	**113**	6	0·178	0	0	12	0·552	0·552	0·718
1GD1	Glyceraldehyde-3-P dehydro., 1·8 Å (Skarzynski *et al.*, 1987)	331	249	34	44	49	376	249	229	309	277	**233**	238	17	0·548	15	0·235	11	0·190	0·389	0·867
1GP1	Glutathione peroxidase, 2·0 Å (Epp *et al.*, 1983)	35	9	1	2	0	12	11	11	12	11	11	**11**	3	0·457	0	0	2	0·171	0·171	0·543
3GRS	Glutathione reductase, 1·54 Å (Karplus & Schulz, 1987)	461	358	47	32	50	487	315	295	382	350	324	**314**	22	0·529	11	0·128	18	0·217	0·330	0·833
1HMQ	Hemerythrin (met), 2·0 Å (Stenkamp *et al.*, 1985)	113	123	9	6	20	158	87	83	111	103	96	**80**	4	0·858	0	0	0	0	0	0·858
1HOE	Amylase inhibitor, 2·0 Å (Pflugrath *et al.*, 1986)	74	35	10	9	8	62	46	46	56	51	**46**	48	3	0·203	0	0	7	0·649	0·649	0·797
1INS	Insulin, 1·5 Å (Baker *et al.*, 1988)	51	39	4	6	2	51	37	31	41	35	**30**	32	3	0·667	0	0	2	0·118	0·118	0·725
2LHB	Hemoglobin v (cyano, met), 2·0 Å (Hendrickson *et al.*, 1973)	149	165	16	16	5	202	119	107	136	120	117	**114**	3	0·893	0	0	0	0	0	0·893
1LZ1	Lysozyme, 1·5 Å (Blake *et al.*, 1983)	130	105	20	16	18	159	96	88	121	108	98	**95**	9	0·815	2	0·100	4	0·146	0·246	0·923
3LZM	Lysozyme, 1·7 Å (Weaver & Matthews, 1987)	164	179	17	20	26	242	128	119	163	144	137	**126**	7	0·860	0	0	4	0·098	0·098	0·927
1MBO	Myoglobin (oxy), 1·6 Å (Phillips, 1980)	153	194	17	13	20	244	131	119	158	143	138	**129**	3	0·941	0	0	0	0	0	0·941
2OVO	Ovomucoid third domain, 1·8 Å (Papamokos *et al.*, 1982)	56	28	9	12	11	60	35	33	46	43	**37**	**37**	3	0·411	0	0	3	0·250	0·250	0·625
9PAP	Papain, 1·65 Å (Kamphuis *et al.*, 1984)	212	132	31	27	31	221	145	132	185	164	**135**	141	11	0·491	4	0·038	9	0·292	0·316	0·731
2PCY	Apo-Plastocyanin, 1·8 Å (Guss & Freeman, 1983)	99	50	9	12	9	80	63	62	75	69	**59**	60	7	0·384	4	0·202	7	0·485	0·586	0·838
4PEP	Pepsin, 1·8 Å (Sielecki *et al.*, 1990)	320	193	36	37	30	296	223	208	259	242	**212**	216	23	0·377	10	0·160	22	0·460	0·555	0·828
1PPT	Avian pancreatic polypeptide, 1·37 Å (Glover *et al.*, 1983)	36	33	1	0	1	35	21	20	22	20	21	**20**	1	0·694	0	0	0	0	0	0·694
5PTI	Trypsin inhibitor, 1·0 Å (Wlodawer *et al.*, 1987)	58	27	4	6	2	39	29	26	32	31	29	**28**	3	0·362	0	0	2	0·293	0·293	0·638
1RDG	Rubredoxin, 1·4 Å (Pierrot *et al.*, 1976)	52	24	6	9	2	41	32	27	38	34	**28**	**28**	5	0·731	0	0	4	0·365	0·365	0·923
2RHE	Ig Bence-Jones protein, 1·6 Å (Furey *et al.*, 1983)	114	61	13	12	11	97	76	69	89	80	**68**	70	8	0·377	4	0·114	6	0·526	0·614	0·886
3RNT	Lys 25-ribonuclease T1, 1·8 Å (Koepke *et al.*, 1989)	104	65	15	12	12	104	65	62	82	76	69	**61**	7	0·452	0	0	7	0·346	0·346	0·750
7RSA	Ribonuclease A, 1·26 Å (Wlodawer *et al.*, 1982)	124	74	25	13	18	130	86	85	110	105	89	**82**	5	0·379	2	0·032	6	0·419	0·444	0·790
1SN3	Scorpion neurotoxin, 1·8 Å (Almassy *et al.*, 1983)	65	34	5	6	3	48	35	32	40	39	**30**	32	5	0·477	0	0	3	0·338	0·338	0·754
1SNC	Staphylococcus nuclease, 1·65 Å (Loll & Lattman, 1989)	135	101	13	19	18	151	103	89	123	109	**92**	100	6	0·530	2	0·060	6	0·396	0·396	0·858
3TLN	Thermolysin, 1·6 Å (Holmes & Matthews, 1982)	316	265	31	39	61	396	249	225	303	281	252	**240**	14	0·595	5	0·098	12	0·218	0·282	0·839
1TPP	Beta-trypsin, 1·4 Å (Bode & Schwager, 1975)	220	123	25	26	16	190	121	111	171	154	**136**	140	12	0·386	0	0	12	0·427	0·427	0·709
1UBQ	Ubiquitin, 1·8 Å (Vijay-Kumar *et al.*, 1987)	76	52	9	11	4	76	49	50	59	57	53	**50**	6	0·579	4	0·276	5	0·539	0·592	0·895
2WRP	Trp repressor, 1·65 Å (Zhang *et al.*, 1987)	105	137	9	7	3	156	82	75	93	82	86	**79**	3	0·905	0	0	0	0	0	0·905
		6734	4970	792	760	777	7299	4695	4383			4515			0·556		0·087		0·245	0·308	0·811

Summary of numbers and types of hydrogen bonds in 42 high-resolution proteins from the Brookhaven (Bernstein *et al.*, 1977) protein data base (PDB), analyzed as described in Materials and Methods. The Table contains 22 columns. Columns 1 to 3 identify each protein and include: (1) PDB identifier, (2) protein name and resolution of structure, and (3) number of residues in the protein. Columns 4 to 8 list the number of hydrogen bonds: (4) backbone donor to backbone acceptor (N:O), (5) side-chain donor to backbone acceptor (R:O), (6) backbone donor to side-chain acceptor (N:R), and (7) side-chain donor to side-chain acceptor (R:R), and (8) total hydrogen bonds (Σ columns 4 to 7). Columns 9 to 14 list the count of donors (D) and acceptors (A): (9) number of donor residues, (10) number of acceptor residues, (11) number of donor atoms, (12) number of acceptor atoms, (13) reduced number of donors, and (14) reduced number of acceptors. The lesser values of columns 13 and 14, shown in boldface, is $\mathfrak{R}$(protein). Columns 15 to 22 list secondary structure by type: (15) number of contiguous segments of helix and/or hydrogen bonded turns, (16) fraction (f) of protein in helix and/or hydrogen-bonded turns, (17) number of contiguous segments of parallel β-sheet (PBS), (18) fraction of protein in parallel β-sheet, (19) number of contiguous segments of antiparallel β-sheet (ABS), (20) fraction of protein in parallel β-sheet, (21) fraction of protein in sheet, the logical-or of columns 18 and 20 (i.e. antiparallel β-sheet *versus* parallel β-sheet), and (22) fraction of protein in helix and sheet, the logical-or of columns 16 and 22 (i.e. helix *versus* sheet). Note: residues at the interface between 2 elements of secondary structure may be counted twice, once in each segment. For this reason, the logical-or of β-sheet, in column 21, and the logical-or of all secondary structure, in column 22, are typically less than the arithmetic sum of their components.