

Ligand-free model N°	01	02	03	04	05	06	07	08	09	10
Favored (98%)	93.0%	95.3%	94.0%	95.3%	94.5%	94.0%	94.3%	93.8%	91.3%	91.8%
Allowed (2%)	4.2%	3.0%	4.5%	3.0%	3.2%	3.5%	4.0%	4.5%	6.2%	5.7%
Outlier (0%)	2.7%	1.7%	1.5%	1.7%	2.2%	2.5%	1.7%	1.7%	2.5%	2.5%
Substrate-bound model N°	01	02	03	04	05	06	07	08	09	10
Favored (98%)	97.5%	96.8%	97.5%	97.3%	97.3%	97.3%	95.5%	96.0%	97.3%	96.5%
Allowed (2%)	1.7%	2.5%	2.0%	2.0%	2.2%	2.0%	3.5%	3.0%	2.2%	3.0%
Outlier (0%)	0.7%	0.7%	0.5%	0.7%	0.5%	0.7%	1.0%	1.0%	0.5%	0.5%