

## Supplementary Material.

**Table I.** LCPO parameters. The four parameters ( $P1, P2, P3, P4$ ) employed in the LCPO method are shown. Parameters were derived from a database of 81 proteins by multiple linear regression fitting using equation 7, with solvent surface accessible areas obtained with the analytical method available within the TINKER package (<http://dasher.wustl.edu/tinker/>) as independent variable. The number of atoms employed in the fitting for each atom type, together with the mean and maximum error per atom upon fitting, are also shown.

Atom Type	Bonded Neighbors	# of atoms	$P1$	$P2$	$P3$	$P4$	Mean (max) error in $\text{\AA}^2$ per atom
<b>C sp3</b>	1	11517	0.30742	-0.06915	-1.10E-04	6.70E-05	1.46 (36.86)
	2	22605	0.16897	-0.04215	-6.23E-05	4.28E-05	1.36 (20.34)
	3	21233	0.01408	-0.00283	3.45E-06	1.90E-06	0.12 (6.53)
	4	60	0.18207	-0.04683	-4.73E-05	4.61E-05	0.51 (4.90)
<b>C sp2</b>	2	6718	0.25313	-0.05276	-1.47E-04	5.09E-05	1.45 (29.30)
	3	23767	0.05938	-0.01066	1.31E-05	6.32E-06	0.59 (7.13)
<b>O sp3</b>	1	2495	0.50994	-0.10401	-1.61E-04	9.23E-05	3.33 (53.57)
	2	70	0.39539	-0.09158	-1.15E-04	8.84E-05	1.34 (10.50)
<b>O sp2</b>	1	22033	0.64143	-0.13439	-5.55E-04	1.47E-04	2.84 (71.85)
<b>N sp3</b>	1	1108	0.39530	-0.11093	-2.77E-05	1.11E-04	1.69 (30.34)
	2	97	0.18125	-0.03628	8.07E-04	-2.57E-05	0.56 (9.68)
	3	2	-0.04179	0.00139	1.06E-04	1.04E-05	2.03 (2.37)
<b>N sp2</b>	1	3058	0.51301	-0.13328	-1.72E-04	1.37E-05	2.46 (23.34)
	2	17835	0.15282	-0.03057	8.50E-05	1.79E-05	0.95 (25.28)
	3	797	0.03929	-0.00693	-1.08E-05	4.74E-06	0.28 (2.37)
<b>S</b>	1	233	0.52683	-0.08452	-6.07E-04	8.45E-05	2.26 (11.85)
	2	524	0.56748	-0.13720	2.71E-05	1.26E-04	4.31 (54.12)
	4	7	0.00552	-0.00020	4.76E-05	-3.40E-06	0.20 (0.45)

<b>P</b>	4	4	0.08255	-0.03718	-1.94E-04	6.04E-05	0.00 (0.00)
<b>F</b>	1	12	0.57935	-0.16373	-1.33E-03	2.95E-04	1.82 (3.64)
<b>H</b>		137972	0.37929	-0.07876	-2.90E-04	8.77E-05	1.50 (37.67)
<b>Ca</b>		23	0.07724	-0.01248	4.93E-05	4.76E-06	0.49 (1.98)