Supporting information for: Deep convolutional networks for quality assessment of protein folds

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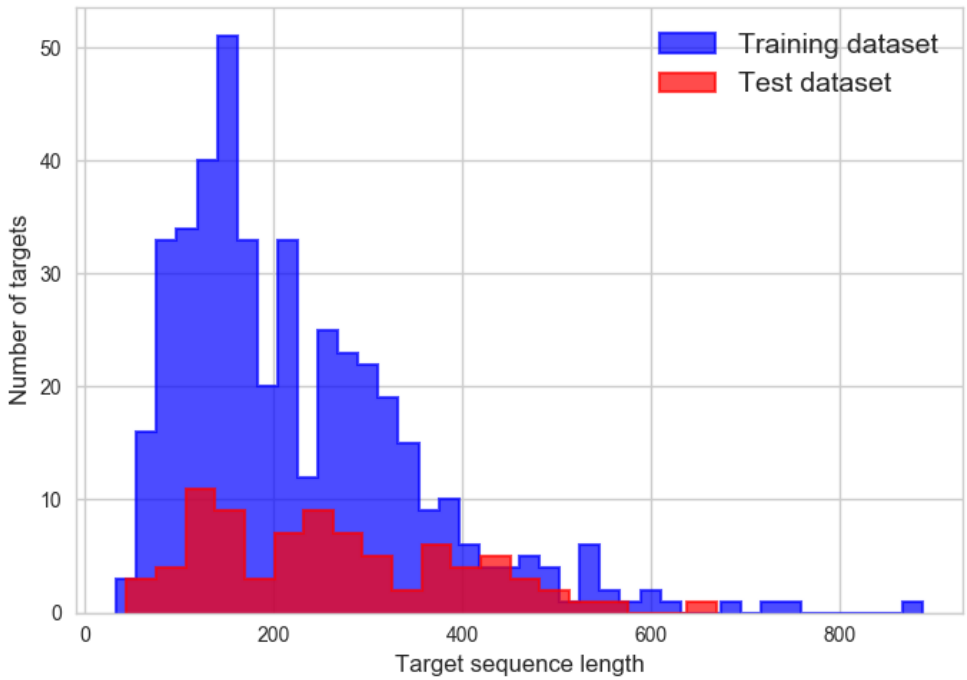


Figure S1: Distributions of sequence lengths for targets in training set (blue) and test set (red).

Table S1: Closest homolog sequences from the training set. A sequence pair is reported if at least one training sequence aligns to a test sequence with a blastp E-value less than 10^{-4}. Only the top alignment is reported for each test sequence.

Test set ID	Closest training set ID	E-value
T0768	T0690	2.70×10^{-13}
T0770	T0645	1.79×10^{-13}
T0772	T0518	1.89×10^{-7}
T0776	T0707	3.98×10^{-5}
T0783	T0699	1.19×10^{-22}
T0798	T0308	9.57×10^{-6}
T0813	T0398	2.45×10^{-5}
T0819	T0636	8.66×10^{-15}
T0854	T0324	2.13×10^{-13}

Table S2: Targets from test and training sets that belong to the same Pfam family [**?**], based on a HMMER search [**?**] with an E-value cutoff of 1.0. With that cutoff, 403 of the 564 training targets and 65 of the 83 test targets could be assigned families. There are 25 families containing at least one test sequence and one training sequence, involving a total of 16 test targets and 42 training targets. Each of the 25 families belongs to a distinct Pfam clan.

Common family	Test set target	Training set targets
PF00795	T0794	T0542
PF13472	T0776	T0448, T0297, T0286, T0750
PF03807	T0813	T0398, T0393, T0702
PF00266	T0801	T0339, T0697
PF01128	T0783	T0699, T0420
PF07949	T0780	T0572
PF13577	T0815	T0752, T0736
PF12804	T0783	T0593, T0699, T0420
PF13242	T0854	T0371, T0341, T0303, T0324, T0330, T0329, T0418
PF13306	T0768	T0690, T0671, T0713, T0653
PF12741	T0770	T0664, T0645, T0532
PF00025	T0798	T0308
PF12872	T0792	T0549
PF03446	T0813, T0851	T0398, T0393, T0702
PF00155	T0801, T0819	T0591, T0636, T0436, T0697
PF13419	T0854	T0371, T0341, T0303, T0379, T0324, T0330, T0329, T0418, T0635
PF12680	T0815	T0451, T0475
PF06439	T0772	T0518
PF12771	T0770	T0664, T0645, T0532
PF08477	T0798	T0308
PF00657	T0776	T0297, T0286, T0679
PF00071	T0798	T0308
PF00702	T0854	T0303, T0324, T0330, T0329, T0418, T0635
PF01926	T0798	T0308
PF12697	T0764	T0672

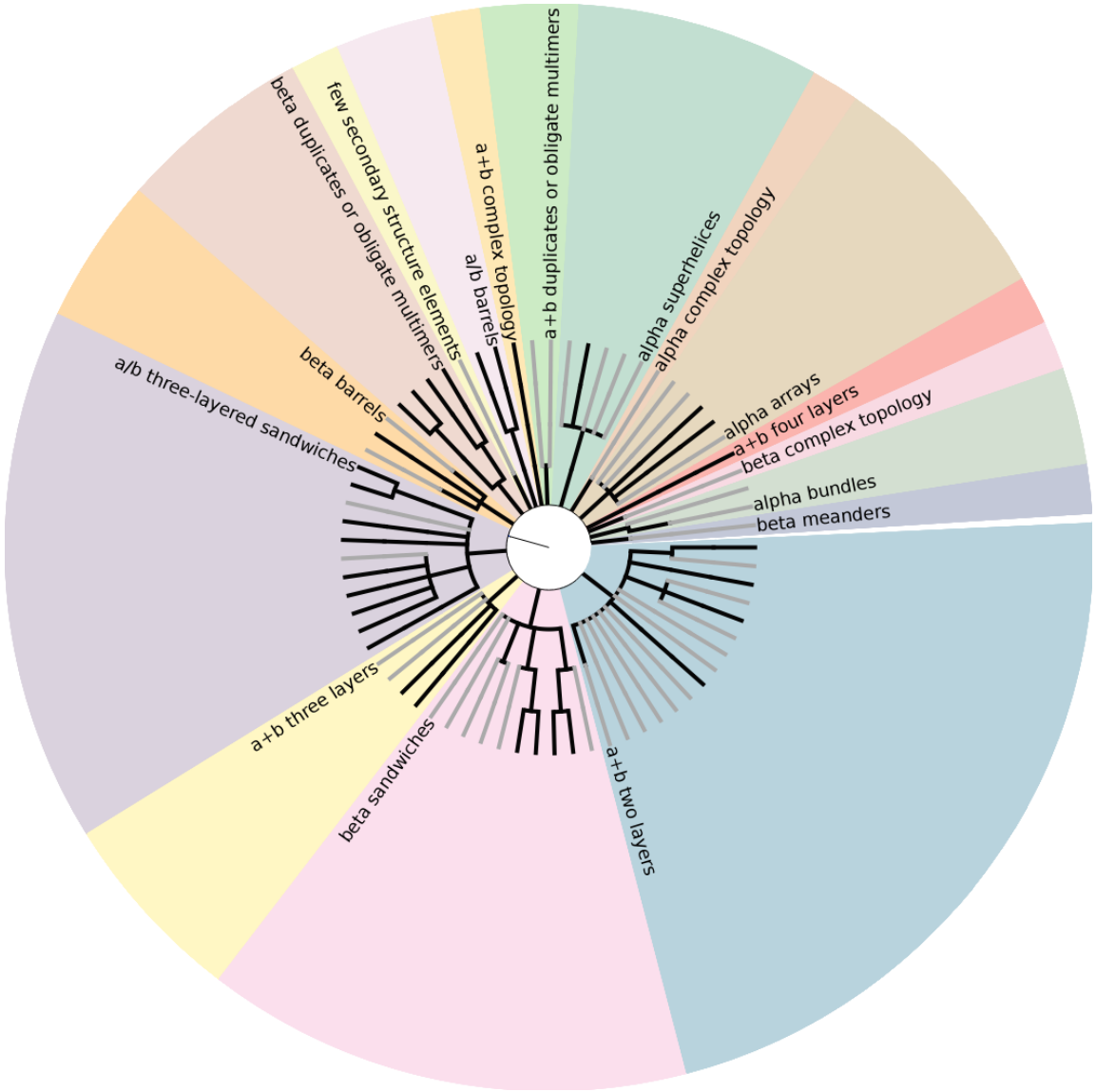


Figure S2: Classification of the test set structures into the top four ECOD structural levels (from the center out): architecture (A), possible homology (X), homology (H), and topology (T). The names of the architecture types are shown in the outer circle of the diagram. Branches drawn in black correspond to groups that have representatives in both training and test sets. Branches drawn in grey correspond to groups unique to the test set. Four architecture groups present overlap at all levels between the training and test sets: "a/b barrels", "beta duplicates or obligate multimers", "a+b complex topology", and "a+b four layers". We do not show the F-groups because they have litle overlap among the training and test sets. Targets T0773, T0797, and T0816 are excluded from the analysis because they have no ECOD classification, and targets T0820, T0823, T0824, T0827, T0835, and T0836 are excluded because they have no structure in the RCSB PDB.

Table S3: Details of the model architecture. Layer 10 is marked with an asterisk to indicate that its output is used in the Grad-CAM analysis reported in Section III.B of the main text.

Layer	Type	Input dimensions	Output dimensions	Parameters
1	3D Convolution	$11 \times 120 \times 120 \times 120$	$16 \times 118 \times 118 \times 118$	Filter size $3 \times 3 \times 3$, stride 1
2	ReLU			
3	Max pooling	$16 \times 118 \times 118 \times 118$	$16 \times 58 \times 58 \times 58$	Filter size $3 \times 3 \times 3$, stride 2
4	3D Convolution	$16 \times 58 \times 58 \times 58$	$32 \times 56 \times 56 \times 56$	Filter size $3 \times 3 \times 3$, stride 1
5	Batch normalization			
6	ReLU			
7	Max pooling	$32 \times 56 \times 56 \times 56$	$32 \times 27 \times 27 \times 27$	Filter size $3 \times 3 \times 3$, stride 2
8	3D Convolution	$32 \times 27 \times 27 \times 27$	$32 \times 25 \times 25 \times 25$	Filter size $3 \times 3 \times 3$, stride 1
9	Batch normalization			
10*	ReLU			
11	3D Convolution	$32 \times 25 \times 25 \times 25$	$64 \times 23 \times 23 \times 23$	Filter size $3 \times 3 \times 3$, stride 1
12	Batch normalization			
13	ReLU			
14	Max pooling	$64 \times 23 \times 23 \times 23$	$64 \times 11 \times 11 \times 11$	Filter size $3 \times 3 \times 3$, stride 2
15	3D Convolution	$64 \times 11 \times 11 \times 11$	$128 \times 9 \times 9 \times 9$	Filter size $3 \times 3 \times 3$, stride 1
16	Batch normalization			
17	ReLU			
18	3D Convolution	$128 \times 9 \times 9 \times 9$	$128 \times 7 \times 7 \times 7$	Filter size $3 \times 3 \times 3$, stride 1
19	Batch normalization			
20	ReLU			
21	3D Convolution	$128 \times 7 \times 7 \times 7$	$256 \times 5 \times 5 \times 5$	Filter size $3 \times 3 \times 3$, stride 1
22	Batch normalization			
23	ReLU			
24	3D Convolution	$256 \times 5 \times 5 \times 5$	$512 \times 3 \times 3 \times 3$	Filter size $3 \times 3 \times 3$, stride 1
25	Batch normalization			
26	ReLU			
27	Max pooling	$512 \times 3 \times 3 \times 3$	$512 \times 1 \times 1 \times 1$	Filter size $3 \times 3 \times 3$, stride 2
28	Reshape	$512 \times 1 \times 1 \times 1$	512	
29	Linear	512	256	
30	ReLU			
31	Linear	256	128	
32	ReLU			
33	Linear	128	1	

Training procedure

Rotations

The rotations were sampled in the following way:

1. Select three random uniform values $u_1, u_2, u_3 \in [0, 1]$
2. Construct quaternion from them

$$q_0 = \sqrt{1 - u_1} \sin(2\pi u_2) \tag{1}$$
$$q_1 = \sqrt{1 - u_1} \cos(2\pi u_2) \tag{2}$$
$$q_2 = \sqrt{u_1} \sin(2\pi u_3) \tag{3}$$
$$q_3 = \sqrt{u_1} \cos(2\pi u_3) \tag{4}$$

3. Construct the corresponding rotation matrix

Translations

The translations were sampled according to the following algorithm:

1. Compute the bounding box of the atoms in the decoy
2. Translate the protein so that the center of the bounding box corresponds to the frame origin
3. Rotate protein using random uniform rotation
4. Calculate the maximum shift along each axis:

$$D_k = \tfrac{1}{2} \max \left[0, \tfrac{1}{2} S_k - \tfrac{1}{2} B_k\right], \quad k \in x, y, z$$

   where S_k are input size along the axes x, y, z and B_k are the bounding box sizes along the same axes.

5. Sample random uniform translation along each axis from the interval $[-\frac{1}{2} D_k, \frac{1}{2} D_k], k \in x, y, z$

Training parameters

The loss function is optimized using the Adam algorithm [**?**], with a learning rate of 0.0003 and a learning rate decay of 0.01.

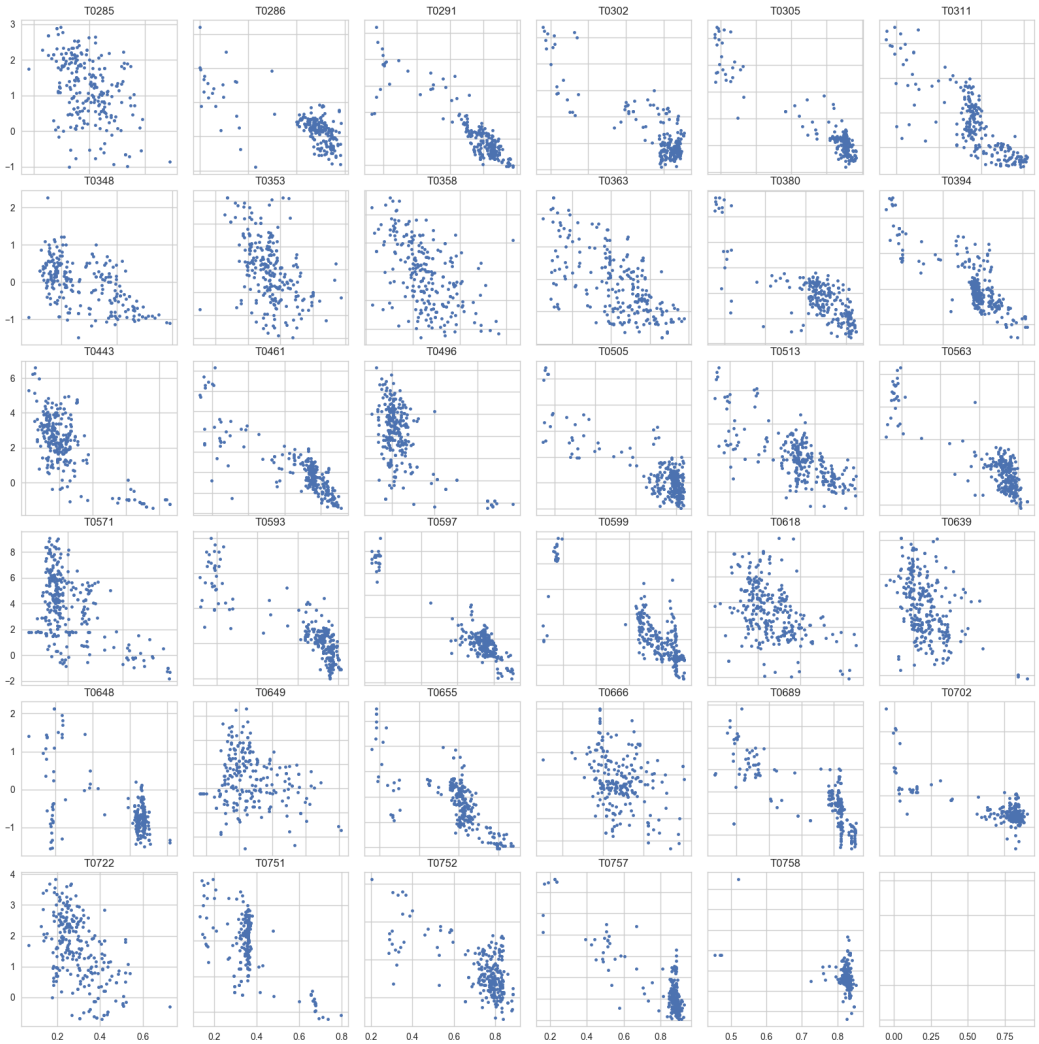


Figure S3: Scoring funnels on the validation set using the 3DCNN model from epoch 40. The x-axis is the GDT_TS score and the y-axis is the s score of a decoy. Each dot represents the score s calculated for a single position and orientation of the decoy structure.

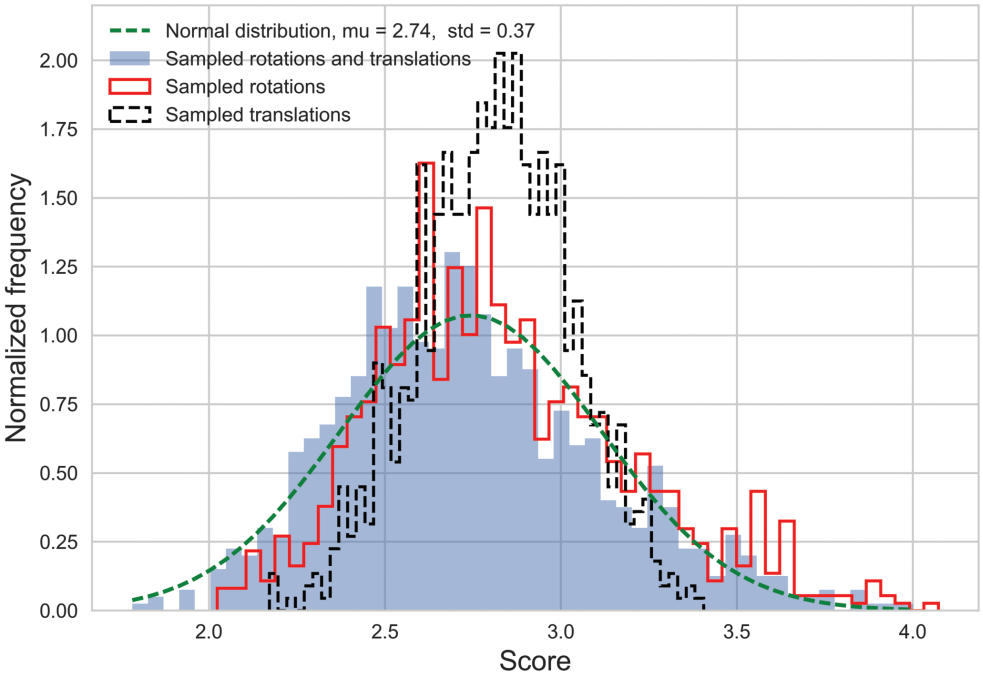


Figure S4: Distribution of the score of decoy FALCON_EnvFold_TS1 for target T0832 under random translations and rotations. The distribution fits a normal distribution with an average $\mu = 2.74$ and a standard deviation $\sigma = 0.37$ (shown in green dashed lines). The figure also shows the distributions of the score under rotations only (red lines) and under translations only (black dashed lines).

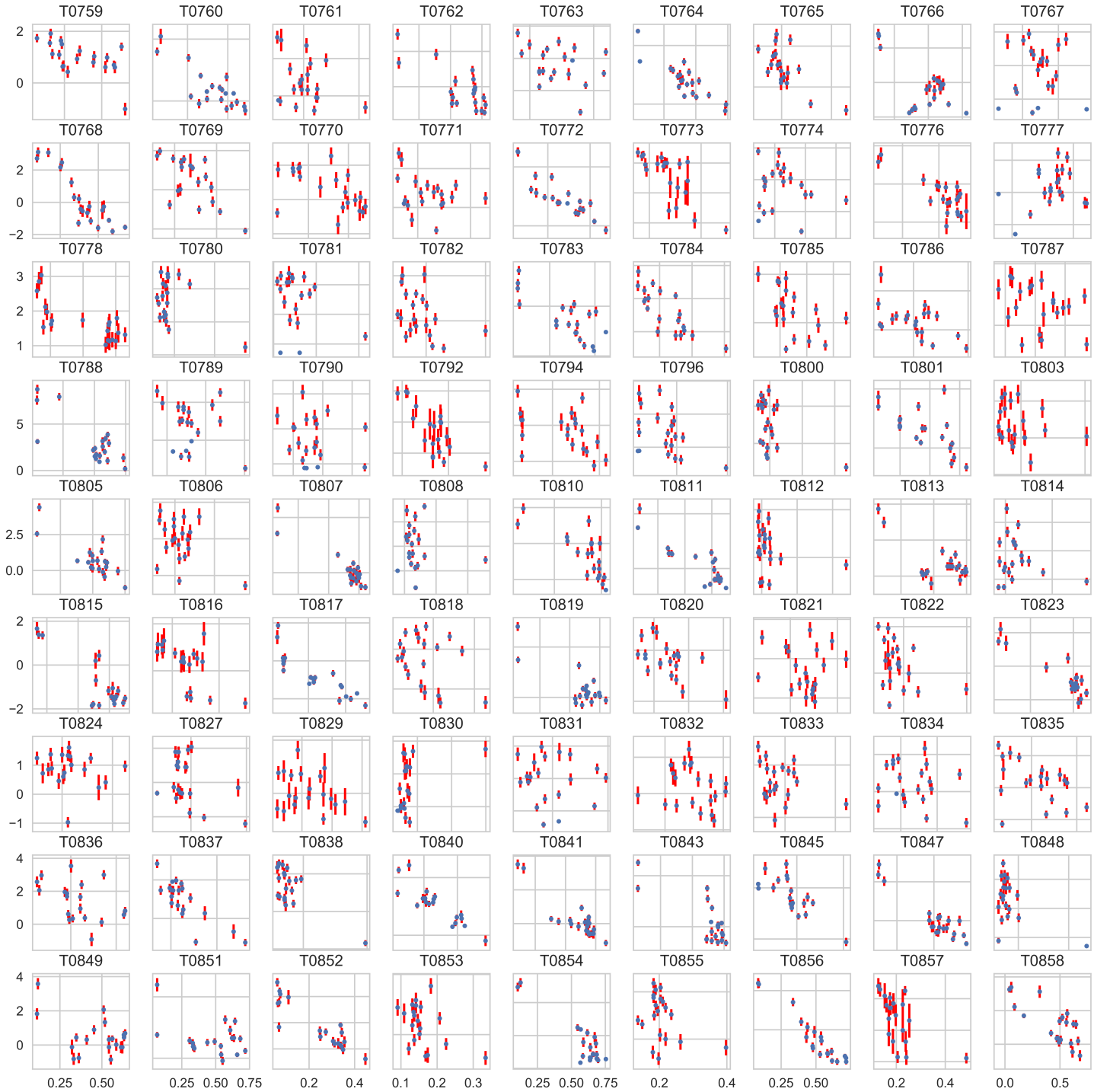


Figure S5: Scoring funnels on stage 1 CASP11 targets. The x-axis is the GDT_TS score and the y-axis is the s score. The score mean (used for ranking) is shown with blue dots and the standard deviation with red error bars.

Figure S6: Scoring funnels on stage 2 CASP11 targets. The x-axis is the GDT_TS score and the y-axis is the s score. The score mean (used for ranking) is shown with blue dots and the standard deviation with red error bars.

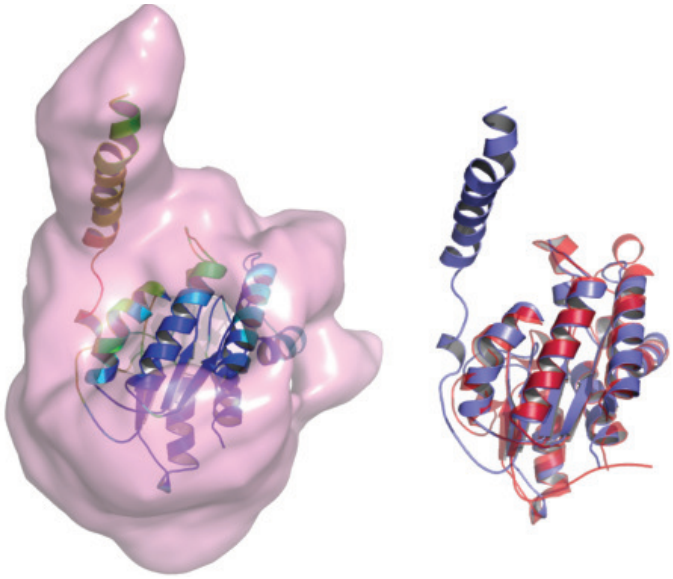


Figure S7: Left: Output of the Grad-CAM analysis for layer 10 of the network projected on candidate structure Distill_TS3 of target T0776. The isosurface shows the scaled outputs at the two-sigma level. The intensities of the outputs at the positions of the protein atoms are color-coded on the cartoon rendering of the structure, from blue (low intensity) to red (high intensity). Right: Cartoon representation of the Distill_TS3 decoy structure (in blue) aligned to the native structure (in red).

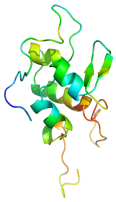
Table S4: (Next page) Output of the Grad-CAM algorithm on representative decoys from the CASP11 test set stage 2. For each target, decoys are divided into four GDT_TS bins of equal width, and one decoy is selected from each bin. The rightmost column shows the native structure. The Grad-CAM output map of each decoy is generated from 30 inputs rotated and translated at random. The 30 output maps are projected on the atoms of the decoys, and the average values of the projections are plotted using Pymol with the "rainbow" color scheme. The 3DCNN score is reported as "average ± standard deviation" over the 30 inputs. Native structures have low scores and low Grad-CAM output values for all targets, except T0787 (PDB code 4tvp; part of a large protein complex), T0797 (PDB code 4ojk; the monomer from a leucine zipper structure), T0821 (PDB code 4r7s), and T0831 (PDB code 4qn1).

T0759

myprotein-me_TS4

GDT_TS = 0.25

Score = 1.31 ± 0.18



T0759

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.31

Score = 0.92 ± 0.22

T0759

FFAS03_TS1

GDT_TS = 0.34

Score = 0.64 ± 0.21

T0759

Seok-server_TS2

GDT_TS = 0.36

Score = 0.79 ± 0.24

T0759

T0759

GDT_TS = 1.00

Score = −1.01 ± 0.16

T0760

FALCON_MANUAL_TS2

GDT_TS = 0.49

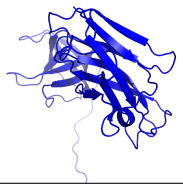
Score = −0.74 ± 0.34

T0760

Seok-server_TS2

GDT_TS = 0.55

Score = 0.22 ± 0.70

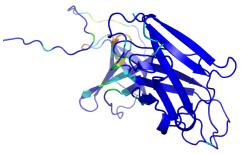


T0760

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.60

Score = −0.50 ± 0.27



T0760

FFAS03_TS1

GDT_TS = 0.62

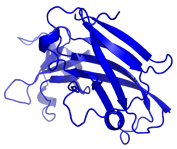
Score = −1.43 ± 0.20

T0760

T0760

GDT_TS = 1.00

Score = −2.14 ± 0.15

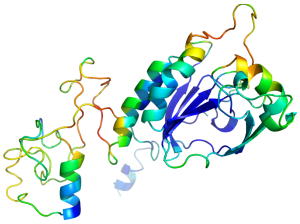


T0761

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.09

Score = 2.60 ± 0.26

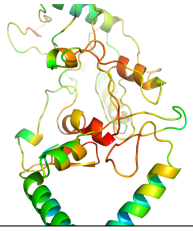


T0761

RBO_Aleph_TS3

GDT_TS = 0.10

Score = 5.61 ± 0.32

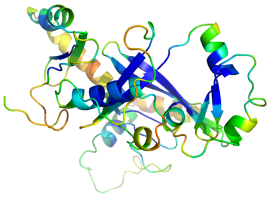


T0761

RBO_Aleph_TS4

GDT_TS = 0.12

Score = 2.87 ± 0.32

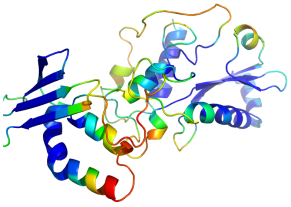


T0761

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.16

Score = 1.32 ± 0.32



T0761

T0761

GDT_TS = 1.00

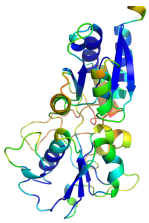
Score = −2.61 ± 0.13

T0762

BhageerathH_TS4

GDT_TS = 0.70

Score = 1.24 ± 0.17

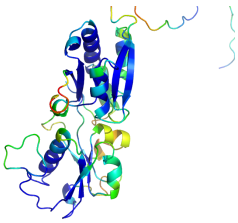


T0762

RBO_Aleph_TS3

GDT_TS = 0.76

Score = 0.86 ± 0.18

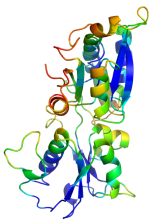


T0762

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.79

Score = 1.78 ± 0.30

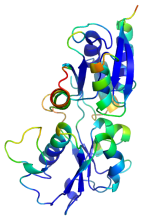


T0762

FFAS03_TS1

GDT_TS = 0.83

Score = 0.21 ± 0.27

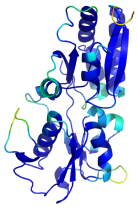


T0762

T0762

GDT_TS = 1.00

Score = −0.95 ± 0.37

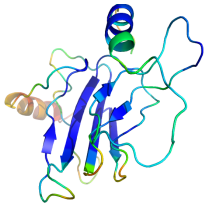


T0763

FALCON_MANUAL_TS2

GDT_TS = 0.12

Score = 1.22 ± 0.25



T0763

Distill_TS3

GDT_TS = 0.13

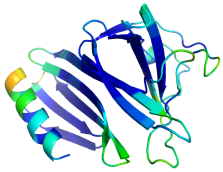
Score = 3.02 ± 0.23

T0763

RBO_Aleph_TS3

GDT_TS = 0.15

Score = 0.30 ± 0.33

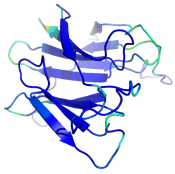


T0763

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.17

Score = 0.06 ± 0.25



T0763

T0763

GDT_TS = 1.00

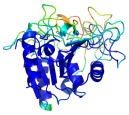
Score = −2.35 ± 0.12

T0764

RBO_Aleph_TS4

GDT_TS = 0.50

Score = 0.74 ± 0.22

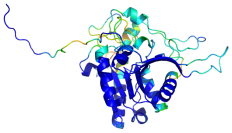


T0764

BioShell-server_TS3

GDT_TS = 0.60

Score = 1.90 ± 0.24

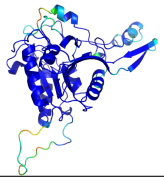


T0764

FFAS03_TS1

GDT_TS = 0.65

Score = 0.67 ± 0.16

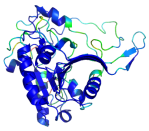


T0764

MUFOLD-Server_TS4

GDT_TS = 0.72

Score = 0.55 ± 0.16

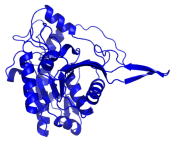


T0764

T0764

GDT_TS = 1.00

Score = −2.04 ± 0.25

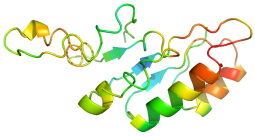


T0765

MUFOLD-Server_TS4

GDT_TS = 0.19

Score = 2.00 ± 0.28

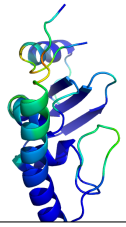


T0765

RBO_Aleph_TS3

GDT_TS = 0.31

Score = −0.25 ± 0.39

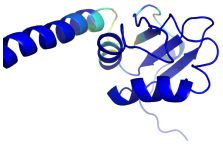


T0765

Distill_TS3

GDT_TS = 0.39

Score = 0.37 ± 0.17

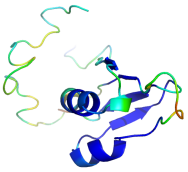


T0765

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.42

Score = 0.84 ± 0.28



T0765

T0765

GDT_TS = 1.00

Score = −1.76 ± 0.13

T0766

RBO_Aleph_TS3

GDT_TS = 0.53

Score = 0.52 ± 0.16

T0766

TASSER-VMT_TS2

GDT_TS = 0.67

Score = −1.41 ± 0.17

T0766

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.78

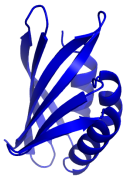
Score = −1.29 ± 0.18

T0766

FFAS03_TS1

GDT_TS = 0.94

Score = −2.06 ± 0.17



T0766

T0766

GDT_TS = 1.00

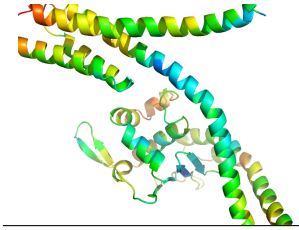
Score = −2.09 ± 0.18

T0767

BioShell-server_TS3

GDT_TS = 0.08

Score = 6.29 ± 0.39

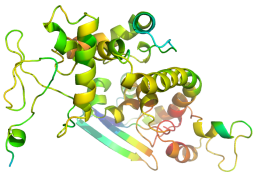


T0767

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.09

Score = 5.77 ± 0.37

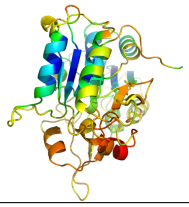


T0767

Pcons-net_TS1

GDT_TS = 0.12

Score = 4.36 ± 0.33

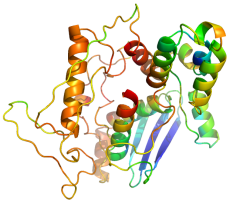


T0767

RBO_Aleph_TS3

GDT_TS = 0.15

Score = 5.27 ± 0.27



T0767

T0767

GDT_TS = 1.00

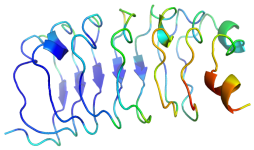
Score = −1.42 ± 0.28

T0768

Distill_TS3

GDT_TS = 0.37

Score = 0.08 ± 0.35

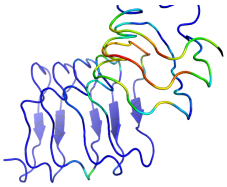


T0768

FFAS03_TS1

GDT_TS = 0.49

Score = −0.81 ± 0.30

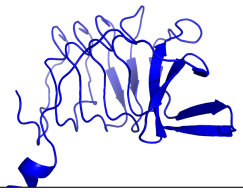


T0768

FALCON_MANUAL_TS2

GDT_TS = 0.65

Score = −1.30 ± 0.23

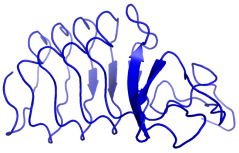


T0768

nns_TS5

GDT_TS = 0.68

Score = −1.83 ± 0.21



T0768

T0768

GDT_TS = 1.00

Score = −2.26 ± 0.16

T0769

MUFOLD-Server_TS4

GDT_TS = 0.44

Score = 0.81 ± 0.21

T0769

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.48

Score = −0.82 ± 0.19

T0769

RBO_Aleph_TS3

GDT_TS = 0.66

Score = −1.86 ± 0.11

T0769

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.68

Score = −1.95 ± 0.14

T0769

T0769

GDT_TS = 1.00

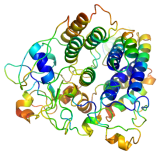
Score = −1.54 ± 0.45

T0770

MUFOLD-Server_TS4

GDT_TS = 0.48

Score = 4.55 ± 0.64

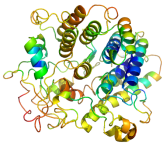


T0770

Distill_TS3

GDT_TS = 0.55

Score = 6.60 ± 0.75

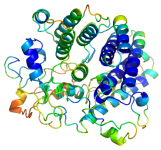


T0770

RBO_Aleph_TS3

GDT_TS = 0.60

Score = 4.03 ± 0.47

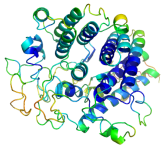


T0770

RBO_Aleph_TS4

GDT_TS = 0.62

Score = 4.98 ± 0.57

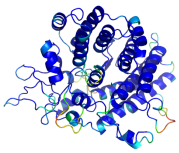


T0770

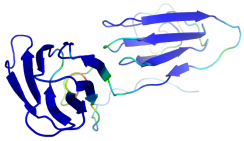
T0770

GDT_TS = 1.00

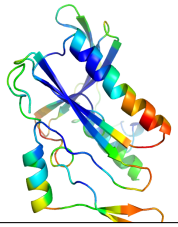
Score = 0.37 ± 0.38



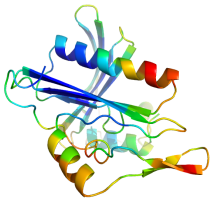
T0771
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.10
Score = 0.69 ± 0.19



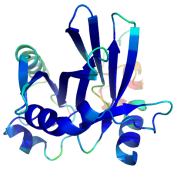
T0771
RBO_Aleph_TS3
GDT_TS = 0.14
Score = 1.30 ± 0.27



T0771
RBO_Aleph_TS4
GDT_TS = 0.15
Score = 1.77 ± 0.26

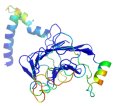


T0771
BAKER-ROSETTASERVER_TS5
GDT_TS = 0.21
Score = 0.94 ± 0.31



T0771
T0771
GDT_TS = 1.00
Score = −1.60 ± 0.22

T0772
Distill_TS3
GDT_TS = 0.45
Score = 1.52 ± 0.28

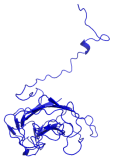


T0772
RBO_Aleph_TS3
GDT_TS = 0.51
Score = 1.95 ± 0.13

T0772
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.56
Score = −0.14 ± 0.37

T0772
FFAS03_TS1
GDT_TS = 0.59
Score = 0.33 ± 0.17

T0772
T0772
GDT_TS = 1.00
Score = −1.01 ± 0.26

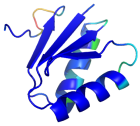


T0773
eThread_TS1
GDT_TS = 0.44
Score = 0.19 ± 0.31

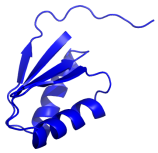
T0773
MULTICOM-CLUSTER_TS2
GDT_TS = 0.57
Score = −1.10 ± 0.19

T0773
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.61
Score = −1.31 ± 0.16

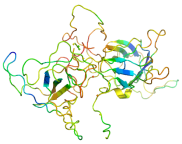
T0773
RBO_Aleph_TS3
GDT_TS = 0.82
Score = −1.14 ± 0.19



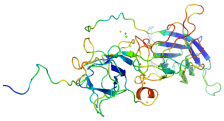
T0773
T0773
GDT_TS = 1.00
Score = −1.15 ± 0.20



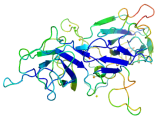
T0774
Seok-server_TS4
GDT_TS = 0.20
Score = 5.80 ± 0.34



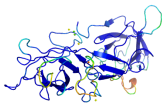
T0774
RBO_Aleph_TS3
GDT_TS = 0.27
Score = 3.19 ± 0.42



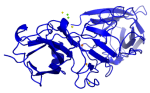
T0774
FFAS03_TS1
GDT_TS = 0.33
Score = 3.50 ± 0.29



T0774
Atome2_CBS_TS3
GDT_TS = 0.43
Score = 0.56 ± 0.15



T0774
T0774
GDT_TS = 1.00
Score = −2.37 ± 0.15

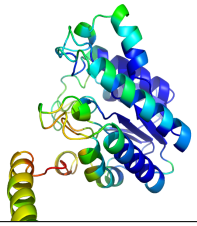


T0776

Distill_TS3

GDT_TS = 0.65

Score = 1.49 ± 0.29

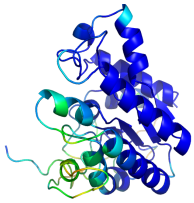


T0776

RBO_Aleph_TS3

GDT_TS = 0.68

Score = 0.33 ± 0.22

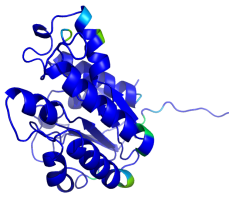


T0776

MUFOLD-Server_TS4

GDT_TS = 0.75

Score = -0.54 ± 0.28



T0776

FFAS03_TS1

GDT_TS = 0.82

Score = -1.65 ± 0.20

T0776

T0776

GDT_TS = 1.00

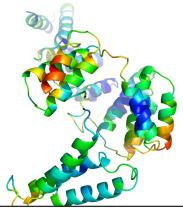
Score = -2.27 ± 0.19

T0777

Atome2_CBS_TS3

GDT_TS = 0.08

Score = 5.44 ± 0.43

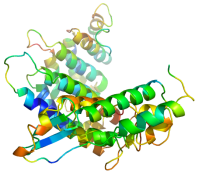


T0777

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.10

Score = 5.15 ± 0.52

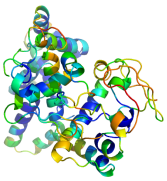


T0777

RBO_Aleph_TS3

GDT_TS = 0.11

Score = 2.69 ± 0.37



T0777

RBO_Aleph_TS4

GDT_TS = 0.13

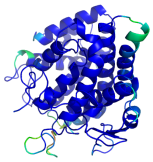
Score = 6.67 ± 0.51

T0777

T0777

GDT_TS = 1.00

Score = -1.25 ± 0.35

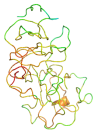


T0780

RBO_Aleph_TS3

GDT_TS = 0.09

Score = 4.88 ± 0.41

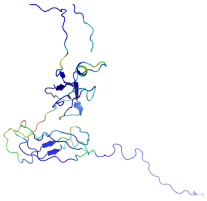


T0780

slbio_TS3

GDT_TS = 0.17

Score = 1.43 ± 0.22



T0780

BioShell-server_TS3

GDT_TS = 0.24

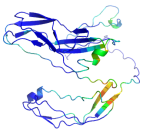
Score = 1.68 ± 0.13

T0780

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.27

Score = 3.06 ± 0.30



T0780

T0780

GDT_TS = 1.00

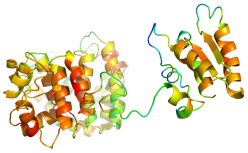
Score = -1.68 ± 0.18

T0781

Distill_TS3

GDT_TS = 0.07

Score = 9.35 ± 0.36

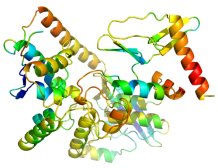


T0781

RBO_Aleph_TS3

GDT_TS = 0.09

Score = 6.76 ± 0.40

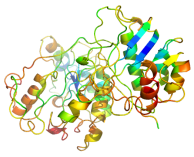


T0781

MULTICOM-CLUSTER_TS2

GDT_TS = 0.12

Score = 6.95 ± 0.35

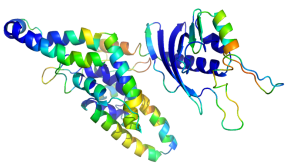


T0781

RaptorX_TS1

GDT_TS = 0.15

Score = 2.73 ± 0.45

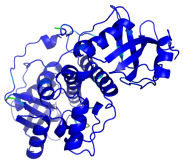


T0781

T0781

GDT_TS = 1.00

Score = -2.04 ± 0.16



T0782

RBO_Aleph_TS3

GDT_TS = 0.26

Score = -0.81 ± 0.20

T0782

FFAS03_TS1

GDT_TS = 0.43

Score = 0.36 ± 0.22

T0782

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.48

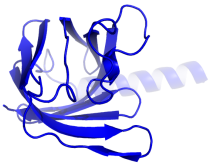
Score = -0.11 ± 0.32

T0782

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.60

Score = -1.01 ± 0.20



T0782

T0782

GDT_TS = 1.00

Score = -2.03 ± 0.15

T0783

MUFOLD-Server_TS4

GDT_TS = 0.30

Score = 2.77 ± 0.36

T0783

FFAS03_TS1

GDT_TS = 0.36

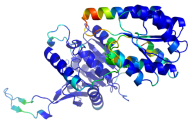
Score = 2.87 ± 0.27

T0783

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.40

Score = 0.78 ± 0.23

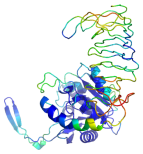


T0783

RBO_Aleph_TS3

GDT_TS = 0.43

Score = 2.45 ± 0.56

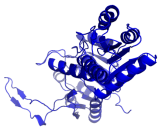


T0783

T0783

GDT_TS = 1.00

Score = -2.20 ± 0.31

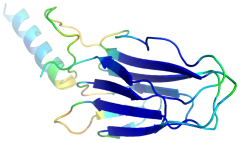


T0784

eThread_TS5

GDT_TS = 0.50

Score = -0.10 ± 0.28

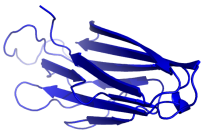


T0784

BioShell-server_TS3

GDT_TS = 0.67

Score = -0.65 ± 0.23

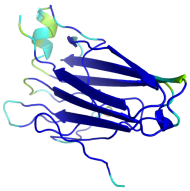


T0784

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.71

Score = -1.07 ± 0.16

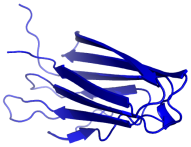


T0784

FFAS03_TS1

GDT_TS = 0.87

Score = -1.59 ± 0.12

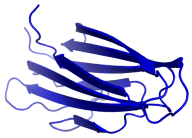


T0784

T0784

GDT_TS = 1.00

Score = -1.76 ± 0.10



T0785

FFAS03_TS1

GDT_TS = 0.14

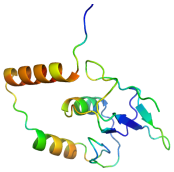
Score = 0.42 ± 0.22

T0785

nns_TS5

GDT_TS = 0.17

Score = 0.62 ± 0.26



T0785

RBO_Aleph_TS3

GDT_TS = 0.21

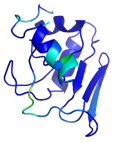
Score = -0.37 ± 0.33

T0785

BAKER-ROSETTASERVER_TS2

GDT_TS = 0.25

Score = -0.88 ± 0.23



T0785

T0785

GDT_TS = 1.00

Score = -2.03 ± 0.16

T0786

eThread_TS2

GDT_TS = 0.32

Score = 3.67 ± 0.29

T0786

FFAS03_TS1

GDT_TS = 0.43

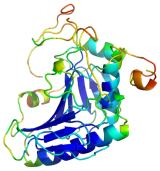
Score = 2.50 ± 0.32

T0786

RBO_Aleph_TS3

GDT_TS = 0.47

Score = 1.85 ± 0.30

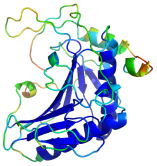


T0786

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.53

Score = 0.93 ± 0.24



T0786

T0786

GDT_TS = 1.00

Score = −2.06 ± 0.18

T0787

MUFOLD-Server_TS4

GDT_TS = 0.16

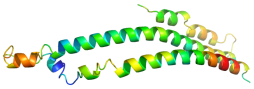
Score = 2.25 ± 0.27

T0787

RBO_Aleph_TS3

GDT_TS = 0.18

Score = 2.22 ± 0.21

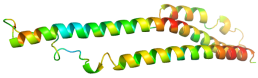


T0787

RBO_Aleph_TS4

GDT_TS = 0.19

Score = 2.33 ± 0.24

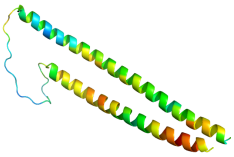


T0787

FFAS03_TS1

GDT_TS = 0.20

Score = 1.75 ± 0.23

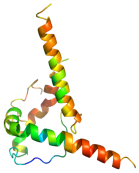


T0787

T0787

GDT_TS = 1.00

Score = 2.13 ± 0.17

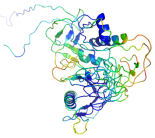


T0788

RBO_Aleph_TS4

GDT_TS = 0.55

Score = 2.32 ± 0.54

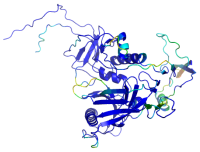


T0788

MULTICOM-CLUSTER_TS2

GDT_TS = 0.60

Score = 1.07 ± 0.33

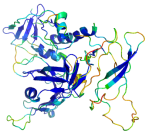


T0788

FFAS03_TS1

GDT_TS = 0.71

Score = 2.11 ± 0.37



T0788

QUARK_TS3

GDT_TS = 0.74

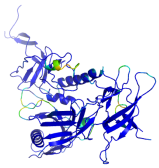
Score = 1.67 ± 0.47

T0788

T0788

GDT_TS = 1.00

Score = −0.68 ± 0.34



T0789

RBO_Aleph_TS3

GDT_TS = 0.09

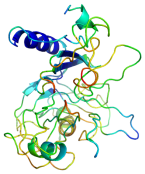
Score = 2.90 ± 0.35

T0789

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.11

Score = 2.93 ± 0.34

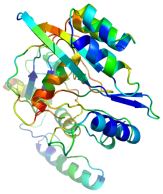


T0789

MULTICOM-NOVEL_TS4

GDT_TS = 0.13

Score = 2.91 ± 0.31

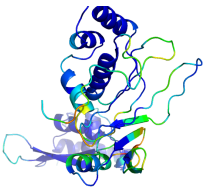


T0789

BAKER-ROSETTASERVER_TS2

GDT_TS = 0.18

Score = 1.16 ± 0.31

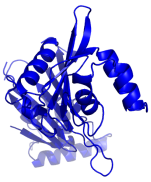


T0789

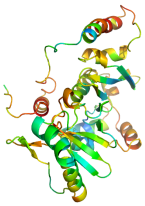
T0789

GDT_TS = 1.00

Score = −2.15 ± 0.18



T0790
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.11
Score = 4.88 ± 0.33



T0790
Distill_TS3
GDT_TS = 0.12
Score = 5.25 ± 0.41

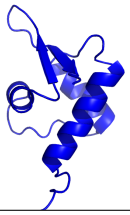
T0790
BAKER-ROSETTASERVER_TS2
GDT_TS = 0.16
Score = 2.77 ± 0.28

T0790
BAKER-ROSETTASERVER_TS3
GDT_TS = 0.22
Score = 1.23 ± 0.25

T0790
T0790
GDT_TS = 1.00
Score = −2.25 ± 0.11

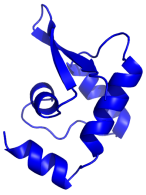
T0792
BioShell-server_TS3
GDT_TS = 0.56
Score = −0.25 ± 0.35

T0792
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.63
Score = −1.09 ± 0.23



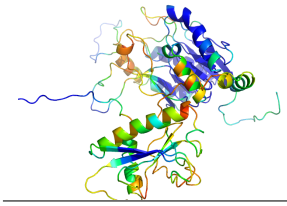
T0792
FFAS03_TS1
GDT_TS = 0.72
Score = −1.32 ± 0.13

T0792
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.79
Score = −1.45 ± 0.16

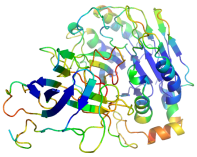


T0792
T0792
GDT_TS = 1.00
Score = −1.70 ± 0.12

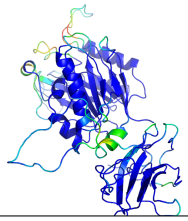
T0794
BioShell-server_TS5
GDT_TS = 0.29
Score = 4.26 ± 0.35



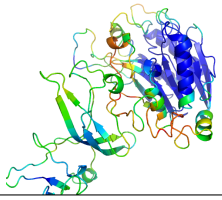
T0794
RBO_Aleph_TS3
GDT_TS = 0.32
Score = 3.22 ± 0.33



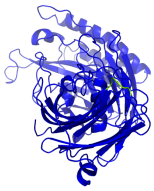
T0794
FALCON_MANUAL_TS2
GDT_TS = 0.38
Score = 1.65 ± 0.24



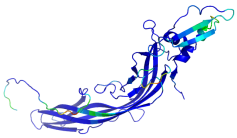
T0794
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.41
Score = 3.07 ± 0.34



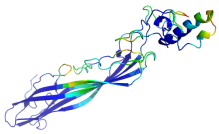
T0794
T0794
GDT_TS = 1.00
Score = −2.30 ± 0.26



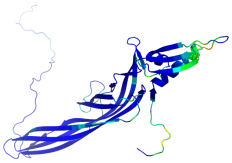
T0796
FALCON_MANUAL_TS2
GDT_TS = 0.32
Score = 0.61 ± 0.14



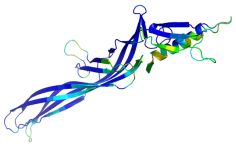
T0796
RBO_Aleph_TS3
GDT_TS = 0.39
Score = 1.35 ± 0.26



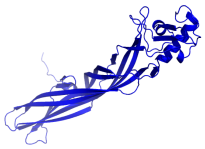
T0796
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.41
Score = 1.22 ± 0.36



T0796
FFAS03_TS1
GDT_TS = 0.53
Score = 0.03 ± 0.23



T0796
T0796
GDT_TS = 1.00
Score = −1.89 ± 0.16



T0797

BAKER-ROSETTASERVER_TS2

GDT_TS = 0.52

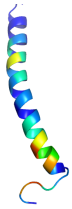
Score = -0.29 ± 0.36

T0797

Alpha-Gelly-Server_TS2

GDT_TS = 0.66

Score = -0.13 ± 0.46

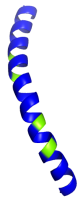


T0797

FFAS03_TS1

GDT_TS = 0.73

Score = -0.37 ± 0.64

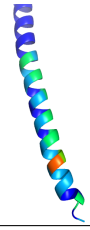


T0797

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.80

Score = -0.40 ± 0.32



T0797

T0797

GDT_TS = 1.00

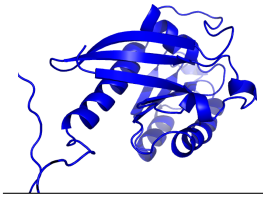
Score = -0.14 ± 0.68

T0798

BioShell-server_TS3

GDT_TS = 0.79

Score = -1.35 ± 0.17



T0798

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.80

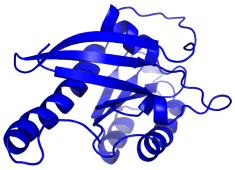
Score = -1.48 ± 0.19

T0798

Atome2_CBS_TS3

GDT_TS = 0.87

Score = -1.70 ± 0.16



T0798

FFAS03_TS1

GDT_TS = 0.89

Score = -1.80 ± 0.15

T0798

T0798

GDT_TS = 1.00

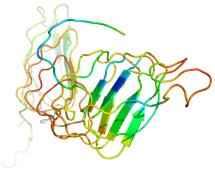
Score = -1.90 ± 0.14

T0800

MUFOLD-Server_TS4

GDT_TS = 0.16

Score = 4.02 ± 0.32

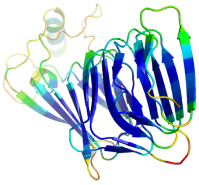


T0800

eThread_TS1

GDT_TS = 0.24

Score = 1.21 ± 0.24

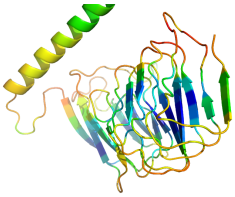


T0800

RBO_Aleph_TS3

GDT_TS = 0.30

Score = 2.70 ± 0.37



T0800

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.37

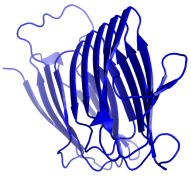
Score = -0.30 ± 0.38

T0800

T0800

GDT_TS = 1.00

Score = -2.54 ± 0.15

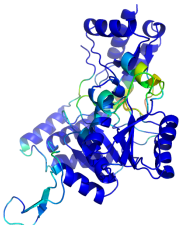


T0801

eThread_TS2

GDT_TS = 0.72

Score = 0.06 ± 0.35



T0801

FFAS03_TS1

GDT_TS = 0.77

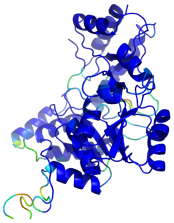
Score = -0.13 ± 0.39

T0801

MUFOLD-Server_TS4

GDT_TS = 0.80

Score = -1.29 ± 0.49

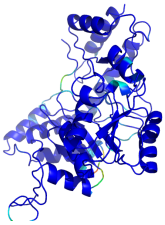


T0801

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.82

Score = -1.69 ± 0.30

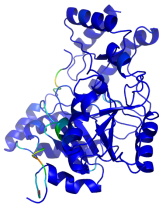


T0801

T0801

GDT_TS = 1.00

Score = -2.04 ± 0.26



T0803

Distill_TS3

GDT_TS = 0.22

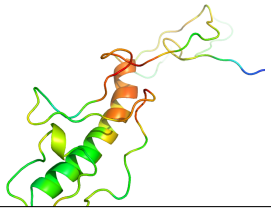
Score = 2.54 ± 0.22

T0803

FALCON_MANUAL_TS2

GDT_TS = 0.33

Score = 2.03 ± 0.23

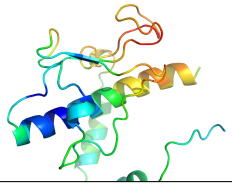


T0803

RBO_Aleph_TS3

GDT_TS = 0.40

Score = 1.95 ± 0.22

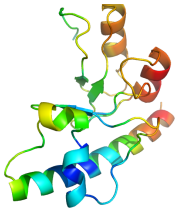


T0803

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.44

Score = 1.47 ± 0.25

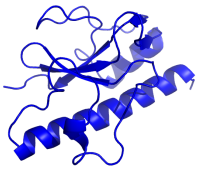


T0803

T0803

GDT_TS = 1.00

Score = −2.15 ± 0.13

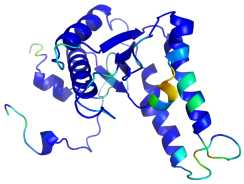


T0805

MUFOLD-Server_TS4

GDT_TS = 0.60

Score = 0.16 ± 0.19

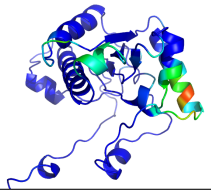


T0805

Seok-server_TS2

GDT_TS = 0.61

Score = 0.47 ± 0.18

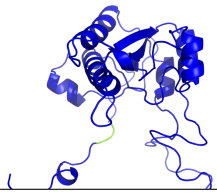


T0805

FFAS03_TS1

GDT_TS = 0.65

Score = 0.36 ± 0.23

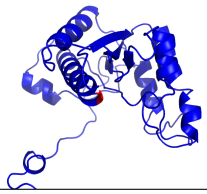


T0805

RBO_Aleph_TS3

GDT_TS = 0.69

Score = −0.03 ± 0.25



T0805

T0805

GDT_TS = 1.00

Score = −1.27 ± 0.22

T0806

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.12

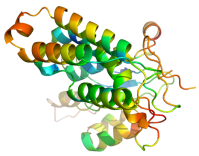
Score = 3.95 ± 0.40

T0806

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.13

Score = 4.38 ± 0.41



T0806

RBO_Aleph_TS3

GDT_TS = 0.19

Score = 1.96 ± 0.29

T0806

BAKER-ROSETTASERVER_TS2

GDT_TS = 0.24

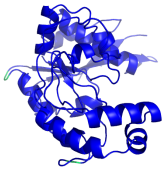
Score = 2.86 ± 0.34

T0806

T0806

GDT_TS = 1.00

Score = −2.21 ± 0.17

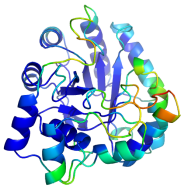


T0807

BioShell-server_TS3

GDT_TS = 0.69

Score = 0.68 ± 0.28



T0807

MUFOLD-Server_TS4

GDT_TS = 0.73

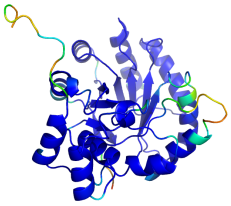
Score = 0.50 ± 0.19

T0807

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.78

Score = −0.59 ± 0.40

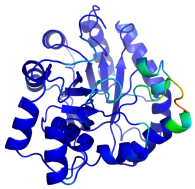


T0807

RBO_Aleph_TS3

GDT_TS = 0.79

Score = −0.67 ± 0.41

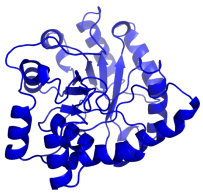


T0807

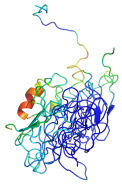
T0807

GDT_TS = 1.00

Score = −2.17 ± 0.17



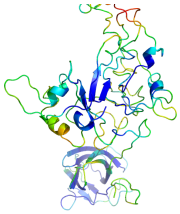
T0808
MUFOLD-Server_TS4
GDT_TS = 0.08
Score = 3.24 ± 0.22



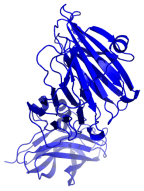
T0808
slbio_TS3
GDT_TS = 0.12
Score = 1.86 ± 0.07

T0808
RBO_Aleph_TS3
GDT_TS = 0.16
Score = 3.66 ± 0.30

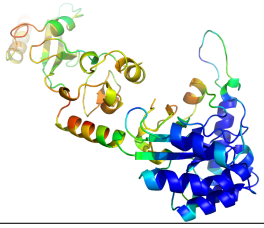
T0808
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.18
Score = 3.71 ± 0.36



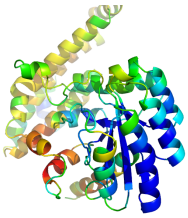
T0808
T0808
GDT_TS = 1.00
Score = −2.28 ± 0.14



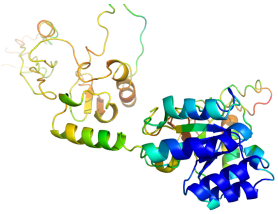
T0810
BioShell-server_TS3
GDT_TS = 0.34
Score = 3.63 ± 0.29



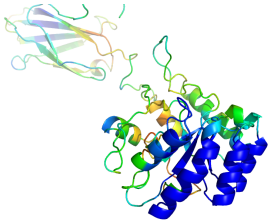
T0810
eThread_TS1
GDT_TS = 0.37
Score = 4.33 ± 0.40



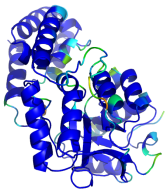
T0810
MUFOLD-Server_TS4
GDT_TS = 0.38
Score = 4.66 ± 0.38



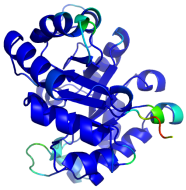
T0810
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.40
Score = 3.75 ± 0.34



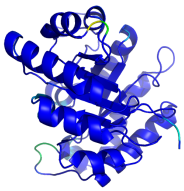
T0810
T0810
GDT_TS = 1.00
Score = −1.78 ± 0.25



T0811
MUFOLD-Server_TS4
GDT_TS = 0.78
Score = −0.88 ± 0.26

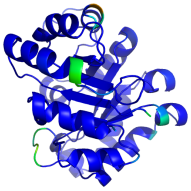


T0811
BioShell-server_TS3
GDT_TS = 0.80
Score = −1.12 ± 0.24

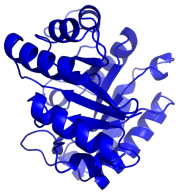


T0811
Distill_TS3
GDT_TS = 0.86
Score = 0.40 ± 0.24

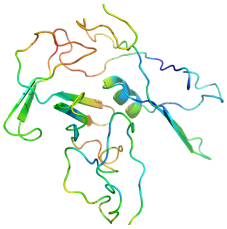
T0811
FFAS03_TS1
GDT_TS = 0.88
Score = −1.29 ± 0.20



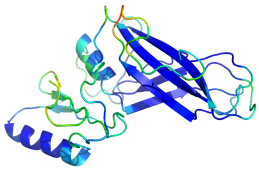
T0811
T0811
GDT_TS = 1.00
Score = −1.99 ± 0.19



T0812
RBO_Aleph_TS3
GDT_TS = 0.11
Score = 2.19 ± 0.30



T0812
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.18
Score = 0.63 ± 0.17

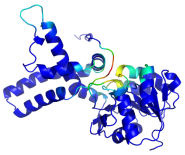


T0812
Pcons-net_TS2
GDT_TS = 0.24
Score = 1.88 ± 0.31

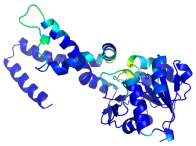
T0812
MUFOLD-Server_TS4
GDT_TS = 0.32
Score = 1.11 ± 0.21

T0812
T0812
GDT_TS = 1.00
Score = −2.04 ± 0.15

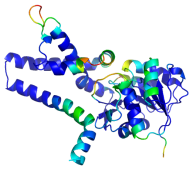
T0813
Pcons-net_TS2
GDT_TS = 0.66
Score = 0.24 ± 0.24



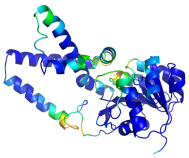
T0813
FFAS03_TS1
GDT_TS = 0.73
Score = -0.09 ± 0.31



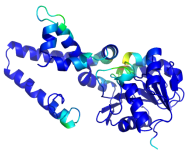
T0813
RBO_Aleph_TS3
GDT_TS = 0.76
Score = 0.59 ± 0.16



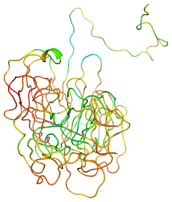
T0813
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.79
Score = -0.03 ± 0.39



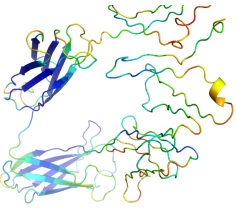
T0813
T0813
GDT_TS = 1.00
Score = -0.50 ± 0.47



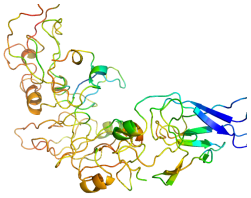
T0814
RBO_Aleph_TS3
GDT_TS = 0.05
Score = 6.57 ± 0.39



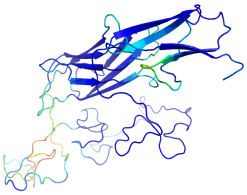
T0814
Distill_TS3
GDT_TS = 0.09
Score = 5.34 ± 0.33



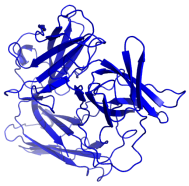
T0814
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.14
Score = 6.70 ± 0.55



T0814
3D-Jigsaw-V5_1_TS4
GDT_TS = 0.18
Score = 3.92 ± 0.28



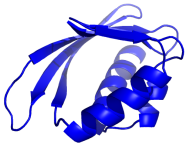
T0814
T0814
GDT_TS = 1.00
Score = -2.27 ± 0.15



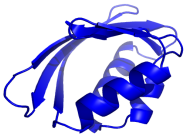
T0815
MUFOLD-Server_TS4
GDT_TS = 0.76
Score = -1.17 ± 0.18

T0815
Seok-server_TS2
GDT_TS = 0.80
Score = -1.67 ± 0.15

T0815
Pcons-net_TS2
GDT_TS = 0.86
Score = -1.73 ± 0.18

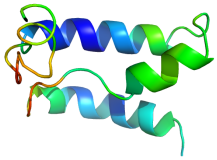


T0815
RBO_Aleph_TS3
GDT_TS = 0.90
Score = -1.82 ± 0.14

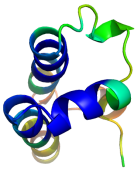


T0815
T0815
GDT_TS = 1.00
Score = -1.92 ± 0.14

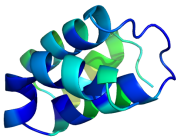
T0816
MUFOLD-Server_TS4
GDT_TS = 0.39
Score = 0.03 ± 0.33



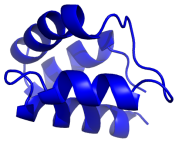
T0816
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.47
Score = -1.19 ± 0.21



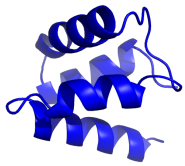
T0816
RaptorX-FM_TS1
GDT_TS = 0.51
Score = -0.89 ± 0.44



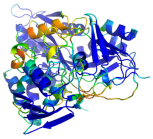
T0816
RBO_Aleph_TS3
GDT_TS = 0.68
Score = -1.52 ± 0.13



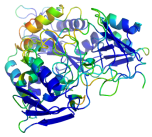
T0816
T0816
GDT_TS = 1.00
Score = -1.75 ± 0.11



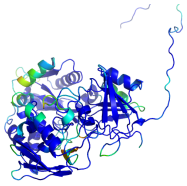
T0817
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.43
Score = 0.41 ± 0.27



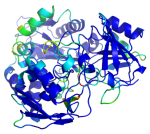
T0817
MUFOLD-Server_TS4
GDT_TS = 0.51
Score = 0.66 ± 0.27



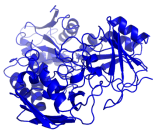
T0817
BioShell-server_TS3
GDT_TS = 0.57
Score = 0.73 ± 0.24



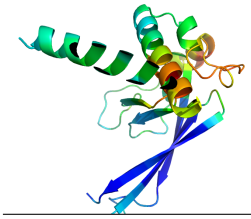
T0817
FFAS03_TS1
GDT_TS = 0.62
Score = −0.63 ± 0.46



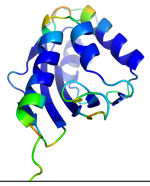
T0817
T0817
GDT_TS = 1.00
Score = −2.54 ± 0.14



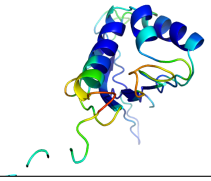
T0818
RBO_Aleph_TS3
GDT_TS = 0.19
Score = 2.20 ± 0.24



T0818
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.26
Score = 0.30 ± 0.26

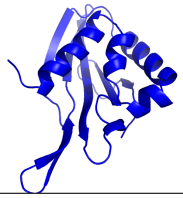


T0818
MUFOLD-Server_TS4
GDT_TS = 0.26
Score = 0.76 ± 0.21

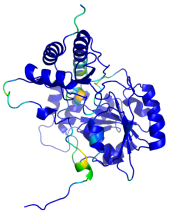


T0818
Alpha-Gelly-Server_TS2
GDT_TS = 0.31
Score = 0.40 ± 0.26

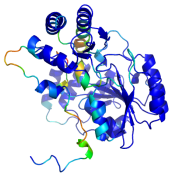
T0818
T0818
GDT_TS = 1.00
Score = −2.08 ± 0.19



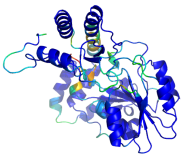
T0819
slbio_TS3
GDT_TS = 0.68
Score = −0.16 ± 0.34



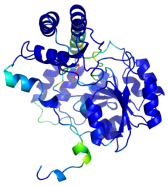
T0819
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.73
Score = 0.16 ± 0.30



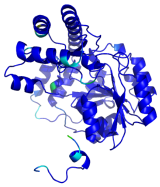
T0819
FFAS03_TS1
GDT_TS = 0.74
Score = −0.09 ± 0.35



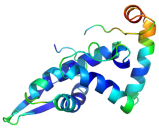
T0819
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.83
Score = −0.17 ± 0.43



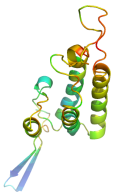
T0819
T0819
GDT_TS = 1.00
Score = −1.48 ± 0.36



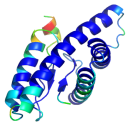
T0820
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.19
Score = 0.66 ± 0.25



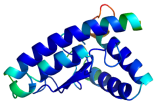
T0820
RBO_Aleph_TS3
GDT_TS = 0.23
Score = 1.85 ± 0.29



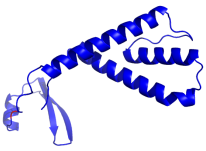
T0820
Zhang-Server_TS1
GDT_TS = 0.28
Score = −0.55 ± 0.30



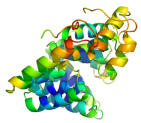
T0820
QUARK_TS4
GDT_TS = 0.31
Score = −0.66 ± 0.26



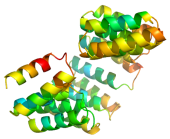
T0820
T0820
GDT_TS = 1.00
Score = −0.11 ± 0.38



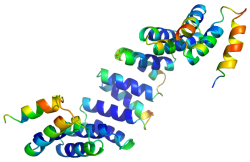
T0821
FFAS03_TS1
GDT_TS = 0.35
Score = 4.04 ± 0.41



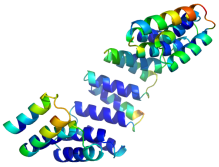
T0821
nns_TS5
GDT_TS = 0.40
Score = 4.53 ± 0.60



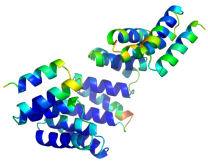
T0821
RBO_Aleph_TS3
GDT_TS = 0.51
Score = 2.38 ± 0.29



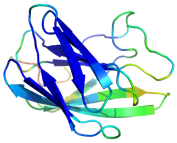
T0821
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.60
Score = 2.40 ± 0.34



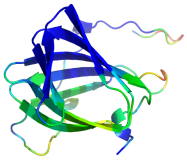
T0821
T0821
GDT_TS = 1.00
Score = 1.56 ± 0.32



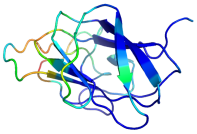
T0822
RBO_Aleph_TS3
GDT_TS = 0.23
Score = −0.67 ± 0.29



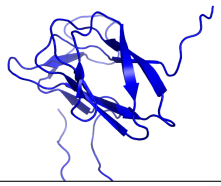
T0822
BioShell-server_TS3
GDT_TS = 0.28
Score = −0.18 ± 0.34



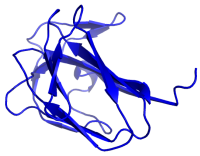
T0822
FALCON_MANUAL_TS2
GDT_TS = 0.40
Score = −0.52 ± 0.32



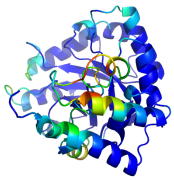
T0822
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.45
Score = −0.27 ± 0.29



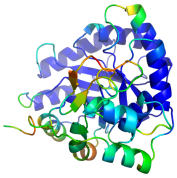
T0822
T0822
GDT_TS = 1.00
Score = −1.91 ± 0.17



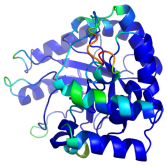
T0823
ZHOU-SPARKS-X_TS5
GDT_TS = 0.52
Score = 0.48 ± 0.22



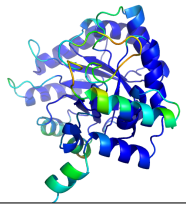
T0823
BioShell-server_TS3
GDT_TS = 0.54
Score = 0.58 ± 0.27



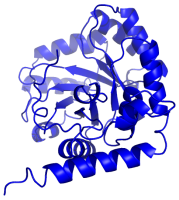
T0823
FFAS03_TS1
GDT_TS = 0.58
Score = −0.26 ± 0.37



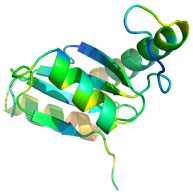
T0823
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.60
Score = 0.65 ± 0.20



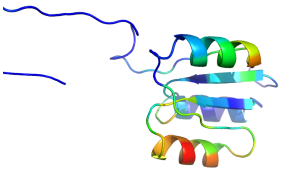
T0823
T0823
GDT_TS = 1.00
Score = −1.93 ± 0.25



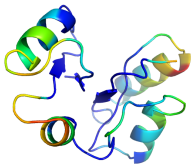
T0824
BioShell-server_TS3
GDT_TS = 0.20
Score = 0.71 ± 0.26



T0824
Distill_TS3
GDT_TS = 0.23
Score = 1.04 ± 0.36

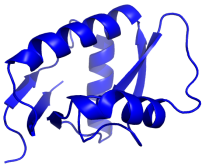


T0824
RBO_Aleph_TS3
GDT_TS = 0.26
Score = −0.27 ± 0.39



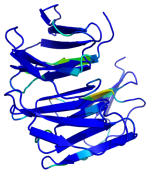
T0824
Zhang-Server_TS1
GDT_TS = 0.29
Score = −0.70 ± 0.28

T0824
T0824
GDT_TS = 1.00
Score = −1.40 ± 0.17



T0825
myprotein-me_TS4
GDT_TS = 0.61
Score = -1.73 ± 0.16

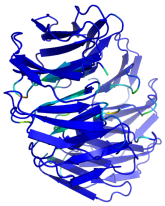
T0825
BioShell-server_TS3
GDT_TS = 0.67
Score = -0.89 ± 0.24



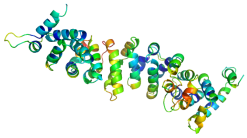
T0825
FFAS03_TS1
GDT_TS = 0.83
Score = -1.54 ± 0.16

T0825
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.84
Score = -1.54 ± 0.17

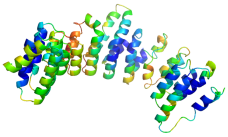
T0825
T0825
GDT_TS = 1.00
Score = -1.95 ± 0.18



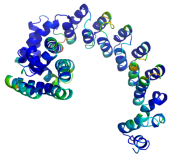
T0827
RBO_Aleph_TS3
GDT_TS = 0.10
Score = 3.47 ± 0.38



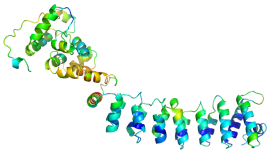
T0827
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.14
Score = 3.87 ± 0.45



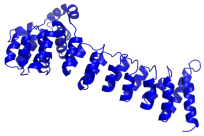
T0827
Zhang-Server_TS1
GDT_TS = 0.21
Score = 2.54 ± 0.35



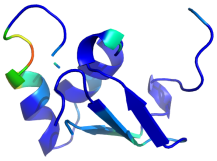
T0827
nns_TS1
GDT_TS = 0.24
Score = 3.64 ± 0.39



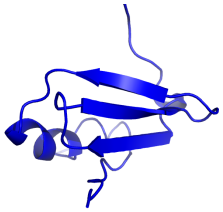
T0827
T0827
GDT_TS = 1.00
Score = -1.72 ± 0.23



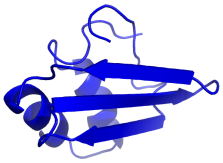
T0829
Alpha-Gelly-Server_TS2
GDT_TS = 0.35
Score = -0.42 ± 0.43



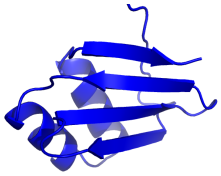
T0829
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.46
Score = -1.37 ± 0.14



T0829
RBO_Aleph_TS3
GDT_TS = 0.56
Score = -1.39 ± 0.17

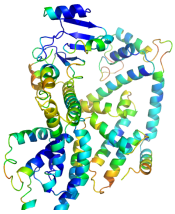


T0829
Zhang-Server_TS1
GDT_TS = 0.62
Score = -1.39 ± 0.13

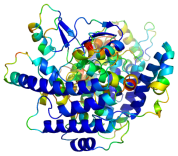


T0829
T0829
GDT_TS = 1.00
Score = -1.70 ± 0.14

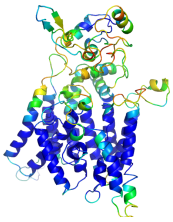
T0830
RBO_Aleph_TS3
GDT_TS = 0.09
Score = 5.20 ± 0.47



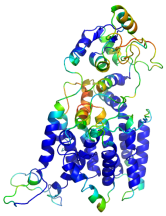
T0830
RBO_Aleph_TS4
GDT_TS = 0.17
Score = 4.44 ± 0.34



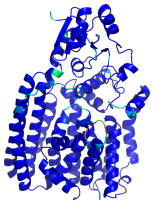
T0830
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.27
Score = 3.34 ± 0.40



T0830
FFAS03_TS1
GDT_TS = 0.33
Score = 3.10 ± 0.42



T0830
T0830
GDT_TS = 1.00
Score = -1.86 ± 0.29

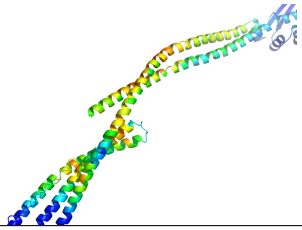


T0831

BioShell-server_TS3

GDT_TS = 0.09

Score = 2.84 ± 0.31

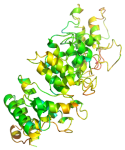


T0831

MUFOLD-Server_TS4

GDT_TS = 0.12

Score = 6.72 ± 0.22



T0831

RBO_Aleph_TS3

GDT_TS = 0.13

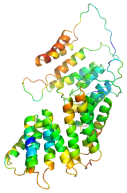
Score = 6.39 ± 0.37

T0831

Pcons-net_TS1

GDT_TS = 0.14

Score = 6.46 ± 0.35

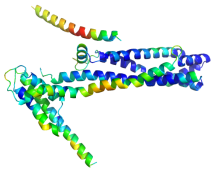


T0831

T0831

GDT_TS = 1.00

Score = 3.07 ± 0.43



T0832

BioShell-server_TS3

GDT_TS = 0.10

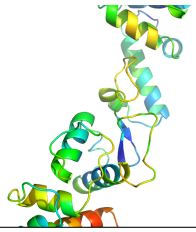
Score = 2.94 ± 0.34

T0832

RBO_Aleph_TS3

GDT_TS = 0.14

Score = 2.34 ± 0.28

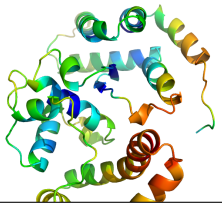


T0832

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.15

Score = 3.97 ± 0.31

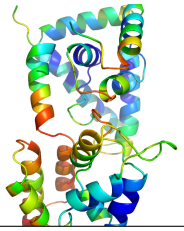


T0832

BAKER-ROSETTASERVER_TS2

GDT_TS = 0.18

Score = 2.50 ± 0.27



T0832

T0832

GDT_TS = 1.00

Score = −2.26 ± 0.13

T0833

BioSerf_TS3

GDT_TS = 0.28

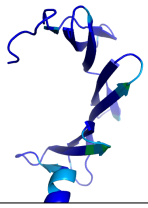
Score = 2.52 ± 0.26

T0833

RBO_Aleph_TS3

GDT_TS = 0.45

Score = 0.36 ± 0.15



T0833

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.50

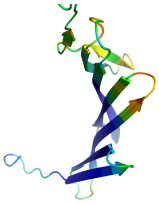
Score = 0.53 ± 0.29

T0833

FFAS03_TS1

GDT_TS = 0.62

Score = 0.19 ± 0.25

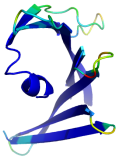


T0833

T0833

GDT_TS = 1.00

Score = −0.73 ± 0.25

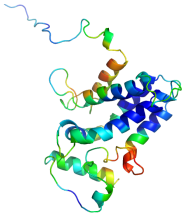


T0834

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.10

Score = 2.34 ± 0.36



T0834

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.11

Score = 3.55 ± 0.34

T0834

RBO_Aleph_TS4

GDT_TS = 0.16

Score = 0.88 ± 0.20

T0834

RBO_Aleph_TS3

GDT_TS = 0.19

Score = 0.86 ± 0.25

T0834

T0834

GDT_TS = 1.00

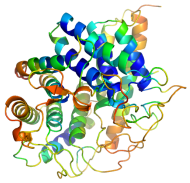
Score = −0.85 ± 0.23

T0835

BioShell-server_TS3

GDT_TS = 0.28

Score = 5.51 ± 0.42



T0835

MUFOLD-Server_TS4

GDT_TS = 0.33

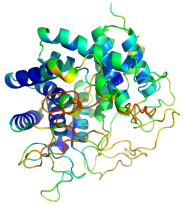
Score = 5.82 ± 0.46

T0835

FFAS03_TS1

GDT_TS = 0.41

Score = 3.95 ± 0.41

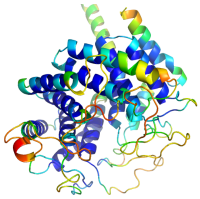


T0835

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.45

Score = 3.28 ± 0.39

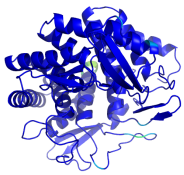


T0835

T0835

GDT_TS = 1.00

Score = −2.55 ± 0.14



T0836

BioShell-server_TS3

GDT_TS = 0.17

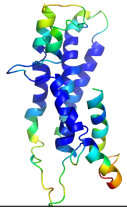
Score = 0.97 ± 0.26

T0836

FFAS03_TS1

GDT_TS = 0.20

Score = 1.75 ± 0.35

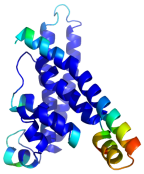


T0836

BAKER-ROSETTASERVER_TS4

GDT_TS = 0.22

Score = 0.71 ± 0.25

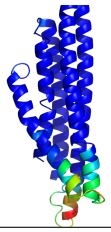


T0836

Zhang-Server_TS3

GDT_TS = 0.30

Score = −0.20 ± 0.40

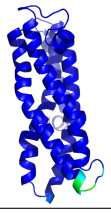


T0836

T0836

GDT_TS = 1.00

Score = −0.59 ± 0.47

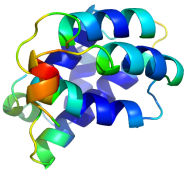


T0837

BioShell-server_TS3

GDT_TS = 0.24

Score = 0.50 ± 0.24

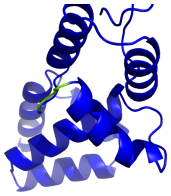


T0837

RBO_Aleph_TS3

GDT_TS = 0.36

Score = −1.25 ± 0.16

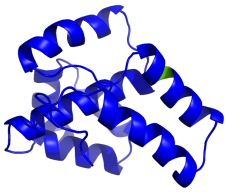


T0837

MULTICOM-CLUSTER_TS2

GDT_TS = 0.47

Score = −1.15 ± 0.21

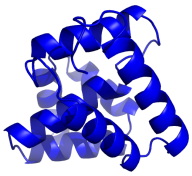


T0837

Zhang-Server_TS2

GDT_TS = 0.58

Score = −1.75 ± 0.17

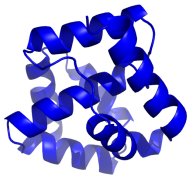


T0837

T0837

GDT_TS = 1.00

Score = −1.87 ± 0.15

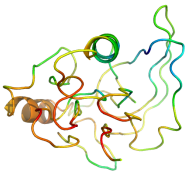


T0838

RBO_Aleph_TS3

GDT_TS = 0.19

Score = 1.50 ± 0.18

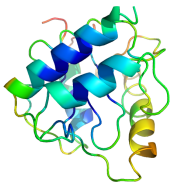


T0838

BioSerf_TS4

GDT_TS = 0.22

Score = 0.86 ± 0.36

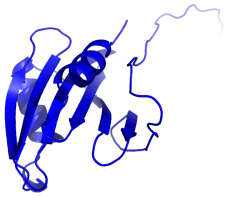


T0838

MULTICOM-CONSTRUCT_TS1

GDT_TS = 0.36

Score = 0.42 ± 0.90

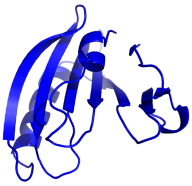


T0838

FFAS03_TS1

GDT_TS = 0.43

Score = −1.32 ± 0.19



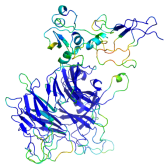
T0838

T0838

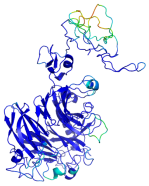
GDT_TS = 1.00

Score = −1.77 ± 0.17

T0840
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.53
Score = 1.55 ± 0.30



T0840
BioSerf_TS4
GDT_TS = 0.67
Score = 1.67 ± 0.71



T0840
RBO_Aleph_TS3
GDT_TS = 0.69
Score = 0.21 ± 0.44

T0840
FFAS03_TS1
GDT_TS = 0.90
Score = -2.27 ± 0.24

T0840
T0840
GDT_TS = 1.00
Score = -1.32 ± 0.36

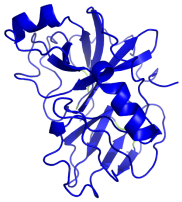
T0841
BioShell-server_TS3
GDT_TS = 0.71
Score = -0.82 ± 0.26

T0841
MUFOLD-Server_TS4
GDT_TS = 0.75
Score = -0.23 ± 0.32

T0841
RBO_Aleph_TS3
GDT_TS = 0.79
Score = -1.33 ± 0.30

T0841
FFAS03_TS1
GDT_TS = 0.90
Score = -1.86 ± 0.18

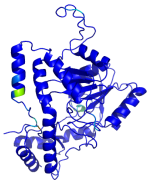
T0841
T0841
GDT_TS = 1.00
Score = -1.38 ± 0.29



T0843
FFAS03_TS1
GDT_TS = 0.71
Score = -0.50 ± 0.40

T0843
MUFOLD-Server_TS4
GDT_TS = 0.72
Score = -0.91 ± 0.35

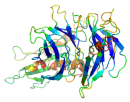
T0843
RBO_Aleph_TS3
GDT_TS = 0.76
Score = -1.43 ± 0.32



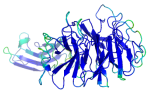
T0843
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.78
Score = -1.48 ± 0.28

T0843
T0843
GDT_TS = 1.00
Score = -2.31 ± 0.23

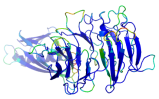
T0845
MUFOLD-Server_TS4
GDT_TS = 0.25
Score = 4.12 ± 0.40



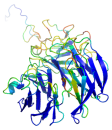
T0845
Atome2_CBS_TS3
GDT_TS = 0.30
Score = 0.80 ± 0.22



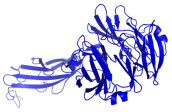
T0845
RBO_Aleph_TS3
GDT_TS = 0.36
Score = 0.38 ± 0.12



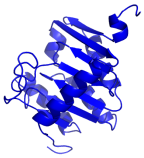
T0845
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.40
Score = 1.50 ± 0.24



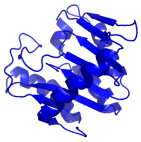
T0845
T0845
GDT_TS = 1.00
Score = -2.42 ± 0.13



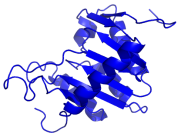
T0847
Pcons-net_TS2
GDT_TS = 0.63
Score = -1.21 ± 0.18



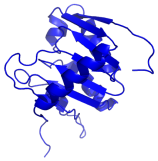
T0847
Seok-server_TS2
GDT_TS = 0.66
Score = -1.46 ± 0.14



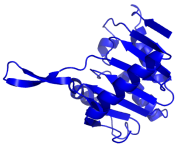
T0847
RBO_Aleph_TS3
GDT_TS = 0.70
Score = -1.04 ± 0.12



T0847
Atome2_CBS_TS3
GDT_TS = 0.72
Score = -1.57 ± 0.13

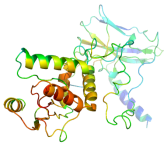


T0847
T0847
GDT_TS = 1.00
Score = -2.14 ± 0.17



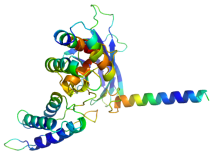
T0848
Alpha-Gelly-Server_TS2
GDT_TS = 0.08
Score = 5.60 ± 0.60

T0848
Distill_TS3
GDT_TS = 0.18
Score = 7.19 ± 0.31

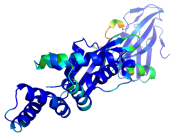


T0848
RBO_Aleph_TS3
GDT_TS = 0.21
Score = 3.47 ± 0.43

T0848
BAKER-ROSETTASERVER_TS4
GDT_TS = 0.29
Score = 2.77 ± 0.36



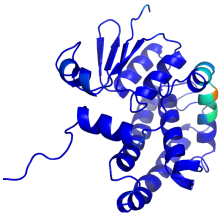
T0848
T0848
GDT_TS = 1.00
Score = -0.73 ± 0.34



T0849
BioShell-server_TS3
GDT_TS = 0.48
Score = 1.11 ± 0.30

T0849
MUFOLD-Server_TS4
GDT_TS = 0.54
Score = 1.19 ± 0.32

T0849
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.62
Score = -0.94 ± 0.25

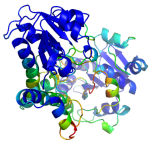


T0849
FFAS03_TS1
GDT_TS = 0.63
Score = 0.88 ± 0.21

T0849
T0849
GDT_TS = 1.00
Score = -2.28 ± 0.17

T0851
BioShell-server_TS3
GDT_TS = 0.55
Score = 0.40 ± 0.18

T0851
Atome2_CBS_TS3
GDT_TS = 0.60
Score = 0.86 ± 0.25

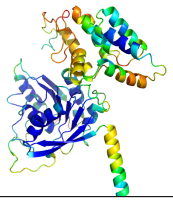


T0851
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.69
Score = 0.44 ± 0.28

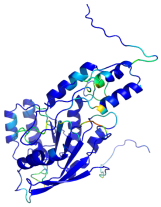
T0851
RBO_Aleph_TS3
GDT_TS = 0.79
Score = -0.43 ± 0.48

T0851
T0851
GDT_TS = 1.00
Score = -1.46 ± 0.28

T0852
RBO_Aleph_TS3
GDT_TS = 0.30
Score = 2.85 ± 0.50

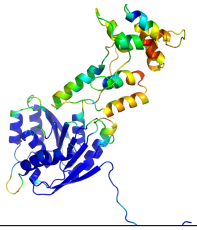


T0852
Alpha-Gelly-Server_TS2
GDT_TS = 0.39
Score = 2.37 ± 0.32

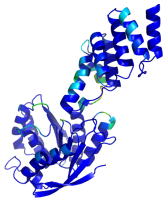


T0852
Distill_TS3
GDT_TS = 0.40
Score = 3.21 ± 0.33

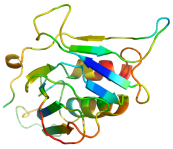
T0852
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.46
Score = 2.93 ± 0.37



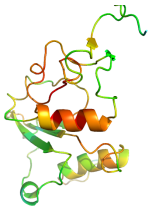
T0852
T0852
GDT_TS = 1.00
Score = −1.68 ± 0.40



T0853
Alpha-Gelly-Server_TS2
GDT_TS = 0.15
Score = 1.38 ± 0.17

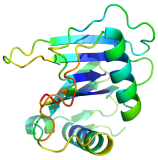


T0853
FALCON_MANUAL_TS2
GDT_TS = 0.23
Score = 2.47 ± 0.28

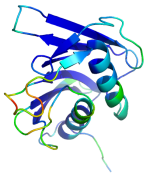


T0853
RBO_Aleph_TS3
GDT_TS = 0.30
Score = 1.30 ± 0.28

T0853
Zhang-Server_TS1
GDT_TS = 0.37
Score = 0.59 ± 0.31



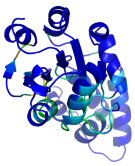
T0853
T0853
GDT_TS = 1.00
Score = −0.85 ± 0.25



T0854
BioShell-server_TS3
GDT_TS = 0.65
Score = −1.04 ± 0.30

T0854
MULTICOM-CONSTRUCT_TS1
GDT_TS = 0.68
Score = −1.42 ± 0.28

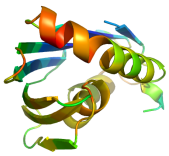
T0854
FFAS03_TS1
GDT_TS = 0.69
Score = −1.35 ± 0.28



T0854
RBO_Aleph_TS3
GDT_TS = 0.74
Score = −1.86 ± 0.18

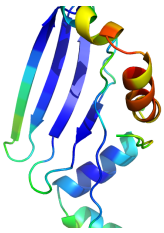
T0854
T0854
GDT_TS = 1.00
Score = −2.10 ± 0.19

T0855
BioShell-server_TS3
GDT_TS = 0.20
Score = 1.30 ± 0.22

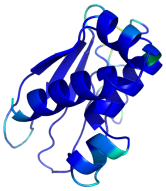


T0855
Pcons-net_TS2
GDT_TS = 0.28
Score = 0.83 ± 0.21

T0855
RBO_Aleph_TS3
GDT_TS = 0.37
Score = 0.19 ± 0.25



T0855
Zhang-Server_TS1
GDT_TS = 0.44
Score = −0.91 ± 0.22



T0855
T0855
GDT_TS = 1.00
Score = −1.59 ± 0.13

Table S5: Performance comparison of our method (3DCNN) with other state-of-the-art MQA methods on the CASP12, CAMEO, and 3DRobot datasets. The table reports the absolute, per-target average values of the correlation coefficients. The CASP12 targets were taken from the December 2, 2017 update and the CAMEO targets were taken from the 6-month period prior to December 10, 2017. CASP12 and CAMEO datasets were optimized with SCWRL4 before scoring.

MQA method	Loss (Eq. 11)	Pearson R	Spearmann ρ	Kendall τ
		CASP12		
3DCNN	0.146	0.607	0.521	0.381
ProQ2D	0.151	0.619	0.607	0.453
VoroMQA	0.161	0.557	0.515	0.380
ProQ3D	0.164	0.609	0.602	0.451
RWplus	0.192	0.313	0.355	0.257
		CAMEO		
3DCNN	0.060	0.586	0.532	0.426
VoroMQA	0.099	0.456	0.427	0.346
RWplus	0.162	0.122	0.095	0.068
		3DRobot		
VoroMQA	0.038	0.891	0.859	0.678
RWplus	0.076	0.844	0.829	0.651
3DCNN	0.083	0.856	0.839	0.652

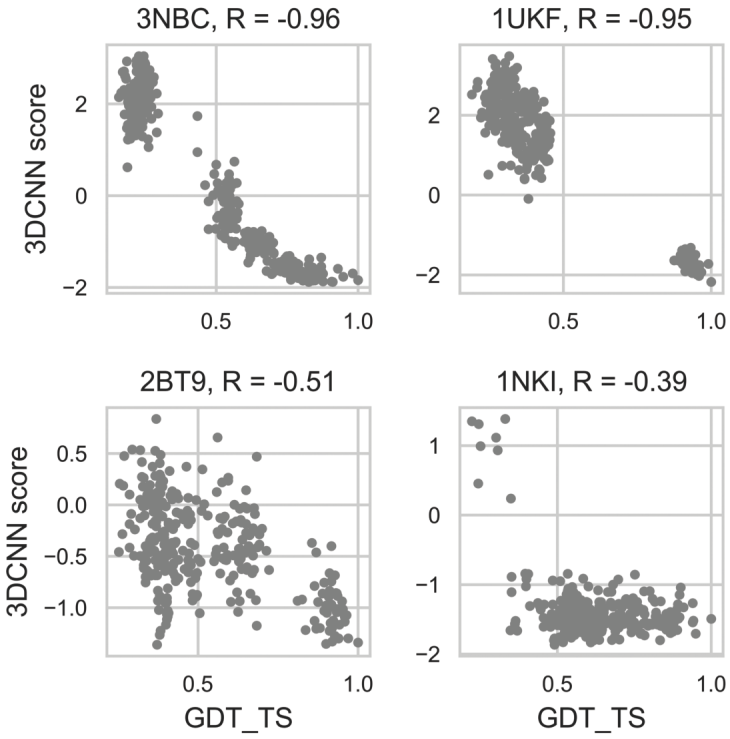


Figure S8: 3DCNN score versus GDT_TS for the two most correlated targets and the two least correlated targets in the 3DRobot benchmark.