

S1 Table. SAXS data collection, analysis and derived structural parameters

Construct	Ig1Ig2 ^{250-444*}	Ig1Ig2 ²⁵⁰⁻⁴⁹⁸	Ig1Ig2 ²²⁰⁻⁴⁵²	Trx-MYOT	Ig1Ig2 ^{220-452†}	Ig1Ig2 ^{220-452 R405K}
Data collection parameters						
Radiation source	ESRF (Grenoble, France)			DESY (Hamburg, Germany)		
			Doris		Petra III	
Beamline	BM29 BioSAXS		EMBL X33		EMBL P12	
Detector	Pilatus 1M		Pilatus 1M-W	Pilatus 2M	Pilatus 6M	
Beam geometry [mm, FWHM]	0.10 × 0.20		n.d.	0.12 × 0.20	0.12 × 0.20	
Wavelength [nm]	0.099		0.126	0.124	0.124	
Sample–detector distance [m]	2.867		2.7	3.1	3.0	
Momentum of transfer <i>s</i> range [nm ⁻¹]	0.04–4.0		0.1–6.0	0.08–3.5	0.15–7.3	
Exposure time [s]	15		15	1 (SEC-SAXS)	0.145	
Temperature [°C]	20		11	20	20	
Buffer	20 mM HEPES, 150 mM NaCl, 5% glycerol, 1 mM DTT, pH 7.4		20 mM MES, 200 mM NaCl, 3% glycerol, pH 6.0	20 mM Tris, 400 mM NaCl, 250 mM arginine, 5% glycerol, pH 7.5	20 mM HEPES, 150 mM NaCl, 5% glycerol, 1 mM DTT, pH 7.4	
Overall parameters						
Conc. range measured [§]	1–14.12 mg/ml (0.05–0.64 mM)	1–42.8 mg/ml (0.04–1.53 mM)	1–52 mg/ml (0.04–1.96 mM)	n.a.	2.1–36.6 mg/ml (0.08–1.38 mM)	2.3–45.5 mg/ml (0.09–1.72 mM)
R _g (Guinier) [Å]	28 (0.64 mM)	32 (0.54 mM) 37 (1.53 mM)	31 (0.04 mM) 37 (0.79 mM) 39 (1.96 mM)	51	30 (0.08 mM) 33 (0.19 mM) 33 (0.37 mM) 34 (0.69 mM) 36 (1.38 mM)	33 (0.09 mM) 34 (0.27 mM) 34 (0.47 mM) 35 (0.82 mM) 36 (1.72 mM)
R _g from PDDF [Å]	29 (0.64 mM)	34 (0.54 mM) 38 (1.53 mM)	32 (0.04 mM) 39 (0.79 mM) 41 (1.96 mM)	53	33 (0.08 mM) 34 (0.19 mM) 35 (0.37 mM) 37 (0.69 mM) 37 (1.38 mM)	34 (0.09 mM) 36 (0.27 mM) 36 (0.47 mM) 37 (0.82 mM) 38 (1.72 mM)
D _{max} [Å]	101 (0.64 mM)	140 (0.54 mM) 152 (1.53 mM)	107 (0.04 mM) 151 (0.79 mM) 152 (1.96 mM)	200	115 (0.08 mM) 125 (0.19 mM) 130 (0.37 mM) 140 (0.69 mM) 140 (1.38 mM)	120 (0.09 mM) 130 (0.27 mM) 140 (0.47 mM) 140 (0.82 mM) 140 (1.72 mM)
Molecular mass (RALLS) [kDa]	n.a.	n.a.	n.a.	70	n.a.	n.a.
Molecular mass (DATMOV) [kDa]	24.3 (0.64 mM)	31.2 (0.54 mM) 44.7 (1.53 mM)	27.3 (0.04 mM) 44.7 (0.79 mM) 58.1 (1.96 mM)	63.7	30.8 (0.08 mM) 30.7 (0.19 mM) 33.7 (0.37 mM) 37.8 (0.69 mM) 43.2 (1.38 mM)	29.1 (0.09 mM) 31.9 (0.27 mM) 35.6 (0.47 mM) 40.6 (0.82 mM) 45.7 (1.72 mM)

(continued)

(continued)

Construct	Ig1Ig2 ^{250-444*}	Ig1Ig2 ²⁵⁰⁻⁴⁹⁸	Ig1Ig2 ²²⁰⁻⁴⁵²	Trx-MYOT	Ig1Ig2 ^{220-452†}	Ig1Ig2 ^{220-452 R405K}
Molecular mass from Porod	21.4 (0.64 mM)	26.4 (0.54 mM)	27.5 (0.04 mM)	77.3	26.9 (0.08 mM)	24.5 (0.09 mM)
volume [kDa]		37.9 (1.53 mM)	36.7 (0.79 mM)		25.9 (0.19 mM)	26.3 (0.27 mM)
			48.2 (1.96 mM)		28.3 (0.37 mM)	29.6 (0.47 mM)
					30.9 (0.69 mM)	33.6 (0.82 mM)
					36.2 (1.38 mM)	38.2 (1.72 mM)
Molecular mass (monomer sequence) [kDa] ^{&}	21.9	28.0	26.5	69.7	26.5	26.5
Software employed						
Primary data red.	SaxsAnalysis pipeline system			SASFLOW	SaxsAnalysis pipeline system	
Data processing	PRIMUS			PRIMUS / Cromixs	PRIMUS	
Calculation and comparison of scattering data	Crysol / Oligomer				n.a.	
<i>Ab initio</i> modelling	DAMMIF				n.a.	
Addition of missing residues	CORAL				n.a.	
Ensemble modelling	EOM				n.a.	
SASDB accession code	SASDF38	SASDF48	SASDF28	SASDFZ7	SASDJH8	SASDJJ8

^{*}, the data for Ig1Ig2²⁵⁰⁻⁴⁴⁴ were already measured and described previously [23]

[§], for Ig1Ig2²⁵⁰⁻⁴⁹⁸ and Ig1Ig2²²⁰⁻⁴⁵² structural parameters at various concentrations, relevant for the comparison, were calculated separately

[&], Molecular mass (monomer sequence) denotes molecular mass calculated from the amino acid sequence of the monomeric species

[†], measured at the same experimental settings/conditions as Ig1Ig2^{220-452 R405K}