Table S1a: Distance constraints in the [2Fe-2S] cluster used in the DYANA program.

Covalent bonds in the newly generated residue:

Cys47 S^{γ}	Cys47 Fe	2.18 Å
Cys47 Fe	Cys47 S^{ε}	2.22 Å
Cys82 S^{γ}	Cys82 Fe	2.18 Å
Cys47 Fe	Cys47 S^{ε}	2.22 Å

Additional distance constraints:

Atom		Atom		lower limits / Å	upper limits / Å
Cys47	S^{γ}	Cys42	S^{γ}	3.30	3.90
Cys82	S^{γ}	Cys50	S^{γ}	3.30	3.90
Cys42	S^{γ}	Cys47	S^{ε}	3.30	3.90
Cys42	S^{γ}	Cys82	S^{ε}	3.30	3.90
Cys50	S^{γ}	Cys47	S^{ε}	3.30	3.90
Cys50	S^{γ}	Cys82	S^{ε}	3.30	3.90
Cys47	Fe	Cys42	S^{γ}	2.00	2.40
Cys82	Fe	Cys50	S^{γ}	2.00	2.40
Cys47	Fe	Cys47	S^{ε}	2.05	2.45
Cys47	Fe	Cys82	S^{ε}	2.05	2.45
Cys82	Fe	Cys82	S^{ε}	2.05	2.45
Cys82	Fe	Cys47	S^{ε}	2.05	2.45
Cys47	Fe	Cys82	Fe	2.40	2.90
Cys47	S^{ε}	Cys82	S^{ε}	3.30	3.90

Table S1b: Distance constraints in the [2Fe-2S] cluster used in the XPLOR program.

Covalent bonds in the newly generated residue:

Cys47 Fe	Cys47 S^{ε}	2.29 Å
Cys47 Fe	Cys82 S^{ε}	2.29 Å
Cys82 Fe	Cys47 S^{ε}	2.29 Å
Cys82 Fe	Cys82 S^{ε}	2.29 Å

Additional distance constraints:

Atom		Atom		lower limits / Å	upper
Cys47	S^{γ}	Cys42	S^{γ}	3.30 -	3.90
Cys82	S^{γ}	Cys50	S^{γ}	3.30 -	3.90
Cys42	S^{γ}	Cys47	S^{ε}	3.30 -	3.90
Cys42	S^{γ}	Cys82	S^{ε}	3.30 -	3.90
Cys47	S^{γ}	Cys47	S^{ε}	3.30 -	3.90
Cys47	S^{γ}	Cys82	S^{ε}	3.30 -	3.90
Cys50	S^{γ}	Cys47	S^{ε}	3.30 -	3.90
Cys50	S^{γ}	Cys82	S^{ε}	3.30 -	3.90
Cys82	S^{γ}	Cys47	S^{ε}	3.30 -	3.90
Cys82	S^{γ}	Cys82	S^{ε}	3.30 -	3.90
Cys47	Fe	Cys42	S^{γ}	2.24 -	2.34
Cys47	Fe	Cys47	S^{γ}	2.24 -	2.34
Cys82	Fe	Cys50	S^{γ}	2.24 -	2.34
Cys82	Fe	Cys82	S^{γ}	2.24 -	2.34

Table S2: Comparison of dihedral angles ϕ (first row) and ψ (first row) for selected residues in the [2Fe-2S] cluster. Amino acids that are identical in MMOR-Fd and the homologous proteins are shown in red. Values in blue denote significant deviations from the respective average values. Proteins are labeled according to their PDB code.

Fd	PDR-Fd (2PIA)	1AWD	1FRR	1FXA	1PFD (NMR)	1QT9 (ox.)	1CZP (red.)
41 SER	45 SER -133.4	36 SER -141.9	37 SER -144.8	40 SER -135.4	38 SER -143.3 ± 98.1	40 SER -139.9	40 SER -139.6 ± 1.6
	-65.0	-78.2	-78.8	-74.0	-23.1 ± 69.2	-74.4	-73.4 ± 2.8
42 CYS	46 CYS -68.6	37 CYS -75.3	38 CYS -66.8	41 CYS -77.0	39 CYS -136.7 ± 66.1	41 CYS -74.5	41 CYS -75.7 ± 0.2
	-37.5	-27.7	-34.3	-30.6	-148.9 ± 51.6	-29.9	-27.7 ± 1.5
43 ARG	47 GLU 54.8	38 ARG 51.1	39 ARG 61.4	42 ARG 57.1	40 ARG -179.6 ± 63.8	42 ARG 56.3	42 ARG 54.1 ± 1.3
	27.8	26.6	17.1	23.9	90.1 ± 54.1	25.1	28.6 ± 1.8
44 GLU	48 SER -134.0	39 ALA -131.6	40 ALA -123.5	43 ALA -131.6	41 ALA 176.6 ± 51.0	43 ALA -131.3	43 ALA -134.2 ± 1.9
	3.8	13.8	4.8	12.2	34.0 ± 69.5	11.9	11.7 ± 0.9
45 GLY	49 GLY 79.3	40 GLY 77.9	41 GLY 78.3	44 GLY 74.0	42 GLY 64.1 ± 65.3	44 GLY 77.0	44 GLY 74.3 ± 0.1
	26.2	14.1	24.6	18.1	25.0 ± 81.7	14.5	17.5 ± 2.5
46 GLY	50 THR -117.1	41 ALA -116.0	42 ALA -121.2	45 ALA -116.8	43 SER -143.5 ± 59.0	45 ALA -120.1	45 ALA -113.4 ± 3.0
	-26.1	21.2	24.2	17.7	54.1 ± 55.9	21.4	5.7 ± 9.9
47 CYS	51 CYS -86.7	42 CYS -150.1	43 CYS -151.3	46 CYS -144.4	44 CYS -118.8 ± 38.2	46 CYS -151.4	46 CYS -135.2 ± 8.1
	-22.7	-167.5	-172.0	-171.2	-163.6 ± 67.0	-173.4	-170.0 ± 0.5
48 ALA	52 GLY 83.5	43 SER -125.9	44 SER -119.3	47 SER -118.5	45 SER -139.2 ± 65.2	47 SER -114.5	47 SER -117.3 ± 1.9
	-3.7	17.8	16.5	0.2	66.9 ± 71.4	4.5	8.6 ± 1.1
49 THR	53 SER -65.8	44 SER -66.2	45 SER -58.0	48 THR -52.1	46 SER -164.4 ± 44.8	48 THR -60.9	48 THR -59.4 ± 0.7
	-38.9	-27.6	-41.8	-49.3	175.0 ± 66.3	-38.1	-38.8 ± 0.0
50 CYS	54 CYS -88.8	45 CYS -100.0	46 CYS -95.2	49 CYS -78.6	47 CYS 71.0 ± 73.6	49 CYS -92.0	49 CYS -91.2 ± 2.3
	16.7	13.0	21.6	2.0	140.7 ± 60.5	15.2	15.8 ± 0.1
80 LEU	80 MET -83.7	73 LEU -94.2	74 LEU -98.0	77 LEU -96.1	75 LEU -71.6 ± 38.7	77 LEU -90.3	77 LEU -90.6 ± 2.0
	97.3	103.7	99.9	101.8	143.2 ± 81.8	101.7	103.5 ± 1.0
81 LEU	81 VAL -60.7	74 THR -63.2	75 THR -59.7	78 THR -57.1	76 THR -80.6 ± 85.0	78 THR -60.7	78 THR -62.4 ± 0.3
	-16.4	-19.5	-22.3	-26.7	-7.4 ± 62.6	-22.6	-22.7 ± 1.3
82 CYS	82 CYS -71.0	75 CYS -71.4	76 CYS -71.6	79 CYS -67.9	77 CYS -89.8 ± 51.3	79 CYS -73.0	79 CYS -71.9 ± 0.8
	-23.5	-19.3	-19.9	-17.9	-72.8 ± 68.8	-14.8	-15.5 ± 1.8
83 ARG	83 VAL -132.9	76 VAL -133.3	77 ILE -116.9	80 VAL -130.0	78 HIS -111.3 ± 87.0	80 VAL -132.0	80 VAL -131.3 ± 0.7
	-30.0	26.3	-14.2	22.9	72.1 ± 23.5	21.6	22.1 ± 1.5

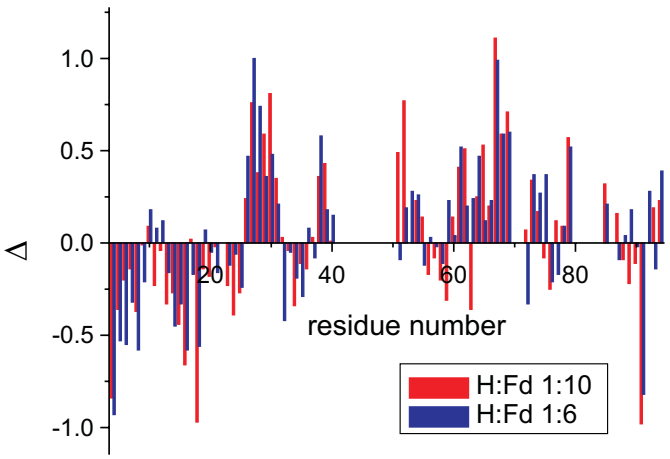

Figure S1: Binding data according to Equation 1.