Supplementary Data

MONOMERIC HUMAN SOLUBLE CD4 DIMERIZES AT PHYSIOLOGICAL TEMPERATURE: SAXS DATA BASED MODELING AND SCREENING OF RETARDANT MOLECULES

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Supplementary Information Attached with this manuscript are:

Supplementary Table S1 Main programs and shape information which was employed to acquire and analyze SAXS data from about 1 mg/ml samples of sCD4 -/+ molecules and matched buffer are tabulated below.

Supplementary Figure S1

Crystal structures of 1WIO vs. 5U1F and 1WIO vs. 3T0E are shown to highlight non-involvement of second chain of sCD4 in interactions as perceived from these crystal structures.

Supplementary Figure S2

The surface and pocket in D4 and D1 domain, respectively have been shown which were used to dock drug molecules.

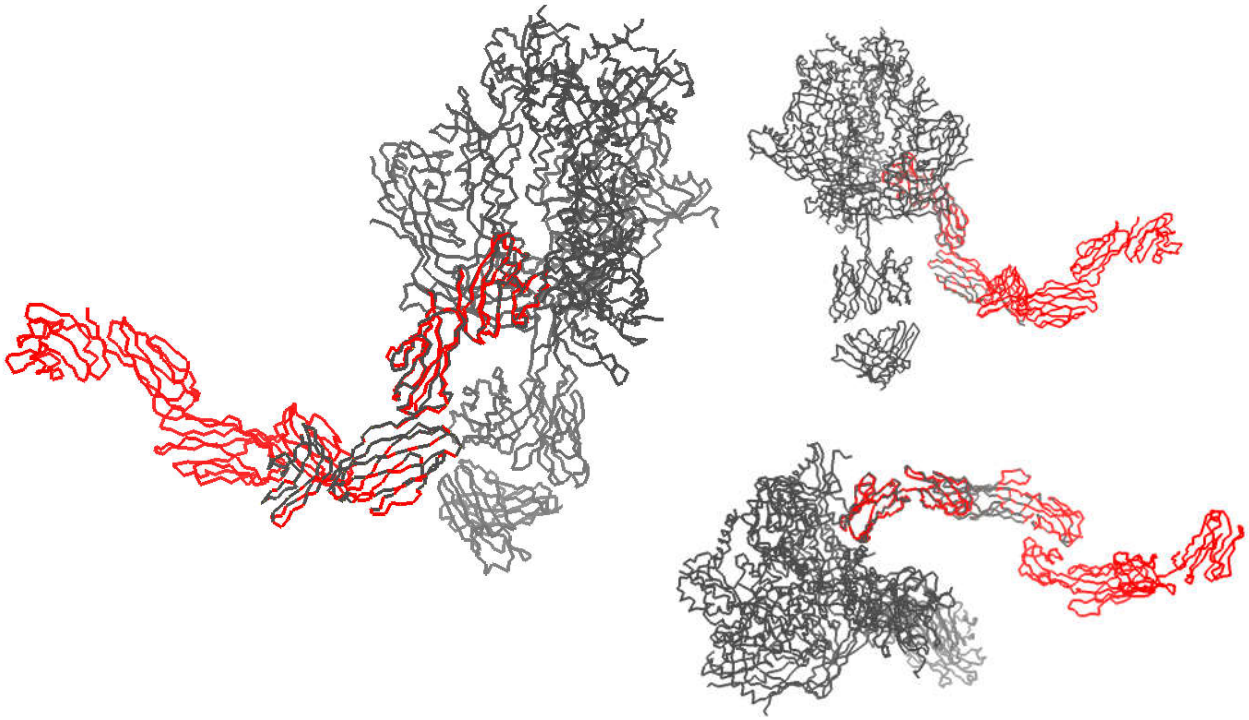
Supplementary Table S1

Main programs and shape parameters which were employed to acquire and analyze SAXS data from about 1 mg/ml samples of sCD4 -/+ molecules and matched buffer are mentioned below.

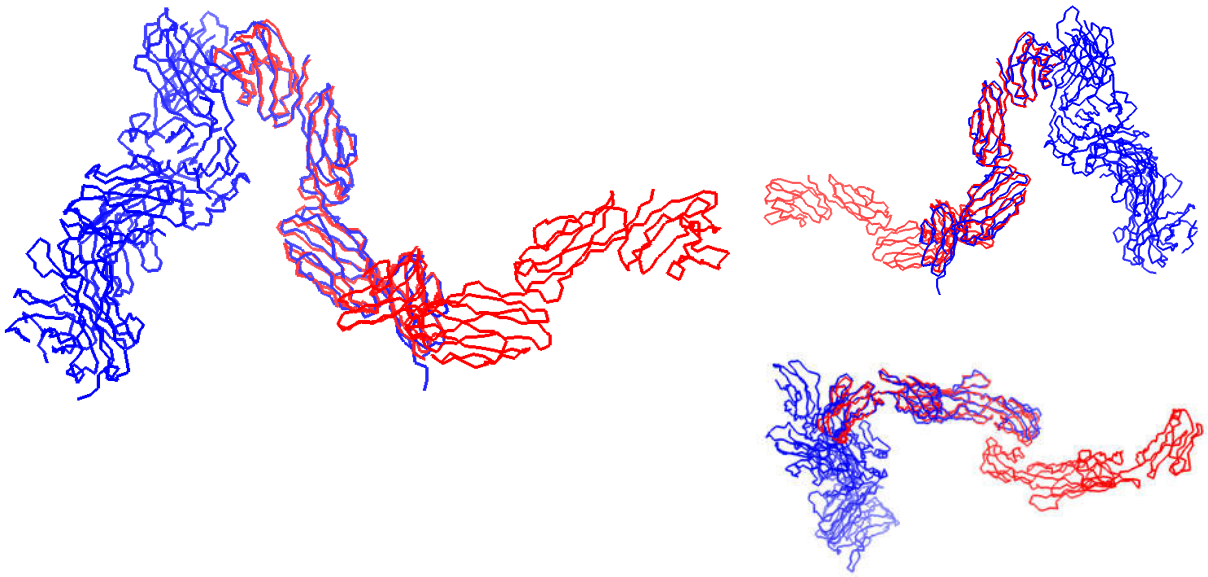
Details	**Information**
SAXS Data Acquisition	
Instrument	SAXSpace (Anton Paar) (At CSIR-IMTECH)
Collimation	Line
Wavelength (nm)	0.154
q range (1/nm) obtained	0.08 – 5
Corresponding real space ($q = 4\pi(\sin\theta/\lambda)) \rightarrow r = 2\pi/q$	78.5 to 1.25 nm
Exposure time	60 minutes (Frame of one)
Temperature	283 to 343 K
Heating/Cooling Gradient	3 K/minute
Holding time at each temperature	1 minute
Programs	
Data Collection Controls	SAXSDrive
Beam position correction	SAXSTreat
Buffer subtraction	SAXSQuant
Desmearing	SAXSQuant
Data Analysis	
All parameter analysis	SAS Data Analysis (ATSAS v 3.0.1) Guinier Analysis, Distance Distribution, Molecular Weight Estimation
Shape Restoration	Online SASREF program to position crystal structure of sCD4 (one chain) into dimeric state using SAXS profile
Inertial Alignment	SUPALM (Pymol), Supcomb (Command Line)
Theoretical SAXS calculation	Online CRYSOL
Normal Mode Analysis with SAXS Profile	Online SREFLEX
3D Graphics	PyMol

Supplementary Figure S1

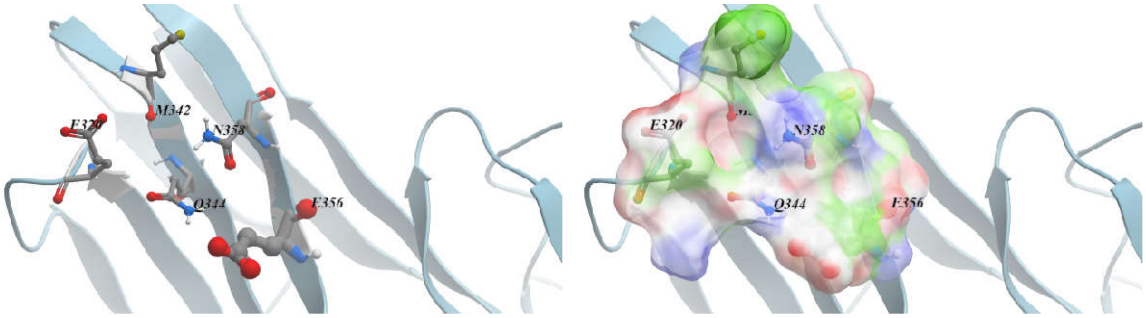
Comparison of 1WIO vs. 5U1F [sCD4 is overlaid in both structures]



Comparison of 1WIO vs. 3T0E [sCD4 is overlaid in both structures]



Supplementary Figure S2
Pocket identified to dock molecules on interacting surface of D4 domain



Pocket identified to dock molecules on apex of D1 domain