Supplementary Table 1. Statistics of data collection and structure refinement of subcomplex I.

Data collection						
Data set	Se1 peak	Se1 inflection	Se1 remote	Se2 peak	Se2 inflection	Se2 remote
Data Collection						
Wavelength (Å)	0.9791	0.9793	0.9641	0.9791	0.9792	0.9641
Resolution (Å)	50-2.70	50-2.70	50-2.70	50-2.10	50-2.10	50-2.10
Outer shell (Å)	2.80-2.70	2.80-2.70	2.80-2.70	2.18-2.10	2.18-2.10	2.18-2.10
Unique reflections	28,053	28,202	28,381	58,588	58,671	58,571
Redundancy	6.5	7.0	7.0	6.4	5.1	4.9
I/σ (outer shell)	12.6 (4.2)	12.2 (3.6)	10.9 (2.7)	11.0 (2.8)	9.4 (2.1)	8.9 (1.8)
Completeness (%) (outer shell)	99.9 (100.0)	99.9 (100.0)	99.9 (100.0)	99.3 (95.4)	98.8 (91.3)	98.6 (90.2)
R_{sym} (outer shell)	0.102 (0.302)	0.097 (0.370)	0.108 (0.513)	0.100 (0.376)	0.093 (0.426)	0.093 (0.479)
Figure of Merit (50-2.7 Å)				0.776		

Refinement	
Resolution (Å)	50-2.1
Reflections (work/free)	55,430/2,931
Data completeness (work + free)	98.8%
No. of atoms (waters)	7,191 (133)
R-work	0.212
R-free	0.259
RMSD bond lengths (Å)	0.0084
RMSD bond angles (^{o})	1.52
RMSD B-factors over bonds	4.5
Average B-factor (Å^2)	36.8
Ramachandran Plot	
within favored (%)	97.4
within allowed (%)	99.2
outliers (%)	0.8

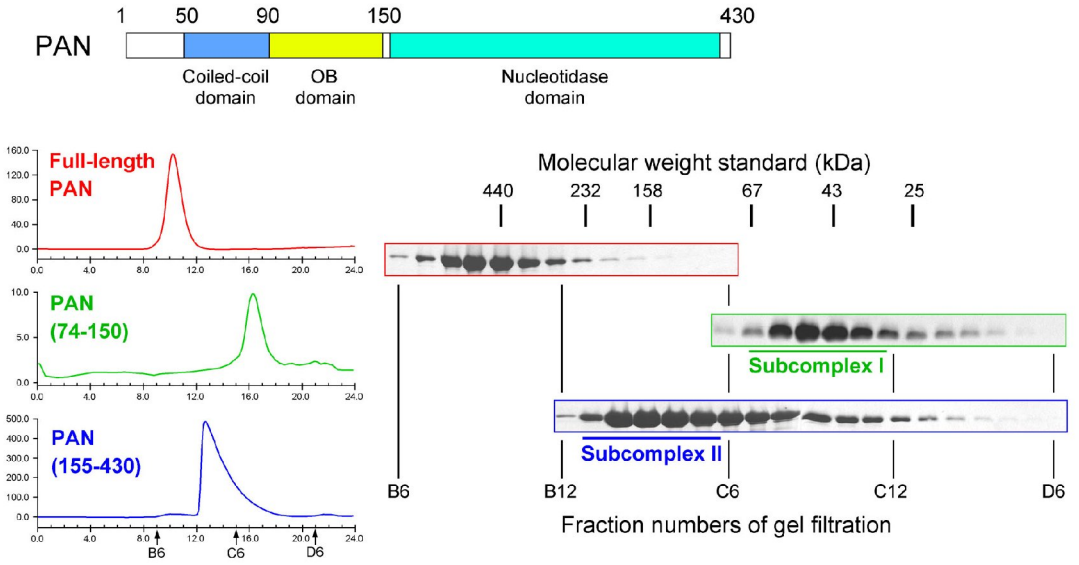
$R_{sym} = \Sigma_h \Sigma_i \; | I_{h,i} - I_h | / \Sigma_h \Sigma_i I_{h,i}$, where I_h is the mean intensity of the i observations of symmetry related reflections of h. $R = \sum | F_{obs} - F_{calc} | / \sum F_{obs}$, where $F_{obs} = F_P$, and F_{calc} is the calculated protein structure factor from the atomic model (R_{free} was calculated with 5% of the reflections). R.m.s.d. in bond lengths and angles are the deviations from ideal values, and the r.m.s.d. deviation in B factors is calculated between bonded atoms. Ramachandran plots were calculated using the program Molprobity, which uses a tougher standard than Procheck.

Supplementary Table 2. Summary of data collection and structure refinement for the nucleotidase domain and the CP.

Data Collection		
Data set	PAN nucleotidase	Core Particle
Wavelength (Å)	1.10	1.08
Resolution (Å)	50-3.10	50-4.10
Outer shell (Å)	3.21-3.10	4.25-4.10
Unique reflections	22,762	54,076
Redundancy	6.6	4.8
I/σ (outer shell)	19.7 (3.1)	9.5 (3.5)
Completeness (%) (outer shell)	99.8 (100.0)	99.8 (100.0)
R_{sym} (outer shell)	0.084 (0.523)	0.126 (0.488)
Refinement		
Resolution (Å)	50-3.1	50-4.1
Reflections (work/free)	19,605/1,092	51,010/2,737
Completeness (%, work+free)	95.8	99.8
No. of atoms	6,162	93,324
R-work	0.221	0.265
R-free	0.277	0.321
RMSD bond lengths (Å)	0.011	0.009
RMSD bond angles (^{o})	1.43	1.26
RMSD B-factors over bonds	1.0	n/a
Average B-factor (Å^2)	101.1	145.0
Ramachandran Plot		
Within favored (%)	89.3	72.5
Within allowed (%)	98.3	93.3
Outliers (%)	1.7	6.7

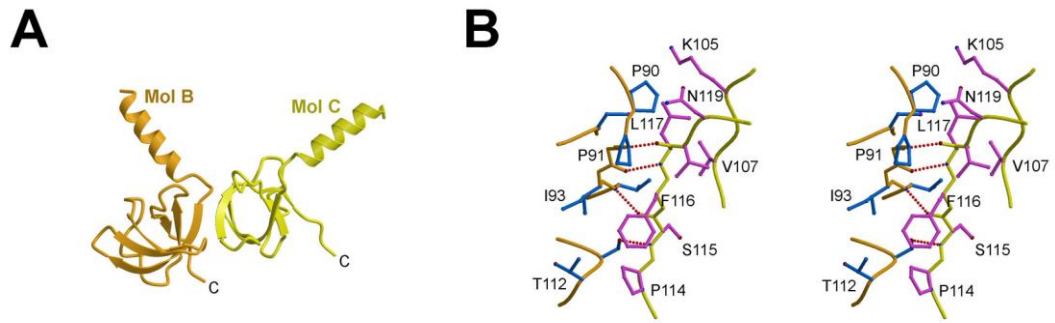
$R_{sym} = \Sigma_h \Sigma_i \ | I_{h,i} - I_h | / \Sigma_h \Sigma_i I_{h,i}$, where I_h is the mean intensity of the i observations of symmetry related reflections of h. $R = \sum | F_{obs} - F_{calc} | / \sum F_{obs}$, where $F_{obs} = F_P$, and F_{calc} is the calculated protein structure factor from the atomic model (R_{free} was calculated with 5% of the reflections). R.m.s.d. in bond lengths and angles are the deviations from ideal values, and the r.m.s.d. deviation in B factors is calculated between bonded atoms. Ramachandran plots were calculated using the program Molprobity, which uses a tougher standard than Procheck.

F) Supplemental Figure 1



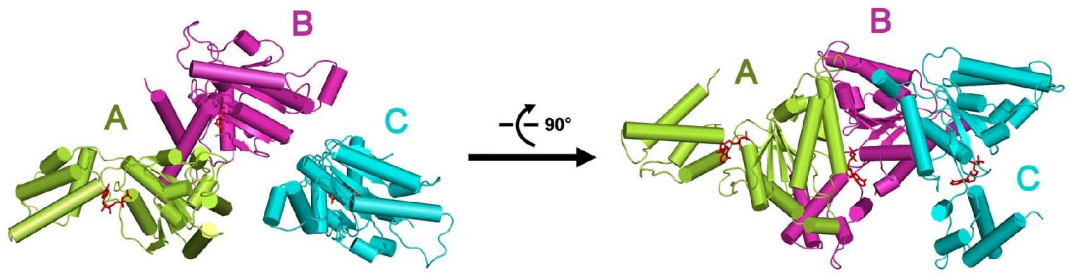
Supplementary Figure 1 The PAN regulatory particle consists of two subcomplexes. The PAN regulatory particle was eluted from gel filtration as a large complex, with an apparent molecular mass in excess of 500-kDa (red chromatogram). Limited proteolysis of the PAN regulatory particle generates two subcomplexes: I and II. Subcomplex I contains amino acids 74-150 and is stable on gel filtration (green chromatogram). Subcomplex II contains residues 155-430 and appears to dissociate on gel filtration (blue chromatogram). Boxed bands show coomassie-stained SDS-PAGE gel of the fractions from the corresponding gel filtration runs on the left. Gel filtration was performed using a Superdex 200 column (10/30, GE Healthcare). The injection volume was 0.5 ml for each gel filtration run. Concentrations of the protein samples prior to injection were: 10 mg/ml for full-length PAN and PAN (74-150), and 20 mg/ml for PAN (155-430).

F) Supplemental Figure 2



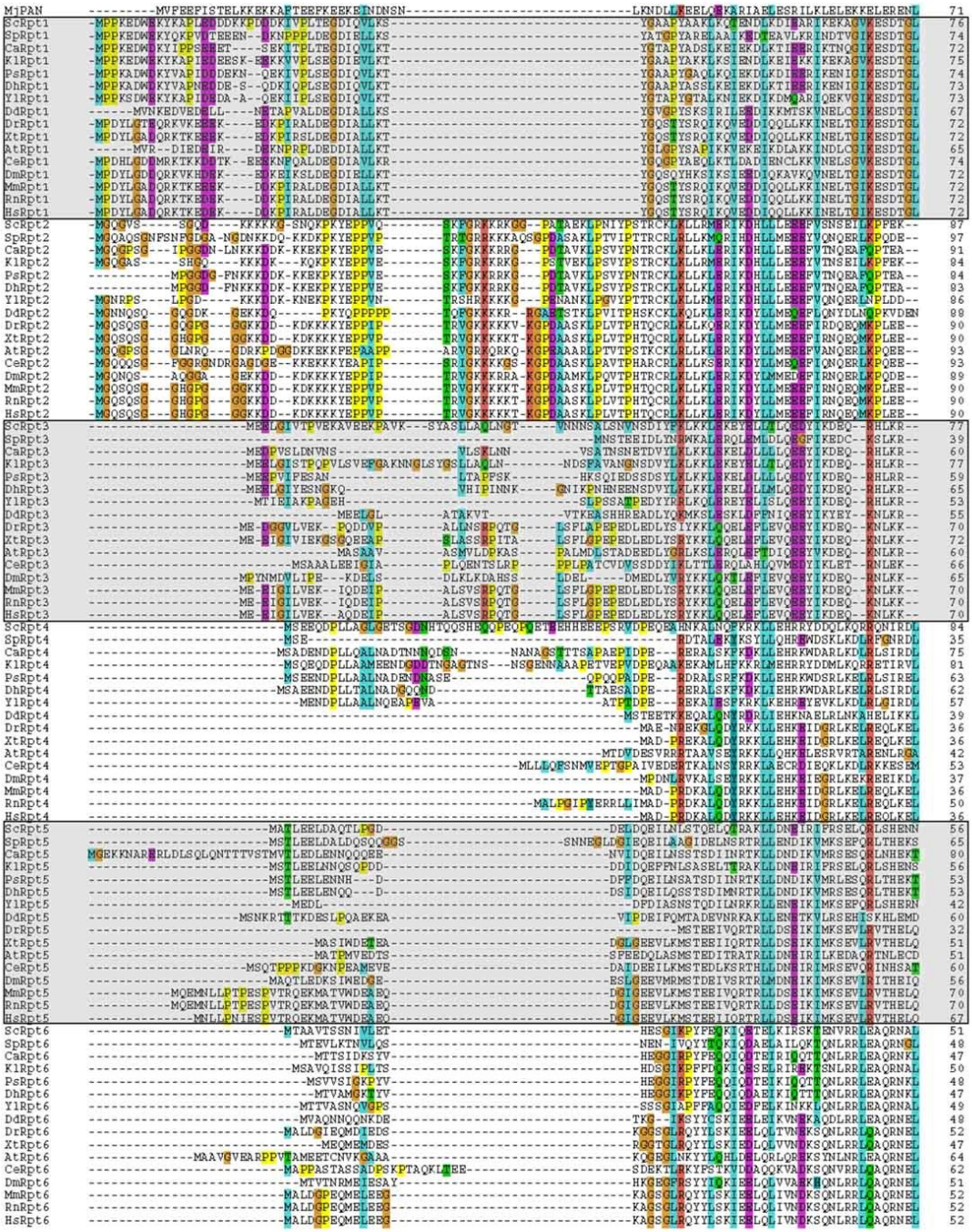
Supplementary Figure 2 The interdimer interface within subcomplex I. (A) Schematic representation of the interdimer interface between molecules B and C. Compared to the A-B interface, the interface between molecules B and C is considerably smaller, involving 820 $Å^2$ surface area. Formation of subcomplex I involves three interfaces of the A-B type and three interfaces of the B-C type. Together, these interactions involve 42 H-bonds and 9100 $Å^2$ surface area in subcomplex I of the PAN regulatory complex. (B) A stereo view of the interdimer interface. Side chains from molecules B and C are colored blue and magenta, respectively. H-bonds are represented by red dashed lines. There are 4 backbone H-bonds and a number of van der Waals contacts.

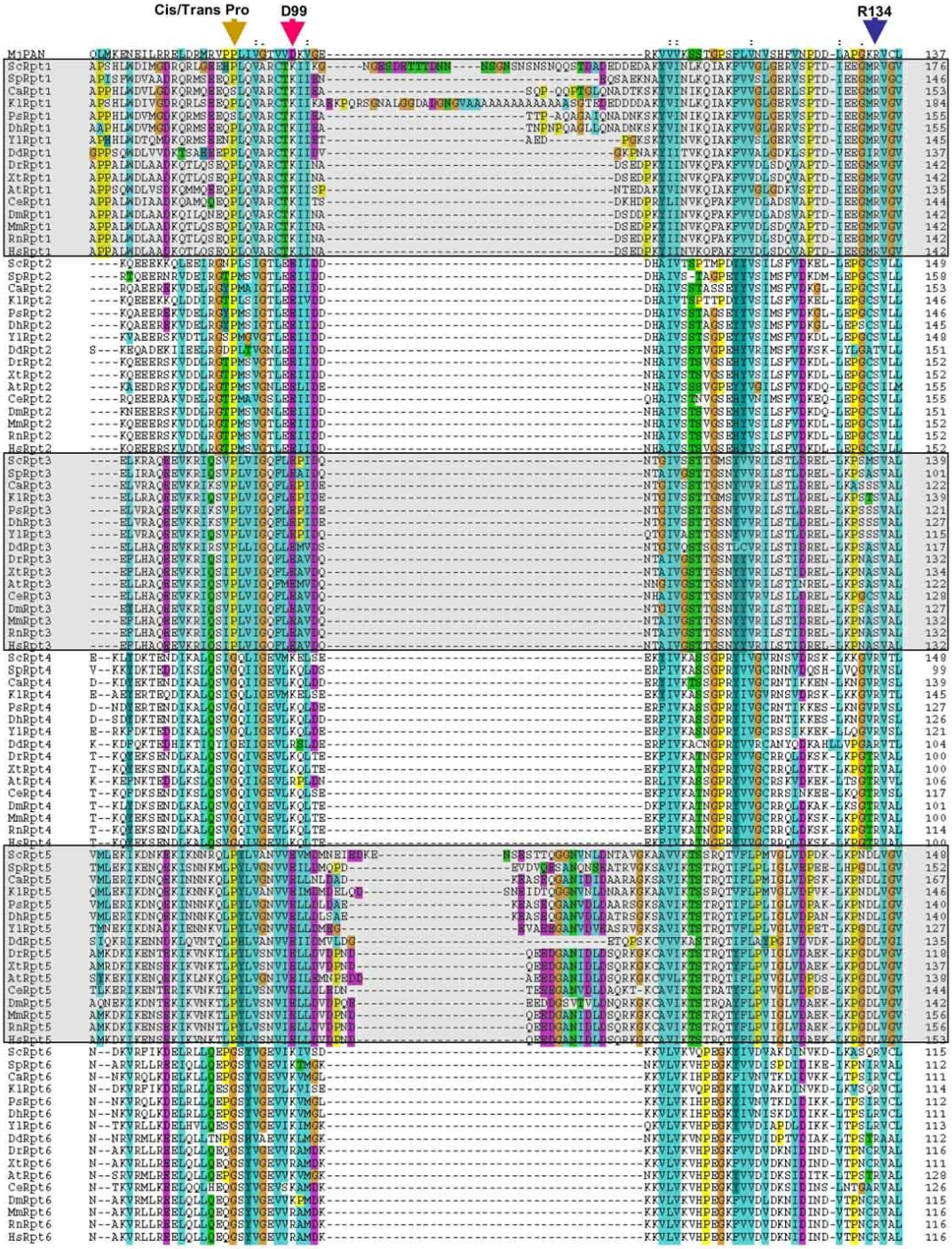
F) Supplemental Figure 3

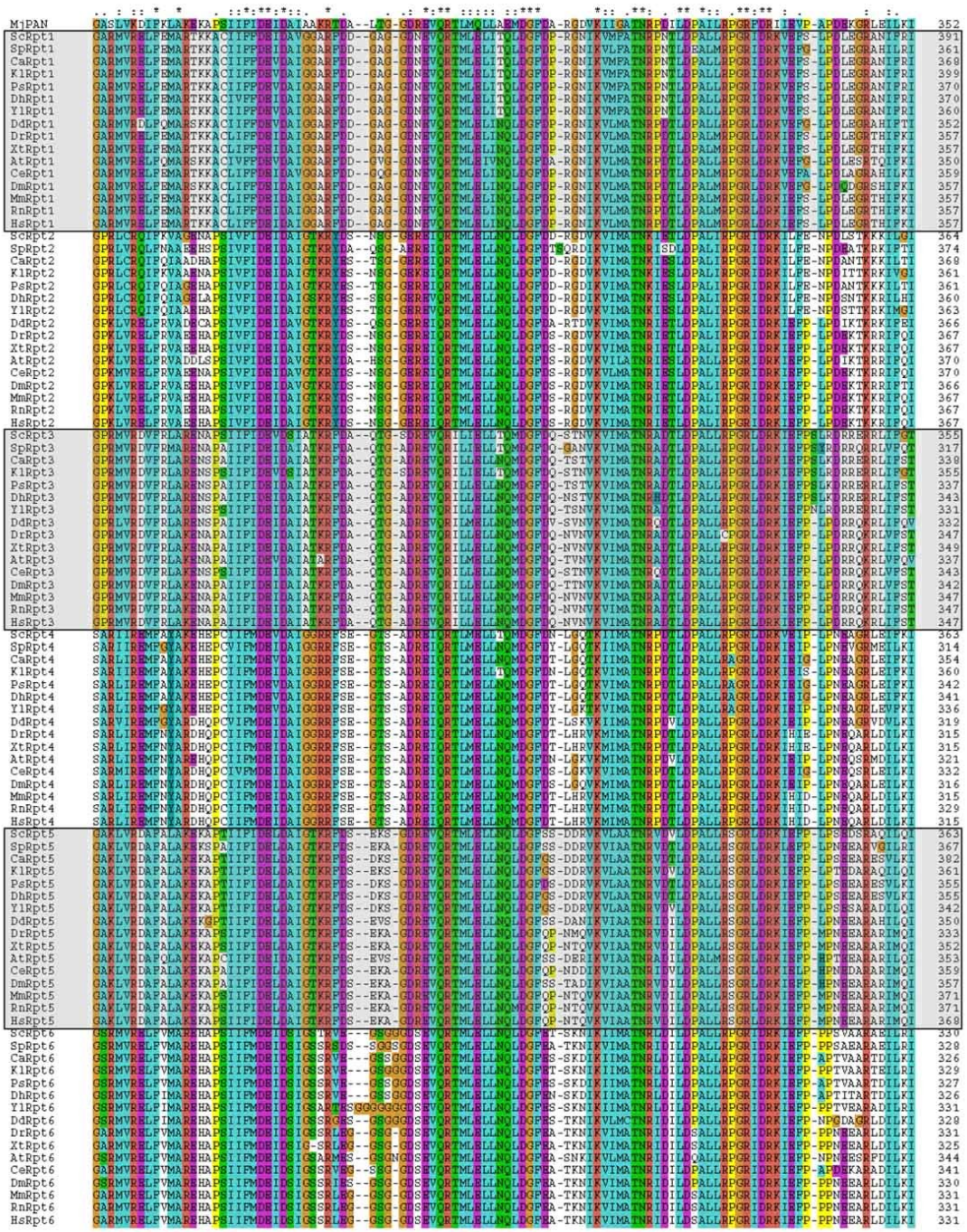


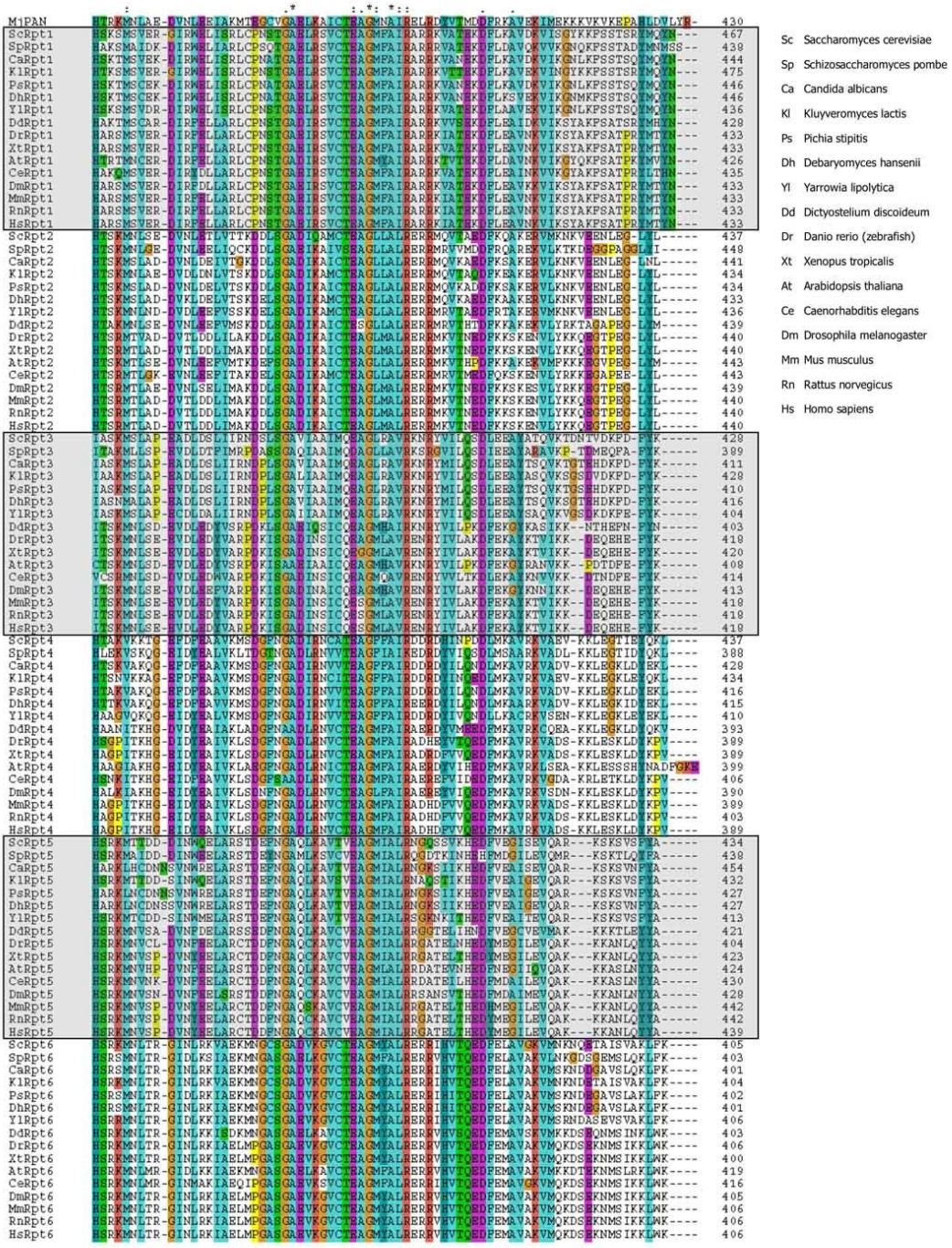
Supplementary Figure 3 Schematic representation of the three molecules of the PAN nucleotidase domain in each asymmetric unit. These three molecules are colored green, magenta, and cyan. The bound ADP molecules are colored red. Two perpendicular views are shown.

F) Supplemental Figure 4



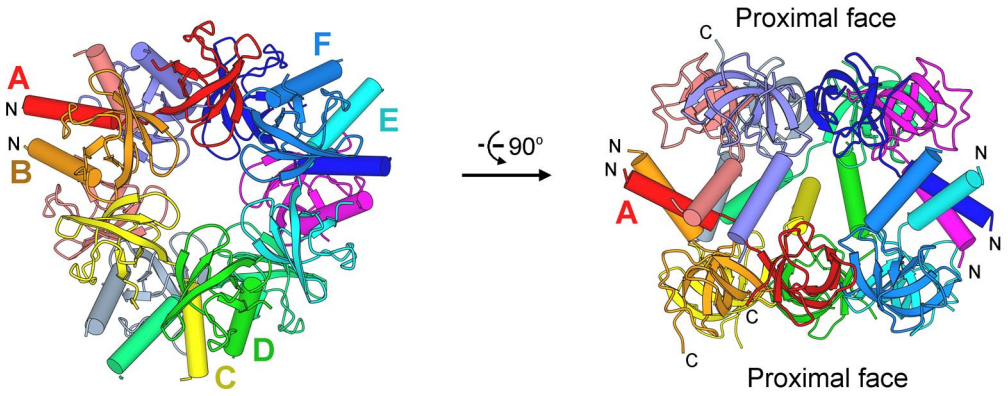

Cis/Trans Pro
D99
R134





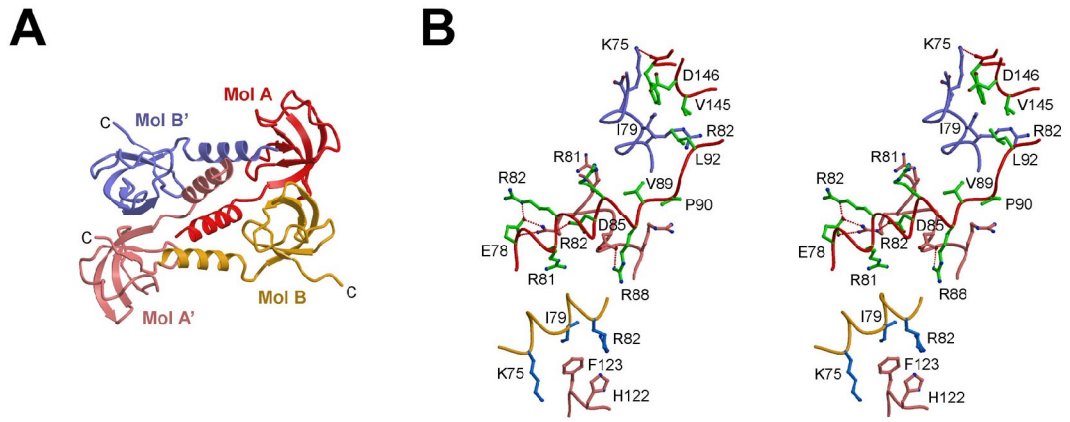
Supplementary Figure 4 Sequence alignment of Rpt subunits from 16 representative species. Sc: *Saccharomyces cerevisiae*; Sp: *Schizosaccharomyces pombe*; Ca: *Candida albicans*; Kl: *Kluyveromyces lactis*; Ps: *Pichia stipitis*; Dh: *Debaryomyces hansenii*; Yl: *Yarrowia lipolytica*; Dd: *Dictyostelium discoideum*; Dr: *Danio rerio* (zebrafish); Xt: *Xenopus tropicalis*; At: *Arabidopsis thaliana*; Ce: *Caenorhabditis elegans*; Dm: *Drosophila melanogaster*; Mm: *Mus musculus*; Rn: *Rattus norvegicus*; Hs: *Homo sapiens*.

F) Supplemental Figure 5



Supplementary Figure 5 Subcomplex I in one asymmetric unit. Two copies of subcomplex I in each asymmetric unit form a cage-shaped structure**.** Two perpendicular views are shown here. Six CC-OB domains within the same subcomplex I are labeled A through F.

F) Supplemental Figure 6



Supplementary Figure 6 The interface between two molecules of subcomplex I. (A) Molecules A and B of subcomplex I interact with molecules A' and B' of an adjacent subcomplex I. Two copies of subcomplex I associate with each other through their respective coiled coils. The coiled coil from molecules A and B interacts with the coiled coil in molecules A' and B' as well as the β domain of molecule A'. (B) A stereo view of the interface. Side chains from molecules A and B are colored green and blue, respectively. Side chains from molecules A' and B' are colored pink and purple, respectively. H-bonds are represented by red dashed lines.