Table S1. Data collection and refinement statistics

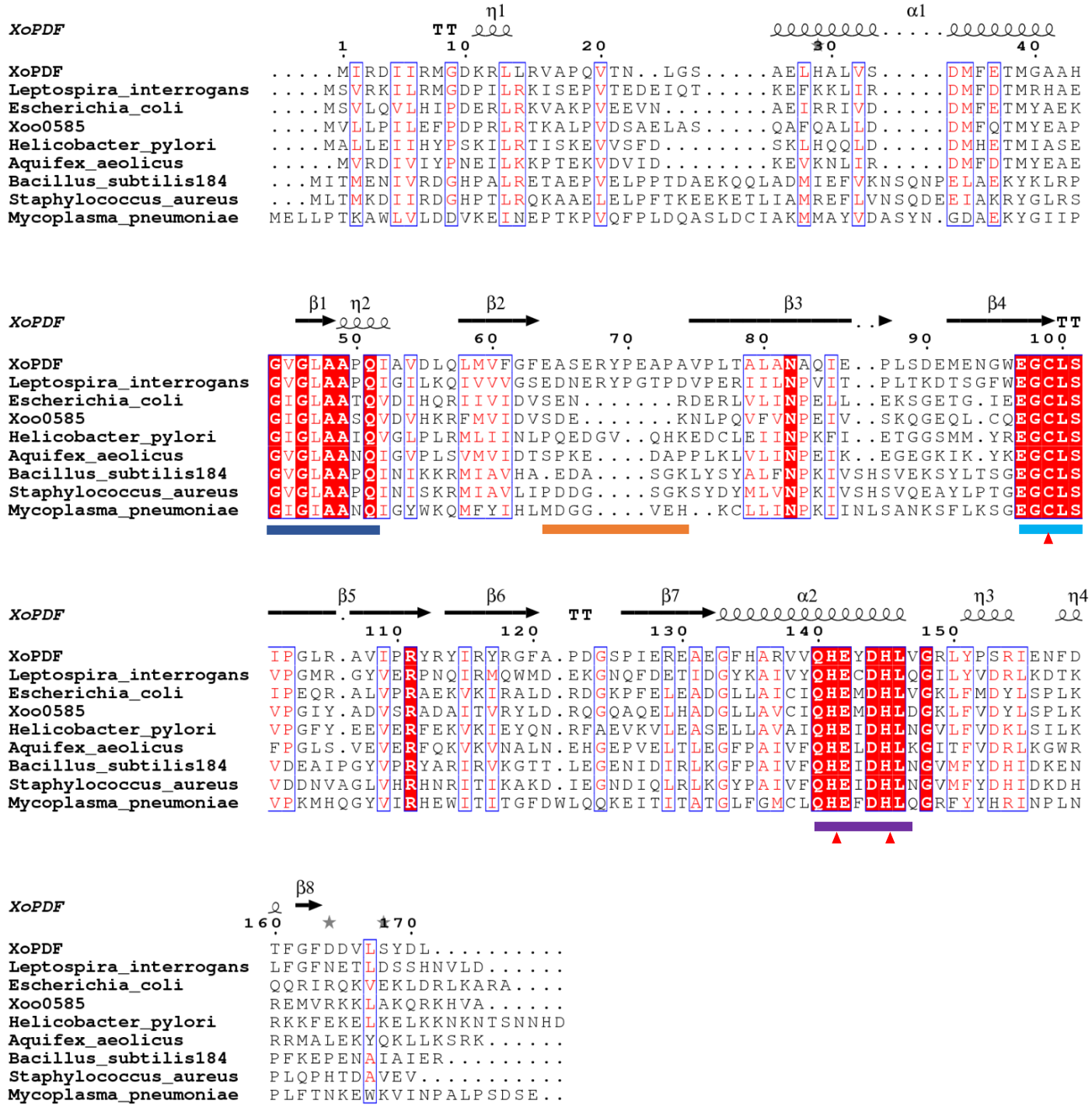
Data collection	Apo 5E5D	MA 5CPD	MAS 5CP0	Actinonin 5CVQ	FCC1 5CY8	FCC2 5CY7	FCC3 5CWY	FCC4 5CVK	FCC5 5CWX	FCC6 5CVP
X-ray source	17A-KEK	PAL4A	PAL4A	PAL4A	PAL4A	PAL4A	PAL4A	PAL4A	PAL4A	PAL4A
Space group	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$	$P6_122$
Unit-cell parameters a(b), c (Å)	58.7, 266.3	58.6, 266.2	58.7, 265.4	58.6, 265.8	58.7, 263.7	58.8, 264.0	58.97, 263.8	59.0, 264.7	58.5, 264.2	58.9, 264.1
Resolution range (Å)	50.0-2.6 (2.69-2.6)	50.0-2.1 (2.14-2.1)	50.0-1.95 (2.02-1.95)	50.0-2.2 (2.24-2.2)	50.0-2.4 (2.47-2.4)	50.0-2.4 (2.47-2.4)	50.0-2.4 (2.47-2.4)	50.0-2.0 (2.03-2.0)	50.0-2.2 (2.24-2.2)	50.0-2.0 (2.03-2.0)
No. of observed reflections (unique)	86,356 (9,011)	159,530 (16,778)	204,372 (20,724)	91,979 (22,857)	113,971 (11,737)	101,079 (11,015)	127,428 (20,246)	151,756 (33,248)	71,918 (25,491)	186,999 (18,979)
Completeness (%)	96.9 (97.4)	98.5(99.6)	98.6 (95.7)	87.6 (83.1)	98.8 (99.1)	95.2 (88.0)	97.9 (96,4)	95.2 (82.7)	98.9 (97.9)	97.1 (84.7)
R_{sym}[†] (%)	15.5 (44.3)	17.7 (59.3)	11.0 (65.2)	18.6 (64.8)	9.1 (42.5)	6.8 (28.9)	9.7 (51.0)	11.1 (48.0)	9.8 (48.4)	8.2 (37.8)
Average I/σ(I)	22.5 (6.6)	9.8 (1.7)	36.2 (4.6)	7.2 (1.6)	25 (4.5)	35.3 (7.4)	18.8 (3.2)	16.9 (2.2)	12.4 (3.2)	31.6 (4.0)
Refinement										
Resolution (Å)	30.4 (2.6)	30.4 (2.2)	29.4 (2.0)	27.8 (2.5)	28.65 (2.38)	30.4 (2.38)	30.4 (2.4)	27.0 (2.1)	30.4 (2.2)	30.4 (2.0)
Number of reflections										
Working set	8,502	13,851	18,225	9,226	4,800	10,401	10,913	15,907	13,777	17,907
Free R set	422	729	979	471	555	524	546	832	729	957
R/R_{free} (%)[c]	18.6 (24.3)	19.1 (24.7)	18.1 (21.7)	17.2 (21.8)	18.7 (22.7)	18.1 (21.2)	18.4 (22.7)	17.6 (22.4)	20.7 (25.9)	17.4 (21.6)
Protein atoms number	1,335	1,317	1,303	1,230	1,335	1,350	1,320	1,328	1,357	1,314
Substrate										
MA	N/D	14	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
MAS	N/D	N/D	20	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Inhibitor				27	13	12	11	15	13	13
Water molecules	116	100	193	88	116	112	113	179	74	172

Cadmium ion	3	3	5	3	3	3	3	5	3	5
Sodium ion	N/D	2	1	N/D	1	1	1	1	N/D	2
Acetate	N/D	4	12	4	4	4	4	1	4	4
Glycerol	N/D	6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
RMS bond lengths (Å)	0.015	0.021	0.026	0.075	0.019	0.018	0.018	0.020	0.019	0.020
RMS bond angles(°)	1,881	2,086	2.337	1,963	2,148	1,919	2,157	2,042	2,146	1,980
Mean B factors (Å^2)										
Main-chain atoms	29.8	27.3	25.0	24.4	30.1	26.2	28.2	22.1	33.5	23.1
Side-chain atoms	33.5	30.8	28.9	27.8	33.8	29.7	32.2	27.4	37.5	29.3
Substrate										
MA	N/D	34.3	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
MAS	N/D	N/D	42.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Inhibitor	N/D	N/D	N/D	25.6	47.8	56.4	53.4	35.3	61.6	45.0
Water atoms	30.4	36.0	36.8	32.0	36.5	31.2	34.3	33.8	40.9	36.0
Cadmium	53.8	33.0	39.7	33.9	41.6	61.8	50.9	27.8	43.5	28.6
Sodium ion	N/D	37.0	32.9	N/D	52.2	45.4	42.9	35.7	N/D	40.3
Acetate	N/D	27.7	46.5	24.4	27.6	26.4	26.1	22.5	31.4	23.9
Glycerol	N/D	65.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Ramachandran plot (%)										
Favored regions	98.2	98.2	97.0	97.4	97.6	98.2	98.8	98.2	96.8	98.7
Allowed regions	1.8	1.8	1.8	2.6	3.4	1.8	1.2	1.8	3.2	1.3
Outlier regions	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Values in parentheses are for the highest resolution shell.

$R_{\text{merge}} = \sum_{hkl}\sum_i \left|\left(I_i(hkl)\right) - \langle I(hkl)\rangle\right| / \sum_{hkl}\sum_i I_i(hkl)$, where $I_i(hkl)$ is the mean intensity of *i*th observation of symmetry-related reflections *hkl*. $R_{\text{free}} = \sum_{hkl}\left||F_{obs}| - |F_{calc}|\right| / \sum_{hkl}|F_{obs}|$, where F_{calc} is the calculated protein structure factor from the atomic model (R_{free} was calculated from a randomly selected 5% sample of all reflections).

Fig. S1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α1
TT
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Escherichia_coli ....MSVLQVLHIPDERLRKVAKPVEEVN.........AEIRRIVD.....DMFETMYAEK
Xoo0585 ....MVLLPILEFPDPRLRTKALPVDSAELAS.....QAFQALLD.....DMFQTMYEAP
Helicobacter_pylori ....MALLEIIHYPSKILRTISKEVVSFD.........SKLHQQLD.....DMHETMIASE
Aquifex_aeolicus .....MVRDIVIYPNEILKKPTEKVDVID.........KEVKNLIR.....DMFDTMYEAE
Bacillus_subtilis184 ...MITMENIVRDGHPALRETAEPVELPPTDAEKQQLADMIEFVKNSQNPELAEKYKLRP
Staphylococcus_aureus ...MLTMKDIIRDGHPTLRQKAAELELPFTKEEKETLIAMREFLVNSQDEEIAKRYGLRS
Mycoplasma_pneumoniae MELLPTKAWLVLDDVKEINEPTKPVQFPLDQASLDCIAKMMAYVDASYN.GDAEKYGIIP
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Leptospira_interrogans GVGLAAPQIGILKQIVVVGSEDNERYPGTPDVPERIILNPVIT..PLTKDTSGFWEGCLS
Escherichia_coli GIGLAATQVDIHQRIIVIDVSEN.......RDERLVLINPELL..EKSGETG.IEEGCLS
Xoo0585 GIGLAASQVDVHKRFMVIDVSDE.......KNLPQVFVNPEIV..SKQGEQL.CQEGCLS
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Aquifex_aeolicus GVGLAANQIGVPLSVMVIDTSPKE....DAPPLKLVLINPEIK..EGEGKIK.YKEGCLS
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XoPDF
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XoPDF IPGLR.AVIPRYRYIRYRGFA.PDGSPIEREAEGFHARVVQHEYDHLVGRLYPSRIENFD
Leptospira_interrogans VPGMR.GYVERPNQIRMQWMD.EKGNQFDETIDGYKAIVYQHECDHLQGILYVDRLKDTK
Escherichia_coli IPEQR.ALVPRAEKVKIRALD.RDGKPFELEADGLLAICIQHEMDHLVGKLFMDYLSPLK
Xoo0585 VPGIY.ADVSRADAITVRYLD.RQGQAQELHADGLLAVCIQHEMDHLDGKLFVDYLSPLK
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Aquifex_aeolicus FPGLS.VEVERFQKVKVNALN.EHGEPVELTLEGFPAIVFQHELDHLKGITFVDRLKGWR
Bacillus_subtilis184 VDEAIPGYVPRYARIRVKGTT.LEGENIDIRLKGFPAIVFQHEIDHLNGVMFYDHIDKEN
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Mycoplasma_pneumoniae VPKMHQGYVIRHEWITITGFDWLQQKEITITATGLFGMCLQHEFDHLQGRFYYHRINPLN
β8
XoPDF
160 170
XoPDF TFGFDDVLSYDL.........
Leptospira_interrogans LFGFNETLDSSHNVLD......
Escherichia_coli QQRIRQKVEKLDRLKARA....
Xoo0585 REMVRKKLAKQRKHVA......
Helicobacter_pylori RKKFEKELKELKKNKNTSNNHD
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Fig. S2

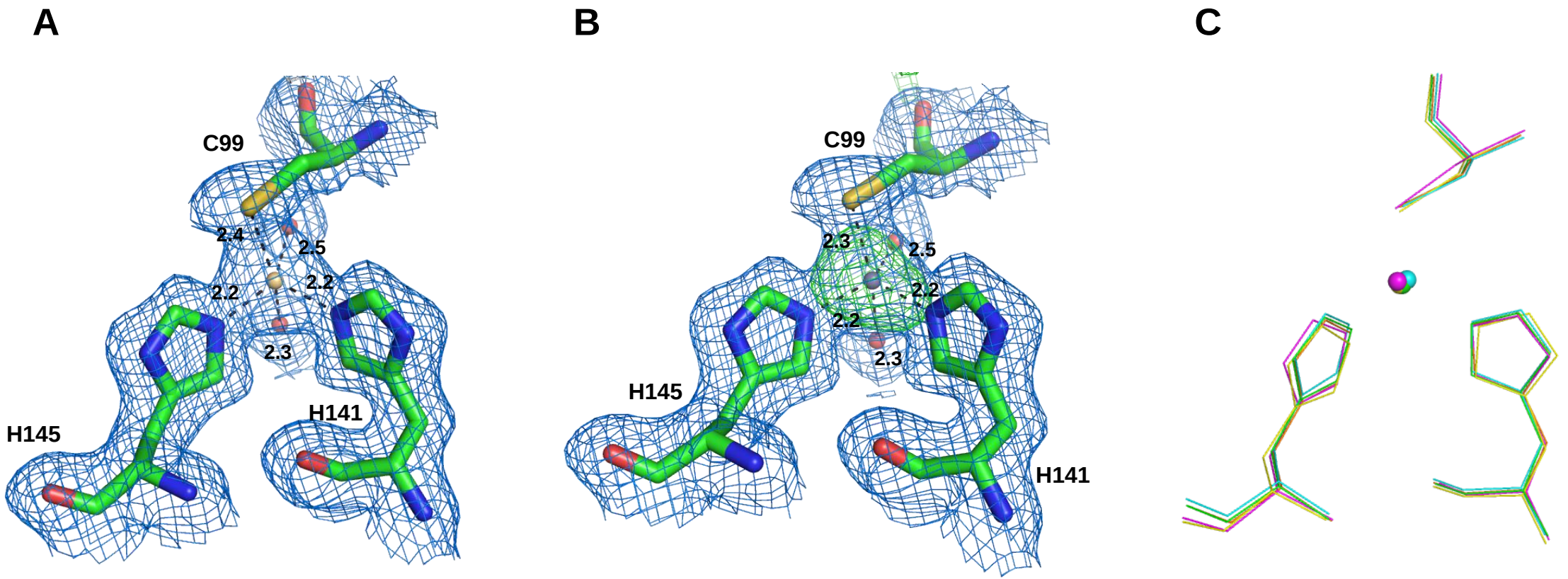


Fig. S3

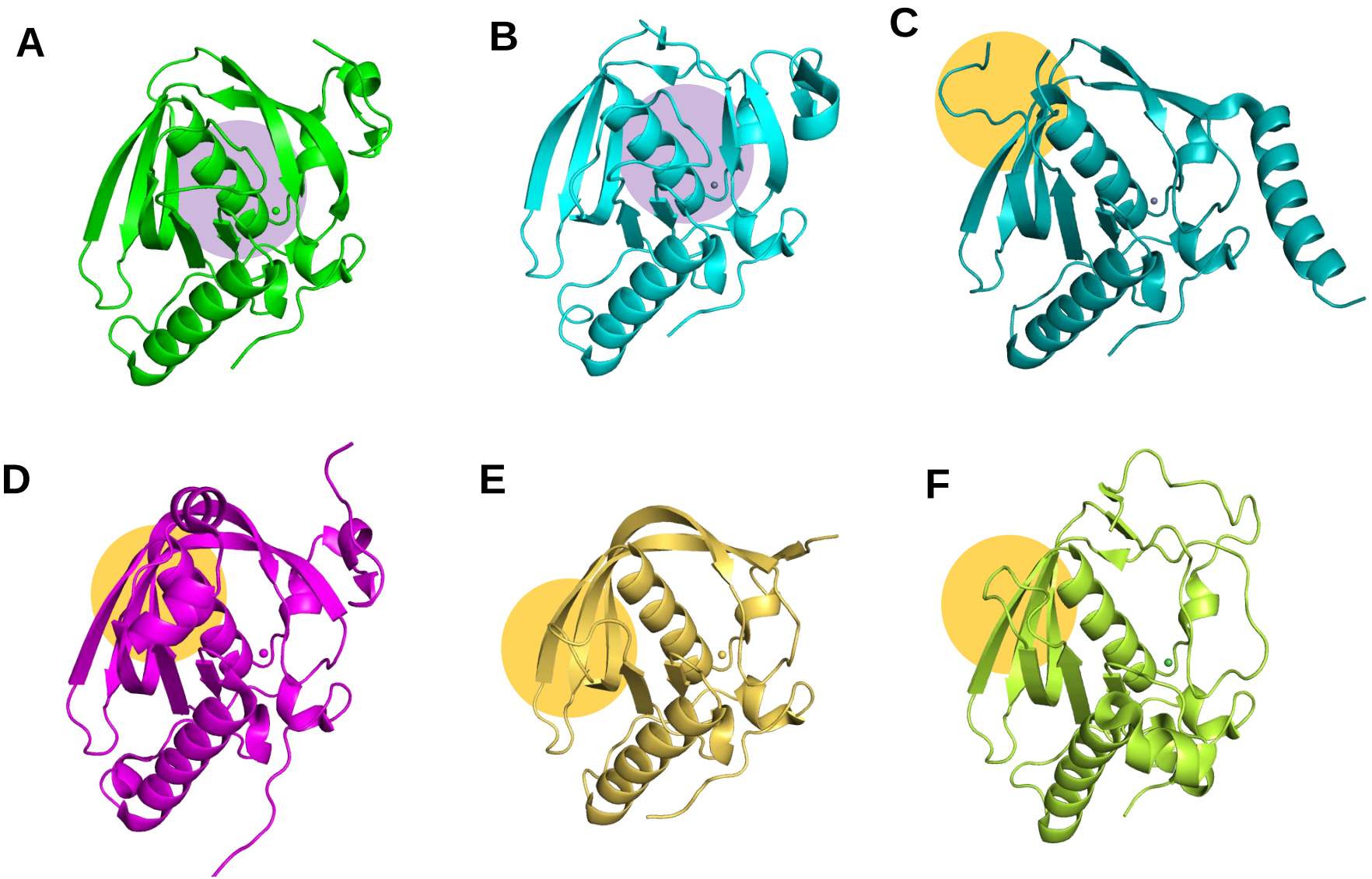
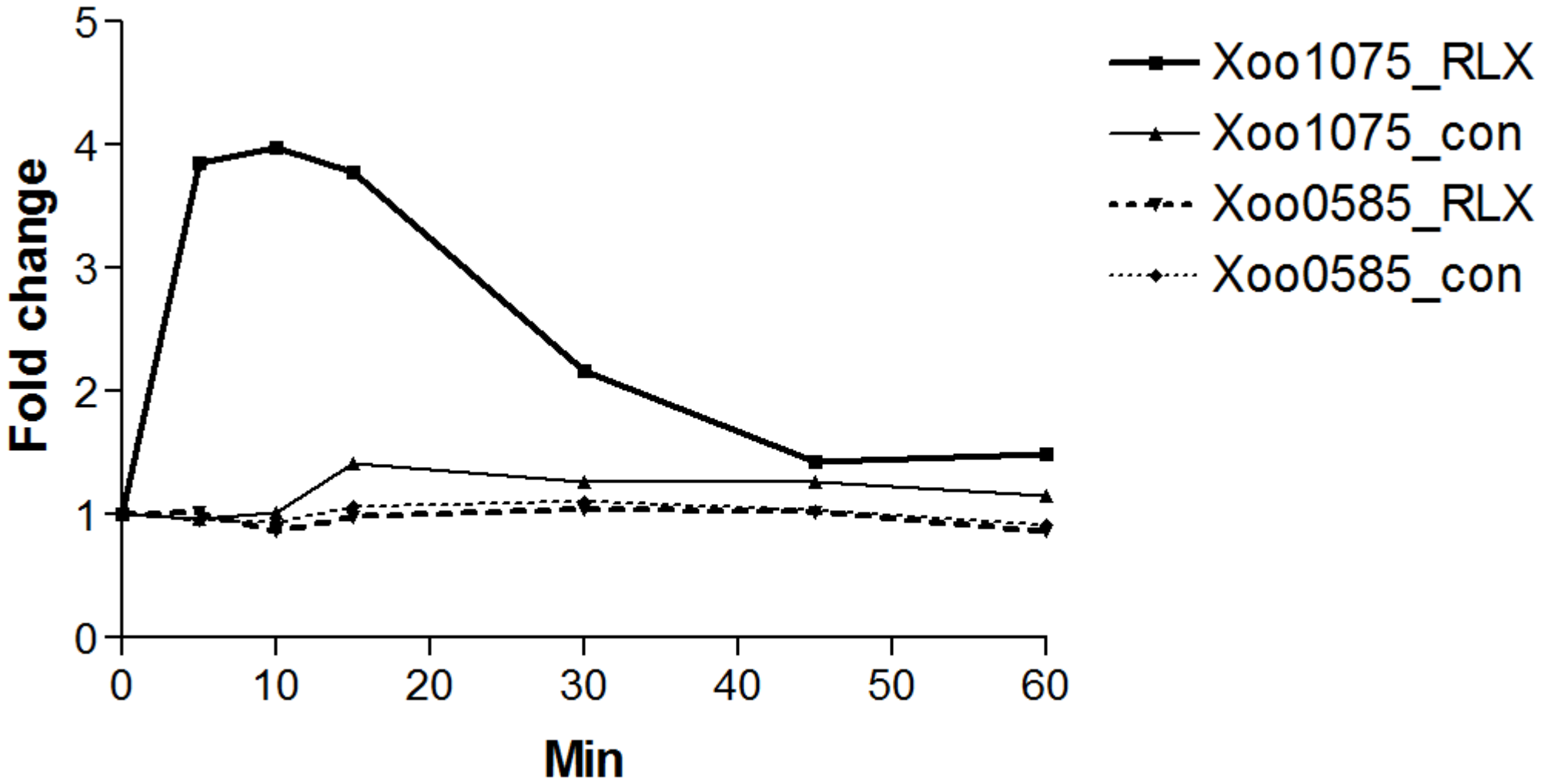


Fig. S4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0
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Min
Xoo1075_RLX
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Fig. S5

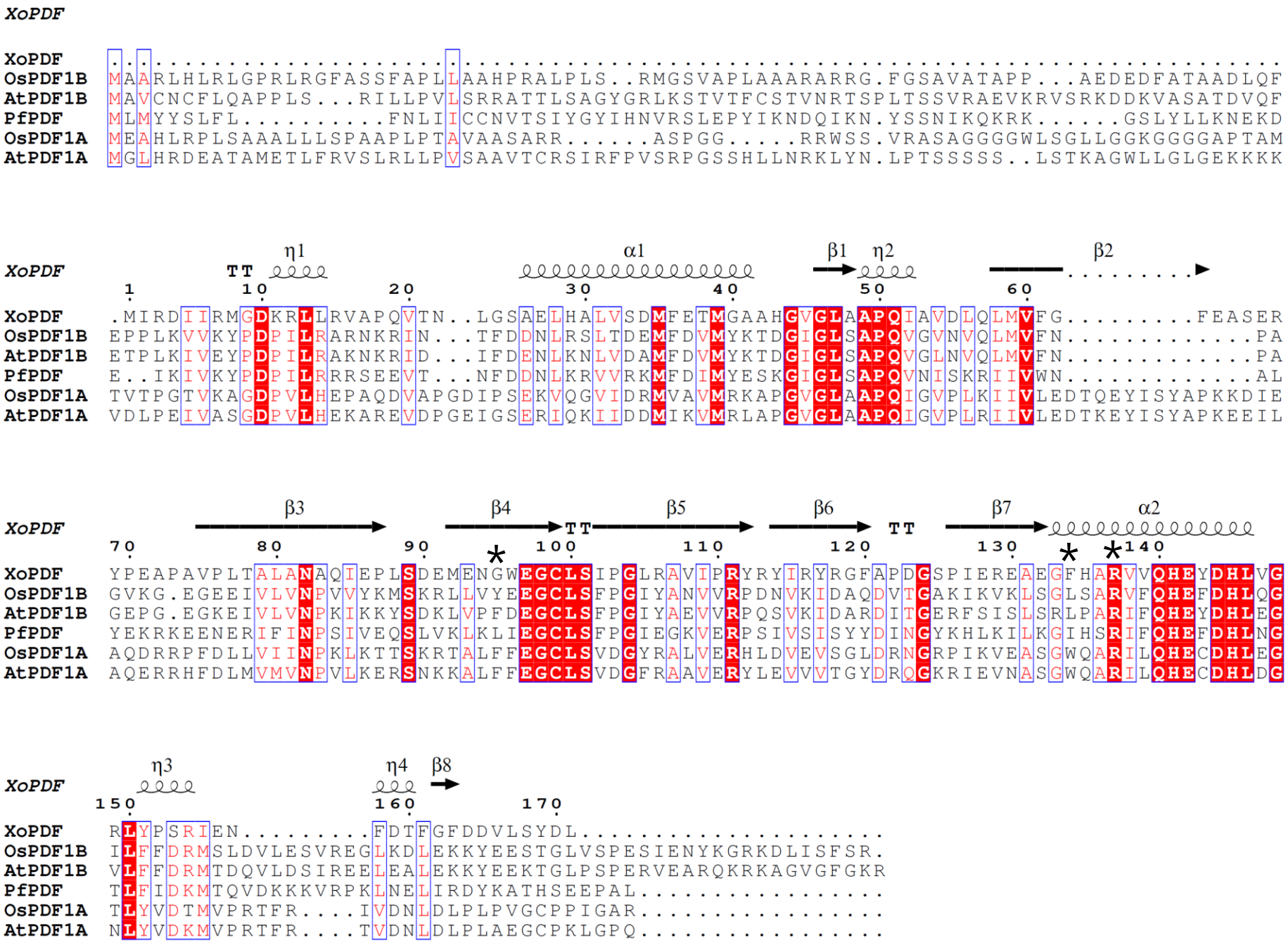
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Fig. S6

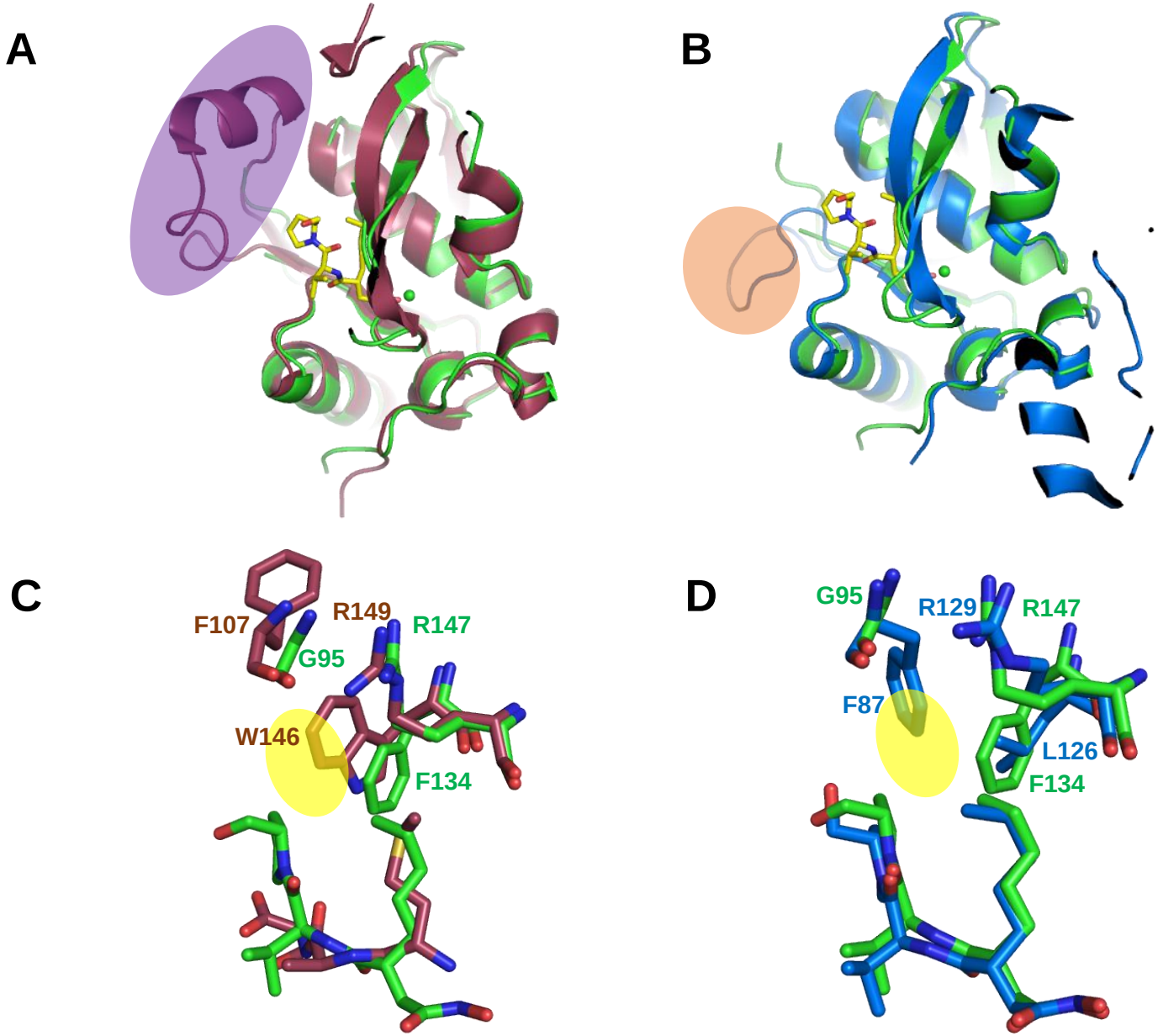


Fig. S7

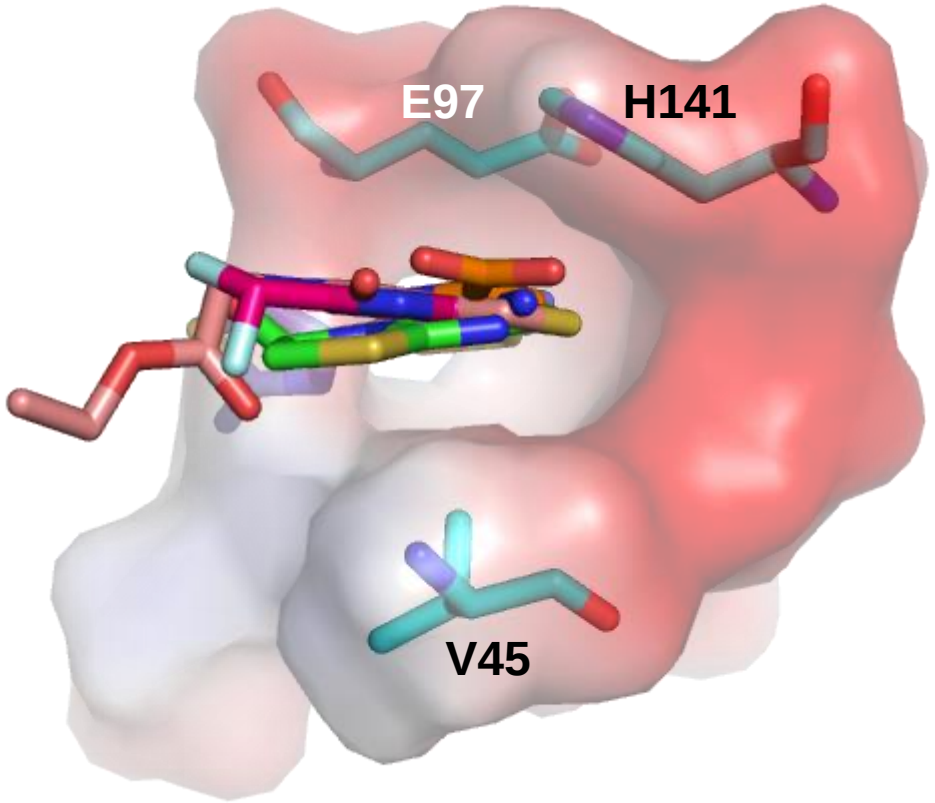


Fig. S8

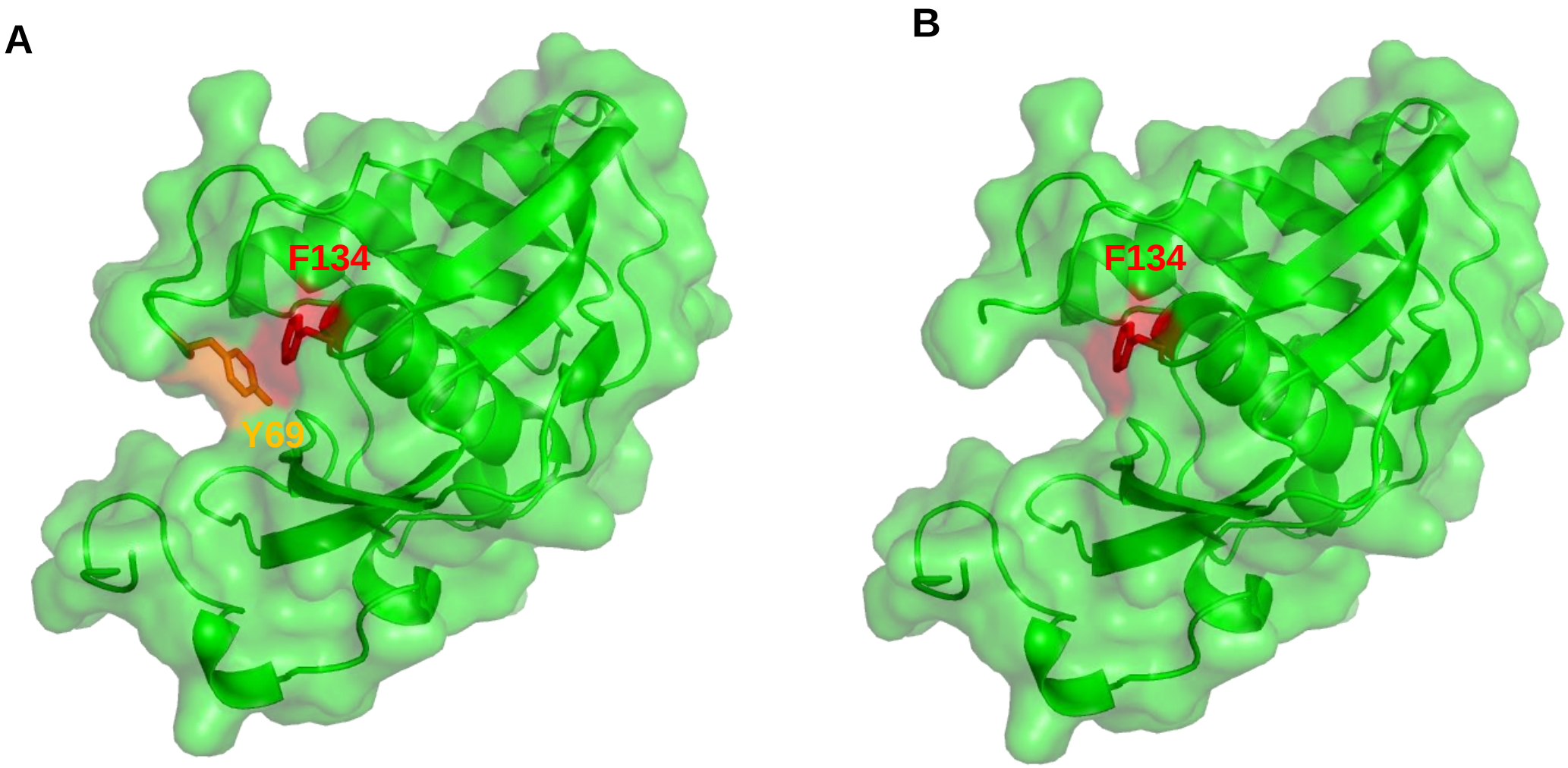
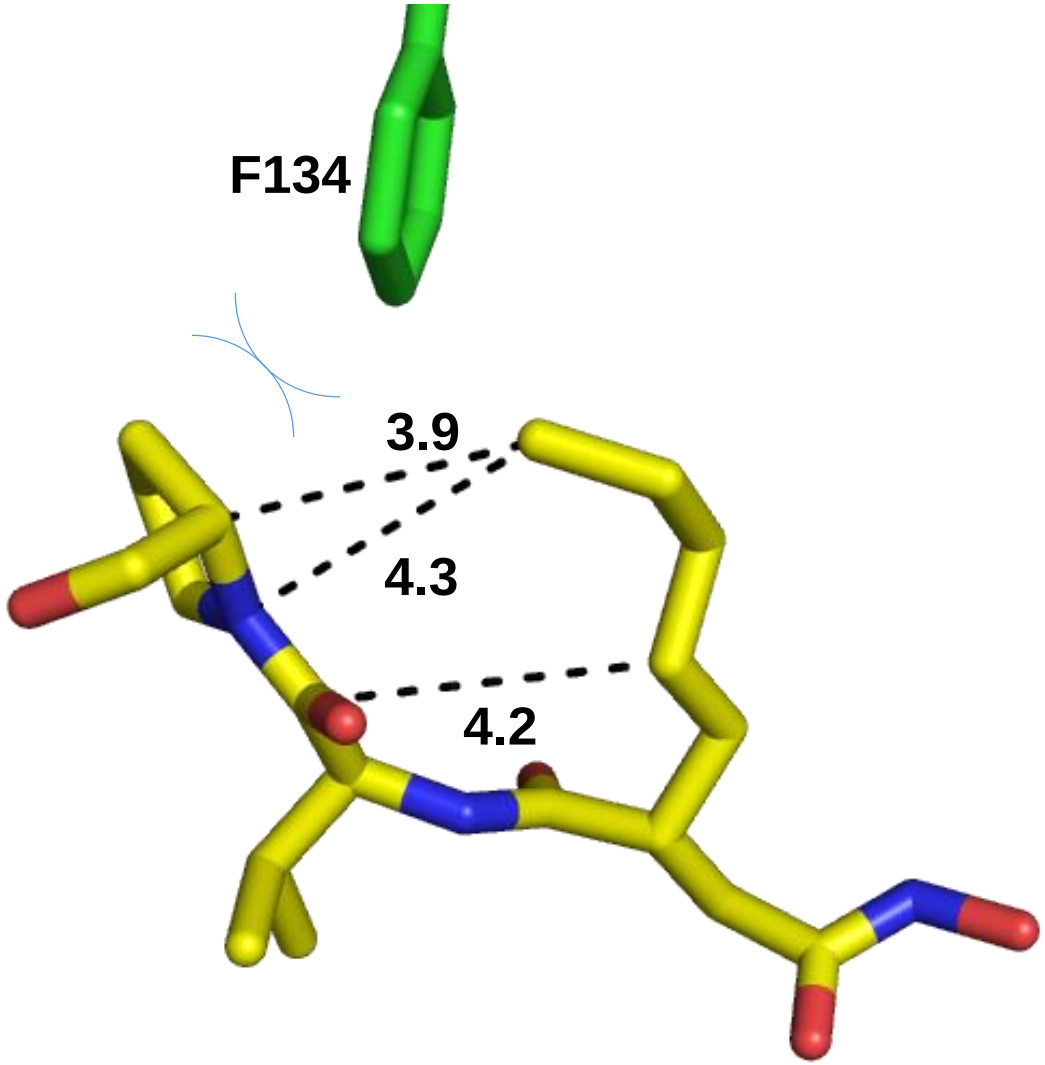


Fig. S9



SUPPLEMENTARY FIGURE LEGENDS

Figure S1. Sequence alignment of bacterial PDFs. The amino acid sequences were aligned with the secondary structure information of XoPDF; XoPDF (Xoo1075; Def) from *Xanthomonas oryzae* pv. *oryzae*, PDF from *Leptospira interrogans*, PDF from *E. coli*, PDF (Xoo0585) from *Xanthomonas oryzae* pv. *oryzae*, PDF from *Helicobacter pylori*, PDF from *Aquifex aeolicus*, PDF from *Bacillus subtilis* 184, PDF from *Staphylococccus aureus* and PDF from *Mycoplasma pneumonia*. Residues coordinating the metal ion in the active site are indicated with red inverted triangles. Signature motif 1 is shown in blue, motif 2 in cyan, motif 3 in purple and CD loop in orange.

Figure S2. Metal binding and coordination of XoPDF. (a) Cd^{2+} ion in the metal site of MAS-bound XoPDF structure with 2Fofc and FoFc maps. (b) Zn^{2+} ion in the metal site of MAS-bound XoPDF structure with 2Fofc and FoFc maps. 2Fofc map (blue mesh) is contoured at 1.0 σ and Fofc map (green mesh) at 5.0 σ. (c) Superimposed metal sites of Cd^{2+}-bound XoPDF (purple), Co^{2+}-bound EcPDF (PDB ID: 4AZ4; cyan), Ni^{2+}-bound EcPDF (PDB ID: 4AL2; yellow), Zn^{2+}-bound EcPDF (PDB ID: 1XEM; green) and Fe^{2+}-bound EcPDF (PDB ID: 1XEN; orange).

Figure S3. Structures of PDF CD-loops. (a) XoPDF. (b) PDF from *Leptospira interrogans* (PDB ID: 1SV2). (c) PDF from *Ehrlichia chaffeensis* (PDB ID: 3OCA). (d) PDF from human (PDB ID: 3G5P). (e) PDF from *Bacillus cereus* (PDB ID: 1WS0). (f) PDF from *Staphylococcus aureus* (PDB ID: 2AI9). CD-loops are shown with purple (closed) and orange (opened) shades.

Figure S4. Time-resolved transcriptional gene expression of *XoPDF* (*Xoo1075, def*) and *Xoo0585* genes Transcriptional gene expression levels of *XoPDF* and *Xoo0585* were measured in a time-resolved manner via RNA-Seq, after the activation of Xoo pathogenicity. Xoo1075_RLX and Xoo1075_con exhibit transcriptional expression of the *XoPDF* gene within 1 hour in the pathogenicity-activated Xoo cell and the control Xoo cell,

respectively. Xoo0585_RLX and Xoo0585_con exhibit transcriptional expression of the *Xoo0585* gene within 1 hour in the pathogenicity-activated Xoo cell and the control Xoo cell, respectively.

Figure S5. Sequence alignment of XoPDF and eukaryotic PDFs: XoPDF (Xoo1075; Def) from *Xanthomonas oryzae* pv. *oryzae*, OsPDF1B from rice, AtPDF1B from *Arabidopsis thaliana*, PfPDF from *Plasmodium falciparum*, OsPDF1A from rice and AtPDF1A from *Arabidopsis thaliana*. Residues in the upper layer of the hydrophobic pocket for substrate methionine side chain are marked with asterisk.

Figure S6. Structure comparison between XoPDF and AtPDFs. (a) Superimposed structures of actinonin-bound XoPDF (green) and MAS-bound AtPDF1A (brown). Actinonin in XoPDF is shown in yellow. CD-loop of AtPDF1A is shaded in purple. (b) Superimposed structures of actinonin-bound XoPDF (green) and actinonin-bound AtPDF1B (pale-blue). Actinonin in XoPDF is shown in yellow. CD-loop of AtPDF1B is shaded in salmon. (c) Superimposed substrate-binding site of actinonin-bound XoPDF (green) and MAS-bound AtPDF1A (brown) with the upper layer residues of the hydrophobic pocket for substrate methionine side chain. (d) Superimposed substrate-binding site of actinonin-bound XoPDF (green) and actinonin-bound AtPDF1B (pale-blue) with the upper layer residues of the hydrophobic pocket for substrate methionine side chain.

Figure S7. Bottom view of substrate methionine-binding site. The fragment chemical compounds (FCCs)-bound structures were superimposed to the MA-bound structure and only FCCs and substrate methionine-binding site are shown in the same bottom view of Fig. 4*b*.

Figure S8. Exposure of Phe134 residue in XoPDF with the flexible open conformation of CD loop. (a) The structure of closed CD loop. (b) The structure of opened CD loop.

Figure S9. Actinonin structure in XoPDF. The hydrophobic van der Waals interactions between the pentyl group and the other chain structure with the pyrrolidine ring are shown as black dashed lines. The hydrophobic van der Waals interactions between Phe134 and the 5-member pyrrolidine ring is shown as blue arcs.