Indones. J. Chem., 2022, 22 (2), 515 - 525

Suppl. **1**

Supplementary Data

This supplementary data is a part of paper entitled "Computational Design of Nanobody Binding to Cortisol to Improve Their Binding Affinity Using Molecular Docking and Molecular Dynamics Simulations".
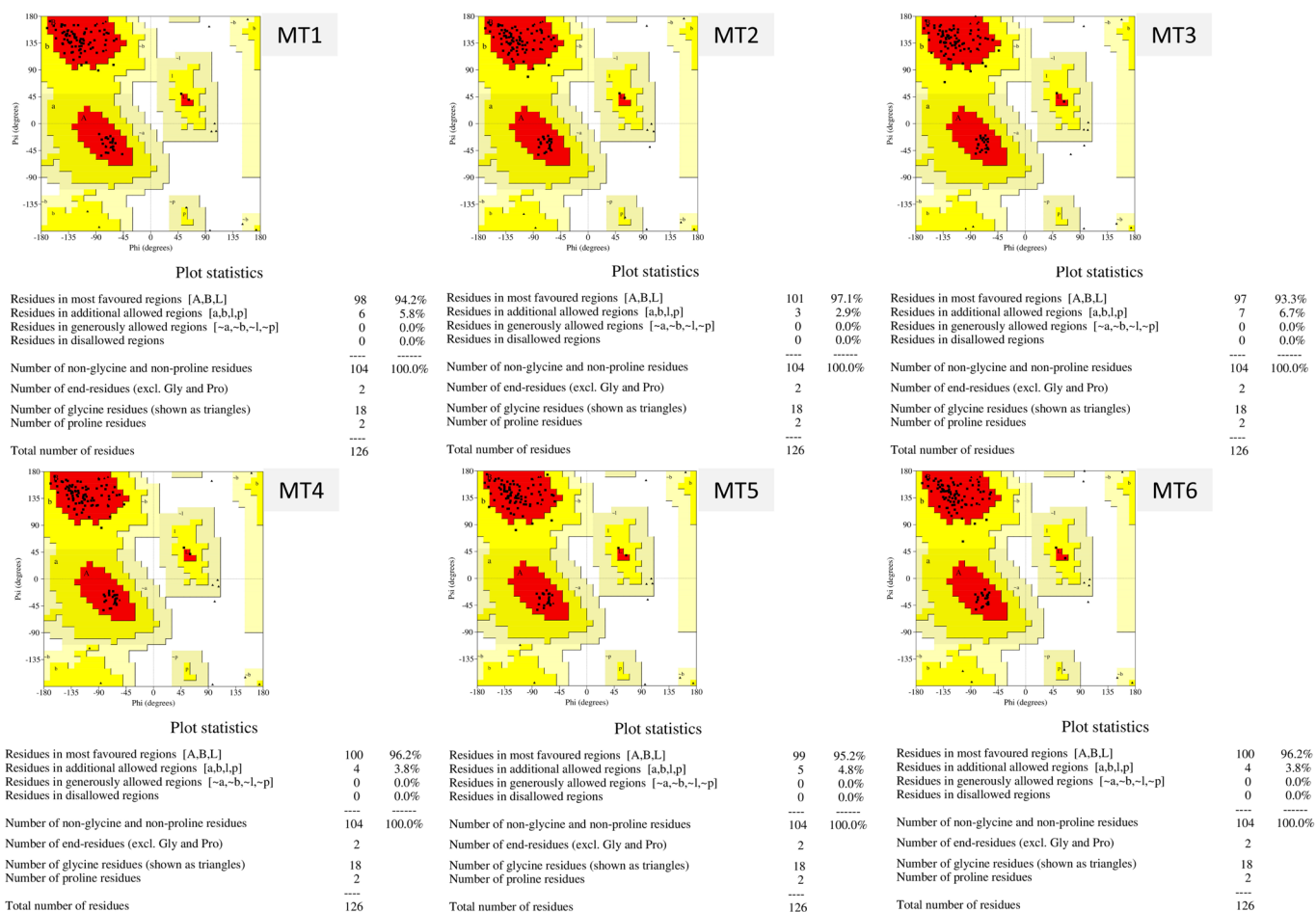

Plot statistics

	MT1			MT2			MT3	
Residues in most favoured regions [A,B,L]	98	94.2%	101	97.1%	97	93.3%
Residues in additional allowed regions [a,b,l,p]	6	5.8%	3	2.9%	7	6.7%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%	0	0.0%	0	0.0%
Residues in disallowed regions	0	0.0%	0	0.0%	0	0.0%
Number of non-glycine and non-proline residues	104	100.0%	104	100.0%	104	100.0%
Number of end-residues (excl. Gly and Pro)	2		2		2	
Number of glycine residues (shown as triangles)	18		18		18	
Number of proline residues	2		2		2	
Total number of residues	126		126		126	

Plot statistics

	MT4			MT5			MT6	
Residues in most favoured regions [A,B,L]	100	96.2%	99	95.2%	100	96.2%
Residues in additional allowed regions [a,b,l,p]	4	3.8%	5	4.8%	4	3.8%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%	0	0.0%	0	0.0%
Residues in disallowed regions	0	0.0%	0	0.0%	0	0.0%
Number of non-glycine and non-proline residues	104	100.0%	104	100.0%	104	100.0%
Number of end-residues (excl. Gly and Pro)	2		2		2	
Number of glycine residues (shown as triangles)	18		18		18	
Number of proline residues	2		2		2	
Total number of residues	126		126		126	

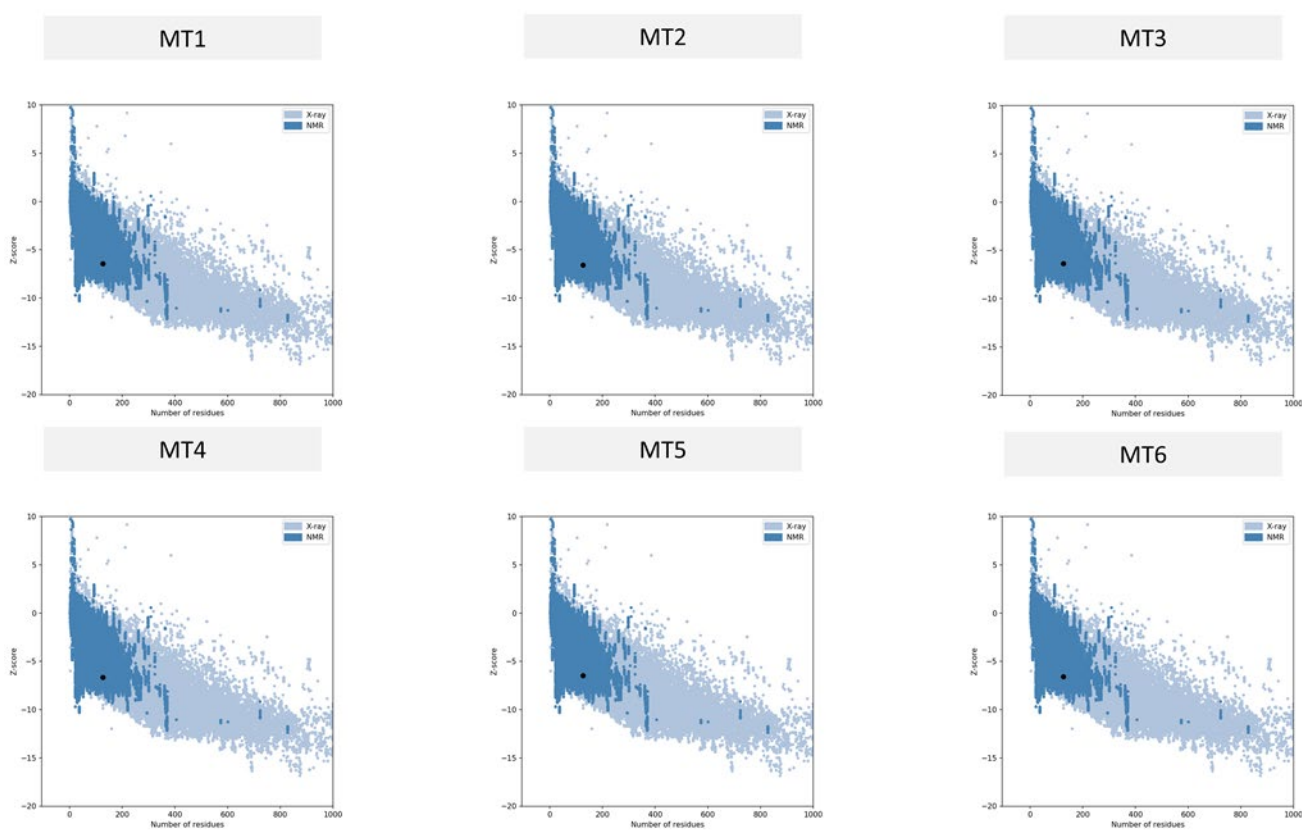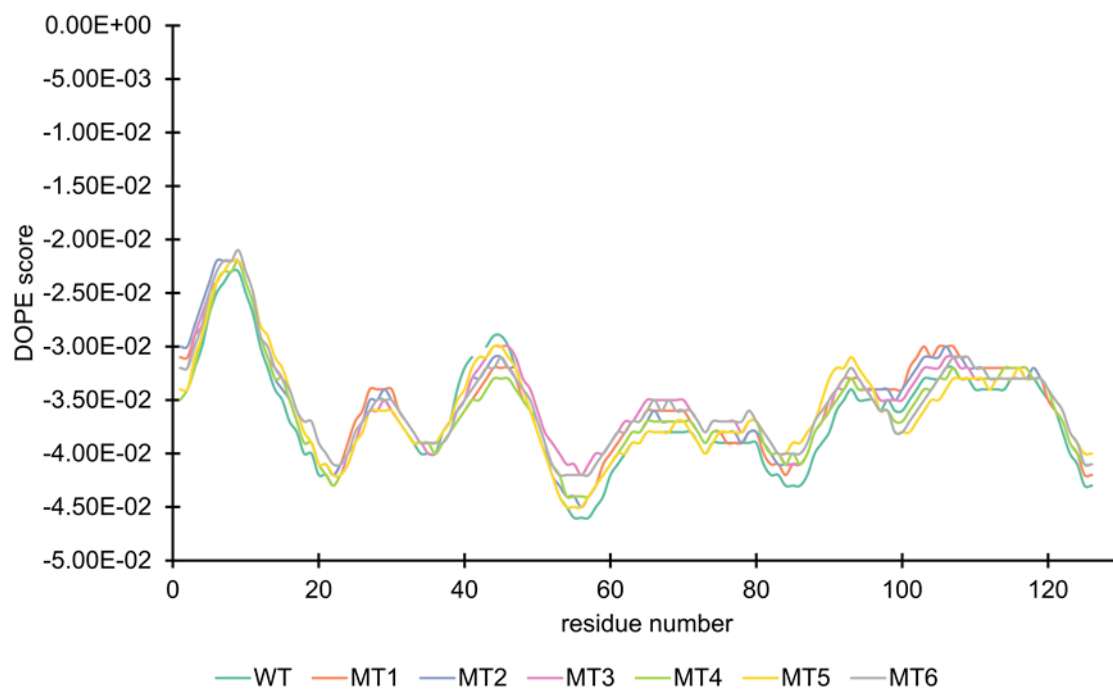**Fig S1.** Ramachandran plot of all models

Fig S2. Z-score off all models

Fig S3. DOPE score of all models and template