Supplementary Information

Domain Motions and Electron Transfer Dynamics in 2Fe-Superoxide Reductase

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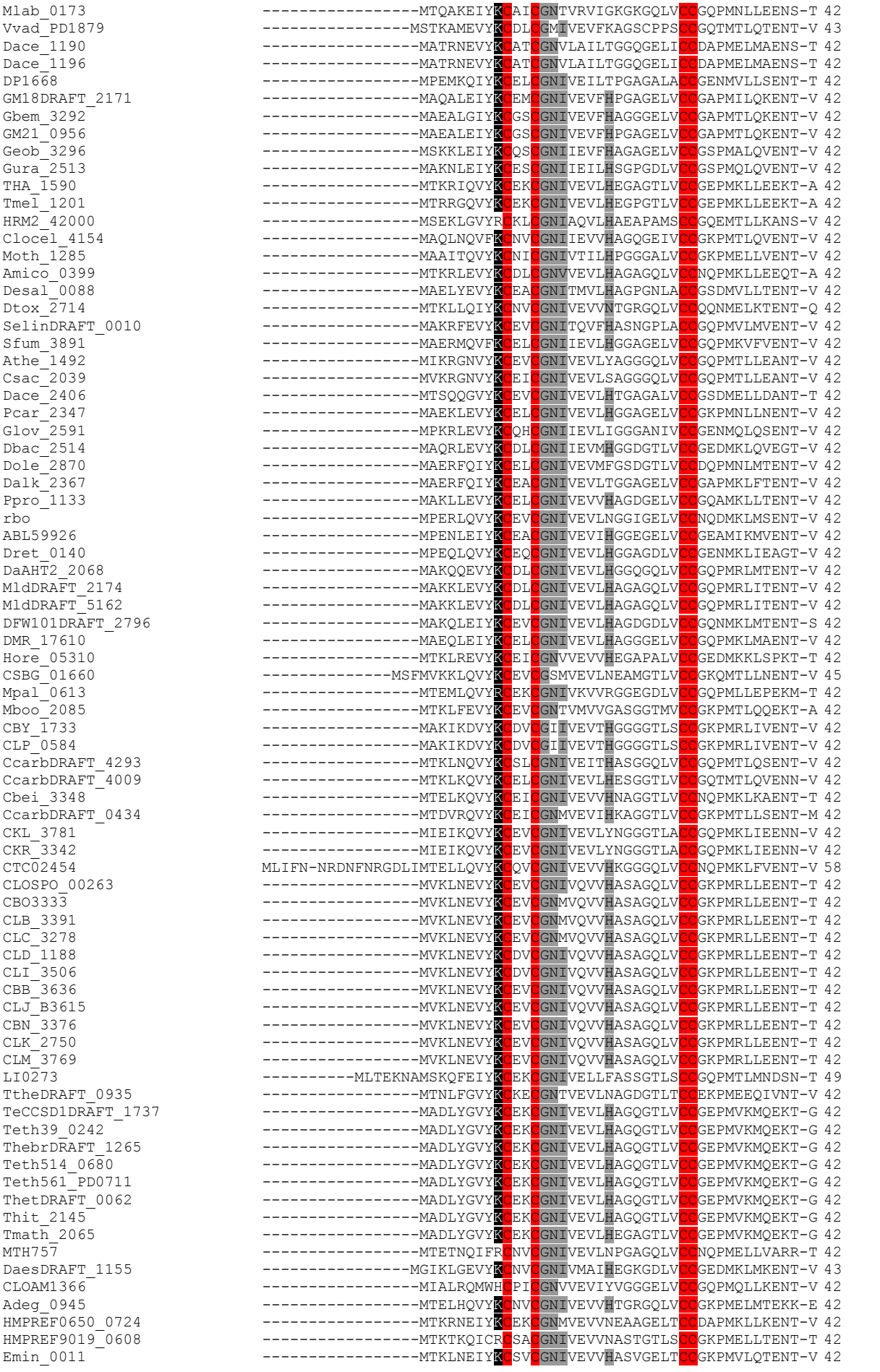
SI 1: Protein Sequence Alignment for (Putative) 2Fe-Superoxide Reductases

In the following, aligned amino acid sequences of (putative) 2Fe-superoxide reductases (2Fe-SORs) are presented. Sequences were obtained from the superoxide reductase gene ontology database (SORGOdb, www.sorgo.genouest.org, accessed 23 September 2015) and labelled according to the locus tags used therein.[1] Apart from one entry (HOLDEFILI_03091, which lacks two of the conserved cysteines forming centre I), all sequences corresponding to canonical 2Fe-SORs were considered.[i] The sequence alignment was performed using Clustal Omega (www.ebi.ac.uk/Tools/msa/clustalo).[2–5]

Strictly conserved amino acids are labelled with an asterisk, while a colon (period) indicates conservation between groups of strongly (weakly) similar properties. Strictly conserved histidines and cysteines involved in the formation of the two metal centres are highlighted in red. Lysine K9 and the *quasi* conserved tyrosine Y115 [1,6,7] are labelled in black and blue, respectively. Other amino acids that appear to be relevant for interdomain electron transfer in *Desulfovibrio desulfuricans* (*Dd*) 2Fe-SOR are indicated by a grey shade. The sequence of this particular enzyme (locus tag Ddes_2010) is set in bold letters.

[i] Within SORGOdb, canonical 2Fe-SORs are termed DX-SORs, where DX indicates the presence of a desulforedoxin domain. Enzymes of this type are also termed Class 1 SORs or desulfoferrodoxins (DFXs).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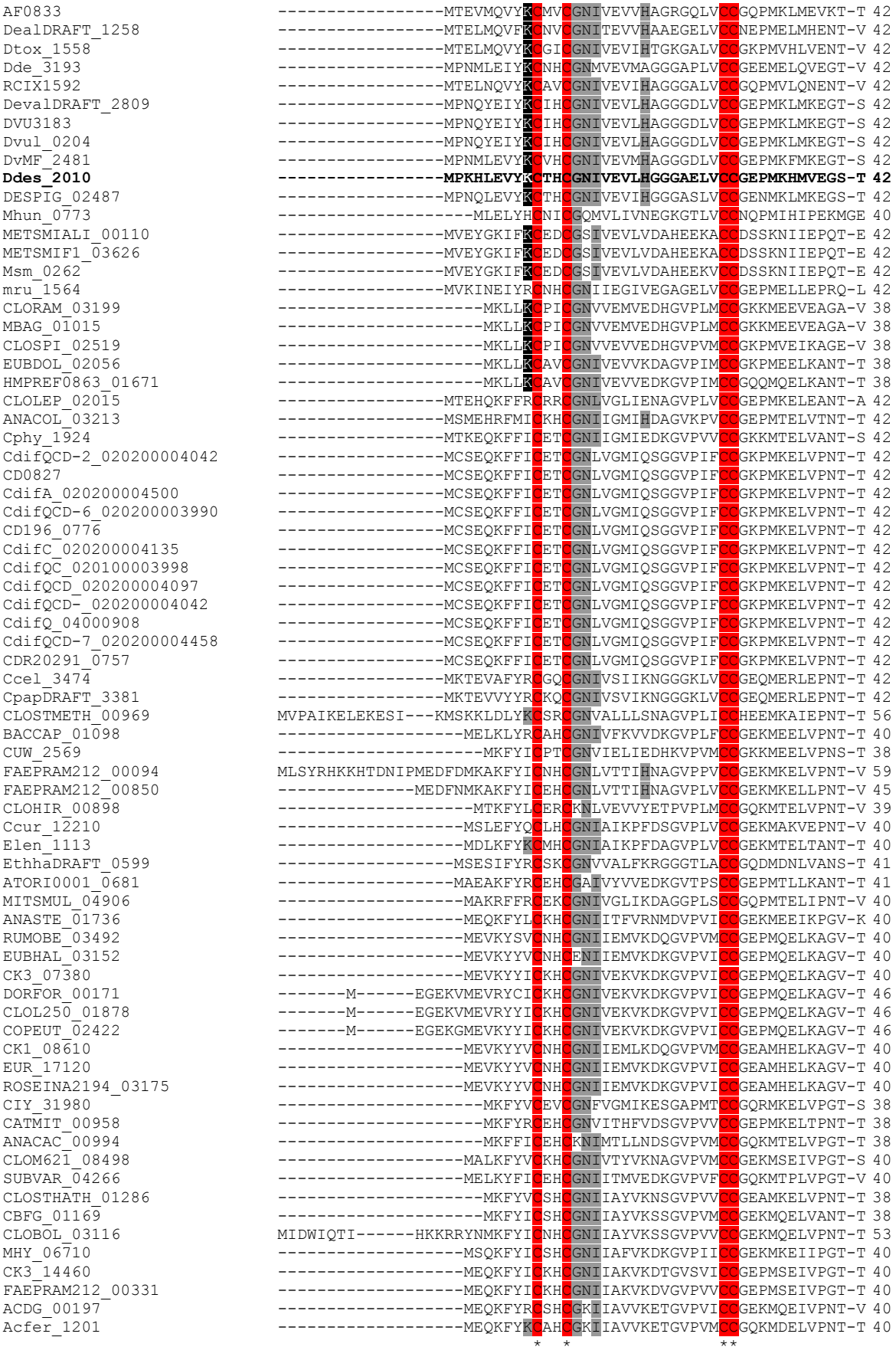
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CcarbDRAFT_4009          DAAKEKHVPIIEK----VKGGVLVKVGEI-EHPMLEKHYIEWIEIQT-KNK--IYRKYLK 94
Cbei_3348                DGATEKHVPVIEK----VEGGVLVKVGSV-EHPMLDNHYIEWIEIHT-ESN--VYKKFLK 94
CcarbDRAFT_0434          DAAVEKHVPVIEK----LQDGIVVKVGEV-EHPMLENHYIEWIEVHT-ANK--VYRKYLK 94
CKL_3781                 DAASEKHVPVIEE----IDGGVVVKVGSV-EHPMLPEHYIQWIEVHT-ENK--IYRKYLK 94
CKR_3342                 DAASEKHVPVIEE----IDGGVVVKVGSV-EHPMLPEHYIQWIEVHT-ENK--IYRKYLK 94
CTC02454                 DAAVEKHVPVIEK----IEGGIRVKIGEA-EHPMIEEHYIEWIEVLT-ENK--VYRKHLK 110
CLOSPO_00263             DAALEKHVPVVEK----TENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CBO3333                  DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLB_3391                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLC_3278                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLD_1188                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLI_3506                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CBB_3636                 DAALEKHVPVVER----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLJ_B3615                DAALEKHVPVVER----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CBN_3376                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLK_2750                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
CLM_3769                 DAALEKHVPVVEK----IENGVKVKVGEK-EHPMEEKHYIEWIEVIT-ENK--VYKKYLK 94
LI0273                   SGAKEKHVPIIEN----NGSGCKVTVSTV-IHPMEEKHWIEWIEIVT-IDG-HHCKKFLN 102
TtheDRAFT_0935           DASKEKHVPVILK----DGDTVTVKVGSV-EHPMEEKHYIEWISILA-DGI--YMRKMLK 94
TeCCSD1DRAFT_1737        DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
Teth39_0242              DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
ThebrDRAFT_1265          DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
Teth514_0680             DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
Teth561_PD0711           DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
ThetDRAFT_0062           DAGTEKHTPVIER----NGNIVTVKVGSI-PHPMEEKHWIEWISLLA-DGV--YMRKVLK 94
Thit_2145                DAGTEKHTPVIER----NGNLVTVKVGSV-PHPMEEKHWIEWISLLA-GGT--YMRKVLK 94
Tmath_2065               DAGTEKHTPVIER----NGNLVTVKVGSV-PHPMEEKHWIEWISLLA-GGT--YMRKVLK 94
MTH757                   DVGPEKHVPVVEE----TGTGIRVKVGEV-PHPMEENHHIQWIEVIA-GDM--VYRKDLN 94
DaesDRAFT_1155           DAAVEKHVPVWTR----DGDKITVKVGSV-AHPMEEKHYIEWIEVMV-GDT--VMTKLLK 95
CLOAM1366                DAAVEKHIPVVTD----LGDKIEVSVGSI-PHPMEEKHYITCIEVLM-EKK--VLRKELK 94
Adeg_0945                DVGQEKHVPVIEP----RNGKIRVHVGEV-PHPMEEAHYIEWIELHM-GDR--VERMHLK 94
HMPREF0650_0724          DAATEKHVPVIEK----IEGGYRVTVGEV-EHPMTEGHYIQWIELIT-PTE--VLRKYLT 94
HMPREF9019_0608          DAATEKHVPVIEK----TDCGYRVTVGEV-EHPMLEAHYIQWIDLIT-ENG--VLRKFLK 94
Emin_0011                DAAKEKHVPFVTK----TADGYKVQIGSV-EHPMTEEHHIEWIELIC-EECNKVMRKHLN 96
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Dtox_1558                   DAAKEKHVPVIEK----SGDSIKVTVGSV-LHPMEEKHYIEWIELIV-DGK--SYRKFLK 94
Dde_3193                    DAAKEKHVPVIEK----TANGFLVKVGAV-EHPMTDKHWIQWIELIA-DGR--SYTKFLN 94
RCIX1592                    DASKEKHVPVIEK----TAAGFKVTVGSV-AHPMEEKHYIEMIEVIA-DGK--TYKKFLK 94
DevalDRAFT_2809             DGAKEKHVPVIEK----TANGYKVTVGSV-AHPMEEKHWIEWIELVA-DGV--SYKKFLK 94
DVU3183                     DGAKEKHVPVIEK----TANGYKVTVGSV-AHPMEEKHWIEWIELVA-DGV--SYKKFLK 94
Dvul_0204                   DGAKEKHVPVIEK----TANGYKVTVGSV-AHPMEEKHWIEWIELVA-DGV--SYKKFLK 94
DvMF_2481                   DGAKEKHVPVIEK----TATGYKVKVGSV-AHPMEETHWIEWIELIA-DGR--SYTRFLK 94
Ddes_2010                   DGAMEKHVPVIEK----VDGGYLIKVGSV-PHPMEEKHWIEWIELLA-DGR--SYTKFLK 94
DESPIG_02487                DGAMEKHVPVIEK----IEGGYKVTVGSV-AHPMDENHYIEWIELLA-DNQ--SLTCFLK 94
Mhun_0773                   EEGTEKHIPVIEK----TNSGIKVKVGSV-PHPMVDDHYIKWIEVIGDTYL---QTSTLK 92
METSMIALI_00110             GDKAPKHVPVISV----DGNEVTVAVGEV-QHPMDDDHFIQFVELIVGDER---YIKHFK 94
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Msm_0262                    GDKAPKHVPVISV----DGNEVTVAVGEV-QHPMDDDHFIQFVELIVGDER---YIKHFK 94
mru_1564                    EEGGVKHIPVVTK----EDGKIVVKMGEV-EHPMLEEHYINFVQLTIGDQV---FRANLK 94
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MBAG_01015                  DAALEKHVPVLKV----EGDCLTAVVGDV-LHPMTPEHLISNIWIEFADGS--NKKVTLT 91
CLOSPI_02519                DAAVEKHVPVVKL----ESDYLVVTVGEV-LHPMTAEHLISNIWVEFSDGS--AMKVTLT 91
EUBDOL_02056                DGALEKHVPVATY----ADGMLKVAVGSV-AHPMLPEHFITDIFVEIDDKV---LRAKLE 90
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CLOLEP_02015                EAAQEKHVPVVTR----KEGQIRVSVGDI-HHPMEEKHFIQWVYLQTKRGG---QRKGLQ 94
ANACOL_03213                DAATEKHVPVVEV----EGNEVRVKVGSA-PHPMSDEHHIAWIYLQTRHGG---QRKALQ 94
Cphy_1924                   DGAQEKHVPVVEV----KDNLVYVSVGTV-VHPMLEEHSIQWVYLRTNQGG---HRKSLA 94
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CpapDRAFT_3381              DAALEKHVPVAER----KDGKIVVQIGSV-DHPMIDAHYIEWVEVAGEEGT---ERIILS 94
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CUW_2569                    EAAVEKHMPVPTV----ENGVLKVSVGEV-EHPSIEKHWIPFVAVKASDLV---MRREIK 90
FAEPRAM212_00094            EASGEKHLPVAEL----SGSRLTVTVGAV-EHPMADVHYIQWIFVETEDGG---QIRYLN 111
FAEPRAM212_00850            EASGEKHLPVAEH----SGSTLTVTVGAV-EHPMVDVHHIQWLFVETENGG---QLRYLA 97
CLOHIR_00898                DAATEKHVPEVTV----EGNVVKAQVGSV-EHPMEEKHYIMFILLETDQGV---RRKDLK 91
Ccur_12210                  DAAREKHLPEVTI----EGNTVRAQVGSV-EHPMEEVHYITFVCLETEKGY---QIAHLT 92
Elen_1113                   DAAVEKHVPVVRV----DGSNVHVEVGST-LHPMTPEHYITFICLVTKNGY---QIVELT 92
EthhaDRAFT_0599             DAAQEKHVPVVTR----DGDTLTVKVGAV-PHPMLEEHYIEWIAIVTGGQV---VIKYLK 93
ATORI0001_0681              DGATEKHVPVVSR----DGFKLTVKVGEV-AHPMLPEHYIVFIALETEQGI---NLKRLN 93
MITSMUL_04906               DAAAEKHVPVITLDR--EGGEVTVQVGTV-AHPMLPEHFIEWIHLETENGA---QIKHLK 94
ANASTE_01736                DAAVEKHIPVVAV----EGNKVEVFIGEV-EHPMVDEHYIEWITLETEKTN---QITHLK 92
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EUBHAL_03152                DAAVEKHVPVYTV----EGSHVHVVVGET-KHPMLEEHFIEWITLSTNQGI---YRKQLN 92
CK3_07380                   DAAVEKHVPVYTV----EGNYVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLS 92
DORFOR_00171                DAAVEKHVPVYTV----EGSHVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLN 98
CLOL250_01878               DAAVEKHVPVYTI----EGSHVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLN 98
COPEUT_02422                DAAVEKHVPVYTI----EGSHVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLN 98
CK1_08610                   DAAVEKHVPVYTV----DKQHVHVVVGEI-KHPMLDNHFIEWITLNTNQGI---YRKQLI 92
EUR_17120                   DAAVEKHVPVYTV----DKQHVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLT 92
ROSEINA2194_03175           DAAVEKHVPVYTV----DKQHVHVVVGET-KHPMLEEHFIEWITLNTNQGI---YRKQLT 92
CIY_31980                   DGAVEKHVPVCKV----EGNKVIVTVGSV-EHPMAPEHYIEWIALETAKGA---QRKVLN 90
CATMIT_00958                DAAVEKHVPVVKV----EDNKVTVSVGSV-EHPMTEAHYITLIVLETKNGT---QFKQLT 90
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SUBVAR_04266                EAAHEKHIPVYTV----DNGVVHVTVGSV-EHPMMDEHYIPWISLQTKQGS---QIKHLK 92
CLOSTHATH_01286             DAAVEKHVPVIHT----DGQKVTVTVGST-SHPMLEEHYIEWIALATKQGN---QRKELK 90
CBFG_01169                  DAAVEKHVPVVTV----DGQKVTVTVGAA-EHPMTPEHYIQWIALATTQGN---QRKELK 90
CLOBOL_03116                DAAVEKHVPVIQI----DGSKVTVTVGSA-EHPMIPEHYIQWIALATRQGN---QRKELQ 105
MHY_06710                   DAAVEKHVPVISQ----EGNIVTVSVGSV-EHPMIPEHYIEWISLETNKGN---QRKVLQ 92
CK3_14460                   DAAVEKHVPVWTV----ENGIVHVKVGSV-EHPMLPEHYIEWVSLHTKQGN---QRKELH 92
FAEPRAM212_00331            DAAVEKHVPVWTV----ENGIVHVKVGSV-EHPMLPEHYIEWVSLQTKQGN---QRKELH 92
ACDG_00197                  DAAQEKHVPVIEV----KENLVTVKVGSV-THPMLDEHYIEWISLETKEGN---QRKELK 92
Acfer_1201                  DAAQEKHVPVVEV----NGSIVTVTVGSV-LHPMQPEHYIEWISLHTKQGN---QRKELK 92
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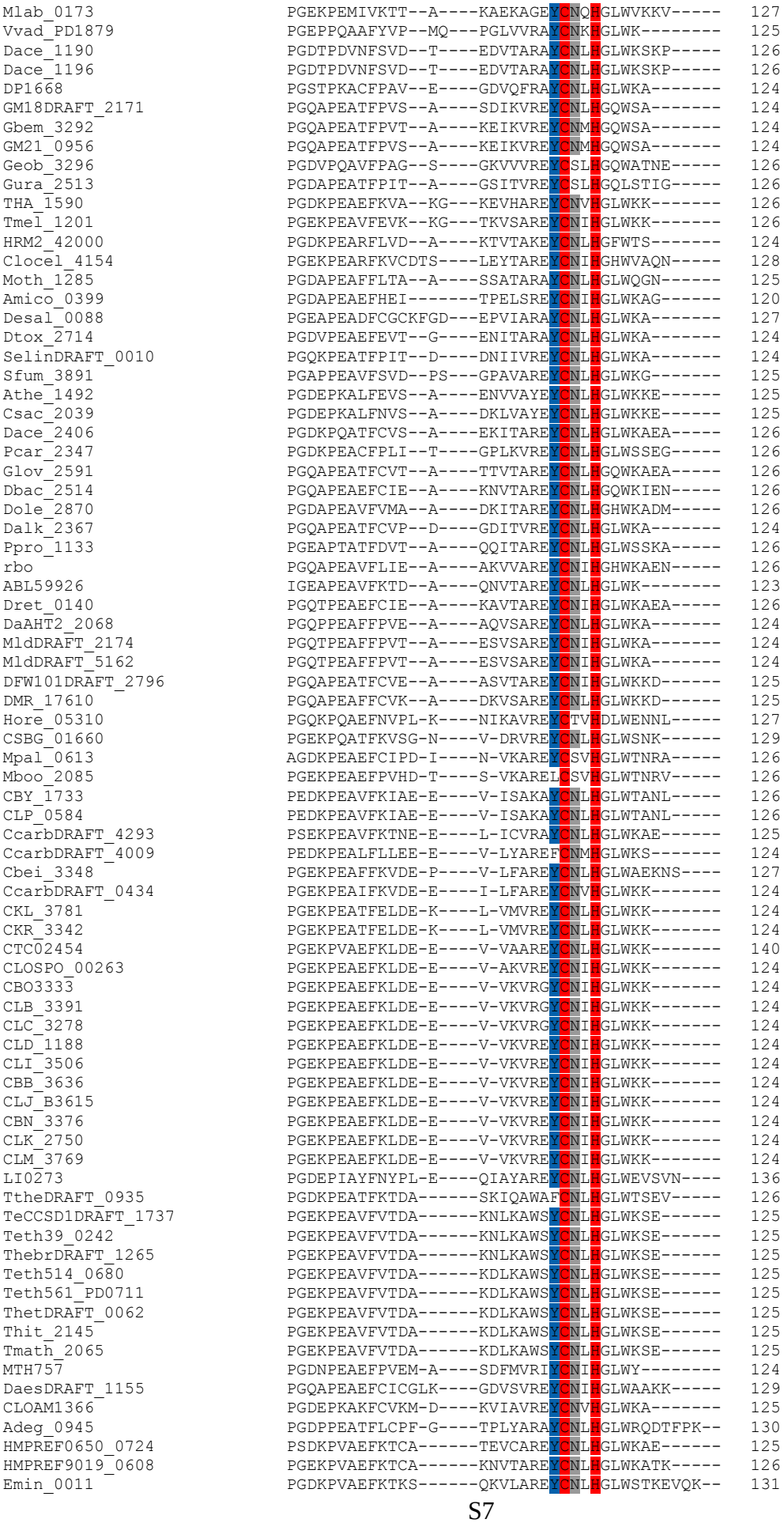
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Vvad_PD1879 PGEPPQAAFYVP--MQ---PGLVVRAYCNKHGLWK-------- 125
Dace_1190 PGDTPDVNFSVD--T----EDVTARAYCNLHGLWKSKP----- 126
Dace_1196 PGDTPDVNFSVD--T----EDVTARAYCNLHGLWKSKP----- 126
DP1668 PGSTPKACFPAV--E----GDVQFRAYCNLHGLWKA------- 124
GM18DRAFT_2171 PGQAPEATFPVS--A----SDIKVREYCNLHGQWSA------- 124
Gbem_3292 PGQAPEATFPVT--A----KEIKVREYCNMHGQWSA------- 124
GM21_0956 PGQAPEATFPVS--A----KEIKVREYCNMHGQWSA------- 124
Geob_3296 PGDVPQAVFPAG--S----GKVVVREYCSLHGQWATNE----- 126
Gura_2513 PGDAPEATFPIT--A----GSITVREYCSLHGQLSTIG----- 126
THA_1590 PGDKPEAEFKVA--KG---KEVHAREYCNVHGLWKK------- 126
Tmel_1201 PGEKPEAVFEVK--KG---TKVSAREYCNIHGLWKK------- 126
HRM2_42000 PGDKPEARFLVD--A----KTVTAKEYCNLHGFWTS------- 124
Clocel_4154 PGEKPEARFKVCDTS----LEYTAREYCNIHGHWVAQN----- 128
Moth_1285 PGDAPEAFFLTA--A----SSATARAYCNLHGLWQGN------ 125
Amico_0399 PGDAPEAEFHEI-------TPELSREYCNIHGLWKAG------ 120
Desal_0088 PGEAPEADFCGCKFGD---EPVIARAYCNLHGLWKA------- 127
Dtox_2714 PGDVPEAEFEVT--G----ENITARAYCNLHGLWKA------- 124
SelinDRAFT_0010 PGQKPEATFPIT--D----DNIIVREYCNLHGLWKA------- 124
Sfum_3891 PGAPPEAVFSVD--PS---GPAVAREYCNLHGLWKG------- 125
Athe_1492 PGDEPKALFEVS--A----ENVVAYEYCNLHGLWKKE------ 125
Csac_2039 PGDEPKALFNVS--A----DKLVAYEYCNLHGLWKKE------ 125
Dace_2406 PGDKPQATFCVS--A----EKITAREYCNLHGLWKAEA----- 126
Pcar_2347 PGDKPEACFPLI--T----GPLKVREYCNLHGLWSSEG----- 126
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Dbac_2514 PGQAPEAEFCIE--A----KNVTAREYCNLHGQWKIEN----- 126
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Mboo_2085 PGEKPEAEFPVHD-T----S-VKARELCSVHGLWTNRV----- 126
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CLP_0584 PEDKPEAVFKIAE-E----V-ISAKAYCNLHGLWTANL----- 126
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Cbei_3348 PGEKPEAFFKVDE-P----V-LFAREYCNLHGLWAEKNS---- 127
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CKL_3781 PGEKPEATFELDE-K----L-VMVREYCNLHGLWKK------- 124
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CLD_1188 PGEKPEAEFKLDE-E----V-VKVREYCNIHGLWKK------- 124
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CBB_3636 PGEKPEAEFKLDE-E----V-VKVREYCNIHGLWKK------- 124
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Tmath_2065 PGEKPEAVFVTDA------KDLKAWSYCNLHGLWKSE------ 125
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Dde_3193                    PGETPEAEFCIKA------DKVTAREYCNLHGHWKTEL-----   126
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CdifQCD-2_020200004042      VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CD0827                      VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifA_020200004500          VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQCD-6_020200003990      VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CD196_0776                  VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifC_020200004135          VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQC_020100003998         VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQCD_020200004097        VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQCD-_020200004042       VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQ_04000908              VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CdifQCD-7_020200004458      VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
CDR20291_0757               VDGEPVVKFALND-DD---KVISAYAYCNLHGLWKAEL-----   128
Ccel_3474                   PGDEPKAVFADKS-------NAEVYAYCNLHGLWMSHVK----   126
CpapDRAFT_3381              PGDEPKAVFADKS-------NAEVYAYCNLHGLWMSHVK----   126
CLOSTMETH_00969             PNEQPVASFSVQP-GE---E-ITVYEYCNLHGVWSAKA-----   141
BACCAP_01098                PGDKPELRTFS---AD---GAVKAYEICNLHGYWKSAD-----   128
CUW_2569                    ATEKPEAIFPIGD-FK---GEVEVYAWCNLHGLWKATITL---   126
FAEPRAM212_00094            PGQAPNVGFELG--SE---KPVAVYAYCNLHGLWMTKL-----   144
FAEPRAM212_00850            PGQAPKAVFELG--SE---KPVAVYAYCNLHGLWMTKL-----   130
CLOHIR_00898                PGEKPVAEFALLE-GE---KPVAVYEYCNLHGLWKKEL-----   125
Ccur_12210                  PGMAPVATFAVAE-GD---KPVAVYEYCNKHGLWKVEL-----   126
Elen_1113                   PEDAPVADFAIAE-GD---EALKVYEYCNLHGLWVAEV-----   126
EthhaDRAFT_0599             PGDAPEKTFSISC-KS-----GTAYAYCNLHGLWKADF-----   125
ATORI0001_0681              PGETPEAHFALPE-NQ---GG-VAYEFCNLHGLWKAEF-----   126
MITSMUL_04906               PGDAPEAVFMLAG-SD---KPVAAFAYCNLHGLWKAEFHED--   131
ANASTE_01736                PGDKPKAEFAIPE-GD---KVISAHEYCNLHGLWKKEL-----   126
RUMOBE_03492                PGQEPVADFCLCN-GE---QVEEVYAYCNLHGLWKC-------   124
EUBHAL_03152                PGQEPVADFCLCD-GE---LVEEVYAYCNLHGLWKC-------   124
CK3_07380                   PGQEPIADFCLCD-GE---QVEEVYAYCNLHGLWKC-------   124
DORFOR_00171                PGQEPVADFCLCD-GE---QVEEVYAYCNLHGLWKC-------   130
CLOL250_01878               PGQEPAADFCLCD-GE---QVEEVYAYCNLHGLWKC-------   130
COPEUT_02422                PGQEPVADFCLCD-GE---QVEEVYAYCNLHGLWKC-------   130
CK1_08610                   PGQEPIADFCLCD-GE---YVEEVYAYCNLHGLWKC-------   124
EUR_17120                   PGQEPVADFSLCD-GE---QVEEVYAYCNLHGLWKC-------   124
ROSEINA2194_03175           PGQEPVADFCLCD-GE---QVEEVYAYCNLHGLWKC-------   124
CIY_31980                   PGDKPCAEFALTD-DD---SVVAVYAYCNLHGLWKA-------   122
CATMIT_00958                PSDKPEAVFYVGE-GD---EVVAAYDYCNLHGLWKA-------   122
ANACAC_00994                PGEKPEAEFLLAD-GE---ELIAAYEYCNLHGLWK--------   121
CLOM621_08498               PGEKPEAEFVLSE-GD---EAVAAYEYCNLHGLWKKEI-----   126
SUBVAR_04266                PGEAPKADFALTA-GD---EVVAVYAYCNLHGLWKA-------   124
CLOSTHATH_01286             PGQEPQAEFMISE-DD---EVLEVYAYCNLHGLWKA-------   122
CBFG_01169                  PGQKPQAEFMVCQ-GD---GVEAVYAYCNLHGLWKA-------   122
CLOBOL_03116                PGQKPQAEFMLCE-GD---EAEAAYAYCNLHGLWKAEP-----   139
MHY_06710                   PNTSPTAQFALLD-GE---EVITAYAYCNLHSLWKA-------   124
CK3_14460                   PGEKPEVCFALCE-GD---AVEAVYAYCNLHSLWKA-------   124
FAEPRAM212_00331            PGEKPEVCFALCE-GD---EVEAVYAYCNLHSLWKA-------   124
ACDG_00197                  PGADPVAVFALAP-SD---DVVAAYAYCNLHGLWKAE------   125
Acfer_1201                  PGDAPKAVFALVD-GD---EVEAAYAYCNLHGLWK--------   123
                                                  *. *
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SI 2: Overview of Animated Figures

Dynamic representations of molecular dynamics (MD) trajectories, normal modes, principal modes, and electron transfer pathways are available as supplementary material in separate files. In the following, an overview of all Animated Figures is given together with a detailed description of the included dynamic representations. For visualization purposes, the number of MD trajectory frames was reduced by a factor of five. In view of file size limits, all animations are provided in medium quality. High quality versions can be supplied on request.

Animation SI 1: Front view dynamic representation of interdomain Fe–Fe stretching mode 11 of *Dd* 2Fe-SOR, as calculated by normal mode analysis based on an elastic network model (ENM-NMA). Fe atoms corresponding to the superoxide reductase (SOR) and desulforedoxin (DX) domain are depicted as blue and red spheres, respectively. The mode amplitude is scaled to an average RMSD of 1 Å.

Animation SI 2: Dynamic representation of domain torsional mode 13 of *Dd* 2Fe-SOR, as calculated by ENM-NMA. The molecule is viewed from the top along the crystallographic C_2 axis (black, also see Figure 1 of the manuscript). Fe atoms corresponding to the SOR and DX domain are depicted as blue and red spheres, respectively. The mode amplitude is scaled to an average RMSD of 1 Å.

Animation SI 3: Front view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory I by essential dynamics analysis (EDA). Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 4: Top view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory I by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 5: Front view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory II by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 6: Top view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory II by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 7: Front view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory III by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 8: Top view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from MD trajectory III by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 9: Front view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from the first 25 ns of MD trajectory III by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 10: Top view dynamic representation of principal mode 1 of *Dd* 2Fe-SOR, as calculated from the first 25 ns of MD trajectory III by EDA. Regions of high and low atomic fluctuations are color-coded in red and blue, respectively. Fe atoms are depicted as green spheres.

Animation SI 11 Front view dynamic representation of MD trajectory I. Electron transfer pathways are visualized in blue for subunit A. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 12: Front view dynamic representation of MD trajectory I. Electron transfer pathways are visualized in red for subunit B. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

Animation SI 13: Front view dynamic representation of MD trajectory II. Electron transfer pathways are visualized in blue for subunit A. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 14: Front view dynamic representation of MD trajectory II. Electron transfer pathways are visualized in red for subunit B. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

Animation SI 15: Front view dynamic representation of MD trajectory III. Electron transfer pathways are visualized in blue for subunit A. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 16: Front view dynamic representation of MD trajectory III. Electron transfer pathways are visualized in red for subunit B. Water molecules were not included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

Animation SI 17: Front view dynamic representation of MD trajectory I. Electron transfer pathways are visualized in blue for subunit A. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 18: Front view dynamic representation of MD trajectory I. Electron transfer pathways are visualized in red for subunit B. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

Animation SI 19: Front view dynamic representation of MD trajectory II. Electron transfer pathways are visualized in blue for subunit A. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 20: Front view dynamic representation of MD trajectory II. Electron transfer pathways are visualized in red for subunit B. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

Animation SI 21: Front view dynamic representation of MD trajectory III. Electron transfer pathways are visualized in blue for subunit A. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit A are depicted in green.

Animation SI 22: Front view dynamic representation of MD trajectory III. Electron transfer pathways are visualized in red for subunit B. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Fe atoms and tyrosine Y115 of subunit B are depicted in green.

SI 3: Data Evaluation of Molecular Dynamics (MD) Trajectory III

For all three trajectories, the time evolution of Fe–Fe distances, the domain dihedral angle, and the root mean square deviation (RMSD) reflects the domain rearrangement described in the manuscript (Figures 4 and SI 2). By visual inspection of the data, this rearrangement is most obvious for trajectory III (Figure 4). In most cases, however, correlations involving these geometric quantities are least pronounced for this particular trajectory, if all data points are included (Figures SI 1 and SI 3 – SI 8). In a similar sense, the contribution of the first principal mode to the overall atomic fluctuation is small (37%) compared to the values obtained for the two other trajectories (56% each). These observations can be explained by the fact that trajectory III reaches a *quasi* stable configuration with respect to the above two internal coordinates (Figure 4) and the eigenvector of the first principal mode after about 25 ns. Thus, the following data points may largely reflect faster and non-correlated fluctuations of atomic coordinates. In terms of essential dynamics and correlation analyses, these statistical motions can be interpreted as noise that reduces the informational content of the obtained results. In addition, essential modes other than the dominating domain rearrangement may contribute stronger to the overall atomic fluctuation after 25 ns. Indeed, normalized eigenvalues of the second to fifth principal mode are increased, if this time span is included in the essential dynamics analysis. Therefore, we have restricted correlation and essential dynamics analyses of trajectory III to the first 25 ns within the manuscript (Figure 5; Animations SI 9 and SI 10). Most results obtained in this way are more similar to the other two simulations, and almost all correlations emerge more clearly, demonstrating the feasibility of this approach. Results from essential dynamics and correlation analyses that consider all data points of trajectory III are available in Figures SI 1 and SI 3 – SI 8 as well as Animations SI 7 and SI 8.

SI 4: Correlations Between Selected Internal Coordinates from MD Simulations

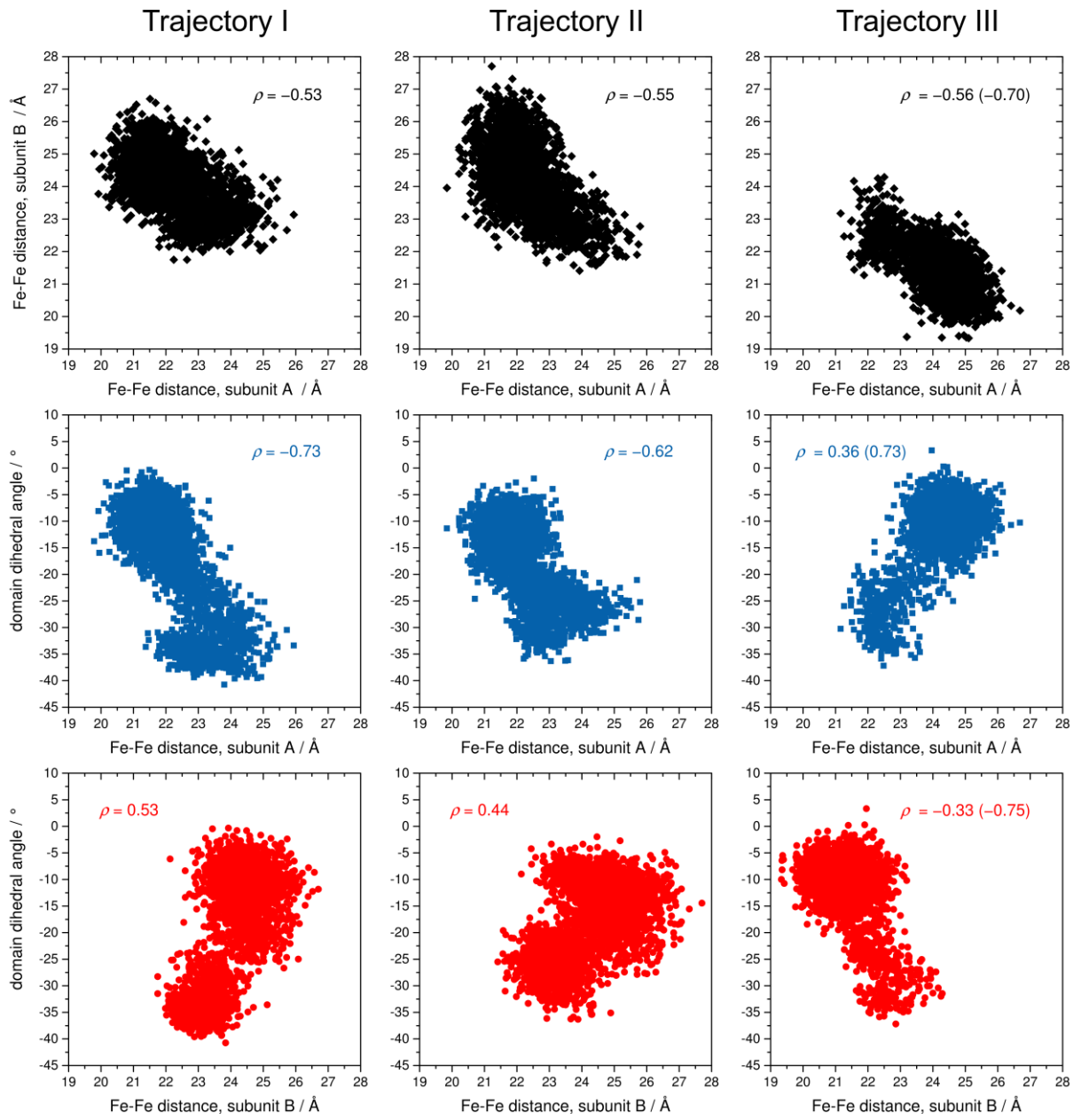

Figure SI 1: Scatter plots visualizing the correlation between different internal coordinates for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. (Top) Correlation between Fe–Fe distances in both subunits. (Centre) Correlation between the domain dihedral angle Fe1–C1'–C2'–Fe2 and the Fe–Fe distance in subunit A. (Bottom) Correlation between the domain dihedral angle Fe1–C1'–C2'–Fe2 and the Fe–Fe distance in subunit B. Fe1 and Fe2 refer to the Fe atoms of centres I and II in one subunit, while C1' (C2') specifies the centroid of the two Fe1 (Fe2) atoms. All correlations are statistically significant at the 0.01 level.

SI 5: Root Mean Square Deviation (RMSD) Values of MD Simulations

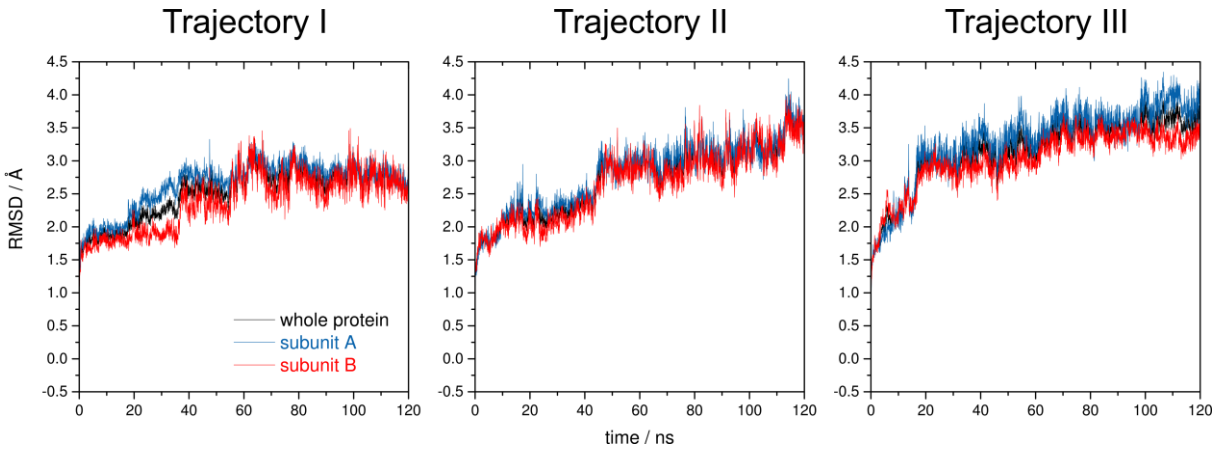

Figure SI 2: Time evolution of all-atom RMSD values of all three MD trajectories, as calculated for subunit A (blue), subunit B (red), and the entire protein (black). All trajectories were aligned to the first-frame reference structure of the protein prior to RMSD calculations.

SI 6: Correlations Between Electronic Couplings and Interdomain Fe–Fe Distances from MD Simulations

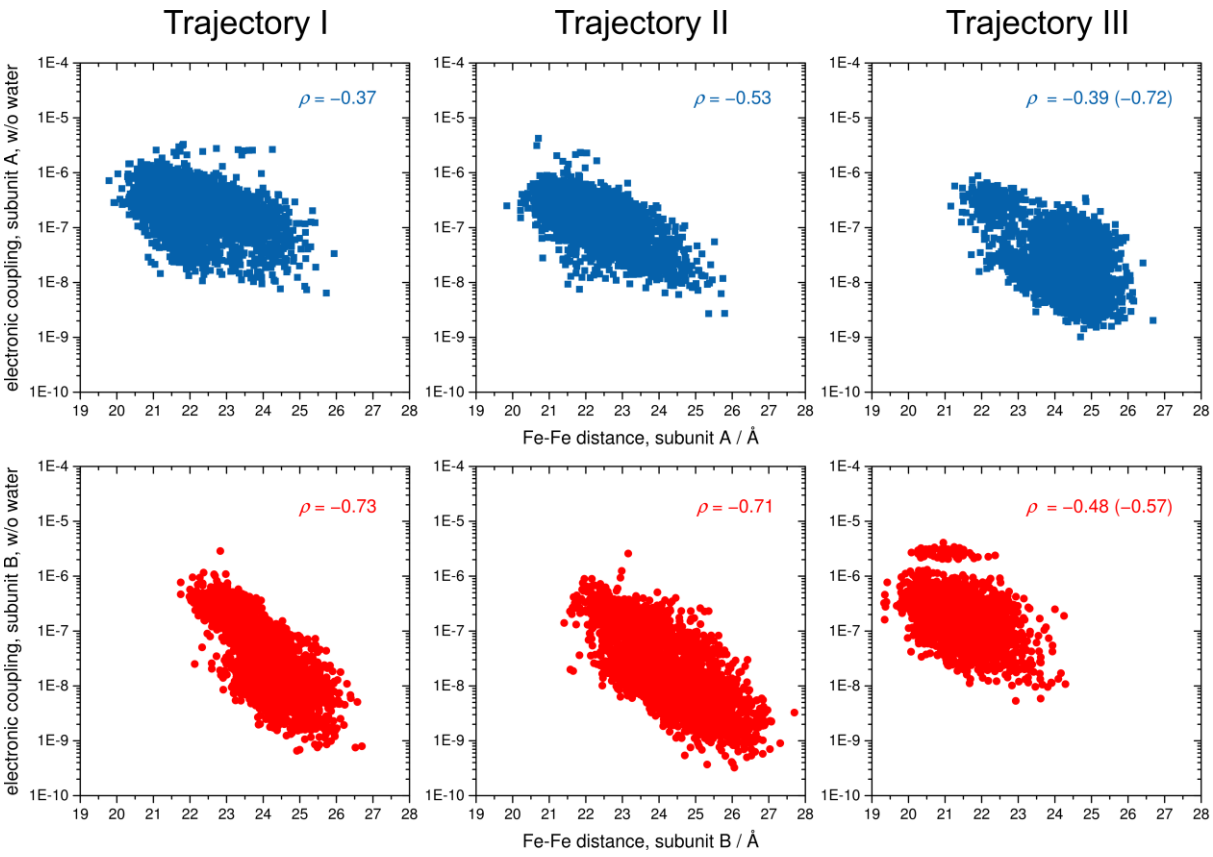

Figure SI 3: Scatter plots visualizing the correlation between electronic couplings and interdomain Fe–Fe distances for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules were not included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). All correlations are statistically significant at the 0.01 level.

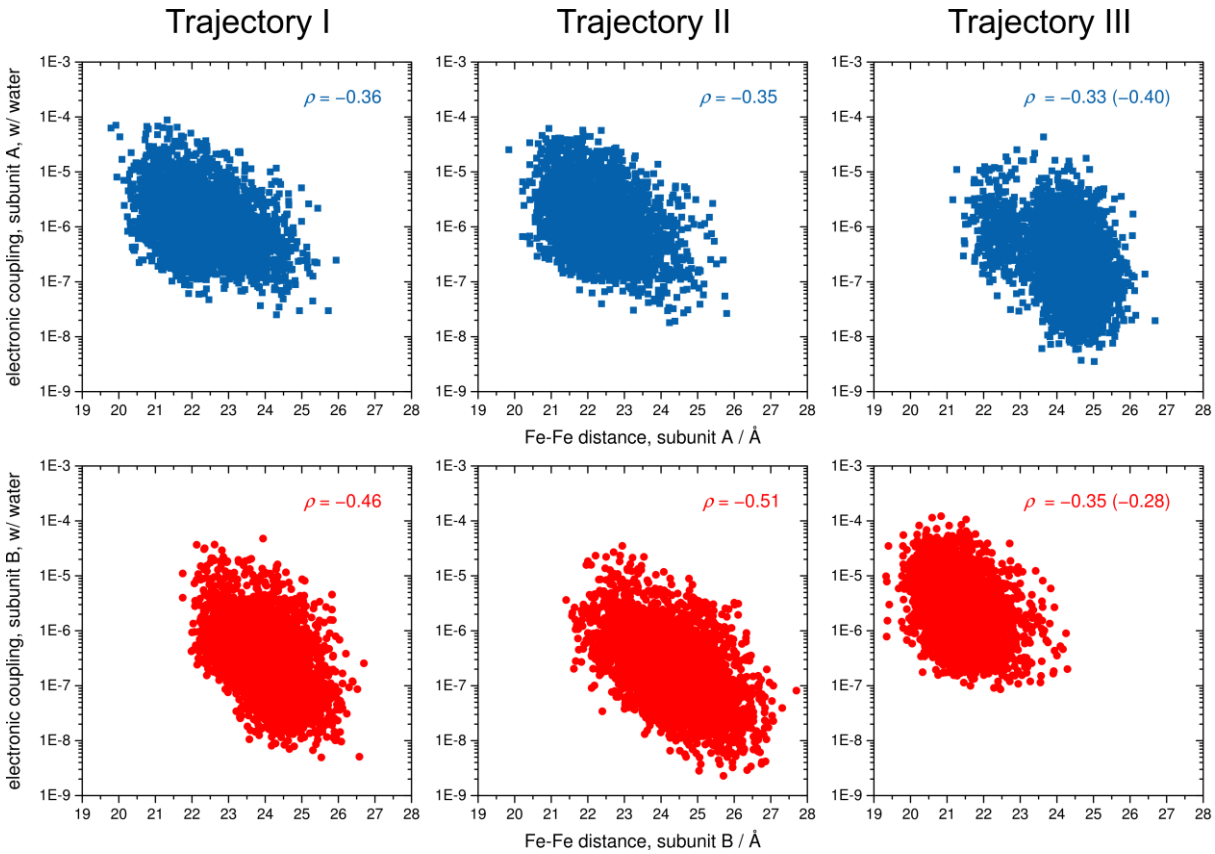

Figure SI 4: Scatter plots visualizing the correlation between electronic couplings and interdomain Fe–Fe distances for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). All correlations are statistically significant at the 0.01 level.

SI 7: Correlations Between Electronic Couplings and the Domain Dihedral Angle from MD Simulations

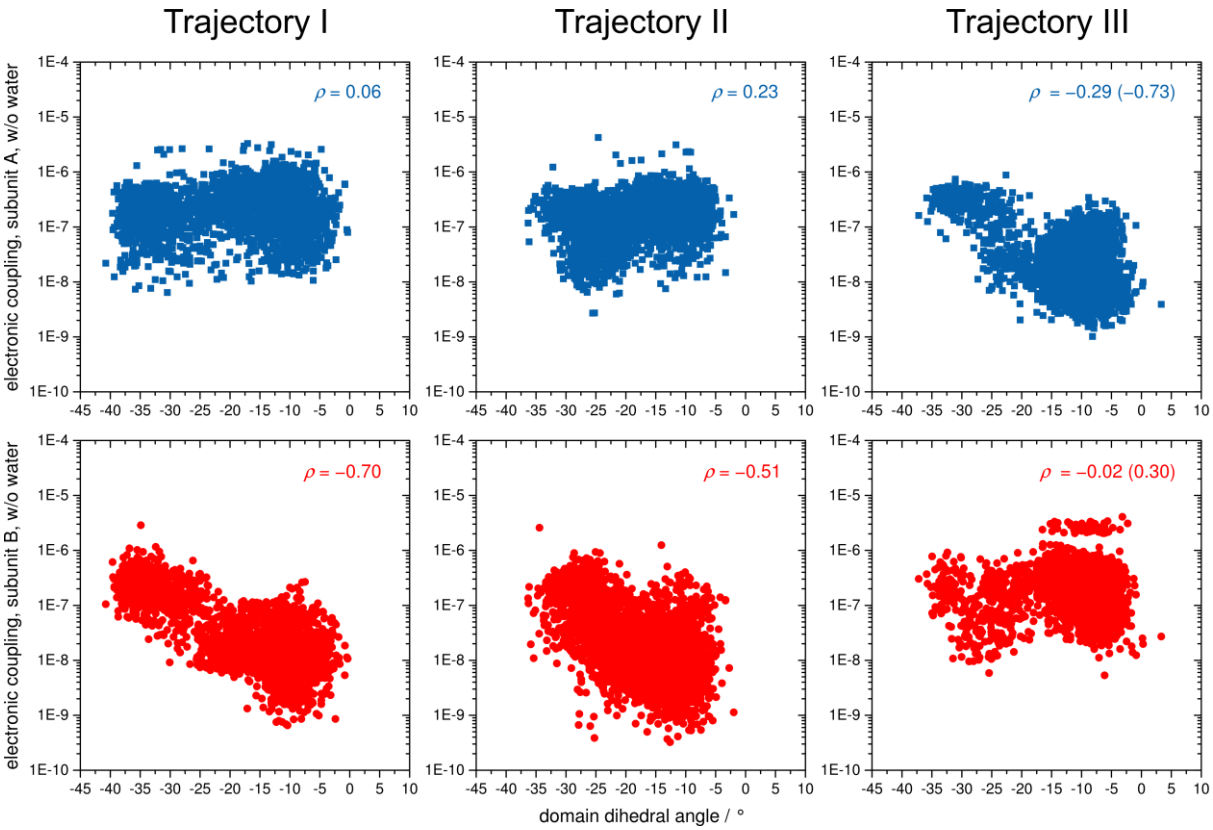

Figure SI 5: Scatter plots visualizing the correlation between electronic couplings and the domain dihedral angle Fe1–C1'–C2'–Fe2 for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules were not included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). Fe1 and Fe2 refer to the Fe atoms of centres I and II in one subunit, while C1' (C2') specifies the centroid of the two Fe1 (Fe2) atoms. All correlations with $|\rho| > 0.05$ are statistically significant at the 0.01 level.

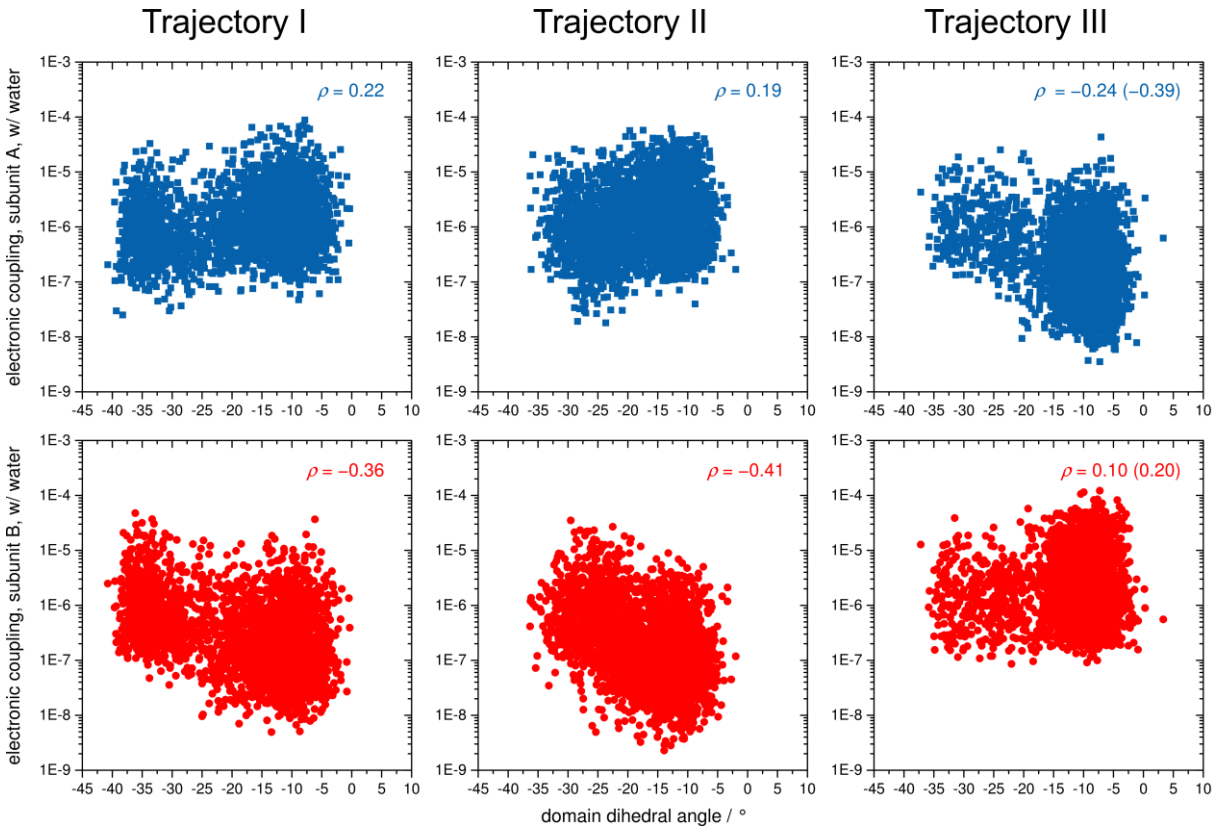

Figure SI 6: Scatter plots visualizing the correlation between electronic couplings and the domain dihedral angle Fe1–C1'–C2'–Fe2 for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). Fe1 and Fe2 refer to the Fe atoms of centres I and II in one subunit, while C1' (C2') specifies the centroid of the two Fe1 (Fe2) atoms. All correlations are statistically significant at the 0.01 level.

SI 8: Correlations Between Electronic Couplings and RMSD Values from MD Simulations

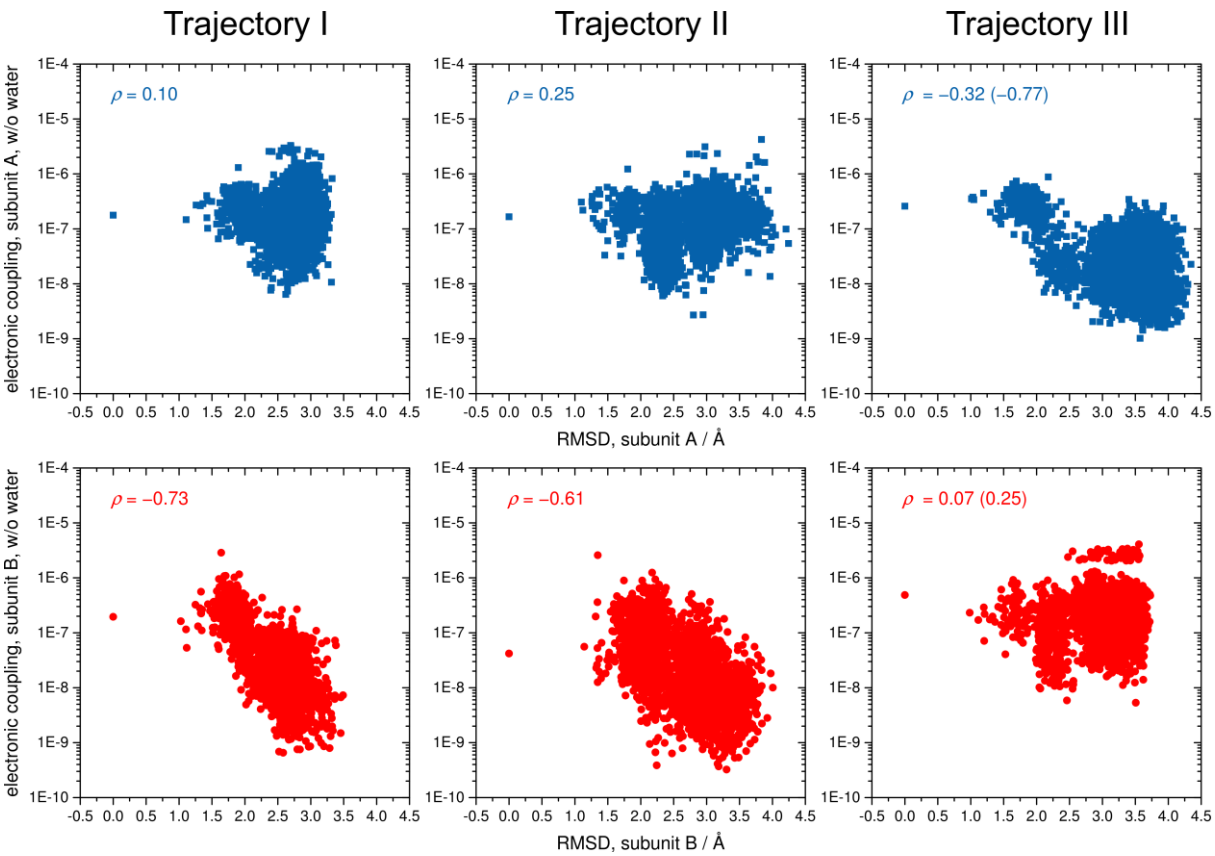

Figure SI 7: Scatter plots visualizing the correlation between electronic couplings and RMSD values for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules were not included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). All correlations are statistically significant at the 0.01 level.

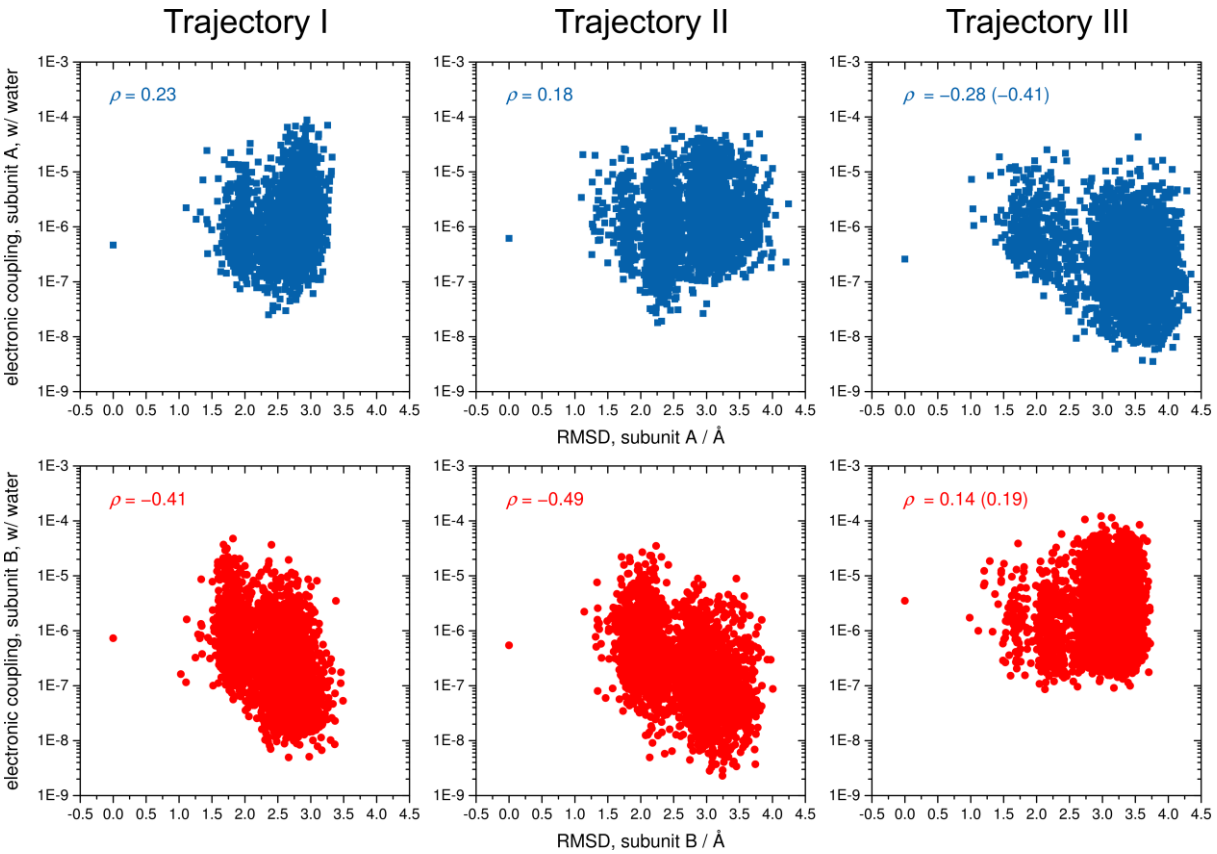

Figure SI 8: Scatter plots visualizing the correlation between electronic couplings and RMSD values for the entire time span of all three MD trajectories. The corresponding Spearman rank correlation coefficients ρ are indicated for all data sets, where values in parentheses reflect the first 25 ns only. Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Data corresponding to subunit A (B) are presented in blue (red) at the top (bottom). All correlations are statistically significant at the 0.01 level.

SI 9: Contributions of Individual Amino Acids to Electron Transfer Pathways from MD Simulations

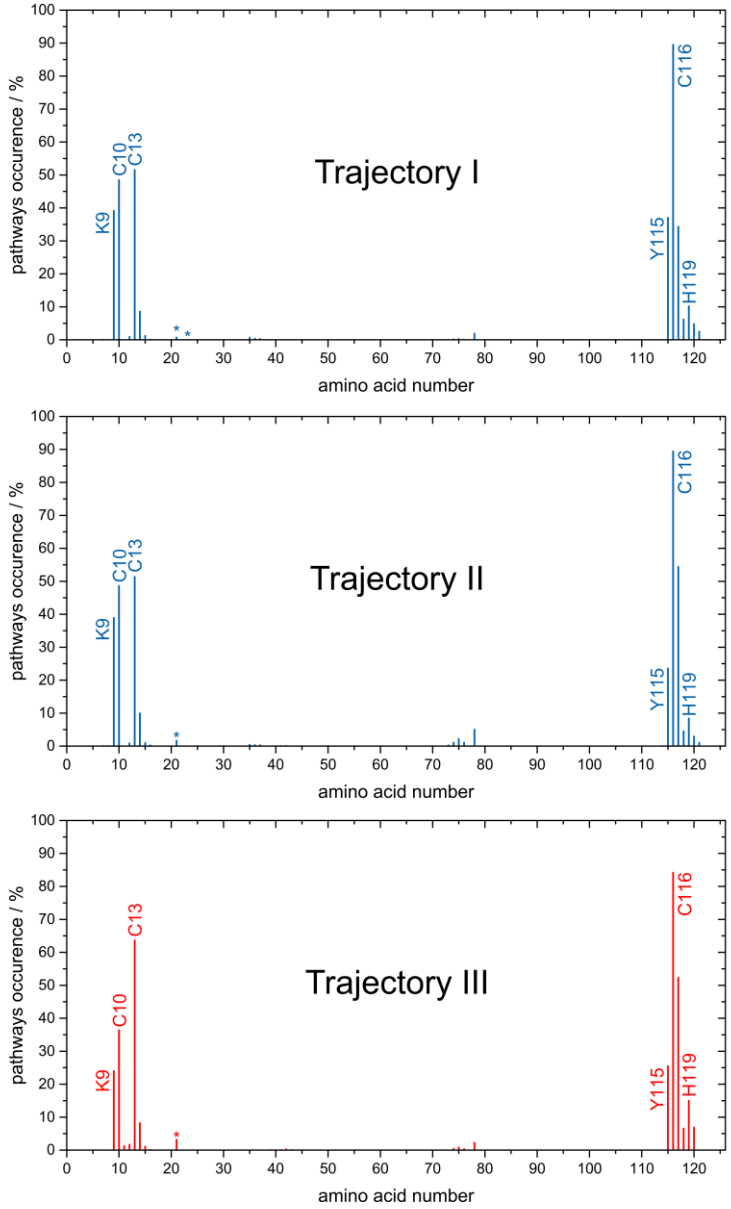

Figure SI 9: Relative contributions of amino acids to electron transfer pathways as calculated by the pathways model for all frames of the three MD trajectories. Data are shown for the subunit assuming a closed configuration during the MD simulations, i.e. subunit A for trajectory I and II (blue) and subunit B for trajectory III (red). Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Amino acids belonging to the respective other subunit are marked by an asterisk, and important residues are labelled in one-letter code.

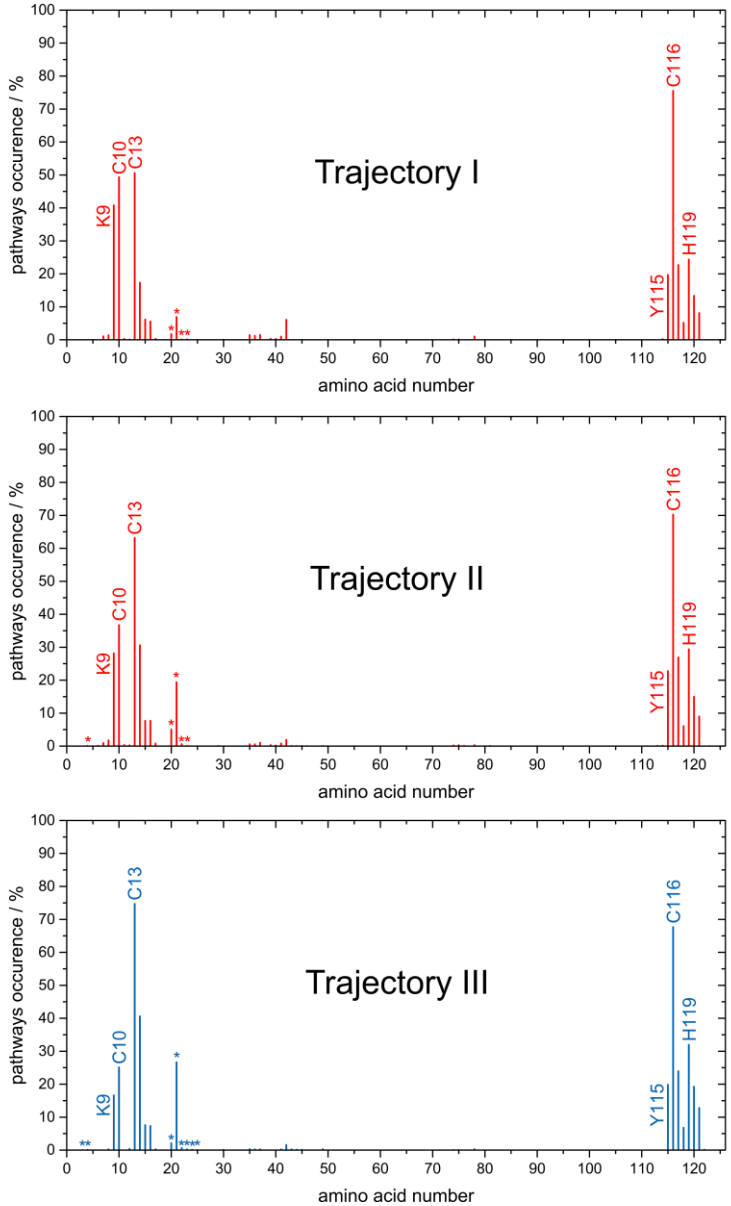

Figure SI 10: Relative contributions of amino acids to electron transfer pathways as calculated by the pathways model for all frames of the three MD trajectories. Data are shown for the subunit assuming an opened configuration during the MD simulations, i.e. subunit B for trajectory I and II (red) and subunit A for trajectory III (blue). Water molecules within a cut-off distance of 5 Å around the protein were included in the analysis. Amino acids belonging to the respective other subunit are marked by an asterisk, and important residues are labelled in one-letter code.

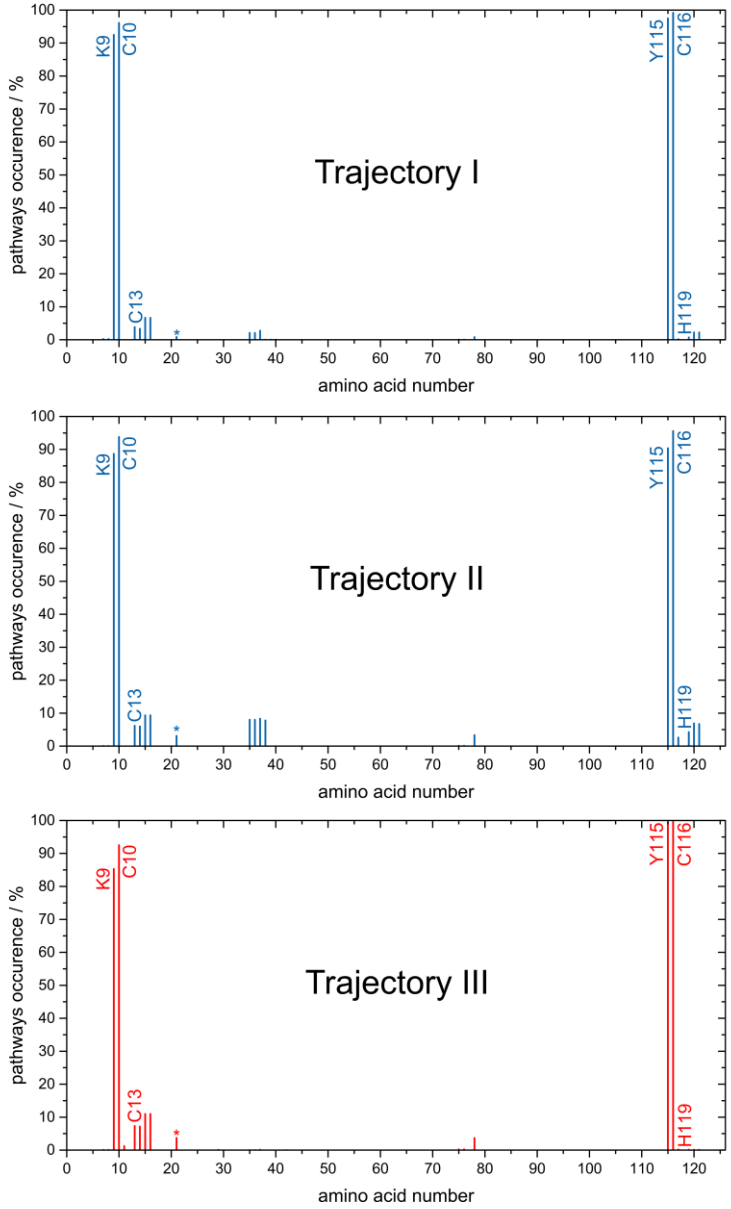

Figure SI 11: Relative contributions of amino acids to electron transfer pathways as calculated by the pathways model for all frames of the three MD trajectories. Data are shown for the subunit assuming a closed configuration during the MD simulations, i.e. subunit A for trajectory I and II (blue) and subunit B for trajectory III (red). Water molecules were not included in the analysis. Amino acids belonging to the respective other subunit are marked by an asterisk, and important residues are labelled in one-letter code.

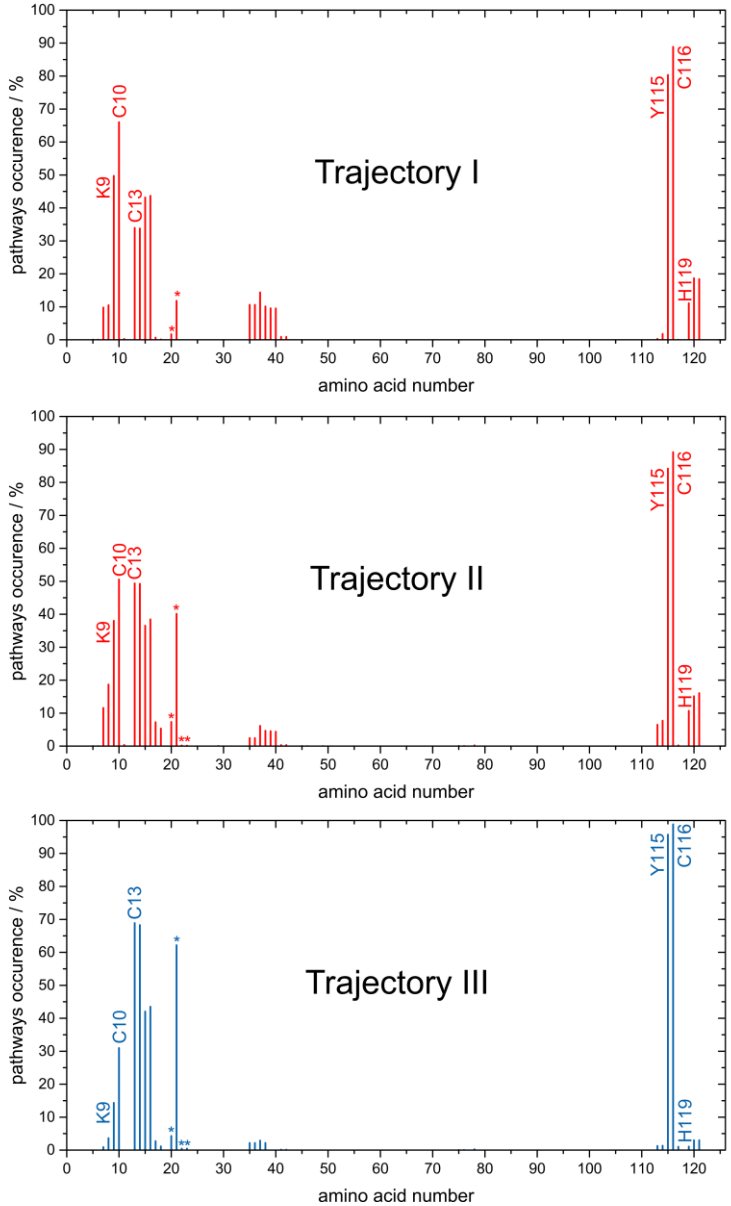

Figure SI 12: Relative contributions of amino acids to electron transfer pathways as calculated by the pathways model for all frames of the three MD trajectories. Data are shown for the subunit assuming an opened configuration during the MD simulations, i.e. subunit B for trajectory I and II (red) and subunit A for trajectory III (blue). Water molecules were not included in the analysis. Amino acids belonging to the respective other subunit are marked by an asterisk, and important residues are labelled in one-letter code.

References

1 C. Lucchetti-Miganeh, D. Goudenege, D. Thybert, G. Salbert and F. Barloy-Hubler, *BMC Microbiol.*, 2011, **11**, 105.

2 M. Goujon, H. McWilliam, W. Li, F. Valentin, S. Squizzato, J. Paern and R. Lopez, *Nucleic Acids Res.*, 2010, **38**, W695-W699.

3 F. Sievers, A. Wilm, D. Dineen, T. J. Gibson, K. Karplus, W. Li, R. Lopez, H. McWilliam, M. Remmert, J. Söding, J. D. Thompson and D. G. Higgins, *Mol. Syst. Biol.*, 2011, **7**, 539.

4 H. McWilliam, W. Li, M. Uludag, S. Squizzato, Y. M. Park, N. Buso, A. P. Cowley and R. Lopez, *Nucleic Acids Res.*, 2013, **41**, W597-W600.

5 W. Li, A. Cowley, M. Uludag, T. Gur, H. McWilliam, S. Squizzato, Y. M. Park, N. Buso and R. Lopez, *Nucleic Acids Res.*, 2015, **43**, W580-W584.

6 M. D. Clay, Jenney,F. E. Jr., H. J. Noh, P. L. Hagedoorn, M. W. Adams and M. K. Johnson, *Biochemistry*, 2002, **41**, 9833–9841.

7 F. Bonnot, S. Duval, M. Lombard, J. Valton, C. Houee-Levin and V. Niviere, *J. Biol. Inorg. Chem.*, 2011, **16**, 889–898.