STRUCTURAL
BIOLOGY

Volume 72 (2016)

Supporting information for article:

Re-evaluation of low-resolution crystal structures via interactive molecular-dynamics flexible fitting (iMDFF): a case study in complement C4

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Table S1 Re-refinement statistics for high-resolution reference models used in C4:MASP-2 refinement

	1q3x	1zjk
Resolution range (Å)	35.58-2.23 (2.31-2.23)	27.97-2.181 (2.259-2.181)
Completeness (%)	95	88
No. of reflections, working set	27014(2359)	18326(924)
No. of reflections, test set	1356(114)	938(45)
Final R_{cryst}	0.1743(0.1991)	0.1901(0.3052)
Final R_{free}	0.2197(0.2634)	0.2260(0.3428)
No. of non-H atoms		
Protein	4885	2991
Ion	2	0
Ligand	42	0
Water	391	104
Total	5320	3095
R.m.s. deviations		
Bonds (Å)	0.003	0.003
Angles (°)	0.59	0.57
Average *B* factors (Å^2)		
Protein	28.19	51.18
Ion	25.04	N/A
Ligand	28.00	N/A
Water	28.21	45.30
Ramachandran plot		
Most favoured (%)	97	95
Allowed (%)	2.9	4.7
Rotamer outliers (%)	0.58	0.94
Clashscore	4.03	2.39
MolProbity Score	1.35	1.34
Number of TLS groups	0	3