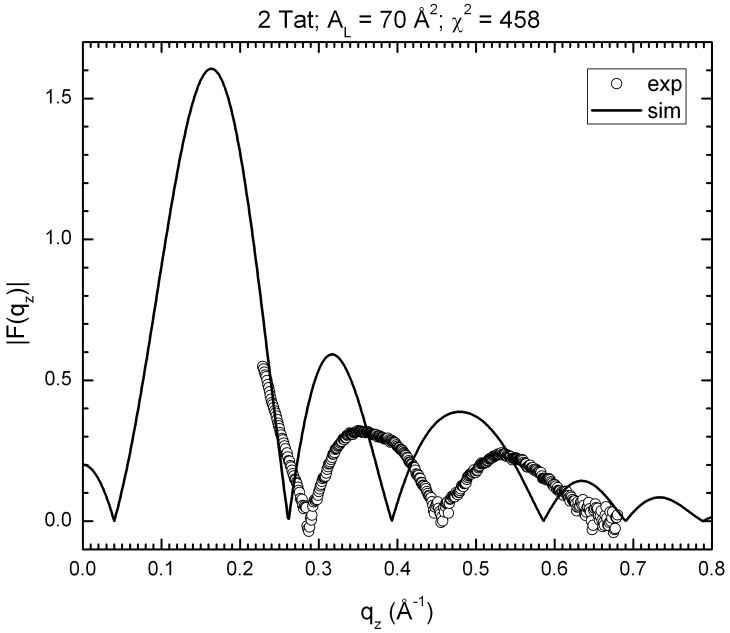
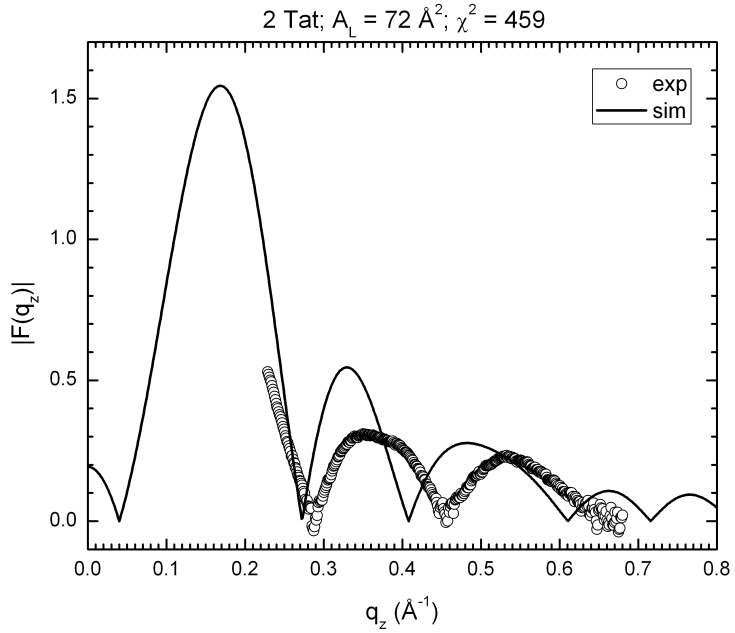
Summary of SIMtoEXP analysis on simulations
4/21/2014

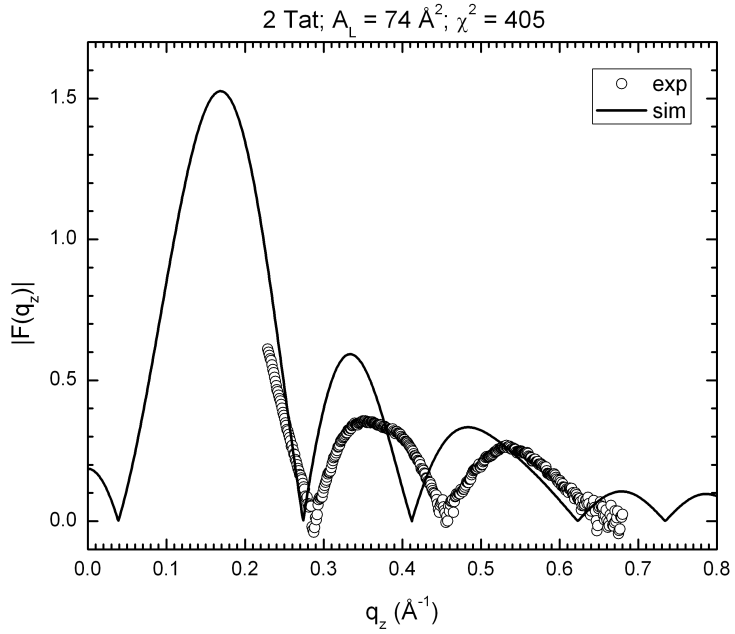
Kun simulated DOPC/Tat systems where Tat center of mass was fixed at 0.5 nm from the bilayer center and the bilayer center was flat (as opposed to the distorted bilayer center simulated earlier). The area per lipid explored is summarized in the table below. In all cases, a pore (pores?) was formed.

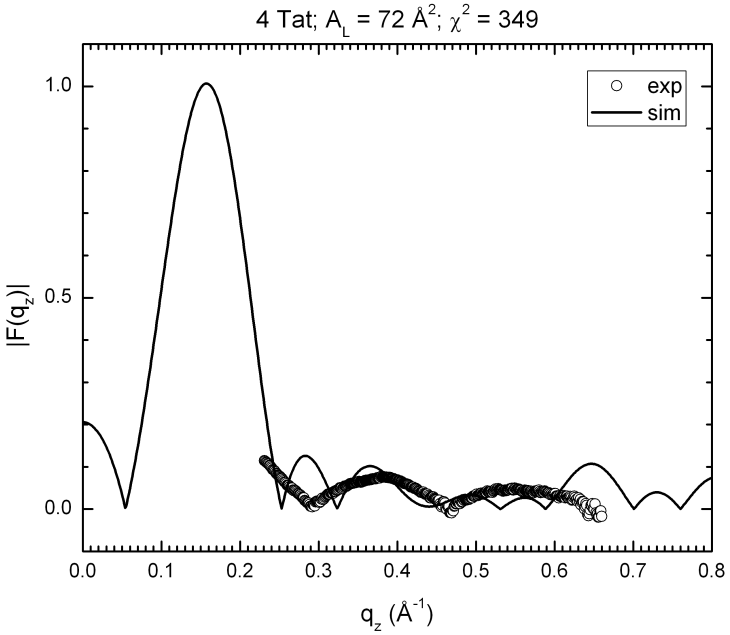
File	A_L (Å^2)	Z_{tat} (Å)	Chi^2
dopc-tat2-a70-6b.sim	70	5	458
dopc-tat2-a72-6b.sim	72	5	459
dopc-tat2-a74-6b.sim	74	5	405
dopc-tat4-a72-6b.sim	72	5	349
dopc-tat4-a74-6b.sim	74	5	110
dopc-tat4-a76-6b.sim	76	5	1664

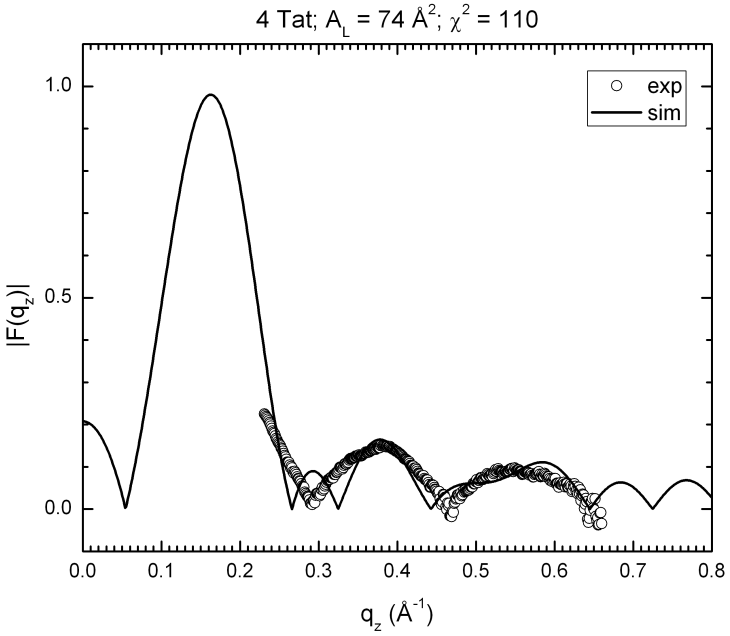
Overall, agreement between experimental and simulated form factors is bad. The chi-squared values of the best matching simulations (Tat fixed at 16 or 18 Å from the bilaye center) are between 18 and 40, far smaller than any chi-squared measured in the current set of simulations.

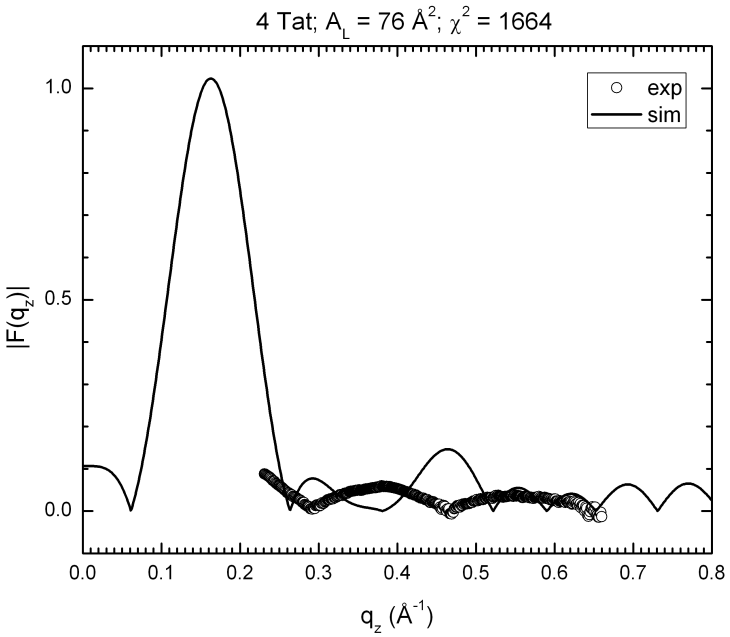



2 Tat; A_L = 72 Å^2; χ^2 = 459
exp
sim
|F(q_z)|
q_z (Å^-1)
0.0
0.5
1.0
1.5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


2 Tat; A_L = 74 Å^2; χ^2 = 405
exp
sim
|F(q_z)|
q_z (Å^-1)
0.0
0.5
1.0
1.5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


4 Tat; A_L = 72 Å^2; χ^2 = 349
exp
sim
|F(q_z)|
q_z (Å^-1)
0.0
0.5
1.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


4 Tat; A_L = 74 Å^2; χ^2 = 110
exp
sim
|F(q_z)|
q_z (Å^-1)
0.0
0.5
1.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


4 Tat; A_L = 76 Å^2; χ^2 = 1664
exp
sim
|F(q_z)|
1.0
0.5
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
q_z (Å^-1)