Small Angle X-ray Scattering
Overview of basic data evaluation and analysis

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Biomoleculare NMR-Spektroskopie

Software

ATSAS Package

Collection of tools for data evaluation
and modeling of SAXS and SANS data

EMBL

https://www.embl-hamburg.de/biosaxs/software.html

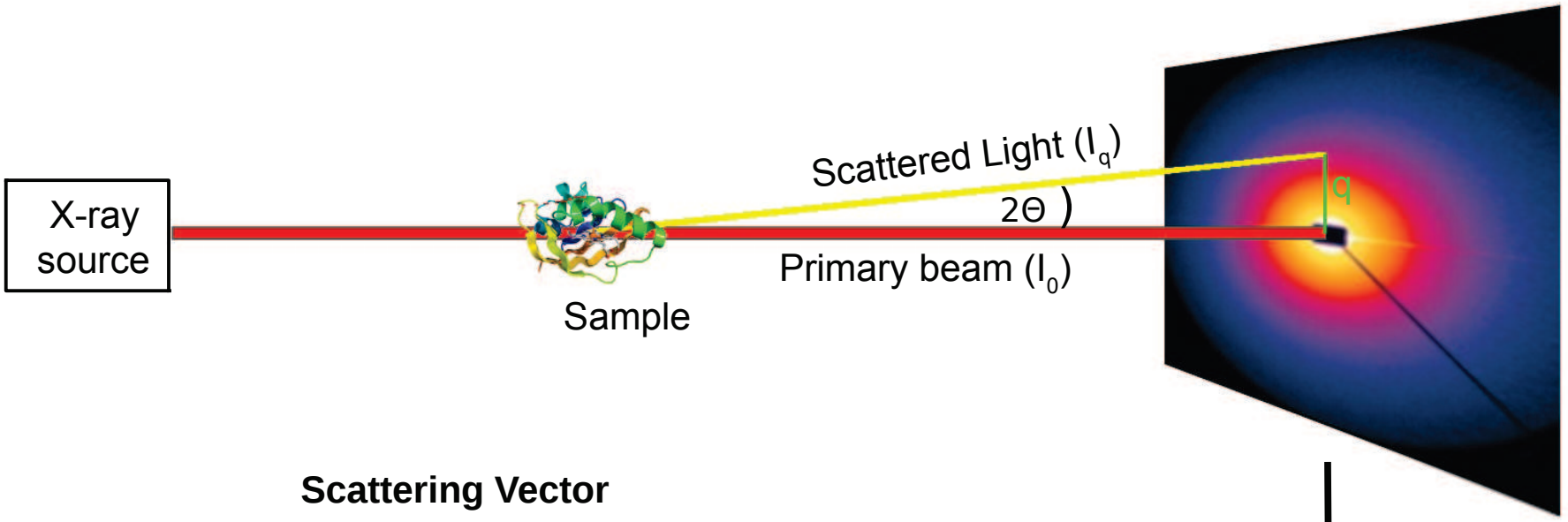
Patforms:
Linux
Windows
Mac OS

For academic use the software is free.

Download:
https://www.embl-hamburg.de/biosaxs/download.html
(Registration required)

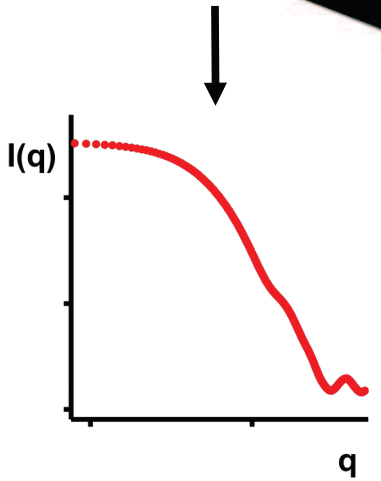
Scattering experiment

Small Angle X-ray Scattering Experiment



Scattering Vector

$$|\vec{q}| = \frac{4\pi}{\lambda} \sin 2\Theta \qquad \vec{q} = (\vec{k}_s - \vec{k}_0)$$

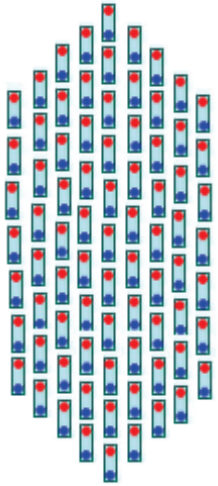


k_0, k_s Wave vectors of incident and scattered beam
λ Wavelength of incident beam

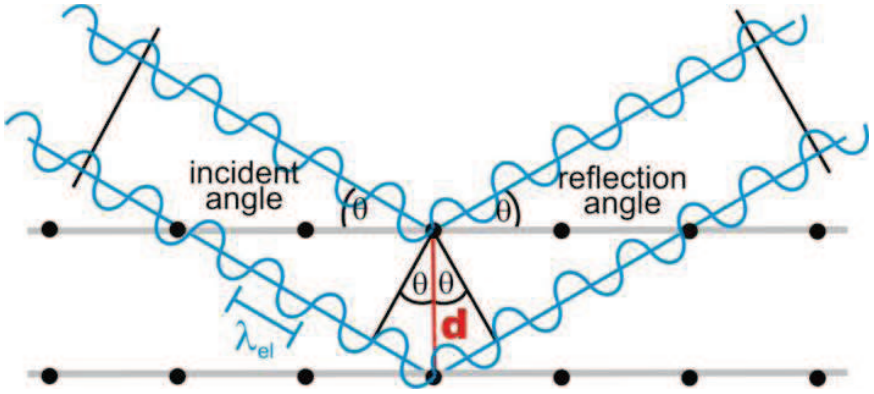
Scattering experiments

Small angle scattering and Single crystal diffraction

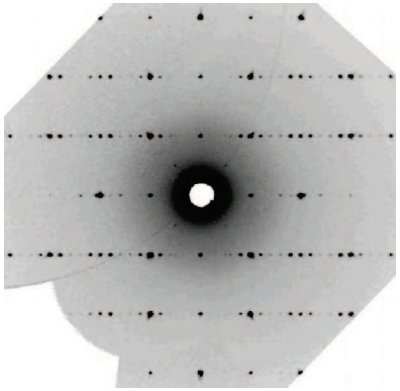
Defined orientation of molecules in a crystal

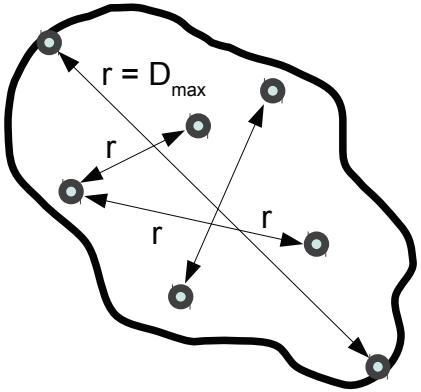


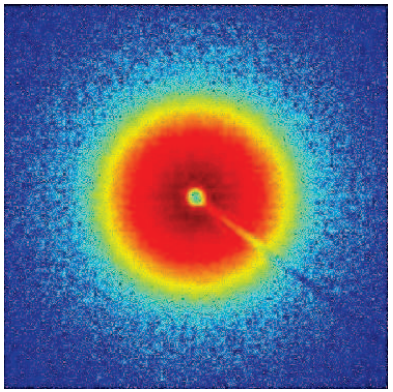
Braggs Law



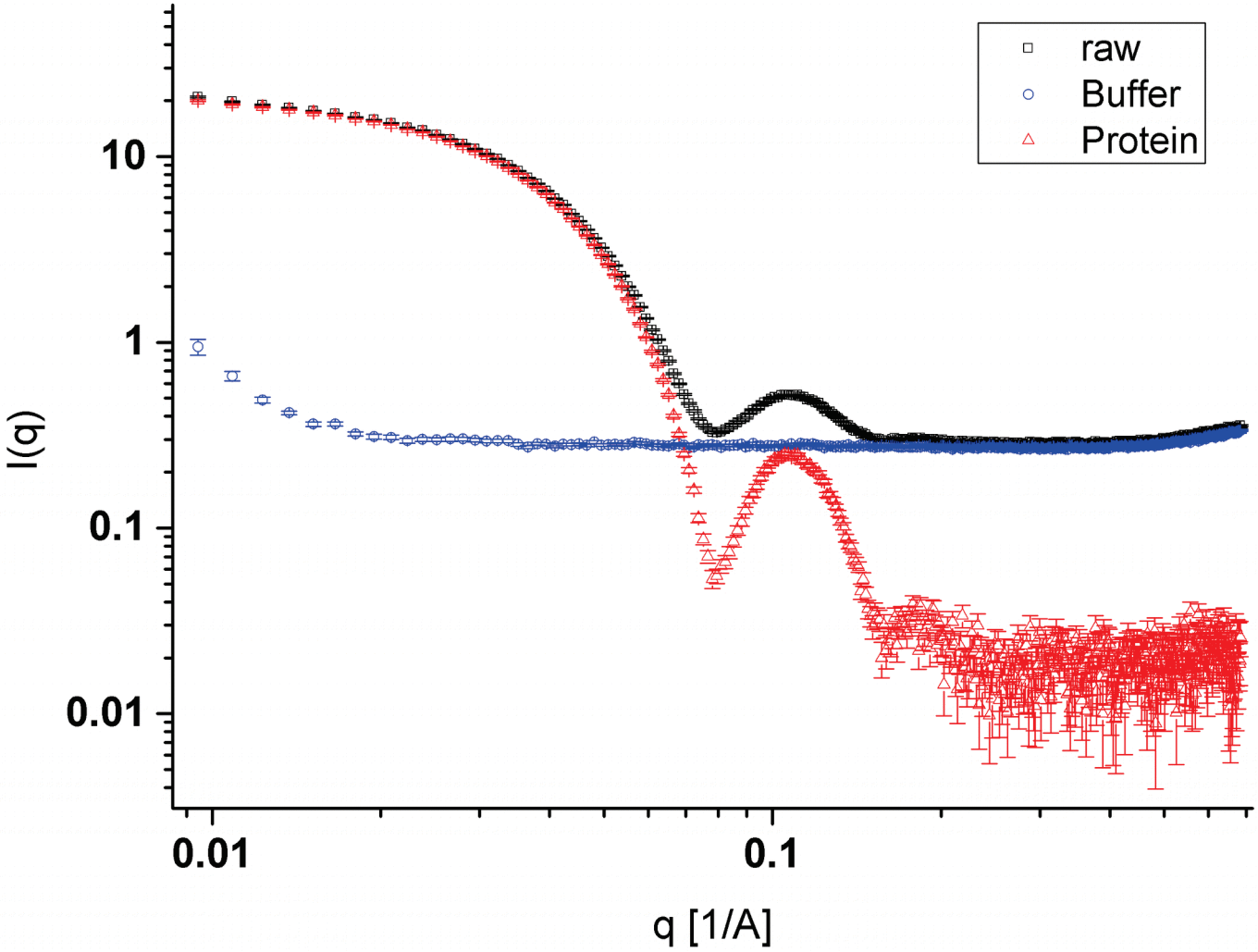
Random orientation of molecules in solution







Measurements



Direct Information

What can we learn from Small Angle X-ray Scattering Curves

What we put in = what we get out

Direct Information

What can we learn from Small Angle X-ray Scattering Curves

Garbage in = Garbage out

Direct Information

What can we learn from Small Angle X-ray Scattering Curves

More secondary information in

=

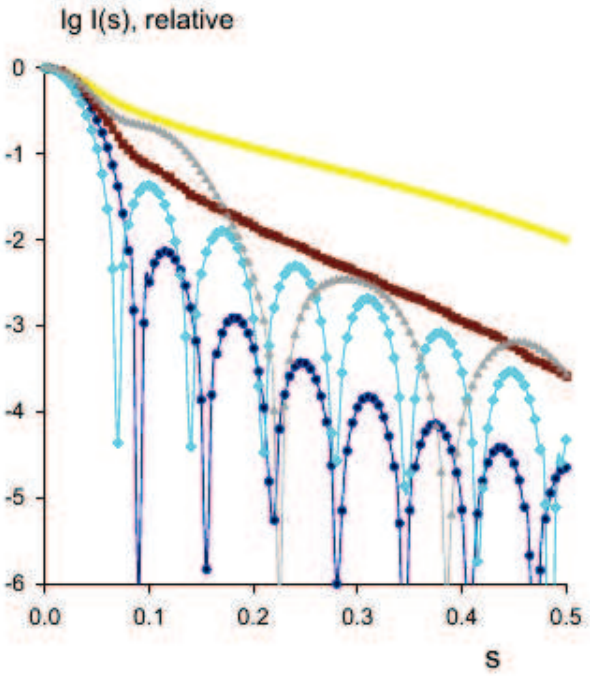
Much more information out

Direct Information

Direct Information

Shape

Solid sphere



Long rod

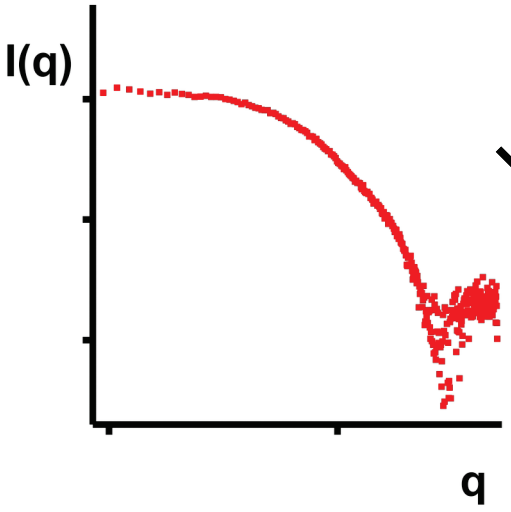
Hollow sphere

Flat disc

Dumbbell

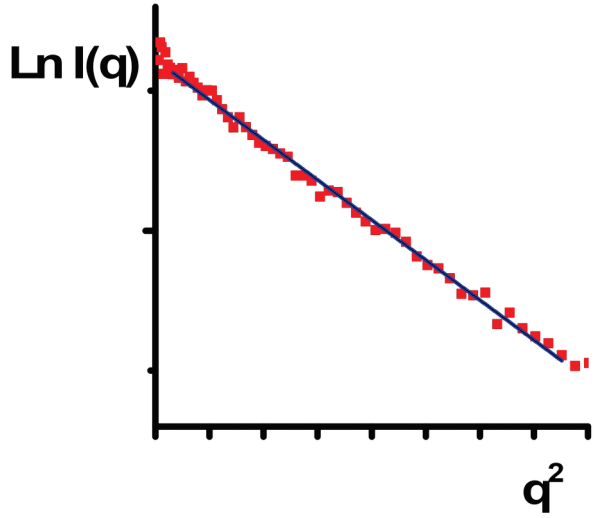
Direct Information

Scattering curve



- Radius of Gyration
- I_0 and Molecular Weight
- Dimerisation or ligand binding

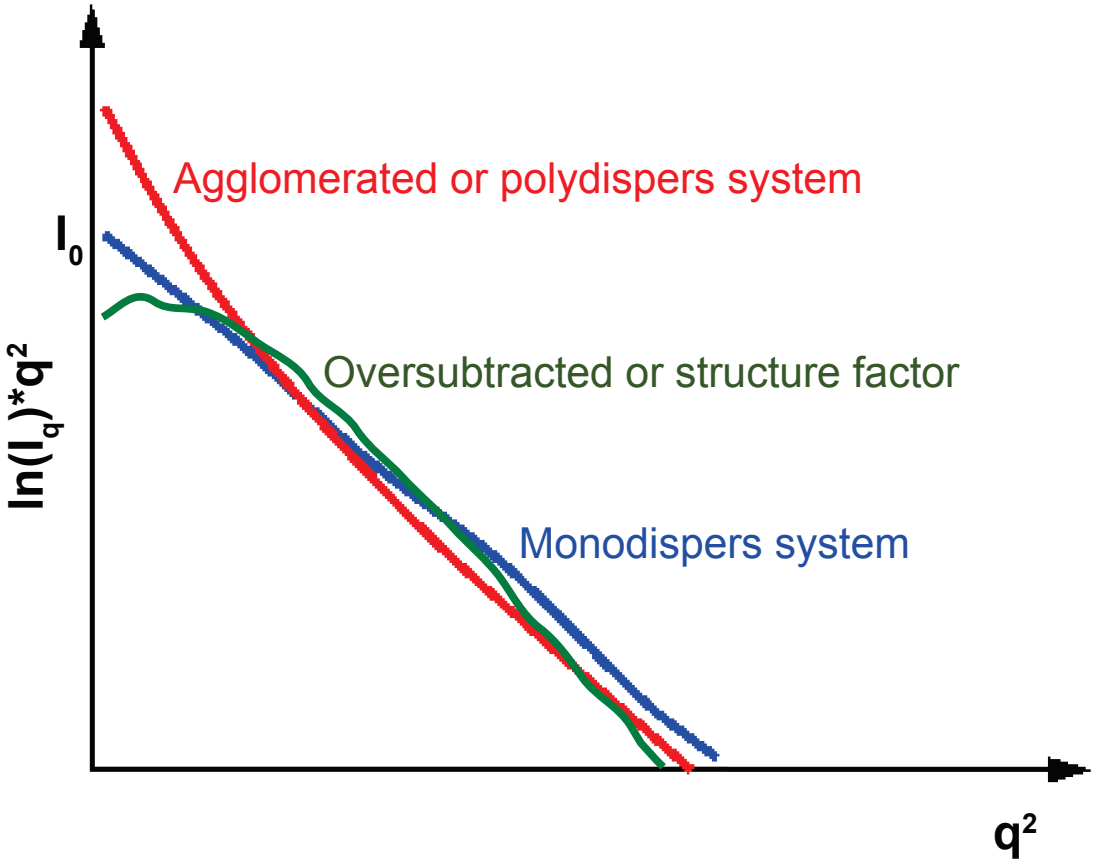
Guinier Plot



Direct Information

Guinier plot

Radius of Gyration (R_g): Average of square centers of mass distances in a particle



Objects of same mass

Guinier Approximation

$$I(q) \approx I_0 \, e^{\frac{-R_g^2}{3} q^2}$$

linearisation

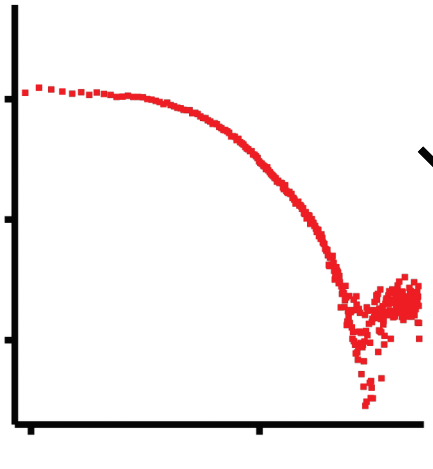
$$\ln(I_q) = -\frac{1}{3} R_g^2 q^2 + I_0$$

Limit: $R_g * q < 1.3$

Direct Information

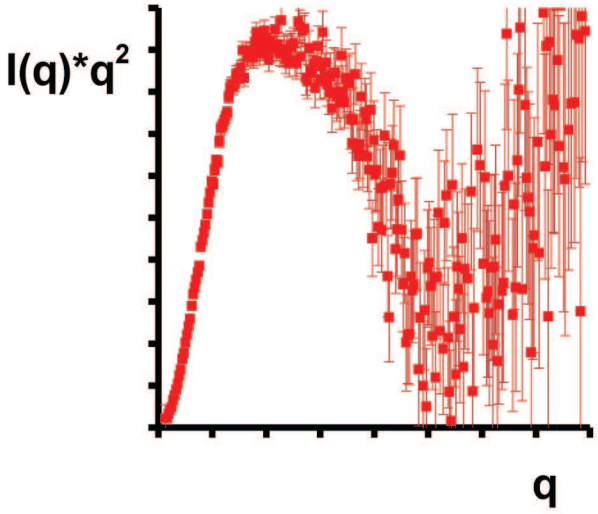
Scattering curve

- State of folding
  - folded
  - unfolded
  - partially folded

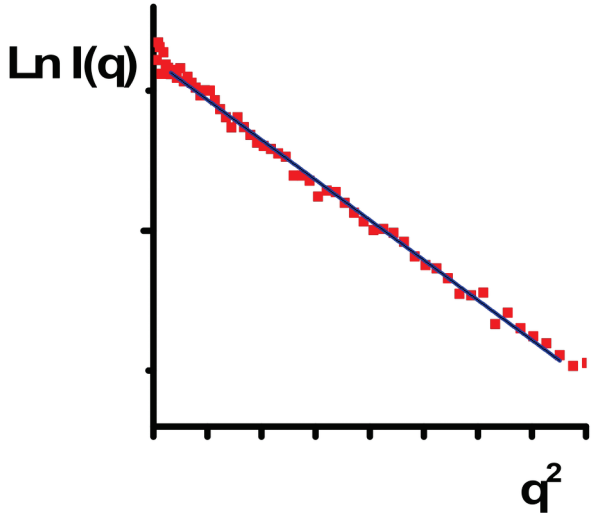


- Radius of Gyration
- I_0 and Molecular Weight
- Dimerisation or ligand binding

Kratky Plot

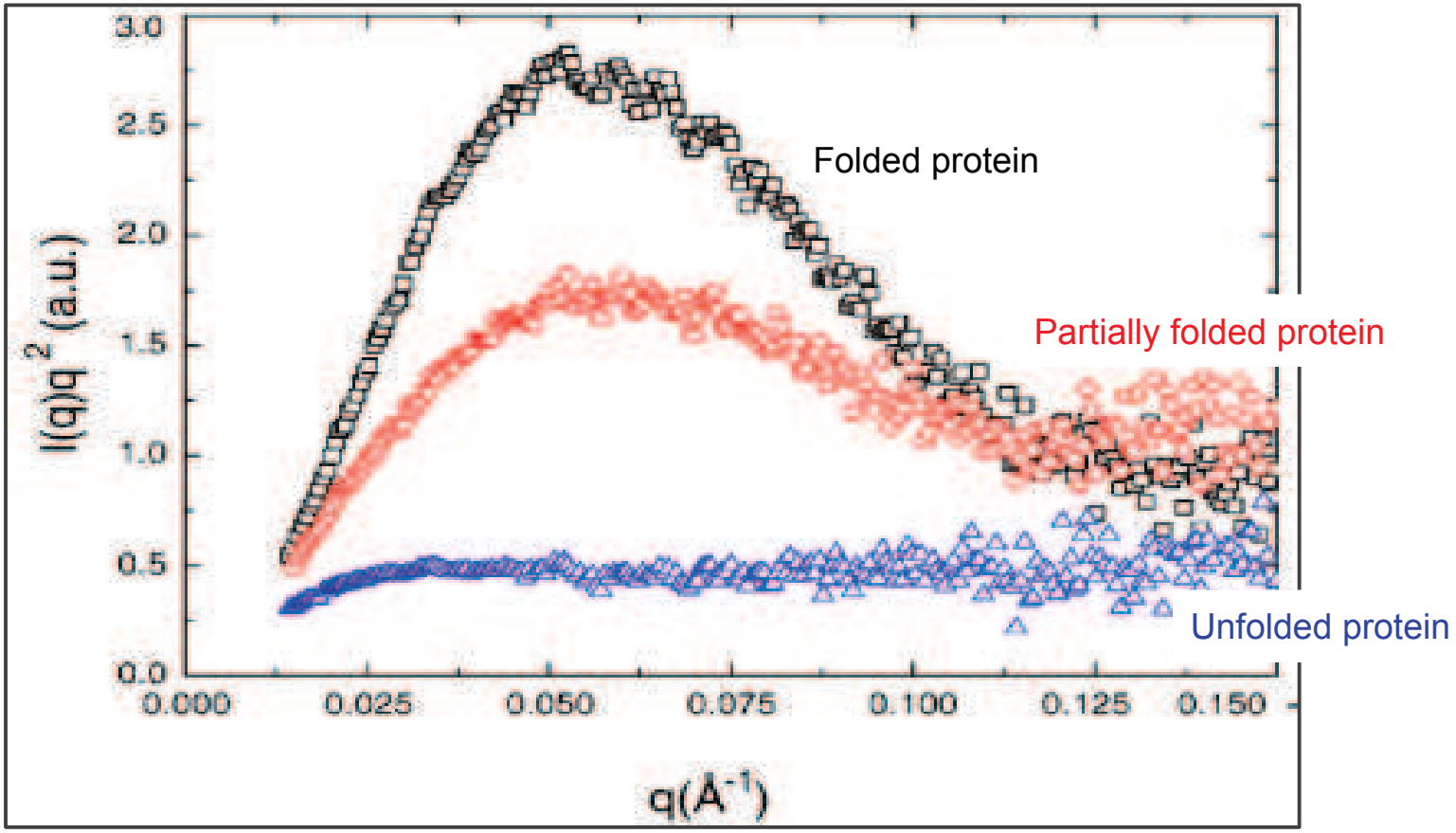


Guinier Plot



Direct Information

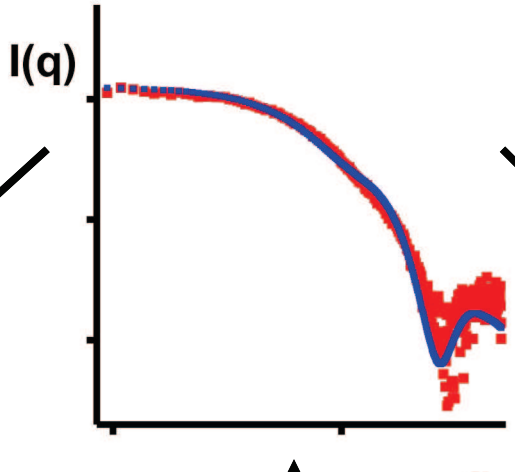
Kratky plot



The Kratky plot shows the state of folding of a protein (BSA with increasing concentrations of urea)

Direct Information

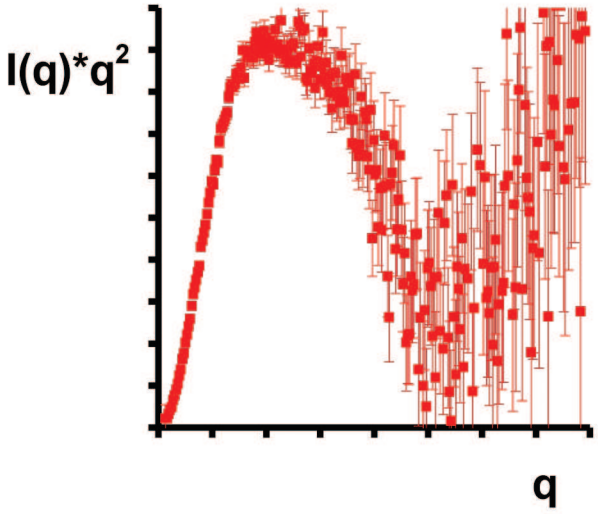
Fit of crystal structure to SAXS data



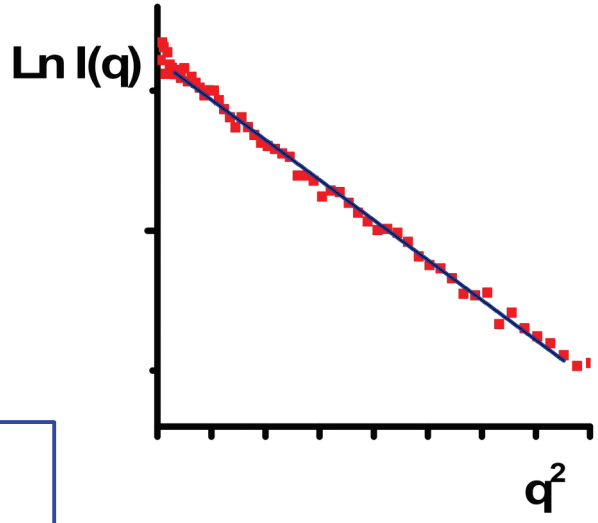
- State of folding
  - folded
  - unfolded
  - partially folded

- Radius of Gyration
- I_0 and Molecular Weight
- Dimerisation or ligand binding

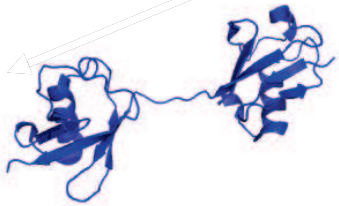
Kratky Plot



Guinier Plot



Crystal Structure

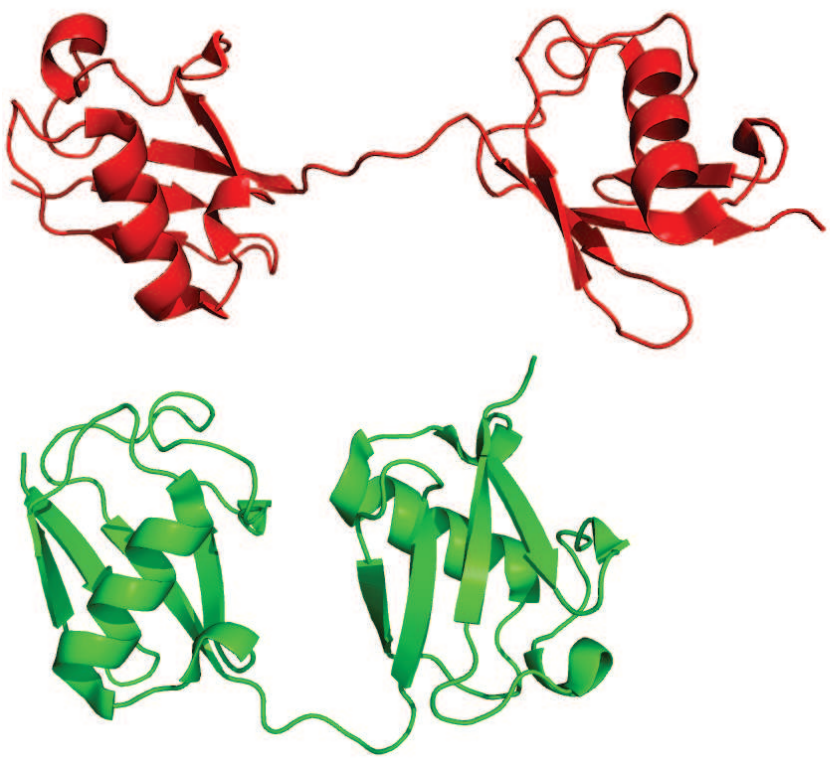


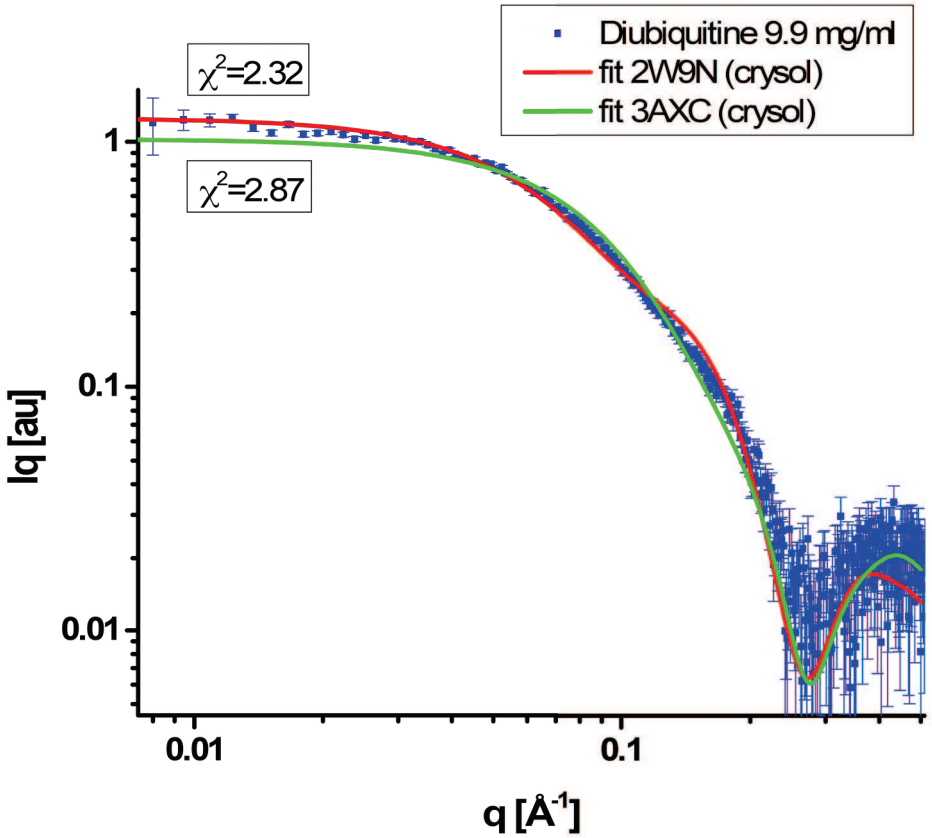
- Difference between crystal structure and structure in solution
- Dimerisation

Direct Information

Combination of high resolution models with SAXS
CRYSOL

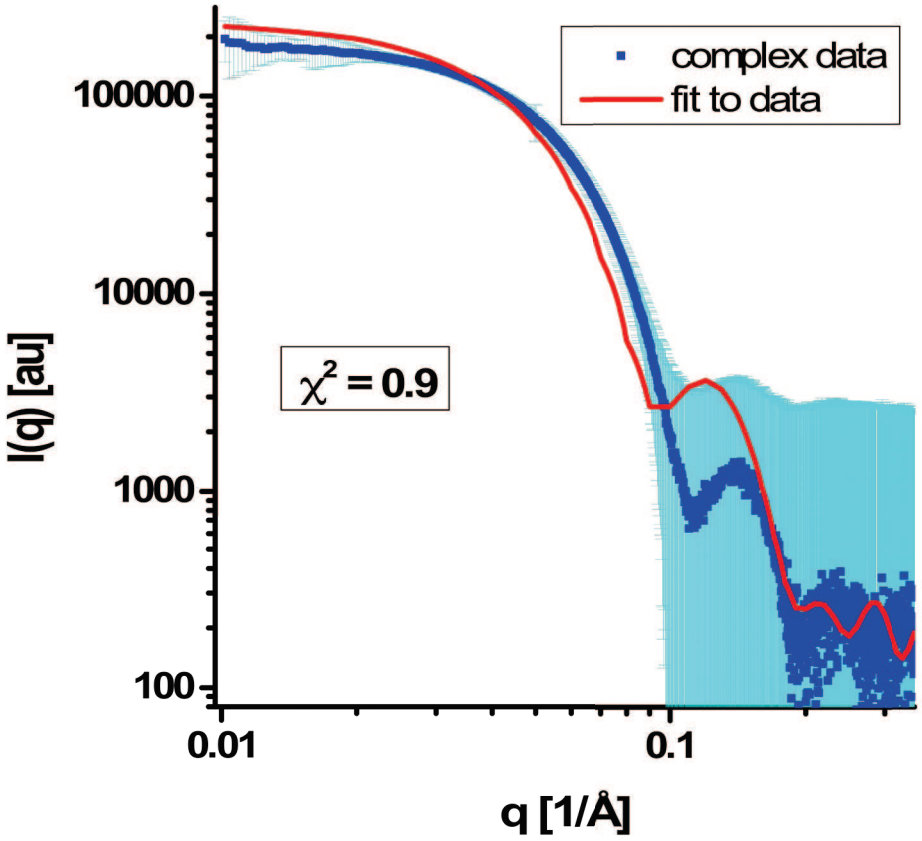
crysol calculates a scattering profile from a high resolution structure and compares to scattering data

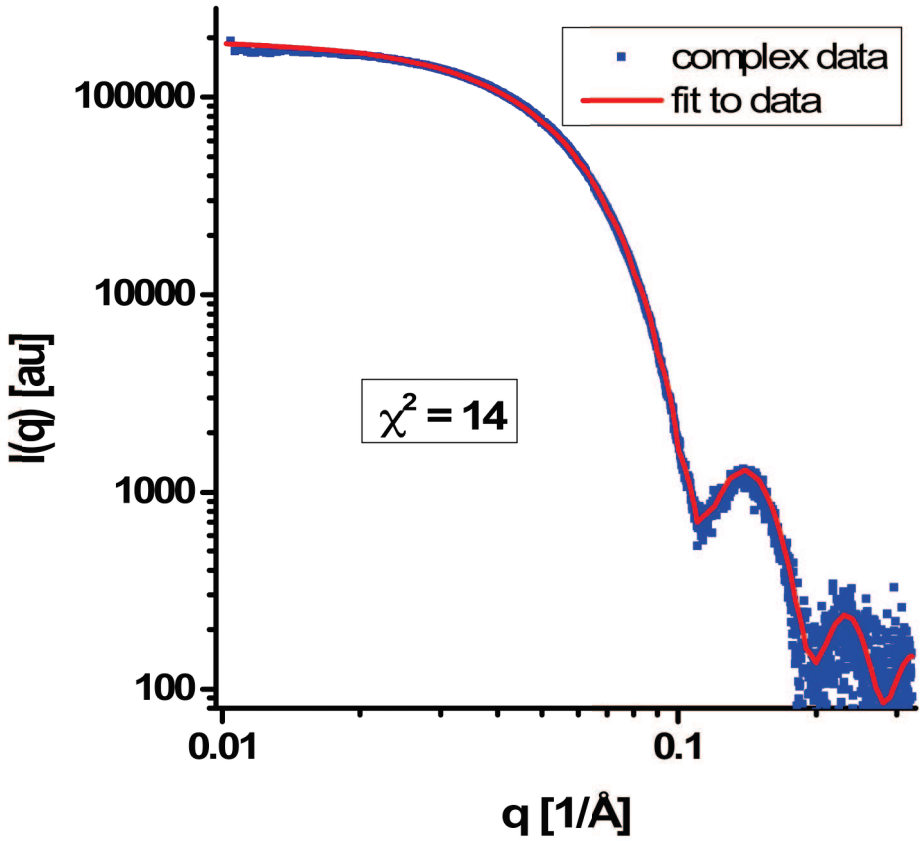




Direct Information

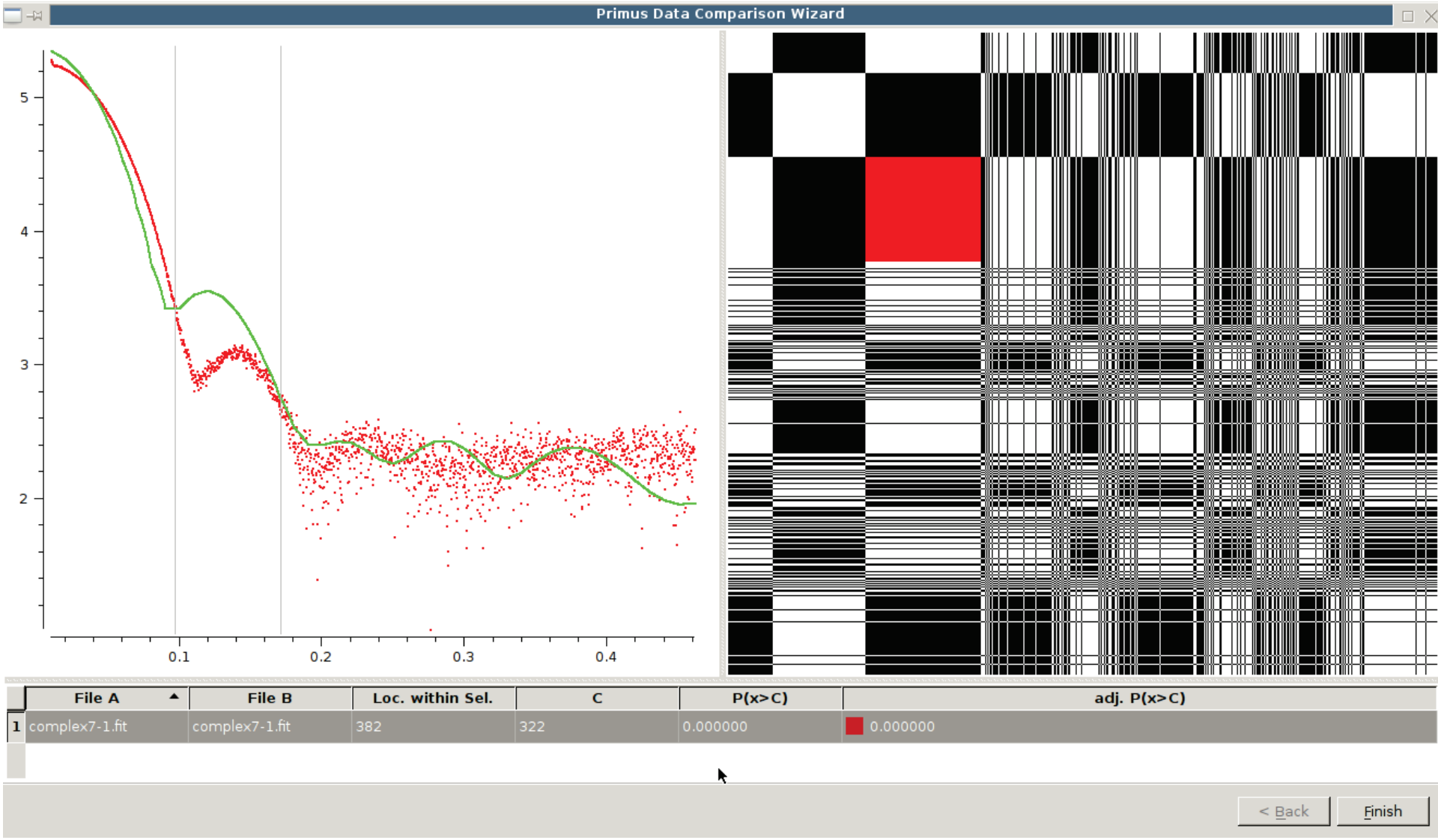
CRYSOL and χ^2 values





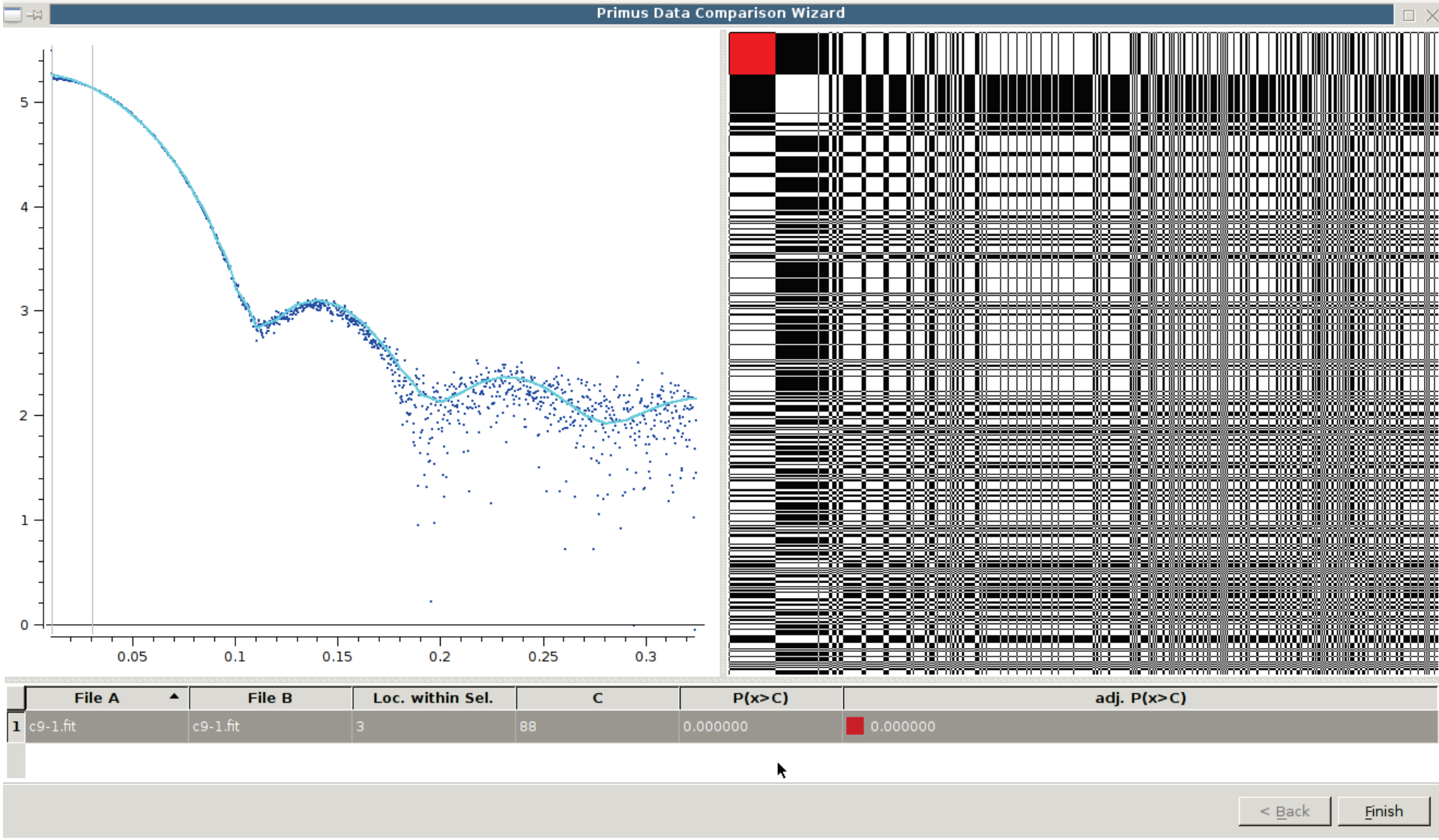
Direct Information

Correlation map primus



Direct Information

Correlation map primus

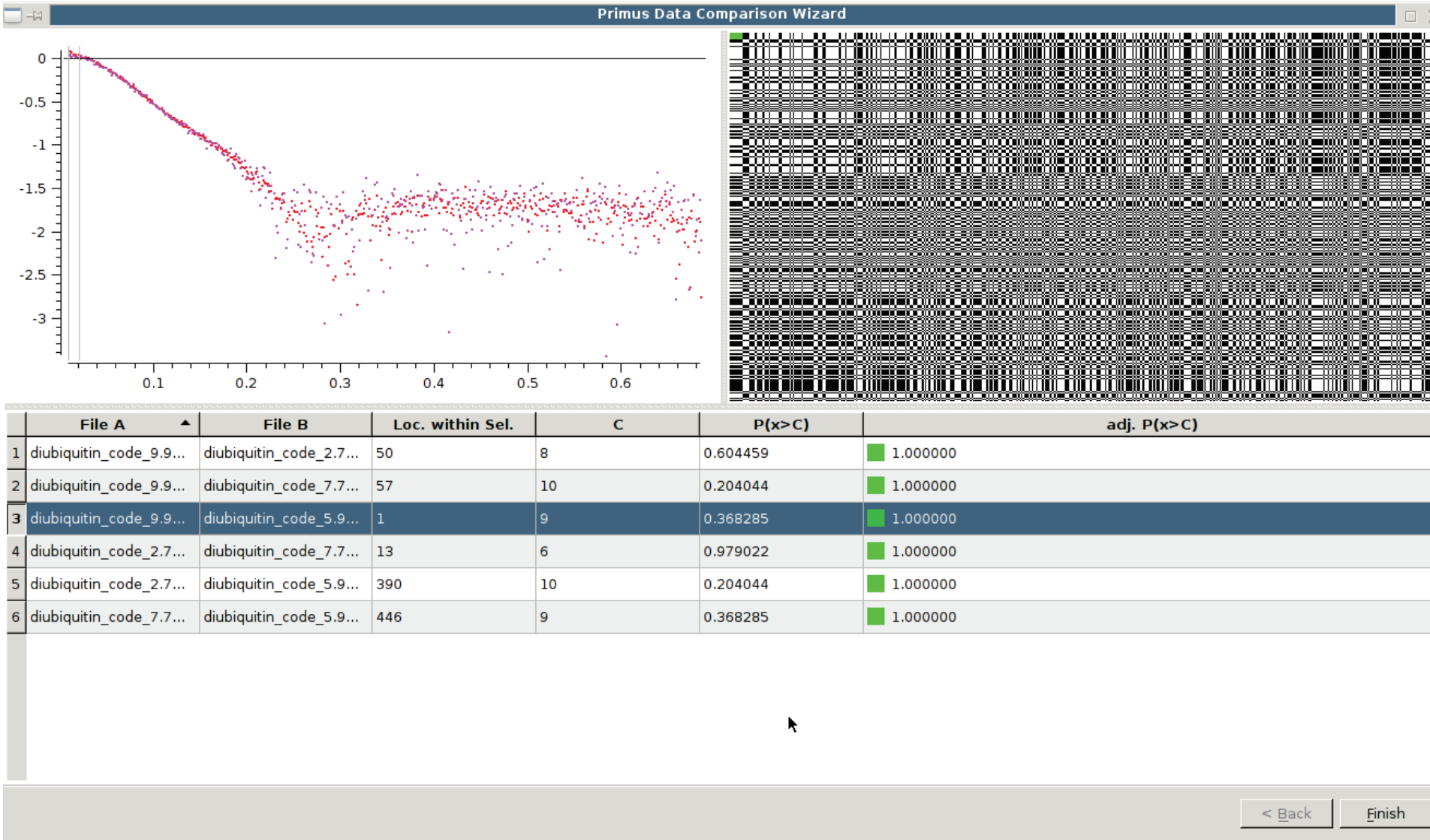


	File A	File B	Loc. within Sel.	C	P(x>C)	adj. P(x>C)
1	c9-1.fit	c9-1.fit	3	88	0.000000	0.000000

< Back | Finish

Direct Information

Correlation map primus



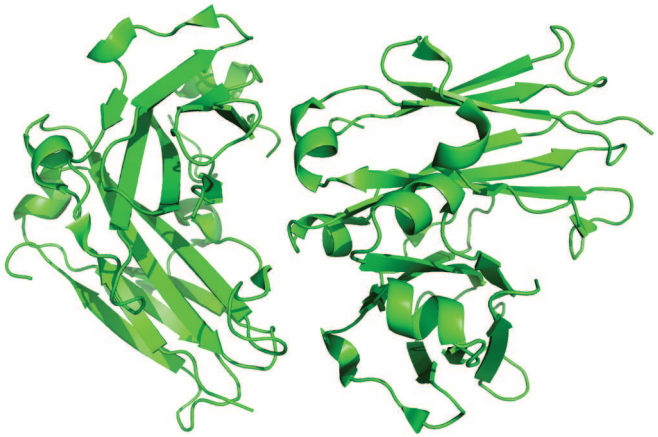
	File A	File B	Loc. within Sel.	C	P(x>C)	adj. P(x>C)
1	diubiquitin_code_9.9...	diubiquitin_code_2.7...	50	8	0.604459	1.000000
2	diubiquitin_code_9.9...	diubiquitin_code_7.7...	57	10	0.204044	1.000000
3	diubiquitin_code_9.9...	diubiquitin_code_5.9...	1	9	0.368285	1.000000
4	diubiquitin_code_2.7...	diubiquitin_code_7.7...	13	6	0.979022	1.000000
5	diubiquitin_code_2.7...	diubiquitin_code_5.9...	390	10	0.204044	1.000000
6	diubiquitin_code_7.7...	diubiquitin_code_5.9...	446	9	0.368285	1.000000

< Back | Finish

Direct Information

Dimerisation oligomer

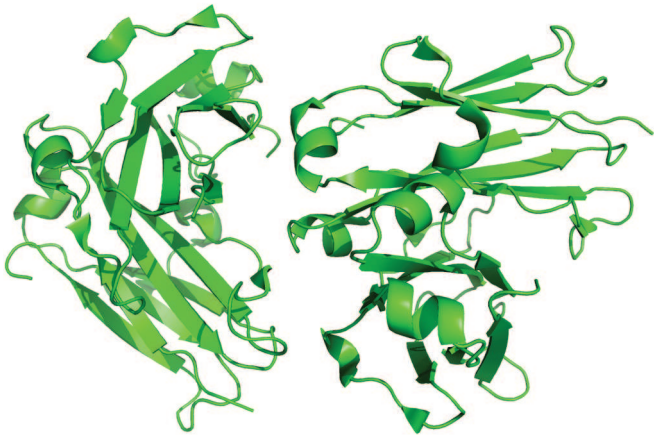
IGMCH4 Dimer

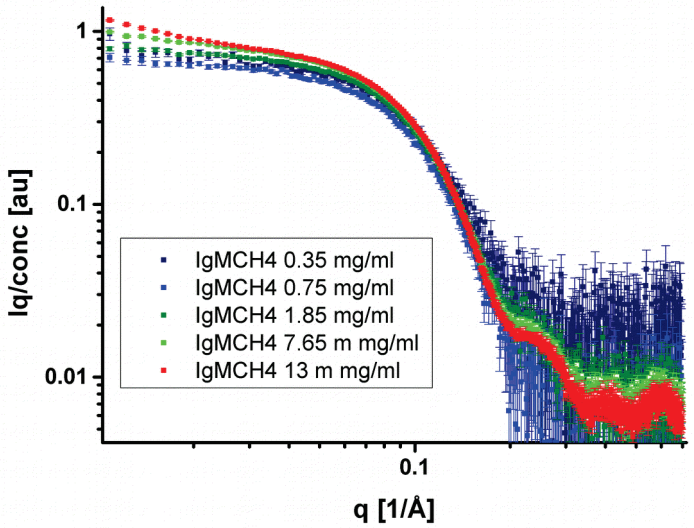


Direct Information

Dimerisation oligomer

IGMCH4 Dimer

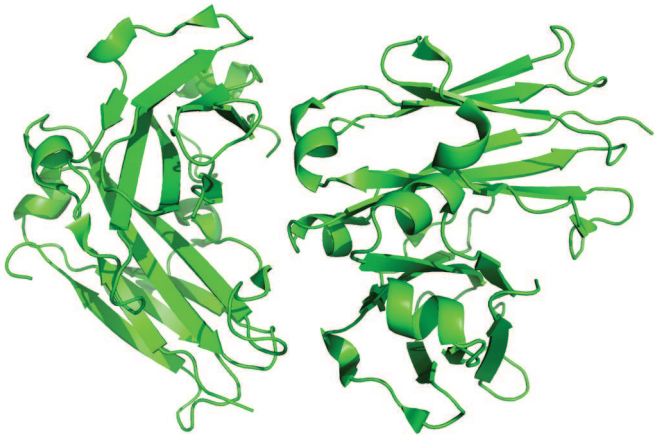


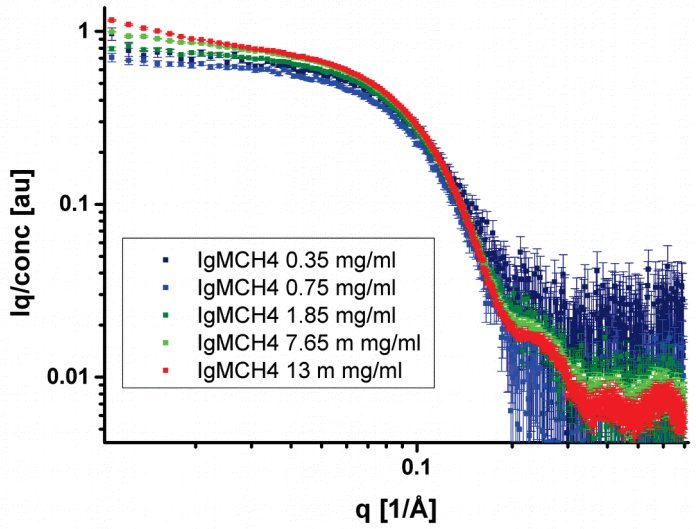


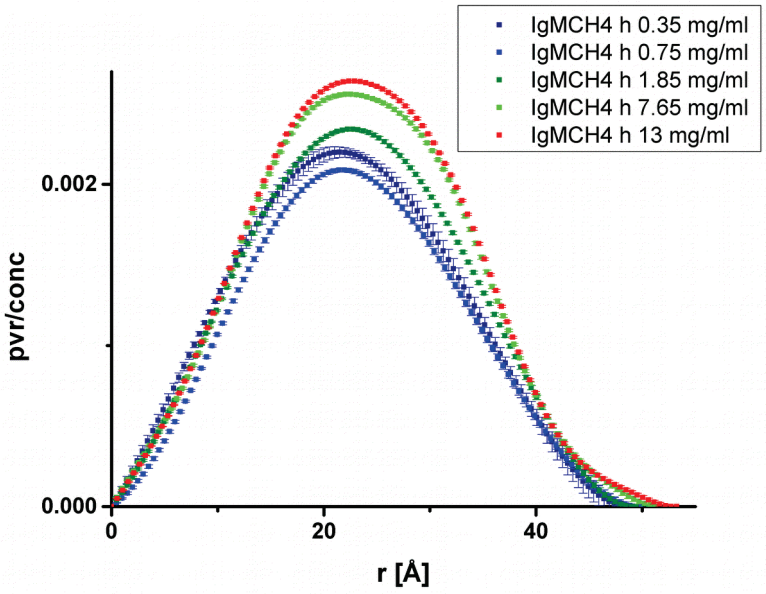
Direct Information

Dimerisation oligomer

IGMCH4 Dimer



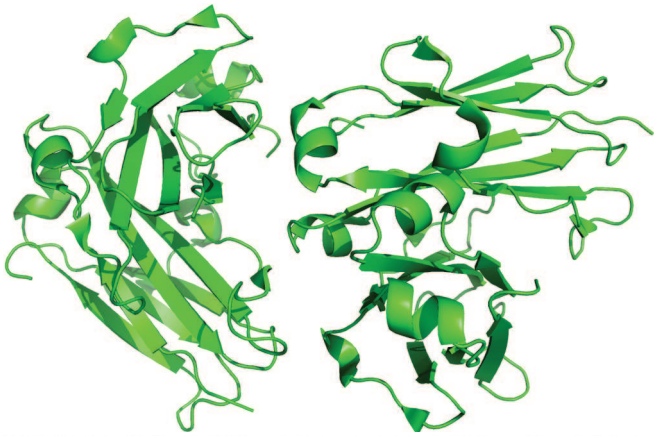


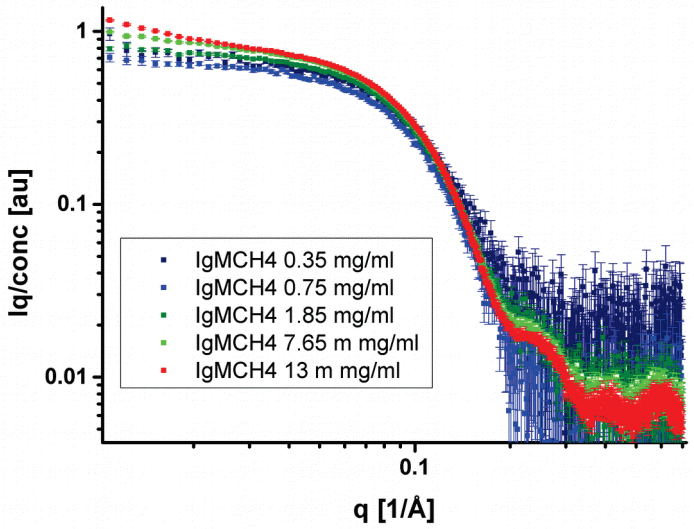


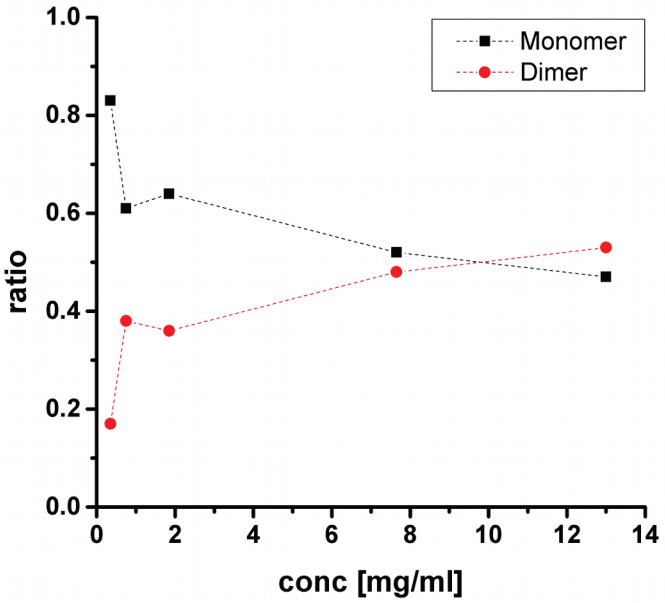
Direct Information

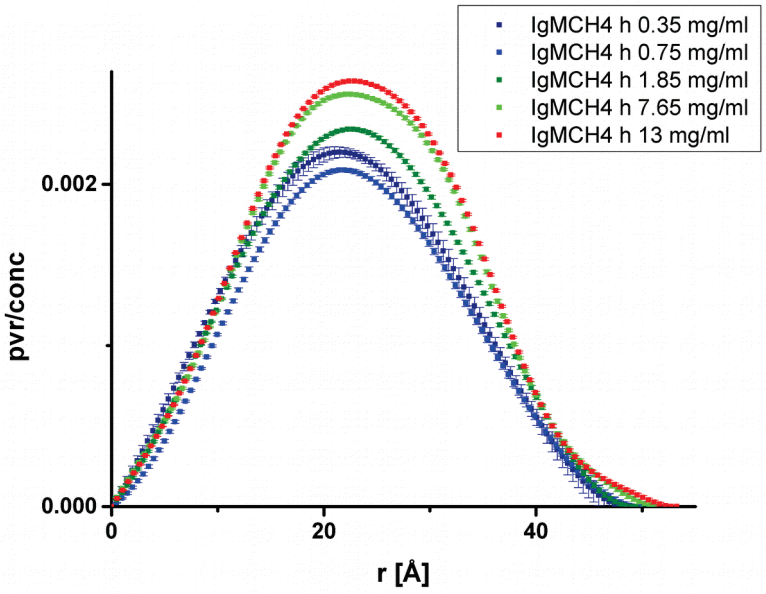
Dimerisation oligomer

IGMCH4 Dimer







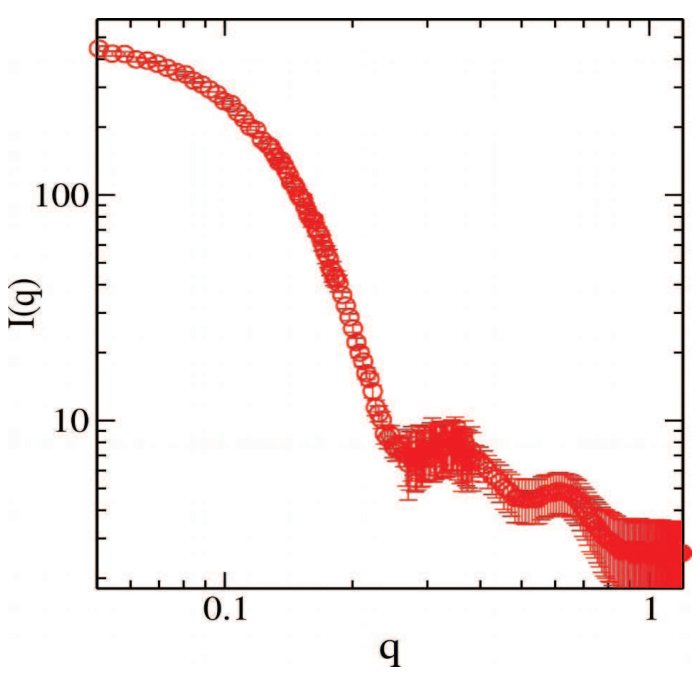


Modeling

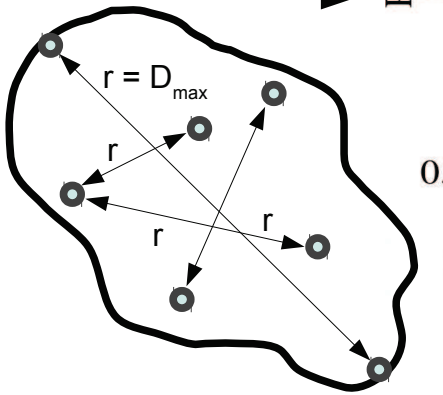
Transformation of scattering curves to real space

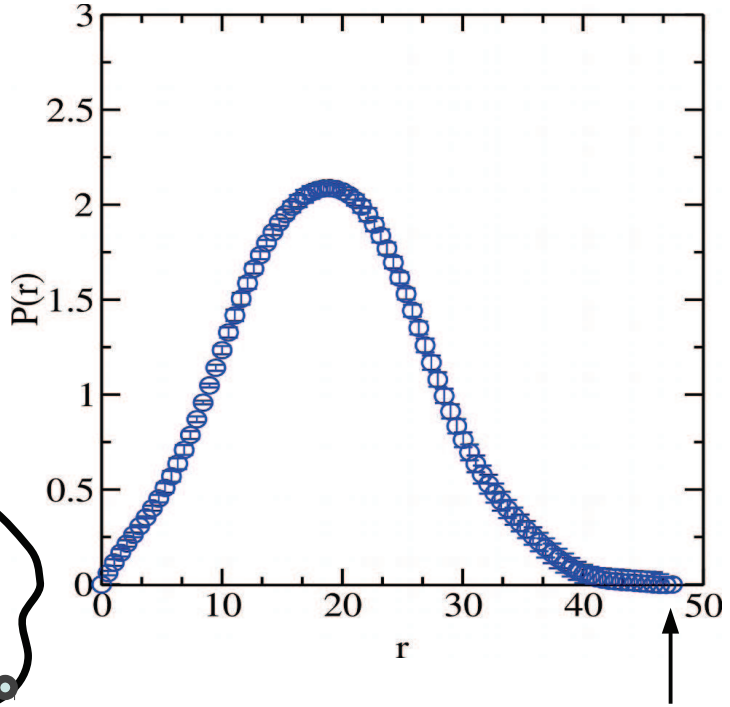
Transformation of the scattering curve from reciprocal space to real space with the programm GNOM to get the

pair distance distribution function p(r) (PDDF)



GNOM

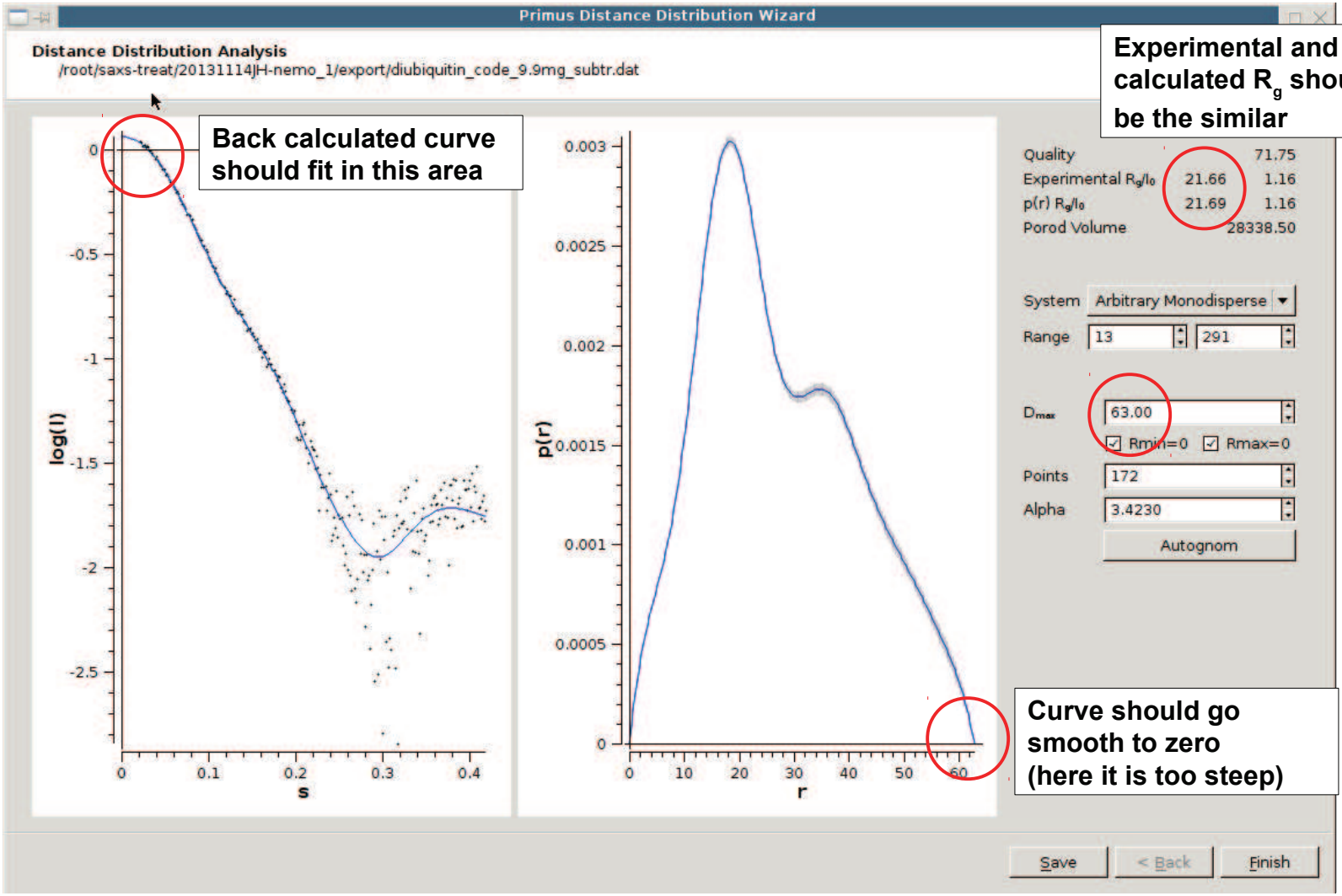




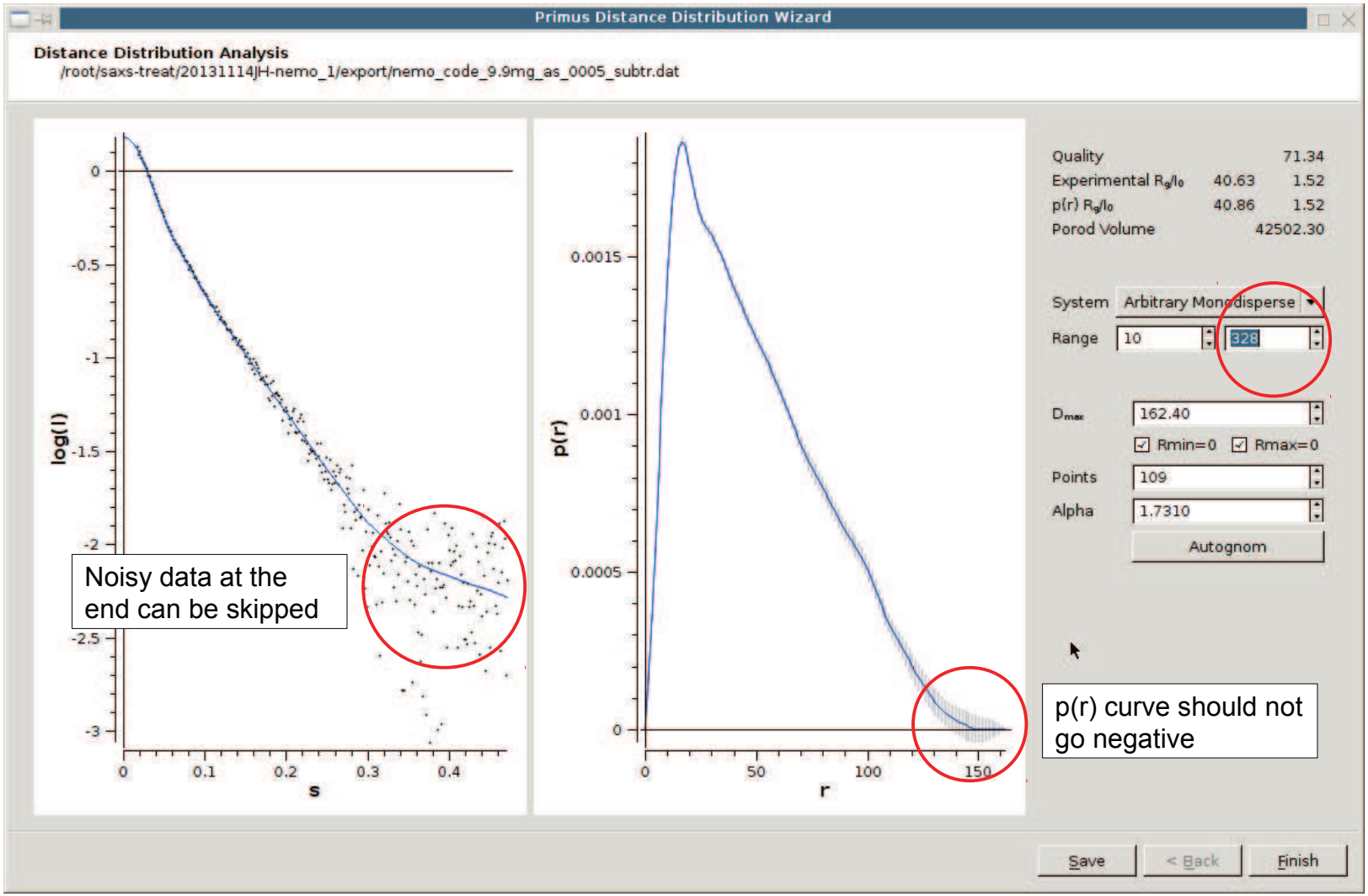
$$p(r) = \frac{r^2}{2\pi^2}\int_0^\infty q^2 I(q)\frac{\sin qr}{qr}dq$$

$$I(0) = 4\pi\int_0^{D\max} p(r)dr$$

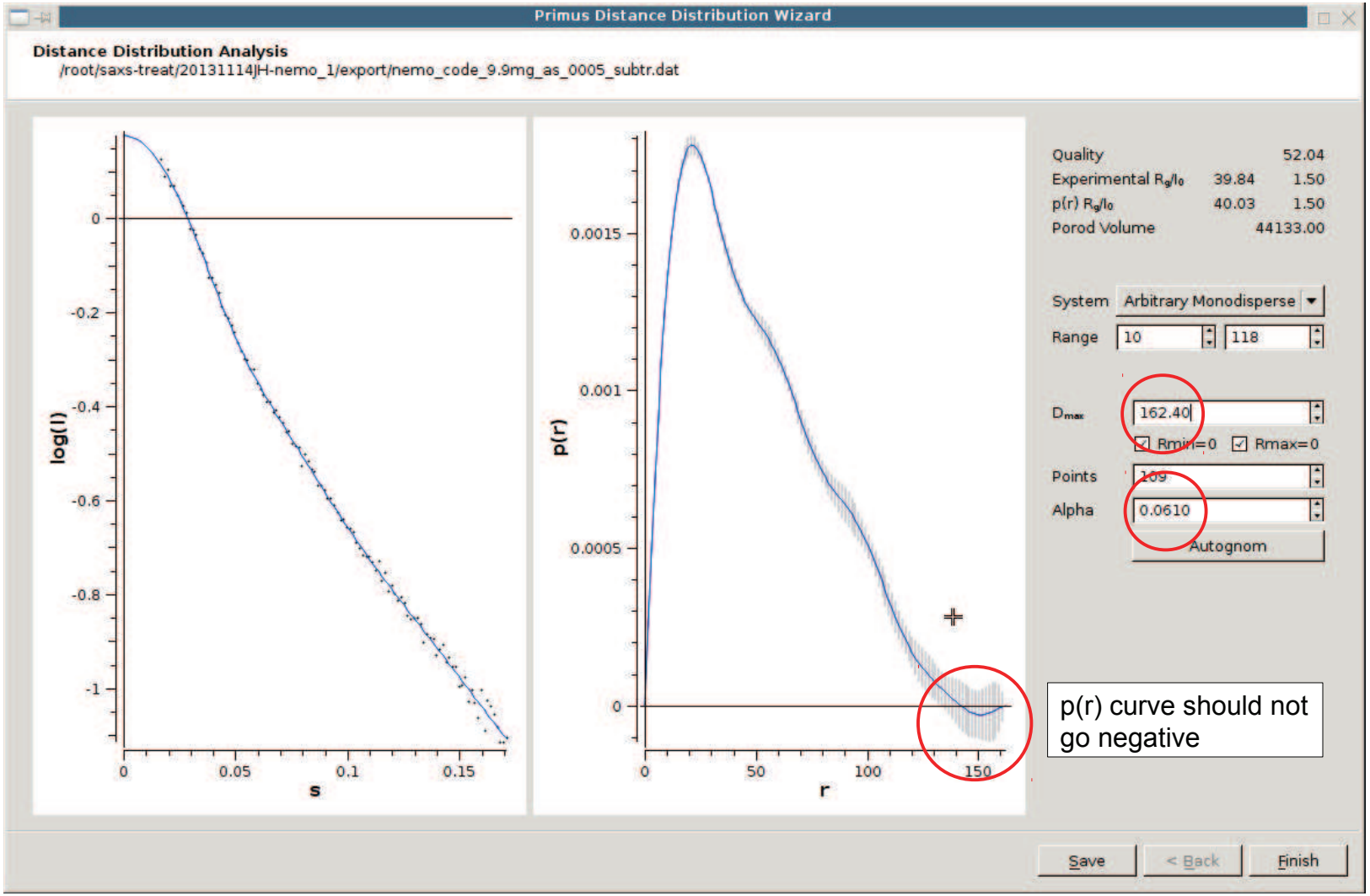
Transformation of scattering curves to real space with GNOM



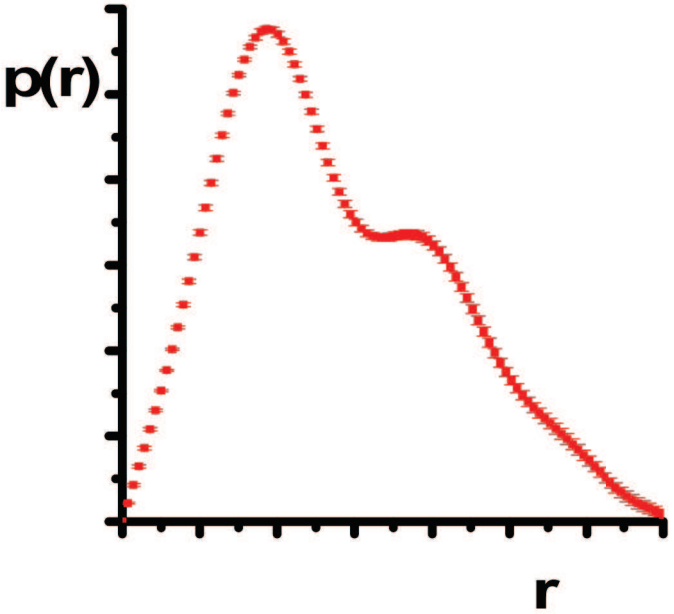
Transformation of scattering curves to real space with GNOM



Transformation of scattering curves to real space with GNOM



Calculating ab initio models

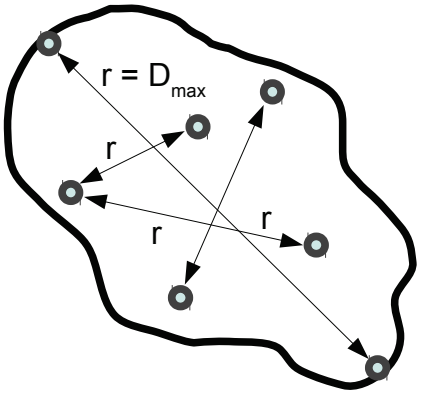


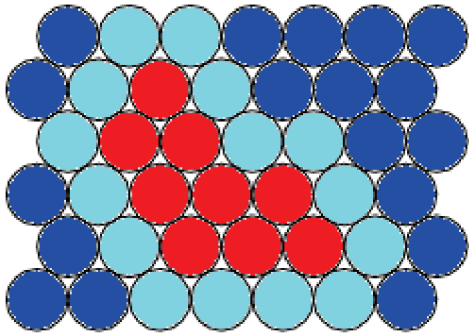
Dammin initially 2000 beads fixed Volume. Each bead can be flipped. Lots of symmetries allowed.

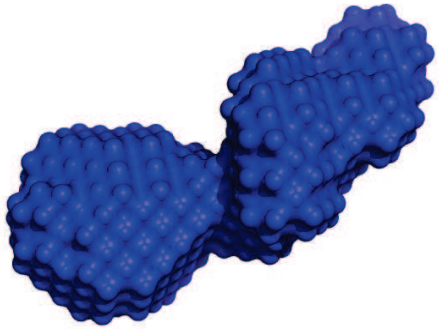
Dammif flexible Volume. Only beads at the phase border can flip. Few symmetries.

Both have problems with flat disks. To avoid this force symmetry (P5, P6)

10-20 models are calculated normally. They are superimposed merged and the result is filtered to the excluded volume of the particle.







Modeling

Ab initio shape determination by simulated annealing using a single phase dummy atom model

Dammin or **Dammif**

Calculation of 10 - 20 models

Damsel

Compare all models, find most probable one and outliers

Damsup

Align all models with the most probable one

Average aligned models and compute probability map

Damaver

Damclust

Sorts similar models into groups

Filters the averaged model at a given cut-off volume

Damfilt

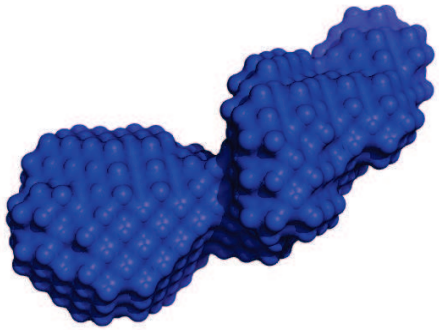
Groups of similar models

Generates an input file from the averaged model with fixed core for dammin

Damstart

Dammin

refined model



Rigid body modeling

Rigid body modeling

Fit of partial structures to SAXS data

sasref fit of complexes. Input multiple chains. Symetry and distance constrains possible.

coral fit of multi domain proteins. Lines up domains to one chain. Flexible linkers are taken from a database. Symetry and distance constrains possible.

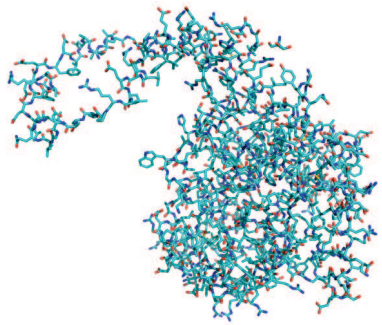
bunch fit of multi domain proteins. Needs a sequence including missing and flexible parts. Domains are rotated around residues of flexible parts. Distance constrains possible.

eom ensemble calculation. Produces 10000 structures clusters them to “chromosomes” and fits them with an evolutionary approach to the experimental data. Lines up domains to one chain. Flexible linkers have to be defined. Symetry and distance constrains possible in a limited way.

Rigid body modeling

Fit of partial structures to SAXS data: sasref

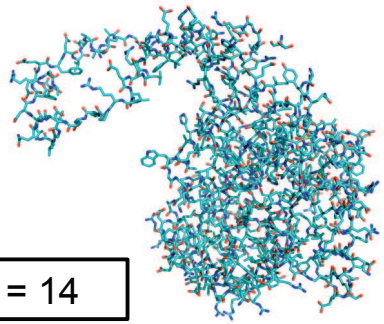
```
$ sasref
  === SASREF06  started at          21-May-2015   10:42:49
Computation mode ..................................... : User
Project identificator ................................ : c9
Project decsription .................................. : c9
Random sequence initialized from ..................... : 104249989
Total number of subunits ............................. : 1
Point symmetry of the particle ....................... : P222
Number of equivalent positions ....................... : 4
Total number of scattering curves .................... : 1
1-st construct, of the first and the last subunits: 1,1
File name, 1-st experimental data .................... : sub_004.dat
Number of experimental points found .................. : 1370
Angular units multiplied by .......................... : 0.1000
Experimental radius of gyration ...................... : 248.0
Number of points in the Guinier Plot ................. : 5
Amplitudes, 1-st subunit ............................. : mon00.alm
Number of points in partial ampliudes ................ : 51
Maximum order of harmonics ........................... : 15
Evaluated from the file .............................. : mon.pdb
Current subunit:   3089 atoms read, center at     0.03   -0.02     0.11
Spatial step in angstroems ........................... : 5.000
Angular step in degrees .............................. : 20.00
Cross value .......................................... : 68.20
Dock value ........................................... : 0.0
Discontiguity value .................................. : 0.0
Cross penalty weight ................................. : 10.00
Disconnectivity penalty weight ....................... : 10.00
Docking penalty weight ............................... : 0.5000
Expected particle anisometry ......................... : Unknown
.
.
```



Rigid body modeling

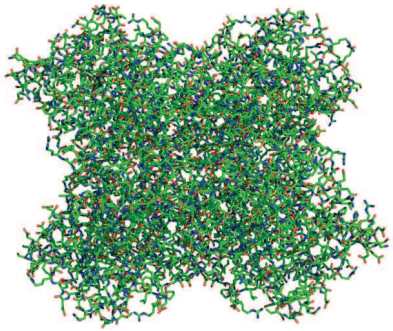
Fit of partial structures to SAXS data: sasref

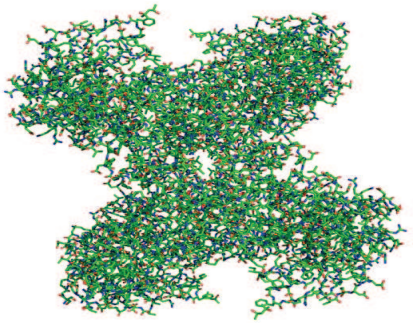
```
$ sasref
  === SASREF06  started at          21-May-2015   10:42:49
Computation mode ..................................... : User
Project identificator ................................ : c9
Project decsription .................................. : c9
Random sequence initialized from ..... : 104249989
Total number of subunits ............................. : 1
Point symmetry of the particle ....................... : P222
Number of equivalent positions ..... : 4
Total number of scattering curves .................... : 1
1-st construct, of the first and the last subunits: 1,1
File name, 1-st experimental data .................... : sub_004.dat
Number of experimental points found ..... : 1370
Angular units multiplied by ..... : 0.1000
Experimental radius of gyration ..... : 248.0
Number of points in the Guinier Plot ..... : 5
Amplitudes, 1-st subunit ............................. : mon00.alm
Number of points in partial ampliudes ..... : 51
Maximum order of harmonics ..... : 15
Evaluated from the file ..... : mon.pdb
Current subunit:   3089 atoms read, center at     0.03   -0.02     0.11
Spatial step in angstroems ..... : 5.000
Angular step in degrees ..... : 20.00
Cross value ..... : 68.20
Dock value ..... : 0.0
Discontiguity value ..... : 0.0
Cross penalty weight ..... : 10.00
Disconnectivity penalty weight ..... : 10.00
Docking penalty weight ..... : 0.5000
Expected particle anisometry ..... : Unknown
.
```

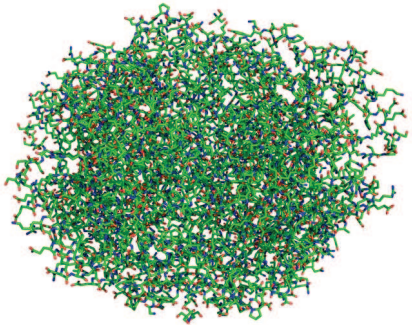


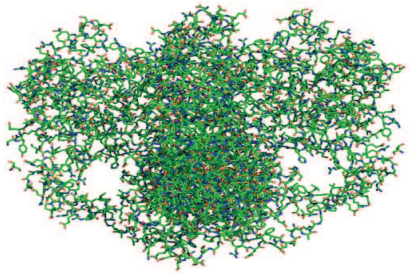
$X^2 = 14$

$X^2 = 0.9$





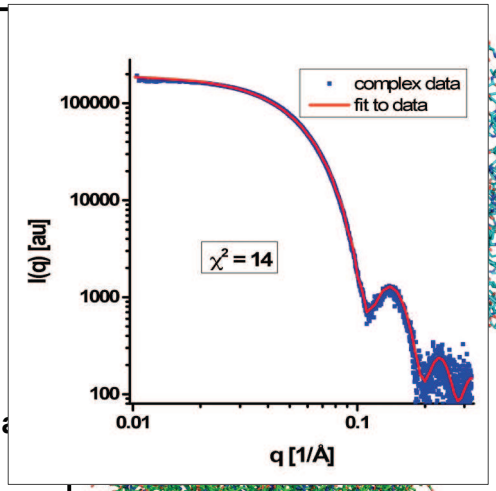


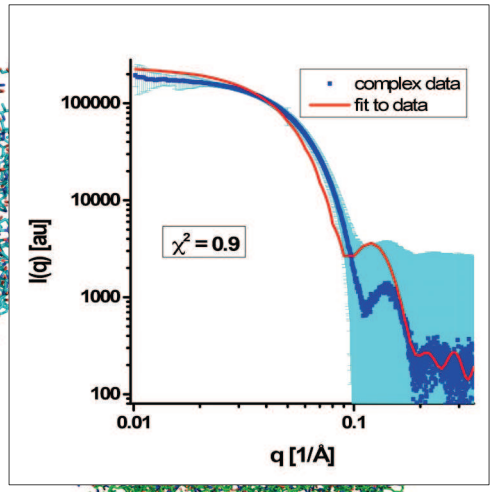


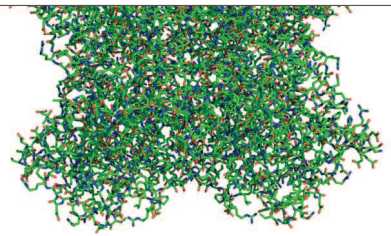
Rigid body modeling

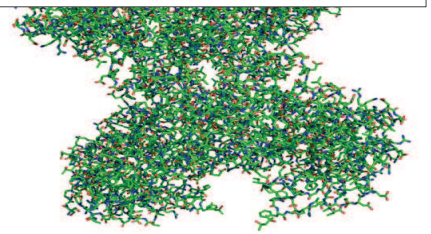
Fit of partial structures to SAXS data: sasref

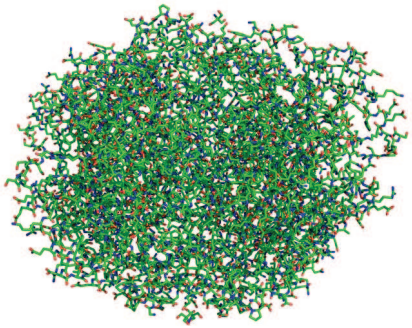
```
$ sasref
  === SASREF06  started at          21-May-2015   10:42:49
Computation mode ..................................... : User
Project identificator ................................ : c9
Project decsription .................................. : c9
Random sequence initialized from ..... : 104249989
Total number of subunits ............................. : 1
Point symmetry of the particle ....................... : P222
Number of equivalent positions ..... : 4
Total number of scattering curves .................... : 1
1-st construct, of the first and the last subunits: 1,1
File name, 1-st experimental data .................... : sub_004.da
Number of experimental points found ..... : 1370
Angular units multiplied by ..... : 0.1000
Experimental radius of gyration ..... : 248.0
Number of points in the Guinier Plot ..... : 5
Amplitudes, 1-st subunit ............................. : mon00.alm
Number of points in partial ampliudes ..... : 51
Maximum order of harmonics ..... : 15
Evaluated from the file ..... : mon.pdb
Current subunit:   3089 atoms read, center at     0.03   -0.02     0.11
Spatial step in angstroems ..... : 5.000
Angular step in degrees ..... : 20.00
Cross value ..... : 68.20
Dock value ..... : 0.0
Discontiguity value ..... : 0.0
Cross penalty weight ..... : 10.00
Disconnectivity penalty weight ..... : 10.00
Docking penalty weight ..... : 0.5000
Expected particle anisometry ..... : Unknown
.
```

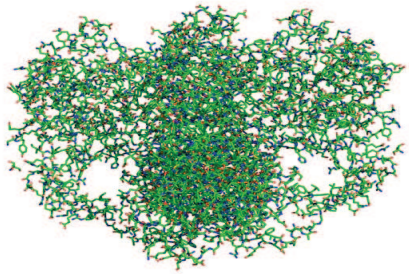








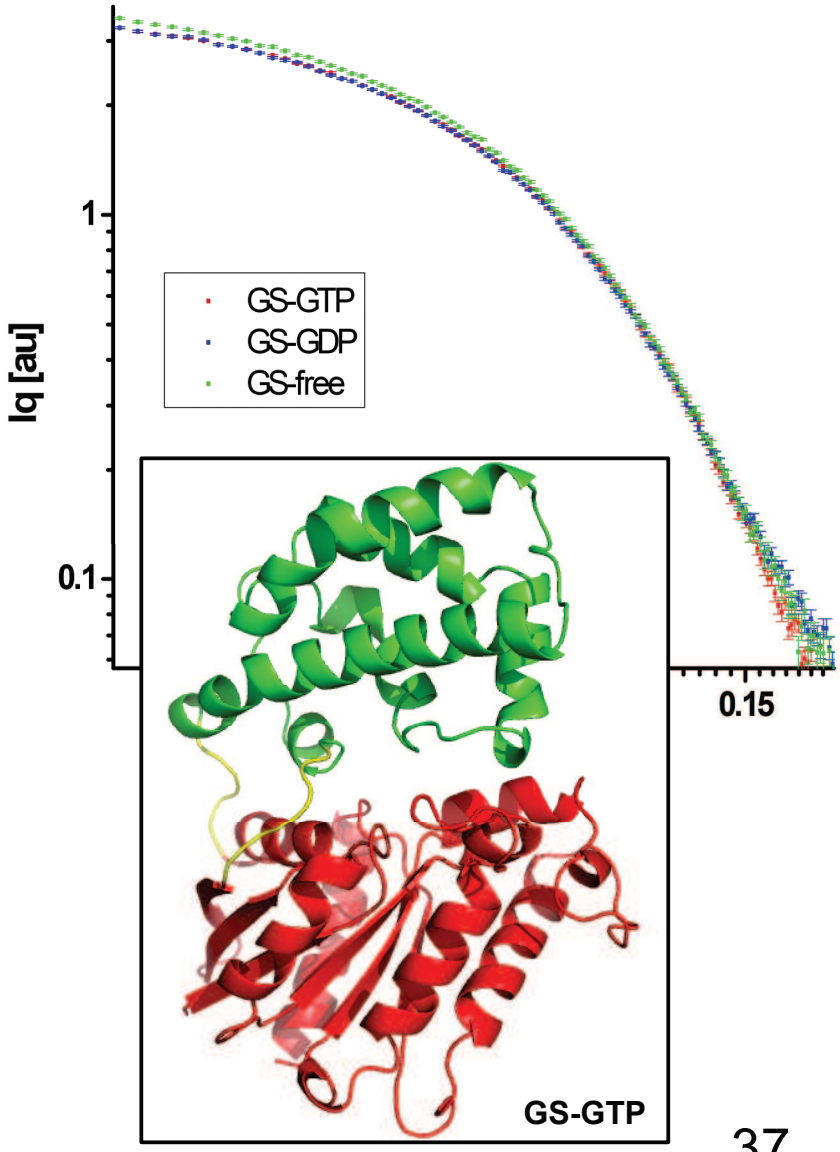




Rigid body modeling

Fit of partial structures to SAXS data: coral

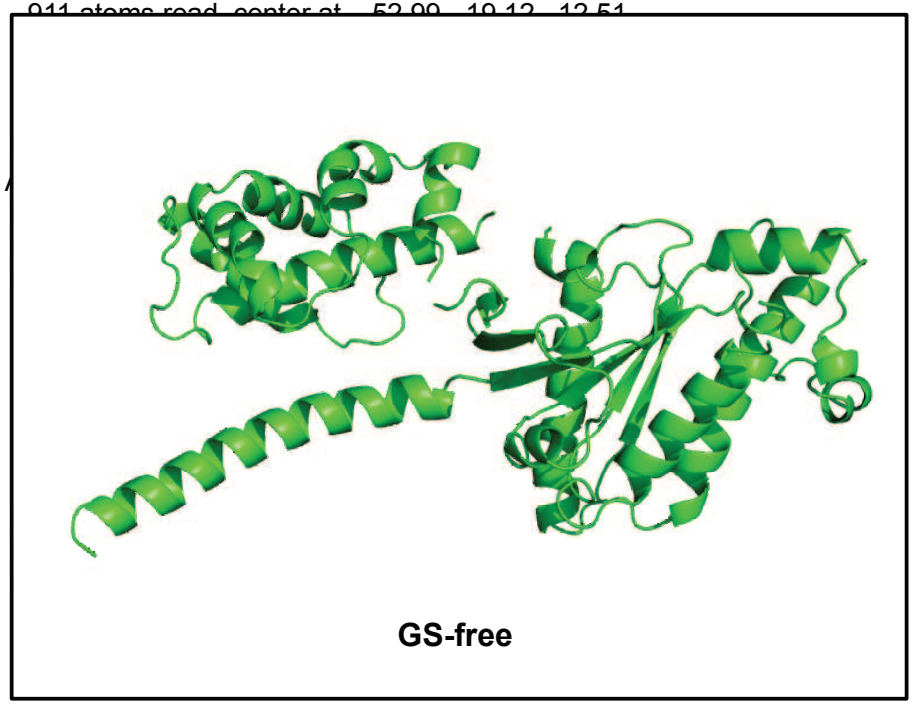
```
$ coral
   === CORAL05  started at          23-Apr-2015   19:35:35
 Computation mode ..................................... : User
 Project identificator ................................ : 2-0a
 Project decsription .................................. : 2-0a
 Random sequence initialized from ..... : 193535
 File name with objects info .......... : c.con
 Coordinates of the 1-st subunit evaluated from ..... : RED1.pdb
   198 atoms read, center at    26.89  -26.80    8.09
 Subunit was fixed
 Coordinates of the 2-nd subunit evaluated from ..... : GREEN.pdb
   911 atoms read, center at    52.99  -19.12   12.51
 Coordinates of the 3-rd subunit evaluated from ..... : RED2.pdb
   1386 atoms read, center at    31.86  -35.37    1.03
 Subunit was fixed
 Number of backbone atoms generated ..... : 316
Averaged formfactors of DRs used
 DR formfactor multiplier ..... : 1.000
 Point symmetry of the particle ..... : P1
 Number of equivalent positions ..... : 1
 Cross penalty ..... : 0.3349
 Cross penalty weight ..... : 100.0
 Shift penalty ..... : 2.376
 Shift penalty weight ..... : 1.000
 Total number of scattering curves ..... : 1
 1-st construct, the first and the last residues: 1   and   316
 File name, 1-st experimental data ..... : GS-GTP-10mg.dat
 Number of experimental points found ..... : 481
 Experimental radius of gyration ..... : 22.20
 .
 .
 .
```

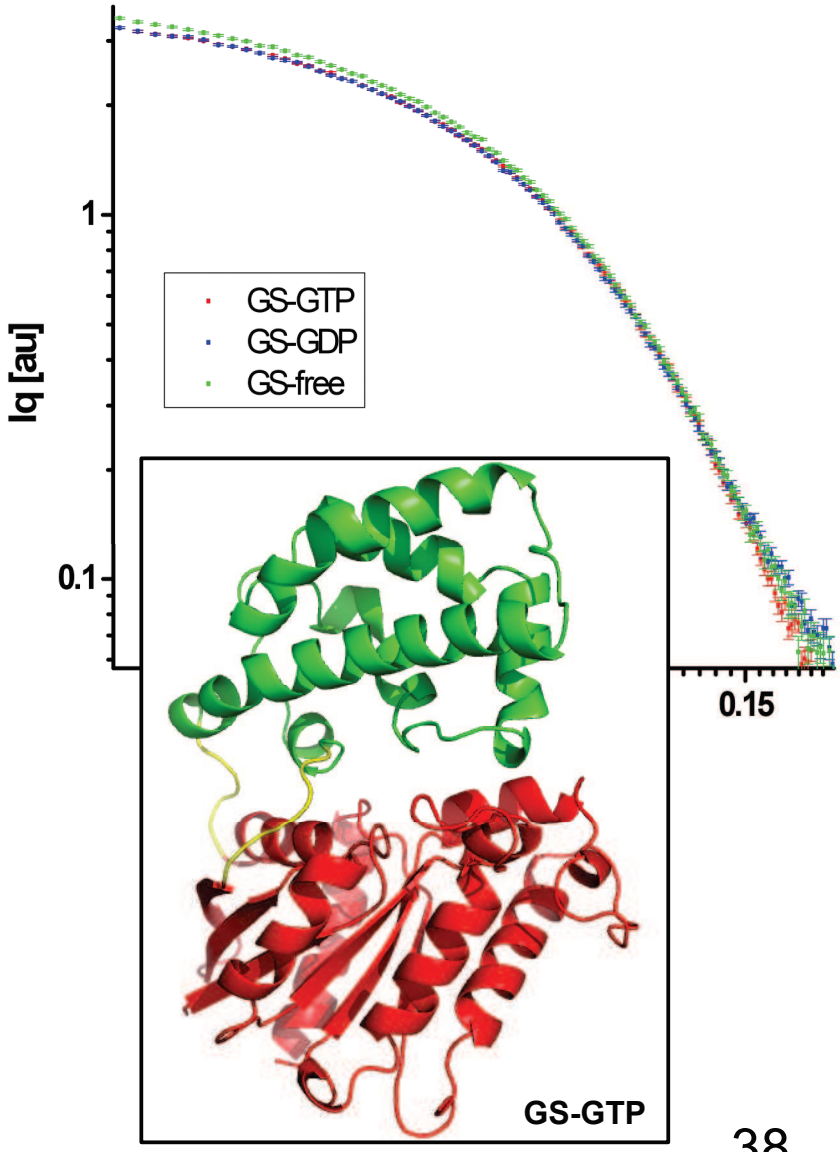


Rigid body modeling

Fit of partial structures to SAXS data: coral

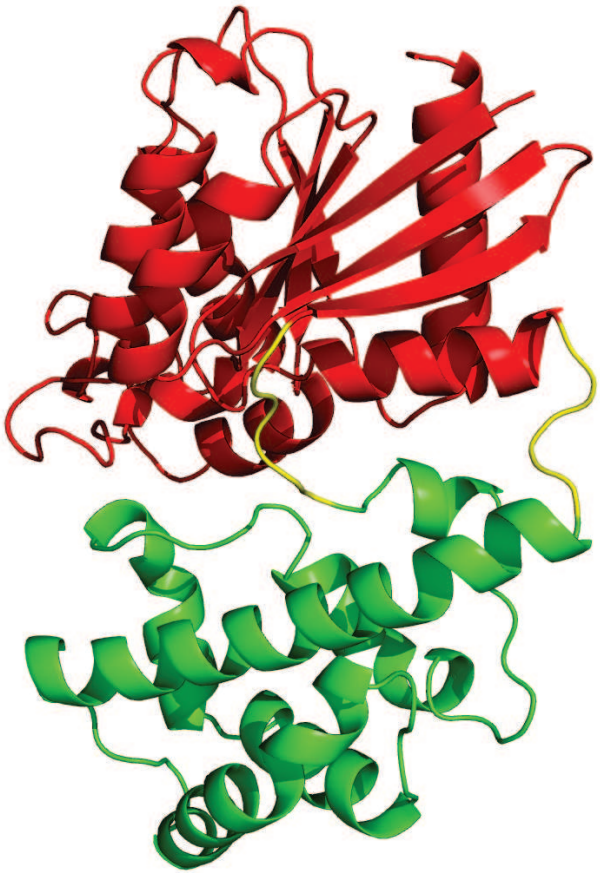
```
$ coral
   === CORAL05  started at          23-Apr-2015   19:35:35
Computation mode ..................................... : User
Project identificator ................................ : 2-0a
Project decsription .................................. : 2-0a
Random sequence initialized from ..................... : 193535
File name with objects info .......................... : c.con
Coordinates of the 1-st subunit evaluated from ..... : RED1.pdb
  198 atoms read, center at    26.89  -26.80    8.09
Subunit was fixed
Coordinates of the 2-nd subunit evaluated from ..... : GREEN.pdb
  911 atoms read, center at    52.99   19.13   12.51
```



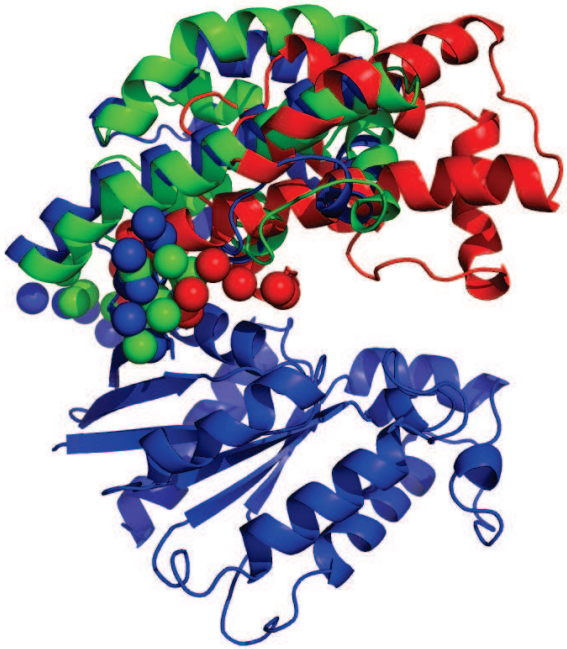


Rigid body modeling

Fit of partial structures to SAXS data: coral

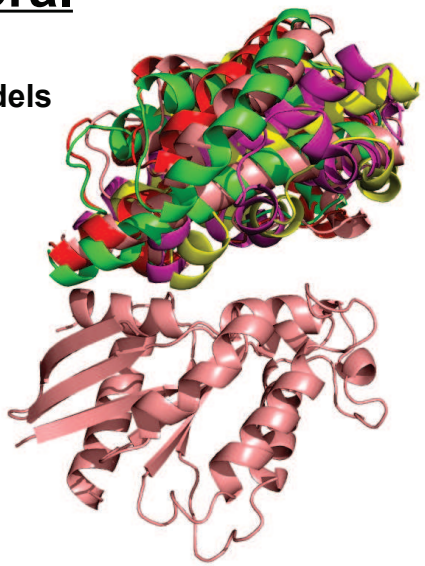


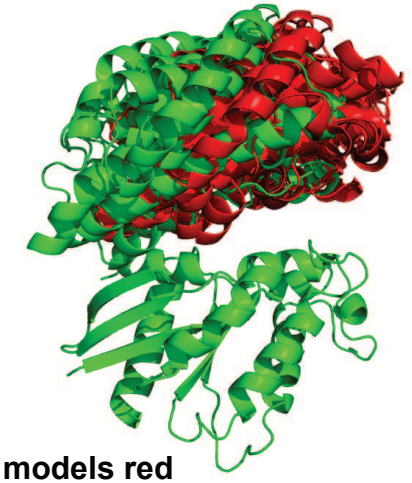
GS-GTP crystal



GS-GTP red
GS-GDP green
GS-free blue

GS-GTP 5 models



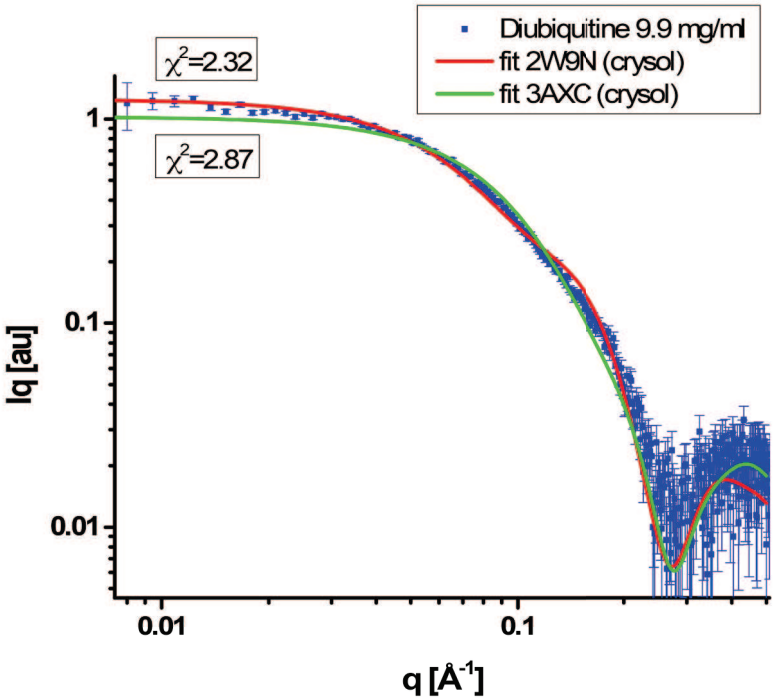


GS-GTP 5 models red
GS-GDP 5 models green

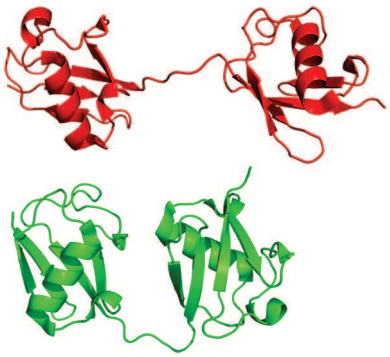
Rigid body modeling

Fit of pieces of structures to SAXS data: eom

```
$ eom
   RANCH  Version 2.0
 Started: ..... : Fri Oct 17 16:06:44 2014
 iSeed ..... : 1934479814
 Chain type ..... : Random
 Sequence file name: ..... : sequence.seq
 Symmetry: ..... : P1
 Symmetry type: ..... : aSymmetric
 Number of residues: ..... : 1142
 Number of domains: ..... : 2
 ----------
 Domain number: ..... : 1
 Path: ..... : diubi1.pdb
 Fixed: ..... : 0
 Oligomer: ..... : 0
 DNA file name: ..... : None
 ----------
 Domain number: ..... : 2
 Path: ..... : diubi2.pdb
 Fixed: ..... : 0
 Oligomer: ..... : 0
 DNA file name: ..... : None
 Contact file name: ..... : None
 Number of structures: ..... : 10000
 Suffix of the pdb files: ..... : eom
 Output Folder Path: ..... : ./
 Number of experimental curves: ..... : 1
 Experimental data filename (curve 1): ..... : diubi_9p9_subtr.dat
.
```



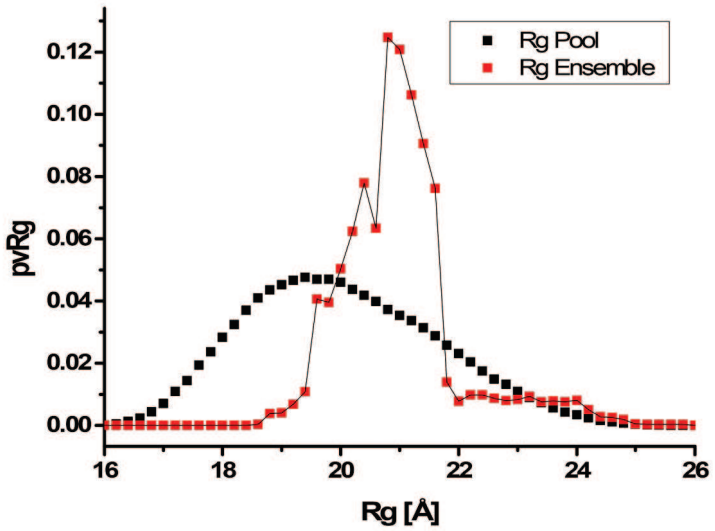
Crystal structures
2W9N (red)
3AXC (green)

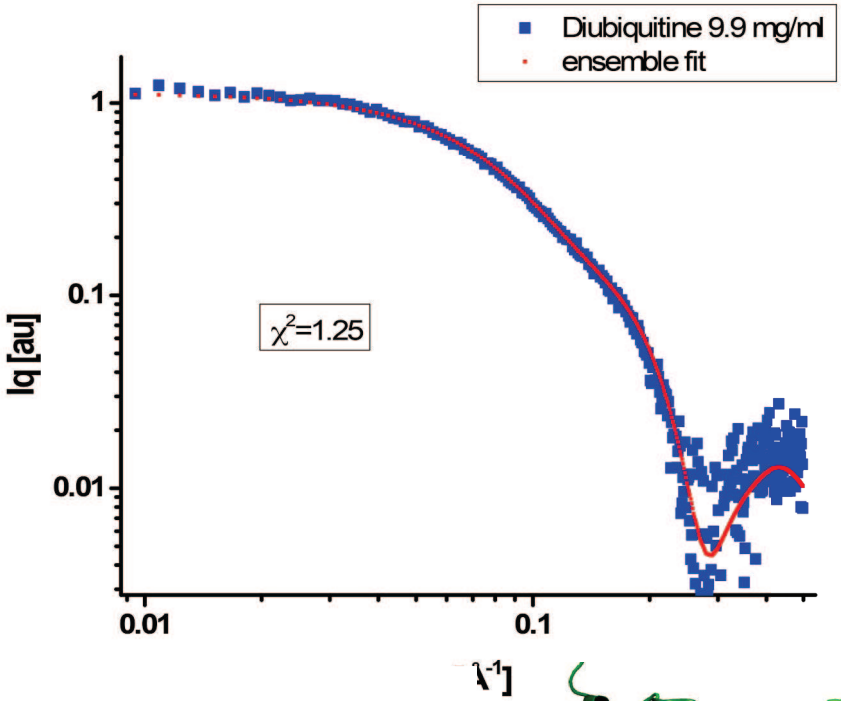


Sequence file has fasta format (without comments and chain information)

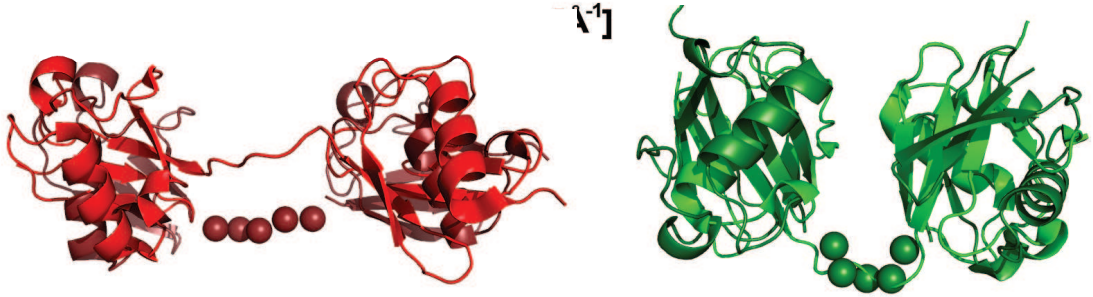
Rigid body modeling

Fit of pieces of structures to SAXS data: eom



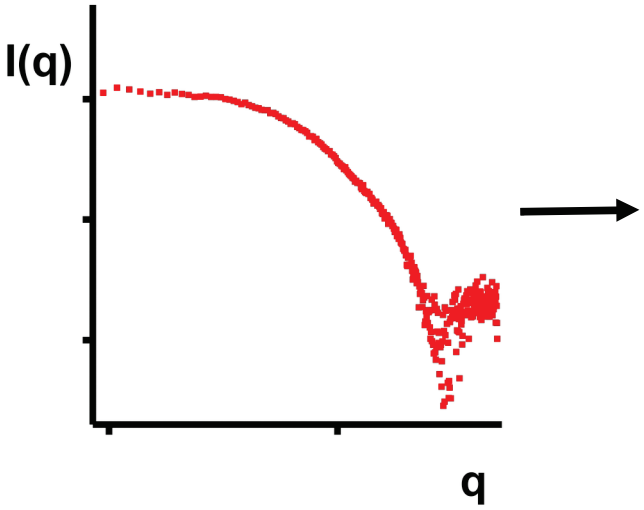


Overlay of Enseble Models and Crystal Structures



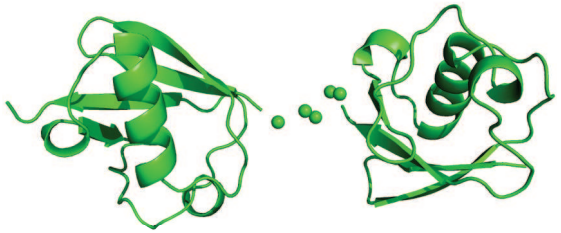
Distance **15 [Å]** **9 [Å]**

Indirect Information

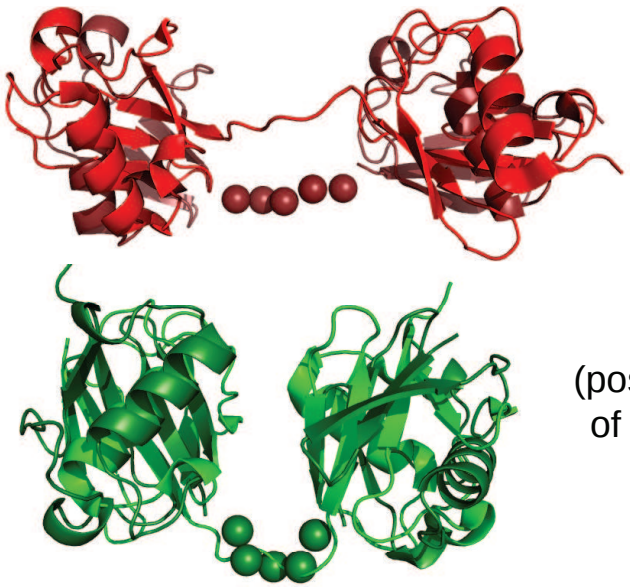


Depending on the initial assumption or question modeling of data with different software leads to different results.

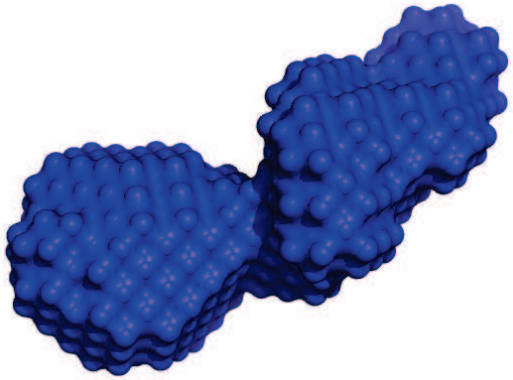
All these results are correct within the limiting factors of the software



Rigid body model
(average structure)

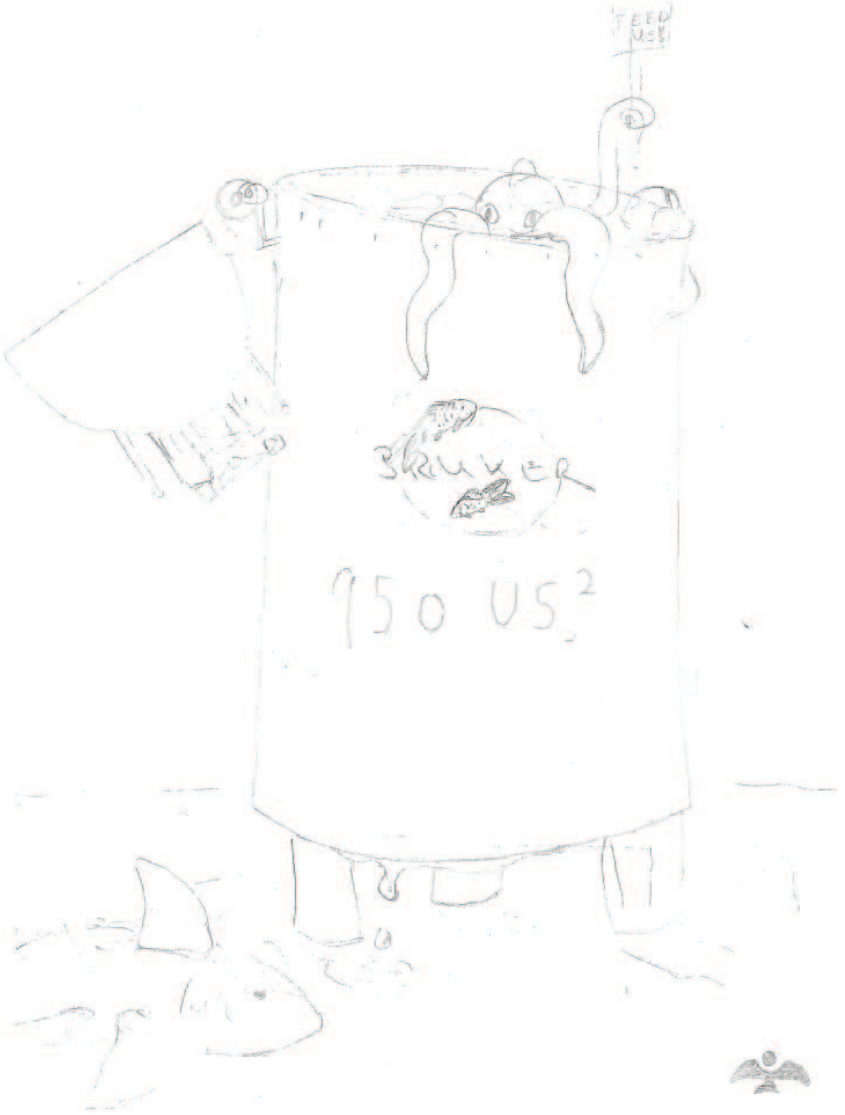


Ensemble
Ratio
38:62
(possible conformations of a flexible molecule)



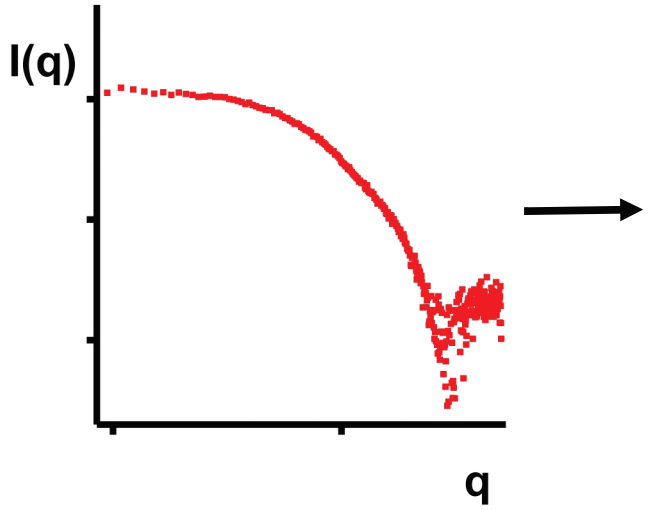
Dummy model
(bead model without any structural information)

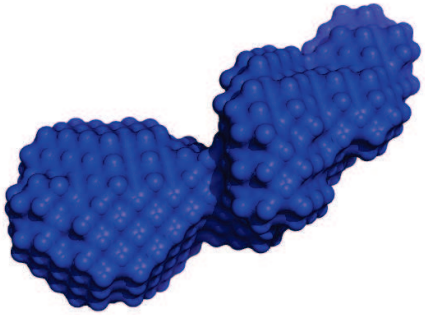
Thanks



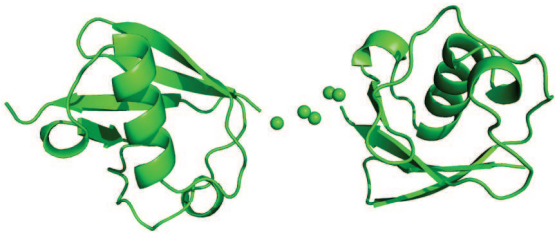
Rigid body modeling

Rigid body modeling





Dummy model



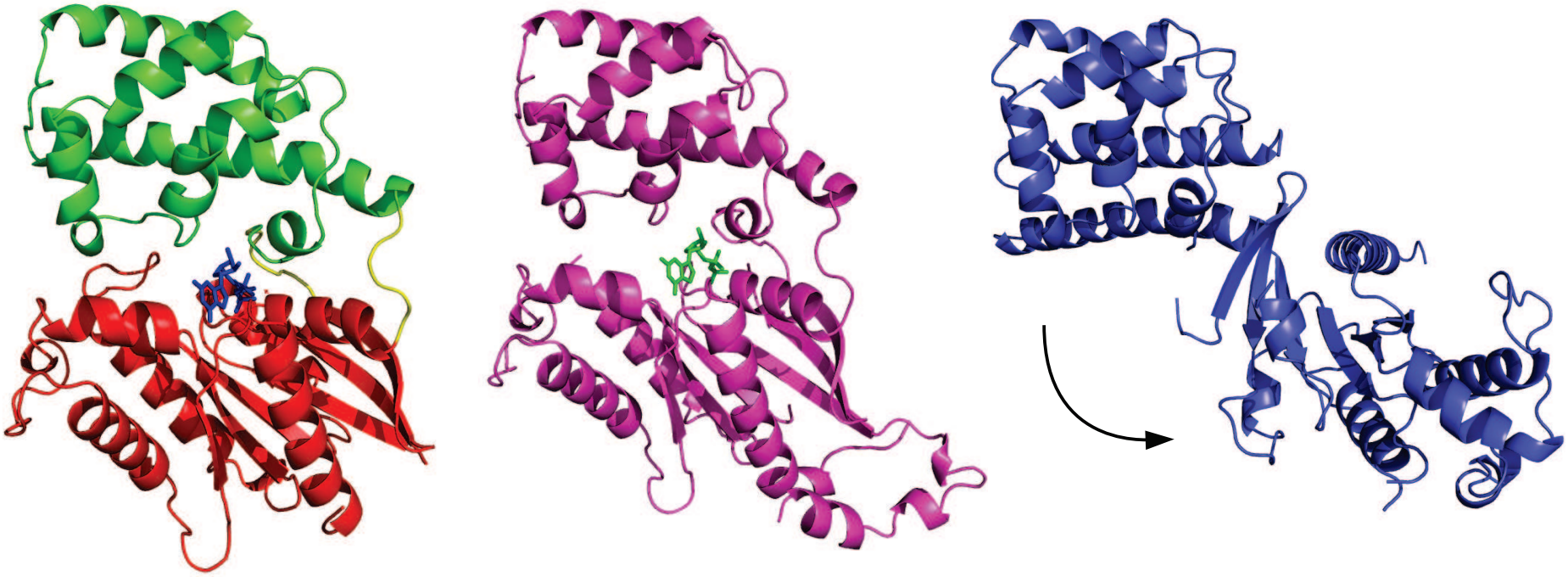
Rigid body model

Crystal Structure

- Arrangement of domains in space

Conformations of a G-protein

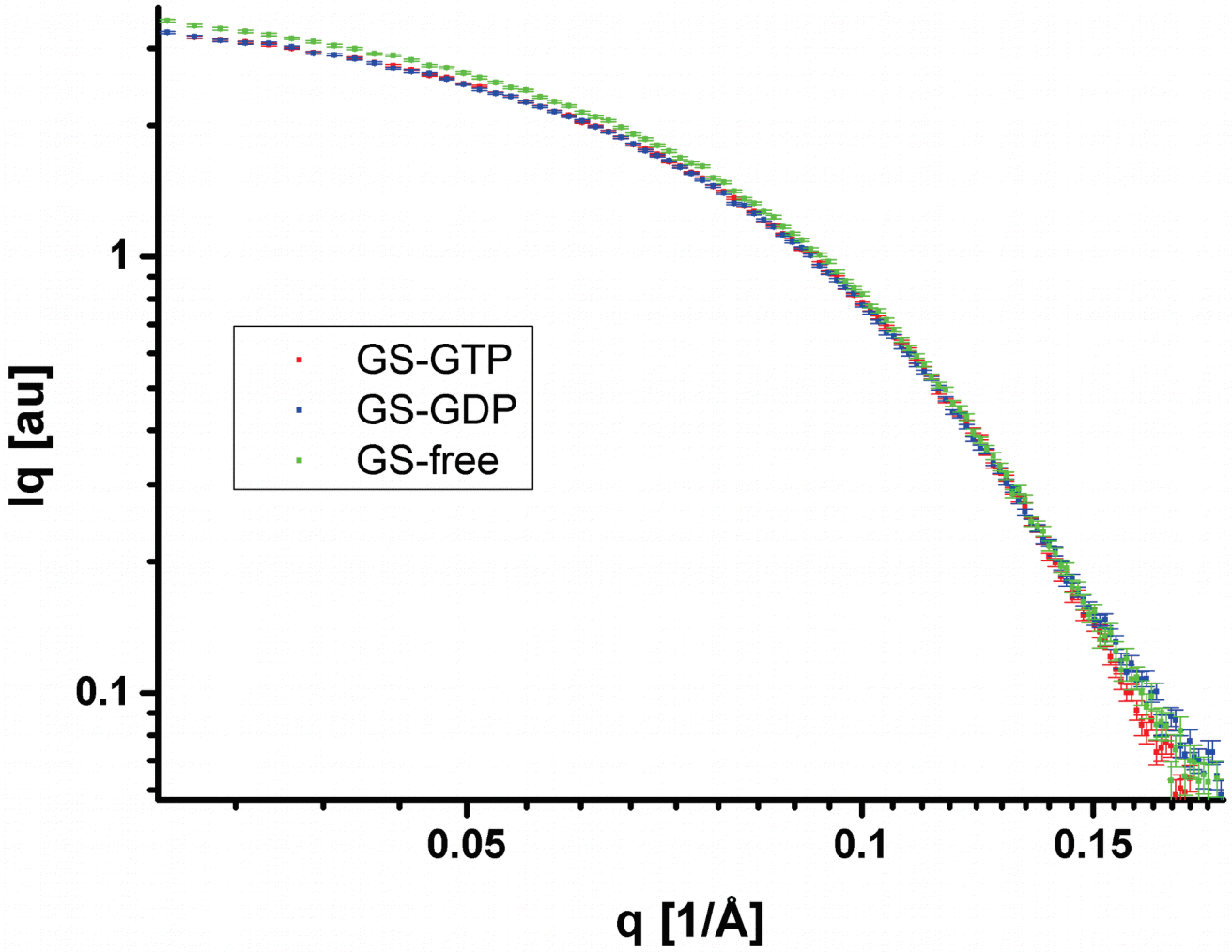
Crystal structures available for all three states



GTP GDP free

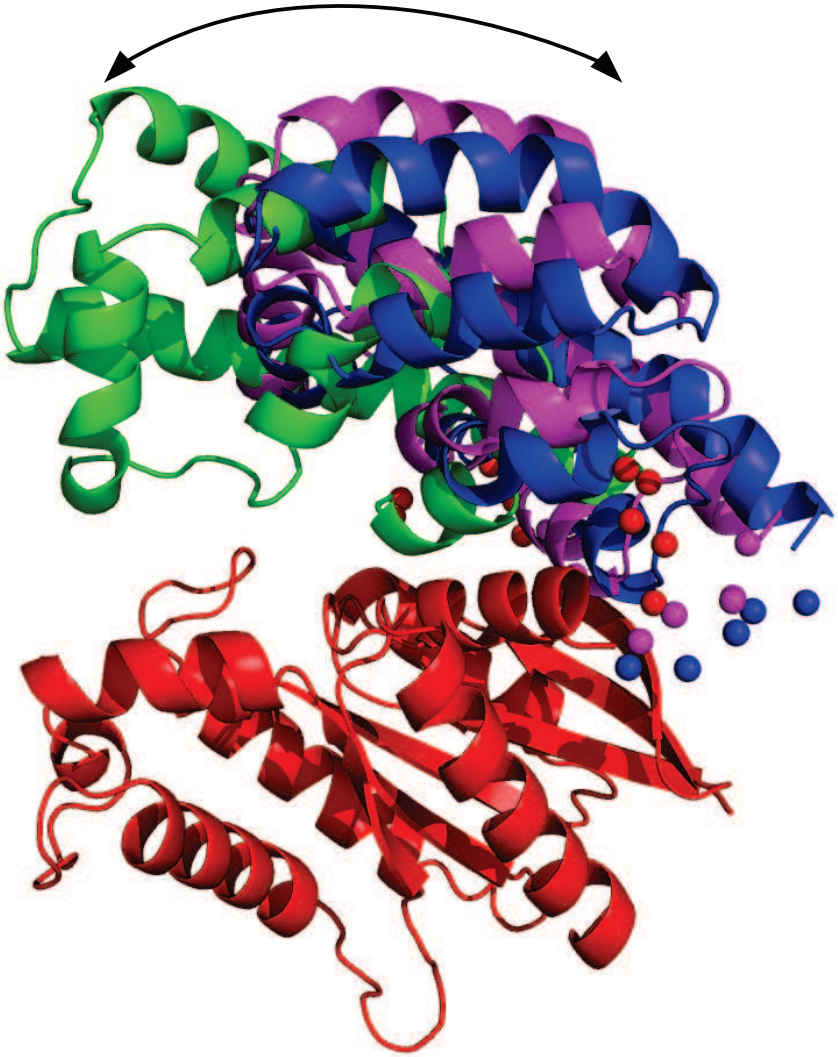
Conformations of a G-protein

Scattering data



Conformations of a G-protein

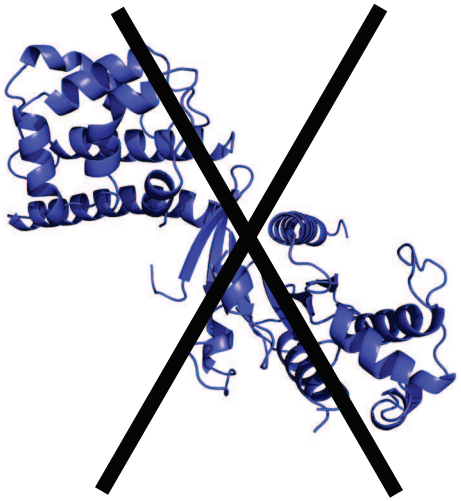
Conformations of the G-protein in solution



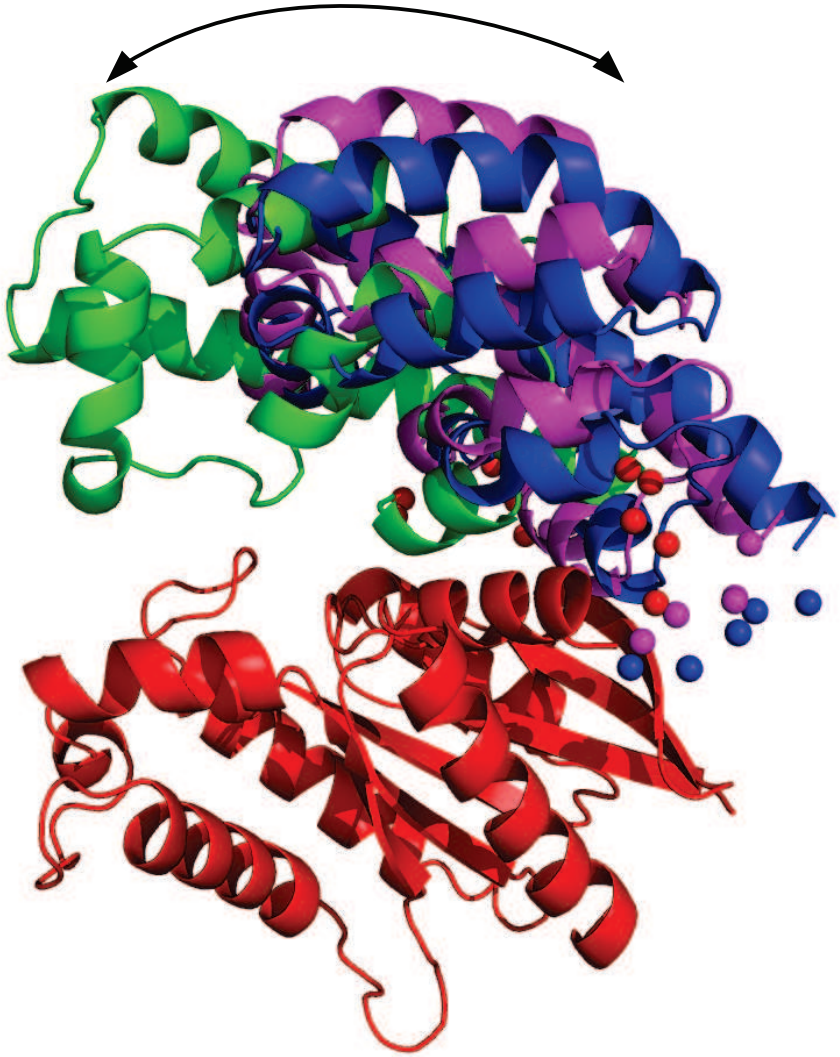
GTP green
GDP magenta
free blue

Conformations of a G-protein

Conformations of the G-protein in solution



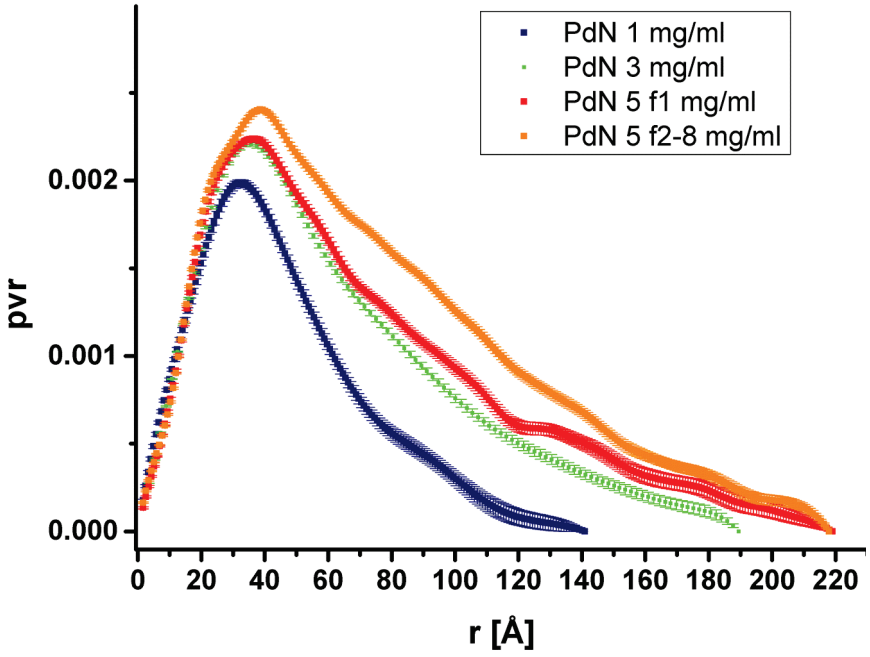
free

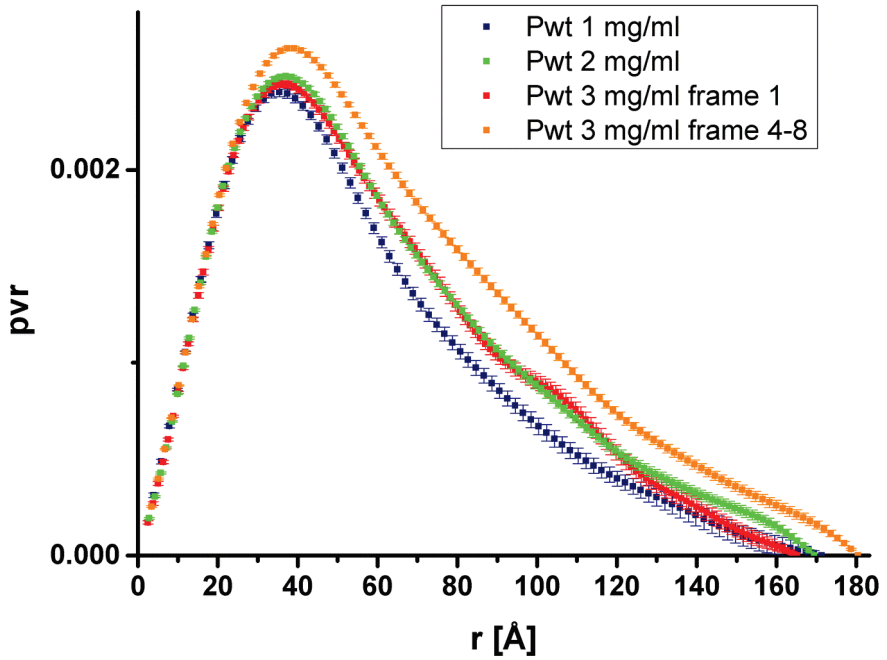


GTP green
GDP magenta
free blue

Protein structural issues

Is the N-terminus unstructured?
Is the N-terminus responsible for dimerisation?



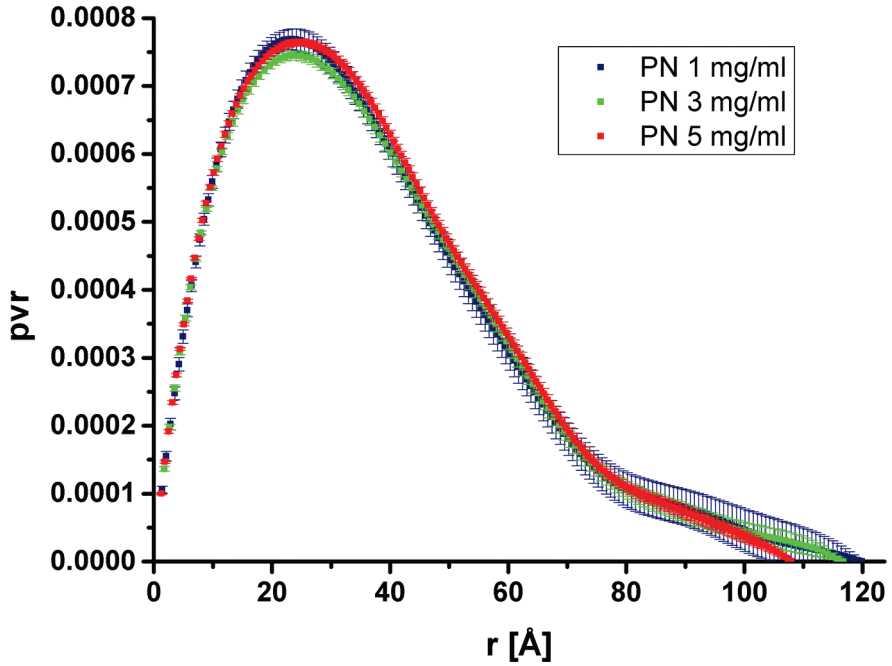


- δN-construct seems unstable
- Concentration dependent growth of size
- Dimerisation or agglomeration

- WT is a bit more stable
- Concentration dependent growth of size
- Dimerisation or agglomeration

Protein structural issues

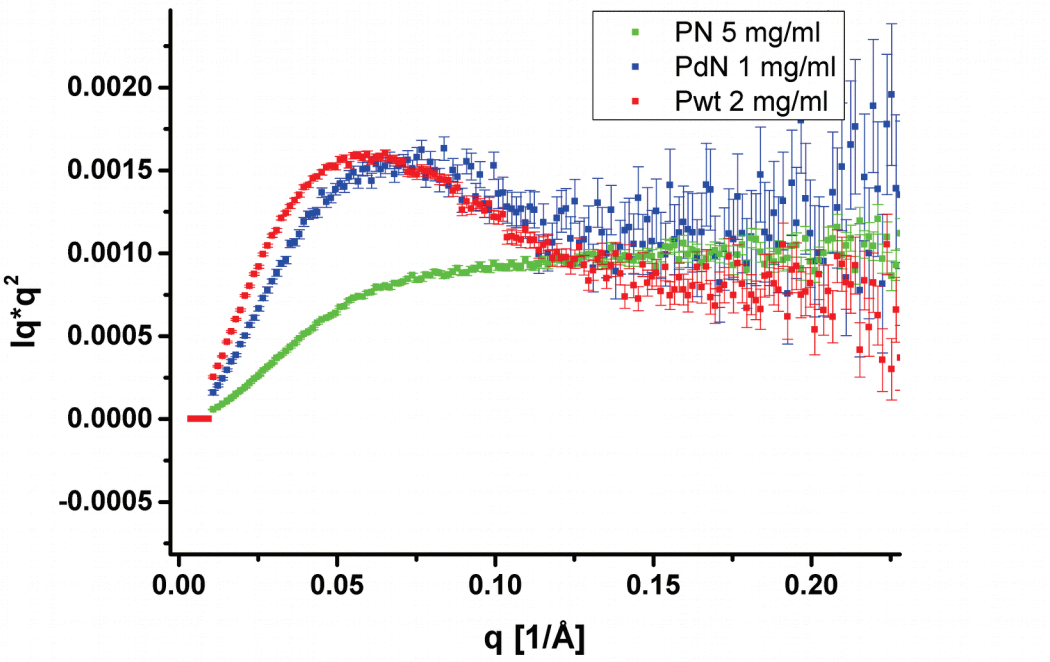
Is the N-terminus unstructured?
Is the N-terminus responsible for dimerisation?



- N-terminal part stable
- No concentration dependent behaviour

Protein structural issues

Is the N-terminus unstructured?
Is the N-terminus responsible for dimerisation?

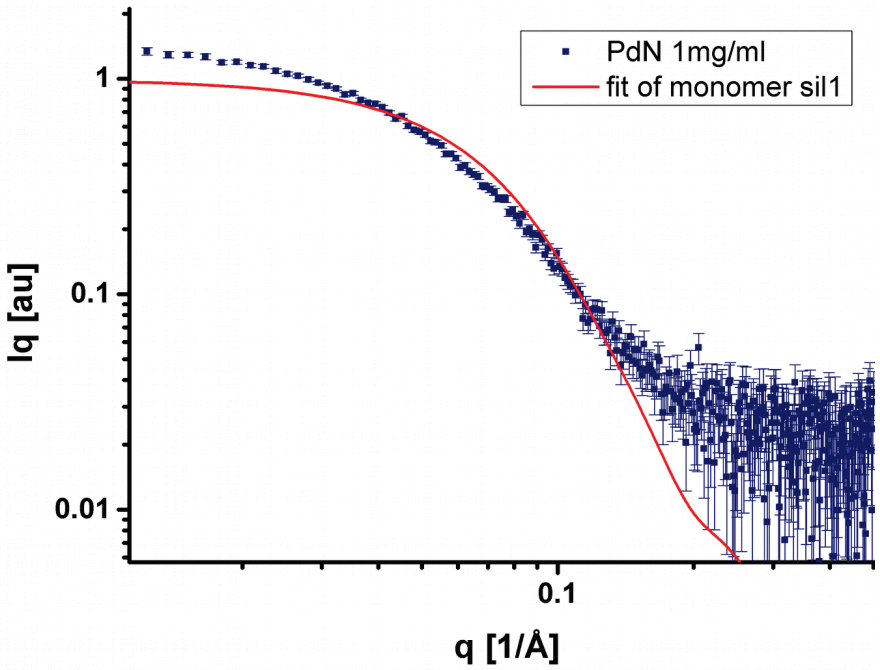


- WT looks more structured than δN
- curves are too noisy artificial increase of intensity due to the noise possible

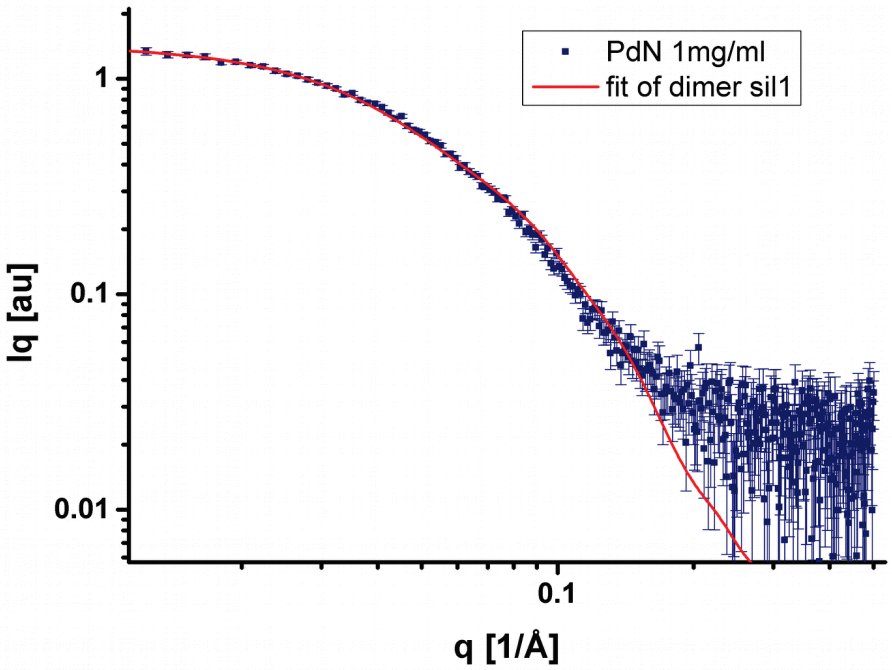
→ **The N-terminal part is unstructured**

Protein structural issues

Is the N-terminus responsible for dimerisation?



- Homology model doesn't fit at all
- Protein is bigger (higher I_0)
- Monomer is more compact (slope)

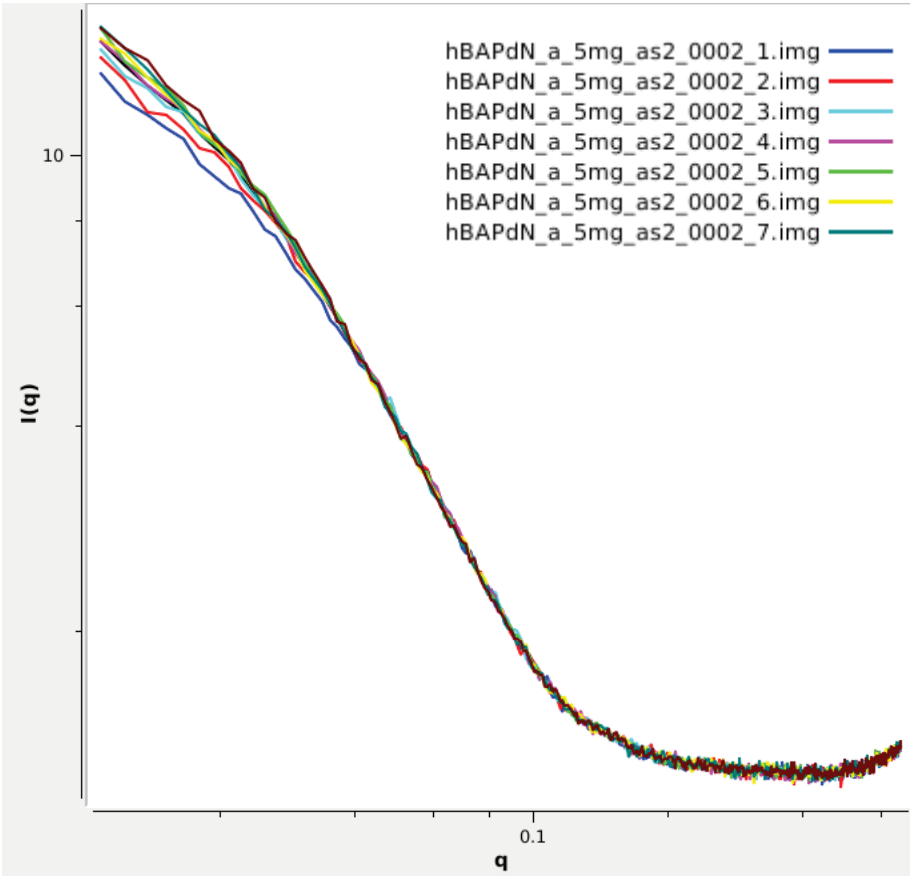


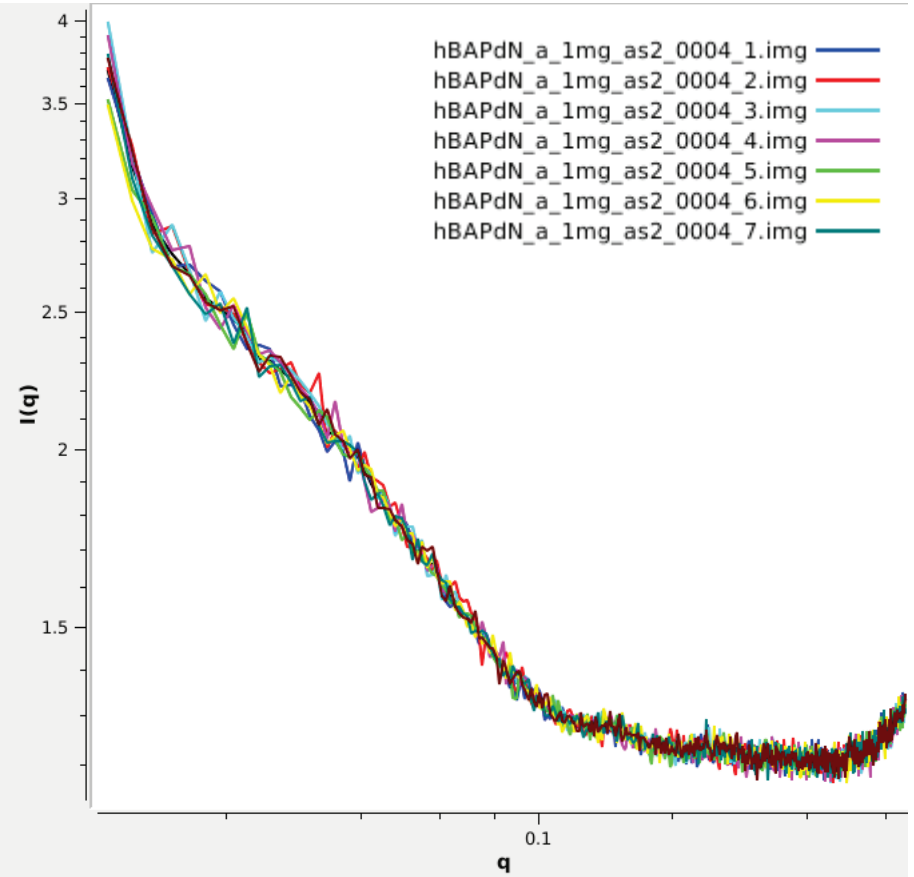
- Dimer of the Homology model fits
- I_0 fits
- Slope fits almost

→ **The protein is a dimer even at the lowes concentration**

Scattering

hBAPdN all frames 5mg/ml (left) 1mg/ml (right)



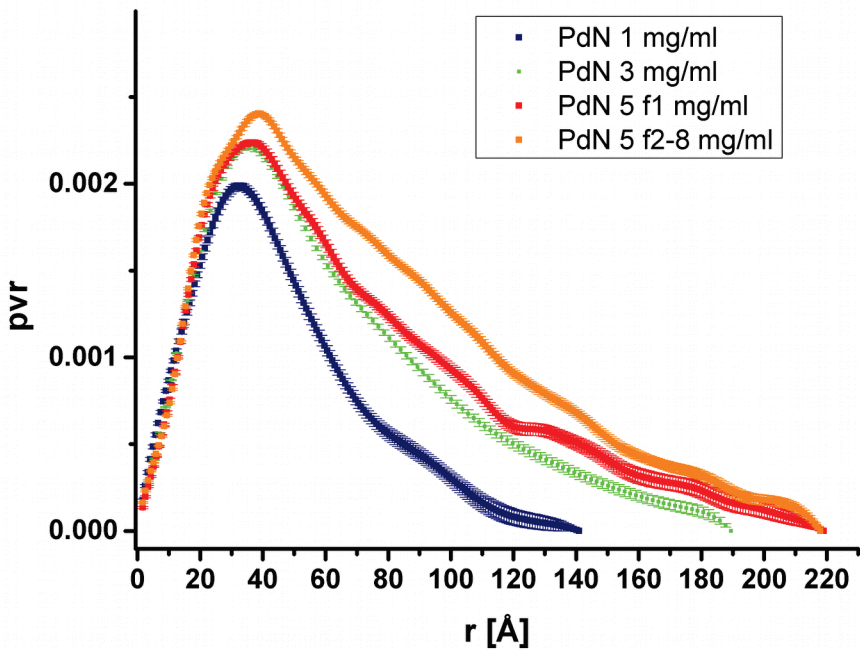


→ High concentration is affected by beamdamage.
Low concentration has no beamdamage.

hBAP

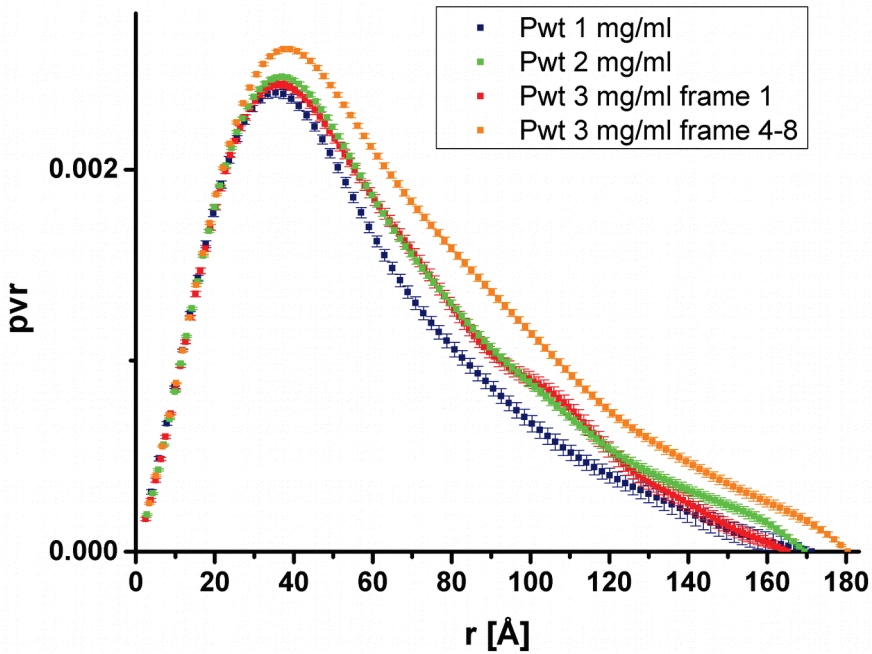
PVR

hBAPdN



Higher concentrations have a much higher molecular weight, show beam damage and have an elongated structure.
The lowest concentration has a Dmax of ~ 140 Å.

hBAPwt

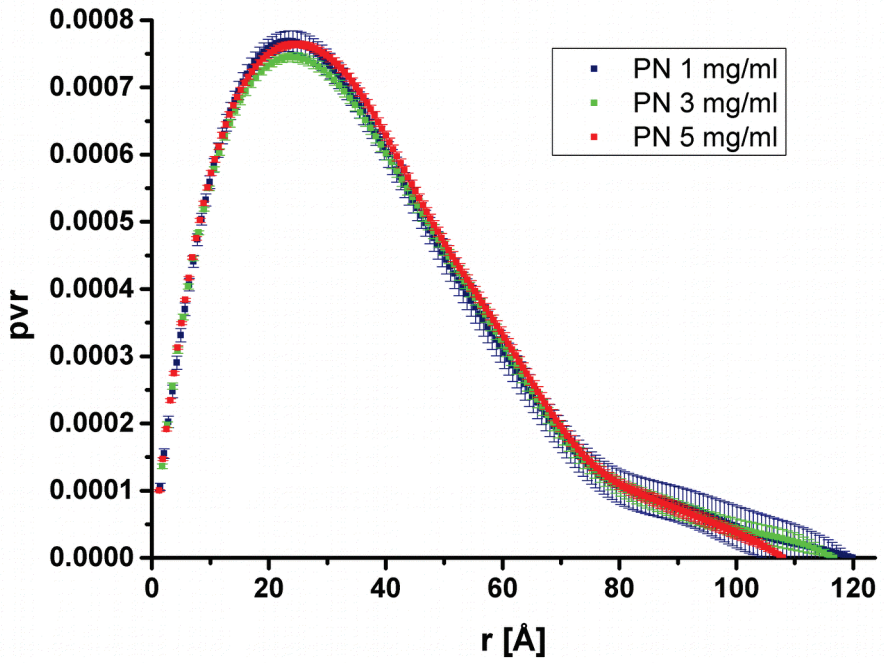


The increase of molecular weight is moderate. The Structure of the Protein is elongated.
All concentrations have a Dmax around ~ 170 Å.

hBAP

PVR

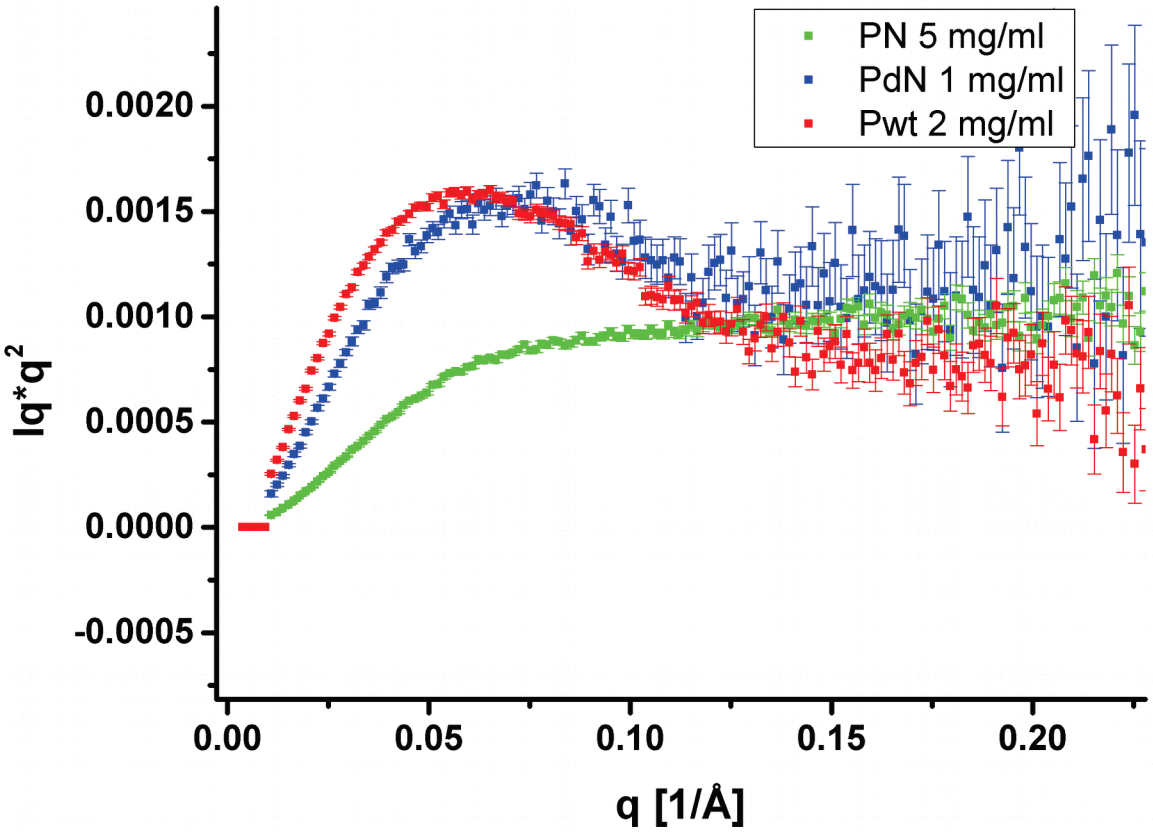
hBAPN



The N-terminus shows no concentration dependent behaviour and has no beamdamage.
All concentrations have a Dmax around ~ 110 Å.

hBAP

Kratky plot



The N-terminus is unfolded.
C-terminus and wt are folded.
The data are too noisy to see if the N-terminus in wt is structured.

Numbers

Radius of gyration

File	Rg	+-
hBAPdN_a_1mg_as2_cnorm.dat	36.59	1.3
hBAPdN_a_3mg_as2_cnorm.dat	49.76	0.9
hBAPdN_a_5mg_as2_0002_f4-8.dat	58.05	0.5
hBAPdN_a_5mg_as2_0002_frame1.dat	54.07	1.2
hBAPwt_b_1mg_as2_cnorm.dat	43	1.3
hBAPwt_b_2mg_as2_cnormf28.dat	47	0.8
hBAPwt_b_3mg_as2_cnorm-f1.dat	46	1.6
hBAPwt_b_3mg_as2_cnorm-f48.dat	51.9	1.0
hBAPN_c_1mg_as2_cnorm.dat	28.4	1.9
hBAPN_c_3mg_as2_cnorm.dat	29.39	0.7
hBAPN_c_5mg_as2_cnorm.dat	29.49	0.5

hBAP

Numbers

Dmax and MW

Sil1 Dmax 70 Å

File	Dmax	Vp	MW
hBAPdN_a_1mg_as2_cnorm_a	97.0	95776.0	77.6
hBAPdN_a_1mg_as2_cnorm_h	141.0	101640.0	82.3
hBAPdN_a_3mg_as2_cnorm_a	165.5	148266.0	120.1
hBAPdN_a_3mg_as2_cnorm_h	189.5	155546.0	126.0
hBAPdN_a_5mg_as2_0002_f4-8_h	218.0	248684.0	201.4
hBAPdN_a_5mg_as2_0002_frame1_h	219.0	196074.0	158.8

hBAPdN 40 kD

File	Dmax	Vp	MW
hBAPwt_b_1mg_as2_cnorm_a	200.3	136833.0	110.8
hBAPwt_b_1mg_as2_cnorm_h	171.3	161053.0	130.5
hBAPwt_b_2mg_as2_cnormf28_h	169.5	191366.0	155.0
hBAPwt_b_3mg_as2_cnorm-f1_a	134.2	157303.0	127.4
hBAPwt_b_3mg_as2_cnorm-f1_h	165.2	177899.0	144.1
hBAPwt_b_3mg_as2_cnorm-f48_a	164.4	232848.0	188.6
hBAPwt_b_3mg_as2_cnorm-f48_h	180.4	194074.0	157.2

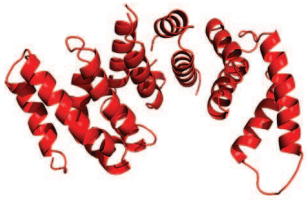
hBAPwt 50 kD

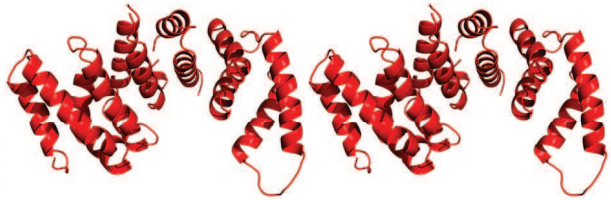
hBAP

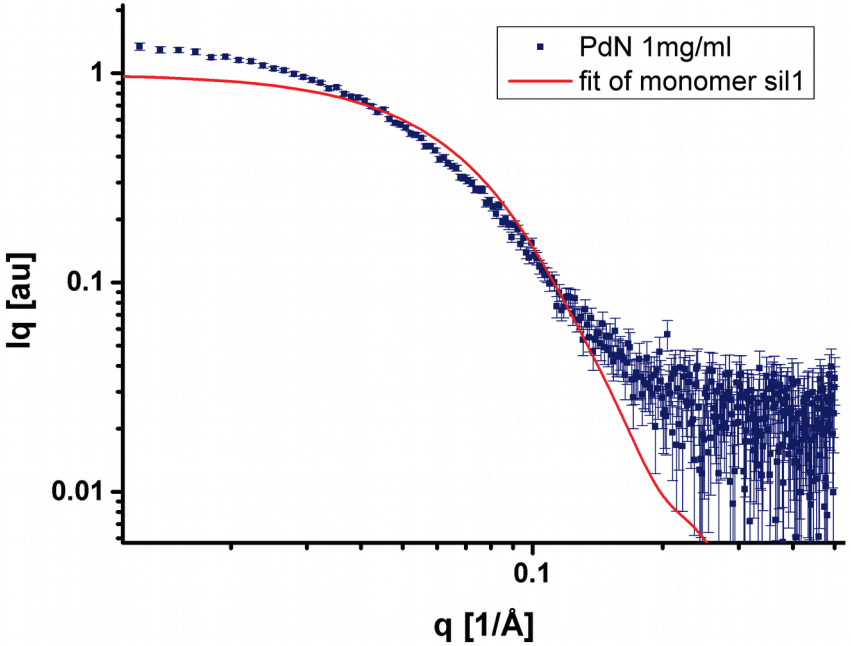
Fits

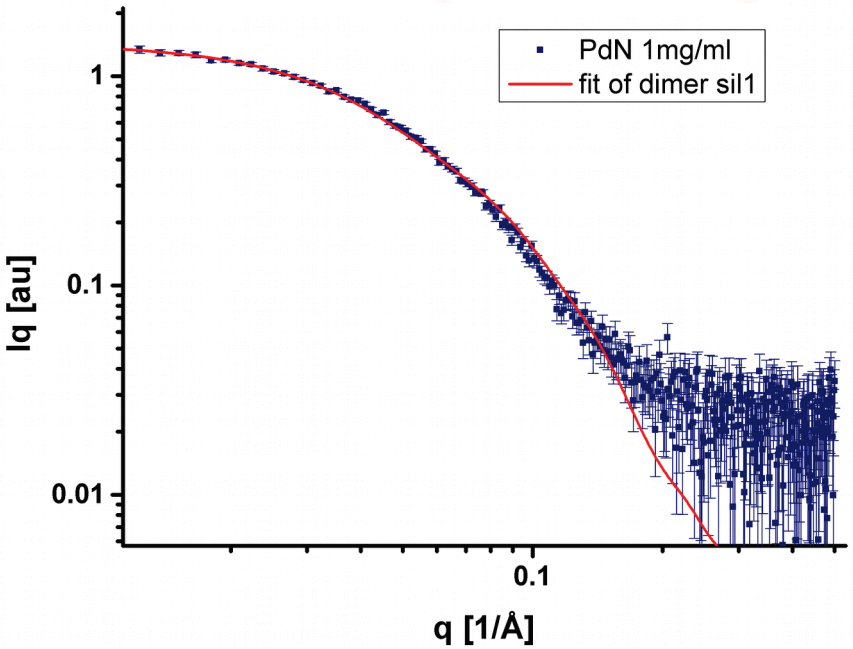
hBAPdN

Sil1









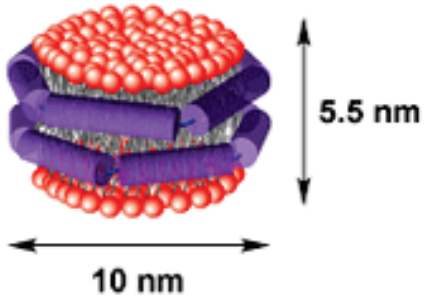
The monomer of Sil1 doesn't fit the scattering curve.
A dimer with dimerisation on the small edge fits the scattering much better.

The dN construct is a dimer, the N-terminus is not responsible for dimerisation.

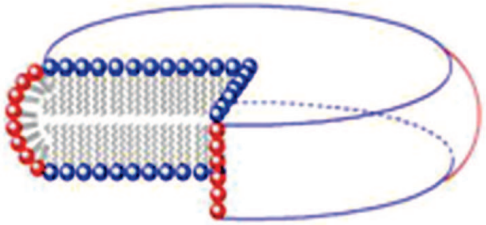
Naodisks

System

Nanodisc



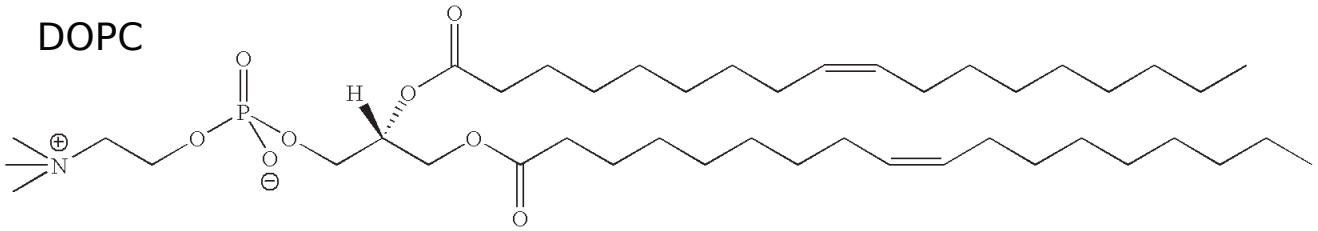
Model for fitting:
Core Shell Bicelle



Bicelle

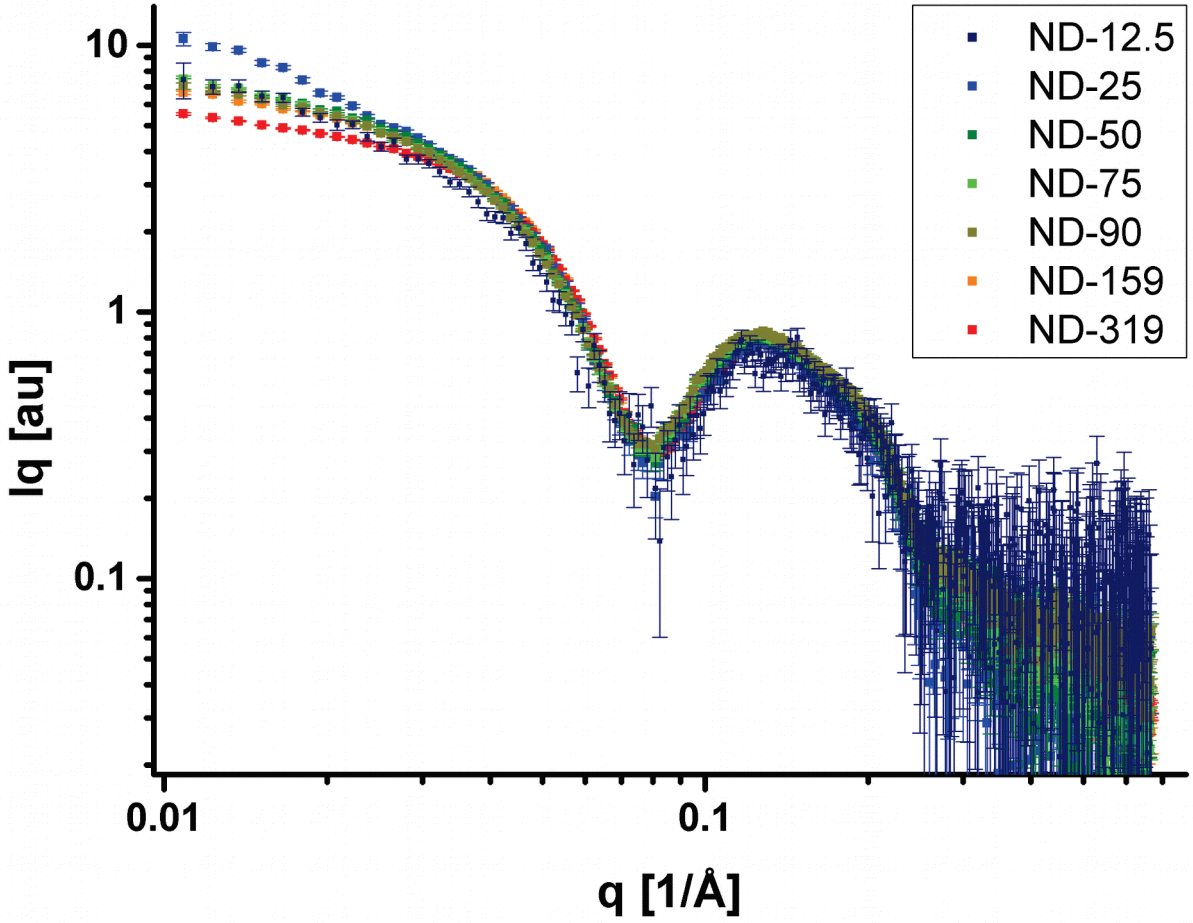
Membrane DOPC
Rim MSP (α-helical, amphipathic membrane scaffold protein)

DOPC



Naodisks

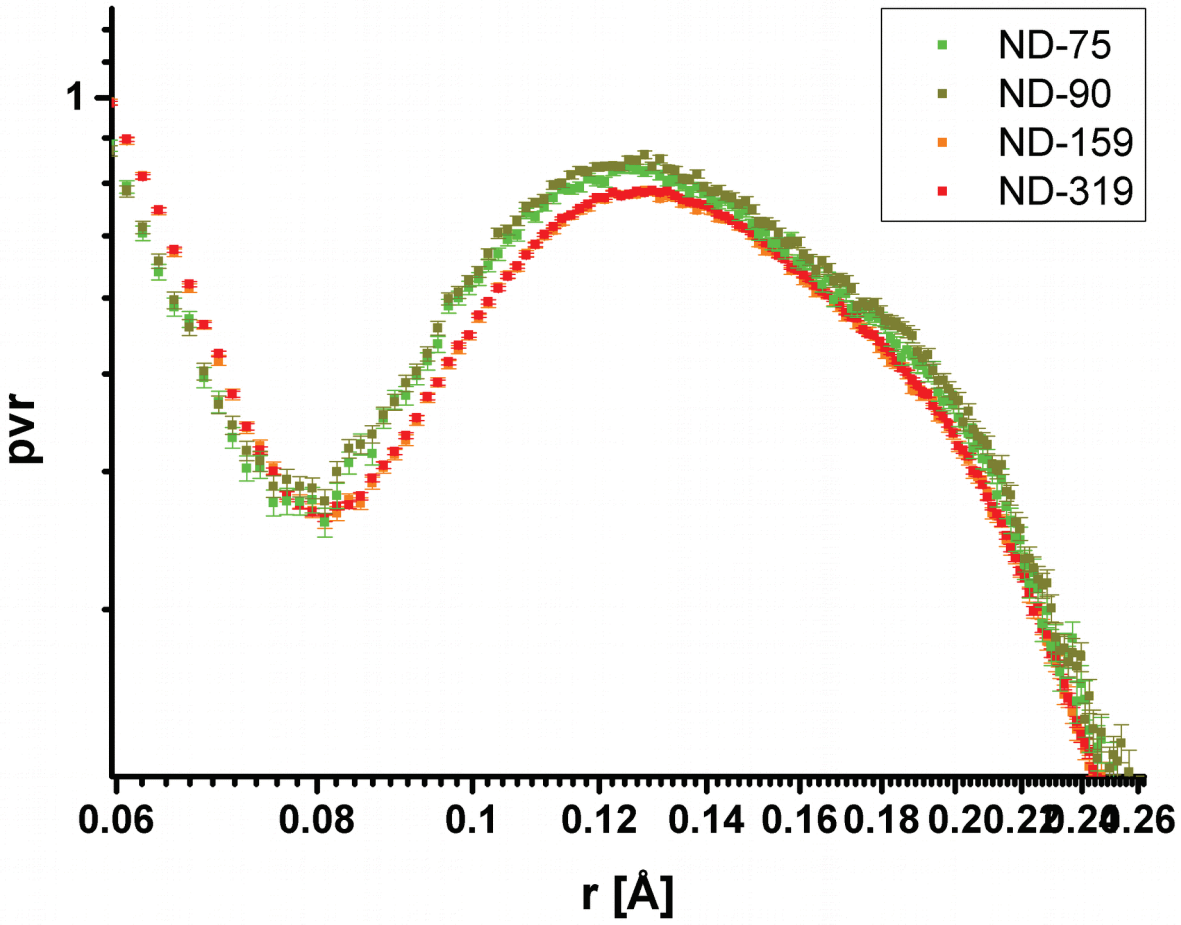
Scattering



319 and 159 µmol are affected by structure factor. 12.5 µmol is too diluted and noisy

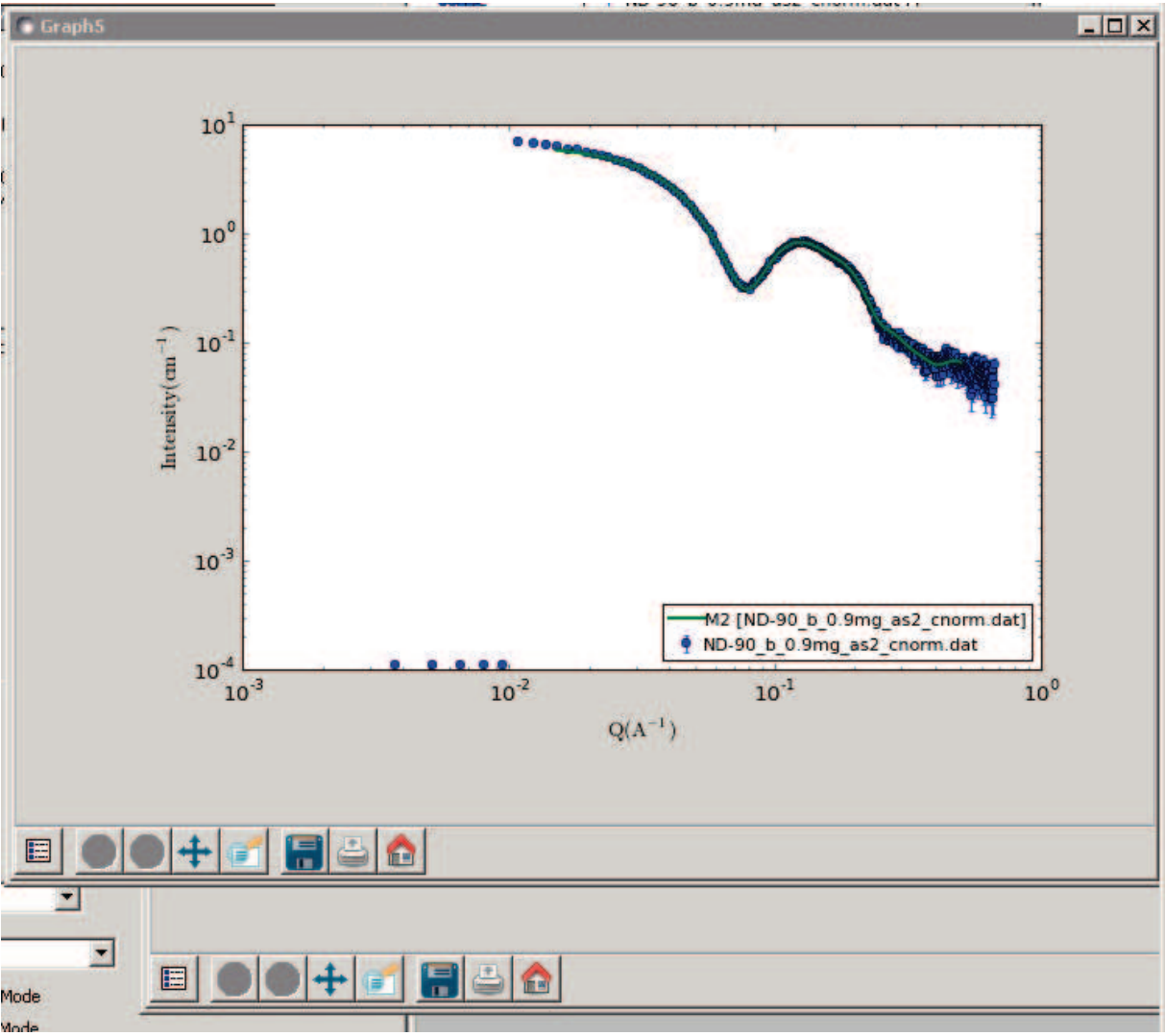
Naodisks

Scattering



319 and 159 µmol are not purified via sec minima are shifted.

Fits



Model Parameters

Select All	Value		Error	Min	Max	[Units]
scale	13.657	+/-	2927.7	0	inf	
background	0.060429	+/-	0.0008639	0	0.3	1/cm
radius	10.004	+/-	0.24226	8	30	Ang
rim_thickness	21.953	+/-	0.15844	12	25	Ang
face_thickness	15.454	+/-	0.50046	3	20	Ang
length	51.298	+/-	0.74995	30	60	Ang
sld_core	8.4061	+/-	111.84	-inf	inf	1e-6/Ang^2
sld_face	10.277	+/-	88.707	-inf	inf	1e-6/Ang^2
sld_rim	9.5749	+/-	13.414	-inf	inf	1e-6/Ang^2
sld_solvent	9.3953	+/-	5.8309	-inf	inf	1e-6/Ang^2

Polydispersity and Orientational Distribution

On Off ?

Fitting

Set Instrumental Smearing

None Use dQ Data Custom Pinhole Smear Custom Slit Smear ?

No smearing is selected...

Set Weighting by Selecting dI Source

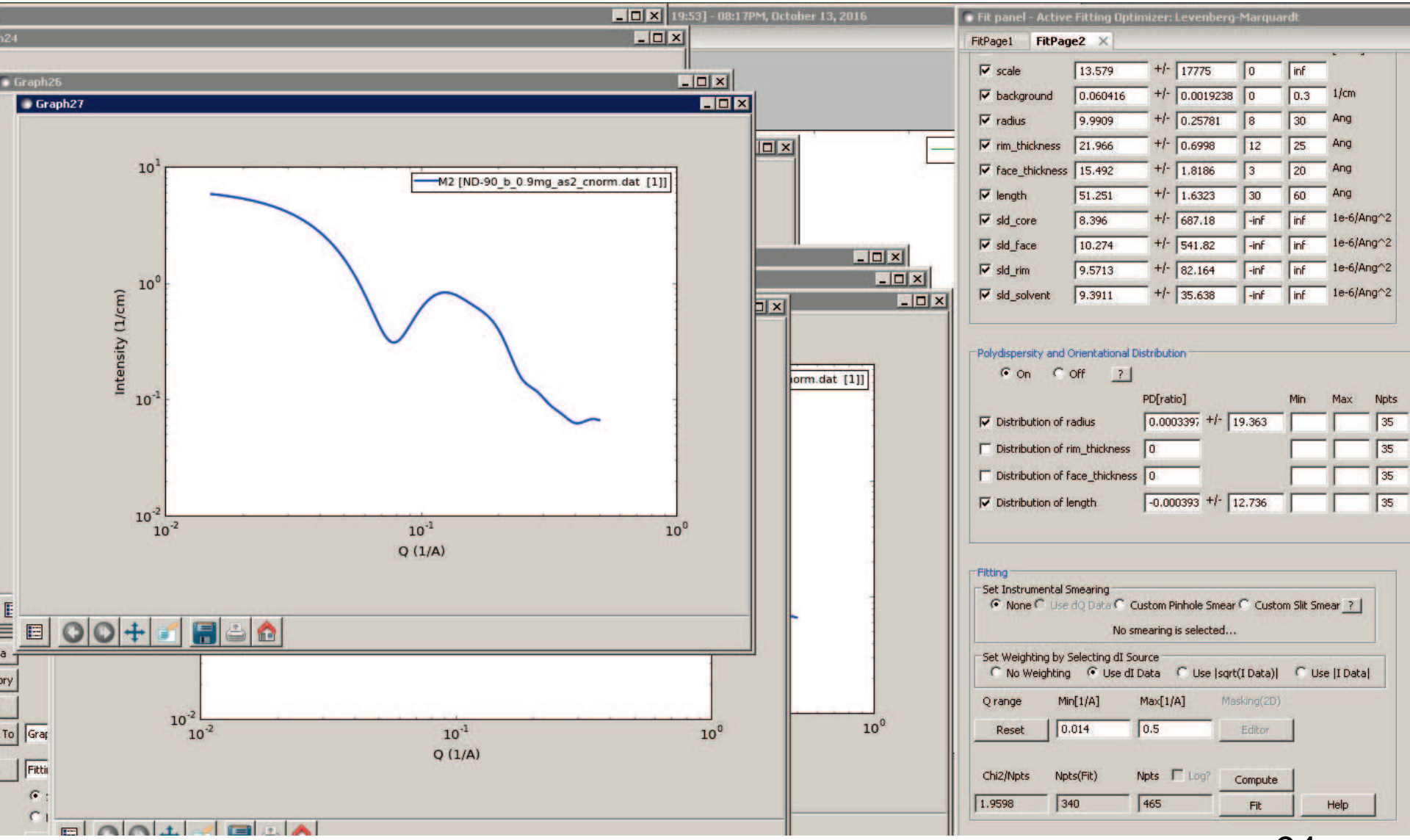
No Weighting Use dI Data Use |sqrt(I Data)| Use |I Data|

Q range	Min[1/A]	Max[1/A]	Masking(2D)
Reset	0.014	0.5	Editor

Chi2/Npts	Npts(Fit)	Npts	Log?	
1.9478	340	465		Compute / Fit / Help

Naodisks

Fits



90 µmol polydispersity added

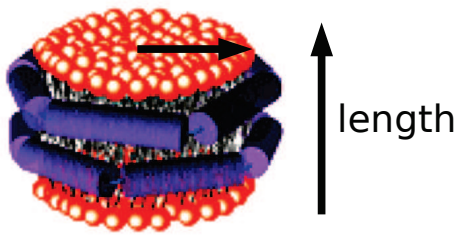
Naodisks

Numbers

file	sc	bg	radius		rim_thickness	face_th	length		sld_core	sld_face	sld_rim	sld_solv	chi
ND319	8.62	0.04	10.25		19.817	17.869	43.46		8.3	10.3	9.69	9.46	15.94
ND159	9.9	0.04	10.044		21.046	16.537	47.426		8.3	10.3	9.62	9.4	1.45
ND159 PD	9.93	0.039	9.71	PD 0.11	21.433	15.62	48.745	PD -2.7e-6	8.25	10.32	9.61	9.39	1.36
ND90	9.79	0.06	9.903		22.11	15.669	51.232		8.25	10.477	9.658	9.44	-
ND90	13.657	0.0604	10.004		21.953	15.454	51.293		8.406	10.277	9.4749	9.39	1.94
ND90 PD	13.579	0.0604	9.9909	PD 0.000339	21.966	15.492	51.251	PD -0.00039	8.396	10.274	9.5713	9.3911	1.95
ND75	10.5	0.05	9.749		22.371	15.811	51.074		7.988	10.177	9.368	9.166	2.045
PD50	8.85	0.04	9.547		22.597	16.297	50.677		8.098	10.515	9.66	9.44	1.47
PD25	12.9	0.02	8.33		24.26	19.324	49.052		8.22	10.51	9.92	9.73	2.56
PD25 rdata	8.79	0.03	9.54		22.747	15.846	50.29		8.24	10.24	9.78	9.56	0.944
PD12p5	0.51	0.0012	10.358		22.366	15.674	53.776		8.00	10.377	9.66	9.37	1.16
PD12p5 rdata	0.51	0.0016	10.358		22.366	15.674	53.776		8.00	10.377	9.66	9.37	1.02

Poly dispersity PD=δr/r

radius = radius of lipid layer



Human HSP90

HSP90
Monomer long axis 124 Å
Dimer open conformation long axis 175 Å
Should be in open conformation.

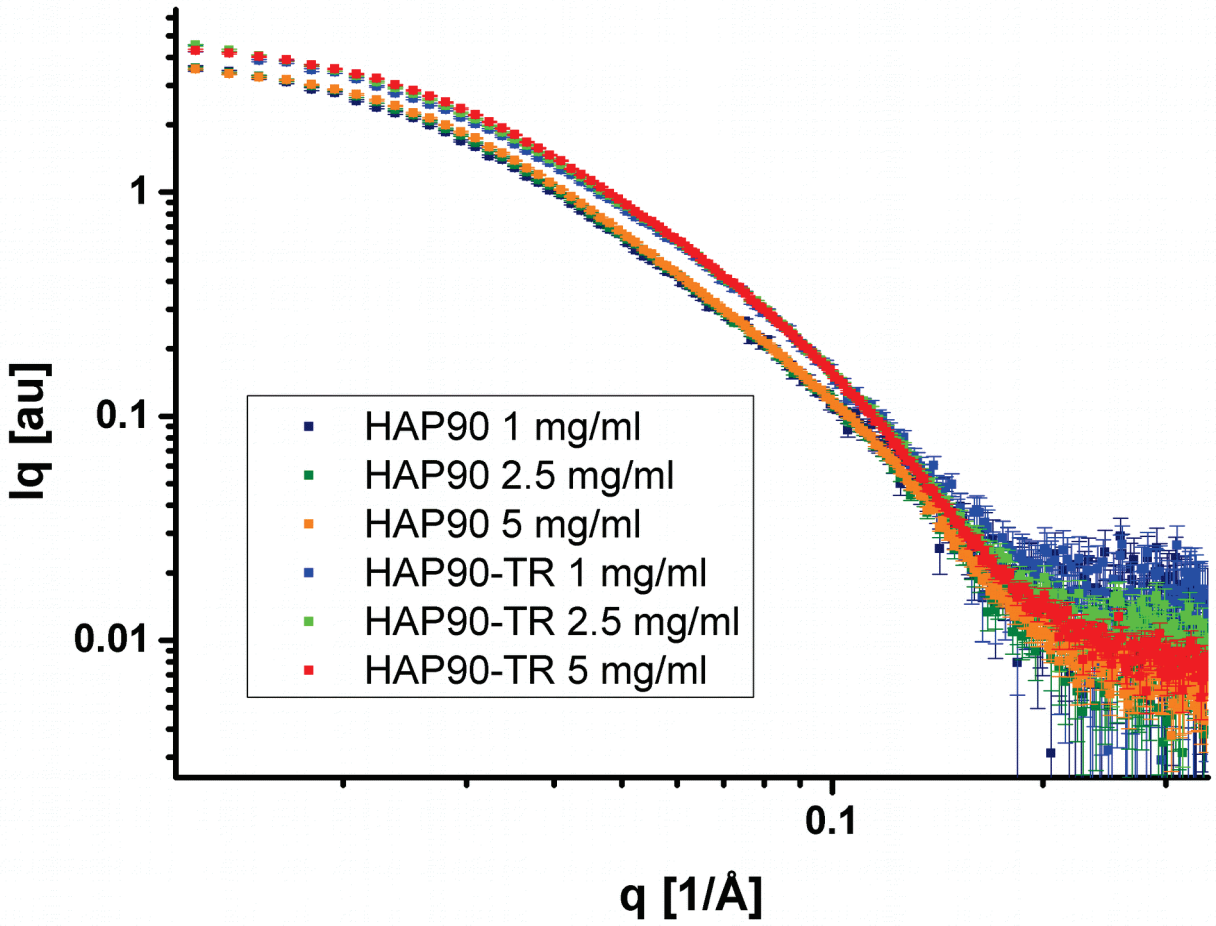
The human HSP90 binds TRb better in the open conformation.
Yeast HSP90 binds better in the closed conformation.

Thyroid hormone receptor (TRb-LBD)
35 kD

Questions:
Is it binding?
Where?
Stoichiometry?

HSP90

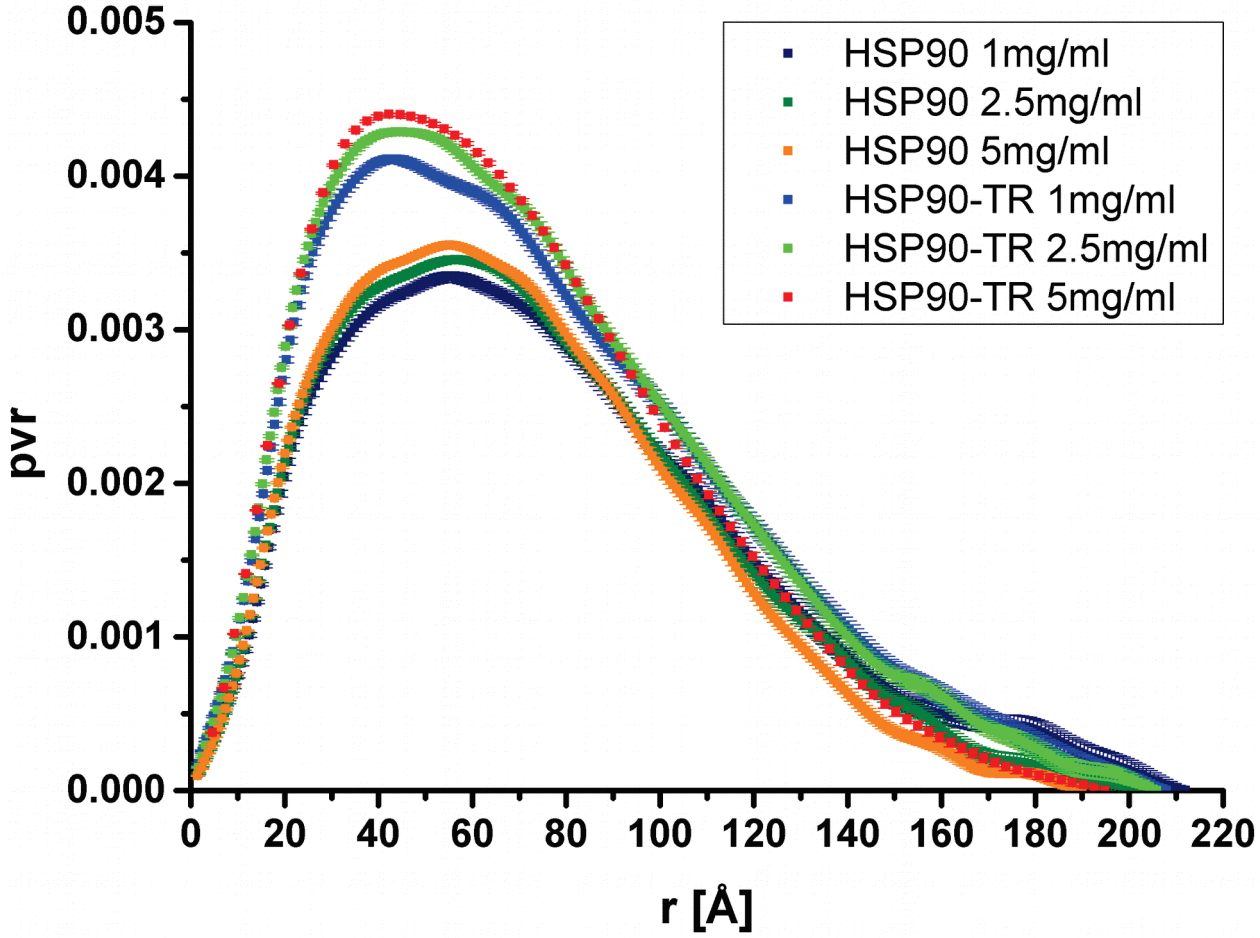
Scattering



Concentration dependent behaviour in the mid q region.

HSP90

Pair distance distribution



Dmax ~200 Å. peak shifted to smaller radius

HSP90

Numbers

File	Rg	+-	I0	+-	datarange	rgl
HSP90_a_1mg_as2_cnorm.dat	59.57	1.44			7-13	1.24
HSP90_a_2.5mg_as2_cnorm.dat	54.42	1			7-14	1.21
HSP90_a_5mg_as2_cnorm.dat	51.9	0.56			7-15	1.23
HSP90-TR_a_1mg_as2_cnorm.dat	56.74	1.15			7-14	1.27
HSP90-TR_a_2.5mg_as2_cnorm.dat	56.76	0.7			7-14	1.27
HSP90-TR_a_5mg_as2_cnorm.dat	50.9	0.24			7-16	1.28

Concentration dependent shift in Rg

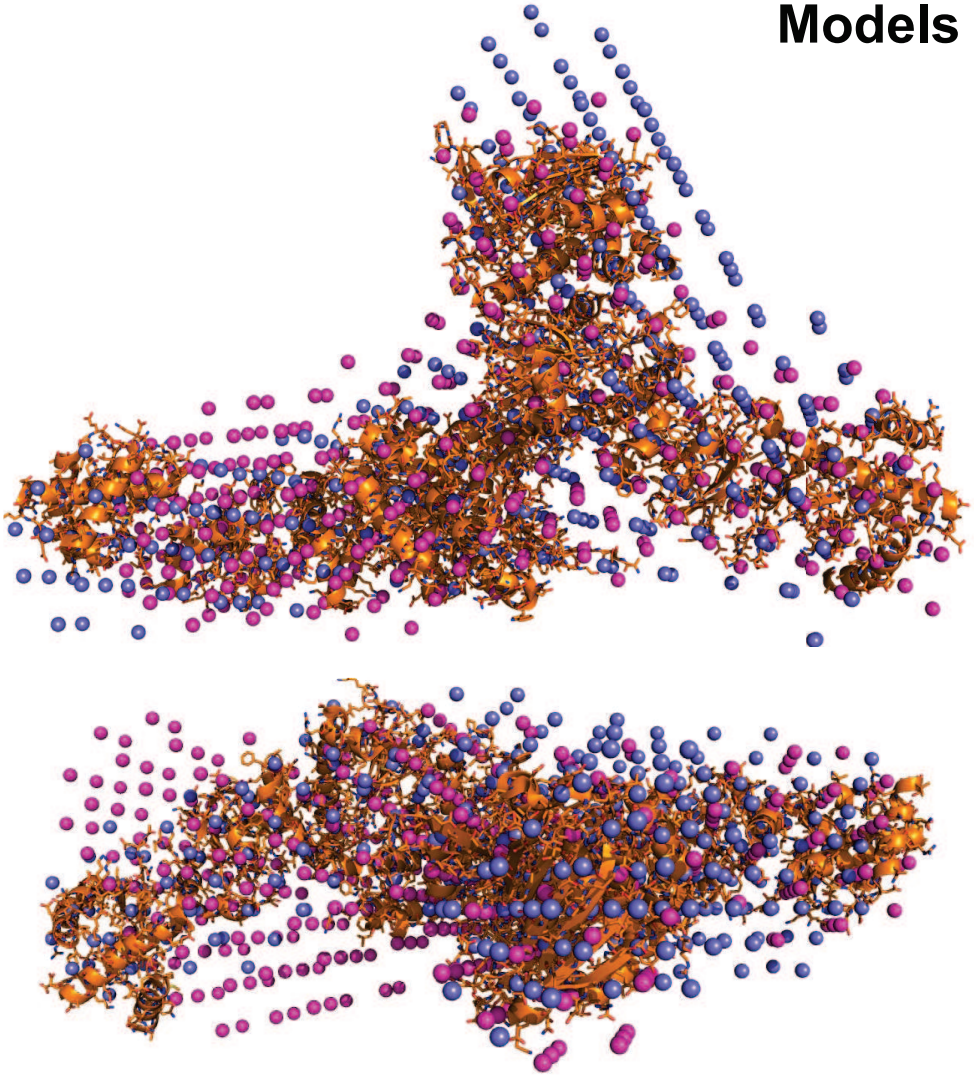
HSP90

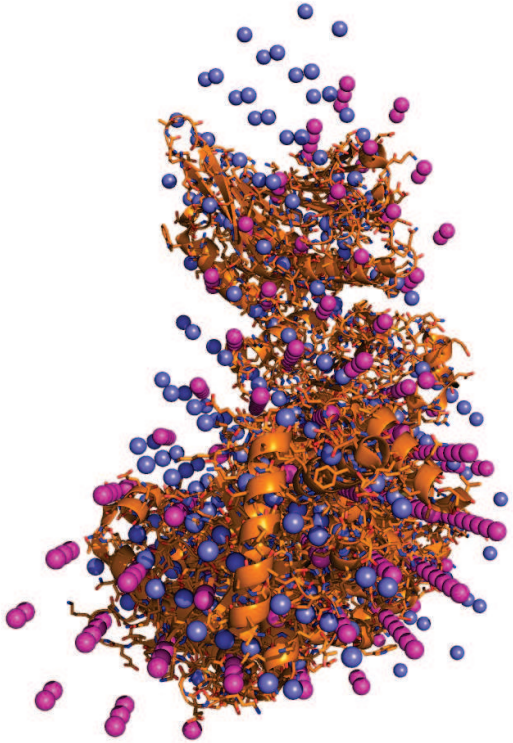
Numbers

File	Dmax	Vp	MW
HSP90_a_1mg_as2_cnorm_h	212.0	432635.0	320.1
HSP90_a_2.5mg_as2_cnorm_h	205.0	395707.0	292.8
HSP90_a_5mg_as2_cnorm_h	190.0	361671.0	267.6
HSP90-TR_a_1mg_as2_cnorm_h	208.0	336122.0	248.7
HSP90-TR_a_2.5mg_as2_cnorm_h	206.0	330489.0	244.6
HSP90-TR_a_5mg_as2_cnorm_a	209.9	294178.0	217.7
HSP90-TR_a_5mg_as2_cnorm_h	194.9	298757.0	221.1

Concentration dependent shift in Dmax and MW

Models





HSP90 5 mg/ml (magenta), HSP90-TR 5 mg/ml (blue)
HSP90 open conformation (2IOQ)

End

Thanks