

Supplementary Material

Structural characterization of the full-length anti-CD20 antibody rituximab

**Benny Danilo Belviso¹, Giuseppe Felice Mangiatordi¹, Domenico Alberga², Vincenzo Mangini¹,
Benedetta Carrozzini¹, Rocco Caliandro^{1*}**

¹Institute of Crystallography, CNR, Bari, Italy

²Cineca, Casalecchio di Reno, Italy

*** Correspondence:**

Corresponding Author: rocco.caliandro@ic.cnr.it

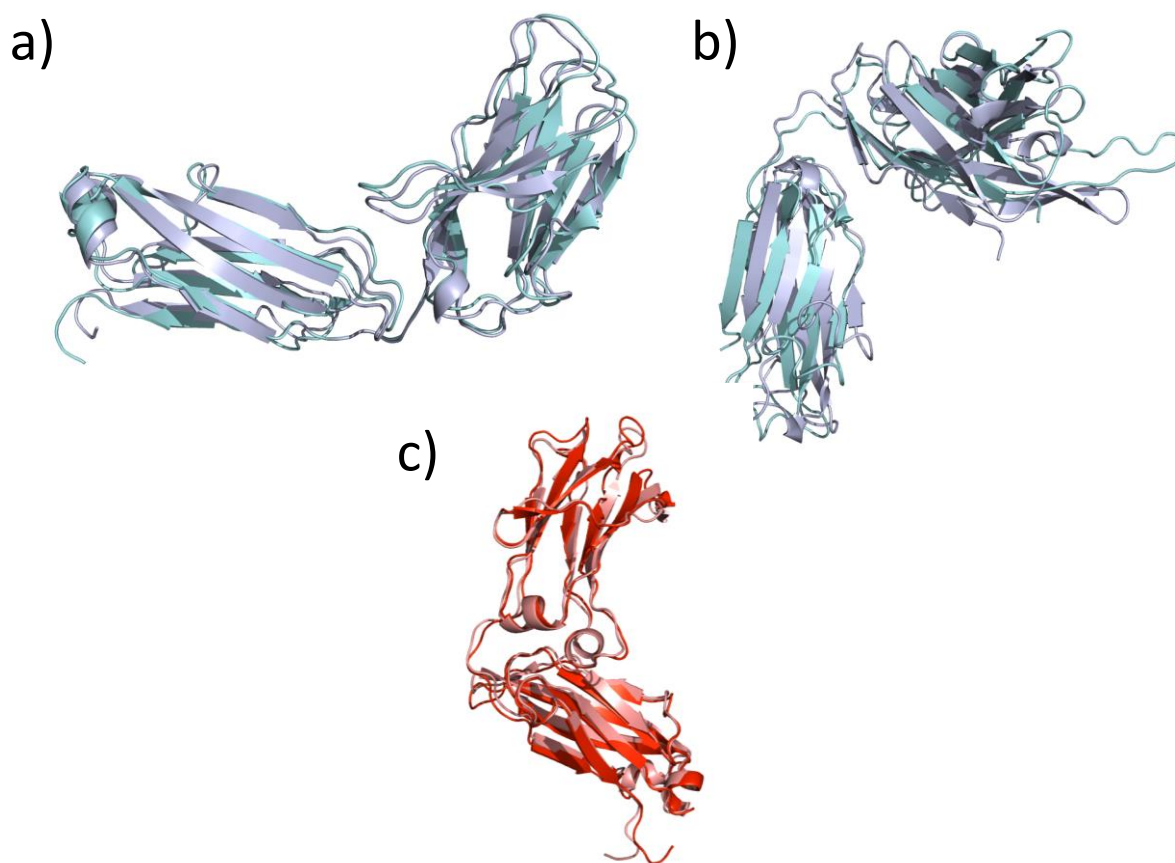


Figure S1. Superposition between the machine learning (lilac and light red) and the homology modelling (cyan and dark red) predictions of the light chain (a), Fab portion heavy chain (b) and Fc portion heavy chain (c).

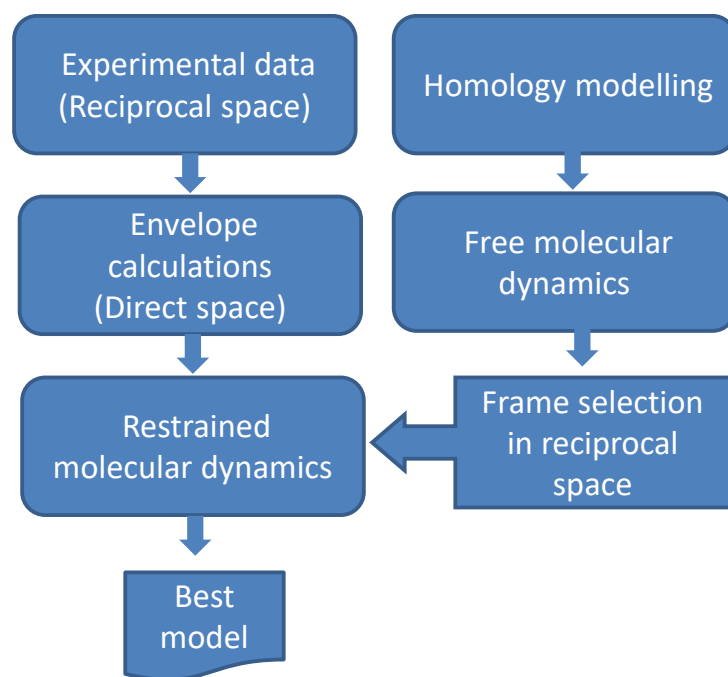


Figure S2. Scheme of the experimental data analysis integrated with computational modelling. Best model is obtained from SAXS data as a result of a procedure that uses experimental information in reciprocal (SAXS radial profiles) and direct (SAXS envelopes) space.

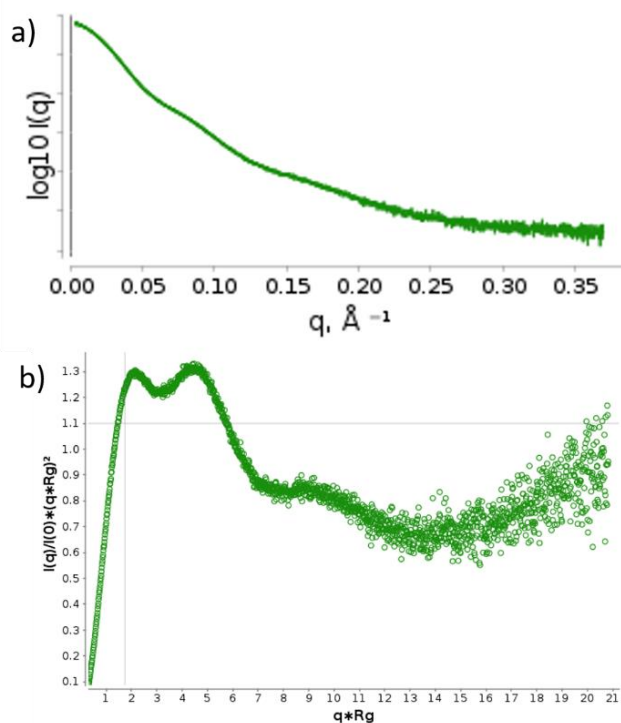
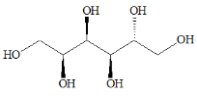
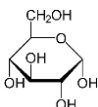
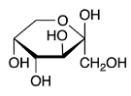
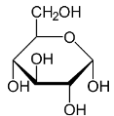
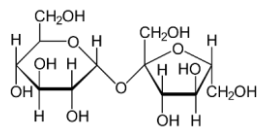
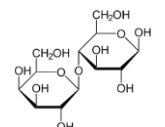
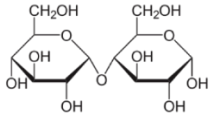
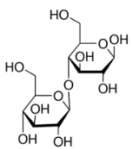


Figure S3. Logarithmic profile (a) and normalized Kratky plot (b) from SAXS measurements on rituximab. The position of the peak expected for compact globular scatters is shown by thin horizontal and vertical lines.

Table S1. Additives tested in solutions containing Rituximab.

Code	Extended name	IUPAC name	Properties
MPD	MPD	2-Methylpentane-2,4-diol	Surfactant and emulsion-stabilizer
ETO	EtOH	Ethanol	Alcohol naturally produced by the fermentation of sugars
BET	Betaine	(Trimethylazaniumyl)acetate	Amino acid derivative occurring in plants
SOB	Sorbitol	(2S,3R,4R,5R)-Hexane-1,2,3,4,5,6-hexol	Sugar alcohol
PRO	Proline	Pyrrolidine-2-carboxylic acid	Proteinogenic amino acid
TAU	Taurine	2-Aminoethane-1-sulfonic acid	Antioxidant, osmoregulator, membrane stabilizer
SAC	Saccharose	β -D-Fructofuranosyl α -D-glucopyranoside	Disaccharide
TWE	Polysorbate 80	Polyoxyethylene (20) sorbitan monooleate	Non-ionic surfactant and emulsifier

Table S2. Sugars of different complexity tested in solutions containing Rituximab.

Name	Type	Chemical formula	Chemical structure
Sorbitol	Monosaccharides	$C_6H_{14}O_6$	
Glucose	Monosaccharides	$C_6H_{12}O_6$	
Fructose	Monosaccharides	$C_6H_{12}O_6$	
Galactose	Monosaccharides	$C_6H_{12}O_6$	
Sucrose	Disaccharides	$C_{12}H_{22}O_{11}$	
Lactose	Disaccharides	$C_{12}H_{22}O_{11}$	
Maltose	Disaccharides	$C_{12}H_{22}O_{11}$	
Cellobiose	Disaccharides	$C_{12}H_{22}O_{11}$	
Raffinose	Trisaccharides	$C_{18}H_{32}O_{16}$	