Supplementary Information for

Real-Time Structure Search and Structure Classification for AlphaFold Protein Models Tunde Aderinwale^{1,†}, Vijay Bharadwaj^{1,†}, Charles Christoffer¹, Genki Terashi², Zicong Zhang¹, Rashidedin Jahandideh¹, Yuki Kagaya² & Daisuke Kihara^{1,2,*}

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Supplementary Table 1. Fold classification accuracy by 3DZD and the deep neural network.

Method	3DZD Type	Threshold	Accuracy	Precision	Recall	F-Measure
		0.1	0.903	0.839	0.997	0.911
		0.2	0.929	0.881	0.993	0.933
		0.3	0.943	0.908	0.987	0.945
		0.4	0.951	0.928	0.977	0.952
	Full Atom	0.5	0.954	0.945	0.964	0.954
		0.6	0.953	0.959	0.945	0.952
		0.7	0.946	0.971	0.919	0.944
		0.8	0.930	0.983	0.875	0.926
		0.9	0.879	0.994	0.763	0.863
3DZD-NN						
		0.1	0.928	0.877	0.996	0.933
		0.2	0.95	0.913	0.994	0.952
		0.3	0.962	0.936	0.991	0.963
	Main Chain	0.4	0.969	0.951	0.988	0.969
		0.5	0.974	0.964	0.984	0.974
		0.6	0.977	0.974	0.979	0.977
		0.7	0.976	0.982	0.97	0.976
		0.8	0.969	0.989	0.948	0.968
		0.9	0.941	0.993	0.888	0.938
		0.05	0.500	0.500	1.000	0.667
		0.1	0.508	0.504	0.998	0.670
		0.15	0.624	0.604	0.717	0.656
		0.2	0.622	0.823	0.312	0.452
		0.3	0.523	0.999	0.047	0.089
		0.4	0.507	1.000	0.014	0.028
	Full Atom	0.5	0.503	1.000	0.005	0.010
		0.6	0.501	1.000	0.002	0.004
		0.7	0.500	1.000	0.001	0.002
		0.8	0.500	1.000	0.000	0.000
		0.9	0.500	1.000	0.000	0.000
3DZD		0.05	0.500	0.500	1 000	0.((7
		0.05	0.500	0.500	1.000	0.66/
		0.1	0.616	0.571	0.939	0./10
		0.15	0.679	0.739	0.553	0.632
		0.2	0.608	0.966	0.223	0.363
	Main Chain	0.3	0.527	0.999	0.055	0.104
		0.4	0.511	1.000	0.022	0.043
		0.5	0.505	1.000	0.010	0.019
		0.6	0.502	1.000	0.004	0.008
		0.7	0.500	1.000	0.001	0.002
		0.8	0.500	1.000	0.000	0.000
		0.9	0.500	1.000	0.000	0.000

Fold classification accuracy using different score cutoff values. The classifications were computed on a dataset of 167,872 protein pairs constructed from 2,521 protein domain structures from SCOPe. Positive and negative pairs were balanced. First, we made all possible protein pairs from the same fold, which turned out to be 83,936. Then we downsampled negative pairs to match the number of the positive pairs. Protein pairs were input to 3DZD-NN or 3DZD to obtain a probability (3DZD-NN) or a score (3DZD) that the protein pair belong to the same fold. In Table 3, we reported results obtained by using cutoff values of 0.6, 0.5, and 0.1 for 3DZD-NN mainchain, 3DZD-NN full-atom, and 3DZD, respectively, because these cutoffs gave the best F-scores among other cutoff values tried. In this table, cutoffs of 0.05 and 0.15 were used only for 3DZD to confirm that 0.1 is the best cutoff.





Fold recognition accuracy of 3DZD and 3DZD-NN were compared with SPalignNS. 5,000 protein pairs are randomly sampled with 2500 positive (i.e. the same fold pairs) and negative pairs, respectively. The pairs were ranked based on the scores of pairs computed by each method. The evaluation was made on 4,228 pairs where SPalignNS did not fail to run. For the rest of 772 cases, SPalignNS encountered an error and did not run.

Supplementary Figure 2. Database search results for examples shown in Fig. 4.



From two structures presented as examples of false positives in Fig. 4, d2jj2f2 and 5mko-a, the entire PDB was searched using 3DZD-NN with the main-chain representation. All structures retrieved within the top 25 for each query have the same fold as the query. Thus, although particular structure pairs with these queries were misrecognized as the same fold by 3DZD-NN and 3DZD as shown in Fig. 4, such relatively weak false positives do not affect the top hits in a database search.

Supplementary Table 2: Top-10 folds of AlphaFold2 models for individual species.

Methanocaldococcus jannaschii	Mycobacterium tuberculosis
1. TIM beta/alpha-barrel (c.1)	1. BAR/IMD domain-like (a.238)
2. Non-globular all-alpha subunits of globular prote	ins (a.137) 2. ROP-like (a.30)
3. L-aspartase-like (a.127)	3. TIM beta/alpha-barrel (c.1)
4 Perinlasmic binding protein-like II (c. 94)	4 Non-globular all-alpha subunits of globular proteins (a 137)
5 P-loop containing pucleoside triphosphate hydrol	ases (c 37) 5 PI P-dependent transferase-like (c 67)
6 ROP-like (2.30)	6 Intrinsically disordered proteins (a 88)
0. ROI-like $(a.50)$ 7. alpha alpha superbalix $(a, 118)$	7. NAD(D) hinding Desember fold domains (c. 2)
7. alpha-alpha superiority (a.116) 8. DI D demondent transformed life (a.(7))	7. $\frac{\text{NAD}(\mathbf{r}) - \text{offiding Rossinalini-tota domains (c.2)}}{1 - \frac{1}{2}}$
8. PLP-dependent transferase-like (0.07)	$\begin{array}{ccc} 0 & \mathbf{L} - \mathbf{a} \mathbf{spartase} - \mathbf{i} \mathbf{k} \mathbf{c} \left(\mathbf{a} \cdot 1 2 \right) \\ 0 & \mathbf{N} - \mathbf{i}^{T} \mathbf{c} \mathbf{c} 1 \\ 1 & 1 \\ 1 & 1 \mathbf{c} 1 \\ 1 & 1 \\ 1 & 1 \mathbf{c} 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 $
9. Knabdovirus nucleoprotein-like (a.260)	9. Mediator ninge subcomplex-like $(a.252)$
10. Bacillus chorismate mutase-like (d. 79)	10. <u>alpha/beta-Hydrolases (c.69)</u>
Staphylococcus aureus	Escherichia coli
1. ROP-like (a.30)	1. <u>TIM beta/alpha-barrel (c.1)</u>
2. Non-globular all-alpha subunits of globular prote	ins (a.137) 2. L-aspartase-like (a.127)
3. <u>TIM beta/alpha-barrel (c.1)</u>	3. <u>Periplasmic binding protein-like II (c.94)</u>
4. L-aspartase-like (a.127)	4. Non-globular all-alpha subunits of globular proteins (a.137)
5. PLP-dependent transferase-like (c.67)	5. PLP-dependent transferase-like (c.67)
6. Acyl-CoA N-acyltransferases (Nat) (d.108)	6. ROP-like (a.30)
7. S-adenosyl-L-methionine-depdt methyltransferas	es (c.66) 7. Mediator hinge subcomplex-like (a.252)
8. BAR/IMD domain-like (a.238)	8. Penicillin binding protein dimerisation domain (d.175)
9 Rhabdovirus nucleoprotein-like (a 260)	9 InaD-like (a 250)
10 Periplasmic binding protein-like II (c 94)	10 $Flavodovin-like (c 23)$
10. Templasinie bildnig protein-like ii (0.94)	10. <u>114/0407/m-mkc (0.25)</u>
Saccharomyces cerevisiae	Candida albicans
1. Non-globular all-alpha subunits of globular prote	ins (a.137) 1. Non-globular all-alpha subunits of globular proteins (a.137)
2. ROP-like (a.30)	2. ROP-like (a.30)
3. Mediator hinge subcomplex-like (a.252)	3. Mediator hinge subcomplex-like (a.252)
4. Intrinsically disordered proteins (g.88)	4. N-terminal domain of bifunctional PutA protein (a.176)
5. N-terminal domain of bifunctional PutA protein ((a.176) 5. Intrinsically disordered proteins (g.88)
6. BAR/IMD domain-like (a.238)	6. BAR/IMD domain-like (a.238)
7 L27 domain (a 194)	7 Spectrin repeat-like (a 7)
8 Histone-fold (a 22)	8 SRF-like (d 88)
9 L-aspartase-like $(a \cdot 127)$	9 $I_{aspartase-like}$ (a 127)
10 Spectrin repeat-like (a 7)	10. Tetracyclin repressor like C terminal domain (a 121)
Sebizosaechanomyees nombe	Diatuestalium dissoideum
1 Non globular all alpha gubunita of globular prote	ing (a 127) 1 Non-globular all alpha gubunita of globular protaing (a 127)
1. Non-globular an-alpha subulitis of globular prote $2 - p_{OD} = \frac{1}{1 - a} \left(- \frac{20}{a} \right)$	(a.157) 1. Non-globular an-alpha subulitis of globular proteins $(a.157)$
2. $ROP-like (a.30)$	2. $ROP-like (a.30)$
5. Niediator hinge subcomplex-like (a.252)	3. Mediator hinge subcomplex-like $(a.252)$
4. N-terminal domain of bifunctional PutA protein ($(a.1/6) \qquad 4. \text{BAR/IMD domain-like } (a.238)$
5. BAR/IMD domain-like (a.238)	5. Intrinsically disordered proteins (g.88)
6. <u>alpha-alpha superhelix (a.118)</u>	6. N-terminal domain of bifunctional PutA protein (a.176)
7. Intrinsically disordered proteins (g.88)	7. CsrA-like (b.151)
8. Spectrin repeat-like (a.7)	8. L27 domain (a.194)
9. L-aspartase-like (a.127)	9. SRF-like (d.88)
10. SRF-like (d.88)	10. Histone-fold (a.22)
Plasmodium falciparum	Trypanosoma cruzi
1. Non-globular all-alpha subunits of globular protein	ns (a.137) 1. Non-globular all-alpha subunits of globular proteins (a.137)
2. ROP-like (a.30)	2. ROP-like (a.30)
3. Mediator hinge subcomplex-like (a.252)	3. Mediator hinge subcomplex-like (a.252)
4. N-terminal domain of bifunctional PutA protein (a	. 176) 4. N-terminal domain of bifunctional PutA protein (a. 176)
5 BAR/IMD domain-like (a 238)	5 Intrinsically disordered proteins (g 88)
6 I 27 domain (a 194)	6 L.27 domain (a 194)
7 SRF_like $(d. 88)$	7 BAR/IMD domain-like (a 238)
7. SIXI-IIK (0.00) 8. Intrinsically disordered protoins (a 99)	$\begin{array}{c} 7. & \text{Driving domain-nkc} (a.230) \\ 8. & \text{A} = 2221 \text{ like} (d.227) \end{array}$
o. munisically disordered proteins (g.88)	0. AT_{2331} -11KC (U.337)

9.	Histone-fold (a.22)	9.	SRF-like (d.88)	
10.	Triple beta-spiral (b.83)	10	. CsrA-like (b.151)	
Leishmania infantum		Caenorhabditis elegans		
1.	Non-globular all-alpha subunits of globular proteins (a.137)	1.	ROP-like (a.30)	
2.	ROP-like (a.30)	2.	Non-globular all-alpha subunits of globular proteins (a.137)	
3.	Mediator hinge subcomplex-like (a.252)	3.	Mediator hinge subcomplex-like (a.252)	
4.	Intrinsically disordered proteins (g.88)	4.	BAR/IMD domain-like (a.238)	
5.	N-terminal domain of bifunctional PutA protein (a.176)	5.	Intrinsically disordered proteins (g.88)	
6.	BAR/IMD domain-like (a.238)	6.	Ferritin-like (a.25)	
7.	L27 domain (a.194)	7.	N-terminal domain of bifunctional PutA protein (a.176)	
8.	CsrA-like (b.151)	8.	L-aspartase-like (a.127)	
9.	Spectrin repeat-like (a.7)	9.	Spectrin repeat-like (a.7)	
10.	Histone-fold (a.22)	10.	P-domain of calnexin/calreticulin (b.104)	
Dre	psophila melanogaster	Dar	nio rerio	
1.	Non-globular all-alpha subunits of globular proteins (a.137)	1.	Non-globular all-alpha subunits of globular proteins (a.137)	
2.	ROP-like (a.30)	2.	ROP-like (a.30)	
3.	Intrinsically disordered proteins (g.88)	3.	BAR/IMD domain-like (a.238)	
4.	Mediator hinge subcomplex-like (a.252)	4.	Mediator hinge subcomplex-like (a.252)	
5.	BAR/IMD domain-like (a.238)	5.	Intrinsically disordered proteins (g.88)	
6.	N-terminal domain of bifunctional PutA protein (a.176)	6.	N-terminal domain of bifunctional PutA protein (a.176)	
7.	alpha-alpha superhelix (a.118)	7.	Immunoglobulin-like beta-sandwich (b.1)	
8	L_{27} domain (a 194)	8	L27 domain (a 194)	
9	Laspartase-like (a 127)	9. 9	P-domain of calnexin/calreticulin (b 104)	
10	Snectrin reneat-like (a 7)	10	alpha-alpha superhelix (a 118)	
Mu	s musculus	Rat	tus norvegicus	
1	Non-globular all-alpha subunits of globular proteins (a 137)	1	Non-globular all-alpha subunits of globular proteins (a 137)	
1. 2	ROP like $(a, 30)$	1. 2	ROP like $(2, 30)$	
2.	Immunoglobulin-like beta-sandwich (b 1)	2. 3	BAR/IMD domain like (a 238)	
5. 1	BAD/IMD domain like (a 238)	5. 1	Mediator hinge subcomplex like (a 252)	
4. 5	Madiator hinga subcomplex like (a 252)	4. 5	Immunoglobulin like bete sendwich (h 1)	
5. 6	International proteins (a.2.52)	5. 6	Infinunogiobulin-like bela-sandwich (b.1)	
0. 7	alaba alaba superbaliy (a 118)	0. 7	Tax NI terminal masian like (a 204)	
/. 0	<u>aipina-aipina superneinx (a.118)</u>	/. 0	aluba aluba sumarkalia (a. 119)	
ð. 0	L 27 domain (a 104)	ð. 0	L 27 domain (a 104)	
9. 10	L27 domain (a.194)	9. 10	L2/ domain (a.194)	
10.	N-terminal domain of offunctional PutA protein (a.176)	10.	N-terminal domain of bifunctional PutA protein (a.1/6)	
1	mo sapiens	Ory	$za \ sanva$	
1.	Non-globular all-alpha subunits of globular proteins (a.137)	1.	Non-globular all-alpha subunits of globular proteins (a.137)	
2.	ROP-like (a.30)	2.	ROP-like (a.30)	
3.	BAR/IMD domain-like (a.238)	3.	Mediator hinge subcomplex-like (a.252)	
4.	Immunoglobulin-like beta-sandwich (b.1)	4.	Leu-rich repeat, LRR (right-handed beta-alpha superhelix) (c.10)	
5.	Mediator hinge subcomplex-like (a.252)	5.	SRF-like (d.88)	
6.	Intrinsically disordered proteins (g.88)	6.	CsrA-like (b.151)	
7.	N-terminal domain of bifunctional PutA protein (a.176)	7.	YetM-like (d.306)	
8.	Pyruvate kinase C-terminal domain-like (c.49)	8.	<u>alpha-alpha superhelix (a.118)</u>	
9.	Interferon-induced guanylate-binding protein 1 (GBP1), C-te	9.	Histone-fold (a.22)	
	rminal domain (a.114)	10.	L27 domain (a.194)	
10.	L27 domain (a.194)			
Zea	n mays	Ara	bidopsis thaliana	
1.	Non-globular all-alpha subunits of globular proteins (a.137)	1.	Non-globular all-alpha subunits of globular proteins (a.137)	
2.	ROP-like (a.30)	2.	ROP-like (a.30)	
3.	Mediator hinge subcomplex-like (a.252)	3.	Mediator hinge subcomplex-like (a.252)	
4.	YheA-like (a.281)	4.	alpha-alpha superhelix (a.118)	
5.	SRF-like (d.88)	5.	Leu-rich repeat, LRR (right-handed beta-alpha superhelix) (c.10)	
6.	CsrA-like (b.151)	6.	SRF-like (d.88)	
7.	L27 domain (a.194)	7.	CsrA-like (b.151)	
8.	alpha-alpha superhelix (a.118)	8.	Histone-fold (a.22)	

9. N-terminal domain of bifunctional PutA protein (a.176)	9. N-terminal domain of bifunctional PutA protein (a.176)
10. triple barrel (b.65)	10. Spectrin repeat-like (a.7)
Glycine max	
1. Non-globular all-alpha subunits of globular proteins (a.137)	
2. ROP-like (a.30)	
3. Mediator hinge subcomplex-like (a.252)	
4. Leu-rich repeat, LRR (right-handed $\beta - \alpha$ superhelix) (c.10)	
5. <u>alpha-alpha superhelix (a.118)</u>	
6. SRF-like (d.88)	
7. Spectrin repeat-like (a.7)	
8. CsrA-like (b.151)	
9. L27 domain (a.194)	
10. N-terminal domain of bifunctional PutA protein (a.176)	

Commonly appeared folds with the SUPERFAMILY2.0 statistics shown in Supplementary Table 4 are underlined. Folds in α -class has a SCOP ID stating from a., an ID of a β -class fold starts from b., α/β and $\alpha+\beta$ class folds have ID with c. and d. respectively, folds with g. are small proteins.

Species	SUPERFAMILY ID	# Sequences	# sequence with assignment	# domains with assignment
Arabidopsis thaliana	at	35,381	22,134	32,197
Caenorhabditis elegans	cl	30,250	16,476	29,666
Candida albicans	al	6,165	3,795	5,360
Danio rerio	da	43,153	31,400	67,350
Dictyostelium discoideum	dt	13,263	6,955	11,119
Drosophila melanogaster	dd	26,950	17,699	38,800
Escherichia coli	ec	4,141	3,010	4,434
Glycine max	уg	55,787	36,697	51,734
Homo sapiens	hs	99,458	60,672	115,355
Leishmania infantum	lh	8,216	4,294	6,092
Methanocaldococcus jannaschii	jМ	1,771	1,177	1,614
Mus musculus	mm	52,998	34,563	68,456
Mycobacterium tuberculosis	7EO	3,994	2,814	3,984
Oryza sativa	AnK	66,338	32,867	51,632
Plasmodium falciparum	pl	5,385	2735	4,219
Rattus norvegicus	rn	25,724	18,941	36,627
Saccharomyces cerevisiae	XS	6,692	3,654	5,383
Schizosaccharomyces pombe	po	5,035	3,356	5,024
Staphylococcus aureus	brP	1,981	1,512	2,375
Trypanosoma cruzi	uz	10,320	4,719	6,449
Zea mays	e0I	63,540	34,145	45,617

Supplementary Table 3. Statistics of SUPERFAMILY 2.0 of the 21 species.

The statistics from the SUPERFAMILY 2.0 database for the same 21 species in Table 1. The annotations were downloaded on December 10, 2021. The SCOP superfamily assigned for each domain by SUPERFAMILY was counted for individual species in the SCOP fold level.

Supplementary Table 4. Top-10 Folds in SUPERFAMILY 2.0 for individual species.

Methanocaldococcus jannaschii (jM)	Mycobacterium tuberculosis (7EO)
1. P-loop cont. nucleoside triphosphate hydrolases (c.37)	1. P-loop containing nucleoside triphosphate hydrolases (c.37)
2. Ferredoxin-like (d.58)	2. Ferritin-like (a.25)
3. TIM beta/alpha-barrel (c,1)	3. DNA/RNA-binding 3-helical bundle (a.4)
4 DNA/RNA-binding 3-belical bundle (a 4)	4 NAD(P)-binding Rossmann-fold domains (c. 2)
5 S-a -I -methionine-dent methyltransferases (c. 66)	5 TIM beta/alpha-barrel (c 1)
6. Adenine nucleotide alpha hydrolase like (c.26)	6 Ferredovin like (d 58)
0. Addinic indeconde alpha invertilase-like (0.20)	0. Ferredoxin-like (0.36)
$\begin{array}{c} 7. \text{OB-1010} (0.40) \\ 8. \text{NAD}(\mathbf{P}) 1 \stackrel{!}{,} 1 \stackrel{!}{,} \mathbf{P} \\ \end{array}$	7. $\underline{\text{alpha/beta-Hydrolases}(c.09)}$
8. NAD(P)-binding Rossmann-fold domains (c.2)	8. S-aL-methionine-dependent methyltransferases (c.66)
9. Flavodoxin-like (c.23) a	9. FAD/NAD(P)-binding domain (c.3)
10. Homing endonuclease-like (d.95)	10.Thiolase-like (c.95)
Staphylococcus aureus (brP)	Escherichia coli (ec)
1. P-loop cont. nucleoside triphosphate hydrolases (c.37)	1. P-loop cont. nucleoside triphosphate hydrolases (c.37)
2. immunoglobulin/albumin-binding domain-like (a.8)	2. DNA/RNA-binding 3-helical bundle (a.4)
3. TIM beta/alpha-barrel (c.1)	3. TIM beta/alpha-barrel (c.1)
4. DNA/RNA-binding 3-helical bundle (a.4)	4. Ferredoxin-like (d.58)
5. NAD(P)-binding Rossmann-fold domains (c.2)	5. NAD(P)-binding Rossmann-fold domains (c.2)
6 Ferredoxin-like (d 58)	6 Ribonuclease H-like motif (c 55)
7 $OB_{\text{fold}}(b 40)$	7 Flavodovin-like (c 23)
8 Elavadovin like (c 23)	8 Devialesmie hinding gratein like II (201)
0. MES general substrate transporter (f 28)	8. <u>Peripiasine binding protein-like II (C.94)</u>
9. MITS general substrate transporter (1.56)	9. MFS general substrate transporter (1.38)
10.FAD/NAD(P)-binding domain (c.3)	10.OB-fold (b.40)
Saccharomyces cerevisiae (xs)	Candida albicans (al)
1. P-loop cont. nucleoside triphosphate hydrolases (c.37)	1. P-loop containing nucleoside triphosphate hydrolases (c.37)
2. alpha-alpha superhelix (a.118)	2. alpha-alpha superhelix (a.118)
3. 7-bladed beta-propeller (b.69)	3. Ferredoxin-like (d.58)
4 Ferredoxin-like (d 58)	4 7-bladed beta-propeller (b 69)
5 Ribonuclease H-like motif (c 55)	5 TIM beta/alpha-barrel (c 1)
6 Protein kinase-like (PK-like) (d 144)	6 NAD(P)-binding Rossmann-fold domains (c 2)
7 TIM beta/alpha-barrel (c 1)	7 Protein kinase-like (PK-like) (d 144)
8 DNA/DNA hinding 2 helical hundle $(a A)$	8 MES general substrate transporter (f 28)
0. NAD(D) binding Desembra fold domains (a 2)	0. Dihonualaasa H lika matif (a 55)
10 MES concered substrate transmoster (f 28)	10 DNA/DNA hinding 2 haliaal hundla (a 4)
10. MFS general substrate transporter (1.58)	10. DINA/KINA-binding 5-nencai bundie (a.4)
Schizosaccharomyces pombe (po)	Dictyostelium discoideum (dt)
1. P-loop cont. nucleoside triphosphate hydrolases (c.37)	1. P-loop containing nucleoside triphosphate hydrolases (c.37)
2. <u>alpha-alpha superhelix (a.118)</u>	2. alpha-alpha superhelix (a.118)
3. 7-bladed beta-propeller (b.69)	3. Protein kinase-like (PK-like) (d.144)
4. Ferredoxin-like (d.58)	4. Ferredoxin-like (d.58)
5. Protein kinase-like (PK-like) (d.144)	5. 7-bladed beta-propeller (b.69)
6. TIM beta/alpha-barrel (c.1)	6. Immunoglobulin-like beta-sandwich (b.1)
7. DNA/RNA-binding 3-helical bundle (a.4)	7. Leu-rich repeat, LRR (right-handed $\beta - \alpha$ superhelix) (c.10)
8. Ribonuclease H-like motif (c.55)	8 NAD(P)-binding Rossmann-fold domains (c. 2)
9 NAD(P)-binding Rossmann-fold domains (c 2)	9 Ribonuclease H-like motif (c 55)
10 OB-fold (b 40)	10 $\operatorname{RING/U-hov}(\mathfrak{g} 44)$
Fusmouum Jaiciparum (pi)	1 Place cont multiplication triplication between the second structures (2.27)
1. r -noop cont. nucleoside tripnosphate hydroiases (C.57) 2. Duffy hinding domain life (= 264)	1. r-toop cont. nucleoside improsphate nydrolases (c.37)
2. Durity binding domain-like $(a.264)$	2. 0 -biaded beta-propener (0.08)
5. aipna-aipha supernelix (a.118)	\star Lonconovolin // like lecting/gluconogeg (h. /U)
$1/1$ Herredovin Like (d, \mathbf{X})	5. Concanavann A-nke recuns/glucanases (0.23)
$\begin{array}{c} 4. \text{Ferredoxin-like} \left(0.56 \right) \\ 5. 7.11 1.11 $	 4. alpha-alpha superhelix (a.118) 5. Concatavanii Arike fectilis/glucatases (0.29) 4. alpha-alpha superhelix (a.118)
5. 7-bladed beta-propeller (b.69)	 4. alpha-alpha superhelix (a.118) 5. Protein kinase-like (PK-like) (d.144)
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9. Ribonuclease H-like motif (c.55) 9. Single-stranded right-handed beta-helix (b.80) 10. Long alpha-hairpin (a.2) 10. Leur-rich repeat, LRR (right-handed β-α superhelix (c.10) 2 alpha-alpha superhelix (a.118) 2. Class A G protein-coupled receptor (GPCH): like (f.13) 3. Protein kinase-like (PK-like) (d.144) 3. Protein kinase-like (VK-like) (d.144) 5. Terredoxin-like (d.58) 6. Ferredoxin-like (d.58) 6. Leur-cith repeat, LRR (right-handed β-α superhelix) (c.10) 6. Ferredoxin-like (d.58) 7. Ribbonuclease H-like motif (c.55) 6. Ferredoxin-like (d.58) 8. Long alpha-hairpin (a.2) 8. South alpha-siphin superhelix (a.118) 9. Star_L-methionine-dpt methyltransferases (c.60) 10. DNA/RNA-binding 3-helical bundle (a.4) 7. Brobaptic like (d.58) 10. DNA/RNA-binding 3-helical bundle (a.4) 7. Bradendpas superhelix (a.118) 10. Entropotic like (d.58) 8. Protorin kinase-like (VK-like) (d.144) 10. SH3-hile barrel (b.34) 7. Bradendpas superhelix (a.118) 8. Protorin kinase-like (VK-like) (d.144) 8. Protorin kinase-like (VK-like) (d.144) 10. SH3-hile barrel (b.34) 7. Brodendpas superhelix (a.118) 8. Protorin kinase-like (VK-like) (d.144) 8. Protorin kinase-like (VK-like) (d.144) 10. SH3-hile barrel (b.34)	8.	EF Hand-like (a.39)	8.	Zincin-like (d.92)
10. Log alpha-hairpin (a.2) 10. Lear-rich repeat, LRR (right-handed β-α superhelix) (c.10) Leishmania infiantum (h) Caenorhabditis degans (cl) 1. P-loop continuing nucleoside triphosphate hydrolases (c.37) Ploop continuing nucleoside triphosphate hydrolases (c.37) 2. Tables Alpha-alpha superhelix (a.118) Ploop continuing nucleoside triphosphate hydrolases (c.37) 3. Protein kinase-like (PK-like) (d.144) Ploop continuing nucleoside triphosphate hydrolases (c.37) 4. Troblade bete-propeller (b.69) Sau-armethionine-dpdit methyltransferases (c.66) 7. Ribonuclease H-like metrif (c.5) Sinotrain (small inhibitors, toxins, lectins) (g.3) 8. Long alpha-hairpin (a.2) Danio zerio (d.a) 10. TTM betazidha-barel (c.1) Downorthick (d.58) 7. alpha-alpha superhelix (a.118) Beta-beta-alpha zinc fingers (g.37) 10. Brain serie (f.42) Danio zerio (d.a) 11. Immunoglobulin-like beta-samdwich (b.1) Beta-beta-alpha zinc fingers (g.37) 2. Beta-beta-alpha zinc fingers (g.37) Seloop cont.nucleoside triphosphate hydrolases (c.37) 3. Shatis ke (k K-like) (d.144) Seconaravating (h.c) 3. Brotoni Kinase-like (PK-like) (d.144) Seconaravating nucleoside triphosphate hydrolases (c.37) 3. Class A G protein-coupled receptor (GPCR)-like (f.13) Class A G protein-coupled receptor (GPCR)-like (f.13) 3. Class A G protein-coupled receptor (GPCR)-like (f.144) Suba-alpha superhelix (a	9.	Ribonuclease H-like motif (c.55)	9.	Single-stranded right-handed beta-helix (b.80)
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5. P-loop cont. nucleoside triphosphate hydrolases (c.37) 6. Ferredoxin-like (d.58) 7. Protein kinase-like (PK-like) (d.144) 9. Glucocorticoid receptor-like (DNA-bdg domain) (g.39) 1. Immunoglobulin-like beta-sandwich (b.1) 2. beta-beta-alpha superhelix (a.118) 7. Protein kinase-like (PK-like) (d.144) 9. Protein kinase-like (PK-like) (d.144) 1. Immunoglobulin-like beta-sandwich (b.1) 2. beta-beta-alpha zinc fingers (g.37) 3. alpha-alpha superhelix (a.118) 6. Knottins (small inhibitors, toxins, lectins) (g.3) 7. Ferredoxin-like (d.58) 8. DNA/RNA-binding 3-helical bundle (a.4) 9. Protein kinase-like (PK-like) (d.144) 10.PH domain-like barrel (b.55) 11. Immunoglobulin-like barrel (b.55) 12. beta-beta-alpha zinc fingers (g.37) 3. P-loop cont. nucleoside triphosphate hydrolases (c.37) 4. Knottins (small inhibitors, toxins, lectins) (g.3) 7. Ferredoxin-like (PK-like) (d.144) 10.PH domain-like barrel (b.55) 11. Immunoglobulin-like bares (b.55) 12. beta-beta-alpha zinc fingers (g.37) 3. P-loop cont. nucleoside triphosphate hydrolases (c.37) 4. Leu-rich repeat. LRR (ri-handed β - α superhelix (a.118) 4. P-loop containing nucleoside triphosphate hydrolases (c.37) 5. Japha-alpha superhelix (a.118) 5. Knottins (small inhibitors, toxins, lectins) (g.3) 6. Ferredoxin-like (cf.55) 1. Inmunoglobulin-like bares (b.55) 1. Inmunoglobulin-like bares (b.50) 8. SH3-like barel (b.34) 9. DNA/RNA-binding 3-helical bundle (a.4) 10.PH domain-like barel (b.54) 8. SH3-like barel (b.34) 9. DNA/RNA-binding 3-helical bundle (a.4) 10.PH domain-like barel (b.54) 10. Protein kinase-like (PK-like) (d.144) 10. PH domain-like barel (b	4.	Spectrin repeat-like (a.7)	4.	Knottins (small inhibitors, toxins, lectins) (g.3)
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 9. Ferredoxin-like (d.58) 9. Ferredoxin-like (d.58) 10. PH domain-like barrel (b.55) 9. Ferredoxin-like (d.58) 10. Cysteine proteinases (d.3) Arabidopsis thaliana (at) 1. P-loop containing nucleoside triphosphate hydrolases (c.37) 2. P-loop cont. nucleoside triphosphate hydrolases (c.37) 3. <u>alpha-alpha superhelix (a.118)</u> 4. Ferredoxin-like (d.58) 5. DNA/RNA-binding 3-helical bundle (a.4) 6. TIM beta/alpha-barrel (c.1) 9. Ferredoxin-like (d.58) 6. DNA/RNA-binding 3-helical bundle (a.4) 	ð. 0	SH3-like darrel (0.54) DNA/DNA hinding 2 haliaal hundla (a.4)	8.	alpha-alpha superhelix (a.118)
10.111 domain-ince barrer (0.55) 10.Cysteline proteinases (d.5) 2i Protein kinase-like (PK-like) (d.144) 1. P-loop containing nucleoside triphosphate hydrolases (c.37) 2. P-loop cont. nucleoside triphosphate hydrolases (c.37) 2. Protein kinase-like (PK-like) (d.144) 3. alpha-alpha superhelix (a.118) 3. alpha-alpha superhelix (a.118) 4. Ferredoxin-like (d.58) 4. Leu-rich repeat, LRR (rhanded β-α superhelix) (c.10) 5. DNA/RNA-binding 3-helical bundle (a.4) 5. Ferredoxin-like (d.58) 6. TIM beta/alpha-barrel (c.1) 6. DNA/RNA-binding 3-helical bundle (a.4)	2. 10	PH domain_like barrel (b 55)	9. 10	Custaina protainasas (d.3)
<i>Lea mays</i> (e01) <i>Arabidopsis thaliana</i> (at) 1. Protein kinase-like (PK-like) (d.144) 1. P-loop containing nucleoside triphosphate hydrolases (c.37) 2. P-loop cont. nucleoside triphosphate hydrolases (c.37) 2. Protein kinase-like (PK-like) (d.144) 3. <u>alpha-alpha superhelix (a.118)</u> 4. Ferredoxin-like (d.58) 5. DNA/RNA-binding 3-helical bundle (a.4) 5. Ferredoxin-like (d.58) 6. TIM beta/alpha-barrel (c.1) 6. DNA/RNA-binding 3-helical bundle (a.4)	70.		10	Cysteme proteinases (d.5)
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 4. Ferredoxin-like (d.58) 5. DNA/RNA-binding 3-helical bundle (a.4) 6. TIM beta/alpha-barrel (c.1) 5. alpha-alpha superhelix (a.116) 4. Leu-rich repeat, LRR (rhanded β-α superhelix) (c.10) 5. Ferredoxin-like (d.58) 6. DNA/RNA-binding 3-helical bundle (a.4) 	3	alpha-alpha superhelix (a 118)	2. 3	alpha-alpha superhelix (a 118)
 5. DNA/RNA-binding 3-helical bundle (a.4) 6. TIM beta/alpha-barrel (c.1) 7. <u>Leu-Hen repeat, Erec (1handed p=0 superior (c.10)</u> 6. DNA/RNA-binding 3-helical bundle (a.4) 	4	Ferredoxin-like (d 58)	<u></u>	Leu-rich repeat I RR (r-handed R-a superhelix) (c 10)
6. TIM beta/alpha-barrel (c.1) 6. DNA/RNA-binding 3-helical bundle (a.4)	5	DNA/RNA-binding 3-helical bundle (a 4)	- 1 . 5	Ferredoxin-like (d 58)
	6.	TIM beta/alpha-barrel (c.1)	6.	DNA/RNA-binding 3-helical bundle (a.4)

7. RING/U-box (g.44)	7. RING/U-box (g.44)
8. Leu-rich repeat, LRR (r-handed $\beta - \alpha$ superhelix) (c.10)	8. F-box domain (a.158)
9. NAD(P)-binding Rossmann-fold domains (c.2)	9. Cysteine-rich domain (g.49)
10.7-bladed beta-propeller (b.69)	10.TIM beta/alpha-barrel (c.1)
Glycine max (yg)	
1. P-loop cont. nucleoside triphosphate hydrolases (c.37)	
2. Protein kinase-like (PK-like) (d.144)	
3. Leu-rich repeat, LRR (rhanded β - α superhelix) (c.10)	
4. alpha-alpha superhelix (a.118)	
5. Ferredoxin-like (d.58)	
6. DNA/RNA-binding 3-helical bundle (a.4)	
7. RING/U-box (g.44)	
8. TIM beta/alpha-barrel (c.1)	
9. NAD(P)-binding Rossmann-fold domains (c.2)	
10.7-bladed beta-propeller (b.69)	

The Genome ID used in SUPERFAMILY is noted after each species name. Folds commonly appeared in the Alphafold2 models in Supplementary Table 2 and in this SUPERFAMILY database are underlined.

Eschanishin coli (E()	Sacahanamusas agnavisias (SC)
	1 D1 C () NTD H 1 1 (24)
1. NAD(P)-binding Rossmann Fold (c.18)	1. P-loop Containing NTP Hydrolases (c.24)
2. <u>Flavodoxin-like (c.13)</u>	2. Ribonuclease H-like motif (c.38)
3. <u>TIM-Barrel (c.1)</u>	3. NAD(P)-binding Rossmann Fold (c.18)
4. Like Ferrodoxin (d.31)	4. TIM-Barrel (c.1)
5. Ribonuclease H-like motif (c.38)	5. Like Ferrodoxin (d.31)
6. P-loop Containing NTP Hydrolases (c.24)	6. Long Alpha-hairpin (a.2)
7. Thiamin-binding (c.23)	7. Thiamin-binding (c.23)
8. FAD/NAD(P)-binding (c.4)	8. GroES-like (b.21)
9. GroES-like (b.21)	9. Thioredoxin-like (c.30)
10. OB-fold (b.24)	10.FAD/NAD(P)-binding (c.4)
Methanocaldococcus jannaschii (MJ)	
1. Like Ferrodoxin (d.31)	
2. <u>P-loop containing NTP Hydrolases (c.24)</u>	
3. <u>TIM-Barrel (c.1)</u>	
4. FAD/NAD(P)-binding (c.4)	
5. Thiamin-binding (c.23)	
6. NAD(P)-binding Rossman Fold (c.18)	
7. ATP Pyrophosphatases (c.15)	
8. Flavodoxin-like (c.13)	
9. Reductase/Elongation Factor Domain (b.27)	
10. Asp-carbomoyltransferase, Catchain (c.56)	

Supplementary Table 5. The top 10 most abundant folds by Gerstein (1998)

The top 10 most abundant folds in the three species taken from Fig. 1. in the paper by M. Gerstein, Patterns of protein-fold usage in eight microbial genomes: a comprehensive structural census. *Proteins* **33**, 518-534, (1998). Among eight species analyzed in their work, three species that are common with Supplementary Table 2 are listed. Folds with underline are those which are in common with Supplementary Table 2. In the parentheses, SCOP codes are shown.

Supplementary Table 6. The top 5 most abundant folds by Kihara & Skolnick (2004).

Escherichia coli	Saccharomyces cerevisiae		
1. Rossmann fold (3.40.50)	1. Rossmann fold (3.40.50)		
2. Alpha-Betta plaits (3.30.70)	2. Alpha-Betta plaits (3.30.70)		
3. <u>TIM barrel (3.20.20)</u>	3. Immunoglobin-like (2.60.40)		
4. Arc repressor mutant subunit A (1.10.10)	4. Arc repressor mutatant subunit A (1.10.10)		
5. Immunoglobin-like (2.60.40)	5. Kinase (3.30.200)		

The top 5 most abundant folds in the two species from Table IIIB in the paper by D. Kihara & J. Skolnick, Microbial genomes have over 72% structure assignment by the threading algorithm PROSPECTOR_Q, *Proteins*, **55**, 464-473, 2004. Only top 5 folds are listed here because their work only showed top 5. Among five species analyzed in their work, these two species were in common with Supplementary Table 2. Folds with underline are commonly appeared in Supplementary Table 2. In the parentheses, CATH codes are shown.