ALPHA-CARBON COORDINATES FOR BOVINE CU,ZN SUPEROXIDE DISMUTASE

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Summary Preliminary α-carbon and metal coordinates are given for a subunit of the bovine erythrocyte Cu^{++},Zn^{++} superoxide dismutase. The coordinates are averaged from 5 sets of measurements made on electron density maps at 3Å resolution: one set from an averaged map and one set from each of the 4 crystallographically independent subunits (2 dimeric molecules) in the asymmetric unit of the crystal. The 3-dimensional structure of the polypeptide backbone is illustrated and briefly described.

The methods and the general results of the x-ray crystallographic investigation of bovine Cu^{++},Zn^{++} superoxide dismutase to 3Å resolution have been described elsewhere (1). The course of the polypeptide backbone chain has been traced and the metal ligands identified. Although the crystallographic work will be continued to higher resolution, preliminary α-carbon coordinates are listed here for the use of anyone wishing to make backbone models, drawings, or approximate distance calculations.

Bovine Cu,Zn superoxide dismutase crystallizes in space group C2, with 4 subunits (2 molecules) per asymmetric unit. At 3Å resolution the backbone conformation appears to be identical for all 4 crystallographically independent subunits. α-carbon, copper, and zinc coordinates were measured from the electron density map for each of the 4 subunits. An averaged map was calculated by transforming, interpolating, and averaging the numerical output of the Fourier calculation, and a set of coordinates was measured from the averaged map. All 5 coordinate sets were transformed to a common Cartesian coordinate system with the local twofold axis of the dimer along the y axis. The 5 sets were averaged,and dis-

	x	y	z		x	y	z		x	y	z
Ala 1	8.1	-13.8	4.1	Asn 51	-7.1	3.5	-1.5	Leu 101	-2.0	-14.9	15.3
Thr 2	9.1	-12.7	6.7	Thr 52	-9.6	4.8	-3.2	Ile 102	-1.2	-13.3	12.8
Lys 3	8.9	-8.6	6.7	Gln 53	-12.2	6.0	-1.4	Ser 103	0.0	-14.7	9.8
Ala 4	6.8	-5.5	7.0	Gly 54	-10.1	7.0	1.0	Leu 104	1.9	-13.6	7.2
Val 5	5.7	-2.2	5.7	Cys 55	-9.4	5.3	3.9	Ser 105	1.6	-16.4	5.2
Cysh 6	3.3	0.0	6.8	Thr 56	-12.7	4.8	3.4	Gly 106	-1.0	-17.6	4.3
Val 7	2.5	3.4	6.2	Ser 57	-12.4	2.1	1.7	Glu 107	-4.4	-17.6	5.3
Leu 8	0.5	5.7	7.3	Ala 58	-11.1	0.0	3.5	Tyr 108	-3.6	-15.2	7.5
Lys 9	-0.9	8.4	6.0	Gly 59	-13.1	-1.9	5.2	Ser 109	-2.2	-12.6	5.9
Gly 10	-3.7	11.2	5.8	Pro 60	-13.8	-3.8	7.5	Ile 110	-2.0	-9.2	6.4
Asp 11	-6.3	13.8	5.9	His 61	-12.4	-5.6	10.1	Ile 111	-0.9	-8.2	3.2
Gly 12	-5.0	15.4	8.3	Phe 62	-10.6	-9.0	9.8	Gly 112	-2.7	-6.2	1.4
Pro 13	-2.6	15.3	11.0	Asn 63	-12.1	-11.2	10.7	Arg 113	-4.1	-5.0	3.8
Val 14	-1.2	12.1	11.2	Pro 64	-12.1	-13.9	9.7	Thr 114	-4.9	-2.4	5.7
Gln 15	1.7	9.8	10.6	Leu 65	-13.8	-16.6	10.9	Met 115	-3.7	-0.9	8.7
Gly 16	3.3	6.8	10.3	Ser 66	-16.5	-14.9	12.0	Val 116	-5.6	1.3	10.8
Thr 17	5.5	4.2	10.5	Lys 67	-16.2	-13.3	14.9	Val 117	-5.6	4.2	13.0
Ile 18	5.2	0.6	10.6	Lys 68	-16.7	-10.6	17.3	His 118	-8.6	5.6	14.9
His 19	7.0	-2.3	11.4	His 69	-14.8	-8.0	18.8	Glu 119	-9.8	8.4	17.3
Phe 20	6.1	-5.8	11.0	Gly 70	-12.6	-8.1	20.7	Lys 120	-10.8	6.9	20.1
Glu 21	8.0	-9.3	11.8	Gly 71	-9.5	-7.6	22.1	Pro 121	-10.3	4.6	22.0
Ala 22	8.1	-12.8	11.5	Pro 72	-6.1	-8.4	21.7	Asp 122	-11.1	1.2	22.0
Lys 23	9.2	-14.6	14.0	Lys 73	-6.2	-11.3	23.4	Asp 123	-13.2	-0.8	24.0
Gly 24	7.6	-17.6	14.3	Asp 74	-9.5	-12.8	23.8	Leu 124	-12.0	-3.9	23.7
Asp 25	4.2	-18.1	15.5	Glu 75	-11.3	-15.6	22.5	Gly 125	-15.1	-5.6	23.6
Thr 26	4.3	-15.1	16.9	Glu 76	-13.1	-13.5	20.9	Arg 126	-17.5	-4.9	25.8
Val 27	3.8	-11.8	15.1	Arg 77	-10.9	-12.1	19.0	Gly 127	-19.2	-2.1	25.6
Val 28	5.6	-8.9	16.3	His 78	-10.9	-10.8	15.9	Gly 128	-23.3	-2.5	25.4
Val 29	5.0	-5.4	16.1	Val 79	-8.0	-11.0	13.5	Asn 129	-23.6	-1.7	22.3
Thr 30	6.7	-2.5	15.9	Gly 80	-7.6	-8.0	13.4	Glu 130	-23.9	-2.7	18.9
Gly 31	6.6	1.0	15.7	Asp 81	-7.6	-6.8	16.3	Glu 131	-20.7	-1.2	18.3
Ser 32	5.9	4.4	15.6	Leu 82	-5.4	-5.6	17.8	Ser 132	-19.0	-3.3	19.7
Ile 33	3.3	6.8	15.5	Gly 83	-5.4	-2.6	20.0	Thr 133	-19.4	-5.7	18.2
Thr 34	2.9	10.8	15.4	Asn 84	-4.7	0.3	21.6	Lys 134	-18.3	-4.4	15.4
Gly 35	0.1	13.4	15.1	Val 85	-2.3	2.5	21.2	Thr 135	-16.0	-1.8	16.7
Leu 36	-2.1	12.8	18.0	Thr 86	-1.1	5.0	23.6	Gly 136	-15.2	-0.1	19.2
Thr 37	-4.7	13.0	20.2	Ala 87	-0.3	8.6	23.2	Asn 137	-16.0	2.7	19.2
Glu 38	-4.2	12.0	23.8	Asp 88	2.0	12.4	23.9	Ala 138	-13.1	3.6	17.6
Gly 39	-4.2	9.0	23.9	Lys 89	1.7	15.9	24.3	Gly 139	-14.0	5.7	15.2
Asp 40	-5.6	6.4	23.1	Asn 90	3.4	16.7	22.0	Ser 140	-12.9	7.1	13.0
His 41	-6.1	4.8	20.0	Gly 91	2.4	13.8	19.8	Arg 141	-10.4	6.8	11.1
Gly 42	-6.7	2.5	17.8	Val 92	3.4	10.6	19.7	Leu 142	-7.2	8.5	10.5
Phe 43	-5.8	-0.2	16.1	Ala 93	3.3	6.6	19.8	Ala 143	-4.4	7.2	9.6
His 44	-6.9	-2.2	14.5	Ile 94	4.8	3.4	20.4	Cys 144	-3.9	4.8	7.2
Val 45	-6.5	-3.9	11.1	Val 95	4.5	0.2	18.9	Gly 145	-2.2	2.6	5.4
His 46	-8.9	-3.9	7.9	Asp 96	4.4	-2.8	20.8	Val 146	-1.1	-0.3	3.0
Glu 47	-9.9	-6.1	4.9	Ile 97	2.9	-6.0	19.9	Ile 147	0.8	-3.3	4.1
Phe 48	-8.8	-4.4	2.3	Val 98	3.1	-9.9	20.0	Gly 148	3.6	-4.6	2.8
Gly 49	-6.8	-2.5	0.9	Asp 99	0.5	-11.4	18.4	Ile 149	6.2	-6.8	2.2
Asp 50	-8.0	0.1	-1.3	Pro 100	-0.5	-14.5	18.0	Ala 150	9.9	-6.5	3.6
								Lys 151	13.6	-7.0	3.5
Cu	-10.4	-0.6	13.2	Zn	-12.2	-5.7	15.4				

Table I - Averaged α-carbon and metal coordinates for a subunit of bovine Cu,Zn superoxide dismutase. Coordinates are orthogonal and in Å. The transformation to obtain coordinates for the second subunit of a dimer molecule is: x'=-x, y'=y, z'=-z.

crepancies were reexamined on the individual electron density maps. The root mean square errors between the individual coordinate sets and the averaged coordinates given in Table I are between 0.8 and 0.9Å. No attempt has been made to refine these co-

	dihedral angle	bend angle	Cα-Cα dist. Å
	(180°)		
Ala 1		(71°)	
	0°		3.1
Thr 2		70°	
	78°		4.0
Lys 3		33°	
	306°		3.8
Ala 4		30°	
	123°		3.7
Val 5		50°	
	288°		3.4
Cysh 6		44°	
	117°		3.6
Val 7		40°	
	324°		3.2
Leu 8		46°	
	119°		3.3
Lys 9		28°	
	161°		4.0
Gly 10		2°	
	197°		3.6
Asp 11		85°	
	185°		3.2
Gly 12		36°	
	177°		3.6
Pro 13		70°	
	284°		3.5
Val 14		31°	
	120°		3.7
Gln 15		23°	
	347°		3.4
Gly 16		14°	
	130°		3.5
Thr 17		45°	
	326°		3.6
Ile 18		39°	
	152°		3.5
His 19		50°	
	333°		3.7
Phe 20		46°	
	164°		4.1
Glu 21		33°	
	19°		3.5
Ala 22		61°	
	164°		3.3
Lys 23		65°	
	91°		3.5
Gly 24		54°	
	73°		3.6
Asp 25		90°	
	151°		3.3
Thr 26		53°	
	4°		3.8
Val 27		62°	
	209°		3.6
Val 28		47°	
	61°		3.6
Val 29		39°	
	241°		3.4
Thr 30		32°	
	246°		3.5
Gly 31		9°	
	242°		3.5
Ser 32		35°	
	62°		3.5
Ile 33		42°	
	237°		4.0
Thr 34		42°	
	294°		3.9
Gly 35		75°	
	117°		3.7
Leu 36		19°	
	324°		3.4
Thr 37		62°	
	247°		3.8
Glu 38		71°	
	201°		2.9
Gly 39		33°	
	266°		3.1
Asp 40		48°	
	63°		3.5
His 41		20°	
	356°		3.3
Gly 42		28°	
	161°		3.2
Phe 43		38°	
	288°		2.8
His 44		37°	
	174°		3.8
Val 45		51°	
	22°		4.0
His 46		40°	
	269°		3.8
Glu 47		77°	
	298°		3.3
Phe 48		26°	
	163°		3.2
Gly 49		59°	
	298°		3.6
Asp 50		51°	
	135°		3.6
Asn 51		78°	
	226°		3.3
Thr 52		64°	
	262°		3.4
Gln 53		88°	
	165°		3.3
Gly 54		55°	
	126°		3.4
Cys 55		104°	
	217°		3.4
Thr 56		83°	
	279°		3.1
Ser 57		71°	
	9°		3.1
Ala 58		65°	
	208°		3.2
Gly 59		26°	
	206°		3.2
Pro 60		39°	
	122°		3.5
His 61		56°	
	18°		3.8
Phe 62		65°	
	164°		2.9
Asn 63		52°	
	341°		2.9
Pro 64		52°	
	16°		3.3
Leu 65		83°	
	297°		3.3
Ser 66		62°	
	73°		3.4
Lys 67		22°	
	330°		3.6
Lys 68		41°	
	261°		3.5
His 69		49°	
	22°		3.0
Gly 70		21°	
	319°		3.4
Gly 71		35°	
	233°		3.5
Pro 72		83°	
	253°		3.4
Lys 73		64°	
	1°		3.7
Asp 74		42°	
	251°		3.5
Glu 75		93°	

Table II - The bend angles and α-carbon to α-carbon distances needed to construct a wire backbone model (2) of the bovine Cu,Zn superoxide dismutase subunit. Such a model is shown in Fig. 4.

ordinates or to adjust them to give standard Cα-Cα distances.

Table I lists these averaged coordinates for the 151 α-carbons, the copper, and the zinc of one subunit of Cu,Zn superoxide dismutase; Table II lists the bend angles, dihedral angles,

	dihedral angle	bend angle	Cα-Cα dist. Å
	313°		3.2
Glu 76		78°	
	99°		3.3
Arg 77		43°	
	315°		3.3
His 78		56°	
	198°		3.7
Val 79		87°	
	248°		3.1
Gly 80		70°	
	0°		3.1
Asp 81		49°	
	136°		2.9
Leu 82		48°	
	1°		3.6
Gly 83		13°	
	5°		3.5
Asn 84		49°	
	206°		3.3
Val 85		52°	
	72°		3.7
Thr 86		49°	
	291°		3.7
Ala 87		25°	
	146°		4.5
Asp 88		36°	
	25°		3.6
Lys 89		83°	
	60°		3.0
Asn 90		85°	
	338°		3.8
Gly 91		50°	
	106°		3.4
Val 92		20°	
	312°		4.1
Ala 93		27°	
	164°		3.6
Ile 94		46°	
	22°		3.5
Val 95		58°	
	177°		3.5
Asp 96		53°	
	322°		3.7
Ile 97		32°	
	142°		4.0
Val 98		68°	
	328°		3.3
Asp 99		46°	
	177°		3.4
Pro 100		69°	
	210°		3.1
Leu 101		57°	
	326°		3.1
Ile 102		53°	
	173°		3.5
Ser 103		43°	
	359°		3.4
Leu 104		81°	
	51°		3.5
Ser 105		55°	
	34°		3.0
Gly 106		41°	
	40°		3.6
Glu 107		93°	
	97°		3.3
Tyr 108		71°	
	248°		3.4
Ser 109		45°	
	84°		3.5
Ile 110		81°	
	203°		3.6
Ile 111		58°	
	226°		3.1
Gly 112		86°	
	348°		3.0
Arg 113		29°	
	252°		3.3
Thr 114		43°	
	92°		3.7
Met 115		56°	
	306°		3.5
Val 116		33°	
	128°		3.7
Val 117		53°	
	310°		3.7
His 118		36°	
	192°		3.9
Glu 119		73°	
	226°		3.4
Lys 120		36°	
	147°		3.0
Pro 121		44°	
	34°		3.5
Asp 122		47°	
	237°		3.5
Asp 123		74°	
	96°		3.3
Leu 124		81°	
	48°		3.5
Gly 125		60°	
	123°		3.3
Arg 126		59°	
	247°		3.3
Gly 127		64°	
	137°		4.0
Gly 128		82°	
	231°		3.3
Asn 129		32°	
	122°		3.6
Glu 130		92°	
	195°		3.6
Glu 131		81°	
	259°		3.0
Ser 132		76°	
	318°		2.8
Thr 133		85°	
	345°		3.3
Lys 134		79°	
	327°		3.7
Thr 135		36°	
	223°		3.1
Gly 136		62°	
	134°		3.0
Asn 137		90°	
	268°		3.5
Ala 138		75°	
	93°		3.3
Gly 139		40°	
	119°		2.8
Ser 140		44°	
	7°		3.3
Arg 141		42°	
	152°		3.6
Leu 142		51°	
	198°		3.2
Ala 143		55°	
	28°		3.4
Cys 144		23°	
	196°		3.4
Gly 145		15°	
	71°		3.9
Val 146		57°	
	302°		3.7
Ile 147		49°	
	134°		3.3
Gly 148		18°	
	32°		3.5
Ile 149		54°	
	242°		4.0
Ala 150		26°	
	(62°)		3.7
Lys 151		(71°)	

and Cα-Cα distances needed for constructing a wire backbone model (2) such as the one shown in Fig. 4. The amino acid sequence is from Steinman, Naik, Abernethy, and Hill (3).

Figures 1-3 illustrate the α-carbon backbone conformation of the Cu,Zn superoxide dismutase subunit from the averaged coordi-

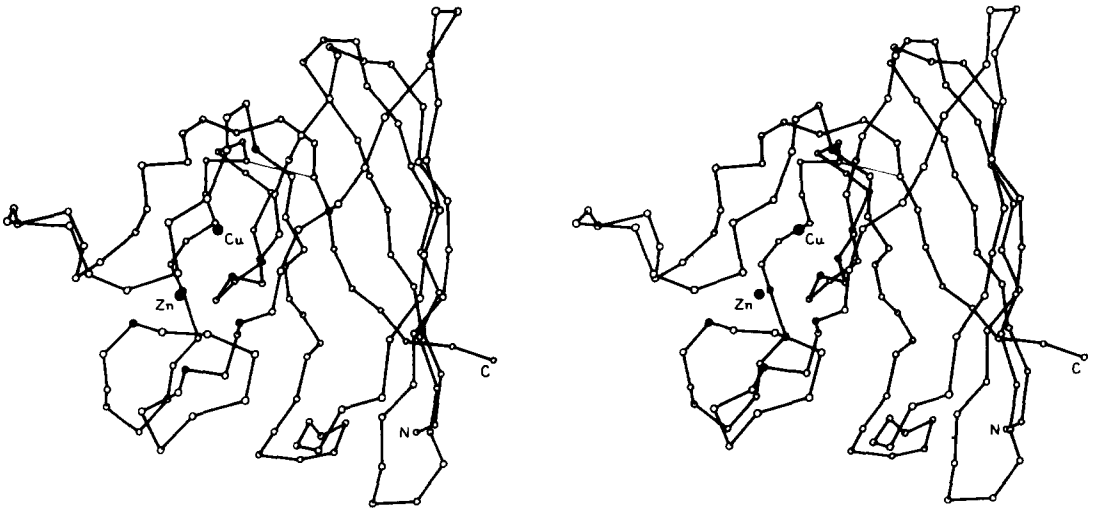

Fig. 1 - Stereo drawing of the α-carbon backbone of the Cu,Zn superoxide dismutase subunit, viewed down the +z coordinate axis. Both here and in Fig. 2 the disulfide bridge is indicated by a thin line, and the α-carbons of the 7 residues which contribute ligands to the metals are shown as solid circles.

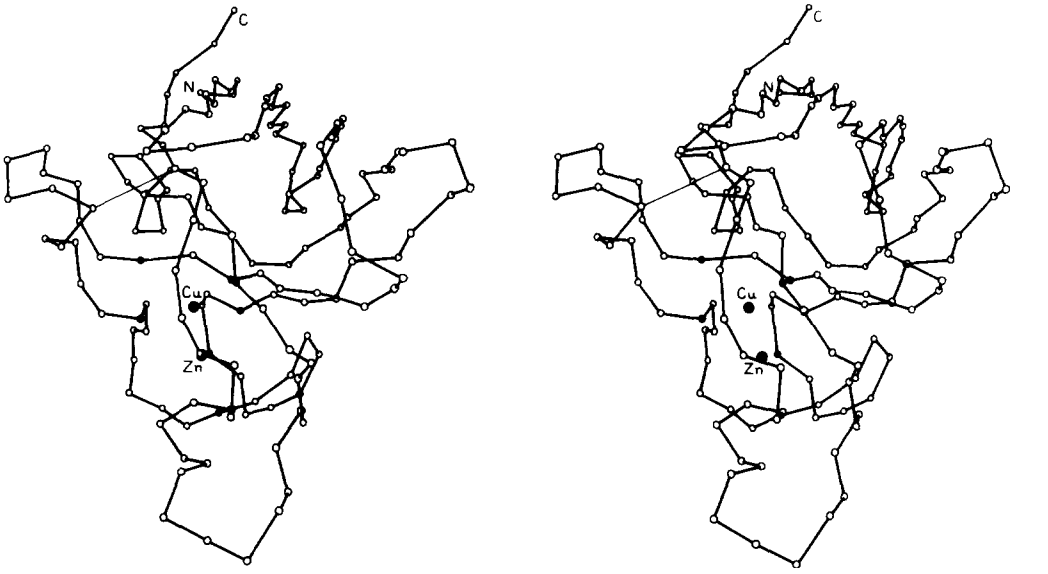

Fig. 2 - Stereo drawing of the α-carbon backbone of the Cu,Zn superoxide dismutase subunit. The direction of view is about 20° away from the +y coordinate axis (the local twofold axis of the dimer) and approximately down the axis of the β barrel.

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nates. They are redrawn from plots produced by Carroll Johnson's ORTEP program. The dominant structural feature of this molecule

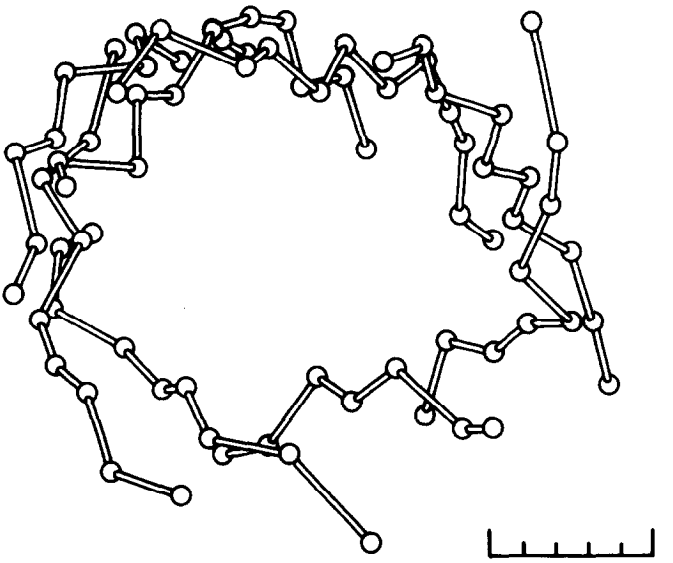

Fig. 3 - The 8 strands of antiparallel β structure in Cu,Zn superoxide dismutase, viewed from one end of the β barrel. The line at the lower right is a scale in Å. The residues included are 2-11, 13-24, 25-35,38-46,80-88,91-100,113-118, and 142-150.

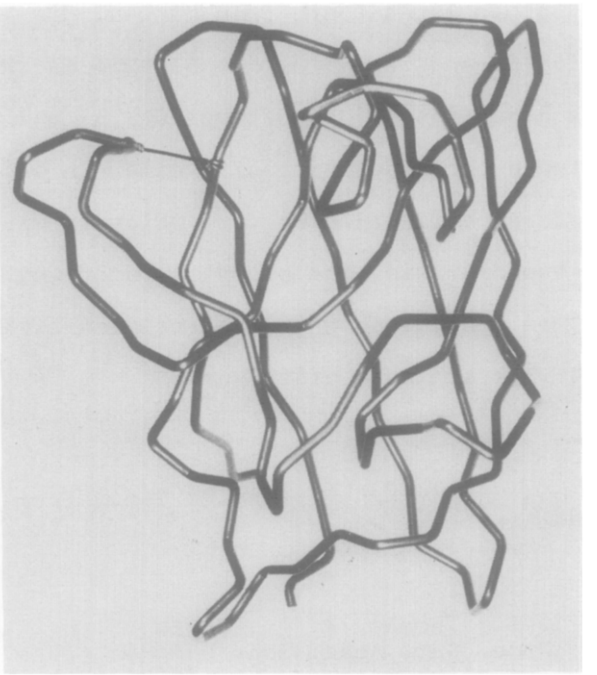

Fig. 4 - Photograph of a wire backbone model of the Cu,Zn superoxide dismutase produced from the bend angles and distances listed in Table II. The disulfide bridge (at upper left) is indicated by a thin wire. The direction of view is approximately down the -x coordinate axis, perpendicular to the views in Fig. 1 and 2.

is an 8-stranded barrel of antiparallel β structure, which is viewed from one end in Fig. 3, showing the fairly smooth curvature and the slight flattening from top to bottom. In Fig. 1, where the barrel is shown from one side, it can be seen that the spacing between most of the β strands is quite close and uniform (probably indicating extensive hydrogen bonding), but that the 2 strands in front are rather far apart. Diamond-shaped patterns are produced in Fig. 4 by the characteristic twist of the β sheet, which causes the front set of 4 β strands to cross the back set of 4 β strands at an angle of about 45° in that projection.

The one very short section of α-helix is directly below the Zn in Fig. 2, on one of the two exposed external loops. The copper and zinc are only 6Å apart, with a common histidine ligand, and they are bound between the external loops and one side of the β barrel. The copper ligands are from His 44, His 46, His 61, and His 118; the zinc ligands are from His 61, His 69, His 78, and Asp 81. There is a disulfide bridge between Cys 55 and Cys 144. The interaction between the 2 subunits of a dimer is discussed and illustrated in reference (1). In Fig. 2, which is viewed almost down the local twofold axis, the second subunit would lie above and to the left of the one shown, with residues 1, 5-7, 17, 47-52, 105-113, and 145-151 at the contact surface.

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