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Supporting information for article:

Crystal structures of Scone: pseudosymmetric folding of a symmetric designer protein

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Table S1: Amino acid and DNA sequences

Protein	Amino Acid sequence	DNA sequence
SconeE	GSHMDGTEKWRFKTNDAI TSAASIGKDGTIYFGSDKV YAINPDGTEKWNFYAGYW TVTRPAISEDGTIYVTSLDG HLYAINPDGTEKWRFKTEK RIESSPVIGNTDTIYFGSYD GHLYAINPDGTEKWRFKT NDAITSAASIGKDGTIYFGS DKVYAINPDGTEKWNFYA GYWTVTRPAISEDGTIYVT SLDGHLYAINPDGTEKWR FKTEKRIESSPVIGNTDTIY FGSYDGHLYAINPDGTEK WRFKTNDAITSAASIGKDG TIYFGSDKVYAINPDGTEK WNFYAGYWTVTRPAISED GTIYVTSLDGHLYAINPDG TEKWRFKTEKRIESSPVIG NTDIYFGSYDGHLYAINP	ATGGACGGTACTGAGAAGTGCGCTTCA AAACTAACGATGCGATTACATCAGCTGCT TCAATTGGAAAAGGATGGAACAATTTACTT TGGGTCTGACAAGGTCTACGCCATCAAC CCAGACGGTACGGAGAAGTGGAATTTTT ACGCCGGATATTGGACCGTAACCCGTCC CGCGATTTCCAGAAGACGGTACAATCTAT GTTACGTGCGTTGACGGTTCATCTTTATGC GATCAACCCAGATGGTACGGAAAAGTGG CGCTTTAAGACGGAAAACGATTGAAA GTAGTCCCGTAATCGGCAACACAGACAC GATCTATTTCCGGATCCTATGACGGGCAC TTATATGCTATTAACCCTGATGGGACTGA GAAATGGCGCTTTAAGACGAACGATGCT ATTACCAGCGCGCTAGTATCGGTAAGG ATGGCACGATTTACTTCGGCTCGGACAA AGTATATGCAATTAATCCGGATGGGACG GAAAAATGGAACCTTCTATGCAGGGTACT GGACCGTAACCTCGCCAGCAATCAGTGA AGACGGAAACCATTTACGTGACGTCATTG GACGGACATTTATACGGCATCAATCCAG ACGGTACCGAAAAGTGGCGTTTCAAAC GGAAAAGCGTATCGAATCAAGCCCGCTA ATTGGTAACACTGACACCATTTATTTTGG ATCGTATGATGGACATCTTTATGCTATCA ATCCCAGCGGGACAGAAAAGTGGCGCTT CAAGACCAATGATGCTATCACAAGTGCT GCCAGCATCGGGAAAAGTGGCACAATTT ATTTTGGCTCGGATAAAGTGTACGCCAT CAACCCAGACGGTACCGAGAAATGGAAT TTTTACGGGGATATTGGACTGTAACCC GCCAGCAATCAGCGAGGATGGGACGA TCTACGTGACCTCCCTGGATGGTCATTT GTACGCCATCAATCCCGACGGAACCTGAA AAATGGCGCTTCAAGACAGAGAAAGCGCA TTGAATCTCCCTGTATCGGAAACAC CGACACAATCTACTTCGGATCCTACGAT GGGCACCTGTATGCGATTAACCCCTAA
SconeR	GSHMDGTEKWRFKTNKAI ESTPVIGNDGTIYFGSNHL YAINPDGTEKWNFYAGYW TVTRPAISEDGTIYVTSLDG HLYAINPDGTEKWRFKTG KRIESSPVIGNTDTIYFGSY DGHLYAINPDGTEKWRFK TNKAIESTPVIGNDGTIYFG SNHLYAINPDGTEKWNFY AGYWTVTRPAISEDGTIYV TSLDGHLYAINPDGTEKW RFKTKRIESSPVIGNTDTI YFGSYDGHLYAINPDGTEK WRFKTNKAIESTPVIGNDGT TIYFGSNHLYAINPDGTEK WNFYAGYWTVTRPAISED GTIYVTSLDGHLYAINPDG TEKWRFKTKRIESSPVIG NTDIYFGSYDGHLYAINP	ATGGACGGGACCGAGAAGTGGCGTTTCA AGACCAACAAGGCTATCGAGTCCACTCC AGTGATTGGTAATGATGGTACTATCTACT TTGGATCCAACCACCTGTATGCTATCAAC CCTGATGGCACCGAGAAGTGGAATTTTT ACGCCGGTATTGGACTGTTACACGCCCC TGCAATCTCTGAAGATGGGACGATTTAT GTAACATCACTTGATGGACATTTATATGC GATCAATCCTGACGGAACCGAAAAGTGG CGCTTCAAACCGGTAAGCGTATTGAGT CATCGCCTGTTATCGGAAATACGGATAC TATTTACTTTGGCTCATACGATGGGCATT TATATGCGATCAACCCTGATGGAACAGA AAAGTGGCGCTTTAAGACAAATAAGGCA ATCGAGAGTACGCCCGTATCGGCAACG ATGGAACTATTTACTTCGGCTCAAACCAC TTATACGCCATTAACCCCGATGGTACTGA GAAGTGGAAATTTCTACGCTGGACTG ACCGTAACCGGCCCGCGATTTCTGAGG ACGGGACAATTTACGTTACTAGTTTGGAC GGACATTTGATGCGATTAATCCGGACG GGACTGAGAAATGGCGCTTTAAGACAGG GAAGCGTATCGAAAGTTCACCCCGTAATT GGAAACACGGACACGATCTATTTCCGAT CTTATGACGGCCATCTGTACGGATCAA TCCTGACGGTACTGAGAAGTGGCGTTTC AAAACCAACAAAGCCATTGAATCTACGC CAGTCATTGGTAATGATGGGACAATTTAT TTCCGGATCCAACCATCTGTACGCAATTA TCCAGATGGTACCGAGAAATGGAACCTC TATGCTGGGTATTGGACGGTGACGCGCC CGGCTATCTCCGAGGACGGGACAATCTA CGTGACCTCCCTGACGGCCACTTATAT CGGATCAACCCCGACGGGACAGAAAAGT GGCGTTTCAAACAGGAAAACGCATCGA GAGTAGTCTGTATCGGCAACACAGAT ACCATCTATTTCCGGTCTTATGATGGACA TCTGTACGCTATTAATCCCTAA

Table S2: Crystallization conditions

Name	Protein Concentration (mg/ml)	STA concentration (mM)	Reservoir solution
Scone-R	10	0	0.1M Magnesium Acetate 0.1M Sodium Acetate 4% (w/v) PEG8000
Scone-E	10	3.5	0.1M MES pH 6.0 40% (v/v) MDP
Scone-E + STA a	10	3.5	1.8M Na/K phosphate, pH 7.5
Scone-E + STA b	10	3.5	1.9M Sodium malonate, pH 6.0

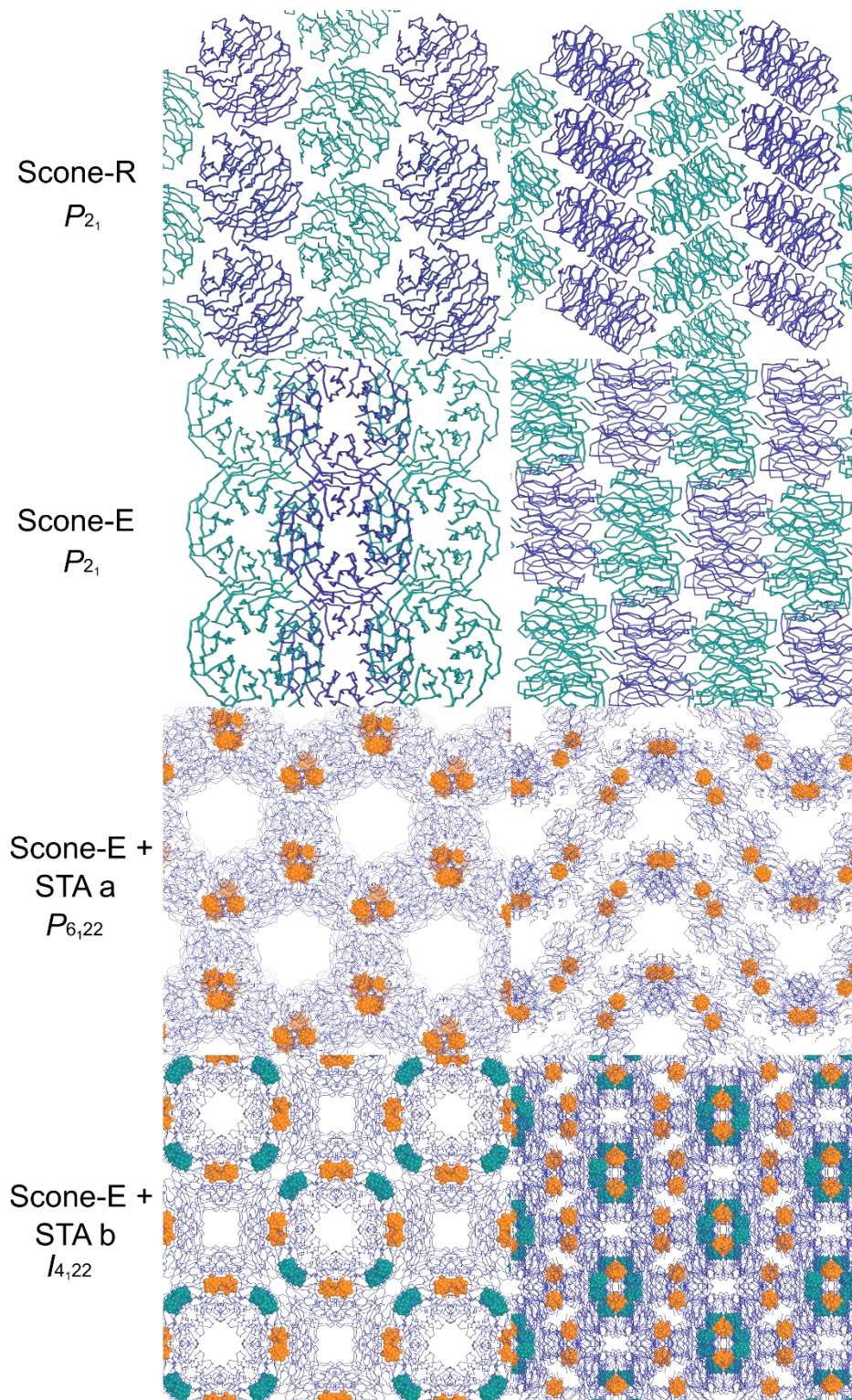


Figure S1: The crystals without bound POM have the same spacegroup but are not isomorphous

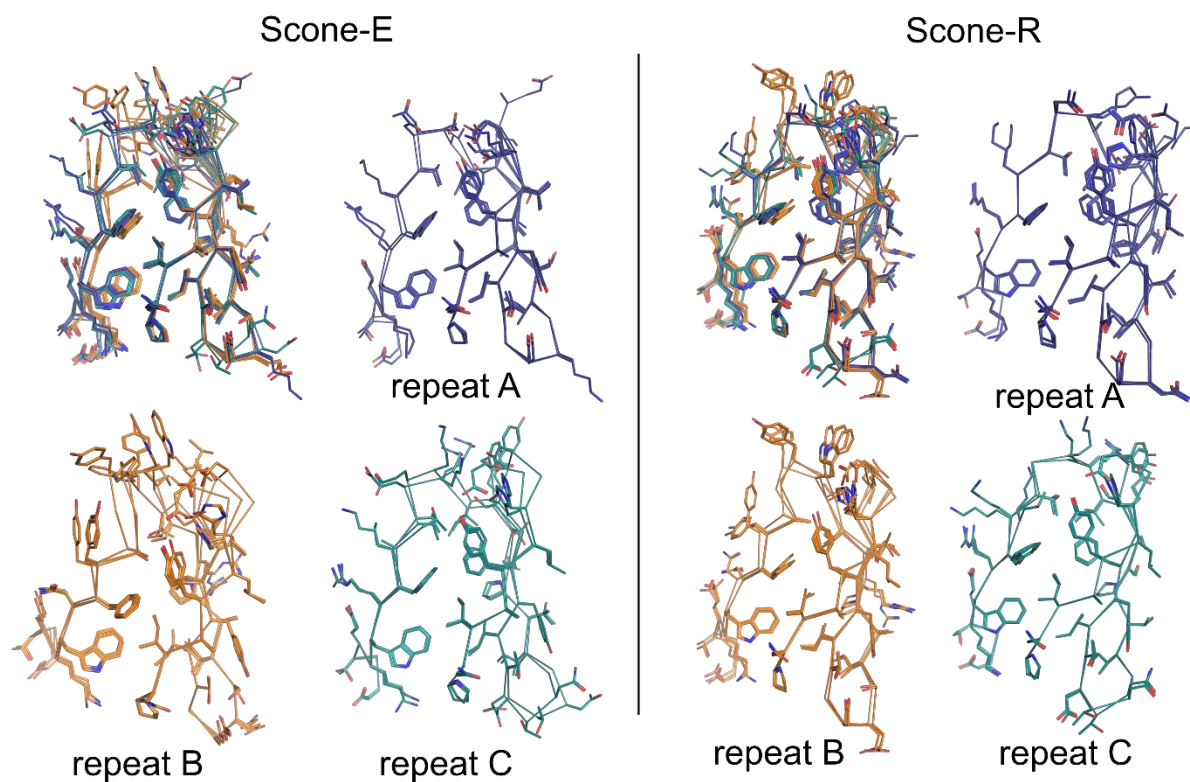


Figure S2: Structural Alignment of repeats: Each repeat is aligned, all together an with the identical sequence repeats separately.

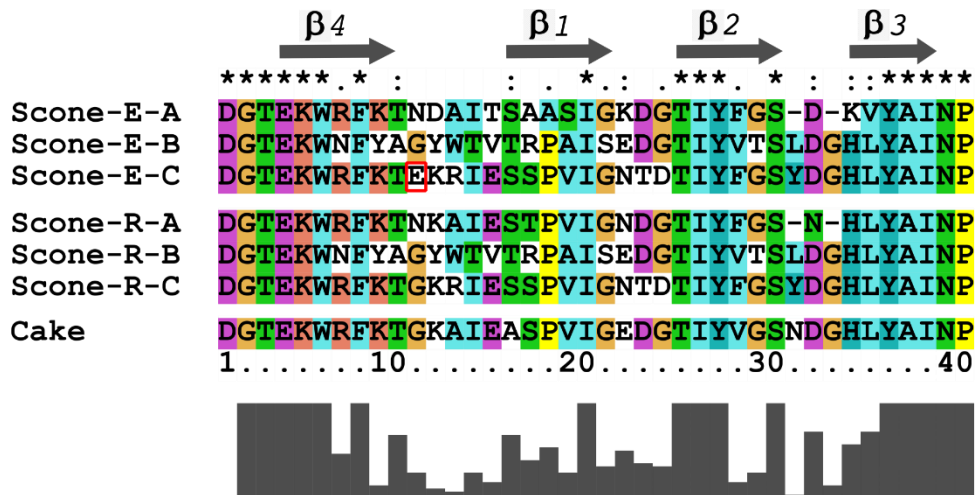


Figure S3: Sequence alignment of repeats: The sequences of the designed Cake protein (PDB:6tjh) is included. On top the location of β -strands in the repeat is shown. The marked glutamate is the only non-extant residue included in the sequences.



Figure S4: C-A interface: An alignment between the designed C-A interface (grey) and the crystal C (teal) - A (blue) interface shows the clear difference caused by the different fold. The C-blade of the design is aligned on the C blade of the crystal structure.

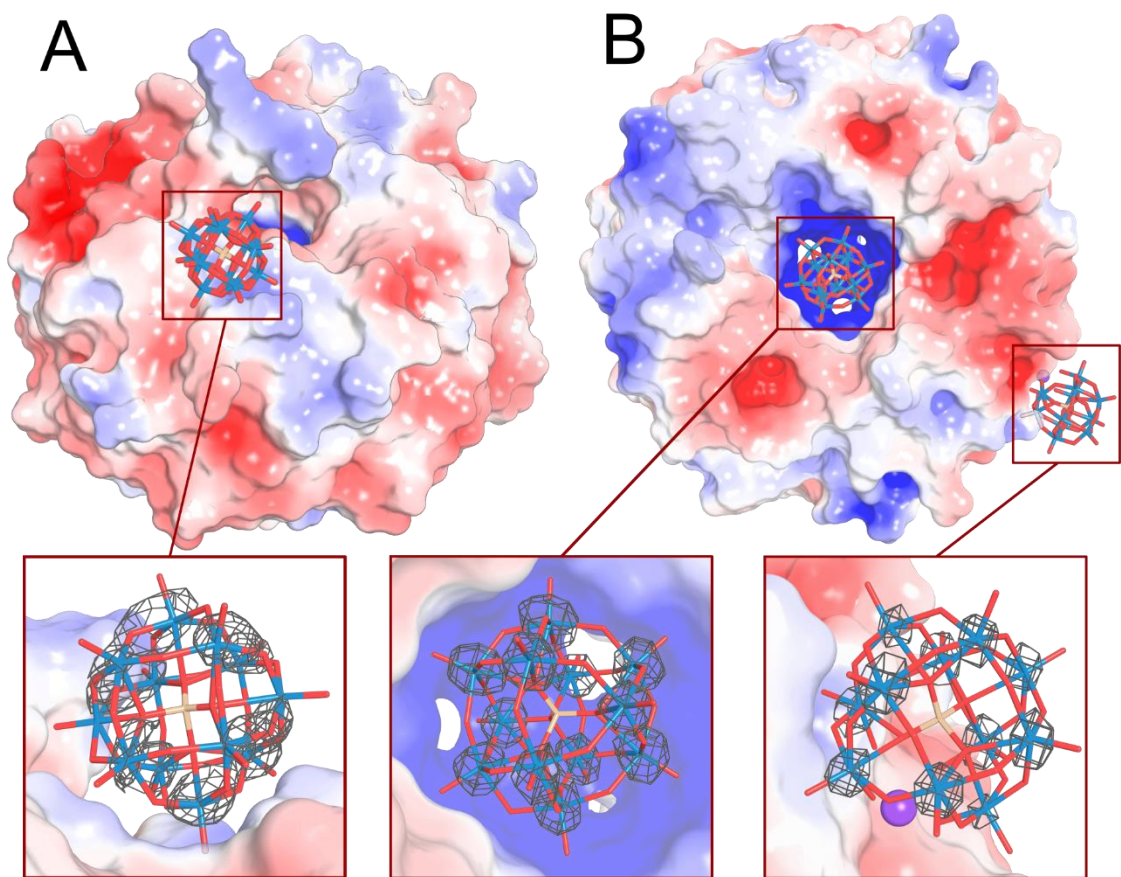


Figure S5: Electrostatic potential map of Scone-E with STA: The electrostatic potential map was calculated with the APBS plugin in PyMOL. Zoom-in on the STA binding site is shown. The anomalous map at sigma 5.5 clearly shows the location of the tungsten atoms.