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Supporting information for article:

Coiled-coil deformations in crystal structures: the measles virus phosphoprotein multimerization domain as an illustrative example

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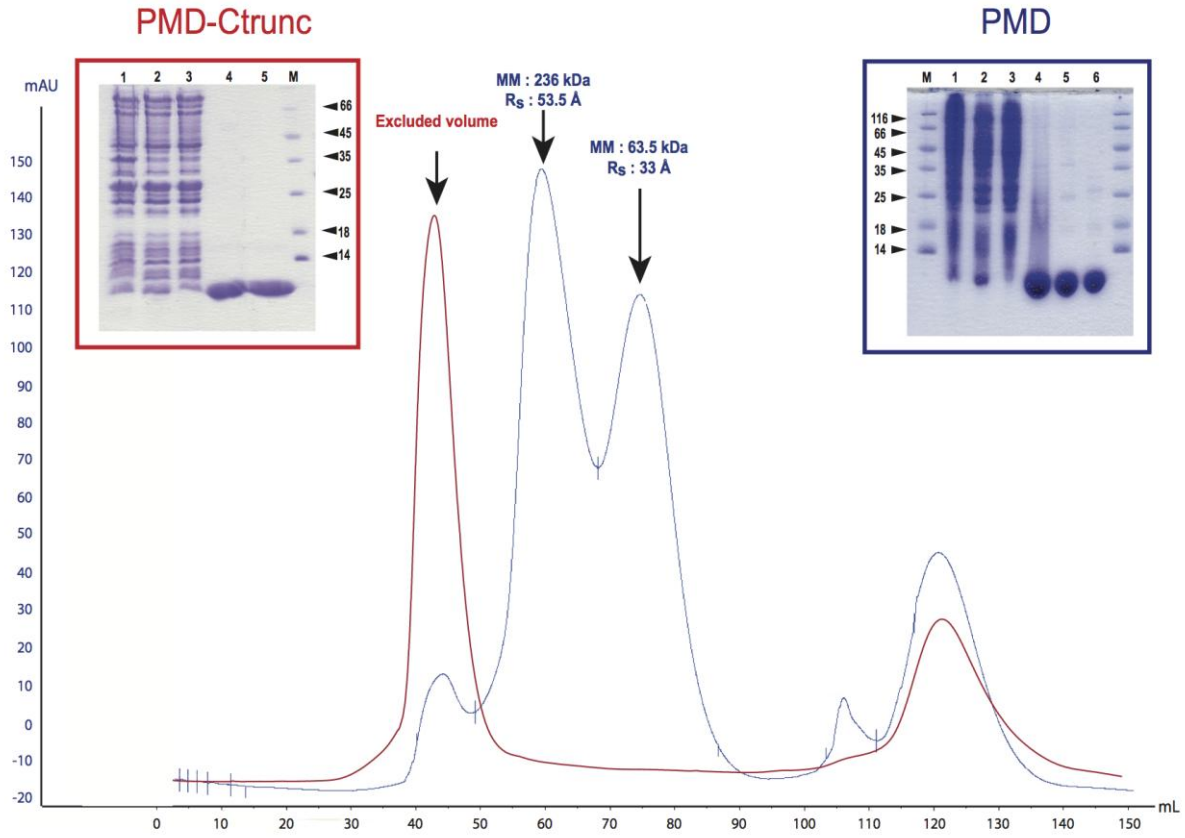


Figure S1 Size exclusion chromatography profile of MeV PMD loaded onto an S200 column. Gel filtration profiles are shown in red and blue for PMD-Ctrunc and PMD, respectively. The left and right insets show a Coomassie Blue staining of a 18% SDS-PAGE loaded with total fraction (lane 1), clarified cell lysate (lane 2), unbound fraction of the Ni-NTA column (lane 3), Ni-NTA elution (lane 4) and peaks 1 and 2 from the gel filtration column (lane 5 and 6 respectively). Molecular mass markers are indicated.

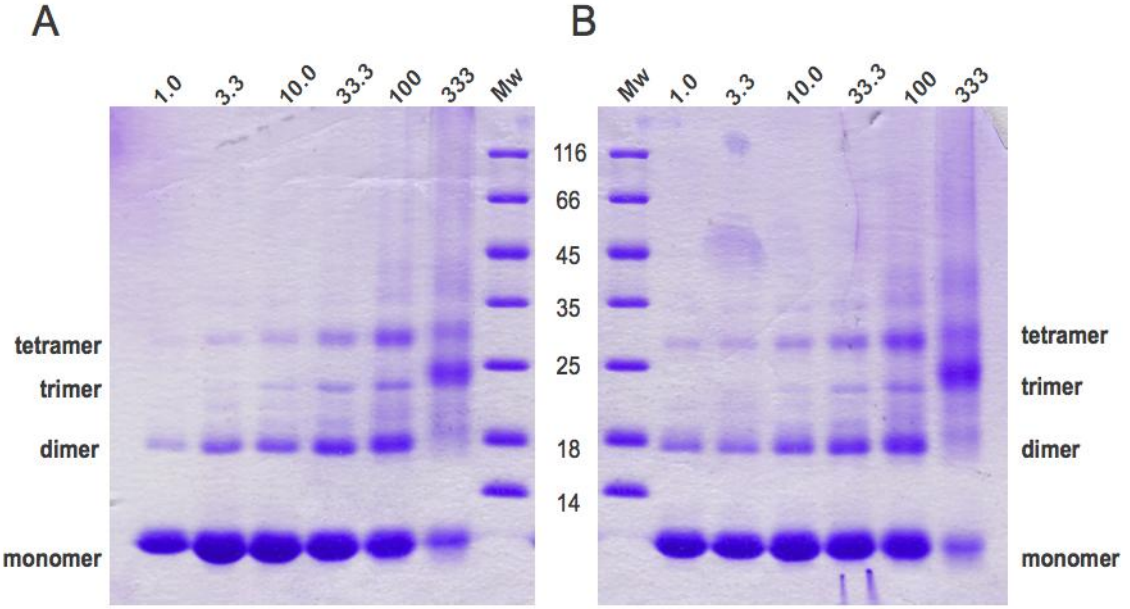
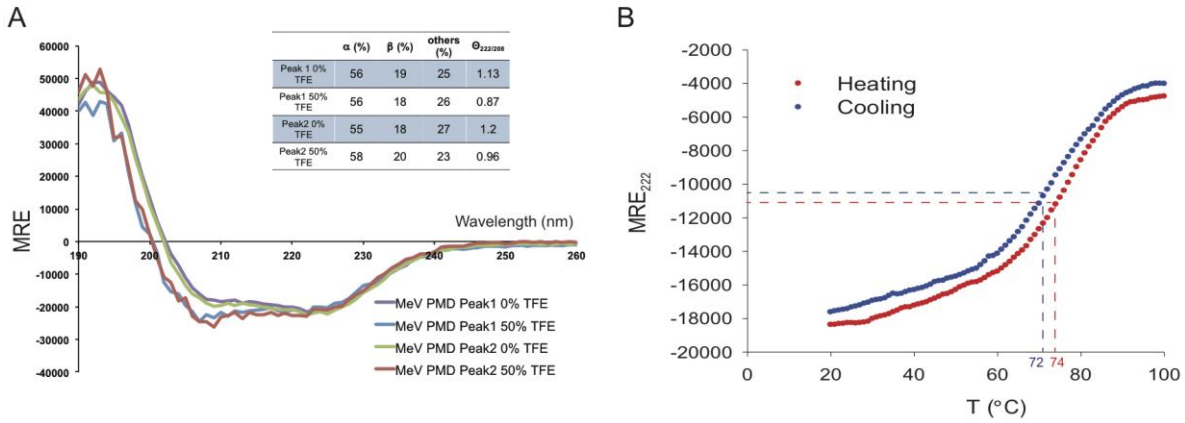


Figure S2 Cross-linking experiments of MeV PMD. Coomassie stained 18% SDS-PAGE showing the results of cross-linking with SAB (see Experimental Procedures) of peak 1 (A) and peak 2 (B). The concentration of SAB (μM) is indicated above the gel.



	α (%)	β (%)	others (%)	$\Theta_{222/208}$
Peak 1 0% TFE	56	19	25	1.13
Peak1 50% TFE	56	18	26	0.87
Peak2 0% TFE	55	18	27	1.2
Peak2 50% TFE	58	20	23	0.96

Figure S3 **Analysis of MeV PMD by far-UV circular dichroism. (A)** Far-UV CD spectra of MeV PMD peaks 1 and 2 at 0.1 mg/mL in 10 mM sodium phosphate pH 7 either in the absence or presence of 50% TFE at 20°C. Data are representative of one out of three independent acquisitions. The inset shows the relative secondary structure content along with the ellipticity ratio at 222 and 208 nm ($\Theta_{222/208}$). **(B)** Mean residue ellipticity at 222 nm (MRE_{222}) of MeV PMD peak 2 as a function of the T. Data are representative of one out of three independent experiments. Protein and buffer concentrations were the same as described above. The blue and red lines show the variation of MRE_{222} during heating and cooling, respectively.

Table S1 Knobs into holes analysis in all protomers of the three PMD structures

4BHV				4C5Q				3ZDO			
A	B	C	D	A	B	C	D	A	B	C	D
asp 314	asp 314	asp 314	asp 314			asp 314			asp 314	asp 314	asp 314
ile 318	ile 318	ile 318	ile 318	ile 318	ile 318	ile 318	ile 318	val 315			
leu 322	leu 322	leu 322	leu 322	leu 322	leu 322	leu 322	leu 322	ile 318	ile 318	ile 318	ile 318
ile 325	ile 325	ile 325	ile 325	ile 325	ile 325	ile 325	ile 325	leu 322	leu 322	leu 322	leu 322
asp 328	asp 328	asp 328	asp 328	his 326	his 326	his 326	his 326		ile 325	ile 325	ile 325
asn 329	asn 329	asn 329	asn 329	asp 328	asp 328	asp 328	asp 328		asp 328	asp 328	asp 328
ile 332	ile 332	ile 332	ile 332	asn 329	asn 329	asn 329	asn 329	asn 329	asn 329	asn 329	asn 329
ile 333	ile 333	ile 333	ile 333	ile 332	ile 332	ile 332	ile 332	ile 332	ile 332	ile 332	
lys 335	lys 335	lys 335	lys 335	ile 333	ile 333	ile 333	ile 333	ile 333		ile 333	ile 333
leu 336	leu 336	leu 336	leu 336	lys 335	lys 335	lys 335	lys 335		lys 335	lys 335	
		leu 339		leu 336	leu 336	leu 336	leu 336	leu 336	leu 336	leu 336	leu 336
val 346	val 346	val 346	val 346	val 346	val 346	val 346	val 346	leu 339	leu 339		
	ile 349	ile 349		ile 349	ile 349	ile 349	ile 349			lys 343	
	lys 350			lys 350		lys 350			glu 345		
	gln 352	gln 352		gln 352			gln 352	Val 346	val 346	val 346	val 346
ile 353	ile 353	ile 353	ile 353	ile 353	ile 353	ile 353	ile 353	ile 349	ile 349		ile 349
	gln 356							lys 350			
											gln 352
								ile 353	ile 353	ile 353	ile 353
								gln 356	gln 356	gln 356	gln 356
								asn 357		asn 357	
								ile 360	ile 360	ile 360	ile 360
								leu 363	leu 363	leu 363	leu 363
											glu 364
									his 366		leu 367