

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

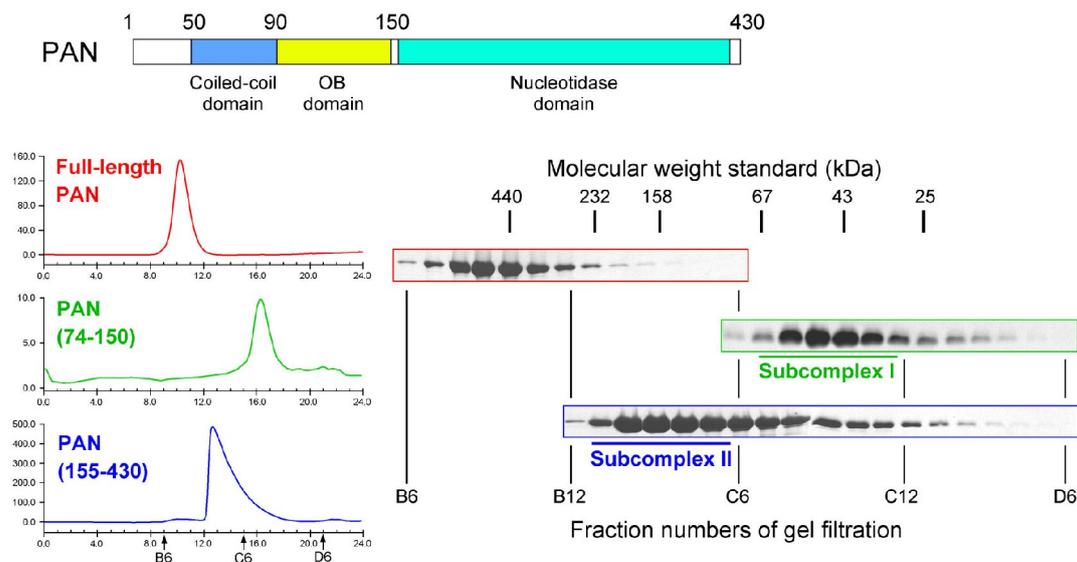
<u>Data collection</u>						
Data set	Se1 peak	Se1 inflection	Se1 remote	Se2 peak	Se2 inflection	Se2 remote
Data Collection						
Wavelength (Å)	0.9791	0.9793	0.9641	0.9791	0.9792	0.9641
Resolution (Å)	50-2.70	50-2.70	50-2.70	50-2.10	50-2.10	50-2.10
Outer shell (Å)	2.80-2.70	2.80-2.70	2.80-2.70	2.18-2.10	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		
<hr/>						
<u>Refinement</u>						
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 (°)				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		

$R_{\text{sym}} = \frac{\sum_h \sum_i |I_{h,i} - I_h|}{\sum_h \sum_i I_{h,i}}$, where I_h is the mean intensity of the i observations of symmetry related reflections of h . $R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum F_{\text{obs}}}$, where $F_{\text{obs}} = F_p$, 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 Molprobit, which uses a tougher standard than Procheck.

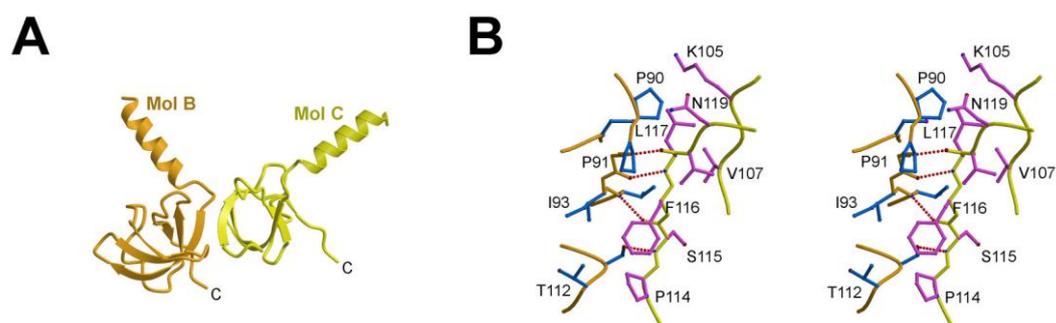
Supplementary Table 2. Summary of data collection and structure refinement for the nucleotidase domain and the CP.

<u>Data Collection</u>		
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)
<u>Refinement</u>		
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 (°)	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

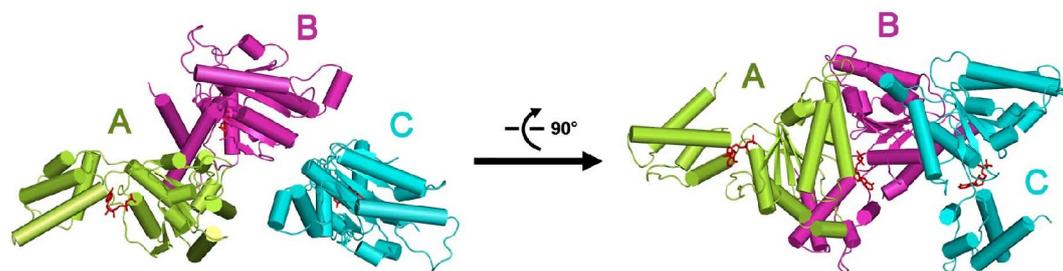
$R_{\text{sym}} = \frac{\sum_h \sum_i |I_{h,i} - I_h|}{\sum_h \sum_i I_{h,i}}$, where I_h is the mean intensity of the i observations of symmetry related reflections of h . $R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum F_{\text{obs}}}$, where $F_{\text{obs}} = F_p$, and F_{calc} is the calculated 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 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).



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 \AA^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 \AA^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.

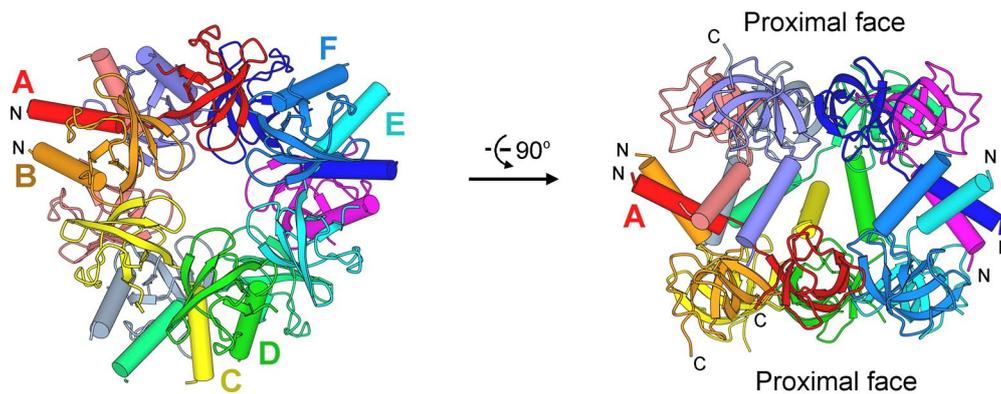


Supplementary Figure 3 Schematic representation of the three molecules of the PAN nucleotidase domain in each asymmetric unit. These three molecules are colored green, magenta, and cyan. The bound ADP molecules are colored red. Two perpendicular views are shown.

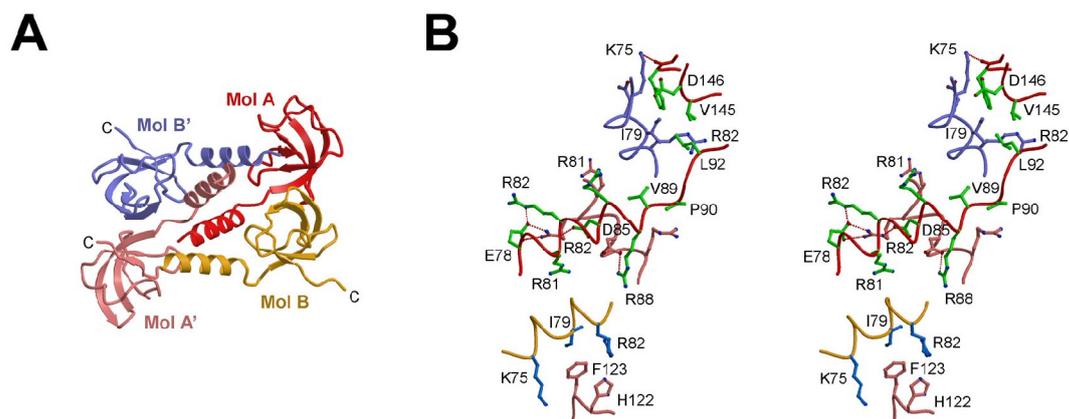
Cis/Trans Pro D99

R134

M1PAN	QINKENIILRRERDPMRVPDQVSTVAVKVGSR	RFVVVKSSTQPSFVNVSHFWNDD	LAPGKRVCI	137	
ScRpt1	APSHLMDIMRQRRLGHEPPLQVARCKIITG	NGRSDPVMVAVLN	MGNSNSNSNQSS	EDDEDAKVINLQIAKFPVVLGERVSPD	176
SpRpt1	APSPMDVAAIRQRMSRQPLQVARCKIITG			QSAEKNAIVINLQIAKFPVVLGERVSPD	146
CaRpt1	APPHLMDVLCRQRMSRQPLQVARCKIITG			SQP	153
K1Rpt1	APSHLMDVLRQRRLSREPLQVARCKIITG	KPQRSNALGGDA	GGVAAAAA	EDDDAKVINLQIAKFPVVLGERVSPD	134
PsRpt1	APPHLMDVMCRQRMSRQPLQVARCKIITG			TTP	155
DhRpt1	APSHLMDVMCRQRMSRQPLQVARCKIITG			TNPNQAGLL	155
Y1Rpt1	APSHLMDTQMKQRMSRQPLQVARCKIITG			ABD	145
DdRpt1	APPSMDLVVVKRSMRQPLQVARCKIITG			PKSKYVINVKQIAKFPVVLGERVSPD	137
DrRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DFNAKILITVKQIAKFPVVLGERVSPD	142
ZtRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DSBDPKIINVKQPAKFPVVLSDQVAFD	142
AtRpt1	APPSMDLVVVKRSMRQPLQVARCKIITG			NTEDAIVINVKQIAKFPVVLGERVSPD	135
CeRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DKHDFALINVKQPAKFPVVLSDQVAFD	144
DmRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DSDDPKIINVKQPAKFPVVLSDQVAFD	142
MmRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DSBDPKIINVKQPAKFPVVLSDQVAFD	142
RnRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DSBDPKIINVKQPAKFPVVLSDQVAFD	142
HsRpt1	APPALMDLAAIKQTLQSRQPLQVARCKIITG			DSBDPKIINVKQPAKFPVVLSDQVAFD	142
ScRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVSTPMPDMSVLSLSPVKKL	149
SpRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVS	158
CaRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVS	153
K1Rpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVSTPMPDMSVLSLSPVKKL	146
PsRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVS	146
DhRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVS	145
Y1Rpt2	---KQEEERKQLEBIRNPLSITGLEIITD			DHAIVS	148
DdRpt2	S---KQADKXILEBIRNPLSITGLEIITD			NHAIVS	151
DrRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	152
ZtRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	153
AtRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	155
CeRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	155
DmRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	151
MmRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	152
RnRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	152
HsRpt2	---KQEEERKQLEBIRNPLSITGLEIITD			NHAIVS	152
ScRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	139
CaRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	122
K1Rpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	139
PsRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	121
DhRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	127
Y1Rpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	115
DdRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	117
DrRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	104
ZtRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	134
AtRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	122
CeRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NHAIVSSTTMSNVVRLSILRE	120
DmRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	127
MmRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	132
RnRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	132
HsRpt3	---ELVRAQHEVVKRISVPLVIGQPLAIPIDE			NTGIVSSTTMSNVVRLSILRE	132
ScRpt4	E-KLIDKTEINDIKALSVGQIIGEVVKQLTE			EKPIVKA	148
SpRpt4	V-KKIDKTEINDIKALSVGQIIGEVVKQLTE			ERP	99
CaRpt4	D-KIDKTEINDIKALSVGQIIGEVVKQLTE			ERL	139
K1Rpt4	E-ABERTQDIDKALSVGQIIGEVVKQLTE			EKPIVKA	145
PsRpt4	D-NDERTENDIKALSVGQIIGEVVKQLTE			ERP	127
DhRpt4	D-SIDKTEINDIKALSVGQIIGEVVKQLTE			ERP	126
Y1Rpt4	E-RKIDKTEINDIKALSVGQIIGEVVKQLTE			ERP	121
DdRpt4	K-KIDKTEINDIKALSVGQIIGEVVKQLTE			ERP	104
DrRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	100
ZtRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	100
AtRpt4	K-KENKTEINDIKALSVGQIIGEVVKQLTE			ERL	106
CeRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	117
DmRpt4	T-KLIDKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	101
MmRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	100
RnRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	114
HsRpt4	T-KQEKSENDIKALSVGQIIGEVVKQLTE			EKPIVKA	100
ScRpt5	VMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			NSSTTQGGVNL	148
SpRpt5	TMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			EVDV	152
CaRpt5	VMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			KBAS	167
K1Rpt5	QMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			SNE	146
PsRpt5	VMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			KBAS	140
DhRpt5	VMLERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			KBAS	140
Y1Rpt5	TMNERIKDNKFKIKNNKQLPVLVNVVILMDDLRB			VVA	127
DdRpt5	SIQKRIKENNKFKIQNTQCPVLVNVVILMDDLRB			ETQSKCVVKA	135
DrRpt5	AMKDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			QERD	110
ZtRpt5	AMRDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			QERD	137
AtRpt5	SIQKRIKENNKFKIKNNKQLPVLVNVVILMDDLRB			AERD	130
CeRpt5	TLEKRIKENTRERIKNNKQLPVLVNVVILMDDLRB			TEBGA	144
DmRpt5	AMKDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			EEL	142
MmRpt5	AMKDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			QERD	156
RnRpt5	AMKDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			QERD	156
HsRpt5	AMKDKIKENNKFKIKNNKQLPVLVNVVILMDDLRB			QERD	153
ScRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	115
SpRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			NKVLV	112
CaRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	111
K1Rpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	114
PsRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	112
DhRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	111
Y1Rpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			QKVLV	113
DdRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			NKVLV	112
DrRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	116
ZtRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	111
AtRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			NKVLV	128
CeRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	126
DmRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	115
MmRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	116
RnRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	116
HsRpt6	N--AKVRLLELQLLRQESVGEVVRAMDK			FKVLV	116



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.



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.