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Electron Density Based Analysis of N-H···O=C Hydrogen Bonds and Electrostatic Interaction Energies in High-resolution Secondary Protein Structures: Quantum Crystallographic Approaches

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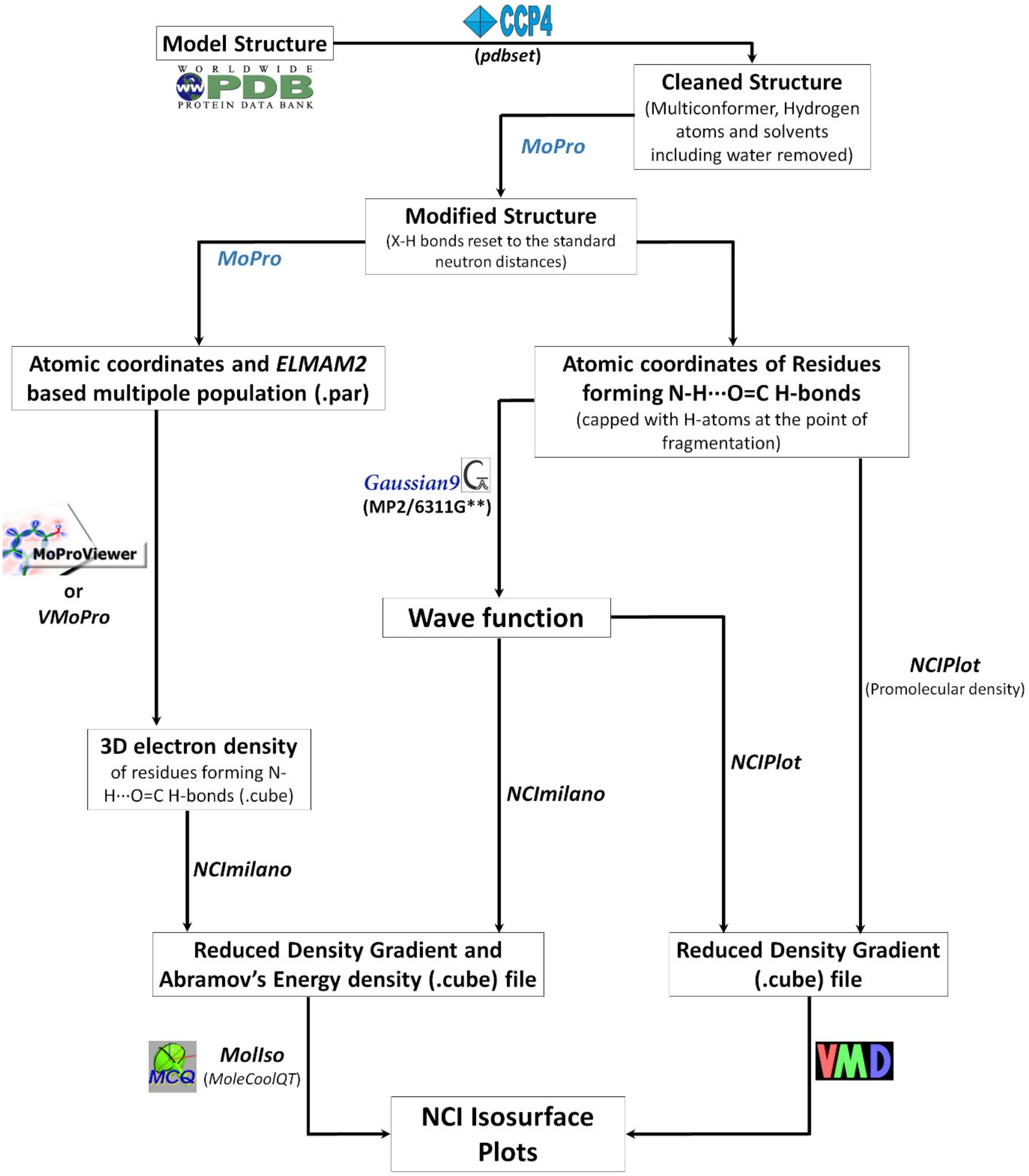
Supporting information



Scheme S1 Flowchart and methodologies for the generation of NCI isosurfaces

Table S1: Showing the presence of metal ions/atoms and other heavy atoms in the protein structures selected for this study.

Protein Name	**Metal Ions**	**Other heavy Atoms**	**Remark**
5D8V	4-Fe	-	Fe_4S_4-Cys_4 complex in protein
1EJG	-	-	-
2VB1	-	-	-
1US0	-	P, Br, F	NADPH and IDD594 Ligands
1YK4	Fe	-	Fe-Cys_4 Complex in protein
4REK	-	P	FAD Ligand
1GCI	Ca	-	Ca^{2+} ion
5GV8	-	P	FAD Ligand
1PQ7	-	-	-
3UI4	-	-	-
2H5C	-	-	-
2VXN	-	P	Ligand 2-Phosphoglycolic Acid
2PWA	Ca	-	Ca^{2+} ion
2O9S	-	-	-
4EIC	Fe	-	Heme (Protoporphyrin-9 containing Fe) in Protein
1MC2	-	-	-
1PJX	Ca	-	Ca^{2+} ion
4AYO	Ca, Na	-	Ca^{2+}, Na^{+} ions
4O8H	-	-	-
4HS1	-	-	-
5AKR	Cu	-	Cu-Cys-Met-His_2 Complex in protein
4TJZ	-	-	-

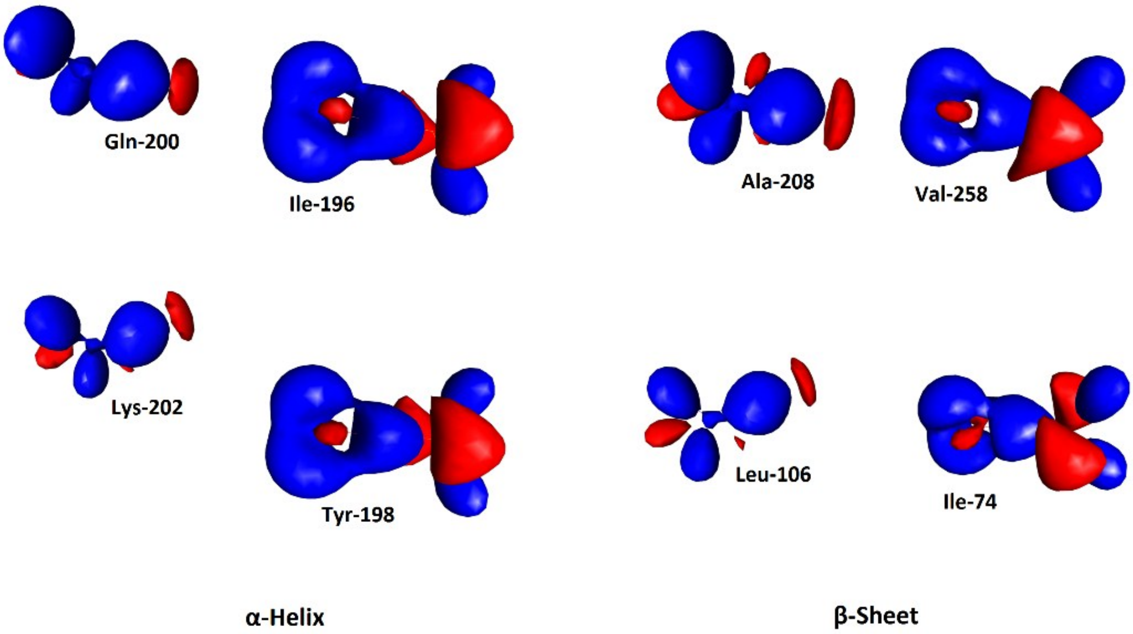


Figure S1 3D deformation density map of α-helices and β-sheets in protein human Aldose Reductase (hAR). The +ve and –ve contours at ± 0.1 eÅ^{-3} are shown in blue and red, respecitively

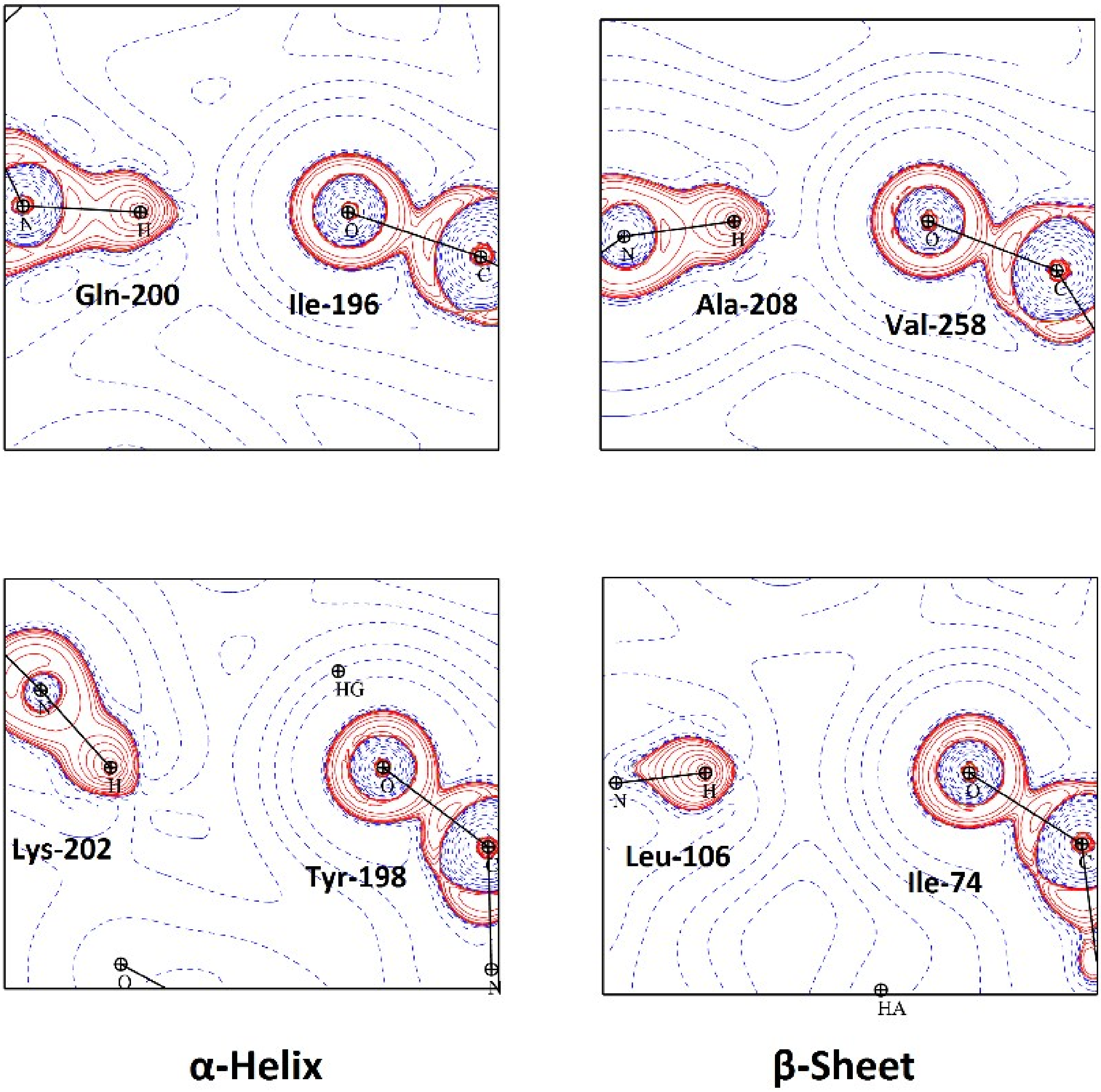


Figure S2 2D Laplacian map of strong and weak H-bonds in α-helices and β-sheets in hAR. +ve and –ve contours are drawn at logarithmic interval of $-\nabla^2\rho_{bcp}$ shown in solid red and dashed blue line, respectively.

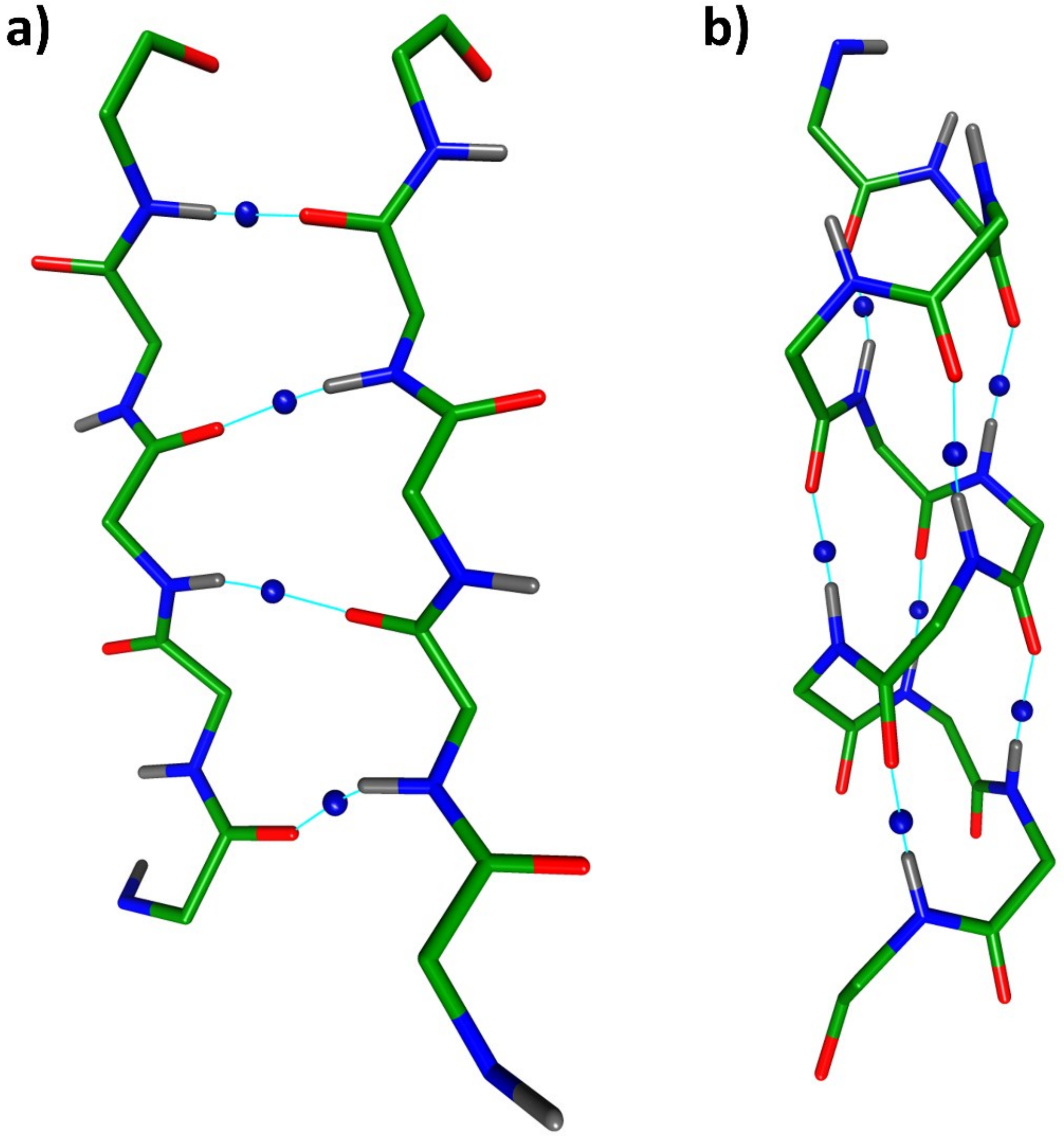


Figure S3 Succession of HBs in **(a)** β-sheets and **(b)** α-helix of hAR are shown interms of the bond path (cyan solid line) and bond critical point (black circles).

Table S2 Topological properties, E_{elec} and ∠C=O···H and ∠N-H···O of the i→i+4 α-helix hydrogen bonds in the 22 protein systems (estimated error on ρ_{BCP} is 0.05 eÅ^{-3}, E_{elec} is 2.32 kCal/mol and $\nabla^2\rho_{BCP}$ is 0.32 eÅ^{-5})

Sl. No.	**Protein**	**Residue O**	**Residue H**	**R_{ij} (Å)**	**ρ_{BCP} (eÅ^{-3})**	**E_{elec} (kCal/mol)**	**$\nabla^2\rho_{BCP}$ (eÅ^{-5})**	**Angles (°)**	
								C=O···H	**N-H···O**
1	**NrDH (4HS1)**	cys_11	ser_15	1.97	0.17	-9.79	1.41	162.9	163.1
2		val_12	ala_16	1.90	0.20	-11.23	1.58	151.9	165.3
3		gln_13	thr_17	2.09	0.13	-7.42	1.24	131.4	152.1
4		cys_14	ser_18	2.00	0.16	-9.27	1.34	152.4	163.2
5		ser_15	lys_19	1.96	0.18	-9.93	1.47	151.7	160.6
6		ala_16	ala_20	1.95	0.18	-9.98	1.49	148.7	160
7		thr_17	leu_21	1.93	0.19	-10.66	1.48	156.7	166.7
8		ser_18	asp_22	1.91	0.20	-11.13	1.54	151.7	166.4
9		lys_19	lys_23	1.98	0.17	-9.31	1.47	148.6	155.7
10		ala_20	gln_24	2.41	0.07	-4.81	0.69	141.1	154.3
11		asp_36	arg_40	2.08	0.14	-7.88	1.26	146.5	154.6
12		ser_37	asp_41	1.87	0.21	-11.55	1.76	140.8	159.4
13		glu_38	tyr_42	2.03	0.15	-8.42	1.36	144.3	154.9
14		ala_39	val_43	2.04	0.15	-8.60	1.22	154.2	165.4
15		arg_40	met_44	1.87	0.21	-11.81	1.74	155.7	161.1
16		asp_41	ala_45	1.81	0.24	-13.26	1.98	149.4	160.6
17		tyr_42	leu_46	2.06	0.15	-8.26	1.25	150.2	158.4
18		val_43	gly_47	2.20	0.10	-5.89	1.26	136	136.6
19		arg_65	ile_69	2.08	0.14	-8.07	1.23	157.5	157.5
20		pro_66	lys_70	1.98	0.17	-9.54	1.40	148.1	161.8
21		asp_67	ala_71	2.21	0.10	-6.19	1.01	139.6	150
22		ala_71	ala_75	2.43	0.07	-4.56	0.72	145.3	144.1
23	**Human Parvulin 14 (3ui4)**	lys_47	ile_51	2.12	0.13	-7.45	1.13	155.5	158.6
24		his_48	met_52	2.08	0.14	-7.63	1.25	151.7	153.3
25		gly_49	glu_53	2.18	0.11	-6.29	1.09	140.2	148.8
26		lys_50	ala_54	2.07	0.14	-7.87	1.24	152.6	156.2
27		ile_51	met_55	1.93	0.19	-10.06	1.66	144.7	155

28		met_52	glu_56	2.01	0.16	-8.66	1.42	146.2	154.3
29		glu_53	lys_57	2.19	0.11	-6.39	1.04	146.3	152.2
30		ala_54	leu_58	2.06	0.15	-8.26	1.26	156.1	159.2
31		met_55	lys_59	1.99	0.17	-9.21	1.48	151.8	155.5
32		glu_56	ser_60	2.31	0.08	-4.58	1.15	140.5	127.8
33		arg_63	val_67	2.10	0.13	-7.52	1.23	153.8	153.6
34		phe_64	ala_68	1.91	0.20	-10.92	1.62	153.9	161.7
35		asn_65	ala_69	1.96	0.18	-9.44	1.53	139.4	156
36		glu_66	gln_70	2.18	0.11	-6.35	1.05	138.8	151.9
37		val_67	tyr_71	2.02	0.15	-8.28	1.60	153.6	144.8
38		ala_68	ser_72	1.86	0.23	-12.10	1.97	124.1	155.2
39		val_91	gln_95	1.94	0.18	-10.00	1.58	155.7	157.6
40		gly_92	glu_96	2.07	0.14	-8.19	1.16	161.8	166.8
41		pro_93	ala_97	2.18	0.11	-6.56	0.98	138.3	159.6
42		phe_94	ala_98	1.91	0.20	-10.57	1.89	152	150
43		gln_95	phe_99	2.04	0.15	-8.74	1.19	159.8	170.4
44		glu_96	ala_100	2.63	0.04	-3.22	0.51	133.7	134.2
45	**HEWL (2VB1)**	gly_4	leu_8	1.88	0.21	-11.25	1.67	154.7	162.8
46		arg_5	ala_9	1.89	0.20	-10.81	1.79	139.5	155.3
47		cys_6	ala_10	1.99	0.17	-9.04	1.40	144.6	159.4
48		glu_7	ala_11	2.07	0.14	-7.89	1.19	147.4	162.3
49		leu_8	met_12	1.77	0.27	-14.98	2.01	159.9	169.3
50		ala_9	lys_13	1.95	0.18	-9.51	1.60	146.2	154.6
51		ala_10	arg_14	1.95	0.18	-9.82	1.48	147.9	162.2
52		ala_11	his_15	2.17	0.11	-6.30	1.15	143.3	146.3
53		ser_24	trp_28	2.45	0.06	-4.49	0.65	149.6	154.7
54		leu_25	val_29	1.96	0.18	-9.96	1.44	160.1	165.5
55		gly_26	cys_30	1.89	0.20	-11.00	1.63	145.8	163.1
56		asn_27	ala_31	1.97	0.17	-8.98	1.57	138.5	152.4
57		trp_28	ala_32	2.06	0.14	-7.93	1.21	144	160.9
58		val_29	lys_33	1.94	0.19	-9.97	1.57	152	158.3
59		cys_30	phe_34	2.18	0.11	-6.59	1.00	155.4	158.8
60		ala_31	glu_35	1.87	0.21	-11.04	1.93	150.9	152.4

61		ala_32	ser_36	2.02	0.16	-8.51	1.32	143.1	160
62		ile_88	val_92	1.90	0.20	-11.28	1.56	170.9	169.5
63		thr_89	asn_93	1.95	0.18	-10.06	1.44	154.3	166.5
64		ala_90	cys_94	1.97	0.17	-9.32	1.52	144.6	155.8
65		ser_91	ala_95	1.87	0.21	-11.47	1.74	146.1	161.1
66		val_92	lys_96	1.93	0.19	-10.28	1.56	153.3	161.2
67		asn_93	lys_97	2.14	0.12	-6.71	1.12	140.8	153.5
68		cys_94	ile_98	1.92	0.19	-10.43	1.59	158.2	160.7
69		ala_95	val_99	2.25	0.10	-5.93	0.87	148.3	162.3
70		lys_96	ser_100	1.96	0.18	-9.25	1.72	146.3	148.7
71		lys_97	asp_101	2.16	0.11	-5.82	1.47	142.2	132.5
72		trp_108	arg_112	2.10	0.13	-7.59	1.11	161.4	164.3
73		val_109	asn_113	2.14	0.12	-6.81	1.14	146.1	152.8
74		ala_110	arg_114	2.23	0.10	-5.11	1.47	136	125.4
75		trp_111	cys_115	2.04	0.15	-7.69	1.58	133.9	143.2
76	**HiPIP (5D8V)**	asp_11	ile_15	1.92	0.19	-10.86	1.61	160.2	159.9
77		pro_12	ala_16	1.95	0.18	-10.09	1.47	144.3	162
78		thr_13	leu_17	1.95	0.18	-9.76	1.61	149	153.4
79		glu_27	ala_31	2.16	0.12	-7.00	1.05	156.9	156.2
80		arg_28	ala_32	2.28	0.08	-5.29	0.97	143.9	139.7
81	**Cytochrome c6 (4eic)**	asp_2	gly_6	2.01	0.16	-8.69	1.54	147.1	148.5
82		ala_3	ala_7	2.38	0.07	-4.54	0.94	145.4	130.4
83		gly_6	phe_10	1.93	0.19	-10.53	1.57	155	160.1
84		ala_7	ala_11	2.00	0.16	-9.18	1.40	144.6	157.1
85		gln_8	ala_12	2.22	0.10	-6.12	1.02	144	146.6
86		phe_10	cys_14	1.97	0.17	-9.46	1.70	150.1	147.1
87		cys_14	his_18	2.13	0.12	-6.58	1.58	142.7	132.3
88		lys_32	leu_36	1.93	0.19	-10.91	1.48	167.4	168
89		ala_33	lys_37	2.20	0.11	-6.56	0.94	144	160.9
90		asp_34	thr_38	2.43	0.06	-4.28	0.78	137	135.9
91		ala_35	tyr_39	2.08	0.13	-7.44	1.63	155.9	136.9
92		leu_36	leu_40	1.95	0.18	-10.67	1.41	137.9	169.6
93		ser_49	ala_53	1.93	0.19	-10.77	1.48	153.9	166.3

94		leu_50	val_54	1.91	0.20	-11.25	1.57	160.5	164.9
95		glu_51	ala_55	1.93	0.19	-10.64	1.48	151.6	165.8
96		glu_52	tyr_56	1.91	0.19	-10.73	1.66	151.1	157
97		ala_53	gln_57	2.05	0.15	-8.39	1.21	146.7	161.7
98		val_54	val_58	1.85	0.22	-12.62	1.71	161	167.5
99		ala_55	thr_59	1.96	0.18	-9.97	1.48	146.3	160.6
100		tyr_56	asn_60	2.00	0.16	-8.94	1.57	148.7	148.6
101		gln_57	gly_61	1.99	0.16	-8.45	1.97	138	135.7
102		ser_73	ile_77	2.03	0.15	-8.85	1.26	158	163
103		asp_74	ala_78	1.97	0.18	-10.04	1.37	152.5	167.4
104		ala_75	asn_79	1.85	0.22	-12.31	1.85	151.3	159
105		asp_76	val_80	1.90	0.20	-11.08	1.58	148.8	163.2
106		ile_77	ala_81	2.09	0.14	-7.92	1.16	148.8	160
107		ala_78	ala_82	2.07	0.14	-8.06	1.23	146.5	156.8
108		asn_79	tyr_83	2.01	0.16	-8.89	1.50	148.5	151.1
109		val_80	ile_84	1.95	0.18	-10.30	1.47	156.3	163.1
110		ala_81	ala_85	1.99	0.17	-9.55	1.33	150.9	165.7
111		ala_82	asp_86	1.91	0.20	-11.01	1.62	149.1	160.8
112		tyr_83	gln_87	1.85	0.22	-12.62	1.65	160	172.2
113		ile_84	ala_88	1.93	0.19	-10.53	1.51	152.6	162.3
114		ala_85	glu_89	1.82	0.24	-13.41	1.75	151.4	171.6
115		asp_86	asn_90	2.17	0.11	-6.63	1.04	141.3	151.9
116	**1,2-alpha mannosidase (4ayo)**	asp_32	leu_36	2.11	0.13	-7.46	1.19	149.3	154.2
117		trp_33	ala_37	1.88	0.21	-11.63	1.71	151	161.1
118		lys_34	ala_38	2.04	0.15	-8.32	1.34	145.1	154.7
119		ala_35	asp_39	2.08	0.14	-7.55	1.32	144.8	149.2
120		leu_36	val_40	1.98	0.17	-9.57	1.46	154.6	158.8
121		ala_37	arg_41	1.97	0.18	-9.85	1.41	153.8	164.2
122		ala_38	ser_42	1.94	0.19	-10.14	1.55	145.3	158.9
123		asp_39	glu_43	1.90	0.20	-11.19	1.61	155.3	163.8
124		val_40	phe_44	1.93	0.19	-10.28	1.70	148.9	153.8
125		arg_41	gln_45	1.90	0.20	-11.11	1.58	153.6	164.5
126		ser_42	trp_46	1.98	0.17	-9.51	1.41	145.8	160.6

127		glu_43	ala_47	1.92	0.19	-10.49	1.60	146.9	159.4
128		phe_44	trp_48	1.85	0.23	-12.43	1.78	152.5	163.5
129		gln_45	gln_49	1.97	0.17	-9.58	1.52	149.4	156.5
130		trp_46	gly_50	2.22	0.10	-6.25	0.98	146.8	152.7
131		ala_47	tyr_51	2.01	0.16	-8.90	1.39	154	157.1
132		trp_48	val_52	1.90	0.20	-11.07	1.66	159	160.5
133		gln_49	ala_53	2.05	0.14	-7.94	1.36	143	150.7
134		gly_50	lys_54	2.11	0.12	-6.92	1.47	148.4	137.8
135		tyr_51	ala_55	1.87	0.21	-11.50	1.95	144.9	152.1
136		gly_79	val_83	1.99	0.17	-9.46	1.37	164	163.2
137		leu_80	glu_84	1.87	0.22	-11.90	1.74	157.7	161.8
138		ser_81	ala_85	2.10	0.13	-7.12	1.39	139.5	142.3
139		ala_85	leu_89	1.95	0.18	-10.22	1.48	164.6	162.3
140		leu_86	trp_90	2.10	0.13	-7.77	1.13	157.4	161.7
141		asp_87	ile_91	1.92	0.19	-10.80	1.50	156.5	166.7
142		thr_88	met_92	2.06	0.14	-8.01	1.26	151.9	155.6
143		leu_94	phe_98	1.89	0.21	-11.59	1.58	155.7	169.2
144		asp_95	gln_99	1.88	0.21	-11.47	1.66	152.5	162.9
145		ala_96	ala_100	1.97	0.17	-9.42	1.49	146.2	156.1
146		glu_97	gly_101	2.03	0.15	-8.67	1.31	153.5	159.1
147		phe_98	val_102	1.84	0.23	-12.87	1.79	158.2	166.2
148		gln_99	asp_103	1.84	0.23	-12.49	1.82	147.2	161.7
149		ala_100	trp_104	2.11	0.13	-7.36	1.19	140.5	153.3
150		gly_101	val_105	2.01	0.16	-9.01	1.35	153.9	160.1
151		val_102	lys_106	1.96	0.18	-9.97	1.51	155	159.8
152		asp_103	ala_107	2.16	0.12	-6.74	1.09	144.1	152.5
153		trp_104	asn_108	2.13	0.12	-6.56	1.54	150.9	133.3
154		val_105	leu_109	1.99	0.17	-9.68	1.30	133.6	172.1
155		val_119	asn_123	1.96	0.18	-10.03	1.42	152.8	164.4
156		phe_120	ile_124	2.09	0.14	-7.90	1.09	156.8	169.4
157		glu_121	arg_125	2.03	0.15	-8.33	1.33	144.5	154.8
158		thr_122	leu_126	2.06	0.14	-7.85	1.38	130.7	148.1
159		leu_126	leu_130	1.97	0.17	-9.60	1.37	148	164.9

160		val_127	leu_131	1.97	0.17	-9.52	1.51	150	156.2
161		gly_128	ser_132	2.01	0.16	-8.87	1.31	149.8	161.7
162		gly_129	ala_133	2.18	0.11	-6.62	0.95	137.8	163.7
163		leu_130	his_134	1.87	0.21	-11.40	1.84	144.9	155.3
164		leu_131	leu_135	1.90	0.20	-10.96	1.74	151.7	156.4
165		ser_132	ala_136	2.05	0.14	-8.08	1.35	149.7	152
166		ala_133	ser_137	2.23	0.10	-5.75	1.07	141.3	142.4
167		his_134	gly_138	1.85	0.22	-11.45	2.24	149.3	145.3
168		pro_140	ala_144	1.93	0.19	-10.51	1.53	155.5	162.8
169		val_141	lys_145	2.00	0.16	-9.04	1.40	149.3	157.1
170		leu_142	ala_146	2.05	0.15	-8.31	1.23	141.4	161.4
171		leu_143	arg_147	1.92	0.19	-10.60	1.59	156.5	160.3
172		ala_144	asp_148	1.93	0.19	-10.39	1.51	148.6	162.3
173		lys_145	leu_149	2.06	0.15	-8.29	1.21	149.8	162.1
174		ala_146	ala_150	1.95	0.18	-10.07	1.48	146.6	161.8
175		arg_147	asp_151	1.97	0.17	-9.47	1.52	151.1	155.4
176		asp_148	arg_152	2.29	0.09	-5.45	0.91	143.5	147.3
177		leu_149	leu_153	1.99	0.16	-9.18	1.46	153.9	155.4
178		ala_150	ala_154	1.99	0.16	-8.42	1.90	144.7	138.3
179		ala_154	glu_158	2.06	0.14	-8.12	1.27	154.3	156.6
180		lys_155	ala_159	2.41	0.06	-4.20	0.85	137.5	131.4
181		tyr_189	phe_193	1.81	0.24	-13.74	1.81	170.9	171.4
182		leu_190	gly_194	1.80	0.24	-12.84	2.28	129.5	150.3
183		ser_191	val_195	2.02	0.16	-8.68	1.28	142.1	162
184		glu_192	leu_196	1.91	0.20	-10.82	1.56	147.5	163.8
185		phe_193	ser_197	1.95	0.18	-9.68	1.69	145.2	151.1
186		gly_194	gln_198	2.02	0.16	-8.75	1.40	146.8	155.3
187		val_195	leu_199	1.93	0.19	-10.50	1.58	160.4	160
188		leu_196	thr_200	1.87	0.22	-11.88	1.71	155.2	163.6
189		ser_197	gly_201	2.06	0.14	-7.42	1.50	137.1	140.8
190		arg_203	asp_207	2.01	0.16	-9.21	1.27	163.1	168
191		lys_204	met_208	1.99	0.17	-9.24	1.41	146.4	158.6
192		tyr_205	ala_209	2.07	0.14	-8.18	1.15	160.2	166

193		phe_206	lys_210	1.93	0.19	-10.64	1.48	160.5	166.7
194		asp_207	arg_211	2.02	0.16	-8.84	1.33	147.9	158.2
195		met_208	ala_212	2.54	0.05	-4.18	0.53	146.2	157.8
196		ala_209	met_213	2.49	0.06	-4.47	0.60	149.1	157.6
197		lys_210	arg_214	1.92	0.19	-10.85	1.53	161.5	165.3
198		arg_211	his_215	2.20	0.10	-6.13	1.08	144	145.9
199		met_213	leu_217	2.09	0.14	-8.06	1.11	157.7	170.2
200		arg_214	asp_218	1.88	0.21	-11.32	1.76	154.2	157.3
201		ser_250	tyr_254	2.01	0.16	-8.89	1.48	150.9	152
202		phe_251	leu_255	2.36	0.07	-4.98	0.80	147.2	145.6
203		glu_253	asp_257	1.87	0.22	-12.00	1.80	153.5	160.2
204		tyr_254	ala_258	2.10	0.13	-7.07	1.28	136.1	146.7
205		leu_255	trp_259	2.42	0.07	-4.84	0.65	147.8	161.4
206		trp_256	ala_260	1.98	0.17	-9.55	1.48	153.3	157.6
207		asp_257	leu_261	1.83	0.23	-12.52	1.99	148.2	156.7
208		ala_258	phe_262	1.97	0.17	-9.09	1.56	131.4	150.8
209		trp_259	gly_263	1.99	0.16	-8.60	1.71	125.6	142.4
210		asp_264	lys_268	2.13	0.12	-7.16	1.12	147.4	155.9
211		glu_265	arg_269	2.11	0.13	-7.56	1.09	146.2	164.1
212		asp_266	trp_270	1.83	0.24	-13.26	1.80	159	168.1
213		cys_267	ala_271	1.88	0.21	-11.35	1.79	148	156.5
214		lys_268	val_272	2.40	0.07	-5.00	0.67	145.1	165.8
215		arg_269	glu_273	1.92	0.19	-10.87	1.48	157.3	168.9
216		trp_270	cys_274	1.88	0.21	-11.61	1.65	150.2	164.3
217		ala_271	val_275	2.17	0.11	-6.84	0.97	144.3	163.9
218		val_272	asp_276	1.87	0.21	-11.89	1.62	155.2	168.7
219		glu_273	ala_277	2.07	0.14	-7.91	1.26	149.9	154.6
220		cys_274	gln_278	2.09	0.13	-7.66	1.19	145.4	156.4
221		val_275	leu_279	1.85	0.23	-11.58	1.86	157.4	159.5
222		asp_276	ala_280	2.07	0.14	-7.60	1.36	142.7	147.4
223		ala_277	his_281	2.15	0.11	-6.37	1.33	143.9	138
224		gln_278	gln_282	1.80	0.25	-13.53	2.17	132.5	155.1
225		tyr_313	leu_317	2.20	0.11	-6.47	0.99	145.3	156.7

226		tyr_314	leu_318	1.86	0.22	-12.26	1.69	153.5	167.4
227		ala_315	gly_319	2.42	0.07	-4.74	0.66	139	159.2
228		gly_316	gln_320	2.00	0.16	-9.15	1.42	151.5	157.6
229		leu_317	val_321	2.08	0.13	-7.67	1.28	160	150.8
230		arg_323	gly_327	2.01	0.16	-9.02	1.44	150	155.5
231		lys_324	asp_328	1.83	0.23	-12.78	1.88	161.2	161.2
232		ala_325	asp_329	2.02	0.16	-8.63	1.37	144.3	155.9
233		gln_326	tyr_330	1.96	0.18	-9.64	1.57	149.8	154.6
234		gly_327	leu_331	1.85	0.23	-12.53	1.74	151.8	166.2
235		asp_328	ala_332	2.04	0.15	-8.15	1.37	145.3	152.1
236		asp_329	ser_333	2.63	0.04	-3.45	0.51	139.6	137
237		leu_331	thr_335	1.90	0.20	-11.00	1.85	150.1	152.9
238		ala_332	tyr_336	2.00	0.16	-8.93	1.37	145.1	158.5
239		ser_333	leu_337	2.31	0.09	-5.36	0.86	137.1	150.5
240		phe_334	gln_338	1.93	0.19	-10.27	1.62	153.1	156.9
241		thr_335	ala_339	1.89	0.20	-11.20	1.64	151	161.7
242		tyr_336	thr_340	2.04	0.15	-8.06	1.47	147.3	147.2
243		leu_337	phe_341	1.86	0.22	-12.13	1.73	150.7	162.4
244		gln_338	gly_342	1.98	0.16	-8.74	1.83	129	140.5
245		pro_364	asp_368	2.15	0.12	-7.04	1.06	152.1	157.6
246		glu_365	ala_369	2.04	0.15	-8.45	1.22	145.4	163.5
247		tyr_366	cys_370	1.96	0.18	-9.97	1.47	152.8	161
248		pro_367	leu_371	1.89	0.21	-11.35	1.59	148.3	166
249		asp_368	asn_372	2.00	0.17	-9.42	1.30	158.1	168.9
250		ala_369	leu_373	1.93	0.19	-10.66	1.49	158.2	166
251		cys_370	trp_374	1.91	0.19	-10.67	1.60	146.8	160.4
252		leu_371	leu_375	2.01	0.15	-8.45	1.56	152.7	146.5
253		trp_374	arg_378	1.80	0.25	-13.49	2.35	145.5	150.8
254		pro_380	arg_384	2.06	0.15	-8.35	1.23	157.6	161.6
255		arg_381	leu_385	2.08	0.14	-7.89	1.23	151.8	156.6
256		tyr_382	ala_386	2.00	0.16	-8.92	1.35	141.8	159.2
257		arg_383	ala_387	1.95	0.18	-9.66	1.70	148.7	150
258		arg_384	ile_388	2.27	0.09	-5.80	0.87	145.5	155.6

259		leu_385	his_389	2.28	0.09	-5.67	0.87	141.7	154.4
260		ala_386	tyr_390	1.88	0.21	-11.54	1.69	153.3	161.8
261		ala_387	arg_391	1.92	0.19	-10.87	1.45	151.4	171.9
262		ile_388	glu_392	1.92	0.19	-10.44	1.76	148.9	152.4
263		his_389	met_393	1.98	0.17	-9.37	1.46	148.6	157
264		tyr_390	lys_394	2.02	0.16	-8.72	1.31	154.3	160
265		arg_391	ala_395	2.13	0.12	-6.68	1.36	140.1	140.4
266		met_393	ser_397	1.87	0.21	-12.00	1.65	152.5	167.3
267		tyr_423	glu_427	1.91	0.19	-10.43	1.92	159.2	147.6
268		glu_427	tyr_431	1.87	0.21	-11.70	1.83	157.9	157.6
269		gln_428	tyr_432	1.86	0.22	-12.17	1.64	158.6	170.8
270		met_429	tyr_433	1.95	0.18	-10.07	1.47	145	162.3
271		lys_430	leu_434	1.78	0.26	-14.26	1.98	157.8	166.3
272		tyr_431	leu_435	1.95	0.18	-9.93	1.51	150.3	158.8
273		tyr_432	phe_436	2.24	0.09	-5.39	1.31	146.8	130
274		tyr_433	ser_437	1.95	0.18	-9.58	1.72	153.8	148.4
275	**Acutohaemonlysin (1mc2)**	ser_1001	leu_1005	2.08	0.14	-8.11	1.13	159.8	169.5
276		leu_1002	gly_1006	1.88	0.21	-11.48	1.61	144	167.4
277		phe_1003	lys_1007	2.11	0.13	-7.39	1.10	143.5	162.5
278		glu_1004	met_1008	1.93	0.19	-10.41	1.50	158.3	165
279		leu_1005	ile_1009	1.96	0.18	-9.97	1.45	157.5	163.4
280		gly_1006	trp_1010	1.95	0.18	-10.06	1.44	155.4	165.5
281		lys_1007	gln_1011	1.84	0.23	-12.57	1.83	154.8	163.2
282		met_1008	glu_1012	1.93	0.19	-10.06	1.60	151.6	157.2
283		ile_1009	thr_1013	1.94	0.18	-9.81	1.70	151.5	151.9
284		trp_1010	gly_1014	1.88	0.21	-11.02	1.93	131.2	150.9
285		asn_1016	asn_1020	2.15	0.12	-6.81	1.09	150	154.3
286		asp_1039	arg_1043	1.98	0.17	-9.20	1.53	148.9	153.9
287		ala_1040	cys_1044	2.08	0.14	-7.61	1.27	149.6	152.5
288		thr_1041	cys_1045	2.33	0.08	-5.11	0.83	145.3	148.8
289		asp_1042	phe_1046	2.02	0.16	-8.51	1.47	149.2	151.4
290		arg_1043	val_1047	1.91	0.20	-11.06	1.50	164.8	172
291		cys_1044	his_1048	2.03	0.15	-8.36	1.38	144.7	154

292		cys_1045	lys_1049	2.05	0.15	-8.34	1.21	148.4	164.2
293		phe_1046	cys_1050	1.96	0.18	-9.83	1.39	156.1	167
294		val_1047	cys_1051	1.93	0.19	-9.77	1.94	146.5	145.4
295		his_1048	tyr_1052	2.19	0.11	-6.23	1.07	149	148.9
296		gln_1089	gln_1093	1.95	0.18	-9.70	1.71	160.5	150.8
297		pro_1090	glu_1094	2.09	0.14	-7.68	1.16	149.7	161.1
298		cys_1091	met_1095	2.02	0.16	-8.52	1.39	146.1	155
299		met_1092	cys_1096	1.91	0.20	-10.79	1.57	149.6	163.9
300		gln_1093	glu_1097	1.93	0.19	-10.23	1.60	152.5	158.2
301		glu_1094	cys_1098	1.95	0.18	-9.76	1.55	149.6	157.7
302		met_1095	asp_1099	2.01	0.16	-8.91	1.37	152.3	158.8
303		cys_1096	lys_1100	1.84	0.23	-12.52	1.84	155.8	162.5
304		glu_1097	ala_1101	2.14	0.12	-7.18	1.00	144.8	169.9
305		cys_1098	phe_1102	2.20	0.11	-6.32	1.00	141.3	154.9
306		asp_1099	ala_1103	1.96	0.18	-9.94	1.47	155.7	161.5
307		lys_1100	ile_1104	2.06	0.14	-8.21	1.15	158.1	169
308		ala_1101	cys_1105	1.92	0.19	-10.38	1.59	146.1	159.9
309		phe_1102	leu_1106	1.93	0.19	-10.29	1.61	156.6	158.2
310		ala_1103	arg_1107	2.10	0.13	-7.51	1.13	147.3	161.1
311		ile_1104	glu_1108	1.94	0.19	-10.14	1.55	154.9	160.1
312		cys_1105	asn_1109	2.54	0.05	-3.28	0.74	140.7	124.4
313	**Triose-Phosphate Isomerase (2vxn)**	thr_17	ile_21	1.91	0.20	-11.03	1.52	158.4	168.8
314		thr_18	glu_22	1.92	0.19	-10.49	1.52	151	163.9
315		ala_19	lys_23	2.15	0.12	-6.97	1.03	146.5	161.6
316		ser_20	leu_24	1.98	0.17	-9.28	1.41	148.6	160.7
317		ile_21	val_25	1.80	0.25	-13.76	1.81	158.9	174
318		glu_22	gln_26	2.09	0.13	-7.49	1.15	142.7	158.7
319		lys_23	val_27	2.16	0.12	-6.82	1.06	147.4	157.5
320		leu_24	phe_28	1.97	0.17	-9.46	1.51	151.9	156.8
321		val_25	asn_29	1.82	0.24	-12.76	2.04	152	156.6
322		gln_26	glu_30	2.05	0.14	-7.81	1.44	149.1	147.2
323		val_27	his_31	2.65	0.04	-2.85	0.59	139.2	123.2
324		his_47	val_51	2.04	0.15	-8.63	1.21	162.3	168.7

325		ile_48	gln_52	1.83	0.24	-12.86	1.87	161.1	163.3
326		pro_49	ala_53	2.09	0.13	-7.17	1.46	143.5	141.8
327		leu_50	lys_54	2.28	0.09	-4.94	1.21	145.2	129.6
328		val_51	leu_55	1.84	0.23	-12.80	1.71	151.7	170.9
329		ser_79	leu_83	2.05	0.15	-8.31	1.26	153.3	160.5
330		met_80	lys_84	1.95	0.18	-10.20	1.43	160.9	167.4
331		pro_81	asp_85	1.99	0.17	-9.15	1.37	148	161.3
332		ile_82	ile_86	2.24	0.10	-5.77	0.99	145.7	147.5
333		his_95	arg_99	2.01	0.16	-8.85	1.39	152	158.2
334		ser_96	thr_100	2.00	0.16	-8.28	1.78	146.2	140.7
335		glu_97	tyr_101	1.84	0.23	-12.37	1.76	139.7	164.8
336		thr_105	val_109	1.87	0.22	-11.96	1.64	166.7	170.4
337		asp_106	ala_110	1.84	0.23	-12.47	1.74	148.8	166.8
338		glu_107	gln_111	1.95	0.18	-9.93	1.53	149	159.2
339		ile_108	lys_112	1.99	0.17	-9.34	1.36	150.7	164.5
340		val_109	val_113	1.88	0.21	-11.66	1.68	160.8	164.4
341		ala_110	ser_114	2.00	0.16	-9.02	1.38	148.8	159.4
342		gln_111	glu_115	1.96	0.18	-9.86	1.43	154.6	163.6
343		lys_112	ala_116	1.90	0.20	-11.00	1.69	151.8	159.4
344		val_113	cys_117	1.93	0.19	-10.33	1.53	154	161.7
345		ser_114	lys_118	2.03	0.15	-8.56	1.30	148.5	160.6
346		glu_115	gln_119	2.16	0.11	-6.32	1.23	143.6	142.6
347		thr_130	arg_134	1.93	0.19	-10.49	1.55	158.2	162.3
348		leu_131	glu_135	2.01	0.16	-8.86	1.34	153	161.3
349		gln_132	ala_136	2.16	0.11	-6.34	1.23	145.4	142.8
350		gln_138	val_142	1.91	0.20	-10.95	1.61	165.9	162.7
351		thr_139	val_143	1.97	0.18	-9.84	1.35	163.1	171.8
352		ala_140	leu_144	1.91	0.20	-11.00	1.52	156.9	168.3
353		lys_141	ser_145	1.98	0.17	-9.21	1.48	141.6	156.3
354		val_142	gln_146	1.93	0.19	-10.26	1.56	156.3	160.4
355		val_143	thr_147	2.00	0.16	-8.82	1.39	142.7	158.4
356		leu_144	ser_148	1.82	0.24	-12.86	1.90	145.2	161.6
357		ser_145	ala_149	2.08	0.13	-7.42	1.25	142.2	152.3

358		gln_146	ile_150	2.36	0.08	-5.14	0.73	142.7	162.8
359		thr_147	ala_151	1.88	0.21	-11.39	1.71	151.9	161.3
360		ser_148	ala_152	2.10	0.13	-6.98	1.33	147	144.4
361		thr_179	ala_183	1.91	0.20	-11.00	1.50	168.8	170.4
362		pro_180	gln_184	1.86	0.22	-12.12	1.65	149	168.6
363		glu_181	glu_185	2.08	0.14	-7.67	1.17	145.7	158.9
364		ala_183	his_187	1.91	0.20	-10.89	1.55	160.1	165.7
365		gln_184	leu_188	1.86	0.22	-11.99	1.74	154.2	163.1
366		glu_185	leu_189	2.26	0.10	-5.77	0.88	139.9	157.5
367		val_186	leu_190	1.93	0.19	-10.37	1.53	155.8	162.8
368		his_187	arg_191	1.93	0.19	-10.52	1.51	150.8	164.4
369		leu_188	lys_192	2.00	0.16	-8.99	1.34	150.1	161.6
370		leu_189	trp_193	2.06	0.14	-8.10	1.20	144.2	162.4
371		leu_190	val_194	1.94	0.19	-10.38	1.49	154.9	164.7
372		arg_191	ser_195	1.85	0.23	-12.42	1.91	150.3	158.3
373		lys_192	glu_196	2.05	0.15	-8.15	1.29	153.3	157.2
374		trp_193	asn_197	1.94	0.18	-9.66	1.79	153.5	148
375		val_194	ile_198	1.87	0.21	-11.42	1.87	138.8	154.8
376		thr_200	ala_204	2.16	0.12	-6.56	1.12	141.7	150.5
377		asp_201	lys_205	2.38	0.07	-4.60	0.79	146.3	142.1
378		val_202	leu_206	2.35	0.08	-4.38	1.28	148.4	122.8
379		asn_218	leu_222	2.40	0.07	-4.91	0.67	152.3	163.2
380		ala_219	tyr_223	1.93	0.19	-10.25	1.60	156.2	158.1
381		ala_220	ala_224	2.24	0.09	-5.29	1.18	141.6	134
382		glu_241	ile_245	2.32	0.08	-5.24	0.84	149	151
383		phe_242	ile_246	1.98	0.17	-9.53	1.39	159.4	163.6
384		arg_243	asp_247	2.04	0.15	-8.20	1.29	145.3	158.1
385		asp_244	ala_248	2.16	0.11	-5.87	1.59	136.1	130
386	**hAR (1us0)**	pro_23	val_27	2.15	0.11	-6.17	1.62	160.5	129.9
387		gln_26	ala_30	2.09	0.14	-7.61	1.24	145.4	154.2
388		val_27	val_31	1.95	0.18	-9.89	1.45	150.2	162.9
389		thr_28	lys_32	1.97	0.18	-9.77	1.40	153.1	165.8
390		glu_29	val_33	1.84	0.23	-12.69	1.69	158.8	172.9

391		ala_30	ala_34	1.88	0.21	-11.36	1.70	144.6	161.2
392		val_31	ile_35	1.92	0.19	-10.73	1.50	154.2	167.6
393		lys_32	asp_36	1.96	0.18	-9.94	1.46	148.9	162.5
394		val_33	val_37	2.10	0.13	-7.08	1.49	153.1	139.5
395		ala_34	gly_38	2.54	0.06	-3.45	0.99	143.6	120.5
396		asn_50	val_54	2.00	0.17	-9.27	1.34	157.2	164.7
397		glu_51	gly_55	1.84	0.23	-12.40	1.83	148.3	161.9
398		asn_52	val_56	2.10	0.13	-7.17	1.43	142.3	142.3
399		glu_53	ala_57	2.47	0.06	-4.41	0.61	144.4	157
400		val_54	ile_58	2.06	0.14	-8.23	1.22	154.5	161.7
401		gly_55	gln_59	1.85	0.23	-12.67	1.67	157.2	173
402		val_56	glu_60	2.01	0.16	-8.71	1.36	144.4	157.6
403		ala_57	lys_61	2.03	0.15	-8.57	1.28	152.1	160.9
404		ile_58	leu_62	1.95	0.18	-10.04	1.53	155.7	159.9
405		gln_59	arg_63	1.83	0.23	-12.61	1.90	149.2	160.4
406		glu_60	glu_64	1.82	0.24	-13.36	1.80	151.4	170.9
407		leu_87	ala_91	2.06	0.14	-8.03	1.25	152.7	157.5
408		val_88	cys_92	1.98	0.17	-9.38	1.37	154.8	163.1
409		lys_89	gln_93	1.81	0.24	-13.12	1.98	153.8	160.6
410		gly_90	lys_94	1.93	0.19	-9.92	1.68	146.1	153
411		ala_91	thr_95	2.15	0.12	-7.16	1.01	149.2	167.3
412		cys_92	leu_96	1.85	0.22	-12.16	1.85	152.9	159.9
413		gln_93	ser_97	1.82	0.24	-13.02	1.90	148.2	162.5
414		lys_94	asp_98	1.89	0.21	-11.30	1.65	152.7	163.1
415		thr_95	leu_99	1.89	0.21	-11.23	1.65	154.8	162.4
416		asn_136	thr_140	2.14	0.12	-7.13	1.07	147.7	162.4
417		ile_137	trp_141	1.91	0.20	-10.38	1.72	137	154.6
418		leu_138	ala_142	2.04	0.15	-8.15	1.37	146.8	153.2
419		asp_139	ala_143	2.22	0.10	-6.16	0.97	145.3	154.6
420		thr_140	met_144	2.07	0.14	-7.75	1.34	148.7	151.3
421		trp_141	glu_145	1.93	0.19	-10.19	1.69	156.6	153.9
422		ala_142	glu_146	2.25	0.09	-5.69	0.97	143.1	147.3
423		ala_143	leu_147	2.62	0.04	-3.50	0.52	137.7	140.3

424		met_144	val_148	2.59	0.05	-3.80	0.52	147.8	148
425		glu_145	asp_149	2.23	0.10	-6.08	0.93	149	157.7
426		glu_146	glu_150	2.34	0.08	-4.53	1.40	142.8	122.1
427		asn_162	val_166	1.87	0.22	-11.98	1.72	166.5	164.4
428		his_163	glu_167	1.97	0.18	-9.79	1.33	154.1	172.9
429		leu_164	met_168	2.07	0.14	-7.32	1.42	135.8	144.7
430		gln_165	ile_169	2.05	0.15	-8.47	1.18	150.4	170.2
431		val_166	leu_170	1.97	0.18	-9.67	1.48	154.5	159.4
432		glu_167	asn_171	1.99	0.16	-8.52	1.75	147.9	142.6
433		gln_192	ile_196	1.94	0.19	-10.55	1.43	165.5	170.3
434		glu_193	gln_197	1.99	0.17	-9.24	1.32	148.9	165.6
435		lys_194	tyr_198	2.06	0.14	-8.18	1.17	151.7	165.4
436		leu_195	cys_199	1.91	0.20	-10.99	1.47	156.2	173.9
437		ile_196	gln_200	1.80	0.25	-13.99	1.82	161.5	176.9
438		gln_197	ser_201	1.95	0.18	-9.67	1.55	145.4	156.4
439		tyr_198	lys_202	2.58	0.05	-3.31	0.62	143	129.6
440		asp_230	lys_234	1.93	0.19	-10.66	1.48	161.9	169.2
441		pro_231	ala_235	2.04	0.15	-7.77	1.54	134.7	143.5
442		arg_232	ile_236	2.47	0.06	-4.28	0.62	134.7	153.3
443		ile_233	ala_237	1.99	0.17	-9.40	1.35	156.8	165.2
444		lys_234	ala_238	1.86	0.22	-12.02	1.74	152.1	162.6
445		ala_235	lys_239	2.13	0.12	-6.92	1.16	142.7	151.5
446		ile_236	his_240	2.31	0.08	-5.25	0.87	147	147.9
447		thr_243	val_247	2.09	0.13	-7.63	1.19	154.1	156.6
448		thr_244	leu_248	1.96	0.18	-9.87	1.53	152.9	158.5
449		ala_245	ile_249	2.10	0.13	-6.91	1.51	147.4	138.2
450		gln_246	arg_250	1.91	0.20	-10.63	1.58	149.4	161.9
451		val_247	phe_251	2.00	0.16	-8.78	1.48	150.2	151.6
452		arg_250	gln_254	2.16	0.11	-6.68	1.16	157.1	147.9
453		thr_265	ile_269	1.90	0.20	-11.11	1.64	162.4	162.7
454		pro_266	ala_270	2.11	0.13	-7.55	1.07	152.2	166.9
455		glu_267	glu_271	1.94	0.19	-10.08	1.56	140.1	159.4
456		arg_268	asn_272	1.79	0.25	-13.89	2.04	158.5	162.4

457		ser_281	met_285	1.92	0.19	-10.41	1.64	153.3	157.7
458		ser_282	thr_286	1.87	0.21	-11.74	1.70	152.8	164
459		gln_283	thr_287	1.86	0.22	-11.79	1.82	148	159.2
460		asp_284	leu_288	1.86	0.22	-12.04	1.72	151.7	164.1
461		met_285	leu_289	1.92	0.19	-10.45	1.59	149.4	159.9
462		thr_286	ser_290	2.23	0.09	-5.21	1.28	137.6	130.8
463	**Rubredoxin (1yk4)**	lys_29	leu_33	2.67	0.04	-3.03	0.61	144.5	120.7
464	**Cyclophilin D (4o8h)**	val_29	ala_33	1.87	0.22	-12.07	1.62	164.1	171.8
465		pro_30	glu_34	1.98	0.17	-9.13	1.48	140.7	155
466		lys_31	asn_35	2.16	0.12	-6.95	1.00	141.5	163.5
467		thr_32	phe_36	2.23	0.10	-6.33	0.88	151.2	166.1
468		ala_33	arg_37	1.87	0.21	-11.84	1.63	157.6	168.5
469		glu_34	ala_38	1.95	0.18	-10.18	1.39	155.1	170.1
470		asn_35	leu_39	2.02	0.16	-8.63	1.41	151.3	154.1
471		phe_36	cys_40	2.05	0.14	-7.94	1.44	149.7	147.2
472		arg_37	thr_41	2.11	0.13	-7.34	1.22	150	151.8
473		ala_38	gly_42	2.13	0.12	-6.44	1.51	137.4	134.5
474		gly_135	val_139	2.16	0.12	-6.94	1.08	151.4	156.5
475		met_136	lys_140	1.88	0.21	-11.37	1.82	154.4	155.8
476		asp_137	lys_141	2.10	0.13	-7.38	1.20	140.6	153.8
477		val_138	ile_142	1.94	0.19	-10.46	1.47	158.4	166.4
478		val_139	glu_143	1.84	0.23	-12.60	1.74	155	166.9
479		lys_140	ser_144	2.14	0.12	-6.69	1.19	140.6	147.1
480	**Serine Protease (1gci)**	trp_6	arg_10	1.92	0.19	-10.35	1.84	145	149.4
481		ala_13	his_17	1.99	0.17	-9.41	1.36	158.1	164.2
482		pro_14	asn_18	2.01	0.16	-8.47	1.52	147.6	148.8
483		ala_15	arg_19	2.66	0.04	-3.16	0.49	131.3	135
484		his_64	val_68	1.93	0.19	-10.80	1.43	160.5	176.2
485		gly_65	ala_69	1.94	0.19	-10.03	1.56	142.7	158.3
486		thr_66	gly_70	2.16	0.11	-6.54	1.10	140.6	150
487		his_67	thr_71	2.31	0.08	-5.37	0.85	151.5	149.9

488		val_68	ile_72	2.29	0.09	-5.80	0.83	153.8	161.1
489		ala_69	ala_73	2.04	0.14	-7.70	1.73	143.6	137.6
490		val_104	ala_108	1.90	0.20	-10.87	1.66	144.2	159.3
491		ser_105	gln_109	1.91	0.20	-10.76	1.70	147.6	157
492		ser_106	gly_110	2.07	0.14	-7.79	1.28	143	153.5
493		ile_107	leu_111	2.00	0.16	-9.17	1.44	151.2	156.3
494		ala_108	glu_112	1.87	0.21	-11.76	1.68	154.7	164.1
495		gln_109	trp_113	1.93	0.19	-10.23	1.58	143.3	158.6
496		gly_110	ala_114	2.00	0.16	-8.91	1.46	141.4	153.9
497		leu_111	gly_115	2.13	0.13	-7.24	1.10	147.4	158.6
498		glu_112	asn_116	2.14	0.12	-6.46	1.46	144.8	135.8
499		ala_133	gln_137	1.97	0.17	-9.68	1.37	148.6	165.8
500		thr_134	ala_138	2.34	0.08	-5.22	0.76	142.6	156.6
501		leu_135	val_139	1.93	0.19	-10.64	1.54	157	163.1
502		glu_136	asn_140	1.93	0.19	-10.57	1.50	155	165.2
503		gln_137	ser_141	1.92	0.19	-10.38	1.70	143.9	154.8
504		ala_138	ala_142	1.91	0.20	-10.95	1.48	148.8	170.6
505		val_139	thr_143	2.02	0.16	-8.61	1.35	144.5	157.5
506		asn_140	ser_144	1.96	0.18	-9.53	1.54	146.4	155.5
507		ser_141	arg_145	2.26	0.09	-5.58	1.03	145.8	142.3
508		thr_220	thr_224	2.09	0.14	-7.81	1.13	153.1	165.1
509		thr_224	ala_228	1.98	0.17	-9.64	1.41	151	162.6
510		pro_225	gly_229	1.88	0.21	-11.28	1.64	140.1	163.4
511		his_226	ala_230	2.04	0.15	-8.09	1.38	133.8	151.5
512		val_227	ala_231	1.86	0.22	-12.03	1.77	152.4	161.3
513		ala_228	ala_232	2.21	0.10	-6.21	1.01	142.3	151.5
514		gly_229	leu_233	2.11	0.13	-7.50	1.18	150.3	155.4
515		ala_230	val_234	2.03	0.15	-8.56	1.29	152	160.7
516		ala_231	lys_235	1.93	0.19	-10.32	1.63	148.2	157
517		ala_232	gln_236	2.02	0.15	-8.59	1.34	145.9	157
518		leu_233	lys_237	2.11	0.13	-7.44	1.11	146.7	161
519		asn_243	arg_247	1.92	0.19	-11.08	1.47	154.2	170.9
520		val_244	asn_248	1.87	0.22	-11.97	1.64	153.2	168.5

521		gln_245	his_249	2.04	0.15	-8.08	1.33	140.7	153.6
522		ile_246	leu_250	1.93	0.19	-10.68	1.48	157.7	167.8
523		arg_247	lys_251	2.09	0.14	-7.80	1.15	151	161.8
524		asn_248	asn_252	1.86	0.22	-11.85	1.90	148.9	156.3
525	**Proteinase K (2pwa)**	pro_7	ala_11	2.21	0.11	-6.52	0.93	158	163.5
526		trp_8	arg_12	1.90	0.20	-10.46	2.03	144.4	146.1
527		gly_9	ile_13	2.18	0.11	-6.44	1.14	144.1	145.7
528		gly_68	his_72	1.93	0.19	-10.39	1.69	158.4	154.4
529		his_69	cys_73	1.95	0.18	-10.32	1.44	157.1	165.8
530		gly_70	ala_74	1.85	0.23	-12.57	1.71	149	168.4
531		thr_71	gly_75	1.98	0.17	-8.90	1.57	139.2	149.7
532		his_72	thr_76	2.16	0.11	-6.68	1.20	150.1	145.4
533		cys_73	val_77	2.11	0.13	-7.49	1.22	150.9	152.8
534		ala_74	gly_78	2.03	0.15	-8.15	1.51	149.5	145.9
535		gln_103	ile_107	2.07	0.14	-8.27	1.22	154	160.9
536		tyr_104	ile_108	1.83	0.24	-13.20	1.76	159.9	170.9
537		ser_105	ala_109	2.04	0.15	-8.28	1.29	136.6	157.2
538		thr_106	gly_110	1.97	0.17	-9.55	1.52	149.5	155.6
539		ile_107	met_111	2.13	0.12	-7.18	1.14	148.8	153.9
540		ile_108	asp_112	1.99	0.17	-9.55	1.36	159.9	164.2
541		ala_109	phe_113	1.87	0.22	-11.60	1.90	149.7	154.6
542		gly_110	val_114	2.13	0.12	-7.16	1.14	145.8	154.9
543		met_111	ala_115	2.13	0.12	-7.28	1.07	154.1	160.5
544		asp_112	ser_116	2.31	0.08	-5.39	0.84	147.7	150.6
545		phe_113	asp_117	1.72	0.30	-16.75	2.19	162.6	171.6
546		val_114	lys_118	2.11	0.13	-7.53	1.12	151.4	158.9
547		ser_138	asn_142	1.99	0.17	-9.41	1.33	153.8	165.4
548		ser_139	ser_143	1.89	0.21	-11.18	1.77	144.3	156.4
549		ser_140	ala_144	2.06	0.14	-8.00	1.26	144.9	155.7
550		val_141	ala_145	2.09	0.14	-7.81	1.19	151.5	157.1
551		asn_142	ala_146	1.88	0.21	-11.58	1.74	153	159.8
552		ser_143	arg_147	1.89	0.21	-11.08	1.85	148.6	153.5
553		ala_144	leu_148	2.01	0.16	-8.90	1.39	147.7	157

554		ala_145	gln_149	2.03	0.15	-8.89	1.23	152.8	167.5
555		ala_146	ser_150	1.87	0.22	-11.88	1.68	150.3	165.3
556		arg_147	ser_151	2.03	0.15	-8.08	1.64	151.3	141.9
557		gly_222	ala_226	2.49	0.06	-4.19	0.64	139.6	143.7
558		thr_223	thr_227	2.05	0.15	-8.25	1.26	153.9	159.3
559		ala_226	val_230	2.36	0.08	-5.14	0.77	151.8	151.9
560		thr_227	ala_231	1.92	0.19	-10.57	1.64	150.6	158
561		pro_228	gly_232	1.85	0.22	-12.35	1.67	139.1	168.6
562		his_229	leu_233	1.94	0.18	-9.94	1.65	137.5	153.6
563		val_230	ala_234	1.87	0.22	-11.93	1.73	152	162.1
564		ala_231	ala_235	2.04	0.15	-8.54	1.24	151.1	162.3
565		gly_232	tyr_236	1.91	0.20	-11.05	1.52	152.4	167.5
566		leu_233	leu_237	1.92	0.19	-10.53	1.68	153.2	156.1
567		ala_234	met_238	1.86	0.22	-12.02	1.85	154.7	158.4
568		ala_235	thr_239	1.93	0.19	-10.42	1.49	152.7	164
569		tyr_236	leu_240	2.20	0.11	-6.36	1.02	140.1	152.1
570		ser_247	tyr_251	1.91	0.20	-10.95	1.63	155.5	160.3
571		ala_248	ile_252	1.82	0.24	-13.35	1.84	153.8	166.6
572		cys_249	ala_253	1.92	0.19	-10.66	1.59	151	160.4
573		arg_250	asp_254	1.83	0.23	-12.45	1.99	147.7	156.3
574		tyr_251	thr_255	2.19	0.11	-6.04	1.32	143.5	136.3
575	**Trypsin (1pq7)**	ala_55	ser_59	1.91	0.20	-10.55	1.92	171.1	148.7
576		ser_161	cys_165	1.88	0.21	-11.46	1.67	156.2	163.4
577		arg_162	arg_166	1.87	0.21	-11.28	1.87	147.6	154.5
578		ala_163	ala_167	2.07	0.14	-7.67	1.33	143.3	150.5
579		thr_164	gln_168	2.15	0.12	-6.61	1.23	146.2	144.8
580		cys_165	tyr_169	2.05	0.15	-8.04	1.48	148.5	147
581		arg_166	gly_170	1.95	0.17	-8.98	2.07	126.4	138.1
582		leu_231	ile_235	2.22	0.11	-6.48	0.90	153.4	169.7
583		arg_232	asp_236	1.80	0.25	-13.59	1.95	147.5	164
584		ser_233	thr_237	2.05	0.15	-7.95	1.40	144.1	149.7
585		phe_234	tyr_238	2.27	0.09	-5.61	0.91	151.3	149
586		ile_235	ala_239	1.94	0.18	-9.66	1.85	153.5	145.7

587	**Cholesterol Oxidase (4rek)**	gly_19	ala_23	1.86	0.22	-11.85	1.90	152.7	155.9
588		tyr_20	val_24	2.09	0.14	-7.97	1.07	156.6	175.7
589		gly_21	ser_25	2.14	0.12	-7.04	1.05	143.4	162
590		ala_22	ala_26	1.88	0.21	-11.71	1.65	154.6	165.8
591		ala_23	leu_27	2.07	0.14	-8.05	1.16	147.5	164.3
592		val_24	arg_28	2.13	0.13	-7.37	1.05	156.9	165.6
593		ser_25	leu_29	1.88	0.21	-11.69	1.62	157	168.1
594		ala_26	gly_30	1.91	0.20	-10.91	1.54	148.7	164.9
595		leu_27	glu_31	1.93	0.19	-10.33	1.52	152.6	162.3
596		arg_28	ala_32	2.17	0.11	-6.10	1.23	139.3	140.2
597		ser_78	leu_82	1.92	0.19	-10.36	1.82	156.4	150.5
598		phe_79	asp_83	2.12	0.12	-7.25	1.14	132.7	154.6
599		lys_127	phe_131	1.91	0.20	-10.86	1.60	159.1	161.8
600		arg_128	glu_132	1.95	0.18	-9.88	1.54	154.7	157.4
601		ser_129	glu_133	2.32	0.08	-4.95	0.89	131	142.4
602		tyr_130	ile_134	2.01	0.16	-8.77	1.48	158.1	151.7
603		phe_131	leu_135	2.04	0.15	-8.10	1.43	151.8	148.2
604		asp_139	met_143	2.53	0.06	-4.23	0.55	142.4	160.9
605		ser_140	tyr_144	2.01	0.16	-8.97	1.33	156	161.6
606		ser_141	asp_145	1.80	0.25	-13.48	2.18	152.9	155.6
607		glu_142	arg_146	2.01	0.15	-8.35	1.52	136.3	147.1
608		arg_146	arg_150	2.16	0.12	-6.78	1.06	144.3	155.1
609		tyr_147	ala_151	1.97	0.17	-9.69	1.37	152.5	165.9
610		phe_148	asn_152	1.99	0.17	-9.38	1.38	158.9	161.5
611		pro_149	ser_153	2.13	0.12	-7.14	1.09	150.9	158.4
612		arg_150	met_154	2.01	0.16	-9.14	1.27	155.1	168.8
613		ala_151	leu_155	1.91	0.20	-10.93	1.60	156	161.9
614		asp_161	phe_165	1.95	0.18	-10.20	1.38	157.5	171.1
615		thr_162	glu_166	2.04	0.15	-8.16	1.42	144	150.2
616		lys_163	asp_167	2.30	0.08	-5.06	1.01	145.2	136.7
617		trp_164	thr_168	2.18	0.11	-6.17	1.32	159	135.9
618		tyr_171	arg_175	2.21	0.11	-6.50	0.99	155	156.9
619		lys_172	val_176	1.97	0.17	-9.52	1.50	161.1	156.2

620		phe_173	ser_177	2.38	0.07	-5.05	0.69	142.3	165.4
621		ala_174	arg_178	1.97	0.17	-9.54	1.46	149.7	158.7
622		arg_175	glu_179	2.04	0.15	-8.28	1.29	150.5	157.6
623		val_176	gln_180	2.03	0.15	-8.59	1.29	154.2	160.4
624		ser_177	ala_181	1.81	0.25	-13.61	1.82	153.7	170.2
625		arg_178	gly_182	1.99	0.17	-9.06	1.47	145	154.3
626		glu_179	lys_183	2.53	0.05	-3.82	0.61	141	138.2
627		asp_196	met_200	2.11	0.13	-7.29	1.25	142.6	150.3
628		phe_197	gln_201	2.12	0.12	-7.05	1.20	142	149.6
629		gly_198	arg_202	2.21	0.11	-6.42	0.97	148.9	158.1
630		tyr_199	glu_203	1.93	0.19	-10.01	1.82	152.1	148.7
631		met_200	ala_204	2.21	0.11	-6.32	1.00	148.9	152.8
632		gln_201	ala_205	2.32	0.08	-5.01	0.89	140.8	142.1
633		thr_231	ala_235	2.08	0.14	-8.09	1.14	159.8	166.2
634		tyr_232	ala_236	1.91	0.20	-10.60	1.82	144.6	152.1
635		leu_233	leu_237	1.90	0.20	-11.24	1.56	157.4	167.1
636		ala_234	gly_238	2.05	0.14	-7.87	1.42	141.5	147.9
637		gly_290	ser_294	1.83	0.23	-12.96	1.88	145.5	161.9
638		leu_292	glu_296	1.97	0.17	-9.56	1.45	146.7	159.1
639		gly_293	leu_297	2.12	0.13	-7.28	1.06	142.4	163.4
640		ser_294	leu_298	2.16	0.12	-6.82	1.09	150.6	154.2
641		thr_295	val_299	1.85	0.22	-12.44	1.68	166.8	170.2
642		glu_296	arg_300	1.94	0.19	-10.36	1.41	151.1	169.3
643		leu_297	ala_301	2.00	0.16	-8.92	1.43	139.1	155.5
644		leu_298	arg_302	1.90	0.20	-11.05	1.57	153	164.5
645		val_299	asp_303	1.92	0.19	-10.52	1.57	153.9	161.2
646		arg_300	thr_304	1.94	0.18	-9.91	1.73	154.2	151.1
647		asn_406	val_410	1.94	0.19	-10.50	1.48	165.3	165.3
648		ala_407	asn_411	1.85	0.22	-12.35	1.84	153.5	160.4
649		pro_408	ala_412	2.09	0.13	-7.55	1.21	142	154.6
650		ala_409	ala_413	1.96	0.18	-10.08	1.36	157.6	172.1
651		val_410	lys_414	1.78	0.26	-14.33	1.99	158.7	165.9
652		asn_411	ala_415	2.00	0.16	-8.92	1.43	144.3	155

653		ala_412	leu_416	2.26	0.10	-5.89	0.89	147.8	156.4
654		ala_413	phe_417	1.96	0.18	-10.01	1.36	161.1	171.3
655		lys_414	asp_418	1.82	0.23	-12.36	2.13	147.5	152.1
656		ala_415	arg_419	2.42	0.07	-4.55	0.70	137.4	148.6
657		leu_416	ile_420	2.47	0.06	-4.35	0.65	142.6	147.8
658		phe_417	asn_421	1.86	0.22	-12.22	1.75	154.5	164.1
659		asp_418	lys_422	1.87	0.21	-11.58	1.76	148.9	159.3
660		arg_419	ala_423	2.10	0.13	-7.55	1.17	144.7	157
661		ile_420	asn_424	2.44	0.06	-4.01	0.81	143.2	130.5
662		pro_486	ile_490	2.11	0.13	-7.62	1.13	157.6	161.6
663		phe_487	thr_491	1.92	0.19	-10.44	1.57	149.6	161.3
664		val_488	ala_492	1.86	0.22	-11.96	1.69	153.7	165.8
665		thr_489	leu_493	1.86	0.22	-12.34	1.62	156.3	174.7
666		ile_490	ala_494	1.99	0.16	-9.01	1.47	143.3	154.1
667		thr_491	glu_495	1.98	0.17	-9.10	1.58	147.9	151
668		ala_492	arg_496	2.06	0.14	-8.23	1.21	149.7	162.6
669		leu_493	asn_497	1.90	0.20	-10.93	1.76	151.1	155.8
670		ala_494	val_498	1.93	0.19	-10.54	1.40	152.4	174.1
671		glu_495	glu_499	2.22	0.10	-6.26	0.91	142.7	161.1
672		arg_496	arg_500	2.28	0.09	-5.81	0.83	147.3	161.4
673		asn_497	ile_501	1.92	0.19	-10.56	1.58	153.9	160.7
674		val_498	ile_502	1.80	0.25	-13.70	1.88	155.1	167.7
675		glu_499	lys_503	2.16	0.12	-6.83	1.05	141.4	157
676		arg_500	gln_504	1.92	0.19	-10.59	1.63	157.8	158.2
677		ile_501	asp_505	1.97	0.17	-9.58	1.50	145.5	156.1
678	**α-Lytic protease (2H5C)**	leu_184	leu_188	2.03	0.15	-8.67	1.26	163	165
679		gln_185	ser_189	2.07	0.14	-8.18	1.14	161.7	170.6
680		pro_186	gln_190	1.96	0.17	-9.14	1.55	133.5	153.3
681		ile_187	tyr_191	2.28	0.09	-5.39	0.87	146.9	150.2
682	**Fatty acid-binding protein**	asn_15	tyr_19	2.13	0.12	-7.27	1.09	152.9	159.8
683		phe_16	met_20	1.87	0.22	-12.11	1.62	161.1	172.1
684		asp_17	lys_21	1.79	0.26	-14.09	1.95	157.1	166.8
685		asp_18	ser_22	1.99	0.17	-9.21	1.44	148.2	156.7

686	**(4tjz)**	tyr_19	leu_23	2.22	0.10	-6.07	1.01	147.7	149.5
687		gly_26	arg_30	1.96	0.18	-10.06	1.44	159.2	164
688		phe_27	gln_31	2.06	0.14	-7.96	1.39	146.6	149.4
689		ala_28	val_32	2.19	0.11	-6.68	0.95	149.9	165.4
690		thr_29	ala_33	1.87	0.21	-11.93	1.57	158.5	174
691		arg_30	ser_34	2.06	0.14	-7.36	1.57	145.1	139.8
692	**Cytochrome b5 reductase (5gv8)**	gly_1096	gln_1100	2.32	0.08	-5.20	0.78	129.8	154
693		lys_1097	tyr_1101	2.10	0.13	-7.39	1.22	140.8	152.9
694		met_1098	leu_1102	1.81	0.25	-13.62	1.85	155.3	168.9
695		ser_1099	glu_1103	2.08	0.14	-7.82	1.18	141.4	159.5
696		gln_1100	ser_1104	2.28	0.09	-5.08	1.08	138.5	134
697		ile_1155	leu_1159	1.88	0.21	-11.67	1.60	163	168.6
698		thr_1156	gln_1160	2.05	0.14	-8.15	1.24	150.4	158.8
699		pro_1157	val_1161	2.48	0.06	-4.38	0.59	136.7	160
700		met_1158	ile_1162	1.83	0.24	-13.35	1.75	163.2	173.4
701		leu_1159	arg_1163	1.93	0.19	-10.29	1.59	149.6	158.4
702		gln_1160	ala_1164	2.16	0.11	-6.62	1.05	139.3	154.7
703		val_1161	ile_1165	1.99	0.17	-9.40	1.33	156.8	165.6
704		ile_1162	met_1166	1.89	0.20	-11.29	1.60	156.6	165.3
705		arg_1163	lys_1167	2.01	0.16	-8.97	1.38	159.2	158
706		leu_1189	leu_1193	1.97	0.17	-9.63	1.42	157.4	161.2
707		arg_1190	glu_1194	1.92	0.19	-10.46	1.61	155.6	159
708		pro_1191	glu_1195	1.94	0.18	-9.92	1.74	146.8	150.4
709		glu_1192	leu_1196	2.21	0.11	-6.43	0.93	146.1	163.1
710		leu_1193	arg_1197	1.98	0.17	-9.36	1.43	147.8	158.9
711		glu_1194	asn_1198	1.91	0.20	-10.46	1.78	140.8	152.8
712		glu_1195	glu_1199	2.16	0.11	-6.55	1.21	147.6	144.4
713		leu_1196	his_1200	2.13	0.12	-6.31	1.83	146.6	127.2
714		asn_1225	ile_1229	2.01	0.16	-9.14	1.24	161.1	172.5
715		glu_1226	arg_1230	1.96	0.18	-9.87	1.42	154.9	163.4
716		glu_1227	asp_1231	1.99	0.17	-8.78	1.81	144.6	142.4
717		met_1228	his_1232	2.32	0.09	-4.66	1.49	138.7	121.4
718		ile_1229	leu_1233	2.35	0.07	-4.83	0.85	134	139.5

719		pro_1247	ile_1251	2.16	0.12	-7.13	1.02	160.8	163.1
720		pro_1248	gln_1252	1.95	0.18	-10.16	1.47	155.5	162.7
721		pro_1249	tyr_1253	1.98	0.17	-9.05	1.47	135.8	154.5
722		met_1250	ala_1254	2.15	0.12	-6.32	1.35	120.4	137.3
723		cys_1255	leu_1259	1.80	0.25	-14.05	1.89	170.8	169.1
724		leu_1256	glu_1260	2.05	0.15	-8.37	1.19	150.5	165.6
725		pro_1257	arg_1261	2.05	0.15	-8.17	1.32	137.6	155.3
726		asn_1258	val_1262	2.17	0.11	-6.52	1.08	143.8	151.2
727		leu_1259	gly_1263	2.37	0.07	-4.51	0.90	137.4	134.3
728	**Cu-containing nitrite reductase (5akr)**	met_141	his_145	2.36	0.08	-5.39	0.73	157.3	159.9
729		val_142	val_146	2.11	0.13	-7.80	1.07	161.5	168
730		pro_143	thr_147	1.87	0.22	-12.15	1.62	151.8	170.1
731		thr_198	ala_202	2.31	0.08	-5.27	0.95	144	139.4
732		ala_202	ala_206	1.89	0.21	-11.36	1.82	156.8	154.6
733		tyr_203	val_207	1.93	0.19	-10.53	1.63	154.9	156.7
734		glu_204	lys_208	1.86	0.22	-12.10	1.73	148.3	163
735		asp_205	ala_209	1.76	0.27	-14.95	2.10	150.8	164.1
736		ala_206	met_210	1.89	0.21	-11.43	1.61	152.1	164.2
737		val_207	arg_211	1.95	0.18	-9.91	1.64	151.7	152.7
738		asn_307	ala_311	2.00	0.16	-8.97	1.59	145.6	148.4
739		leu_308	phe_312	1.87	0.21	-11.79	1.60	140.7	168.2
740		ile_309	glu_313	1.96	0.18	-9.69	1.61	131.2	151.7
741	**Crambin (1ejg)**	ser_6	arg_10	2.18	0.11	-6.84	1.00	149.4	157.7
742		ala_9	phe_13	1.91	0.20	-10.71	1.78	144.4	152.4
743		arg_10	asn_14	1.95	0.18	-10.07	1.57	155	156.2
744		ser_11	val_15	2.18	0.11	-6.78	1.01	148	156.1
745		asn_12	cys_16	1.90	0.20	-11.39	1.55	150.9	167
746		phe_13	arg_17	2.12	0.12	-7.07	1.35	147.7	141.7
747		glu_23	ala_27	1.89	0.20	-10.68	2.09	148.8	145
748		ala_24	thr_28	2.22	0.10	-6.46	0.90	147	162.5
749		cys_26	thr_30	2.30	0.08	-5.07	1.06	138.4	133.4
750		ala_27	gly_31	1.98	0.16	-9.16	1.76	162.1	143.2

Table S3 Topological properties, E_{elec} and ∠C=O···H and ∠N-H···O of parallel (p) and antiparallel (a) β-sheet hydrogen bonds in the 22 protein systems (estimated error on ρ_{BCP} is 0.05 eÅ^{-3}, E_{elec} is 2.32 kCal/mol and $\nabla^2\rho_{BCP}$ is 0.33 eÅ^{-5}).

Sl. No.	Protein	Type	Residue O	Residue H	R_{ij} (Å)	ρ_{bcp} (eÅ^{-3})	E_{elec} (kCal/mol)	$\nabla^2\rho_{bcp}$ (eÅ^{-5})	Angles (°)	
									C=H···O	N-H···O
1	**NrDH (4HS1)**	p	val_3	gln_29	1.86	0.22	-12.35	1.77	164.7	162.6
2		a	thr_4	val_55	1.89	0.21	-11.52	1.66	154.8	162.5
3		a	val_55	thr_4	1.88	0.21	-11.76	1.71	153.6	161.3
4		p	val_5	val_31	1.87	0.22	-11.98	1.75	150.4	161.4
5		p	gln_29	val_5	1.82	0.24	-13.09	1.98	159.9	159.2
6		a	tyr_6	val_53	2.11	0.13	-7.74	1.21	138.1	154.2
7		a	val_53	tyr_6	1.79	0.26	-14.34	2.05	159.9	162.7
8		p	val_31	thr_7	1.87	0.21	-11.59	1.69	145.1	162.7
9		a	val_54	trp_61	2.01	0.16	-8.97	1.60	145.5	147.6
10		a	trp_61	val_54	1.83	0.23	-13.10	1.73	159.3	170.5
11		a	ala_56	asp_59	1.90	0.20	-11.10	1.55	135.8	166.5
12		a	asp_59	ala_56	1.87	0.21	-11.69	1.65	141.6	165
13	**Human Parvulin 14 (3ui4)**	a	val_38	met_85	1.85	0.22	-12.09	1.98	148.9	155
14		a	met_85	val_38	2.04	0.15	-8.38	1.32	150.6	155.9
15		a	lys_39	glu_128	1.84	0.23	-12.05	1.99	148.7	155.1
16		a	gly_129	lys_39	1.91	0.20	-10.56	1.63	121	159.3
17		a	val_40	leu_82	1.92	0.19	-10.38	1.70	147.7	154.6
18		a	gly_83	val_40	2.07	0.14	-8.04	1.18	139.4	161.4
19		a	arg_41	met_126	1.95	0.18	-10.19	1.53	155.4	160.3
20		a	met_126	arg_41	1.99	0.17	-9.46	1.38	158.5	162.1
21		a	ile_43	ile_124	1.97	0.17	-9.57	1.61	145.7	152.4
22		a	ile_124	ile_43	1.93	0.19	-10.38	1.67	148.2	155.1
23		a	cys_45	tyr_122	1.82	0.24	-13.17	1.74	144.7	172.3
24		a	tyr_122	cys_45	1.94	0.19	-10.42	1.59	152.4	158.9
25		a	val_116	his_123	1.86	0.22	-12.05	1.91	136.2	156.9
26		a	his_123	val_116	1.85	0.23	-12.79	1.81	150	164.4
27		a	gly_121	thr_118	1.86	0.22	-12.43	1.75	156.2	165.5
28	**HEWL**	a	asn_44	asp_52	1.82	0.25	-13.52	1.83	146.1	169.7

29	**(2VB1)**	a	asp_52	asn_44	2.03	0.15	-8.60	1.42	141.8	153.6
30		a	tyr_53	ile_58	2.10	0.13	-7.46	1.23	133.3	153
31		a	ile_58	tyr_53	1.93	0.19	-9.93	1.81	122	149.8
32	**HiPIP (5DV8)**	a	gln_50	gly_60	2.53	0.05	-4.30	0.59	142.6	140.9
33		a	gly_60	gln_50	1.75	0.28	-15.49	1.99	122.6	174.6
34		a	glu_55	trp_58	2.11	0.13	-7.48	1.15	132.6	157
35		a	trp_58	glu_55	1.91	0.19	-10.68	1.89	160.3	148.5
36		a	lys_59	ile_69	1.79	0.26	-14.63	1.86	167.8	174.4
37		a	ile_69	lys_59	2.06	0.14	-7.70	1.45	144.8	143.5
38	**Ponsin (2o9s)**	a	glu_825	lys_881	2.18	0.11	-6.70	1.11	146.3	150.1
39		a	lys_881	glu_825	1.91	0.20	-10.98	1.84	134.1	152.8
40		a	ile_848	ala_826	2.06	0.14	-7.65	1.63	149.4	139.1
41		a	ile_827	asp_878	1.85	0.23	-12.69	1.7	159.4	170.4
42		a	asp_878	ile_827	2.01	0.16	-9.07	1.46	148	153.9
43		a	thr_849	arg_862	2.03	0.15	-8.52	1.5	141.6	148.6
44		a	arg_862	thr_849	1.95	0.17	-9.37	1.95	171.3	141.2
45		a	glu_860	leu_851	1.89	0.21	-10.96	1.94	139.7	151
46		a	arg_852	glu_860	1.86	0.22	-12.12	1.87	162.6	158.2
47		a	glu_860	arg_852	2.33	0.08	-5.41	0.85	142.3	148.9
48		a	tyr_859	phe_872	2.07	0.14	-7.93	1.47	150.8	144.8
49		a	phe_872	tyr_859	1.91	0.19	-10.77	1.66	174.4	158.4
50		a	gly_861	gly_870	2.01	0.16	-8.87	1.4	153.8	155.8
51		a	gly_870	gly_861	1.91	0.20	-10.82	1.62	157.3	159.9
52	**1,2-alpha mannose-dase (4ayo)**	a	glu_60	arg_69	1.92	0.19	-10.58	1.73	145.7	153.4
53		a	arg_69	glu_60	2.10	0.13	-7.61	1.30	156.5	148.3
54		a	asn_62	thr_67	2.24	0.10	-6.16	0.99	140.7	149.1
55		a	thr_67	asn_62	1.76	0.27	-15.21	1.97	146	176.2
56		a	ala_117	val_169	2.06	0.14	-8.27	1.28	146	156.6
57		a	val_169	ala_117	1.88	0.21	-11.75	1.62	145.4	167.3
58		a	tyr_168	ser_177	2.14	0.12	-7.02	1.14	135.3	152
59		a	ser_177	tyr_168	2.18	0.11	-6.69	1.08	164.7	149
60		a	ile_230	thr_181	2.04	0.14	-8.08	1.65	161.5	140.1
61		a	ala_242	val_295	2.27	0.09	-5.85	0.93	139.7	149.6

62		a	val_295	ala_242	1.87	0.21	-11.49	1.96	176.8	152.1
63		a	lys_284	trp_291	1.87	0.22	-12.15	1.65	162.3	168.6
64		a	trp_291	lys_284	1.93	0.19	-10.82	1.47	161.2	168.8
65		a	tyr_286	arg_289	1.94	0.19	-10.07	1.38	121.9	171.4
66		a	arg_289	tyr_286	1.99	0.17	-9.52	1.52	150.1	154.6
67		a	gln_307	ile_348	1.92	0.19	-10.77	1.61	152.4	160.1
68		a	ile_348	gln_307	1.98	0.17	-9.50	1.47	147.7	156.9
69		a	gly_402	ala_399	1.84	0.23	-12.46	2.06	174.9	153.6
70		a	thr_415	lys_407	1.91	0.20	-10.17	1.96	120.9	147.4
71		a	asp_408	thr_415	2.37	0.07	-4.84	0.90	137.3	134.5
72		a	thr_415	asp_408	2.32	0.08	-5.50	0.81	132.6	153.7
73		a	gln_448	leu_456	1.96	0.18	-9.67	1.47	143.3	159.5
74		a	arg_457	gln_448	2.13	0.12	-7.31	1.19	135.9	151.2
75	**Acutohaemonlysin (1mc2)**	a	lys_1076	val_1083	1.92	0.19	-10.77	1.59	155.2	161.5
76		a	val_1083	lys_1076	2.00	0.16	-9.03	1.41	138.4	157.3
77		a	ala_1081	lys_1078	1.96	0.18	-10.06	1.49	152.6	161.4
78	**Triose-Phosphate Isomerase (2vxn)**	p	ala_8	val_40	2.05	0.14	-7.98	1.50	148.1	145.6
79		p	gln_38	ala_8	2.09	0.13	-7.24	1.28	139.2	149.3
80		p	ala_9	val_233	1.87	0.21	-11.38	1.91	158	153.6
81		p	ala_10	ala_42	1.84	0.23	-12.38	1.95	169.3	156.9
82		p	val_40	ala_10	1.78	0.26	-14.10	2.04	146.8	163.9
83		p	val_233	asn_11	1.86	0.22	-11.58	1.93	147.4	154.3
84		p	cys_39	val_61	2.05	0.15	-7.94	1.47	142.1	147
85		p	val_41	ser_63	1.89	0.21	-11.16	1.69	137.3	161.3
86		p	val_61	val_41	2.05	0.14	-8.08	1.36	155.4	152.2
87		p	ala_64	ile_92	1.93	0.19	-10.20	1.51	146.8	162.8
88		p	trp_90	ala_64	2.05	0.15	-8.23	1.32	142.9	155.8
89		p	val_91	ile_124	1.94	0.18	-9.91	1.59	145.6	156.8
90		p	met_122	val_91	2.12	0.12	-6.92	1.29	155.4	144.5
91		p	leu_93	cys_126	1.98	0.17	-9.58	1.42	167.7	161.2
92		p	ile_124	leu_93	1.93	0.19	-10.21	1.54	151.7	160.9
93		p	val_123	val_163	1.86	0.22	-11.89	1.89	177.1	156.5
94		p	ala_125	ala_165	1.90	0.20	-10.92	1.65	144.2	160.8

95		p	val_163	ala_125	1.86	0.22	-12.17	1.77	174.6	162.7
96		p	ala_165	ile_127	1.98	0.17	-9.45	1.41	159.5	161.1
97		p	leu_164	leu_209	1.77	0.27	-14.69	2.05	160.1	166.1
98		p	arg_207	leu_164	2.10	0.13	-7.27	1.30	160.5	147.1
99		p	leu_209	tyr_166	1.87	0.21	-11.26	2.00	173	150.4
100	**hAR**	a	ile_4	met_12	1.87	0.22	-12.10	1.82	142.5	159.3
101	**(1us0)**	a	met_12	ile_4	1.90	0.20	-11.18	1.75	140.7	157.2
102		p	leu_17	asp_43	1.86	0.22	-12.03	1.59	147.6	170.6
103		p	his_41	leu_17	1.97	0.17	-9.37	1.64	142	152.7
104		p	ile_42	val_75	2.06	0.14	-8.42	1.17	174.5	167.3
105		p	phe_73	ile_42	2.32	0.08	-5.10	0.88	146.4	144.1
106		p	ile_74	leu_106	2.47	0.06	-4.38	0.67	147.7	144.3
107		p	ser_76	leu_108	2.01	0.16	-8.73	1.55	137.1	150.6
108		p	leu_106	ser_76	2.19	0.11	-6.31	1.08	156.2	147.8
109		p	leu_108	leu_78	1.81	0.24	-13.02	2.09	161.8	156.6
110		p	tyr_107	gly_157	2.06	0.14	-7.88	1.46	143.4	145.9
111		p	gly_157	ile_109	2.00	0.16	-8.90	1.52	139	151.6
112		p	ile_158	gln_183	2.02	0.16	-8.54	1.47	138.5	151.9
113		p	val_181	ile_158	1.89	0.21	-11.35	1.62	154.8	165.8
114		p	asn_182	thr_207	2.22	0.10	-5.70	1.03	125	147.3
115		p	val_205	asn_182	2.07	0.14	-7.44	1.43	146.5	144.2
116		p	ile_184	tyr_209	1.87	0.21	-11.46	1.68	134.6	163.8
117		p	thr_207	ile_184	1.90	0.20	-11.12	1.76	173.4	156.8
118		p	val_206	val_258	2.02	0.16	-8.75	1.37	149.2	157.7
119		p	val_258	ala_208	1.74	0.28	-15.66	2.19	159.1	165.6
120	**Rubredoxin**	a	lys_3	ile_52	1.93	0.19	-10.88	1.42	143.3	176.3
121	**(1yk4)**	a	leu_4	tyr_13	1.91	0.19	-10.62	1.99	167	145.9
122		a	tyr_13	leu_4	1.90	0.20	-10.91	1.78	141.8	154
123		a	ser_5	glu_50	2.08	0.14	-8.19	1.21	142.4	158
124		a	glu_50	ser_5	1.96	0.17	-9.61	1.74	160	146.7
125	**Cyclophilin**	a	val_6	leu_22	1.87	0.21	-11.73	1.71	148.3	162.5
126	**D**	a	leu_22	val_6	1.95	0.18	-10.41	1.51	153.9	161.6
127	**(4o8h)**	a	tyr_7	gly_162	2.27	0.09	-5.75	0.98	142.9	143.6

128		a	gly_162	tyr_7	1.97	0.17	-9.40	1.58	146.6	152.4
129		a	leu_8	val_20	1.85	0.23	-12.84	1.79	156.8	164.6
130		a	val_20	leu_8	1.90	0.20	-11.28	1.72	151.3	158.4
131		a	asp_9	thr_159	2.07	0.13	-7.18	1.76	147.3	133.6
132		a	asp_160	asp_9	1.83	0.23	-13.31	1.71	152.2	174.3
133		a	val_10	leu_17	1.75	0.28	-15.74	2.06	155.5	172.2
134		a	gly_18	val_10	2.07	0.14	-8.30	1.18	171.6	162.8
135		a	asp_11	val_157	2.02	0.16	-8.72	1.44	137.7	153
136		a	val_157	asp_11	1.85	0.22	-12.34	1.91	156.6	157.8
137		a	lys_15	ala_12	1.96	0.18	-9.86	1.62	153.9	153.4
138		a	val_21	ile_133	1.86	0.22	-11.57	1.96	140.4	153.6
139		a	val_21	glu_134	2.51	0.06	-4.40	0.59	128.6	159.1
140		a	glu_134	val_21	1.91	0.20	-10.94	1.54	142.2	165.9
141		a	glu_23	his_131	2.26	0.09	-5.81	1.02	143.2	142.5
142		a	his_131	glu_23	2.02	0.15	-8.70	1.42	166.8	152.5
143		a	gln_63	his_54	2.56	0.05	-3.40	0.87	142.1	121.4
144		a	arg_55	gln_63	1.86	0.22	-11.65	2.00	154.9	151.7
145		a	gln_63	arg_55	2.47	0.06	-4.68	0.60	139.2	172.2
146		a	ile_57	met_61	2.37	0.07	-4.89	0.85	140.2	139.8
147		a	met_61	ile_57	1.95	0.18	-10.39	1.39	171.3	172.6
148		a	cys_62	ile_114	1.93	0.19	-10.38	1.62	147.5	157.1
149		a	ile_114	cys_62	1.97	0.17	-9.70	1.47	143.4	158.8
150		a	ala_64	phe_112	1.99	0.16	-9.10	1.45	140.2	155.5
151		a	phe_112	ala_64	1.96	0.18	-9.94	1.47	160.7	160.9
152		a	val_97	cys_115	1.91	0.20	-11.19	1.70	152.1	158.8
153		a	leu_98	phe_129	1.93	0.19	-10.51	1.48	153.4	166.5
154		a	leu_98	gly_130	2.62	0.04	-3.66	0.60	142	132.3
155		a	gly_130	leu_98	1.96	0.18	-9.75	1.37	128.3	168.1
156		a	ser_99	phe_113	1.89	0.21	-11.28	1.85	155.8	153.8
157		a	phe_113	ser_99	2.03	0.15	-8.60	1.36	155	155
158	**Serine Protease (1gci)**	p	lys_27	val_121	2.23	0.10	-6.10	0.99	157.4	149.1
159		p	val_28	tyr_91	2.01	0.16	-8.96	1.46	155.6	152.9
160		p	glu_89	val_28	1.84	0.23	-12.81	1.67	160	174.8

161		p	ala_29	asn_123	1.79	0.25	-14.33	1.86	174.2	174.5
162		p	val_121	ala_29	1.90	0.20	-11.29	1.56	157.4	166.7
163		p	val_30	val_93	2.02	0.15	-8.76	1.36	147.7	154.6
164		p	tyr_91	val_30	1.87	0.22	-12.22	1.61	171	173.9
165		p	asn_123	leu_31	1.98	0.17	-9.73	1.44	159.8	159.2
166		p	val_93	asp_32	2.16	0.11	-6.58	1.13	149.1	147.5
167		p	leu_90	arg_45	1.80	0.25	-13.76	2.07	159.2	159.9
168		p	gly_46	ala_92	1.92	0.20	-11.03	1.60	150	163.1
169		p	ala_48	lys_94	1.96	0.18	-9.62	1.69	153.8	149.9
170		p	ala_92	ala_48	2.07	0.14	-7.73	1.38	146.6	147.2
171		p	ala_122	val_150	1.87	0.22	-12.08	1.63	175.3	169.4
172		p	leu_148	ala_122	1.87	0.22	-11.92	1.63	146.8	169.1
173		p	leu_124	ala_152	2.21	0.10	-6.50	1.00	155.1	152.8
174		p	val_150	leu_124	1.79	0.26	-14.17	1.97	171.9	166.1
175		p	val_149	met_175	1.77	0.27	-15.03	1.94	156.4	176.8
176		p	ala_151	val_177	1.96	0.17	-9.61	1.64	161	151
177		p	met_175	ala_151	1.87	0.21	-11.80	1.63	152.3	167.8
178		p	ala_176	asp_197	2.07	0.14	-7.71	1.37	128	148.2
179		p	ala_176	ile_198	2.43	0.06	-4.42	0.76	159.7	136.5
180		p	gly_178	ala_200	2.08	0.14	-7.62	1.32	143.3	149.3
181		p	ile_198	gly_178	1.98	0.17	-9.63	1.41	149.5	163.1
182		p	ala_200	thr_180	1.93	0.19	-10.17	1.55	129.5	160.5
183		a	val_205	leu_217	2.07	0.14	-8.06	1.25	132.5	156.7
184		a	leu_217	val_205	2.06	0.14	-8.27	1.19	145.7	162.3
185		a	ser_207	ala_215	1.99	0.17	-9.36	1.46	153.5	155.5
186		a	ala_215	ser_207	1.97	0.17	-9.41	1.52	144.7	154.5
187		a	tyr_209	thr_213	2.12	0.13	-7.59	1.04	153.5	169.3
188		a	thr_213	tyr_209	2.17	0.11	-6.39	1.37	138.3	134.7
189	**Proteinase K (2pwa)**	a	gln_3	tyr_23	1.96	0.18	-10.04	1.63	144.5	153.6
190		a	tyr_23	gln_3	1.85	0.23	-12.76	1.79	145.4	164.2
191		p	ser_33	gln_89	2.16	0.12	-7.10	0.96	144.6	173.6
192		p	cys_34	val_128	1.92	0.19	-10.52	1.73	155	153.8
193		p	gly_126	cys_34	2.12	0.12	-7.10	1.30	151.3	144.2

194		p	val_35	phe_91	1.92	0.20	-10.80	1.59	144.8	161.5
195		p	gln_89	val_35	1.82	0.24	-13.15	1.93	166	161
196		p	tyr_36	ser_130	1.85	0.23	-12.62	1.82	167.9	162.4
197		p	val_128	tyr_36	1.86	0.22	-12.06	1.87	157.1	157.6
198		p	val_37	val_93	2.08	0.14	-8.06	1.13	151.4	165.7
199		p	phe_91	val_37	1.87	0.21	-11.78	1.83	158.7	157.8
200		p	ser_130	ile_38	2.07	0.14	-8.40	1.12	166.1	171.7
201		p	val_93	asp_39	1.96	0.18	-9.77	1.52	159.6	156.9
202		p	gln_54	gly_92	1.87	0.22	-11.72	1.84	140.3	157.2
203		p	leu_90	gln_54	2.11	0.13	-7.12	1.30	143.6	146.1
204		p	gly_92	val_56	1.89	0.21	-11.86	1.54	150.1	176.5
205		p	lys_57	lys_94	1.89	0.21	-11.45	1.69	146.5	161
206		p	gly_92	lys_57	2.58	0.05	-3.85	0.58	155.2	139.4
207		p	val_127	met_154	1.92	0.20	-10.89	1.59	145	162.5
208		p	ala_129	ala_156	1.91	0.20	-11.12	1.49	169.7	169.7
209		p	met_154	ala_129	1.83	0.23	-12.86	1.91	147.2	160.5
210		p	leu_131	ala_158	2.17	0.11	-6.71	1.11	159	147.8
211		p	ala_156	leu_131	1.92	0.19	-10.56	1.74	157.6	153.3
212		a	gly_135	ser_170	1.96	0.17	-9.44	1.57	135.9	153.5
213		a	ser_170	gly_135	2.29	0.08	-5.44	1.05	160.6	135.2
214		p	val_155	cys_178	1.92	0.19	-10.44	1.64	150.9	156.2
215		p	val_157	val_180	1.96	0.17	-9.60	1.68	166.9	149.7
216		p	cys_178	val_157	1.85	0.22	-12.22	1.83	156.6	160.1
217		p	thr_179	ile_201	2.62	0.04	-3.71	0.52	160.4	138.9
218		p	gly_181	gly_203	1.92	0.19	-10.53	1.61	154.2	158.3
219		p	ile_201	gly_181	1.94	0.18	-10.23	1.66	151.1	154.9
220		p	gly_203	ser_183	2.03	0.15	-8.19	1.46	139.4	148
221		a	ile_208	ile_220	2.26	0.09	-5.89	0.93	134	149.6
222		a	ile_220	ile_208	1.89	0.20	-11.51	1.52	149.5	172.4
223		a	ser_210	arg_218	2.08	0.13	-7.67	1.36	154.8	147.1
224		a	arg_218	ser_210	2.07	0.14	-7.97	1.23	143	156.9
225		a	trp_212	ser_216	2.28	0.09	-5.25	0.91	124.1	146
226		a	ser_216	trp_212	1.97	0.17	-9.14	1.59	124.4	151.3

227		a	asn_257	leu_272	1.98	0.17	-9.41	1.59	143	151.2
228		a	leu_272	asn_257	2.09	0.13	-7.53	1.55	161.5	138.9
229	**Trypsin (1pq7)**	a	thr_20	lys_154	1.90	0.20	-11.15	1.83	152.2	153.6
230		a	lys_154	thr_20	1.91	0.20	-11.12	1.66	156.4	159.7
231		a	val_31	gly_43	2.11	0.12	-7.21	1.47	149.6	138.4
232		a	gly_43	val_31	1.92	0.20	-10.74	1.43	131.7	176.5
233		a	ser_32	arg_69	2.04	0.15	-8.59	1.36	147.2	155.1
234		a	arg_69	ser_32	2.14	0.12	-6.90	1.30	152.4	142.1
235		a	ile_33	cys_41	1.97	0.18	-10.07	1.35	150.5	174
236		a	cys_41	ile_33	2.00	0.16	-9.04	1.35	134.9	160.2
237		a	ser_34	gln_67	2.02	0.16	-8.70	1.31	132.9	160
238		a	gln_67	ser_34	1.96	0.18	-9.74	1.63	161.8	152.5
239		a	arg_35	gly_38	1.98	0.17	-9.08	1.33	120.7	165.5
240		a	gly_38	arg_35	1.93	0.19	-10.66	1.59	149.4	160.3
241		a	ser_44	leu_52	1.81	0.25	-14.02	1.90	153.4	168.2
242		a	leu_52	ser_44	1.96	0.18	-9.80	1.67	143.2	151.2
243		a	thr_50	leu_46	1.86	0.22	-11.82	1.82	146.9	158.5
244		a	val_51	leu_103	1.79	0.26	-14.42	1.92	161.6	171.4
245		a	leu_103	val_51	1.91	0.20	-11.07	1.56	144.2	165.6
246		a	thr_53	ala_101	1.90	0.20	-11.09	1.66	143.2	160.5
247		a	ala_101	thr_53	1.99	0.17	-9.59	1.30	154.8	170.2
248		a	ile_68	ser_82	1.97	0.17	-9.68	1.54	140.8	155.1
249		a	ser_82	ile_68	1.87	0.22	-12.14	1.74	168.5	163.2
250		a	ala_70	ile_80	1.94	0.19	-10.52	1.53	149.6	162
251		a	ile_80	ala_70	1.87	0.22	-12.02	1.59	155.7	174
252		a	lys_104	ser_85	1.80	0.25	-13.46	2.08	138.4	159.4
253		a	ser_86	lys_104	1.99	0.17	-9.11	1.37	134.5	161
254		a	lys_104	ser_86	2.50	0.06	-4.42	0.60	127.2	159.6
255		a	arg_88	ile_102	1.87	0.22	-12.01	1.85	159.8	157.6
256		a	ile_102	arg_88	1.97	0.17	-9.31	1.65	149.9	149.8
257		a	ala_133	val_157	1.90	0.20	-11.06	1.74	153.9	156.9
258		a	val_157	ala_133	1.88	0.21	-11.39	1.63	149.9	164.6
259		a	thr_134	val_200	1.81	0.25	-13.62	1.86	152.1	168

260		a	val_200	thr_134	1.93	0.19	-10.51	1.55	144.5	160.9
261		a	val_135	val_155	1.97	0.17	-9.64	1.54	157.4	154.8
262		a	val_155	val_135	1.91	0.20	-11.13	1.55	162.9	166.4
263		a	pro_198	ala_136	2.33	0.08	-5.36	0.80	165.2	149
264		a	gly_137	leu_153	2.13	0.12	-7.30	1.02	144.3	167.2
265		a	leu_153	gly_137	1.99	0.16	-9.19	1.48	149.9	153.7
266		a	cys_180	val_160	1.90	0.21	-10.93	1.54	121.2	168.5
267		a	phe_179	tyr_225	1.88	0.21	-11.35	1.93	164.6	152
268		a	tyr_225	phe_179	2.01	0.16	-9.06	1.42	143.9	156
269		a	ala_181	gly_223	2.16	0.11	-6.39	1.43	156.7	133.9
270		a	gly_223	ala_181	2.04	0.15	-8.57	1.39	147.2	153
271		a	ile_199	ile_207	2.01	0.16	-8.62	1.57	142	148.4
272		a	ile_199	gly_208	2.31	0.08	-5.39	0.95	150.7	139.9
273		a	gly_208	ile_199	2.07	0.14	-7.98	1.09	130.4	176
274		a	ala_209	ala_226	2.08	0.13	-7.65	1.38	160.1	145.6
275		a	ala_226	ala_209	2.15	0.12	-7.08	1.13	136.9	152.5
276		a	val_224	ser_211	2.43	0.06	-4.39	0.78	152.3	133.2
277		a	trp_212	val_224	1.92	0.19	-10.27	1.87	172	147.3
278		a	val_224	trp_212	2.06	0.15	-8.32	1.19	137	164.8
279	**DFPase (1pjx)**	p	ile_6	arg_264	2.00	0.16	-9.11	1.41	170.8	156.1
280		p	arg_262	ile_6	1.98	0.17	-9.61	1.51	159.5	155.7
281		a	thr_11	lys_294	1.99	0.16	-9.03	1.79	141.7	143
282		a	lys_294	thr_11	1.88	0.21	-12.01	1.69	156.9	164.3
283		a	val_292	val_13	1.84	0.23	-12.84	1.86	144.3	161.9
284		a	thr_14	val_292	1.94	0.19	-10.50	1.45	150.4	165.9
285		a	val_292	thr_14	2.33	0.08	-5.37	0.82	125.8	153.4
286		a	glu_21	val_34	1.93	0.19	-10.50	1.45	135.3	167.6
287		a	val_34	glu_21	2.13	0.12	-6.87	1.54	150.9	134
288		a	val_24	tyr_32	1.97	0.17	-9.83	1.55	159.9	155.1
289		a	tyr_32	val_24	2.19	0.11	-6.49	1.19	149.5	140.9
290		a	phe_31	ile_51	1.90	0.20	-11.20	1.54	150.6	168.3
291		a	ile_33	leu_49	1.81	0.24	-13.62	1.84	173.3	167.3
292		a	leu_49	ile_33	2.08	0.14	-7.77	1.28	138.1	151.6

293		a	glu_47	ala_35	1.79	0.26	-14.22	1.98	153	165
294		a	val_40	lys_43	2.08	0.14	-7.66	1.15	121.3	162
295		a	lys_43	val_40	2.01	0.16	-9.15	1.46	152.8	153.9
296		a	ile_48	ile_61	2.02	0.15	-8.34	1.69	147.1	142.3
297		a	ile_48	cys_62	2.42	0.07	-4.93	0.7	143.3	151.3
298		a	cys_62	ile_48	1.85	0.23	-12.62	1.87	162.2	160
299		a	arg_50	thr_59	1.95	0.18	-10.27	1.51	157	160.2
300		a	thr_59	arg_50	1.98	0.17	-9.22	1.74	158.1	145.1
301		a	val_66	tyr_69	2.01	0.16	-8.73	1.27	121.8	164.4
302		a	tyr_69	val_66	2.07	0.14	-8.11	1.34	138.7	151.3
303		a	ala_88	ala_74	1.79	0.25	-14.24	1.94	168.4	167.7
304		a	gly_75	ala_88	1.93	0.19	-9.85	1.99	136.6	144.4
305		a	ala_88	gly_75	2.50	0.06	-4.28	0.68	137.7	140.1
306		a	gln_77	phe_86	1.82	0.24	-13.13	1.99	170.7	159.2
307		a	phe_86	gln_77	1.96	0.18	-9.83	1.61	149.7	153.1
308		a	leu_85	val_97	1.81	0.25	-13.61	2.02	150.4	160.1
309		a	val_97	leu_85	1.87	0.22	-12.24	1.67	155.7	167.1
310		a	val_87	leu_95	1.82	0.24	-13.63	1.84	148.1	168.1
311		a	leu_95	val_87	1.87	0.22	-11.94	1.75	142.6	160.9
312		a	asp_89	gly_93	1.98	0.17	-9.30	1.51	134.5	153.1
313		a	gly_93	asp_89	1.81	0.25	-13.64	1.92	147.6	164.6
314		a	val_96	glu_104	2.01	0.16	-9.05	1.5	147.5	151.7
315		a	glu_104	val_96	1.98	0.17	-9.66	1.48	152	156.7
316		a	asp_121	thr_133	1.98	0.17	-9.33	1.47	145.2	155.8
317		a	ala_123	trp_131	1.87	0.22	-12.03	1.57	143.8	175.1
318		a	trp_131	ala_123	1.95	0.18	-9.87	1.96	146.1	143.4
319		a	leu_130	phe_158	1.82	0.24	-13.53	2.02	150.5	159.6
320		a	phe_158	leu_130	1.94	0.19	-10.53	1.43	145.2	168
321		a	ile_132	tyr_156	1.90	0.21	-11.46	1.66	145.9	161.8
322		a	tyr_156	ile_132	1.93	0.19	-10.38	1.79	147.7	149.7
323		a	ala_134	ser_154	1.93	0.19	-10.49	1.59	129.2	158.9
324		a	ser_154	ala_134	1.91	0.19	-10.45	2.03	166.6	144.1
325		a	gly_153	phe_171	1.90	0.20	-11.58	1.52	137.3	174.2

326		a	phe_171	gly_153	1.89	0.20	-11.47	1.91	153.7	152
327		a	ile_155	val_167	1.83	0.24	-12.82	1.9	142.8	161.5
328		a	ile_155	asp_168	2.38	0.08	-5.17	0.74	130.4	156.7
329		a	asp_168	ile_155	1.96	0.18	-9.86	1.48	138.7	159.1
330		a	cys_157	ile_165	1.90	0.20	-11.35	1.48	144.4	174.4
331		a	ile_165	cys_157	1.87	0.22	-11.88	1.9	147	154.8
332		a	ala_193	asn_175	2.10	0.13	-7.22	1.68	143.9	133.6
333		a	gly_176	ala_193	1.89	0.20	-11.16	1.59	136.9	164.3
334		a	ala_178	ile_191	1.88	0.21	-11.85	1.6	156.5	168.6
335		a	ile_191	ala_178	2.13	0.12	-7.16	1.3	147.2	143.8
336		a	arg_180	tyr_188	1.91	0.20	-11.12	1.52	166.3	168.2
337		a	arg_180	gln_189	2.39	0.08	-5.11	0.75	137.9	153.9
338		a	gln_189	arg_180	1.85	0.22	-12.39	1.82	150.6	160.8
339		a	leu_190	tyr_203	2.03	0.15	-8.52	1.54	145	146.3
340		a	tyr_203	leu_190	1.96	0.18	-10.00	1.52	145.8	158.6
341		a	val_192	trp_201	1.81	0.25	-13.90	1.82	150.9	170.6
342		a	trp_201	val_192	1.88	0.21	-11.74	1.86	145.7	155.2
343		a	lys_199	glu_194	2.01	0.16	-9.32	1.22	157.2	176
344		a	leu_200	trp_217	1.99	0.17	-8.79	1.96	140.6	139
345		a	leu_200	gly_218	2.12	0.13	-7.59	1.16	131.7	157.3
346		a	gly_218	leu_200	1.93	0.19	-10.73	1.45	134.6	169.4
347		a	ser_202	lys_215	2.10	0.13	-7.49	1.49	149.4	140.1
348		a	lys_215	ser_202	1.88	0.21	-11.76	1.85	148.7	156.3
349		a	asp_204	glu_212	2.08	0.13	-7.81	1.34	144.1	148.6
350		a	glu_212	asp_204	1.98	0.16	-8.94	1.9	157.1	140.1
351		a	lys_210	lys_206	1.87	0.21	-11.55	1.87	150	155.1
352		a	gly_207	lys_210	2.04	0.15	-8.38	1.44	139.7	148.7
353		a	lys_210	gly_207	2.65	0.04	-3.71	0.5	134.5	142.8
354		a	gly_227	trp_244	2.10	0.13	-7.12	1.63	148.6	134
355		a	trp_244	gly_227	2.12	0.13	-7.31	1.33	135.7	145.3
356		a	ala_242	asp_229	1.90	0.20	-11.31	1.69	158.8	159.4
357		a	gly_230	ala_242	1.93	0.19	-10.26	1.72	158.2	152.2
358		a	asp_232	leu_240	1.87	0.21	-12.04	1.64	162	167.9

359		a	leu_240	asp_232	2.12	0.12	-7.37	1.25	147.8	147.9
360		a	leu_239	phe_252	1.83	0.24	-13.26	1.79	149.9	167.7
361		a	phe_252	leu_239	1.94	0.18	-10.33	1.79	140.1	149.2
362		a	val_241	glu_250	1.86	0.22	-12.00	1.96	153.4	154.2
363		a	glu_250	val_241	1.93	0.19	-10.37	1.88	148.6	147.7
364		a	his_248	asn_243	2.08	0.14	-8.15	1.19	153.2	158
365		a	ile_249	ile_263	1.81	0.24	-13.45	2.08	152.4	157.6
366		a	ile_263	ile_249	1.97	0.17	-9.86	1.57	145	154.6
367		a	val_251	met_261	2.53	0.05	-4.28	0.59	140	147.8
368		a	met_261	val_251	1.95	0.18	-9.87	1.65	165.7	151.1
369		a	thr_285	ser_271	1.82	0.24	-13.36	1.8	145.3	169.4
370		a	asn_272	thr_285	1.91	0.19	-10.70	1.66	142.3	157.4
371		a	his_274	phe_283	1.84	0.23	-12.57	1.84	160	161.5
372		a	phe_283	his_274	2.07	0.14	-7.63	1.64	145.1	137.8
373		a	ile_282	phe_295	2.05	0.14	-8.21	1.43	143.7	148.1
374		a	phe_295	ile_282	1.86	0.22	-12.34	1.69	172.7	167
375		a	val_284	trp_293	1.91	0.20	-11.10	1.7	149.6	157.7
376		a	trp_293	val_284	1.83	0.23	-12.68	1.91	142.3	159.7
377		a	glu_286	ala_291	2.16	0.11	-6.90	1.15	146.4	148.5
378		a	ala_291	glu_286	2.15	0.11	-6.75	1.37	159.8	137.5
379	**Cholesterol Oxidase (4rek)**	p	ser_281	val_11	1.97	0.17	-9.48	1.51	152.4	155.6
380		p	pro_12	arg_283	2.02	0.15	-8.29	1.60	125.6	144.9
381		p	pro_12	tyr_284	1.98	0.17	-9.47	1.41	157.5	160.9
382		p	ala_13	leu_37	1.98	0.17	-9.38	1.52	151.6	154.9
383		p	val_14	phe_286	1.87	0.22	-12.13	1.67	163	167.4
384		p	tyr_284	val_14	2.10	0.13	-7.67	1.22	161.9	153.9
385		p	val_15	leu_39	1.98	0.17	-9.25	1.54	160.3	153
386		p	leu_37	val_15	1.91	0.20	-10.86	1.69	143.1	157.9
387		p	phe_286	ile_16	1.89	0.21	-11.32	1.74	164.4	158.6
388		p	thr_36	thr_243	2.09	0.13	-7.71	1.26	156.8	152.3
389		p	met_38	gln_245	1.89	0.20	-11.35	1.64	171.1	163.4
390		p	thr_243	met_38	1.80	0.25	-13.91	1.88	156.5	169.3
391		p	gln_245	glu_40	1.92	0.19	-10.91	1.48	162.7	169.6

392		a	asp_97	val_108	1.99	0.17	-9.15	1.52	137.9	152.9
393		a	val_108	asp_97	1.81	0.25	-13.86	1.81	166.3	172.6
394		a	val_99	val_106	1.92	0.19	-10.79	1.73	148.7	155.2
395		a	val_106	val_99	1.74	0.28	-15.76	2.05	149.4	173.4
396		p	ser_105	cys_445	2.21	0.10	-5.88	1.52	155.7	128
397		p	cys_445	tyr_107	1.87	0.21	-11.89	1.68	172.7	165.3
398		a	val_189	gly_347	1.97	0.17	-9.71	1.49	153.4	157.6
399		a	gly_347	val_189	1.94	0.19	-10.11	1.73	147.8	151.6
400		a	gln_249	glu_266	1.97	0.17	-9.77	1.54	152.1	155.8
401		a	glu_266	gln_249	1.92	0.19	-10.73	1.67	151.5	157.4
402		a	thr_264	lys_251	1.83	0.24	-13.26	1.75	157.3	172.2
403		a	thr_252	thr_264	2.23	0.10	-5.68	1.04	127	143.2
404		a	arg_254	ala_262	1.95	0.18	-10.09	1.56	147.4	158.4
405		a	ala_262	arg_254	1.99	0.17	-9.50	1.46	154.6	157.6
406		a	tyr_261	cys_282	2.07	0.14	-7.62	1.57	153.6	139.8
407		a	cys_282	tyr_261	2.01	0.16	-8.80	1.36	143.1	158
408		a	leu_263	ile_280	2.07	0.14	-8.14	1.29	141.8	155.9
409		a	ile_280	leu_263	1.80	0.25	-13.31	2.27	153.3	152.6
410		a	val_265	lys_278	1.81	0.25	-13.73	1.92	149.4	165.3
411		a	lys_278	val_265	1.97	0.17	-9.35	1.78	152.4	145.1
412		a	gln_267	leu_275	1.76	0.27	-15.16	2.12	152.1	165.1
413		a	gln_267	ala_276	2.44	0.06	-4.68	0.70	140.6	147.7
414		a	ala_276	gln_267	1.85	0.22	-12.31	1.73	153.3	165.8
415		p	leu_285	tyr_471	1.95	0.18	-9.61	1.75	159.6	148.2
416		p	tyr_471	leu_287	1.78	0.26	-14.22	2.09	148	162.4
417		a	ile_324	ala_378	1.81	0.24	-13.09	2.20	174.5	153.1
418		a	ala_378	ile_324	2.06	0.14	-8.09	1.40	143.7	149.1
419		a	met_325	ala_441	1.92	0.19	-10.38	1.82	148.8	150.3
420		a	ala_441	met_325	2.28	0.09	-5.78	0.88	131.9	154.7
421		a	thr_326	tyr_376	1.95	0.18	-9.81	1.75	168.8	148.3
422		a	tyr_376	thr_326	2.09	0.14	-7.84	1.24	147.6	154.2
423		a	arg_328	ser_374	1.94	0.18	-10.34	1.50	157.4	162.5
424		a	ser_374	arg_328	1.95	0.18	-9.95	1.73	147.6	150.4

425		a	ile_427	ala_329	1.95	0.18	-10.21	1.41	162.9	167.7
426		a	ile_348	ala_360	1.92	0.20	-10.85	1.61	143.7	160.9
427		a	ala_360	ile_348	1.81	0.25	-13.39	2.10	147.2	157.1
428		a	val_358	ala_350	1.95	0.18	-9.65	1.88	160.5	143.2
429		a	phe_359	ile_379	1.88	0.21	-11.10	1.71	137.4	158.5
430		a	ile_379	phe_359	1.94	0.19	-10.34	1.59	146.3	158.3
431		a	leu_377	glu_361	2.13	0.12	-6.82	1.48	157	135.1
432		a	leu_375	ala_363	1.88	0.21	-11.48	1.71	140.7	161
433		a	lys_398	val_389	1.91	0.19	-10.81	1.77	159.3	153.7
434		a	asp_391	arg_396	2.41	0.07	-4.75	0.75	138.2	144
435		a	arg_396	asp_391	1.80	0.25	-13.82	1.84	153.9	170.8
436	**ALP (2H5C)**	p	ile_3	leu_76	2.62	0.04	-3.26	0.57	146.3	127.2
437		p	thr_74	ile_3	1.84	0.23	-12.79	1.77	165.4	166.7
438		p	gly_5	ala_80	1.78	0.26	-14.57	1.92	152.8	175.6
439		p	arg_78	gly_5	1.85	0.23	-12.41	1.81	146.6	163.6
440		a	tyr_9	cys_17	1.98	0.17	-9.59	1.34	163.9	168.4
441		a	cys_17	tyr_9	1.95	0.18	-10.01	1.43	146.8	165.7
442		a	ser_10	arg_45	2.05	0.15	-8.37	1.29	138.3	157.8
443		a	arg_45	ser_10	1.94	0.19	-10.28	1.54	145.5	160.7
444		a	ser_15	ile_11	1.98	0.17	-9.16	1.64	152.7	148.3
445		a	phe_21	val_32	2.02	0.15	-8.72	1.43	152.2	153.1
446		a	val_32	phe_21	2.56	0.05	-3.80	0.56	122.4	144.2
447		a	val_23	gly_30	2.10	0.13	-7.19	1.53	163.6	137.1
448		a	gly_30	val_23	1.93	0.19	-10.37	1.49	138.3	165.6
449		a	thr_24	ser_194	1.88	0.21	-11.87	1.62	153.5	169.3
450		a	ser_194	thr_24	1.91	0.20	-11.07	1.68	147.9	159.4
451		a	arg_25	thr_28	2.03	0.15	-8.15	1.36	129.6	153.5
452		a	thr_28	arg_25	1.83	0.23	-12.90	1.90	151	161.4
453		a	lys_29	leu_69	1.84	0.23	-12.74	1.71	144	172.3
454		a	phe_31	val_67	1.83	0.24	-13.23	1.77	162.9	170.9
455		a	val_67	phe_31	2.07	0.14	-7.92	1.36	141.1	150.1
456		a	thr_33	ala_65	2.25	0.09	-5.48	1.20	148.5	132.3
457		a	ala_65	thr_33	2.03	0.15	-8.41	1.29	145.7	159

458		a	ala_44	val_51	1.86	0.22	-12.12	1.63	150.1	174.9
459		a	gly_52	ala_44	1.88	0.21	-11.32	1.63	141.6	165.1
460		a	ala_49	ile_46	2.06	0.14	-8.00	1.38	160.9	149.6
461		a	thr_53	ser_68	1.95	0.18	-9.53	1.88	172.7	144
462		a	ser_68	thr_53	2.05	0.15	-8.38	1.28	148.2	158.1
463		a	trp_66	ala_55	1.95	0.18	-9.79	1.64	147	154.4
464		a	val_58	arg_64	1.99	0.17	-9.31	1.34	149.7	164.4
465		a	arg_64	val_58	1.86	0.22	-11.98	1.76	149.6	161.8
466		a	val_79	val_86	1.81	0.25	-13.62	1.88	151.2	167.1
467		a	val_86	val_79	1.98	0.17	-9.33	1.60	145.3	151.6
468		a	asn_81	ser_84	2.04	0.14	-7.71	1.72	139	137.4
469		a	ser_84	asn_81	1.93	0.19	-10.33	1.42	127.1	171.9
470		a	val_100	gly_112	1.84	0.23	-12.71	1.82	170.1	164.1
471		a	gly_112	val_100	1.95	0.18	-9.75	1.43	135.6	163.9
472		a	arg_102	gln_110	1.93	0.19	-10.56	1.55	154.8	162.6
473		a	gln_110	arg_102	1.86	0.22	-11.80	2.01	154.7	152.6
474		a	ser_146	ser_103	1.97	0.17	-9.29	1.72	152.6	147
475		a	gly_104	gly_108	2.27	0.09	-4.96	1.22	137.1	128.2
476		a	gln_133	thr_115	1.81	0.25	-13.11	1.99	141.5	160.9
477		a	ala_116	gln_133	1.81	0.24	-13.38	1.83	148.3	169.4
478		a	gln_133	ala_116	2.39	0.07	-5.01	0.73	135.2	157.1
479		a	val_119	leu_131	2.01	0.16	-8.84	1.49	143.2	151.9
480		a	leu_131	val_119	1.79	0.26	-14.45	1.96	146	170
481		a	ala_121	val_128	1.85	0.23	-12.58	1.77	153.9	165
482		a	val_128	ala_121	1.87	0.21	-11.81	1.81	159.3	158.9
483		a	gly_126	tyr_123	2.35	0.07	-4.58	0.93	135	132.7
484		a	thr_132	phe_181	1.81	0.25	-13.67	1.90	155.6	166.7
485		a	phe_181	thr_132	1.93	0.19	-10.50	1.61	162.1	158.7
486		a	gly_134	ser_179	2.11	0.13	-7.39	1.22	161.8	150.7
487		a	ser_179	gly_134	1.79	0.26	-14.38	1.88	159.5	176.2
488		a	gly_145	met_158	1.93	0.19	-10.16	1.81	136.9	150
489		a	trp_147	gln_155	1.78	0.26	-14.14	2.05	145	163.9
490		a	trp_147	gly_156	2.55	0.05	-4.04	0.57	136.3	146.9

491		a	gly_156	trp_147	1.96	0.17	-9.57	1.54	154.1	155.2
492		a	val_157	glu_182	1.94	0.18	-10.05	1.66	162.3	154.1
493		a	glu_182	val_157	1.98	0.17	-9.50	1.55	142.8	153.9
494		a	leu_180	ser_159	1.90	0.20	-10.93	1.82	147	153.7
495		a	gly_160	leu_180	1.77	0.26	-14.61	2.10	171	163.4
496		a	leu_180	gly_160	2.18	0.11	-6.83	1.00	141.8	162.1
497	**Fatty acid-binding protein (4tjz)**	a	thr_60	thr_53	1.91	0.20	-10.94	1.61	138.5	161.9
498		a	thr_53	thr_60	1.89	0.21	-11.48	1.81	147.3	155.8
499		a	ile_62	leu_51	1.88	0.21	-11.58	1.74	157.2	159.4
500		a	leu_51	ile_62	2.05	0.15	-8.27	1.26	143.3	158.3
501		a	phe_64	leu_49	1.81	0.25	-13.77	1.86	167.7	169
502		a	leu_49	phe_64	1.97	0.17	-9.37	1.73	150.8	146.8
503		a	ile_48	asn_45	1.91	0.20	-10.90	1.73	150.7	155.9
504		a	asn_45	ile_48	2.02	0.16	-8.74	1.23	130.3	167.7
505		a	thr_50	glu_43	1.93	0.19	-10.61	1.52	155.6	163.1
506		a	glu_43	thr_50	1.86	0.22	-12.19	1.77	150.7	162
507		a	lys_52	ile_41	1.89	0.21	-11.31	1.78	140.5	156.4
508		a	ile_41	lys_52	1.83	0.24	-13.21	1.87	152.4	164.1
509		a	his_54	thr_39	1.93	0.19	-10.61	1.63	148.8	158.2
510		a	thr_39	his_54	1.83	0.24	-13.17	1.94	151.2	160.4
511		a	thr_40	trp_8	1.95	0.18	-9.27	2.02	146	140.3
512		a	trp_8	thr_40	1.91	0.19	-10.56	1.85	143	150.7
513		a	ile_42	gly_6	1.92	0.20	-10.79	1.73	140.1	155.4
514		a	gly_6	ile_42	1.88	0.21	-11.72	1.73	152	160.7
515		a	thr_7	glu_131	1.84	0.23	-12.45	1.86	140.7	161.2
516		a	lys_9	glu_129	1.98	0.17	-9.56	1.56	147.5	153.3
517		a	glu_129	lys_9	1.89	0.21	-11.45	1.79	144.1	157
518		a	thr_127	val_11	1.76	0.27	-15.42	1.97	161	177.5
519		a	asp_12	thr_127	1.83	0.24	-13.00	1.84	142.4	164.6
520		a	thr_127	asp_12	2.45	0.06	-4.46	0.76	138.7	138.1
521		a	lys_14	thr_125	2.09	0.13	-7.48	1.42	138.1	143.6
522		a	thr_125	lys_14	1.96	0.17	-9.27	1.75	141.6	146.6
523		a	ala_122	his_119	2.16	0.12	-6.89	1.14	144.2	149.8

524		a	his_119	ala_122	2.08	0.13	-7.43	1.56	149.5	138.6
525		a	cys_124	leu_117	1.86	0.22	-12.34	1.85	145.8	159.8
526		a	leu_117	cys_124	1.85	0.23	-12.90	1.76	151.6	167.2
527		a	arg_126	leu_115	1.76	0.27	-15.41	1.97	163.9	177.1
528		a	leu_115	arg_126	1.80	0.25	-14.08	1.97	151.2	165
529		a	tyr_128	leu_113	1.95	0.18	-10.05	1.50	149.4	160.6
530		a	leu_113	tyr_128	1.79	0.25	-14.07	2.02	151	163.5
531		a	lys_112	ile_109	1.95	0.18	-10.18	1.55	152.5	158.5
532		a	ile_109	lys_112	1.90	0.21	-11.05	1.56	125.9	166.5
533		a	ile_114	glu_107	2.01	0.16	-8.75	1.52	139.7	150
534		a	glu_107	ile_114	1.77	0.27	-15.10	1.97	165.4	172.6
535		a	thr_116	val_105	1.86	0.22	-12.17	1.72	143.9	164.7
536		a	val_105	thr_116	1.81	0.25	-13.77	2.06	149	160
537		a	thr_118	thr_103	2.25	0.09	-6.00	0.95	145.3	149.7
538		a	thr_103	thr_118	2.02	0.16	-8.95	1.39	151.9	156.1
539		a	gln_100	trp_97	2.13	0.12	-7.09	1.14	134	153.9
540		a	trp_97	gln_100	1.83	0.23	-12.31	2.16	135.8	151.2
541		a	thr_102	gln_95	1.93	0.19	-10.99	1.42	164.5	171.5
542		a	gln_95	thr_102	2.08	0.14	-7.85	1.32	145.2	150.5
543		a	leu_104	his_93	1.89	0.21	-11.34	1.60	145.3	165.1
544		a	his_93	leu_104	1.85	0.23	-12.65	1.89	151	159.6
545		a	arg_106	leu_91	1.96	0.17	-9.52	1.78	148.8	146.7
546		a	leu_91	arg_106	1.87	0.22	-11.98	1.70	147.8	164.7
547		a	lys_90	asp_87	1.91	0.20	-10.99	1.84	144.3	152.3
548		a	val_92	thr_85	2.07	0.14	-7.76	1.41	138.2	145.7
549		a	thr_85	val_92	1.78	0.26	-14.58	1.88	160.6	175.6
550		a	leu_94	ile_83	2.12	0.12	-6.37	1.25	148.4	148
551		a	ile_83	leu_94	1.90	0.20	-11.41	1.62	167.8	164.6
552		a	lys_96	lys_81	1.86	0.22	-12.62	1.69	151.2	168.6
553		a	lys_81	lys_96	2.00	0.16	-8.71	1.69	138.2	145
554		a	val_80	glu_72	2.09	0.13	-7.75	1.22	152.8	153.7
555		a	glu_72	val_80	1.84	0.23	-13.02	1.75	162.2	169.2
556		a	ser_82	phe_70	1.92	0.19	-10.50	1.80	144.6	151.1

557		a	phe_70	ser_82	1.87	0.21	-11.77	1.75	155.2	160.1
558	**Cyto-chrome b5 reductase (5gv8)**	a	tyr_1014	phe_1113	1.87	0.22	-11.72	1.58	129.5	172.7
559		a	phe_1113	tyr_1014	1.80	0.25	-13.97	1.93	149.5	166.6
560		a	leu_1016	ile_1111	2.16	0.12	-7.05	1.08	141	155.6
561		a	ile_1111	leu_1016	1.89	0.21	-11.37	1.55	144.7	169.9
562		a	arg_1017	ala_1034	1.92	0.19	-10.78	1.67	161.2	156.7
563		a	arg_1032	ile_1019	1.83	0.24	-13.05	1.83	155.6	165.9
564		a	asp_1020	arg_1032	1.86	0.22	-12.42	1.63	149.4	177.3
565		a	arg_1032	asp_1020	2.37	0.07	-5.13	0.78	140.1	149.6
566		a	glu_1022	arg_1030	1.98	0.17	-9.61	1.48	137	157.7
567		a	arg_1030	glu_1022	1.81	0.25	-14.09	1.83	153.6	173.8
568		a	thr_1028	val_1024	2.15	0.12	-6.33	1.36	133.4	137.6
569		a	thr_1028	asn_1025	2.43	0.07	-4.88	0.66	125.1	168.3
570		a	arg_1029	ile_1081	1.85	0.22	-12.54	1.73	154.8	166.4
571		a	ile_1081	arg_1029	1.91	0.20	-11.14	1.54	153.2	166.7
572		a	phe_1031	leu_1079	1.86	0.22	-11.71	1.70	155.8	169.2
573		a	leu_1079	phe_1031	1.81	0.25	-13.78	1.92	162.5	165.4
574		a	phe_1033	val_1077	1.94	0.19	-10.46	1.54	151.4	160.4
575		a	val_1077	phe_1033	1.87	0.22	-12.25	1.62	160.4	173.1
576		a	his_1049	asn_1117	1.98	0.17	-9.12	1.74	151.9	144.8
577		a	asn_1117	his_1049	1.85	0.23	-12.84	1.73	155.3	168.9
578		a	ile_1050	tyr_1065	1.88	0.21	-11.61	1.62	149.1	166.3
579		a	tyr_1065	ile_1050	1.97	0.17	-9.71	1.42	165.5	161.9
580		a	tyr_1051	arg_1114	2.15	0.12	-6.34	1.67	143.7	130.5
581		a	arg_1114	tyr_1051	2.01	0.16	-8.97	1.39	134	157.3
582		a	leu_1052	arg_1063	2.01	0.16	-9.29	1.38	154.3	159.7
583		a	arg_1063	leu_1052	1.96	0.17	-9.72	1.60	169.9	153.2
584		a	glu_1112	ser_1053	2.17	0.11	-6.89	1.09	145.7	152.7
585		a	ala_1054	val_1061	1.92	0.19	-10.61	1.62	161.8	158.5
586		a	val_1061	ala_1054	2.07	0.14	-8.15	1.26	152.5	155.5
587		a	ile_1056	asn_1059	2.03	0.15	-8.49	1.17	122	174.3
588		a	asn_1059	ile_1056	1.82	0.24	-13.34	1.79	150.6	169.7
589		a	val_1121	ala_1129	1.81	0.25	-13.89	1.79	163.6	178

590		a	ala_1129	val_1121	1.95	0.18	-10.22	1.46	150.5	163.6
591		a	lys_1127	gln_1123	1.83	0.23	-12.44	2.14	153.7	152
592		a	phe_1128	lys_1141	1.90	0.21	-11.50	1.59	158.7	167.4
593		a	lys_1141	phe_1128	1.81	0.24	-13.75	1.77	158.8	178.1
594		a	ile_1130	val_1139	1.79	0.25	-13.85	2.09	139.5	159.9
595		a	val_1139	ile_1130	1.98	0.17	-9.41	1.40	135.8	160.9
596		p	ser_1145	leu_1241	2.36	0.07	-5.05	0.81	157.9	142.1
597		p	val_1146	his_1176	1.85	0.22	-12.40	1.70	169	168
598		p	val_1174	val_1146	1.89	0.20	-11.36	1.67	155	161.2
599		p	gly_1147	leu_1243	1.84	0.23	-12.81	1.69	149.9	173.5
600		p	leu_1241	gly_1147	1.94	0.18	-9.58	1.96	150.9	143.1
601		p	met_1148	leu_1178	1.79	0.25	-14.20	1.86	167.1	173.4
602		p	his_1176	met_1148	1.81	0.24	-13.36	1.96	165.7	160.2
603		p	ile_1149	cys_1245	1.97	0.17	-9.62	1.50	159.4	156.1
604		p	leu_1243	ile_1149	1.86	0.22	-12.28	1.79	154.3	162.2
605		p	ala_1150	ala_1180	1.76	0.27	-15.27	2.02	164.6	171.6
606		p	leu_1178	ala_1150	2.04	0.15	-8.41	1.29	151.2	157.9
607		p	cys_1245	gly_1151	1.91	0.20	-11.14	1.61	148.7	162.7
608		p	cys_1175	lys_1205	1.83	0.24	-13.28	1.80	160.4	168.8
609		p	leu_1177	trp_1207	2.09	0.13	-7.10	1.51	150.1	138.7
610		p	lys_1205	leu_1177	1.78	0.26	-14.52	1.87	157.6	177
611		p	phe_1179	thr_1209	1.99	0.17	-9.12	1.41	132.8	158.2
612		p	trp_1207	phe_1179	1.97	0.17	-9.24	1.60	146.5	151.1
613		p	thr_1209	asn_1181	2.15	0.12	-6.62	1.21	142.4	145.1
614		p	tyr_1208	ser_1220	2.09	0.13	-7.87	1.14	159.3	163.2
615		p	ser_1220	val_1210	2.23	0.10	-5.86	0.97	130.4	150.4
616		p	val_1242	phe_1270	1.85	0.22	-12.55	1.77	168.3	164.6
617		p	phe_1270	met_1244	1.95	0.18	-9.40	2.07	158.6	139.7
618	**Cu-containing nitrite reductase (5akr)**	p	val_38	val_15	2.07	0.14	-8.12	1.28	155.4	153.6
619		p	val_15	glu_40	1.81	0.24	-13.73	1.83	152.7	169.1
620		a	glu_46	thr_63	2.15	0.11	-6.34	1.21	124	142.5
621		a	thr_63	glu_46	1.93	0.19	-10.35	1.64	137	155.8
622		a	lys_48	ala_61	1.89	0.20	-11.04	2.04	160	146.7

623		a	ala_61	lys_48	2.09	0.13	-7.85	1.20	140.8	155.4
624		a	leu_50	ile_59	1.93	0.19	-10.73	1.59	151.9	159.2
625		a	ile_59	leu_50	1.98	0.17	-9.53	1.55	148.8	152.8
626		a	glu_118	asn_87	1.88	0.21	-11.89	1.59	165.6	167.3
627		a	thr_120	leu_85	1.84	0.23	-12.75	1.86	163.2	161
628		a	leu_85	thr_120	2.10	0.13	-7.42	1.35	143.7	144.3
629		a	leu_122	leu_83	1.92	0.19	-10.63	1.88	160.8	148.6
630		a	leu_83	leu_122	2.00	0.16	-9.32	1.48	150.5	153.5
631		a	phe_124	val_81	1.84	0.23	-12.57	1.99	166.5	155.7
632		a	val_81	phe_124	2.01	0.16	-9.03	1.53	147.4	149.6
633		p	tyr_80	val_39	1.78	0.26	-14.65	1.91	166.5	171.9
634		p	val_39	glu_82	1.90	0.20	-11.47	1.51	153.6	171.1
635		p	glu_82	phe_41	1.90	0.20	-11.21	1.58	151.1	164.1
636		p	phe_41	arg_84	1.89	0.21	-11.60	1.70	157.8	160.9
637		p	arg_84	met_43	2.01	0.16	-8.99	1.45	163.4	152.3
638		p	met_43	ile_86	2.00	0.16	-9.35	1.43	157.1	156.3
639		p	ile_86	ile_45	1.87	0.22	-12.21	1.66	176.2	167.4
640		p	ala_153	met_73	2.19	0.11	-6.74	1.00	143.6	156.8
641		p	met_73	met_155	1.76	0.27	-15.04	2.28	164.1	158.6
642		p	met_155	val_75	1.93	0.19	-10.79	1.57	162.6	160.5
643		p	val_75	leu_157	1.86	0.22	-12.27	1.80	150.9	161
644		a	tyr_134	gly_152	1.89	0.20	-11.41	1.68	145.7	160.3
645		a	ile_154	phe_132	1.92	0.19	-10.17	1.96	147.3	144.9
646		a	phe_132	ile_154	1.87	0.21	-11.87	1.88	151.8	155.3
647		a	val_156	gly_130	1.88	0.21	-11.57	1.97	133.8	151.4
648		a	gly_130	val_156	1.72	0.30	-16.99	2.14	159.4	176.8
649		a	his_135	asp_98	1.82	0.24	-12.93	1.95	144.1	159.2
650		a	asp_98	his_135	1.98	0.17	-9.47	1.61	145.3	150
651		a	leu_162	leu_170	1.95	0.18	-10.10	1.41	125.5	167.3
652		a	his_217	phe_183	1.89	0.20	-11.40	1.59	148.8	165.6
653		a	phe_183	his_217	2.53	0.05	-4.38	0.56	134.7	158.2
654		a	val_219	gln_181	1.86	0.22	-12.66	1.86	152.2	159.1
655		a	gln_181	val_219	2.01	0.16	-8.97	1.51	136.4	150.5

656		p	arg_240	lys_174	2.26	0.09	-6.04	0.95	154.3	149.7
657		p	lys_174	leu_242	1.98	0.17	-9.78	1.46	154	158.4
658		p	leu_242	tyr_176	2.01	0.16	-9.11	1.43	159.7	154.8
659		p	tyr_176	val_244	1.92	0.19	-10.84	1.71	169	154.9
660		p	val_244	val_178	1.82	0.23	-13.19	1.97	171.2	159.1
661		p	val_178	ser_246	2.17	0.11	-6.76	1.16	148.5	145.7
662		p	ser_246	glu_180	2.00	0.16	-9.48	1.27	158.4	168.5
663		a	val_241	tyr_293	1.97	0.17	-9.67	1.54	148	154
664		a	tyr_293	val_241	1.84	0.23	-12.95	1.81	151.5	164.1
665		a	val_243	ala_291	2.03	0.15	-8.59	1.33	135.4	156
666		a	ala_291	val_243	1.82	0.24	-13.47	1.95	157.4	161.1
667		a	his_245	gly_289	1.86	0.22	-12.58	1.76	161.9	163.8
668		a	gly_289	his_245	1.92	0.19	-10.71	1.54	146.6	161.9
669		a	gln_247	thr_287	2.38	0.07	-5.02	0.76	150.4	144.1
670		a	thr_287	gln_247	2.12	0.12	-7.51	1.08	157.3	159.8
671		a	ala_290	trp_265	1.89	0.20	-11.45	1.78	165.8	156
672		a	trp_265	ala_290	2.11	0.13	-7.47	1.17	133.9	154.2
673		a	phe_292	tyr_263	2.21	0.11	-6.68	0.98	141.7	157
674		a	tyr_263	phe_292	1.80	0.25	-14.02	1.96	158.5	164.2
675		a	gly_261	gln_278	2.11	0.12	-7.32	1.71	157.4	132.2
676		a	gln_278	gly_261	1.91	0.20	-10.94	1.70	142.1	156.9
677		a	val_264	asp_275	1.86	0.21	-11.95	2.06	156.3	150.6
678		a	asp_275	val_264	1.91	0.19	-10.41	2.10	138.4	143.2
679		p	his_319	leu_233	2.04	0.14	-8.30	1.63	168.3	141.1
680		p	leu_233	lys_321	1.86	0.22	-11.86	1.94	154.6	154
681		p	lys_321	ala_235	2.36	0.08	-5.24	0.79	142	148.9
682		p	ala_235	thr_323	2.02	0.16	-8.88	1.47	144.6	151.7
683		a	gly_318	tyr_303	1.84	0.23	-12.35	1.85	133.1	160
684		a	tyr_303	gly_318	1.83	0.23	-13.24	1.79	157.3	166.6
685		a	phe_320	tyr_301	1.94	0.19	-10.38	1.56	140.9	159
686		a	tyr_301	phe_320	2.03	0.15	-8.06	1.51	127.3	145.6
687		a	val_322	gly_299	1.85	0.23	-13.02	1.78	135.5	166.1
688		a	gly_299	val_322	1.95	0.18	-9.85	1.61	131.1	153.7

689		a	ala_302	ile_257	1.72	0.30	-16.71	2.24	152.6	168.1
690		a	val_304	his_255	2.19	0.11	-6.13	1.60	152.1	127.1
691		a	his_255	val_304	1.94	0.18	-10.39	1.56	152.2	158.7
692	**Crambin (1ejg)**	a	cys_3	ile_33	1.88	0.21	-11.72	1.88	155.5	153.9
693		a	ile_33	cys_3	1.97	0.17	-9.77	1.54	146.6	154.5

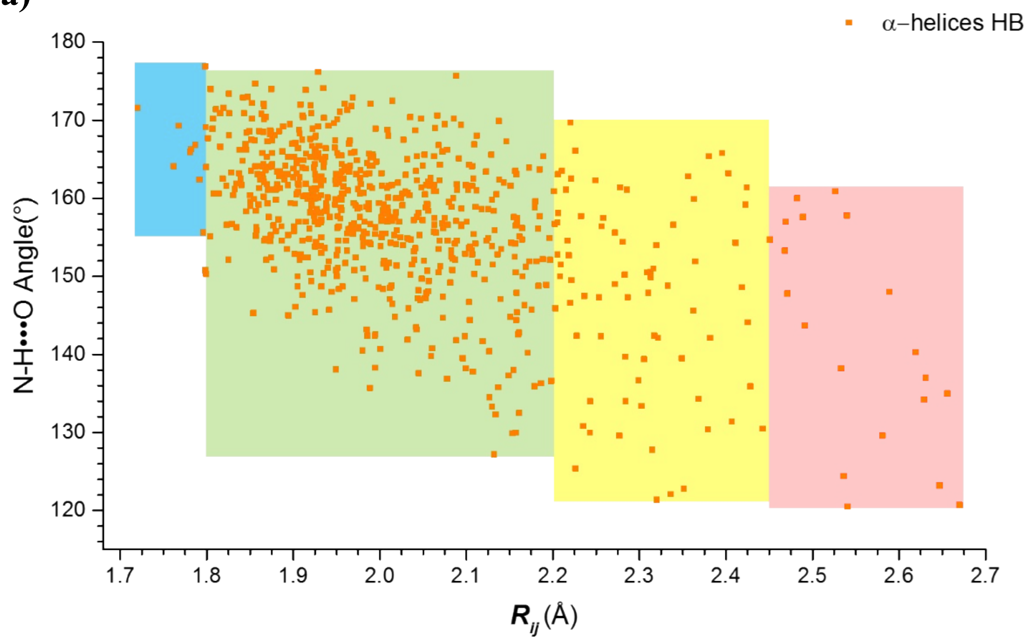
Estimated Error

These estimated errors are the standard deviation from the average (mean) of the entire population of ρ_{BCP}, E_{elec} and $\nabla^2\rho_{\text{BCP}}$ and obtained using the *STDEV.P* function in Microsoft Excel. These estimated errors provide some idea about the accuracy of the methodology as discussed in an earlier report.[1]

N-H···O and C=O···H angles of the α-helices and the β-sheets hydrogen bonds

The distributions of the ∠N-H···O and the ∠C=O···H across the ranges of R_{ij} and E_{elec} for the α-helices and the β-sheets hydrogen bonds as listed in **Table S1** and **Table S2** are also shown in **Figure S4 – S7**. The gradual deviation of the angles from its linearity with the increase of R_{ij} and decrease of E_{elec}, especially for the α-helices hydrogen bonds, is evident from these plots. Some outliers are also noticed.

(a)



(b)

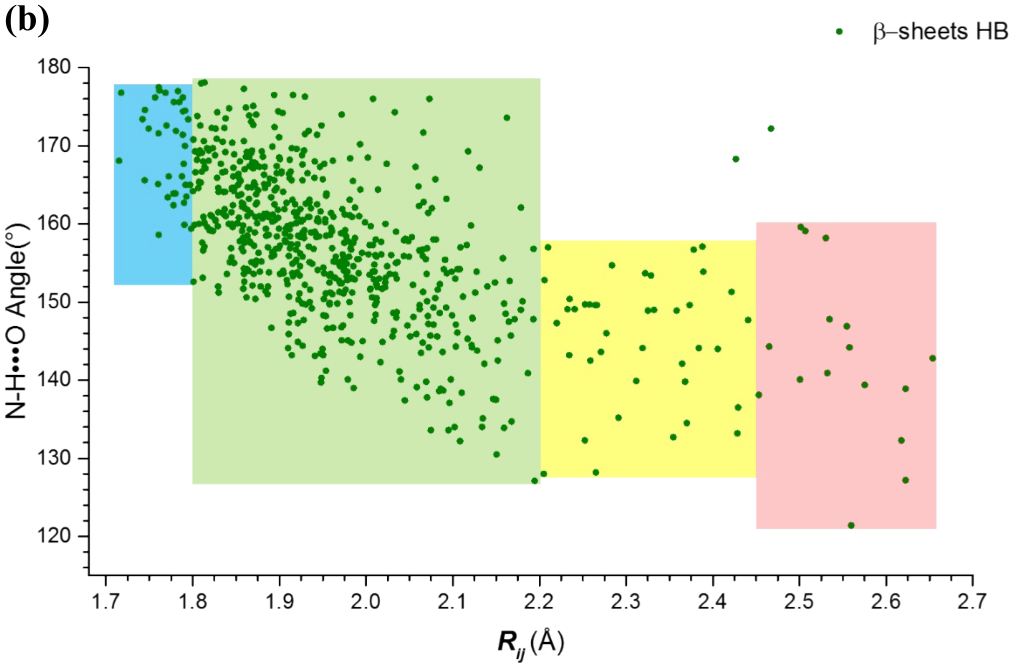
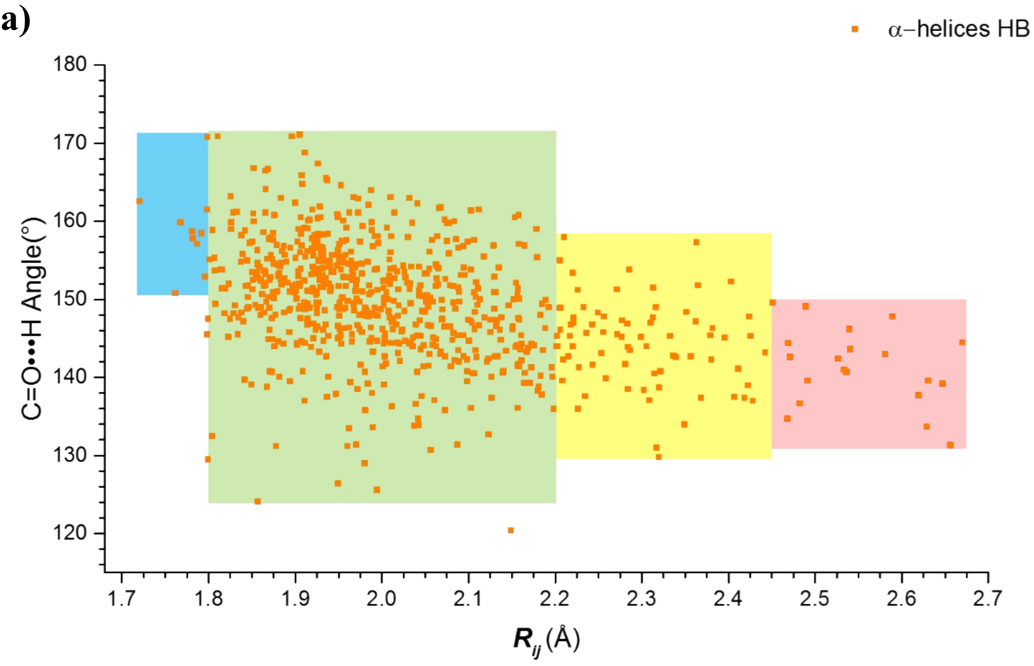


Figure S4: Distribution of the ∠N-H···O across the ranges of R_{ij} for **(a)** the α-helices and **(b)** the β-sheets HBs. The regions of the strongest, most populated, weaker and weakest HBs are highlighted using blue, green, yellow and pink colors, respectively.

(a)



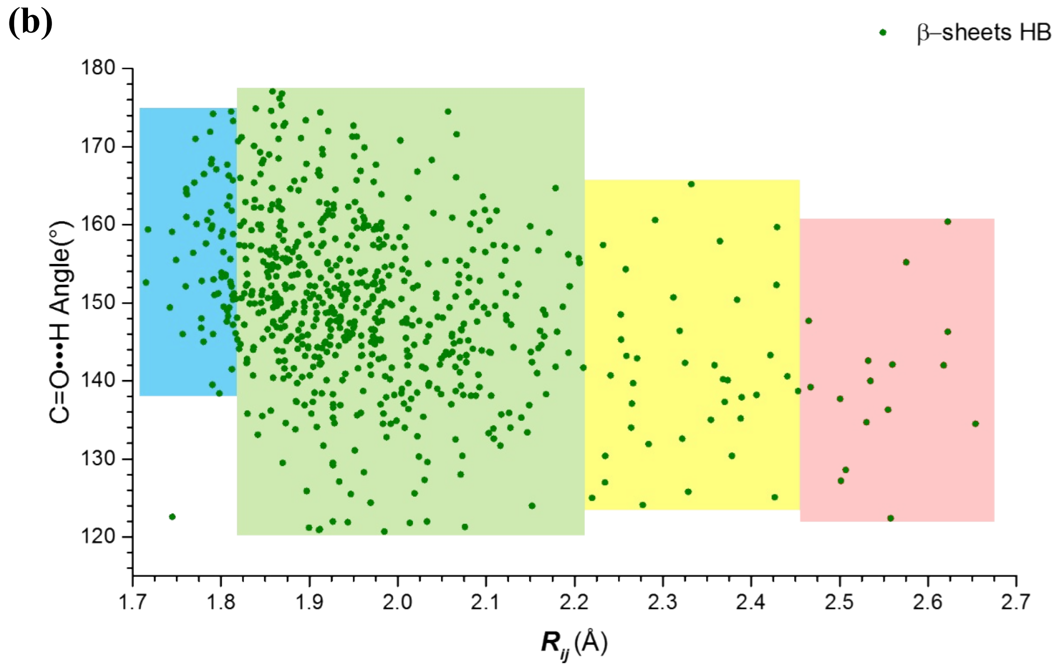
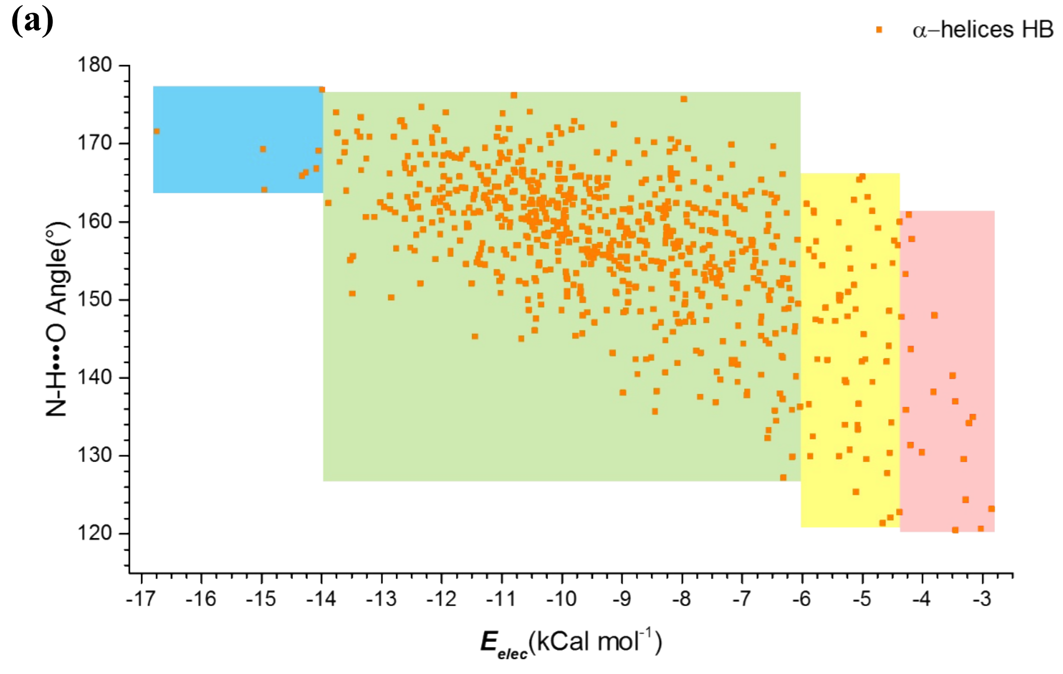


Figure S5: Distribution of the ∠C=O···H across the ranges of R_{ij} for **(a)** the α-helices and **(b)** the β-sheets HBs. The regions of the strongest, most populated, weaker and weakest HBs are highlighted using blue, green, yellow and pink colors, respectively.



(b)

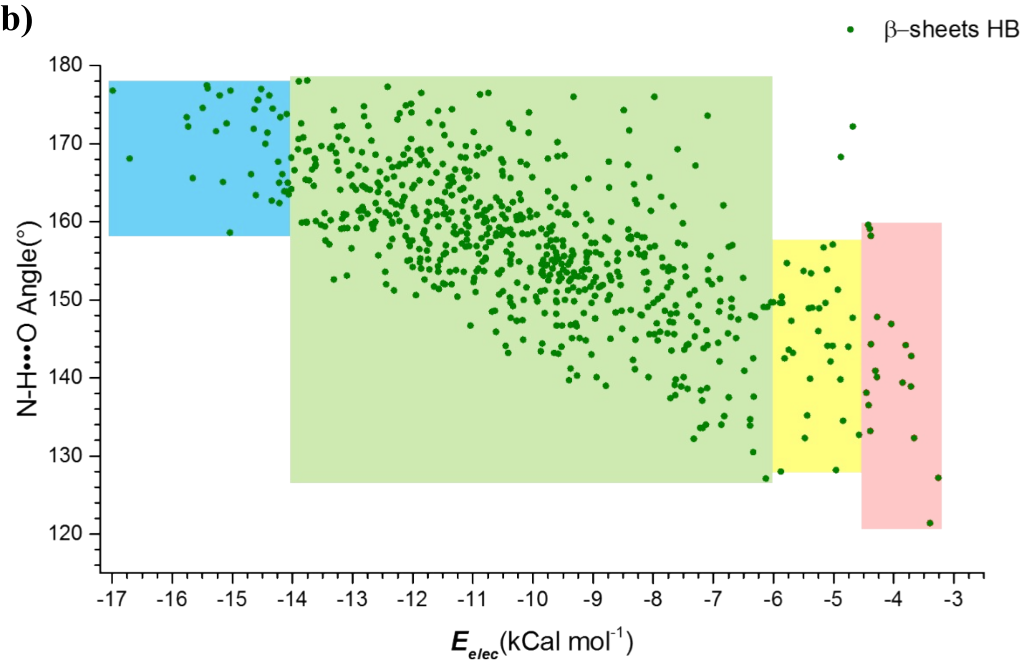
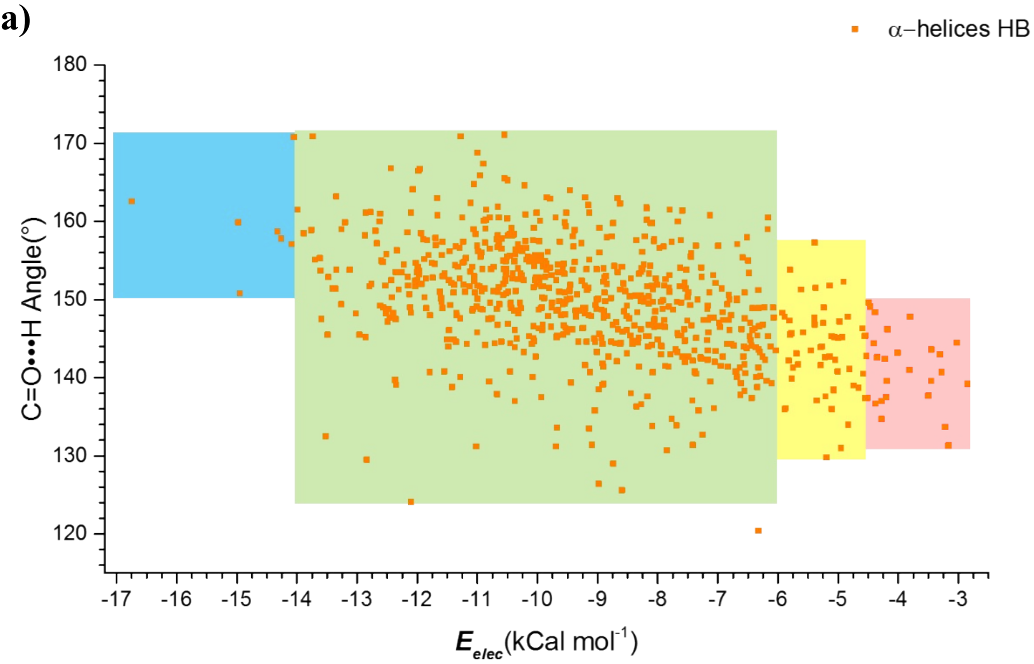


Figure S6: Distribution of the ∠N-H···O across the ranges of E_{elec} for **(a)** the α-helices and **(b)** the β-sheets HBs. The regions of the strongest, most populated, weaker and weakest HBs are highlighted using blue, green, yellow and pink colours, respectively.

(a)



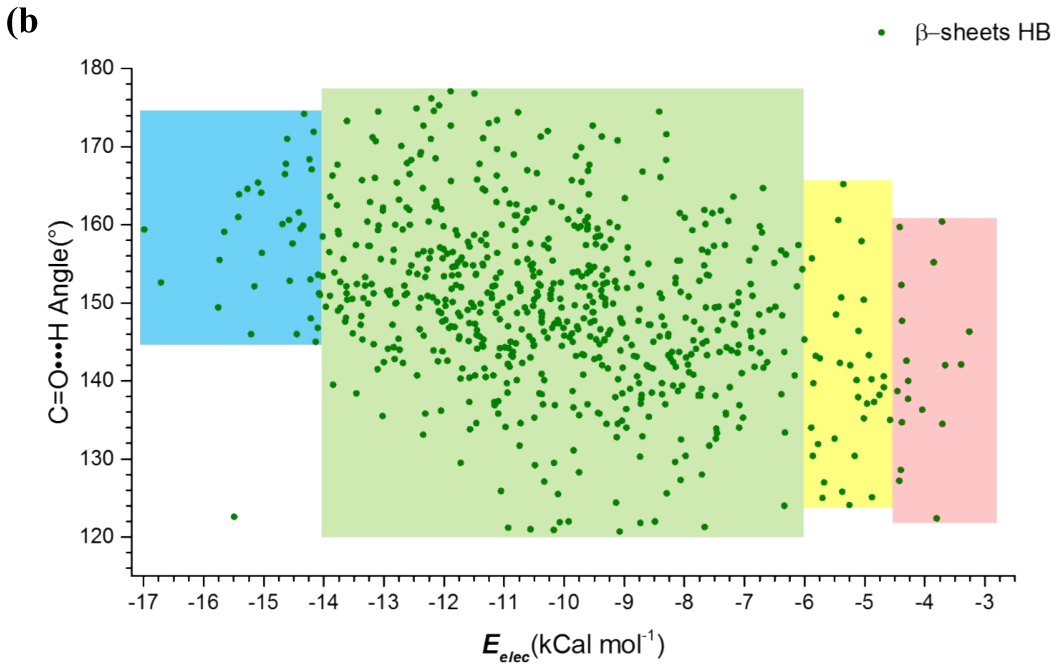


Figure S7: Distribution of ∠C=O···H across the ranges of E_{elec} **(a)** the α-helices and **(b)** the β-sheets HBs. The regions of the strongest, most populated, weaker and weakest HBs are highlighted using blue, green, yellow and pink colours, respectively.

Table S4: Ranges of ∠N-H···O and ∠C=O···H across the different regions of R_{ij} of the α-helices and the β-sheets HBs

Ranges of R_{ij}	∠N-H···O (°)		∠C=O···H (°)	
	α-helices HB	β-sheets HB	α-helices HB	β-sheets HB
<1.8 Å	156-177	152-178	151-171	138-175
1.8-2.2 Å	127-176	127-178	124-171	121-177
2.2-2.45 A	122-170	128-157	130-158	124-165
>2.45 Å	120-161	121-160	131-150	122-160

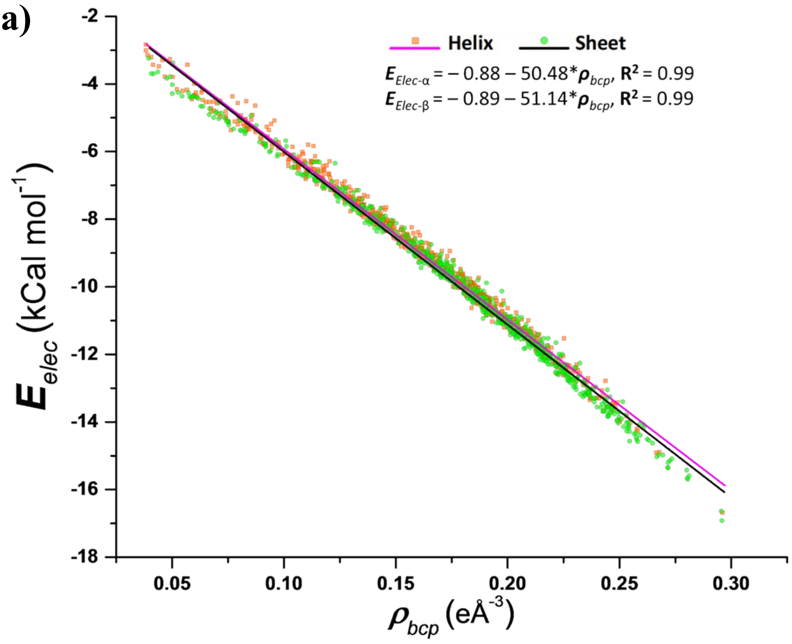
Table S5: Range of ∠N-H···O and ∠C=O···H across the different regions of E_{elec} of the α-helices and the β-sheets HBs

Ranges of E_{elec}	∠N-H···O (°)		∠C=O···H (°)	
	α-helices HB	β-sheets HB	α-helices HB	β-sheets HB
< -14 kCal mol^{-1}	164-177	158-178	151-171	145-174
-14 to -14 kCal mol^{-1}	127-176	127-178	124-171	121-177
-6 to -4.5 kCal mol^{-1}	122-166	128-157	130-157	124-165
> -4.5 kCal mol^{-1}	120-161	121-160	131-150	122-160

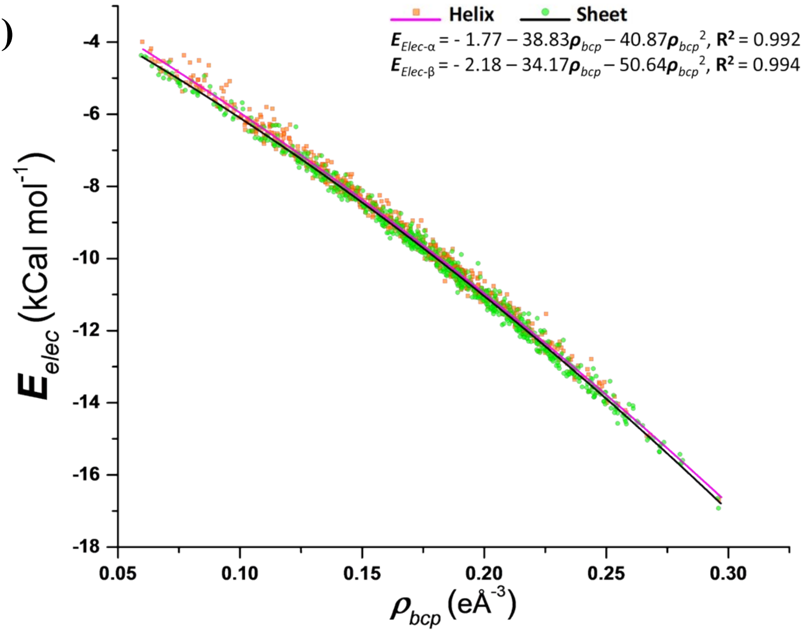
Table S6: The overall ranges of ∠N-H···O and ∠C=O···H for the α-helices, β-sheets and both (α-helices and β-sheets together) HBs.

Ranges of HBs	∠N-H···O (°)			∠C=O···H (°)		
	α-helices HB	β-sheets HB	both HBs	α-helices HB	β-sheets HB	both HBs
Strongest	156-177	152-178	152-178	151-171	138-175	138-175
Most Populated	127-176	127-178	127-178	124-171	121-177	121-177
Weaker	122-170	128-157	122-170	130-158	124-165	124-165
Weakest	120-161	121-160	120-161	131-150	122-160	122-160

(a)



(b)



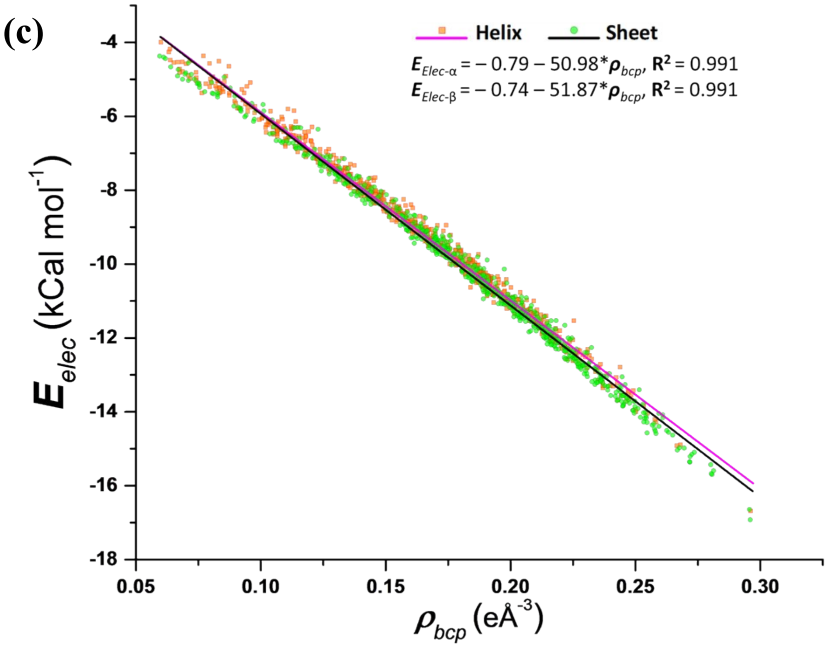


Figure S8 (a) Linear relationship between the ρ_{BCP} (eÅ^{-3}) and E_{elec} (kCal mol^{-1}) values of 1443 N-H···O=C HBs; **(b)** Quadratic and **(c)** Linear relationship between the ρ_{BCP} (eÅ^{-3}) and E_{elec} (kCal mol^{-1}) values of N-H···O=C HBs with $\rho_{BCP} > 0.06$ eÅ^{-3}

Table S7: Details of the terminal N-H…O=C HBs in the α-helices

PDB ID	**N-terminal HB**	**C-terminal HB**	**Weaker 2.2 Å < $R_{ij} \leq 2.45$ Å**	**Weakest ($R_{ij} \geq 2.45$ Å)**
5D8V	2	2	0	0
1EJG	2	2	0	0
2VB1	4	4	2	1
1US0	9	10	3	2
1YK4	1	0	0	1
4REK	10	11	1	3
1GCI	7	6	1	1
5GV8	5	6	3	0
1PQ7	3	2	0	0
3UI4	3	3	1	1
2H5C	1	1	1	0
2VXN	11	11	5	1
2PWA	6	6	1	1
2O9S	-	-	-	-
4EIC	5	4	0	0
1MC2	4	3	0	1
1PJX	-	-	-	-
4AYO	13	14	1	0
4O8H	2	2	0	0
4HS1	3	3	2	0
5AKR	3	3	2	0
4TJZ	2	2	1	0
Total	96	95	24	12

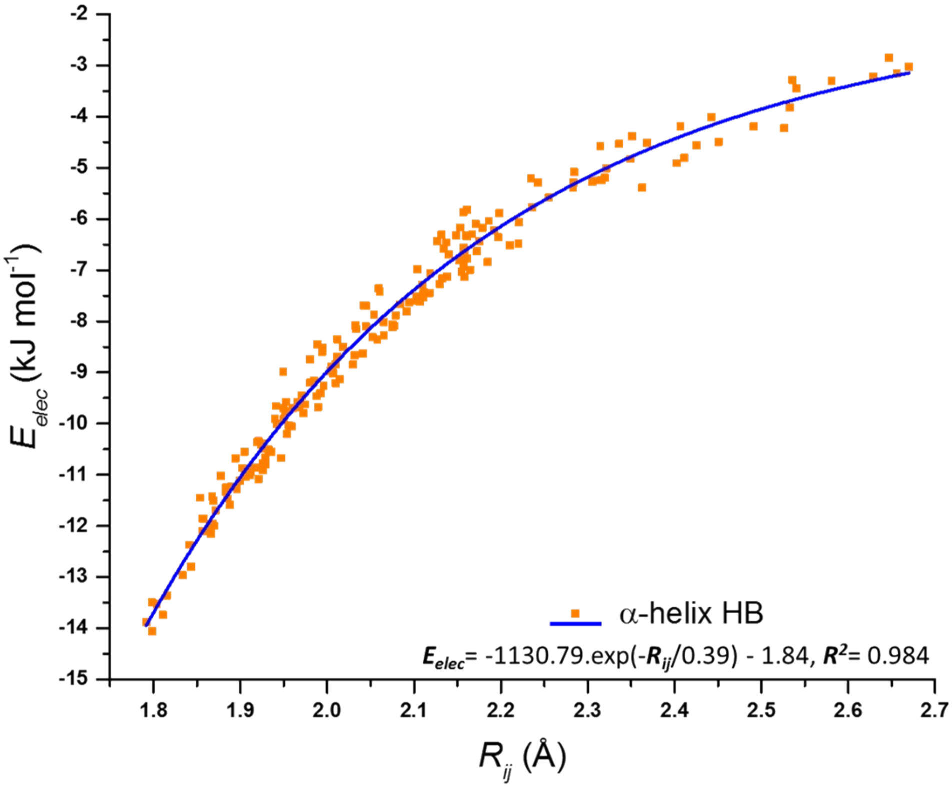


Figure S9: R_{ij} vs E_{elec} plot for the terminal HBs (total 191) of the α-helices.

Table S8: Percentage distributions of the HB populations in HEWL and glutaredoxin NrdH in the different regions of HBs.

Protein/ Resolution	HBs in	Regions of HBs (based on R_{ij})				Regions of HBs (based on E_{elec})			
		Strongest (%)	Most Populated (%)	Weaker (%)	Weakest (%)	Strongest (%)	Most Populated (%)	Weaker (%)	Weakest (%)
HEWL (2vb1)/ **0.65 A**	α-helices	3.23	87.10	6.45	3.23	3.23	83.87	9.68	3.23
	β-sheets	0.00	100.00	0.00	0.00	0.00	100.00	0.00	0.00
	overall	**2.86**	**88.57**	**5.71**	**2.86**	**2.86**	**85.71**	**8.57**	**2.86**
Glutaredoxin NrdH (4hs1)/ **0.87 A**	α-helices	0.00	86.36	13.64	0.00	0.00	86.36	13.64	0.00
	β-sheets	8.33	91.67	0.00	0.00	8.33	91.67	0.00	0.00
	overall	**2.94**	**88.24**	**8.82**	**0.00**	**2.94**	**88.24**	**8.82**	**0.00**

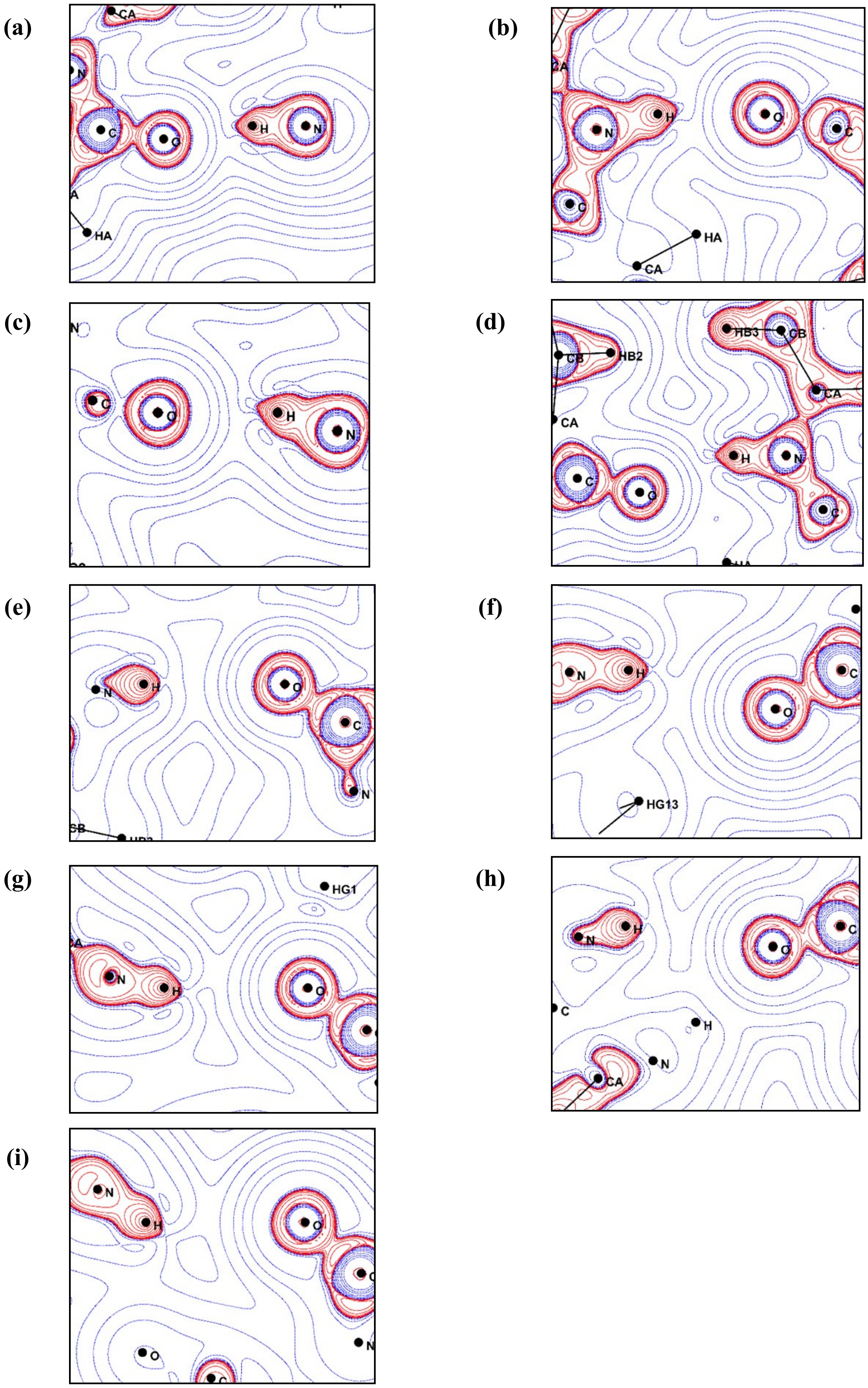
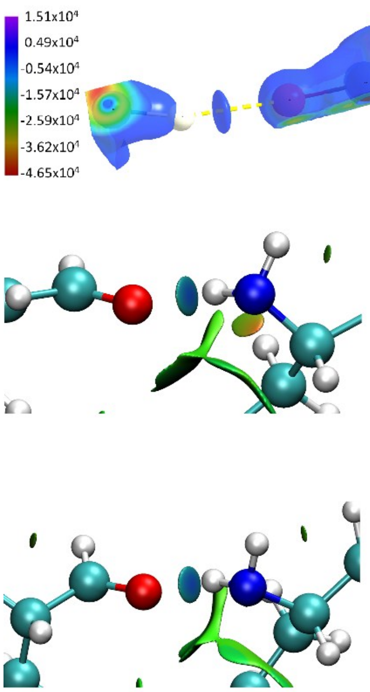


Figure S10 2D Laplacian drawn at logarithmic interval of -$\nabla^2\rho_{bcp}$ for N-H···O=C hydrogen bonds **(a)** in the strongest region (~1.72 Å) in one of the α-helices of proteinase K (2pwa), **(b)** in the strongest region (~1.74 Å) in one of the β-sheets of human aldose reductase (1us0), **(c)** from the most populated region (~1.95 Å) in one of the α-helices of 1us0, **(d)** from the most populated region (~1.95 Å) in one of the β-sheets of DFP-ase (1pjx), **(e)** from the weaker region (~2.44 Å) in one of the β-sheets of 1us0, **(f)** at the interface of weaker and weakest regions (~2.45 Å) in one of the α-helices of 1us0, **(g)** at the interface of weaker and weakest regions (~2.46 Å) in one of the α-helices of 1us0, **(h)** from the weakest region (~2.55 Å) in one of the β-sheets of 2pwa and **(i)** from the weakest (~2.6 Å) regions in one of the α-helices of 1us0.

Comparison of NCI Isourfaces

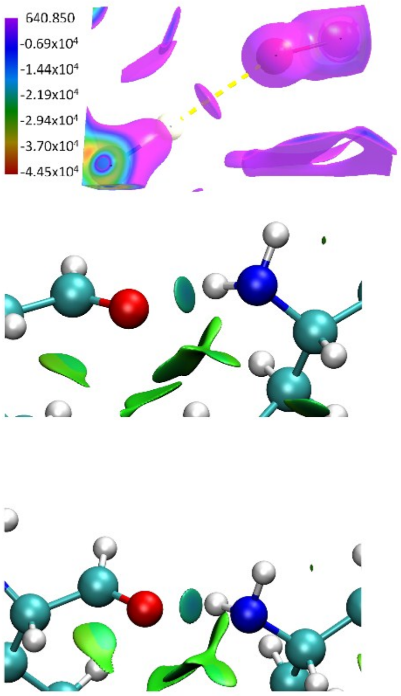
The *ELMAM2* based NCI isosurfaces of six representative H-bonds across the strongest to the weakest regions (three each of α-helices and β-sheets) plotted using *NCIMilano* are compared with those from the fully quantum mechanical calculation using MP2/6-311G(*d,p*) and promolecular electron densities. Latter isosurfaces were plotted using *NCIPlot*.

ELMAM2 based NCI isosurfaces were generated using the density cubes calculated for the N-H and C=O pairs forming the N-H···O=C HBs using *VMoPro*. Whereas, for the isosurface generation using the other two approaches, the fragment based method - Kernel Energy Method (KEM)[2] was employed. For this, the main-chain protein was fragmented to include only one residue and the N- and C-terminals were then capped with H-atoms placed at the same geometry as that of the C- and N-atoms, respectively, which were present in the peptide prior to the fragmentation. This approach was adopted in some earlier studies.[2,3] Subsequently, wavefunctions were calculated on two such residues forming the N-H···O=C HBs dimer. These wavefunctions were then used to generate the corresponding NCI isosurfaces,



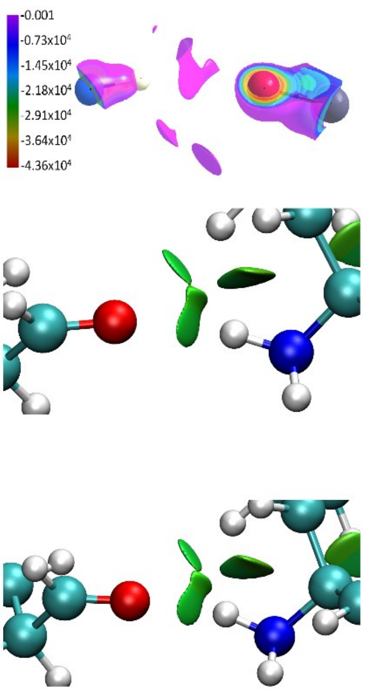
Strongest

R_{ij} = 1.79 Å
E_{elec} = -13.89 kCal/mol



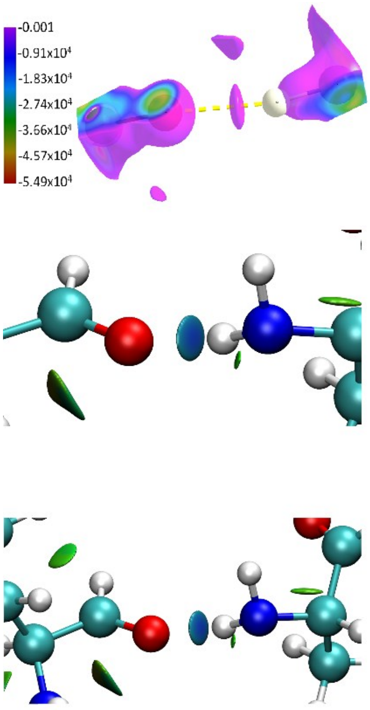
Most Populated

R_{ij} = 1.89 Å
E_{elec} = -11.23 kCal/mol



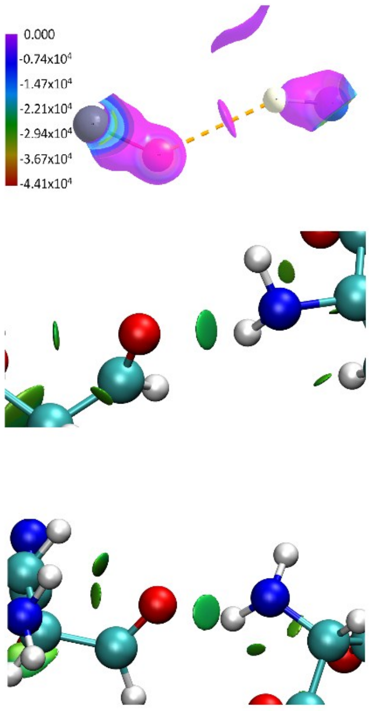
Weakest

R_{ij} = 2.62 Å
E_{elec} = -3.50 kCal/mol



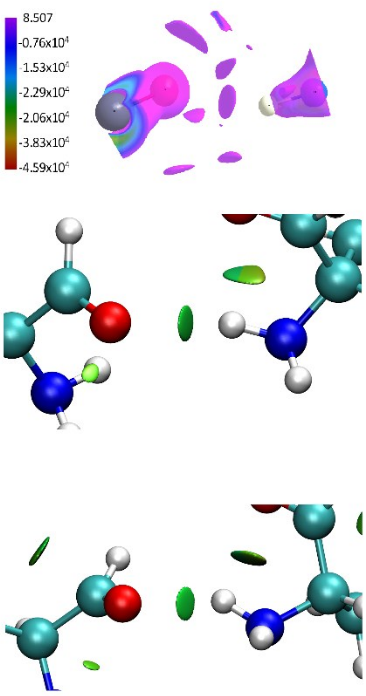
Strongest

R_{ij} = 1.74 Å
E_{elec} = -15.66 kCal/mol



Most Populated

R_{ij} = 1.90 Å
E_{elec} = -11.20 kCal/mol



Weakest

R_{ij} = 2.47 Å
E_{elec} = -4.38 kCal/mol

Figure S11 For the α-helices (up) and β-sheets (down), the NCI isosurfaces based on the electron densities derived from the multipolar analysis (top row, using *ELMAM2* and *NCIMilano*), fully quantum mechanical calculation (middle row, using Gaussian and *NCIPLOT*) and promolecular density (last row, using *NCIPLOT*) for the. For the former approach, the colour scale for sign(λ_2)ρ *au* is given on the left and for the latter approaches, the isosurfaces were generated at s=0.5 *au* and a colour scale of -0.03 < sign(λ_2)ρ < +0.03 *au*.

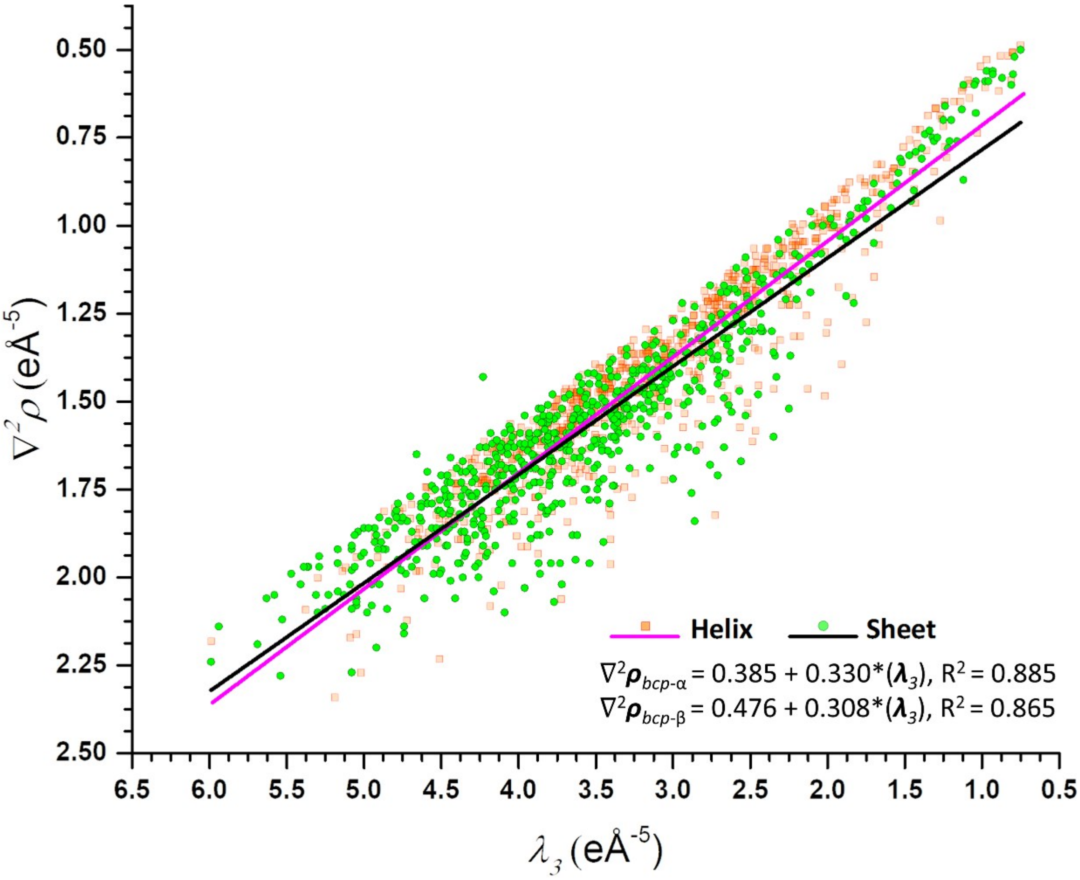


Figure S12. Linear relationship between the λ_3 (eÅ^{-5}) and $\nabla^2\rho_{BCP}$ (eÅ^{-5})

References:

1 D. Liebschner, C. Jelsch, E. Espinosa, C. Lecomte, E. Chabrière and B. Guillot, *J. Phys. Chem. A*, 2011, **115**, 12895–12904.

2 L. Huang, L. Massa and J. Karle, *Int. J. Quantum Chem.*, 2005, **103**, 808–817.

3 S. K. Mandal, P. Saha, P. Munshi and N. Sukumar, *Struct. Chem.*, 2017, **28**, 1537–1552.