

Supplemental Information

An unusual dimeric structure and assembly for RP105/MD-1, a regulator for the TLR4 response to LPS

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Supplementary Table 1

Supplementary Figures 1-7

Supplementary Table 1. Data collection and refinement statistics

	sRP105-VLR/MD-1	sRP105/MD-1
Data Collection		
Space group	P 2 ₁ 2 ₁ 2 ₁	P 1
Cell parameters		
<i>a</i> , <i>b</i> , <i>c</i> (Å)	89.58, 137.52, 141.67	101.51, 141.58, 141.95
α , β , γ (°)	90, 90, 90	94.00, 91.66, 91.37
Wavelength (Å)	1.0718	1.0333
Resolution (Å)	20.00 - 3.10 (3.21-3.10)*	20.00 - 2.91 (3.00-2.91)
No. observations	261,804	332,433
No. unique reflections	32,274	160,125
<i>R</i> _{merge} (%)	9.0 (80.3)	6.3 (45.7)
<i>I</i> / σ <i>I</i>	34.3 (2.8)	18.2 (1.8)
Completeness (%)	98.9 (93.1)	93.5 (73.0)
Redundancy	8.1 (7.1)	2.1 (1.9)
Refinement		
Resolution (Å)		20.00 - 2.91
No. reflections (total / test)		152,067 / 8,030
<i>R</i> _{cryst} / <i>R</i> _{free} (%)		23.86 / 27.53
No. atoms		
Protein		42,570
Carbohydrate		1,064
Pseudoligand		124
Water		37
<i>B</i> -values (Å ²)		
Protein		76.4
Carbohydrate		49.4
Pseudoligand		81.8
Water		42.8
R.m.s. deviations		
Bond lengths (Å)		0.013
Bond angles (°)		1.44

*Numbers in parenthesis are for the highest resolution shell.

Supplementary References

1. Yoon, S.I., Hong, M., Han, G.W. & Wilson, I.A. Crystal structure of soluble MD-1 and its interaction with lipid IVa. *Proc Natl Acad Sci U S A* **107**, 10990-10995 (2010).
2. Harada, H., Ohto, U. & Satow, Y. Crystal structure of mouse MD-1 with endogenous phospholipid bound in its cavity. *J Mol Biol* **400**, 838-846 (2010).