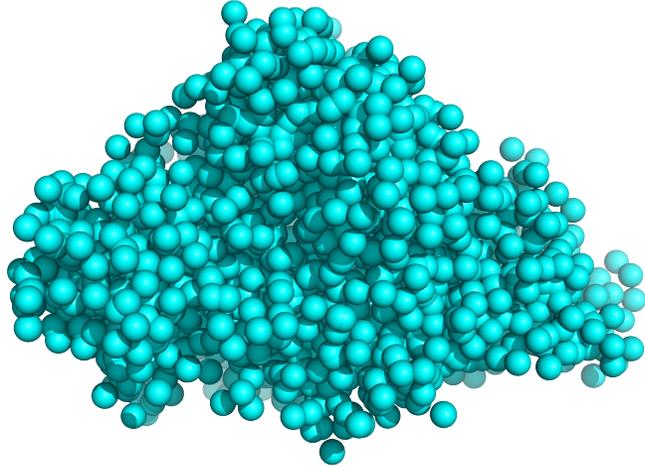
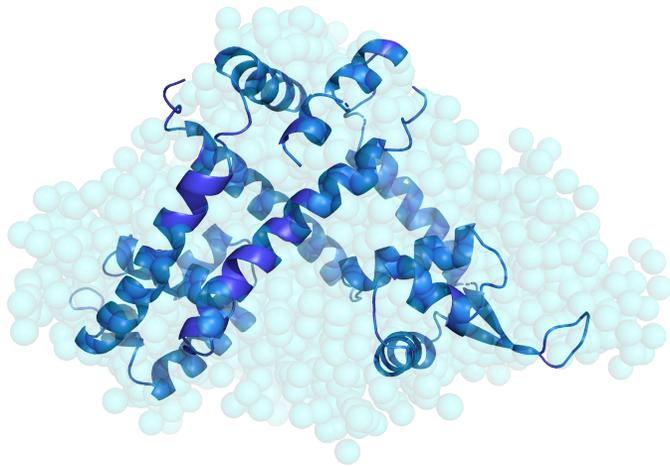


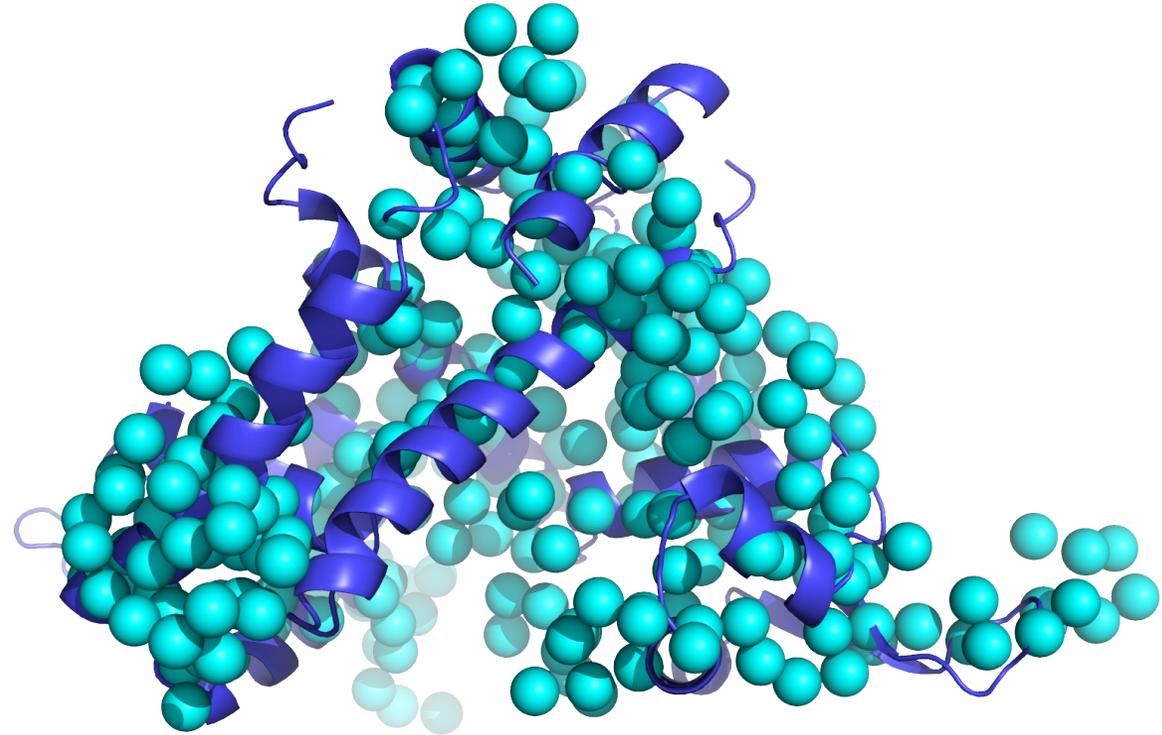
# GASBOR MexR Modelling Summary – P1 symmetry.



GASBOR model cohort alignment

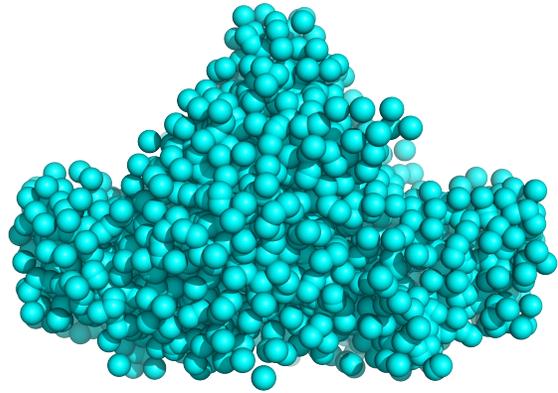


GASBOR model cohort alignment compared to MexR dimer model

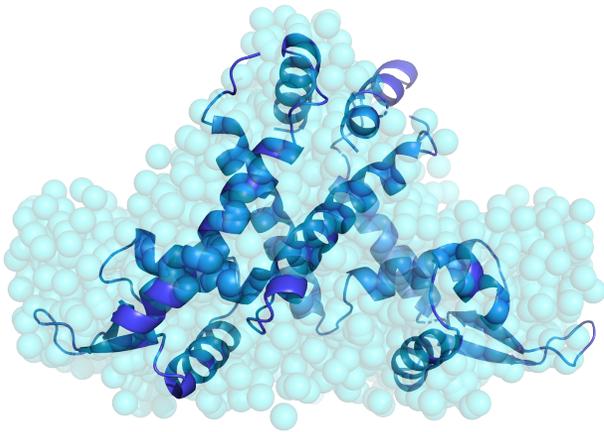


Spatial alignment of GASBOR model D (lowest NSD) compared to the refined asymmetric MexR dimer model

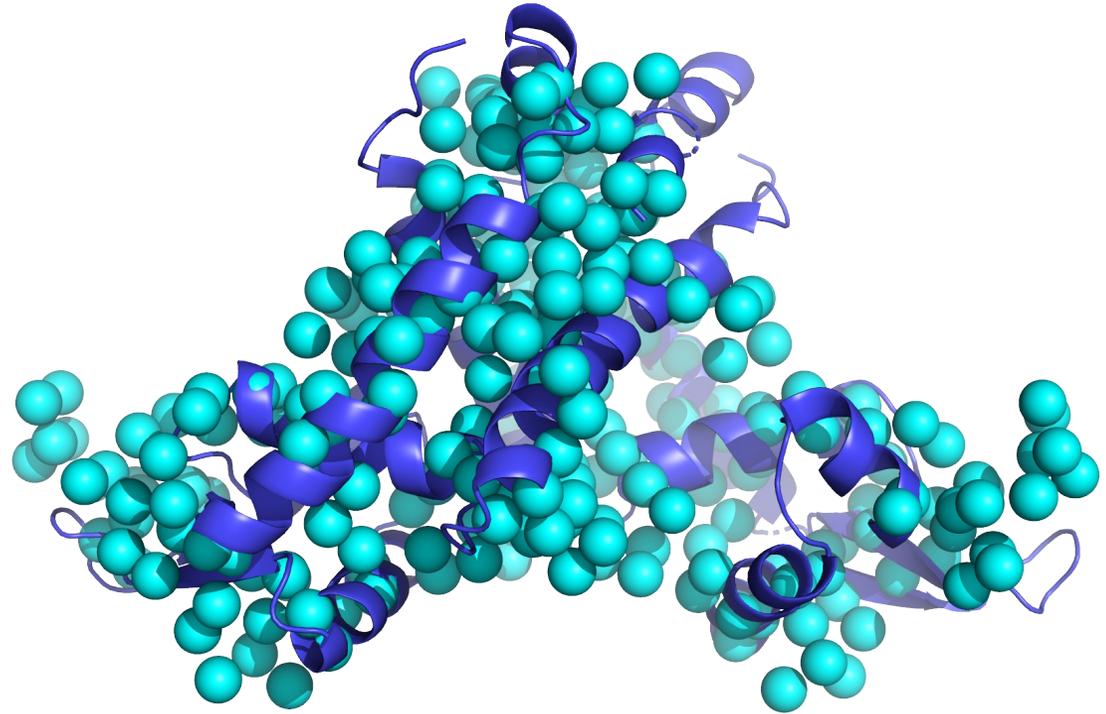
# GASBOR MexR Modelling Summary – P2 symmetry enforced.



GASBOR model cohort alignment in P2



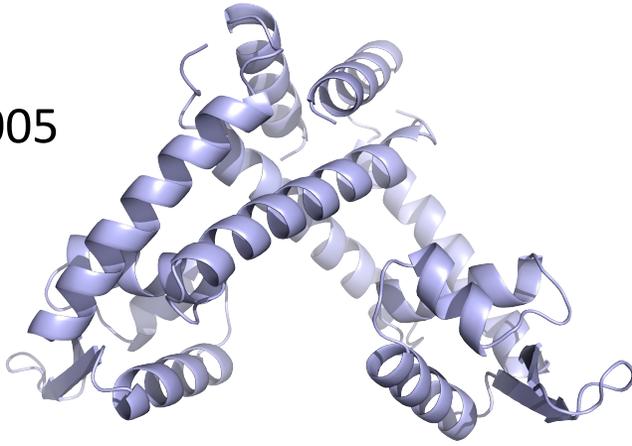
GASBOR model cohort alignment in P2,  
compared to MexR dimer model



Spatial alignment of GASBOR model J (lowest  
NSD) calculated in P2 symmetry, compared to  
the asymmetric refined MexR dimer model

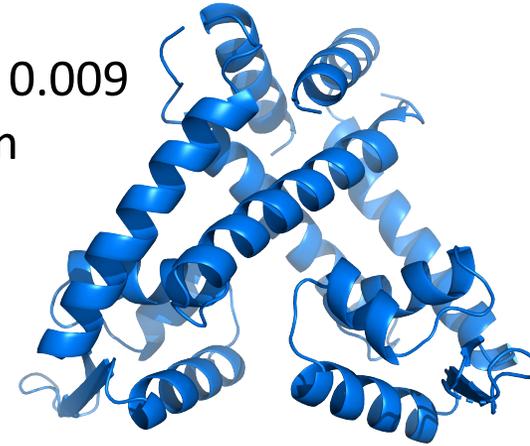
It is possible to construct 3 dimers from the 1LNW X-ray crystal structure, and a predicted model dimer (extended version) based on 6C2S. Note! The  $R_g$  from POR, experimental, is 2.31 nm.

$\chi^2 = 1.5$   
CorMap P = 0.005  
 $R_g = 2.34$  nm



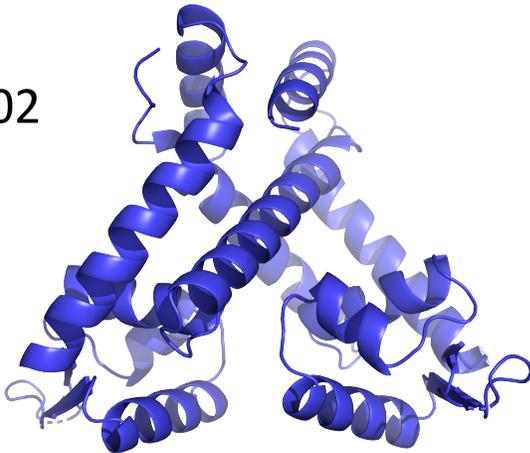
1LNW Dimer 1 model

$\chi^2 = 1.6$   
CorMap P = 0.009  
 $R_g = 2.18$  nm



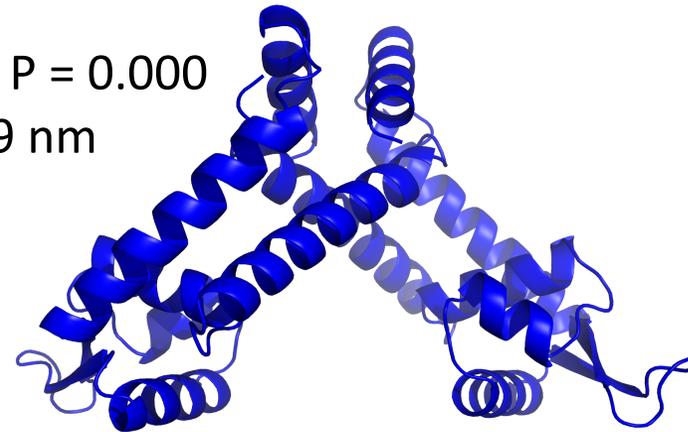
1LNW Dimer 2 model

$\chi^2 = 1.7$   
CorMap P = 0.002  
 $R_g = 2.16$  nm



1LNW Dimer 3 model

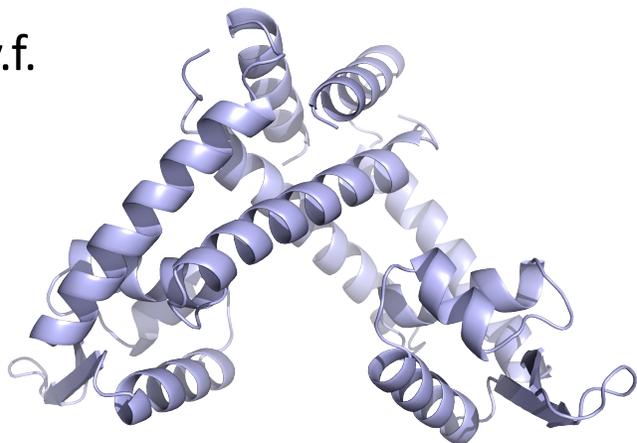
$\chi^2 = 2.9$   
CorMap P = 0.000  
 $R_g = 2.49$  nm



6C2S Dimer model – AlphaFold2 predicted dimer superposed onto the 6C2S X-ray crystal structure

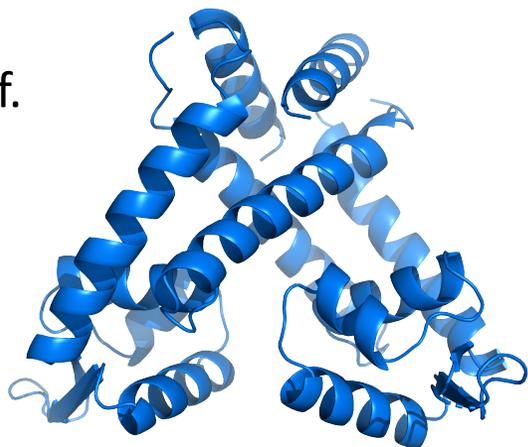
OLIGOMER can be used to describe the scattering data as a volume fraction weighted mixture of dimers that sample ,open' and ,closed' states in solution.

60% v.f.



1LNW Dimer 1 model

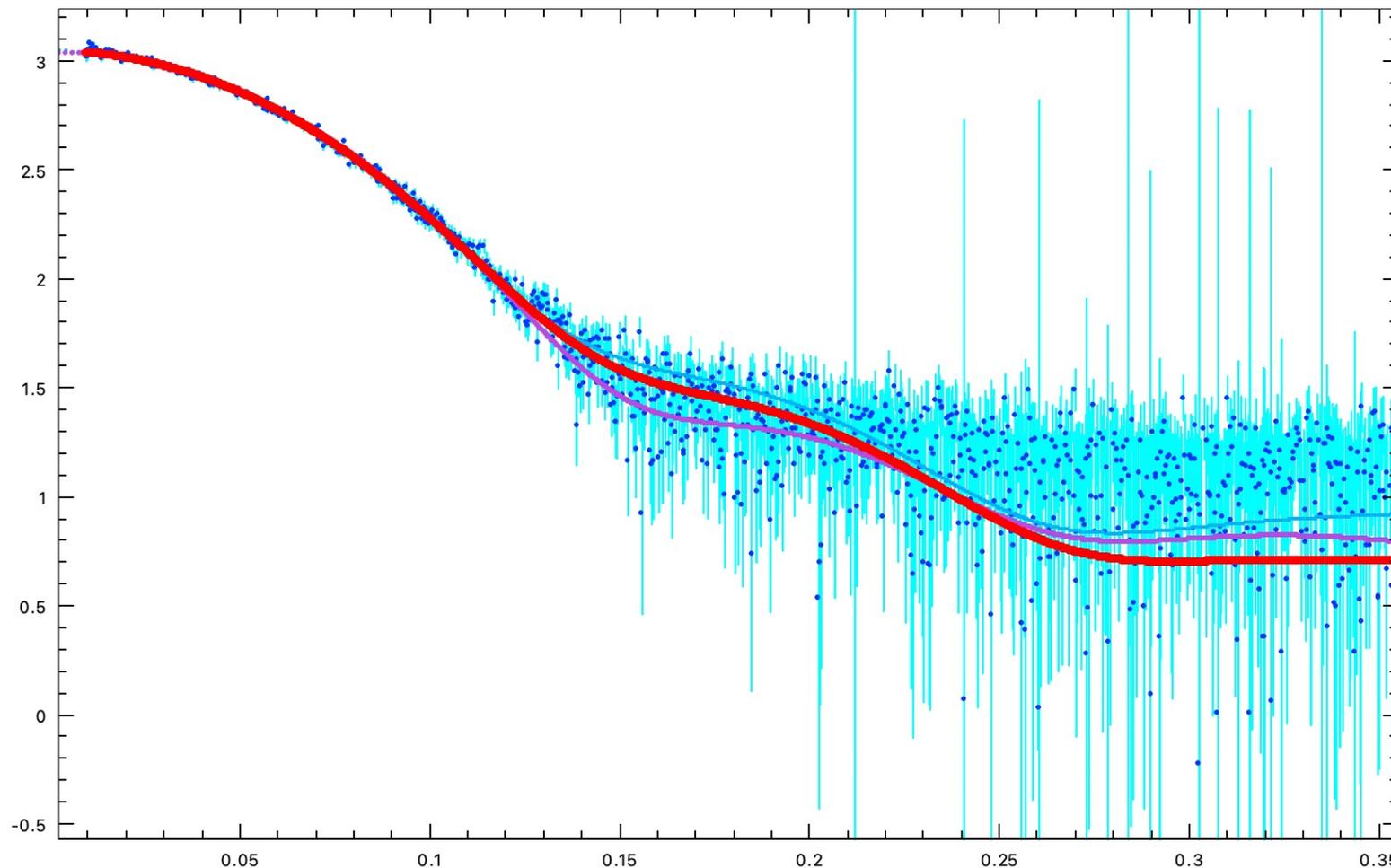
40% v.f.



1LNW Dimer 2 model

$$\chi^2 = 1.5$$

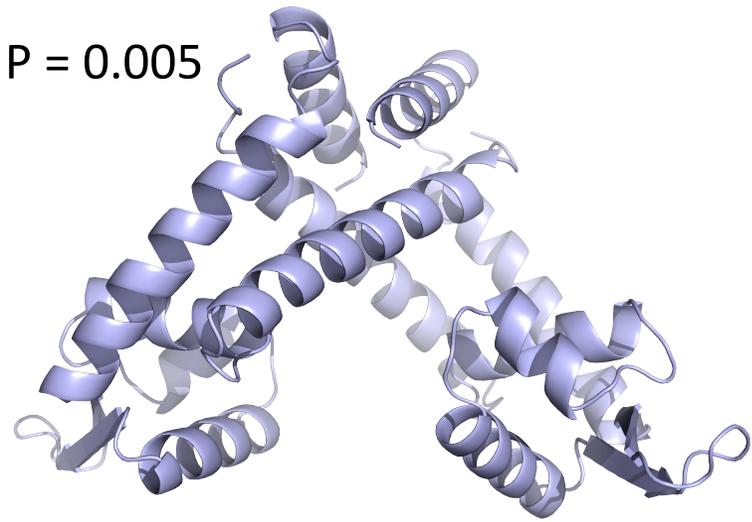
**CorMap P = 0.26**



The RED fit shows the result from OLIGOMER, the light blue for Dimer 1 and darker blue for Dimer 2. The mid-s region between 1.30 and 2.24 nm<sup>-1</sup> appears to be sensitive to the 'open' and 'closed' and/or 'twisted' status of the dimer.

Building the final single model representation of the MexR dimer representing an averaged spatial disposition.

$\chi^2 = 1.5$   
CorMap P = 0.005

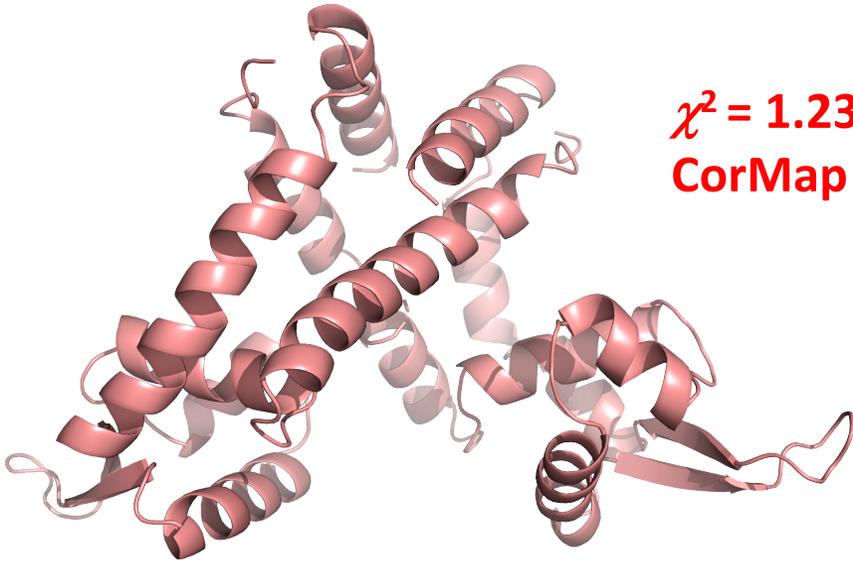


1LNW Dimer 1 model

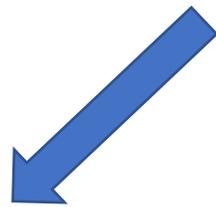
SREFLEX



$\chi^2 = 1.23$   
CorMap P = 0.26

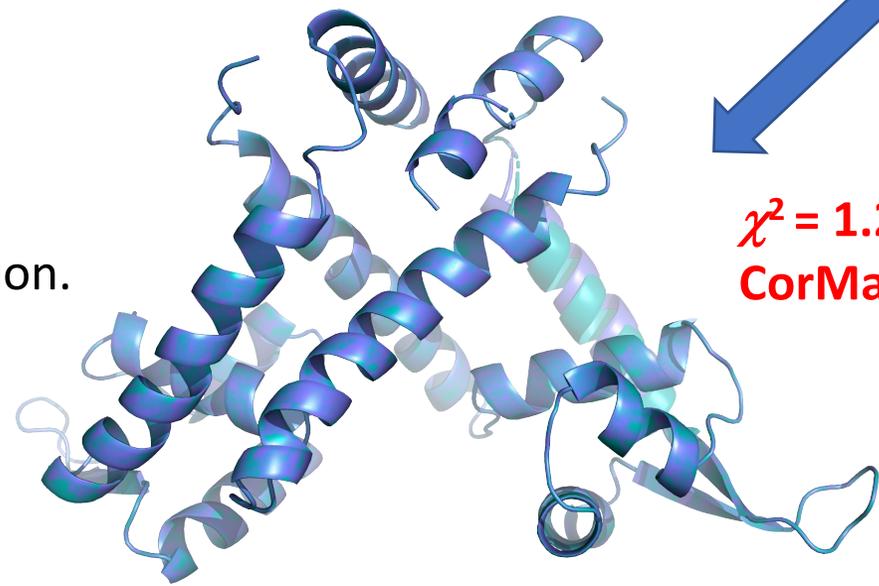


Fix up breaks and clashes as best as possible

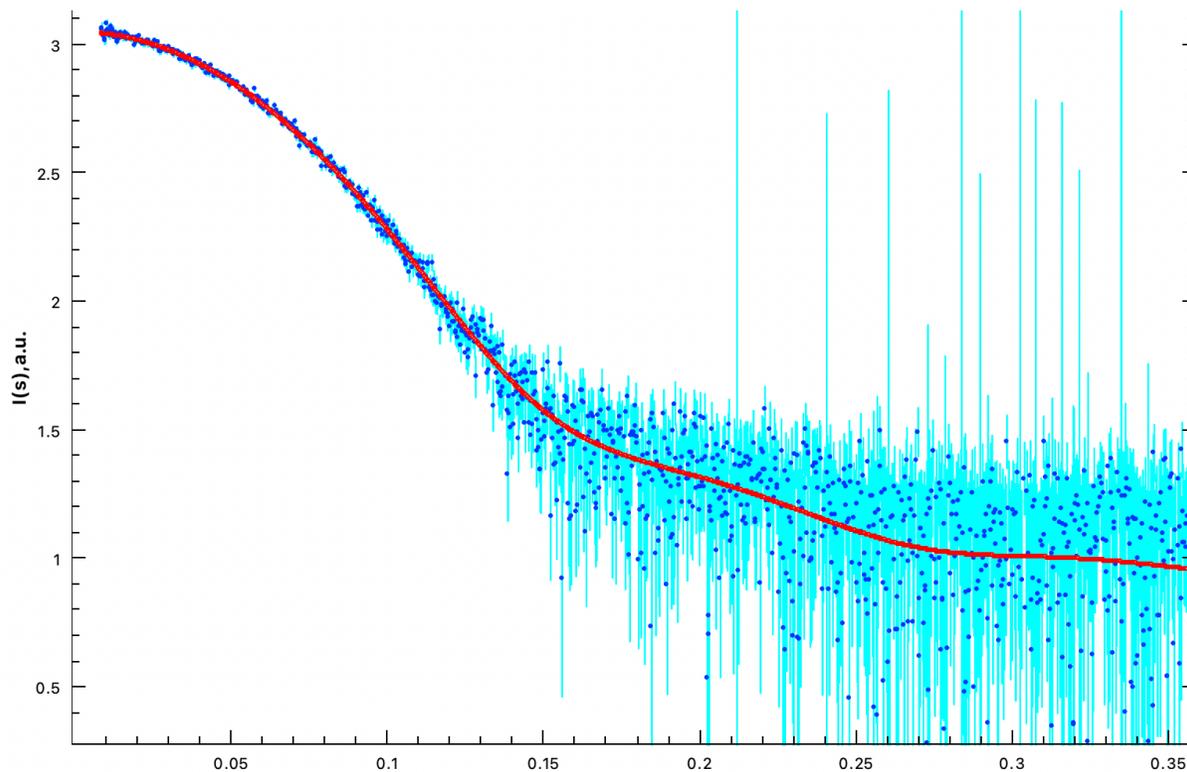


Final single model representation.  
 $R_g = 2.32$  nm.

$\chi^2 = 1.25$   
CorMap P = 0.26 (dimerS)/0.76(dimerQ)



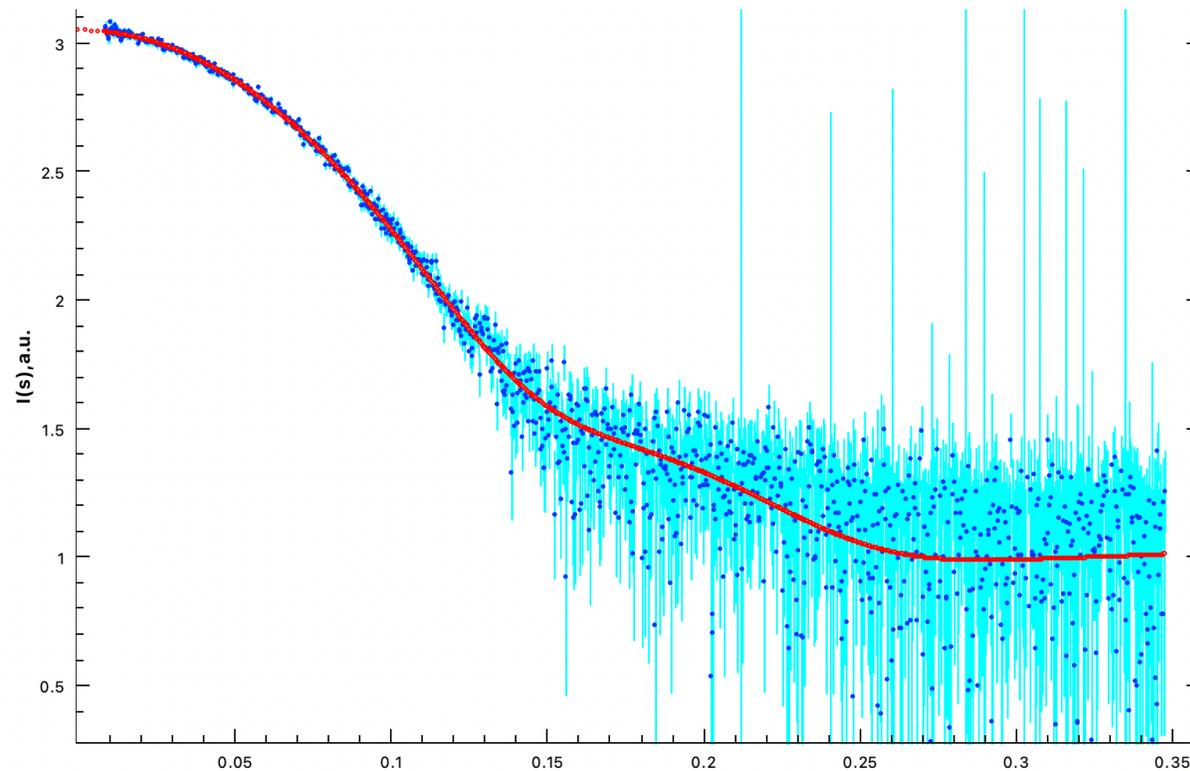
# GASBOR and refined dimer S/Q model fit examples



GASBOR model:

$\chi^2$ , 1.23 - 1.25, CorMap P = 0.71

CRY SOL fit. 30 harmonics and 256 points



Asymmetric Dimer model:

$\chi^2$ , 1.25, CorMap P = 0.26